المملكة العربية السعودية
وزارة التعليم
جَامِعَةُ أمّ القُرىٰ

البحث العلمي بكلية العلوم التطبيقية

أرقام وإحصائيات

إعداد

وكالة كلية العلوم التطبيقية
للدراسات العليا والبحث العلمي

إشراف

عميد كلية العلوم التطبيقية

١٤٤٠هـ | ٢٠١٩م

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انطلاقاً من الرؤية الطموحة للمملكة 2030 وبرنامج التحول الوطني 2020 والتي وضعت البحث العلمي على رأس الأولويات التي توليها حكومة خادم الحرمين الشريفين وولي عهده الأمين -حفظهم الله- اكبر اهتمام فأصبح لزاماً على الجامعات والكليات ان تسعى لذات الهدف لينعكس هذا الاهتمام إيجاباً على جودة البحث العلمي وربطه بقضايا العصر الحديث والتي تركز على ان تكون المعرفة والبحث العلمي أدوات لحل العديد من التحديات المعاصرة بهدف رفع كفاءة الحياة وجودتها. وتأتي كلية العلوم التطبيقية في طليعة الكليات بجامعة ام القرى وبدعم وتوجيه من رئيس الجامعة ووكالة الجامعة للدراسات العليا والبحث العلمي أن تهتم بتطوير أدواتها البحثية بمجالاتها الواسعة والمتداخلة ليس فيما بينها فقط بل تتداخل مع شتى العلوم الاخرى في الصناعة والهندسة والطب والبيئة. وعليه فقد قامت وكالة كلية العلوم التطبيقية للدراسات العليا والبحث العلمي مشكورةً بتعميق فكرة الشراكة البحثية ونشر ثقافة التخصصات المتعددة عن طريق تجميع بيانات البحث العلمي لمختلف تخصصات الكلية وتهيئة الفرصة للباحثين بالكلية للاطلاع على نتاج زملائهم العلمي. ويعد هذا الكتيب احد إصدارات كلية العلوم التطبيقية لعام 1440هـ - 2019 م لعرض ملخص وتقريرعن النتاج العلمي بوجود 134 بحثا ضمن ال ISI و 133 بحثا لها عامل تأثير (IF) بالإضافة الى المشاريع المدعومة والكتب المختلفة المنشورة لتكون مرجعاً للباحثين من الكلية وخارجها ولمعرفة الاهتمامات البحثية للباحثين في كلية العلوم التطبيقية ونشاطهم البحثي.

عميد كلية العلوم التطبيقية
د. حاتم بن محمد الطس

الحمد لله رب العالمين، والصلاة والسلام على نبينا محمد وعلى آله وصحبه أجمعين، أما بعد:
فإن الاعتناء بجانب البحث العلمي لعضو هيئة التدريس بكليات الجامعة يُعد من أهم المهمات، التي ينبغي أن تُحاط بكامل العناية والاهتمام وبما يتواكب مع رؤية المملكة الطموحة 2030. وقد أدركت عمادة كلية العلوم التطبيقية بتوجيهات معالي رئيس الجامعة وبإشراف سعادة عميد الكلية د. حاتم بن محمد الطس، هذا الأمر وبما يتوافق مع رؤية الكلية وأهدافها وتحقيق جانبا من جوانب رسالتها، فبدأت الكلية بإجراء عدد من الأنشطة والفعاليات وعكفت على انتاج عدد من المخرجات ومنها تجميع كل ما يتعلق بالبحث العلمي وجوانبه لعام واحد وبإنشاء رابط خاص بنتاج البحث العلمي بالموقع الالكتروني الخاص بكلية العلوم التطبيقية والذي ساعد أعضاء الكلية بالدخول لهذا الرابط وتعبئة نتاجهم البحثي العلمي المختلف وتمت إضافته بعد ذلك في هذا التقرير. فالحمد الله ان وفقنا في إصدار التقرير الحالي والخاص بعام 2019 م والذي اشتمل على ملخص كامل بجميع الأبحاث العلمية والكتب والمشاريع الممولة من عمادة البحث العلمي ومدينة الملك عبدالعزيز للعلوم والتقنية لجميع اعضاء هيئة التدريس بالكلية لهذا العام والتي بلغ فيها عدد المخرجات العلمية المنشورة 153 بحثا منشورا و7 كتب و 25مشروعا بحثيا مدعوما لجميع أقسام الكلية. وأخيرا أتقدم بالشكر الجزيل لسعادة العميد والوكلاء والوكيلات ورؤساء ووكيلات الاقسام ولكافة أعضاء هيئة التدريس بالكلية ولكل من ساهم في انجاز هذا التقرير. والله نسأل أن يجعل هذا العمل خالصا لوجه الكريم، وأن يكلل دائماً اعمالنا بالنجاح والتوفيق والسداد.

وكيل الكلية للدراسات العليا والبحث العلمي
أ. د. باسم بن حسين أصغر

بسم الله والحمد لله والصلاة والسلام على نبي الرحمة، ومنار الهدى محمد بن عبد الله وعلى آله وصحبه ومن والاه

ان الحاجة الى الدراسات والبحوث والتعلم لهي اليوم اشد منها في أي وقت مضى. فالعلم والعالم في سباق للوصول الى أكبر قدر ممكن من المعرفة الدقيقة المستمدة من العلوم التي تكفل الرفاهية للإنسان، وتضمن له التفوق. وإذا كانت الدول المتقدمة تولي اهتمامًا كبيرًا للبحث العلمي فذلك يرجع الى انها أدركت ان عظمة الامم تكمن في قدرات ابنائها العلمية والفكرية والسلوكية. والبحث العلمي ميدان خصب ودعامة اساسية لاقتصاد الدول وتطورها وبالتالي تحقيق رفاهية شعوبها. وقد اصبحت منهجية البحث العلمي واساليب القيام بها من الامور المسلم بها في المؤسسات الاكاديمية ومراكز البحوث، بالإضافة الى انتشار استخدامها في معالجة المشكلات التي تواجه المجتمع بصفة عامة.

وهناك العديد من فوائد البحث العلمي التي تنعكس إيجابًا على المجتمع، ومنها ما يأتي:

- رفع مستوى الوعي لدى أفراد المجتمع ممّا يُساهم في تطويره.
- نمو المجتمع اقتصادياً ممّا يُحقّق رفاهية أفراده.
- حلّ المشكلات على كافة المستويات الاقتصادية، والسياسية، والصحية، وغيرها.
- إيجاد تفسيرات للظواهر الطبيعية والتنبّؤ بها.
- تتبّع الإنجازات الفكرية للإنسان في مختلف المجالات.
- وتهدف الجامعة الى ربط البحث العلمي بأهداف الجامعة وخطط التنمية، والبعد عن الازدواجية والتكرار والإفادة من الدراسات السابقة.

وكيلة كلية العلوم التطبيقية
أ.د. رجاء بنت طاهر معتوق

الشكر والتقدير والامتنان لإصحاب السعادة على الجهد المبذول لتجميع بيانات هذا التقرير

تأتي أهمية البحث العلمي في المساهمة الفاعلة في حل المشـــاكل من خلال الجمع بين الملاحظات والمعرفـة والبيـانـات مما يجعل ابتكار الحلول وخلق منتجات جديدة أمراً ممكنا و قسم الكيميـــاء أحد أهم الاقسـام التي تدفع عجلة البحث العلمي في مختـلـف تخصصات الكيمياء الدقيقة و التي يهتـم الباحثون فيه بالتركيز على الأولويات البحثيـة التطبيقية المتوافقـة مع الخطة الاستراتيجية للجامعة .

د. اسماعيل بن ابراهيم الثقفي

رئيس قسم الكيمياء

مما لا شك فيه أن تقدم الدول و تطورها يبتديء بتعزيز الأبحاث العلمية و تشجيع طلبة العلم و دعمهم في زيادة إنتاج الأبحاث التنموية العلمية المتوافقة مع الرؤية الوطنية 2030 لإثراء مجالات العلم والمعرفة بشتى حقولها.

د. ياسر بن عايش المروعي

رئيس قسم الاحياء

بلا شك ان فائدة البحث العلمي تساعد على تطور العلوم بصفة عامة سواءً الإنسانية منها أو العلمية، في كلا الحالتين يضيف شيئاً جديداً للبشرية. ولكي تصل الدولة إلى أهدافها، في رؤية 2030، في أسرع وقت ممكن فإن البحث العلمي هو أحد السبيل .

د. تركي بن عثمان المعطاني

رئيس قسم الفيزياء

يولي قسم العلوم الرياضية للنشاط البحثي أهميته ويعمل على تحقيق رسالة الكلية والجامعة من خلال عقد لقاءات علمية وحلقات نقاش خلال العام ينخرط فيها اعضاء هيئة التدريس وطلاب الدراسات العليا بالإضافة الى تشجيع الباحثين لحضورالموتمرات التخصصية وتكوين مجموعات بحثية يلتقي فيها الباحث الجديد مع الأساتذة المتميزين في البحث العلمي لاكتساب مهارات البحث العلمي والنشر.

د. عبدالله بن عوض الاحمري

رئيس قسم العلوم الرياضية

الأعلى نشرا من أعضاء هيئة التدريس بكلية العلوم التطبيقية وفقا ل Scopus الى عام 2019 م :

أ.د. متولي عبدالله محمد عبد السيد

أ.د. صالح عبدالمجيد احمد صالح

أ.د. محمد اسماعيل محمد عواد

أ.د. ثريا عبدالرحيم فرغلي محمد

الأعلى نشرا من أعضاء هيئة التدريس بكلية العلوم التطبيقية وفقا ل ISI الى عام 2019 م :

أ.د. ثريا عبدالرحيم فرغلي محمد

أ.د. صالح عبدالمجيد احمد صالح

أ.د. متولي عبدالله محمد عبد السيد

أ.د. أحمد فوزي سعد سيد

أ. د. محمد ربيع شعبان جنيدي

الأكثر نشرا للأبحاث في عام 2019 بكلية العلوم التطبيقية وفقا لتقرير النشر العلمي لعمادة البحث العلمي بالجامعة :

د. إسماعيل إبراهيم الثقفي
(قسم الكيمياء – 21 بحثاً)

أ.د. ثريا عبدالرحيم فرغلي محمد
(قسم الكيمياء – 20 بحثاً)

أ.د. صالح عبدالمجيد احمد صالح
(قسم الكيمياء – 12 بحثاً)

أ.د. نشوه محمود المتولي محمد
(قسم الكيمياء – 11 بحثاً)

د. هدى ابوالفتوح أحمد الغمري
(قسم الكيمياء – 7 أبحاث)

د. حسين حسن أبوالريش
(قسم الأحياء – 7 أبحاث)

أ. د. محمد ربيع شعبان جنيدي
(قسم الكيمياء – 7 أبحاث)

أ.د. جمال ابراهيم هريدي عثمان
(قسم الأحياء – 7 أبحاث)

د. أحمد محمد الحربي
(قسم الكيمياء – 6 أبحاث)

د.هنادي أحمد كتوعة
(قسم الكيمياء – 6 أبحاث)

أ.د. متولي عبدالله محمد عبدالسيد
(قسم الكيمياء – 6 أبحاث)

الكيمياء

أولا: الأبحاث المنشورة بقسم الكيمياء :

م	عنوان البحث	المشاركين	المجلة	دار النشر	ISI/ NON-ISI	معامل التأثير IF
1	Design, synthesis, and biological evaluation of novel N-4substituted sulfonamides: acetamides derivatives as dihydrofolate reductase (DHFR) inhibitors	Essam M. Hussein, Munirah M. Al-Rooqi, Shimaa M. Abd El-Galil, Saleh A. Ahmed	BMC Chemistry	Springer	ISI	2.09
2	Bioactive fluorenes. part I. Synthesis, pharmacological study and molecular docking of novel dihydrofolate reductase inhibitors based-2,7-dichlorofluoren	Essam M. Hussein, Reem I. Alsantali, Shimaa M. Abd El-Galil, Rami J. Obaid, Ahmed Alharbi, Mohamed A.S. Abourehab, Saleh A. Ahmed	Heliyon	Elsevier	ISI	1.65
3	MCM-SO3H catalyzed synthesis of environment-sensitive fluorophores incorporating pyrene moiety: Optimization, fluorescence emission and theoretical studies	Nizar El Guesmi, Essam M. Hussein, Saleh A. Ahmed	Journal of Photochemistry & Photobiology A: Chemistry	Elsevier	ISI	3.26
4	Competent inhibitor for the corrosion of zinc in hydrochloric acid based on -2,6bis-[-2)-1 phenylhydrazono)ethyl]pyridine	Metwally Abdallah, Saleh A. Ahmed, Hatem M. Altass, Ishaq A. Zaafarany, M. Salem, A. I. Aly, Essam M. Hussein	Chemical engraining communications	Taylor& Francis	ISI	1.43
5	Nano-synthesis, biological efficiency and DNA binding affinity of new homo-binuclear metal complexes with sulfa azo dye based ligand for further pharmaceutical applications	Fawaz A. Saad, Hoda El-Ghamry, Mohammed A. Kassem, Abdalla M. Khedr	Journal of Inorganic and Organometallic Polymers and Materials	Springer	ISI	1.90
6	Novel series of nanosized mono- and homobi-nuclear metal complexes of sulfathiazole azo dye ligand: Synthesis, characterization, DNA-binding affinity, and anticancer activity	Abdalla M. Khedr Hoda El-Ghamry Mohammed A. Kassem Fawaz A. Saad Nizar El-Guesmi	Inorganic Chemistry Communications	Elsevier	ISI	1.80
7	Enhanced Electrocatalytic Oxidation of Paracetamol at DNA Modified Gold Electrode	Ismail I. Althagafi Mohammed A. Kassem, Mohamed I. Awad	Electroanalysis	Wiley	ISI	2.30
8	Synthesis, structural characterization and DNA binding affinity of new bioactive nano-sized transition metal complexes with sulfathiazole azo dye for therapeutic applications	Fawaz A. Saad Hoda A. El-Ghamry Mohammed A. Kassem	Applied Organometallic Chemistry	Wiley	ISI	3.25

3.05	ISI	RSC	RSC Advances	Essam M. Hussein, Nizar El Guesmi and Saleh A. Ahmed	Exploiting a multicomponent domino reaction strategy for the tailoring of versatile environmentally sensitive fluorophore-based nicotinonitriles incorporating pyrene and fluorene moieties	9
-	-	Oriental Scientific Publishing Company	ORIENTAL JOURNAL OF CHEMISTRY	,Amr Lotfy Saber, Wael Abd-Allah Zordok, Ahmed Alharbi and Abdu Subaihi	Characterization of Palladium Chelates and their Interactions with Z-N›-(benzo(d)thiazol-2-yl)-N,N-dimethylformimidamide using the Spectrophotometric and Computational Methods	10
1.28	ISI	-	Int. J. Electrochem. Sci.	Gharam I. Mohammed and Amr L.Saber	Study of the Electrochemical Behavior of Melatonin on Different Electrodes in Aqueous Solution	11
1.28	ISI	-	Int. J. Electrochem. Sci.	Fawzy A, Abdallah M, Alfakeer M, Ali H M	Corrosion Inhibition of Sabic Iron in Different Media Using Synthesized Sodium N-dodecyl Arginine Surfactant	12
1.90	ISI	Springer	Journal of Inorganic and Organometallic Polymers and Materials	Takroni K M, El-Ghamry H A, Fawzy A	Evaluation of the Catalytic Activities of Some Synthesized Divalent and Trivalent Metal Complexes and Their Inhibition Efficiencies for the Corrosion of Mild Steel	13
4.56	ISI	Elsevier	Journal of Molecular Liquids	Ahmed Fawzy	Removal of toxic tellurium (IV) compounds via bioreduction using flucloxacillin in aqueous acidic medium: A kinetic and mechanistic approach	14
1.90	ISI	Springer	Journal of Inorganic and Organometallic Polymers and Materials	Bawazeer T M, El-Ghamry H A, Farghaly T A, Fawzy A	Novel -1,3,4Thiadiazolethiosemic arbazones Derivatives and Their Divalent Cobalt-Complexes: Synthesis, Characterization and Their Efficiencies for Acidic Corrosion	15
0.12	ISI	-	Journal of Pure and Applied Microbiology	Chandra Mohan Singh Bisht, S.M. Shakeel Iqubal, Aejaz A. Khan, Tasneem Mohammed, Areej Dawoud, Mohammed Gamal, S.K. Singh and Basim H. Asghar	Natural Products in Drug Discovery: Antibacterial and Antifungal Activity of Essential Oil of Compound Isolated from Senecio royleanus	16

3.05	ISI	RSC	RSC Advances	Jessica A. Kretzman , RuiLu Fengb, Alaa M. Munshi a, Diwei Hoa, Anna M. Ranieric, Massimiliano Mass, Martin Saundersd, Marck Norreta, K. Swaminathan Iyer and Cameron W. Evans	A facile methodology using quantum dot multiplex labels for tracking co-transfection	17
0.10	ISI	Elsevier	Heliyon	Khormi A. Y., Farghaly T. A. , Shaaban M. R.	Pyrimidyl formamidine palladium(II) complex as a nanocatalyst for aqueous Suzuki-Miyaura coupling	18
1.90	ISI	Springer	Journal of Inorganic and Organometallic Polymers and Materials	BawazeerT. M. , El-Ghamry H. A. , Farghaly T. A. , Fawzy A.	Novel 1,3,4Thiadiazolethiosemicarbazones Derivatives and Their Divalent CobaltComplexes: Synthesis, Characterization and Their Efficiencies for Acidic Corrosion Inhibition of Carbon Steel	19
1.24	ISI	Wiley	J. Heterocyclic Chem.	Althagafi. I. , Abouzied A. S. , Farghaly T. A. , Al-Qurashi N. T. , Alfaifi M. Y. , Shabaan M. R. , Abdel Azizd M. R.	Novel Nano-sized bis-indoline Derivatives as Antitumor Agents	20
2.12	ISI	Elsevier	Journal of Molecular Structure	N. El-Metwaly , T. A. Farghaly , I. Althagafi , Marwa G.Elghalban	Synthesis for novel VO(II)-triazole complexes; spectral, analytical characterization and catalytic usage for biodiesel synthesis from waste oil	21
3.25	ISI	Wiley	Applied Organometallic Chemistry	Ismail Althagafi , Nashwa M. El-Metwaly , Thoraya Farghaly	Characterization of new Pt(IV)–thiazole complexes: Analytical, spectral,molecular modeling and molecular docking studies and applications in two opposing pathways	22
2.04	ISI	Springer	Research on Chemical Intermediates	M. M. Alsharekh, I. I. Althagafi, M. R. Shabaan, Thoraya Farghaly	Microwave-assisted and thermal synthesis of nanosized thiazolyl-phenothiazine derivatives and their biological activities	23
4.56	ISI	Elsevier	Journal of Molecular Liquids	H.S. Gadowa, Thoraya A. Farghaly , A.M. Eldesoky	Experimental and theoretical investigations for some spiropyrazoles derivatives as corrosion inhibitors for copper in 2 M HNO3 solutions	24
3.09	ISI	MDPI	Molecules	I. Althagafi , N. El-Metwaly , T. A. Farghaly	New Series of Thiazole Derivatives: Synthesis, Structural Elucidation, Antimicrobial Activity, Molecular Modeling and MOE Docking	25

3.09	ISI	MDPI	Molecules	A. M. R. Alsaedi , T. A. Farghaly , M. R. Shaaban	Synthesis and Antimicrobial Evaluation of Novel Pyrazolopyrimidines Incorporated with Mono- and Diphenylsulfonyl Groups	26
2.60	ISI	Bentham Science Publishers	Mini-Reviews in Medicinal Chemistry	Z. A. Muhammad., M. A.A. Radwan., T.A. Farghaly., H.M. Gaber, Mahmuod M. Elaasser	Synthesis and Antitumor Activity of Novel [1,2,4,5]-tetrazepino[-6,7b] indole Derivatives: Marine Natural Product Hyrtioreticuline C and D Analogues	27
2.76	ISI	Bentham Science Publishers	Medicinal Chemistry	D. H. Dawood.., E. M. H. Abbas., T. A. Farghaly., M. M. Ali., .M. F. Ibrahim	ZnO Nanoparticles Catalyst in the Synthesis of Bioactive Fused Pyrimidines as Anti-breast Cancer Agents Targeting VEGFR2-	28
2.60	ISI	Bentham Science Publishers	Mini-Reviews in Medicinal Chemistry	T. Ben Hadda., A. Rauf., H. Zgou., F. S. Senol., I. E. Orhan., Y. N. Mabkhot., I. I. Althagafi., T. A. Farghaly,, S, Alterary	Drug Design of Inhibitors of Alzheimer's Disease (AD): POM and DFT Analyses of Cholinesterase Inhibitory Activity of β-amino di-Carbonyl Derivatives	29
2.60	ISI	Bentham Science Publishers	Mini-Reviews in Medicinal Chemistry	H. A. El-Ghamry. , M. Gaber ., T. A. Farghaly	Synthesis, structural characterization, molecular modeling and DNA binding ability of CoII, NiII, CuII, ZnII, PdII and CdII complexes of benzocycloheptenone	30
5.07	ISI	Elsevier	Materials Science & Engineering C	Hanadi A. Katouah, Jabir H. Al-Fahemi, Marwa G.Elghalban, Fawaz A. Saad, Ismail A. Althagafi , Nashwa M. El-Metwaly, Abdalla M. Khedr	Synthesis of new Cu(II)-benzohydrazide nanometer complexes, spectral, modeling, CT-DNA binding with potential anti-inflammatory and antiallergic theoretical features	31
2.20	ISI	Springer	Research on Chemical Intermediates	Layla Almazroia, Reem Shah, Thoryaa Farghaly, Nashwa El-Metwaly	New catalytic approach for nanosized V(IV), Cr(III), Mn(II) and Fe(III)triazole complexes: detailed spectral, electrochemical and analytical studies	32
1.90	ISI	Springer	Journal of Inorganic and Organometallic Polymers and Materials	Ismail Althagafi, Marwa G. Elghalban ,Nashwa M. El-Metwaly	Novel Synthesized Benzesulfonamide Nanosized Complexes; Spectral Characterization, Molecular Docking, Molecular Modeling and Analytical Application	33
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ثانيا: المشاريع الممولة من عمادة البحث العلمي ومدينة الملك عبد العزيز للعلوم والتقنية بقسم الكيمياء :

	Projects	Researcher	Fund
1	Catalytic studies on V(IV), Cr(III), Mn(IV) and Fe(III) nano-meter complexes extracted from triazole derivative and analytical, electrochemical and spectral characterization especially with ESR spectra	أ.د. ثريا عبدالرحيم فرغلي	KACST 127000 SR
2	Chemotherapy and industrial catalysis implementations for new nanometer Pt (II) complexes for thiazole derivatives have elaborated study	أ.د. ثريا عبدالرحيم فرغلي	DSR Umm Al-Qura University 212000 SR

3	Elaborated study to synthesize a novel series of VO(II) nanometer complexes extracted from triazole derivatives and their utilization as catalyst in synthesis of economic materials	أ.د. ثريا عبدالرحيم فرغلي	DSR Umm Al-Qura University 120800
4	Cancer therapeutics: Imidazole –urea/thiourea pharmacophores based novel chemical entities as tubulin inhibitors.	د. محمد شهير مالك	GPURC -KACST 750000 SAR
6	Designing Heterogeneous gold based bimetallic nano-alloy catalysts for the one pot synthesis of phthalic anhydride from oxylene oxidation Project code -18SCI0010-01-1-	د. معتزهاشم مراد	DSR Umm Al-Qura University 199,760 SR
7	Development of advanced Nano-Hybrids with enhanced medicinal efficacy, project no. -18SCI-1-0024-01,	أ.د. صالح عبد المجيد أحمد	DSR Umm Al-Qura University 190000 SR
8	Design and synthesis of novel thiazolidinedione derivatives for anti-diabetic, antioxidant and antiglycation activities	أ.د. صالح عبد المجيد أحمد	DSR Umm Al-Qura University 198000 SR
9	New Observations of Acid-catalysed Accretion Reaction of Aldehydes	د. أحمد حميد د. أحمد الحربي د. علي صيقل	DSR Umm Al-Qura University 99000 SR
10	Corrosion inhibition of carbon steel using composite of nanostructured materials and ecofriendly corrosion inhibitors	أ.د. متولي عبدالله د. حاتم الطس أ.د. محمد عواد	DSR Umm Al-Qura University 70000 SR
11	Novel electrocatalyst with high tailoring against poisoning in fuel cells	د. محمد قاسم د. بدرية الجحدلي د. معتز مراد أ.د. محمد عواد	DSR Umm Al-Qura University 70000 SR

ثالثا: الكتب المنشورة بقسم الكيمياء :

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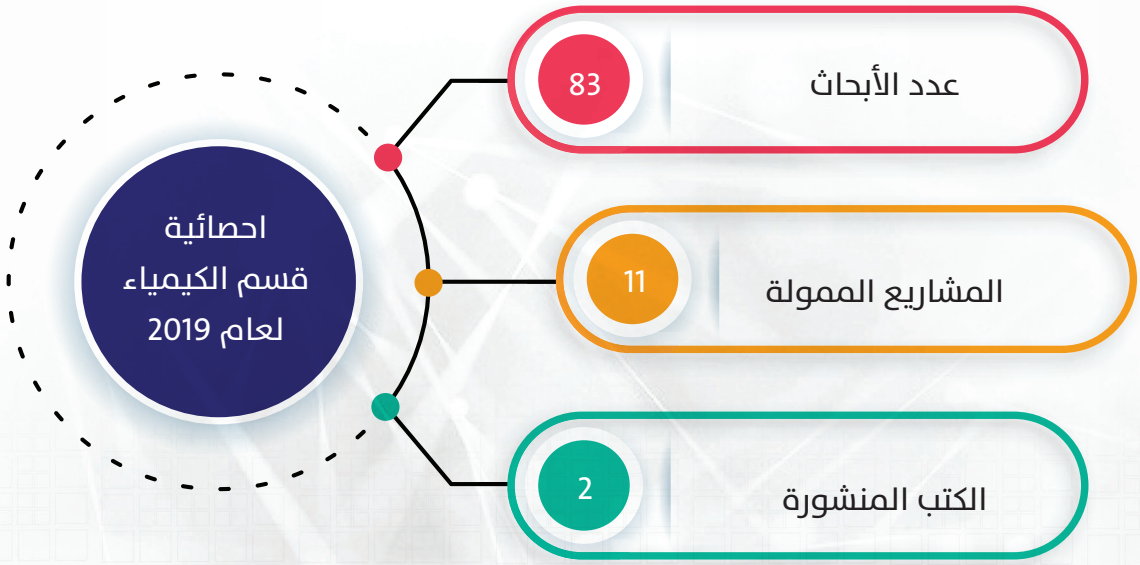
1	Non-Enzymatic Exogenous and Endogenous Antioxidants	Ziad Moussa, Zaher M. A. Judeh, Saleh A. Ahmed	IntechOpen
2	An Efficient Route for Synthesis of Macrocyclic Gadolinium Complexes and Their Role in Medical Applications	Rasha E. El-Mekawy	Intech open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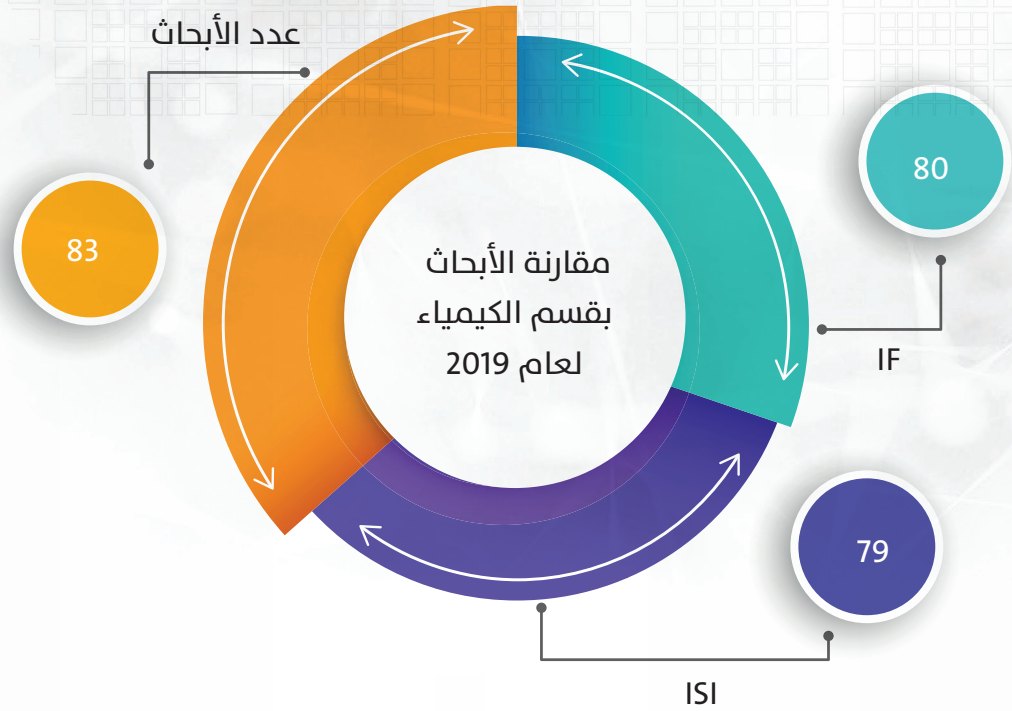
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ARTICLE IN PRESS

Heliyon 5 (2019) e01982

Contents lists available at ScienceDirect

Heliyon

journal homepage: www.heliyon.com

Bioactive fluorenes. part I. Synthesis, pharmacological study and molecular docking of novel dihydrofolate reductase inhibitors based-2,7-dichlorofluorene

Essam M. Hussein[a,b,*], Reem I. Alsantali[a,c,1], Shimaa M. Abd El-Galil[d], Rami J. Obaid[a], Ahmed Alharbi[a], Mohamed A.S. Abourehab[e,f], Saleh A. Ahmed[a,b,**]

[a] Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, 21955, Makkah, Saudi Arabia
[b] Chemistry Department, Faculty of Science, Assiut University, 71516, Assiut, Egypt
[c] Department of Pharmaceutical Chemistry, Pharmacy College, Taif University, 888, Taif, Saudi Arabia
[d] Department of Pharmaceutical Organic Chemistry, Faculty of Pharmacy (girls), Al-azhar University, Nasr City, Cairo, Egypt
[e] Department of Pharmaceutics, Faculty of Pharmacy, Umm Al-Qura University, Makkah, Saudi Arabia
[f] Department of Pharmaceutics and Industrial Pharmacy, Faculty of Pharmacy, Minia University, Minia, Egypt

ARTICLE INFO

Keywords:
Organic chemistry
Fluorene
Anti-cancer
Antimicrobial
DHFR inhibitors
Molecular docking

ABSTRACT

In this study, a new series of 2,7-dichloro-4-(2-substituted-amino acetyl)fluorene derivatives were synthesized, characterized and evaluated for their antimicrobial activity and screened for cytotoxic activity against human lung carcinoma (A-549) and human breast carcinoma (MCF-7) cell lines. Most of the synthesized compounds displayed significant activity against A-549 and MCF-7 cell lines when compared to 5-fluorouracil (5-FU), which was used as a reference drug. In addition, some of these reported novel compounds exhibited promising antibacterial and antifungal properties. A molecular docking study was performed to identify the mechanism of action of the synthesized compounds, which suggested binding interactions with the active sites of dihydrofolate reductase (DHFR).

1. Introduction

Fluorene and its derivatives are versatile reagents which are used in wide range of synthetic applications [1]. Fluorene-based aromatic ketones are of profound interest as building blocks for the production of drugs, pharmaceuticals and industrial fine chemicals [2, 3] particularly in the production of lubricating and thermosetting plastic materials. Furthermore, fluorene-based polymers and copolymers are of interest owing to their unusual optical and electrical properties and therefore are usually used in organic light-emitting diodes, flat panel displays and in solar cells [4, 5, 6].

Benflumetol is a racemic fluorene derivative, which mimics the structure and reactivity of the arylamino alcohol group of antimalarial drugs such as quinine, mefloquine, and halofantrine (Fig. 1) and is used as antimalarial agent in combination treatment with artemether [7]. In the synthesis of benflumetol, 2,7-dichloro-4-(chloroacetyl)fluorene is an important intermediate [8]. Interestingly, *N*-arylaminoacetyl, *N*-alkylaminoacetyl, and *N*-dialkylaminoacetyl derivatives are reported to exhibit a wide spectrum of pharmacological activities such as antitumor, anti-inflammatory, antibacterial, antiviral, antituberculer and anti-arrhythmic activity [9, 10, 11].

In cellular functions, dihydrofolate reductase (DHFR) is an enzyme that reduces 7,8-dihydrofolate (DHF) to 5,6,7,8-tetrahydrofolate (THF) using NADPH as electron donor: $DHF + NADPH + H^+ \rightarrow THF + NADP^+$, which is the precursor of the co-factors required for the biosynthesis of purine nucleotides, thymidine (precursor for DNA replication) and several amino acids [12]. Thus, inhibition of DHFR can lead to the disruption of DNA synthesis and the death of the cancer cells [12, 13]. In addition to this, bacteria also need DHFR to grow and multiply and hence inhibitors selective for bacterial vs. host DHFR have found application as antibacterial agents [14]. These two important factors make the enzyme a key target for both antibacterial and antitumor drug design in cancer

* Corresponding author.
** Corresponding author.
E-mail addresses: essam.hussein78@yahoo.com (E.M. Hussein), saahmed@uqu.edu.sa, saleh_63@hotmail.com (S.A. Ahmed).
[1] This work is a part of Ph. D thesis of R.I. Alsantali.

https://doi.org/10.1016/j.heliyon.2019.e01982
Received 2 May 2019; Received in revised form 18 May 2019; Accepted 19 May 2019
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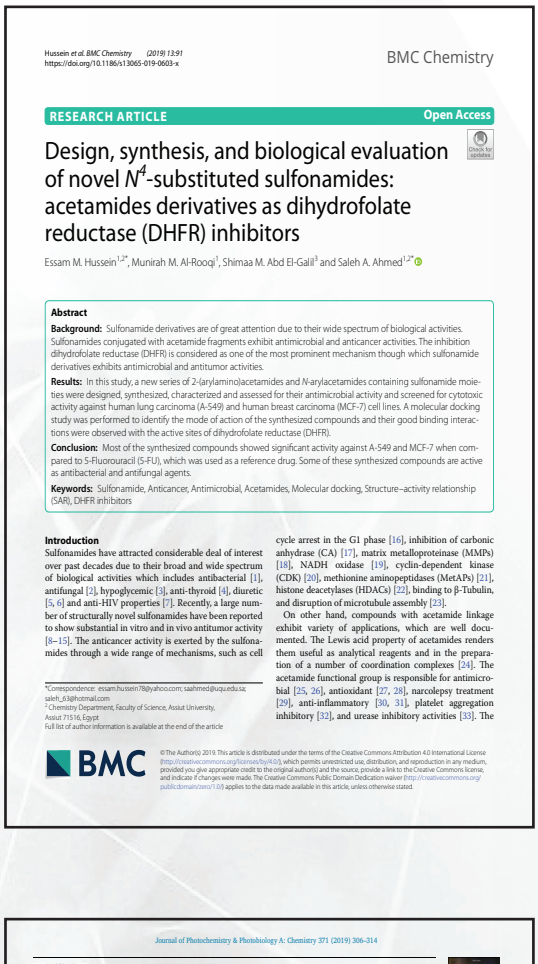
Please cite this article as: E.M. Hussein et al., Bioactive fluorenes. part I. Synthesis, pharmacological study and molecular docking of novel dihydrofolate reductase inhibitors based-2,7-dichlorofluorene, Heliyon, https://doi.org/10.1016/j.heliyon.2019.e01982



Hussein et al. BMC Chemistry (2019) 13:91
https://doi.org/10.1186/s13065-019-0603-x

BMC Chemistry

RESEARCH ARTICLE Open Access

Design, synthesis, and biological evaluation of novel N^4-substituted sulfonamides: acetamides derivatives as dihydrofolate reductase (DHFR) inhibitors

Essam M. Hussein[1,2*], Munirah M. Al-Rooqi[1], Shimaa M. Abd El-Galil[3] and Saleh A. Ahmed[1,2*]

Abstract

Background: Sulfonamide derivatives are of great attention due to their wide spectrum of biological activities. Sulfonamides conjugated with acetamide fragments exhibit antimicrobial and anticancer activities. The inhibition dihydrofolate reductase (DHFR) is considered as one of the most prominent mechanism though which sulfonamide derivatives exhibits antimicrobial and antitumor activities.

Results: In this study, a new series of 2-(arylamino)acetamides and *N*-arylacetamides containing sulfonamide moieties were designed, synthesized, characterized and assessed for their antimicrobial activity and screened for cytotoxic activity against human lung carcinoma (A-549) and human breast carcinoma (MCF-7) cell lines. A molecular docking study was performed to identify the mode of action of the synthesized compounds and their good binding interactions were observed with the active sites of dihydrofolate reductase (DHFR).

Conclusion: Most of the synthesized compounds showed significant activity against A-549 and MCF-7 when compared to 5-Fluorouracil (5-FU), which was used as a reference drug. Some of these synthesized compounds are active as antibacterial and antifungal agents.

Keywords: Sulfonamide, Anticancer, Antimicrobial, Acetamides, Molecular docking, Structure–activity relationship (SAR), DHFR inhibitors

Introduction

Sulfonamides have attracted considerable deal of interest over past decades due to their broad and wide spectrum of biological activities which includes antibacterial [1], antifungal [2], hypoglycemic [3], anti-thyroid [4], diuretic [5, 6] and anti-HIV properties [7]. Recently, a large number of structurally novel sulfonamides have been reported to show substantial in vitro and in vivo antitumor activity [8–15]. The anticancer activity is exerted by the sulfonamides through a wide range of mechanisms, such as cell cycle arrest in the G1 phase [16], inhibition of carbonic anhydrase (CA) [17], matrix metalloproteinase (MMPs) [18], NADH oxidase [19], cyclin-dependent kinase (CDK) [20], methionine aminopeptidases (MetAPs) [21], histone deacetylases (HDACs) [22], binding to β-Tubulin, and disruption of microtubule assembly [23].

On other hand, compounds with acetamide linkage exhibit variety of applications, which are well documented. The Lewis acid property of acetamides renders them useful as analytical reagents and in the preparation of a number of coordination complexes [24]. The acetamide functional group is responsible for antimicrobial [25, 26], antioxidant [27, 28], narcolepsy treatment [29], anti-inflammatory [30, 31], platelet aggregation inhibitory [32], and urease inhibitory activities [33]. The

*Correspondence: essam.hussein78@yahoo.com; saahmed@uqu.edu.sa; saleh_63@hotmail.com
[2] Chemistry Department, Faculty of Science, Assiut University, Assiut 71516, Egypt
Full list of author information is available at the end of the article

CHEMICAL ENGINEERING COMMUNICATIONS
2019, VOL. 206, NO. 2, 137–148
https://doi.org/10.1080/00986445.2018.1477761

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Competent inhibitor for the corrosion of zinc in hydrochloric acid based on 2,6-bis-[1-(2-phenylhydrazono)ethyl]pyridine

M. Abdallah[a,b], S. A. Ahmed[a,c], H. M. Altass[a], I. A. Zaafarany[a], M. Salem[d], A. I. Aly[b], and E. M. Hussein[a,c]

[a]Department of Chemistry, Faculty of Applied Sciences, Umm Al-Qura University, Makkah, Saudi Arabia; [b]Department of Chemistry, Faculty of Science, Benha University, Benha, Egypt; [c]Department of Chemistry, Faculty of Science, Assiut University, Assiut, Egypt; [d]Department of Chemistry, College of Science, Majmaah University, Majmaah, Saudi Arabia

ABSTRACT

A novel compound, 2,6-bis-[1-(2-phenylhydrazono)ethyl]pyridine (BPEP), was synthesized and confirmed by NMR and IR spectroscopy. BPEP was examined as an inhibitor for the corrosion of zinc electrode in 1.0 M HCl. The inhibition efficiency of BPEP was assessed through various techniques such as hydrogen evolution, galvanostatic polarization, potentiodynamic anodic polarization, and electrochemical impedance spectroscopy. The inhibiting action of BPEP was explained in terms of the formation of a stable complex between zinc ions and BPEP and then adsorbed onto the zinc surface. The formation of the complex was established by FT-IR spectroscopy. A conductometric titration indicated that the stoichiometry of Zn^{+2}-BPEP (metal:ligand) is 1:1. The adsorption follows the Langmuir isotherm. The Galvanostatic polarization measurements have shown that the BPEP molecule acts as a mixed-type inhibitor. The pitting potential shifted in the noble direction, indicating that the inhibition of pitting corrosion of zinc in the presence of BPEP. The activation energy and thermodynamic parameters of the adsorption process were calculated and have been explained.

KEYWORDS
Adsorption; 2,6-Bis-[1-(2-phenylhydrazono)ethyl]pyridine; Corrosion inhibitor; Zinc

Introduction

Zinc metal is used in many industrial applications such as the manufacture defensive coatings for steel, vehicle, shipbuilding industries, household electrical appliances, batteries and other light industries. HCl solutions are used for pickling and cleaning zinc surfaces, which are highly susceptible to corrosion when exposed to acid solutions, especially HCl. Corrosion inhibitors are used to reduce the aggressive attack of acid (Agrawal et al., 2004). The most common corrosion inhibitors are nitrogen-, oxygen-, and/or sulfur-based organic compounds. These compounds inhibit zinc corrosion in the acidic medium by absorption on the zinc surface (Troquet et al., 1981; Abdallah, 2003; Wang et al., 2003; El-Sherbini et al., 2005; Abdallah et al., 2009b; Abiola and James, 2010; Fouda et al., 2006, 2010; Shanbhag et al., 2011; Abdallah et al., 2011, 2012a, 2013b, 2014, 2016b; Suedile et al., 2014).

The adsorbed layer isolates the zinc surface from the corrosive acidic solution. The adsorption force depends on the chemical composition of the organic compound (Stupnisek-Lisac et al. 1994). The importance of zinc metal and its corrosion motivated us to explore the inhibiting effect of a new synthetic organic compound, 2,6-bis-[1-(2-phenylhydrazono)ethyl]pyridine (BPEP), on the dissolution of zinc in 1.0 M HCl. Numerous chemical techniques such as evolution of hydrogen reaction and electrochemical techniques such as galvanostatic and potentiodynamic anodic polarization and electrochemical impedance spectroscopy (EIS) were used to estimate the percentage inhibition efficacy of this compound. The adsorption isotherm, the stoichiometry of the complex formed between Zn^{+2} and BPEP, and the mechanism of inhibition were also elucidated.

Experimental methods

The purity of the Zn metal used in this study as a working electrode is 99.99%. For the hydrogen evolution reaction, test Zn sheets with dimensions $1.0 \times 1.0 \times 0.2\ cm^3$ were used. To obtain a smooth

CONTACT M. Abdallah metwally555@yahoo.com Department of Chemistry, Faculty of Science, Benha University, Benha, Egypt.
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Journal of Photochemistry & Photobiology A: Chemistry 371 (2019) 306–314

Contents lists available at ScienceDirect

Journal of Photochemistry & Photobiology A: Chemistry

journal homepage: www.elsevier.com/locate/jphotochem

MCM-SO_3H catalyzed synthesis of environment-sensitive fluorophores incorporating pyrene moiety: Optimization, fluorescence emission and theoretical studies

Nizar El Guesmi[a,b], Essam M. Hussein[a,c], Saleh A. Ahmed[a,c,*]

[a] Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, 21955, Makkah, Saudi Arabia
[b] Département de chimie, Faculté des Sciences de Monastir, Avenue de l'Environnement, 5019, Monastir, Tunisia
[c] Department of Chemistry, Faculty of Science, Assiut university, 71516, Assiut, Egypt

ARTICLE INFO

Keywords:
MCM-SO_3H
Pyrene
Fluorophores
Solvatochromic properties
2-Pyrazolines
Eco-friendly

ABSTRACT

Six new highly fluorescent 5-(aryl)-1-phenyl-3-(pyren-1yl)-2-pyrazolines were synthesized by reaction of various (*E*)-3-aryl-1-(pyren-1-yl)prop-2-en-1-ones with phenyl hydrazine in the presence of sulfonated mesoporous silica (MCM-SO_3H) as efficient and eco-friendly acidic catalyst. The chemical structures of all synthesized compounds were illustrated on the basis of spectral data (IR, ^{1}H NMR and ^{13}C NMR). This was followed by photophysical properties-based absorption and emission studies of the target compounds in solutions of different solvent polarities. The microenvironment-sensitive fluorescent pyrazolines labeled with pyrene exhibited valuable fluorescence properties with emission in the range of 600–700 nm with a marked response to change in the environmental polarities. A significant and pronounced red shift was observed in the emission spectrum of 5-(aryl)-1-phenyl-3-(pyren-1yl)-2-pyrazolines Δλ ~ 50 nm compared to the absorption spectrum Δλ ~ 10 nm upon increasing the solvent polarity. This indicated the presence of higher dipole moment in the excited state than in the ground state and the transition involved are π-π* transition through the charge transfer phenomena. The fundamental understanding of solvatochromic properties were analyzed through Lippert-Mataga and Reichardts correlations in order to estimate the change in dipole moments (Δμ) which suggested the emissive state of designed fluorescent 2-pyrazoline derivatives is of strong ICT character.

1. Introduction

Pyrene is a well-known polynuclear aromatic hydrocarbon, which recently become one of the most widely studied organic molecules in the field of photochemistry and photophysics. Because of its unique properties, it has emerged as an outstanding area of areas in many scientific fields. The highly fluorescence properties of pyrene has rendered it to a fluorophore of first choice in both applied and fundamental photochemical and photophysical research [1–10]. Interestingly, pyrene is one of few polycyclic aromatic hydrocarbons that perform vibronic structure in its monomer fluorescence spectrum in solution [11]. Its derivatives have been extensively expended in many applications such as fluorescent sensors [12,13] or fluorescent probes [14] based on virtue of their excellent fluorescence properties. Pyrene monomer emission typically occurs between 370 and 420 nm exhibiting a characteristic violet color and is considered as one of the most useful frameworks for the construction of fluorogenic chemosensors by conjugating with numerous and diverse chemical species [15]. This has encouraged the development of new synthetic methodologies for the synthesis of pyrene type substances. Some of these compounds can be used as useful key intermediates for the synthesis of precious heterocyclic ring systems. Among them, 1-cinnamoylpyrenes synthesized through the Claisen-Schmidt condensation of 1-acetylpyrene and aromatic aldehydes [16,17] has proved to be particularly important. 1-Cinnamoylpyrenes have been used for the synthesis of functionalized pyrrolidines [16], pyrrolizidines [17] and other nitrogen-based heterocycles. Furthermore, pyrazolines are important nitrogen-containing five membered heterocyclic compounds. Literature survey revealed that many pyrazoline derivatives are known to exhibit a wide range of biological activities such as antimicrobial [18], antimalarial [19], antitumor [20], anti-inflammatory [20], anticonvulsant and antidepressants activities [21].

2 -Pyrazoline derivatives are the most commonly studied pyrazoline-type compounds and numerous methods have been reported for

* Corresponding author at: Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, 21955, Makkah, Saudi Arabia.
E-mail address: saahmed@uqu.edu.sa (S.A. Ahmed).

https://doi.org/10.1016/j.jphotochem.2018.11.026
Received 18 October 2018; Received in revised form 22 November 2018; Accepted 24 November 2018
Available online 26 November 2018
1010-6030/

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ELECTROANALYSIS

DOI: 10.1002/elan.201900141

Enhanced Electrocatalytic Oxidation of Paracetamol at DNA Modified Gold Electrode

Ismail I. Althagafi,[b] Mohammed A. Kassem,[a,b] and Mohamed I. Awad[a,c]

Abstract: Cysteine monolayer has been assembled onto bare gold electrode (SAM/Au), and subsequently deoxyribonucleic acid (DNA) has been successfully immobilized at the SAM/Au electrode. The thus modified electrode is assigned DNA/SAM/Au. Modification steps of the electrode were followed electrochemically using $K_4[Fe(CN_6)]$ electrochemical marker. Also, the build-up of the modified electrode composition is followed using EDX and the crystallographic orientation is inspected using XRD. The electrochemical behavior of paracetamol (PC) at DNA/SAM/Au electrode is investigated. Interestingly, the sluggish irreversible behavior of PC at the bare gold electrode is converted to a quasi-reversible one at DNA/SAM/Au electrode pointing to some interaction between the immobilized DNA and PC. The enhanced electrochemical behavior of PC at modified DNA/SAM/Au electrode is successfully used for a sensitive electrochemical determination of PC. Square wave voltammetry (SWV) was used for this purpose. The concentration of PC was in linear relation with the peak current at the optimum conditions within the range 10.0–110.0 μg mL^{-1} with correlation coefficient (R^2) of 0.998. Also, the standard deviation (SD) and relative standard deviation (RSD) were calculated and found to be 0.817 and 1.52, respectively, indicating the significance of the present method.

