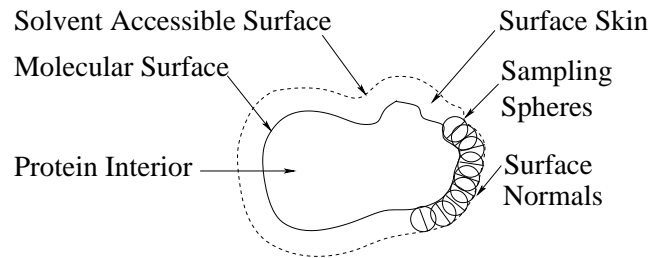


## 3D protein shape density representation in Hex

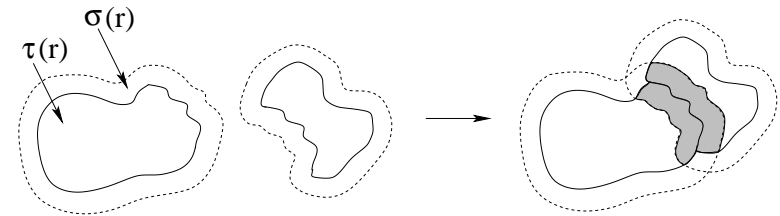


$$\sigma(\underline{r}) = \begin{cases} 1; & \underline{r} \in \text{surface skin} \\ 0; & \text{otherwise} \end{cases} \quad \tau(\underline{r}) = \begin{cases} 1; & \underline{r} \in \text{protein atom} \\ 0; & \text{otherwise} \end{cases}$$

[Ritchie & Kemp (2000) Proteins **39:178–194**]

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## Protein shape complementarity



$$\text{Favourable:} \quad \int (\sigma_A(\underline{r}_A)\tau_B(\underline{r}_B) + \tau_A(\underline{r}_A)\sigma_B(\underline{r}_B))dV$$

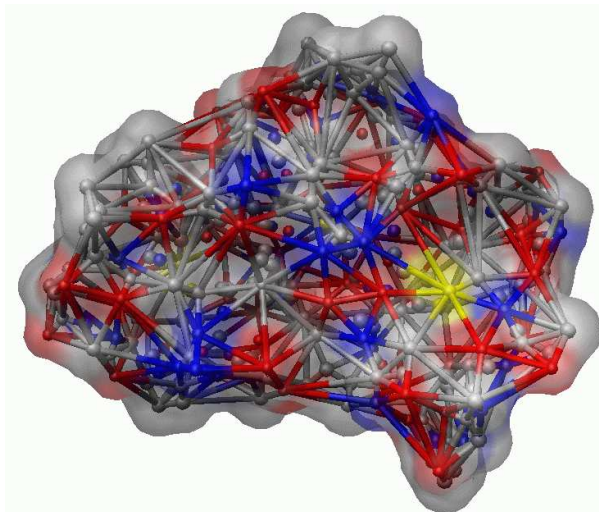
$$\text{Unfavourable:} \quad \int \tau_A(\underline{r}_A)\tau_B(\underline{r}_B)dV$$

$$\text{Score:} \quad S_{AB} = \int (\sigma_{ATB} + \tau_{A\sigma B} - Q_{TATB})dV$$

$$\text{Penalty Factor:} \quad Q = 11$$

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## Surface representation

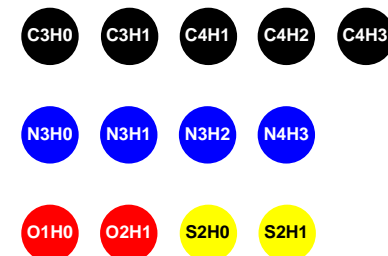


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## Atomic group in proteins

Classification proposed by Tsai et al. (J. Mol. Biol., 1999, 290:253-266), based on:

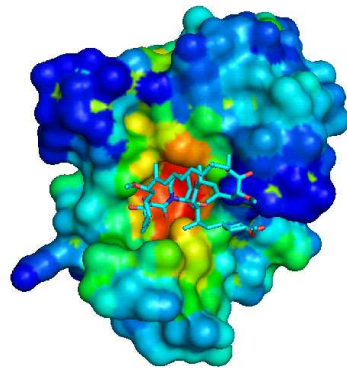
- ▶ heavy-atom types,
- ▶ the number of covalently attached hydrogen atoms, and
- ▶ the number of all covalently attached atoms.



