

Combinatorics Seminar

Friday, September 24, 2004

3:00 pm in Hume 331

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Graph generation for predictive chemistry

ABSTRACT

Graph theoretical methods have long been used to enumerate the isomers of organic compounds. There are few practical tools, however, for generating a listing of all isomers with a specific chemical formula. This talk will discuss a current project to develop such a generator. I will address questions such as the following: Once we get them, how will we use graphs to predict chemical reactions? Why is exhaustive generation hard? What limiting properties would make it easy? How can we apply algebraic methods? What other methods have been successfully applied?

This project is a collaboration with Dr. Greg Tschumper of the Chemistry and Biochemistry department, and will also involve Dr. Bahram Alidaee of MIS/POM.