

Table S3a. The inference time of the models with the PDBbind 2016 core set (290 complexes)

	Model ^a					
	Adj-float	Adj-1	Adj-2	Adj-4	Adj-8	Pafnucy
dataset1	58.65 (0.09)	0.80 (0.15)	1.61 (0.32)	2.68 (0.19)	5.45 (0.52)	2.14 (0.04)
dataset2	58.63 (0.19)	0.94 (0.06)	1.36 (0.14)	3.09 (0.36)	5.59 (0.18)	2.13 (0.05)
dataset3	58.80 (0.13)	0.92 (0.07)	1.42 (0.18)	3.02 (0.21)	5.55 (0.52)	2.18 (0.05)
dataset4	58.55 (0.11)	0.85 (0.04)	1.62 (0.17)	3.09 (0.19)	6.00 (0.85)	2.19 (0.07)

^aComputing time were measured in second scale.

Table S3b. The data preparation time of the models with the CSAR NRC-HiQ set (51 and 36 complexes)

	GraphBAR	Pafnucy
CSAR NRC-HiQ set 1	26.65 (0.08)	61.26 (0.24)
CSAR NRC-HiQ set 2	10.77 (0.07)	17.51 (0.11)

Computing time were measured in second scale.