

Table 1. Performance Benchmarks for ROCS on All 40 Targets Using Different Query Conformations.^a

target	mode	AUC	EF_max ^b	with_% ^c	EF1	DUD EF1	EF5	EF10	EF20	DUD EF20
ACE	corina	0.65	25.6	1	25.6		7.8	4.7	2.6	
ACE	omega_highestE	0.65	27.7	1	27.7		8.2	4.3	2.7	
ACE	omega_lowestE	0.68	29.8	1	29.8		9.9	4.9	2.8	
ACE	sybyl	0.67	25.6	1	25.6		7.8	4.3	2.9	
ACE	xtal	0.70	27.7	1	27.7	40.4	8.2	4.7	3.2	3.7
ACHE	corina	0.76	23.0	1	23.0		10.7	6.7	3.8	
ACHE	omega_highestE	0.76	22.0	1	22.0		9.6	6.9	3.8	
ACHE	omega_lowestE	0.76	22.0	1	22.0		10.7	7.3	3.8	
ACHE	sybyl	0.77	23.0	1	23.0		14.0	7.6	3.8	
ACHE	xtal	0.77	26.8	1	26.8	1.9	12.6	7.4	3.9	2.0
ADA	corina	0.75	9.2	1	9.2		5.2	4.8	2.8	
ADA	omega_highestE	0.80	13.8	1	13.8		3.5	2.2	2.4	
ADA	omega_lowestE	0.85	13.8	1	13.8		4.4	4.4	3.3	
ADA	sybyl	0.83	18.3	1	18.3		7.0	4.4	2.6	
ADA	xtal	0.86	13.8	1	13.8	12.9	3.5	3.9	3.5	2.4
ALR2	corina	0.59	4.0	1	4.0		3.1	3.1	2.5	

ALR2	omega_highestE	0.73	12.1	1	12.1		3.9	4.2	3.1	
ALR2	omega_lowestE	0.65	4.9	4	4.0		4.6	3.9	2.1	
ALR2	sybyl	0.57	4.0	1	4.0		3.1	3.1	1.5	
ALR2	xtal	0.57	8.1	1	8.1	38.1	3.1	3.1	1.5	2.3
AMPC	corina	0.84	35.9	1	35.9		13.6	7.2	3.8	
AMPC	omega_highestE	0.88	35.9	1	35.9		14.5	7.6	4.1	
AMPC	omega_lowestE	0.86	35.9	1	35.9		14.5	7.2	3.8	
AMPC	sybyl	0.83	35.9	1	35.9		13.6	7.2	3.6	
AMPC	xtal	0.82	35.9	1	35.9	17.1	13.6	7.2	3.6	4.7
AR	corina	0.76	21.6	1	21.6		8.9	5.3	2.9	
AR	omega_highestE	0.76	25.7	1	25.7		9.5	5.4	3.0	
AR	omega_lowestE	0.76	25.7	1	25.7		9.5	5.4	3.0	
AR	sybyl	0.76	16.2	1	16.2		7.8	4.7	3.0	
AR	xtal	0.79	27.0	1	27.0	33.5	9.5	5.1	3.0	3.8
CDK2	corina	0.66	26.4	1	26.4		6.4	3.4	2.5	
CDK2	omega_highestE	0.67	22.4	1	22.4		6.4	3.4	2.1	
CDK2	omega_lowestE	0.69	28.5	1	28.5		6.4	3.4	2.2	
CDK2	sybyl	0.67	26.4	1	26.4		6.4	3.4	2.3	

