Enabling the Best Structure-Based Design Engine: an Expert Scientist

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Drug discovery scientists need interactive and intuitive software to enable design and hypothesis testing, driven by increasingly powerful, but still qualitative computational methods. We have many useful computational tools: molecular modeling, SAR visualization, physicochemical property prediction, DMPK prediction, database searching for crystal structures, conformational profiles, intermolecular interactions, in-house and commercially available compounds, virtual libraries of synthetically accessible compounds, and patents. Improvements in compute price/performance, modular software components, web services, and GUI technology are bringing "best of breed" tools to the drug discovery scientist's desktop. But drug discovery is done by teams: desktop modeling also needs to facilitate teams brainstorming and designing together. I will describe where desktop modeling is today and its likely next steps.