**Gordon Chalmers**

I am a hard-working, motivated, and career minded computational scientist who has worked in several areas doing 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 machine learning. Please understand that it is difficult for me to concisely explain my background, knowledge, expertise, and ability in these areas. In chemistry I have worked much 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 others, and in molecular software. I would very much like a job having to do with molecules, machine learning, and/or in a high performance computing (HPC) environment. I am willing to work in any of these broad areas.

Responsibilities requiring experience working in molecular protein-protein and protein-ligand interactions, screening, or data mining with a goal of finding new molecules for a purpose, is in my area, also in the use of CSD GOLD. I have much experience in both proteins and carbohydrates, and in the last 2 years, in general small molecules. I have much experience in molecular modeling from work at the UGA Complex Carb. Res. Center (CCRC) and RPI Center for Biotech. and Inter-disciplinary Studies.

My work in molecular chemistry is heavily grounded in software pertaining to molecular structures, MD, force fields, structure files and analysis, and in NMR experimental data. I can go to the BMRB, Protein Data Bank, protein databases such as PDBe, or molecule databases to get structures, experimental data, and other statistical measures and firmly understand it. I have performed statistical analysis of BMRB data of NOESY and HSQC data, and I have also produced an (unpublished) database of publicly available measurements and back calculated RDC’s from a set of over 150 proteins, 20 snapshots of the protein dynamics (models in the pdb), and statistical analysis of >300,000 RDCs. I have worked a variety of computational topics in NMR including trajectory based modeling of NMR observables and simulated spectra (1D, 2D, 3D of different types), automated assignment and automated peak-picking, and in my brief position at RPI in database analysis and in creation of one database, and protein structure building from NMR data, as well as further analysis of NMR relaxation data.

The next 9 sentences describe the timeline of my career. I started my research career in physics at the age of 19 at UCLA having co-published my first papers then and starting graduate classes, both in physics. I went 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. There are employment gaps and during these periods I continued research in quantum field and string theory and also attempted a startup concerned with creating educational software for better teaching of advanced physics, although other options were available.

I decided to enroll for another Ph.D., one that is closer to practicality, 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. The 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 in several research groups at the CCRC.

I have experience in collaborating, speaking in public, and work well in a team. ~20 PPT presentations (~30 talks) in chemistry are available, 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.

A recent paper, in review at J Comp-Aided Mol Design, is very relevant and applicable to modern day small molecule and drug design and listed with a link in my CV. It is a genetic algorithm approach to generating high scoring small molecule binders to proteins, i.e. therapeutics or anti-virals, with or without the use of known databases of molecules or fragments. The project is ongoing and, discussed in the software documentation folder and paper. A 2nd paper, Computational Study of Paxlovid in Ligand GA, is in review at J Comp-Aided Mol Design and uses Ligand GA to find in silico inhibitors of SARS-Cov-2 3CL main protease and a thorough examination of these. A generalization of the software using a multi-objective function, Ligand Multi-Protein GA, is soon to be released. The Ligand GA molecular design project and software has wide applications, also in materials science.

I appreciate the opportunity to be examined as a serious, knowledgeable, and experienced individual for what your job requires in computation and molecular chemistry. My work in chemistry has been in fruitful, enjoyable, and productive collaborations. My CV is attached, and it has details of work areas, topics, and information about my background and work pertaining to employment.