



HBIGS Lecture

by

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Rational Design for Crop Protection

Date: Wednesday, 03 March 2010

Time: 2 pm

Venue: INF 282 (ZMBH), R001

Abstract:

The plethora of new experimental techniques, like combinatorial chemistry or robot controlled high-throughput screening, has significantly increased the capacity of biochemical assays for the search of new active ingredients. But unfortunately, they did not deliver the expected high quality output but just dramatically increased the number of data points and the costs. Therefore computer-assisted virtual techniques were established to reduce the infinite chemical space to a finite number of potentially active compounds. The presentation will introduce BASF's crop protection research in general, and focuses on the integrated computational chemistry support. Furthermore, identification of a natural product and the following optimization cycles will be demonstrated yielding a successful market product.