**Gordon Chalmers**

I am a motivated, and career minded computational scientist who has worked in cutting-edge research and for many years. My current interests and work are in molecular chemistry, protein and ligand-protein modeling and design, small molecules including carbohydrates and modeling/design, software/scientific computation, and in machine learning. I have worked in computation, molecular modeling and analysis, NMR, molecular scientific software, and machine learning. I am up to date in modern developments in these areas and in molecular software. I am targeting a job investigating molecules, pharmaceutical design and/or development, machine learning, and/or in a high performance computing (HPC) environment.

My experience includes working in molecular protein-protein and protein-ligand interactions, screening, or data mining with a goal of finding new molecules, and also in the use of CSD GOLD. I have much experience working with both proteins and carbohydrates at the computational and atomic scale, and in the last 2 years, in general with small molecules pertaining to drug design and development. I have considerable experience in molecular modeling from a decade of collaborative research work at the UGA Complex Carbohydrate Research Center (CCRC) and RPI Center for Biotech. and Inter-disciplinary Studies. Recently I have worked in an industrial environment in the role of molecular modeling with a team of synthetic and medicinal chemists.

My work in molecular chemistry is heavily grounded in software pertaining to molecular analysis and computational understanding of small molecules, proteins, and their interactions. This uses a large amount of technical experience in computational tools using structures, MD, force fields, NMR experimental data, and importantly SAR data and screening. I utilize the protein databases Protein Data Bank, Uniprot, PDBe, AlphaFold and small molecule PubChem, Zinc, and many others, to get structures, experimental data, and other statistical and biochemical measures and firmly understand their use. I also am very familiar with and use many molecular software packages and tools. Please examine the github link in my CV and folders in it, such as presentations for some details. I have experience, in using and creating, databases in molecular work. In the past year I have worked with a focus on drug discovery and design, and this has involved collaborations with medicinal and synthetic chemists both at UGA CCRC and at a small company. I have worked in a laboratory setting at UGA and a company for both hit discovery and hit-to-lead optimization of small molecule therapeutics.

At 19 I started my research career in physics at UCLA where I co-published my first papers and started graduate classes, both in physics. I advanced into theoretical particle physics after working in condensed matter physics. Since obtaining my PhD in theoretical physics in 1995 I began a long attempt to find a permanent career in theoretical particle physics and string theory. During gaps in employment I continued research in quantum field and string theory, and in software design for a start-up.

I decided to enroll for another Ph.D., due to my interest in computer science. I obtained my Ph.D. in CS at UGA, which has a very extensive curriculum, in the fall of 2019. The core of the CS PhD work was in approximation algorithms of NP hard or complete problems, optimization algorithms, genetic algorithms, machine learning, and complexity theory. My Ph.D. is in CS, but I spent more than 70% of my time working in molecular chemistry, computation, software, molecular modeling, nuclear magnetic resonance, and in both protein and carbohydrate science. This was within several research groups at the CCRC.

I have experience in collaborating, speaking in public, and work well in a team. For example,~20 PPT presentations (~30 talks) in chemistry are available for review, including my 2019 Ph.D. dissertation, at <https://github.com/gordonchalmers/GRC_Presentations>. During my physics career I gave more than 100 seminars in 14 countries.

Some of my previous research, being published in Scientific Reports and Journal of Comp Chem, is very relevant and applicable to modern day small molecule and drug design and listed with a link in my CV. This work uses is a genetic algorithm approach to generating high scoring small molecule binders with specificity to proteins, i.e. therapeutics or anti-virals, with or without the use of known databases of molecules or fragments. The project was ongoing and further discussion is in the software documentation folder and paper; Multiple papers have been generated in this avenue. The tools generated in that software, and its unreleased up-to-date version Ligand Multi-Protein GA, are applicable to general large scale molecular analysis in drug design, and potent for both computational hit and hit-to-lead design without the use of databases. The Ligand GA molecular design project and software has wide applications, also in materials science. In this project I have used the software and also just the scripts and techniques to advance several small molecules to potential therapeutic candidates. This is recent work and I have worked in a broader context of proteins and molecules in varying ways including analyzing large datasets from both in public databases.

I have worked on a variety of proteins, in their ligand properties, in NMR, and in software development in several projects, one of which with J.H. Prestegard helped generate an R01 grant. The software that I have written can be found linked in my CV. I have been using scientific software such as Matlab for more than 20 years and appreciate the algorithmic development. Due to my background in particle physics I bring a large number of techniques to scientific computing work in molecular biochemistry such as those based in graph theory or efficient techniques for large scale computation.

My 2nd PhD and much work during and after this used different machine learning approaches, and genetic algorithms are in my expertise and I have written many of these. I am up to date on machine learning algorithms in general and can use genetic algorithms or other techniques in computational modeling. This includes the areas of small molecule design and developing protein structures. I have an ideal mixture of molecular chemistry, computer experience, machine learning, and physics to solve hard and specific molecular problems. I am used to using large datasets and finding correlations of information, this skill is applicable to applying my knowledge to analyze bioinformatics information.

I appreciate the opportunity to be considered for a molecular computational position. My CV is attached, and it has details of work areas, topics, and information about my background and work pertaining to this position. It is difficult for me to summarize all of the work that I have participated in or completed, have done partially in short snippets in this cover letter, and I do feel that I can contribute in the role to which I applied.