Keywords: Self-assembly monolayer · DNA · Paracetamol · Electrocatalysis

1 Introduction

Deoxyribonucleic acid (DNA) is the information source controlling all life processes of the organism. Transcription and replication, which are the main functions of the DNA, are vital to functioning of all body processes in the proper way. DNA interactions with drugs have become an active area of research as DNA is the major target of drug interactions. These interactions have been utilized as a base for the estimation of DNA and/or drugs [1–3]. Such interactions are a fundamental issue in life process, for gene delivery systems. On the other hand, analytical determination based on DNA is an essential for clinical diagnosis in discovering the different ways which develop the disease, and consequently to find suitable ways of remediation. Several analytical methods have been reported, as for instance, flow injection chemiluminescence, capillary electrophoresis, ion pairing liquid, micellar electrokinetic chromatography and laser-induced fluorescence detection [4–10]. Also, interactions of DNA with some drugs have been utilized in the analysis of these drugs at DNA modified electrodes. For instance, the analysis of didanosine [11] and 6-mercaptopurine [12] using voltammetric techniques, which are sensitive, simple and compatible with micro fabrication technology. It offers advantages over conventional used biological and chemical assays. Signal amplification strategies have been used to increase the electrochemical biosensors sensitivity. In this correspondence, electro-active polymer as the transduction element has been reported [13–21]. The electroactivity of DNA at those electrodes is controlled by the structure and conformation of DNA as well as its damage [18,19]. Electroactivity of DNA is due to the presence of adenine, cytosine and guanine [22,13–20]. In the present work, the DNA modified gold electrode is utilized in the enhanced electrocatalytic oxidation and the subsequent electroanalysis of paracetamol (PC). PC is a main component in plentiful cold and flu medications. It is widely used over-the-counter analgesic and antipyretic for the relief of headaches and other minor pains. A rapid simple method for the analysis of PC is needed for pharmaceutical control. Several methods have been reported for assaying PC in pharmaceutical preparations [23–31]. Among these methods, chromatographic methods

[a] I. I. Althagafi, M. A. Kassem, M. I. Awad
Chemistry Department, Faculty of Applied Science, Umm Al-Qura University, Makkah, Kingdom Saudi Arabia
Tel: 00966595491550
E-mail: mawad700@yahoo.com
miawad@uqu.edu.sa
[b] M. A. Kassem
Chemistry Department, Faculty of Science, Benha University, Benha, 13518, Egypt
Tel: 00966532175442
E-mail: maa_kassem@hotmail.com
makassem@uqu.edu.sa
[c] M. I. Awad
Chemistry Department, Faculty of Science, Cairo University, Cairo, Egypt
E-mail: mawad700@yahoo.com
miawad@uqu.edu.sa

Supporting information for this article is available on the WWW under https://doi.org/10.1002/elan.201900141

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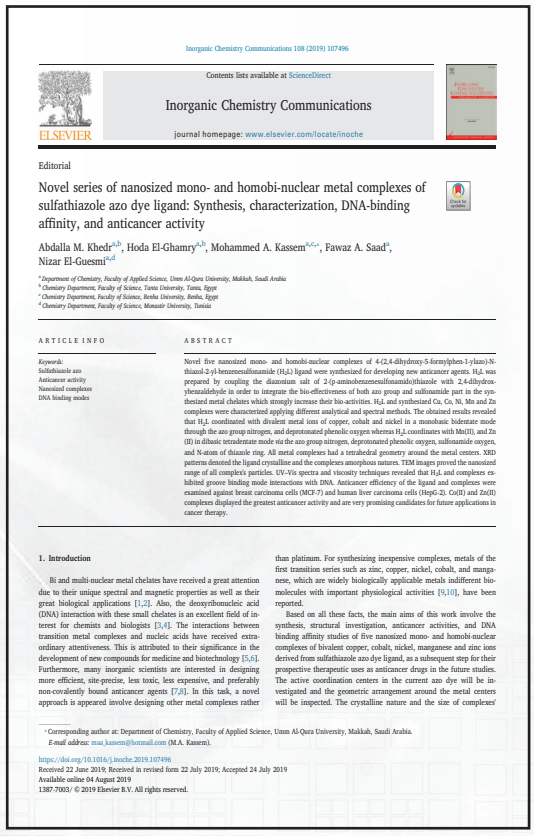


Inorganic Chemistry Communications 108 (2019) 107496

Contents lists available at ScienceDirect

Inorganic Chemistry Communications

journal homepage: www.elsevier.com/locate/inoche

Editorial

Novel series of nanosized mono- and homobi-nuclear metal complexes of sulfathiazole azo dye ligand: Synthesis, characterization, DNA-binding affinity, and anticancer activity

Abdalla M. Khedr[a,b], Hoda El-Ghamry[a,b], Mohammed A. Kassem[a,c,*], Fawaz A. Saad[a], Nizar El-Guesmi[a,d]

[a] Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia
[b] Chemistry Department, Faculty of Science, Tanta University, Tanta, Egypt
[c] Chemistry Department, Faculty of Science, Benha University, Benha, Egypt
[d] Chemistry Department, Faculty of Science, Monastir University, Tunisia

ARTICLE INFO

Keywords:
Sulfathiazole azo
Anticancer activity
Nanosized complexes
DNA binding modes

ABSTRACT

Novel five nanosized mono- and homobi-nuclear complexes of 4-(2,4-dihydroxy-5-formylphen-1-ylazo)-*N*-thiazol-2-ylbenzenesulfonamide (H_2L) ligand were synthesized for developing new anticancer agents. H_2L was prepared by coupling the diazonium salt of 2-(p-aminobenzenesulfonamido)thiazole with 2,4-dihydroxybenzaldehyde in order to integrate the bio-effectiveness of both azo group and sulfonamide part in the synthesized metal chelates which strongly increase their bio-activities. H_2L and synthesized Cu, Co, Ni, Mn and Zn complexes were characterized applying different analytical and spectral methods. The obtained results revealed that H_2L coordinated with divalent metal ions of copper, cobalt and nickel in a monobasic bidentate mode through the azo group nitrogen, and deprotonated phenolic oxygen whereas H_2L coordinates with Mn(II), and Zn (II) in dibasic tetradentate mode via the azo group nitrogen, deprotonated phenolic oxygen, sulfonamide oxygen, and N-atom of thiazole ring. All metal complexes had a tetrahedral geometry around the metal centers. XRD patterns denoted the ligand crystalline and the complexes amorphous natures. TEM images proved the nanosized range of all complex's particles. UV–Vis spectra and viscosity techniques revealed that H_2L and complexes exhibited groove binding mode interactions with DNA. Anticancer efficiency of the ligand and complexes were examined against breast carcinoma cells (MCF-7) and human liver carcinoma cells (HepG-2). Co(II) and Zn(II) complexes displayed the greatest anticancer activity and are very promising candidates for future applications in cancer therapy.

1. Introduction

Bi and multi-nuclear metal chelates have received a great attention due to their unique spectral and magnetic properties as well as their great biological applications [1,2]. Also, the deoxyribonucleic acid (DNA) interaction with these small chelates is an excellent field of interest for chemists and biologists [3,4]. The interactions between transition metal complexes and nucleic acids have received extraordinary attentiveness. This is attributed to their significance in the development of new compounds for medicine and biotechnology [5,6]. Furthermore, many inorganic scientists are interested in designing more efficient, site-precise, less toxic, less expensive, and preferably non-covalently bound anticancer agents [7,8]. In this task, a novel approach is appeared involve designing other metal complexes rather than platinum. For synthesizing inexpensive complexes, metals of the first transition series such as zinc, copper, nickel, cobalt, and manganese, which are widely biologically applicable metals indifferent biomolecules with important physiological activities [9,10], have been reported.

Based on all these facts, the main aims of this work involve the synthesis, structural investigation, anticancer activities, and DNA binding affinity studies of five nanosized mono- and homobi-nuclear complexes of bivalent copper, cobalt, nickel, manganese and zinc ions derived from sulfathiazole azo dye ligand, as a subsequent step for their prospective therapeutic uses as anticancer drugs in the future studies. The active coordination centers in the current azo dye will be investigated and the geometric arrangement around the metal centers will be inspected. The crystalline nature and the size of complexes'

* Corresponding author at: Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia.
E-mail address: maa_kassem@hotmail.com (M.A. Kassem).

https://doi.org/10.1016/j.inoche.2019.107496
Received 22 June 2019; Received in revised form 22 July 2019; Accepted 24 July 2019
Available online 04 August 2019
1387-7003/

Received: 10 December 2018 | Revised: 22 January 2019 | Accepted: 1 April 2019
DOI: 10.1002/aoc.4965

FULL PAPER

WILEY Applied Organometallic Chemistry

Synthesis, structural characterization and DNA binding affinity of new bioactive nano-sized transition metal complexes with sulfathiazole azo dye for therapeutic applications

Fawaz A. Saad[1] | Hoda A. El-Ghamry[1,2] | Mohammed A. Kassem[1,3]

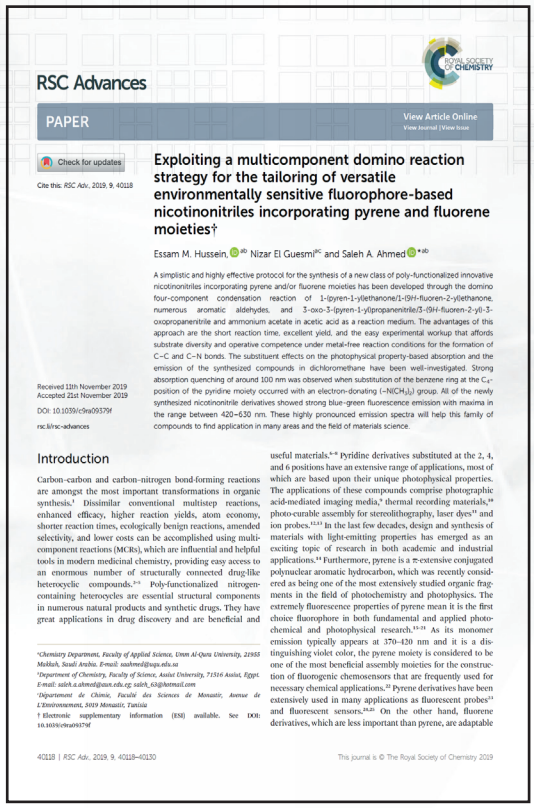
[1]Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia
[2]Chemistry Department, Faculty of Science, Tanta University, Tanta, Egypt
[3]Chemistry Department, Faculty of Science, Benha University, Benha, Egypt

Correspondence
Hoda El-Ghamry, Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia.
Email: helghamrymo@yahoo.com

Funding information
King Abdulaziz City for Science and Technology (KACST), Grant/Award Number: 37-175

The azo dye ligand 4-(5-chloro-2-hydroxyphenylazo)-*N*-thiazol-2-ylbenzenesulfonamide (H_2L) formed by the coupling reaction of sulfathiazole and *p*-chlorophenol was synthesized and characterized using elemental analysis and Fourier transform infrared (FT-IR) as well as UV–visible spectra. Nano-sized divalent Cu, Co, Ni, Mn and Zn complexes of the synthesized azo dye ligand were prepared and investigated using various spectroscopic and analytical techniques. Elemental and thermal analyses indicated the formation of the Cu(II), Ni(II) and Mn(II) complexes in a molar ratio of 1:2 (L:M) while Co(II) and Zn(II) complexes exhibited a 1:1 (M:L) ratio. FT-IR spectral studies confirmed the coordination of the ligand to the metal ions through the phenolic hydroxyl oxygen, azo nitrogen, sulfonamide oxygen and/or thiazole nitrogen. The geometric arrangements around the central metal ions were investigated applying UV–visible and electron spin resonance spectra, thermogravimetric analysis and molar conductance measurements. X-ray diffraction patterns revealed crystalline nature of H_2L and amorphous nature of all synthesized complexes. Transmission electron microscopy images confirmed nano-sized particles and their homogeneous distribution over the complex surface. Antibacterial, antifungal and antitumour activities of the investigated complexes were screened compared with familiar standard drugs to confirm their potential therapeutic applications. The Cu(II) complex showed IC_{50} of 3.47 μg ml^{-1} (5.53 μM) against hepatocellular carcinoma cells, which means that it is a more potent anticancer drug compared with the standard cisplatin (IC_{50} = 3.67 μg ml^{-1} (12.23 μM)). Furthermore, the Co(II), Ni(II), Cu(II) and Zn(II) complexes displayed IC_{50} greater than that of an applied standard anticancer agent (5-flurouracil) towards breast carcinoma cells. Hence, these complexes can be considered as promising anticancer drugs. The mode of binding of the complexes with salmon serum DNA was determined through electronic absorption titration and viscosity studies.

KEYWORDS
anticancer, characterization, DNA binding, nano-sized complexes, sulfthiazole



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Cite this: *RSC Adv.*, 2019, 9, 40118

Exploiting a multicomponent domino reaction strategy for the tailoring of versatile environmentally sensitive fluorophore-based nicotinonitriles incorporating pyrene and fluorene moieties†

Essam M. Hussein, Nizar El Guesmi and Saleh A. Ahmed *

A simplistic and highly effective protocol for the synthesis of a new class of poly-functionalized innovative nicotinonitriles incorporating pyrene and/or fluorene moieties has been developed through the domino four-component condensation reaction of 1-(pyren-1-yl)ethanone/1-(9*H*-fluoren-2-yl)ethanone, numerous aromatic aldehydes, and 3-oxo-3-(pyren-1-yl)propanenitrile/3-(9*H*-fluoren-2-yl)-3-oxopropanenitrile and ammonium acetate in acetic acid as a reaction medium. The advantages of this approach are the short reaction time, excellent yield, and the easy experimental workup that affords substrate diversity and operative competence under metal-free reaction conditions for the formation of C–C and C–N bonds. The substituent effects on the photophysical property-based absorption and the emission of the synthesized compounds in dichloromethane have been well-investigated. Strong absorption quenching of around 100 nm was observed when substitution of the benzene ring at the C_4-position of the pyridine moiety occurred with an electron-donating (–$NICH_3)_2$) group. All of the newly synthesized *nicotinonitrile* derivatives showed strong blue–green fluorescence emission with maxima in the range between 420–630 nm. These highly pronounced emission spectra will help this family of compounds to find application in many areas and the field of materials science.

Received 11th November 2019
Accepted 21st November 2019
DOI: 10.1039/c9ra09379f
rsc.li/rsc-advances

Introduction

Carbon–carbon and carbon–nitrogen bond-forming reactions are amongst the most important transformations in organic synthesis.[1] Dissimilar conventional multistep reactions, enhanced efficacy, higher reaction yields, atom economy, shorter reaction times, ecologically benign reactions, amended selectivity, and lower costs can be accomplished using multicomponent reactions (MCRs), which are influential and helpful tools in modern medicinal chemistry, providing easy access to an enormous number of structurally connected drug-like heterocyclic compounds.[2–5] Poly-functionalized nitrogen-containing heterocycles are essential structural components in numerous natural products and synthetic drugs. They have great applications in drug discovery and are beneficial and useful materials.[6–8] Pyridine derivatives substituted at the 2, 4, and 6 positions have an extensive range of applications, most of which are based upon their unique photophysical properties. The applications of these compounds comprise photographic acid-mediated imaging media,[9] thermal recording materials,[10] photo-curtable assembly for stereolithography, laser dyes[11] and ion probes.[12,13] In the last few decades, design and synthesis of materials with light-emitting properties has emerged as an exciting topic of research in both academic and industrial applications.[14] Furthermore, pyrene is a π-extensive conjugated polynuclear aromatic hydrocarbon, which was recently considered as being one of the most extensively studied organic fragments in the field of photochemistry and photophysics. The extremely fluorescence properties of pyrene mean it is the first choice fluorophore in both fundamental and applied photochemical and photophysical research.[15–18] As its monomer emission typically appears at 370–420 nm and it is a distinguishing violet color, the pyrene moiety is considered to be one of the most beneficial assembly moieties for the construction of fluorogenic chemosensors that are frequently used for necessary chemical applications.[19] Pyrene derivatives have been extensively used in many applications as fluorescent probes[13] and fluorescent sensors.[20,21] On the other hand, fluorene derivatives, which are less important than pyrene, are adaptable

[a]Chemistry Department, Faculty of Applied Science, Umm Al-Qura University, 21955 Makkah, Saudi Arabia. E-mail: saahmed@uqu.edu.sa
[b]Department of Chemistry, Faculty of Science, Assiut University, 71516 Assiut, Egypt. E-mail: saleh.a.ahmed@aun.edu.eg; saleh_63@hotmail.com
[c]Département de Chimie, Faculté des Sciences de Monastir, Avenue de L'Environnement, 5019 Monastir, Tunisia

† Electronic supplementary information (ESI) available. See DOI: 10.1039/c9ra09379f

ORIENTAL JOURNAL OF CHEMISTRY
An International Open Access, Peer Reviewed Research Journal
www.orientjchem.org
Est. 1984
ISSN: 0970-020 X
CODEN: OJCHEG
2019, Vol. 35, No.(2):
Pg. 626-636

Characterization of Palladium Chelates and their Interactions with Z-N'-(benzo(d)thiazol-2-yl)-N,N-dimethylformimidamide using the Spectrophotometric and Computational Methods

AMR LOTFY SABER[1,2*], WAEL ABD-ALLAH ZORDOK[1,3], AHMED ALHARBI[2] and ABDU SUBAIHI[2]

[1]Department of Chemistry, Faculty of Science, Zagazig University, Zagazig, Egypt.
[2]Department of Chemistry, Faculty of Applied Science, Umm Al Qura University, Makkah, Kingdom of Saudi Arabia.
[3]Department of Chemistry, Al-Qunfidhah University College, Kingdom of Saudi Arabia.
*Corresponding author E-mail: alshefny@yahoo.com

http://dx.doi.org/10.13005/ojc/350217

(Received: December 10, 2018; Accepted: March 24, 2019)

ABSTRACT

A rapid, selective and sensitive method for the quantification of Pd (II) using spectrophotometric technique associated with Z-N'-(benzo(d)thiazol-2-yl)-N,N-dimethylformimidamide BTDF as new chelating agent is described. Yellow colored complex of Pd (II) with BTDF is formed in Britton-Robinson universal buffer of pH 9 and extracted with chloroform. The formed complex clearly illustrate an absorption at ~384 nm and follw Beer's law in the range of concentration between 0.5–18.0 µg ml^{-1} of Pd (II) with absorbance of 3.62 × 10^4 L mol^{-1} cm^{-1} and limit of detection (LOD) of Pd (II) 0.07 µg ml^{-1}. The effects of different experimental parameters have been established by study the optimum conditions for the extraction and quantification of palladium ion. Density functional theory (DFT) have also been employed to compute the influence of the cation on theoretical parameters of Pd^{2+} complexes. The effect of donating centers was investigated theoretically which prove that Pd^{2+} favor coordinated with two molecules of Z-N'-(benzo(d)thiazol-2-yl)-N,N-dimethylformimidamide through two nitrogen atoms. The performance of the examined method was estimated to detect the impact of current method over the presented methods in the literature without interference effect of cations and anions. The examined method has successfully demonstrated the quantification of Pd(II) in natural and spiked water samples.

Keywords: Spectrophotometry, Palladium ion, Dimethylformimidamide, DFT.

INTRODUCTION

Recently, the use of nitrogen containing heterocyclic derivatives in biological processes has attracted a lot of considerable attention, due to it snatural abundance, chemistry coordinating ability for a trace metal ion and promising application in industry[1]. The synthesis of platinum pyrimidine has

Inorganic Chemistry Communications 108 (2019) 107496

Contents lists available at ScienceDirect

Inorganic Chemistry Communications

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Editorial

Novel series of nanosized mono- and homobi-nuclear metal complexes of sulfathiazole azo dye ligand: Synthesis, characterization, DNA-binding affinity, and anticancer activity

Abdalla M. Khedr[a,b], Hoda El-Ghamry[a,b], Mohammed A. Kassem[b,c,*], Fawaz A. Saad[d], Nizar El-Guesmi[a,d]

[a] Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia
[b] Chemistry Department, Faculty of Science, Tanta University, Tanta, Egypt
[c] Chemistry Department, Faculty of Science, Benha University, Benha, Egypt
[d] Chemistry Department, Faculty of Science, Monastir University, Tunisia

ARTICLE INFO

Keywords:
Sulfathiazole azo
Anticancer activity
Nanosized complexes
DNA binding modes

ABSTRACT

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1. Introduction

Bi and multi-nuclear metal chelates have received a great attention due to their unique spectral and magnetic properties as well as their great biological applications [1,2]. Also, the deoxyribonucleic acid (DNA) interaction with these small chelates is an excellent field of interest for chemists and biologists [3,4]. The interactions between transition metal complexes and nucleic acids have received extraordinary attentiveness. This is attributed to their significance in the development of new compounds for medicine and biotechnology [5,6]. Furthermore, many inorganic scientists are interested in designing more efficient, site-precise, less toxic, less expensive, and preferably non-covalently bound anticancer agents [7,8]. In this task, a novel approach is appeared involve designing other metal complexes rather than platinum. For synthesizing inexpensive complexes, metals of the first transition series such as zinc, copper, nickel, cobalt, and manganese, which are widely biologically applicable metals indifferent biomolecules with important physiological activities [9,10], have been reported.

Based on all these facts, the main aims of this work involve the synthesis, structural investigation, anticancer activities, and DNA binding affinity studies of five nanosized mono- and homobi-nuclear complexes of bivalent copper, cobalt, nickel, manganese and zinc ions derived from sulfathiazole azo dye ligand, as a subsequent step for their prospective therapeutic uses as anticancer drugs in the future studies. The active coordination centers in the current azo dye will be investigated and the geometric arrangement around the metal centers will be inspected. The crystalline nature and the size of complexes'

* Corresponding author at: Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia.
E-mail address: maa_kassem@hotmail.com (M.A. Kassem).

https://doi.org/10.1016/j.inoche.2019.107496
Received 22 June 2019; Received in revised form 22 July 2019; Accepted 24 July 2019
Available online 04 August 2019
1387-7003/

Journal of Inorganic and Organometallic Polymers and Materials
https://doi.org/10.1007/s10904-019-01153-9

Evaluation of the Catalytic Activities of Some Synthesized Divalent and Trivalent Metal Complexes and Their Inhibition Efficiencies for the Corrosion of Mild Steel in Sulfuric Acid Medium

Khadiga M. Takroni[1] · Hoda A. El-Ghamry[1,2] · Ahmed Fawzy[1,3]

Received: 26 February 2019 / Accepted: 8 April 2019

Abstract
The divalent copper, cobalt, nickel and cadmium in addition to the trivalent iron complexes of the ligand named (E)-1-((4,6-dimethylpyrimidin-2-ylimino)methyl)naphthalen-2-ol were synthesized by the reaction of the ligand with different metal chlorides. The Structures and geometry of the metal chelates have been successfully deduced applying various analytical and spectroscopic tools such as elemental analysis, molar conductance, TGA, magnetic moment measurements, IR, ^{1}H-NMR, EI-mass and UV–Vis spectral studies. The X-ray single crystal structure of the ligand has been also discussed. Spectral studies and analytical results supported the monobasic bidentate behavior of the ligand connecting the metal ion centers via deprotonated phenolic OH and imine nitrogen. In the case of Cu(II) complex, the pyrimidine nitrogen took part in coordination to the Cu center. The results ensured the monometallic character of the chelates having 1:2 (M:L) ratio for copper, cobalt and nickel and 1:1 (M:L) ration for iron and cadmium complexes. The molar conductance data ensured that all the metal complexes are non-electrolytic type of complexes. All the complexes have been proved to have octahedral geometry. The antimicrobial activities of the synthesized metal chelates were evaluated against different bacterial and fungal strains. The synthesized ligand and its complexes were also examined as inhibitors for the corrosion of mild steel in 1.0 M H_2SO_4 at 25 °C using various techniques. The experimental outcomes indicated that the inhibition efficiencies of the tested compounds increased as their concentrations increase. The obtained inhibition efficiencies were interpreted on the basis of strong adsorption of the inhibitor molecules on the surface of mild steel and composing good protection films. The adsorption was found to obey Langmuir adsorption isotherm. The results achieved from all applied techniques are obviously compatible.

Keywords Schiff base · Metal chelates · Structural identification · Corrosion · Inhibitors

1 Introduction

The extensive usefulness of pyrimidine-based compounds is fundamentally due to their implementations in alternative fields such as pharmaceutical, agrochemical, and phytosanitary industries [1, 2]. Recently, there is a great interest in the synthesis of pyrimidine metal complexes due to biological activity including antiviral, antimalarial, antibacterial and antitumor activities [3]. Moreover, numerous number of therapeutics dependent on luminescent heterocyclic metal chelates with interesting characteristics has illustrated in literature, and related complexes may be used in the area of materials science as optical material preparations [4]. Eventually, such compounds may be also employed as significant design for bioinorganic systems, such as metalloproteins, photosensitizers and catalysts [5]. Schiff base metal complexes, as a class of inorganic compounds, are classified as a

Electronic supplementary material The online version of this article (https://doi.org/10.1007/s10904-019-01153-9) contains supplementary material, which is available to authorized users.

✉ Hoda A. El-Ghamry
helghamrymo@yahoo.com

[1] Chemistry Department, Faculty of Applied Science, Umm Al-Qura University, Mecca, Saudi Arabia
[2] Chemistry Department, Faculty of Science, Tanta University, Tanta, Egypt
[3] Chemistry Department, Faculty of Science, Assiut University, Assiut, Egypt

Published online: 16 April 2019

Springer

Int. J. Electrochem. Sci., 15 **(2020)** xx – yy

International Journal of
ELECTROCHEMICAL
SCIENCE
www.electrochemsci.org

Study of the Electrochemical Behavior of Melatonin on Different Electrodes in Aqueous Solution

G. I. Mohammed[1], A.L.Saber[1,2,]*

[1] Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, P.O. Box 16722, Makkah 21955, Saudi Arabia

[2] Department of Chemistry, Faculty of Science, University of Zagazig, Zagazig, Egypt

[*]E-mail: alshefny@yahoo.com

Received: 1 xxx 2019 / *Accepted:* 1 xxx 2019 / *Published:* 1 xxx 2019

The electrochemical investigation of melatonin was researched utilizing cyclic, linear sweep voltammetry at a glassy carbon (GC), gold (Au) and platinum (Pt) terminals. The aim of this work was to study the behavior of melatonin at different electrodes. The cyclic voltammetry (CVs) of melatonin (1.0 ×10^{-4} mol L^{-1}) were critically investigated at various sweep rate (10-1000 mV/s) at GCE, AuE and PtE in B-R buffer solution of pH 7. The repeatability,

Bisht *et al. J Pure Appl Microbiol,* **13**(3), 1611-1617 | September 2019
Article 5750 | https://doi.org/10.22207/JPAM.13.3.34
Print ISSN: 0973-7510; E-ISSN: 2581-690X

JPAM

RESEARCH ARTICLE OPEN ACCESS

Natural Products in Drug Discovery: Antibacterial and Antifungal Activity of Essential Oil of Compound Isolated from *Senecio royleanus*

Chandra Mohan Singh Bisht[1], S.M. Shakeel Iqubal[2]*, Aejaz A. Khan[2], Tasneem Mohammed[2], Areej Dawoud[2], Mohammed Gamal[3,4], S.K. Singh[5] and Basim H. Asghar[6]

[1]Department of Applied Science, IIMT College of Engineering, Greater Noida - 201 301, India. [2]Department of General Science (Chemistry), Ibn Sina National College, Jeddah, Saudi Arabia. [3]Pharmaceutical Chemistry Department, Faculty of Pharmacy, Jouf University, Skaka 2014, Kingdom of Saudi Arabia. [4]Pharmaceutical Analytical Chemistry Department, Faculty of Pharmacy, Beni-Suef University, AlshaheetShehata Ahmed Hegazy St., 62574 Beni-Suef, Egypt. [5]Department of Chemistry, GGV (Central University), Bilaspur, Chhattisgarh - 495 009, India. [6]Department of Chemistry, Faculty of Science, Umm Al-Qura, University, Makkah, Saudi Arabia.

Abstract

Natural products are an excellent source of therapeutic products which has led to the discovery of many important drugs that play an important role in the treatment of various human diseases. In this current study two compounds has been isolated from *Senecio royleanus* DC. (Asteraceae) were undertaken for antibacterial and antifungal activity against five bacterial and fungal pathogens. The compounds isolated from *Senecio royleanus*, viz; 1,10β-epoxy 6-oxo-furanoeremophilan and 1β, 10-epoxy-furanoeremophilan displayed a very important role against all bacterial and fungal strains. 1,10 β-epoxy 6-oxo-furanoeremophilan showed maximum antibacterial activity against *Agrobacterium tumefaciens* (13 mm). While it showed maximum fungal activity against *Fusarium oxysporum* (15 mm). 1β,10-Epoxy-furanoeremophilan was found inactive in antibacterial activity against *Escherichia coli*, and showed maximum zone of inhibiton against bacterial strain of *Bacillus subtilis* (12 mm) . It showed 12 mm zone against *Rhizoctonia solani* during antifungal activity. The fractions which showed significant antimicrobial activity i.e. (zoi ≥ 10 mm), were further tested to find out minimuminhibitory concentration and minimum bactericidal concentration at different concentrations.

Keywords: Asteraceae/aenecio, royleanus, Antifungal activity, Antibacterial activity.

***Correspondence:** shakeeliqubal@gmail.com; +919891308291; +966570158198

(Received: 29 July 2019; accepted: 06 September 2019)

Citation: Chandra Mohan Singh Bisht, S.M. Shakeel Iqubal Aejaz A. Khan, Tasneem Mohammed, Areej Dawoud, Mohammed Gamal, S.K. Singh and Basim H. Asghar, Natural Products in Drug Discovery: Antibacterial and Antifungal Activity of Essential Oil of Compound Isolated from *Senecio royleanus*, *J Pure Appl Microbiol.*, 2019; **13**(3): 1611-1617. https://doi.org/10.22207/JPAM.13.3.34

Journal of Molecular Liquids 292 (2019) 111436

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

Removal of toxic tellurium (IV) compounds via bioreduction using flucloxacillin in aqueous acidic medium: A kinetic and mechanistic approach

Ahmed Fawzy

Chemistry Department, Faculty of Applied Sciences, Umm Al-Qura University, Makkah, Saudi Arabia
Chemistry Department, Faculty of Science, Assiut University, Assiut, Egypt

ARTICLE INFO

Article history:
Received 1 June 2019
Received in revised form 20 July 2019
Accepted 23 July 2019
Available online 29 July 2019

Keywords:
Removal
Tellurium (VI)
Flucloxacillin
Bioreduction
Kinetics
Mechanism

ABSTRACT

This paper describes a novel method for the removal of potassium tellurite (Te^{4+}), a toxic tellurium (IV) compound, via its bioreduction using the drug flucloxacillin (Flx) in an aqueous sulfuric acid solution. The kinetics of the bioreduction process were monitored using (UV–Vis absorption spectra at an ionic strength of 2.0 mol dm^{-3} and 298 K. The reaction between Te^{IV} and Flx was set at a 1:1 stoichiometry. The reduction reaction followed first-order kinetics for [Flx] and fractional-first-order kinetics for [Te^{IV}] and [H^+]. The effects of ionic strength and relative permittivity of the reaction medium were also explored. Supplementation with divalent transition metal ions enhanced the reduction rate. The reaction products were identified, in order of their stoichiometric results, spot tests and FT-IR spectra as 3-(2-chloro-6-fluorophenyl)-5-methylisoxazol-4-carbocylic acid, 5,5-dimethyl-thiazolidine-2,4-dicarboxcilic acid, ammonium ion, carbon dioxide and elemental tellurium (Te^0). The reaction rate dependence on temperature was studied, and the activation and thermodynamic parameters were assessed and discussed. The derived rate-law expression was found to be in excellent accordance with the acquired investigational outcomes. A conceivable reaction mechanism has been provided, which includes a reaction between the protonated flucloxacillin (Flx^+) and tellurous acid (H_2TeO_3) as the essential reactive species, resulting in the construction of an intermediate complex. Such complex decays in the rate-determining step to yield the final reaction products.

1. Introduction

Tellurium is a harmful and essential rare metalloid present in a trace amounts in the earth's crust [1]. It exists in nature in several forms, including the nontoxic, elemental state (Te^0), telluride (Te^{2-}), and as the oxyanions tellurite (TeO_3^{2-}) and tellurate (TeO_4^{2-}), which are toxic for a variety of life forms [2,3]. In humans, tellurium is one of the most abundant trace elements in bone. It is a critical element utilized in energy and defence applications [4]. Tellurium compounds have several applications in the manufacture of ceramics, glass, semiconductors, and metals [3]. Tellurium oxyanions are strong oxidants that can be produced by their reductive precipitation to form insoluble elemental tellurium (Te^0) [5]. Tellurium oxyanions have also been investigated as potential antibacterial agents [6,7]. Tellurite ($Te^{IV}O_3^{2-}$) is highly toxic to a variety of microorganisms [4] and is an extremely stable compound, although it can be reduced to Te^0 by electrolysis, by using a powerful reducing agent [2,4,8], by living cells [9] or by some bacteria [10]. The reduction of highly toxic soluble tellurite, which has detrimental impacts on the environment and human health, to the nontoxic insoluble Te^0 is important due to the increasing employment of tellurium in several industries. Additionally, this process could be a treatment for the removal of toxic tellurite from polluted areas to address serious pollution problems. Therefore, the development of a biochemical reduction method for toxic tellurite for environmental clean-up purposes is of interest.

Antibiotics are a group of pharmaceutical drugs used to treat bacterial and fungal infections in both humans and animals. They are not only used in medicine but also in food industries and in scientific research activities [11]. However, antibiotics are chemical substances that are foreign to the human body; hence, the body eliminates them through drug metabolism processes, which may result in pharmacologically active, inactive, or toxic metabolites. Antibiotics are introduced into the environment through many routes, including human or animal excreta, wastewater effluent and industrial wastes and processes [12,13]. The presence of such chemicals, which contain complex organic compounds, even at low environmental concentrations may negatively affect the ecosystem and human health and have toxic impacts on the soil, water resources and organisms. Therefore, they are designated as a dangerous environmental pollutant [13]. There has been increasing concern for the removal of these compounds to protect the human health and the environment [14]. Several well-known methods or

E-mail addresses: afsaad139@yahoo.com, afsayed@uqu.edu.sa.

https://doi.org/10.1016/j.molliq.2019.111436
0167-7322/

Heliyon

ELSEVIER

Received:
30 January 2019
Revised:
1 March 2019
Accepted:
13 March 2019

Cite as: Afaf Y. Khormi, Thoraya. A. Farghaly, Mohamed R. Shaaban. Pyrimidyl formamidine palladium(II) complex as a nanocatalyst for aqueous Suzuki-Miyaura coupling. Heliyon 5 (2019) e01367. doi: 10.1016/j.heliyon.2019.e01367

Pyrimidyl formamidine palladium(II) complex as a nanocatalyst for aqueous Suzuki-Miyaura coupling

Afaf Y. Khormi[a,*], Thoraya. A. Farghaly[a,b], Mohamed R. Shaaban[a,b,*]

[a] *Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Makkah Almukarramah, Saudi Arabia*

[b] *Department of Chemistry, Faculty of Science, Cairo University, Giza 12613, Egypt*

* Corresponding author.
E-mail address: rabiemohamed@hotmail.com (M.R. Shaaban).

Abstract

Synthesis of a new phosphene-free nano-size formamidine-based palladium complex have been achieved. The molecular structure of novel palladium complex have been confirmed using spectroscopic methods of analysis as well as physical characterizations. The synthesized complex has been used as a catalyst for microwave assisted aqueous Suzuki-Miyaura Cross-coupling (SMC) of aryl bromides with phenylboronic acid. The formamidine-based Pd(II)-complex exhibited excellent catalytic activity to obtain biaryls using mild reaction conditions.

Keyword: Organic chemistry

1. Introduction

Cross-coupling reactions with transition-metal-catalysts are considerably useful synthetic process for C-C bonds formation [1, 2, 3]. The Suzuki-Miyaura cross-coupling (SMC) [4], has become charming standard procedure for the synthesis of biaryls, which have an assorted spectrum of implementations, extending from pharmaceuticals to materials science [5]. Traditionally, palladium intermediates were stabilized by using phosphine ligands [6]. The air-susceptibility of these kinds of ligands, however,

https://doi.org/10.1016/j.heliyon.2019.e01367

RSC Advances

PAPER View Article Online View Journal | View Issue

Check for updates

Cite this: *RSC Adv.*, 2019, 9, 20053

A facile methodology using quantum dot multiplex labels for tracking co-transfection†

Jessica A. Kretzmann,[a] RuiLu Feng,[b] Alaa M. Munshi,‡[a] Diwei Ho,[a] Anna M. Ranieri,[c] Massimiliano Massi,[c] Martin Saunders,[d] Marck Norret,[a] K. Swaminathan Iyer[a] and Cameron W. Evans[a]

Advances in the field of genome engineering demand the development of efficient non-viral transfection agents capable of delivering multiple distinct nucleic acids efficiently to cells (co-transfection). However, current delivery methods result in lower co-transfection efficiency than single plasmid transfections, and the efficiency decreases further with increasing numbers of plasmids. The development of a high-throughput methodology is required for the validation of co-transfection platforms to facilitate independent tracking of not only the multiple DNA plasmids during transfection but also the localisation of transfection agents. This is pivotal to determine the bottlenecks in achieving high transfection efficiencies at various stages of the cell internalisation and plasmid expression process. Herein we demonstrate that this can be achieved using a facile methodology in which quantum dots (QDs) are used to label two different plasmid DNA assemblies that are delivered to cells simultaneously using a dendronised polymer system. Multispectral confocal imaging can be used to separate signals from each polyplex as well as the expressed fluorescent reporter proteins to determine whether co-transfection difficulties result from poor internalisation or the inability of DNA to escape from polyplexes. The results demonstrate the utility of this facile approach to label polyplexes without interfering with gene expression, and enable high-throughput screening of transfection reagents for achieving optimal co-transfection.

Received 10th May 2019
Accepted 18th June 2019

DOI: 10.1039/c9ra03518d

rsc.li/rsc-advances

Introduction

Transfection is an important route for the introduction of genetic material into cells to facilitate gene-based therapies.[1] In contrast to viral transduction, which is associated with severe toxicity and immunogenicity problems,[2] non-viral transfection employs synthetic carriers to condense plasmid DNA (pDNA) into compact nanoparticles which are then taken up by cells *via* endocytosis.[3] However, non-viral transfection remains a relatively poorly understood route, prone to failure and low transfection efficiency.[4] Non-viral delivery materials can be divided into two main groups: those that use lipids to form liposomes (lipoplexes), and those that use synthetic polymers (polyplexes).[5] Previous work has shown that polyplexes are internalised *via* endocytosis with trafficking through the endolysosomal pathway,[3,6] which results in a low efficiency with which pDNA escapes from endosomal compartments.[6] A separate study established that transgene expression does not necessarily require cell division to translocate the pDNA into the nuclei.[7] Therefore, cell surface binding, endosomal escape, translocation to the nucleus, and intracellular polyplex decomposition may all be rate-limiting in the process of successful transfection.[8,9]

The advent of genomic editing tools such as CRISPR/Cas9, which is usually delivered as a mixture of pDNA components, has drawn attention to the inefficiency of non-viral transfection, particularly because such platforms require the delivery and expression of multiple plasmids simultaneously.[10] Questions addressing bottlenecks in plasmid co-transfection, whether of similar or different size, are important for this reason, and have been overlooked. For transfection agents with only moderate efficiency, the likelihood of transfecting a given cell with multiple different plasmids simultaneously is low, and in previous studies this has necessitated the use of cell sorting to select for specific cellular populations.[11,12] Consequently, identifying limiting steps in the transfection pathway and improving current understanding of the transfection process are paramount if successful non-viral delivery of genetic therapies is to be realised, and the technology progressed towards a clinical setting.

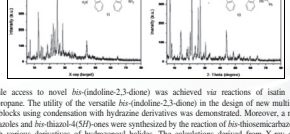
[a]*School of Molecular Sciences, The University of Western Australia, 35 Stirling Hwy, Crawley, WA 6009, Australia. E-mail: swaminathn.iyer@uwa.edu.au; cameron.evans@uwa.edu.au*
[b]*University of Science and Technology of China, 1129 Huizhou Ave, Baohe Qu, Hefei Shi, Anhui Sheng, China, 230000*
[c]*Department of Chemistry, Nanochemistry Research Institute, Curtin University of Technology, Kent St, Bentley, WA 6102, Australia*
[d]*Centre for Microscopy, Characterisation and Analysis, The University of Western Australia, 35 Stirling Hwy, Crawley, WA 6009, Australia*

† Electronic supplementary information (ESI) available: Detailed chemical synthesis, QD characterisation. See DOI: 10.1039/c9ra03518d

‡ Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Taif Road, 21955, Mecca, Makkah Province, Saudi Arabia.

Ismail I. Althagafi,[a] Amr S. Abouzied,[b,c] Thoraya A. Farghaly,[c,d] Nadia T. Al-Qurashi,[a] Mohammad Y. Alfaifi,[e] Mohamed R. Shaaban,[a,d] and Mohamed R. Abdel Aziz[d]

[a]Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Makkah Al mukkarramah, Kingdom of Saudi Arabia
[b]National Organization for Drug Control and Research (NODCAR), Cairo, Egypt
[c]Department of Pharmaceutical Chemistry, College of Pharmacy, University of Hail, Hail, Kingdom of Saudi Arabia
[d]Department of Chemistry, Faculty of Science, University of Cairo, Giza 12613, Egypt
[e]Biology Department, Faculty of Science, King Khalid University, Abha 9004, Kingdom of Saudi Arabia
*E-mail: thoraya-f@hotmail.com
Received August 7, 2018
DOI: 10.1002/jhet.3410
Published online 22 November 2018 in Wiley Online Library (wileyonlinelibrary.com).



A facile access to novel *bis*-(indoline-2,3-dione) was achieved *via* reactions of isatin with 1,3-dibromopropane. The utility of the versatile *bis*-(indoline-2,3-dione) in the design of new multifunctional building blocks using condensation with hydrazine derivatives was demonstrated. Moreover, a new series of *bis*-thiazoles and *bis*-thiazol-4(5*H*)-ones were synthesized by the reaction of *bis*-thiosemicarbazone derivative with various derivatives of hydrazonoyl halides. The calculations derived from X-ray diffraction patterns indicated the nanosize of the newly designed compounds. The spectral data of the formed compounds were established their structures. Also, the cytotoxic activity of the produced derivatives was screened against line MCF-7 (breast cancer cell). It was found that four derivatives from nine investigated compounds showed activity more potent than the standard drug used by 20 times in some cases.

J. Heterocyclic Chem., **56**, 391 (2019).

INTRODUCTION

The prominence of substituted thiazoles in the biochemistry is exceedingly known. Thiazole derivatives display abroad spectrum of inhibitory activities covering antimicrobial [1], anti-inflammatory [2], antitumor [3], antitubercular [4] and antiviral activities [5], and also enzymes and human platelet aggregation inhibitors [6]. *Bis*-heterocyclic ring systems have a special role in different implementation fields as electrical materials [7], chelating agents, and metal ligands [8]. They also manifest different biological activities having tuberculostatic, antibacterial, plant growth regulative, and fungicidal properties [9]. Several literature reports [10–12] proved that compounds bearing more than one thiazole ring unit exhibit good biological activities. For example, myxothiazol (Fig. 1) which is the mitochondrial cytochrome bc1 complex inhibitor, and bleomycin is an antitumor agent, containing 2,4′-*bis*-thiazole system. Thiazol ring was synthesized *via* several methods the common one is the reaction of thiosemicarbazone with haloketone compounds [13,14]. Thiosemicarbazone derivatives have been reported as antitumor [15,16], antiviral [17], antibacterial [18], antimalarial [19], antifungal [20], anti-inflammatory [21], and anti-HIV activities [22]. Furthermore, certain thiosemicarbazones showed an inhibition of herpessimplex virus infection *in vitro* [23], and also they were active inhibitors of *in vivo* herpessimplex virus genital infection [24]. Moreover, the biological and pharmacological properties of isatin and its derivatives have led to extensive use of these compounds as key intermediates in organic synthesis [25]. Isatin is a core constituent of many alkaloids [26] and drugs [27] as well as dyes [28], pesticides, and analytical reagents. From all the earlier findings, we were interested here in to design new *bis*-heterocyclic compounds having indoline derivatives (isatins) and/or *bis*-thiazoles in nanometer size using rapid re-precipitation method [29–31] and investigate their antitumor activity. This is due to nanoparticles are emerging materials that have broad range of applications and notable characteristics different from those of bulk materials. They often have specific optical and electronic properties and chemical reactivity [32,33]. In addition, the compounds in nanosize have potent biological activities and less toxicity than bulk derivatives due to it can penetrate the DNA and the cell membrane easily [34,35].

Journal of Inorganic and Organometallic Polymers and Materials
https://doi.org/10.1007/s10904-019-01308-8

Novel 1,3,4-Thiadiazolethiosemicarbazones Derivatives and Their Divalent Cobalt-Complexes: Synthesis, Characterization and Their Efficiencies for Acidic Corrosion Inhibition of Carbon Steel

Tahani M. Bawazeer[1,2] · Hoda A. El-Ghamry[1,3] · Thoraya A. Farghaly[4] · Ahmed Fawzy[1,5]

Received: 28 June 2019 / Accepted: 29 August 2019

Abstract
Two newly synthesized ligands based on 1,3,4-thiadiazolethiosemicarbazone have been isolated by the condensation reaction of 2,3-disubstituted-5-acetyl-1,3,4-thiadiazole derivatives with thiosemicarbazide in acidic medium in addition to their Co(II) chelates. The synthesized cobalt chelates that have been obtained by the reaction of each ligand with cobalt acetate were confirmed to have the formulae [(**LM**)Co(OAc)$(H_2O)_2$]H_2O (**LM–Co**) and [(**LN**)Co(OAc)$(H_2O)_2$]$0.5CH_3OH$ (**LN–Co**); where **LM** and **LN** are 1,3,4-thiadiazolethiosemicarbazone ligands with methyl and nitro substituents, respectively. Comparison of the IR spectrum of each ligand with that of its cobalt complex implied that both ligands acted as monobasic tridentate connecting to the cobalt ion through N atoms of both azomethine group and thiadiazole ring and S atom of deprotonated SH group as well. The two complexes have been proved to have octahedral geometrical structures. The synthesized compounds were studied as corrosion inhibitors for carbon steel in molar hydrochloric acid solution using several chemical and electrochemical techniques. The investigational outcomes displayed that the inhibition efficiencies of the examined compounds were found to augment as the concentrations of such compounds raised. At comparable inhibitors concentration, the inhibition efficiency was a little increased following the order: **LM > LM–Co > LN > LN–Co**. The acquired high inhibition efficiencies of the explored compounds were ascribed to the potent adsorption of the molecules on the steel surface and construction of adherent layers. Such adsorption was found to accord with Langmuir adsorption isotherm. There is a good correlation in the results obtained from the different measurements used.

Keywords Thiadiazoles · Thiosemicarbazone · Cobalt chelates · Acidic corrosion · Inhibition

1 Introduction

Heterocyclic ligands with more than one hetero-atom as sulfur and nitrogen are versatile multi-donor in coordination chemistry [1–3], among them, polyfunctional electron rich-1,3,4-thiadiazoles. In the last two decades, ligands carrying thiadiazole moiety revealed a considerable number of publications concerned with the preparation, structural elucidation and implementations of metal complexes of this type of ligands [4–7]. As for instance, copper and nickel complexes based on 1,3,4-thidiazole ligands display potent antimicrobial activity and were found to be able to protect tomato against Verticillium wilt [8, 9].

It was stated [10–12] that thiadiazole ring itself was used for steel corrosion protection and showed a high efficiency in different acidic media, while, the application of their complexes in the area of corrosion inhibition is limited [2]. Researchers are paying much attention to the search for

✉ Hoda A. El-Ghamry
helghamrymo@yahoo.com

[1] Chemistry Department, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia
[2] Medical Applications of Nanobiotechnology Research Group, King Fahad Medical Research Center, King Abdulariz University, Jeddah, Saudi Arabia
[3] Chemistry Department, Faculty of Science, Tanta University, Tanta, Egypt
[4] Chemistry Department, Faculty of Science, Cairo University, Giza, Egypt
[5] Chemistry Department, Faculty of Science, Assiut University, Assiut, Egypt

Published online: 05 September 2019

Send Orders for Reprints to reprints@benthamscience.ae
Mini-Reviews in Medicinal Chemistry, **2019**, *19*, 79-86 79

RESEARCH ARTICLE

Synthesis and Antitumor Activity of Novel [1,2,4,5]-tetrazepino[6,7-*b*] indole Derivatives: Marine Natural Product Hyrtioreticuline C and D Analogues

Zeinab A. Muhammad[1], Mohamed A.A. Radwan[2,3*], Thoraya A. Farghaly[4,5*], Hatem M. Gaber[1] and Mahmuod M. Elaasser[6]

[1]*National Organization for Drug Control and Research (NODCAR), P.O.Box 29, Cairo, Egypt;* [2]*Applied Organic Chemistry Department, National Research Centre, Dokki, Giza, Egypt;* [3]*Department of Chemistry, Faculty of Science, Qassim University, Saudi Arabia;* [4]*Department of Chemistry, Faculty of Science, Cairo University, Giza, 12613, Egypt;* [5]*Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Makkah Almukkarramah, Saudi Arabia;* [6]*The Regional Center for Mycology and Biotechnology, Al-Azhar University, Cairo, Egypt*

ARTICLE HISTORY
Received: July 18, 2017
Revised: September 21, 2017
Accepted: December 27, 2017
DOI: 10.2174/1389557517666161072094244

Abstract: ***Background***: Several biologically active indole alkaloids have been isolated from marine organisms over the previous few years. Many scientists interested in synthesis of the marine azepinoindole alkaloids due to their wide range of biological activies.

Objective: We interested herein to synthesize a new series of some analogues of new naturally occurring azepinoindole alkaloids.

Method: A novel series of [1,2,4,5]tetrazepino[6,7-*b*]indoles, Marine natural product *Hyrtioreticuline* C and D analogues, were synthesized *via* the reaction of 3-hydrazonoindolin-2-one with hydrzaonoyl chlorides in basic medium.

Results: The spectral data of the products proved their structure. All new derivatives were tested against two carcinoma cell lines ((A-549 & HepG2)) in comparison with the well-known anticancer standard drug (cisplatin) and two derivatives from the tested compounds showed activity more potent than the reference drug.

Conclusion: We succeeded in synthesis of new antitumor active azepinoindole alkaloids.

Keywords: Hydrazonoyl halides, isatin, [1,2,4,5]tetrazepino[6,7-*b*]indoles, *Hyrtioreticuline*, antitumor agents, SAR study.

1. INTRODUCTION

Marine living beings are a source of exceptional bioactive molecules and antitumor compounds. Several biologically active indole alkaloids have been isolated from marine organisms over the previous few years [1-4]. Azepinoindoles have been isolated from varied natural sources (Fig. 1). This set of alkaloids comprises of aurantioclavine, which was extracted from the fungus Penicillium aurantiovirens [5], clavicipitic acid from the fungus Claviceps fusiformis [6], the diastereomeric alkaloids hyrtioreticuline C and D from the marine sponge *Hyrtios reticulatus* [7], and fargesine from the roots and stems of Evodia fargesii [8]. Furthermore, cimitrypazepine was recognized in the roots and rhizomes of black cohosh (Cimicifuga racemosa) [9]. This forms the basis for the intention of the synthesis of the marine azepinoindole alkaloids. Here, we describe a direct procedure for the effective synthesis of small tricyclic compounds. Biological evaluation of the novel synthesized derivatives indicated their kinase inhibitory activities and revealed promising selectivity profiles against two kinase targets (A-549 & HepG2). Guided by the above descriptions, and in the extension of our earlier effort in the direction of the synthesis of indole alkaloid derivatives [10-12], and bioactive compounds [13-20], we report here a convenient synthesis of some analogues of new naturally occurring azepinoindole alkaloids.

*Address correspondence to these authors at the Applied Organic Chemistry Department, National Research Centre, Dokki, Giza, Egypt;
E-mail: m1radwan@yahoo.com; and Department of Chemistry, Faculty of Science, Cairo University, Giza, 12613, Egypt. Tel: 00201006745618;
E-mail: thoraya-f@hotmail.com

1389-5575/19 $58.00+.00

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Synthesis and Antimicrobial Evaluation of Novel Pyrazolopyrimidines Incorporated with Mono- and Diphenylsulfonyl Groups

Amani M. R. Alsaedi [1], Thoraya. A. Farghaly [2,*] and Mohamed R. Shaaban [1,2,*]

[1] Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Makkah Almukaramah 21514, Saudi Arabia; ams_ksa85@hotmail.com
[2] Department of Chemistry, Faculty of Science, Cairo University, Giza 12613, Egypt
* Correspondence: thoraya-f@hotmail.com (T.A.F.); mrgenidi@uqu.edu.sa (M.R.S.); Tel.: +966545917568 (M.R.S.)

Received: 30 September 2019; Accepted: 31 October 2019; Published: 5 November 2019

Abstract: A novel series of pyrazolo[1,5-*a*]pyrimidine ring systems containing phenylsulfonyl moiety have been synthesized via the reaction of 2-(phenylsulfonyl)-1-(4-(phenylsulfonyl) phenyl)ethan-1-one, 2-benzenesulfonyl-1-(4-benzenesulfonyl-phenyl)-3-dimethylamino-propenone and 3-(dimethylamino)-1-(4-(phenylsulfonyl)phenyl)prop-2-en-1-one each with various substituted aminoazopyrazole derivatives in one pot reaction strategy. The proposed structure as well as the mechanism of their reactions were discussed and proved with all possible spectral data. The results of antimicrobial activities of the new sulfone derivatives revealed that several derivatives showed activity exceeding the activity of reference drug. Contrary to expectations, we found that derivatives containing one sulfone group are more effective against all bacteria and fungi used than those contain two sulfone groups.

