SMAP: Software for Functional Site Characterization and Analysis (ligand binding site comparison)

Tech ID: 22670 / UC Case 2010-823-0

TECHNOLOGY DESCRIPTION

SMAP software package is designed for the comparison and the similarity search of protein three-dimensional motifs independent on the sequence order. It is based on the works published in:

- L. Xie, and P.E. Bourne 2007 "A Robust and Efficient Algorithm for the Shape Description of Protein Structures and Its Application in Predicting Ligand Binding Sites". *BMC Bioinformatics*, 8(Suppl 4):S9 [PDF].
- L. Xie and P.E. Bourne 2008 "Detecting Evolutionary Relationships Across Existing Fold Space, Using Sequence Order Independent Profile-profile Alignments". *PNAS*, 105(14):5441 [PDF]
- L. Xie, L. Xie and P.E. Bourne 2009 "A unified statistical model to support local sequence order independent similarity searching for ligand binding sites and its application to genome-based drug discovery". *Bioinformatics*, 25(12):i305-i312 [PDF].

SYSTEM REQUIREMENTS

- **Windows XP or Linux Operating system**: SMAP can be executed on both Windows and Linux operating system. For windows users, it is strongly recommended to install cygwin.
- **1G Memory**: For the most of PDB chains, at least 1G RAM should be allocated to the software. Some comparisons needs more memory than 1G.
- **Java 1.6**: Java 1.6 is required to run SMAP.

SUGGESTED USES

SMAP has been successfully applied to studying fundamental biological problems and rationally designing polypharmacology drugs. The cases include:

Detecting evolutionary relationships across existing fold spaces
L. Xie and P.E. Bourne 2008 "Detecting Evolutionary Relationships Across Existing Fold Space, Using Sequence Order Independent Profile-profile Alignments". *PNAS*, 105(14):5441 [PDF]

Elucidating molecular mechanisms defining drug side effects
L. Xie, J. Wang and P.E. Bourne 2007 "In Silico Elucidation of the Molecular Mechanism Defining the Adverse Effect of Selective Esterogen Receptor Modulators". *PLoS Comp. Biol.*, 3(11):e217 [PDF]

Repositioning safe pharmaceuticals to treat different diseases
S. Kinnings, N. Liu, N. Buchmeier, P.J. Tonge, L. Xie and P.E. Bourne 2009 "Drug discovery using chemical systems biology: repositioning the safe medicine Comtan to treat multi-drug and extensively drug resistant tuberculosis". *PLoS Comp Biol.,* 5(7):e1000423 [PDF]

Revealing complex biological networks using small molecules as probes

L. Xie, L. Xie and P.E. Bourne 2009 "Drug Discovery Using Chemical Systems Biology: Identification of the Protein-Ligand Binding Network To Explain the Side Effects of CETP Inhibitors". *PLoS Comp. Biol.*, 5(5):e1000387 [PDF]

STATE OF DEVELOPMENT

Download SMAP for academic (non-profit or non-commercial users). Commercial users please contact UC San Diego Office of Innovation and Commercialization (innovation@ucsd.edu) for license information.

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OTHER INFORMATION

CATEGORIZED AS
- **Biotechnology**
  - Bioinformatics
- **Computer**
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