Mauricio L. Cafiero
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School of Chemistry, Food and Pharmacy
Reading, UK

Professional Experience

Sept. 2022 – Present: **University of Reading,** Reading, UK.
Lecturer, Physical Chemistry
- School lead for Wellbeing, Inclusion, Diversity and Equity

Sept. 2020 – Aug, 2022: **University of Wolverhampton,** Wolverhampton, UK.
Aug. 2021 – Aug. 2022 **Programme Leader, Chemistry**
Sept. 2020 – Aug. 2022 **Senior Lecturer, Physical Chemistry**

Aug. 2004 – Aug. 2020 **Rhodes College,** Memphis, TN, USA.
Aug. 2017 – Aug. 2020 **Professor, Chemistry**

Aug. 2016 – July 2019 **Director of Fellowships and Undergraduate Research**

May 2015 – Aug 2016 **Special Assistant to the Dean**

Aug. 2013 – May 2019 **Chair, Department of Chemistry**

Sept. 2011 – Aug. 2017 **James H. Daughdrill Professor of Natural Sciences.**

Aug. 2010 – Aug. 2017 **Associate Professor, Chemistry**

Aug. 2004 – July 2010 **Assistant Professor, Chemistry**

July 2019 – Dec. 2020: **Queens University**, Belfast, UK
Visiting Research Professor, Atomistic Simulation Centre
- Research on multiscale methods

Feb. 2016 – Dec. 2018: **Consultant/Expert Witness in Medicinal Chemistry**
- Expert Witness on Drug Patent case: prepared report, prepared response report to opposition expert witness, gave deposition.
- Consultant on six drug patent projects: found prior art and prepared reports.

Dec. 2002 – Aug. 2004:	**National Institute of Standards and Technology**, Gaithersburg, MD. **Post-Doctoral Research Chemist**. • Advisor: Carlos Gonzalez.	
Aug. 1998 – Dec. 2002:	**University of Arizona**, Tucson, AZ.	**Teaching Assistant**.
Jan. 1998 – July 1998:	**University of S. Florida**, Tampa, FL.	**Teaching Assistant**.
Aug. 1996 – Dec. 1997:	**University of N. Florida**, Jax, FL.	**Adjunct Instructor**.

Education

2002	**Ph.D, Chemistry** with emphasis in Theoretical Chemistry. • Thesis Advisor: Ludwik Adamowicz. • Thesis: *High Accuracy Calculations on Coulombic Few Particle Systems in a Basis of Explicitly Correlated Gaussian Functions.* University of Arizona, Tucson, AZ.
2000	**M.A., Chemistry** with emphasis in Physical Chemistry. University of Arizona, Tucson, AZ.
1997	**B.S., Chemistry**. University of North Florida, Jacksonville, FL.

Funded Grants

2021	RSC Research Enablement Grant, "A novel dynamic Density Functional Theory method for analysing multi-scale ligand/protein interactions."
2016	NSF CHE-1626238, "MRI: Addition of High Performance Computers for the Molecular Education and Research Consortium in Undergraduate Computational ChemistRY (MERCURY)." *As part of the MERCURY consortium.*
2013	Faculty International Curricular Grant, Rhodes College.
2012	NSF CHE-1229354, "MRI: Acquisition of a High Performance Computer for the Molecular Education and Research Consortium in Undergraduate computational chemistRY (MERCURY)." *As part of the MERCURY consortium.*
2010	Mellon Cluster Grant, "Workshops focused on modernizing General Chemistry Laboratories."
2010	Rhodes College Faculty Development Grant.
2009	Rhodes College Faculty Development Grant.
2008	Spence Wilson faculty International Travel Grant.

2008	NSF CHE-0821581, "MRI: Acquisition of a High Performance Computer for the Molecular Education and Research Consortium in Undergraduate computational chemistRY (MERCURY)." *As part of the MERCURY consortium.*
2007	Faculty Internationalization Grant, Rhodes College.
2007	Cottrell College Science Award, Research Corporation, "The application of Density Functional Theory and *ab initio* methods to aromatic protein/ligand binding."
2007	Spence Wilson faculty International Travel Grant.
2006	Faculty Development Grant, Rhodes College.
2006	Pittsburg Conference Memorial National College Grant.
2005	National Science Foundation Cyber-Infrastructure Grant.
2005	Rhodes College Hill Grant**.**
2005	Faculty Development Grant, Rhodes College.
2005	Passer Education Fund (American Chemical Society).
2005	Associated Colleges of the South Teaching with Technology Fellowship.
2004	NPACI Expedited Supercomputing Grant.