Keywords: antimicrobial activity; pyrazolopyrimidine; aminopyrazoles; microwaves; structure-activity relationship (SAR)

1. Introduction

Pyrazolo[1,5-*a*]pyrimidine is known to be purine analog that has protruded a vital building block for pharmaceutical drugs. It has several potent biological implementations as antischistosomal, antimetabolites in purine bio-chemical interactions, sedative and antitrypanosomal [1], AMP phosphodiesterase inhibitors [2], anxiolytic [3], benzodiazepine receptor ligands [4], KDR (kinase insert domain receptor) kinase inhibitors [5], HMG-CoA (3-hydroxy-3-methyl-glutaryl-coenzyme A reductase) reductase inhibitors [6], COX-1 (cyclooxygenase-1) , COX-2 (cyclooxygenase-2) selective inhibitors [7], HCV (hepatitis C virus) inhibitors [8], serotonin 5-HT6 (5-hydroxytryptamine) receptor antagonists [9], PET (positron emission tomography) tumor imaging agents [10], kinase inhibitors [11], CCR1 (C-C chemokine receptor type 1) antagonists [12], HIV (human immunodeficiency viruses) reverse transcriptase inhibitors [13], and antifungal and antimalarial activities [14]. Many marketed drugs have pyrazolo[1 ,5-*a*]pyrimidine nucleus such as indiplon, zaleplon, dorsomorphin, dinaciclib, anagliptin, pyrazophos, loreciplon, and ocinaplon [15] are showed in Figure 1. Another important scaffold is benzene-sulfone moiety which present in several important pharmaceutical and agrochemical molecules due to their distinctive structural and electronic features. As for instance, molecules used as gamma-secretase inhibitors (I) [16], in migraine and prostate cancer, or as the herbicides mesotrione and cafenstrole, all feature aryl sulfone units [17] (Figure 1). Due to the specific physical and chemical properties as well as the biological activities of azobenzene dyes, they have found wide applications in the cosmetic, pharmaceutical, dyeing/textile industry, food, and analytical

Research on Chemical Intermediates (2019) 45:1943–1971
https://doi.org/10.1007/s11164-018-03714-y

New catalytic approach for nano-sized V(IV), Cr(III), Mn(II) and Fe(III)-triazole complexes: detailed spectral, electrochemical and analytical studies

Layla Almazroia, et al. *[full author details at the end of the article]*

Received: 3 October 2018 / Accepted: 14 December 2018 / Published online: 1 January 2019

Abstract
A new series of metal ion complexes from a triazole-Schiff base was synthesized and fully characterized. The tridentate mode of coordination was the only mode of bonding in a 1:1 (M:L) molar ratio. Octahedral geometry was the only structural form proposed for all chelating compounds. This geometry was established based on UV–Vis, magnetic moments and ESR studies. The nanometer feature for all complexes was extracted from SEM images and XRD data. CV electrochemical study over Fe(III) and Mn(II) complexes (examples) displayed a $i_{p,c}/i_{p,a}$ ratio over 1, which points to irreversible electrode couples. TGA and kinetic parameters reflect a best view about the thermal stability of all tested compounds. Molecular modeling was achieved through an advanced program, to optimize the structural forms and estimate significant parameters. All features concluded from all implemented studies orient us towards the best compounds serving in the intended catalytic application. Proceeding from this, Fe(III) and Mn(II) complexes were chosen for their heterogeneous catalytic application, as they can be used without treatment. Moreover, amounts from such complexes were ignited in open air (calcinations) to produce their corresponding oxides, Fe_2O_3 and MnO_2. The synthesized oxides were fully analyzed to establish their chemical formula, as well as extract their morphological characters, which are the main players in the catalytic field. The surface characteristic and particulate sizes show promise in a catalytic role compared to other similar purchased oxides. The original complexes and their synthesized oxides were utilized separately to synthesize biodiesel from waste oils through heterogenous catalytic process. This process was conducted through a comparative study with other referenced methods. The catalytic role of prepared oxides was clearly observed whenever their original complexes did not display catalytic features as desired. Moreover, this comparative study was prolonged versus purchased oxides (Fe_2O_3 and MnO_2) and the differentiation based on reaction yields after verification of physical features.

Electronic supplementary material The online version of this article (https://doi.org/10.1007/s11164-018-03714-y) contains supplementary material, which is available to authorized users.

Materials Science & Engineering C 96 (2019) 740–756

Contents lists available at ScienceDirect

Materials Science & Engineering C

journal homepage: www.elsevier.com/locate/msec

Synthesis of new Cu(II)-benzohydrazide nanometer complexes, spectral, modeling, CT-DNA binding with potential anti-inflammatory and anti-allergic theoretical features

Hanadi A. Katouah[a], Jabir H. Al-Fahemi[a], Marwa G. Elghalban[a,b], Fawaz A. Saad[a], Ismail A. Althagafi[a], Nashwa M. El-Metwaly[a,b,c,*], Abdalla M. Khedr[b,c]

[a] Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia
[b] Chemistry Department Faculty of Science, Mansoura University, Mansoura, Egypt
[c] Chemistry Department, Faculty of Science, Tanta University, Tanta, Egypt

ARTICLE INFO

Keywords:
Nanometer Cu(II) complexes
DFT/B3LYP
Anti-inflammatory
Anti-allergic docking and DNA binding

ABSTRACT

New nanometer Cu(II)-benzohydrazide complexes were synthesized and characterized. Mono negative tetradentate mode is the general feature proposed for all coordinating ligands. Variable structural forms were established, square-planer, tetrahedral and octahedral arrangements around copper centers. XRD and TEM studies displayed a nanometer size for crystalline compounds. TGA analysis of new complexes showed low thermal stability due to the presence of crystal water molecules. Kinetic parameters were calculated using two comparative methods for assertion. ESR study was performed on three chosen complexes to estimate essential spectral parameters and assert on proposed geometries. Gaussian09 software program and applying DFT/B3LYP method was used for optimizing all structures to give the best arrangement for atoms. Essential indexes were extracted from log files as well as other indexes were computed based on frontier energy gaps. Potential theoretical anti-inflammatory, antitumor and anti-allergic studies were executed using Autodock 4.2 tools. Essential energies were calculated over docking complexes corresponding to 5HN1, 5AV1 and 4H1L protein receptors for three pathogens (inflammation, liver cancer and allergy, respectively). H_2L^1 ligand displays significant activity towards inflammation and allergy diseases. Such potential feature will give a well insight about their biological attitude in future experimentation.

1. Introduction

Hydrazides and derivatives are well known to display a great range of biological activities, including antifungal, antimycobacterial, antibacterial, anti-tumoral, anti-inflammatory and antioxidant [1]. These compounds have excellent ability to readily coordinate to great number of transition metals. Indeed, great number hydrazide complexes have been synthesized and inspected [2–4]. Several compounds of this class display remarkable biological characteristics, mainly antitumoral [5,6]. Recently, there is a magnificent attention in the application of copper complexes in cancer chemotherapy [7]. A considerable number of Cu (II) complexes containing N,N-donors ligands have been prepared and applied as synthetic nucleases, after reporting that $[Cu(phen)_2]^{+}$ complex have the ability to cleave DNA [8]. Furthermore, several Cu(II) complexes have been depicted to inhibit tumoral cell growth [9–11]. Touching the clinical advantage of these complexes, two of them reported by L. Ruiz and co-workers, are advised for their clinical trials as antitumor drugs [12,13]. For instance, the influence of Cu(II) complexes containing hydrazide ligands on the growth of tumor cells has been evaluated. Recently, Bortolotto et al. reported that under UV-light exposure, this type of complexes promote DNA cleavage activity [14]. Certainly, these results show distinctly that ternary Cu(II) complexes with hydrazides are very promising as anticancer agents. Aiming to continue our research on bio-active promising compounds [15,16], we reported herein the synthesis and characterization of novel series for Cu (II) complexes involving hydrazide ligands. A full characterization will be in concern applying analytical, spectral and theoretical tools. CT-DNA binding study will be tested over ligand derivatives. The biological investigation will focus on computational referenced method in drug designing (Docking process).

* Corresponding author at: Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia.
E-mail address: n_elmetwaly00@yahoo.com (N.M. El-Metwaly).

https://doi.org/10.1016/j.msec.2018.11.034
Received 11 November 2017; Received in revised form 5 October 2018; Accepted 23 November 2018
Available online 26 November 2018
0928-4931/

Journal of Inorganic and Organometallic Polymers and Materials
https://doi.org/10.1007/s10904-019-01124-0

Synthesis, Characterization for New Nanometric VO(II)–Thioacetanilide Complexes by, Spectral, Thermal, Molecular Computations and DNA Interaction Study Beside Promising Antitumor Activity

Fawaz Saad[1] · Nashwa El-Metwaly[1,2] · Abdalla M. Khedr[1,3]

Received: 4 January 2019 / Accepted: 27 February 2019

Abstract
A novel series, of thioacetanilide derivatives (4a–e), was synthesized and fully characterized. Their corresponding VO(II) complexes, were prepared and inspected by all analytical, spectral and computational techniques. From IR spectral analysis, poly dentate mode of bonding, was proposed for all organic ligands towards two central atoms. The octahedral arrangement configuration, was suggested for all complexes, based on; UV–Vis, ESR and magnetic measurements. TGA and DTA analysis, built a good assertion on the presence of solvent molecules, attached with the complex particles. The molecular modeling technique, excreted the best structural forms for all tested compounds. Moreover, essential computational parameters were estimated, to verify the molecular formulae. Molecular docking study, was concerning with the inhibition feature against 3s7s and 3gcw proteins, belonging to breast and liver cancer cells, respectively. The computed parameters introduced a promising activity for some tested derivatives. Furthermore, the experimental antitumor screening for VO(II) complexes, versus HepG-2 and MCF-7 cell lines, displayed superiority for $[(VO)_2(SO_4)_2(AETA)(H_2O)_2]3H_2O$ complex in comparing to cisplatin (standard drug). As well as, the genotoxicity results, coincide excellently with antitumor result.

Keywords Vanadyl complexes · Thioacetanilides · DNA binding · Genotoxicity · Docking · Antitumor activity

1 Introduction

Vanadium compounds, chiefly VO(II) coordination chemistry, have attracted agreat attention for several substantial reasons in recent years specially in the designing of long-acting drugs in metabolism [1]. Research solicitude in VO(II) compounds originates from its utility in various industrial and biological applications such as insulin mimetic [2], antitumor, antioxidant, spermicidal, antimicrobial and DNA binding [3]. The animated role of vanadium in diverse biological and chemical systems has stimulated the progress of chemistry of vanadium compounds. The coordination number, geometry, and biological efficacy of VO(II) are extremely ligand dependent. Also, it is well known that VO^{2+} is less toxic than the vanadate ion (VO_4^{3-}). Due to all these unique characteristics, the VO^{2+} complexes display potential therapeutic uses [4]. The authentic factor in the leverage of anti-cancer reagents is their capability to interact with the DNA of the cancer cell which prohibit the cell division until it dies [5, 6]. Furthermore, arylhydrazone derivatives have been vastly applied as a building block in various antitumor agents especially in presence of both acceptors and donors of hydrogen as well as flexible skeleton [7]. Most of the antitumor hydrazone derivatives have been spotted through motivating apoptosis in diversified carcinogenic cells [8, 9]. In addition, cancer remains one of the farthest current reasons for death in the worldwide. In spite of fast changes in the cancer therapy and the widespread research, nevertheless there is a rising indigence for novel therapeutic agents [10, 11]. Discovery of unprecedented chemotherapeutic agents are of significant importance due to the substantial

Electronic supplementary material The online version of this article (https://doi.org/10.1007/s10904-019-01124-0) contains supplementary material, which is available to authorized users.

✉ Nashwa El-Metwaly
n_elmetwaly00@yahoo.com

[1] Chemistry Department, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia
[2] Chemistry Department Faculty of Science, Mansoura University, Mansoura, Egypt
[3] Chemistry Department, Faculty of Science, Tanta University, Tanta, Egypt

Published online: 11 March 2019

Journal of Molecular Structure 1194 (2019) 86–103

Contents lists available at ScienceDirect

Journal of Molecular Structure

journal homepage: http://www.elsevier.com/locate/molstruc

Synthesis and characterization for novel Cu(II)-thiazole complexes-dyes and their usage in dyeing cotton to be special bandage for cancerous wounds

Nashwa El-Metwaly [a, b, *], Ismail Althagafi [a], Abdalla M. Khedr [a, c], Jabir H. Al-Fahemi [a], Hanadi A. Katouah [a], Aisha S. Hossan [d], Aisha Y. Al-Dawood [a], Gamil A. Al-Hazmi [d, e]

[a] Department of Chemistry, Faculty of Applied Sciences, Umm Al-Qura University, Makkah, Saudi Arabia
[b] Department of Chemistry Faculty of Science, Mansoura University, Mansoura, Egypt
[c] Department of Chemistry, Faculty of Science, Tanta University, Tanta, Egypt
[d] Department of Chemistry, Faculty of Science, King Khalid University, P.O. Box 9004, Abha, Saudi Arabia
[e] Department of Chemistry, Faculty of Applied Sciences, Taiz University, P.O. Box 82, Taiz, Yemen

ARTICLE INFO

Article history:
Received 14 April 2019
Received in revised form
15 May 2019
Accepted 19 May 2019
Available online 23 May 2019

Keywords:
Cu(II)-thiazole complexes
Bandage for cancerous wounds
CT-DNA
Molecular docking
DFT/B3LYP

ABSTRACT

New series of Cu(II)-thiazole complexes were synthesized using variable p-substituted, *N*-aryl-2-oxo-2-(thiazol-2-ylamino)-acetohydrazonoyl cyanide. All new syntheses were elucidated by, analytical, spectral and conformational study. The binuclear feature (2M:1L), was proposed for all complexes, through mono-negative tetra-dentate chelation mode in octahedral or square-planer geometry. The formulae of chosen compounds, were confirmed by, ^{1}HNMR and mass spectral analysis. The ideal distribution for atomic-skeletons, was performed utilizing Gaussian09 software, to confirm the bonding mode. Also, substantial parameters were extracted from output-files (log &chk), beside others calculated based on frontier energy gaps. The superiority of Cu(II) complexes, was predicated from such conformational study. Also and by applying MOE module, the docking process was performed for most syntheses against selected pathogen proteins (1miu, 4k9g and 5jm5), which have been tested practically in application. The extracted docking-data, showed clear superiority and promising efficiency for Cu(II) complexes as anticancer drugs compared to free derivatives. Traditional screening was conducted over new complexes against three carcinoma cell lines (HCT-116, MCF-7 & HepG-2) as well as healthy cell line (HSF). IC_{50} values showed considerable toxicity of Cu(II)-4e complex versus HCT-116 cell line. The antitumor screening was conducted over cotton fabric after dyeing by complexes, to test the degree of success to be used as a special bandage for cancerous wounds. The most lighted observation was, the effect of released-pigmenting complex on colon cancer cell line, while the absence of any effect on healthy cell. Also, the released-pigment, controlled the pH of cancerous wound, which is significantly preferable.

1. Introduction

For many years, the heterocyclic compounds containing O, N, and S, displayed magnificent importance in medicinal and chemical applications [1,2]. They are widely applied as cosmetics, perfumes, food additives, pharmaceuticals, optical brighteners, laser and fluorescent and dyes [3]. Thiazole derivatives have enhanced antimicrobial activities towards various pathogens including *Helicobacter pylori* and *Mycobacterium tuberculosis* [4]. These thiasole compounds, have also good anti-cholinesterase, anti-cancer, anti-analgesic, anti-inflammatory activities [5]. Transition metals have incorporated with numerous biological processes that are animated to life processes [6]. Hence, they can coordinate with N- or O-terminals from proteins in a assortment of models, and so, play a peppy role biological system such as the utility and conformation of living macromolecules [7]. Schiff bases involving imino moieties (>C=N–) and their complexes have been exceedingly reported to display a distinction of motivating biological effectiveness such as anti-inflammatory, antimicrobial, antifungal, antitumor, analgesic effects, anti-proliferative, and anticancer

* Corresponding author. Department of Chemistry, Faculty of Applied Sciences, Umm Al-Qura University, Makkah, Saudi Arabia
E-mail address: n_elmetwaly00@yahoo.com (N. El-Metwaly).

https://doi.org/10.1016/j.molstruc.2019.05.080
0022-2860/

Received: 23 April 2019 | Revised: 9 June 2019 | Accepted: 14 June 2019
DOI: 10.1002/aoc.5095

FULL PAPER

WILEY Applied Organometallic Chemistry

Synthesis of novel VO (II)-thaizole complexes; spectral, conformational characterization, MOE-docking and genotoxicity

Nashwa El-Metwaly[1,2] | Ismail Althagafi[1] | Hanadi A. Katouah[1] | Jabir H. Al-Fahemi[1] | Tahani M. Bawazeer[1] | Abdalla M. Khedr[3]

[1]Department of chemistry, Faculty of Applied Sciences, Umm Al-Qura University, Makkah, Saudi Arabia
[2]Department of chemistry Faculty of Science, Mansoura University, Mansoura, Egypt
[3]Department of chemistry, Faculty of Science, Tanta University, Tanta, Egypt

Correspondence
Prof. Nashwa M. El-Metwaly, Department of chemistry, Faculty of Applied Sciences, Umm Al-Qura University. Makkah, Saudi Arabia.
Email: n_elmetwaly00@yahoo.com

Funding information
Deanship of Scientific Research at Umm Al-Qura University, Grant/Award Number: project ID: 17-SCI-1-03-0001

New VO (II)-thaizolyl hydrazine complexes were synthesized and characterized by analytical, spectral and theoretical techniques. Bi-nuclear complexes were suggested for all synthesizes upon neutral poly-dentate mode of bonding. UV–Vis and EPR spectra, proposed two structural geometries as, square-planer and octahedral. TGA confirmed the contribution of solvent molecules through physical and/or coordinate-bonding. XRD parameters calculated, displayed outstanding nanometer-sizes for all nano-crystalline compounds, which suffering slight imperfections. Also, SEM images showed, spherical-shape that observed for most topographic particulates. Conformational study executed for all new synthesizes, demonstrated their optimized structural-forms. Furthermore, important physical parameters were computed that predict essential characteristics as, biological efficiency. Predictable parameters as softness and electrophilicity, point to priority of VO (II)-4d complex. Genotoxic study, was already examined, for all new synthesizes, against CT-DNA and displayed complete deterioration for DNA, by influence of most tested compounds. Moreover, MOE-docking technique, was executed against receptors of Y-family DNA-polymerase (4irk) and Key-Enzyme Linking-Metabolic Inflammation (4cyf). This docking study displayed the following ascending order; VO (II)-4c,4irk ˃ VO (II)-4d,4cyf ˃ VO (II)-4c, 4cyf ˃ VO (II)-4b, 4cyf, based on scoring-energy values. This study concluded with promising prediction of these complexes in relation to DNA-polymerase as well as inflammation enzyme that compared with known anti-inflammatory drug (meloxicam).

KEYWORDS
conformational analysis, genotoxicity, MOE-docking, VO (II) complexes

1 | INTRODUCTION

Recently hydrazone derivatives display a key important role in medicinal, organic and inorganic chemistry as a result of their structural varieties, preparative accessibilities structures and meaningful biological activities.[1] Hydrazone compounds are primarily a Schiff-base group of materials having a secondary amine proton including a gorgeous family of derivatives in a variance of research areas, such as chemical and biosensors, nonlinear optics, and a variety of medical applications.[2–4] Moreover, hydrazones are well known to exhibit a great ability to

Journal of Inorganic and Organometallic Polymers and Materials
https://doi.org/10.1007/s10904-019-01233-w

Docking Approach to Predict Inhibition Activity of New Pt(II) Complexes Against Kinase Protein and Human DNA: Full Characterization, HF-FC Modeling and Genotoxicity

Nashwa El-Metwaly[1,2] · Jabir H. Al-Fahemi[1] · Ismail Althagafi[1] · Abdalla M. Khedr[1,3] · Hanadi A. Katouah[1]

Received: 20 April 2019 / Accepted: 17 June 2019

Abstract
New series of Pt(II)–azaindazole complexes, were synthesized and also characterized by, analytical, spectral and computational tools. All synthesized Pt(II)-complexes, appeared as mononuclear with bi-dentate mode of bonding. Octahedral arrangement as well as square-planer, were proposed geometries around platinum atoms in all complexes. The best atomic-skeletons, were demonstrated by using Gaussian09 program. Applying MOE module (V. 2015), extensive molecular docking process was executed upon all new synthesizes. This docking study was interested in kinase protein (3ce3) and health cell–DNA (5ahr), to predict the degree of cancer-inhibition and also the mode of interaction. A significant inhibition activity, was clearly predicted with Pt(II)–**4b** and Pt(II)–**4c** complexes, against 3ce3 protein-receptors. While the absence of any significant effect towards 5ahr, which is favorable trend of therapeutic agent. Various backbone receptors (amino acids) were attacked through H-bonding, from most tested inhibitors, especially of 3ce3 protein. DNA-degradation study, which executed in vitro, displayed a complete degradation for DNA with most screened compounds except **4d** and **4e** derivatives. This feature points to the promising antitumor activity of most synthesizes, especially the Pt(II) complexes, as a predicted role of its complexes.

Keywords Pt(II)–triaazene complexes · Docking against kinase protein · CT–DNA · HF-FC · B3LYP-FC

1 Introduction

The advancement of metallo-drugs and the inspection of their action modes have attracted many inorganic chemistry scientists as a very important field of research, especially after the discovery of great antitumor efficiency of cisplatin in the 1960s [1]. In the cancer chemotherapy, the most applied metal-based drugs were cisplatin and its successors [2, 3]. The cisplatin altitude toxicity which motivates serious side-effects, such as neurotoxicity, nephrotoxicity, emetogenesis, and ototoxicity [4], predetermines the designing of new antitumor metal-based chemotherapeutic agents. In addition to the toxicity of platinum drugs problems, another limitation of their clinical efficiency is their ability to stimulate the resistance of the cells [5]. The resistance to cisplatin is mostly multi-factorial and can be assigned to reduced accumulation of the drug, inactivation of drugs trough interaction with sulfur and nitrogen containing organic compounds, and alterations in the proteins included in apoptosis [6]. Oxaliplatin and carboplatin were the second generation of platinum-based drugs which developed in order to get more antitumor activity, lower toxic side effects, and increased solubility in comparison with cisplatin [7]. The responsible interactions for Pt-based drugs antitumor activity are the covalent binding to N7 atoms of guanine and/or intercalation of DNA cells with the aromatic ligands [2]. The cancer cell death is generally attributed to the resulting changes in the tertiary structure of DNA through apoptosis [8]. Although these important drawbacks, the first-line chemotherapy for 12 diversified neoplasms which exceeding 50% clinically used anticancer regimens includes a platinum(II)-based derivatives [9, 10].

Electronic supplementary material The online version of this article (https://doi.org/10.1007/s10904-019-01233-w) contains supplementary material, which is available to authorized users.

✉ Nashwa El-Metwaly
n_elmetwaly00@yahoo.com

[1] Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Mecca, Saudi Arabia
[2] Department of Chemistry, Faculty of Science, Mansoura University, Mansoura, Egypt
[3] Department of Chemistry, Faculty of Science, Tanta University, Tanta, Egypt

Published online: 22 June 2019

Springer

Received: 7 January 2019 | Revised: 12 June 2019 | Accepted: 14 June 2019
DOI: 10.1002/aoc.5099

FULL PAPER

WILEY Applied Organometallic Chemistry

Characterization of new Pt(IV)–thiazole complexes: Analytical, spectral, molecular modeling and molecular docking studies and applications in two opposing pathways

Ismail Althagafi[1] | Nashwa M. El-Metwaly[1,2] | Thoraya Farghaly[1,3]

[1] Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia
[2] Department of Chemistry, Faculty of Science, Mansoura University, Mansoura, Egypt
[3] Department of Chemistry, Faculty of Science, Cairo University, Cairo, Egypt

Correspondence
Ismail Althagafi and Nashwa M. El-Metwaly, Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Makkah. Saudi Arabia.
Email: iithagafi@uqu.edu.sa; n_elmetwaly00@yahoo.com

Funding information
Deanship of Scientific Research at Umm Al-Qura University, Grant/Award Number: (project ID: 17-SCI-1-01-0004) project ID: 17-SCI-1-01-0004

New thiazole derivatives were synthesized and fully characterized, then coordinated with $PtCl_4$ salt. Also, the newly synthesized Pt(IV) complexes were investigated analytically (elemental and thermogravimetric analyses), spectrally (infrared, UV–visible, mass, ^1H NMR, ^{13}C NMR, X-ray diffraction) as well as theoretically (kinetics, modeling and docking). The data extracted led to the establishment of the best chemical and structural forms. Octahedral geometry was the only formula proposed for all complexes, which is favorable for d^6 systems. The molecular ion peaks from mass spectral analysis coincide with all analytical data, confirming the molecular formula proposed. X-ray diffraction (XRD) and scanning electron microscopy (SEM) allowed discrimination of features between crystalline particles and other amorphous morphology. By applying Gaussian09 as well as HyperChem 8.2 programs, the best structural forms were obtained, as well as computed significant parameters. Computed parameters such as softness, hardness, surface area and reactivity led us towards application in two opposing pathways: tumor inhibition and oxidation activation. The catalytic oxidation for CO was conducted over PtO_2, which was yielded from calcination of the most reactive complex. The success of catalytic role for synthesized PtO_2 was due to its particulate size and surface morphology, which were estimated from XRD patterns and SEM images, respectively. The antitumor activity was tested versus HCT-116 and HepG-2 cell lines. Mild toxicity was recorded for two of the derivatives and their corresponding complexes. This degree of toxicity is more favorable in most cases, due to exclusion of serious side effects, which is coherently attached with known antitumor drugs.

KEYWORDS
antitumor activity, catalytic oxidation, docking, modeling, Pt(IV)–thiazole complexes

1 | INTRODUCTION

Over the last decade, platinum complexes have become well known for their high potential anticancer activity and as industrial catalysts.[1–3] For example, *cis*-diamminedichloroplatinum(II) (known as cisplatin) is a commercially available drug for human malignancies. This may be attributed to crosslinking of DNA strands by metal complexes via coordination of nucleic acid bases, which then encourages apoptosis of cancer cells.[4] Also,

Journal of Inorganic and Organometallic Polymers and Materials
https://doi.org/10.1007/s10904-019-01326-6

Green Synthesis for 3-(2-Benzoylhydrazono)-*N*-(pyridin-2-yl) butanamide Complexes: Spectral, Analytical, Modelling, MOE Docking and Biological Studies

Gamil A. A. Al-Hazmi[1,2] · Khlood S. Abou-Melha[1] · Nashwa M. El-Metwaly[3,4] · Ismail Althagafi[3] · Rania Zaki[4] · Fathy Shaaban[5]

Received: 19 June 2019 / Accepted: 13 September 2019

Abstract
Applying ball-milling green synthesis strategy process, Hg(II), Cd(II), Cu(II), Co(II) and Ni(II) complexes, were prepared for 3-(2-benzoylhydrazono)-*N*-(pyridin-2-yl)butanamide (H_2BHAH) ligand. All synthesized complexes were characterized using, analytical, spectral and conformational techniques. Octahedral geometry was proposed for all complexes, which mainly based on electronic spectral-data and magnetic moments. TGA was performed for Cu(II) and Ni(II) complexes to elucidate the chemical formula. Also, Coats–Redfern method was utilized to calculate thermodynamic parameters for all degradation stages, to assert on nonspontaneous kinetic behavior of metal–ligand bonds. XRD study was executed for three complexes to assure on their discriminated purity. Material studio program was used to build the best atomic-skeletons for all investigated complexes by DFT method. Significant physical parameters were also calculated by using standard equations. Using MOE module (Vs. 2015), the docking process was executed towards three essential proteins (1bqb, 1p6f and 4cl7). This aims to predicate a suitable view towards the biological feature of new synthesized complexes, to strengthen in vitro study. Antimicrobial, antioxidant and cytotoxic activities of H_2BHAH and its complexes were examined, to raise the value of new synthesis.

Keywords Hydrazone complexes · Ball milling · DFT studying · MOE docking · Antioxidant · Cytotoxic

1 Introduction

Main confront of current chemistry is to develop new method to help the chemical industry in managing shortage of raw materials, the global problems of pollution and growing energy demand [1–3]. The ball-milling technique showed great potential when compared to other traditional methods in preparing compounds in solid state with high purity and yield. This environmentally-friend technique, which is carried out in absence of solvent, effortless and also short reaction times. Schiff-base complexes have wide spectrum of applications in pharmacological and biological areas as analgesic, anticancer, anti-inflammatory, antifungal, antibacterial, and anticonvulsant agents [4–6]. The modern biochemistry associated with metallic complexes played significant role in coordination biochemistry [7–9]. They are used for applications, which dealing with many diseases such as mental disorder, leprosy, anti-tumor and tuberculosis and also used as synthetic and analytical reagents [10–12]. In this study Schiff bases complexes of 3-(2-benzoylhydrazono)-*N*-(pyridin-2-yl)butanamide were

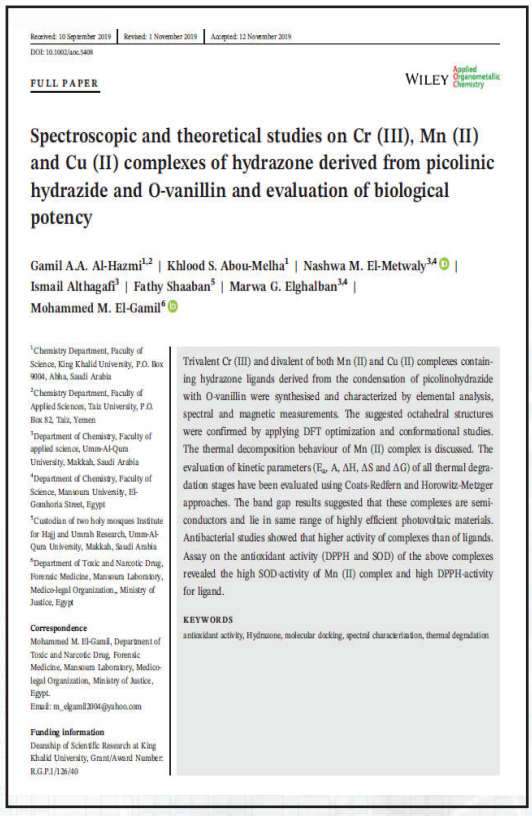
Electronic supplementary material The online version of this article (https://doi.org/10.1007/s10904-019-01326-6) contains supplementary material, which is available to authorized users.

✉ Nashwa M. El-Metwaly
n_elmetwaly00@yahoo.com

[1] Chemistry Department, Faculty of Science, King Khalid University, P.O. Box 9004, Abha, Saudi Arabia
[2] Chemistry Department, Faculty of Applied Sciences, Taiz University, P.O. Box 82, Taiz, Yemen
[3] Department of Chemistry, Faculty of Applied Science, Umm-Al-Qura University, Mecca, Saudi Arabia
[4] Department of Chemistry, Faculty of Science, Mansoura University, Mansoura, Egypt
[5] Custodian of Two Holy Mosques Institute for Hajj and Umrah Research, Umm-Al-Qura University, Mecca, Saudi Arabia

Published online: 20 September 2019

Springer



Received: 10 September 2019 | Revised: 1 November 2019 | Accepted: 12 November 2019
DOI: 10.1002/aoc.5408

FULL PAPER

WILEY Applied Organometallic Chemistry

Spectroscopic and theoretical studies on Cr (III), Mn (II) and Cu (II) complexes of hydrazone derived from picolinic hydrazide and O-vanillin and evaluation of biological potency

Gamil A.A. Al-Hazmi[1,2] | Khlood S. Abou-Melha[1] | Nashwa M. El-Metwaly[3,4] | Ismail Althagafi[3] | Fathy Shaaban[5] | Marwa G. Elghalban[3,4] | Mohammed M. El-Gamil[6]

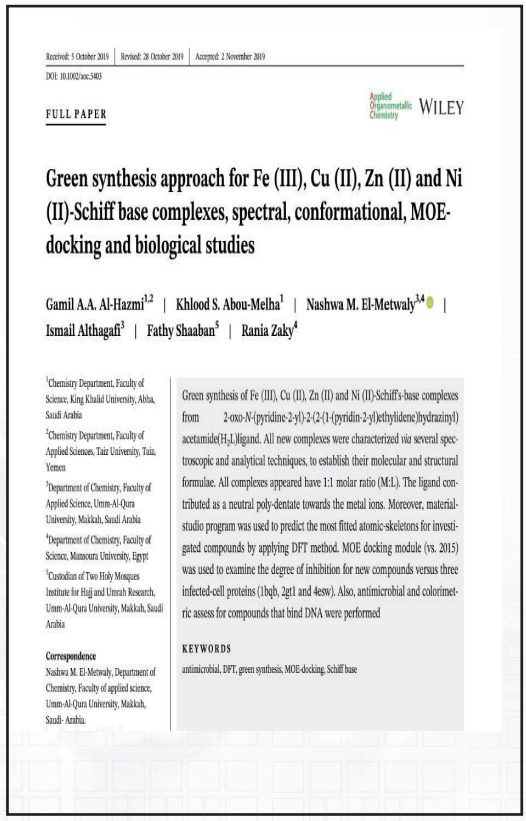
[1]Chemistry Department, Faculty of Science, King Khalid University, P.O. Box 9004, Abha, Saudi Arabia
[2]Chemistry Department, Faculty of Applied Sciences, Taiz University, P.O. Box 82, Taiz, Yemen
[3]Department of Chemistry, Faculty of applied science, Umm-Al-Qura University, Makkah, Saudi Arabia
[4]Department of Chemistry, Faculty of Science, Mansoura University, El-Gomhoria Street, Egypt
[5]Custodian of two holy mosques Institute for Hajj and Umrah Research, Umm-Al-Qura University, Makkah, Saudi Arabia
[6]Department of Toxic and Narcotic Drug, Forensic Medicine, Mansoura Laboratory, Medico-legal Organization., Ministry of Justice, Egypt

Correspondence
Mohammed M. El-Gamil, Department of Toxic and Narcotic Drug, Forensic Medicine, Mansoura Laboratory, Medico-legal Organization, Ministry of Justice, Egypt.
Email: m_elgamil2004@yahoo.com

Funding information
Deanship of Scientific Research at King Khalid University, Grant/Award Number: R.G.P.1/126/40

Trivalent Cr (III) and divalent of both Mn (II) and Cu (II) complexes containing hydrazone ligands derived from the condensation of picolinohydrazide with O-vanillin were synthesised and characterized by elemental analysis, spectral and magnetic measurements. The suggested octahedral structures were confirmed by applying DFT optimization and conformational studies. The thermal decomposition behaviour of Mn (II) complex is discussed. The evaluation of kinetic parameters (E_a, A, ΔH, ΔS and ΔG) of all thermal degradation stages have been evaluated using Coats-Redfern and Horowitz-Metzger approaches. The band gap results suggested that these complexes are semiconductors and lie in same range of highly efficient photovoltaic materials. Antibacterial studies showed that higher activity of complexes than of ligands. Assay on the antioxidant activity (DPPH and SOD) of the above complexes revealed the high SOD-activity of Mn (II) complex and high DPPH-activity for ligand.

KEYWORDS
antioxidant activity, Hydrazone, molecular docking, spectral characterization, thermal degradation



Received: 5 October 2019 | Revised: 26 October 2019 | Accepted: 2 November 2019
DOI: 10.1002/aoc.5403

FULL PAPER

Applied Organometallic Chemistry WILEY

Green synthesis approach for Fe (III), Cu (II), Zn (II) and Ni (II)-Schiff base complexes, spectral, conformational, MOE-docking and biological studies

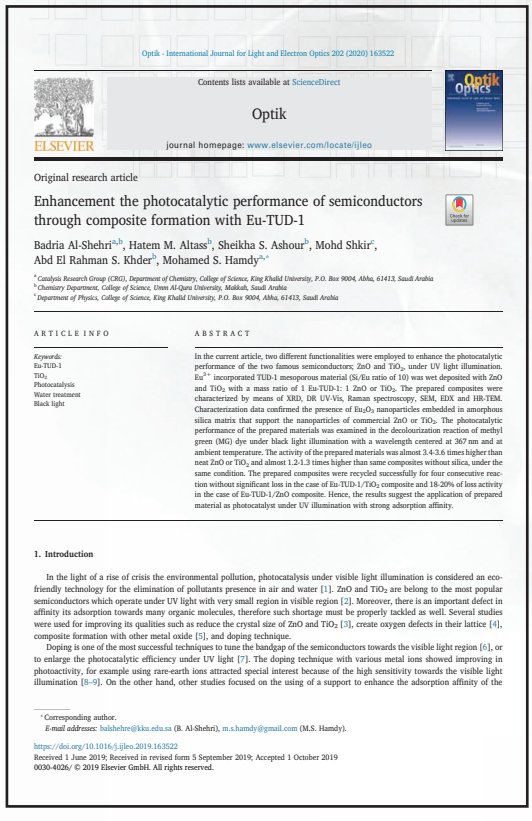
Gamil A.A. Al-Hazmi[1,2] | Khlood S. Abou-Melha[1] | Nashwa M. El-Metwaly[3,4] | Ismail Althagafi[3] | Fathy Shaaban[5] | Rania Zaky[4]

[1]Chemistry Department, Faculty of Science, King Khalid University, Abha, Saudi Arabia
[2]Chemistry Department, Faculty of Applied Sciences, Taiz University, Taiz, Yemen
[3]Department of Chemistry, Faculty of Applied Science, Umm-Al-Qura University, Makkah, Saudi Arabia
[4]Department of Chemistry, Faculty of Science, Mansoura University, Egypt
[5]Custodian of Two Holy Mosques Institute for Hajj and Umrah Research, Umm-Al-Qura University, Makkah, Saudi Arabia

Correspondence
Nashwa M. El-Metwaly, Department of Chemistry, Faculty of applied science, Umm-Al-Qura University, Makkah, Saudi- Arabia.

Green synthesis of Fe (III), Cu (II), Zn (II) and Ni (II)-Schiff's-base complexes from 2-oxo-*N*-(pyridine-2-yl)-2-(2-(1-(pyridin-2-yl)ethylidene)hydrazinyl) acetamide(H_2L),ligand. All new complexes were characterized *via* several spectroscopic and analytical techniques, to establish their molecular and structural formulae. All complexes appeared have 1:1 molar ratio (M:L). The ligand contributed as a neutral poly-dentate towards the metal ions. Moreover, material-studio program was used to predict the most fitted atomic-skeletons for investigated compounds by applying DFT method. MOE docking module (vs. 2015) was used to examine the degree of inhibition for new compounds versus three infected-cell proteins (1hqb, 2gt1 and 4esw). Also, antimicrobial and colorimetric assess for compounds that bind DNA were performed

KEYWORDS
antimicrobial, DFT, green synthesis, MOE-docking, Schiff base



Optik - International Journal for Light and Electron Optics 202 (2020) 163522

Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.com/locate/ijleo

Original research article

Enhancement the photocatalytic performance of semiconductors through composite formation with Eu-TUD-1

Badria Al-Shehri[a,b], Hatem M. Altass[b], Sheikha S. Ashour[b], Mohd Shkir[c], Abd El Rahman S. Khder[b], Mohamed S. Hamdy[a,*]

[a] Catalysis Research Group (CRG), Department of Chemistry, College of Science, King Khalid University, P.O. Box 9004, Abha, 61413, Saudi Arabia
[b] Chemistry Department, College of Science, Umm Al-Qura University, Makkah, Saudi Arabia
[c] Department of Physics, College of Science, King Khalid University, P.O. Box 9004, Abha, 61413, Saudi Arabia

ARTICLE INFO

Keywords:
Eu-TUD-1
TiO_2
Photocatalysis
Water treatment
Black light

ABSTRACT

In the current article, two different functionalities were employed to enhance the photocatalytic performance of the two famous semiconductors; ZnO and TiO_2 under UV light illumination. Eu^{3+} incorporated TUD-1 mesoporous material (Si/Eu ratio of 10) was wet deposited with ZnO and TiO_2 with a mass ratio of 1 Eu-TUD-1: 1 ZnO or TiO_2. The prepared composites were characterized by means of XRD, DR UV-Vis, Raman spectroscopy, SEM, EDX and HR-TEM. Characterization data confirmed the presence of Eu_2O_3 nanoparticles embedded in amorphous silica matrix that support the nanoparticles of commercial ZnO or TiO_2. The photocatalytic performance of the prepared materials was examined in the decolourization reaction of methyl green (MG) dye under black light illumination with a wavelength centered at 367 nm and at ambient temperature. The activity of the prepared materials was almost 3.4-3.6 times higher than neat ZnO or TiO_2 and almost 1.2-1.3 times higher than same composites without silica, under the same condition. The prepared composites were recycled successfully for four consecutive reaction without significant loss in the case of Eu-TUD-1/TiO_2 composite and 18-20% of loss activity in the case of Eu-TUD-1/ZnO composite. Hence, the results suggest the application of prepared material as photocatalyst under UV illumination with strong adsorption affinity.

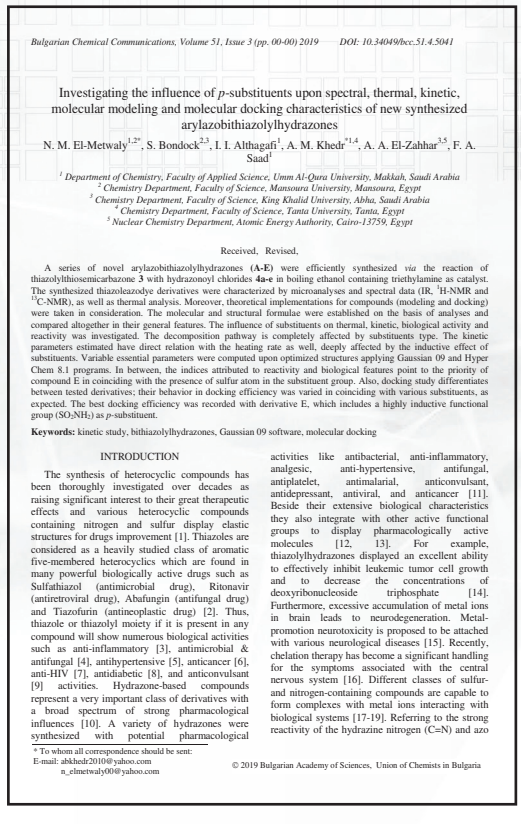
1. Introduction

In the light of a rise of crisis the environmental pollution, photocatalysis under visible light illumination is considered an eco-friendly technology for the elimination of pollutants presence in air and water [1]. ZnO and TiO_2 are belong to the most popular semiconductors which operate under UV light with very small region in visible region [2]. Moreover, there is an important defect in affinity its adsorption towards many organic molecules, therefore such shortage must be properly tackled as well. Several studies were used for improving its qualities such as reduce the crystal size of ZnO and TiO_2 [3], create oxygen defects in their lattice [4], composite formation with other metal oxide [5], and doping technique.

Doping is one of the most successful techniques to tune the bandgap of the semiconductors towards the visible light region [6], or to enlarge the photocatalytic efficiency under UV light [7]. The doping technique with various metal ions showed improving in photoactivity, for example using rare-earth ions attracted special interest because of the high sensitivity towards the visible light illumination [8–9]. On the other hand, other studies focused on the using of a support to enhance the adsorption affinity of the

* Corresponding author.
E-mail addresses: balshehre@kku.edu.sa (B. Al-Shehri), m.s.hamdy@gmail.com (M.S. Hamdy).

https://doi.org/10.1016/j.ijleo.2019.163522
Received 1 June 2019; Received in revised form 5 September 2019; Accepted 1 October 2019
0030-4026/



Bulgarian Chemical Communications, Volume 51, Issue 3 (pp. 00-00) 2019 DOI: 10.34049/bcc.51.4.5041

Investigating the influence of *p*-substituents upon spectral, thermal, kinetic, molecular modeling and molecular docking characteristics of new synthesized arylazobithiazolylhydrazones

N. M. El-Metwaly[1,2*], S. Bondock[2,3], I. I. Althagafi[1], A. M. Khedr[*1,4], A. A. El-Zahhar[3,5], F. A. Saad[1]

[1] *Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia*
[2] *Chemistry Department, Faculty of Science, Mansoura University, Mansoura, Egypt*
[3] *Chemistry Department, Faculty of Science, King Khalid University, Abha, Saudi Arabia*
[4] *Chemistry Department, Faculty of Science, Tanta University, Tanta, Egypt*
[5] *Nuclear Chemistry Department, Atomic Energy Authority, Cairo-13759, Egypt*

Received, Revised,

A series of novel arylazobithiazolylhydrazones (**A-E**) were efficiently synthesized *via* the reaction of thiazolylthiosemicarbazone **3** with hydrazonoyl chlorides **4a-e** in boiling ethanol containing triethylamine as catalyst. The synthesized thiazoleazodye derivatives were characterized by microanalyses and spectral data (IR, ^{1}H-NMR and ^{13}C-NMR), as well as thermal analysis. Moreover, theoretical implementations for compounds (modeling and docking) were taken in consideration. The molecular and structural formulae were established on the basis of analyses and compared altogether in their general features. The influence of substituents on thermal, kinetic, biological activity and reactivity was investigated. The decomposition pathway is completely affected by substituents type. The kinetic parameters estimated have direct relation with the heating rate as well, deeply affected by the inductive effect of substituents. Variable essential parameters were computed upon optimized structures applying Gaussian 09 and Hyper Chem 8.1 programs. In between, the indices attributed to reactivity and biological features point to the priority of compound E in coinciding with the presence of sulfur atom in the substituent group. Also, docking study differentiates between tested derivatives; their behavior in docking efficiency was varied in coinciding with various substituents, as expected. The best docking efficiency was recorded with derivative E, which includes a highly inductive functional group (SO_2NH_2) as *p*-substituent.

Keywords: kinetic study, bithiazolylhydrazones, Gaussian 09 software, molecular docking

INTRODUCTION

The synthesis of heterocyclic compounds has been thoroughly investigated over decades as raising significant interest to their great therapeutic effects and various heterocyclic compounds containing nitrogen and sulfur display elastic structures for drugs improvement [1]. Thiazoles are considered as a heavily studied class of aromatic five-membered heterocyclics which are found in many powerful biologically active drugs such as Sulfathiazol (antimicrobial drug), Ritonavir (antiretroviral drug), Abafungin (antifungal drug) and Tiazofurin (antineoplastic drug) [2]. Thus, thiazole or thiazolyl moiety if it is present in any compound will show numerous biological activities such as anti-inflammatory [3], antimicrobial & antifungal [4], antihypertensive [5], anticancer [6], anti-HIV [7], antidiabetic [8], and anticonvulsant [9] activities. Hydrazone-based compounds represent a very important class of derivatives with a broad spectrum of strong pharmacological influences [10]. A variety of hydrazones were synthesized with potential pharmacological activities like antibacterial, anti-inflammatory, analgesic, anti-hypertensive, antifungal, antiplatelet, antimalarial, anticonvulsant, antidepressant, antiviral, and anticancer [11]. Beside their extensive biological characteristics they also integrate with other active functional groups to display pharmacologically active molecules [12, 13]. For example, thiazolylhydrazones displayed an excellent ability to effectively inhibit leukemic tumor cell growth and to decrease the concentrations of deoxyribonucleoside triphosphate [14]. Furthermore, excessive accumulation of metal ions in brain leads to neurodegeneration. Metal-promotion neurotoxicity is proposed to be attached with various neurological diseases [15]. Recently, chelation therapy has become a significant handling for the symptoms associated with the central nervous system [16]. Different classes of sulfur- and nitrogen-containing compounds are capable to form complexes with metal ions interacting with biological systems [17-19]. Referring to the strong reactivity of the hydrazine nitrogen (C=N) and azo

* To whom all correspondence should be sent:
E-mail: abkhedr2010@yahoo.com
n_elmetwaly00@yahoo.com

European Journal of Medicinal Chemistry 165 (2019) 502–513

Contents lists available at ScienceDirect

European Journal of Medicinal Chemistry

journal homepage: http://www.elsevier.com/locate/ejmech

Review article

Role of PPAR receptor in different diseases and their ligands: Physiological importance and clinical implications

Agha Zeeshan Mirza [a, b, *], Ismail I. Althagafi [a, b], Hina Shamshad [c]

[a] Chemistry Department, Faculty of Applied Sciences, Umm Al-Qura University, Makkah, Saudi Arabia
[b] Research Laboratories Centre, Faculty of Applied Sciences, Umm Al-Qura University, Makkah, Saudi Arabia
[c] Research Institute of Pharmaceutical Sciences, Faculty of Pharmacy, University of Karachi, Karachi, 75270, Pakistan

ARTICLE INFO

Article history:
Received 4 October 2018
Received in revised form
27 January 2019
Accepted 28 January 2019
Available online 1 February 2019

Keywords:
Peroxisome proliferator-activated receptors
Thiazolidinediones

ABSTRACT

The peroxisome proliferator-activated receptors (PPAR-α, PPAR-β/δ, and PPAR-γ) are members of the nuclear receptor super-family, acting as ligand-inducible transcription factors and play crucial roles in glucose and lipid metabolism. These are a well-known receptor for diabetic therapy, not only influence the cardiovascular systems but are also expressed in many human solid tumors. For atherosclerosis, inflammation, and hypertension, the PPARs are considered as important therapeutic targets. Furthermore, it has been suggested that careful designing of partial agonists for PPARs, may show improvement with the side effects and also increase the therapeutic value for different diseases as cancer, inflammation and cardiovascular etc. This review summaries structural features of PPAR receptors, illustrates the method of PPAR modulator design, then analyzes recent dual- and pan-agonist with different therapeutic outcomes of the receptor to be used as a target for drugs in future. The advances in PPARs antagonists, their classification and structure-activity relationship are also summarized.

