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I combine machine learning, biomolecular modelling, and statistical mechanics approaches, to understand how proteins move and interact with small molecules.

PROFESSIONAL EXPERIENCE

Academic

04/2021 — now	**Chancellor's Fellow** University of Edinburgh, School of Chemistry (SoC)
01/2020 — 03/2021	**Christina Miller Research Fellow** University of Edinburgh, SoC
04/2015 — 12/2019	**Postdoctoral Research Associate** with Prof. Julien Michel University of Edinburgh, SoC
	April 2019 - August 2019 Acting Group Leader during parental leave cover for Prof. Julien Michel
01/2013 — 03/2015	**Post-Doctoral Research Scientist** Computational Molecular Biology Group, Prof. Frank Noé School of Mathematics and Computer Science, Freie Universität Berlin

Other professional experience

03/2023 — now	**Consultant Redesign Science Ltd.**
03/2014 — now	**Freelance Project manager for IMAGINARY gGmbH**
12/2020 — 12/2022	**Consultant Exscientia Plc.**

EDUCATION

Jul 2013	**PhD in Physics,** University of Nottingham, Nottingham, UK
Jul 2007	**BSc Hons. in Physics with Chemistry** 1st Class Honours Keele University, Keele, UK

AWARDS, GRANTS, SCHOLARSHIPS AND PRIZES

2023	**Establishing the Accessible Computational Regimes for Biomolecular Simulations at Exascale (ExaBioSim)** Co-I, £620,045 (2023-2025 EPSRC)
2022	**Redesign Science PhD studentship,** ~£90k (2022-2025, UK)
2021	**Redesign Science 1 year postdoctoral position (50%),** £76k (2021- 2022, UK)
2021	**RSC Enablement Grant** (£9k) Understanding β-lactamase dynamics (Mar 2022-Feb 2023, UK)
2021	**Biomedical AI CDT Case PhD Studentship,** £40k, Exscientia (2021-2023, UK)
2020	**Chancellor's Fellowship** 5 year fellowship, ~£500k (2021-2026, UK)
2020	**SUPA Short term visit funding,** for visits to University of Florida and MSKCC £2500 (USA)
2019	**Christina Miller Research Fellowship** 3 year fellowship, ~£250k (2020-2023, UK)
2019	**RSC Outreach grant,** £1600 for *Chemistry in Focus* (2019-2020, UK)
2018	**Co-Investigator on**: EPSRC Flagship Software - BioSimSpace: A shared space for the community development of biomolecular simulation workflows Grant: EP/P022138/1, ~£524k (2018-2020, UK)

2017	**Institute for Academic Development New Network Award:** Edinburgh MD Simulation day, £1000 (UK)
2016	**Computing time worth $10000** on Amazon Web services (AWS) (UK)
2016	**Poster prize** at the 1st UK Research Software Engineering conference (UK)
2014	**1st prize** in the 'Fast-forward Science' short film competition (https://youtu.be/cyKb-P3mwDk) joint with G. Jouvet, Glacial mysteries (Germany)
2014	**Computing time** at the HLRN worth 3 million CPU hours (Germany)
2013	**3rd prize** in a competition of the "Math of Planet Earth 2013" initiative (http://imaginary.org/film/the-future-of-glaciers) (France)
2009	**BESTS travelling scholarship,** £3000 to fund research visit to UC Berkeley (USA)
2007	**DESY summer student** programme (Germany)
2006	**Nuffield undergraduate research bursary** (UK)