CDK2	xtal	0.68	26.4	1	26.4	13.9	6.4	4.0	2.5	1.4
COMT	corina	0.39	30.1	1	30.1		7.3	3.6	1.8	
COMT	omega_highestE	0.38	30.1	1	30.1		5.5	3.6	1.8	
COMT	omega_lowestE	0.35	30.1	1	30.1		5.5	2.7	1.4	
COMT	sybyl	0.36	30.1	1	30.1		5.5	2.7	1.4	
COMT	xtal	0.32	30.1	1	30.1	0.0	5.5	2.7	1.4	3.3
COX1	corina	0.50	17.5	1	17.5		5.7	2.8	1.4	
COX1	omega_highestE	0.52	21.9	1	21.9		5.7	2.8	2.0	
COX1	omega_lowestE	0.51	17.5	1	17.5		4.9	2.8	1.4	
COX1	sybyl	0.50	17.5	1	17.5		4.9	2.8	1.6	
COX1	xtal	0.53	17.5	1	17.5	4.0	5.7	2.8	2.0	1.6
COX2	corina	0.94	35.1	1	35.1		16.8	8.7	4.5	
COX2	omega_highestE	0.94	36.2	1	36.2		16.7	8.7	4.5	
COX2	omega_lowestE	0.94	36.2	1	36.2		16.9	8.6	4.5	
COX2	sybyl	0.94	34.5	1	34.5		16.7	8.7	4.5	
COX2	xtal	0.93	35.7	1	35.7	20.1	17.1	8.7	4.5	3.3
DHFR	corina	0.96	34.5	1	34.5		16.7	9.3	4.8	
DHFR	omega_highestE	0.97	33.0	1	33.0		15.9	9.2	4.8	

DHFR	omega_lowestE	0.92	31.0	1	31.0		12.3	7.3	4.3	
DHFR	sybyl	0.93	34.0	1	34.0		15.7	8.7	4.6	
DHFR	xtal	0.92	33.5	1	33.5	21.7	14.0	8.2	4.4	3.5
EGFR	corina	0.96	33.4	1	33.4		17.3	9.1	4.6	
EGFR	omega_highestE	0.97	33.6	1	33.6		18.4	9.3	4.8	
EGFR	omega_lowestE	0.95	33.6	1	33.6		17.4	9.1	4.7	
EGFR	sybyl	0.90	31.8	1	31.8		14.3	7.7	4.1	
EGFR	xtal	0.95	33.0	1	33.0	2.1	16.9	8.9	4.7	2.4
ER_AGONIST	corina	0.93	28.6	1	28.6		15.8	8.8	4.6	
ER_AGONIST	omega_highestE	0.93	30.1	1	30.1		16.1	8.8	4.6	
ER_AGONIST	omega_lowestE	0.93	30.1	1	30.1		16.1	8.8	4.6	
ER_AGONIST	sybyl	0.94	30.1	1	30.1		16.4	8.7	4.6	
ER_AGONIST	xtal	0.94	27.1	1	27.1	19.2	16.1	9.0	4.6	4.5
ER_ANTAGONIST	corina	0.98	18.8	3	13.1		15.5	9.8	5.0	
ER_ANTAGONIST	omega_highestE	0.98	18.0	3	13.1		16.1	9.8	5.0	
ER_ANTAGONIST	omega_lowestE	0.98	18.8	3	15.8		16.6	10.0	5.0	
ER_ANTAGONIST	sybyl	0.97	18.0	3	13.1		12.9	9.5	5.0	
ER_ANTAGONIST	xtal	0.98	18.8	3	5.3	12.7	15.0	9.8	5.0	1.3

FGFR1	corina	0.40	4.3	1	4.3		2.2	1.4	1.2	
FGFR1	omega_highestE	0.45	4.3	2	3.4		1.9	2.4	1.4	
FGFR1	omega_lowestE	0.46	3.8	2	3.4		1.9	1.8	1.3	
FGFR1	sybyl	0.47	3.8	2	3.4		3.7	2.5	1.6	
FGFR1	xtal	0.49	2.4	7	0.0	0.0	2.4	2.0	1.7	0.2
FXA	corina	0.64	4.3	1	4.3		2.3	1.7	1.5	
FXA	omega_highestE	0.42	4.3	1	4.3		0.9	0.5	0.5	
FXA	omega_lowestE	0.66	5.8	1	5.8		1.4	1.4	2.1	
FXA	sybyl	0.39	4.3	1	4.3		0.9	0.7	0.5	
FXA	xtal	0.39	4.3	1	4.3	14.6	1.0	0.8	0.5	3.8
GART	corina	0.92	7.4	2	0.0		6.8	6.2	5.0	
GART	omega_highestE	0.91	10.5	1	10.5		5.8	4.8	4.8	
GART	omega_lowestE	0.92	6.4	3	5.3		4.8	5.3	5.0	
GART	sybyl	0.89	5.3	1	5.3		3.9	3.3	4.5	
GART	xtal	0.93	7.4	2	0.0	42.4	3.9	5.7	5.0	3.3
GPB	corina	0.89	36.6	1	36.6		15.4	8.1	4.2	
GPB	omega_highestE	0.89	36.6	1	36.6		15.4	7.7	4.1	
GPB	omega_lowestE	0.89	36.6	1	36.6		15.4	7.7	4.1	