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* Corresponding author.Chemistry Department, Faculty of Applied Sciences, Umm Al-Qura University, Makkah, Saudi Arabia.
E-mail address: azmirza@uqu.edu.sa (A.Z. Mirza).

https://doi.org/10.1016/j.ejmech.2019.01.067
0223-5234/

Environmental Technology

ISSN: 0959-3330 (Print) 1479-487X (Online) Journal homepage: https://www.tandfonline.com/loi/tent20

Microwave-assisted synthesis of gold nanoparticles supported on Mn_3O_4 catalyst for low temperature CO oxidation

Moataz Morad, Mohammad A. Karim, Hatem M. Altass & Abd El Rahman S. Khder

To cite this article: Moataz Morad, Mohammad A. Karim, Hatem M. Altass & Abd El Rahman S. Khder (2019): Microwave-assisted synthesis of gold nanoparticles supported on Mn_3O_4 catalyst for low temperature CO oxidation, Environmental Technology, DOI: 10.1080/09593330.2019.1709988

To link to this article: https://doi.org/10.1080/09593330.2019.1709988

Journal of Saudi Chemical Society (2019) 23, 503–513

King Saud University

Journal of Saudi Chemical Society

www.ksu.edu.sa
www.sciencedirect.com

Multicomponent access to novel proline/cyclized cysteine tethered monastrol conjugates as potential anticancer agents

M. Shaheer Malik [a,b,*], Zaki S. Seddigi [c], Shaik Bajee [d], Shaik Azeeza [d], Syed Riyaz [d], Saleh A. Ahmed [a,b], Ismail I. Althagafi [a,b], Qazi M. Sajid Jamal [e], Ahmed Kamal [d,*]

[a] Central Research Laboratories, Faculty of Applied Sciences, Umm Al-Qura University, 21955 Makkah, Saudi Arabia
[b] Department of Chemistry, Faculty of Applied Sciences, Umm Al-Qura University, 21955 Makkah, Saudi Arabia
[c] Department of Environmental Health, College of Public Health and Health informatics, Umm Al-Qura University, 21955 Makkah, Saudi Arabia
[d] Department of Medicinal Chemistry and Pharmacology, CSIR-Indian Institute of Chemical Technology, Hyderabad-500007, India
[e] Department of Health Information Management, College of Applied Medical Sciences, Buraydah Colleges, Al Qassim, Saudi Arabia

Received 28 November 2018; revised 6 January 2019; accepted 8 January 2019
Available online 18 January 2019

KEYWORDS
Monastrol;
Amino acids;
Multicomponent Biginelli's reaction;
Anticancer agents;
Docking studies

Abstract The versatility of multicomponent Biginelli's reaction is exploited in the development of proline and cyclized cysteine tethered conjugates of monastrol, a kinesin Eg5 inhibitor. Ten new conjugates are synthesized focusing on structural replacement of the ester moiety (C-5 position) of the monastrol backbone with amino acid based amide moieties. On cytotoxic evaluation, conjugate **24** has shown promising in vitro cytotoxic activity against leukemia. Molecular docking studies revealed that the conjugates **19** and **24** exhibit better interaction at kinesin Eg5 receptor compared to monastrol. Moreover, computational calculations and predictions of important molecular properties suggest that these new amino acid based conjugates could be further improved to provide potential anticancer agents.

1. Introduction

In the quest for a sustainable approach in organic synthesis, the multicomponent reactions are indispensable tools in the repertoire of chemists because of their near perfect atom economy and higher efficiency [1]. The rapid access to structural diversity provided by the multicomponent reaction is well exploited in the drug design and discovery programs [2,3]. One of the interesting multicomponent reactions is Biginelli's

* Corresponding authors.
E-mail addresses: msmalik@uqu.edu.sa (M. Shaheer Malik), ahmedkamal@iict.res.in (A. Kamal).
Peer review under responsibility of King Saud University.

Production and hosting by Elsevier

https://doi.org/10.1016/j.jscs.2019.01.003
1319-6103 © 2019 King Saud University. Production and hosting by Elsevier B.V.

Materials Research Bulletin 113 (2019) 215–222

Contents lists available at ScienceDirect

Materials Research Bulletin

journal homepage: www.elsevier.com/locate/matresbu

Preparation and characterization of highly active Pd nanoparticles supported Mn_3O_4 catalyst for low-temperature CO oxidation

Abd El Rahman S. Khder[a,b,*], Hatem M. Altass[b], Mohamed I. Orif[c], Sheikha S. Ashour[b], Layla S. Almazroai[b]

[a] Faculty of Science, Chemistry Department, Mansoura University, Mansoura, Egypt
[b] Faculty of Applied Science, Chemistry Department, Umm Al Qura University, Makkah, Saudi Arabia
[c] Faculty of Marine Science, Marine Chemistry Department, King Abdulaziz University, PO Box 80207, Jeddah 21589, Saudi Arabia

ARTICLE INFO

Keywords:
Pd
Mn_3O_4
H_2-TPR
XPS
CO oxidation

ABSTRACT

Two methods were used to prepare Mn_3O_4 followed by deposition of Pd nanoparticles with 2 and 4 wt.%. The textural and structural properties were characterized by several methods. The XRD results showed the participation of MnO_2 phase with small amount with tetragonal Mn_3O_4 due to hydrothermal treatment at 150 °C. Moreover, no changes in the textural properties of Mn_3O_4 due to the difference in preparation method or Pd nanoparticles deposition. TEM images showed different morphologies such as cubic, spheroid and plate-shaped structures. The XPS study confirmed the distribution of both Pd^0 and Pd^{2+} species on the Mn_3O_4 surface. The reducibility of pure Mn_3O_4 was greatly enhanced and shifted to lower temperatures after incorporation of Pd nanoparticles. The presence of Pd^{2+} may facilitate the providing of reactive lattice oxygen for CO oxidation by the support. The performance of the catalysts towards CO oxidation was much more enhanced as the Pd content increased to 4 wt. %. The results showed good stability and durability during the CO oxidation.

1. Introduction

Many environmental hazard materials were emitted into the atmosphere in the last decades due to the industrial revolution and the millions of tons of industrial waste left over. In this issue, heterogeneous catalysis plays a very important role in order to reduce environmental pollution and hazard pollutants [1]. Lots of authors were using solid acid catalysts in catalyzing of many organic reactions to overcome homogeneous catalysis and industrial liquid pollutants problems [2–7]. On the other hand, in the gas phase, carbon monoxide (CO) is one of the most dangerous components. The main sources of carbon monoxide (CO) in the atmosphere are the incomplete combustion of carbonaceous materials, industrial processes exhaust and automobile exhausts. The dangerous effects of carbon monoxide are due to it is colorless and odorless gas and at the ppm level is fatal. Therefor lots of authors were interested in CO elimination. Therefore, heterogeneous catalytic oxidation is a clever solution for environmental pollution control. However, the development of the current catalytic processes implies great development in the catalytic materials. Those materials must be active, selective, stable and cost-effective. In this field, good improvements have been reached using Nobel metals nanoparticles [8–10].

Palldium supported catalysts exhibited very high catalytic activities for various applications [11–13]. Generally, when Pd nanoparticles supported on active supports highly active and durable catalysts obtained. Transition metal oxides are considered to very active supports which may be due to the diversity of their oxidation numbers. Such transition metal oxides can adsorb oxygen easily which leads to the formation of mobile oxygen moiety which can oxidize CO [14,15].

Moreover, Manganese oxides are very important components in heterogeneous catalysis [16–19]. Many preparation methods and skills have been used to obtain active supported catalysts. Generally, Mn_3O_4 is synthesized by heating salts of manganese at about 1000 °C in the air [20], co-precipitation [21], sol-gel methods [22], hydrothermal [23], solvothermal [24] microwave irradiation [25], and ultrasonic irradiation [26]. These preparation methods may affect the properties of the support which in turn may result in strong Pd nanoparticles support interactions, that strongly enhance the catalytic properties of the catalyst.

In the present work, we study the effect of preparation method as well as Pd nanoparticles deposition over the Mn_3O_4 surface. We prepared Mn_3O_4 through simple chemical precipitation method at room temperature followed by hydrothermal treatment at 150 °C. The relationship between the catalysts structure, reducibility and their

* Corresponding Author.
E-mail address: aakhder2244@yahoo.com (A.E.R.S. Khder).

https://doi.org/10.1016/j.materresbull.2019.02.011
Received 27 June 2018; Received in revised form 9 November 2018; Accepted 7 February 2019
Available online 08 February 2019
0025-5408/

NUCLEOSIDES, NUCLEOTIDES AND NUCLEIC ACIDS
https://doi.org/10.1080/15257770.2019.1615623

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Advancement in the development of heterocyclic nucleosides for the treatment of cancer - A review

Agha Zeeshan Mirza[a,b]

[a]Chemistry Department, Faculty of Applied Sciences, Umm Al-Qura University, Makkah, Saudi Arabia; [b]Research Laboratories Centre, Faculty of Applied Sciences, Umm Al-Qura University, Makkah, Saudi Arabia

ABSTRACT

Cancer diseases are widely recognised as an important medical problem and killing millions of people in a year. Chemotherapeutic drugs are successful against cancer in many cases and different compounds, including the analogues of natural substances, may be used for anticancer agents. Nucleoside analogues also have become a necessity for the treatment of cancer diseases. Nucleoside, nucleotide and base analogues have been utilised for decades for the treatment of viral pathogens, neoplasms and in anticancer chemotherapy. This review focuses on the different types of nucleosides and their potential role as anticancer agents. It also discusses the nucleoside analogues approved by FDA and in process of approval. The effect of the substitution on the nucleoside analogues and their pharmacological role is also discussed in the review. Owing to the advances in computational chemistry, it concludes with the future advancement and possible outcome of the nucleoside analogues. Also, it depicts the development of heterocyclic nucleoside analogues, explores the QSAR of the synthesised compounds and discusses the 3 D QSAR pharmacophore modelling in order to examine their potential anti-cancer activities.

ARTICLE HISTORY
Received 12 November 2018
Accepted 2 May 2019

KEYWORDS
Heterocyclic nucleoside; cancer; isoxazolidine; chemotherapeutic drugs

Introduction

Cancer, a serious worldwide disease, including more than 150 different diseases together, is responsible for killing millions of people in a year.[1,2] Chemotherapeutic agents for cancer treatment have gained a lot of popularity but it has some major drawbacks to be addressed.

One of the responsibilities of a medicinal organic chemist is to design and synthesise compounds which may be potent and efficient against diseases.

For almost 50 years, nucleoside analogues are in use and have become a necessity for the treatment of cancer and viral diseases.[3] These compounds have poor bioavailability after oral administration because of low intestinal permeability and due to rapid change into the inactive metabolite

CONTACT Agha Zeeshan Mirza dr.zeeshan80@gmail.com
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Current Computer-Aided Drug Design, **2019**, *15*, 167-181 167

RESEARCH ARTICLE

QSAR and Docking Studies on Piperidyl-cyclohexylurea Derivatives for Prediction of Selective and Potent Inhibitor of Matriptase

Agha Zeeshan Mirza[1,2,*] and Hina Shamshad[3]

[1]*Chemistry Department, Faculty of Applied Sciences, Umm Al-Qura University, Makkah, Saudi Arabia;* [2]*Research Laboratories Centre, Faculty of Applied Sciences, Umm Al-Qura University, Makkah, Saudi Arabia;* [3]*Research Institute of Pharmaceutical Sciences, Faculty of Pharmacy, University of Karachi, Karachi-75270, Pakistan*

ARTICLE HISTORY
Received: January 26, 2018
Revised: May 03, 2018
Accepted: May 11, 2018

DOI:
10.2174/1573409914666180516162349

Abstract: ***Background:*** QSAR models as PLS, GFA, and 3D were developed for a series of matriptase inhibitors using 35 piperidyl-cyclohexylurea compounds. The training and test sets were divided into a set of 28 and 8 compounds, respectively and the pki values of each compound were used in the analysis.

Methods: Docking and alignment methodologies were used to develop models in 3D QSAR. The best models among all were selected on the basis of regression statistics as r2, predictive r2 and Friedman Lack of fit measure. Hydrogen donors and rotatable bonds were found to be positively correlated properties for this target. The models were validated and used for the prediction of new compounds. Based on the predictions of 3D-QSAR model, 17 new compounds were prepared and their activities were predicted and compared with the active compound. Prediction of activities was performed for these 18 compounds using consensus results of all models. ADMET was also performed for the best-chosen compound and compared with the known active.

Results and Conclusion: The developed model was able to validate the obtained results and can be successfully used to predict new potential and active compounds.

Keywords: QSAR, docking studies, piperidyl-cyclohexylurea derivatives, matriptase, ADMET, GFA.

1. INTRODUCTION

Matriptase (type II transmembrane serine protease) has been established as cancer associated protein since its substrates (prourokinase plasminogen activator and pro-hepatocyte growth factor) are involved in cancer processes. An imbalance between the protease and its cognate inhibitor hepatocyte growth factor activator inhibitor-1 (HAI-1) has been reported to be involved in cancer [1]. Matriptase is attached to the cell surface by signal anchor trans-membrane domain and it is believed that it not only facilitates cellular invasiveness but may also activate oncogenic pathways [2]. Matriptase was first characterized in human breast cancer cells and was named membrane-type serine proteinase (MT-SP1) having 855-residue with the presence in different types of cancers as prostate, breast, and colorectal cancers. Its role in breast cancer was found to be variable and cell context dependent [3]. It was also established that expression of matriptase and prostasin was related to breast cancer cell lines [4]. Matriptase is also a target for ovarian cancer as it expresses and activates proteins that play a role in ovarian cancer [5]. Not limited to ovarian cancer, matriptase is also involved in different signaling pathways and abnormal activity of matriptase may lead to different diseases. Matriptase exists in zymogen form or with hepatocyte growth factor activator lipophilicity inhibitor [6]. It was observed that its inhibition reduced metastasis and tumor growth in a prostate cancer of rat model [7]. Selectivity is the major issue for matriptase inhibitors, as a lot of inhibitors were not suitable due to interference with signaling pathways and processes.

Hence, a highly selective inhibitor of matriptase may have a number of advantages [8]. Small molecules used as inhibitors of matriptase were found to be more beneficial as they possess selectivity over other serine proteases also such as thrombin. Matriptase like another protease consists of eight loops and its active site of matriptase is much more negatively charged [8].

Few compounds having 3-amidinophenylalanine were found not only to be the inhibitor of matriptase but also selective for thrombin [9].

Theoretical methods have been employed to assist in a number of complex diseases like cancer since they are fast and efficient. The application of Quantitative Structure-activity Relationship (QSAR) models are important in finding potent molecule by evaluating chemical information of the molecules into molecular descriptors [10].

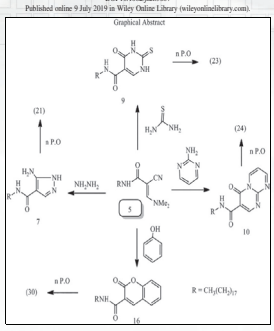
*Address correspondence to this author at the Science and Technology Unit (STU), Umm Al-Qura University, Makkah, Saudi Arabia; E-mail: dr.zeeshan80@gmail.com

1573-4099/19 $58.00+.00

Refat El-Sayed[a,b]* and Hanadi A. Katouah[a]

[a]Chemistry Department, College of Applied Sciences, Umm Al-Qura University, Makkah 21955, Saudi Arabia
[b]Chemistry Department, Faculty of Science, Benha University, Benha, Egypt
*E-mail: ref_ja9@hotmail.com
Received October 23, 2018
DOI 10.1002/jhet.3607
Published online 9 July 2019 in Wiley Online Library (wileyonlinelibrary.com).

Graphical Abstract



This study aims to synthesis of condensed and non-condensed heterocyclic rings with long fatty chains as surface active biological compounds. 2-Cyano-3-(dimethylamino)-*N*-octadecylacrylamide (**5**) was used to synthesize pyrimidine, pyran, and other condensed products by interacting with appropriate chemical reagents. These compounds were transferred to nonionic surface-active agents by condensation with propylene oxide. The surface and biological properties showed that these compounds have a high solubility that helps them in easy absorption and adsorption with other compounds. In addition, they have a high ability to decrease the surface tension of the liquids, good wetting, and emulsification power, which can be used at different temperatures without losing their surface or biological properties and enable them for use in industrial and pharmaceutical purposes easily.

J. Heterocyclic Chem., **56**, 2134 (2019).

INTRODUCTION

The primary means of obtaining chemical products that have practical applications such as pharmaceuticals, photosensitizers, dyes, plant protection agents, monomers, and other applications is organic synthesis [1]. Heterocyclic derivatives containing one or more atoms in their structure are of great importance in our daily lives because of their biological effects. Therefore, it enters into wide range of applications such as pharmaceuticals, agrochemicals, disinfectants, developers, corrosion inhibitors, and polymers as they are used in the synthesis of other organic compounds where the most majority of new drugs contains heterocycles interface between chemistry and biology [2,3]. Nemours compounds containing isoxazole, pyrazole, pyrazole, and pyrimidine moieties are bioactive molecules, which play an important role in the medicinal fields because of their diverse biological and pharmacological activities as antibacterial, antifungal, antioxidant, antipyretics, anti-inflammatory, antiviral, cytotoxic, anticancer agent, antihypertensive, muscle-relaxant, hypnotic, antidepressant, analgesic, and

Journal of Photochemistry & Photobiology A: Chemistry 371 (2019) 306–314

Contents lists available at ScienceDirect

Journal of Photochemistry & Photobiology A: Chemistry

journal homepage: www.elsevier.com/locate/jphotochem

MCM-SO_3H catalyzed synthesis of environment-sensitive fluorophores incorporating pyrene moiety: Optimization, fluorescence emission and theoretical studies

Nizar El Guesmi[a,b], Essam M. Hussein[a,c], Saleh A. Ahmed[a,c,*]

[a] *Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, 21955, Makkah, Saudi Arabia*
[b] *Département de chimie, Faculté des Sciences de Monastir, Avenue de l'Environnement, 5019, Monastir, Tunisia*
[c] *Department of Chemistry, Faculty of Science, Assiut university, 71516, Assiut, Egypt*

ARTICLE INFO

Keywords:
MCM-SO_3H
Pyrene
Fluorophores
Solvatochromic properties
2-Pyrazolines
Eco-friendly

ABSTRACT

Six new highly fluorescent 5-(aryl)-1-phenyl-3-(pyren-1yl)-2-pyrazolines were synthesized by reaction of various (*E*)-3-aryl-1-(pyren-1-yl)prop-2-en-1-ones with phenyl hydrazine in the presence of sulfonated mesoporous silica (MCM-SO_3H) as efficient and eco-friendly acidic catalyst. The chemical structures of all synthesized compounds were illustrated on the basis of spectral data (IR, ^{1}H NMR and ^{13}C NMR). This was followed by photophysical properties-based absorption and emission studies of the target compounds in solutions of different solvent polarities. The microenvironment-sensitive fluorescent pyrazolines labeled with pyrene exhibited valuable fluorescence properties with emission in the range of 600–700 nm with a marked response to change in the environmental polarities. A significant and pronounced red shift was observed in the emission spectrum of 5-(aryl)-1-phenyl-3-(pyren-1yl)-2-pyrazolines $\Delta\tilde{\nu}_{\sim}$ 50 nm compared to the absorption spectrum $\Delta\tilde{\nu}_{\sim}$ 10 nm upon increasing the solvent polarity. This indicated the presence of higher dipole moment in the excited state than in the ground state and the transition involved are π-π^* transition through the charge transfer phenomena. The fundamental understanding of solvatochromic properties were analyzed through Lippert-Mataga and Reichardts correlations in order to estimate the change in dipole moments ($\Delta\mu$) which suggested the emissive state of designed fluorescent 2-pyrazoline derivatives is of strong ICT character.

1. Introduction

Pyrene is a well-known polynuclear aromatic hydrocarbon, which recently become one of the most widely studied organic molecules in the field of photochemistry and photophysics. Because of its unique properties, it has emerged as an outstanding area of area in many scientific fields. The highly fluorescence properties of pyrene has rendered it to a fluorophore of first choice in both applied and fundamental photochemical and photophysical research [1-10]. Interestingly, pyrene is one of few polycyclic aromatic hydrocarbons that perform vibronic structure in its monomer fluorescence spectrum in solution [11]. Its derivatives have been extensively expended in many applications such as fluorescent sensors [12,13] or fluorescent probes [14] based on virtue of their excellent fluorescence properties. Pyrene monomer emission typically occurs between 370 and 420 nm exhibiting a characteristic violet color and is considered as one of the most useful frameworks for the construction of fluorogenic chemosensors by conjugating with numerous and diverse chemical species [15]. This has encouraged the development of new synthetic methodologies for the synthesis of pyrene type substances. Some of these compounds can be used as useful key intermediates for the synthesis of precious heterocyclic ring systems. Among them, 1-cinnamoylpyrenes synthesized through the Claisen-Schmidt condensation of 1-acetylpyrene and aromatic aldehydes [16,17] has proved to be particularly important. 1-Cinnamoylpyrenes have been used for the synthesis of functionalized pyrrolidines [16], pyrrolizidines [17] and other nitrogen-based heterocycles. Furthermore, pyrazolines are important nitrogen-containing five membered heterocyclic compounds. Literature survey revealed that many pyrazoline derivatives are known to exhibit a wide range of biological activities such as antimicrobial [18], antimalarial [19], antitumor [20], anti-inflammatory [20], anticonvulsant and antidepressants activities [21].

2 -Pyrazoline derivatives are the most commonly studied pyrazoline-type compounds and numerous methods have been reported for

* Corresponding author at: Department of Chemistry, Faculty of Applied Science, Umm Al-Qura University, 21955, Makkah, Saudi Arabia.
E-mail address: saahmed@uqu.edu.sa (S.A. Ahmed).

https://doi.org/10.1016/j.jphotochem.2018.11.036
Received 18 October 2018; Received in revised form 22 November 2018; Accepted 24 November 2018
Available online 26 November 2018
1010-6030/

RSC Advances

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Cite this: *RSC Adv.*, 2019, 9, 35549

Probing relaxation dynamics of a cationic lipid based non-viral carrier: a time-resolved fluorescence study

Priya Singh,†[a] Diparjan Mukherjee,†[a] Subhankar Singha,[b] V. K. Sharma,[c] Ismail I. Althagafi,[d] Saleh A. Ahmed,[b] R. Mukhopadhyay,[c] Ranjan Das[a] *[e] and Samir Kumar Pal[a] *[e]

Lipid vesicles composed of cationic dioctadecyldimethylammonium bromide (DODAB) and neutral 1-monooleoyl-rac-glycerol (MO) are promising non-viral carriers of nucleic acids for delivery into cells. Among them, higher cell transfection efficiency was displayed by DODAB-rich vesicles than those enriched with MO. Structural relaxation of these mixed lipid vesicles plays a key role in their cell transfection efficiency because structural organization of the DODAB-rich vesicles are different from that of the MO-rich vesicles. Polarization-gated anisotropy in conjunction with picosecond resolved emission transients of a novel fluorophore 6-acetyl-(2-((4-hydroxycyclohexyl)(methyl)amino) naphthalene) (ACYMAN) has been employed to probe relaxation dynamics in pure DODAB vesicles, and in mixed vesicles of DODAB with varying content of MO. Both orientational relaxation of ACYMAN and relaxation dynamics of its local environment are retarded significantly in mixed lipid vesicles with increasing MO content, from a mole fraction (χ_{MO}) of 0.2 to that of 0.8 which is consistent with increased rigidity of the MO-rich ($\chi_{MO} > 0.5$) vesicles relative to the DODAB-rich ($\chi_{MO} < 0.5$) vesicles. Therefore, higher structural rigidity of the MO-rich vesicles ($\chi_{MO} > 0.5$) gives rise to their lower cell transfection efficiency than the more flexible DODAB-rich ($\chi_{MO} < 0.5$) vesicles as observed in previous *in vivo* studies (*Biochim. Biophys. Acta, Biomembr.*, 2014, **1838**, 2555–2567).

Received 28th August 2019
Accepted 18th October 2019

DOI: 10.1039/c9ra06824d

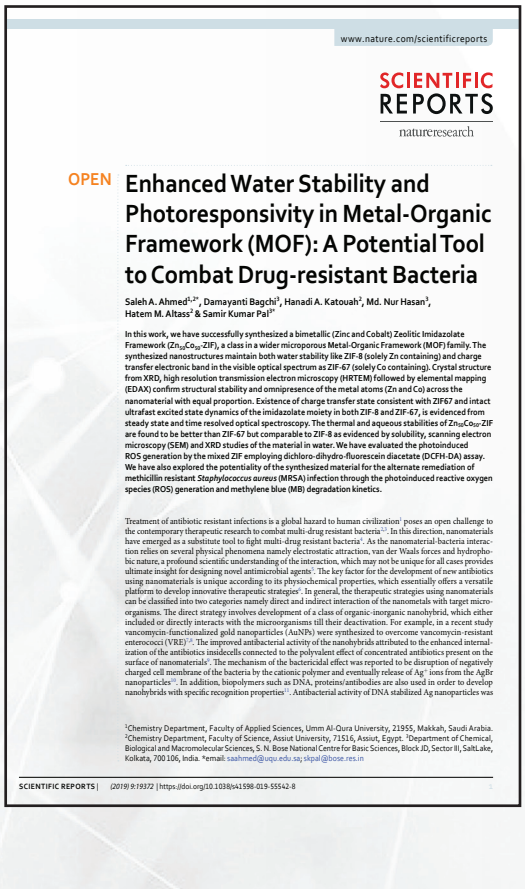
rsc.li/rsc-advances

Introduction

Vesicles, based on cationic lipids, are one of the most promising carriers among non-viral vectors in gene therapy.[1] The headgroups of the cationic lipids interact with the negatively charged phosphates of DNA forming lipoplexes, and the nucleic acid can be untied from these DNA-cationic lipid complexes (lipoplexes) for release into the cytoplasm which is crucial to successful delivery of DNA into the cell. The addition of neutral lipids to cationic lipid vesicles favours fusion of the lipoplexes with cell membranes, due to their propensity to form non-lamellar structures which are akin to membrane fusion intermediates and therefore, act as important mediators in cell transfection.[2–5]

Recent studies[5,6] have revealed that tuning the content of MO in vesicles composed of a cationic lipid dioctadecyldimethylammonium bromide (DODAB, Scheme 1) and a neutral lipid 1-monooleoyl-rac-glycerol or monolein (MO, Scheme 1) not only alters the structural organization of the lipoplexes between multilamellar and inverted non-lamellar structures, but, also modulates the cell transfection efficiency of these non-viral carriers. For example, lipid vesicles of DODAB with higher MO content ($\chi_{MO} > 0.5$) were found to exhibit lower cell transfection efficiency than those enriched with DODAB ($\chi_{MO} < 0.5$).[6] The low transfection efficiency of the MO-rich vesicles was thought to be related to their higher stability conferred by the non-lamellar inverted phases, which are advantageous regarding DNA encapsulation and protection, but have a drawback in efficient release of DNA into the cell cytosol.[6] On the other hand, several reports[5–8] have established a correlation between the membrane fluidity and improved *in vitro* transfection activity, where cationic lipids characterized by increased acyl chain fluidity and high interfacial elasticity were found to demonstrate high *in vitro* transfection activity hinting to the role of membrane dynamics in cell transfection. Lipid structural dynamics plays a key role in membrane fluidity and is

[a]Department of Chemical, Biological & Macromolecular Sciences, S. N. Bose National Centre for Basic Sciences, Block JD, Sector III, Salt Lake, Kolkata 700106, India. E-mail: skpal@bose.res.in
[b]Centre of Health Science &Technology, JIS Institute of Advanced Studies, Kolkata, India
[c]Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India
[d]Chemistry Department, Faculty of Applied Sciences, Umm Al-Qura University, 21955 Makkah Al-Mukarramma, Saudi Arabia
[e]Chemistry Department, Faculty of Science, Assiut University, 71516 Assiut, Egypt
[f]Department of Chemistry, West Bengal State University, Barasat, Kolkata 700126, India. E-mail: ranjan.das66@gmail.com
† Authors made equal contribution.



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Enhanced Water Stability and Photoresponsivity in Metal-Organic Framework (MOF): A Potential Tool to Combat Drug-resistant Bacteria

Saleh A. Ahmed[1,2*], Damayanti Bagchi[3], Hanadi A. Katouah[1], Md. Nur Hasan[3], Hatem M. Altass[2] & Samir Kumar Pal[3*]

In this work, we have successfully synthesized a bimetallic (Zinc and Cobalt) Zeolitic Imidazolate Framework ($Zn_{50}Co_{50}$-ZIF), a class in a wider microporous Metal-Organic Framework (MOF) family. The synthesized nanostructures maintain both water stability like ZIF-8 (solely Zn containing) and charge transfer electronic band in the visible optical spectrum as ZIF-67 (solely Co containing). Crystal structure from XRD, high resolution transmission electron microscopy (HRTEM) followed by elemental mapping (EDAX) confirm structural stability and omnipresence of the metal atoms (Zn and Co) across the nanomaterial with equal proportion. Existence of charge transfer state consistent with ZIF67 and intact ultrafast excited state dynamics of the imidazolate moiety in both ZIF-8 and ZIF-67, is evidenced from steady state and time resolved optical spectroscopy. The thermal and aqueous stabilities of $Zn_{50}Co_{50}$-ZIF are found to be better than ZIF-67 but comparable to ZIF-8 as evidenced by solubility, scanning electron microscopy (SEM) and XRD studies of the material in water. We have evaluated the photoinduced ROS generation by the mixed ZIF employing dichloro-dihydro-fluorescein diacetate (DCFH-DA) assay. We have also explored the potentiality of the synthesized material for the alternate remediation of methicillin resistant *Staphylococcus aureus* (MRSA) infection through the photoinduced reactive oxygen species (ROS) generation and methylene blue (MB) degradation kinetics.

Treatment of antibiotic resistant infections is a global hazard to human civilization[1] poses an open challenge to the contemporary therapeutic research to combat multi-drug resistant bacteria[2,3]. In this direction, nanomaterials have emerged as a substitute tool to fight multi-drug resistant bacteria[4]. As the nanomaterial-bacteria interaction relies on several physical phenomena namely electrostatic attraction, van der Waals forces and hydrophobic nature, a profound scientific understanding of the interaction, which may not be unique for all cases provides ultimate insight for designing novel antimicrobial agents[5]. The key factor for the development of new antibiotics using nanomaterials is unique according to its physicochemical properties, which essentially offers a versatile platform to develop innovative therapeutic strategies[6]. In general, the therapeutic strategies using nanomaterials can be classified into two categories namely direct and indirect interaction of the nanometals with target microorganisms. The direct strategy involves development of a class of organic-inorganic nanohybrid, which either included or directly interacts with the microorganisms till their deactivation. For example, in a recent study vancomycin-functionalized gold nanoparticles (AuNPs) were synthesized to overcome vancomycin-resistant enterococci (VRE)[7,8]. The improved antibacterial activity of the nanohybrids attributed to the enhanced internalization of the antibiotics insidecells connected to the polyvalent effect of concentrated antibiotics present on the surface of nanomaterials[9]. The mechanism of the bactericidal effect was reported to be disruption of negatively charged cell membrane of the bacteria by the cationic polymer and eventually release of Ag^+ ions from the AgBr nanoparticles[10]. In addition, biopolymers such as DNA, proteins/antibodies are also used in order to develop nanohybrids with specific recognition properties[11]. Antibacterial activity of DNA stabilized Ag nanoparticles was

[1]Chemistry Department, Faculty of Applied Sciences, Umm Al-Qura University, 21955, Makkah, Saudi Arabia. [2]Chemistry Department, Faculty of Science, Assiut University, 71516, Assiut, Egypt. [3]Department of Chemical, Biological and Macromolecular Sciences, S. N. Bose National Centre for Basic Sciences, Block JD, Sector III, SaltLake, Kolkata, 700 106, India. *email: saahmed@uqu.edu.sa; skpal@bose.res.in

Journal of Molecular Liquids 291 (2019) 111356

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

Newly synthesized indolium-based ionic liquids as unprecedented inhibitors for the corrosion of mild steel in acid medium

Saleh A. Ahmed [a,b,*], Mohamed I. Awad [a,c,**], Ismail I. Althagafi [a], Hatem M. Altass [a], Moataz Morad [a], Ahmed Alharbi [a], Rami J. Obaid [a]

[a] Chemistry Department, Faculty of Applied Sciences, Umm Al-Qura University, 21955 Makkah, Saudi Arabia
[b] Chemistry Department, Faculty of Science, Assiut University, 71516 Assiut, Egypt
[c] Chemistry Department, Faculty of Science, Cairo University, Giza, Egypt

ARTICLE INFO

Article history:
Received 20 March 2019
Received in revised form 20 June 2019
Accepted 11 July 2019
Available online 12 July 2019

Keywords:
Ionic liquids
Corrosion inhibitor
Langmuir isotherm
Mild steel
Adsorption

ABSTRACT

New indolium-based ionic liquids (IILs) of chemical formula 5-methoxy-1,2,3,3-tetramethyl-3H-indolium iodide (IIL-I), 1-(2-carboxyethyl)-2,3,3-trimethyl-3H-indolium iodide (IIL-II), 2,3,3-trimethyl-1-(pyren-2-ylmthyl)-3H-indolium iodide (IIL-III), 1-(3-ethoxy-3-oxopropyl)-2,3,3-trimethyl-3H-indolium bromide (IIL-IV) and 1-(2-ethoxy-2-oxoethyl)-2,3,3-trimethyl-3H-indolium bromide (IIL-V) have been synthesized and characterized. The adsorption and corrosion inhibition effect of these IILs have been studied using polarization measurements and cyclic voltammetry. It has been found that the inhibitive effect of the corrosion of mild steel in 0.5 M H_2SO_4 is inherently dependent on the structure of the studied IILs; IILs with bromide as an anionic head are more efficient than those with iodide. Thermodynamic calculations indicated that the adsorption on steel surface accords with Langmuir adsorption isotherm. Electrochemical measurements showed that the IIL-IV, with the highest inhibition efficiency, acted mainly as a mixed type inhibitor, albeit the inhibition of the anodic branch is larger than the cathodic one. Cyclic voltammetric measurements at polycrystalline gold electrode gave an insight into the mechanism of corrosion inhibition by the studied ionic liquids.

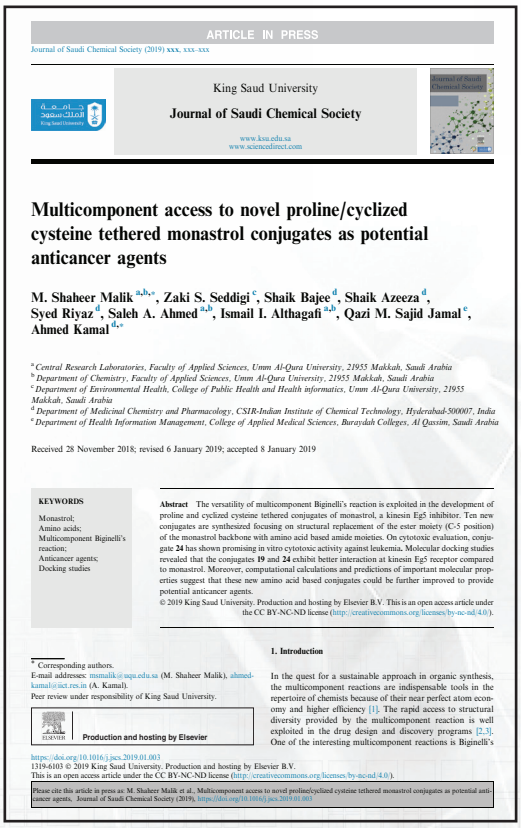
1. Introduction

Acid solutions are widely used in industry for several purposes including, for instance, acid pickling and descaling [1–3]. To avoid metal dissolution, organic inhibitors containing heteroatoms of large adsorption affinity are often added to this harsh environment. Most organic inhibitors contain a heteroatom which enhances the adsorption of those compounds on the metal surface forming a barrier between the metal surface and the corroding environment [4]. Recently researchers are interested to replace toxic traditional inhibitors with an eco-friendly corrosion inhibitor. Among those inhibitors ionic liquids received increasing attention as green corrosion inhibitors for several metals in various media [5,6]. Ionic liquids hold eco-friendly properties as they are characterized by low vapor pressure, recyclability, product recovery and moisture-stability and non-flammability in addition to the thermal and chemical stability [7–9]. Ionic liquids have a general molecular structure fulfilling the requirement of an efficient corrosion inhibitor. Generally, it is organic salts which composed generally from an organic cation (common typical cations: ammonium, imidazolium, pyrolidinium, phosphonium, piperidinium, sulfonium) and a complex anion (common typical anions: bromide, chloride, hexafluorophosphate, tetrafluoroborate). The former one contains heterocyclic rings which are well-reported to significantly adsorb on metals surface [10–14]. Ionic liquids with imidazolium, pyridinium and pyridazinium based-cationic part have been reported as an efficient inhibitor for the corrosion of copper and mild steel [15,16]. Imidazolium-based ionic liquids have been reported as efficient inhibitors for aluminum and iron, and their inhibition efficiency have been attributed to the presence of C=N bond, where a forward donation is given from the imidazolium ring to the iron in addition to the back donation from the iron to the d-orbital of the iron [17].

Recently, research on green inhibitors, of low or "zero" environmental impact, [18] became the hottest point of research in the area of metal protection. However, literatures still have scarce studies about using ionic liquids as green corrosion inhibitors [16,17]. Green corrosion inhibitors in various corrosive media [19,20] include for examples amino acids and derivatives [21,22], and extracts of natural substances [23–28] Extract of natural compounds are not so stable (biodegradable) and evaluating the inhibitive effect is tedious [19]. Thus, using ionic

* Correspondence to: S. A. Ahmed, Chemistry Department, Faculty of Science, Assiut University, 71516 Assiut, Egypt.
** Correspondence to: M. I. Awad, Chemistry Department, Faculty of Science, Cairo University, Giza, Egypt.
E-mail addresses: saahmed@uqu.edu.sa (S.A. Ahmed), miawad@uqu.edu.sa (M.I. Awad).

https://doi.org/10.1016/j.molliq.2019.111356
0167-7322/



ARTICLE IN PRESS
Journal of Saudi Chemical Society (2019) xxx, xxx–xxx

King Saud University
Journal of Saudi Chemical Society
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Multicomponent access to novel proline/cyclized cysteine tethered monastrol conjugates as potential anticancer agents

M. Shaheer Malik [a,b,*], Zaki S. Seddigi [c], Shaik Bajee [d], Shaik Azeeza [d], Syed Riyaz [d], Saleh A. Ahmed [a,b], Ismail I. Althagafi [a,b], Qazi M. Sajid Jamal [e], Ahmed Kamal [d,*]

[a] Central Research Laboratories, Faculty of Applied Sciences, Umm Al-Qura University, 21955 Makkah, Saudi Arabia
[b] Department of Chemistry, Faculty of Applied Sciences, Umm Al-Qura University, 21955 Makkah, Saudi Arabia
[c] Department of Environmental Health, College of Public Health and Health informatics, Umm Al-Qura University, 21955 Makkah, Saudi Arabia
[d] Department of Medicinal Chemistry and Pharmacology, CSIR-Indian Institute of Chemical Technology, Hyderabad-500007, India
[e] Department of Health Information Management, College of Applied Medical Sciences, Buraydah Colleges, Al Qassim, Saudi Arabia

Received 28 November 2018; revised 6 January 2019; accepted 8 January 2019

KEYWORDS
Monastrol;
Amino acids;
Multicomponent Biginelli's reaction;
Anticancer agents;
Docking studies

Abstract The versatility of multicomponent Biginelli's reaction is exploited in the development of proline and cyclized cysteine tethered conjugates of monastrol, a kinesin Eg5 inhibitor. Ten new conjugates are synthesized focusing on structural replacement of the ester moiety (C-5 position) of the monastrol backbone with amino acid based amide moieties. On cytotoxic evaluation, conjugate **24** has shown promising in vitro cytotoxic activity against leukemia. Molecular docking studies revealed that the conjugates **19** and **24** exhibit better interaction at kinesin Eg5 receptor compared to monastrol. Moreover, computational calculations and predictions of important molecular properties suggest that these new amino acid based conjugates could be further improved to provide potential anticancer agents.

* Corresponding authors.
E-mail addresses: msmalik@uqu.edu.sa (M. Shaheer Malik), ahmedkamal@iict.res.in (A. Kamal).
Peer review under responsibility of King Saud University.

Production and hosting by Elsevier

https://doi.org/10.1016/j.jscs.2019.01.003
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Please cite this article in press as: M. Shaheer Malik et al., Multicomponent access to novel proline/cyclized cysteine tethered monastrol conjugates as potential anticancer agents, Journal of Saudi Chemical Society (2019), https://doi.org/10.1016/j.jscs.2019.01.003

1. Introduction

In the quest for a sustainable approach in organic synthesis, the multicomponent reactions are indispensable tools in the repertoire of chemists because of their near perfect atom economy and higher efficiency [1]. The rapid access to structural diversity provided by the multicomponent reaction is well exploited in the drug design and discovery programs [2,3]. One of the interesting multicomponent reactions is Biginelli's

Chromatographia (2020) 83:53–64
https://doi.org/10.1007/s10337-019-03814-w

ORIGINAL

Simultaneous Analysis of Drugs in Forensic Cases by Liquid Chromatography–High-Resolution Orbitrap Mass Spectrometry

Siti U. Mokhtar[1] · Chadin Kulsing[2,3,4] · Jalal T. Althakafy[2,5] · Alex Kotsos[6] · Olaf H. Drummer[6,7] · Philip J. Marriott[2]

Received: 10 May 2019 / Revised: 23 September 2019 / Accepted: 15 October 2019 / Published online: 31 October 2019

Abstract
In the present study, liquid chromatography coupled to an Orbitrap mass spectrometer (HPLC–Q-Orbitrap MS) was used as an approach for identification and quantification of 113 drugs simultaneously in biological samples (whole blood/plasma/serum). Samples were prepared using liquid–liquid extraction conducted using a trizma/isopropanol/butyl chloride buffer system. Reversed-phase separation employing a column (50 × 2.1 mm) packed with 2.6-µm C18 particles was then performed under gradient elution with mobile phase composition consisting of acetic acid and aqueous-acetonitrile mixtures with the acetonitrile content ranging from 10 to 100% v/v. Compounds were detected with high-resolution MS operated in full scan mode having a mass accuracy < 5 ppm. In this study, isobaric compounds (same nominal mass) were easily distinguished and identified by their different retention times. Extracted ion chromatograms (XICs) with narrow mass tolerance window (5 ppm) provided analysis with acceptable linearity (r^2) ranged from 0.9530 to 1, low limits of detection (LOD) (0.02–39 ng mL^{-1}) and low limit of quantification (LOQ) (0.1–130 ng mL^{-1}). The developed method was applied to successfully analyse drugs in 26 blood samples from positive forensic cases and proved that this technique was able to detect analytes at trace level.

Electronic supplementary material The online version of this article (https://doi.org/10.1007/s10337-019-03814-w) contains supplementary material, which is available to authorized users.

✉ Siti U. Mokhtar
umairah@ump.edu.my

[1] Faculty of Engineering Technology, Universiti Malaysia Pahang, 26300 Pahang, Malaysia
[2] Australian Centre of Research on Separation Science, School of Chemistry, Faculty of Science, Monash University, Clayton, VIC 3800, Australia
[3] Chromatography and Separation Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand
[4] Center of Molecular Sensory Science, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand
[5] Department of Chemistry, Faculty of Applied Sciences, Umm Al-Qura University, Mecca 21955, Saudi Arabia
[6] Victorian Institute of Forensic Medicine, Southbank, VIC 3006, Australia
[7] Department of Forensic Medicine, Monash University, Clayton, VIC 3800, Australia

الأحياء

أولا: الأبحاث المنشورة بقسم الاحياء :

م	عنوان البحث	المشاركين	المجلة	دار النشر	ISI/ NON-ISI	معامل التأثير IF
1	Isolation, haracterization, cloning and bioinformatics analysis of a novel receptor from black cut worm (Agrotis ipsilon) of Bacillus thuringiensis vip 3Aa toxins	Gamal Osman Raya Soltane Ibrahim Saleh Hussein h. Abulreesh Khaled Gazi Ibrahim A. Arif Ahmaed M. Ramadan Hussien Almeldin Yahia Osman Mamdouh Idress	Saudi Journal of Biological Sciences	Elsevier	ISI	3,18
2	Bioactive extracts of Carum copticum L. enhances efficacy of ciprofloxacin against MDR enteric bacteria	Meenu Maheshwari Adbullah Safar Althubiani Hussein H. Abulreesh Faizan Abul Qais Mohd Shavez Khan Iqbal Ahmad	Saudi Journal of Biological Sciences	Elsevier	ISI	3,18
3	Recent progress in metal-microbe interactions: prospects in bioremediation	Gamal Osman Hussein H. Abulreesh Khaled Elbanna Mohammed R. Shabaan Samreen Iqbal Ahmad	J Pure Appl Microbiol	-	ISI	0,70
4	Phenotypic and genotypic characterizationof exopolysaccharide producing bacteria isolated from fermented fruits, vegetables and dairy products	Salah Abdalrahim Abdel Naser A. Zohri Manal Khider Adel M. Kamal El-Dean Hussein H. Abulreesh Iqbal Ahmad Khaled Elbanna	J Pure Appl Microbiol	-	ISI	0,70
5	Phytoremediation Capacity of Some Forage Plants Grown on a Metals-Contaminated Soil	Mamdouh A. Eissa , Yaser A. Almaroai	Soil and Sediment Contamination: An International Journal	Taylor&Francis	ISI	0.99
6	Exogenous spermidine enhances expression of Calvin cycle genes and photosynthetic efficiency in sweet sorghum seedlings under salt stress	A.I. El Sayed, M.A.M. El-Hamahmy, M.S. Rafudeen, M.K.H. Ebrahim	Biologia Plantarum	-	ISI	1.38
7	Diversity, Virulence Factors, and Antifungal Susceptibility Patterns of Pathogenic and Opportunistic Yeast Species in Rock Pigeon (Columba livia) Fecal Droppings in Western Saudi Arabia	Hussein H. Abulreesh Sameer R. Organji Khaled Elbanna Gamal E. H. Osman Meshal K.H. Almalki Ahmed Y. Abdel-Malek Abdullah A. K. Ghauthuddin Iqbal Ahmad	Polish Journal of Microbiology	Polish Society of Microbiologists	ISI	0.77

2.85	ISI	Taylor&Francis	Biofouling	Meenu Maheshwari Faizan Abul Qais Abdullah Safar Althubiani Hussein H. Abulreesh Iqbal Ahmad	Bioactive extracts of Carum copticum and thymol inhibit biofilm development by multidrug-resistant extended spectrum β-lactamase producing enteric bacteria	8
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2.80	ISI	Elsevier	Saudi Journal of Biological Sciences	Lamiaa El-Gaied, Alshimaa Mahmoud, Reda Salem, Wael Elmenofy, Ibrahim Saleh, Hussein H. Abulreesh, Ibrahim A. Arif, Gamal Osman	Characterization, Cloning, Expression and bioassay of vip3 gene isolated from an Egyptian Bacillus thuringiensis against whiteflies. Saudi Journal of Biological Sciences.	10
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2.20	ISI	Elsevier	Journal of Food Bioactives	Albishi, T., Banoub, J. H., de Camargo, A. C., & Shahidi, F.	Wood extracts as unique sources of soluble and insoluble-bound phenolics: reducing power, metal chelation and inhibition of oxidation of human LDL-cholesterol and DNA strand scission	19
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1.66	ISI	Wiley	Journal of food biochemistry	Albishi, Tasahil, Joseph H. Banoub, Adriano Costa de Camargo, and Fereidoon Shahidi.	Date palm wood as a new source of phenolic antioxidants and in preparation of smoked salmon	21

ثانيا: المشاريع الممولة من عمادة البحث العلمي ومدينة الملك عبدالعزيز للعلوم والتقنية بقسم الاحياء :

	Projects	Researcher	Fund
1	Development of an improved, Foot and Mouth Disease Virus FMDV) veterinarian vaccine in plants)	أ.د. جمال ابراهيم هريدي	Deanship of Scientific Research 0007-01-1 -SCI-18 SR 180000
2	Screening the activity of different parasporin proteins as antiviral agent against human and animal viruses	أ.د. جمال ابراهيم هريدي	Deanship of Scientific Research SR 120000
3	Osmotic-Priming as A Smart Approach to Develop Wheat Tolerant Genotypes for Salinity	أ.د. جمال ابراهيم هريدي	University of Tabuk Deanship of scientific Research SR 30000

ثالثا: الكتب المنشورة بقسم الاحياء :

م	عنوان الكتاب	المشاركين	دار النشر
1	Antibacterial drug discovery: perspective insights	Iqbal Ahmad Faizan Abul Qais Samreen Hussein H. Abulreesh Shameem Ahmad Kendra p. Rumbaugh	Springer Nature Singapore Pte Ltd
2	Antibiotic resistance in Campylobacter jejuni: mechanisms, status and public health significance	Javed Ahamad Khan Hussein H. Abulreesh Ramesh Kumar Samreen Iqbal Ahmad	Springer Nature Singapore Pte Ltd
3	Actinomycetes as continued source of new antibacterial leads	Iqbal Ahmad Abdullah S. Althubiani Muzammil S. Dar Samreen Faizan Abul Qais Hussein H. Abulreesh Majed A. Bamaga Saled B. Al-Ghamdi Fatimah Alshehrei	Springer Nature Singapore Pte Ltd


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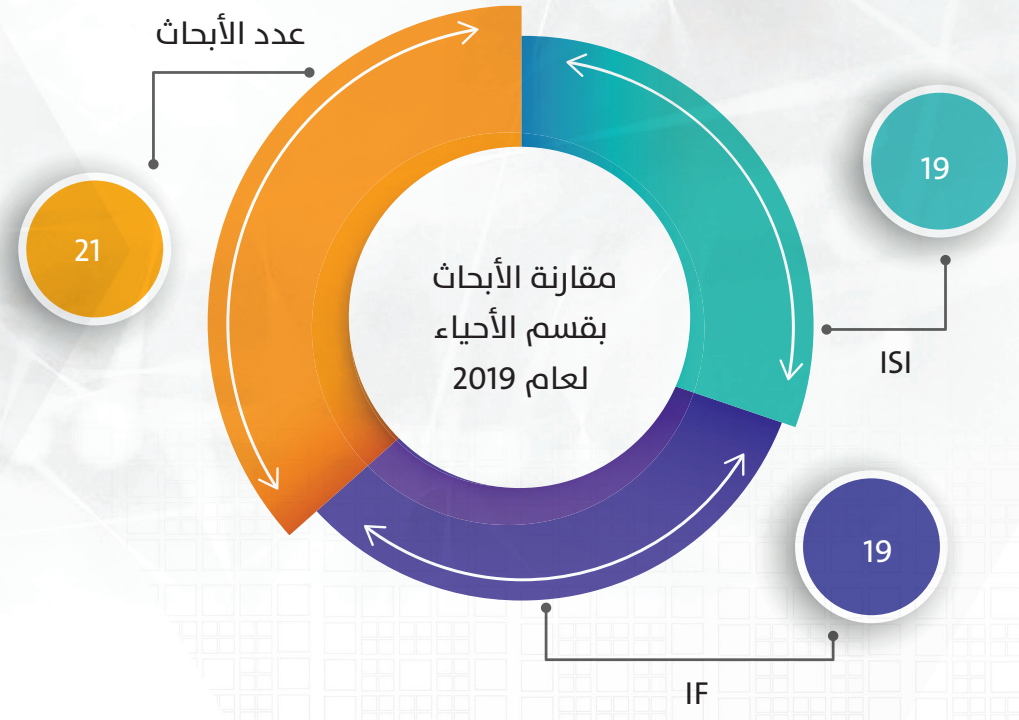
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ملخصات الأوراق العلمية المنشورة بقسم الأحياء:

Saudi Journal of Biological Sciences 26 (2019) 1848–1855

Contents lists available at ScienceDirect

Saudi Journal of Biological Sciences

journal homepage: www.sciencedirect.com

Original article

Bioactive extracts of *Carum copticum* L. enhances efficacy of ciprofloxacin against MDR enteric bacteria

Meenu Maheshwari [a], Abdullah Safar Althubiani [b], Hussein Hasan Abulreesh [b], Faizan Abul Qais [a], Mohd Shavez Khan [a], Iqbal Ahmad [a,*]

[a] Department of Agricultural Microbiology, Aligarh Muslim University, Aligarh 202002, India
[b] Department of Biology, Faculty of Applied Science, Umm Al Qura University, Makkah, Saudi Arabia

ARTICLE INFO

Article history:
Received 5 April 2017
Revised 11 December 2017
Accepted 20 December 2017
Available online 22 December 2017

Keywords:
ESβL producing enteric bacteria
Carum copticum
Plant extracts
Synergy
Ciprofloxacin
GC/MS

ABSTRACT

The widespread occurrence of extended spectrum β-lactamases (ESβLs) producing enteric bacteria and their co-resistance with fluoroquinolones has impaired the current antimicrobial therapy. This has prompted the search for new alternatives through synergistic approaches with herbal extracts. In this study *Carum copticum* (seeds) was extracted first in methanol and then subsequently extracted in different organic solvents. MIC of plant extracts, ciprofloxacin and thymol was determined by broth microdilution method using TTC. Synergism between plant extracts and ciprofloxacin was assayed by the checkerboard method. Chemical constituents of active extracts were analyzed by GC-MS. Methanolic, hexane and ether extract of *Carum copticum* exhibited significant antibacterial activity with MIC values ranged from 0.25 mg/ml to 2.0 mg/ml. Synergy analysis between *Carum copticum* extracts and ciprofloxacin combinations revealed FIC index in the range of 0.093–0.25. About 81% ciprofloxacin resistant ESβL producing enteric bacteria were re-sensitized in the presence of 15.6–250 μg/ml of methanolic extract of *Carum copticum*. Moreover, ciprofloxacin showed 8 to 64 folds reduction in MIC in presence of 250 and 500 μg/ml of hexane extract. Whereas, 4–32 folds reduction in MIC of ciprofloxacin was achieved in the presence of 31.25 and 62.5 μg/ml of ether extract, indicating synergistic enhancement of drug activity. The chemical analysis of hexane and ether extracts by GC-MS revealed the common occurrence of one or more phenolic hydroxyl at different locations on benzene ring. This study demonstrated the potential use of herbal extract of *Carum copticum* in combination therapy against ESβL producing bacteria.

