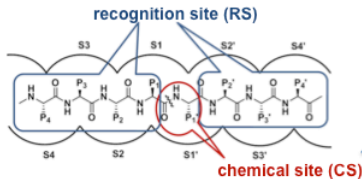
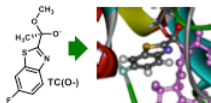
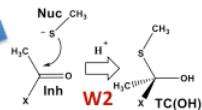
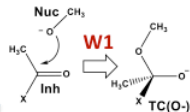


# EMBM – Enzyme Mechanism Based Method for the Design of TS analog enzyme Inhibitors

Separate treatment of **CS** and **RS** parts of inhibitors



**W1** and **W2** are covalent descriptors  
quantum mechanically calculated  
on a reaction core model.  
Saved in databank



Structure-based  
design



Ligand-based  
design

