# **Explorations in Fold Space COPS - Classification of Protein Structures Stefan J. Suhrer and Manfred J. Sippl**

**University of Salzburg** 

Center of Applied Molecular Engineering / Department of Molecular Biology / Division of Bioinformatics Hellbrunnerstr. 34 / 5020 Salzburg / Austria









# Motivation

Classification of protein structures implies several intricate tasks like the characterization of the classification unit or the definition of the properties to organize these units. But perhaps the most important aspect of any structure classification is

that the complete repertoire of available structures is represented in a way that is accessible and comprehensible to consumers who are not necessarily experts in domain decomposition and structure comparison. This requires appropriate user interfaces for navigation in fold space and the instant visualization of structural similarities.

The COPS web service (Classification Of Protein Structures) provides an example of current developments in this area (1,2,3,4).

# **Availability**

http://cops.services.came.sbg.ac.at/



# **The COPS Hierarchy**

Protein domains in COPS are organized as a tree where the domains correspond to tree nodes and pairwise structural similarities among domains correspond to tree edges. The edges represent relative similarities among protein domains derived from structure superpositions (2). The classification layers of COPS are obtained by cutting the tree at constant relative similarity (3,4). Currently, the Fold Space Navigator of COPS displays five layers called distant (30% relative similarity), remote (40%), related (60%), similar (80%) and equivalent (99%).

# **COPS Examples**

Recently, Leiman et al. (2009) reported the amazing structural similarities of proteins from the bacterial secretion system VI (T6SS) with proteins from the cell-puncturing device of bacteriophage T4. The authors identified the similarities by elaborate sequence and structure searches. Using COPS, the reported similar protein domains are available within seconds (a, c). Moreover, the structures can instantly be visualized and superimposed with a few mouse clicks (b, the query is in blue, the target in green and the regions of similar structure are colored red (query) and orange (target)).

### References

(1) Sippl, M. J. (2009) Fold space unlimited. Curr Opin Struct Biol., 19 (3), 312-320. (2) Sippl, M. J. (2008) On distance and similarity in fold space. Bioinformatics, 24, 872–873. (3) Sippl, M. J., Suhrer, S. J., Gruber, M. and Wiederstein, M. (2008) A discrete view on fold space. Bioinformatics, 24, 870–871. (4) Suhrer, S. J., Wiederstein, M., Gruber, M. and

Sippl M. J. (2009) COPS - A Novel Workbench for Explorations in Fold Space. Nucleic Acids Research, 37 (Web Server Issue), Advance Access published May 22, 2009