1. Introduction

The emergence and spread of multidrug resistance among bacteria has created an immense clinical global problem and threat to human health. Extended spectrum β-lactamases (ESβLs) is one of the most influential cephalosporin resistance mechanisms among enterobacteriaceae. It is recognized that ESβL producing enteric bacteria harbour transferable plasmids which also confer resistance to other non β-lactam antibiotics, such as fluoroquinolones, aminoglycosides, and chloramphenicol etc. thereby positioning themselves as resistant to almost all available antibiotics (Brolund and Sandegren, 2016).

In the past few years, the growing co-existence of ESβL production and fluoroquinolone resistance has been documented worldwide and considered as serious public health challenge. Recently a global survey on antimicrobial resistance by world health organization has analyzed the data on resistance to third-generation cephalosporins, including resistance conferred by ESβLs, and to fluoroquinolones in *E. coli*, which has been reported higher resistance rates to fluoroquinolones than for the third-generation cephalosporins (WHO, 2014). Another report of SMART study in the Asia-Pacific region have shown greater incidence of fluoroquinolones resistance (ciprofloxacin 82.5% and levofloxacin 79.3%) among ESβL producers than resistance in non-ESβL producing isolates to those agents (31.2% and 28.6%, respectively) (Lu et al., 2012).

Abbreviations: **FIC**, fractional inhibitory concentration; **Ca-CIP**, *Carum copticum*-ciprofloxacin; **Th-CIP**, thymol-ciprofloxacin; **MDR**, multi-drug resistant; **ESβL**, extended spectrum β-lactamase; **PE**, plant extract; **TH**, thymol.

* Corresponding author.
E-mail address: ahmadiqbal84@yahoo.co.in (I. Ahmad).

Peer review under responsibility of King Saud University.

Production and hosting by Elsevier

https://doi.org/10.1016/j.sjbs.2017.12.008
1319-562X/© 2017 Production and hosting by Elsevier B.V. on behalf of King Saud University.

Saudi Journal of Biological Sciences 26 (2019) 1078–1083

Contents lists available at ScienceDirect

Saudi Journal of Biological Sciences

journal homepage: www.sciencedirect.com

Isolation, characterization, cloning and bioinformatics analysis of a novel receptor from black cut worm (*Agrotis ipsilon*) of *Bacillus thuringiensis* vip 3Aa toxins

Gamal H. Osman [a,b,c,*], Raya Soltane [c,d], Ibrahim Saleh [e,*], Hussein H. Abulreesh [a], Khaled S. Gazi [f], Ibrahim A. Arif [e], Ahmed M. Ramadan [g,h], Hussien F. Alameldin [i,j], Yehia A. Osman [k], Mamdouh Idriss [l]

[a] Department of Biology, Faculty of Applied Science, Umm Al-Qura University, Makka, Saudi Arabia
[b] Microbial Genetics Department, Agricultural Genetic Engineering Research Institute (AGERI), Giza, Egypt
[c] Faculty of Sciences of Tunis, Tunis El Manar University, Tunisia
[d] Department of basic sciences, Alhum University college, Umm Al-Qura University, Saudi Arabia
[e] Prince Sultan Research Chair for Environment and Wildlife, Department of Botany & Microbiology, College of Sciences, King Saud University (KSU), Riyadh, Saudi Arabia
[f] Department of Biology, Faculty of Arts and Sciences in Almasnaa, Albaha University, Saudi Arabia
[g] Department of Biological Sciences, Faculty of Science, King Abdulaziz University (KAU), Jeddah 80203, Saudi Arabia
[h] Plant Molecular Biology Department, Agricultural Genetic Engineering Research Institute (AGERI), Agriculture Research Center (ARC), Giza, Egypt
[i] Department of Energy - Plant Research Laboratory, Michigan State University, East Lansing, MI 48824, USA
[j] Department of Bioinformatics, Agricultural Genetic Engineering Research Institute (AGERI), Agricultural Research Center (ARC), Giza, Egypt
[k] Microbiology Department, Faculty of Science, Mansoura University, Mansoura, Egypt
[l] Department of Entomology, Faculty of Agriculture, Alexandria University, Egypt

ARTICLE INFO

Article history:
Received 5 February 2018
Revised 3 May 2018
Accepted 12 June 2018
Available online 13 June 2018

Keywords:
Receptor
Vip3A
Bacillus thuringiensis
BBMV

ABSTRACT

Black cutworm (BCW) is an economically important lepidopteran insect. The control of this insect by a Bt toxin and the understanding of the interaction between the Bt toxin and its receptor molecule were the objectives of this research work. A gene coding for a Vip3A receptor molecule was identified, characterized, and cloned, from the brush border membrane vesicles (BBMV) of the BCW. The nucleotide sequence analysis of the cloned putative Vip3A-receptor gene revealed that the gene was 1.3-kb long and exhibited no homology with any gene in the gene bank. We succeeded in identifying and characterizing most of the Vip3A-receptor gene sequence; and the nucleotide sequence analysis of the cloned putative Vip3A-receptor gene (accession no. KX858809) revealed about 92% of the expected sequence was recovered, which exhibited no homology with any gene in the GenBank.

1. Introduction

The primary action of Bt toxin occurs in the midgut of susceptible insects. The insect larval midgut is composed of outer longitudinal and circular muscle layers, bordered by a basal lamina and a monolayer of epithelial cells overlaid by the peritrophic membrane (Knowles, 1989; Sinu et al., 2010). The epithelial cell layer mainly consists of columnar and goblet cells. The columnar epithelial cells maintain an apical brush border of microvilli exposed to the midgut lumen. Goblet cells do not have microvilli; however, they contain an apical pore through which digestive enzymes are secreted into the midgut lumen (Du et al., 2013). These two epithelial cell types are held together by tight junctions to form a single layer of cells. Both the cell types communicate through electrochemical coupling within the tight junctions (Moffett and Koch, 1992). This coupling helps the epithelial cell layer to maintain a potassium gradient between hemolymph (blood) and the gut lumen. A potassium pump that creates an approximate 180 mV potential across the epithelial cell layer preserves the gradient. This large membrane potential is responsible for the symport of nutrients to the basement membrane using K^+ as the functional cation (Vasilyeva and Forgac, 1998). The insect's digestive tract,

* Corresponding authors at: Department of Biology, Faculty of Applied Science, Umm Al-Qura University, Makkah 21955, Saudi Arabia (G.H. Osman).
E-mail addresses: gmosman@uqu.edu.sa (G.H. Osman), isaleh@ksu.edu.sa (I. Saleh).

Peer review under responsibility of King Saud University.

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https://doi.org/10.1016/j.sjbs.2018.06.002
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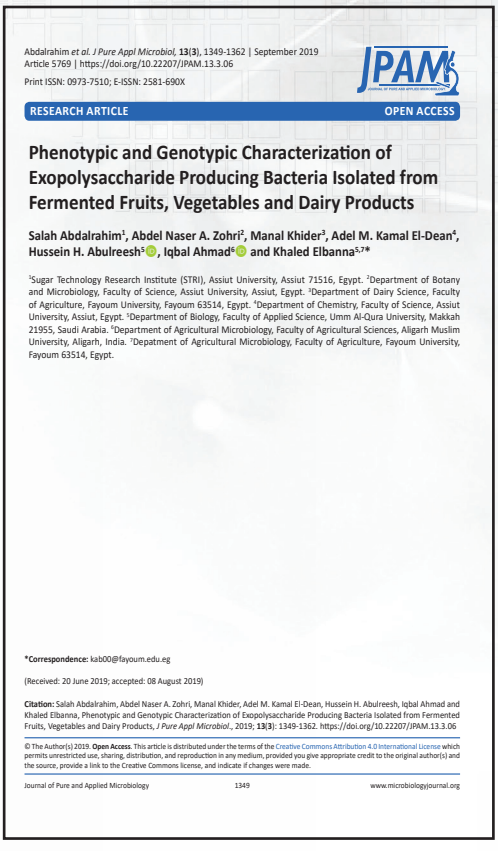

Abdalrahim *et al. J Pure Appl Microbiol*, **13**(3), 1349-1362 | September 2019
Article 5769 | https://doi.org/10.22207/JPAM.13.3.06
Print ISSN: 0973-7510; E-ISSN: 2581-690X

RESEARCH ARTICLE OPEN ACCESS

Phenotypic and Genotypic Characterization of Exopolysaccharide Producing Bacteria Isolated from Fermented Fruits, Vegetables and Dairy Products

Salah Abdalrahim[1], Abdel Naser A. Zohri[2], Manal Khider[3], Adel M. Kamal El-Dean[4], Hussein H. Abulreesh[5], Iqbal Ahmad[6] and Khaled Elbanna[5,7]*

[1]Sugar Technology Research Institute (STRI), Assiut University, Assiut 71516, Egypt. [2]Department of Botany and Microbiology, Faculty of Science, Assiut University, Assiut, Egypt. [3]Department of Dairy Science, Faculty of Agriculture, Fayoum University, Fayoum 63514, Egypt. [4]Department of Chemistry, Faculty of Science, Assiut University, Assiut, Egypt. [5]Department of Biology, Faculty of Applied Science, Umm Al-Qura University, Makkah 21955, Saudi Arabia. [6]Department of Agricultural Microbiology, Faculty of Agricultural Sciences, Aligarh Muslim University, Aligarh, India. [7]Depatment of Agricultural Microbiology, Faculty of Agriculture, Fayoum University, Fayoum 63514, Egypt.

***Correspondence:** kab00@fayoum.edu.eg

(Received: 20 June 2019; accepted: 08 August 2019)

Citation: Salah Abdalrahim, Abdel Naser A. Zohri, Manal Khider, Adel M. Kamal El-Dean, Hussein H. Abulreesh, Iqbal Ahmad and Khaled Elbanna, Phenotypic and Genotypic Characterization of Exopolysaccharide Producing Bacteria Isolated from Fermented Fruits, Vegetables and Dairy Products, *J Pure Appl Microbiol.*, 2019; **13**(3): 1349-1362. https://doi.org/10.22207/JPAM.13.3.06

Osman *et al. J Pure Appl Microbiol*, **13**(1), 13-26 | March 2019
Article 5460 | https://dx.doi.org/10.22207/JPAM.13.1.02
Print ISSN: 0973-7510; E-ISSN: 2581-690X

REVIEW ARTICLE

Recent Progress in Metal-Microbe Interactions: Prospects in Bioremediation

Gamal E.H. Osman[1,2], Hussein H. Abulreesh[1]*, Khaled Elbanna[1,3], Mohammed R. Shaaban[1,4], Samreen[5] and Iqbal Ahmad[5]

[1]Department of Biology, Faculty of Applied Science, Umm Al-Qura University, Makkah 21955, Saudi Arabia. [2]Microbial Genetics Department, Agricultural Genetic Engineering Research Institute (AGERI), ARC, Giza 12619, Egypt. [3]Department of Agricultural Microbiology, Faculty of Agriculture, Fayoum University, Fayoum, Egypt. [4]Department of Chemistry, Faculty of Science, Cairo University, Cairo, Egypt. [5]Department of Agricultural Microbiology, Faculty of Agricultural Sciences, Aligarh Muslim University, Aligarh - 202 002, India.

Abstract

Heavy metal contamination due to natural and anthropogenic source is a major environmental problem. Release of metal from use of agrochemicals, industrial effluents and wastewater residues and their accumulation in food causes serious dilemma to animal and human health concern. On the other hand microbial population gets affected from metal toxicity at elevated concentration. With the result microbes develops various resistance mechanism to cope with metal toxicity. Both physiological and genetic mechanisms are involved in developing such resistance. Recent advances on metal-bacteria interaction has led to better understanding of metal accumulation/detoxification or biotransformation and bioremediation of metals through application of such bacteria. Role of various transport protein families involved in heavy metal metabolism are now explored. This article provides insights of metal-bacteria interaction in terms of resistance mechanisms and role of various transport proteins and its potential application in bioremediation of metal pollution.

Keywords: Heavy metal resistance; bioremediation; public health; efflux pump; genes. Transport proteins.

*Correspondence: hhabulreesh@uqu.edu.sa, +966555519597

(Received: 28 December 2018; accepted: 31 January 2019)

Citation: Gamal E. H. Osman, Hussein H. Abulreesh, Khaled Elbanna, Mohammed R. Shaaban and Samreen, Iqbal Ahmad, Recent Progress in Metal-Microbe Interactions: Prospects in Bioremediation, *J Pure Appl Microbiol.*, 2019; **13**(1):13-26 doi: 10.22207/JPAM.13.1.02

DOI: 10.32615/bp.2019.046 BIOLOGIA PLANTARUM 63: 511-518, 2019

Exogenous spermidine enhances expression of Calvin cycle genes and photosynthetic efficiency in sweet sorghum seedlings under salt stress

A.I. EL SAYED[1]*, M.A.M. EL-HAMAHMY[2], M.S. RAFUDEEN[3], and M.K.H. EBRAHIM[4,5]

Biochemistry Department, Faculty of Agriculture, Zagazig University, 44519 Zagazig, Egypt[1]
Department of Agricultural Botany, Faculty of Agriculture, Suez Canal University, 41522 Ismailia, Egypt[2]
Department of Molecular and Cell Biology, University of Cape Town, Private Bag, 7701 Rondebosch, South Africa[3]
*Biology Department, Faculty of applied sciences, Umm Al- Qura University, **postal code?** Makkah Al-Mukarramah, KSA[4]*
Botany Department, Faculty of Science, Tanta University, 31257 Tanta, Egypt [5]

Abstract

Salinity adversely affects plants resulting in disruption to plant growth and physiology. Previously, it has been shown that these negative effects can be alleviated by various exogenous polyamines. However, the role of spermidine (Spd) in conferring salinity tolerance in sorghum is not well documented. The effect of exogenous Spd on the responses of sweet sorghum (*Sorghum bicolor* L.) seedlings to salt stress (150 mM NaCl) was investigated by measuring photosynthetic carbon assimilation, Calvin cycle enzyme activities, and the the expression of respective genes. Application of 0.25 mM Spd alleviated the negative effects of salt stress on efficiency of photosystem II and CO_2 assimilation and increased the activities of ribulose 1,5-bisphosphate carboxylase/oxygenase (Rubisco) and aldolase. Salt stress significantly lowered the transcriptions of genes encoding Rubisco large subunit, Rubisco small subunit, 3-phosphoglyceric acid kinase, glyceraldehyde-3-phosphate dehydrogenase, triose-3-phosphate isomerase, fructose-1,6-bisphosphate aldolase, fructose-1,6-bisphosphate phosphatase, and sedoheptulose-1,7-bisphosphatase. However, transcriptions of genes encoding phosphoribokinase and Rubisco were up-regulated. The Spd application enhanced expressions of most of these genes. It appears Spd conferred salinity tolerance to sweet sorghum seedlings by enhancing photosynthetic efficiency through regulation of gene expressions and activities of key CO_2 assimilation enzymes.

Additional key words: aldolase, CO_2 assimilation rate, NaCl, photosystem II, phylogenetic analysis, Rubisco.

Introduction

Salinity is a major environmental factor inhibiting crop growth and productivity (Parida and Das 2005). It has been observed that in various plants, salinity induces an increase in endogenous polyamines (Das *et al.* 1995, Chattopadhayay *et al.* 2002). Polyamines, such as putrescine (Put), spermidine (Spd), and spermine (Spm) are involved in various physiological and biochemical processes related to the regulation of plant responses to different environmental stresses (Takahashi *et al.* 2010, Roychoudhury *et al.* 2011). This allows the plant to be protected from these stresses by scavenging free radicals, stabilizing membranes, maintaining a cation-anion balance, and stimulation of ATP synthesis (Bouchereau *et al.* 1999, Ioannidis *et al.* 2006). Furthermore, polyamines have pivotal roles in many other cellular processes including gene expression, DNA and protein synthesis, regulation of ion channels, and providing protection from oxidative damage (Duan *et al.* 2008). Several studies reported that application of exogenous polyamines is an effective approach for enhancing salinity tolerance of plants and for protecting plant cell structure; they could be used to improve the productivity of many crops under salinity

Submitted 8 November 2018, *last revision* 21 January 2019, *accepted* 29 January 2019.
Abbreviations: Φ_{PSII} – photosynthetic quantumyield; Chl - chlorophyll; FBA - fructose-1,6-bisphosphate aldolase also known as aldolase (ALD); FBPase - fructose-1,6-bisphosphate phosphatase; GAPDH - glyceraldehyde-3-phosphate dehydrogenase; MDA - malondialdehyde; PGK - 3-phosphoglyceric acid kinase; PRK - ribulose-5-phosphate kinase; PS - photosystem; Put - putrescine; RbcL - ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit; RbcS - ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit; RCA - ribulose bisphosphate carboxylase/oxygenase activase; Rubisco - ribulose bisphosphate carboxylase/oxygenase; SBPase - sedoheptulose-1,7-bisphosphatase; Spd - spermidine; Spm - spermine; TPI - triose-3-phosphate isomerase.
Acknowledgement: The author thanks the Zagazig University for supporting the research.
* Corresponding author: e-mail: aelsayed@zu.edu.eg

SOIL AND SEDIMENT CONTAMINATION
2019, VOL. 28, NO. 6, 569–581
https://doi.org/10.1080/15320383.2019.1634674

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Phytoremediation Capacity of Some Forage Plants Grown on a Metals-Contaminated Soil

Mamdouh A. Eissa[a] and Yaser A. Almaroai[b]

[a]Department of Soils and Water, Faculty of Agriculture, Assiut University, Assiut, Egypt; [b]Department of Biology, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia

ABSTRACT

Phytoremediation is a good strategy for metals-contaminated soils where the removal of contaminates is not a viable solution. Little is known about the quality of halophyte forage plants grown on metal-contaminated soils. A two-year field experiment was conducted to study the growth and elemental composition of three *Atriplex* species, maize and sorghum plants grown on metal-contaminated soil. Maize and sorghum plants significantly ($P< 0.05$) produced higher yields compared to *Atriplex* species. The fresh yield of the conventional forage plants and *Atriplex* species ranged between 3.4-3.6 and 1.1-1.4 tonnes ha^{-1}, respectively. Concentrations of Zn, Cu, Pb and Cd in maize and sorghum plants were significantly higher than those of *Atriplex* species. The nutritive value of the studied *Atriplex* plants was higher than that of maize and sorghum; moreover, the forage material of *Atriplex* species was safer. It was also observed that higher Zn, Cu, Cd and Pb content were accumulated in the roots than those of plant shoots; with low translocation factor (TF). The roots of *Atriplex* plants contained higher concentrations of SO_4, PO_4, Cl and oxalaterather than maize and sorghum plants. In metal-contaminated soils *Atriplex* plants are able to produce more safe forage materials than maize and sorghum.

KEYWORDS
Forage plants; halophytes; maize; sorghum; Atriplex

1. Introduction

Metal-contaminated soils have become a global environmental problem due to intensively increasing industrialization and agricultural activities (Ashraf et al. 2019). Heavy metals are highly toxic because, unlike organic matter, they are not biodegradable but can only change their oxidation state and are highly persistent in nature with a half-life more than 20 years (Hadia-e-Fatima 2018). Fifty-three elements are documented as heavy metals and are considered as universal pollutants with densities greater than 5 g/cm3 (Ashraf et al. 2019; Prieto, Acevedo, and Prieto 2018).Trace elements are a part of the soil ecosystem. However, the accumulation of these elements in the soil or reaching the groundwater may be harmful to people, animals, plants and other organisms (Dembitsky 2003). Geological and anthropogenic activities are sources of heavy metal contamination (Dembitsky 2003). Remediation methods of metal-contaminated soils e.g., washing, vitrification, and solidification are not effective in agriculture lands, they are expensive and cause soil disturbances, and are not accepted by the general public (Martin and Ruby 2004; Saifullah et al. 2009). Phytostabilization is the use of

CONTACT Mamdouh A. Eissa mamdouhessa@gmail.com Department of Soils and Water, Faculty of Agriculture, Assiut University, Assiut 71526, Egypt.

BIOFOULING
2019, VOL. 35, NO. 9, 1026–1039
https://doi.org/10.1080/08927014.2019.1688305

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Bioactive extracts of *Carum copticum* and thymol inhibit biofilm development by multidrug-resistant extended spectrum β-lactamase producing enteric bacteria

Meenu Maheshwari[a], Faizan Abul Qais[a], Abdullah Safar Althubiani[b], Hussein Hasan Abulreesh[b,c] and Iqbal Ahmad[a,b,c]

[a]Department of Agricultural Microbiology, Aligarh Muslim University, Aligarh, India; [b]Faculty of Applied Science, Department of Biology, Umm Al-Qura University, Makkah, Saudi Arabia; [c]Faculty of Applied Science, Research Laboratories Centre, Umm Al-Qura University, Makkah, Saudi Arabia

ABSTRACT

The emergence and spread of multidrug-resistant (MDR) pathogenic bacteria is a clinical problem that requires novel anti-infective agents. Targeting pathogenic biofilms is considered a promising strategy to control bacterial infections. In this study, bioactive extracts of *Carum copticum* were investigated for their anti-biofilm efficacy against extended spectrum β-lactamase (ESβL) producing MDR enteric bacteria. Thymol was also tested for its anti-biofilm properties, as gas chromatography-mass spectrometry revealed a high content (65.8%) of this phytochemical in the *C. copticum* methanolic extract. Biofilm inhibition was assessed in microtitre plates and further validated by light, electron and confocal laser microscopy. Sub-inhibitory concentrations of bioactive extracts of *C. copticum* and thymol significantly prevented biofilm development, ranging from 78.6 to 83.9% reductions. Microscopic analysis revealed that biofilms made by ESβL producing MDR enteric bacteria had a weakened structure, scattered microcolonies, and reduced cell density and thickness after exposure to the bioactive extracts and thymol.

ARTICLE HISTORY
Received 8 April 2019
Accepted 29 October 2019

KEYWORDS
Multidrug resistance; anti-biofilm activity; *Carum copticum*; thymol; ESβL

Introduction

Extended spectrum β-lactamase (ESβL) producing enteric bacteria have been recognized globally as one of the major problematic groups of multidrug-resistant (MDR) bacteria (USCDC 2013; WHO 2014; Hawken and Snitkin 2019). ESβLs are the group of β-lactamase enzymes that confer resistance to oxyimino-cephalosporins, such as cefotaxime, aztreonam, and ceftazidime due to their broad-spectrum hydrolytic activities. ESβL producing enteric bacteria are commonly MDR, leaving limited antibacterial options (Rupp and Fey 2003; Tacão et al. 2014). Treatment of infections caused by ESβL producing MDR bacteria becomes more complicated when they establish biofilms in the host. Biofilms are communities of surface-attached microorganisms enclosed in a self-produced extracellular matrix. Biofilms protect bacteria from antibiotics and other toxic chemical stresses in a variety of environments, e.g. from a wastewater to a host organism (Vogeleer et al. 2014).

The role of biofilms in chronic and persistent infections such as pneumonia in cystic fibrosis patients, chronic wounds, chronic implants and catheter-associated infections is well recognized (Costerton 1999; Hall-Stoodley et al. 2004). The high mortality rates due to biofilm-related infections have been reported and compared to other infections (Barsoumian et al. 2015). Furthermore, in biofilm related infections, planktonic bacteria released from the biofilm can spread into the blood stream around the source of the infection and increase the risk of recurrence (Ferreira et al. 2018).

ESβL genes are mainly plasmid encoded and such plasmids are often self-transferable and disseminated among enteric bacteria (Rupp and Fey 2003). In the biofilm mode of growth, genetic exchange of plasmids carrying drug-resistant genes has been reported with high frequency, facilitating the widespread dissemination of MDR genes (Maheshwari et al. 2016; Nesse and Simm 2018). Furthermore, the expression of drug-resistant genes and virulence factors is many folds higher in biofilms in comparison to planktonic

CONTACT Iqbal Ahmad ahmadiqbal@yahoo.co.in
Supplemental data for this article is available online at https://doi.org/10.1080/08927014.2019.1688305.

Polish Journal of Microbiology
2019, Vol. 68, No 4, 493–504
https://doi.org/10.33073/pjm-2019-049

ORIGINAL PAPER

Diversity, Virulence Factors, and Antifungal Susceptibility Patterns of Pathogenic and Opportunistic Yeast Species in Rock Pigeon (*Columba livia*) Fecal Droppings in Western Saudi Arabia

HUSSEIN H. ABULREESH[1,2]*, SAMEER R. ORGANJI[1,2], KHALED ELBANNA[1,2,3], GAMAL E.H. OSMAN[1,2,4], MESHAL H.K. ALMALKI[1,2], AHMED Y. ABDEL-MALEK[5], ABDULLAH A.K. GHYATHUDDIN[6,7] and IQBAL AHMAD[8]

[1]Department of Biology, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia
[2]Research Laboratories Center, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia
[3]Department of Agricultural Microbiology, Faculty of Agriculture, Fayoum University, Fayoum, Egypt
[4]Microbial Genetics Department, Agricultural Genetic Engineering Research Institute (AGERI), Giza, Egypt
[5]Botany and Microbiology Department, Faculty of Science, Assiut University, Assiut, Egypt
[6]Fakieh Poultry Farms, Makkah, Saudi Arabia
[7]Department of Biological Sciences, King Abdulaziz University, Jeddah, Saudi Arabia
[8]Department of Agricultural Microbiology, Faculty of Agricultural Sciences, Aligarh Muslim University, Aligarh, India

Submitted 19 June 2019, revised 28 September 2019, accepted 29 September 2019

Abstract

Bird fecal matter is considered a potential source of pathogenic microbes such as yeast species that contaminate the environment. Therefore, it needs to be scrutinized to assess potential environmental health risks. The aim of this study was to investigate the diversity of the yeasts in pigeon fecal droppings, their antifungal susceptibility patterns, and virulence factors. We used culturing techniques to detect the yeasts in pigeon fecal droppings. The isolates were then characterized based on colony morphologies, microscopic examinations, and biochemical reactions. The molecular identification of all yeast isolates was performed by sequencing of the amplified ITS gene. Genes encoding virulence factors *CAP1*, *CAP59*, and *PLB* were also detected. Antifungal susceptibility patterns were examined by the disk diffusion method. A total of 46 yeast-like isolates were recovered, and they belonged to nine different genera, namely, *Cryptococcus*, *Saccharomyces*, *Rhodotorula*, *Candida*, *Meyerozyma*, *Cyberlindnera*, *Rhodosporidium*, *Millerozyma*, and *Loddaromyces*. The prevalence of two genera *Cryptococcus* and *Rhodotorula* was high. None of the yeast isolates exhibited any resistance to the antifungal drugs tested; however, all pathogenic *Cryptococcus* species were positive for virulence determinants like urease activity, growth at 37°C, melanin production, the *PLB* and *CAP* genes. This is the first report on the molecular diversity of yeast species, particularly, *Cryptococcus* species and their virulence attributes in pigeon fecal droppings in Saudi Arabia.

Key words: *Cryptococcus*, pigeon, fecal droppings, antifungal susceptibility, virulence genes, yeast

Introduction

Free-living wild birds are regarded as one of the indicators of a healthy environment. However, they also may be regarded as potential carriers of human-pathogenic viral, bacterial, fungal, and protozoan agents. Free-living rock pigeons (*Columba livia*), are found in large flocks within major cities around the world. They live in close proximity to humans, particularly in public parks, on rooftops, and sometimes close to catering establishments. Numerous reports highlight that pigeon fecal droppings in public areas are a source of bacterial infectious agents, such as *Salmonella*, *Campylobacter*, and *E. coli* O157, and that they may significantly affect public health (Abulreesh et al. 2007; Abulreesh 2014).

Carriage of pathogenic yeast in pigeon feces is a matter of growing interest and has been investigated worldwide, with much focus on the *Cryptococcus* species. Wu et al. (2012) reported the presence of eight different genera of yeast, such as *Cryptococcus*, *Candida*,

* Corresponding author: H.H. Abulreesh, Department of Biology, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia; **e-mail: hhabulreesh@uqu.edu.sa**

Alshehri et al. J Pure Appl Microbiol, 13(4), 2035-2044 | December 2019
Article 5923 | https://doi.org/10.22207/JPAM.13.4.15
Print ISSN: 0973-7510; E-ISSN: 2581-690X

JPAM

RESEARCH ARTICLE OPEN ACCESS

DNA-barcoding and Species Identification for some Saudi Arabia Seaweeds using *rbcL* Gene

Mohammed Ali Alshehri[1,2], Al Thabiani Aziz[1], Othman Alzahrani[1,2], Abdulrahman Alasmari[1], Shafik Ibrahim[3], Gamal Osman[3,4*] and Omar Bahattab[1]

[1]Biology Department, Faculty of Science, University of Tabuk, Tabuk, Saudi Arabia. [2]Genome and Biotechnology Unit, Faculty of Sciences, University of Tabuk, Tabuk, Saudi Arabia. [3]Agricultural Genetic Engineering Research Institute (AGERI), Agriculture Research Center (ARC), Giza, Egypt. [4]Department of Biology, Faculty of Applied Sciences, Umm Al-Qura University, Makkah, Saudi Arabia.

Abstract

Among the different biological sources, seaweeds have lot of biotechnological applications. Saudi Arabia is bounded by three bodies of water. With a coastal border of almost 1,800 km. This area high species richness caused by its complex geological history has encompassed genetic and morphological diversity studies for decades. The DNA-barcoding using *rbcL* gene has proved its usefulness in studying seaweeds phylogenetic diversity, multiple cryptic introductions, environmental modulation the geographical distribution and species identification in different seaweed species. Eight algae samples were collected from different locations in Saudi Arabia. The *rbcL* gene was used through PCR protocol for species identification. A total number of 8 sequences were obtained with a total sequence length of 5263 bp. where it ranged from 610 to 753 with an average length of 658 bp. The species identification revealed that the specimens samples 1,2,3,4,5,6,7 and 8 belongs to *Padina pavonica*, *Turbinaria gracilis*, *Carpomitra costata*, *Pterocladiella capillacea*, *Cladostephus spongiosus*, *Ulva lactuca*, *Sporochnus comosus* and *Sargassum muticum* respectively. The *rbcL*-based DNA bar-coding was almost successful to identify different seaweeds specimens according to species and genus. Some specimens *rbcL* was not adequate to identify genus level and failed to differentiate between highly similar species. We suggest to use more DNA barcoding techniques in addition to *rbcL* to ad more resolution to the species identification.

***Correspondence:** geosman@uqu.edu.sa; +966530760365

(Received: 21 September 2019; accepted: 30 October 2019)

Citation: Mohammed Ali Alshehri, Al Thabiani Aziza, Othman Alzahrani, Abdulrahman Alasmari Shafik Ibrahim, Gamal Osman and Omar Bahattab, DNA-barcoding and Species Identification for some Saudi Arabia Seaweeds using rbcL Gene, *J Pure Appl Microbiol.*, 2019; **13**(4):2035-2044. https://doi.org/10.22207/JPAM.13.4.15

Journal of Mammalogy, XX(X):1–13, 2019
DOI:10.1093/jmammal/gyz081

Characterizing wing tears in common pipistrelles (*Pipistrellus pipistrellus*): investigating tear distribution, wing strength, and possible causes

Rana Osama S. Khayat, Kirsty J. Shaw, Gary Dougill, Louise M. Melling, Glenn R. Ferris, Glen Cooper, and Robyn A. Grant*

School of Science and the Environment, John Dalton Building, Manchester Metropolitan University, Chester Street, Manchester, M1 5GD, United Kingdom (ROSK, KJS, GD, LMM, RAG)
School of Healthcare Science, John Dalton Building, Manchester Metropolitan University, Chester Street, Manchester, M1 5GD, United Kingdom (GRF)
School of Mechanical, Aerospace and Civil Engineering, George Begg Building, University of Manchester, Manchester, M1 3BB, United Kingdom (GC)

** Correspondent: robyn.grant@mmu.ac.uk*

Bats have large, thin wings that are particularly susceptible to tearing. Anatomical specializations, such as fiber reinforcement, strengthen the wing and increase its resistance to puncture, and an extensive vasculature system across the wing also promotes healing. We investigated whether tear positioning is associated with anatomy in common pipistrelles (*Pipistrellus pipistrellus*). Wing anatomy was described using histological techniques, imaging, and material testing. Tear information, including type, position, time in rehabilitation, and possible causes, was collected from rehabilitators of injured bats across the United Kingdom. Results suggest that the position of the plagiopatagium (the most proximal wing section to the body), rather than its anatomy, influenced the number, location, and orientation of wing tears. While material testing did not identify the plagiopatagium as being significantly weaker than the chiropatagium (the more distal sections of the wing), the plagiopatagium tended to have the most tears. The position of the tears, close to the body and toward the trailing edge, suggests that they are caused by predator attacks, such as from a cat (*Felis catus*), rather than collisions. Consistent with this, 38% of *P. pipistrellus* individuals had confirmed wing tears caused by cats, with an additional 38% identified by rehabilitators as due to suspected cat attacks. The plagiopatagium had the lowest number of blood vessels and highest amounts of elastin fibers, suggesting that healing may take longer in this section. Further investigations into the causes of tears, and their effect on flight capabilities, will help to improve bat rehabilitation.

Key words: bat wing, collagen, elastin, healing, material testing, plagiopatagium, wing tear

Bats have thin wing membranes well adapted to generate appropriate lift and thrust to be maneuverable during flight (Vaughan 1970; Swartz et al. 1996; Neuweiler 2000). However, the large area and the thin membranous material of the wings make them particularly susceptible to injuries, such as holes and tears (Ceballos-Vasquez et al. 2015). Davis (1968) found over 40% of pallid bats (*Antrozous pallidus*) in one rural roost had wing injuries or abnormalities. While bats can fly with large wing tears (Davis 1968; Voigt 2013), hundreds of bats are taken to rescue centers for rehabilitation annually in the United Kingdom, especially the common pipistrelle, *Pipistrellus pipistrellus* (Kelly et al. 2008). Indeed, 748 *Pipistrellus* spp. were admitted to just one rescue center in the United Kingdom between 1997 and 2006 (Kelly et al. 2008). Tears are considered significant and severe injuries (Molony et al. 2007; Kelly et al. 2008). Rehabilitation in captivity can also result in increased stress (Moorhouse et al. 2007); therefore, the tear and resulting rehabilitation can significantly affect animal health and welfare (Molony et al. 2007; Kelly et al. 2008). Even though several studies have investigated wing tears in bats (Davis 1968; Powers et al. 2013; Voigt 2013; Greville et al. 2018), there is little characterization of their form (position, orientation, size) and what causes them, although collisions (Davis 1968), fungal infections (Reichard and Kunz 2009; Cryan et al. 2010; Fuller

Saudi Journal of Biological Sciences 27 (2020) 279–287

Contents lists available at ScienceDirect

Saudi Journal of Biological Sciences

journal homepage: www.sciencedirect.com

Piriformospora indica promotes cucumber tolerance against Root-knot nematode by modulating photosynthesis and innate responsive genes

Mohamed A.M. Atia [a], Emad A. Abdeldaym [b,1], Mohamed Abdelsattar [a,e], Dina S.S. Ibrahim [c], Ibrahim Saleh [d], Mohamed Abd Elwahab [b], Gamal H. Osman [f,g,h,*], Ibrahim A. Arif [d], Mohamed E. Abdelaziz [b,*]

[a]Agricultural Genetic Engineering Research Institute (AGERI), Agricultural Research Center (ARC), 12619 Giza, Egypt
[b]Faculty of Agriculture, Cairo University, 12613 Giza, Egypt
[c]Nematology Department, Plant Pathology Institute, Agricultural Research Center (ARC), 12619 Giza, Egypt
[d]Prince Sultan Research Chair for Environment and Wildlife, Department of Botany & Microbiology, College of Sciences, King Saud University (KSU), Riyadh, Saudi Arabia
[e]Department of Biology, Faculty of Applied Science, Umm Al-Qura University, Makka, Saudi Arabia
[f]Microbial Genetics Department, Agricultural Genetic Engineering Research Institute (AGERI), Giza, Egypt
[g]Research Laboratories Center, Faculty of Applied Science, Umm Al-Qura University, Mecca, Saudi Arabia

ARTICLE INFO

Article history:
Received 10 May 2019
Revised 1 September 2019
Accepted 9 September 2019
Available online 11 September 2019

Keywords:
Piriformospora indica
Root-knot nematode
Cucumber
Salicylic acid

ABSTRACT

Root Knot Nematode (RKN, *Meloidogyne incognita*) is one of the greatest damaging soil pathogens causes severe yield losses in cucumber and many other economic crops. Here, we evaluated the potential antagonistic effect of the root mutualistic fungus *Piriformospora indica* against RKN and their impact on vegetative growth, yield, photosynthesis, endogenous salicylic acid (SA) and its responsive genes. Our results showed that *P. indica* dramatically decreased the damage on shoot and root architecture of cucumber plants, which consequently enhanced yield of infested plants. Likewise, *P. indica* colonization clearly improved the chlorophyll content and delimited the negative impact of RNK on photosynthesis. Moreover, *P. indica* colonization exhibited a significant reduction of different vital nematological parameters such as soil larva density, amount of egg/eggmass, eggmasses, females and amount of galls at cucumber roots. Additionally, the results showed that SA level was significantly increased generally in the roots of all treatments especially in plants infested with RKN alone as compared to control. This suggests that *P. indica* promoting SA levels in host cucumber plant roots to antagonize the RKN and alleviate severity damages occurred in its roots. This higher levels of SA in cucumber roots was consistent with the higher expressional levels of SA pathway genes PR1 and PR5. Furthermore, *P. indica* colonization reduces PR1, PR5 and increased NPR1 in roots of RKN infested cucumber plants when compared to non-colonized plants. Interestingly, our in vitro results showed that direct application of *P. indica* suspension against the J2s exhibited a significant increase in mortality ratio. Our results collectively suggest that *P. indica* promoting morphological, physiological and SA levels that might together play a major important role to alleviate the adverse impact of RKN in cucumber.

* Corresponding authors at: Faculty of Applied Science, Umm Al-Qura University, Makka, Saudi Arabia (G.H. Osman). Agricultural Genetic Engineering Research Institute, Agricultural Research Center (M. Abdelsattar). Faculty of Agriculture, Cairo University (M. E. Abdelaziz).
E-mail addresses: matia@ageri.sci.eg (M.A.M. Atia), emad.abdeldaym@agr.cu.edu.eg (E.A. Abdeldaym), mtreina@ageri.sci.eg (M. Abdelsattar), mcsky@ymail.com (D.S.S. Ibrahim), mohamed.mahmoud@agr.cu.edu.eg (M.A. Elwahab), geosman@uqu.edu.sa (G.H. Osman), iaarif@ksu.edu.sa (I.A. Arif), mohamed.ewis@agr.cu.edu.eg (M.E. Abdelaziz).
[1] Equal contribution with the 1st author.

Peer review under responsibility of King Saud University.

Production and hosting by Elsevier

https://doi.org/10.1016/j.sjbs.2019.09.007
1319-562X/© 2019 Production and hosting by Elsevier B.V. on behalf of King Saud University.
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1. Introduction

Cucumber (*Cucumis sativus* L.) is vital economical vegetal crops (Mukhtar et al., 2013). In addition it consider a typical plant for vascular biology and sex determination studies with a draft genome size 243.5 Mb (~30% smaller than estimated genome size 367 Mb) (Huang et al., 2009). Root-knot nematodes (RKNs; *Meloidogyne* spp.) are endoparasites causing a dangerous hazard to agricultural sector. RKN includes more than 80 species, with a diverse devastating ability. Globally, root knot nematode is soil pathogens producing severe yield damages in numerous crops due to their ability to infest many of plant taxa (Abad and Williamson, 2010; Kayani et al. 2017). RKN species cause an estimated yearly damage of $157 billion

biology

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Article

Impact Effect of Methyl Tertiary-Butyl Ether "Twelve Months Vapor Inhalation Study in Rats"

Osama M. Sarhan [1,2], Antrix Jain [3], Hamed M. A. Mutwally [1], Gamal H. Osman [1,4,5,*], Sung Yun Jung [6], Tawfik Issa [7] and Mohamed Elmogy [8]

1 Biology Department, Faculty of Science, Umm Al-Qura University, Makkah 673, Saudi Arabia; sarhanomm59756@gmail.com (O.M.S.); pmmutwally@uqu.edu.sa (H.M.A.M.)
2 Zoology Department, Faculty of Science Fayoum University, Fayoum 63514, Egypt
3 Advanced Technology Cores, Baylor College of Medicine, Houston, TX 77030, USA; antrixj@bcm.edu
4 Microbial Genetics Department, Agricultural Genetic Engineering Research Institute (AGERI), Giza, Cairo 12619, Egypt
5 Research Laboratories Center, Faculty of Applied Science, Umm Al-Qura University, Mecca 24381, Saudi Arabia
6 Department of Biochemistry and Molecular Biology, Baylor College of Medicine, Houston, TX 77030, USA; syjung@bcm.edu
7 Department of Ophthalmology, Baylor College of Medicine, Houston, TX 77030, USA; Tawfik.Issa@bcm.edu
8 Entomology Department, Cairo University, Giza 12613, Egypt; osmangamal@hotmail.com
* Correspondence: geosman@uqu.edu.sa

Received: 29 October 2019; Accepted: 13 December 2019; Published: 20 December 2019

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Simple Summary: The detection of major blood-based markers for cancer requires expensive blood tests. Therefore, finding simple and effective blood-based markers is of great interest. The present results suggested that CA II, CA I, and peroxiredoxin2 could be utilized as potential biomarkers for the early detection of tracheal and lung cancer.

Abstract: We investigated the early risk of developing cancer by inhalation of low doses (60 µL/day) of methyl tertiary butyl ether (MTBE) vapors using protein SDS-PAGE and LC-MS/MS analysis of rat sera. Furthermore, histological alterations were assessed in the trachea and lungs of 60 adult male Wistar rats. SDS-PAGE of blood sera showed three protein bands corresponding to 29, 28, and 21 kDa. Mass spectroscopy was used to identify these three bands. The upper and middle protein bands showed homology to carbonic anhydrase 2 (CA II), whereas the lower protein band showed homology with peroxiredoxin 2. We found that exposure to MTBE resulted in histopathological alterations in the trachea and the lungs. The histological anomalies of trachea and lung showed that the lumen of trachea, bronchi, and air alveoli packed with free and necrotic epithelial cells (epithelialization). The tracheal lamina propria of lung demonstrated aggregation of lymphoid cells, lymphoid hyperplasia, hemorrhage, adenomas, fibroid degeneration, steatosis, foam cells, severe inflammatory cells with monocytic infiltration, edema, hemorrhage. Occluded, congested, and hypertrophied lung arteries in addition, degenerated thyroid follicles, were observed. The hyaline cartilage displayed degeneration, deformation, and abnormal protrusion. In conclusion, our results suggest that inhalation of very low concentrations of the gasoline additive MTBE could induce an increase in protein levels and resulted in histopathological alterations of the trachea and the lungs.

Keywords: MTBE; LC-MS/MS analysis; histopathology; cancer biomarker

Egypt. Acad. J. Biolog. Sci., 11(1): 105– 122 (2019)
Egyptian Academic Journal of Biological Sciences
F. Toxicology & Pest control
ISSN: 2090 - 0791
http://eajbsf.journals.ckb.eg/

Genome-wide DNA Mutability and Biochemical Effects of Novel Insecticides in the Control of Date Palm Fruit Pest *Ephestia cautella* (Walker)

Fouad A. Ahmed[1], Mohamed M.Rashed[1], Hala M. Abou-Yousf[2], Emam A. Abdel-Rahim[1], Shaimaa M. Mahdi[2],Gamal H. Osman[3,4,5]* and Mohamed A. Omar[4]

[1]*Biochemistry Department, Faculty of Agricultural, Cairo University, Egypt.*
[2]BioassayDepartment, Central Agricultural Pesticide Laboratory (CAPL), Agriculture Research Center (ARC). Egypt.
[3] Biology Department, Faculty of Applied Sciences, Umm Al-Qura University, Makkah, 21955, PO Box 715, Saudi Arabia.
[4] Agriculture Genetic Engineering Research Institute (AGERI), Agriculture Research Center (ARC). Egypt.
[5]Research Laboratories Center, Faculty of Applied Science, Umm Al-Qura University, Mecca, Saudi Arabia.
E-mail: geosman@uqu.edu.sa

ARTICLE INFO
Article History
Received:3/2/2019
Accepted:5/4/2019

Keywords:
Toxicological.
Ephestia cautella.
Insecticides.
RAPD. Date palm

ABSTRACT

Different pests attack date palm fruits during all the stages of maturity. Almond moth (*Ephestia cautella*) is a destructive insect of stored products, such as dates, wheat flour, and nuts. In the present study, the usage of novel groups of insecticides (Spinosyns, Diamide, Pyridalyl, and Azadirachtin) that are safe for humans and exert a relatively lower effect on the environment was assessed. In particular, the toxicological and biochemical impacts of five insecticides (Tracer, Radiant, Coragen, Pleo, and Achook) on the control of *E. Cautella* were evaluated, and the genome-wide DNA mutability caused by these insecticides was screened. A bioassay was performed in order to determine the LC_{50}value for each insecticide, the results of which revealed that Coragen with an LC_{50} value of 0.49 ppm was the most potent insecticide, followed by Radiant and Achook (with LC_{50} values of 1.51 and 1.73 ppm, respectively). In addition, the effect of these insecticides on vital enzymes was investigated. The data from this investigation revealed that the treatment with Radiant demonstrated stimulation in AST, ACP, ALP, and GST activity, and inhibition in AChE, ALT, and protease activity. The insects treated with Coragen exhibited an elevation in the activities of AChE, GST, ALP, ACP, ALT, and protease. Finally, DNA-level mutability caused by the insecticides was assessed by using RAPD-PCR analysis, and the results indicated Radiant as a genotoxic insecticide that caused large changes at the genomic-DNA level. On the other hand, Coragen exhibited the lowest mutability effect on insect DNA.

Citation: *Egypt. Acad. J. Biolog. Sci. (F. Toxicology & Pest control) Vol. 11(1) pp. 105- 122 (2019)*

www.nature.com/scientificreports

SCIENTIFIC REPORTS

OPEN

Construction, Expression and Evaluation of Recombinant VP2 Protein for serotype-independent Detection of FMDV Seropositive Animals in Egypt

Received: 2 October 2018
Accepted: 25 June 2019
Published online: 12 July 2019

Reda Salem[1], Alaa A. El-Kholy[2], Omar A. Omar[2], Mohamed N. Abu el-naga[3], Mohamed Ibrahim[4] & Gamal Osman[1,5,6]

Foot-and-mouth disease virus (FMDV) is one of the most devastating viral pathogens of cloven-hoofed animals. The detection of antibodies (Ab) against FMDV structural proteins (SP) using virus neutralization test (VNT) and liquid-phase blocking ELISA (LPBE) is the standard procedure in use for monitoring seroconversion in animals post vaccination, the prevalence of infection-surveillance, proving clinical cases and seronegative status of FMDV-free/naïve-animals prior transportation. However, due to variations within SP of FMDV serotypes, each serotype-specific Ab should be detected separately which is laborious and time-consuming. Accordingly, it is crucial to develop a sensitive, rapid, and accurate test capable of detecting FMDV-specific Ab, regardless its serotype. This study describes the heterologous expression of VP2 protein in *E. coli*, and its evaluation as a capture antigen in a simple indirect ELISA for serotype-independent detection of anti-FMDV Ab. Sequence analysis revealed that the VP2-coding sequence is considerably conserved among FMDV serotypes. The recombinant VP2 (rVP2), a 22 kDa polypeptide, was purified to near homogeneity by affinity chromatography under native conditions. Immunoreactivity of the rVP2 was confirmed by using a panel of positive sera including sera from animals vaccinated with the local trivalent vaccine and guinea pig FMDV antiserum, which is routinely used as tracing/detecting Ab in LPBE testing. The results obtained from the VP2-based ELISA were comparable to those determined by VNT and LPBE standard diagnostic assays. Specificity and sensitivity of rVP2 in capturing anti-FMDV Ab were 98.3% and 100%, respectively. The developed VP2-ELISA is proved reliable and time-efficient assay for detection of FMDV seropositive animals, regardless the FMDV serotype that can be implemented in a combination with VNT and/or LPBE for rapid diagnosis of an ongoing FMDV infection.

Foot-and-mouth disease (FMD) is a severe ailment affecting livestock. There are seven antigenically and genetically divergent serotypes of the etiological agent FMD virus (FMDV): O, A, C, Asia 1, and the Southern African Territories SAT 1, SAT 2, and SAT 3[1]. FMDV particles are made up of an icosahedral capsid each consisting of sixteen repeats of four structural proteins (SPs) VP1, VP2, VP3, and VP4, encapsulating a single-stranded, positive-sense RNA genome[2]. In addition to the structural proteins, during viral infection, a number of non-structural viral proteins (NSP) are also made in the infected cells[3].

