
Prof. Dr. rer. nat. Holger Gohlke



born April 07th 1972 in Langen / Hessen

Position Professor (W2) of Pharmaceutical and Medicinal Chemistry at the Heinrich Heine University Düsseldorf

Contact Institute for Pharmaceutical and Medicinal Chemistry Heinrich Heine University Düsseldorf, Universitätsstr. 1, 40225 Düsseldorf

E-mail Gohlke@uni-duesseldorf.de

Phone +49-(0)211-81-13662

Academic studies and degrees

1997 - 2000 PhD thesis, Philipps University Marburg, Dr. rer. nat. (2000)

1997 - 2001 Applied Informatics, University Hagen

1992 - 1997 Chemistry, Technical University Darmstadt, Diploma (Dipl.-Ing.) 1997

Professional Career

since 2015 Managing director, Institute for Pharmaceutical and Medicinal Chemistry, Heinrich Heine University Düsseldorf

since 2009 Professor of Pharmaceutical and Medicinal Chemistry (W2), Heinrich Heine University, Düsseldorf, Germany

2008 - 2009 Professor of Pharmaceutical and Medicinal Chemistry (W2), Christian Albrechts University, Kiel, Germany

2003 - 2008 Juniorprofessor of Molecular Bioinformatics (W1), Goethe University, Frankfurt, Germany

2001 - 2003 Research Associate, The Scripps Research Institute, La Jolla, CA, USA

2000 - 2001 Postdoctoral Fellow, Philipps University, Marburg, Germany

Academic distinctions, honors and other activities

2012 Novartis Chemistry Lectureship

2009 Hansch Award of The Cheminformatics and QSAR Society

2005 “Innovationspreis” in Medicinal/Pharmaceutical Chemistry of German Chemical Society (GDCh) and German Pharmaceutical Society (DPhG)

2003 PhD thesis award of Philipps University, Marburg

2001 Feodor-Lynen fellowship of Alexander von Humboldt foundation

1999 Fellowship of ESCOM Science foundation

1995 Awardee of Dr. Anton Keller foundation, Technical University, Darmstadt

Academic activities

since 2017 PI in FOR 2518

since 2016 Co-speaker of the iGK, SFB 974

since 2016 Member of the steering committee, SFB 1208

since 2016 PI in SFB 1208

since 2016 PI in GRK 2158

since 2012 PI in the Bioeconomy Science Center (BioSC)

2012 - 2016 PI in SFB 974

since 2010 Member of the Faculty of CLIB Graduate Cluster Industrial Biotechnology

2009 - 2013 Member of the Board of Directors of NRW Research School Biostruct

Editorial activities

2013 Member of the Editor Search Committee of J. Chem. Inf. Model.

since 2011 Member of the Editorial Advisory Board of J. Med. Chem.

2011 Member of the Computational Pre-Review Panel of J. Med. Chem.

Patents

Pending Inhibitors of NHR2 and/or RUNX1/ETO-tetramerization.
EP Appl. 13165993.0, 2014.

Most important original publications

1. Frieg B, Görg B, Homeyer N, Keitel V, Häussinger D, **Gohlke H**. Molecular Mechanisms of Glutamine Synthetase Mutations that Lead to Clinically Relevant Pathologies. *PLoS Comput Biol*. 2016 Feb 2;12(2):e1004693. doi:10.1371/journal.pcbi.1004693. PubMed PMID: 26836257; PubMed Central PMCID:PMC4737493.
IF 4.326; 5-Year-IF 5.017
2. Fulle S, Saini JS, Homeyer N, **Gohlke H**. Complex long-distance effects of mutations that confer linezolid resistance in the large ribosomal subunit. *Nucleic Acids Res*. 2015 Sep 18;43(16):7731-43. doi: 10.1093/nar/gkv729. PubMed PMID: 26202966; PubMed Central PMCID: PMC4652758.
IF ; 9.202 5-Year-IF 8.647
3. Homeyer N, **Gohlke H**. Extension of the free energy workflow FEW towards implicit solvent/ implicit membrane MM-PBSA calculations. *Biochim Biophys Acta*. 2015 May; 1850(5):972-82. doi: 10.1016/j.bbagen.2014.10.013. PubMed PMID:25450172.
IF 2.590; 5-Year-IF N.N.
4. Homeyer N, Stoll F, Hillisch A, **Gohlke H**. Binding Free Energy Calculations for Lead Optimization: Assessment of Their Accuracy in an Industrial Drug Design Context. *J Chem Theory Comput*. 2014 Aug 12;10(8):3331-44. doi: 10.1021/ct5000296. PubMed PMID: 26588302.
IF 4.353; 5-Year-IF 5.756
5. Pflieger C, **Gohlke H**. Efficient and robust analysis of biomacromolecular flexibility using ensembles of

network topologies based on fuzzy noncovalent constraints. *Structure*. 2013 Oct 8;21(10):1725-34. doi: 10.1016/j.str.2013.07.012. PubMed PMID: 23994009.

IF 5.237; 5-Year-IF 5.622

6. **Gohlke H**, Schmitz B, Sommerfeld A, Reinehr R, Häussinger D. $\alpha 5 \beta 1$ -integrins are sensors for tauroursodeoxycholic acid in hepatocytes. *Hepatology*. 2013 Mar;57(3):1117-29. doi: 10.1002/hep.25992. PubMed PMID: 22865233.

IF 11.149; 5-Year-IF 11.854

7. Kalinin S, Peulen T, Sindbert S, Rothwell PJ, Berger S, Restle T, Goody RS, **Gohlke H**, Seidel CA. A toolkit and benchmark study for FRET-restrained high-precision structural modeling. *Nat Methods*. 2012 Dec;9(12):1218-25. doi: 10.1038/nmeth.2222. PubMed PMID: 23142871.

IF 25.328; 5-Year-IF 35.028

8. **Gohlke H**, Schlieper D, Groth G. Resolving the negative potential side (n-side)water-accessible proton pathway of F-type ATP synthase by molecular dynamics simulations. *J Biol Chem*. 2012 Oct 19;287(43):36536-43. doi: 10.1074/jbc.M112.398396. PubMed PMID: 22942277; PubMed Central PMCID: PMC3476320.

IF 4.258; 5-Year-IF 4.403

9. Metz A, Pflieger C, Kopitz H, Pfeiffer-Marek S, Baringhaus KH, **Gohlke H**. Hot spots and transient pockets: predicting the determinants of small-molecule binding to a protein-protein interface. *J Chem Inf Model*. 2012 Jan 23;52(1):120-33. doi: 10.1021/ci200322s. PubMed PMID: 22087639.

IF 3.657; 5-Year-IF 4.170

10. **Gohlke H**, Kiel C, Case DA. Insights into protein-protein binding by binding free energy calculation and free energy decomposition for the Ras-Raf and Ras-RalGDS complexes. *J Mol Biol*. 2003 Jul 18;330(4):891-913. PubMed PMID: 12850155.

IF 3-959 ; 5-Year-IF 3.795