TEACHING EXPERIENCE AND TRAINING

2022 — now	**Machine learning for chemistry,** Course content designer and lecturer as part of 4th year course on Advanced Topics in Chemical Physics, 2 lectures & three 4-hour workshops and assessment — UoE
2022 —now	**CCP5 Summer school: MDAnalysis and machine learning workshop** Course content design and lecturer — Durham
2022	**2 day joint MDAnalysis and machine learning workshop (MGMS funded)** Course content design and lecturer and event organiser — UoE
2021 — now	**Chemistry 1A, 6 lectures on chemical yhermodynamics** Lecturer
2020 — now	**Data-Driven Chemistry,** Course content co-designer and lecturer compulsory year 2 course on programming and data analysis — UoE
2020	**Certified Software Carpentries Instructor,** online
2019 — now	**Phases and Interfaces** Tutorials for year 3 course — UoE
2019	**Two 1-Day workshops at the CCP BioBioSim Training Week** Course content design on alchemical molecular simulations, using BioSimSpace and course instructor for Markov State modelling using pyemma here — Bristol
2019 — 2021	**Taught and organised 5 Software or Data Carpentries workshops** — Various places
2018 — now	**Introduction to molecular dynamics lecture** as part of SUPA Computational Chemistry course —UoE
2018	**1-Day workshop at the CCP BioBioSim Training Week** Course content design on alchemical molecular simulations, as well as course instructor, using a cloud based teaching infrastructure with material available here
2015 — 2017	**Chemistry 1A and 1B co-tutor,** Running tutorials covering mainly introductory university level physical and quantum chemistry concepts — UoE
2014 — 2017	**PyEMMA workshop lecturer**, Freie Universität Berlin and King's College London Lecturer and tutor for 1-day courses on Markov State Modelling using PyEMMA software
2014	**MSc course organiser, Freie Universität Berlin** Co-organiser and lecturer for "Computational Molecular Physics and Methods of molecular simulations" MSc module for students across chemistry, physics and mathematics
2010 — 2011	**Private tutor** Private tuition for A-Level and AS-Level mathematics and physics
2008 — 2011	**Tutor for problem classes University of Nottingham** Subjects included: quantum mechanics, solid state physics, and mathematics for physicists

Teaching and Leadership Training

2022 **Fellow of the Higher Education Academy (FHEA)** through the Edinburgh Teaching Award

2020 **Aurora leadership training award** Aurora training supported by the School of Chemistry Edinburgh

2020 **Research leaders training program** from the Institute of Academic Development UoE

2013 **Higher education pedagogics training week**
One week training workshop on higher education pedagogics at the Freie Universität Berlin

Supervision

2015 — now **1 Postdoc, 9 PhD students, 5 MChem, 1 MSc, and 6 BSc students, 3 summer project students**

Postdoc

2021 — 2022 *Rob Arbon (50%),* ReDesign Science funded

PhD students

2023 — now *Marco Mattia,* Sofi CDT, (Primary supervisor)
2023 — now *Saabir Petker*, Sofi CDT (Co-supervisor)
2022 — now *Ryan Zhu,* ReDesign Science funded PhD (Primary supervisor)
2022 — now *Esra Nur Soysal* (Primary supervisor)
2022 — now *Dominic Philips*, Biomedical AI CDT, IBM funded (Co-supervisor)
2021 — now *Jasmin Güven* (Primary supervisor)
2021 — now *Rohan Gorantla,* Biomedical AI CDT, Exscientia funded (Primary supervisor)
2021 — now *Katerina Karoni*, Mag-Mics CDT student, IBM funded (Co-Supervisor)
2018 — 2022 *Jenke Scheen*, Cresset funded (Co-supervisor)
Applications of AI to alchemical free energy calculations for contemporary drug design

Supervision of master and bachelor students at the University of Edinburgh

2022/23 *Li Horowitz*, Undergraduate visiting research student, Relative binding free energy calculations using AlphaFold protein structures (School of Chemistry)

2022/23 Beth Killen, MChem year abroad student (School of Chemistry)
Project at University of Sydney with Dr Meredith Jordon

2021/22 *Yifan Wu, MSc student,* Comparison of Binding Affinities from Crystal and AlphaFold2 Protein structures (School of Chemistry)