[1]Agricultural Genetic Engineering Research Institute (AGERI), ARC, 12619, Giza, Egypt. [2]Veterinary Sera and Vaccines Research Institute (VSVRI), ARC, Abbassia, Cairo, Egypt. [3]Radiation microbiology department, National Center for Radiation Research and Technology, Atomic Energy Authority, 11787, Cairo, Egypt. [4]Department of Molecular and Cell Biology, University of Texas at Dallas, Richardson, TX, 75083, USA. [5]Biology Department, Faculty of Science, Umm-Al-Qura University, Mecca, 673, Saudi Arabia. [6]Research Laboratories Center, Faculty of Applied Science, Umm Al-Qura University, Mecca, Saudi Arabia. Correspondence and requests for materials should be addressed to R.S. (email: redasalem@ageri.sci.eg) or G.O. (email: geosman@uqu.edu.sa)

| (2019) 9:10135 | https://doi.org/10.1038/s41598-019-46596-9

Steroids 141 (2019) 1–8

Contents lists available at ScienceDirect

Steroids

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Control of β-sitosterol biosynthesis under light and watering in desert plant *Calotropis procera*

Ahmed M. Ramadan[a,b,c], Ahmed Abdel Azeiz[c], Saeed Baabad[a], Sameh Hassanein[c,d], Nour O. Gadalla[e,f], Sabah Hassan[b,g], Mardi Algandaby[a], Salwa Bakr[h,i], Thana Khan[a], Heba H. Abouseadaa[j], Hani Mohammed Ali[a], Areej Al-Ghamdi[k], Gamal Osman[l,m,*], Sherif Edris[n,o], Hala Eissa[b,c], Ahmed Bahieldin[n,o]

Most scientific studies on *Calotropis procera* refer to the plant as an important source of pharmaceutical compounds and its valuable benefits in medicine. One of the most important substances in this plant is the potential immunostimulant β-sitosterol (BS) that acts in improving human health. This study focused on the effects of lighting before and after irrigation on the BS accumulation pathway namely sterol biosynthesis. Studying the enzymes in BS biosynthetic pathway indicated the upregulation at dawn and predusk of the *SMT2* and *SMT3* genes encoding sterol methyltransferase 2 and methylsterol monooxygenase, two key enzymes in BS accumulation in *C. procera*. The results almost indicated no regulation at the different time points of the *CYP710A* gene encoding sterol 22-desaturase, an enzyme that acts in depleting β-sitosterol towards the biosynthesis of stigmasterol. RNA-Seq data was validated via quantitative RT-PCR and results were positive. The data of ultra-performance liquid chromatography-tandem mass spectrometry analysis with regard to BS accumulation also aligned with those of RNA-Seq analysis. We focused on the effects of light before and after watering on BS accumulation in *C. procera*. Our results show that BS accumulation is high at dawn in both dehydrated and well-watered condition. While, the BS was dramatically decrease at midday in well-watered plants. This increase/decrease in BS content is correlated with rates of expression of *SMT2* gene. This gene is a key converter between the different branches in the cardiac glycoside biosynthesis. Accordingly, it could be suggested that BS (or one of the descendent product) may play an important role in *C. procera* tolerance to drought/light intensity conditions.

1. Introduction

Calotropis procera is a poisonous flowering plant from the family Apocynaceae. This plant is native to and grows in the dry lands of North Africa, Tropical Africa, Western Asia, South Asia, and Indochina [1]. Most scientific studies on *Calotropis* regarding the plant as an important source of pharmaceutical compounds and indicated its valuable benefits in medicine [2,3]. Despite the severe toxicity that can be caused by

* Corresponding authors at: Department of Biological Sciences, Faculty of Science, King Abdulaziz University (KAU), P.O. Box 80141, Jeddah 21589, Saudi Arabia (A. Ramadan). Department of Biology, Umm Al-Qura University, Makkah, Saudi Arabia (G. Osman).
E-mail addresses: asmara@kau.edu.sa (A.M. Ramadan), geosman@uqu.edu.sa (G. Osman).

https://doi.org/10.1016/j.steroids.2018.11.003
Received 12 September 2018; Received in revised form 23 October 2018; Accepted 2 November 2018
Available online 07 November 2018
0039-128X/

Osman *et al. J Pure Appl Microbiol*, **13**(2), 767-778 | June 2019
Article 5559 | https://dx.doi.org/10.22207/JPAM.13.2.12
Print ISSN: 0973-7510; E-ISSN: 2581-690X

RESEARCH ARTICLE OPEN ACCESS

Photocatalytic Bacterial Disinfection using Ag^{o}/Ag^{+1} Immobilized on CNT Modified TiO_2 Nanomaterials

Gamal Osman[1,2,3], Mohamed M. Mohamed[4]* and Khalid S. Khairou[5]

[1]Department of Biology, Faculty of Applied Sciences, Umm Al Qura University, Makkah- 21955, Kingdom of Saudi Arabia. [2]Agricultural Genetic Engineering Research Institute (AGERI), Giza, Egypt. [3]Research Laboratories Center, Faculty of Applied Science, Umm Al-Qura University, Mecca, Saudi Arabia. [4]*Department of Chemistry, Faculty of Science, Benha University, Benha- 13518, Egypt. [5]Department of Chemistry, Faculty of Applied Sciences, Umm Al Qura University, Makkah - 21955, Kingdom of Saudi Arabia.

Abstract

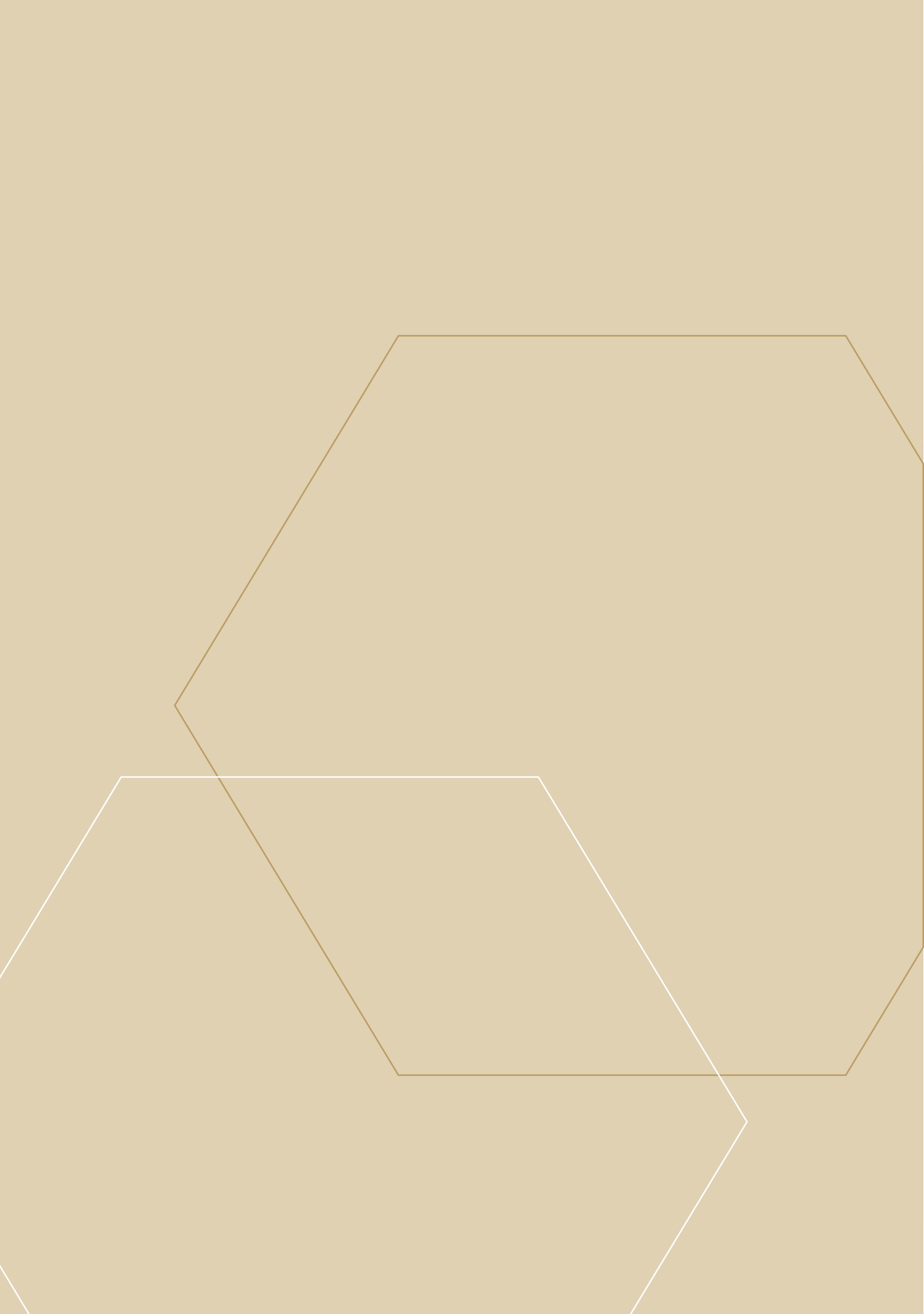
Different loading of Ag nanoparticles (2 and 6%) modified TiO2 synthesized by employing polymeric template; comprises of polyvinyl alcohol and polyethylene glycol (Tev), were utilized to react hydrothermally (433 K for 48 h) with functionalized SWCNT and MWCNT. Several characterization techniques, including UV-visible diffuse reflectance spectroscopy, X-ray diffraction, HRTEM-ASED, and N2 sorptiometry were utilized for obtaining information about surface texturing, morphology, optical properties and crystalline phases. The synthesized photocatalysts were tested for their antibacterial activity against Escherichia coli (Gram negative bacterium) and Staphylococcus aureus (Gram positive bacterium) through agar well diffusion method under visible light irradiation (λ > 450 nm, 60 mWcm-2). It has been revealed that the photocatalyst TevAg6-SWCNT exhibited the maximum lethal action thereby inhibiting the growth of bacteria as compared to rest of the catalysts; this was due to increase in surface area value with delay in electrons and holes recombination as well as the diameter of Ago nanoparticles which was reduced to 3 nm. It has been evidenced that the nanocomposites attack mechanism on while disinfecting bacteria indicates the formation of O2•− and ·OH radicals, those played significant role in inactivation of cellular process. The TEM images revealed the role of Ag+ ions, and the presence of TevAg6-SWCNT were thoroughly studied and correlated to identify the disinfection mechanisms induced through irradiation of visible light.

Keywords: Ag/TiO_2-CNTs nanocomposites, Bacterial disinfection; DNA damage; Surface active species, morphology change.

***Correspondence:** mohmok2000@yahoo.com

(Received: 12 March 2019; accepted: 07 May 2019)

Citation: Gamal Osman, Mohamed M. Mohamed and Khalid S. Khairou, Photocatalytic Bacterial Disinfection using Ag^{o}/Ag^{+1} Immobilized on CNT Modified TiO_2 Nanomaterials, *J Pure Appl Microbiol.*, 2019; **13**(2):767-778. doi: 10.22207/JPAM.13.2.12



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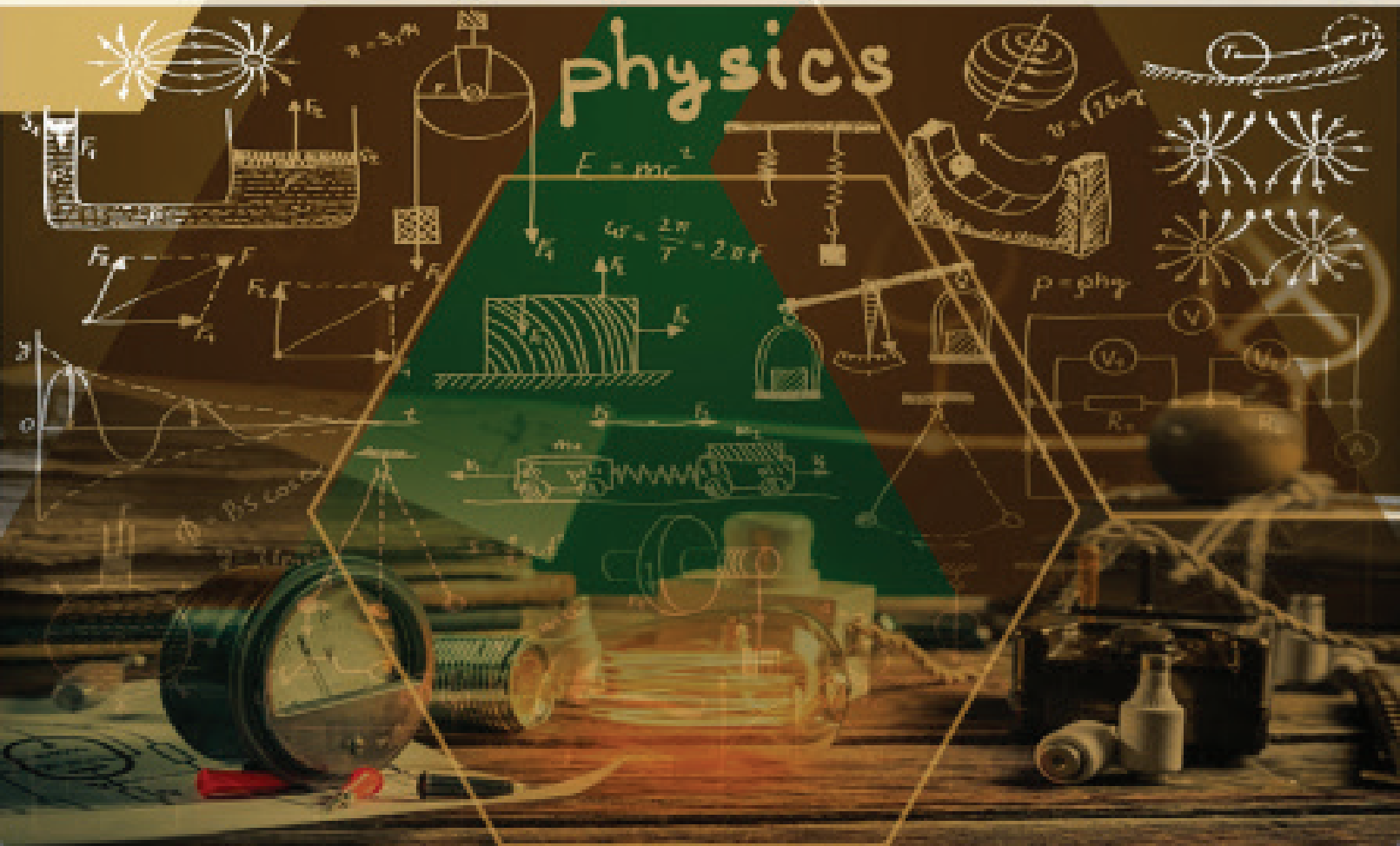

أولا: الأبحاث المنشورة بقسم الفيزياء :

م	عنوان البحث	المشاركين	المجلة	دار النشر	ISI/ NON-ISI	معامل التأثير IF
1	Interactions between a water molecule and C60 in the endohedral fullerene H2O@ C60	Effat Rashed and Janette L. Dunn	Phys. Chem. Chem. Phys	RSC	ISI	3.57
2	Orientations and Crystallinities of Drawn Fibers Using Two Beam Interferometry	A. M. Ali	Egypt. J. Phys	National Information and Documentation Center	-	-
3	The impact of processing conditions on the structural and optical properties of the as-spun polyamides fibers	Afaf M. Ali	Microsc Res Tech	Wiley	ISI	1.33
4	An insight on the process–property relationships of melt spun Polylactic acid fibers.	AM Ali and HM El-Dessouky	Textile Research Journal	SAGE	ISI	1.61
5	Improving the efficiency of the organic solar cell (CuPc/ C60) via PEDOT: PSS as a photoconductor layer doped by silver nanoparticles	A. M. Ali , D. A. Said, M. M. Khayyat, M. Boustimi, R. Seoudi	Results in Physics	Elsevier	ISI	3.04
6	Energies, Wavelengths, and Transition Probabilities in Sc XIII	Fatma El-Sayed, S. M. Attia	Physics of Atomic Nuclei	Pleiades Publishing, Ltd	ISI	0.46
7	Multifunctional curcumin-loaded mesoporous silica nanoparticles for cancer chemoprevention and therapy	,Nihal S. Elbialy ,Samia Faisal Aboushoushah ,Balsam Fahad Sofi Abdulwahab Noorwali	Microporous and Mesoporous Materials	Elsevier	ISI	4.18
8	Concentrated Photovoltaic/ Thermal Hybrid System Coupled with a Thermoelectric Generator	Abdelrahman Lashin, Mohammad Al Turkestani and Mohamed Sabry	Energies	MDPI	ISI	2.70
9	Energy Levels and Transition Rates for Ti XIV	Fatma El-Sayed, Z. S. Mattar	Physics of Particles and Nuclei Letters	Pleiades Publishing, Ltd	ISI	0.58
10	Improving the efficiency of the organic solar cell (CuPc/ C60) via PEDOT:PSS as a photoconductor layer doped by silver nanoparticles	Ali A M, Said D A, Khayyat M, Boustimi M, Seoudi R	Results in Physics	Elsevier	ISI	3.04
11	A study of the influence of plasmonic resonance of gold nanoparticle doped PEDOT: PSS on the performance of organic solar cells based on CuPc/C60	Said D A, Ali A M, Khayyat M M, Boustimi M, Loulou M, Seoudi R	Heliyon	Elsevier	ISI	1.66
12	Approaches of Energy-Saving Facades – Review Article	Mohamed Sabry	The Umm Al-Qura University Journal of Applied Sciences	-	-	-

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ثانيا: المشاريع الممولة من عمادة البحث العلمي ومدينة الملك عبدالعزيز للعلوم والتقنية بقسم الفيزياء :

	Projects	Researcher	Fund
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3	تراكيب الكربون النانوية المنتجة من الرماد المتطاير لاحتراق الوقود الأحفوري وتنشيط مراكز الانبعاث الضوئي الطيفي لها لغرض استخدامها في الطاقة	د. صالح مرزوق اللقماني	KACST برنامج الأبحاث التطبيقية SR 700,000
4	Grain Size Effects on the Mechanical Properties of ZnO nanoparticles- Based Varistor Ceramics	د. رباب خالد سندي د. عفاف معوض علي	DSR Umm Al -Qura University 100000 SR
5	Improvingtheefficiencyoftheorganicsolarcell(CuPc/C60)viaPEDOT:PSS as a photoconductor layer doped by silver nanoparticle A study of the influence of plasmonic resonance of gold nanoparticle doped PEDOT: PSS on the performance of organic solar cells based on CuPc/C60	أ.د. رشدي سعودي عوض	DSR Umm Al -Qura University 215,000
6	Nitrogen Doped Carbon Quantum Dots Derived from Oil Fly Ash for Green Solar Cells	د. محرز الشرياني لولو د. جلال الناصر الورفلي	DSR Umm Al -Qura University 287800 SR
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ثالثا: الكتب المنشورة بقسم الفيزياء :

م	عنوان الكتاب	المشاركين	دار النشر
1	أساسيات كيمياء الجوامد 2	أ.د. يسري محمد مصطفى د/ الحسيني الطاهر محمد	دار النوارس ترقيم دولي 978 - 977 - 6588 - 45 - 5 رقم ايداع 13522 / 2017
2	Nanomaterials: Science and Technology	Seoudi R, Said D, Mostafa Y	Dar Obaid for printing, publishing, ,and distribution Egypt 978 - 977 - 6646 - 21 - 6


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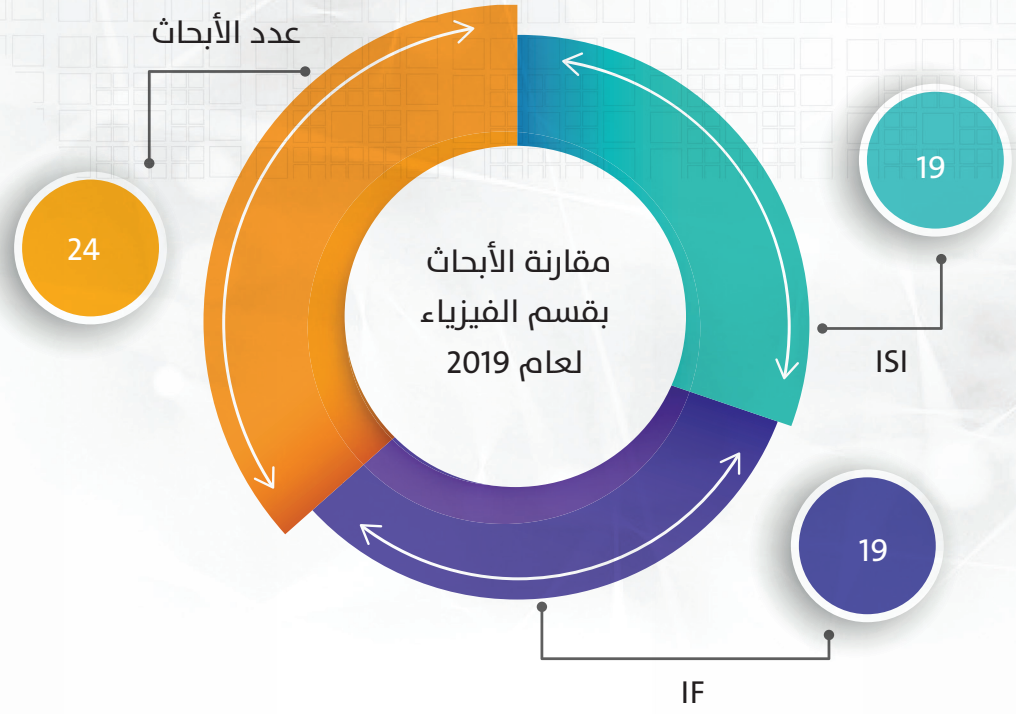
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ملخصات الأوراق العلمية المنشورة بقسم الفيزياء:

Received: 11 April 2019 | Revised: 19 July 2019 | Accepted: 28 July 2019
DOI: 10.1002/jemt.23360

RESEARCH ARTICLE

MICROSCOPY RESEARCH TECHNIQUE WILEY

The impact of processing conditions on the structural and optical properties of the as-spun polyamides fibers

Afaf M. Ali[1,2]

[1]Physics Department, Faculty of Science, Mansoura University, Mansoura, Egypt
[2]Physics Department, Faculty of Science, Umm Al-Qura University, Makkah, Saudi Arabia

Correspondence
Afaf M. Ali, Physics Department, Faculty of Science, Mansoura University, Mansoura, Egypt.
Email: afafmawsed@gmail.com

Review Editor: Mingying Yang

Funding information
Deanship of Scientific Research at Umm Al-Qura University, Grant/Award Number: Grant Code: 17-SCI-1-3-0002

Abstract

The development of crystallinity and orientation during the melt spinning of polyamides (nylon 66) was investigated. This study reports the question of the orientation and crystallinity determination of nylon 66 by means of differential scanning calorimetry, optical polarized microscope, and X-ray diffraction techniques during the cold drawing process. The different structural properties such as crystallinity, crystal size, birefringence, and different orientation functions were measured as a function of the draw ratio. From the obtained thermogram, it is clear that the melting temperature of the drawn nylon 66 fibers did not show a significant change due to the cold drawing process. As the draw ratio increase, the crystallinity and crystal size increase. The drawing process improves the chain orientations along the fiber axis of nylon 66 fibers. The orientations of the chain segments enhanced due to the cold drawing process of nylon 66 fibers.

KEYWORDS
birefringence, crystallinity, drawing, melt spinning, nylon 66 fibers, orientation

1 | INTRODUCTION

The structure of semicrystalline polymers is strongly sensitive to the processing conditions. The crystallinity is depending on texturing and chain orientation effects (Galeski, 2003; Patlazhan & Remond, 2012). Nylon 66 fibers are classified as a semicrystalline polymer. Nylon 66 fibers are common used in plastic engineering and fibers due to its high strength and toughness.

To get complete view about the different physical properties of semicrystalline fiber, the crystallinity of the fiber after thermo-mechanical treatment must be measured. Different techniques were used to measure the degree of crystallinity such as differential scanning calorimetry (DSC), X-ray diffraction, Raman and infrared spectroscopy (Ataf & El-Dessouky, 2015; Coraline Millot, Lame, Sotta, & Seguela, 2015; Wunderlich, 2001). DSC is the simplest and widely used technique for the determination of degree of crystallinity in fibers. This method depends on measuring the amount of heat should be provided to the fibers. That heat used to melt its crystalline phase during the thermal treatment at constant rate of heating.

X-ray diffraction (XRD) technique has been used to characterize the different polymeric materials from a long time. XRD technique is still the most prominent method used to determine the different materials crystallinity due to its professed strength, nondestructive technique, and availability (Afaf & El-Dessouky, 2019; Kim & Chang-Doo, 2014; Lindner, Petridis, Langan, & Smith, 2015; Patrik Ahvenainen, 2016). The crystal structures of different nylon 66 fibers were studied (Puiggali´, Franco, Aleman, & Subirana, 2009).

The birefringence measurement is powerful indicator for the study of different characteristics of semicrystalline polymers. Also it can be used to investigate the physical structure accurately (Hamza, Sokkar, El-Bakary, & Ali, 2010a; El-Dessouky et al., 2010; Hamza, Sokkar, El-Bakary, & Ali, 2002; Hamza, Sokkar, El-Farahaty, & El-Dessouky, 2004; Sokkar, El-Farhaty, El-Bakary, Ali, & Ahmed, 2018; Sokkar, El-Tonsy, El-Bakary, El-Morsy, & Ali, 2009). In particular, the birefringence is mainly used to measure the degree of the molecular alignment in uniaxial oriented fibers that utilized in several structure techniques (Hamza, Sokkar, El-Farahaty, & El-Dessouky, 2005).

Egypt. J. Phys. **Vol. 47,** pp. 31- 43 (2019)

Orientations and Crystallinities of Drawn Fibers Using Two Beam Interferometry

A. M. Ali[1,2]
[1]*Physics Department, Faculty of Science, Umm Al- Qura University, KSA*
[2]*Physics Department, Faculty of Science, Mansoura University, Egypt*

IN this work, the Pluta interference microscope was used to study the effect of drawing process on the optical, structural, and mechanical properties of polyethylene terephthalate (PET) fibers. The orientational behavior of drawn PET fibers to different draw ratios was investigated using the calculated values of the refractive indices and the double refraction. Changing the draw ratio resulted in changes in optical parameters, which were used to determine the mechanical factors of orientation. Different orientation functions, such as $f_1(\theta)$, $f_2(\theta)$, $f_3(\theta)$, f_c, f_a, and f_{av} were calculated. Molecular reorientation during the cold drawing process can be considered the main reason for the major variations in the properties of PET fibers. It can be concluded that double refraction related to the total overall orientation of the crystalline and amorphous phases. The different crystallinities parameters were measured. Microinterferograms were utilized to illustrate these variations.

Keywords: Orientation, Crystallinity, Drawing and PET fibers.

Introduction

Polyethylene terephthalate (PET), a semi crystalline polymer, can be used in a wide range of commercial applications due to its desirable physical and chemical properties, such as clearness, light weight, high strength, stiffness, high chemical resistance, elastic nature, and low price [1-3]. A drawing process should be applied to make PET fibers acceptable for textile and other industrial applications. The polymer tensile deformations are always accompanied by advance alignment of chains along the drawing direction. The amorphous and crystalline molecular orientation is related to the induced strain in the sample. There are two different models that explain the orientation as a function of draw ratio the pseudo- affine and affine models. The application of one these model depends on the drawing conditions [4]. Many authors studied the effect of drawing process on the mechanical and structural behavior of PET [5-9].

To enhance the behavior of the final polymeric products, the orientation amount and crystallinity degree should be completely characterized. Different experimental methods, such as wide-angle X-ray scattering, X-ray scattering, and density measurement, can be used to monitor these properties (Kolb et al., 2000). Several methods, such as molten fiber stretching, rapid cooling, and hot or cold drawing process, can be utilized to produce orientation in the polymers. Fiber properties can be changed by the drawing process. This change is due to the molecular arrangement, which is vital in characterizing the orientation, crystallinity, and other structural properties. When polymers, such as PET, are mechanically drawn above or close to their glass transition temperatures, an induced strain crystallinity can be formed.

Birefringence is a physical indicator that correlates the mechanical and optical properties of fiber. Measuring the birefringence and correlating it to other physical properties shed light on the characteristics of a bulk polymer. An external force is applied to the fiber during the cold drawing process so that the polymer chains become highly oriented along the drawing direction [11,12]. Birefringence measurement can be used as a significant indicator to characterize the amount of orientation and anisotropy. The birefringence of polymeric fibers has been extensively investigated because it is related to the polarizability of the molecules and the orientation function of these fibers. Birefringence and refractive indices provide an orientation measure, which is an average of the amorphous

DOI : 10.21608/ejphysics.2018.6032.1013

ISSN 1063-7796, Physics of Atomic Nuclei, 2019, Vol. 82, No. 6, pp. 583–588. © Pleiades Publishing, Ltd., 2019.

NUCLEI
Theory

Energies, Wavelengths, and Transition Probabilities in Sc XIII

Fatma El-Sayed[1),2)]* and S. M. Attia[1),2)]

Received June 27, 2019; revised June 27, 2019; accepted June 27, 2019

Abstract—The fine-structure energy levels and lifetimes are calculated for the lowest 218 levels of the $2s^22p^6$, $2s2p^6$, $2s^22p^53s$, $2s^22p^53p$, $2s^22p^43d$, $2s2p^53s$, $2s2p^53d$, $2p^63s$, $2p^63d$, $2s^22p^54s$, $2s^22p^54p$, $2s^22p^44d$, $2s2p^54s$, $2s2p^54p$, and $2s2p^54d$ configurations in Sc XIII using the general-purpose relativistic atomic structure package (GRASP). The atomic data of the electric dipole ($E1$), electric quadrupole ($E2$), magnetic dipole ($M1$), and magnetic quadrupole ($M2$) transitions from the levels of $2s^22p^6$, $2s2p^6$, $2s^22p^53s$, $2s^22p^53p$, $2s^22p^43d$, $2s2p^53s$, $2s2p^53p$, $2s2p^53d$, $2p^63s$, $2p^63p$, and $2p^63d$ configurations to the levels of the $2s^22p^5$ and $2s2p^6$ configurations are presented. The GRASP results are compared with the other calculations and measurements.

DOI: 10.1134/S1063778819060061

1. INTRODUCTION

The atomic data of highly ionized atoms are needed for several fields, such as astrophysics, laser physics, and plasmas physics. The magnetic-dipole transitions in the $2s^22p^5$ configuration are an important tool for the diagnostics of high-temperature plasmas [1]. The atomic data for ions in the F-like ions have been reported [1–23].

Cohen et al. [2] have observed the lines of the $2s^22p^5$–$2s^22p^43s$, $2s^22p^5$–$2s^22p^43d$, and $2s2p^6$–$2s2p^53s$ transitions of F-like ions from Sc XIII to Cu XXI. Chapman and Shadmi [3] have calculated the energy levels and oscillator strengths for transitions from the levels of the $2s^22p^43s$, $2s^22p^43d$, $2s2p^53p$, $2p^63s$, and $2p^63d$ configurations to $2s^22p^{5}P_{3/2}$,$2s^22p^{5}P_{1/2}$, and $2s^22p^{5}P_{1/2}$ levels for the Sc XIII, Fe XVIII, and Cu XXI. The lines of the $2s^22p^5$–$2s^22p^43d$ transitions for the F-like ions with $19 \leqslant Z \leqslant 27$ have been observed by Feldman et al. [4].

The general-purpose relativistic atomic structure package code has been used in the calculation of the atomic data for transitions among the lowest 113 levels of the $2s^22p^5$, $2s2p^6$, $2s^22p^43l$, $2s^23p^43l$, and $2s^23l^2$ ($l = s, p, d$) configurations for F-like ions with $37 \leqslant Z \leqslant 53$ [19], and for ions with $55 \leqslant Z \leqslant 73$ [22]. Recently, Zhang et al. [23] have calculated the atomic data for $E1$, $E2$, $M1$, and $M2$ transitions between the lowest 200 levels of $2s^22p^5$, $2s2p^63s$, $2s2p^63p$, $2s2p^63d$, $2s2p^64s$, $2s2p^64p$, $2s2p^64d$, and $2s2p^64f$ configurations in Kr XXVIII.

In this work, we calculate the energy levels, lifetimes, wavelengths, transition probabilities, oscillator strengths, and line strengths for $E1$, $E2$, $M1$, and $M2$ transitions in Sc XIII using the general-purpose relativistic atomic structure package.

2. CALCULATION AND RESULTS

2.1. Energy Levels

The atomic data of Sc XIII of the lowest 218 levels of $2s^22p^5$, $2s2p^6$, $2s^22p^43s$, $2s^22p^53p$, $2s^22p^43d$, $2s2p^53s$, $2s2p^53p$, $2s2p^53d$, $2p^63p$, $2p^63d$, $2s^22p^44s$, $2s^22p^44p$, $2s^22p^44d$, $2s2p^54s$, $2s2p^54p$, and $2s2p^54d$ configurations are calculated using the GRASP code [24].

In Table 1, we present the energy levels (in Ryd), and the mixing coefficients for 218 fine-structure levels of the $2s^22p^5$, $2s2p^6$, $2s^22p^43l$, $2s2p^53l$, $2p^63l$, $2s^22p^44l$, and $2s2p^54l$ ($l = s, p, d$) configurations obtained from GRASP with and without Breit and QED effects for Sc XIII. The Breit and QED energies (GRASP$^{\text{BQ}}$) are lower than the corresponding Coulomb energies (GRASP$^{\text{N}}$) by up to 0.04 Ryd (~0.1%), except for the $2s^22p^{1/2}P_{1/2}$ level is 0.01 Ryd (~3.2%). The comparison between the present energy levels results and the compiled data from NIST [25] shows the level orderings are the same and the differences are within 0.4%, except for the $2s2p^{1/2}S_{1/2}$ level is 2%.

The lifetime of excited level j is given by $1/(\sum_i A_{ji})$ and the summation includes A-values from all types

[1)]Physics Department, Faculty of Science, Kafrelsheikh University, Kafr El-Sheikh, Egypt.
[2)]Physics Department, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia.
*E-mail: Fatma_aathrous@yahoo.com

Textile Research Journal

Original article

An insight on the process–property relationships of melt spun polylactic acid fibers

Textile Research Journal
2019, Vol. 89(23-24) 4959–4966

DOI: 10.1177/0040517519845684
journals.sagepub.com/home/trj
SAGE

AM Ali[1,2] **and HM El-Dessouky**[2,3]

Abstract
Polylactic acid (PLA) fibers are receiving growing interest as one of the recent innovative materials being developed for various applications. The inherent biodegradability of PLA makes it highly attractive for the biomedical and health care sectors. PLA fibers need to be partially and/or highly oriented to allow high performance and readiness for a wide range of manufacturability. In this study, the structure and properties of PLA fibers, manufactured at different spinning speeds, were studied. Laser diffractometry, polarized light microscopy, differential scanning calorimetry (DSC) and X-ray diffraction (XRD) were used to determine the diameter, birefringence, molecular orientation, enthalpy and degree of crystallinity of as-spun and drawn PLA fibers. The results of DSC and XRD showed that the degree of crystallinity of the PLA fibers is significantly improved for the drawn PLA fibers compared to the as-spun fibers and leveled off in the case of changing the take-up speeds of drawn fibers.

Keywords
biodegradable, crystallinity, orientation, polylactic acid, structure–properties, fibers

Biodegradable materials have been given increasing attention in the last few decades. The biodegradable polymers degradation feature offers attractive advantage in contrast with the low recycling ratio of most plastics, such as polyethylene (PE) or polypropylene (PP). Also, the obtained products from biodegradable polymers fit in the natural recycling processes.[1,2]

Polylactic acid (PLA) is the first feasible thermoplastic fiber that can be produced from plant-based renewable resources, such as corn and sugar cane, and extruded by conventional melt-spinning processing technologies. PLA successfully bridges the gap between synthetic and natural fibers, thereby expanding its application range, from medical and pharmaceutical to environmentally benign films and fibers for packaging, houseware and clothing. PLA fibers have particularly attracted attention in commercial textiles due to their various advantages, such as ease of melt processing, unique property spectrum, renewable source origin and ease of compositing and recycling at the end of their useful life.[3,4] PLA has been intensively studied due to its biocompatibility, sustainability and environmentally friendly characteristics, as well as its desirable physical and mechanical properties.[5]

PLA is a biodegradable polymer with excellent mechanical properties, easy processability and reasonable price. Many products, such as shopping bags, mulch films, cutleries, office utensils, flower pots, yoghurt cans and toothbrush handles, can be made from PLA, which may also be used in medical and engineering applications.[4,6]

The building block of PLA is lactic acid, which exists as optically active D- or L-enantiomers.[7] The decomposition of PLA occurs by hydrolysis,

[1]Physics Department, Faculty of Science, Umm Al- Qura University, KSA
[2]Physics Department, Faculty of Science, Mansoura University, Egypt
[3]Composite Centre, Advanced Manufacturing Research Centre-AMRC, University of Sheffield, UK

Corresponding author:
AM Ali, Faculty of Science, Mansoura University, Makkah, 111123, Saudi Arabia.
Email: afafmawsed@gmail.com

ISSN 1547-4771, Physics of Particles and Nuclei Letters, 2019, Vol. 16, No. 6, pp. 713–728. © Pleiades Publishing, Ltd., 2019.

PHYSICS OF ELEMENTARY PARTICLES AND ATOMIC NUCLEI. THEORY

Energy Levels and Transition Rates for Ti XIV

Fatma El-Sayed[a, b, *], [**], [***] and Z. S. Matar[b, **]**

[a] *Physics Department, Faculty of Science, Kafrelsheikh University, Kafr El-Sheikh, 33516 Egypt*
[b] *Physics Department, Faculty of Applied Science, Umm Al-Qura University, Makkah, 21955 Saudi Arabia*
*e-mail: fatma_mahrous@yahoo.com
**e-mail: fatmamahrous@sci.kfs.edu.eg
***e-mail: feuhman@uqu.edu.sa
****e-mail: zsmatar@uqu.edu.sa

Received July 15, 2019; revised August 8, 2019; accepted August 9, 2019

Abstract—Energy levels, wavelengths, oscillator strengths, transition probabilities, line strengths, and lifetimes are calculated for transitions in Ti XIV. The $2s^22p^5$, $2s2p^6$, $2s^22p^43l$, $2s2p^53l$, $2s^22p^44l$, and $2s2p^54l$ ($l = s, p, d$) configurations are used in the calculations and 218 fine-structure levels are obtained using the general-purpose relativistic atomic structure package (GRASP). The results for the electric dipole, electric quadrupole, magnetic dipole, and magnetic quadrupole transitions from the levels of the $2s^22p^5$, $2s2p^6$, $2s^22p^43l$, $2s2p^53l$, and $2s^22p^44l$ ($l = s, p, d$) configurations to the levels of $2s^22p^6$ and $2s2p^6$ configurations are presented. Comparisons are made with the available experimental and the other calculations.

Keywords: energy levels, transition probabilities, oscillator strengths, F-like ions

DOI: 10.1134/S1547477119060451

INTRODUCTION

The spectra of highly ionized atoms are needed in astrophysics, laser physics, and in diagnostic of high-temperature plasmas [1]. The atomic data for the F-like ions have been studied experimentally and theoretically [1–20]. The observed and calculated wavelengths and wavenumbers of the lines of the $2s^22p^5$–$2s^22p^43s$, $2s^22p^5$–$2s^22p^43d$, and $2s2p^6$–$2s2p^53s$ transitions of the F-like ions with $21 \le Z \le 29$ have been presented [2]. The observed wavelengths of the lines of the $2s^22p^5$–$2s^22p^43d$ transitions for the F-like ions with $19 \le Z \le 27$ [4], and for the $2s^22p^5$–$2s2p^6$ transitions for ions from Ne II to Ni XX [5] have been reported.

The energy levels, wavelengths and weighted oscillator strengths for the transitions from the levels of $2s2p^6$, $2s^22p^43s$, and $2s^22p^43d$ to the levels of $2s^22p^5$ for the F-like ions with $12 \le Z \le 28$ have been calculated using the Hartree–Fock Relativistic (HFR) program [7]. The many-body perturbation theory (MBPT) approach in combined with the configuration interaction (CI) have been used in the calculation of the energy levels of $2s^22p^5$ and $2s2p^6$ configurations for the F-like ions with $Z \le 60$, by M.F. Gu [13].

The energy levels, lifetimes, and radiative rates for transitions among the lowest 113 levels of the $2s^22p^5$, $2s2p^6$, $2s^22p^43l$, $2s^23p^33l$, and $2s^63l$ ($l = s, p, d$) configurations have been calculated using the general-purpose relativistic atomic structure package (GRASP) code for 17 F-like ions with $37 \le Z \le 53$ [16], and for 19 F-like ions with $55 \le Z \le 73$ [19].

In this paper, the energy levels, lifetimes, wavelengths, transition probabilities, oscillator strengths, and line strengths are calculated for the electric dipole (E1), electric quadrupole (E2), magnetic dipole (M1), and magnetic quadrupole (M2) transitions in Ti XIV, using the general-purpose relativistic atomic structure package (GRASP).

1. CALCULATION AND RESULTS

1.1. Energy Levels and Lifetimes

The energy levels (in Ryd), lifetimes (τ in s), and the mixing coefficients for the lowest 218 levels of $2s^22p^5$, $2s2p^6$, $2s^22p^43s$, $2s^22p^43p$, $2s^22p^43d$, $2s2p^53s$, $2s2p^53p$, $2s2p^53d$, $2p^53s$, $2p^53p$, $2p^53d$, $2s^22p^44s$, $2s^22p^44p$, $2s^22p^44d$, $2s2p^54s$, $2s2p^54p$, and $2s2p^54d$ configurations in Ti XIV are calculated using the general purpose relativistic atomic structure package (GRASP) [21]. The energy levels obtained from GRASP with and without Breit and QED effects are presented in Table 1. The Breit-and QED energies (GRASP[a]) are lower than the corresponding Coulomb energies (GRASP[a]) by up to 0.05 Ryd (−0.1%), except the $2s^22p^5\ ^2P_{1/2}$ level is 0.01 Ryd (−3.3%). Furthermore, the inclusion of the Breit- and QED corrections has resulted in slightly different level orderings for 34/35, 67/68, and 94/95 levels.

Microporous and Mesoporous Materials 291 (2020) 109540

Contents lists available at ScienceDirect

Microporous and Mesoporous Materials

journal homepage: www.elsevier.com/locate/micromeso

Multifunctional curcumin-loaded mesoporous silica nanoparticles for cancer chemoprevention and therapy

Nihal S. Elbialy[a,b,*], Samia Faisal Aboushoushah[a], Balsam Fahad Sofi[b,c], Abdulwahab Noorwali[d]

[a] *Medical Physics Program, Physics Department, Faculty of Science, King Abdulaziz University, Jeddah, 21589, Saudi Arabia*
[b] *Biophysics Department, Faculty of Science, Cairo University, 12613, Giza, Egypt*
[c] *Medical Physics, Department of Physics, College of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia*
[d] *Medical School, King Abdulaziz University (KAU), Jeddah, Saudi Arabia*

ARTICLE INFO

Keywords:
Cancer
Curcumin-loaded mesoporous silica nanoparticles
Drug delivery system
Cancer chemoprevention

ABSTRACT

This study aims to synthesize smart mesoporous silica nanocarrier for curcumin (Cur) as a nutraceutical anticancer agent. Multifunctional PEG-MSNPs-Cur were synthesized to enhance curcumin bioavailability for the purpose of preventing and treating cancer. It can also serve as auto-fluorescence probe for molecular imaging (image guided therapy).

The prepared nanocarrier has been characterized using transmission electron microscope (TEM), Fourier transform infrared spectroscopy (FTIR), Dynamic light scattering (DLS) and zeta potential.

In vitro, the antitumor activity of PEG-MSNPs-Cur and Cur was investigated on two human cancer cell lines: liver cancer (HepG2) and cervical cancer (HeLa). Compared with free-Cur, PEG-MSNPs-Cur showed higher cellular uptake and significant cytotoxicity against HepG2 and HeLa cells. Furthermore, PEG-MSNPs-Cur-treated HepG2 cells exhibited marked cell cycle arrest at G2/M compared to free-Cur-treated cells.

In vivo, cancer chemoprevention and therapeutic efficacy of PEG-MSNPs-Cur as well as Cur, have been evaluated using two treatment protocols: Tumor Chemoprevention Protocol (TCP) and Tumor Reduction Protocol (TRP). The results demonstrated that TCP exhibited high therapeutic efficacy over TRP.

The toxicity of PEG-MSNPs-Cur were assessed by serum biochemical analysis and histopathological examination for certain vital body organs to address the biosafety issue of PEG-MSNPs-Cur.

The integrated results indicated that smart multifunctional MSNPs greatly enhanced curcumin bioavailability. PEG-MSNPs-Cur offered pH-triggered drug release in an acidic pH (tumor microenvironment). Additionally, PEG-MSNPs-Cur is utilized as self-fluorescence probe that allow their tracing in the cells without the need of dyes. PEG-MSNPs-Cur could be effectively used as a safe chemopreventive and therapeutic agent.

1. Introduction

Cancer is a significant healthcare problem, which is characterized by an abnormal and uncontrolled increase in cell proliferation. It is the most serious life-threatening disease worldwide [1]. According to the World Health Organization (WHO), it is expected that cancer death rates will increase to 12 million cases by 2030. Whereas, the rate of cancer diagnoses is expected to reach 24 million globally by 2035 [2].

The most conventional strategy used for cancer therapy is chemotherapy. Most cancer patients receive chemotherapy either alone or in combination with other oncological modalities. However, this approach has several limitations including the non-specific distribution of drugs in the body thus effecting both cancerous and normal cells, resulting in dose related side effects combined with low drug concentration in the tumor site [3].

As a consequence, the use of natural products, that have anticancer properties such as induction of apoptosis and inhibition of tumor growth without harming normal cells, is pressing. A natural substance that is a food or food ingredient and offers a health or medical benefit is known as a nutraceutical [4]. One of the promising nutraceutical ingredients is curcumin, it is a hydrophobic polyphenol which is derived from the turmeric spice (curcuma longa plant). Turmeric spice is a popular south Asian spice that belongs to the ginger family and its active ingredient is curcumin [5]. Through the past decades, curcumin has attracted the attention of the scientific community due to its high therapeutic potential towards cancer. Curcumin has been found to inhibit carcinogenesis [6], cause disturbances in mitosis thus leading to cell cycle arrest [7], inhibit tumor initiation and progression (invasion

* Corresponding author. Medical Physics Program, Physics Department, Faculty of Science, King Abdulaziz University, Jeddah, 21589, Saudi Arabia
E-mail addresses: mmohamad@kau.edu.sa, n_elbialy@hotmail.com (N.S. Elbialy).

https://doi.org/10.1016/j.micromeso.2019.06.002
Received 23 February 2019; Received in revised form 29 May 2019; Accepted 3 June 2019
Available online 08 June 2019

Received: 27 June 2018 | Accepted: 13 October 2018
DOI: 10.1002/maco.201810382

ARTICLE

Materials and Corrosion

High temperature corrosion of Fe-6 wt% Si steel in various atmospheres

Eva Švábenská[1] | Pavla Roupcová[1,2] | Martin Vondráček[3] | Abdel R. Lashin[4,5] | Oldřich Schneeweis[1,2]

[1] Institute of Physics of Materials of the CAS, Žižkova 22, Brno 616 00, Czech Republic
[2] CEITEC BUT, Brno, Czech Republic
[3] Institute of Physics of the CAS, Prague 182 21, Czech Republic
[4] Faculty of Applied Science, Umm Al-Qura University, Makkah 219 55, Saudi Arabia
[5] Faculty of Science, Mansoura University, Mansoura 355 16, Egypt

Correspondence
Eva Švábenská, Institute of Physics of Materials of the CAS, Žižkova 22, Brno 616 00, Czech Republic.
Email: svabenska@ipm.cz

Funding information
Ministry of Education, Youth and Sports of the Czech Republic, Grant number: LQ1601

Corrosion of Fe-6Si steel during heat treatment at 500 and 700 °C in air, argon, and vacuum was studied. Phase and structure analysis were carried out using Mössbauer spectroscopy, X-ray diffraction, scanning electron microscopy, Glow discharge optical emission spectrometry, and X-ray photoelectron spectroscopy. Measurement of magnetic hysteresis loops were used to follow changes in magnetic properties. Structure and phase composition of surface layers change in dependence on annealing conditions. Besides the content of hematite, magnetite, and fayalite an increase in silicon content at the surface was detected namely after annealing at 700 °C. Our results show that good magnetic properties of the studied Fe-6 wt% Si steel are not deteriorated substantially by annealing at 500 and 700 °C in air, argon, and vacuum. Therefore this steel can be applied in magnetic circuits working at high temperatures.

KEYWORDS
corrosion, Fe-6Si steel, magnetic properties, phase analysis, structure, surface

1 | INTRODUCTION

Silicon steels are widely used as soft magnetic materials in several applications, e.g., transformer cores, electrical engines, etc. With increasing Si content hysteresis losses at high frequencies decrease and at 6 wt% Si the alloy exhibits zero magnetostriction.[1] However, as Si content increases the material workability deteriorates. Above 7 at% Si (~3.65 wt%), the materials are too brittle to be rolled without appearing of cracks.[2] This lack of ductility has been attributed to structural decomposition into at least two phases known as B2 (Fe-Si) and DO3 (Fe_3Si).[3] Several methods for preparation material with a high Si content have been developed, such as a special thermochemical routing,[4] hot dipping process followed by diffusion annealing,[5] chemical vapor deposition,[6] or mechanical alloying.[7,8] Recently the Fe-Si steel with 6.5 wt% Si has been developed namely for electrical engines applied in electrical vehicles.[9]

Studies of the corrosion of Fe-Si alloy have been done in various atmospheres of chemical composition and pressures. Yanagihara and Yamazaki[10] annealed the samples of Fe-Si with 3 wt% Si alloy at 850 °C in 75% H_2-25% N_2. Sidor and Kovac[11] annealed Fe-Si (0.9, 1.5, and 2.4 wt% Si) alloy in N_2–H_2–H_2O atmosphere in temperature range 800–960 °C, Li et al.[12] annealed the alloy with 1, 2, 3 wt% Si in Ar-CO_2 atmosphere at 800 °C. An effect of combustion gas containing 72% N_2–17% H_2O–8% CO_2–1% O_2 applied at 1100 °C and 1200 °C were studied in Ref. [13]. Liu et al.[14] studied corrosion behaviors of 5.9 and 13 at% Si alloy in H_2-H_2S–CO_2 mixture at 700 °C. Influence of oxidation atmosphere in

energies

MDPI

Article

Concentrated Photovoltaic/Thermal Hybrid System Coupled with a Thermoelectric Generator

Abdelrahman Lashin [1,2], Mohammad Al Turkestani [1] and Mohamed Sabry [1,3,*]

[1] Physics Department, College of Applied Science, Umm Al Qura University, Makkah 21955, Saudi Arabia; aylashin@uqu.edu.sa (A.L.); mkturkestani@uqu.edu.sa (M.A.T.)
[2] Physics Department, Faculty of Science, Mansoura University, Mansoura 35516, Egypt
[3] Solar Physics Lab, National Research Institute of Astronomy and Geophysics, Cairo 11421, Egypt
* Correspondence: mmsalaheldin@uqu.edu.sa

Received: 13 May 2019; Accepted: 4 July 2019; Published: 8 July 2019

Abstract: Concentrator photovoltaic (CPV) systems have displayed an important cost reduction and in the next few years could offer a competitive cost advantage compared to that of flat plate PV systems. Such CPV systems require some cooling methods to overcome high operating temperatures, which reduces their efficiency significantly. On the other hand, thermoelectric generators (TEG) are devices that convert thermal energy directly to electrical energy, provided that there is a temperature difference between its two faces. A hybrid concentrator photovoltaic/thermal (CPV/T) system is proposed in this work. Such a system uses TEG in a two-fold manner: to passively cool down the CPV cell in order to maintain its power conversion efficiency in such high temperature conditions, and to use the accumulated thermal energy to generate electrical energy, which is added to the system's total power output. Two types of solar cells were investigated, namely, $Ga_{0.35}In_{0.65}P/Ga_{0.83}In_{0.17}As$ with efficiency an of 28% at 250X, and a Laser Grooved Buried Contact (LGBC) silicon concentrator PV cell with an efficiency of 18.3% at 40X. These cells are assumed to be coupled with two TEGs of the same type but with a different number of junctions. Experimental results showed that coupling TEG modules to a CPV system could be a useful method for enhancing the overall output power, provided that PV cells are chosen with a low efficiency temperature coefficient and high PV performance. Also, TEG modules have to be chosen with a high figure of merit. Moreover, the operating optical concentration ratio, as well as the covered area of the TEG, have to be optimized in order to maximize the total system output.

