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CAChe Software Drug Discovery Training Seminars

April 1, 2004

Join UCSD Extension for two CAChe Software hands-on training seminars:

Structure-Guided Drug Design
9:00 a.m. - 12:00 noon

Quantitative Structure-Activity Relati
1:00 a.m. - 4:00 p.m.

Schedule • Fee • Location • Register • Accommodations • Information

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Structure-Guided Drug Design

April 1, 2004
Training Session: 9:00 a.m. - 12:00 noon
Lunch and Networking Break: 12:00 p.m. – 1:00 p.m.

Registration Closed - Event Full

This 3-hour course starts with a 40 minute overview presentation of the basic principles examples of software tools for structure-guided drug design, including analyzing protei identifying active-sites, comparing ligand-protein interactions, and automated docking. course is designed for the experimental chemist or biochemist and requires no special knowledge of computational chemistry or modelling techniques. Some familiarity with V based computers is assumed.

The remainder of the 3 hour session is devoted to hands-on exercises in using the BioMedCAChe software on a Windows computer to: import, clean-up, and analyze prote crystal structures, ligands, and their complexes from the Protein Data Bank; dock ligan proteins; identify active sites in homologues by automatic sequence alignment; use aut docking to screen libraries of potential inhibitors. The student has the choice of working the examples at their own pace with the step-by-step written notes or, following along instructor demonstrating the exercises on the projection screen. There will be one or tv students per computer.

Fee: $50.00 (includes cost of instruction and lunch)

Quantitative Structure-Activity Relationships

April 1, 2004
Lunch and Networking Break: 12:00 p.m. – 1:00 p.m.
Training Session: 1:00 p.m. - 4:00 p.m.

Registration Closed - Event Full

This 3-hour course starts with a 40 minute overview presentation of the basic principles application of Quantitative Structure-Property (and Activity) Relationships (QSAR & QSI predicting almost any physical, chemical or biological property, e.g. water solubility, re rates, rodent carcinogenicity, etc. The course is designed for the experimental chemist

biochemist and requires no special knowledge of computational chemistry or modelling techniques. Some familiarity with Windows-based computers is assumed.

The remainder of the 3 hour session is devoted to hands-on exercises in using the CAC software on a Windows computer to develop and create QSARs to predict various prope such as Lipinski's Rule-of-5, pKa, reaction rates, human intestinal absorption (HIA), an antibacterial activity. The student has the choice of working through the examples at th pace with the step-by-step written notes or, following along with the instructor demons the exercises on the projection screen. There will be one or two students per computer

Fee: $50.00 (includes cost of instruction and lunch)

Schedule

April 1, 2004

Structure-Guided Drug Design

- 9:00 a.m. - 12:00 noon
- Lunch Break and Networking Session 12:00noon - 1:00pm

Quantitative Structure-Activity Relationship

- Lunch Break and Networking Session 12:00noon - 1:00pm
- 1:00 a.m. - 4:00 p.m.

Fee

Each single session is $50.00. This includes cost of instruction and lunch break and networking session from 12:00noon - 1:00pm. Join us for both sessions and pay only (includes cost of instruction and lunch). **Registration Closed - Event Full**.

Location

Lecture Location: UCSD Extension; Sorrento Mesa Center, 6925 Lusk Blvd., San Diego, 92121.

Hotel Accommodations
Several hotels are within a few miles of the UCSD Extension Sorrento Mesa Center to s students from out of town. Click on this link for a list of recommended hotels. Check C Shuttle for shuttle service between the San Diego Airport and your hotel. You will rece 15% discount if you book online. Click on this link for other nearby hotels.

About CAChe Software
CAChe Group is a leading provider of computer-aided chemistry software and services predicting molecular structure, properties, spectra, reactions, thermodynamics, and kir Find out more online at cachesoftware.com or call 877 962 2243.

Information

Call (858) 964-1347 or e-mail unexbio2@ucsd.edu.

Complete details on all Bioscience programs offered by UCSD Extension at http://bioscience.ucsd.edu