

Einladung zu einem Seminarvortrag

Cheminformatics for Practical Organic Chemistry

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Seminarraum 1 des Instituts für Angewandte Synthesechemie, BI EG B06 (Erdgeschoß)

Abstract. In a cheminformatics laboratory of NII, we have been conducting several cheminformatics research projects concerning the development of new methodologies for representation, classification, and organization of chemical information, and their applications to practical problems in chemistry, including chemical reaction prediction, NMR chemical shift estimation, and chemical structural elucidation, to meet the requirements of state-of-the-art of organic chemistry. In this lecture, I will give a brief introduction of our recent activities on these cheminformatics topics especially for organic chemistry with some demonstrations.

References

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