Honors and Awards

2011 – 2017	James H. Daughdrill Professor of Natural Sciences.
2002 - 2004	National Research Council Postdoctoral Fellowship (at the National Institute of Standards and Technology).
2002	Sloan Foundation NACME Scholarship.
2001	Gregson Fellowship, University of Arizona Department of Chemistry.
1998	Incoming Graduate Student Fellowship, University of Arizona Department of Chemistry.
1994 - 1997	National Merit Scholarship.
1994 - 1997	Florida Academic Scholars Scholarship.
1994 - 1997	Florida State University System Minority Scholarship.

Intramural Service at Rhodes College (2004 – 2020), University of Wolverhampton(2020 – 2022) and University of Reading

2024 – Present	UoA3 REF output committee.

2022 – Present	School lead, Wellbeing, Inclusion, Diversity, and Equity
2022 – Present	Member, School Management Board
2021 – 2022	Member, Faculty Staff Wellbeing committee
2021 – 2022	Member, Learning, Teaching and Assessment Sub-committee
2017 – 2019	Parliamentarian, Faculty meetings
2016 – 2019	Member of First Year Seminar planning committee.
2011 – 2019	Member, Neuroscience Programme Committee.
2011 – Present	Faculty Advisor, Gamma Sigma Epsilon Chemistry Honor Society.
2015 – 2016	Member, Howard Hughes Medical Institute grant proposal steering committee
2014 – 2016	Natural Sciences Rep., Faculty Governance Committee.
2015	Chair, Search Committee for Rhodes College Dean of the Faculty and Vice President for Academic Affairs.
2012 – 2015	Member, Rhodes College Fellowships Committee.
2012 – 2015	Member, Rhodes/St. Jude Partnership Committee.
2014/2015	Chair, Chemistry Department Search Committee (Biochemistry)
2014/2015	Chair, Chemistry Department Search Committee (Inorganic)
2011 – 2014	Admissions Policy Committee (Chair 2012 - 2014).
2013/2014	Chair, Chemistry Department Search Committee (Organic)
2005 – 2013	Faculty Advisor, Student Affiliate American Chemical Society. (Honorable mention in 2008/2009 and 2009/2010 by the ACS).
2006 – 2012	Chair, Barry Goldwater Scholarship Selection Committee. (Excluding 2010/11; 3 scholars selected from Rhodes, 2008).
2011/2012	Member, Mathematics Department Faculty Search Committee.
2011/2012	Member, Biology Department Faculty Search Committee.
2005/06, 2007/08, 2011/12	Chemistry Department Seminar Coordinator.
2007 - 2010	Member, Faculty Development Committee.
2007/2008	Chair, Chemistry Department Faculty Search Committee.
2006	Chair, Chemistry Department Faculty Search Committee.
2005	Member, Barry Goldwater Scholarship Selection Committee.
2005	Member, Chemistry Department Faculty Search Committee.

Extramural Service

Journal Referee:	Reviewed sixty seven (67) manuscripts for *Journal of Chemical Theory and Computation, Computational and Theoretical Chemistry (*formerly *THEOCHEM), Journal of Physical Chemistry B, Journal of Chemical Physics, Journal of Physical Chemistry C, Journal of Physical Chemistry A, Chemical Physics Letters, ACS Omega, European Journal of Medicinal Chemistry, PLOS One, Canadian Journal of Chemistry,*

