**Gordon Chalmers**

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Results-oriented and passionate computational scientist with a background in molecular chemistry, physics and computer science. Adept in continuing work in computational chemistry, molecular modeling and analysis with strong background in NMR (nuclear magnetic resonance) data. Possessing excellent analytical skills in math, physics, and science. General work areas span molecular chemistry (computational, modeling, and NMR related data), computer science, and physics. Much work has been in machine learning and within this area in particular, genetic algorithms.

Participates in research projects innovating, applying intellectual ability and in-depth knowledge of the application of molecular modeling, computation, and interpretation relevant to the function of proteins and small molecules including carbohydrates, calculating NMR observables from molecular models, and molecule design. Work in the last 2 years has focused on small molecules, inhibitor (drug) design and development.

Have worked in pharmaceutical setting on more than half dozen potential oral drug candidates and am familiar with the drug discovery and development pipeline. Both in a company setting and in a pharmacy dept academic setting. Some, small part, of this work cannot be discussed for legal reasons.

**AREAS OF EXPERTISE**

computational chemistry

molecular dynamics

theoretical particle physics

quantum field and string th.

numerical algorithms

nuclear magnetic resonance

NP-Hard, NP-complete

databases

mathematics

cluster computing

complexity theory

real-time systems

software dev.

carbohydrates, proteins

genetic algorithms

optimization algorithms

system administration

machine learning

neural networks

**SEVERAL HIGHLIGHTS**

* My contributed software at the Glycam site (glycam.org) has been uniquely downloaded more than 2,400 times.
* Programming work involved the use of many specialized scientific software systems, primarily in molecular dynamics simulations, modeling, and analysis.
* Extensive use of computer science, molecular chemistry, machine learning, mathematics, physics.
* Department of Education fellowship, research assistantships, and teaching assistants during the 1st PhD.
* Graduate research assistantship during the 2nd PhD from the Complex Carbohydrate Research Center.
* Work with Prestegard generated an awarded R01 NIH grant, 2019.
* Software and other content at: <http://github.com/gordonchalmers>
* Some of the C++ and Matlab software used in published work is available at sites of the Robert J. Woods group, the James H. Prestegard group, and the Gaetano T. Montelione group:

<http://glycam.org/docs/othertoolsservice/downloads/downloads-software/>

<http://tesla.ccrc.uga.edu/software/>

<http://montelionelab.chem.rpi.edu>

**EDUCATION & CREDENTIALS**

UNIVERSITY OF GEORGIA **2019**

**PhD Computer Science**: *Genetic Algorithms in Different Areas of Science*

**(Doctoral Minor in Statistics)**

UNIVERSITY OF CALIFORNIA, LOS ANGELES (UCLA) – Los Angeles, CA **1991 & 1995**

**PhD Physics** – *1995 •* **M.S. Physics** & **B.S. Physics** – *1991 – Outstanding Graduate Student Award 1995*

**ACADEMIC EXPERIENCE**

UNIVERSITY OF GEORGIA (UGA), COMPLEX CARBOHYDRATE RESEARCH CENTER (CCRC) **2021**

**Visiting Scholar**

* Research in molecule design.

RENSSELAER POLYTECHNIC INSTITUTE (RPI), CENTER FOR BIOTECHNOLOGY AND INTERDISCIPLINARY STUDIES (CBIS) **2020-2021**

**Staff Research Scientist**, Montelione Lab

* Research and calculations of proteins in the areas of computational chemistry, NMR, machine learning, generating software including data mining. Supported group computer usage including software, sys-admin.
* Remote work mostly.

UNIVERSITY OF GEORGIA (UGA), COMPLEX CARBOHYDRATE RESEARCH CENTER (CCRC) **2013-2019**

**Research Assistant**, Prestegard Lab, Woods Lab

* Research and calculations with proteins and carbohydrates in the areas of computational chemistry, NMR, and various. Collaborative and independent research.
* Software development in both labs.
* Completed graduate work in computer science, computational chemistry, and statistics.

UNIVERSITY OF CALIFORNIA – LOS ANGELES (UCLA) – Los Angeles, CA **2001-2009**

**Lecturer** – *2001-2002 •* **Postdoctoral Associate** – *2006-2009*

* Research and teaching, undergraduate and graduate level in physics.
* Continued research in theoretical particle physics.

