### $13^{\text{th}}$ International Conference on

# **Structural and Molecular Biology: Techniques & Market Analysis** October 22-23, 2018 | Ottawa, Canada

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#### Normal modes, what do they tell us about the protein dynamics?

Normal Mode Analysis (NMA) is a method to calculate proteins' motions, in which the trajectory of the protein is approximated by the sum of its internal vibrations. The interest of NMA is to provide the essential motions of the protein and therefore, to allow us to observe easily its collective movements. In this presentation, we will explain the method and show its usefulness and limitations. We will also see that NMA tells us that the most collective motions depend on the protein shape rather than its composition or function. This concept was extended to 2D images, as for microtubule.

#### Biography

Liliane Mouawad was always interested in understanding the mechanism of action of proteins or protein assemblies. This understanding may be based on either molecular simulations or on experiments like NMR. But her expertise is primarily in molecular dynamics simulations and more precisely in normal mode analysis (NMA). She has developed several methods going from the calculation of normal modes of very large systems or of images, to the calculation of the pathway between two protein conformations, or to the prediction of the compactness of a calcium-binding protein. Recently she was also involved in docking and virtual screening themes, where she has acquired enough expertise to develop a new consensus methodology to overcome some issues observed in these approaches.

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