	Monatshefte fur Chemie, Journal of Molecular Graphics and Modeling, Journal of Chemical Information and Modeling, Journal of Molecular Structure, International Journal of Quantum Chemistry, Spectrochimica Acta A, International Journal of Molecular Sciences, African Journal of Pure and Applied Chemistry, The International Conference on Computational Science, Molecules, Biomolecules, Open Bioinformatics, Marine Drugs, Jove, Pharmaceuticals, and *International Journal of Scientific Research (IJSRU) at UAE University*.
Proposal Referee:	Reviewed nine (9) grant proposals for *Research Corporation for Science Advancement, ACS Petroleum Research Fund,* and the *National Science Foundation*.
Editorial Textbook reviews:	*Quanta, Matter and Change* (by Atkins and Freidman, W.H. Freeman and Co); *Mathematics for Physical Chemistry* (by R. Mortimer, Elsevier); *How can you measure a reaction enthalpy without going into the lab?"* (by Reeves *et al*, ACS Books).
Officer:	Local Memphis chapter of the American Chemical Society, 2006—2007.
Chair, Southern Chemist Selection Committee:	Local Memphis chapter of the American Chemical Society, 2016-2018.
Television Interviews:	"Hot Fuel, Cold Facts" for WREG Channel 4 (aired July 16, 2009). "Truth or Scare" for BBC Breakfast (aired September 2, 2021).
Session Chair:	MERCURY conference 2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015, 2016, 2017. Conference on Current Tends in Computational Chemistry 2012, 2013.

Teaching Highlights

- Supervised *summer research Fellowships* in summers of 2011 – 2020: "Design, synthesis, and evaluation of drug-like molecules," (2 students in 2011, 3 students in 2012, 2 students in 2013, 3 students in 2014, 6 students in 2015, 4 students in 2016, 5 students in 2017, 6 students in 2018, 6 students in 2019; 3 students in 2020)
- Supervised the final year theses of 29 students from 2004 to 2024.
- Modules Taught/UK
    - Chemistry for Foundations (Spring 2021)
    - Chemistry for Forensic Science (Fall 2020, 2021)
    - Skills for Chemistry (Fall/Spring 2020/2021,2021/2022)
    - Principles of Physical Chemistry (Spring 2021, 2022)
    - Physical Chemistry (Fall 2020, 2021)
    - Advanced Physical and Materials Chemistry (Spring 2021, 2022)
    - Chemistry Research (Fall/Spring 2020/2021, 2021/2022)
    - Advanced Topics in Physical Chemistry (Fall/Spring 2020/2021)

- Modules Taught/United States
    - Physical Chemistry sequence with lab (2004–present, excluding Fall 2010, 2019)
    - Foundations of Chemistry (Fall 2011, 2012, 2013, 2014, 2015, 2016, 2017; Summer 2019)
    - Molecular Shapes (for non-majors) (Spring 2013, Summer 2020)
    - General Chemistry I (Fall 2005, 2006, 2007, 2008, 2009).
    - General Chemistry II (Spring 2006, 2007, 2009, 2011).
    - Chemistry Senior Seminar (2004/2005, 2007/2008, 2018).
    - Chemistry Research (2005 – present).
    - Honors Chemistry Research (2005 -- present).
- Developed and wrote general chemistry lab experiments: "Calorimetric measurements of enthalpy of reaction," "Introduction to spectroscopy" and "Rate constant and energy of activation for the bleaching of a food dye."
- Co-PI for a series of workshops dedicated to improvement of general chemistry labs. This Mellon Foundation funded work involves faculty from Rhodes, Vassar, Middlebury, Claremont, and Denison colleges.
- Class evaluation scores (using the IDEA evaluation instrument) for Physical and General Chemistry classes have been at or above the mean scores for all classes at Rhodes College.

Research Highlights

- Published forty six (46) manuscripts in peer-reviewed journals.
- PhD supervision: supervisor for one current PhD student (started 2023); second supervisor/internal assessor for three PhD students.
- Supervised over fifty (60+) undergraduate research students from 2004-2024
- Presented research in oral sessions, poster sessions and invited talks twenty one (21) times from 2000-2023.
- Undergraduate students have presented collaborative research over one hundred (100+) times at international, national and regional conferences in oral and poster sessions from 2005-2019.
- Member of the MERCURY consortium of computational chemists at primarily undergraduate institutions (2006 - 2021).

Invited Talks and Poster Sessions—Self

2024	MMM Conference, **Talk** (London, UK). "Transformer-based GPT models for creating virtual screening libraries of molecules with tuned properties"
2024	Integrating AI in Computational Chemistry, **Talk** (Sheffield, UK). "Using GPT and other Deep Neural Network Models to Create Virtual Screening Libraries for Docking and DFT-based Protein-ligand Analysis."
2024	PCCP 25th Anniversary Symposium, **Poster** (Amsterdam, Netherlands). "Evaluation of exact exchange in Density Functional Theory methods for ligand/protein binding: pairwise additivity and two and three-body interactions."

