CRANK – New Methods for Automated Structure Solution

Steven R. Ness, RAG de Graaff, Jan Pieter Abrahams and Navraj S. Pannu. *Department of Biophysical Structural Chemistry, Leiden University, Leiden, The Netherlands*

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CRANK is a novel suite for automated macromolecular structure solution in crystallography that uses new programs for substructure detection (CRUNCH2) (de Graaff 2001), and substructure refinement and phasing (BP3) (Pannu 2003, 2004). CRANK combines these new methods for determining and refining substructures with existing programs for density modification and model building with iterative refinement into an easy-to-use CCP4i graphical interface. CRANK uses a flexible and extensible decision making system, extensively using the widely used XML markup language to store, manipulate and compare data from a variety of different sources. The CRANK system is very amenable to parallelization and contains a data model that is very useful to classify, store and manipulate the large amount of data produced in macromolecular structure determination. We have applied CRANK to a variety of different test cases which has yielded very promising results: CRANK often outperforms existing automated substructure solution packages, and can lead to solutions where existing methods fail.

For more information, please visit CRANK's web site: http://www.bfsc.leidenuniv.nl/software/crank.

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