Interaction energies between PIN1 protein and different ligands

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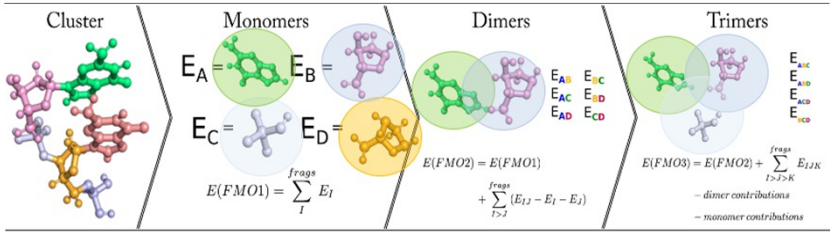
Purpose To identify preferential binding of ligands to PIN1 protein

Outline Utilised the Fragment Molecular Orbital method (FMO) as a cost saving approach to study interaction energies between different ligands and the active site of PIN1 protein.

Result Based on the calculated energies, it is possible to determine preferential binding between certain ligands to PIN1

Computing system:	SQUID General Purpose CPU nodes
node-hour	10000 node-hour
memory used	96 GB
parallelize	1 nodes



Using FMO to speed up protein calculations