2021/22 *Matthew Bowley,* MChem Chemistry, Modelling small peptides with machine learning potentials (School of Chemistry)

2021/22 *Ryan Zhu*, BSc Chemistry, Predict Protein-Ligand Binding Affinity Using Neural Networks: A Comparative Study (School of Chemistry)

2020/21 *Victor Principe* MChem Chemistry, The role transition metal in amyloid beta formation in Altzheimer's disease (School of Chemistry)

2020/21 *Junhao Wang* BSc Chemistry, Graph Convolutional Networks for binding affinity prediction of Covid Moonshot Folding@Home data

2019/20 *Jonathan Alvis* BSc Biochemistry, Searching the PDB how to select the right protein structures for simulation (School of Biological Sciences)

2019/20 *Cameron Marshall* BSc Biotechnology, Computational study of New Delhi beta-lactamase inhibitors (School of Biological Sciences)

2018/19 *Calum Smart* BSc Chemistry, Comparative study of different docking tools, Flare and VINA and their performance on BACE-1 as part of the D3R Grand Challenge 4 (School of Chemistry)

2016/17 *Jason Klebes* MSc Physics Investigating dynamics in small intrinsically disordered peptides using enhanced sampling methods and TRAM. (School of Physics)

2016/17 *Clara Kelly* BSc Chemistry Charging corrections in alchemical free energy protocols as part of the D3R Grand Challenge 2. (School of Chemistry)

2015/16 *David Tiemessen* MSc PhysicsLooking at coarse grained modelling of BSLA - a protein playing vital parts in Bacterial raincoats. (School of Physics)

2015/16 *Alexis Hennessy* MChem Chemistry Docking calculations and simple MD simulations of ligand molecules biding to HSP90 as part of the D3R Grand Challenge 2015. (School of Chemistry)

OTHER RESPONSIBILITIES, COMMITTEES & MEMBERSHIPS

Conferences and other organisational work

2024 **Organiser for recent appointees in physical chemistry conference,** UoE

2023 **Co-organiser for the early careers in SMTG RSC interest group meeting,** UoE

2022 **Organiser MDAnalysis and machine learning workshop,** UoE

2022 **Co-organiser of the 8th Annual CCPBioSim Conference**, UoE

2021 — now **Organiser of the Physical Chemistry Seminar series,** UoE

2020 **Chair of the 5th EaStChem** early careers researcher conference committee, UoE, Edinburgh

2018 **Organiser of the 3rd EaStChem** early careers researcher conference (ECECR2018), UoE, Edinburgh

2018 **Organiser of '2018 Workshop on Free Energy Methods, Kinetics and Markov State Models in Drug Design',** at Silicon Therapeutics and Novartis, Boston

2017 **Organiser of 'Edinburgh MD Simulation Day'**, a college of Science wide simulation day to encourage cross-departmental collaborations at UoE, Edinburgh

2016 **Organiser of joint physical chemistry meeting** between UoE and Heriot-Watt University, Edinburgh

2016 **Co-organiser of IMAGINARY conference 2016**, bringing mathematics outreach enthusiasts together, Berlin

2015-2018 **Chair of the Physical Chemistry Section Committee** at the University of Edinburgh, organising seminars and social events for PhD students and postdocs, Edinburgh

2010 **Organiser of a 1-day CUDA training workshop University of Nottingham,** Nottingham

2009 — 2011 **Founder and organiser of a "Scientific Computing Seminar"** for PhD students across various departments at the University of Nottingham, Nottingham

2009 — 2011 **Postgraduate committee** member at the University of Nottingham, Nottingham

Committees

2023 — now Co-opted member of the **Faraday Council**

2023 — now Member of the **Information security committee**, Chemistry UoE

2023 — now Member of the **CCPBioSim Management Group**

2022 — now **Statistical mechanics and thermodynamic**s RSC interest group committee