2023	MMM Conference, **Talk** (London, UK). “Pairwise additivity and three-body interactions for protein-ligand binding energies using Density Functional Theory.”
2021	Research Institute for Health Sciences, University of Wolverhampton, **Seminar** (Wolverhampton, UK), “Using quantum chemical methods in Drug Design: Applications to Parkinson’s Disease.”
2021	The Third International Virtual Conference on Trends in Chemical, Nano and Synthetic Biology, **Seminar,** (online), “Computational Drug Design.”
2019	Department of Chemistry and Chemical Engineering, Queens University Belfast, **Seminar** (Belfast, UK), “Using quantum chemical methods in Drug Design: Theory and Experiment,”
2019	Physics Department, University of Memphis, **Seminar** (Memphis, TN), “Using quantum chemical methods in Drug Design: Theory and Experiment,”
2018	Mississippi College Chemistry Department, **Seminar** (Clinton, MS), “Novel inhibitors of enzymes in the dopamine pathway: Modelling and synthesis”
2017	INBRE Conference **plenary speaker**, University of Arkansas (Fayetteville, AR), “Novel inhibitors of enzymes in the dopamine pathway: Modelling and synthesis”
2013	University of Tennessee Health Science Center (Memphis, TN), Department of Pharmaceutical Sciences **seminar**, “Investigating the selectivity of human cytosolic sulfotransferase SULT1A3: A computational and experimental study.”
2011	Bowdoin College (Brunswick, ME), Department of Chemistry **seminar**, “The Role of pi-Interactions in Ligand-Protein and Ligand-DNA Complexes.”
2008	University of Memphis (Memphis, TN), Department of Chemistry **seminar**, “Developing a truly non-local Density Functional Theory method for predicting dispersion interactions: problems in protein-ligand chemistry.”
2008	Heriot-Watt University (Edinburgh, Scotland), Department of Chemistry **seminar**, “Using new and old Density Functional Theory methods for dispersion interactions: applications to the biosynthesis of neurotransmitters.”
2007	University of Mississippi (Oxford, MS), Department of Chemistry **seminar**, “Can a true non-local DFT method describe dispersion?”
2006	Austin Symposium on Molecular Structure (Austin, TX), **Talk**: "Molecular Structure in Non-Born-Oppenheimer Quantum Chemistry."
2006	American Chemical Society Super-Regional Meeting (Memphis, TN), **Talk**: "Molecular Structure in Non-Born-Oppenheimer Quantum Chemistry."

2004	Canadian Theoretical Chemistry Conference (Montreal, Canada), **Poster**: "Non-Born-Oppenheimer Quantum Chemistry"
2004	Canadian Theoretical Chemistry Conference (Montreal, Canada), **Poster**: "Scaled DFT Correlation Functionals for use with Exact Exchange"
2003	American Chemical Society National Meeting (New York, NY), **Poster**: "The Role of Exact Exchange and Correlation Functionals in Chemical Reactions."
2003	Southeast Theoretical Chemistry Conference (Clemson, South Carolina), **Talk**: "The Role of Exact Exchange and Correlation Functionals in Thermochemical Properties."
2002	Rocky Mountain regional American Chemical Society meeting (Albuquerque, NM), **Talk**: "Nonadiabatic Calculations of Dipole Moments and Polarizabilities of Molecules."
2000	West Coast Theoretical Chemistry Conference (Salt Lake City, UT), **Poster**: "Analytical Gradients for Explicitly Correlated Gaussian Functions."

Peer Reviewed Publications Since 2001 (undergraduates underlined)

1. M. Cafiero and L. Adamowicz, "Analytical Gradients for Singer's Molecular n-electron Explicitly Correlated Gaussians", *Int. J. Quantum. Chem*., **82**, 151, (2001).

2. M. Cafiero and L. Adamowicz, "Simultaneous Optimization of Molecular Geometry and the Wave Function in a Basis of Singer's n-electron Explicitly Correlated Gaussians", *Chem. Phys. Lett.*, **335,** 404, (2001).

