W0289

Application Programming with Crystallographic Concept/Protocol Libraries (CCL™/CPL™). Zhong Ren[†], X. Yang[†¶] & W. F. Anderson[¶], [†]Renz Research, Inc., Westmont, IL 60559, USA, http://renzresearch.com. [¶]Dept. of Molecular Pharmacology & Biological Chemistry, Northwestern Univ. Medical School, Chicago, IL 60611, USA.

CCL contains a collection of object-oriented C++ classes that reflects the fundamental concepts in crystallography, such as space group and structure factor. In contrast, CPL utilizes the abundant resources of crystallographic computing from the existing software packages, and integrates them into a set of uniform-looking programming interfaces in Python modules and classes that perform more complex processes such as data scaling and substructure solution. CPL offers high-level, generic protocols without data and control format specific to the underlying computational engines. Using these libraries, a new generation of Laue data processing software Precognition™ is developed, which greatly simplifies this difficult task. Two programs Nasymm and NCSymm detecting non-crystallographic symmetry at very early stage of structure determination help to ease the major bottleneck in MAD/SAD process. These libraries can be integrated into other software systems such as those at synchrotron facilities. We welcome academic collaboration and business partnership in further development and application of these libraries. CCL/CPL are trademarks of Renz Research, Inc.