Computational tools to aid crystallization

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Many of the techniques used for, or in association with, crystallization produce such large amounts of (often unreadable) data that it is difficult to extract an appropriate interpretation without over-interpretation. Systematic (automated) data analyses are crucial to obtaining consistent interpretation of results, particularly for techniques which a researcher only uses intermittently. Current computational analysis tools are sparse due to the complex nature of most output data. Single results that consist of multiple points (for example, a visible spectrum) require functional analysis to make curve-to-curve rather than point-to-point comparisons.

In the Collaborative Crystallisation Centre (C3), the creation of computer software which considers data as functional sets of points has allowed us to simplify and speed up numerous data analyses. We have created automated analyses of both thermal melt experiments [1, 2] and pH experiments that produce spectral output. By allowing easier understanding of machine output, different techniques are made more useful and accessible to the end users of the analyses.

1. N. Rosa, M. Ristic, S. A. Seabrook, D. Lovell, D. Lucent, J. Newman, *J Biomol Screening,* **20**, (2015), 898-905.

2. M. Ristic, N. Rosa, S. A. Seabrook, J. Newman, *Acta Cryst,* **F71**, (2015), 1359-1364.