

Prof. Dr. Holger Gohlke



1 General information

Holger Gohlke, Prof. Dr., *7.4.1972

Institute for Pharmaceutical and Medicinal Chemistry
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Current positions

- Professor (W3) of Pharmaceutical and Medicinal Chemistry, Heinrich Heine University Düsseldorf
- Director, Institute of Bio- and Geosciences (IBG-4: Bioinformatics), Forschungszentrum Jülich

2 University education with degree

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

3 Scientific degrees

2000 Thesis, PhD, topic: Development of a knowledge-based scoring function to predict the structure and affinities of protein-ligand complexes, Philipps University Marburg, mentor: Prof. Dr. G. Klebe

4 Professional career since final degree

since 2021	Director, Institute of Bio- and Geosciences (IBG-4: Bioinformatics), Forschungszentrum Jülich
since 2020	Professor of Pharmaceutical and Medicinal Chemistry (W3), Heinrich Heine University, Düsseldorf, Germany
2017 - 2022	Head, NIC Research Group Computational Biophysical Chemistry, Forschungszentrum Jülich
2021 - 2023 & 2015 - 2017	Managing director, Institute for Pharmaceutical and Medicinal Chemistry, Heinrich Heine University Düsseldorf
2009 - 2020	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

5 Other

Awards

2023 Phoenix Pharmacy Science Award in Pharmaceutical Chemistry for the publication Bhatia*, ..., Gohlke*, Kurz*, "Development of a First-in-Class Small-Molecule Inhibitor of the C-Terminal Hsp90 Dimerization", ACS Cent Sci 2022, 8, 636-655

2023 John von Neumann Institute for Computing (NIC) Excellence Project awarded for the Project "Structural dynamics of apo, agonist-, and antagonist-bound full-length ETR1"

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 2023 Member of the ad hoc working group of the DFG senate for topics of digital transformation

since 2023 Member of the DFG Committee for Scientific Equipment and Information Technology ("WGI-Ausschuss")

since 2022 Head of the International Advisory Panel, DASHH – Data Science in Hamburg (Helmholtz Graduate School for the Structure of Matter)

since 2019 Speaker, Research training group "Natural products and natural product analogs against therapy-resistant tumors and microorganisms: new lead structures and modes of action" (GRK 2158)

2018 - 2022 Member of the Board of Directors of the John von Neumann Institute for Computing (NIC)

2016 - 2024 Member of the Steering Committee, Collaborative research center „Identität und Dynamik von Membransystemen – Von Molekülen zu zellulären Funktionen“ (SFB 1208)

2016 - 2019 Co-Speaker "integriertes Graduiertenkolleg" (iGK), Collaborative research center „Kommunikation und Systemrelevanz bei Leberschädigung und Regeneration“ (SFB 974)

since 2015 Member of the "Fakultätsrat der Mathematisch-Naturwissenschaftlichen Fakultät der Heinrich-Heine-Universität"

2012 - 2016 Member of the Faculty of the "Graduiertenkolleg" iGRASPseed

2010 - 2016 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.