3. M. Cafiero and L. Adamowicz, "Non-Adiabatic Calculations of the Dipole Moments of LiH and LiD", *Phys. Rev. Lett*., **88**, 33002 (2002).

4. M. Cafiero and L. Adamowicz, "Non-Adiabatic Calculations of the Polarizability of LiH in a Basis of Explicitly Correlated Gaussian Functions", *J. Chem. Phys*, **116**, 5557 (2002).

5. M. Cafiero and L. Adamowicz, "Non-Born-Oppenheimer Isotope Effects on the Polarizabilities of H2", *Phys. Rev. Lett.*, **89**, 073001 (2002).

6. M. Cafiero, L. Adamowicz, M. Duran, and J.M. Luis, "Nonadiabatic and Born-Oppenheimer Calculations of the Polarizabilites of LiH and LiD", *J. Mol. Struct. (THEOCHEM*), **633**, 113 (2003).

7. M. Cafiero, S. Bubin, and L. Adamowicz," Non-Born-Oppenheimer Calculations of atoms and molecules", *Phys. Chem. Chem. Phys*., invited review, **5**, 1491 (2003).

8. M. Cafiero and L. Adamowicz, "Molecular Structure in Non-Born-Oppenheimer Quantum Mechanics", *Chem. Phys. Lett.*, **387**, 136 (2004).

9. S. Bubin, M. Cafiero, and L. Adamowicz, "Quantum Mechanical Calculations on Molecules Containing Positrons", *Fundamental World of Quantum Chemistry, A Tribute Volume to the Memory of Per-Olov Lowdin, Vol. 3*, Cluwer, Dordrecht, (2004).

10. S. Bubin, L. Adamowicz, and M. Cafiero, "Non-Born-Oppenheimer Calculations of Atoms and Molecules with Explicitly Correlated Gaussian Functions", *Electronic Encyclopedia of Computational Chemistry (eECC)*, (2004).

11. M. Cafiero and L. Adamowicz, "Non-Born-Oppenheimer Calculations of H3", *Comp. Meth. Sci.Technolog. (CMST)*, **9**, 23-30 (2004).

12. M. Cafiero and C. Gonzalez, "Approximate self-consistent potentials for use in DFT XC functionals " *Phys. Rev. A.*. **71**, 42505 (2005).

13. M. Cafiero and L Adamowicz, "Nuclear Densities for DH_2+," *J. Chem. Phys.* **122**, 1 (2005).

Publications below for work done while at Rhodes College

14. M. Cafiero "Scaled Gradient Corrected Correlation Functionals for use with Exact Exchange," *Chem. Phys. Lett* .**418**, 126 (2006).

15. A. Godfrey_Kittle, M. Cafiero "Interaction energies for mono-substituted benzene ring dimers using DFT", *Int. J. Quantum Chem.,* **106**, 2035 (2006).

16. K. Van Sickle, L.M. Culberson, J.L. Holzmacher and M. Cafiero, "Evaluation of Density Functional Theory methods for the electronic interactions between indole and substituted benzene: Applications to Horseradish Peroxidase". *Int. J. Quantum Chem.* **107**, 1523-1531 (2007).

17. M. E. Hofto , A. Godfrey_Kittle, and M. Cafiero " Substrate-Protein interaction energy in the enzyme Phenylalanine Hydroxylase: DFT and *ab initio* Results ", *THEOCHEM,* **809**, 125 (2007).

18. M Cafiero and L. Adamowicz, "Non-Born-Oppenheimer calculations of the ground state of H_3" *Int. J. Quantum Chem.*, **107**, 2679 (2007).

19. L. R. Hofto, K. Van Sickle, and M. Cafiero, "Evaluation of sandwich-type electronic interactions in fourteen polyaromatic molecules." *Int. J. Quantum Chem.*, **108**, 112 (2008).

20. M. E. Hofto, J.N. Cross, and M. Cafiero "Interaction energies between tetrahydrobiopterin analogues and phenylalanine residues in tyrosine hydroxylase and phenylalanine hydroxylase.", *J. Phys. Chem. B*,**32**, 111 (2007).

