Citizenship: UK
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Expertise

Molecular dynamics (MD)
Coarse-grained MD
Brownian dynamics
Homology modelling
Drug docking
Mathematical modelling
Reaction-diffusion
Machine learning
Markov modelling
Enhanced sampling
GPU computing
High-performance computing

Research Experience

Macromolecular self-assembly
Synthetic biology
RNA biophysics
Polymer physics
Binding affinities/kinetics
Protein conformation change
Protein folding
Drug discovery
Personalized medicine
Enzyme (auto)catalysis
HIV structural biology

Skills

Project management
Teamwork & supervision
Grant & paper writing
Scientific refereeing
Communication
Teaching

KASHIF SADIQ PhD

Theoretical and Computational Biophysicist

Experience

Data Scientist in Computational Biology
European Molecular Biology Laboratory, Heidelberg | 2020-current

Senior Research Fellow
Heidelberg Institute for Theoretical Studies | 2016 – 2020

- Principal investigator of Volkswagen Foundation grant – modelling multiscale physics of sub-cellular polymer-protein condensates, capsid assembly and retroviral infectivity. ***Responsibilities:*** project lead, planning, implementing, interpreting, disseminating and supervising.
- Senior research fellow in EU-collaboration: Kinetics for drug discovery (k4dd.eu). Developed enhanced sampling methods in all-atom molecular dynamics (MD) and Brownian dynamics (BD) for drug-protein binding kinetics. ***Responsibilities:*** project planning, implementing, delivery, reporting, disseminating, supervising students and postdocs; undergraduate and graduate teaching.

Research Fellow
Universitat Pompeu Fabra, Barcelona, Spain | 2009 – 2015

- Principal investigator of American foundation for AIDS Research (amfAR) grant. Developed a computational drug-discovery pipeline including high-throughput virtual screening, all-atom MD and coarse-grained reaction diffusion. Led collaboration with experimental virologists, biochemists and medicinal chemists exploring novel HIV interference pathways for AIDS eradication**.** ***Responsibilities:*** budget planning, GPU cluster assembly and maintenance, student supervision, developing collaboration, full project delivery.
- Marie Curie postdoc: developed high-throughput MD methods for protein folding kinetics; distributed GPU computing (GPUGRID.net). ***Responsibilities:*** project design, planning, implementing and data interpreting.

Education

PhD Computational Biophysics
University College London, UK | 2008

- Developed the Binding Affinity Calculator, a molecular dynamics-based software to compute accurate drug binding affinities for HIV-1 protease as part of the EU-funded Virolab project (http://www.virolab.org). Extensive use and development of high-performance computing

BA MSci Natural Sciences (Theoretical Physics)
University of Cambridge, UK | 2001

AWARDS & FUNDING

- Volkswagen Foundation "Experiment!" Grant: €120,000 + €80,000 ext
- Marie Curie Career Integration Grant (awarded but declined): €100,000
- American Foundation for AIDS Research (amfAR) Grant: $150,000
- Marie Curie Intra-European Fellowship

TEACHING

- University of Heidelberg, Master's Course, Computational Molecular Biophysics | 2019
- University of Heidelberg, Bachelor's Course, Bioinformatics | 2019
- University of Heidelberg 4th Semester Bachelor's Lecture Course: Structure and dynamics of biological macromolecules | 2018 - 2019
- Heidelberg Biosciences International Graduate School (HBIGS) Lecture Course: Computational analysis of protein binding properties | 2017

STUDENT MENTORING & SUPERVISION

- 2 MSc students, 3 BSc students and 2 interns | 2016 - 2019
- 2 PhD students, 1 BSc student | 2009 – 2014

PUBLICATION & PRESENTATION SUMMARY

- 30 papers (18 as first author, 10 as corresponding author)
- Citations: 1060, H-index: 16, I10-index: 16
- Over 40 oral/poster presentations at conferences, meetings and invited seminars

SELECTED INVITED TALKS

- CECAM: Challenges in Large Scale Biomolecular Simulation, Cargèse, 2019
- Viruses and Cells: Computational Challenges and Approaches, Heidelberg, 2017
- Solvay Workshop on Multiscale Modelling in Physics, Chemistry and Biology, 2016
- Big Debate on Synthetic Biology, Barcelona, 2015

COMMISSIONS OF TRUST

- Scientific referee for Partnership for Advanced Computing in Europe (PRACE)
- Scientific referee for the following journals: European Biophysics Journal, Journal of Computational Physics, Journal of Chemical Theory and Computation, Philosophical Transactions of the Royal Society A, Molecular Biosystems, PLoS Computational Biology, PLoS One, Scientific Reports.

