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Education

- ✓ PhD, Physical Chemistry,sherbrooke - 2013
- ✓ B.Sc, , - 2011
- ✓ MS, , - 2012

Courses

- | | |
|--|------------------------------------|
| 1. Bio Molecular Systems Modeling | 2. physical chemistry 3 |
| 3. The Application of Computer in Chemistry | 4. physical chemistry 2 |
| 5. General Chemistry1 | 6. physical chemistry laboratory 1 |
| 7. General chemistry in chemical engineering | 8. quantom chemical |
| 9. Advanced physical chemistry | 10. molecular spectroscopy |
| 11. physical chemistry 1 | 12. Biophysical Chemistry |

Master Thesis

Journals Papers

2023

1. [Synthesis, Characterization, Cytotoxicity and DNA/ BSA Interaction of Pd\(II\) Complexes with AlkylAmine and 1,10-Phenanthroline](#)

Farahnaz Mohamadlo, Hassan Mansouri Torshizi, Effat Dehghanian, Khatereh Abdi

POLYCYCLIC AROMATIC COMPOUNDS Volume: (43) 6730 - 6749

2. [A new zinc\(II\) complex of 2-benzoimidazoledisulfide ligand: synthesis, X-ray crystallographic structure, investigation of CT-DNA and BSA interaction by spectroscopic techniques and molecular docking](#)

Farahnaz Mohamadlo, Hassan Mansouri Torshizi, Effat Dehghanian, Mahboubeh Eslami-Moghadam, Michal Du

JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY Volume: (443) 114830-1 - 114830-15

3. [Au\(III\) complexes of symmetrical tetradentate Schiff base ligands: Synthesis, characterization, anticancer/antioxidant potency, in silico prediction, and catalase binding properties](#)

Alireza Oveisikeikha, Somaye Shahraki, Hassan Mansouri Torshizi, Effat Dehghanian, Mostafa Heidari M

APPLIED ORGANOMETALLIC CHEMISTRY Volume: (37) e7139-1 - e7139-17

4. [Zn\(II\) and Pd\(II\) Complexes Derived from Novel Benzohydrazide-based Schiff Base Ligand as Multi-target Agents](#)

Alireza Oveisikeikha, Hassan Mansouri Torshizi, Somaye Shahraki, Effat Dehghanian

JOURNAL OF MOLECULAR LIQUIDS Volume: (391) 123272-1 - 123272-16

5. [Exploring the Interaction Between the Newly Designed Antitumor Zn\(II\) Complex and CT-DNA/BSA: Spectroscopic Methods, DFT Computational Analysis, and Docking Simulation](#)

ASHRAF SADAT DORAFSHAN TABATABAEI, Effat Dehghanian, Hassan Mansouri Torshizi

APPLIED BIOCHEMISTRY AND BIOTECHNOLOGY Volume: (195) 6276 - 6308

6. [Spectroscopy, docking and molecular dynamics studies on the interaction between cis and trans palladium-alanine complexes with calf-thymus DNA and antitumor activities](#)

Asma Izadyar, Hassan Mansouri Torshizi, Effat Dehghanian, Somaye Shahraki

JOURNAL OF COORDINATION CHEMISTRY Volume: (76) 519 - 542

2022

7. [Probing the interaction of new and biologically active Pd\(II\) complex with DNA/BSA via joint experimental and computational studies along with thermodynamic, NLO, FMO and NBO analysis](#)

ASHRAF SADAT DORAFSHAN TABATABAEI, Effat Dehghanian, Hassan Mansouri Torshizi

BIOMETALS Volume: (35) 245 - 266

8. Probing the biomolecular (DNA/BSA) interaction by new Pd(II) complex via in-depth experimental and computational perspectives: synthesis, characterization, cytotoxicity, and DFT approach

Mehran Feizi, Effat Dehghanian, Hassan Mansouri Torshizi

Journal of the Iranian Chemical Society JICS Volume: (19) 3155 - 3175

9. Biological activity of bis-(morpholineacetato)palladium(II) complex: Preparation, structural elucidation, cytotoxicity, DNA-/serum albumin-interaction, density functional theory, in-silico prediction and molecular modeling

Mehran Feizi, Effat Dehghanian, Hassan Mansouri Torshizi

SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY Volume: (281) 121543-1 - 121543-17

10. Diverse coordination of dipicolinic acid to Pd(II) ion result antitumor complexes, their interaction with CT-DNA by spectroscopic experiments and computational methods

Ameneh Heidari, Hassan Mansouri Torshizi, Maryam Saeidifar, Effat Dehghanian, Khatereh Abdi, Hojat S

JOURNAL OF MOLECULAR STRUCTURE Volume: (1261) 132937-1 - 132937-12

11. In-silico and in-detail experimental interaction studies of new antitumor Zn(II) complex with CT-DNA and serum albumin

ASHRAF SADAT DORAFSHAN TABATABAEI, Effat Dehghanian, Hassan Mansouri Torshizi

JOURNAL OF BIOMOLECULAR STRUCTURE and DYNAMICS Volume: () 1 - 18

12. Synthesis, characterization, cytotoxicity and DNA/ BSA binding of two amino acid palladium(II) complexes derived from alanine and valine

