A Modified ACORN to Solve Protein Structures at Resolutions of 1.7 Å or better

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The first development of ACORN provided an efficient density modification procedure for the *ab initio* solution of protein structures with diffraction data to better than 1.3 Å starting with poor phases. An initial phase set could be obtained from a variety of sources such as the position of a heavy atom, a set of scatterers such as Sulphur atoms that had been positioned from anomalous dispersion measurements, a fragment or a very low homology model placed from a molecular replacement search. New procedures have been developed that yield good quality maps with data sets of resolution down to 1.7 Å. These new developments involve the artificial extension of data to atomic resolution and novel density-modification processes that develop density at atomic positions that was previously suppressed. The several known protein structures have been tested starting from a heavy atom, small α-helix and a model from molecular replacement search. The F-map from ACORN can be trace easily and the E-map can show most atom positions with the data extended to atomic resolution.

Keywords: data extension, density modification, Sayre equation refinement