# Curriculum Vitae

*Mazen Yousef Hamed*

## *Personal information*

**Marital status**: Married,

## *Contact Information*

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EDUCATION

**PhD**. Chemistry, (Bio-inorganic) 1983 Chemistry department, University of Essex, Wivenhoe Park, Colchester, CO4 3SQ, **UK**

**B.Sc**. Chemistry, 1978 Chemistry Department, University of **Jordan**

## *Academic and Professional Positions Held*

• **Current: Associate professor Chemistry/BZU**

**Visiting Scholar2008/2009 , Nanoengineering, Atkinson Hall, 9500 Gilman, University of California at Sandiego(UCSD), Lajolla, California (Aug2008-**

• Associate professor, Chemistry Department, Birzeit University 1992- 2008

* Chairman of Department 1994-1997

* Research Associate, Biochemistry Department, University of California (Berkeley) 1989-1990.

* Assistant Professor Chemistry Department, Birzeit University 1983-1989

* Teaching assistant, Inorganic chemistry, University of Essex, UK 1979-1983

## Honors & Awards

- 1979: British Council Award, Ph.D. study
- 1984, 1985,1991 British Council Awards for research
- 1989: *Fulbright* Award, Research and teaching, USA

- 1992: Associate of *International center for theoretical physics* (ICTP)
- 1994: Associate of the International *Center for Theoretical Physics*/Biophysics (ICTP), Triest, Italy.
- 2008: Fulbright, UCSD, California, USA

## Research Grants

- Grants for research From International Centre for Theoretical Physics (ICTP) 1994
- Research grant from The Board of Research (Council of Higher Education) 1995
- support of the *Board for Higher Education research Committee*
- Research grant from *Third World Academy of Sciences* TWAS. 1996
- Research Grants from Birzeit University 1998
- Research Grant from BZU 2006,2007

## • Membership in Scientific Organizations

- Royal Chemical Society(UK)
- New York Academy of sciences
- Society for Biological inorganic chemistry

## Fields of Interest and Current Research

**Current: Molecular dynamics and binding energy calculations on zinc finger proteins as transcription factors: studying DNA recognition by DNA binding residues**

**Research**: Study of the DNA binding repressor proteins (i.e Ferric uptake regulation protein) and the role of co-repressors in the activation deactivation mechanism.

Both experimentally and using theoretical approach

Computer aided Molecular design: the work involves establishing the mode of action of Fur protein and its conformational tuning upon its binding to metal ions and to the DNA.

**Background:** Protein folding and the 3 D structure of proteins is one of the most challenging problems in biochemistry
, given the amino acid sequence, the 3-dimensional structure of the protein can be predicted. This technique is rich in mathematical modelling, numerical analysis and other mathematical techniques. **Computational chemistry** is an outgrowth of theoretical chemistry, the role of which involves the creation of infrastructure for the chemical science at the atomic and molecular levels. The significance and widespread applicability of computational chemistry may not always be obvious to people who are not frequently concerned with the activity. It is central to **drug design**, it contributes to **selection and synthesis of new materials** and guides the design of catalysts.. Applications which are heavily used: ESP for Molecular Dynamics, Gaussian for Quantum chemistry AMBER, ARGOS for molecular dynamics**.**

Using computation to identify the binding sites on the DNA binding protein *(Fur*), and any possible conformational changes in both the protein and DNA **iron box** upon the repressor binding – the role of transition metal ions. Molecular modelling proved to be an efficient tool in such studies involving protein molecules [see reference1 &2].
**Theory: Techniques I use**: Alignment, Energy minimization Molecular dynamics, Docking.

- QSAR on organic molecules as potential drugs for the treatment of Alzheimer's' disease: modeling (ChemDraw, HyperChem), Energy Minimization ( AMBER,Hyperchem, Gaussian), Descriptors (Dragon), LOGP, Docking techniques and Matlab.
- **Research interest**:

  Understanding the protein- specific binding to DNA in transcription factors like zinc finger proteins
  The known crystal structures and theoretical work done on the DNA recognition code has achieved progress but the problem is not resolved:
  Some researchers go to the independent specific binding between certain residues and certain DNA bases, for example R known to bind G, E binds C, but other researchers tend to go for cooperative binding for example the alpha-helix residues R binds G, E bind C on the 5'-3' strand while E or D in the same helix binds an A (in neighboring triplet) from the opposite strand (3'-5') . Other work gives importance to the phosphate binding, and water mediated binding.
  Many zinc finger proteins were prepared and were bound to different triplets , thousands of combinations and the strength of binding was analyzed by Segel and co-workers and Kd values were reported

Different studies gave different importance to which set of residues prefer which set of bases, several affinities and specificities were reported .
This problem is very challenging , I am currently analyzing the Zinc finger protein DNA binding using energy minimization and molecular modeling, I will proceed to mutating what is thought to be crucial residues in the helices and study their effect on binding of the whole protein, then vary the bases and study their effect. I am currently studying parts of the protein and going down in the number of helices and calculating the binding energy and other parameters.
I would like at later stages to build triplets and helices and combine and study in order to single out the most significant combination.

