

## Using thrombin to study protein-ligand interactions.

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X-ray structures of closely similar inhibitors may be used to develop an accurate experimental estimate of the energetics of ligand receptor interactions. This requires a well-diffracting crystal system of sufficient interest to be attractive for synthetic chemistry. I will describe in detail the use of the blood coagulation enzyme Thrombin for this purpose, drawing examples both from the literature and from my own work. In particular, the substitution of fluorine for hydrogen has been examined recently in the context of medicinal chemistry, as this can contribute both to improved binding and to improved molecular properties.

### References:

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