

Prime

cutoff

0.95 kcal/mol

1.77 kcal/mol

2.72 kcal/mol

axitinib

		Prediction	
		s	r
Experiment	S	20	6
	R	0	0

		Prediction	
		s	r
Experiment	S	23	3
	R	0	0

		Prediction	
		s	r
Experiment	S	24	2
	R	0	0

bosutinib

		Prediction	
		s	r
Experiment	S	13	4
	R	1	3

		Prediction	
		s	r
Experiment	S	16	4
	R	0	1

		Prediction	
		s	r
Experiment	S	16	5
	R	0	0

dasatinib

		Prediction	
		s	r
Experiment	S	11	2
	R	2	6

		Prediction	
		s	r
Experiment	S	14	2
	R	1	4

		Prediction	
		s	r
Experiment	S	17	3
	R	1	0

imatinib

		Prediction	
		s	r
Experiment	S	7	7
	R	5	2

		Prediction	
		s	r
Experiment	S	10	7
	R	3	1

		Prediction	
		s	r
Experiment	S	18	2
	R	0	0

nilotinib

		Prediction	
		s	r
Experiment	S	8	8
	R	4	1

		Prediction	
		s	r
Experiment	S	11	7
	R	2	1

		Prediction	
		s	r
Experiment	S	14	6
	R	0	1

ponatinib

		Prediction	
		s	r
Experiment	S	14	6
	R	1	0

		Prediction	
		s	r
Experiment	S	18	3
	R	0	0

		Prediction	
		s	r
Experiment	S	21	0
	R	0	0

FEP+

0.95 kcal/mol

1.77 kcal/mol

2.72 kcal/mol

		Prediction	
		s	r
Experiment	S	20	6
	R	0	0

		Prediction	
		s	r
Experiment	S	23	3
	R	0	0

		Prediction	
		s	r
Experiment	S	26	0
	R	0	0

		Prediction	
		s	r
Experiment	S	13	4
	R	2	2

		Prediction	
		s	r
Experiment	S	18	1
	R	2	0

		Prediction	
		s	r
Experiment	S	21	0
	R	0	0

		Prediction	
		s	r
Experiment	S	11	2
	R	3	5

		Prediction	
		s	r
Experiment	S	16	0
	R	1	4

		Prediction	
		s	r
Experiment	S	19	1
	R	0	1

		Prediction	
		s	r
Experiment	S	13	1
	R	4	3

		Prediction	
		s	r
Experiment	S	17	0
	R	2	2

		Prediction	
		s	r
Experiment	S	19	1
	R	0	0

		Prediction	
		s	r
Experiment	S	10	6
	R	3	2

		Prediction	
		s	r
Experiment	S	18	0
	R	1	2

		Prediction	
		s	r
Experiment	S	20	0
	R	0	1

		Prediction	
		s	r
Experiment	S	17	3
	R	1	0

		Prediction	
		s	r
Experiment	S	21	0
	R	0	0

		Prediction	
		s	r
Experiment	S	21	0
	R	0	0