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Author <b>Adolfo Orro Graña</b>		
Title (English) <b>Examination of the role of binding site water molecules in molecular recognition</b>		
Title (Swedish)		
Abstract <p>A set of algorithms were designed, implemented and evaluated in order to, first, identify clusters of conserved waters in binding pockets, i.e. hydration sites. Then, their contribution to the free energy of binding in a ligand-protein association was quantified by calculating their enthalpy and entropy. The information obtained by using these algorithms could contribute to the development of new drugs by generating new ligands that target specific high-energy, unfavorable waters. Evaluation tests show that our algorithms can indeed provide relevant data about how hydration sites influence ligand-protein binding.</p>		
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Supervisors <b>Jens Carlsson</b> <b>Stockholm University</b>		
Scientific reviewer <b>Erik Lindahl</b> <b>Royal Institute of Technology</b>		
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<b>Biology Education Centre</b> Box 592 S-75124 Uppsala	Biomedical Center Tel +46 (0)18 4710000	Husargatan 3 Uppsala Fax +46 (0)18 471 4687