SOFTWARE & PROGRAMMING SKILLS

- *Operating Systems:* Linux, Windows, Mac OS
- *Programming & Scripting Languages:* C++, Python, Perl, Bash, Tcl
- *HPC, GPU and Distributed Computing:* AHE Middleware, CUDA, BOINC
- *Data Analytics & Deep Learning:* Matlab, R, Theano, TensorFlow
- *Molecular Dynamics:* NAMD, AMBER, ACEMD, Gromacs
- *Brownian Dynamics:* SDA, ReaDDy
- *Visualization:* VMD, PyMol, Chimera
- *Quantum Chemistry:* Gaussian
- *Docking:* Autodock, Vina
- *Writing & Presentation:* MS Office, EndNote, Mendeley, LaTeX, BibTeX, Keynote (Mac)

PUBLICATIONS

1. **S.K. Sadiq‡**, A. Muñiz Chicharro, P. Friedrich and R. Wade (2021) *bioRxiv,* A multiscale approach for computing gated ligand binding from molecular dynamics and Brownian dynamics simulations.

2. G. Balogh, T. Gyöngyösi, I. Timári, M. Herczeg, A. Borbás, **S. K. Sadiq‡**, K. Fehér‡ and K. E. Kövér‡ (2021) *J Chem Inf Model,* Conformational analysis of heparin-analogue pentasaccharides by nuclear magnetic resonance spectroscopy and molecular dynamics simulations, 61 (6) 2926-2936.

3. **S.K. Sadiq‡** (2020) *Catalysts,* Fine-tuning of sequence-specificity by near attack conformations in enzyme-catalyzed peptide hydrolysis, 10 (6) 684.

4. S. Lyonnais*‡, **S.K. Sadiq*‡** C. Lorca-Oró, L. Dufau, S. Nieto Marquez, T. Escriba, N. Gabrielli, X. Tan, M. Ouizougun-Oubari, J. Okoronkwo, M. Reboud-Ravaux, J. M. Gatell, R. Marquet, J.-C. Paillart, A. Meyerhans, C. Tisné, R. J.Gorelick, and G. Mirambeau*‡ (2019) *bioRxiv*, The HIV-1 ribonucleoprotein dynamically regulates its condensate behavior and drives acceleration of protease activity through membrane-less granular phase separation, 528638.

5. **S.K. Sadiq‡**, G. Mirambeau and A. Meyerhans. (2018) *AIDS Research and Human Retroviruses*. Equilibrium model of drug-modulated GagPol-embedded HIV-1 reverse transcriptase dimerization to enhance premature protease activation, 34 (9) 804-807.

6. R.G. Douglas, P. Nandekar, J.-E. Aktories, H. Kumar, R. Weber, J. M. Sattler, M. Singer, S. Lepper, **S.K. Sadiq**, R.C. Wade and F. Frischknecht. (2018) *PLoS Biology*, Inter-subunit interactions drive divergent dynamics in mammalian and *Plasmodium* actin filaments, 16 (7) e2005345.

7. N.J. Bruce*, G. K. Ganotra*, D. B. Kokh*, **S. K. Sadiq*** and R. C. Wade*. (2018), *Current Opinion in Structural Biology*. New approaches for computing ligand-receptor binding kinetics, 49:1-10.

8. D. A. Schuetz, W. E. A. de Witte, Y. Ch. Wong, B. Knasmueller, L. Richter, R. Bosma, D. B. Kokh, **S. K. Sadiq**, I. Nederpelt, E. Segala, M. Amaral, D. Guo, D. Andres, L. A. Stoddart, S. Hill, R. M. Cooke, R. Leurs, M. Frech, R. C. Wade, E. C. M. de Lange, A. P. IJzerman, A. Müller-Fahrnow, G. F. Ecker, (2017) *Drug Discovery Today*. Kinetics for Drug Discovery – An industry driven effort to target drug residence time. 22 (6) 896-911.

9. E Fleta-Soriano, K Smutná, JP Martinez, CL Oró, **SK Sadiq**, G Mirambeau, C Lopez-Iglesias, M Bosch, A Pol, M Brönstrup, J Diez and A Meyerhans (2017) *Antimicrobial Agents and Chemotherapy*, The myxobacterial metabolite Soraphen A inhibits HIV-1 by reducing virus production and altering virion composition. AAC-00739.

*10.***Sadiq, S.K. ‡** (2016). *Phil Trans R Soc A.* Reaction-diffusion basis of retroviral infectivity 374:20160148.

*11.***Sadiq, S.K. ‡** and Coveney P.V. (2015). *J Chem Theor Comput.* Computing the role of near attack conformations in an enzyme-catalyzed nucleophilic bimolecular reaction. 11 (1), pp 316–324

*12.*Venken, T., Voet, A., De Maeyer, M., De Fabritiis, G. and **Sadiq, S.K. ‡** (2013). *J Chem Theor Comput.* Rapid conformational fluctuations of disordered HIV-1 fusion peptide in solution. *9* (7), 2870–2874.

*13.*B. Konnyu, **S. K. Sadiq,** T. Turanyi, R. Hirmondo, B. Muller, J. Konvalinka, P. V. Coveney, H.-G. Krausslich, V. Muller. (2013). *PLoS Comp Biol.* Gag-Pol Processing during HIV-1 Virion Maturation: A Systems Biology Approach. 9(6): e1003103.

