Prof. Dr. Awwad Abdoh Radwan

Salama Ph.D., Computer-Aided Drug Design

E-mail: dhna_2001@hotmail.com

Major research field:

Molecular modelling and computer-aided drug design.

Synthesis and characterisation of biologicaly active heterocyclic

compounds.

Permanent Job and Address

Professor (Full) of Pharmaceutical Organic Chemistry, Faculty of Pharmacy, Assiut University, Assiut, Egypt. **Tel**: +2-(0)88-241-1312 (**work**) Home tel: +2-(0)88-2320294 (**tel**) +2(0)88-233-2776 (**fax**)

Email: dhna_2001@hotmail.com

Current Job and contact:

Associate professor at kayyali's Chair of Pharmaceutical Technology Center (PCT), King Saud University, El-Riyadh, Saudi Arabia. Office tel. 046-70562; Mob. Tel. 0505193925

Personal Details

Sex: Male

- Date of Birth: 30-09-1965
- Nationality: Egypt
- Marital Status: Married (5 children)

Personal Profile

I am a patient, perceptive and thorough researcher with a clear understanding of both the perceived and actual role of computational chemistry, Pharmaceutical Organic Chemistry, Medicinal Chemistry. I believe that I am skilful at evaluating problems and communicating possible solutions as well as capable of making a significant contribution to the efficiency of any research team. I am a good team worker with a healthy sense of humour who works well under pressure. **I got two** **awards** From 'ACDIMA Award for best research from ACDIMA drug company (Oman, Jordanian' years 2008 and 2012. **I got two European patents**; EP 2540746 B1

(3/03/2013) and EP 2 527 335 A1 (28.11.2012). I got one United States patents; US 8,829,016 B2. I got Silver Medal from Geneva Innovation Salon (Swizerland, 2-6 April 2014).

I got four research project-funds three of 45,000 SR, 150,000 SR and 1,000,000.0 SR were finished and published and the fourth project is of 450,000 SR is going on. I have 34 publications. In addition to my PhD degree obtained from Kitasato University, Japan 2002, I had two visiting professor travels, one at Medicinal Chemistry Institute of Pharmacy Martin-Luther-Universität Halle (Saale), Germany'20/6/2012-10/8/2012' and the second was at Dept of drug design and molecular modelling, School of Pharmaceutical Sciences, Kitasato University, Tokyo, Japan '15/7/2010-14/9/2010'. (All details of the profile are below).

Key Qualifications and Skills

- Ph.D. in Pharmaceutical Chemistry (Computer-Aided Drug Design)
- MSc. Chemical Research (Pharmaceutical organic chemistry)
 BSc. (Hons)
 pharmaceutical sciences.
- Member of the Pharmacy syndicate.

Teaching skills for Undergraduates

2002–2008 -(Full time) Department of Pharmaceutical Organic Chemistry, Faculty of Pharmacy, Assiut University, Egypt

-(Secondment 2 days/week) Department of Organic Chemsitry, Faculty of Pharmcy, AlAzhar University, Teach first , second and third year student class (2 days

- Teach physical chemistry including atom structure, molecular orbital, bond formation, bond energy in addition to organic chemistry including aliphaic and aromatic hydrocarbons, Alicycles and heterocycles, alcohols, carboxylic cids, phenols, carbonyl compounds, carbohydrates, amino acids, stereochemistry and spectroscopy (IR, ¹H NMR, ¹³C NMR, and Mass spectroscopy).
- Supervise the student laboratory and tutorials.
- Supervise an examination committee that manage final exam of a student class.
- Supervise the tutorial work of first year student class.
- Participated as a member of Faculty council.

• Participated in student social activities in the university.

Teaching skills for Postgraduates

- 1-Supervise master students (Successfully graduated and obtained their degrees) □ 2-Teach advanced spectrometry including 2D NMR, ¹³C NMR.
- 3- Teach advanced Organic Chemsity.
- 4- Teach computer-aided drug design methods including Ligand-based and Structurebased drug design such as 2D-and-3D QSAR, Dock, DeNovo Design and receptor mapping methods.

Research skills of synthesis

Synthesis of biologically active heterocyclic compounds (pyrimidinones, thiadiazinethiones, quinazolinones, thiazolidinones, pyrazolopyrimidines, triazoles, thiadiazoles, pyrazoles, thienoquinolines and pyrdinoquinolines).

Research skills of molecular modeling

- Professional use of Molecular Modelling packages including: Cerius² (Catalyst, hiphop and hypogen molules).
- Professional use of SYBYL8.2 package and all its modules (CoMFA, CoMSIA, surflexdock, flexdock.....etc).
- Professional use of Maestro which is the graphical user interface (GUI) for all of Schrödinger's computational programs: CombiGlide, Confgen, Desmond, Epik, Glide, Impact, Jaguar, Liaison, LigPrep, MacroModel, Phase, Prime, PrimeX, QikProp, QSite, SiteMap, Strike, and WaterMap.
- Professional use of QSAR software, midas, Amber 6, Dock 6.4, Autodock and LigandScout.
- Use of basic UNIX operating systems and Linux operating system in addition to PC operating systems including Word, Excel, PowerPoint, Access.
- Basic skills in shell scripts writing and basic skills in programming languages such as fortran, C++ and visual C++ languages.