2021 — now **Technical advisory committee:** Open Free energy consortium

2021 — 2023 Member of the **Studentship allocation committee** (21/22), **Chair** (22/23)

2020 — now Member of the **Widening participation committee**

2019 — 2022 Member of the **Software Carpentry organisational committee** for Edinburgh

2019 — 2021 Member of the **Equality, diversity and inclusion committee,** Chemistry UoE

Editorial work

2022 — now Editor for the **Journal of Open Source Scientific Software**

2022 — now Editor for the **Living Journal of Computational Molecular Science**

PhD examination

2023 **External examiner PhD** for Alexander van Teijling, University of Strathclyde

Member of the Institute of Physics (IOP), **Royal Society of Chemistry** (RSC), **Biophysical Society** (PBS), and **Molecular modelling and graphics society (**MGMS**)**

INVITED TALKS & CONFERENCES (SELECTED)

1. **Invited seminar,** King's College London (Date TBC, postponed due to illness)
2. **Invited talk**, Society of Chemical Industry's Young Chemists' Panel (YCP) (October 2023)
3. **Invited seminar**, Department of Chemistry ETH Zürich (October 2023)
4. **Plenary talk**, WiFo2023 of the German Chemical Society (September 2023)
5. **Invited seminar,** Abbvie, internal CAAD seminar (September 2023)
6. **Invited talk**, CECAM workshop FU Berlin (June 2023)
7. **Invited seminar** Departmental Chemistry Seminar University of Manchester (May 2023)
8. **Panel member**, The future of AI in drug discovery, OMSF symposium, Boston (May 2023)
9. **Invited webinar** Statistical Mechanics and Thermodynamics RSC interest group (April 2023)
10. **Invited seminar,** Warwick Chemistry department Computational chemistry seminar (Feb 2023)
11. **Invited talk**, BioDocSoc informal networking seminar (October 2022)
12. **Invited talk**, 9th Heidelberg Laureate Forum, I am A.I. explaining artificial intelligence (September 2022)
13. **Invited seminar**, Statistical Physics and Complexity Webinar Series, online (May 2022)
14. **Invited talk**, DigiDrug, online (April 2022)
15. **Invited seminar**, UC Berkeley, Berkely (April 2022)
16. **Invited seminar,** Flatiron Institute, New York (April 2022)
17. **Invited seminar**, Carnegie Mellon - Pittsburgh Computational Biology PhD Program, online (December 2021)
18. **Invited talk**, Scotchem Women's Day, online (March 2021)
19. **Invited talk**, British Crystallography Association Meeting, online (March 2021)
20. **Invited talk**, ChemBio Cluster Meeting, Edinburgh (February 2020)
21. **Invited seminar**, Adrea Volkamer Research group, Charité Berlin (February 2020)
22. **Invited talk**, *Alchemical Free Energy Workshop,* Göttingen (May 2019),
23. **Invited seminar,** Mathematics Seminar, Nottingham Trent University, Nottingham (February 2019)
24. **Invited talk,** PyData, Edinburgh (September — 2018)
25. Conference Talk, *Europython*, Edinburgh (July — 2018)
26. **Invited talk**, *Cresset User Meeting,* Cambridge (June — 2018)
27. **Invited talk**, *Kinetics and Markov State Models in Drug Design,* Boston (May — 2018)
28. **Invited talk**, *CECAM Multi-scale modelling meeting*, Université Paris-Est, Paris (May—2017)
29. **Invited talk**, Institute for Condensed Matter and Complex Systems, UoE, Edinburgh (January — 2017)
30. **Invited talk**, *IOP Workshop: Self-Assembly, Recognition, and Application,* UoE, Edinburgh (December — 2016)
31. **Invited lecturer** at *CCPBiosim Molecular Kinetics workshop,* King's College London, London (September — 2016)
32. **Invited talk**, *Kinetics and Markov State Models in Drug Design,* Boston (May — 2016)
33. Seminar talk, A. Mulholland group, University of Bristol, Bristol (April — 2016)
34. Conference talk, *ACS Annual Meeting*, San Diego (March — 2016)
35. **Invited talk**, *D3R Workshop*, UCSD, San Diego (March — 2016)

