***elNémo*: Using Normal Mode Analysis in Molecular Replacement**

Karsten Suhre[a], Yves-Henri Sanejouand[b], [a]*Information Génomique & Structurale, UPR CNRS 2589, Marseille, France.* [b] *Laboratoire de Physique, Ecole Normale Supérieure, Lyon, France.* E-mail: karsten.suhre@igs.cnrs-mrs.fr

Normal mode analysis (NMA) is a powerful tool for predicting the possible movements of a given macromolecule. A newly emerging field of NMA in X-ray crystallography is the utilization of normal mode perturbed models as templates for diffraction data phasing through molecular replacement (MR), thus accounting for conformational changes arising for example from ligand binding or different crystallogenic conditions [1]. Given that half of the known protein movements can be modelled by displacing the studied structure using at most two low-frequency normal modes, NMA may have the potential to break tough MR problems in up to 50% of cases. Moreover, even in situations where a MR solution is available, NMA can be used to further improve the starting model prior to refinement, eventually reducing the time spent on manual model construction (i.e. when working with low resolution data sets). Here we present this approach at a number of examples where screening for MR solutions using NMA perturbed templates allowed to obtain a MR solution, whereas MR using the original template failed to yield a model that could ultimately be refined. We outline possible protocols of using NMA in MR and present the web- server *elNémo* [2] for online NMA template generation http://igs-server.cnrs-mrs.fr/elnemo/index.html.

[1] Suhre K., Sanejouand Y.H., *Acta Cryst.*, 2004, D**60**, 796-799. [2] Suhre K., Sanejouand Y.H., *Nucleic Acids Research*, 2004, **32**, W610-W614.

Keywords: crystallography, phasing, normal mode analysis