GPB	sybyl	0.90	36.6	1	36.6		15.0	8.1	4.1	
GPB	xtal	0.92	36.6	1	36.6	22.8	14.6	8.1	4.4	4.1
GR	corina	0.81	15.8	1	15.8		6.7	5.4	3.5	
GR	omega_highestE	0.78	17.1	1	17.1		5.7	5.3	3.1	
GR	omega_lowestE	0.78	17.1	1	17.1		5.9	5.3	3.1	
GR	sybyl	0.77	15.8	1	15.8		5.4	4.4	2.9	
GR	xtal	0.79	15.8	1	15.8	8.9	5.2	5.7	3.2	1.4
HIVPR	corina	0.32	1.9	1	1.9		0.8	0.6	0.5	
HIVPR	omega_highestE	0.40	3.2	3	0.0		2.3	1.5	1.1	
HIVPR	omega_lowestE	0.45	3.8	1	3.8		1.5	1.3	1.3	
HIVPR	sybyl	0.59	7.7	1	7.7		2.7	2.1	1.9	
HIVPR	xtal	0.56	5.8	1	5.8	3.7	2.3	1.5	1.2	2.2
HIVRT	corina	0.74	21.1	1	21.1		4.6	2.8	2.4	
HIVRT	omega_highestE	0.65	21.1	1	21.1		4.0	2.8	1.8	
HIVRT	omega_lowestE	0.70	21.1	1	21.1		5.1	2.5	1.8	
HIVRT	sybyl	0.66	21.1	1	21.1		4.6	2.5	1.8	
HIVRT	xtal	0.66	21.1	1	21.1	5.0	4.6	2.5	1.8	3.0
HMGA	corina	0.90	36.5	1	36.5		15.6	8.0	4.3	

HMGA	omega_highestE	0.97	36.5	1	36.5		17.4	9.2	4.7	
HMGA	omega_lowestE	0.93	36.5	1	36.5		17.4	8.9	4.4	
HMGA	sybyl	0.92	36.5	1	36.5		15.0	8.0	4.6	
HMGA	xtal	0.92	36.5	1	36.5	33.9	15.6	8.3	4.6	2.1
HSP90	corina	0.88	36.8	1	36.8		10.0	5.4	3.3	
HSP90	omega_highestE	0.75	36.8	1	36.8		9.2	4.6	2.3	
HSP90	omega_lowestE	0.68	36.8	1	36.8		9.2	4.6	2.3	
HSP90	sybyl	0.75	36.8	1	36.8		9.2	4.6	2.9	
HSP90	xtal	0.66	36.8	1	36.8	8.6	9.2	4.6	2.3	2.0
INHA	corina	0.66	30.8	1	30.8		7.8	4.1	2.5	
INHA	omega_highestE	0.70	35.5	1	35.5		10.6	5.3	2.8	
INHA	omega_lowestE	0.73	36.7	1	36.7		10.1	5.3	2.8	
INHA	sybyl	0.64	10.7	1	10.7		5.2	3.3	2.0	
INHA	xtal	0.72	36.7	1	36.7	0.0	9.9	5.1	2.8	0.3
MR	corina	0.85	29.3	1	29.3		16.3	8.0	4.0	
MR	omega_highestE	0.87	29.3	1	29.3		16.3	8.0	4.0	
MR	omega_lowestE	0.87	36.7	1	36.7		16.3	8.0	4.0	
MR	sybyl	0.86	30.0	2	29.3		16.3	8.0	4.0	

