Title: Analyzing crystals to help fight cancer

Summary: Behind-the-scenes work continues on the Help Conquer Cancer project – the team is analyzing millions of protein crystallization images that you processed, with the hope of finding patterns that will help them build better cancer screening tools. Read their new article for team news and a list of recent publications, then check back for a detailed update in the next few months.

Dear World Community Grid volunteers:

We continue to analyze the millions of protein-crystallization images that you processed as part of Help Conquer Cancer (http://www.cs.toronto.edu/~juris/WCG/wcg-hcc.html) (HCC), with the end goal of gaining insight into the crystallization process. In turn, this will enable to crystalize cancer- (and other disease-) related proteins, determine their structure, function, and design drugs as needed. We aim to identify non-trivial, interesting and ultimately useful patterns in this large and valuable data set.

We strive to integrate more detailed data we have received from Hauptman Woodward Institute (http://www.hwi.buffalo.edu). This will enable us to interpret patterns we are identifying and linking properties of proteins, conditions, and temporal data to specific images that were process on the WCG. Work is ongoing, albeit more slowly at present, as the Post Doctoral Fellow working on the integration and data mining had to take a leave of absence to expand her teaching skills. Christian continues to dedicate some of his time to the HCC project, but also had to expand on the analysis and streamline infrastructure to support our Mapping Cancer Markers (http://www.worldcommunitygrid.org/research/mcm1, and http://www.cs.utoronto.ca/~juris/MCM.htm project. We expect to be able to give you more detailed results in the next HCC update, which we will provide in a few months. We have been working on some novel analysis angle with a visiting student from Denmark, and a new student is expected to start working on the project in the Fall 2015.

In the meantime, here are some recent cancer-related publications and media coverage by our group. While they are not directly related to data from HCC or MCM, they all relate to our effort to identify better algorithms for determining prognostic/predictive signatures and work towards finding and validating novel treatment options for cancer patients. Combined, results from these papers feeds into our new work units for the MCM project, and in turn, results from the MCM projects feed into this research.

Publications
- Navab, R., **Strumpf, D.,** … **Jurisica, I.**, Walker, C. G., Gullberg, D., Tsao, M.S. Integrin a11b1 regulates cancer stromal stiffness and promotes tumorigenecity in non-small cell lung cancer, *Oncogene,* 2015. In press.

- Stewart, E.L., Mascaux, C., Pham, N-A, Sakashita, S., Sykes, J., Kim, L., Yanagawa, N., Allo, G., Ishizawa, K., Wang, D., Zhu, C.Q., Li, M., Ng, C., Liu, N., Pintilie, M., Martin, P., John, T., **Jurisica, I.**, Leighl, N.B., Neel, B.G., Waddell, T.K., Shepherd, F.A., Liu, G., Tsao, M-S. Clinical Utility of Patient Derived Xenografts to Determine Biomarkers of Prognosis and Map Resistance Pathways in EGFR-Mutant Lung Adenocarcinoma, *J Clin Oncol*, 2015. In press. CJCO/2014/601492.

- Camargo, J. F., Resende, M., Zamel, R., Klement, W., Bhimji, A., Huibner, S., Kumar, D., Humar, A., **Jurisica, I.,** Keshavjee, S., Kaul, R., Husain, S. Potential role of CC chemokine receptor 6 (CCR6) in prediction of late-onset CMV infection following solid organ transplant. *Clinical Transplantation*, 2015. In press. doi: 10.1111/ctr.12531

- Fortney, K., **Griesman, G., Kotlyar, M., Pastrello, C., Angeli**, M., Tsao, M.S., **Jurisica, I.** Prioritizing therapeutics for lung cancer: An integrative meta-analysis of cancer gene signatures and chemogenomic data, *PLoS Comp Biol*, **11**(3): e1004068, 2015.

- Starmans, M.H., Pintilie, M., Chan-Seng-Yue, M., Moon, N.C., Haider, S., Nguyen, F., Lau, S.K., Liu, N., Kasprzyk, A., Wouters, B.G., Der, S.D., Shepherd, F.A., **Jurisica, I.**, Penn, L.Z., Tsao, M.S., Lambin, P., Boutros, P.C. Integrating RAS status into prognostic signatures for adenocarcinomas of the lung. *Clin Cancer Res*, **21**(6): 1477-86, 2015.