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## Surface Triplet Propensities

Mehio, W., Kemp, G.J.L., Taylor P. and Walkinshaw, M.D. (2010) Identification of Protein Binding Surfaces using Surface Triplet Propensities. *Bioinformatics*



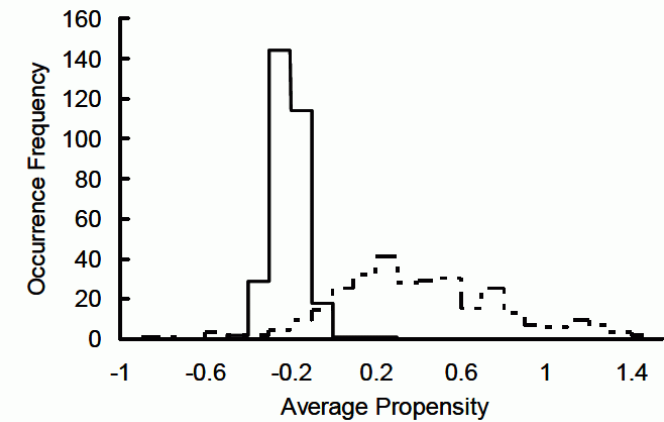
Navigation icons

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## Surface Triplet Propensities

### A Distribution of Average Propensities in the Protein - Ligand Interaction Dataset

— Entire Surface — - Binding Sites



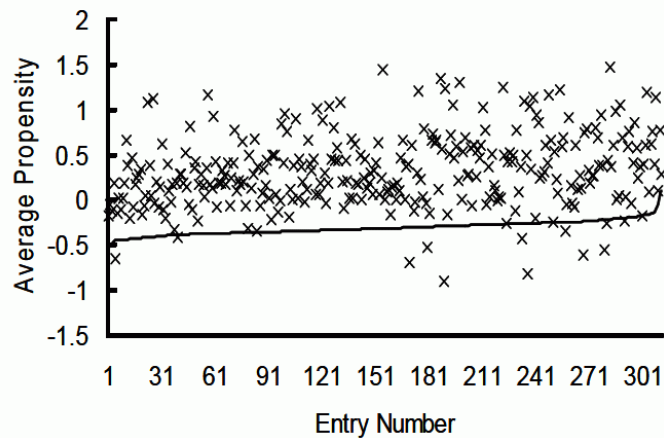
Navigation icons

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## Surface Triplet Propensities

### B Average Propensity: Entire Surface vs Binding Sites

— Entire Surface × Binding Sites

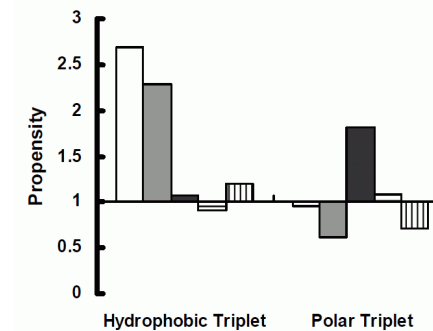


Navigation icons

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## Surface Triplet Propensities

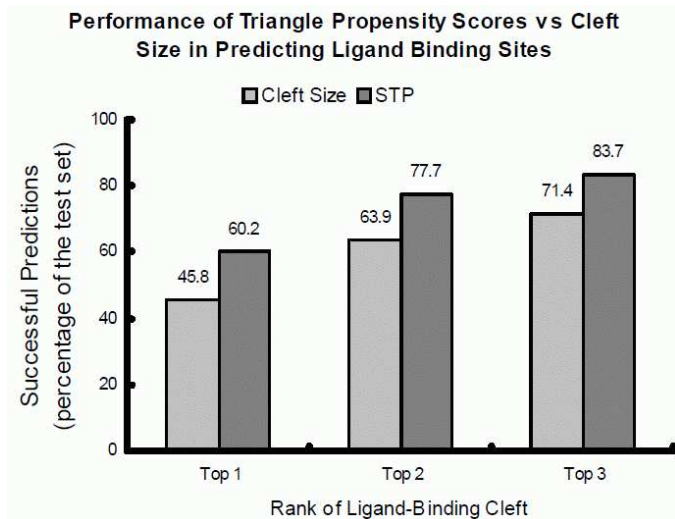
□ Halogen Atom □ Hydrophobic Atom  
■ Polar Atom □ Water Molecule  
□ Empty