21. L.R. Hofto, M.E. Hofto, J.N. Cross, and M. Cafiero, "Using simple molecular orbital calculations to predict disease: fast DFT methods applied to enzymes implicated in PKU, Parkinson's diseas, and obsessive compulsive disorder." *AIP Conf. Proc.*, **940**, 127-136 (2007).

22. M. Pavanello, M. Cafiero, S. Bubin, and L. Adamowicz, "Born--Oppenheimer calculations of the low-lying $^3\Sigma^+_g$ and $^3\Sigma^+_u$ excited states of the Helium Dimer." *Int. J. Quantum Chem.* **108**, 2291 (2008)

23. L.R. Hofto, C.E. Lee, and Mauricio Cafiero "Scaling gradient dependant corrections to LSDA DFT methods for aromatic interactions: applications to Tryptophan hydroxylase" *J. Comp. Chem.* **30**, 1111 (2009).

24. E. A. Kee, M. C. Livengood, E. E. Carter, M. L. McKenna, and M. Cafiero, "Aromatic Interactions in the Binding of Ligands to HMGCoA Reductase." *J. Phys. Chem. B.* **113**, 14810 (2009)

25. K. Van Sickle, M. C. Shroyer, and M. Cafiero, "Relative stability of complexes of six-carbon-rings with variable numbers of double bonds: DFT and ab initio results" *Journal of Molecular Structure: THEOCHEM*, **941**, 78 (2010).

26. H.E. Utkov, M. C. Livengood, and M. Cafiero, "Using Density Functional Theory methods for modeling induction and dispersion interactions in ligand-protein complexes." *Annual Reports in Computational Chemistry*, **6** (2010).

27. H.E. Utkov, A.M. Price, and M. Cafiero, "MP2, Density Functional Theory, and Semi-empirical calculations of the interaction energies between a series of statin-drug-like molecules and the HMG-CoA reductase active site." *Computational and Theoretical Chemistry*, **967**, 171 (2011).

28. K.M. DiGiovanni, A. Katherine Hatstat, Jennifer Rote and M. Cafiero, "MP2//DFT Calculations of Interaction Energies Between Acetaminophen and Acetaminophen Analogues and the Aryl Sulfotransferase Active Site." *Computational and Theoretical Chemistry*,**1007,** 41 (2013).

29. K. Copeland, Kari; S. Pellock; J. Cox; M. Cafiero; G. Tschumper. "Examination of Tyrosine/Adenine Stacking Interactions in Protein Complexes." *J. Phys. Chem. B*, **117**, 14001 (2013).

30. D. J. Bigler, L. W. Peterson, M. Cafiero. "Effects of Implicit Solvent and Relaxed Amino Acid Side Chains on the MP2 and DFT Calculations of Ligand-protein Structure and Electronic Interaction Energies of Dopaminergic Ligands in the SULT1A3 Enzyme Active Site." *Computational and Theoretical Chemistry*, **1051,** 79 (2015).

31. D.J. Bigler, L.W. Peterson, M. Cafiero. "DFT and MP2 study of the effects of point mutations on the binding of ligands within the SULT1A3 active site," *Computational and Theoretical Chemistry*, **1068**, 63 (2015).

32. A. K. Hatstat, M. Morris, L.W. Peterson, M. Cafiero. "Ab initio study of electronic interaction energies and desolvation energies for dopaminergic ligands in the catechol-O-methyltransferase active site" *Computational and Theoretical Chemistry*, **1078**, 146 (2016).

33. J. C. Rote, S. N. Malkowski, C. S. Cochrane, G. E. Bailey, N. S. Brown, M. Cafiero and L. W. Peterson "Catechol reactivity: Synthesis of dopamine derivatives substituted at the 6-position," *Synthetic Communications* **47,** 435 (2017).

34. S. N. Malkowski, C. F. Dishuck, G. G. Lamanilao, C. P. Embry, C. S. Grubb, M. Cafiero and L. W. Peterson, "Design, Modeling and Synthesis of 1,2,3-Triazole-Linked Nucleoside-Amino Acid Conjugates as Potential Antibacterial Agents," *Molecules*, **22**, 1682 (2017).

35. J. C. Dewar, A. S. Thakur, W. W. Brennessel, M. Cafiero, L. W. Peterson, W. T. Eckenhoff, "Simple Zinc Complex to Model Substrate Binding to Zinc Enzymes," *Inorganica Chimica Acta*, **24,** 473:15-19 (2018).