Detailed Professional Experience

- O5/2013 Until now Professor (full) of Pharmaceutical Organic Chemistry, Assiut University, Egypt
- 1/2008 05/2013 Associate professor at Alkayyali's Chair of Pharmaceutical Technology Center (PTC)-King Saud University, Saudi Arabia
- □ 04/2008 11/2008 Associate professor of Pharmaceutical Organic Chemistry, Assiut

University, Egypt

- 04/2002 04 / 2008 Lecturer, Ph.D., of Pharmaceutical Organic Chemistry, Assiut University, Egypt
- 04/2002 04 / 2008 Postgraduate Teaching Assistant Advanced medicinal chemistry, Advanced Organic chemistry and Computer application Course for drug design and synthesis. 03 / 1990 – 05/1997: Demonstrator and assistant lecturer –Pharmaceutical Organic Chemistry.

Academic education and research Fellowships.

7/7/2013-until now Professor of Pharm. Org. Chem., Fac. Of Pharmacy, Assiut

University, Assiut, Egypt.

- 20/6/2012-10/8/2012. Visiting professor, Medicinal Chemistry Institute of Pharmacy Martin-Luther-Universität Halle-Wittenberg Wolfgang-Langenbeck-Str. 4 06120 Halle (Saale), Germany. Project title: "Structure-based design and optimization of inhibitors of the histone lysine methyltransferase SET7/9".
- □ 15/7/2010-14/9/2010. Visiting professor, School of Pharmaceutical Sciences, Dept of drug design and molecular modelling, Tokyo, Japan. Project title "*In silico screening and structure-based molecular design of D-aspartate oxidase inhibitors*".
- 21/5/2008- until now: Assiut University, Faculty of Pharmacy, Dept Pharm Org Chemistry, Assiut, Egypt. Associate Professor.
- 21/4/2002-21/5/2008: Faculty of Pharmacy, Dept Pharm Org Chemistry, Assiut, Egypt. Assistant Professor.
- 21/4/2002: Ph.D. graduate; Kitasato University, school of pharmaceutical sciences, Dept physical chemistry for drug design and molecular modelling, Tokyo, Japan. 05/1997 4/2002 Ph. D student at Kitasato University, Tokyo, Japan

Major field: Computer aided drug design

Ph.D. Title: "Rational Procedure for 3D QSAR Analysis Using TRNOE Experiments and

Computational Methods: Application to Thermolysin Inhibitors"

To develop rational procedure that combines the advantage of structure based drug design with the advantage of ligend based drug design in 3D QSARs. The work was completed using the 2D NMR techniques to find the binding conformation constraint (structure based drug design). These constraints are included in exhaustive conformational analysis and alignment to find the binding conformations. These binding conformations are included in CoMFA and CoMSIA to find the 3D QSAR between these conformers (ligend based drug design). The method was applied on thermolysin inhibitors.

- 04/1995: Master degree, Msc.D., Assiut University, Faculty of Pharmacy, Dept Pharm Org Chemistry, Assiut, Egypt.
- 04/1990 05/1995: Demonstrator for undergraduate students at Assiut University, Faculty of Pharmacy, Dept Pharm Org Chemistry, Assiut, Egypt.

Major field: Design and synthesis of biologically active heterocyclic compounds. <u>MSc.</u>

Title: "Synthesis and evaluation of the cytotoxic and anti viral activities of

5,6disubstituted isocytosine derivatives".

- □ To develope new anticancer compounds, isocytosine derivatives (Bropirimine analogues) and its biological evaluation as cytotoxic agents.
- □ 12/1988 03/1990 Obligatory National army service.
- 05/1988 Assiut University, Faculty of Pharmacy, Dept Pharm Org Chemistry, Assiut, Egypt.

BSc. (Hons) Of pharmaceutical sciences.

 09/1983-05/1988 Undergraduate student. Assiut University, Faculty of Pharmacy, Dept Pharm Org Chemistry, Assiut, Egypt.

Current Ongoing and Funded Project: Project 1: (450,000 SR)

2015-2017 **Design and synthesis of new compounds as multi-receptor targeting for treatment of Alzheimer's Disease**. Kingdome of Saudi Arabia, National Plan for Science, Technology and innovation. (**Project ID:** 14-MED622-02; PI: Awwad A Radwan; Co-I: Fares K Al-Anazy).

