



Molecular Biotechnology Programme
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Title (English) EXCAVAT: A program for the calculation of solvent accessible surface area and the identification of cavities in proteins		
Title (Swedish)		
Abstract A program for the calculation of solvent accessible surface area (SASA) and the identification of putative binding sites in proteins has been developed based on the classification of grid points depending upon their shortest distance to the protein surface and their accessibility. Simple descriptors related to geometrical properties of these cavities are also calculated. Input to the program are the atomic coordinates in PDB format. The cavity finding algorithm was validated using a test set of 31 proteins from different functional classes. It was possible to identify the experimentally observed binding site for all test cases. An analysis of the ability of the descriptors to cluster these groups showed that different descriptors might be relevant for different groups of proteins.		
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