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*Breaking the structure complexity limits for powder based structure solution*

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There exist theoretical predictions trying to determine how much complex crystal structure can be solved from perfect powder diffraction data [1]. The theoretical limit for perfect synchrotron data is about 300 DOF (degree of freedom) while one of the current record solves only 42 DOF problem simplified by heavy atom presence [2]. We have tried to determine a realistic DOF limit based on perfect simulated powder diffraction data. For the simulation we have chosen structures from CSD with 1 single peptide molecule in asymmetric unit cell, 2-8 amino acids, 10-39 DOF. The parameters of the simulated powder diffractogram used were close to typical perfect measurement on ID31 of ESRF - wavelength 0.5 Å, range 0.5º-15º, step 0.002º, FWHM 0.01º. The structure solution tests were done by SA (simulated annealing) in DASH 3.2 software [3]. To speed up the computation we have used parallel processing obtained by MDASH extension. Influence of Mogul CSD based torsion angles bias on the calculation effectiveness was investigated as well. The results demonstrate the required number of SA steps depends exponentially on the problems DOF. This requires for problems close to 30 DOF about 10E+10 SA steps and years of single CPU computational time. The Mogul based bias can significantly help for compounds like peptides - e.g. for simulation based on compound CSD code AHAREH (4 peptides, DOF 24) the Mogul based calculation gives 50 times more often correct result than non-restricted SA run. We believe the 40 DOF structures can be solved routinely on 16-32 CPU clusters from perfect data not influenced by preferred orientation when the Mogul CSD torsion angles bias will be used. Without developing a more efficient algorithm than SA solution we do not see a way how to get really close to the 300 DOF theoretical limit.   Acknowledgement: This work was supported by the Grant Agency of Czech Republic, Grant No. 106/14/03636S.   Fig. caption: Dependence of required simulated annealing steps required to get one solution on DOF and the use of Mogul based bias.

[1] W.I.F. David, K. Shankland, Acta Cryst.,2013, A64, 52-64, [2] P. Fernandes, K. Shankland, A. Florence at all, Journal of Pharmaceutical Science, 2013, 96-5, 1192-1202, [3] W.I.F David, K. Shankland, J. Streek at all , J. Appl. Cryst., 2006, 39, 910-915
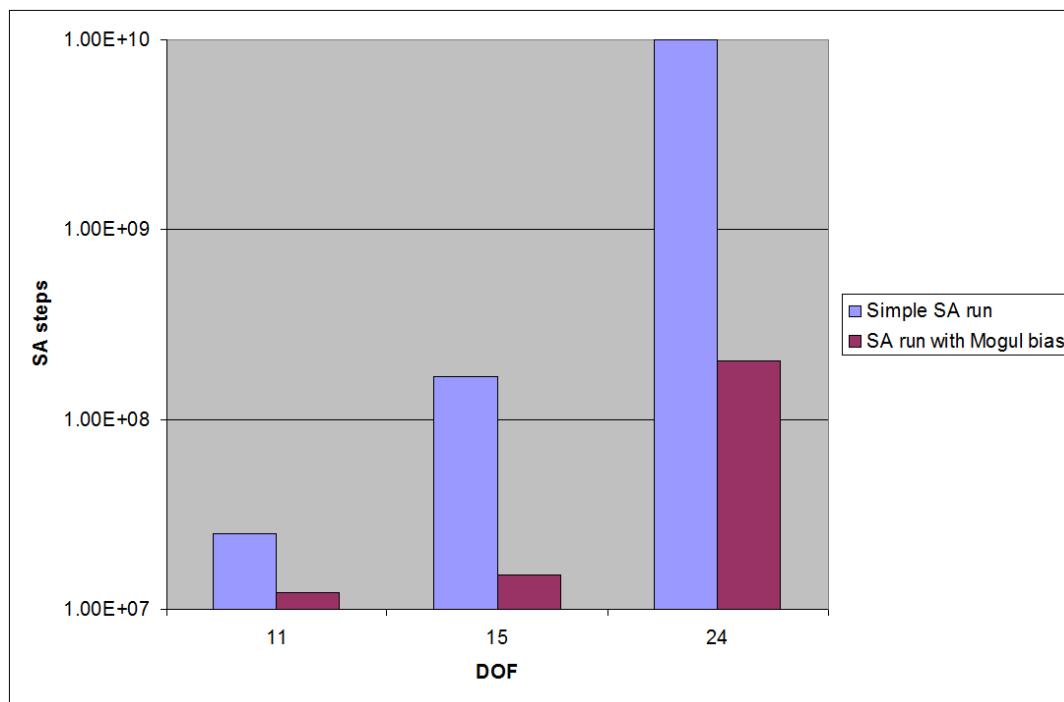
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