# Poster Presentations

**[MS04-P02]  Nucleic  Acid  Auto-Tracing with knuspr and RCrane.** Tim Gruene, S. MoritzWette, George M. Sheldrick

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The building of nucleic acids lacks behind the degree of completion that can be achieved for protein models. In the past years, important advances have been made in the field of auto tracing of nucleic acids, with a wide number of available programs, e.g. NUT/DHL/RSR [1, 2], arp/warp [3], NAFIT/NABUILD [4] nautilus [5], knuspr [6], RCrane [7].

The program knuspr [6] places phosphates and bases into electron density maps at a high degree of reliability even at moderate resolution ( 3 ☐ 4Å). This output is a suitable starting point for the program RCrane. Via its GUI for Coot, RCrane automatically builds an RNA strand from an existing trace of phosphates and bases.

In order to improve the usability of knuspr, we have developed a GUI for coot. It creates the input script for knuspr from the user's selection consisting of the electron density map to use from a pull-down menu, optionally a PDB file as mask in case a preliminary protein trace exists, the nucleic acid sequence, and type (A-, B-, or Z- DNA or RNA).

Via this GUI knuspr can be used alone, or interface to RCrane with the phosphates and bases placed by knuspr as backbone for RCrane. In the latter case the phosphates and putative bases are automatically loaded into coot and passed to RCrane. One important amendment to the RCrane work-flow consists of the search for phosphate or C1' atom candidates around the current centre by the crystallographic distance function. This makes running RCrane independent from where knuspr placed their positions in crystal space.

The high ratio of true positives vs. false positives achieved by knuspr [6] and the combination with RCrane a strand of RNA can be generated quickly and by means of only few clicks on the "Next" button of RCrane.

knuspr is available for download from TG's web page to be found on the shelx server. The python code for the GUI is currently at  testing stage and available upon request from TG.

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[4] K. Yamashita, Y. Zhou, I. Tanaka, and M. Yao. New model-fitting and model-completion programs for automated iterative nucleic acid refinement. Acta Crystallogr., D69:1–9, 2013.
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