MR	xtal	0.87	36.7	1	36.7	46.2	16.3	8.0	4.0	3.7
NA	corina	0.88	30.2	1	30.2		13.2	7.8	4.2	
NA	omega_highestE	0.93	30.2	1	30.2		14.4	8.6	4.4	
NA	omega_lowestE	0.91	30.2	1	30.2		14.0	7.6	4.3	
NA	sybyl	0.87	32.3	1	32.3		14.0	7.4	3.9	
NA	xtal	0.97	32.3	1	32.3	20.2	18.5	9.6	4.8	3.3
P38	corina	0.45	10.2	1	10.2		2.7	1.6	1.2	
P38	omega_highestE	0.47	9.0	1	9.0		2.3	1.3	1.1	
P38	omega_lowestE	0.46	13.3	1	13.3		2.9	1.5	1.1	
P38	sybyl	0.47	10.2	1	10.2		2.7	1.8	1.3	
P38	xtal	0.52	10.2	1	10.2	2.1	2.8	2.0	1.4	2.4
PARP	corina	0.43	3.1	1	3.1		0.6	0.3	0.3	
PARP	omega_highestE	0.38	3.1	1	3.1		0.6	0.3	0.2	
PARP	omega_lowestE	0.58	3.7	10	3.1		1.8	3.7	2.4	
PARP	sybyl	0.61	3.7	10	3.1		1.8	3.7	2.4	
PARP	xtal	0.58	4.2	8	3.1	6.0	3.1	3.7	2.4	3.6
PDE5	corina	0.43	18.2	1	18.2		4.8	2.8	1.4	
PDE5	omega_highestE	0.49	22.3	1	22.3		5.5	2.8	1.4	

PDE5	omega_lowestE	0.51	20.3	1	20.3		4.8	2.6	1.5	
PDE5	sybyl	0.49	12.2	1	12.2		2.4	1.6	1.2	
PDE5	xtal	0.53	16.2	1	16.2	11.8	4.0	2.4	1.6	2.3
PDGFRB	corina	0.30	7.7	1	7.7		1.5	0.8	0.5	
PDGFRB	omega_highestE	0.33	7.7	1	7.7		1.5	0.8	0.6	
PDGFRB	omega_lowestE	0.23	7.7	1	7.7		1.7	1.0	0.6	
PDGFRB	sybyl	0.34	7.7	1	7.7		1.7	1.1	0.6	
PDGFRB	xtal	0.34	7.7	1	7.7	0.0	1.7	1.1	0.6	0.6
PNP	corina	0.90	17.1	4	16.1		16.9	8.9	4.4	
PNP	omega_highestE	0.91	21.5	3	16.1		17.7	9.3	4.6	
PNP	omega_lowestE	0.90	16.1	1	16.1		12.9	9.3	4.6	
PNP	sybyl	0.86	16.1	1	16.1		6.4	7.3	4.4	
PNP	xtal	0.91	22.2	2	20.2	31.7	16.9	9.3	4.6	4.4
PPAR_GAMMA	corina	0.90	21.6	1	21.6		13.1	8.2	4.2	
PPAR_GAMMA	omega_highestE	0.94	25.6	2	20.3		17.6	9.0	4.6	
PPAR_GAMMA	omega_lowestE	0.94	30.6	2	30.5		18.6	9.3	4.6	
PPAR_GAMMA	sybyl	0.94	25.0	2	20.3		16.8	9.0	4.6	
PPAR_GAMMA	xtal	0.92	21.6	1	21.6	0.0	15.8	8.3	4.4	0.0

