

## Prof. Dr. Holger Gohlke



### 1 General information

Holger Gohlke, Prof. Dr., \*7.4.1972

Institute for Pharmaceutical and Medicinal Chemistry  
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Institute of Bio- and Geosciences (IBG-4: Bioinformatics) &  
John von Neumann Institute for Computing (NIC),  
Jülich Supercomputing Centre (JSC), and  
Institute of Biological Information Processing (IBI-7: Structural Biochemistry)  
Forschungszentrum Jülich  
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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
- Head, NIC Research Group Computational Biophysical Chemistry, 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

since 2017      Head, NIC Research Group Computational Biophysical Chemistry,  
Forschungszentrum Jülich

since 2021 &  
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

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 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)  
since 2018      Member of the Board of Directors of the John von Neumann Institute for Computing (NIC)  
since 2016      Member of the Steering Committee, Collaborative research center „Identität und Dynamik von Membransystemen – Von Molekülen zu zellulären Funktionen“ (SFB 1208)  
since 2016      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.