ITbM Nagoya University

IGER Nagoya University

Nagoya University

RCMS Research Center for Materials Science, Nagoya University

Theoretical Chemistry Colloquium

March 10, 2015 (Tue), 14:00-16:00

Room no. SA322, Science and Agricultural Building

Identification And Optimization Of Synthesizable Lead Candidates

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Tripos – Pharsight - SimCYP
Implementing Translational Science

Abstract: Identification And Optimization Of Synthesizable Lead Candidates by using Muse® Invent™. It is a molecular design workflow designed to accelerate the identification and optimization of lead candidates. It enables researchers to create drug candidates with novel structures, scaffolds or side-chains that are not only synthesizable, but it also describes the necessary synthesis pathway.
Core functionality:

- *Generate drug design ideas that include synthetic chemistry considerations alongside other design criteria*
- *Explore Lead- and Scaffold-Hopping*
- *Invent New R-Groups around a fixed scaffold*
- *Elaborate fragments in the context of a protein binding site for fragment based drug design*
- *Easily integrate in-house or 3rd party scoring methods for use as design criteria*

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