Joseph M. Hayes

Curriculum Vitae & Publication List

Name: Joseph M. Hayes
Address: Institute of Organic & Pharmaceutical Chemistry, National Hellenic Research Foundation, 48 Vas. Constaintinou Ave., Athens 11635, Greece
Date of Birth: 18 November 1970
Place of Birth: Ennis, Co. Clare, Ireland.
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Current position

Since Mar'07 — **Researcher Position**
Institute of Organic and Pharmaceutical Chemistry, National Hellenic Research Foundation,
48 Vas. Constantinou Ave, Athens 11635, Greece

DRUGDESI and EUROSTRUCT EU projects:
Simulation of biological environments to extract and exploit valuable information from experimental data obtained using X-ray crystallography to design improved inhibitors of glycogenolysis, potential hypoglycaemic agents for the treatment of Diabetes II, in collaboration with the Structural Biology & Chemistry Group.

Previous positions

Nov '05 – Jan'07 — **Post-doctoral Position within EU Framework Program 5**
Unitat de Química Física, Departament de Química, Universitat Autònoma de Barcelona, Spain

Hydrochem:
Application of computational chemistry methodology to hydride chemistry. Use of Density Functional Theory (DFT) and hybrid Quantum Mechanics/ Molecular Mechanics (QM/MM) methods to study reaction mechanisms in organometallic catalysis. Rational design of new chiral ligands for use in enantioselective catalysis.

Oct '02 – Nov '05 — **Post-doctoral Position within EU Framework Program 5**
anterio consult & research GmbH., Mannheim, Germany.

Enantioselective Recognition: Towards the Separation of Racemates
Rational design and virtual screening of synthetic receptors for large scale chiral separations of amino acids and drug-like molecules. Conformational analysis is performed by means of Monte Carlo methods or molecular dynamics in implicit or explicit solvent models, respectively. Binding free energies are calculated using either the MINTA or free enery perturbation (FEP) approaches. Deficient forcefield parameters are corrected by fitting to ab initio data.

Jan '01 – Aug '02 — **Post-doctoral Position & Part-time Faculty**
Dept. of Chemistry, Trinity University, San Antonio, Texas, USA.

Nucleophilic Substitution at Sulfur
Use of quantum chemical computations (DFT, HF, MP2, MP4(SDTQ), G2) to determine the mechanisms of nucleophilic substitution at sulfur in di- and trisulfides. Consideration of electronic and steric effects. Inclusion of micro (semi-solvated) and bulk (PCM) H_2O solvation.

Teaching Responsibilities & Research Coordination
"Organic Chemistry" to Freshman students.
Assistant in coordination and supervision of undergraduate computational chemistry research.

Oct '93 – Nov '00 — **Part-time Secondary School Teacher**
Sandymount High School; Ard Scoil Rois, Griffith Avenue; Loreto Secondary School, Bray; Manor House, Raheny; Templeogue College; Mercy College, Coolock; Sutton Park; Temple House, Malahide Road; St. Marks Community College, Tallaght; CBS, Synge St.; Loreto Convent; Oatlands College, Stillorgan; Terenure College; Blackrock College (All Dublin, Ireland).

Teacher of Chemistry, Biology, Physics and Mathematics

Nov '98 – Dec '98 — **Chemistry Tutor**
School of Nursing, Department of Physiology, University of Dublin, Trinity College, Dublin, Ireland.

Jun '92 – Oct '92 — **Research Chemist (summer placement)**

Syntex Ireland Ltd. (now Roche Pharmaceuticals), Ennis, Co. Clare, Ireland.

Education

Jan '96 – Nov '00 **Doctor of Philosophy (PhD.)**
Department of Chemistry, University of Dublin, Trinity College, Dublin, Ireland

PhD. Thesis: ***Computational Studies of Lithium Complexes and Alkanes*** *– structural and energetic study of lithium complexes and their formation. Mechanistic study of the role of lithium bases in organic synthesis. Design and implementation of the PAROPT program for extraction of forcefield parameters from quantum chemical data. Application to the study of alkanes under high pressure conditions.*

Oct '93 – Jan '96 **Registered for Masters in Computational Chemistry**
Department of Chemistry, Univerisity of Dublin, Trinity College, Dublin, Ireland

Transfer to PhD program Jan '96

Oct '88 – Oct '93 **B.Sc(Hons.) Chemistry**
University College Dublin, Dublin, Ireland

Research Interests

Computational biophysics; chiral chemistry; receptor/ligand design; free energy calculations; catalysis; modelling solvation effects; development & testing of forcefield parameters; statistical & quantum mechanics; theoretical organic and organometallic chemistry; QSAR.