36. **Invited lecturer**, *CECAM Macromolecular Simulation Software Workshop,* Jülich (October — 2015)
37. Conference talk, *ScotChem*, Strathclyde University, Glasgow (June — 2015)
38. **Invited talk,** *the Non-linear Science Colloquium,* Münster (November —2014)
39. Seminar talk, Schrödinger, New York (September — 2014)
40. Seminar talk, MSKCC, John Chodera Lab, New York (September — 2014)
41. Conference talk, *Exploring energy landscapes Conference*, Durham (August — 2014)
42. Seminar talk, UoE, (August — 2014)
43. **Invited talk**, *Roland Netz Group,* Freie Universität Berlin, Berlin (July — 2014)
44. Conference Talk, *Open Statistical Physics,* The Open University, Milton Keynes (March — 2013)
45. Conference Talk, *CCP BioSim Annual Meeting*, Nottingham (March — 2013)
46. Conference Talk, *Computer Simulations and Theory of Macromolecules*, Hünfeld (April — 2012)
47. Seminar talk, *Center for Soft Matter Research,* New York University, NY (September — 2011)
48. Conference Talk, *Open Statistical Physics,* Open University, Milton Keynes (March — 2011)
49. *MDnet conference*, University of Bath, Bath (November — 2010) (attended)
50. Autumn School, *Core Algorithms for High Performance Scientific Computing,* University of Warwick, Warwick (October — 2009) (attended)
51. 3-day meeting: *Aspects of Complexity,* University of Manchester, Manchester (July — 2009)

RESEARCH VISITS

Apr 2022 MSKCC, Prof. Chodera machine learning for binding affinity predictions

Aug 2014 University of Edinburgh, Dr Marieke Schor Collaboration on investigating the dock-lock mechanism for fibril formation

2011— 2012 Freie Universität Berlin, Dr Frank Noé visit that initiated the development of Multi-ensemble transition based free energy estimators.

Jul-Aug 2010 UC Berkeley, Dr Chodera Collaborative visit to explore entropy in trajectory ensembles.

Apr 2010 Université Paris VII, Prof. van Wijland: mathematical foundations in stochastic

Oct-Dec 2009 UC Berkeley, Prof. Geissler Collaborative visit, funded by the BESTS traveling scholarship understanding complex dynamical phases in lattice protein models.

PUBLIC ENGAGEMENT & OUTREACH

2019 — 2022 **Science Ceilidh RSC funded YTPT:**
Development of teaching resources for primary school children on topics around **proteins and drug discovery** (https://www.scienceceilidh.com).

2019 — now **Chemistry in Focus,** a RSC funded project for the production of 3 short movies highlighting recent publications of PhD students in the Physical Chemistry section at Edinburgh Chemistry

2019 — 2022 **STEM Ambassador with various 1-day activities, e.g. Edinburgh Science Festival**

2014 — now **Freelance project manager for IMAGINARY gGmbH** (www.imaginary.org)
IMAGINARY is a non-profit outreach organisation popularising modern mathematics, through exhibitions, workshops, and online-material

Selected List of outreach activities conducted as part of Freelance work with IMAGINARY:

2022 **Talk at Heidelberg Laureate Forum,** I am A.I. explaining artificial intelligence

2022 **Maths of Planet Earth** exhibition for the Maths of Planet Earth CDT at Imperial College London

2022 **AI explorable for schools MOOG** for secondary school available on KI-Campus