- Previous Research **(experimental)**

1. Preparation and characterization of Copper oxide based ceramic superconductors.

2. Electrochemical Studies of Iron (III) and Iron (II) thiol and ascorbate with heme

3. **DNA binding proteins: Repressor proteins which acquire metal ion co-repressor**.

4. Equilibrium and kinetic studies on Cu(II) complexes with anticancer and anti-inflammatory drugs and their reaction with molecular oxygen

- **Molecular Biology Techniques**:
- Protein preparation from Bacteria ( *E.coli)*
- Protein characterization and metal binding using nmr and esr and equilibrium dialysis

The project aims at understanding the repressor activity of the ferric uptake regulation protein in E.Coli: This protein was found to bind the DNA (iron box) at elevated Iron(II) levels using the metal ion as co-repressor to regulate the synthesis of Entrobactin

**Techniques**: column chromatography, gel electrophoresis, metal ion analysis using atomic absorption and ICP, equilibrium dialysis. Metal ion binding studied by electron paramagnetic resonance spectroscopy, $Fe^{57}$Mossbauer spectroscopy.

**Facilities for Computations**

HP cluster

work stations ( dell ) loaded with Amber and docking software running Linux and windows

Molecular Dynamics: Amber 9 and mmpbsa energy calculation

Docking: protein-protein, protein-ligand, protein-DNA

Descriptor calculations Dragon

*Experimental:

Coordination chemistry of biologically important thioles and peptides with Iron(II) and Iron(III)

Techniques: Rapid kinetics, EPR, Mossbauer spectroscopy and thermodynamic equilibrium measurements are used to study the electron transitions which take place and the coordination of metal ion. Important systems under study are Glutathione and cysteine.

*Coordination and electron transfer reactions in the L-ascorbic acid iron(III) and iron(II) complex formation process

Copper complexes with carboxylate and imidazole: Equilibrium studies using potentiometric titration and the SUPERQUAD software. Rapid kinetics for electron transfer and oxygen binding

I have gained experience in employing and teaching the following techniques:

- Spectroscopic techniques: UV-Visible, infrared, nuclear magnetic resonance (nmr)

- Mossbuer spectroscopy in all its aspects, starting with sample preparation, to fitting and interpreting the $^{57}$Fe Mossbuer spectra. I have gained experience in using the

- ***electron paramagnetic resonance*** (epr) spectroscopy and interpreting the results for *transition metal ions like* copper, iron and manganese.

- Chromatographic and analytical techniques: ion analysis, automatic titrator, ICP,

- Gas chromatography, HPLC

I used chemistry related programs like: *ENZfitter* for kinetic studies and DNA binding, , *SUPERQUAD* for Thermodynamic Equilibrium studies I, also, did some successful inter-phasing between my old spectrophotometer and the computer using RS232 communication port and simple software

## *Teaching*

During my work in Birzeit University I have taught

- Inorganic chemistry, where I taught *coordination chemistry, electronic structure of the atom, bonding, reaction mechanism, symmetry and main group chemistry, both experimental and theory .*

- general chemistry for both science and Engineering students,

- Analytical chemistry,

- physical chemistry
- X-ray crystallography,
- Bio-inorganic chemistry,
- industrial chemistry lab and theory
- spectroscopic techniques

Industrial inorganic Chemistry

Advanced Inorganic Chemistry for grad. students

- **graduate courses**: -
- CAMP (computer Aided molecular design) for M.Sc students in Scientific computing
- **Water Quality** for M.sc students in Water Engineering both theory and experiments,
- **Instrumental methods of analysis: using various analytical techniques in water analysis, GC, HPLC, ion analysis, atomic absorption,….**

- ***External examiner for M.sc students in other Palestinian universities***

- Supervising M.Sc. students in scientific computing

Examiner for Msc students working on protein molecular dynamics
Thesis:
MD study of some proteins, Energy minimization studies on proteins, MM on iron carbonyls

## *Administrative Positions and Other Work*

During my chairmanship of the chemistry department ( 14 academic members of staff plus 4 teaching assistants plus 4 technicians and 80 to 100 students) my duties included running the chemistry department in all aspects. Chair the meetings, assign committees and receive reports, Putting the teaching loads, decide the needs of the department from staff, office equipment, instruments, chemicals. In addition to the usual duties I have made improvements on the department curricula by introducing new applied courses and specialization and made cooperation with institutes outside the country.

