Patrick Penner

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Education

Novartis — Basel
Innovation Postdoc GDC/CADD, Advisor: Dr. Anna Vulpetti — 2022–Current

University of Hamburg — Hamburg
Doctorate in Computer Science, Advisor: Prof. Dr. Matthias Rarey — 2018–2023
- Thesis: "Interactive Pocket Exploration and Fragment Growing"

University of Vienna — Vienna
Mag. Pharm. in Pharmaceutical Science, Advisor: Univ.-Prof. Mag. Dr. Thierry Langer — 2012–2018
- Thesis: "Bulk Processing of Patent Molecule Associations"

Professional Experience

Inte:Ligand — Vienna
Project Work — Winter Semester 2017/18
- Pharmacophore Features for Halogen Bonding

Boehringer Ingelheim — Vienna
Internship in the CompChem Department — Summer 2017

Projects

- **FastGrow** (2022)
  Integrated in BioSolveIT SeeSAR
- **Halogen Bonding in Pharmacophores** (2018)
  Integrated in Inte:Ligand LigandScout
- **Torsion Library** (2022)
  Used in RDKit, Roche, OE etc.
- **Patent Molecule Associations** (2017)
  Integrated in Inte:Ligand KNIME nodes

Domain Knowledge

- **Structure-based Design** Advanced knowledge in development and application of structure-based methods
- **Statistical Modelling** Advanced knowledge in classical statistics/models and initial experience with emerging methods
- **Cheminformatics** In-depth knowledge of concepts, algorithms and design of systems
- **Pharmacophore Modelling** Advanced knowledge in development and application of pharmacophore methods, with or without receptor structure contributions
- **Chemical Patent Information** Experience with concepts specific to chemical and pharmaceutical patents
- **Quantum Chemistry** Experience in concepts and application
- **Drug Discovery** Initial experience in collaborative drug discovery projects

Programming

- **C++ (>100.000 Lines, >5 Years)**
- **Javascript (>10.000 Lines, >3 Years)**
- **Python (>10.000 Lines, >6 Years)**
- **Java (>10.000 Lines, >2 Years)**
- **Linux Environments and Configuration**
- **Data Science Packages**
- **Database Optimization**
- **Containerization**
- **Development Operations**
- **COBOL**

Publications

[1] **P. Penner** and A. Vulpetti, "QM assisted ML for 19f NMR chemical shift prediction", Oct. 2023. DOI: 10.26434/chemrxiv-2023-sd3vq-v2.

[2] **P. Penner**, W. Guba, R. Schmidt, A. Meyder, M. Stahl, and M. Rarey, "The torsion library: Semiautomated improvement of torsion rules with smartscompare", *Journal of Chemical Information and Modeling*, Mar. 2022. DOI: 10.1021/acs.jcim.2c00043.

[3] **P. Penner**, V. Martiny, L. Bellmann, F. Flachsenberg, M. Gastreich, I. Theret, C. Meyer, and M. Rarey, "Fastgrow: On-the-fly growing and its application to dyrk1a", *Journal of Computer-Aided Molecular Design*, vol. 36, no. 9, pp. 639–651, Aug. 2022. DOI: 10.1007/s10822-022-00469-y.

[4] K. Schöning-Stierand, K. Diedrich, C. Ehrt, F. Flachsenberg, J. Graef, J. Sieg, **P. Penner**, M. Poppinga, A. Ungethüm, and M. Rarey, "ProteinsPlus: a comprehensive collection of web-based molecular modeling tools", *Nucleic Acids Research*, Apr. 2022. DOI: 10.1093/nar/gkac305.

[5] L. Bellmann, **P. Penner**, and M. Rarey, "Topological similarity search in large combinatorial fragment spaces", *Journal of Chemical Information and Modeling*, vol. 61, pp. 238–251, 1 Oct. 2021. DOI: 10.1021/acs.jcim.0c00850.

[6] F. Flachsenberg, A. Meyder, K. Sommer, **P. Penner**, and M. Rarey, "A consistent scheme for gradient-based optimization of protein–ligand poses", *J. Chem. Inf. Model.*, vol. 60, pp. 6502–6522, 12 Dec. 2020. DOI: 10.1021/acs.jcim.0c01095.

[7] **P. Penner**, V. Martiny, A. Gohier, M. Gastreich, P. Ducrot, D. Brown, and M. Rarey, "Shape-based descriptors for efficient structure-based fragment growing", *J. Chem. Inf. Model.*, vol. 60, pp. 6269–6281, 12 Nov. 2020. DOI: 10.1021/acs.jcim.0c00920.

Conference Participation/Contributions

12th International Conference on Chemical Structures (ICCS) Noordwijkerhout, Netherlands
Improving Torsion Library Patterns with SMARTScompare 2022

16th German Conference on Cheminformatics and SAMPL Satellite Workshop Online
Research Talk: Fragment Growing Validation Dataset 2020

2019 GRS/GRC Computer Aided Drug Design West Dover VT, USA
GRC Poster: Next Generation Methods for Structure-Based Fragment Growing 2019
GRS Talk: Next Generation Methods for Structure-Based Fragment Growing

6th Strasbourg Summer School in Chemoinformatics Strasbourg, France
Participant 2018