QuantumBio Inc. announces: SBGrid Lunch Break Discussion and Webinar with Lance Westerhoff on September 22nd

STATE COLLEGE, PA, USA, September 21, 2015 /EINPresswire.com/ -- QuantumBio Inc. and the SBGrid Consortium have entered into an agreement that will allow for the distribution of QuantumBio's DivCon Discovery Suite software to non-profit, SBGrid members. Dr. Lance Westerhoff, QuantumBio's President and General Manager, will present a webinar on September 22nd to introduce SBGrid members to Phenix/DivCon, a tool for accurate macromolecular crystallographic refinement and active site protonation state determination using linear scaling, semiempirical quantum mechanics.

To learn more about the Phenix/DivCon, visit our website.

Webinar Topic Summary

Phenix/DivCon: accurate macromolecular crystallographic refinement using linear scaling, semi empirical quantum-mechanics

Date/Time: Tuesday, September 22nd at 12pm EDT

Conventional, biomolecular crystallographic refinement relies on often-dubious stereochemical restraints and rudimentary energy functionals to ensure the correct geometry of the X-ray model of the biomolecule and any bound ligand(s) and cofactors. The ligand stereochemical restraint file (CIF) - along with tools based on molecular mechanics - requires an a priori understanding of the ligand geometry within the active site, and creation of the CIF is often an error-prone process owing to the great variety of potential ligand chemistry and structure. At the same time, crucial interactions such as hydrogen bonds, electrostatics, and so on are absent from the conventional refinement functional. Recently, we have completely replaced these stereochemical restraints with a more robust functional through the integration of the linear-scaling, semiempirical quantum mechanics (SE-QM) program DivCon with the Phenix X-ray refinement engine. Unlike with conventional refinement, Phenix/DivCon does not utilize CIF(s), link restraints, atom types, and other refinement parameters and hence it allows one to make fewer assumptions about the model. With the addition of accurate energy and density scoring tools, this work has been further expanded to include not only refinement but tautomer/protomer and "flip state" determination as well.

The DivCon plugin to the Phenix package is available within the SBGrid environment and it may be used in non-profit research. Separate permission may be obtained in order to use the method for commercial applications.

For connection instructions and additional information about SBGrid, please visit the webinar website:

https://sbgrid.org/news/sbgrid-lunch-break-lance-westerhoff-2015-08-27

About: QuantumBio is a leader in providing a next generation of Computer Assisted Drug Design (CADD) and Computer Assisted Molecular Modeling (CAMM) solutions to Pharmaceutical, Biotech, Materials and Nanotechnology companies. QuantumBio is working with leading pharmaceutical, biotech companies, government and academic research organizations. For further information about QuantumBio Inc., please visit our website at http://www.QuantumBioInc.com

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