14. **Sadiq, S.K.*,** Guixà-González, R.*, Dainese E., Pastor, M., De Fabritiis, G. and Selent, J. (2013). *Curr Med Chem.* Molecular modeling and simulation of membrane lipid-mediated effects on GPCRs. 20 (1), 22-38.

15. **Sadiq, S. K.‡,** Noé, F. and De Fabritiis, G. (2012). *Proc Natl Acad Sci USA.* Kinetic characterization of the critical step in HIV-1 protease maturation. 109 (50), 20449-20454.

16. Wright, D.W.*****, **Sadiq, S.K.***, De Fabritiis, G. and Coveney, P.V. (2012). *J Am Chem Soc.* Thumbs down for HIV: Domain level rearrangements do occur in the NNRTI bound HIV-1 Reverse Transcriptase. 134 (31), 12885–12888.
17. **Sadiq, S. K.** ‡ Konnyu, B., Muller, V. and Coveney, P.V. (2011) *J Phys Chem B.* Reaction Kinetics of Catalyzed Competitive Heteropolymer Cleavage, 115, 11017– 11027.
18. Buch, I.*****, **Sadiq, S. K.*** and De Fabritiis, G. (2011). *J Chem Theor Comput.* Optimizing potential of mean force calculations of standard binding free energy, 7, 1765–1772.
19. **Sadiq, S. K.**‡ and De Fabritiis, G. (2010). *Proteins: Struct Funct Bioinf.* Explicit solvent dynamics and energetics of HIV-1 protease flap-opening and closing, 78: 2873–2885.
20. **Sadiq, S. K.**, Wright, D. W., Kenway, O. A. and Coveney, P. V. (2010). *J Chem Inf Model.* Accurate ensemble molecular dynamics binding free energy ranking of multidrug-resistant HIV-1 proteases, 50(5), 890–905.
21. R. S. Saksena, B. Boghosian, L. Fazendeiro, O. A. Kenway, S. Manos, M. D. Mazzeo, **S. K. Sadiq**, J. L. Suter, D. Wright, and P. V. Coveney, (2009). *Phil Trans R Soc A.* 367, *1897,* 2557-2571.
22. **Sadiq, S. K**., Mazzeo, M. D., Zasada, S. J., Manos, S., Stoica, I., Gale, C. V., Watson, S. J., Kellam, P., Brew, S. and Coveney, P. V. (2008). *Phil Trans R Soc A.* Patient-specific simulation as a basis for clinical decision making. 366, 3199-3219.
23. **Sadiq, S. K.,** Zasada, S. J., Wright, D., Stoica, I., and Coveney, P. V. (2008). *J Chem Inf Model.* Automated molecular simulation based binding affinity calculator for ligand- bound HIV-1 proteases. 48, 1909-1919.
24. Stoica, I., **Sadiq, S. K.** and Coveney, P. V. (2008). *J Am Chem Soc.* Rapid and accurate prediction of binding free energies for saquinavir-bound HIV-1 proteases. 130, 2639-2648.
25. Stoica, I., **Sadiq, S. K.**, Gale, C. V. and Coveney., P. V. (2008). *Future HIV Ther.* Virtual physiological human research initiative; the future for rational HIV treatment design? 2(5), 419-425.
26. **Sadiq, S. K.**, Wan, S. and Coveney, P. V. (2007). *Biochemistry.* Insights into a mutation-assisted lateral drug escape mechanism from the HIV-1 protease active site. 46 (51), 14865 - 14877.
27. **Sadiq, S. K.**, Zasada, S. J. and Coveney, P. V. (2006). *Lecture Notes in Computer Science.* Grid assisted ensemble molecular dynamics simulations of HIV-1 proteases reveal novel conformations of the inhibitor saquinavir. LNBI 4216, Berthold, M.R., Glen, R. and Fischer I. (eds.) CompLife 2006, Springer-Verlag, pp.150–161.
28. **S. K. Sadiq,** S. Wan, and P. V. Coveney (2006). *Antiviral Ther.* Ensemble molecular dynamics of HIV-1 protease with the inhibitor saquinavir: Insights into the molecular basis of drug resistance caused by the G48V and L90M mutations. 11:S151.
29. P. V. Coveney, **S. K. Sadiq,** R. S. Saksena, M. Thyveetil, S. J. Zasada, M. McKeown and S. Pickles (2006). *Proceedings of the UK e-Science All Hands Meeting.* A lightweight application hosting environment for grid computing. pp.217–224.
30. P. V. Coveney, **S. K. Sadiq**, R. S. Saksena, S. J. Zasada (2006). *Proceedings of the UK e-Science All Hands Meeting.* Constructing chained molecular dynamics simulations of HIV-1 protease using the application hosting environment. pp.428–431.

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