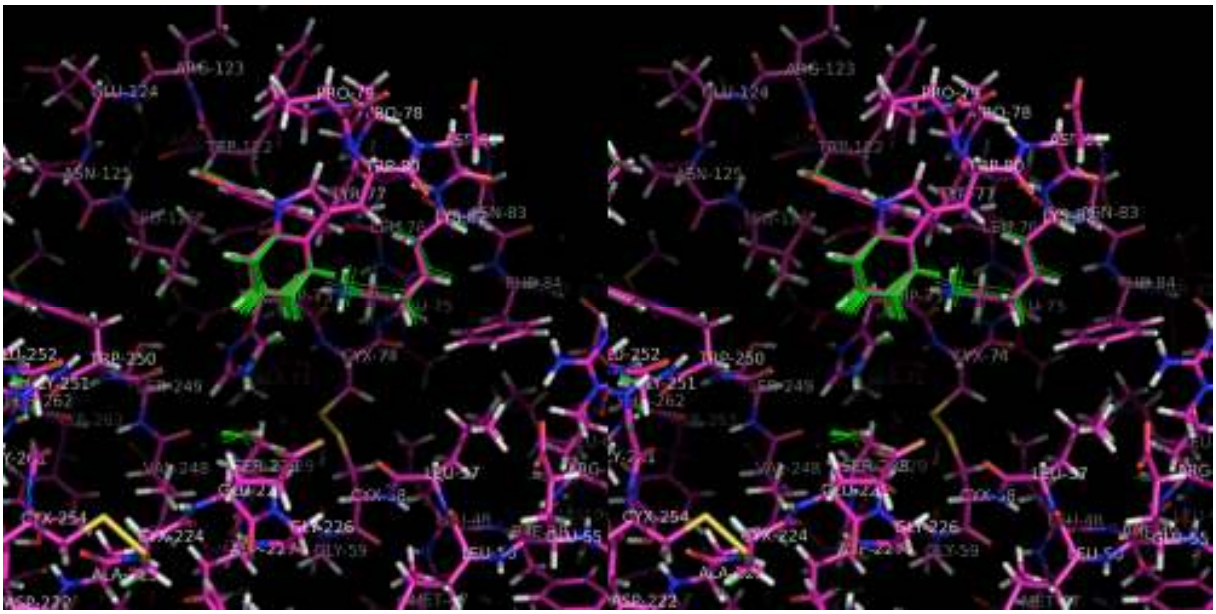
01.06.2006

~/report/zope/2006-05/

Analysis of the thrombin model2_260406, Combine model output-A91-A82

thrombin model 2

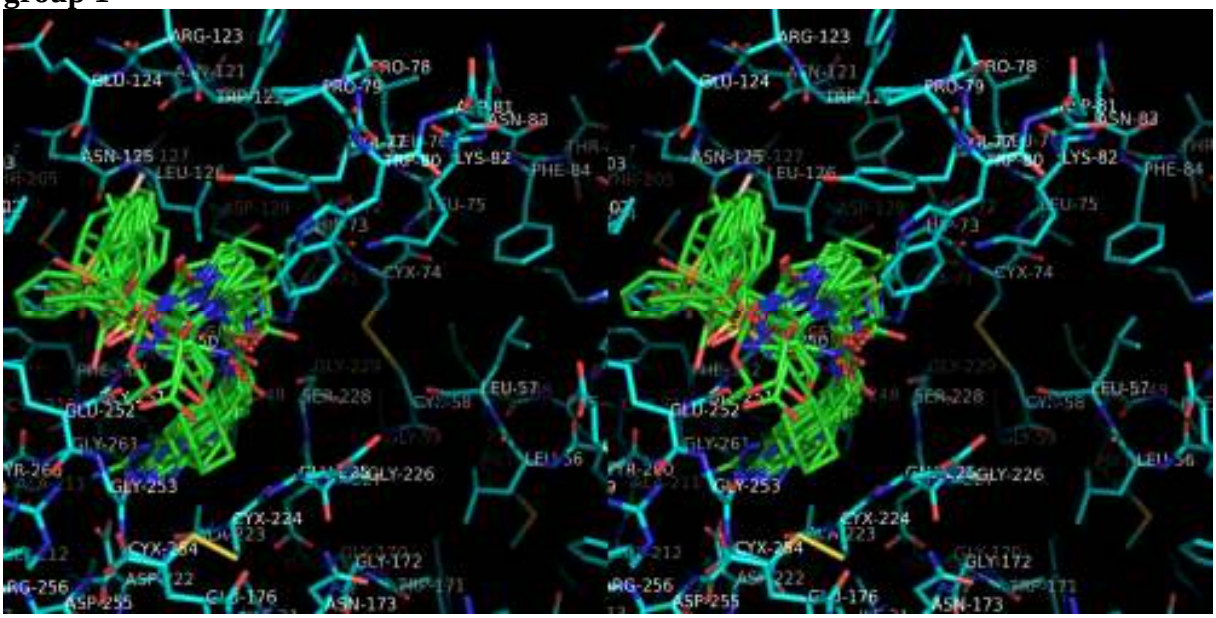


thrombin_model2_min_shift_Y80_K82.png
pink: thrombin model 2
green: 29 receptor conformations of minimization with different ligands.
It can be seen that Lys82 and Tyr80 moves a lot during minimization.