- Tu, W.B., Helander, S., Pilstål, R., Hickman, K.A., Lourenco, C., **Jurisica**, I., Raught, B., Wallner, B., Sunnerhagen, M., Penn, L.Z. Myc and its interactors take shape. *Biochim Biophys Acta,* **1849**(5): 469-483, 2015.

- Dingar, D., Kalkat, M., Chan, M. P-K, Bailey, S.D., Srikumar, T., Tu, W.B., Ponzielli, R., **Kotlyar, M., Jurisica, I.,** Huang, A., Lupien, M., Penn, L.Z., Raught, B. BioID identifies novel c-MYC interacting partners in cultured cells and xenograft tumors, *J Proteomics*, 2015. doi: 10.1016/j.jprot.2014.09.029

- Wong, S. W. H., Cercone, N., **Jurisica**, I. Comparative network analysis via differential graphlet communities, Special Issue of Proteomics dedicated to Signal Transduction, *Proteomics,* **15**(2-3):608-17, 2015. E-pub 2014/10/07. doi: 10.1002/pmic.201400233

- **Kotlyar M., Pastrello C.,** Pivetta, F., Lo Sardo A., **Cumbaa, C., Li, H.,** Naranian, T., Niu Y., Ding Z., Vafaee F., **Broackes-Carter F.,** Petschnigg, J., Mills, G.B., Jurisicova, A., Stagljar, I., Maestro, R., & **Jurisica, I**. *In silico* prediction of physical protein interactions and characterization of interactome orphans, *Nat Methods*, **12**(1):79-84, 2015. E-pub 2014/11/18.

Editorial

- Hoeng J, Peitsch MC, Meyer, P. and **Jurisica, I.** Where are we at regarding Species Translation? A review of the sbv IMPROVER Challenge, *Bioinformatics*, **31**(4):451-452, 2015.

Presentations

- Keynote: Life of an orphan protein, *Symposium on Computational Biology, eScience approaches for biomedical data analysis, University of Southern Denmark*, Odense, June 10-12

- Invited highlight presentation: *In silico* prediction of physical protein interactions and characterization of interactome orphans, *[BC]2 Basel Computational Biology Conference*, Basel, June 7-10

- Invited presentation: High-performance computing in integrative cancer informatics. Fathoming cancer by data-driven medicine, *Advanced Computing and Analytics in Medical Research Symposium, University of Ottawa*, May 11-12.

- Invited presentation: Scalable visual data mining. HPC and "big data" in integrative cancer informatics. *OCE Discovery Conference*, the Metro Toronto Convention Centre, April 28.

- Invited presentation: High-performance computing in integrative cancer informatics. Challenges and opportunities in intelligent molecular medicine, *Systems Biology Ireland Seminar Series, University College Dublin, The College of Health Sciences*, Dublin, Ireland, March 6

- Keynote presentation: Integrative cancer informatics - moving personalized medicine to preventive interventions, *Cancer Care Ontario Workshop* - Prevention Intervention Studies to Improve the Health of Adult Cancer Survivors.

- Scalable visual data mining video and demo, *Compute Ontario highlight at OCE Discovery Conference*, Toronto, April 27-28

- Scalable visual data mining video, *High Performance Computing Conference*, Montreal, June

Media

- The Jurisica lab and the MCM1 project scientists were recently interviewed for a Drug Discovery News article about the difficulties of cancer biomarker discovery and validation: Signs of intelligent biomarkers, by Randall C Willis, DDNews. (www.ddn-news.com/index.php?newsarticle=9227)

- Igor was also interviewed for the NewsTalk Radio 1010 in June 2015 about the work on discovering prognostic and predictive cancer signatures.

- The World Community Grid project was also covered by Genevieve Roberts in *Independent: In 10 years, 'crowdsourced computing' has changed the world; now it's tackling Ebola, Genevieve Roberts, Independent, June 10; http://www.independent.co.uk/life-style/health-and-families/features/in-10-years-crowdsourced-computing-has-changed-the-world-now-its-tackling-ebola-10311574.html*

As we continue to work through these analyses and results, we're constantly reminded of how much you all have supported our research, and given us the opportunity to expand the anti-cancer arsenal. Big thank you to all our volunteers for your invaluable contributions.

The HCC team