Keywords: concentrator photovoltaic; thermoelectric generator; PV/T hybrid system

1. Introduction

Photovoltaic energy conversion has already become one of the most reliable energy resources. Further reduction of the system costs is a must in order to fulfill the increasing demand for energy all over the world. In order to achieve such a cost reduction, the solar cell output power could be increased by the use of either stationary or tracking solar concentrator subsystems [1]. One disadvantage of concentrator photovoltaic systems (CPV) is that they require direct sunlight as they cannot operate effectively with diffuse radiation, meaning some sort of sun-tracking system is required, which adds to the system complexity and total cost of the operation. The operating temperature of PV cells plays an important role in determining their electrical output because part of the incident solar energy is converted into electricity while the remaining part is converted into heat [2–5]. This adds another disadvantage to using such concentrating systems because of the elevated PV cell's temperature. While the generated current of the PV cells increases slightly with temperature, the corresponding voltage decreases considerably with temperature elevation. This reduces the fill factor, output power, and electrical conversion efficiency accordingly.

Results in Physics 16 (2020) 102819

Contents lists available at ScienceDirect

Results in Physics

journal homepage: www.elsevier.com/locate/rinp

Improving the efficiency of the organic solar cell ($CuPc/C_{60}$) via PEDOT: PSS as a photoconductor layer doped by silver nanoparticles

A.M. Ali[a,b], D.A. Said[c], M. Khayyat[d], M. Boustimi[a], R. Seoudi[b,e,*]

[a] Department of Physics, College of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia
[b] Department of Physics, Faculty of Science, Mansoura University, Mansoura, Egypt
[c] Physics Department, Faculty of Women for Art, Sciences and Education, Ain Shams University, Cairo, Egypt
[d] King Abdulaziz City for Science and Technology, Riyadh 11442, Saudi Arabia
[e] Spectroscopy Department, Physics Division, NRC, Dokki, Cairo 12622, Egypt

ARTICLE INFO

Keywords:
Silver nanoparticles
Organic solar cell
Copper phthalocyanine
C_{60}
Thin film

ABSTRACT

In this work, the efficiency of organic photovoltaic cells (OPV) based on copper phthalocyanine (CuPc) as donor/fullerene (C_{60}) as an acceptor was improved via Poly(3,4-ethylene dioxythiophene):Polystyrene sulfonate (PEDOT:PSS) as (photoconductor transport layer) embedded by silver nanoparticles. Silver nanoparticles (AgNPs) were prepared using a thermochemical method. The change of the surface plasmonic band positions of AgNPs has been explained by the Un-Vis spectra. Different sizes and shapes of AgNPs have been confirmed from images of a transmission electron microscope (TEM). Thin films of PEDOT: PSS embedded by different sizes and shapes of AgNPs were made on glass/ITO using Spin Coater. The last two layers of CuPc and C_{60} were precipitated using a vacuum evaporation technique. The study of the prepared junction film using AFM showed a morphological smooth on the surface layers due to the good distribution of AgNPs. Cell efficiency of OPV was improved from 0.663 to 0.925 with increasing the particle sizes of AgNPs from 43 nm to 57 nm. The increase in V_{oc}, I_{sc}, and fill factor with increasing the particle size can be attributed to the increase in scattering light and the built-in electric field that generate due to surface plasmon resonance around AgNPs embedded in PEDOT:PSS. The scattering increases the excitons (e-h) generation and built-in electric field dissociation these excitons to e^- and h^+ and move to terminal connection and improved the cell efficiency.

Introduction

Photovoltaic cells have earned more study because they are clean, renewable, and low-cost sources [1,2]. Artificial OPV cells on organic semiconductors have achieved widespread interest in current years due to the low production costs, the facility of manufacturing, and tunable optical properties such as color and transparency [3,4]. Recently, the efficiency of converting light into electricity from OPV has been increased significantly [5,6]. Phthalocyanine has a significant advantage for carrier movement and optical properties by changing the molecular structures with different central metals. Copper phthalocyanines CuPc consists of π-conjugated and used as a hole transporting material [7,8]. Besides, CuPc has been used as active material in the OPV devices, as a donor and dominant absorbent material, so that it used in charge transport. Fullerene is performed as an acceptor in OPV because it has a high electron mobility, absorbing light, related to primary donor materials, and long exciton diffusion length [9–13]. Solar cells based on phthalocyanine/fullerene have been investigated, and the conversion efficiency was achieved [14–16]. Different constituents can be interested in the power conversion efficiency of OPV devices such as cathode and electrode, barrier layer, donor/acceptor heterojunction. ITO on a glass substrate is utilized as an anode in OPV applications due to its high optical transmittance in the visible range. Also, a top-illuminated construction with a thick Ag anode and a thin Ag single layer as the semi-transparent cathode followed with a capping layer was reported [9]. The deposition of the capping layer above the cathode increases the incidental photons into the active layer and increasing the absorption of the active substances. Also, this capping layer could be applied to improve the optical field distribution within the device. A thin layer of organic and inorganic materials is injected between the anode and the donor layer, which called anode barrier layer for enhancing charge transport in the direction between the two electrodes and to progressing the efficiency OPV. Also, the anode barrier layer uses to change the work function (WF) at the anode-donor interface. It decreases the

* Corresponding author at: Spectroscopy Department, Physics Division, NRC, Dokki, Cairo 12622, Egypt.
E-mail address: rsmawed@yahoo.com (R. Seoudi).

https://doi.org/10.1016/j.rinp.2019.102819
Received 18 September 2019; Received in revised form 16 November 2019; Accepted 17 November 2019
Available online 22 November 2019
2211-3797/

Check for updates

Article

JOURNAL OF COMPOSITE MATERIALS

Journal of Composite Materials
2019, Vol. 53(16) 2305–2314

DOI: 10.1177/0021998319826348
journals.sagepub.com/home/jcm
SAGE

The role of polyaniline and plasticizer on the development of the electrical conductivity of PHB composites

Ahmed M El-hadi[1,2], Ahmed M Abd Elbary[3] and Saleh M Alluqmani[1]

Abstract

This work is aimed to use polyaniline (PAni) as the conductive filler with a different weight percentage for the development of the electrical conductivity in poly (3-hydroxybutyrate) (PHB) to apply in the green electronic devices and biomedical application. PHB is brittle, and for this reason, it has mixed with polypropylene carbonate (PPC)/plasticizer (TEC) to improve its toughness and then mixed with PANI/CB to introduce semi-conductive biopolymer. I-V characteristics of the samples were measured and showed ohmic behaviors, and this is apparent as the temperature rises above 50°C. It observed the semiconductivity properties of all samples. It has been found that increasing in PANI concentration in PHB/PPC matrix leads to increase in the value of the AC conductivity, dielectric permittivity (ε') and dielectric loss (ε''). The AC conductivity of the PHB blends is improved from 10 to 16 $S\,cm^{-1}$ (pure PHB) to 1 $S\,cm^{-1}$ (composite 4), and this depends on the PANI concentration. These enhance in the electrical conductivity was due to the improved miscibility between all the components as shown in DSC, the single Tg, and Tm, which was supported too by SEM where PANI/CB is good dispersion in the PHB/PPC matrix.

Keywords

Poly (3-hydroxybutrate), polypropylene carbonate, biopolymer composites, DC- and AC conductivity

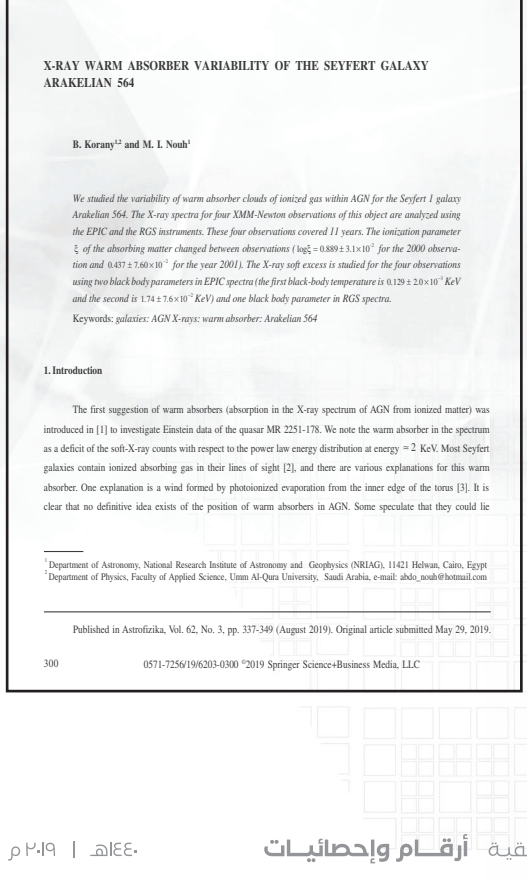
Introduction

Poly (3-hydroxybutyrate) (PHB) is produced from renewable sources like molasses (sugar beet, sugar cane) by bacteria during the fermentation and is also biodegraded by different bacteria.[1] PHB is polyester thermoplastics and can be used in many applications such as surgical sutures, drug delivery and films in food packaging. However, PHB is brittle, compared to commercial synthetic polyester polymers. Therefore, this disadvantage can be overcome in PHB by adding flexible materials like PPC and TEC to improve the elongation at break and elasticity.[1]

Carbon dioxide (CO_2) is released through human pollution by burning the plastic waste and fuel from cars. CO_2 continues to rise and is difficult to recycle, increasing the release of CO_2 into the atmosphere that leads to the global warming. Each year produces tons of CO_2 in the atmosphere and causes pollution of the environment. Interest in the use of carbon dioxide to preparer bioplastics material is increasing, because it is available and renewable. PPC is a biopolymer from carbon dioxide and propylene oxide (PO) using a catalyst.[2] The elasticity of PPC is higher than PHB, therefore we mixed it with PHB, only 20% of PPC to improve the softness and anything more than 20% will give phase transition with undesirable characteristics. It is known that most polymers are used as insulators in electricity cable, because the polymers are lightweight and low cost and easy to manufacture compared

[1]Faculty of Applied Science, Department of Physics, Umm Al-Qura University, Saudi Arabia
[2]Department of Basic Science, Higher Institute of Engineering and Technology, Egypt
[3]Department of Mathematics and Physical Science, Higher Institute of Engineering and Technology, Egypt

Corresponding author:
Ahmed M El-Hadi, Faculty of Applied Science, Department of Physics, Umm Al-Qura University, Al-Abidiyya, P.O. Box, 13174, Makkah 21955, Saudi Arabia.
Email: amabdelaziz@hotmail.com



DOI 10.1007/s10511-019-09583-6
Astrophysics, Vol. 62, No. 3, September, 2019

X-RAY WARM ABSORBER VARIABILITY OF THE SEYFERT GALAXY ARAKELIAN 564

B. Korany[1,2] and M. I. Nouh[1]

We studied the variability of warm absorber clouds of ionized gas within AGN for the Seyfert 1 galaxy Arakelian 564. The X-ray spectra for four XMM-Newton observations of this object are analyzed using the EPIC and the RGS instruments. These four observations covered 11 years. The ionization parameter ξ of the absorbing matter changed between observations ($\log\xi = 0.889 \pm 3.1\times10^{2}$ for the 2000 observation and $0.437 \pm 7.60\times10^{-2}$ for the year 2001). The X-ray soft excess is studied for the four observations using two black body parameters in EPIC spectra (the first black-body temperature is $0.129 \pm 2.0\times10^{-3}$ KeV and the second is $1.74 \pm 7.6\times10^{-2}$ KeV) and one black body parameter in RGS spectra.

Keywords: *galaxies: AGN X-rays: warm absorber: Arakelian 564*

1. Introduction

The first suggestion of warm absorbers (absorption in the X-ray spectrum of AGN from ionized matter) was introduced in [1] to investigate Einstein data of the quasar MR 2251-178. We note the warm absorber in the spectrum as a deficit of the soft-X-ray counts with respect to the power law energy distribution at energy ≈ 2 KeV. Most Seyfert galaxies contain ionized absorbing gas in their lines of sight [2], and there are various explanations for this warm absorber. One explanation is a wind formed by photoionized evaporation from the inner edge of the torus [3]. It is clear that no definitive idea exists of the position of warm absorbers in AGN. Some speculate that they could lie

[1] Department of Astronomy, National Research Institute of Astronomy and Geophysics (NRIAG), 11421 Helwan, Cairo, Egypt
[2] Department of Physics, Faculty of Applied Science, Umm Al-Qura University, Saudi Arabia, e-mail: abdo_nouh@hotmail.com

Published in Astrofizika, Vol. 62, No. 3, pp. 337-349 (August 2019). Original article submitted May 29, 2019.

 0571-7256/19/6203-0300

Heliyon 5 (2019) e02675

Contents lists available at ScienceDirect

Heliyon

journal homepage: www.heliyon.com

Heliyon

Research article

A study of the influence of plasmonic resonance of gold nanoparticle doped PEDOT: PSS on the performance of organic solar cells based on $CuPc/C_{60}$

D.A. Said[a], A.M. Ali[b,c], M.M. Khayyat[d], M. Boustimi[b], M. Loulou[b], R. Seoudi[b,e,*]

[a] Physics Department, Faculty of Women for Art, Sciences and Education, Ain Shams University, Cairo, Egypt
[b] Department of Physics, College of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia
[c] Department of Physics, Faculty of Science, Mansoura University, Mansoura, Egypt
[d] King Abdulaziz City for Science and Technology, Riyadh 11442, Kingdom of Saudi Arabia
[e] Spectroscopy Department, Physics Division, NRC, Dokki, Cairo 12622, Egypt

ARTICLE INFO

Keywords:
Materials science
Materials chemistry
Copper phthalocyanine
Gold nanoparticles
Fullerene
Solar cell
PEDOT:PSS

ABSTRACT

This work studied the role of gold nanoparticles (AuNPs) with different spherical sizes mixed with poly (3, 4-ethylene dioxythiophene): polystyrene sulfonate (PEDOT: PSS) as a hole transfer layer to enhance the efficiency (ITO/PEDOT:PSS (AuNPs)/$CuPc/C_{60}$/Al) organic photovoltaic cell (OPV). AuNPs were synthesized using the thermochemical method and the results of the transmission electron microscope (TEM) images showed that the gold nanoparticles mostly dominated by spherical shapes and sizes were calculated in the range (12–23 nm). Measurements of UV-VIS spectra for AuNPs have shown that the surface plasmon resonance shifted to a higher wavelength with decreasing the particle size. Surface morphology and absorption spectra of OPV cells were studied using atomic force microscope and UV-VIS spectrometer techniques. The efficiency of the OPV cell was calculated without and with AuNPs. Efficiency was increased from 0.78% to 1.02% due to the embedded of AuNPs with (12 nm) in PEDOT/PSS. The increase in the light absorption in CuPc is due to the good transparent conducting of PEDOT:PSS and the increase in the electric field around AuNPs embedded in PEDOT:PSS and inbuilt electric field at the interfacial between CuPc and C_{60} is due to the surface plasmon resonance of AuNPs. The increase in these two factors increase the exciton generation in CuPc, dissociation at the interfacial layer, and charge carrier transfer which increases the collection of electrons and holes at cathode and anode.

1. Introduction

Gold nanoparticles prepared in the range (1–100 nm) have distinct optical and physical properties depending on their size and shape [1, 2, 3]. The characteristic optical properties are due to the absorbance and scattering of incident light at Localized Surface Plasmon Resonance (LSPR). The LSPR is the collective oscillation of electrons in the conduction band in resonance with the incident-specific wavelength [4]. The band absorbance of LSPR increases with increased particle size. Colloidal gold nanoparticles are synthesized by reduction of citrate [5, 6, 7, 8]. In reduction methods, the particle sizes and shapes can be controlled by changing the reaction temperature or the concentration of the reducing agent [9, 10, 11, 12]. More recently, gold nanoparticles have been used in technological applications such as organic photovoltaic cells [13, 14]. Organic semiconductor solar cells have gained widespread attention in recent years due to low production costs, ease of fabrication, flexibility and tunable optical properties. Furthermore, phthalocyanine (Pc) as an organic semiconductor has been widely used as attractive materials for photovoltaic cells [15, 16]. Copper phthalocyanine (CuPc) is one of the most important organic molecules useful for thin organic solar cells [17, 18]. Organic solar cells (OSCs) are suitable for solar light harvesting due to both properties and preparation process. Transparent conductive films (TCF) are materials that must fulfill the requirements of high conductivity and high optical transparency for use in various applications of solar cell device as an anode. Graphene [19], conductive polymer [20], metal nanowires [21], aluminum zinc oxide [22], metal nanostructures consisting of nanowires, nanogrid, nanofibres [23], and carbon nanotubes (CNT) [24, 25] have been applied as transparent conducting films (TCF). Chukaroun et. al. made three-layer anodes of ITO/Au/ITO in $CuPc/C_{60}$ photovoltaic cells to achieve low resistivity of the anode and to improve the fill factor and efficiency [26]. It can be replaced ITO by PEDOT:PSS as a front electrode in organic solar cells because of its high

* Corresponding author.
E-mail address: rsmawed@yahoo.com (R. Seoudi).

https://doi.org/10.1016/j.heliyon.2019.e02675
Received 18 April 2019; Received in revised form 18 August 2019; Accepted 14 October 2019
2405-8440/

Journal of
NUCLEAR
Technology in Applied Science

Examination of Quality Control Parameters in some Diagnostic X-ray Units

ABSTRACT

CAMBRIDGE
INTERNATIONAL ACADEMICS

Journal of
NUCLEAR
Technology in Applied Science
ISSN 2314-8209 e-ISSN 2314-8217

J. Nucl. Tech. Appl. Sci., Vol. 7, No. 14, (2019)

Examination of Quality Control Parameters in some Diagnostic X-ray Units

Alfawwal, T.M.[1,2]; Kuthi, R.A[3]

Received: 14/05/2019
Accepted: 03/07/2019

E-mail: tahaalfawwal@hotmail.com

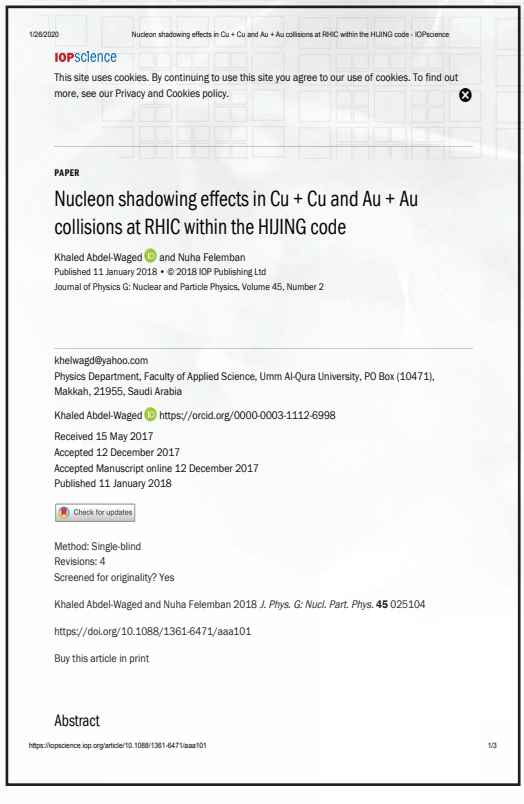
ABSTRACT

Periodical performance of quality control in diagnostic x-ray machines is important to provide minimum dose delivered to patients and high image quality. The current study is aimed to assure the quality control of conventional X-ray machines over some Makkah city hospitals according to quality control protocol and the measured parameters values are compared to the international acceptance limits. Some factors affecting on quality assurance of conventional X-ray machines such as reproducibility of time, applied high voltage, kilo-voltage accuracy, time accuracy, linearity and half value layer of X-ray machines over four hospitals in Makkah city are investigated. These parameters are measured by using the RaySafe solid-state detector connected with suitable ionization chambers located at 100 cm source to image detector. Time Reproducibility ranged from 0.05% to 0.07% and high voltage reproducibility ranged from 0.09% to 0.14 %. Kilo-voltage accuracy ranged from 0.22 to 3.5 % and time accuracy ranged from 0.02 to 4.1% respectively. Coefficients of linearity of diagnostic X-ray units in four hospitals in KSA were 0.02, 0.004, 0.02 and 0.24. This study concluded that quality control examinations are within the tolerance limit of the American Association of Physicist in Medicine, *"(AAPM)"*. It assists in the optimization of a dose delivered to patients.

KEYWORDS

Quality Control, Reproducibility, Accuracy, Linearity and Diagnostic X-ray, RaySafe.

1. Physics Department, Faculty of Applied Sciences, Umm Al-Qura University, KSA, P. Box 21955.
2. Radiation Protection Department, Nuclear Research Center, Atomic Energy Authority, Cairo. P.O.13759, Egypt.
3. The radiology department in KAMC-Jeddah, Department of Medical Physics.



IOPscience

PAPER

Nucleon shadowing effects in Cu + Cu and Au + Au collisions at RHIC within the HIJING code

Khaled Abdel-Waged and Nuha Felemban

Published 11 January 2018 • © 2018 IOP Publishing Ltd
Journal of Physics G: Nuclear and Particle Physics, Volume 45, Number 2

khelwagd@yahoo.com
Physics Department, Faculty of Applied Science, Umm Al-Qura University, PO Box (10471), Makkah, 21955, Saudi Arabia

Khaled Abdel-Waged https://orcid.org/0000-0003-1112-6998

Received 15 May 2017
Accepted 12 December 2017
Accepted Manuscript online 12 December 2017
Published 11 January 2018

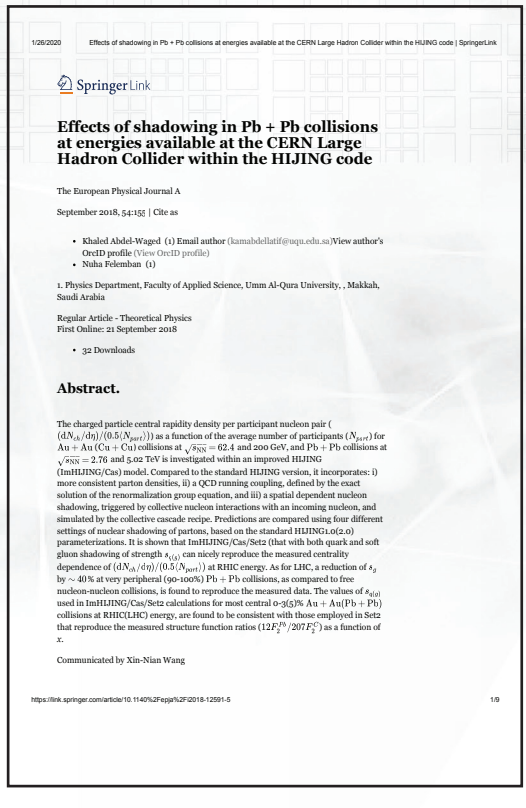
Check for updates

Method: Single-blind
Revisions: 4
Screened for originality? Yes

Khaled Abdel-Waged and Nuha Felemban 2018 *J. Phys. G: Nucl. Part. Phys.* **45** 025104

https://doi.org/10.1088/1361-6471/aaa101

Abstract



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Effects of shadowing in Pb + Pb collisions at energies available at the CERN Large Hadron Collider within the HIJING code

The European Physical Journal A

September 2018, 54:155 | Cite as

- Khaled Abdel-Waged (1) Email author (kamabdellatif@uqu.edu.sa)View author's OrcID profile (View OrcID profile)
- Nuha Felemban (1)

1. Physics Department, Faculty of Applied Science, Umm Al-Qura University, , Makkah, Saudi Arabia

Regular Article - Theoretical Physics
First Online: 21 September 2018

Abstract.

The charged particle central rapidity density per participant nucleon pair ($(dN_{ch}/d\eta)/(0.5\langle N_{part}\rangle)$) as a function of the average number of participants (N_{part}) for Au + Au (Cu + Cu) collisions at $\sqrt{s_{NN}} = 62.4$ and 200 GeV, and Pb + Pb collisions at $\sqrt{s_{NN}} = 2.76$ and 5.02 TeV is investigated within an improved HIJING (ImHIJING/Cas) model. Compared to the standard HIJING version, it incorporates: i) more consistent parton densities, ii) a QCD running coupling, defined by the exact solution of the renormalization group equation, and iii) a spatial dependent nucleon shadowing, triggered by collective nucleon interactions with an incoming nucleon, and simulated by the collective cascade recipe. Predictions are compared using four different settings of nuclear shadowing of partons, based on the standard HIJING1.0(2.0) parameterizations. It is shown that ImHIJING/Cas/Set2 (that with both quark and soft gluon shadowing of strength $s_{A(g)}$ can nicely reproduce the measured centrality dependence of $(dN_{ch}/d\eta)/(0.5\langle N_{part}\rangle)$ at RHIC energy. As for LHC, a reduction of s_g by $\sim 40\%$ at very peripheral (90-100%) Pb + Pb collisions, as compared to free nucleon-nucleon collisions, is found to reproduce the measured data. The values of $s_{A(g)}$ used in ImHIJING/Cas/Set2 calculations for most central 0-3(5)% Au + Au(Pb + Pb) collisions at RHIC(LHC) energy, are found to be consistent with those employed in Set2 that reproduce the measured structure function ratios $(12F_2^{Fe}/207F_2^{Pb})$ as a function of x.

Communicated by Xin-Nian Wang

IOP Publishing Mater. Res. Express 6 (2019) 055103 https://doi.org/10.1088/2053-1591/ab0598

Materials Research Express

PAPER

Study of electrical and dielectric properties of palladium-phthalocyanine (PdPc) in pellet form

RECEIVED 13 November 2018
REVISED 27 January 2019
ACCEPTED FOR PUBLICATION 8 February 2019
PUBLISHED 15 February 2019

A Timoumi[1,2], N Bouguila[1], J Koaib[3], M K Al Turkestani[3] and B Jamoussi[4]

[1] Department of Physics, Faculty of Applied Science, Umm AL-Qura University, 21955 Makkah, Saudi Arabia
[2] LPMS, National Engineering School of Tunis, Belvedere, PO Box 37, 1002 Tunis, Tunisia
[3] Laboratoire de Physique des Matériaux et des Nanomatériaux appliquée à l'environnement, Université de Gabès, Faculté des Sciences, Cité Erriadh, Zrig 6072 Gabes, Tunisia
[4] Laboratoire de Chimie Organique et Analytique, ISEFC, 2000 Bardo, Tunisia

E-mail: timoumiabdelmajid@yahoo.fr

Keywords: palladium phthalocyanine, dielectric response, pellets, photovoltaic

Abstract

A pressed pellet of palladium phthalocyanine (PdPc) was characterized by impedance spectroscopy. The dielectric properties were investigated in a wide frequency (10^2–10^6 Hz) and temperature (300–440 K) ranges. The values of activation energy, the relaxation time, and the critical frequency were closed to each other, indicating that the same type of charge carriers is responsible for electrical conduction and relaxation phenomenon in the samples. According to the values of the frequency exponent *s* and the conductivity, the conduction mechanism was determined for both the as prepared and annealed films. The *AC* conductance obeyed Jonscher's universal power law, and the conduction mechanism was interpreted by the overlapping large polaron tunneling (OLPT) process. Thus, a significant correlation was established between the temperature and activation energy. A metal semiconductor transition of this material was observed at 440 K. The obtained results demonstrate the potential of this material for photovoltaic applications.

1. Introduction

Recently, many research groups from all over the world have focused on studying the various properties of organic semiconductor thin films, in the bulk material or pellet forms. Metal-free and /or metal-substituted phthalocyanine systems are examples of such compounds. Phthalocyanines (Pcs) are aromatic and chemically stable compounds with semiconducting properties, which make them suitable for use in various applications, such as photovoltaic devices, chemical sensors, gas sensors, catalysis, and solar cells [1–9]. They are characterized by a high symmetry, planarity, electron delocalization, and thermal as well as chemical stability, depending on the crystalline structure of the material [10, 11]. Enhancement of the electrical conductivity of phthalocyanines by divalent metal ion complexation is a well-known phenomenon. Therefore, significant attention has been devoted to studying the electrical and optical properties of phthalocyanine and its derivatives. The electrical conductivity and dielectric relaxation process in these compounds play an important role in the suitability of the material for particular device applications. Thus far, only a few studies have reported on the dielectric properties of Pcs. [12, 13]. Dielectric relaxation studies are important to understand the nature and the origin of dielectric losses, which in turn could be useful in the determination of the structure and defects in solids [14]. In a previous work, thin films of palladium (II) phthalocyanine and its derivatives were synthesized and characterized [15].

In this study, some *AC* electrical properties and the dielectric response of a palladium phthalocyanine compound in the pellet form are investigated and analyzed over a range of temperatures (300–440 K) and frequencies (10^2–10^6 Hz) by impedance spectroscopy. The results are analyzed and discussed based on various theoretical models.

Journal of Computational and Theoretical Nanoscience Vol. 16, 1–5, 2019

Effect of Gamma Irradiation on Physical Properties of Spray Deposited SnO_2-F Thin Films

H. Al-Ghamdi[1, *], Shatha A. Aldaghfag[1], J. Bouslimi[2], and J. Ouerfelli[3]

[1]Department of Physics, College of Science, Princess Nourah Bint Abdulrahman University, Saudi Arabia
[2]Department of Physics, College of Science, Taif University, Saudi Arabia
[3]Department of Physics, College of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia

In this study, tin oxide thin films doped Fluor SnO_2-F were deposited on glass substrate by spray pyrolysis, for promoting the sensitivity of the films. The structural, optical and electrical properties of thin films before and after γ-irradiation using ^{60}Co G-ray source (0 to 100 kGy) have been reported. The X-ray diffraction and AFM microscopy analysis revealed that the films before irradiation were polycrystalline with crystallite size of 41 nm and increase with increasing of gamma radiation dose, but dislocation density and micro strain decrease, and the sensible roughness to irradiation dose. UV-VIS Spectroscopy revealed that the transmittance at wavelength 1400 nm decreases as the doses increases and also the optical band gap from 3.91 eV to 2.7 eV. The electrical properties from *I–V* characteristics showed a change on conductivity decrease in resistance with the increase irradiation dose. The changes in the conductivity and optical band gap, shows that SnO_2-F thin films are sensitive to gamma irradiation and it can be used for dosimetric applications and as gamma sensor.

Keywords: Gamma Irradiation, Thin Films, SnO_2-F.

RESEARCH ARTICLE

1. INTRODUCTION

Metal oxide semiconductors have been the topic of intensive research due to their wide range of applications. Among these materials, tin oxide thin films, it is considered as very interesting metal oxides because of their electrical and optical properties, SnO_2 is an n-type material with direct band gap, around 3.6 eV, it have a exciton binding energy (130 MeV) and carrier mobility (250 cm^2/VS).[1–9] Tin oxide (SnO_2) thin films as transparent conductive oxide TCO, is considered as important material, it used in different applications areas: touch screens, thin-film transistors, sensors, wide gap windows, electro luminescent windows, nuclear technology, etc.[10–11] SnO_2 thin films are synthesized by a different techniques such as thermal evaporation,[12] oxidation of tin film, Molecular Beam Epitaxial MBE, chemical deposition, sputtering Radio Frequency RF, by sol gel and spray pyrolysis.[13–19] Several efforts have been devoted to study the γ-irradiation effect on different metal oxide and metal oxide structure thin films.[20–23] but The efforts to study of effect of G-irradiation on optical, electrical and magnetic properties of tin oxide thin film rest limited. Senthil and Sudha, have studied the influence of Gamma irradiation on tin oxide thin films in the range of 0–150 Gy_t for dosimetric applications and irradiation sensors.[22, 23] The electrical measurement shows the films have a low electrical conductivity and low sensitivity.

In this paper, the ^{60}Co γ-irradiation effect of on SnO_2-F layer prepared by spray pyrolysis has been studied (morphology, optical and electrical properties). The prepared thin films, fluorine doped tin oxide with optimum percentage doping have highest electrical conductivity $\sigma = 1.71 \times 10^3$ Scm^{-1}, and studied before and after γ-radiation irradiation. The present results show improvement in the sensitivity due to fluorine doping.

2. EXPERIMENTAL DETAILS

Thin films of tin oxide SnO_2 are deposited by Spray method. The preparation of the solution is based on anhydrous $SnCl_4$ as a precursor, first dissolved in methanol, to which is added an amount of NH_4F dissolved in deionized distilled water (DDW) in order to obtain a crystalline solution.[8] The solution will be in the following proportions: 970 ml of methanol are combined with 23 ml of $SnCl_4$ and 5.5 g of NH_4F dissolved in 7.5 ml of water, which corresponds to an approximate doping of 9% optimized for minimum sheet resistance (R_s). The sheet

*Author to whom correspondence should be addressed.

Journal of Superconductivity and Novel Magnetism
https://doi.org/10.1007/s10948-019-5099-z

ORIGINAL PAPER

Photonic Band Gap Properties of One-dimensional Generalized Fibonacci Photonic Quasicrystal Containing Superconductor Material

Y. Trabelsi[1,2] · N. Ben Ali[2,3] · W. Belhadj[4] · M. Kanzari[2]

Received: 7 February 2019 / Accepted: 1 April 2019

Abstract

In this work, we theoretically investigate the transmission properties of one-dimensional (1D) Fibonacci photonic quasicrystal (PQC) by using the transfer matrix modeling (TMM) method. The PQC structure is composed of alternated layers of isotropic dielectric (SiO_2) and a high-T_c superconductor (YBCO). Frequency-dependent dispersion formula according to the two-fluid Gorter–Casimir theory has been adopted to describe the optical response of the superconducting material. Within the framework of the TMM method, we studied the effect of many parameters such as the thicknesses of the dielectric and superconductor layers, Fibonacci lattice parameters, and the operating temperature on the transmission behaviors of the PQC structure. Our numerical results reveal the transmission cutoff frequency can be tuned efficiently by the operating temperature as well as by the thicknesses of the constituent materials. We found that increasing the temperature and the angle of incidence, maintaining materials thicknesses constant, there is a shift of the cutoff frequency to lower frequency values. Nevertheless, this cutoff frequency is shifted to higher values with increasing the superconductor layer thickness. Moreover, we found that the width and the number of the photonic bandgaps can be controlled by order of Fibonacci sequence. Our results are promising for the design of tunable filtering devices.

Keywords Photonic band gap (PBG) · Fibonacci photonic quasicrystal (PQC) · Superconductor · Transfer matrix method (TMM) · Stop filter

1 Introduction

Photonic crystals (PCs) are a new type of optical materials having a periodic refractive index in one or more directions of the space that have been proposed to control the propagation of electromagnetic waves [1–3]. These materials provide the ability to prevent or allow, in certain frequency ranges, the propagation of light in one or more directions and/or the location of the light at other frequencies. PCs, also, called photonic band gap (PBG) materials, have attracted a lot of attention in recent years due to their remarkable features and the possibility to be used in several applications such as waveguides (PCWs), fibers (PCFs), low threshold lasers, phase retarders, and filters [4–8]. Photonic quasicrystals (PQCs) are a new field of PBG materials that are simply generated by quasiperiodic sequences such as Fibonacci, Thue Morse, Rudin Shapiro, and Cantor [9–15]. One-dimensional PQC is the simplest form of quasicrystal class generated by a recurrence rule of quasiperiodic sequence named "deterministic aperiodic" structure. Furthermore, this intermediate class which is between periodic and random structure exhibits the properties of self-similarity, long-range order, and lack translational symmetry. This kind of quasiperiodic multilayers structures generates various PBGs in which the propagation of electromagnetic waves is prohibited. These photonic quasicrystals have been widely used in various modern applications like optical filters, high reflector, and optical switches [16–18].

Recently, the introduction of dispersive materials, such as semiconductors, metals, plasma, and superconductors in a PBG material has attracted much attention because of their peculiar optical characteristics [19–21]. Actually, the optical

✉ W. Belhadj
wbelhadj@uqu.edu.sa

[1] College of Arts and Sciences in Mahayel Aseer, Physics Department, King Khaled University, Abha, Saudi Arabia
[2] Photovoltaic and Semiconductor Materials Laboratory, University of Tunis El. Manar, PO. Box 37, Belvedere, 1002 Tunis, Tunisia
[3] College of Engineering of Hail, Industrial Engineering Department, University of Hail, 2440 Hail City, Saudi Arabia
[4] Faculty of Applied Sciences, Department of Physics, Umm Al-Qura University, Makkah, Saudi Arabia

Published online: 02 May 2019

International Journal of New Technology and Research (IJNTR)
ISSN: 2454-4116, Volume-5, Issue-12, December 2019 Pages 31-34

Cardiac Phantom for Gated Single Photon Emission Computed Tomography (GSPECT)

R. A. Hassan, S.H.A. Al Lehyani

***Abstract*—Gated single-photon emission computed tomography (GSPECT) is the most important technique for the heart imaging, but the patients instability and the physiological cardiac function variability make studies difficult to evaluation and comparing different imaging techniques. So, a dynamic cardiac phantom (DCP) was constructed at our nuclear medicine unit-National cancer institute, which can be used as a reference to compare the reconstructed volumes & ejection fractions for GSPECT. GSPECT data were acquired using the DCP with a standard dual-head gamma camera, and the reconstructions were carried out using the Mirage software released by Segami. The validity of DCP for GSPECT imaging was evaluated by imaging of 12 different volumes of the phantom. Linear regression analysis was performed to assess the correlation between the real versus the measured volumes & ejection fractions for all the 12 different volumes. Then we assessed the correlation between real EF and the GSPECT-quantified EF for some acquisition parameters as frame/cycle (8 versus 16), and time/projection (40 versus 20 sec). Results obtained in our study showed that the constructed DCP is suitable to GSPECT imaging. Also, the study shown that in the case of acquisition parameters it's enough to using the 8 frames per cardiac cycle with 40 sec time per projection.**

***Index Terms*—Gated, SPECT, cardiac, phantom**

I. INTRODUCTION

The human heart is a 3-D organ with a complex shape and a periodic motion. For a correct evaluation of systolic function, a 4-D reconstruction (3-D volumes as a function of time) seems to be necessary. However, no reference method currently exists for cardiac volume reconstruction; doubtless because of the intrinsic complexity and the recent nature of all multidimensional imaging techniques of the heart. Most of the studies carried out compared two or more modalities: for example, echocardiography vs. gated single-photon emission computed tomography, SPECT (Nichols et al. 2000), 3-D echocardiography vs. nuclear magnetic resonance, NMR (Chuang et al. 2000; Bauer et al. 2001) or vs. Isotopic entriculography (Nosir et al. 1998) or nuclear medicine vs. angiography (Yamazaki et al. 1997).

Results sometimes pointed out differences of volume quantification, but it is often difficult to select one method in preference to another, without an accepted standard. Calibration of methods using a beating cardiac phantom, with known parameters, is an appropriate response to these difficulties, and a necessity before clinical evaluation.

Ramadan Ali Hassan Ali, Physics Department, Faculty of Applied Science, Umm Al-Qura University, Makkha, Saudi Arabia
Saud Hamid Ahmad Al Lehyani, Physics Department, Faculty of Applied Science, Umm Al-Qura University, Makkha, Saudi Arabia.

Many studies have been done on cardiac volume measurement to determine the accuracy and reliability with different modalities (Lowe et al. 1993; Reicheck 1987; Hosland-Carlsen et al. 1984). They were tested mainly on animal or human models (Byrd et al. 1989) (ventricular mass and volume determined postmortem) and sometimes on static phantoms of different materials (Aakhus et al. 1994). Physiological cardiac rhythm and systolic function variability make studies difficult in living subjects. Similarly, static phantoms are very restrictive. Studies on isolated beating hearts have been carried out with US imaging (Smith et al. 1995) but cannot be realized with gated SPECT because the exam depends on radioisotope uptake by a living cell.

II. MATERIALS AND METHODS

A.MATERIALS:

Dynamic cardiac phantom (DCP) (Fig. 1) was constructed in our nuclear medicine unit to studying the heart quantification by Gated single photon emission computed tomography (GSPECT). It was made from a mechanical pump system, which was connected to an ellipsoidal model of left ventricle made from rubber balloon and surrounded by a thorax phantom. At this time, no right ventricle is available to allow two-chamber examinations. Ventricular filling and emptying were achieved by mans of a noncircular motor motion on a reservoir, which withdrew/ added water from/ into the balloon, yielding a sinusoidal filling and emptying pattern. To simulate the ventricular wall, the balloon coated with a mixture of glue and 99mTc, it composes using 5 ml glue add with 99mTc (0.025 mCi/ ml3) and shake the solution to be homogenous, then we coated the cardiac balloon with it. 20 min later we coated the balloon with another layer of free glue (without 99mTc) to prevent the chest phantom contamination, it leaved about 30 min to dry, then we installed the DCP in the thorax phantom replacing the static cardiac phantom of Data-Spectrum, Chapel Hill, NC.

The pump rate was controlled such that we obtained constant heart rate of about 65 beats. min^{-1}. An electrical contact generated a voltage peak when the pump reached its outermost position (end-diastolic (ED) volume of the ventricular cavity) to simulate the patient's electrocardiogram (ECG) trigger. A fixed 33.8 ml3 stroke volume is applied for each ejection fraction, but systolic volume is adjustable, starting from a volume of 22.5 ml3. The diastolic volume was varied from 56.3 to 96.9 ml3, and the systolic volume from 22.5 to 63.4 ml3, using steps of 3.75 ml3, the corresponding ejection fraction varying from 60% (a value close to the mean normal value) to 34% (pathologic cases). Twelve precisely

العلوم الرياضية

أولا: الأبحاث المنشورة بقسم العلوم الرياضية :

م	عنوان البحث	المشاركين	المجلة	دار النشر	ISI/ NON-ISI	معامل التأثير IF
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-	-	Mathematics Subject Classification	Carpathian Math. Publ.	PIRZADA S, GANIE H A, ALGHAMDI A M	ON THE SUM OF SIGNLESS LAPLACIAN SPECTRA OF GRAPHS	11
-	-	House of Rzesz´ow University of Technology	J o u r n a l of Mathematics and Applications	Alahmari, M. Mabrouk, M- A. Taoudi	Fixed Point Theorems for Monotone Mappings in Ordered Banach Spaces Under Weak Topology Features	12
1.51	ISI	Springer	Advances in Difference Equations	Mohammed Fathy Elettreby, Elsayed Ahmed, Muntaser Safan	A simple mathematical model for Guillain–Barré syndrome	13
1.31	ISI	Aimspree	Mathematical Biosciences and Engineering	Muntaser Safan	Mathematical analysis of an SIR respiratory infection model with sex and gender disparity: special reference to influenza A	14
-	-	HIKARI Ltd	Applied Mathematical Sciences	Wajdi Kallel, Amel Hatem	Stability of Perturbed Switched Systems	15
0.32	ISI	Techscience	Fluid Dynamics & Materials Processing	Najat A. Alghamdi, Hamdy M. Youssef	On the Application of the Adomian's Decomposition Method to a Generalized Thermoelastic Infinite Medium with a Spherical Cavity in the Framework Three Different Models	16
0,32	ISI	Techsci ence	Fluid Dynamics & Materials Processing	Najat A. Alghamdi and Hamdy M. Youssef	On the Application of the Adomian's Decomposition Method to a Generalized Thermoelastic Infinite Medium with a Spherical Cavity in the Framework Three Different Models	17
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-	ISI	Springer	International Journal of Applied and Computational Mathematics	Mohamed Safaa Mohamed Osman (M.S. Osman)	Jacobi elliptic function expansion method for solving KdV equation with conformable derivative and dual-power law nonlinearity	21
-	ISI	Springer	Journal of the Egyptian Mathematical Society	Tahani A. Abushal	Bayesian Estimation of the Reliability Characteristic of Shanker Distribution,	22
2.44	ISI	American Physical Society	Physical Review Fluids	Bakhsh, A and Samtaney, Ravi	Incompressible models of magnetohydrodynamic Richtmyer-Meshkov instability in cylindrical geometry	23
0.50	ISI	Tylor and Francis	Communications in Statistics - Simulation and Computation	Doaa Basalamah, Khamis K. Said, Wei Ning & Yubin Tian	Modified information criterion for linear regression change-point model with its applications	24
0.74	ISI	Springer	Complex Analysis and Operator Theory	Bourhim and M. Mabrouk	Maps Preserving the Numerical Radius Distance Between C* -Algebras	25

ثانيا: المشاريع الممولة من عمادة البحث العلمي ومدينة الملك عبدالعزيز للعلوم والتقنية بقسم العلوم الرياضية :

	Projects	Researcher	Fund
1	Propagation of Thermoelastic Waves on Skin Tissue	د. نجاة عتيق الغامدي	الخطة الوطنية الشاملة طويلة الاجل للعلوم والتكنولوجيا والابتكار مدينة الملك عبد العزيز للعلوم والتقنية 500,000 SR
2	Stability of Perturbed Systems	د. وجدي فتحي القلال	Deanship of Scientific Research 93000 SR
3	Propagation of thermoelastic waves on skin tissue	د. نجاة عتيق الغامدي	وحدة العلوم والتقنية بجامعه ام القرى الخطة الوطنية الشاملة طويلة الأجل للعلوم والتكنولوجيا والابتكار SR 500000


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العلوم الرياضية
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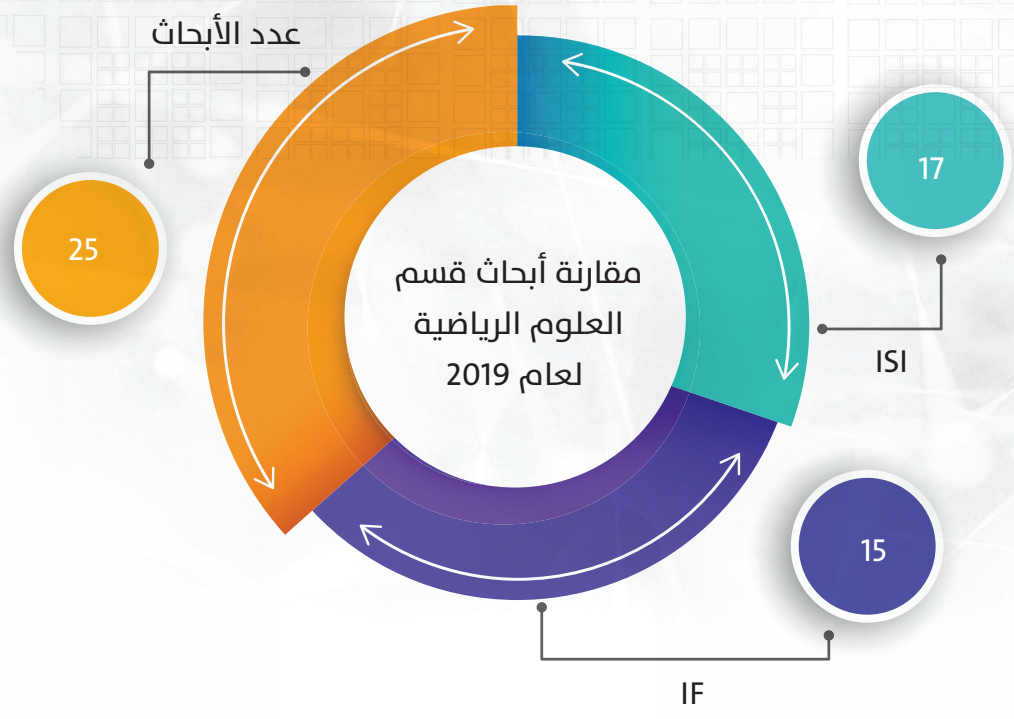
المشاريع الممولة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ملخصات الأوراق العلمية المنشورة بقسم العلوم الرياضية :

Applied Mathematics & Information Sciences 3(1) (2009), 59–77
– An International Journal

Benard Convection in a Horizontal Porous Layer Permeated by a Non-Linear Magnetic Fluid under the Influence of Both Magnetic Field and Coriolis Forces

F. M. Allehiany and A. A. Abdullah
Department of Mathematical Sciences, Faculty of Applied Sciences,
Umm Al-Qura University, Makkah, Saudi Arabia
Email Address: abdullah@uqu.edu.sa
Received May 1, 2007; Revised January 30, 2008

This work examines the Benard convection of an infinite horizontal layer occupied by a porous medium permeated by an incompressible, thermally and electrically conducting viscous fluid heated from below when subjected to both uniform vertical magnetic field and Coriolis forces. A model proposed by P. H. Roberts (1981) in the context of neutron stars is used. We show that the nonlinearity in this model has no effect on the development of instabilities through the mechanism of stationary convection which is the preferred process in terrestrial applications. However, in non-terrestrial applications the non-linearity influences the onset of overstable convection and overstability is the preferred mechanism. Some numerical results are presented for the overstability case when both boundaries are free and rigid.

Keywords: Benard convection, linear stability, porous medium, stationary instability, overstable convection.

1 Introduction

Thermal instability theory has attracted considerable interest and has been recognized as a problem of fundamental importance in many fields of fluid dynamics. The earliest experiments to demonstrate the onset of thermal instability in fluids are attributed to Benard (1900, 1901). Rayleigh (1916) provided a theoretical basis for Benard's experimental results.

Thermal instability theory has been enlarged by the interest in hydrodynamic flows of electrically conducting fluids in the presence of magnetic field. The presence of such fields in an electrically conducting fluid usually has the effect of inhibiting the development of

Advances in Mechanical Engineering

Research Article

Advances in Mechanical Engineering 2019, Vol. 11(11) 1–8
© The Author(s) 2019
DOI: 10.1177/1687814019889480
journals.sagepub.com/home/ade
SAGE

Vibration of circular micro-ceramic (Si_3N_4) plate resonators in the context of the generalized viscothermoelastic dual-phase-lagging theory

Najat A Alghamdi

Abstract
In this article, the analysis and numerical results are represented for the thermoelastic of an isotropic homogeneous, thermally conducting, Kelvin–Voigt-type circular micro-plate in the context of Kirchhoff's Love plate theory of generalized viscothermoelasticity based on the dual-phase-lagging model. The governing equations are obtained for the generalized dual-phase-lagging model and coupled viscothermoelastic plates. The scaled viscothermoelasticity has been illustrated in the case of the circular plate and the axisymmetric circular plate for an aspect ratio for clamped boundary conditions. Laplace transform has been applied, and its inversions have been calculated numerically by using the Tzou method. The results have been carried out for the ceramic (Si_3N_4). It is noted that the temperature increment and lateral deflection are significantly affected by the time, the width, the thickness, and the mechanical relaxation times of the material.