ARGONNE NATIONAL LABORATORY – Chicago, IL **1998-2001**

**Postdoctoral Associate**

* Conducted research in the theoretical particle physics. Collaborative and independent research.
* Refereed journal articles.

STATE UNIVERSITY OF NEW YORK – Stony Brook, NY **1995-1998**

C.N. YANG INSTITUTE FOR THEORETICAL PHYSICS

**Postdoctoral Associate**

* Conducted theoretical particle physics research. Collaborative and independent research.
* Refereed journal articles.

**INDUSTRY EXPERIENCE**

VENENUM BIODESIGN, GENESIS BIOTECHNOLOGY GROUP

**Computational Chemist, Team Leader**

* .Worked with synthetic and medicinal chemists in drug design and hit-to-lead development **2022**(2 mo.)

RAYTHEON AEROSPACE – El Segundo, CA **2002-2004**

**Engineer IV**

* Algorithm and software development pertaining to AESA radars.
* Received Patent for: Instantaneous 3—D target location resolution utilizing only bistatic range measurement in a multistatic system.

**MEMBERSHIP**

GLYCAM SOFTWARE DEVELOPER TEAM in the WOODS GROUP • **Member**

***Compiled languages***: C++, C, Java, Fortran, and others as needed

***Non-compiled languages***: Matlab, Python, Bash, R, Html, Javascript... ***Operating sys***: Linux, Windows, VMs

***Specialty software for computational chemistry***: CCDC GOLD, AM-MN Corina, AutoDock (4.2, Vina), Amber, PyTorch, RDKit, Cyana, AlphaFold, Cpptraj, VMD, Chimera, Glylib, PpmOne, ShiftX2, Cyrange, PdbStat, VinaCarb, Oculus Nanome, Open Babel, and many others

***Web design***: Wordpress, Drupal ***Parallel processing***: Pmemd, Posix threads, CUDA

***Database management***: MySql, Apache **Collaboration**: Git

**PUBLICATIONS**

***Papers in physics***: 88 found at [https://scholar.google.com/citations?user=LOyh-tYAAAAJ&hl=en](about:blank)

***Presentations in molecular work***: <https://github.com/gordonchalmers/GRC_Presentations>

***Software:*** https://github.com/gordonchalmers

***Papers in computational chemistry:***

Gordon Chalmers, Dynamic docking in protein-ligand modelling. Accepted, in revision at Journal of Computational Chemistry. chemRxiv: 10.26434/chemrxiv-2022-6m0q5.

Gordon Chalmers, Computational molecular modelling of Paxlovid binding. Submitted to Journal of European Medicinal Chemistry. chemRxiv: 10.26434/chemrxiv-2022-vfn6t.

Xu Yang, Gordon Chalmers, Asif Shajahan, Stephanie Archer-Hartmann, Christian Heiss, Parastoo Azadi. Rational design of glycopeptides enrichment tool based on boronic acid chemistry and ESI-MS/MS Analysis. Annual meeting at GlycoMIP (2022). Github://gordonchalmers/GRC\_presentations.

Gordon Chalmers. Computational Study of Paxlovid in Ligand GA. Submitted to Journal of Computer-Aided Molecular Design. chemRxiv: doi: 10.26434/chemrxiv-20220p2phq. Found also at, with supplementary information:

https://www.dropbox.com/sh/3vuza1s0gjmy1eo/AADLXPPe2Ve-N3RjMH3GoH5fa?dl=0

Gordon Chalmers. Ligand GA: a genetic algorithm for automated protein inhibitor design. Accepted, in revision at Nature Scientific Reports. bioRxiv: doi: 10.1101/2021.10.11.463970. Software package: https://www.dropbox.com/sh/s5nm3yzsd3l4y5r/AADCjHIymuu0nWSYnD3V0dQRa?dl=0

Sriram Aiyer, G.V.T. Swapna, Li-Chung Ma, Gaohua Liu, Jingzhou Hao, Gordon Chalmers, Brian C. Jacobs, Gaetano T. Montelione, Monica J. Roth. A common binding motif in the ET domain of BRD3 forms polymorphic structural interfaces with host and viral proteins, Structure 2021 Aug 5, 29(8):886-898. bioRxiv 2020.09.21.306696. doi: 10.1101/2020.09.21.306696.