Research Experience

Molecular mechanics & dynamics; docking; free energy calculations; Monte Carlo methods; quantum chemical methods; free energy claculations; QM/MM; solvation modelling; conformational searching; derivation of forcefield parameters; design of synthetic receptors; virtual screening; determination of reaction mechanisms.

Conferences & Workshops Organised

Oct '09 **Structural Biology and Chemistry Symposium**
"Dedicated to the memory of Dr. Nikos G. Oikonomakos"
National Hellenic Research Foundation, Athens, Greece.

Dec '08 **Workshop on Molecular Modelling: Approaches to Computational Biophysics (DRUGDESI)**
National Hellenic Research Foundation, Athens, Greece.

Jun '08 **Workshop on Structure Based Drug Discovery (EURODESY)**
National Hellenic Research Foundation, Athens, Greece.

Jan '02 **Molecular Modelling Training Workshop**
Chiral Recognition EU network meeting, Mannheim, Germany

Conference Presentations (Oral)

Dec '08 **Workshop on Molecular Modelling: Approaches to Computational Biophysics (DRUGDESI)**
Athens, Greece
"Glycogenolysis Control in Type II Diabetes: The Role of Computation in Structure Based Drug Design", J.M. Hayes*, M. Mamais, D. Papageorgiou, K-M. Alexacou, D. Sovantzis, E.D. Chrysina, D.D. Leonidas, S.E. Zographos, T. Gimisis, J-P. Praly, G. Archontis, N.G. Oikonomakos

Mar '08 **13th Panhellenic Conference on Medicinal Chemistry**
Athens, Greece
"Molecular Modelling of the Binding of Inhibitors at the Catalytic Site of Glycogen Phosphorylase b (GPb): The Search for New Antihyperglycaemic Drugs", J. M. Hayes*

Sep '04 **International Conference on Supramolecular Science & Technology**
Prague, Czech Republic
Symposium Lecture "Chiral Separation: Design of Enantioselective Receptors Bases on the Cholic Acid Structural Backbone", J. M. Hayes*, M. Stein and J. Weiser

Oct '03 **Synthetic Receptors 2003**

Lisbon, Portugal
"Design of Chiral Selective Receptors: A Molecular Modelling Approach", J. M. Hayes*, M. Stein and J. Weiser

Sep '03 **9th International Conference on Circular Dichroism**
Budapest, Hungary
"Molecular Modelling Approaches to Chiral Separation: Accurate Computation of Ligand Binding Free Energies", J. M. Hayes*, M. Stein and J. Weiser

Conference Presentations (Poster)

Sep '08 **Hellenic Crystallographic Association 4th Conference**
Athens, Greece
"New Inhibitors of Glycogen Phosphorylase from Docking and Molecular Modelling Calculations" , J. M. Hayes*, M. Mamais, K.-M. Alexacou, E.D. Chrysina, D.D. Leonidas, S.E. Zographos, T. Gimisis, J.-P. Praly, N.G. Oikonomakos

Jul '06 **XXII International Conference on Organometallic Chemistry**
Zaragoza, Spain
"Computational Investigation of a New Iridium Catalyst for Asymmetric Hydrogenation of Ketones: A Mechanistic Study" , J. M. Hayes*, E. Manoury, G. Ujaque, R. Poli and A. Lledos

Apr '02 **223rd ACS National Meeting**
Orlando, Florida
"Computational Investigation of the Solution Phase Mechanism of Nucleophilic Substitution at Sulfur" J. M. Hayes* and S. M. Bachrach

Oct '02 **57th Southwest Regional ACS Meeting**
San Antonio, Texas
"Computational Investigation of the Mechanism of Nucleophilic Substitution at Sulfur in Di- and Trisulfides", J. M. Hayes* and S. M. Bachrach

Apr '97 **CCP5 Spring School**
University of Bristol, U.K.