I have Participated in several academic and Administrative committees in Birzeit University, most important is:

1. the graduate program committee to design and teach M.sc in Scientific computing and follow up the progress of the program Duties include putting the program from scratch, employing staff and accepting students.

2. .Member of the council for graduate program in **Water science& Technology**

3. Member of various University committees on the faculty, department, and University levels.

( member of the council for faculty of science several yearscurricula committeeinstrumentation committeerecruitment committee: the duty is to run the faculty of science in all aspects in cooperation with dean and take crucial academic and administrative decisions, to enhance the faculty's programs and courses and introduce improvements, to study the needs for instruments and study the quotations and to purchase instruments and computers, to study the needs of department in staff and evaluate the staff and contract renewals

**Society and consultations:**

1. Vice Chairman to the **National Committee for Science curriculum**s for Ministry of Education PNA. To put the curricula for science at high schools in Palestine

2. member of the unit for Science & Technology planning: work involved assessing the needs of industry (esp, pharmaceutical industry) for Research and development.

**3.** Consultant to the Palestinian Economic Council for Research and reconstruction (PECDAR) **on Solid waste management**

4. as part of the executive and founding Committee for Palestinian Chemists several workshops and activities were held

5. Founding member of the Palestinian Academic network (PLANET) Connecting all academic institutions in Palestine to the world wide web and together since 1996

*6*. Evaluating graduate and undergraduate Chemistry Programs for QC department in the Ministry of Higher education in Palestine .

**Publications**

*** pending publications: Zinc Finger Protein: Specificity to DNA binding sites calculated by Molecular dynamic simulations, an Energy prospective.**

current work:

# zinc finger protein specificity to DNA fragment: effect of mutating R-1,D2,R6 on the energy of binding of Fingers 1,2 and 3 : in prep

## Effect of F1,F2 and F3 mutations in the wild type zinc finger protein on the specificity of binding as indicated by free energy. in prep

*The Role of metal ion co-repressors in the DNA binding process of EC Fur: Effect of varying metal ion on the process. (Submitted)


1.Hamed, M.Y. and Jabour, S. **The Competition Between Zn(II) and Iron(II) in Binding *E.coli* Fur and the effect on structural and conformational changes of Fur upon DNA binding: an MD study**,

*J. Mol. Graphics and Modeling* (2008). **Accepted:** 3 November 2008 **Published online:** 21 November 2008

2. Hamed, M.Y and Jabour, S. : **Iron(II) Triggered Conformational Changes in *E.coli* Fur upon DNA binding: A study using Molecular dynamics**, *J. Mol. Graphics and Modeling* 25, 234-246(2006)

3.Hamed,M.Y.and Neilands ,J.B.. : **An electron spin resonance study of the Mn(II) and Cu(II) complexes of the Fur repressor protein**, *J. Inorg .Biochem*, 53,235-248 **(1993)**.

4.Hamed,M.Y.,Neilands,J.B., and Huynh,V. :**Binding of the ferric uptake regulation repressor protein(Fur) to Cu(II), Mn(II), Fe(II) and Co(II) ions as co-repressors. Electronic absorption, equilibrium and Fe Mossbauer study.**,*J.Inorg.Biochem*,50,193- 220,(**1993).**

5.Hamed,M.Y.,Wilson,M.T., Silver,J. Keypour,H.: **Studies on the Reactions of Iron(II) Ascorbate mixtures with molecular oxygen in solution**,*Inorg.Chim.Ac*ta,152,227-231 **(1988).**

6.Hamed,M.Y.,Wilson,M.T.,Silver,J.and Keypour,H.: **Studies on the reactions of ferric iron with ascorbic acid. A study of the solution chemistry using Mossbauer spectroscopy and stopped flow techniques**, *Inorg.Chim.Acta,* 125,97-106**(1986)**

7.Hamed,M.Y.,Jensen,P.,Wilson,M.T. and Silver J.: **Electron Spin Resonance study of rapidly frozen solution of iron glutathione,***Inog.Chim.Acta*,125,1-4**(1986).**

8.Hamed,M.Y.,Silver,J.Morrison,I.(In part): **Studies On the reactions of ferric iron with glutathione and some related thiols, part(v). Solid complexes containing Fe(II) and GSH and Fe(III) and GSSG**,*Inorg.Chim.Acta*,107,169-178**(1985**).

