

国家数学与交叉科学中心

Time: 3:00 pm, December 7, 2012

Venue: 蓝白楼 301

Computer-Assisted Discovery of Novel Chemical Reactions



Speaker: Prof. Nikolay Zefirov

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Director of the Institute of Physiologically Active Compounds of the Russian Academy of Sciences

Head of the Laboratory of Organic Chemistry of Moscow State University

Abstract:

Using "formal-logical approach" to recognize the similarity in description of chemical reactions, graph-based approach for search of novel reactions was developed. Success of the approach will be exemplified by real experimental proof.