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Insulin dynameomics of Langmuir-Blodgett and classical insulin with and without insulin receptor

Nicola Bragazzi¹ and Marine Bozdaganyan²

¹Genova University, Italy

²Moscow State University, Russia

A new multi-scale and multi-dimensional approach termed as “dynamomics”, arising from the coupling of protein crystallography and molecular dynamics, has been coined by Daggett. In the present article, we present extensive bioinformatics and molecular dynamics simulations of three insulin proteins that we previously solved (namely, 4ihn, 4i5y and 4i5z). We show that: these proteins, even though being structurally identical, exhibit some slight differences, above all for the side-chain and fluctuation dynamics that become more important and evident when insulin binds to its receptor. The protein obtained with the Langmuir-Blodgett crystallization (4ihn) proves to be more stable both alone and when binding to the receptor than the proteins obtained with classical hanging-drop crystallization technique (4i5y, 4i5z). Implications for the field of molecular endocrinology and drug design will be also envisaged.