Overview:

The project aims to synthesize tacrine derivatives intended to inhibit acetyl chorine esterase activity, chelate metals, amyloid-beta peptide aggregation, and inhibit beta-site APP converting enzyme (BACE) activity. This will be done through a combination of benzofuran moiety, AChE and BChE inhibitor, and 8-hydroxquinoline moiety, iron chelator, linked through substituted piperazine in one molecule. It is thought that the piperazine linker will enhance the molecule crossing the blood-brain barrier (BBB). The proposed compounds are suggested to improve the muscarinic system beside neuroprotection through its iron chelation functionality. The new compound may be applicable to the treatment of multiple neurodegenerative disorders, including Alzheimer's disease (AD).

Funded Projects And Finished successfully:

Project 1: (45,000 SR)

2009-2010 Synthesis and molecular modelling of 1,2,4-triazole derivatives as selective

COX-inhibitors antiinflammatory. Saudi Arabia Basic Industries Company, SABIC (MED30-19) (PI: Awwad A Radwan; Co-I: Fares K Al-Anazy).

Overview:

Slight gastric ulceration occurs on longtime dose of currently COX-2 inhibitors such as Celcoxibe. Therefore, current research challenges with the synthesis of new compounds that are safer for gastrointestinal tissues or in other words more completely selective COX-2 inhibitors. In our work, A series of novel substituted 1,2,4-triazoles are designed for synthesis and evaluation for their inhibition of the two isoforms of human cyclooxygenase (COX-1 and COX2). This series is expected to displays exceptionally selective COX-2 inhibition. Computer-aided molecular modeling is done in order to correlate the biological activity with the threedimensional structure activity relationship and explore the binding mechanism between the test compounds and target site of the cyclooxygenase enzyme

Project 2: (150,000.0 SR)

2009-2010 Design and Synthesis of a Novel Crown Ether-Crosslinked Chitosan for Removal

of Toxic Metal Ions (M⁺ⁿ) from Wastewater: An Industrial Application. Center of

Excellence for Research in Engineering Materials, Center of Excellence Programs, King Saud University, Ministry of Higher Education, (03-CEREM-430) (PI: Ibrahim A Al-Sarra; Co-I: Awwad Aradwan)

Overview:

The water supply in Saudi Arabia has increased dramatically from 1.75 billion m³ in 1975 to 22.93 billion m³ in 1992. In Saudi Arabia, the total amount of wastewater available is around 1.32 million m³/d. In the near future, these amounts of industrial wastewater are of several hundred times-folds larger. The industrial areas of Saudi Arabia generate some of industrial wastewater which is discharged directly into the sea water without extensive treatment. The four main components of wastes in the Saudi Arabia industries are large-volume cooling water, lower volume but high-to-low strength process wastes from refineries and petrochemicals, and sanitary wastes. In addition, future expansion in the refineries and secondary industries in the areas will result in a greater pollution of the seawater and thus affect the productivity and quality of the seawater and environments surrounding the industrial areas.

An unfortunate consequence of industrialization is the generation and the release of toxic waste products which are polluting our environment. Heavy metal contamination of various water resources is of great concern because of the toxic effects of heavy metals on human beings and other animals and plants, even at very low concentrations, and were listed as priority pollutants by the United States Environmental Protection Agency.

Addressing these problems calls out for a tremendous amount of research to be conducted to identify robust new methods of purifying water at lower cost and with less energy consumption, while at the same time minimizing the use of chemicals and impact on the environment. Advanced techniques of the science and technology are being developed to improve the disinfection and decontamination of water, as well as efforts to increase water supplies through the safe re-use of wastewater and efficient desalination of sea and brackish water. Adsorption has been proved to be an excellent way to treat industrial waste effluents, offering significant advantages like the low-cost, availability, profitability, easy of operation and efficiency.

In recent years, biosorption using materials of biological origin as the adsorbents for heavy metal removal has attracted more interest, largely due to the unique properties of these biomaterials being environmentally benign, low cost, effective at low metal concentrations, and easily reusable. Among these biomaterials, chitosan, a derivative from N-deacetylation of chitin (a naturally abundant polysaccharide from crustacean and fungal biomass) has particularly attracted attention because of its capability to chemically or physically adsorb various heavy metal ions.

Chitosan has received considerable interests for heavy metals removal due to its excellent metalbinding capacities and low cost as compared to the activated carbon. Chitosan can be recycled by releasing bound metals with an acid wash leaving the metal waste more highly concentrated in a greatly reduced volume. After rinsing with water, chitosan is available for immediate re-use. However, chitosan usually displayed poor acidic resistance and would gradually dissolve in a solution of pH 4 or less, which is considered a major drawback of chitosan as most industrial wastewater containing heavy metals are almost acidic and eventually, will limit the use of the chitosan, as low-cost recyclable sorpent, in decontamination of industrial wastewater.

