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Piotr Sliz, PhD
Structural Biology Computing Group
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Dear Piotr,

Our laboratory is interested in protein-protein interactions, particularly those mediating immune recognition. We use X-ray crystallography and biochemistry to study purified proteins, and are beginning to include confocal and electron microscopy (EM) to examine protein complexes in cells. Some of our work focuses upon homologs and mimics of class I MHC proteins. These proteins have similar three-dimensional structures, but different functions including immune functions (IgG transport by the neonatal Fc receptor, FcRn; evasion of the immune response by viral MHC mimics), and non-immune functions (regulation of iron or lipid metabolism by HFE and ZAG). We are also comparing the structures and functions of host and viral Fc receptors with FcRn. The structural studies of these compounds have been aided recently by the utilization of the software distribution from SBGrid.

The SBGrid computer farm has the potential to help our laboratory by increasing the processing power required for molecular replacement and refinement calculations on the large multi protein structures that are the focus of our current research efforts. A number of our past efforts could have benefited by using multi threaded calculations. The structure of prostate-specific membrane antigen (PSMA) is a large dimeric protein having over 2800 residues in the asymmetric unit. A large number of molecular replacement trails were conducted with multiple alignments before a final solution was determined. In the process of removing any bias from the structure a number of composite omit map calculations where done with the program suite CNS. Both of the steps in the determination of the PSMA structure could have benefited from a

multiprocessor environment as offered by the SBGrid computer farm. The composite omit map calculations alone could run for a couple of days on a single processor workstation. Having the possibility of running these calculations in a optimized multiprocessor environment would have greatly reduced the time it took in completing the structure.

This letter affirms our commitment to continue our collaboration as members of the SBGrid Consortium project. We look forward to using the new grid enabled software, as it will provide an important tool for our structural biology research. We are also aware of your new General User Program for cluster computing and will utilize it if opportunity arises.

Good luck with your grant. I look forward to working together.

Sincerely,

Pamela J. Bjorkman
Max Delbrück Professor of Biology
and Investigator, HHMI