PR	corina	0.61	4.1	1	4.1		1.5	1.9	1.3	
PR	omega_highestE	0.70	8.2	1	8.2		3.8	2.6	1.9	
PR	omega_lowestE	0.66	5.1	3	4.1		3.0	2.2	1.9	
PR	sybyl	0.67	16.4	1	16.4		5.3	2.6	2.0	
PR	xtal	0.67	16.4	1	16.4	0.0	3.0	2.6	1.5	0.0
RXR_ALPHA	corina	0.91	33.8	2	31.2		17.2	8.6	4.3	
RXR_ALPHA	omega_highestE	0.91	31.2	2	26.0		16.2	8.6	4.3	
RXR_ALPHA	omega_lowestE	0.92	33.8	2	31.2		17.2	8.6	4.3	
RXR_ALPHA	sybyl	0.94	31.2	1	31.2		17.2	8.6	4.3	
RXR_ALPHA	xtal	0.96	31.2	2	26.0	24.8	17.2	8.6	4.3	2.2
SAHH	corina	0.98	32.8	1	32.8		17.1	9.4	4.7	
SAHH	omega_highestE	0.97	20.6	3	16.4		15.9	8.2	4.9	
SAHH	omega_lowestE	0.98	32.8	1	32.8		17.1	9.4	5.0	
SAHH	sybyl	0.98	21.7	3	13.1		16.5	9.4	5.0	
SAHH	xtal	0.97	26.3	1	26.3	78.0	14.7	9.4	4.9	5.0
SRC	corina	0.37	7.2	1	7.2		2.7	1.9	1.3	
SRC	omega_highestE	0.33	6.5	1	6.5		2.7	1.6	1.1	
SRC	omega_lowestE	0.30	5.2	1	5.2		2.1	1.3	0.7	

SRC	sybyl	0.34	3.9	1	3.9		2.1	1.2	0.7	
SRC	xtal	0.38	2.3	2	2.0	1.2	1.6	1.0	0.8	1.5
THROMBIN	corina	0.35	3.7	1	3.7		1.8	1.1	0.5	
THROMBIN	omega_highestE	0.39	3.7	1	3.7		1.5	0.7	0.5	
THROMBIN	omega_lowestE	0.41	3.7	2	1.8		1.5	1.1	0.8	
THROMBIN	sybyl	0.70	3.7	1	3.7		1.1	1.5	1.7	
THROMBIN	xtal	0.66	1.8	1	1.8	13.7	1.1	0.7	1.5	2.9
TK	corina	0.84	5.3	6	0.0		4.6	4.1	4.1	
TK	omega_highestE	0.85	18.3	1	18.3		11.0	5.5	3.2	
TK	omega_lowestE	0.89	18.3	1	18.3		10.1	6.0	3.6	
TK	sybyl	0.86	9.2	2	4.6		6.4	5.0	3.6	
TK	xtal	0.86	13.7	1	13.7	54.0	4.6	6.0	3.6	5.0
TRYPSIN	corina	0.84	4.1	8	0.0		3.5	3.8	3.9	
TRYPSIN	omega_highestE	0.78	5.0	3	0.0		4.0	3.5	2.4	
TRYPSIN	omega_lowestE	0.78	5.0	3	0.0		4.0	3.5	2.4	
TRYPSIN	sybyl	0.73	2.6	1	2.6		0.5	1.0	1.4	
TRYPSIN	xtal	0.78	3.4	16	0.0	22.5	0.0	2.8	3.3	2.6
VEGFR2	corina	0.48	1.2	12	0.0		0.3	1.1	1.0	

VEGFR2	omega_highestE	0.47	1.1	15	0.0		0.3	0.9	0.9	
VEGFR2	omega_lowestE	0.46	1.0	91	0.0		0.0	0.5	0.8	
VEGFR2	sybyl	0.46	1.4	1	1.4		0.5	0.7	0.7	
VEGFR2	xtal	0.43	1.0	84	0.0	1.3	0.3	0.4	0.6	1.4

^a Benchmark values are reported for ROCS in direct relation to the results published by Huang et al. for the DOCK algorithm.

^b Maximum enrichment factor obtained during virtual screening; calculated for each percentage of the rank-ordered hit list.

^c Percentage of the rank-ordered hit list where ROCS obtains highest enrichment.