Regine Bohacek, Med chem 2016, 6:10(Suppl)
http://dx.doi.org/10.4172/2161-0444.C1.027



## "Growing" hydrogen bonding waters in molecular complexes!

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The goal of this work is to use fast algorithms from the *de novo* design program, AlleGrow, to accurately position explicit waters in a protein structure. The best source of precise data on water interactions in organic complexes is found in small molecule X-ray structures. The studies were done using packed X-ray structures which contain water taken from the Crystallographic Open Data Base (COD, 2). To test the growth algorithm, waters were removed one at a time and "regrown". This search algorithm was optimized to ensure that the output contained a water close to the experimental X-ray water. A scoring function was developed to rank order the water positions found in the search with the aim of identifying the water closest to the X-ray structure. The scoring function was optimized to obtain the best possible predictions for a large set of different experimental waters.

### Biography

Regine Bohacek received her PhD in physical chemistry from Rutgers University. She received a post-doctoral fellowship from Ciba-Geigy in Summit, NJ. Subsequently she became a permanent member of the computational chemistry group at Ciba-Geigy where she worked closely with synthetic chemists on a variety of structure based drug design projects. To aid in these projects, she wrote a de novo design computer program called GrowMol. Subsequently, she joined Ariad Pharmaceuticals in Cambridge, MA, as head of the computational chemistry group. Presently, she has her own company, Boston De Novo Design, and has developed a second de novo program called AlleGrow and is consulting for a number of firms and universities. She divides her time between Madison, WI and Boston, MA

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