Objectives:

One goal of this research is to investigate and plan to overcome the above mentioned dilemma through the synthesis of new and novel chitosan derivatives, crown ether crosslinked chitosan. This crown ether crosslinked chitosan is a water insoluble derivative either in a basic or in an acidic medium and still exhibits an excellent heavy metal adsorption capacity. In addition, the crown ethers, which contain a hydrophobic ring of ethylenic groups surrounding a hydrophilic cavity of

ether oxygen atoms, possess the greatest affinities for the alkali and alkaline earth cations. The crown ether crosslinked chitosan proposed to be synthesized will be characterized using analytical and instrumental methods. Also, its adsorptive properties of industrial heavy metals either in basic or acidic industrial waste water will be characterized for large scale usefulness in decontamination of industrial waste water to be re-used in our daily life as in agriculture and in industries that require large amounts of water as in cooling process of nuclear plants or even to be re-used for human being.

(The project finished and published August 2010)

Project 3: (1,000,000.0 SR)

2012-2013 Design and Synthesis of Novel Cholesterol-Conjugated 5-Fluorouracil Compounds: Their Loading in nanocarriers as Novel Delivery System for Cancer Treatment. King Abdulaziz City for Science and Technology 2011 (10-NAN1286-02) (PI:

Awwad A Radwan; Co-I: Fares K Al-Anazi).

Overview:

In this study, cholesterol esters will be conjugated to 5-fluorouracil to generate a series of new cholesterol 5-fluorouracil (5-FU) compounds. These compounds will be loaded to low density lipoprotein (LDL). Also, these compounds will then be packaged into liposomes.

It is proposed that the LDL-loaded with cholesterol-5-FU conjugates will specifically bind, including its loaded anticancer drug, to the LDL receptor (which is highest recognized on cancer cells) and deliver the 5-FU to the tumor cell. Following development of the pro-drug liposomes, they will be tested for their ability to inhibit growth of breast carcinoma cells and in vivo using animal model.

Supervision of postgraduate students

Co-supervising of master degree students, all of them are graduated successfully and the work has been published.

Publications

<u>2021</u>

- Awwad A. Radwan, Fres K. Aanazi, Mohammed AL-AGAMY, Gamal M. Mahrous. Design, synthesis and molecular modeling study of substituted indoline-2-ones and spiro[indoleheterocycles] with potential activity against Gram-positive bacteria. Acta Pharm. 71 (2021) ???– ???. https://acta.pharmaceutica.farmaceut.org/wp-content/uploads/2021/02/Radwan.pdf
- Awwad A Radwan, Gamal A Magrous, Fars K Alanazi. FDA-antiviral drugs as potential candidates against SARS-CoV-2 main protease: structure and ligand-based database screening. J. Enz. Inh. Med. Chem. Submitted February 2nd 2021 (Subm. ID: 213384282).

<u>2020</u>

- Awwad Radwan, Mahrous GM (2020) Docking studies and molecular dynamics simulations of the binding characteristics of waldiomycin and its methyl ester analog to Staphylococcus aureus histidine kinase. PLoS ONE 15(6): e0234215. https://doi.org/10.1371/journal.pone.0234215.
- Ibrahim Darwish, et al. Preparation and characterization of two immunogens and production of polyclonal antibody with high affinity and specificity for darunavir, a potent antiviral drug used for treatment of acquired immunodeficiency syndrome (AIDS). Plosone submitted (January 2020; PONE-D-20-00994)
- Saleh A. Alanazi, Gamaleldin I. Harisa, Mohamed M. Badran, Nazrul Haq, Awwad A. Radwan, Ashok Kumar, Faiyaz Shakeel and Fars K. Alanazi, "Cholesterol-Conjugate as a New Strategy to Improve the Cytotoxic Effect of 5-Fluorouracil on Liver Cancer: Impact of Liposomal Composition", Current Drug Delivery (2020) 17: 1. https://doi.org/10.2174/1567201817666200211095452
- Saleh Alanazi, Mohamed Badran, Gamaleldin Harisa, Nazrul Haq, Awwad Radwan, Ashok Kumar, Faiyaz Shakeel, Fars Alanazi. Consequence of cholesterol conjugation and content on antitumor activity of liposome: Pharmaceutical chattels. Current Drug Delivery. Galey proof accepted Vol. 17 2020.

 Awwad A. Radwan, Fares K.Alanazi, In Silico studies on novel inhibitors of MERS-CoV: Structure-based pharmacophore modeling, database screening and molecular docking. Trop. J. Pharm. Res. 2018, 17(3), 513-517.

