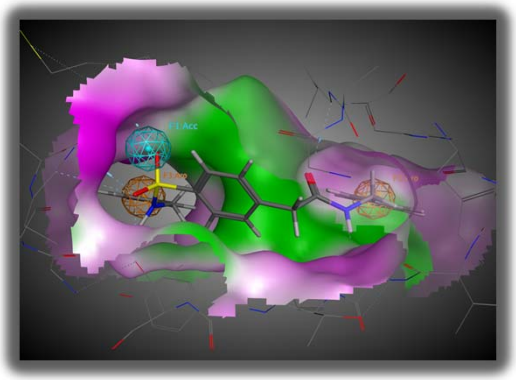
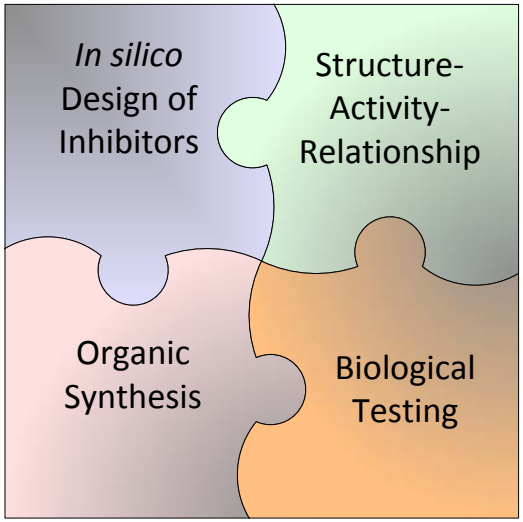
Design and synthesis of novel scaffolds for therapeutically validated drug targets

In order to improve the ***potency*** and ***selectivity*** of inhibitors of validated drug targets, we rationally ***design*** and ***synthesize*** novel scaffolds based on X-ray data of co-crystal structures. The iterative process of ***computational design, organic synthesis*** and ***biological testing*** leads to detailed ***structure activity relationships*** for therapeutically validated drug targets. Ultimately, this allows for the development of novel drug candidates for the treatment of diseases. Our focus is on the ***design*** and ***synthesis part*** of the drug discovery process.





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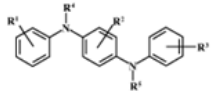
Structure Activity Data



Compd no.	Structure R^1	R^2	R^3	R^4	R^5	IC_{50} (nM)
40	H	H	H	H	H	102
41	H	H	H	Me	H	$> 10^5$
42	H	H	H	H	Me	80
43	H	H	H	Me	Me	$> 10^5$
44	2-OH	H	H	H	Me	62
45	3-OH	H	H	H	Me	5.3
46	4-OH	H	H	H	Me	48
47	H	3-OH	H	H	Me	75
48	3-OH	3-OH	H	H	Me	1.2