2021 — now **Workshop leader for AI-Debunk**
2020 **www.i-am.ai virtual exhibition on AI**
2020 **Maths of Planet Earth** exhibition for the Maths of Planet Earth CDT at Imperial College London
2019 **Contributor to Lala Lab** and exhibition on maths and music and Artificial Intelligence
2015 — now **IMAGINARY coordinator for Snapshots of modern mathematics,** short articles on current mathematical research (https://imaginary.org/snapshots)
2015 — 2022 **Technical Museum Berlin Germany,** Exhibit: Future of Glaciers on display, Berlin
2017 **2-week IMAGINARY exhibition as part of the ENESCU music festival** responsible for setup and training of local staff, Bucharest
2017 **UNESCO funded teacher training workshop in Liberia,** introducing 'Mathematics in a Suitcase' (designed and taught 2-day workshop), Monrovia
2016 **2-day IMAGINARY conference,** bringing together mathematics outreach practitioners around the world, organiser and workshop leader, Berlin
2015/2016 **Glasgow Science festival:** pop-up stand with IMAGINARY exhibitions, Glasgow
2015 **3 month IMAGINARY exhibition at the Weizmann Institute,** project coordinator, set-up, testing, and local staff training, Rehovot
2015 **MATRIX conference,** conference for community of mathematics museums, Dresden
2014/2015 **Long Night of Sciences Berlin: '**Math of Planet Earth' exhibition, Berlin
2014 **3-day IMAGINARY workshop at AIMS Institute South Africa,** coordinator for workshop content, exhibition setup, and local staff training, Cape Town
2014 **Tanzania Pi day — 1**-day pop-up workshop to celebrate 10th anniversary of pi day in Tanzania, Dar es Salaam

Publications:

1. Handbook of Mathematical Science Communication Chapter 8: The IMAGINARY Journey to Open Mathematics Engagement: History and Current Project E. Londaits, A. Matt, **A.S.J.S. Mey**, D. Ramos, C. Stussak, B. Violet World Scientific Series on Science Communication pp. 135-163 (2023) **DOI**
2. Modern Mathematics Communication — An Asian Focus, A.D. Matt, **A.S.J.S. Mey**, B. Violet, *Asia Pacific Mathematics Newsletter*
3. IMAGINARY – Mathematics Communication for the 21st Century, G.-M. Greuel, A.D. Matt, **A.S.J.S. Mey**, *Newsletter of the European Mathematical Society* 92, 3 (2014) [http://www.ems-ph.org/journals/newsletter/pdf/2014-06-92.pdf] [invited contribution]

Funding:

2019: RSC Outreach grant: Chemistry in Focus (£1600)
2017: UNESCO funding for 2-day teacher training workshop (€7000)
2016: Co-author for VW foundation funding for IMAGINARY conference 2016 (€50 000)
2015: Co-author for Leibniz association funding for the founding of IMAGINARY as a non-profit organisation (€200 000)
2015: Co-author for Funding from Ministry of Science and Education, Germany for exhibition in Israel (€50 000)

PEER REVIEW

Journals

European Physics Letters, Journal of Chemical Theory and Computation, PloS One Computational Biology, Journal of Chemical Physics, Journal of Computer Aided Molecular Design, Journal of the American Chemical Society

Grant agencies

Swiss National Science Foundation, French National Research Agency

PUBLICATIONS

Google scholar: goo.gl/PaKuF3
* equal contribution
^ corresponding author

Preprints

1. mRNA interactions with disordered regions control protein activity Y. Luo, S. Pratihar, E. Horste, S. Mitschka, **A.S.J.S. Mey**, H.M. Al-Hashimi, C. Mayr (2023) bioRxiv **DOI**

2. SILVR: Guided Diffusion for Molecule Generation N.T. Runcie, **A.S.J.S. Mey^**, arXiv (2023) **DOI**

Peer Reviewed

3. What geometrically constrained models can tell us about real-world protein contact maps, N. Molkenthin, J.J. Güven, S. Mühle, **A.S.J.S. Mey**^, *Phys. Biol.* **20** 046004 (2023) **DOI**

