EMBM – Enzyme Mechanism Based Method for Rational Design of Chemical Sites of Covalent Inhibitors

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Separate design of CS and RS fragments of inhibitors

W1 and W2 are covalent descriptors quantum mechanically precalculated on reaction core. Saved in databank

QSAR

Ligand-based design
Structure-based design

Databank

[Diagram showing the separation of chemical and recognition sites, with W1 and W2 as covalent descriptors.]