~/report/zope/2006-06/

Trypsin model 1 with 41 ligands (~/combine2go/data/trypsin/model1_010606)

file	command	#	var0	var	LV	r2	q2 (LOO)	D/FFD	var	LV	r2	q2 (LOO)	SDEP
output.dat	all minimized structures	48											
active.dat	with Ki; no double	41	452	210	3 4	0.85 0.92	0.71 0.65	3	97	4	0.88	0.74	1.27
active.dat	with Ki; no double	41	452	210	3 4	0.85 0.92	0.71 0.65	5					
select.dat	structures 1-20 of active.dat	20	452	206	4	0.86	0.56	4	90	3	0.82	0.65	0.86
select1.dat	structures 21-41 of active.dat	21	452	206	7	0.99	0.80	7	100	3	0.92	0.79	1.35

model 1	command	LV	prediction xray	#	SDEP	prediction docking	#	SDEP
active.dat	with Ki; no double	5	active.dat	29	1.57 (1.34@LV3)		510	2.38
select.dat	structures 1-20 of active.dat	3				select1.dat	21	2.33
select1.dat	structures 21-41 of active.dat	7				select.dat	20	1.97

Trypsin model 1 with 43 ligands without calcium and chloride (~/combine2go/data/trypsin/model1_del_ions010606)

file	command	#	var0	var	LV	r2	q2 (LOO)	D/FFD	var	LV	r2	q2 (LOO)	SDEP
active.dat	with Ki	43	448	210	3	0.85	0.72	3	100	3	0.87	0.77	1.26
active-nodbl.dat	with Ki; no double	42	448	210	3	0.84	0.71	3	98	3	0.87	0.74	1.27

model 1	command	LV	prediction xray	#	SDEP	prediction docking	#	SDEP
active.dat	with Ki	3	active.dat	43	0.94	trypsin_all_010606_del_ion.dat	3370	
active-nodbl.dat	with Ki; no double							