

SCHEMATICS OF BEST PERFORMING COMPUTATIONAL METHODS IN CACHE #1

Koes [Score: 18] MD → CE → DLD/HTD/CD

Isayev/Cherkasov [Score: 18] DLD → CD → MD → FEC
AL

Schindler [Score: 17] UHTD → DND → FSS → HTD

Kireev [Score: 16] DLF → HTD

Gorgulla [Score: 16] MD → UHTD → FSS → CE → HTD

Rognan [Score: 16] SPBC → IHS → DND → FSS

Polishchuk [Score: 16] MD → CE → DF → DND → CD → MM → FSS → CD

CE: conformational ensemble

IHS: interaction hot spots

SPBC: similar pocket in PDB
with bound compound

FSS: fingerprint similarity search

DND: de novo design

DLD: deep learning docking

DLF: deep learn. frag. docking

AL: active learning

DF: docking fragments

HTD : high-throughput docking

UHTD: ultra HTD

CD: consensus docking

MM: molecular mechanics

MD: molecular dynamics

FEC: free energy

AI