

## HIGH-THROUGHPUT STRUCTURE DETERMINATION, HIGH-QUALITY STRUCTURE REFINEMENT

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The use of global optimisation methods has increased the size and complexity of molecular organic structures that can now be solved directly from powder diffraction data. However, these methods require many repeat runs to be performed in order to confirm the location of the global minimum in parameter space; this is particularly true of very complex structures, where success rates in locating the minimum may fall to only a few percent. Fortunately, these multiple runs can be performed independently of each other and as such, they are ideally suited to the notion of grid-type computing. We have recently adapted the DASH structure determination package to run under the United Devices GRIDMP system, which is widely used in pharmaceutical industry, mainly in the context of virtual screening. The current setup allows up to eighty DASH runs to be executed in parallel on existing desktop computing resources. The first half of this presentation will focus on results obtained using the DASH and HMC structure determination programs running under GRIDMP. These show not only impressive performance gains but also indicate that new computational routes that were previously closed to us due to their compute-intensive requirements are now open.

Once a structure is solved, structural refinement to *Acta Crystallographica* standards can prove to be a serious bottleneck. In the second half of the talk, the focus will be on refinement strategies that deliver a CIF that is geared for rapid publication in *Acta Crystallographica Section E*. Recent experience gained in publishing in "Acta E" will be used to illustrate problems that are likely to be encountered, such as addressing *checkCIF* warnings. Once the basic 'recipe' for an "Acta E" CIF is understood, the possibility of high-throughput publication for powders becomes a reality. I will argue that, even if publication in "Acta E" is not the aim, it is still well worth refining the structure to *Acta Cryst* standard.