<u>2017</u>

<u>Awwad Abdoh Radwan</u>, Fares Kaed Alanazi, Mohammed Hamed Al-Agamy, 1,3,4Thiadiazole and 1,2,4-triazole-3(4H)-thione bearing salicylate moiety: synthesis and evaluation as anti-Candida albicans. Braz. J. Pharm. Sci. 2017;53(1):e15239

<u>2016</u>

- <u>Awwad A. Radwan</u>, F. Al-Mohanna, Fares K. Alanazi, P.S. Manogaran, Abdullah AlDhfyan. Target β-catenin/CD44/Nanog axis in colon cancer cells by certain *N'*-(2-oxoindolin3-ylidene)-2-(benzyloxy)benzohydrazides. *Bioorg. Med. Chem. Let.* 2016, 1664–1670.
- Faiyaz Shakeel, Nazrul Haq, <u>Awwad A. Radwan</u>, Fars K. Alanazi, Ibrahim A. Alsarra.
 Solubility and thermodynamic analysis of N'-(1-(N-(methyl)benzylaminomethyl)-2-oxoindolin-3-ylidene)-2-(benzyloxy)benzohydrazide in different neat solvents at different temperatures. *Journal of Molecular Liquids* 2016, 220, 108–112.
- Faiyaz Shakeel, Nazrul Haq, <u>Awwad A. Radwan</u>, Fars K. Alanazi, Ibrahim A. Alsarra.
 Solubility and solvation behavior of N'-(1-(N-(methyl)benzylaminomethyl)-2-oxoindolin-3ylidene)-2-(benzyloxy)benzohydrazide in (PEG 400 + water) mixtures. *Journal of Molecular Liquids* 2016, 221, 1225–1230.

<u>2015</u>

Awwad Abdoh Radwan. Pharmacophore elucidation and molecular docking studies on phosphodiesterase-5 inhibitors. *Bioinformation* 2015, 11, 63–66.

- Fars K. Alanazi, Nazrul Haq, Awwad A. Radwan, Ibrahim A. Alsarra, and Faiyaz Shakeel.
 Formulation and evaluation of cholesterol-rich nanoemulsion (LDE) for drug delivery potential of cholesteryl-maleoyl-5-fluorouracil. *Pharm Dev Technol*, 2015, 20, 266–270.
- Mohamed A. IBRAHIM, Gamal M. MAHROUS, Gamal A. SHAZLY, Awwad A.
 RADWAN. Formulation of Theophylline-Loaded Pellets Based on Chitosan: Powder Wet Mass
 Characterization. Lat. Am. J. Pharm. 2015, 34, 797-802.
- Awwad A Radwan. Structure-Based Virtual Screening for Novel EGFR Kinase Inhibitors Using the Zinc Database. *Lat. Am. J. Pharm.* 2015, 34, 1107-12.

<u>2014</u>

- <u>Awwad A. Radwan</u>, Mostafa M. Ghorab, Mansour S. Alsaid, Fares K. Alanazi. Novel ethyl 1,5-disubstituted-1*H*-pyrazole-3-carboxylates as a new class of antimicrobial agents. *Acta Pharm.* 2014, 64, 335–344. DOI: 10.2478/acph-2014-0028.
- A.A. Radwan, T. Aboul-Fadl, A. AL-Dhfyan and W.M. Abdel-Mageed. Synthesis and Characterization of *bis*-3,5-Disubstituted Thiadiazine-2-thione Derivatives as Anticancer Agents. *Asian journal of chemistry* 2014, 26 (23), 8145-8150.
- <u>Awwad A. Radwan</u>, Fares K. Alanazi. Design and Synthesis of New Cholesterol-Conjugated
 5-Fluorouracil: A Novel Potential Delivery System for Cancer Treatment. *Molecules* 2014, *19*, 13177-13187
- <u>Awwad A. Radwan</u>, Wael Abdel-Mageed. In silico studies of quinoxaline-2-carboxamide 1,4di-N-oxide derivatives as antimycobacterial agents. *Molecules* 2014, *19*(2), 2247-2260.
- <u>Awwad A. Radwan</u>, Fares K. Alanazi. Targeting cancer using cholesterol conjugates. *Saudi Pharmaceutical Journal* 2014, 22(1) 3–16.
- Mohamed I Attia, Awwad A Radwan, Azza S Zakaria, Maha S Almutairi, Soraya W Ghoneim. 1-Aryl-3-(1 H-imidazol-1-yl)propan-1-ol esters: synthesis, anti-Candida potential and molecular modeling studies. *Chemistry Central Journal* 2013, 7, 168.

- <u>Awwad A. Radwan</u>, and Kamal El-dein El-Taher. Synthesis and in-silico studies of some diaryltriazole derivatives as potential cyclooxygenase inhibitors. *Archive Pharm Res.*. 36, 2013, 553–563.
- <u>Awwad A. Radwan</u>, Fares K. Alanazi, Abdallah Al-Dhfyan, Synthesis, and docking studies of some fusedquinazolines and quinazolines carrying biological active isatin moiety as cellcycle inhibitors of breast cancer cell lines. *Drug Res* (Arzneimittelforschung) 63, 2013, 129–136.
- Awwad A. Radwan. Design, synthesis, and molecular modelling of novel 4-thiazolidinones of potential activity against Gram-positive bacteria. *Med. Chem. Res.* 2013, 22(3), 11311141.
- Mostafa M. Ghoraba, Zienab H. Ismail, Mohamad Abdalla, <u>Awwad A. Radwan</u>, Synthesis, antimicrobial evaluation and molecular modelling of novel sulfonamides carrying a biologically active quinazoline nucleus. *Arch. Pharm. Res.* 2013, 36(6), 660-70. doi: 10.1007/s12272-013-0094-6.
- Mostafa M. Ghoraba, Zienab H. Ismail, <u>Awwad A. Radwan</u>, Mohamad Abdalla. Synthesis and pharmacophore modeling of novel quinazolines bearing a biologically active sulfonamide moiety. *Acta Pharm*. 2013, 63, 1–18.