Skills & Knowledge

Software: Schrodinger, Cerius^2, GAUSSIAN, GAMESS, Turbomole, MOPAC, DL_POLY, GOLD
Operating Systems: Windows, Linux, UNIX
Programming: FORTRAN, Perl, MPI

Other Experience

Reviewer of articles for:
Journal of Computational Chemistry
European Journal of Medicinal Chemistry
Journal of Molecular Structure
Biosensors & Bioelectronics

Personal Characteristics

Highly motivated
Innovative thinking
Excellent communication skills & good team player

Extra-Curricular Activities

Sport (particularly soccer, gaelic games)
Music (irish traditional)
Play guitar and bodhran

Languages spoken

English
German (basic)
Spanish (basic)

References

Dr. Jörg Weiser
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List of publications

1. Zographos SE,* Drakou CE, Malekkou A, Lederer CW, Hayes JM, Leonidas DD, Lamond AI, Santama N and Oikonomakos NG, "hCINAP is an atypical mammalian nuclear adenylate kinase with ATPase activity: insights into its catalytic mechanism and function" *J. Biol. Chem.* (**2009**), *submitted.*

2. Benltifa M, Hayes JM, Vidal S, Gueyrard D, Goekjian PG, Praly JP,* Kizilis G, Tiraidis C, Alexacou K-M, Chrysina ED*, Zographos SE, Leonidas DD, Archontis G, and Oikonomakos NG, "Glucose-based Spiro-isoxazolines: A New Family of Potent Glycogen Phosphorylase Inhibitors", *Biorg. Med. Chem.* (**2009**), *17*, 7368-7380.

3. Dossi K, Tsirkone VG, Hayes JM, Matousek J, Pouckova, Soucek J, Zadinova M, Zographos SE, Leonidas DD*, "Mapping the ribonucleolytic active site of bovine seminal ribonuclease. The binding of pyrimidinyl phosphonucleotide inhibitors", *Eur. J. Med. Chem.* (**2009**), *44*, 4496-4508.

4. Potamitis C, Zervou M, Katsiaris V, Zoumpoulakis P, Durdagi D, Papadopoulos MG, Hayes JM, Grdadolnik SG, Kyrikou I, Argyropoulos D, Vatougia G, Mavromoustakos T*. "Antihypertensive Drug Valsartan: Conformational Analysis, Dynamic NMR Spectroscopy, *in silico* Docking and Molecular Dynamics Studies" *J. Chem. Inf. Model.* (**2009**), *49*, 726-739.

5. Zographos SE, Leonidas DD, Alexacou KM, Gimisis T, Hayes JM, Oikonomakos NG*, Wen X, Sun H, Liu J, Cheng K, Zhang P, Zhang L, Hao J, Zhang L, Ni P,. "Pentacyclic Triterpenes Inhibitors of Glycogen Phosphorylase as Potential Drugs for Type 2 Diabetes: X-ray Crystallographic Studies", *Planta Medica* (**2008**), *74*, 1146-1147.

6. Somsák L*, Czifrák K, Tóth M, Bokor E, Chrysina ED, Alexacou K-M, Hayes JM, Lazoura E, Leonidas DD, Zographos SE, Oikonomakos NG*. "New Inhibitors of Glycogen Phosphorylase as Potential Antidiabetic Agents", *Current Medicinal Chemistry* (**2008**), *15*, 2933-2983.

7. Wen X, Sun H, Liu J, Cheng K, Zhang P, Zhang L, Hao J, Zhang L, Ni P, Zographos SE, Leonidas DD, Alexacou KM, Gimisis T, Hayes JM, Oikonomakos NG*. "Naturally Occurring Pentacyclic Triterpenes as Inhibitors of Glycogen Phosphorylase: Synthesis, Structure-Activity Relationships and X-ray Crystallographic Studies", *J. Med. Chem.* (**2008**), *51*, 3540-3544.

