

## W0108

**Automated Structure Solution with CRANK.** Steven R. Ness, Rudolph A.G. de Graaff, Jan Pieter Abrahams, Navraj S. Pannu, Biophysical Structural Chemistry, PO Box 9502, Leiden Univ., Leiden, The Netherlands.

Crank [1,2] is a new suite of computer programs for the automated solution of macromolecules containing anomalous and/or heavy atom substructures. By combining programs like CRUNCH2 and SHELXD for substructure determination, BP3 for substructure refinement and phasing, along with DM,SHELXE, and SOLOMON for density modification, Crank enables the user to go from intensity data to a map suitable for automated model building with ARP/wARP with minimal user input. Crank uses the XML extensible markup language for communication, a new standard language in the computing community. XML is used by the PDB in PDBml and is also used by the DNA project, amongst others. Crank has been tested on a number of datasets from a wide variety of sources with different substructure signals from different experiments. The excellent results from these tests show the wide applicability of the algorithms and programs used with Crank for automated structure solution. We present here both our current results, as well as the algorithms and communication methods used within Crank.

[1] Ness, SR, de Graaff, RAG, Abrahams, JP, Pannu, NS (2004) Structure, 12, 1753-1761.

[2] <http://www.bfsc.leidenuniv.nl/software/crank/>