<u>2012</u>

- Tarek Hassan; <u>Awwad Radwan</u>; Mohamad I Attia; Abdullah Al-Dhfyan; Hatem Abdel-Aziz.
 Schiff bases of indoline-2,3-dione (isatin) with potential antiproliferative activity. *Chemistry Central Journal* 2012, 6:49.
- Tarek Aboul-Fadl, <u>Awwad A. Radwan</u>, Hatem A. Abdel-Aziz, Mohd. Baseeruddin, Mohamad I. Attia and Adnan Kadi. Novel Schiff bases of indoline-2,3-dione and nalidixic acid hydrazide: synthesis, *in vitro* antimycobacterial and in silico mycobacterium tuberculosis (mtb) DNA gyrase inhibitory activity. *Digest Journal of Nanomaterials and Biostructures*, 2012, 7, 327 – 336.
- <u>Awwad A. Radwan</u>, Abdullah Al-Dhfyan, Mohammed K. Abdel-Hamid, Abullah Al-Badr and Tarek Aboul-Fadl. 3,5-Disubstituted Thiadiazine-2-Thiones: New Cell-Cycle Inhibitors.

<u>2010</u>

- <u>Awwad A. Radwan</u>, Fars K. Alanazi and Ibrahim A. Alsarra. Microwave irradiation-assisted synthesis of a novel crown ether crosslinked chitosan as a chelating agent for heavy metal ions (M⁺ⁿ). *Molecules* 2010, 15, 6257-6268.
- Fars K. Alanazi, Awwad A. Radwan and Ibrahim A. Alsara, Biopharmaceutical Application of Nanogold, *Saudi Pharmaceutical Journal* 2010, 18, 179-193.
- Marc Lindner, Wolfgang Sippl and <u>Awwad A Radwan</u>. Pharmacophore elucidation and molecular docking studies on 5-phenyl-1-(3-pyridyl)-1H-1,2,4-triazole-3-carboxylic acid derivatives as COX-2 inhibitors. *Scientia Pharmaceutica* 2010, 78, 195-214.

<u>2009</u>

Mohammad A. Shaaban, <u>Awwad A. Radwan,</u> Yaseen A. Mosa and Basel A. Abd-Elwahab, Synthesis and docking study of some pyrazolo[3,4-d]pyrimidin-4(5H)-one derivatives as phosphodiesterase-5 inhibitors, *Saudi Pharmaceutical Journal* 2009, 17, 109-129.

<u>2008</u>

Yaser A.-H. Mostafa, Mostafa A. Hussein, <u>Awwad A. Radwan</u>, and Abd El-Hamid N. Kfafy;
 Synthesis and Antimicrobial Activity of Certain New 1,2,4-Triazolo[1,5-a]Pyrimidine
 Derivatives. *Arch. Pharm. Res.* 2008, 31, 279-293.

<u>2007</u>

- Ahmad M. Ali, Gamal El.-D. Saber, Nadia M. Ahmad, Mahmoud Abdel-F. El-Gendy,
 Awwad <u>A. Radwan</u>, Mohammad Ismail. Synthesis And Three-Dimensional Qualitative Structure Selectivity Relationship Of 3,5-Disubstituted-2,4-Thiazolidinedion Derivatives As COX2 Inhibitors. *Arch. Pharm. Res.* 2007, 30, 1186-1204.
- □ Alaa Hyallah and <u>Awwad A Radwan</u>. Synthesis and Quantitative Structure Activity

Relationship of New 3-Allyl-5-substituted-tetrahydro-2H-1,3,5-Thiadiazine-2-Thiones of Potential Antimicrobial Activity. Bull. Pharm. Sci., Assiut University, 2007, 30, 39-50.

<u>2006</u>

 <u>Awwad A. Radwan</u> and N. A. Hussein. Synthesis and Antimicrobial Activity of Some 3-(1Phenylethyl)-5-Substituted-2H-Tetrahydro-1,3,5-thiadiazine-2-thione Derivatives. *Bull. Pharm. Sci, Assiut* University, 2006, 28, 255-260.

<u>2002</u>

 <u>Awwad A. Radwan</u>, *Doctor thesis* (2002). Rational Procedure for 3D QSAR Analysis Using TRNOE Experiments and Computational Methods: Application to Thermolysin Inhibitors.

