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Targeting protein dynamics in drug design

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The dynamic nature of protein structures provides challenges and opportunities for ligand design. I will first discuss some of the different ways in which protein dynamics can be targeted, giving examples from our experience in the design of inhibitors of thymidylate synthase [1-3]. I will then describe the development of a computational toolbox (TRAPP: TRAnsient Pockets in Proteins) to identify and visualize transient pockets in proteins that may be exploited in ligand design.

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