Crank - New Methods in Automated Structure Solution

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We present Crank[1], a suite to help a user perform automated macromolecular structure solution. In this aim, it uses novel programs, including CRUNCH2 for substructure determination and BP3 for substructure refinement and phasing. In addition, Crank uses other commonly used crystallographic programs including SOLOMON, DM and various programs within the CCP4 suite. Crank uses the CCP4i package for its user interface, this allows for tight integration into the CCP4 suite and presents the user with a familiar interface. Crank uses the XML eXtensible Markup Language to store, manipulate and compare data, this XML can subsequently be used to assist in data deposition. We have tested Crank on a large number of datasets, including datasets from the Joint Center for Structural Genomics, our results show that Crank often outperforms existing automated substructure solution packages, and can lead to solutions where existing methods fail. For more information, please visit the Crank web site: http://www.bfsc.leidenuniv.nl/software/crank.

[1] Ness S. R., de Graaff R.A.G., Abrahams J. P., Pannu N.S., *Structure*, **12**, 1753-1761.

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