8. Alexacou KM, Hayes JM, Tiraidis C, Zographos SE, Leonidas DD, Chrysina ED, Archontis G, Oikonomakos NG*, Paul JV, Varghese B, Loganathan D*, "Crystallographic and computational studies on 4-phenyl-N-(b-D-glucopyranosyl)-1H-1,2,3-triazole-1-acetamide, an inhibitor of glycogen phosphorylase: Comparison with a-D-glucose, N-acetyl-b-D-glucopyranosylamine and N-benzoyl-N0-b-D-glucopyranosyl urea binding", *Proteins: Structure, Function & Bioinformatics* (**2008**), *71*, 301-307.

9. Hayes JM; Viciano M; Peris E; Ujaque G; Lledós A. "Mechanism of Formation of Silver N-Heterocyclic Carbenes using Silver Oxide: A Theoretical Study", *Organometallics* (**2007**), *26*, 6170-6183.

10. A. Ragusa, J. M. Hayes*, Mark E. Light, J. D. Kilburn*, "A Combined Computational and Experimental Approach to Analysis of the Enantioselective Potential of a New Macrocyclic Receptor for Amino Acids" , *Chem. Eur. J.* **(2007)**, 13(9), 2717-2728.

11. A. Ragusa, J. M. Hayes*, Mark E. Light, J. D. Kilburn*, "Chiral Separation: Computation as a New Experimental Tool to Probe Enantioselectivity", *Eur. J. Org. Chem.* **(2006)**, 16, 3545-3549.

12. A. Ragusa, S. Rossi, J. M. Hayes, M. Stein and J. D. Kilburn*, "Novel Enantioselective Receptors for N-protected Glutamate and Aspartate", *Chem. Eur. J.* **(2005)**, 11(19), 5674-5688.

13. S. H. Norton, S. M. Bachrach* and J. M. Hayes, "Theoretical Study of Nucleophilic Substitution at Sulfur in Sulfinyl Derivatives" , *J. Org. Chem.* **(2005)**, 70(15), 5896-5902.

14. J. M. Hayes*, M. Stein, J. Weiser, "Accurate Calculations of Ligand Binding Free Energies: Chiral Separation with Enantioselective Receptors", *J. Phys. Chem. A* **(2004)**, 108, 3572-3580.

15. A. del Rio*, J. M. Hayes, M. Stein, P. Piras and C. Roussel, "Theoretical Reassessment of Whelk-O1 as an Enantioselective Receptor for 1-(4-halageno-phenyl)-1-ethylamine Derivatives", *Chirality* **(2004**), 16, S1-S11.

16. J. M. Hayes*, J. C. Greer and A. Morton-Blake, "A Forcefield Description of Short-Range Repulsions for High Density Alkane Molecular Dynamics Simulations" , *J. Comput. Chem.* **(2004**), 25(16), 1953-1966.

17. J. M. Hayes and S. M. Bachrach*, "Effect of Micro and Bulk Solvation on the Mechanism of Nucleophilic Substitution at Sulfur in Disulfides", *J. Phys. Chem. A* **(2003)**, 107(39), 7952-7961.

18. J. M. Hayes and J. C. Greer*, “Extraction of Analytical Potential Function Parameters from Ab Initio Potential Energy Surfaces and Analytical Forces”, *Comput. Phys. Commun.* **(2002)**, 147, 803.

19. S. M. Bachrach*, J. M. Hayes, T. Dao and J. L. Mynar, “DFT Gas and Solution Phase Study of Nucleophilic Substitution at Di- and Trisulfides”, *Theor. Chem. Acc.* **(2002)**, 107(5), 266.

20. S. M. Bachrach*, J. M. Hayes, C. E. Check and L. S. Sunderlin*, “Potential Energy Surface of $SOCl_3^-$”, *J. Phys. Chem. A* **(2001)**, 105(41), 9595.

21. J. M. Hayes, J. C. Greer and F. S. Mair*, “Amidolithium-Mediated Enolization: Does Proton Transfer Occur via a Dimer Intermediate with Bridging Carbonyls?”, *New J. Chem.* **(2001)**, 25, 262.

22. W. Clegg, J. C. Greer, J. M. Hayes and F. S. Mair*, “Mixed Aggregation between Lithium Diisopropylamide and Lithium Chloride: NMR, Solid-State Structure and Ab Initio Calculations”, *Inorg. Chim. Acta.* **(1997)**, 258, 1.