ANNA LOUISE BOWMAN, PH.D.

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EDUCATION

Ph.D. Computational Chemistry, University of Bristol, United Kingdom, 2005
"Modeling the mechanism & dynamics of hen egg white lysozyme & glutathione S-transferase"
Advisor: Adrian J. Mulholland, Ph.D.

B.S. Chemistry, University of Bristol, United Kingdom, 2001

RESEARCH EXPERIENCE

Research Assistant Professor, Center for Drug Discovery, Northeastern University, Boston, MA, Aug 2011 – Present
Principal Research Scientist, Center for Drug Discovery, Northeastern University, Boston, MA, Feb 2010 – Jul 2011
Associate Research Scientist, Center for Drug Discovery, Northeastern University, Boston, MA, Aug 2009 – Jan 2010
Postdoctoral Research Associate, Center for Drug Discovery, Northeastern University, Boston, MA, Jul 2007 – Jul 2009

- Applied structure-based drug design tools toward the selective inhibition of the endocannabinoid degradation enzymes including homology modeling, molecular dynamics simulations and docking
- Investigated activation of the cannabinoid G-protein coupled receptors following covalent ligand attachment through molecular dynamics simulations in an explicit membrane environment
- Collaborated extensively with synthetic chemists and biochemists to identify potent novel endocannabinoid ligands with methodology including pharmacophore model development, conformational analyses, and pharmaceutically relevant property prediction

Postdoctoral Fellow, University of Michigan, Ann Arbor, MI, Feb 2005 – Jun 2007
Advisor: Prof. Heather A. Carlson

- Discovered potent novel small molecule scaffolds for inhibiting the MDM2 – p53 protein-protein interface through virtual high throughput screening
- Demonstrated that increased dynamic sampling improves the performance of the multiple protein structure (MPS) method
- Developed species-specific, receptor-based pharmacophore models which incorporated protein flexibility for dihydrofolate reductase

Graduate Assistant, University of Bristol, United Kingdom, Oct 2001 – Jan 2005
Advisor: Prof. Adrian J. Mulholland

- Demonstrated the first theoretical proof of a covalent intermediate in the wild type hen egg white lysozyme with QM/MM free energy simulations
- Explored the catalytic effect of three single point mutations in the detoxification enzyme glutathione S-transferase with reaction specific parameterized QM/MM dynamics simulations
- Performed higher-level small model calculations on oligosaccharides and related molecules

PUBLICATIONS

- **A. L. Bowman** & A. Makriyannis (2011) "Approximating protein flexibility through dynamic pharmacophore models: application to fatty acid amide hydrolase (FAAH)" *J. Chem. Inf. Model.* 51: 3247-3253
- S. P. Nikas, S. O. Alapafuja, I. Papanastasiou, C. A. Paronis, V. G. Shukla, D. P. Papahatjis, **A. L. Bowman**, A. Halikhedkar, X. W. Han & A. Makriyannis (2010) "Novel 1 ',1 '-Chain Substituted Hexahydrocannabinols: 9β -1-Hydroxy-3-(1-hexyl-

cyclobut-l-yl)hexahydrocannabinol (AM2389) a Highly Potent Cannabinoid Receptor 1 (CB1) Agonist" *J. Med. Chem.* 53: 6996-7010.

- D. D. Dixon, D. Sethumadhavan, T. Benneche, A. R. Banaag, M. A. Tius, G. A. Thakur, A. L. Bowman, J. T. Wood & A. Makriyannis, A. (2010) "Heteroadamantyl Cannabinoids" *J. Med. Chem.* 53: 5656-5666.
- **A. L. Bowman** & A. Makriyannis (2009) "Refined Homology Model of Monoacylglycerol Lipase: Toward a Selective Inhibitor" *J. Comput. Aided Mol. Des.* 23: 799-806.
- E. K. Tiburu, **A. L. Bowman**, J. O. Struppe, D. R. Janero, H. K. Avraham & A. Makriyannis (2009) "Solid-state NMR and molecular dynamics characterization of cannabinoid receptor-1 (CB1) helix 7 conformational plasticity in model membranes" *Biochim. Biophys. Acta* 1788: 1159-1167.
- **A. L. Bowman**, I. M. Grant & A. J. Mulholland (2008) "QM/MM simulations predict a covalent intermediate in the hen egg white lysozyme reaction with its natural substrate" *Chem. Commun.* 7: 4425-4427. Highlighted as a hot article and with cover image
- D. Lu, J. Guo, R. I. Duclos, **A. L. Bowman** & A. Makriyannis (2008) "Bornyl- and isobornyl-Δ8-tetrahydrocannabinols: A novel class of cannabinergic Ligands" *J. Med. Chem.* 51: 6393-6399.
- F. Yao, C. Li, S. K. Vadivel, **A. L. Bowman** & A. Makriyannis (2008) "Development of novel tail-modified anandamide analogs" *Bioorg. Med. Chem. Lett.* 18: 5912-5915.
- **A. L. Bowman**, Z. Nikolovska-Coleska, H. Zhong, S. Wang & H. A. Carlson (2007) "Small molecule inhibitors of the MDM2-p53 interaction through dynamic pharmacophore modeling" *J. Am. Chem. Soc.* 129: 12809-12814. Highlighted in SciBX January 2008 issue
- **A. L. Bowman**, M. G. Lerner & H. A. Carlson (2007) "Protein flexibility and species specificity in structure-based drug discovery: Dihydrofolate reductase as a test system" *J. Am. Chem. Soc.* 129: 3634-3640
- M. G. Lerner*, **A. L. Bowman*** & H. A. Carlson (2007) "Incorporating dynamics in E. coli dihydrofolate reductase enhances structure-based drug discovery" *J. Chem. Inf. Model.* 47: 2358-2365 *These two authors contributed equally
- **A. L. Bowman**, L. Ridder, I. M. C. M. Rietjens, J. Vervoort & A. J. Mulholland (2007) "Molecular determinants of xenobiotic metabolism: QM/MM simulation of the conversion of 1 - chloro - 2,4 - dinitrobenzene catalyzed by M1-1 glutathione S – transferase" *Biochemistry*, 46: 6353-6363
- J. Żurek, **A. L. Bowman**, W. A. Sokalski & A. J. Mulholland (2004) "MM and QM/MM modeling of threonyl-tRNA synthetase: Model testing and simulations" *Struct. Chem.* 15: 409-418

