In silico technologies in drug discovery

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Recently, computer aided molecular design has come to play a more important role than ever on the discovery phase of medicinal research. This is because outcomes become more and more useful in spite of that fundamental methodologies used in structure based drug design and QSAR have not changed so much. What behind this are rapid increase of information related to proteins and chemical compounds, and the development of computer hardware techniques that can handle those huge information. Especially HTS technique has yielded not only pharmacological activity but also physicochemical properties and ADME/T profiles on quite a number of compounds, which contribute to the improvement of reliability of predicting models for those properties. On the other hand, increasing number of opportunities where protein 3D structure is available let us employing computationally costly methods such as fast docking simulations of hundreds of thousands of compounds and prediction of binding free energy, those are now completed in a reasonable time owing to recent progress of computational techniques like special purpose computers and cluster computing. Since reliability and coverage of computational models have much improved, virtual screenings carried out *in silico* based on these models are now widely used on selecting/prioritizing compounds for an assay or synthesis. We will present a development of computational techniques both on hardware and software at Taisho, together with examples of applying those techniques on drug discovery.