Fragment based drug discovery at Astex

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Fragment based drug discovery at Astex uses a combination of X-ray crystallography and other biophysical techniques including NMR, SPR, ITC and thermal shift (T_m) to detect the binding of low molecular weight fragments. Using our proprietary fragment screening platform, Pyramid™ we have successfully discovered fragments (MW<250Da) that bind to maximize their interaction with the protein target. Fragment hits with suitable vectors are selected and grown to optimize their interaction with the protein target. After several rounds of fast iterative structure-based drug design, fragments are evolved to potent inhibitors highly complementary to the target protein. This talk will describe the key aspects of fragment based drug design and how it has been successfully utilized on different protein targets at Astex.