Navigation icons

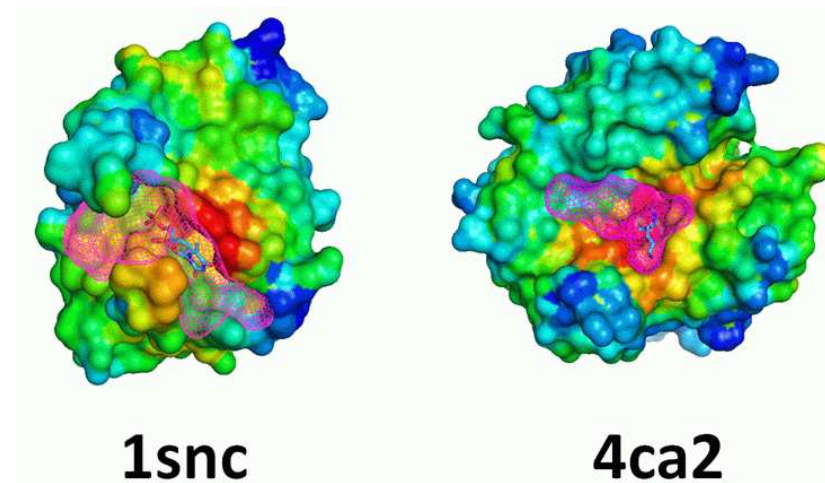
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## Surface Triplet Propensities



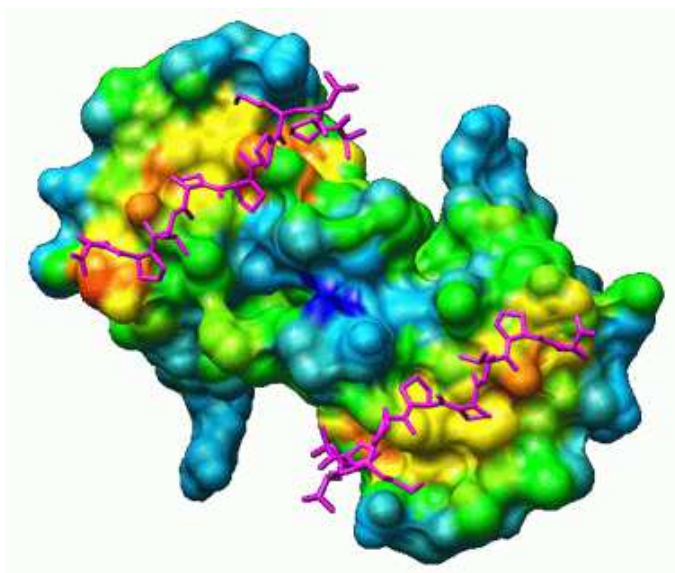
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## Surface Triplet Propensities



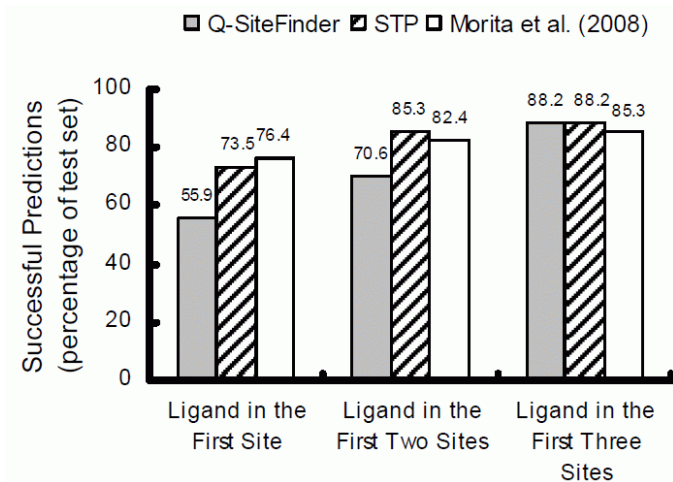
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## Surface Triplet Propensities



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## Surface Triplet Propensities



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