A.

Batch size	Prediction method	Percentage of acquired hits							
		AA2AR		CB2		AmpC		D4	
		"add"	"noadd"	"add"	"noadd"	"add"	"noadd"	"add"	"noadd"
40 000	"LastModel"	18 ± 4	19 ± 4	17 ± 5	17 ± 5	41.2 ± 0.2	41.6 ± 0.1	23.3 ± 0.5	23.5 ± 0.3
	"MeanRank"	18 ± 4	18 ± 4	17 ± 5	17 ± 5	41.3 ± 0.3	41.2 ± 0.2	23.3 ± 0.5	23.4 ± 0.2
	"TopFromEveryModel"	18 ± 3	18 ± 4	17 ± 5	17 ± 5	41.1 ± 0.2	41.2 ± 0.2	23 ± 1	23.3 ± 0.5
	Second docking	53.8 ± 0.4	53.8 ± 0.2	47.57 ± 0.01	47.7 ± 0.3	NA	NA	NA	NA
20 000	"LastModel"	20 ± 8	26 ± 4	31.4 ± 0.3	28 ± 3	74.4 ± 0.4	74 ± 1	37.9 ± 0.1	36.35 ± 0.03
	"MeanRank"	30 ± 7	28 ± 5	29.8 ± 0.5	30.5 ± 0.3	70 ± 1	72 ± 1	36.6 ± 0.2	37.8 ± 0.5
	"TopFromEveryModel"	26 ± 8	25 ± 7	27 ± 2	28 ± 2	69.6 ± 0.4	70.6 ± 0.4	36.0 ± 0.3	35.6 ± 0.3
	Second docking	64.8 ± 0.2	64.9 ± 0.2	61.1 ± 0.2	60.9 ± 0.3	NA	NA	NA	NA
10 000	"LastModel"	50 ± 2	42.1 ± 0.4	43 ± 3	39 ± 2	90.2 ± 0.1	87 ± 1	55.4 ± 0.3	46.7 ± 0.4
	"MeanRank"	45 ± 4	48 ± 4	41 ± 1	44 ± 1	85 ± 1	88.6 ± 0.3	51.6 ± 0.4	54.0 ± 0.5
	"TopFromEveryModel"	47 ± 2	43 ± 1	39 ± 6	36 ± 1	86 ± 1	85.3 ± 0.3	50.7 ± 0.3	47.0 ± 0.3
	Second docking	72.25 ± 0.03	72.3 ± 0.1	70.4 ± 0.1	70.61 ± 0.03	NA	NA	NA	NA
8000	"LastModel"	45 ± 7	42 ± 1	40 ± 20	34 ± 3	92.4 ± 0.1	86 ± 1	61.8 ± 0.1	48.3 ± 0.3
	"MeanRank"	40 ± 10	51 ± 3	39 ± 16	48 ± 3	88 ± 1	91.3 ± 0.4	56.7 ± 0.5	60 ± 1
	"TopFromEveryModel"	40 ± 10	42 ± 3	40 ± 13	38 ± 1	89.2 ± 0.2	87.8 ± 0.3	56 ± 1	49.5 ± 0.4
	Second docking	74.07 ± 0.02	74.1 ± 0.1	73.1 ± 0.1	73.2 ± 0.1	NA	NA	NA	NA

B.

Batch size	Prediction method	Percentage of acquired hits							
		AA2AR		CB2		AmpC		D4	
		"add"	"noadd"	"add"	"noadd"	"add"	"noadd"	"add"	"noadd"
40 000	"LastModel"	58 ± 2	55 ± 3	51 ± 4	56 ± 1	89.1 ± 0.3	90.2 ± 0.4	67.7 ± 0.3	67.2 ± 0.2
	"MeanRank"	58 ± 4	56 ± 4	51 ± 5	53 ± 3	86.8 ± 0.5	87.8 ± 0.5	67 ± 1	68.0 ± 0.3
	"TopFromEveryModel"	54 ± 6	57 ± 2	51 ± 7	53 ± 5	87.3 ± 0.2	88.4 ± 0.3	67 ± 1	67.1 ± 0.1
	Second docking	79.7 ± 0.4	79.5 ± 0.2	78.5 ± 0.5	78.0 ± 1.0	NA	NA	NA	NA
20 000	"LastModel"	50 ± 15	66 ± 1	64 ± 2	60 ± 2	94.19 ± 0.02	93.6 ± 1e-14	76.1 ± 0.5	74.5 ± 0.4
	"MeanRank"	62 ± 14	66 ± 3	63 ± 3	65 ± 3	92.3 ± 0.3	93.2 ± 0.4	74.8 ± 0.2	75.6 ± 0.4
	"TopFromEveryModel"	63 ± 5	65 ± 3	63 ± 2	63 ± 2	93.1 ± 0.3	94.3 ± 0.2	74.6 ± 0.1	74.4 ± 0.4
	Second docking	82.9 ± 0.2	82.7 ± 0.2	83.0 ± 0.1	82.9 ± 0.2	NA	NA	NA	NA
10 000	"LastModel"	79 ± 2	74 ± 2	73 ± 2	71.6 ± 0.4	97.0 ± 0.1	95.6 ± 0.1	85.6 ± 0.3	81 ± 1
	"MeanRank"	70 ± 10	82 ± 1	73 ± 4	76.8 ± 0.2	96.2 ± 0.4	96.2 ± 0.2	84.3 ± 0.1	84.8 ± 0.2
	"TopFromEveryModel"	78 ± 7	78 ± 1	68 ± 10	72 ± 1	96.8 ± 0.1	97.0 ± 0.1	84.1 ± 0.1	81.8 ± 0.2
	Second docking	86.68 ± 0.01	86.80 ± 0.02	87.3 ± 0.1	87.5 ± 0.2	NA	NA	NA	NA
8000	"LastModel"	76 ± 10	78 ± 2	70 ± 20	72 ± 2	97.5 ± 0.1	96 ± 1	88.1 ± 0.4	83.1 ± 0.3
	"MeanRank"	75 ± 6	85 ± 1	70 ± 20	80.3 ± 0.4	96.9 ± 0.1	96.8 ± 0.1	86.7 ± 0.1	87.6 ± 0.3
	"TopFromEveryModel"	77 ± 5	80 ± 2	69 ± 15	75 ± 1	97.3 ± 0.1	97.5 ± 0.1	86.9 ± 0.2	84.0 ± 0.1
	Second docking	88.1 ± 0.1	88.0 ± 0.1	88.8 ± 0.3	88.89 ± 0.01	NA	NA	NA	NA