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STAFF INFORMATION
Professor Kevin A. Lobb
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Lecturer (Physical Organic Chemistry)

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About:

Prof Lobb spent two years as NMR specialist before being appointed as a Lecturer in the department. He teaches NMR and computational chemistry at both the undergraduate and postgraduate levels. As a core member of RUBi [<https://rubi.ru.ac.za/>] he also teaches computational chemistry within the context of the coursework bioinformatics MSc programme. He has supervised and co-supervised 30 MSc and PhD students and has published some 42 papers.

His interests include reaction kinetics and the determination of organic reaction mechanisms (with particular emphasis on carbocations and carbocation rearrangements), and aspects of cheminformatics such as virtual chemical library generation and high throughput virtual screening in the context of drug discovery.

Teaching:

- 1st Year - Atomic Structure and Bonding
- 2nd Year - Nuclear Magnetic Resonance
- 3rd Year - Linear Free Energy Relationships, Molecular Modeling
- Honours and MSc - Nuclear Magnetic Resonance, Molecular Modeling

2019 Publications:

1. **Characterization and computational studies of 2-(benzamido)thiazol-5-yl benzoate.** F. Odame, E. Hosten, R. Betz, K. Lobb and Z. Tshentu, *Journal of Structural Chemistry*, 2019, 60(1), 136-142.
2. **Synthesis of N-Substituted phosphoramidic acid esters as “reverse” fosmidomycin analogues.** Christiana M. Adeyemi, Heinrich C. Hoppe, Michelle Isaacs, Rosalyn Klein, Kevin A. Lobb, Perry T. Kaye, *Tetrahedron*, 2019, 75(16), 2371-2378.

2018 Publications:

1. **A New Synthetic Method for Tetraazatricyclic Derivatives and Evaluation of Their Biological Properties.** Felix Odame, Richard Betz, Eric C. Hosten, Jason Krause, Michelle Isaacs, Heinrich C. Hoppe, Setshaba D. Khanye, Yasien Sayed, Prof Carminita Frost, Kevin A. Lobb, and Zenixole R. Tshentu, *Chemistry Select*, 2018, 3(48), 13613-13618.
2. **Characterization and Computational Studies of a Co-crystal of 2-Aminobenzimidazole and 2-[(Benzolylcarmothioyl)amino]propanoic Acid.** F. Odame, E. C. Hosten, R. Betz, K. Lobb and Z.R. Tshentu. *Journal of Structural Chemistry*, 2018, 59(5), 1240-1244. DOI <https://doi.org/10.1134/S0022476618050268>
3. **The determination of CHARMM force field parameters for the Mg²⁺ containing HIV-1 integrase.** Thommas Musyoka, Özlem Tastan Bishop, Kevin Lobb and Vuyani Moses, *Chemical Physics Letters*, 2018, <https://doi.org/10.1016/j.cplett.2018.09.019>
4. **Iron(III) Porphyrin Electrocatalyzed Enantioselective Carbon-Chloride Bond Cleavage of Hexachlorocyclohexanes (HCHs): A combined Experimental Investigation and Theoretical Calculation.** Xu Liang, Minzhi Li, John Mack, Kevin Lobb and Weihua Zhu, *Dalton Transactions*, 2018, DOI: 10.1039/C8DT02510J.
5. **Synthesis, Characterization and DPPH Scavenging Activity of Some Benzimidazole Derivatives,** Felix Odame, Jason Krause, Eric C. Hosten, Richard Betz, Kevin Lobb, Zenixole R. Tshentu and Carminita L. Frost, *Bull. Chem. Soc. Ethiop.*, 2018, 32(2), 271-284, DOI: <https://dx.doi.org/10.4314/bcse.v32i2.8>
6. **High throughput screening, docking and molecular dynamics studies to identify potential inhibitors of human calcium/calmodulin-dependent protein kinase IV,** Anam Beg, Faez Iqbal Khan, Kevin A. Lobb, Asimul Islam, Faizan Ahmad and Md. Imtaiyaz Hassan, *Journal of Biomolecular Structure and Dynamics*, 2018, <https://doi.org/10.1080/07391102.2018.1479310>
7. **Identification and evaluation of bioactive natural products as potential inhibitors of human microtubule affinity-regulating kinase 4 (MARK4),** Taj Mohammad, Faez Iqbal Khan, Kevin A. Lobb, Asimul Islam, Faizan Ahmad & Md. Imtaiyaz Hassan, *Journal of Biomolecular Structure and Dynamics*, 2018, <http://dx.doi.org/10.1080/07391102.2018.1468282>
8. **Mechanistic insights into the urea-induced denaturation of kinase domain of human integrin linked kinase,** Sunayana Begum Syed, Faez Iqbal Khan, Sabab Hasan Khan, Saurabha Srivastava, Gulam Mustafa Hasan, Kevin A. Lobb, Asimul Islam, Faizan Ahmad, Md. Imtaiyaz Hassan, *International Journal of Biological Macromolecules*, 2018, <https://doi.org/10.1016/j.ijbiomac.2017.12.164>
9. **Exploring molecular insights into the interaction mechanism of cholesterol derivatives with the Mce4A: A combined spectroscopic and molecular dynamic simulation studies,** Shagufta Khan, Faez Iqbal Khan, Taj Mohammad, Parvez Khan, Gulam Mustafa Hasan, Kevin A. Lobb, Asimul Islam, Faizan, Ahmad, Md. Imtaiyaz Hassan, *International Journal of Biological Macromolecules*, 2018, <https://doi.org/10.1016/j.ijbiomac.2017.12.160>
10. **Unravelling the unfolding mechanism of human integrin linked kinase by GdmCl-induced denaturation,** Sunayana Begum Syeda, Faez Iqbal Khan, Sabab Hasan Khan, Saurabha Srivastava, Gulam Mustafa Hasan, Kevin A. Lobb, Asimul Islam, Md. Imtaiyaz Hassan, Faizan Ahmad, *International Journal of Biological Macromolecules*, 2018, <https://doi.org/10.1016/j.ijbiomac.2018.06.025>

