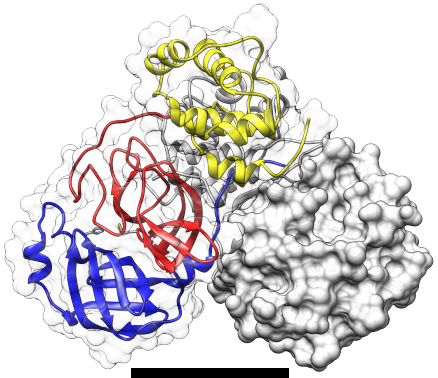
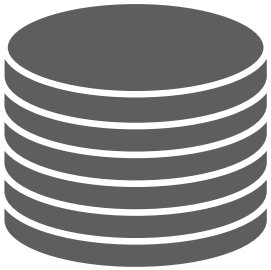
複数の計算手法を用いた統合的創薬計算

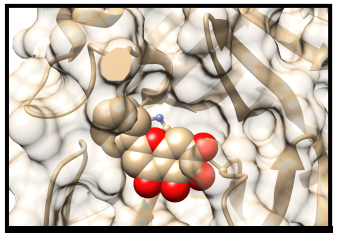


6M2N



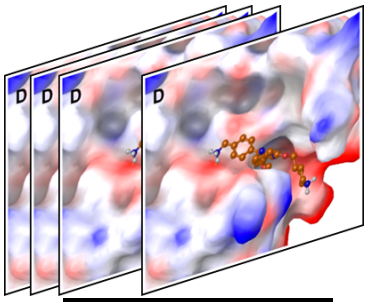
In-house databases

ドッキングシミュレーション



Initial complex

MD計算による構造緩和、
安定構造解析



Trajectories

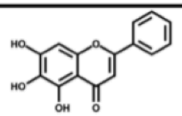
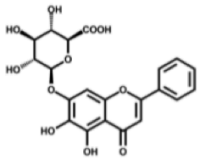
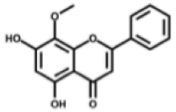
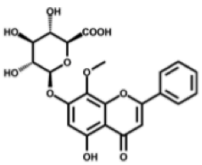
結合自由エネルギー解析
(FMO-MP2/PCM)

阻害剤候補
結合様式の定量評価

SARS-CoV-2 3CLpro に対するドラッグリポジショニング

Baicalein showed the most potent anti- SARS-CoV-2 3CLpro activity with an IC50 of 0.39 μM.

Baicalin inhibited SARS-CoV-2 3CLpro activity for about 41% at 50 μM, while wogonin and wogonoside were not active at this concentration.

Compound	Chemical Structure	IC_{50} (μM)	% Inhibition at 50 μM
Baicalein		0.39 ± 0.12	-
Baicalin		-	41.5±0.6
Wogonin		-	6.1±0.8
Wogonoside		-	**8.5±3.3**

Liu, et al. **bioRxiv**, **DOI**:10.1101/2020.04.10.035824.

Baicalein and halogenated baicalein showed good binding affinity