Book of Abstracts
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(P15) Rational Structure-Based Design of New Lead Compounds.
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Combinatorial and computational chemistry principles combined with high throughput technologies hold the promise to help biologists select new lead compounds, however are currently limited by high cost of compounds and clinical trials. We have implemented a new paradigm in the QSAR, which permit the high throughput analysis of virtual compounds before synthesis. The structure-based prediction of molecular function is based upon using functional reactive groups (descriptors), which determine biological activity of any compound.

Our approaches are significant improvements in the drug (pesticides) discovery process and enable us to evaluate biological activity of any chemical without routing daily testing on existing instrumentation.