Winners and Losers – Ranking Crystals from Diffraction Images. A.R. Criswell, R. Bolotovsky, T. Niemeyer[†], R. Athay, J.W. Pflugrath. *Rigaku/MSC, Inc., 9009 New Trails Dr., The Woodlands, TX 77381 and [†]where's Thad?*. Keywords: high throughput crystallography, crystal ranking, robotics, automation

With the advent of automation, many home labs and beamlines have developed robotic systems for high-throughput evaluation of crystal samples. Ideally, an automated system should provide methods to identify desirable samples. However, most of these systems still depend on human intervention to judge the quality of crystals. We have implemented a method in d*TREK software to evaluate the quality of diffraction images and assign a rank per sample. This ranking procedure evaluates images in terms of several rules and calculates an award or penalty for each rule. The awards and penalties are then summed and updated on a per sample basis. Samples can then be ranked according to these values, and data collected in descending rank order. In general, the ranking rules include the number of Bragg reflections per resolution shell, the <I/sig(I)> of reflections per shell, the spot sharpness, the presence and sharpness of ice rings, crystal mosaicity and unit cell refinement results. We discuss the usefulness of these rules in the evaluation of diffraction images, and highlight those rules which seem most important for ranking of crystals.