High Throughput Technique in Structural Bioinformatics

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As the available macromolecular sequences exceed far in number than the available three-dimensional structures, high throughput techniques are necessary to unravel the 3D-structures of selected macromolecular sequences in the area of Structural Genomics. ACORN program deposited in CCP4 is a comprehensive and efficient phasing procedure for the determination of protein structures when atomic resolution data are available. The structure solution program SHELXD is useful for locating the anomalous scatterers from SIR, SAS, SIRAS or MAD data. SHELXE estimates the native phases and the corresponding weights from SHELXD output. The phases obtained from ACORN and SHELXE are of superb quality to allow automated model building to be carried out in ARP/wARP. Minimal manual model building is required and the structure determination can be completed using maximum likelihood refinement program REFMAC. Attempts are here made in extending the applications to the structure elucidation of Catalase of approximately 57 kDa molecular weight using atomic resolution data (for *ab initio* phasing using ACORN) and Thermolysin of approximately 34 kDa molecular weight using 1.7 Å anomalous scattering data. Detailed presentation will be made on the various options in these in High Throughput structure determination of macromolecules.

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