Molecular Replacement via Normal Mode Analysis and Homology Modelling on the Web

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Molecular replacement (MR) is the method of choice for X-ray crystallography structure determination when structural homologues are available in the Protein Data Bank (PDB). However, the success rate of MR decreases sharply when the sequence similarity between template and target proteins drops below 35% identical residues. Another reason for MR failure are conformational differences between target and template, induced for example by ligand binding or different crystallogenic conditions. It has been found that screening for MR solutions with a large number of different homology models or models that are perturbed in the direction of one or two low frequency normal modes may still produce a suitable solution where the original template failed [1-3]. Here we present the web tools *elNémo* [2] and *CaspR*, [3] that implement such strategies in an automated manner. *elNémo* is accessible at http://igs-server.cnrs-mrs.fr/elnemo/, *CaspR* at http://igs-server.cnrs-mrs.fr/Caspr/.

[1] Suhre K., Sanejouand Y.H., *Acta Cryst. D*, 2004, **60**, 796-799. [2] Suhre K., Sanejouand Y.H., *Nucleic Acids Research*, 2004, **32**, W610-W614. [3] Claude J.B., Suhre K., Notredame C., Claverie J.M., Abergel C., *Nucleic Acids Research*, 2004, **32**, W606-W609.

Keywords: crystallography, phasing, template perturbation