<u>2001</u>

 <u>Awwad A. Radwan</u>, Hiroaki Gouda, Noriyuki Yamaotsu, Hidetaka Torigoe and Shuichi Hirono. Rational Procedure for 3D QSAR Analysis Using TRNOE Experiments and Computational Methods: Application to Thermolysin Inhibitors. *Drug Design and Discovery*, 2001, 17, 265-281.

<u>1995</u>

Awwad A. Radwan, Master thesis (1995). Synthesis and evaluation of the cytotoxic and anti viral activities of 5,6-disubstituted isocytosine derivatives.

<u>1994</u>

Awwad A. Radwan, Abdel-Nasser A. El-Shorbagi, Abdel-Alim M. Abdel-Alim, Nadia M. Mahfouz and Emad K. Nafei. Alex. J. Pharm. Sci., Vol. 8 (3) October 1994/155

Contribution Publication (research activity):

Faiyaz Shakeel, Nazrul Haq, <u>Awwad A. Radwan</u>, Fars K. Alanazi, Ibrahim A. Alsarra.
 Solubility and thermodynamic analysis of N'-(1-(N-(methyl)benzylaminomethyl)-20x0indolin 3-ylidene)-2-(benzyloxy)benzohydrazide in different neat solvents at different

jml_pure016 temperatures.

Journal of Molecular Liquids 2016, 220, 108–112.

 Faiyaz Shakeel, Nazrul Haq, <u>Awwad A. Radwan</u>, Fars K. Alanazi, Ibrahim A. Alsarra.
 Solubility and solvation behavior of N'-(1-(N-(methyl)benzylaminomethyl)-2-oxoindolin-3ylidene)-2-(benzyloxy)benzohydrazide in (PEG 400 + water) mixtures. *Journal of Molecular* jml_peg016

Liquids 2016, 221, 1225–1230.

<u>2015</u>

- F.K. Alanazi, N. Haq, A.A. Radwan, I.A. Alsarra, F. Shakeel. Development and validatedion of UHPLC-DAD method for analysis of cholesteryl-hexahydrophthaloyl-5-fluorouracil in lipid nanoemulsion. *Journal of Analytical Chemistry* 2015, 70(5), 1-7.
- F.K. Alanazi, N. Haq, A.A. Radwan, I.A. Alsarra, F. Shakeel. Validated UHPLC-DAD method for quantification of cholesteryl-succinyl-5-fluorouracil in lipid nanoemu–Submitted to Analytical Letters. (ISI IF 1.02).
- Fars K. Alanazi, Nazrul Haq, Awwad A. Radwan, Ibrahim A. Alsarra, and Faiyaz Shakeel. Formulation and evaluation of cholesterol-rich nanoemulsion (LDE) for drug delivery potential of cholesteryl-maleoyl-5-fluorouracil. Pharm. Dev. Tech. (Online, Epub ahead of print).

 F.K. Alanazi, N. Haq, A.A. Radwan, I.A. Alsarra, F. Shakeel. Potential of lipid nanoemulsions for drug delivery of cholesteryl-hexahydrophthaloyl-5-fluorouracil–Submitted to *The Scientific World Journal. (ISI IF 1.73).*

<u>2014</u>

- Fares K. Alanazi, <u>Awwad A. Radwan</u>, Nazrul Haq, Ibrahim A. Alsarra, Fayaz Shakeel.
 Validated UHPLC-DAD method for quantification of cholesteryl-succinyl-5-fluorouracil conjugate *Bulgarian Chemical Communications*, 2104, 46(4), 806 813.
- Fars K. Alanazia, Nazrul Haq, <u>Awwad A. Radwan</u>, Ibrahim A. Alsarra, Faiyaz Shakeel. Quantification of cholesteryl-maleoyl-5-fluorouracil conjugate in lipid nanoemulsion by validated UHPLCDAD method. *Wulfenia journal* 2014, *21*, 151-172.
- F.K. Alanazi, N. Haq, <u>A.A. Radwan</u>, I.A. Alsarra, F. Shakeel. Cholesterol-rich nanoemulsions (LDE) for drug targeting of cholesteryl-succinyl-5-fluorouracil conjugate.
 Current Nanoscience, 2014, *10*, 287-291.

<u>2013</u>

Nazrul Haq, Faiyaz Shakeel, Fars K. Alanazi, <u>Awwad A. Radwan</u>, Mohammad Ali, Ibrahim
 A. Alsarra. Development and Validation of an Isocratic, Sensitive and Facile RP-HPLC
 Method for Rapid Analysis of 5-Fluorouracil and Stability Studies Under Various Stress
 Conditions. *Asian J. Chem.*, 2013, 25(13), pp 7177-7182.