Keywords
Viscothermoelasticity, dual-phase-lag, relaxation times, circular micro-ceramic

Date received: 5 September 2019; accepted: 16 October 2019

Handling Editor: Mario L Ferrari

Introduction

Heat conduction has been studied using mathematical models such as dual-phase lag (DPL), which was proposed by Tzou.[1,2] The temperature gradient and heat flux were established by this model. Many scientists used this model in heat transfer problems,[3] physical systems,[4–8] and thermoelastic damping vibration.[9,10] Guo et al.[11,12] used the DPL model to analyze the thermoelastic damping theory of micro- and nanomechanical resonators; then, he investigated the dissipation in the circular micro-plate resonator.

The circular plate is a common structural in many micro-and nano-electromechanical resonators. Hao[13] adopted an analytical study to analyze thermoelastic damping in vibrations of micro- and nano-electromechanical circular thin-plate resonators. Sun and Tohmyoh[14] studied thermoelastic damping on axisymmetric out-of-plane vibration of circular plate resonators. Sun and Saka[15] investigated the thermoelastic damping effects on the out-of-plane vibration of circular plate resonators. They added a factor in their formula of thermoelastic damping $K = (1 + v)/(1 - 2v)$, which is different from that of Lifshitz and Roukes,[16] in which v is Poisson's ratio. Li et al.[17] employed an analytical study to analyze thermoelastic damping in

Department of Mathematics, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia

Corresponding author:
Najat A Alghamdi, Department of Mathematics, Faculty of Applied Science, Umm Al-Qura University, Makkah 24235, Saudi Arabia.
Email: najaalghamdi@gmail.com

THERMOSOLUTAL INSTABILITY IN A HORIZONTAL FLUID LAYER AFFECTED BY ROTATION

by

Abdullah Ahmad ABDULLAH[a], Sultana Dafer AL-AHMARI[a], and Ali J. CHAMKHA[b,c]*

[a] Department of Mathematical Sciences, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia
[b] Mechanical Engineering Department, Prince Sultan Endowment for Energy and Environment, Prince Mohammad Bin Fahd University, Al-Khobar, Saudi Arabia
[c] RAK Research and Innovation Center, American University of Ras Al Khaimah, Ras Al Khaimah, United Arab Emirates

Original scientific paper
https://doi.org/10.2298/TSCI171203093A

Thermosolutal convective instability in a horizontal layer affected by rotation is studied. Stationary convection and over-stability cases are considered for different boundary conditions. Analytical solutions were obtained when both boundaries are free and numerical results were obtained for the cases of free and rigid boundaries. The numerical computations of this problem were performed using the method of expansion of Chebyshev polynomials. This method is better suited to the solution of hydrodynamic stability problems than expansions in other sets of orthogonal polynomials. This method not only has high accuracy but also allows stationary and over-stable modes to be treated simultaneously, which is important if perchance the critical eigenvalue flits between the different modes in response to changing parameter values. The results obtained show that the effect of both solute concentration and rotation is to stabilize the system for stationary convection case and for the over-stability case when both boundaries are free. However, when both boundaries are rigid some unexpected behavior are obtained in the case of over-stability.

Key words: *thermal instability, thermosolutal convection, rotation, thermal Rayleigh number, concentration Rayleigh number*

Introduction

Thermal instability theory has attracted considerable interest and has been recognized as a problem of fundamental importance in many fields of fluid dynamics. Rayleigh [1] provided a fundamental theoretical basis for the thermal instability in a fluid layer heated from below. The instability of a layer of fluid heated from below and subjected to Coriolis forces was first studied by Chandrasekhar [2] and Chandrasekhar and Elbert [3] for stationary convection and over-stability respectively. They showed that the effect of Coriolis forces on the instability of the fluid layer is to inhibit the onset of instability. Several other authors discussed the instability of fluids and the effect of rotation, Abdullah [4], Julien *et al.* [5], Chun *et al.* [6], Prosperetti [7], Geurts and Kunnen [8], Horn and Shishkina [9], Khan and Shafie [10], and Sharma *et al.* [11].

* Corresponding author, e-mail: achamkha@pmu.edu.sa

International Mathematical Forum, Vol. 14, 2019, no. 4, 169 - 179
HIKARI Ltd, www.m-hikari.com
https://doi.org/10.12988/imf.2019.9728

Group Action on Quantum Field Theory

Ahmad M. Alghamdi and Roa M. Makki

Department of Mathematical Sciences
Faculty of Applied Sciences
Umm Alqura University
P.O. Box 14035, Makkah 21955, Saudi Arabia

Abstract

The main aim of this paper is to develop some tools for understanding and explaining the concept of group action on a space and group action on algebra by using subgroups with finite index and both restriction and transfer maps. We extend this concept on quantum field theory.

0 Introduction

Group action is a very important tool in mathematics. Namely, if a certain group acts on a certain object, then many results and phenomena can be resolved. Let G be a group, the object can be a set and then we have the notion of a group acts on a set see [7]. Such object can be a vector space which results the so called G-space or G-module see for instance [6]. In some cases, the object can be a group and then we have the notion of group acts on a group see [3]. The topic of a group acting on an algebra can be seen in [5, 9]. This approaches open many gates in the research area called the G-algebras over a field. If we have an action from the group G to an object, then there is a fixed point under this action. This is the key idea in the theory of group action. In fact, by restriction, each subgroup of G acts on the same object too. Therefore, that subgroup has also fixed points.

This theory goes to back the work of Cauchy Frobenius Burnside see [10]. That is the counting lemma which has many application in real life. However, the systematic method which had been initiated by Green in [4] is a very significant approach to unify the study of group action on certain objects.

Electronic Journal of Graph Theory and Applications 7 (2) (2019), 315–328

Electronic Journal of
Graph Theory and Applications

Bounds for graph energy in terms of vertex covering and clique numbers

Hilal A. Ganie[a], U. Samee[b], S. Pirzada[a], Ahmad M. Alghamdi[c]

[a]Department of Mathematics, University of Kashmir, Srinagar, Kashmir, India
[b]Department of Mathematics, Islamia College for Science and Commerce, Srinagar, Kashmir, India
[c]Department of Mathematical Sciences, Umm Alqura University, Makkah, Saudi Arabia

hilahmad1119kt@gmail.com, drumatulsamee@gmail.com, pirzadasd@kashmiruniversity.ac.in, amghamdi@uqu.edu.sa

Abstract

Let G be a simple graph with n vertices, m edges and having adjacency eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$. The energy $\mathbb{E}(G)$ of the graph G is defined as $\mathbb{E}(G) = \sum_{i=1}^{n} |\lambda_i|$. In this paper, we obtain the upper bounds for the energy $\mathbb{E}(G)$ in terms of the vertex covering number τ, the clique number ω, the number of edges m, maximum vertex degree d_1 and second maximum vertex degree d_2 of the connected graph G. These upper bounds improve some of the recently known upper bounds.

Keywords: graph energy, vertex covering number, clique number, maximum degree
Mathematics Subject Classification : 05C30, 05C50
DOI: 10.5614/ejgta.2019.7.2.9

1. Introduction

Let $G(V, E)$ be a finite and simple graph with n vertices and m edges and having vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$. The adjacency matrix $A = (a_{ij})$ of G is a $(0,1)$-square matrix of order n whose $(i,j)^{th}$-entry is equal to 1, if v_i is adjacent to v_j and equal to 0, otherwise. The spectrum of the adjacency matrix is called the adjacency spectrum of the graph G.

Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the adjacency eigenvalues of G. Let $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$ be the

Received: 24 August 2018, Revised: 27 April 2019, Accepted: 21 May 2019.

Novi Sad J. Math. Vol. XX, No. Y, 20ZZ, ???-???
https://doi.org/10.30755/NSJOM.09142

Beale-Kato-Majda's criterion for magneto-hydrodynamic equations with zero viscosity

Ahmad M. Alghamdi[1], Sadek Gala[23] Maria Alessandra Ragusa[4],

Abstract. This paper is concerned to study the blow-up criterion of smooth solutions to the three dimensional magneto-hydrodynamic equations with zero viscosity. We prove that the smooth solution may be extended by standard energy method, provided that the norm of the gradient of velocity in a space much bigger than $\dot{B}^{0}_{\infty,\infty}$. This result obtained in this manuscript improves the former corresponding result.

AMS Mathematics Subject Classification (2010): 35Q35; 35B65; 76D05

Key words and phrases: Magneto-hydrodynamic equations with zero viscosity; $\dot{B}^{0}_{\infty,\infty}$ space, blow-up criterion

1. Introduction

This paper deals with the well-known problem of the breakdown of classical solutions to the incompressible magneto-hydrodynamic equations with zero viscosity in $\mathbb{R}^3$:

$$\begin{cases} \partial_t u + u \cdot \nabla u + \nabla \pi - b \cdot \nabla b = 0, \\ \partial_t b - \Delta b + u \cdot \nabla b - b \cdot \nabla u = 0, \\ \nabla \cdot u = \nabla \cdot b = 0, \\ u(x,0) = u_0(x), \qquad b(x,0) = b_0(x), \end{cases} \tag{1.1}$$

where $u = u(x,t)$ is the velocity of the flows, $b = b(x,t)$ is the magnetic field, $\pi = \pi(x,t)$ is the scalar pressure, while u_0 and b_0 are given initial velocity and initial magnetic field with $\nabla \cdot u_0 = \nabla \cdot b_0 = 0$ in the sense of distribution.

The system (1.1) describes the macroscopic behavior of electrically conducting incompressible fluids (see [10]). In the turbulent flow regime which occurs when the Reynolds numbers is very big, we ignore the viscosity of fluids to haveour system (1.1) (see e.g. [9]). In the extremely high electrical conductivity cases, which occur frequently in the cosmical and geophysical problems, we ignore the resistivity term to have our system (1.1) (see e.g. [4]).

[1] Department of Mathematical Science , Faculty of Applied Science, Umm Alqura University, P. O. Box 14035, Makkah 21955, Saudi Arabia, e-mail: amghamdi@uqu.edu.sa
[2] Department of Mathematics, University of Mostaganem, Algeria;
Dipartimento di Mathematica e Informatica, Università di Catania, Viale Andrea Doria 6, Catania, 95125, Italy, e-mail: sgala793@gmail.com
[3]Corresponding author
[4] Dipartimento di Mathematica e Informatica, Università di Catania, Viale Andrea Doria 6, Catania, 95125, Italy;
RUDN University, 6 Miklukho - Maklay St, Moscow, 117198, Russia,
e-mail: maragusa@dmi.unict.it

DISCRETE AND CONTINUOUS
DYNAMICAL SYSTEMS SERIES B
Volume **24**, Number **9**, September **2019**

doi:10.3934/dcdsb.2019040
pp. **4955–4981**

VERIFICATION ESTIMATES FOR THE CONSTRUCTION OF LYAPUNOV FUNCTIONS USING MESHFREE COLLOCATION

PETER GIESL*
Department of Mathematics
University of Sussex
Falmer BN1 9QH, United Kingdom

NAJLA MOHAMMED†
Department of Mathematical Sciences
Umm Al-qura University, Saudi Arabia

(Communicated by Peter E. Kloeden)

ABSTRACT. Lyapunov functions are functions with negative derivative along solutions of a given ordinary differential equation. Moreover, sub-level sets of a Lyapunov function are subsets of the domain of attraction of the equilibrium. One of the numerical construction methods for Lyapunov functions uses meshfree collocation with radial basis functions (RBF). In this paper, we propose two verification estimates combined with this RBF construction method to ensure that the constructed function is a Lyapunov function. We show that this combination of the RBF construction method and the verification estimates always succeeds in constructing and verifying a Lyapunov function for nonlinear ODEs in $\mathbb{R}^d$ with an exponentially stable equilibrium.

1. **Introduction.** The determination of the domain of attraction of an equilibrium is an important task in the analysis and derivation of dynamical systems, arising in many practical applications. Since it is difficult to determine the exact domain of attraction analytically, researchers have been seeking numerical algorithms to determine subsets of the domain of attraction, see [6]. Most of these methods for computing domains of attraction are based on Lyapunov functions, which are functions that decrease along trajectories of the dynamical system. Sublevel sets of Lyapunov functions are positively invariant subsets of the domain of attraction. The construction of such Lyapunov functions, however, is very challenging. One of the numerical methods to compute Lyapunov functions is the RBF (radial basis function) method, a special case of meshfree collocation. It considers a particular Lyapunov function, satisfying a linear PDE and approximates it using meshfree collocation [3, 7]. For this method, a set of scattered collocation points is used to find an approximation to the solution of the linear PDE. It is computed by solving a linear system of equations, for more details see Section 3. A refinement algorithm, based on Voronoi diagrams, for this method was proposed in [12].

2010 *Mathematics Subject Classification.* Primary: 37B25, 65N15; Secondary: 65N35, 37M99.
Key words and phrases. Meshfree collocation, Lyapunov functions, error estimates.
† The second author acknowledges funding for her PhD studies from the Saudi Government.
* Corresponding author.

AIMS *Mathematics*
http://www.aimspress.com/journal/Math

AIMS Mathematics, 5(1): 359–375.
DOI:10.3934/math.2020024
Received: 15 August 2019
Accepted: 23 October 2019
Published: 21 November 2019

Research article

The anisotropic integrability logarithmic regularity criterion to the 3D micropolar fluid equations

Ahmad Mohammad Alghamdi[1], Sadek Gala[2,3,*], Jae-Myoung Kim[4] and Maria Alessandra Ragusa[3,5]

[1] Department of Mathematical Science , Faculty of Applied Science, Umm Alqura University, P. O. Box 14035, Makkah 21955, Saudi Arabia
[2] Department of Mathematics, ENS of Mostaganem, Box 227, Mostaganem 27000, Algeria
[3] Dipartimento di Matematica e Informatica, Università di Catania, Viale Andrea Doria, 6 95125 Catania - Italy
[4] Department of Mathematical Education, Andong National University, Andong, Gyeongsangbuk-do, 36729, Korea (Republic of)
[5] RUDN University, 6 Miklukho - Maklay St, Moscow, 117198, Russia

* **Correspondence:** Email: sgala793@gmail.com.

Abstract: The aim of this paper is to establish the regularity criterion of weak solutions to the 3D micropolar fluid equations by one directional derivative of the pressure in anisotropic Lebesgue spaces. We improve the regularity criterion for weak solutions previously given by Jia, Zhang and Dong in [21].

Keywords: micropolar fluid equations; regularity criterion; anisotropic Lebesgue spaces; a priori estimates
Mathematics Subject Classification: 35Q35, 35B65

1. Introduction

Let us consider the following Cauchy problem of the incompressible micropolar fluid equations in three-spatial dimensions :

$$\begin{cases} \partial_t u + (u\cdot\nabla)u - \Delta u + \nabla\pi - \nabla\times\omega = 0, \\ \partial_t\omega - \Delta\omega - \nabla(\nabla\cdot\omega) + 2\omega + (u\cdot\nabla)\omega - \nabla\times u = 0, \\ \nabla\cdot u = 0, \\ u(x,0) = u_0(x),\ \omega(x,0) = \omega_0(x), \end{cases} \tag{1.1}$$

International Mathematical Forum, Vol. 14, 2019, no. 4, 169 - 179
HIKARI Ltd, www.m-hikari.com
https://doi.org/10.12988/imf.2019.9728

Group Action on Quantum Field Theory

Ahmad M. Alghamdi and Roa M. Makki

Department of Mathematical Sciences
Faculty of Applied Sciences
Umm Alqura University
P.O. Box 14035, Makkah 21955, Saudi Arabia

Abstract

The main aim of this paper is to develop some tools for understanding and explaining the concept of group action on a space and group action on algebra by using subgroups with finite index and both restriction and transfer maps. We extend this concept on quantum field theory.

0 Introduction

Group action is a very important tool in mathematics. Namely, if a certain group acts on a certain object, then many results and phenomena can be resolved. Let G be a group, the object can be a set and then we have the notion of a group acts on a set see [7]. Such object can be a vector space which results the so called G-space or G-module see for instance [6]. In some cases, the object can be a group and then we have the notion of group acts on a group see [3]. The topic of a group acting on an algebra can be seen in [5, 9]. This approaches open many gates in the research area called the G-algebras over a field. If we have an action from the group G to an object, then there is a fixed point under this action. This is the key idea in the theory of group action. In fact, by restriction, each subgroup of G acts on the same object too. Therefore, that subgroup has also fixed points.

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Applied Mathematical Sciences, Vol. 13, 2019, no. 8, 381 - 388
HIKARI Ltd, www.m-hikari.com
https://doi.org/10.12988/ams.2019.511711

Stability of Perturbed Switched Systems

Wajdi Kallel

Department of Mathematics, Faculty of Applied Sciences
Umm Al-Qura University, 21955 Mekkah, Saudi Arabia
&
Mathematics Department
Faculty of Sciences Gabes, Tunisia

Amel Hatem

Department of Mathematics, Faculty of Applied Sciences
Umm Al-Qura University, 21955 Mekkah, Saudi Arabia

Abstract

In this paper, we focus on the stability of perturbed switched systems. we begin by studying switching systems in the plane, then trying to extend the result in a greater dimension. we will discuss and investigate the stability of such systems using a common lyapunov function. One such process which lead to the identification of a single CLF that is valid to all subsystems.

Mathematics Subject Classification: 93Cxx, 93Dxx

Keywords: Switched systems, Control Lyapunov function

1 Introduction

A switched linear system is a hybrid system which consists of several linear subsystems and a rule that orchestrates and organizes the switching among them ([2]).
Dynamic switching systems can be seen as a particular class of hybrid systems. The behavior of a switched system is determined by the behavior of

ISSN 2075-9827 e-ISSN 2313-0210
Carpathian Math. Publ. 2019, **11** (2), 407–417
doi:10.15330/cmp.11.2.407-417

http://www.journals.pnu.edu.ua/index.php/cmp
Карпатські матем. публ. 2019, Т.11, №2, С.407–417

PIRZADA S.[1], GANIE H. A.[1], ALGHAMDI A. M.[2]

ON THE SUM OF SIGNLESS LAPLACIAN SPECTRA OF GRAPHS

For a simple graph $G(V,E)$ with n vertices, m edges, vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$, the adjacency matrix $A = (a_{ij})$ of G is a $(0,1)$-square matrix of order n whose (i,j)-entry is equal to 1 if v_i is adjacent to v_j and equal to 0, otherwise. Let $D(G) = diag(d_1, d_2, \ldots, d_n)$ be the diagonal matrix associated to G, where $d_i = \deg(v_i)$, for all $i \in \{1,2,\ldots,n\}$. The matrices $L(G) = D(G) - A(G)$ and $Q(G) = D(G) + A(G)$ are respectively called the Laplacian and the signless Laplacian matrices and their spectra (eigenvalues) are respectively called the Laplacian spectrum (L-spectrum) and the signless Laplacian spectrum (Q-spectrum) of the graph G. If $0 = \mu_n \leq \mu_{n-1} \leq \cdots \leq \mu_1$ are the Laplacian eigenvalues of G, Brouwer conjectured that the sum of k largest Laplacian eigenvalues $S_k(G)$ satisfies $S_k(G) = \sum_{i=1}^{k} \mu_i \leq m + \binom{k+1}{2}$ and this conjecture is still open. If $q_1, q_2, \ldots, q_n$ are the signless Laplacian eigenvalues of G, for $1 \leq k \leq n$, let $S_k^+(G) = \sum_{i=1}^{k} q_i$ be the sum of k largest signless Laplacian eigenvalues of G. Analogous to Brouwer's conjecture, Ashraf et al. conjectured that $S_k^+(G) \leq m + \binom{k+1}{2}$, for all $1 \leq k \leq n$. This conjecture has been verified in affirmative for some classes of graphs. We obtain the upper bounds for $S_k^+(G)$ in terms of the clique number ω, the vertex covering number τ and the diameter of the graph G. Finally, we show that the conjecture holds for large families of graphs.

Key words and phrases: signless Laplacian spectra, Brouwer's conjecture, clique number, vertex covering number, diameter.

[1] University of Kashmir, 190006, Srinagar, India
[2] Umm Alqura University, P.O.Box 715, Makkah, Saudi Arabia
E-mail: pirzadasd@kashmiruniversity.ac.in (Pirzada S.), hilahmadl119kt@gmail.com (Ganie H. A.), amghamdi@uqu.edu.sa (Alghamdi A. M.)

INTRODUCTION

Let $G(V,E)$ be a simple graph with n vertices, m edges, having vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$. The adjacency matrix $A = (a_{ij})$ of G is a $(0,1)$-square matrix of order n whose (i,j)-entry is equal to 1 if v_i is adjacent to v_j and equal to 0, otherwise. Let $D(G) = diag(d_1, d_2, \ldots, d_n)$ be the diagonal matrix associated to G, where $d_i = \deg(v_i)$, for all $i \in \{1,2,\ldots,n\}$. The matrices $L(G) = D(G) - A(G)$ and $Q(G) = D(G) + A(G)$ are respectively called the Laplacian and the signless Laplacian matrices and their spectra (eigenvalues) are respectively called the Laplacian spectrum (L-spectrum) and the signless Laplacian spectrum (Q-spectrum) of the graph G. These matrices are real symmetric and positive semi-definite. We let $0 = \mu_n \leq \mu_{n-1} \leq \cdots \leq \mu_1$ and $0 \leq q_n \leq q_{n-1} \leq \cdots \leq q_1$ to be the L-spectrum and Q-spectrum of G, respectively. It is well

УДК 519.17
2010 *Mathematics Subject Classification:* 05C30,05C50.
The research of S. Pirzada (first author) is supported by SERB-DST, New Delhi under the research project number MTR/2017/000084.

Research Article

Advances in Mechanical Engineering

Advances in Mechanical Engineering
2019, Vol. 11(11) 1–8
© The Author(s) 2019
DOI: 10.1177/1687814019889480
journals.sagepub.com/home/ade
SAGE

Vibration of circular micro-ceramic (Si_3N_4) plate resonators in the context of the generalized viscothermoelastic dual-phase-lagging theory

Najat A Alghamdi

Abstract

In this article, the analysis and numerical results are represented for the thermoelastic of an isotropic homogeneous, thermally conducting, Kelvin–Voigt-type circular micro-plate in the context of Kirchhoff's Love plate theory of generalized viscothermoelasticity based on the dual-phase-lagging model. The governing equations are obtained for the generalized dual-phase-lagging model and coupled viscothermoelastic plates. The scaled viscothermoelasticity has been illustrated in the case of the circular plate and the axisymmetric circular plate for an aspect ratio for clamped boundary conditions. Laplace transform has been applied, and its inversions have been calculated numerically by using the Tzou method. The results have been carried out for the ceramic (Si_3N_4). It is noted that the temperature increment and lateral deflection are significantly affected by the time, the width, the thickness, and the mechanical relaxation times of the material.

Keywords
Viscothermoelasticity, dual-phase-lag, relaxation times, circular micro-ceramic

Date received: 5 September 2019; accepted: 16 October 2019

Handling Editor: Mario L Ferrari

Introduction

Heat conduction has been studied using mathematical models such as dual-phase lag (DPL), which was proposed by Tzou.[1,2] The temperature gradient and heat flux were established by this model. Many scientists used this model in heat transfer problems,[3] physical systems,[4–8] and thermoelastic damping vibration.[9,10] Guo et al.[11,12] used the DPL model to analyze the thermoelastic damping theory of micro- and nanomechanical resonators; then, he investigated the dissipation in the circular micro-plate resonator.

The circular plate is a common structural in many micro-and nano-electromechanical resonators. Hao[13] adopted an analytical study to analyze thermoelastic damping in vibrations of micro- and nano-electromechanical circular thin-plate resonators. Sun and Tohmyoh[14] studied thermoelastic damping on axisymmetric out-of-plane vibration of circular plate resonators. Sun and Saka[15] investigated the thermoelastic damping effects on the out-of-plane vibration of circular plate resonators. They added a factor in their formula of thermoelastic damping $K = (1 + v)/(1 - 2v)$, which is different from that of Lifshitz and Roukes,[16] in which v is Poisson's ratio. Li et al.[17] employed an analytical study to analyze thermoelastic damping in

Department of Mathematics, Faculty of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia

Corresponding author:
Najat A Alghamdi, Department of Mathematics, Faculty of Applied Science, Umm Al-Qura University, Makkah 24235, Saudi Arabia.
Email: najaralghamdi@gmail.com

International Journal of GEOMATE, Sept., 2019 Vol.17, Issue 61, pp. 1 - 7
ISSN: 2186-2982 (P), 2186-2990 (O), Japan, DOI: https://doi.org/10.21660/2019.61.4642
Special Issue on Science, Engineering & Environment

NONLINEAR BEHAVIOR AND THERMAL DAMAGE OF THERMAL LAGGING IN CONCENTRIC LIVING TISSUES SUBJECTED TO GAUSSIAN DISTRIBUTION SOURCE

Hamdy M. Youssef [1, 2,*], Najat A. Al-Ghamdi[3]

[1,*] Alexandria University, Dept. of Mathematics, Faculty of Education, Alexandria, Egypt
[2,*] Umm Al-Qura University, Dept. of Mechanics, Faculty of Engineering, Makkah, KSA
[3] Umm Al-Qura University, Dept. of Mathematics, Faculty of Science, Makkah, KSA

*Corresponding Author, Received: 27 Oct. 2018, Revised: 24 Dec. 2018, Accepted: 21 Feb. 2019

ABSTRACT: The effects of thermal lagging with high-order became essential to describe non-equilibrium heating in tissues. This paper studies the temperature rise behavior in living tissues theoretically during the treatment by magnetic tumor hyperthermia based on the non-linear form of the dual-phase-lag model. Experimentally, it was found that the concentration of magnetic particles is in Gaussian distribution through the radial direction when magnetic fluid is injected into the living tissue space. Hence, the governing partial differential equation in concentric spherical space is solved in the Laplace transform domain. Some comparisons between the non-linear and linear effects of phase-lag time's parameters on bio-heat transfer have been studied and discussed. The thermal damage quantity for the tumor has been calculated with different values of the phase-lag times. The results show that the non-linear and linear effects of phase-lag times on bio-heat transfer have significant effects on the tumor, the tissue, and the thermal damage quantity.

Keywords: Nonlinear Behavior; Thermal Lagging; Thermal Damage; Living Tissue; Gaussian distribution Source

1. INTRODUCTION

Hyperthermia (also called thermal therapy or thermotherapy) is a kind of medical treatment in cancer therapy; it is elevated body temperature to 40–44 C. Hyperthermia is used with radiation therapy and chemotherapy to treat cancer [1]. Cells in these areas are often cell cycle arrest and so most resistant to growth prohibiting drugs. It remains unclear whether these cells are sensitive to heat damage; moreover, heat can motivate vascularization and increase oxygenation of the tissue, thermotherapy make cancer cells more motivate to radiation or harm other cancer cells that radiation cannot damage [2, 3]. These studies have been certain in a number of clinical studies [4, 5] which indicate that elevation of the temperature within a tumor has a cytotoxic influence on radio resistant cells when heated to temperatures above 42 C. There is a variety of techniques [3, 6] to increase the temperature within the human body. Hyperthermia for the processing of cancer is under study, including all body hyperthermia, partial or regional hyperthermia, and local hyperthermia. In several biologists studying the behavior of bio-heat transfer in tissues during magnetic fluid hyperthermia management, the distribution of the magnetic particles was always regarded as homogenous in a limited spherical domain [7-11]. Furthermore, Salloum et al. [12] experimentally evaluated magnetic nan-ofluid transport and heat distribution stimulated by commercially available magnetic nanoparticles injected into the extracellular area of biological tissue using agarose gel with porous structures alike to human tissue. Pennes model [13] described temperature distribution in the living biological tissues. The connection between [14] arterial blood and the heat transfer in a living tissue are taken. The model known as the bioheat equation remains used today. Pennes inserted a medium response term to the basic heat equation that accounts for the mitigating effect of blood flow. This convective term depicts heat transport by means other than propagation. Wissler [15] explicated the validity of Pennes' model connected to normal thermal distribution in living tissue. supposed mixed boundary conditions in resting tissue, Pennes' model strictly describes the decay of temperature from the core of the body to the surface [14]. The Pennes bio-heat transfer equation (PBT) is based on the classical Fourier's law, taken into account a blood perfusion term, which is proportionate to the volumetric rate of blood perfusion and the difference between the average arterial blood and tissue temperatures. Pennes bio-heat model is true only if when the venous blood flows from the capillary bed to the main supply vein, its temperature remains the same as the tissue temperature disregard the size of the vessel and the

Fluid Dynamics & Materials Processing FDMP, vol.15, no.5, pp.597-611, 2019

On the Application of the Adomian's Decomposition Method to a Generalized Thermoelastic Infinite Medium with a Spherical Cavity in the Framework Three Different Models

Najat A. Alghamdi[1] and Hamdy M. Youssef[2, 3, *]

Abstract: A mathematical model is elaborated for a thermoelastic infinite body with a spherical cavity. A generalized set of governing equations is formulated in the context of three different models of thermoelasticity: the Biot model, also known as "coupled thermoelasticity" model; the Lord-Shulman model, also referred to as "generalized thermoelasticity with one-relaxation time" approach; and the Green-Lindsay model, also called "generalized thermoelasticity with two-relaxation times" approach. The Adomian's decomposition method is used to solve the related mathematical problem. The bounding plane of the cavity is subjected to harmonic thermal loading with zero heat flux and strain. Numerical results for the temperature, radial stress, strain, and displacement are represented graphically. It is shown that the angular thermal load and the relaxation times have significant effects on all the studied fields.

Keywords: Adomian's decomposition method, generalized thermoelasticity, relaxation time, iteration method.

Nomenclature

λ , μ	Lame's constants
ρ	Density
C_E	Specific heat at constant strain
α_T	Coefficient of linear thermal expansion
γ	$=(3\lambda+2\mu)\alpha_T$
t	Time
T	Temperature
T_o	Reference temperature

[1] Mathematics Department, Faculty of Science, Umm Al-Qura University, Makkah, Saudi Arabia.
[2] Mathematics Department, Faculty of Education, Alexandria University, Alexandria, Egypt.
[3] Mathematics Department, Faculty of Engineering, Umm Al-Qura University, Makkah, Saudi Arabia.
* Corresponding Author: Hamdy M. Youssef. Email: youssefanme2005@gmail.com.

FDMP. doi: 10.32604/fdmp.2019.05131 www.techscience.com/fdmp

Journal of Computational and Theoretical Nanoscience
Vol. 16, 1–5, 2019

Effect of Gamma Irradiation on Physical Properties of Spray Deposited SnO_2-F Thin Films

H. Al-Ghamdi[1, *], Shatha A. Aldaghfag[1], J. Bouslimi[2], and J. Ouerfelli[3]

[1] *Department of Physics, College of Science, Princess Nourah Bint Abdulrahman University, Saudi Arabia*
[2] *Department of Physics, College of Science, Taif University, Saudi Arabia*
[3] *Department of Physics, College of Applied Science, Umm Al-Qura University, Makkah, Saudi Arabia*

In this study, tin oxide thin films doped Fluor SnO_2-F were deposited on glass substrate by spray pyrolysis, for promoting the sensitivity of the films. The structural, optical and electrical properties of thin films before and after γ-irradiation using ^{60}Co G-ray source (0 to 100 kGy) have been reported. The X-ray diffraction and AFM microscopy analysis revealed that the films before irradiation were polycrystalline with crystallite size of 41 nm and increase with increasing of gamma radiation dose, but dislocation density and micro strain decrease, and the sensible roughness to irradiation dose. UV-VIS Spectroscopy revealed that the transmittance at wavelength 1400 nm decreases as the doses increases and also the optical band gap from 3.91 eV to 2.7 eV. The electrical properties from *I–V* characteristics showed a change on conductivity decrease in resistance with the increase irradiation dose. The changes in the conductivity and optical band gap, shows that SnO_2-F thin films are sensitive to gamma irradiation and it can be used for dosimetric applications and as gamma sensor.

Keywords: Gamma Irradiation, Thin Films, SnO_2-F.

RESEARCH ARTICLE

1. INTRODUCTION

Metal oxide semiconductors have been the topic of intensive research due to their wide range of applications. Among these materials, tin oxide thin films, it is considered as very interesting metal oxides because of their electrical and optical properties, SnO_2 is an *n*-type material with direct band gap, around 3.6 eV, it have a exciton binding energy (130 MeV) and carrier mobility (250 cm^2/VS).[1-9] Tin oxide (SnO_2) thin films as transparent conductive oxide TCO, is considered as important material, it used in different application areas: touch screens, thin-film transistors, sensors, wide gap windows, electro luminescent windows, nuclear technology, etc.[10-11] SnO_2 thin films are synthesized by a different techniques such as thermal evaporation,[12] oxidation of tin film, Molecular Beam Epitaxial MBE, chemical deposition, sputtering Radio Frequency RF, by sol gel and spray pyrolysis.[13-19] Several efforts have been devoted to study the γ-irradiation effect on different metal oxide and metal oxide structure thin films,[20,21] but The efforts to study of effect of G-irradiation on optical, electrical and magnetic properties of tin oxide thin film rest limited. Senthil and Sudha, have studied the influence of Gamma irradiation on tin oxide thin films in the range of 0–150 Gy, for dosimetric applications and irradiation sensors.[22,23] The electrical measurement shows the films have a low electrical conductivity and low sensitivity.

In this paper, the ^{60}Co γ-irradiation effect of on SnO_2-F layer prepared by spray pyrolysis has been studied (morphology, optical and electrical properties). The prepared thin films, fluorine doped tin oxide with optimum percentage doping have highest electrical conductivity $\sigma = 1.71 \times 10^3$ Scm^{-1}, and studied before and after γ-radiation irradiation. The present results show improvement in the sensitivity due to fluorine doping.

2. EXPERIMENTAL DETAILS

Thin films of tin oxide SnO_2 are deposited by Spray method. The preparation of the solution is based on anhydrous $SnCl_4$ as a precursor, first dissolved in methanol, to which is added an amount of NH_4F dissolved in deionized distilled water (DDW) in order to obtain a crystalline solution.[8] The solution will be in the following proportions: 970 ml of methanol are combined with 23 ml of $SnCl_4$ and 5.5 g of NH_4F dissolved in 7.5 ml of water, which corresponds to an approximate doping of 9% optimized for minimum sheet resistance (R_s). The sheet

*Author to whom correspondence should be addressed.

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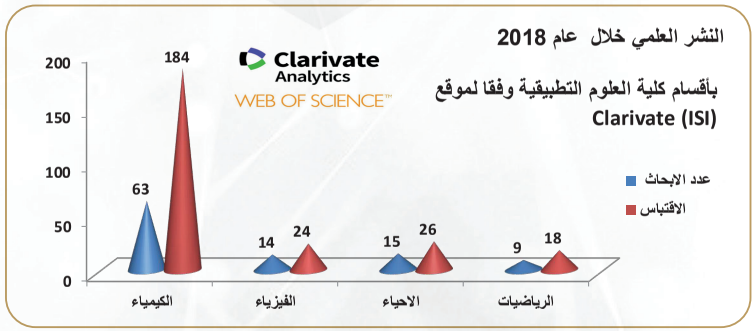

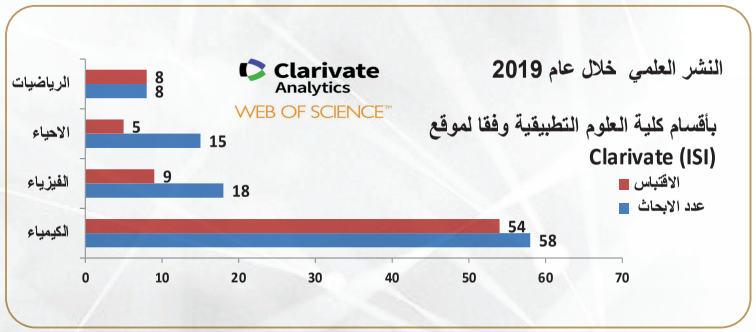

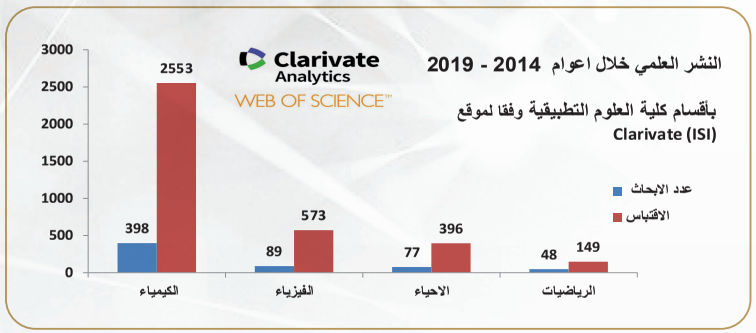

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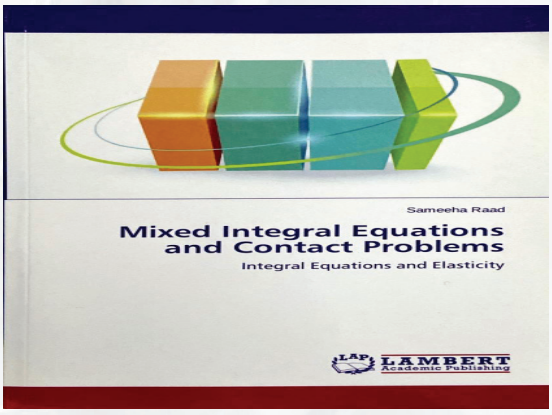

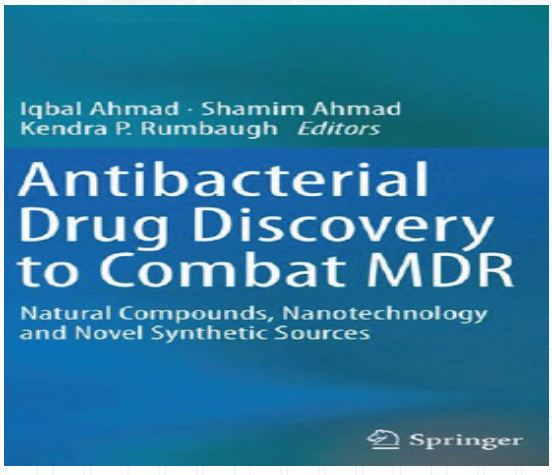

Antibiotic Resistance in *Campylobacter jejuni*: Mechanism, Status, and Public Health Significance

Javed Ahamad Khan, Hussein Hasan Abulreesh, Ramesh Kumar, Samreen, and Iqbal Ahmad

Abstract

Emergence of antibiotic resistance is a never-ending process in the bacteria due its vast capacity to resist and acquire various resistance mechanisms against antibacterial drugs. *Campylobacter* is a well-known pathogenic bacteria to human and animals and survive in different environment including foods. Species of campylobacters is responsible of gastritis and diarrheal and other diseases. Common resistance mechanisms present in Gram-negative bacteria include modification in the target site of antibiotic, inability of the antibiotic to reach its target by expressing major outer membrane proteins (MOMPs), efflux action of the antibiotic through CmeABC pumps, and inactivation or modification of the antibiotic. The plasmid along with chromosomal encoded genes are responsible for resistance. Mutation and acquisition of resistance genes are the common genetic mechanism found in *Campylobacter* spp.; considering the widespread occurrence of drug-resistant campylobacters in the environment, specific strategies to control the emergence and spread are needed. In this chapter, we have reviewed the recent literature on the mechanism of resistance and current status of prevalence of *Campylobacter jejuni* in the environment and its significance in human health.

J. A. Khan
School of Graduate Studies, Quantum University, Roorkee, Uttrakhand, India

H. H. Abulreesh (✉)
Department of Biology, Faculty of Applied Science, Umm Al-Qura University, Makkah, Kingdom of Saudi Arabia
e-mail: hhabulreesh@uqu.edu.sa

R. Kumar
Division of Biochemistry, Indian Veterinary Research Institute, Bareilly, Uttar Pradesh, India

Samreen · I. Ahmad
Department of Agricultural Microbiology, Faculty of Agricultural Sciences, Aligarh Muslim University, Aligarh, Uttar Pradesh, India

I. Ahmad et al. (eds.), *Antibacterial Drug Discovery to Combat MDR*,
https://doi.org/10.1007/978-981-13-9871-1_4

Actinomycetes as Continued Source of New Antibacterial Leads

Iqbal Ahmad, Abdullah Safar Althubiani, Muzammil Shareif Dar, Samreen, Faizan Abul Qais, Hussein Hasan Abulreesh, Majid Abdullah Bamaga, Saleh Bakheet Al-Ghamdi, and Fatimah Alshehrei

Abstract

Early antibiotic discovery program has witnessed significant role of mainly *Streptomyces* in antibiotic/drug discovery program. Due to various constraints, both academic and industry levels, the discovery of new antibiotics with novel mode of action is drastically slowed down in the last three decades. Rapid development and spread of multidrug-resistant bacteria globally have reduced the utility and effectiveness of old antibiotics. Therefore, the discovery of novel antibacterial compounds is urgently needed to combat antimicrobial resistance. However, natural product-based academic research could prove to be a sustained mine of novel antimicrobial leads. According to an estimate among the bioactive compounds that have been obtained so far from microbes, 45% are produced by actinomycetes, 38% by fungi, and 17% by unicellular eubacteria. This has become possible because of great diversity of actinomycetes in different habitat and their extraordinary capacity to synthesize new antibiotics. The development in the screening strategies and the use of modern biochemical and molecular approaches have made possible to detect new compounds. In this chapter, we have focused on general characteristics of soil and marine actinomycetes and

I. Ahmad · M. S. Dar · Samreen · F. A. Qais
Department of Agricultural Microbiology, Faculty of Agricultural Sciences, Aligarh Muslim University, Aligarh, India

A. S. Althubiani (✉) · H. H. Abulreesh · F. Alshehrei
Department of Biology, Faculty of Applied Science, Umm Al-Qura University, Makkah, Kingdom of Saudi Arabia
e-mail: asthubiani@uqu.edu.sa

M. A. Bamaga
Department of Medical Laboratory Sciences, Fakeeh College for Medical Sciences, Jeddah, Saudi Arabia

S. B. Al-Ghamdi
Department of Biology, Faculty of Science, Al-Baha University, Baha, Saudi Arabia

I. Ahmad et al. (eds.), *Antibacterial Drug Discovery to Combat MDR*,
https://doi.org/10.1007/978-981-13-9871-1_16

Antibacterial Drug Discovery: Perspective Insights

Iqbal Ahmad, Faizan Abul Qais, Samreen, Hussein Hasan Abulreesh, Shamim Ahmad, and Kendra P. Rumbaugh

Abstract

Over the last two decades, the development of new antibacterial drugs has been very limited due to many reasons. In light of the alarming situation of antimicrobial resistance (AMR), it is now vital to act promptly to develop new ways to combat the resistance problem through an integrated approach. Despite the slow progress of drug discovery by pharmaceutical companies, natural products have definitely provided an abundant source of new antibacterial leads. On the other hand, genomics- and proteomics-based drug discovery approaches have been more disappointing when it comes to the discovery of new antibacterials with novel modes of action. In the recent past, improved screening strategies and developments in target identification and validation, combinatorial chemistry, and the use of biochemical synthetic-based approaches have provided hope for the development of new antibacterial leads. Other approaches like novel anti-infective and anti-virulence target-based strategies such as quorum sensing, biofilm, virulence, and pathogenicity inhibitors are gaining popularity among drug discovery researchers. Similarly, nanotechnology-based drug delivery has seemingly unlimited application for improving the efficacy of antibiotics, where metallic and natural nanomaterials with antibacterial efficacy are under scrutiny

I. Ahmad (✉) · F. A. Qais · Samreen
Department of Agricultural Microbiology, Faculty of Agricultural Sciences, Aligarh Muslim University, Aligarh, Uttar Pradesh, India

H. H. Abulreesh
Department of Biology, Faculty of Applied Science, Umm Al-Qura University, Makkah, Kingdom of Saudi Arabia

S. Ahmad
Division of Microbiology, Institute of Ophthalmology, JN Medical College, Aligarh Muslim University, Aligarh, Uttar Pradesh, India

K. P. Rumbaugh
School of Medicine, Texas Tech University Health Sciences Center, Lubbock, TX, USA

I. Ahmad et al. (eds.), *Antibacterial Drug Discovery to Combat MDR*,
https://doi.org/10.1007/978-981-13-9871-1_1

اللقاءات العلمية الخارجية بكلية العلوم التطبيقية:

اللقاء العلمي الأول: زيارة الأستاذ الدكتور: زين بن حسن يماني (يوم الأربعاء الموافق 8-6-1440هـ):

ضمن سلسلة اللقاءات العلمية التي تنظمها كلية العلوم التطبيقية، تحت إشراف سعادة عميد كلية العلوم التطبيقية الدكتور حاتم بن محمد الطس، استضافت الكلية سعادة الأستاذ الدكتور: زين بن حسن يماني الأستاذ بقسم الفيزياء بكلية العلوم ومدير مركز التميز البحثي لتقنية النانو بجامعة الملك فهد للبترول والمعادن، وذلك يوم الأربعاء الموافق 8-6-1440هـ، حيث تخللت الزيارة لقسم الفيزياء، واطلع سعادته على معامل الطلاب المختلفة، بعدها أتحف سعادته الحضور بمحاضرة بعنوان « :تطوير المواد للتطبيقات البترولية والبتروكيميائية: برنامج التحسس في مركز التميّز البحثي لتقنية النانو بجامعة الملك فهد للبترول والمعادن أنموذجاً»، وبحضور عددٍ من منسوبي ومنسوبات كلية العلوم التطبيقية، ومن المهتمين بهذا اللقاء العلمي. وقد بدأ اللقاء بكلمة ترحيبية وتعريفية من سعادة وكيل كلية العلوم للدراسات العليا والبحث العلمي الأستاذ الدكتور باسم حسين أصغر، والتي حملت نبذة مختصرة عن سعادته، شملت اهتماماته البحثية، بالإضافة إلى حصوله على وسام الملك عبدالعزيز من الدرجة الأولى في عام 2006م، وعلى جائزة المخترعين من خادم الحرمين الشريفين عام 2017م. بعد ذلك بدأ اللقاء والذي تضمن فكرة إنشاء مركز التميّز في عام 1428هـ، والذي حدد مسار تميّز أبحاثه في مجال التطبيقات المتعلقة بصناعة البترول والبتروكيماويات، ثم أسهب الأستاذ الدكتور زين في عرض أمثلة متعلقة بأبحاث المركز لتطوير المواد النانوية في مجال التحسس للمواد الكيميائية؛ ومن ذلك تصنيع المواد التي تحسس لوجود الماء في مكامن البترول حيث المسامات قد لا تتجاوز مجرد 700 نانومتر، فأنتج المركز حبيبات كمية مشعة ضوئياً ملبسة بأغلفة من مادة أكسيد السيلكون مع مستحضرات أخرى تجعل هذه الحبيبات النانوية (كبرها حوالي 50 نانومتر)، وفي نفس الوقت هي مُحبّة للزيت (البترول) أو محبة للماء أو لكليهما، ولهذه الحبيبات القدرة على كشف مناطق وصول الماء إلى الزيت في مكامن البترول. كما أعطى أ. د. يماني أمثلة أخرى لأنشطة المركز في مجال تحسس الغازات الملوّثة في الهواء أو الماء، وعرض قائمة من الأبحاث العلمية المنشورة في المجلات العالمية المميزة، فاقت الـ (33) بحثاً منشورًا. وختم أ. د. زين لقاءه بالتأكيد على أهمية التعاضد البحثي وزيادة كفاءة الأداء في البحوث تحقيقاً للمصلحة الوطنية. وبعد اللقاء العلمي دار نقاش علمي بين الحضور من منسوبي ومنسوبات الكلية والأستاذ الدكتور زين حول هذا الموضوع. وفي نهاية اللقاء العلمي تم تكريم سعادته من قبل عميد كلية العلوم التطبيقية د. حاتم محمد الطس، وقدم له درع شكر وتقدير نظير مشاركته في تقديم هذا اللقاء العلمي.


أسرتك
#لن_تفقدها


عميد الكلية

اللقاء العلمي الثاني: زيارة الأستاذ الدكتور: عبدالرحمن بن عبدالله الورثان (يوم الأربعاء الموافق: 17-2-1441هـ):

ضمن سلسلة اللقاءات العلمية التي تنظمها كلية العلوم التطبيقية تحت إشراف سعادة عميد كلية العلوم التطبيقية الدكتور حاتم بن محمد الطس، حيث استضافة الكلية سعادة الاستاذ الدكتور: عبدالرحمن بن عبدالله الورثان الأستاذ بقسم الكيمياء بكلية العلوم بجامعة الملك سعود وعضو الجمعية الكيميائية السعودية ورئيس تحرير المجلة العربية الكيميائية وذلك يوم الأربعاء الموافق: 17-2-1441هـ، حيث تخللت الزيارة جولة لكلية العلوم التطبيقية، بعدها أتحف سعادته الحضور بمحاضرة علمية بعنوان: ((الاوراق العلمية والنشر العلمي المميز في مجلات علميه ذات معامل تأثير عالي)) وبحضور عددا من منسوبي ومنسوبات كلية العلوم التطبيقية ومن المهتمين بهذا اللقاء العلمي. وقد بدا اللقاء بكلمة ترحيبية وتعريفية من سعادة وكيل كلية العلوم للدراسات العليا والبحث العلمي الاستاذ الدكتور: باسم حسين أصغر، والتي شملت نبذه مختصرة عن سيرته الذاتية واهتماماته البحثية المختلفة بعد ذلك تطرق الاستاذ الدكتور الورثان الى الأوراق العلمية البحثية وأنها من أهم الأدوات التي يوظفها الباحث العلمي لإيصال أفكاره ونظرياته واكتشافاته في مجال من مجالات المعرفة. بعد ذلك أشار الى المعايير التي تعتمدها المجلات المحكمة، وأهم الأسباب الشائعة لرفض نشر الأوراق البحثية من طرف المحكمين، والأخطاء التي تحرم الباحث من نشر الأوراق البحثية في المجلات العلمية المحكمة. وإن المصداقية التي تحظى بها المجلات العلمية المحكمة، تدفع لقبول نشر الأوراق العلمية البحثية. والتي يجب على الباحث أخذها بعين الاعتبار قبل الشروع في كتابة ورقته البحثية ليضمن قبول نشرها. وأشار أيضا ان الرفض لا يعود دائما لعيب في الورقة البحثية، وقد يكون السبب احيانا في هذه الحالة كثرة الأوراق البحثية الواردة للمجلة، لذلك يجب عدم اعتبار رفض النشر معيارا للحكم على الورقة البحثية، والحرص على إرسالها إلى مجلات أخرى، بعد التأكد من مطابقتها للمعايير المطلوبة. وختم أ. د. الورثان لقاءه بالتأكيد على البحث في النشر العلمي على المجلات المعروفة والمصنفة عالميا والتابعة للجمعيات او للجامعات الأكاديمية. وبعد ذلك دار نقاش علمي بين الحضور من منسوبي ومنسوبات الكلية والأستاذ الدكتور: عبد الرحمن حول هذا الموضوع. وفي نهاية اللقاء العلمي تم تكريم سعادته من قبل سعادة عميد كلية العلوم التطبيقية د. حاتم محمد الطس وقدم له درع شكر وتقدير نظير مشاركته في تقديم هذا اللقاء العلمي.








تم سحب

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