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Application of |ρ| - based direct methods to the solution of anomalous scatterers substructures from SAD data of protein crystals

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Owing to the importance of the *SAD* technique, |ρ|-based direct methods in the form of the recent *SMAR* (= SM,|ρ|) phasing algorithm incorporating the inner-pixel-preservation (*ipp*) procedure [Rius, J.& Torrelles, X. (2021) Acta Cryst A77, 489-493] have been adapted to the determination of anomalous scatterers substructures. Their applicability has been tested on a series of representative experimental data sets, mostly retrieved from Protein Data Bank. The suitability of the data sets is indicated by two main indicators. The dominant anomalous scatterers are either SeMet or S atoms, or metals/clusters incorporated by soaking. The test results indicate that the adapted *SMAR* algorithm (*S-SMAR*) solves the substructures of the protein crystals quite efficiently provided that the Fourier peaks of the anomalous scatterers have spherical symmetry at the working resolution.

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No

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