4. Course Materials for an Introduction to Data-Driven Chemistry, J. Cumby, V. Erastova, M.T. Degiacomi, J.J. Güven, C.L. Hobday, **A.S.J.S. Mey**^, H. Pollak, R. Szabla *Journal of Open Source Education*, **6**, 192 (2023) **DOI**

5. Efficient Purification of Cowpea Chlorotic Mottle Virus by a Novel Peptide Aptamer, G. Tscheuschner, M. Ponader, C. Raab, P. S. Weider, R. Hartfiel, J. O. Kaufmann, J. L. Völzke, G. Bosc-Bierne, C. Prinz, T. Schwaar, P. Andrle, H. Bäßler, K. Nguyen, Y. Zhu, **A.S.J.S. Mey**, A. Mostafa, I. Bald, M. G. Weller *Viruses*, **15**, 697 (2023) **DOI**

6. Best practices for constructing, preparing, and evaluating protein-ligand binding affinity benchmarks, D.F. Hahn, C.I. Bayly, H.E. Bruce Macdonald, J.D. Chodera, **A.S.J.S. Mey**, et al. *Living J. Comp. Mol. Sci.* **4**, 1497 (2022) **DOI**

7. Dynamic Profiling of β-Coronavirus 3CL M^{pro} Protease Ligand-Binding Sites, E. Cho, M. Rosa, Ruhi Anjum, S. Mehmood, M. Soban, M. Mujtaba, K. Bux, S.T. Moin, M. Tanweer, S. Dantu, A. Pandini, J. Yin, H. Ma, A. Ramanathan, B. Islam, **A.S.J.S. Mey**, D. Bhowmik, S. Haider, *J. Chem. Inf. Model.* **61**, 3058 (2021) **DOI**

8. Implementation of the QUBE Force Field in SOMD for High-Throughput Alchemical Free-Energy Calculations L. Nelson, S. Bariami, C. Ringrose, J. Horton, V. Kurdekar, **A.S.J.S. Mey**, J. Michel, D. Cole *J. Chem. Inf. Model.* **61**, 2124 (2021) **DOI**

9. Best Practices for Alchemical Free Energy Calculations*,* **A.S.J.S. Mey**^*, et al. Living J. Comp. Mol. Sci.* **2**, 18378 (2020) **DOI**

10. Hybrid Alchemical Free Energy/Machine-Learning Methodology for the Computation of Hydration Free Energies, J. Scheen, W. Wu, **A.S.J.S. Mey** et al. *J. Chem. Inf. Model.* **60***,* 5331 (2020) **DOI**

11. Assessment of binding affinity via alchemical binding free energy calculations, M. Kuhn, S. Firth-Clark, P. Tosco, **A.S.J.S. Mey**, M. Mackey, J. Michel, *J. Chem. Inf. Model.* **60**, 3120 (2020) **DOI**

12. Geometric constraints in protein folding, N. Molkenthin, S. Mühle, **A.S.J.S. Mey**, M. Timme, *PloS One* **15** e0229230 (2020) **DOI**

13. Dynamic design: manipulation of millisecond timescale motions on the energy landscape of Cyclophilin A, J. Juárez-Jiménez, A. Gupta, G. Karunanithy, **A.S.J.S. Mey**, et al. *Chem. Sci,* **11**, 2670 (2020) **DOI**

14. BioSimSpace: An interoperable Python framework for biomolecular simulation, L.O. Hedges, **A.S.J.S. Mey**, et al., *JOSS*, **4**, 1831 (2019) **DOI**

15. Allosteric effects in a catalytically impaired variant of the enzyme Cyclophilin A may be explained by changes in nano-microsecond time scale motions, P. Wapeesittipan, **A.S.J.S. Mey**, M. Walkinshaw, J. Michel, *Comms. Chem*. **2**, 41 (2019) **DOI**

