

NCS and Normal Modes Ensembles Solve Difficult MR Problem
Jorge Navaza, *LVMS, CNRS, 91980 Gif-sur-Yvette, France*. E-mail:
jnavaza@vms.cnrs.gif.fr

We describe a strategy that has been used to push further the molecular replacement limits by taking advantage of the oligomerisation state of a given molecule both in solution and in the crystal.

This strategy combines the information coming out from experimental data such as the existence of a non crystallographic symmetry in the crystal, reinforced by electronic microscopy data of the oligomeric structure in solution.

Computational methods are then used to extract the orientations and relative positions of each molecule in the oligomer in order to build an oligomeric model to search for a molecular replacement solution.

The closest monomer model in the PDB has 26% identity and, although accurate enough to detect the crystal structure, more contrasted results are obtained by using normal mode analysis to generate a series of models, including NMR-like ensembles.

Keywords: **molecular replacement, normal modes, non-crystallographic symmetry**