

Table S3. Energies for the top-ranked cyclodextrins against the active site and the two allosteric sites of M^{pro}.

	Molecule	Binding Energy (kcal/mol)
Active site	γ -CD	-91.87
	HP- β -CD	-86.86
	Methyl- β -CD	-86.63
	β -CD	-81.77
	α -CD	-65.47
Allosteric site I	β -CD	-92.69
	Methyl- β -CD	-78.76
	γ -CD	-69.74
	α -CD	-65.65
Allosteric site II	HP- β -CD	-84.51
	Methyl- β -CD	-83.61
	γ -CD	-78.39
	β -CD	-78.32
	α -CD	-65.92