2017 Publications:

1. [Synthesis and anti-parasitic activity of C-benzylated \(N-arylcarbamoyl\)alkyl-phosphonate esters](#), Christiana M. Adeyemi, Michelle Isaacs, Dumisani Mnkandhla, Rosalyn Klein, Heinrich C. Hoppe, Rui W.M. Krause, Kevin A. Lobb, Perry T. Kaye, *Tetrahedron*, 2017, 73,1661. <http://dx.doi.org/10.1016/j.tet.2017.01.045>
2. **The Evaluation and Validation of Copper (II) Force Field Parameters of the Auxiliary Activity Family 9 Enzymes**, Vuyani Moses, Özlem Tastan Bishop and Kevin Lobb, *Chemical Physics Letters*, 2017, 678, 91 <http://dx.doi.org/10.1016/j.cplett.2017.04.022>
3. **Investigation of molecular mechanism of recognition between citral and MARK4: A newer therapeutic approach to attenuate cancer cell progression**, Farha Naz, Faez Iqbal Khan, Taj Mohammad, Parvez Khan, Saaliqa Manzoor, Gulam Mustafa Hasan, Kevin A. Lobb, Suaib Luqman, Asimul Islam, Faizan Ahmad, Md. Imtaiyaz Hassan, *International Journal of Biological Macromolecules*, 2017, 107, Part B, 2580. <https://doi.org/10.1016/j.ijbiomac.2017.10.143>
4. **¹H NMR-based kinetic and theoretical studies of the simultaneous formation of two discrete rotameric systems of a novel difenchyl sulfite ester**, Alicia Singh, Perry T. Kaye, Kevin A. Lobb, *Tetrahedron*, 2017, <https://doi.org/10.1016/j.tet.2017.10.059>



Interrogation of the Solution Dynamics of Eukaryotic Initiation Factor 5A by Coupling Simulation Dynamics with NMR Observables, Lester T. Sigauke, Rosemary A. Dorrington and Kevin A. Lobb, *Proceedings of the International Conference on Bioinformatics Research and Applications 2017*, Pages 20-26, Barcelona, Spain — December 08 - 10, 2017, ACM New York, NY, USA ©2017
<https://doi.org/10.1145/3175587.3175602>