, Hassan Mansouri Torshizi, Maryam Saeidifar, Effat Dehghanian, Eliska Skorepova, Michal Dusek, Khat

NUCLEOSIDES NUCLEOTIDES and NUCLEIC ACIDS Volume: (41) 97 - 122

13. A couple of antitumor Pd(II) complexes make DNA-refolding and HSAunfolding: Experimental and docking studies

, Hassan Mansouri Torshizi, Khatereh Abdi, Effat Dehghanian, Maryam Saeidifar,

JOURNAL OF MOLECULAR LIQUIDS Volume: (349) 118450-1 - 118450-18

2021

14. Synthesis and characterization of Pd(II) antitumor complex, DFT calculation and DNA/BSA binding insight through the combined experimental and theoretical aspects

Mehran Feizi, Effat Dehghanian, Hassan Mansouri Torshizi

JOURNAL OF MOLECULAR STRUCTURE Volume: (1240) 130535-1 - 130535-15

15. A novel palladium(II) antitumor agent: Synthesis, characterization, DFT perspective, CT-DNA and BSA interaction studies via in-vitro and in-silico approaches

Mehran Feizi, Effat Dehghanian, Hassan Mansouri Torshizi

SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY Volume: (249) 119215-1 - 119215-17

16. A modified binary particle swarm optimization with a machine learning algorithm and molecular docking for QSAR modelling of cholinesterase inhibitors

Elaheh Shamsi, Amin Rahati, Effat Dehghanian

SAR AND QSAR IN ENVIRONMENTAL RESEARCH Volume: (32) 745 - 767

17. DNA/BSA binding affinity studies of new Pd(II) complex with S-S and N-N donor mixed ligands via experimental insight and molecular simulation: Preliminary antitumor activity, lipophilicity and DFT perspective

Mehran Feizi, Effat Dehghanian, Hassan Mansouri Torshizi

JOURNAL OF MOLECULAR LIQUIDS Volume: (344) 117853-1 - 117853-17

2019

18. Enhanced GROMACS: toward a better numerical simulation framework

Hojjat Rakhshani, Effat Dehghanian, Amin Rahati

JOURNAL OF MOLECULAR MODELING Volume: (25) 355 - 363

2018

19. A multiobjective approach in constructing a predictive model for Fischer-Tropsch synthesis

Effat Dehghanian,

JOURNAL OF CHEMOMETRICS Volume: (32) 1 - 20

2017

20. PRODUCTS DISTRIBUTION MODELING OF FISCHER-TROPSCH SYNTHESIS ON FE-K-SIO₂ CATALYST USING DIFFERENTIAL EVOLUTION OPTIMIZATION ALGORITHM

Effat Dehghanian,

Volume: (12) 131 - 145

2016

21. Hierarchy cuckoo search algorithm for parameter estimation in biological systems

Hojat Rakhshani, Effat Dehghanian, Amin Rahati

CHEMOMETRICS AND INTELLIGENT LABORATORY SYSTEMS Volume: (159) 97 - 107

22. Hierarchy Cuckoo Search Algorithm for parameter estimation in biological systems

Hojat Rakhshani, Effat Dehghanian, Amin Rahati

CHEMOMETRICS AND INTELLIGENT LABORATORY SYSTEMS Volume: (159) 97 - 107

2015

23. Comparison of single best artificial neural network and neural network ensemble in modeling of palladium micro-extraction

Effat Dehghanian, Massoud Kaykhaii

MONATSHEFTE FUR CHEMIE Volume: (146) 1217 - 1227

24. مقایسه روش های شبکه عصبی تکی و جمعی جهت مدل کردن میکرو استخراج پالادیوم

Effat Dehghanian, Massoud Kaykhaii,

MONATSHEFTE FUR CHEMIE Volume: (146) 1217 - 1227

2013

25. Enhanced ionization of the non-symmetric HeH molecule driven by intense ultrashort laser pulses

Effat Dehghanian, A.D Bandrauk,

JOURNAL OF CHEMICAL PHYSICS Volume: (139) 1 - 15

Conferences Papers

2019

1. Investigation of Beta- Secretase inhibitors interactions in the treatment of Alzheimer disease

8th Iranian Conference on Bioinformatics

Eghbal Joobeh, Effat Dehghanian

2. Disquisition of interaction between anti-alzheimer drugs and bovin serum albumin; a computational study

8th Iranian Conference on Bioinformatics

Mehran Feizi, Effat Dehghanian

2018

3. Investigation of some inhibitors of Alzheimer associated amyloid beta aggregation by quantum optimization and molecular docking simulation

21st ICS Physical Chemistry Conference

Ashraf Dorafshantabatabei, Effat Dehghanian, Milad Lagzian

2017

4. Computational modeling of liquid phase microextraction of malondialdehyde from human blood plasma by multi-layer perceptron

6th Iranian Biennial Chemometrics Seminar

Saeideh Sanchooli, Effat Dehghanian, Massoud Kaykhaii

5. Modeling of reversed-phase direct immersion microextraction of acrylamide by feed forward neural network

6th Iranian Biennial Chemometrics Seminar

Effat Dehghanian, Massoud Kaykhaii, Hasan Keykha