16. Effect of automation on the accuracy of alchemical free energy calculation protocols over a set of ACK1 inhibitors, J.M. Granadino-Roldan, **A.S.J.S. Mey,** J.J. Perez, S. Bosisio, J. Rubio-Martinez, J. Michel, *PloS One* **14**, e0213217 (2019) **DOI**

17. Impact of domain knowledge on blinded predictions of binding energies by alchemical free energy calculations, **A.S.J.S. Mey**, J. Juárez-Jiménez, J. Michel, *J. Comput. Aided. Mol. Des.* **32**, 199 (2018) **DOI**

18. Blinded predictions of host-guest standard free energies of binding in the SAMPL5 challenge, S. Bosisio, **A.S.J.S. Mey**, J. Michel, *J. Comput. Aided. Mol. Des.* **31**, 61 (2017) **DOI**

19. Analytical methods for structural ensembles and dynamics of intrinsically disordered proteins, M. Schor, **A.S.J.S. Mey**, C.E. MacPhee, *Biophys. Rev.* **8,** 429 (2016) **DOI**

20. Blinded predictions of distribution coefficients in the SAMPL5 challenge, S. Bosisio, **A.S.J.S. Mey**, J. Michel, *J. Comput. Aided. Mol. Des.* **30,** 1101 (2016) **DOI**

21. Blinded predictions of binding modes and energies of HSP90-α ligands for the 2015 D3R Grand Challenge, **A.S.J.S. Mey***, J. Juárez-Jiménez*, A. Hennessy, J. Michel, *Bioorg. Med. Chem.* **24,** 4890 (2016) **DOI**

22. Elucidation of Non-Additive Effects in Protein-Ligand Binding Energies: Thrombin as a Case Study, G. Calabrò, C.J. Woods, F. Powlesland, **A.S.J.S Mey**, A.J. Mulholland, J. Michel, *J. Phys. Chem. B* **120,** 5340 (2016) **DOI**

23. Shedding light on the dock-lock mechanism in amyloid fibril growth using Markov State Models, M. Schor, **A.S.J.S. Mey**, F. Noé, C.E. MacPhee, *J. Phys. Chem. Lett.* **6**, 1076 (2015) **DOI**

24. Dynamic Properties of Forcefields, F. Vitalini*, **A.S.J.S. Mey***, F. Noé and B.G. Keller, *J. Chem. Phys.* **142**, 084101 (2015) **DOI**

25. Statistically optimal analysis of state-discretized trajectory data from multiple thermodynamic states, H. Wu, **A.S.J.S. Mey**, E. Rosta, F. Noé, *J. Chem. Phys.* **141,** 214106 (2014) **DOI**

26. xTRAM: Estimating equilibrium expectations from time-correlated simulation data at multiple thermodynamic states, **A.S.J.S. Mey**, H. Wu, and F. Noé, *Phys. Rev. X* **4,** 041018 (2014) **DOI**

27. Rare-event trajectory ensemble analysis reveals metastable dynamical phases in lattice proteins, **A.S.J.S. Mey**, P.L. Geissler and J.P. Garrahan, *Phys. Rev. E* **89**, 032109 (2014) **DOI**

28. Variational approach to molecular kinetics, F. Nüske, B.G. Keller, G. Pérez-Hernández, **A.S.J.S. Mey**, F. Noé, *J. Chem. Theory Comput.* **10**, 1739 (2014) **DOI**

29. EMMA - A software package for Markov model building and analysis, M. Senne, B. Trendelkamp-Schroer, **A.S.J.S. Mey**, C. Schütte, F. Noé, *J. Chem. Theory Comput.* **8**, 2223 (2012) **DOI**

30. Thermodynamics of trajectories of the one-dimensional Ising model, E.S. Loscar, **A.S.J.S. Mey**, J.P. Garrahan, *J. Stat. Mech.* **2011,** P12011 (2011) **DOI**