

April 2023

SAMPL11

GDCCs

Small molecule membrane permeabilities

SAMPL11
challenge open

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Drug binding to acyclic CB[n] host

Cosolvent effects on affinities for hosts 1,2

Binding to mutant HSA

Binding to mutants of new system 1

Binding to mutants of new system 2

Binding to new system 2

Binding to mutants of new system 3

Binding in new system 4

Joint D3R/SAMPL workshop

* - Our current plan is to provide pKa values, as in SAMPL6, which is currently in progress. But this may be adjusted to require prediction of pKa values, depending on SAMPL6 outcomes..