9.Hamed,M.Y.,Silver,J.,and Wilson,M.T.: **A study of iron catalyzed oxidation of glutathione by molecular oxygen,** *Inorg.Chim.Acta,80,237-244**(1983)***.

10.Hamed,M.Y.and Silver,J.: **Studies on the reaction of Ferric iron with Glutathione and some related thioles, part(II): Complexes in the pH range 3-7**,*Inorg.Chim.Acta,80,115-122**(1983***).**

11.Hamed,M.Y., Wilson,M.T., and Silver,J.: S**tudies on the reactions of ferric iron with Glutatione and some related thioles,** *Inorg.Chim.Acta, 78,1-11**(1983)***

12.Hamed,M.Y.,Hider,R.C. and Silver,J.: **The competition between *Entrobactin* and glutathione for iron,***Inorg.Chim.Acta,66,13-18**(1982)***

## Conferences

*Protein structure and dynamics (Scripps institute 10/ 2008) , LaJolla, California

* AutoDock workshop on Ligand protein Docking Techniques 2/2008 Scripps Institute, MGL labs, LaJolla, California

1.*Building Interactive Media For Technical Education, Unisco, Birzeit, June 1998*

2. Hamed,M.Y.,*Copper complexes with biologically significant ligands: Rapid kinetic and thermodynamic equilibrium Study of the Cu(II) complexes with glutatione,L-cystein and D-pencillamine,8th.Int.Conf Bioinorganic Chemistry*, Yokohama, Japan,1997, *appeared in* J.Inorg.Biochem,67,(3/4) 1997

3. Hamed, M.Y. Fur*/DNA binding and the role of metal ion,7th Int C. B.I.C Germany*, Aug 1993.

4. *Computers in Chemistry, organized by UNISCO, nov 1996. Hashemite University* Jordan

4.Hamed,M.Y. and Jisrawi, N.M.: *Tunneling Studies and Anomalous behavior of Specially annealed YBCO samples ,CTAP First Symposium on Magnetics,Irbid,Jordan,22-24 Nov. 1993.*

5.Hamed,M.Y.*Binding of the ferric uptake regulation protein (fur)Fe(II) complex to DNA, Sixth International Conf. Bioinorganic Chemistry, Univ. California, Santiago, USA ,Aug. 1993.*

6.Hamed,M.Y., *The Role of Divalent metal ions as co-repressors for the repressor protein FUR: A study of the Co(II) complexes, Fifth International conference on Bioinorganic Chemistry, Augast 4-10,1991,Oxford,UK, J.Inorg.Biochem, 43(3),512 (1991).*

7.Hamed,M.Y.: *The Role of Mn(II) and Cu(II) as co-repressors for the repressor protein FUR, Chemistry and Genetics(Workshop on structure and function of mutated proteins, Florence,Italy,25-30 Aug 1991*

8.Hamed,M.Y.: R*eaction of u-OXO BIS[Trichloroferrate(III) ion with L-Ascorbic acid: Fourth Int.Conf. on Bioinorganic Chemistry,MIT,Cambridge,Boston USA,23-28 Jul 1989, J.Inorg.Biochem.36(4),L 037,1989.*

9.Hamed,M.Y.: *DNA Binding proteins which need metal ion co-repressor, School on Experimental Techniques and Theory of Biophysics, Int.Cent.for theoretical Physics, Triest, Italy 23 Sep.-27 Oct 1992.*

## References


- Prof Jack Mustaklim, Chairman, Chemistry Department, Birzeit University, Palestine e-mail: jackm@birzeit.edu

- Prof. R. C. Hider Department of Pharmacy, King's College, University of London, Manresa Rd., London, SW3 6LX, U.K. http://www.kcl.ac.uk/schools/biohealth/research/pharmsci/groups/drug/hider-rc.html Job title: Professor of Medicinal Chemistry Telephone: 0207 848 6979 Fax: 0207 848 6394 Email: robert.hider@kcl.ac.uk

- Prof.. J. B. Neilands Biochemistry Department, University of California, Berkeley , CA 94720, USA.e-mail: iron@uclink4.berkeley.edu

- Prof. M. T. Wilson Chemistry Department, University of Essex, Wivenho Park ,, Colchester, CO 3SQ, UK.

**http://www.essex.ac.uk/BS/staff/wilson/index.shtm .**

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- Prof Ziad el-MiMi Chairman of the department of water science and technology, Faculty of engineering, Birzeit University: ZMIMI@birzeit.edu

- **Dr Gaurav Arya, Department of Nanoengineering, Atkinson Hall, 9500 Gilman, UCSD,** garya@ucsd.edu