

April 2018

April 2019

April 2020

April 2021

April 2022

April 2023

SAMPL7

SAMPL8

SAMPL9

SAMPL10

SAMPL11

Aim 1

Physical properties

log D in octanol-water,
and cyclohexane-water,
providing* pKa

log D in octanol-water and
cyclohexane-water, predicting pKa

log D in alternate solvents, predicting pKa

Solubilities for drug-like compounds and fragments

Small molecule membrane permeabilities

SAMPL7
challenge open



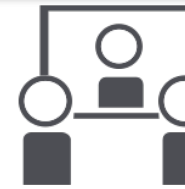
SAMPL8
challenge open



SAMPL9
challenge open



SAMPL10
challenge open



SAMPL11
challenge open

Aim 2

Host-guest binding

Cucubiturils

GDCCs

SAMPL7
challenge open



SAMPL8
challenge open



SAMPL9
challenge open



SAMPL10
challenge open



SAMPL11
challenge open

Me₄CB[8] binding affinities

New compound binding to Me₄CB[8]

Drug binding to glycoluril hexamer

New compound binding to glycoluril hexamer

Drug binding to acyclic CB[n] host

Affinities for hosts 1-2

Affinities for hosts 1,3

Ion effects on affinities for host 1

Ion effects on affinities for host 3

Cosolvent effects on affinities for hosts 1,2

Aim 3

Protein-ligand binding

Binding to wild type HSA

Binding to mutant HSA

Binding to new system 1

Binding to mutants of new system 1

SAMPL9
challenge open



SAMPL7
challenge open



Binding to new system 2

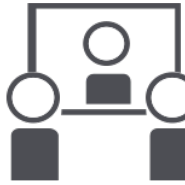
Binding to mutants of new system 2

SAMPL10
challenge open



SAMPL11
challenge open

SAMPL8
challenge open



Binding to new system 3

Binding to mutants of new system 3

Binding in new system 4

Overall events

Key

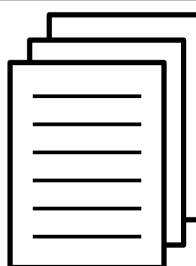
Experimental data collection
Submission window



SAMPL special issue preparation
(approximate 4-5month duration)



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..