ΕΙΧΗΜΥΘ-ΙΤΕ

ΣΕΜΙΝΑΡΙΟ

ΟΜΙΛΗΤΗΣ: Dr. Δημήτρης Αγραφιώτης
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ΘΕΜΑ: Virtual screening of combinatorial libraries

ΤΟΠΟΣ: Αίθουσα Σεμιναρίων ΕΙΧΗΜΥΘ-ΙΤΕ

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ΠΕΡΙΛΗΨΗ

Among all the tools available to the medicinal chemist, combinatorial chemistry is one of the most powerful and best suited for exploring chemical space in search of new pharmaceutical leads. It provides access to millions of novel compounds from a limited number of building blocks using simple synthetic sequences that work reliably across a wide range of starting materials. Unfortunately, despite the ever-increasing throughput of parallel synthesis and screening technologies, in most cases the number of compounds that are accessible from commercially available reagents is too large to permit their physical synthesis in their entirety. A common solution to this problem is to _virtualize_ the combinatorial libraries and apply appropriate selection techniques in order to identify a smaller subset of compounds for synthesis and biological testing. While this approach is straightforward for relatively small collections, there are many combinatorial libraries that defy enumeration, let alone any form of systematic analysis. The effective mining of such libraries necessitates a fundamental shift in methodology and requires algorithms that scale favorably with respect to library size. In this talk, we present novel, efficient and scalable techniques for the construction, analysis, and *in silico* screening of massive virtual combinatorial libraries. Some of the algorithms presented address long-standing problems in computational data analysis with a broad spectrum of applications in many disciplines of science.

BIOGRAPHY

Dr. Dimitris K. Agrafiotis is Senior Director of the DirectedDiversity® group at 3-Dimensional Pharmaceuticals, Inc. Dr. Agrafiotis holds a B.S. in chemistry from the University of Patras, Greece (1985), and a Ph.D. in theoretical organic chemistry from Imperial College, University of London (1988). Following post-doctoral training in the laboratories of Prof. A. Streitwieser at the University of California, Berkeley, and Nobel Laureate E. J. Corey at Harvard, he joined Parke-Davis Pharmaceutical Research as a Senior Scientist in the Computer-Aided Drug Design group. In 1994, he moved to 3-Dimensional Pharmaceuticals, Inc. where he has focused on the development of intelligent computational tools for combinatorial chemistry, high-throughput screening, and structure-based drug design. He is a co-inventor of 3DP_s proprietary DirectedDiversity® technology and serves on the Editorial Board of the Journal of Molecular Graphics and Modelling. More information can be found at his web site: http://www.geocities.com/dimitris_agrafiotis.