MS3-P16 TakeTwo: an indexing algorithm suited to still images with known crystal parameters

Helen Ginn[1], Helen M. Ginn[1,2], Philip Roedig[3], Anling Kuo[4], Gwyndaf Evans[2], Nicholas K. Sauter[5], Oliver Ernst[4,6], Alke Meents[3], Henrike Mueller-Werkmeister[4,7,8], Dwayne Miller[7,8,9], David I. Stuart[1,2]

1. Division of Structural Biology, Wellcome Trust Centre for Human Genetics, Roosevelt Drive, Oxford, Oxfordshire, OX3 7BN England
2. Diamond House, Harwell Science and Innovation Campus, Fermi Avenue, Didcot, Oxfordshire, OX11 0QX England
3. Deutsches Elektronen-Synchrotron, Notkestrasse 85, 22607 Hamburg, Germany
4. Department of Biochemistry, University of Toronto, King's College Circle, Toronto, Ontario M5S 1A8, Canada
5. Molecular Biophysics and Integrated Bioimaging Division, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, California 94720 USA
6. Department of Molecular Genetics, University of Toronto, King's College Circle, Toronto, Ontario M5S 1A8, Canada
7. Departments of Physics Chemistry, University of Toronto, 80 St. George Street, Toronto, Ontario, M5S 1H6, Canada
8. Atomically Resolved Dynamics, Max-Planck-Institute for Structure and Dynamics of Matter, Luruper Chaussee 149, Hamburg, Germany
9. Hamburg Centre for Ultrafast Imaging, University of Hamburg, Hamburg, Germany

email: helen@strubi.ox.ac.uk

Indexing algorithms suited to classical goniometer-based crystallography rely heavily on three-dimensional information from a wedge of reciprocal space. For still shots from serial crystallography, the limited sampling of Bragg peaks can lead to substantial indexing failure rates. In cases where the unit cell parameters are known, we present the TakeTwo algorithm, which seeks to maximally exploit the information contained on a single image diffraction pattern.

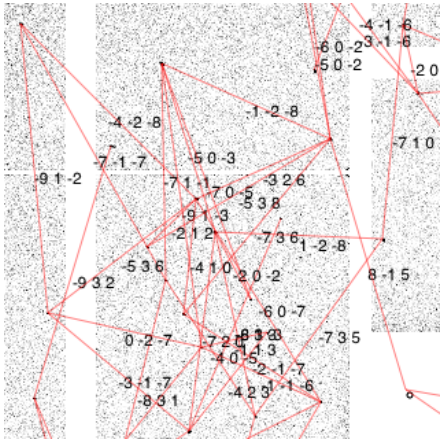

Figure 1. Confirmed Miller index translations between spots on a single thermolysin diffraction pattern, after searching for a self-consistent network of vectors. Red lines indicate an identified inter-spot vector with their corresponding Miller index translation written in black near the mid-point.

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