Gordon Chalmers, Shelby H. Funk, Genetic Algorithms in Real-Time Systems, submitted to the Journal of Real-Time Systems, 2020.

Gordon Chalmers, Alexander Eletsky, Laura Morris, Jeong-Yeh Yang, Fang Tian, Robert J. Woods, Kelley W. Moremen and James H. Prestegard. NMR resonance assignment methodology: characterizing large sparsely labeled glycoproteins, J Mol Biol. 2019 May 3, 431(12):2369-2382. doi: 10.1016/j.jmb.2019.04.029. PMID: 31034888. PMCID: PMC6554063.

Gordon Chalmers, Shelby H. Funk, Adjusting Real-Time Mode Transitions via Genetic Algorithms, 2017 16th IEEE International Conference on Machine Learning and Applications. (presented at conference)

Sheikh, Mohammed, Thieker, David, Chalmers, Gordon, Schafer, Christopher, Ishihara, Mayumi, Azadi, Parastoo, J. Woods, Robert, N. Glushka, John, Bendiak, Brad, H. Prestegard, James, M. West, Christopher. O2 sensing associated glycosylation exposes the F-box combining site of the Dictyostelium Skp1 subunit in E3 ubiquitin ligases, Journal of Biological Chemistry 2017 Nov 17, 292(46):18897-18915. doi:10.1074/jbc.M117.809160. PMID: 28928219. PMCID: PMC5704474.

Kari Pederson, Gordon R. Chalmers, Qi Gao, Daniel Elnatan, Theresa A. Ramelot, Li-Chung Ma, Gaetano T. Montelione, Michael A. Kennedy, David A. Agard, James H. Prestegard. NMR characterization of HtpG, the E. coli Hsp90, using sparse labeling with 13C-methyl alanine. J Biomol NMR, 2017 Jul, 68(3):225-236. doi:10.1007/s10858-017-0123-8. PMID: 28653216. PMCID: PMC5546222.

Qi Gao,Gordon R. Chalmers, Kelley W. Moremen, James H. Prestegard. NMR assignments of sparsely labeled proteins using a genetic algorithm. Journal of Biomolecular NMR, 2017 April, 67:283–294. doi: 10.1007/s10858-017-0101-1.

G. Chalmers, J.N. Glushka, Bethany Foley, R.J. Woods, J.H. Prestegard. Direct NOE simulation from long MD trajectories. Journal of Magnetic Resonance, 2016 Jan 21, 265:1-9. doi: 10.1016/j.jmr.2016.01.006. PMID: 26826977. PMCID: PMC4818662.

~20 presentations (~30 talks) about topics regarding my work at the CCRC (UGA) and CBIS (RPI) are available at [https://github.com/gordonchalmers/GRC\_Presentations](about:blank) or upon request.

**REFERENCES**

Christian Heiss, Senior Research Scientist, Complex Carbohydrate Research Center, University of Georgia, 315 Riverbend Road, Athens, GA 30605, [cheiss@ccrc.uga.edu](mailto:cheiss@ccrc.uga.edu) 706 542 3008

James H. Prestegard, Professor, Complex Carbohydrate Research Center, University of Georgia, 315 Riverbend Road, Athens, GA 30605, [jpresteg@ccrc.uga.edu](mailto:jpresteg@ccrc.uga.edu) 706 542 6281

David Crich, College of Pharmacy and Complex Carbohydrate Research Center, University of Georgia, 110 West Green Street, Athens, GA 30605, [David.crich@uga.edu](mailto:David.crich@uga.edu) 706 542 5605

Robert J. Woods, Professor, Complex Carbohydrate Research Center, University of Georgia, 315 Riverbend Road, Athens, GA 30605, [rwoods@ccrc.uga.edu](mailto:rwoods@ccrc.uga.edu) 706 542 4454

Alan H. Darvill, Director of the CCRC, Professor, Complex Carbohydrate Research Center, University of Georga, 315 Riverbend Road, Athens, GA 30605, [adarvill@ccrc.uga.edu](mailto:adarvill@ccrc.uga.edu) 706 542 4411