MS01-P06 | Better SAUC -- Improving the Identification of Nearby Cells

Bernstein, Herbert J. (Ronin Institute for Independent Scholarship, Upton, NY, USA)

As we move to faster data collection from very large numbers of small crystals, rapid identification of previously solved structures that have similar cells can be helpful both in identifying molecular replacement candidates and in sorting out images that may be suitable for clustering [1][2]. The PDB/COD cell search program SAUC has been speeded up by use of the new S6 cell metric [3] [4].

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[3] L. C. Andrews, H. J. Bernstein, N. K. Sauter. "Selling reduction versus Niggli reduction for crystallographic lattices." Acta Cryst. A75:1 (2019): 115 -- 120.
[4] L. C. Andrews, H. J. Bernstein, N. K. Sauter. "A space for lattice representation and clustering." Acta Cryst. to appear.