36. R. Evans, L. Peterson and M. Cafiero, "Evaluation of hybrid and pure DFT methods for the binding of novel ligands in the tyrosine hydroxylase enzyme." *Computational and Theoretical Chemistry*, **1140,** 145-151 (2018).

37. M.C. Perchik, L.W. Peterson and M. Cafiero, "The Effects of Ligand Deprotonation on the Binding Selectivity of the Phenylalanine Hydroxylase Active Site." *Computational and Theoretical Chemistry,* **1153**, 19-24 (2019).

38. R.J. Roldan, A. O. Pajarillo, J. D. Greenberg, J. E. Karlinsey, M. Cafiero, E. R. Frawley and L. W. Peterson, "Propargylglycine-based antimicrobial compounds are targets of TolC-dependent efflux systems in Escherichia coli." *Bioorganic & Medicinal Chemistry Letters*. **30**, 126875 (2020).

39. C.A. Magee, L.W. Peterson and M. Cafiero, "The effects of ligand charge, orientation and size on the binding of potential inhibitors for Aldehyde Dehydrogenase," *Computational and Theoretical Chemistry,* DOI: 10.1016/j.comptc.2020.112868

40. R.G. Evans, M. C. Perchik, C. A. Magee, and M. Cafiero, "Undergraduate women empowering women in computational chemistry: three perspectives," *Int. J. Quantum Chem.* DOI:10.1002/qua.26354.

Publications below for work done while at University of Wolverhampton

41. D. Safarian, M. Simons, R. G. Evans, L. W. Peterson, and M. Cafiero, "DFT study of ligand binding in the β1 adrenergic receptor," *Computational and Theoretical Chemistry,* **1199**, 113208 (2021).

Publications below for work done while at University of Reading

42. A. Katherine Hatstat, Grace M. Kennedy, Trevor Squires, Gisela Xhafkollari, C. Skyler Cochrane, Mauricio Cafiero, Larryn W. Peterson. "Synthesis and analysis of novel catecholic ligands as inhibitors of catechol-*O*-methyltransferase," *Bioorganic & Medicinal Chemistry Letters*, 88, 129286 (2023).
43. J. Harle, C. Slater, and M. Cafiero, "Investigating Paracetamol's Role as a Potential Treatment for Parkinson's Disease: Ab Initio Analysis of Dopamine, L-DOPA, Paracetamol, and NAPQI Interactions with Enzymes Involved in Dopamine Metabolism," *ACS Omega*, 8, 38053 (2023).
44. Charlotte Armida Elisabeth Schulze, and Mauricio Cafiero, "Pairwise Additivity and Three-Body Contributions for Density Functional Theory-Based Protein/Ligand Interaction Energies," *Journal of Physical Chemistry B*, 12, 2326 (2024).
45. Mauricio Cafiero, "Role of Exact Exchange and Empirical Dispersion in Density Functional Theory-Based Three-Body Noncovalent Interactions," *Journal of Physical Chemistry A*, 128, 8777 (2024).
46. Mauricio Cafiero, "Transformer-decoder GPT models for generating virtual screening libraries of HMGCR inhibitors: effects of temperature, prompt-length and transfer-learning strategies," *Journal of Chemical Information and Modeling*, https://doi.org/10.1021/acs.jcim.4c01309.

Other Publications (undergraduates underlined)

1. D.J. Bigler, L. Peterson, M. Cafiero. "DFT and MP2 Study of the Binding of Salbutamol within the SULT1A3 Active Site." *Rhodes Journal of the Biological Sciences.* **2015**, 30, 13-17.

2. A.K. Hatstat, and M. Cafiero. "Role of Solvation on the binding of Morphine, Met-Enkephalin, and Other Ligands to the u-Opiod receptor and Acetylcholine binding Protein." *Rhodes Journal of the Biological Sciences.* **2015**, 30, 32-36.

3. D. F. Wilson, L. Peterson and M. Cafiero. "Activation energies for the sulfation of ligands in sulfotranserfase enzyme 1A1." *Rhodes Journal of the Biological Sciences.* **2017**, 32, 10-13.