Patents:

1- EP 2540746 (3/03/2013)

Title: Chitosan derivative, a method for its preparation and its use as an adsorption agent (application number EP11171632.0, Date of application 28 June 2011)

2- EP 2 527 335 A1 (28.11.2012)

Title: Triazole compounds as anti-inflammatory agents
 (application number EP 11163672.6, Date of application 26.04.2011).

3. US 8,829,016 B2 (Sep. 9, 2014)

□ Triazole compounds as potential anti-inflammatory agents.

Awards:

- ACDIMA Award for best research in 2008 from ACDIMA drug company (Oman, Jordanian, 2008). Synthesis and Three-dimensional Qualitative Structure Selectivity Relationship of 3,5-Disubstituted-2,4Thiazolidinedione Derivatives As COX2 Inhibitors.
- ACDIMA Award for best research in 2008 from ACDIMA drug company (Oman, Jordanian, 2012).
 3,5-disubstituted thiadiazine-2-thiones: New cell cycle inhibitors.

Achievements:

The research work had been presented in several conferences.

02-2104 Novel Quinazoline Derivatives as Cell-cycle Inhibitors of Breast Cancer Cell Lines: Design, Synthesis, and Molecular Modelling Studies. 6th International Conference on Drug Discovery and Therapy February 10th- 12th, 2014 (Dubai, UAE)

04-2013 Cholesterol-based Cancer treatment (lecture) Future University International Conference on Pharmaceutical Science, APRIL 13-15, 2013, Cairo International Conference Centre, Cairo, Egypt.

09-2012 The Saudi International Biotechnology Conference, September 18-19, 2012, KACST Headquarter-Conference Hall-Building 36 King Abdullah Road – Riyadh, Kingdom of Saudi Arabia (attendance).

04-2010 The 8th Saudi International pharmaceutical Conference and Exhibiton, April 25-28, 2010, Prince Sultan Hall at Alfaisaliah Tower, Al-Rhiyadh/Saudi Arabia p ... (poster).

03-2010 Awwad A Radwan and Fars K Alanazi. Synthesis and molecular modelling of 1,2,4triazole derivatives as selective cox-2 inhibitors anti-inflammatory. 7th International Pharmaceutical Sciences Conference, March 17-18th, 2010, Assiut University, Assiut, Egypt. P 77 (poster).

02-2009 1st International Conference in Biotechnology, February 16-18, 2009, King Fahd Cultural Center, Riyadh, Saudi Arabia (Audience).

07-2007 Mohamed Abdel Rahman Shaaban, <u>Awwad A. Radwan</u>, Yaseen A. Mosa. Synthesis and Docking Study of New Pyrazolo[3, 4-d]pyrimidine-4-one Derivatives as Phosphodiesterase5 Inhibitors. 6th AFMC International Medicinal Chemistry Symposium, July 08-11, 2007, Istanbul/Turkey. p 78 (**poster**).

02-2007 Mamdouh F. Ahmed, <u>Awwad A. Radwan</u> and Abdel-Gaber N. Osman. Synthesis of some new quinoline derivatives of potential anti-inflammatory and analgesic activities. 10th Ibn Sina International Conference on Pure and Applied Heterocyclic Chemistry, February 17-20, 2007, p 191. (**poster**).

02-2007 Awwad A. Radwan, Marc Lindner and Wolfgang Sippl. Pharmacophore elucidation and molecular docking studies on 5-phenyl-1-(3-pyridyl)-1H-1,2,4triazole-3-carboxylic acid derivatives as cox2 inhibitors.. 10th Ibn Sina International Conference on Pure and Applied Heterocyclic Chemistry, February 17-20, 2007, p 191, Luxor, Egypt.

(poster).

03-2006Alaa M. Hayallah and <u>Awwad A. Radwan</u>. Quantitative StructureActivity Relationship (QSAR) Analysis of Some Thiadiazine Thione Derivatives As AntifungalAgents Against Scopulariopsis Brevicaulis Fungi. Assiut University 5th Pharmaceutical SciencesConference, Faculty of Pharmacy, Assiut, March 7-8th , 2006, p 282. (poster)

12-2004 <u>Awwad A. Radwan</u> and Naemat A. Husein. Synthesis and Antimicrobial activity of Some 3,5-Disubstituted Tetrahydro-2H-1,3,5-Thiadiazine-2-Thione Derivatives. 9th Ibn Sina International Conference on Pure and Applied Heterocyclic Chemistry, December, 11-14, 2007, p 167. Sharm El-Sheikh, Egypt. (**poster**).

10-2000Awwad A. Radwan, Hiroaki Gouda, Noriyuki Yamaotsu, HidetakaTorigoe and Shuichi Hirono (2001):Rational Procedure for 3D QSAR Analysis Using TRNOEExperiments and Computational Methods:Application to Thermolysin Inhibitors. 28th Symposiumon Structure-Acitivity Relationships, Kyoto, Japan, October 2000, pp. 282-285. (poster)

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