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Dear Roy,

the Open Science Grid (OSG) would like to acknowledge and thank Cancer Computer for their ongoing contributions of computing resources to benefit and accelerate cancer research. While much cancer research requires medical and biological resources, an increasing share of the work is performed on computers — from biochemical simulations and analyses of potential therapeutic compounds to genetic analyses of cancer tissues to improved medical imaging and radiological techniques. Cancer Computer makes available vast amounts of computing to researchers who otherwise might lack the resources to make significant progress on one of our most pressing health issues.

The OSG facilitates access to distributed high throughput computing for open science research. The resources accessible through the OSG are contributed by the community, organized by the OSG, and governed by the OSG Consortium for use by researchers via local or OSG-supported submission points. In the collaboration with Cancer Computer, OSG helps to label certain computing work as supporting cancer research (based on identification from researchers themselves), then directs that work to compute resources provided by Cancer Computer as available.

To date, Cancer Computer has provided over 4.4 million hours of computing within the last year to six projects via OSG, detailed below. SPLInter has been the most aggressively "hungry" project, having work in queue virtually at all times, and as a result consumed close to 80% of these compute hours. The remaining 20% were used by the others.

- The **Structural Protein-Ligand Interactome** (SPLInter) project, led by Prof. Samy Meroueh (Indiana University), is an online database that predicts interactions of small organic molecules with proteins through structure-based molecular docking and scoring. The more compounds that are docked and scored, the greater the diversity of the interactome, or the set of molecular interactions in a given cell. This increases the chances of making promising discoveries and speeds the research process from simulation, to ordering, to wet lab testing in a more efficient manner. Small molecule therapeutics, such as the anti-cancer drug Gleevec, work by binding to a specific protein in the body and modulating its function. Cancer researchers work to pinpoint proteins in cancer cells, and find compounds that target those proteins, all in hopes of shutting them down.

- **BioGraph**, a project led by Prof. Alex Feltus (Clemson University) is focused on gene interaction graphs with the ultimate goal to reveal the genomic mechanisms underlying phenotype expression. A core aspect of this approach to identify biomarkers that are able to group interesting biological states (e.g., normal kidney versus renal tumor somatic mutation and/or transcriptome profiles).

- **SSGAforCSP**, a project led by Prof. Julio Facelli (University of Utah) plans to demonstrate the feasibility a new steady state genetic algorithm (SSGA) to predict the crystal structures of molecules of pharmaceutical interest.

- **PainDrugs**, a project led by Prof. Pei Tang (University of Pittsburgh and Carnegie Mellon University) is interested in the molecular mechanisms of general anesthesia.

- **PNGTemplate** is a project in the Magnetic Resonance Biomedical Engineering Lab (MRBEL), led by Dr. Joseph Rispoli. The lab develops and applies novel technology and methodologies to better exploit magnetic resonance imaging and spectroscopy for clinical and research use. Dr. Rispoli is also a member of the Purdue Center for Cancer Research (PCCR), facilitating ongoing collaborations with medical scientists to study breast cancer biology using emerging high-field MRI techniques.

- The **SBGrid** Consortium is a research computing group financially supported by participating research laboratories and operated out of Harvard Medical School. SBGrid provides the global structural biology community with support for research computing as a gateway to back-end computing capacity like that in OSG. It provides two portals, "Wide Search Molecular Replacement" and "Deformable Elastic Network" that use Cancer Computer resources within the OSG.

In addition, Cancer Computer made an infrastructure donation of 10 servers to OSG that we are using to improve our overall core infrastructure that hosts all the services the science community needs to make use of the distributed resources available via OSG, including but not limited to the Cancer Computer resources.

The OSG is delighted to continue this fruitful collaboration with Cancer Computer, and thus is wholly supportive of their ongoing efforts to provide computing resources that can transform and propel research in the fight against cancer. #ComputingForTheCure

Sincerely,

Frank Würthwein
Professor of Physics, UCSD
Executive Director, Open Science Grid