Andrzej Koliński's Research Group

HEAD:

Prof. Andrzej Koliński*, PhD DSc

GROUP MEMBERS:

Dominik Gront, PhD DSc; Sebastian Kmiecik, PhD DSc; Maciej Błaszczyk, PhD; Maksim Kouza, PhD; Mateusz Kurciński, PhD

RESEARCH PROFILE:

Theoretical Chemistry. Theory of polymers and biopolymers. Theoretical structural biology. Theory of protein folding. Theory of protein structure and function. Computer simulations of complex biopolymer systems. Structural bioinformatics. Computational biology. Molecular docking in drug design.

CURRENT RESEARCH ACTIVITIES:

Our research areas include:

- coarse-grained modeling and multiscale modeling of proteins and their complexes
- prediction of protein structure: from comparative modeling to de novo folding
- simulations of protein dynamics
- prediction of protein interactions/ molecular docking
- bioinformatics and biological statistics
- computer aided drug design/ structure-based drug design
- modeling and predicting of biomacromolecular interactions: prediction of protein function
- development of software for molecular modeling and computational analysis of experimental data on biomacromolecules

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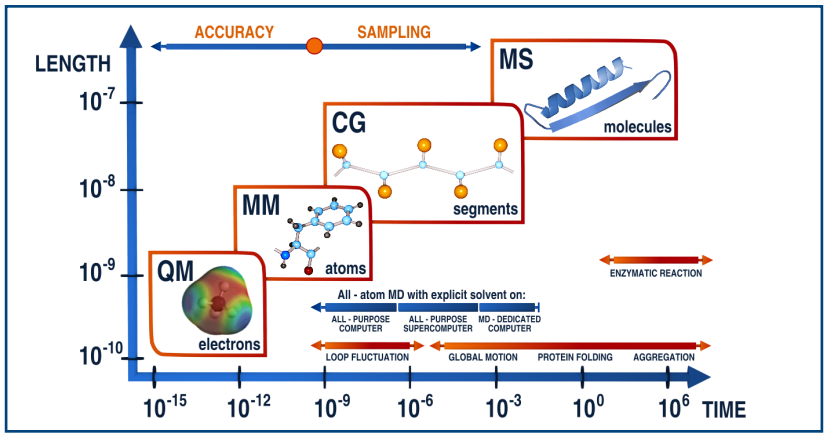

Fig. 1. Application ranges for molecular modeling at different resolutions: quantum, all-atom, coarse-grained, and mesoscale. The plot shows approximate ranges of time scales and system sizes (lengths). The presented application ranges can be expanded by merging tools of different resolution into multiscale schemes.

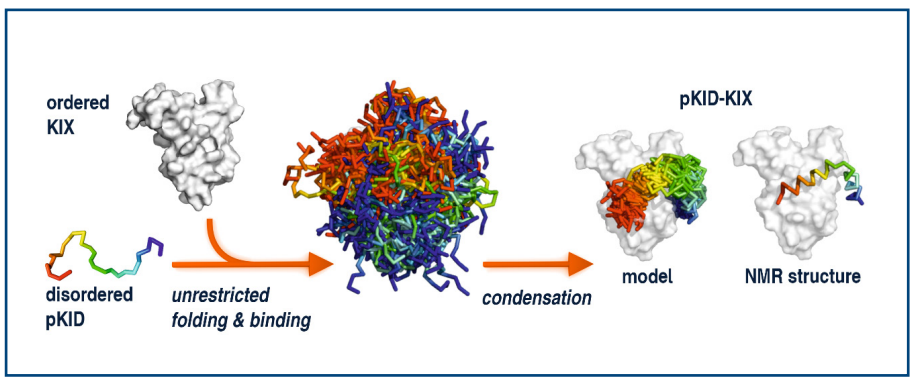

Fig. 2. Mechanism of coupled folding and binding of the pKID/KIX complex as revealed by coarse-grained modeling. Docking simulations allowed full flexibility of the disordered pKID during a blind search for the binding site onto the KIX surface. During docking, the movement of the KIX backbone was limited to near-native fluctuations.

SELECTED PUBLICATIONS:

1. M.P. Ciemny, M. Kurciński, K. Kamel, A. Koliński, N. Alam, O. Schueler-Furman, S. Kmiecik, Protein-peptide docking: opportunities and challenges, Drug Discovery Today. 23(3) (2018) 1530-37.
2. A.E. Dawid, D. Gront, A. Koliński, Coarse-grained modeling of the interplay between secondary structure propensities and protein fold assembly, J. Chem. Theory Comp. 14(4) (2018) 2277-2278.
3. A.E. Dawid, D. Gront, A. Koliński, SURPASS low–resolution coarse–grained protein modeling, J. Chem. Theory Comp. 13(11) (2017) 5766–5779.
4. S. Kmiecik, D. Gront, M. Koliński, L. Wieteska, A. Dawid, A. Koliński, Coarse-grained protein models and their applications, Chemical Reviews. 116(14) (2016) 7898–7936.
5. M.P. Ciemny, A. Dębiński, M. Paczkowska, A. Koliński, M. Kurciński, S. Kmiecik, Protein-peptide molecular docking with large-scale conformational changes: the p53-MDM2 interaction, Scientific Reports – Nature. 6 (2016) 37532.
6. M. Błaszczyk, M. Kurciński, M. Kouza, L. Wieteska, A. Dębiński, A. Koliński, S. Kmiecik, Modeling of protein-peptide interactions using the CABS-dock web server for binding site search and flexible docking, Methods. 93 (2016) 72-83.
7. M. Kurciński, M. Jamróz, M. Błaszczyk, A. Koliński, S. Kmiecik, CABS-dock: web server for flexible docking of peptides to proteins without prior knowledge of the binding site, Nucleic Acids Research. 43(W1) (2015) W419-W424.