BOOK CHAPTERS

- **A. L. Bowman** & A. J. Mulholland (2005) "Simulating enzyme-catalyzed reactions" in *The Handbook of Theoretical and Computational Nanotechnology*, eds. M. Rieth & W. Schommers (American Scientific Publishers, Los Angeles), Vol. 6, pp. 305-359

ABSTRACTS

- A. L. Bowman & A, Makriyannis "Developing dynamic pharmacophore models of monoacylglycerol lipase and related enzymes" Celebrating Computational Biology, Oxford, United Kingdom (2010) poster presentation
- A. L. Bowman & H. A. Carlson "Small molecular inhibitors of the MDM2-p53 interaction discovered through the multiple protein structure (MPS) method" Applied Pharmaceutical Chemistry, Boston, MA (2009) invited speaker
- A. L. Bowman, I. Karageorgos & A. Makriyannis "Refined homology model of monoacylglycerol lipase: Toward a selective inhibitor" ACS 236th National Meeting, Philadelphia, PA (2008) poster presentation
- A. L. Bowman & A. Makriyannis "Human monoacylglycerol lipase: Biochemical, molecular and computational studies toward a therapeutic inhibitor" Current Trends in Drug Abuse Research 5th Annual Symposium, Boston, MA (2008) invited speaker
- A L. Bowman, K. L. Meagher, H. A. Carlson "Targeting protein-protein inhibition with the multiple protein structure method" ACS 232nd National Meeting, San Francisco, CA (2006) poster presentation

- A L. Bowman, K. L. Meagher, H. A. Carlson "Targeting protein-protein inhibition with the multiple protein structure method" GRC on Medicinal Chemistry, USA (2006) poster presentation
- A. L. Bowman & A. J. Mulholland "Conformation and Catalysis in Lysozyme: A 'Textbook' Enzyme?" ISQBP President's Meeting, Como, Italy (2004) poster presentation
- A. L. Bowman & A. J. Mulholland "Conformation and Catalysis in Lysozyme: A 'Textbook' Enzyme?" MGMS Young Modelers' Forum, London, United Kingdom (2003) oral presentation
- A. L. Bowman, L. Ridder, I. M. C. M. Rietjens, J. Vervoort & A. J. Mulholland "Investigating the Specificity of Glutathione S – Transferase Isoenzymes through Mechanistic Modeling" GRC on Computer Aided Drug Design, USA (2003) poster presentation
- A. L. Bowman, L. Ridder, I. M. C. M. Rietjens, J. Vervoort & A. J. Mulholland "Investigating the Specificity of Glutathione S – Transferase Isoenzymes through Mechanistic Modeling" Conformational Approaches to the Understanding of ADMET Properties and Problems, Oxford, United Kingdom (2003) poster presentation

RESEARCH SUPPORT

- **R03 Grant National Institutes of Health, NIDA** A. L. Bowman (PI)
  1R03DA027965-01 "Virtual Screening to identify novel, selective monoacylglycerol lipase inhibitors"

PROFESSIONAL EXPERIENCE

- Reviewer for *J. Am. Chem. Soc.*, *J. Chem. Inf. Model., Proteins*, *Chem. Biol. Drug Des.*, *Biochimie*, *FEBS Lett.*, & *J. Mol. Model.*
- American Chemical Society – Cleveland Section, Secretary (2012 – 2014)

TEACHING & MENTORING EXPERIENCE

- University of Bristol, Designed syllabus and coordinated "Mathematics for Chemists", duties included liaising with faculty, teaching, developing homework and grading assignments
- University of Michigan, Supervised two graduate students and one professional (PharmD) student
- Northeastern University, Mentor to one computation chemistry and two biophysics graduate students

MEMBERSHIPS

- American Chemical Society, ACS, 2005 – Present, *Computers in Chemistry Division*
- American Association for the Advancement of Science, AAAS, 2007 – Present
- Molecular Graphics and Modeling Society, MGMS, 2001 – Present
- Royal Society of Chemistry, RSC, 1999 – 2005

HONORS & AWARDS

- Gordon Conference Chair's Funding to present at the GRC on Medicinal Chemistry, USA (2006)
- MGMS Bursary to present at the ISQBP President's Meeting, Como, Italy (2004)
- First Place Award at MGMS Young Modelers' Forum, London, United Kingdom (2003)
- Gordon Conference Chair's Funding to present at the GRC on Computer Aided Drug Design, USA (2003)
- Bristol University Alumni Foundation Award (2003)
- Chemical Computing Group Bursary (2003)