The training set is falling into two main groups:

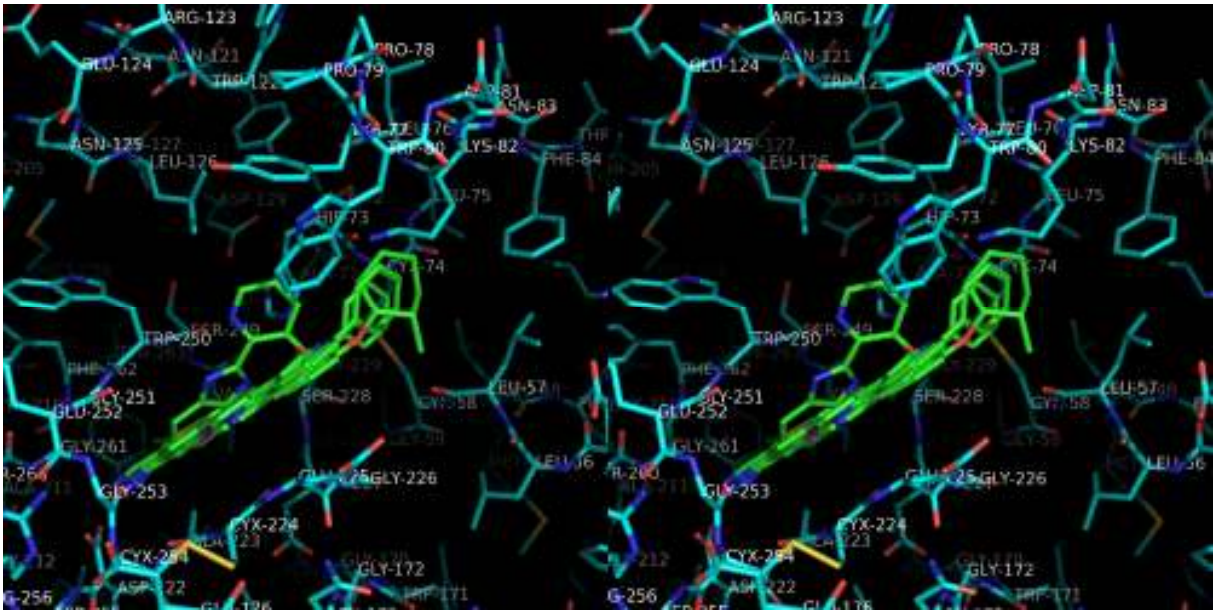
ID	residue	group	netcharge	acceptors	donors	weight	thrombin	PDB_thrombin
347	**A87**	**1**	1	4	4	420.5	0.281838293	**1ae8**
348	**A88**	**1**	1	3	3	335.4	16.21810097	**1afe**
313	**A45**	**1**	1	5	4	468.6	0.147910839	**1bhx**
314	**A46**	**1**	1	6	5	504.6	0.07943	**1bmm**
315	**A48**	**1**	1	6	5	530.6	0.00371535	**1bmn**
349	**A89**	**1**	1	4	3	582.5	0.00004365	**1c4u**
350	**A90**	**1**	1	4	3	527.6	0.000016218	**1c4v**
322	**A62**	**1**	1	6	2	525.6	1.122	**1d6w**
323	**A63**	**1**	1	4	2	475.6	0.0008	**1d9i**
316	**A47**	**1**	1	3	4	522.6	0.00675	**1ets_1dwd**
332	**A72**	**1**	0	7	5	436.5	0.004	**1k21**
333	**A73**	**1**	0	6	5	429.5	0.002	**1k22**
328	**A68**	**1**	1	3	2	496.4	0.003	**1ta2**
354	**A94**	**1**	1	3	3	387.5	0.00501187	**1tom**
344	**A84**	**1**	2	5	6	538.7	40.73802778	**7kme**
288	**A19**	**2**	1	1	2	303.1	20.4	**1c5n**
291	**A22**	**2**	1	5	4	254.3	45	**1ghv**
10	**A12**	**2**	1	4	4	253.3	63	**1ghw_1ghx**
13	**A09**	**2**	1	5	4	254.3	8.5	**1ghy**
2	**A18**	**2**	1	3	4	362.8	85	**1gj4**
20	**A14**	**2**	1	4	4	329.4	11	**1gj5**
21	**A04**	**2**	1	3	4	328.4	0.76	**1o2g**
8	**A17**	**2**	1	6	4	383.4	11	**1o5g**
353	**A93**	**3**	1	6	4	614.8	1.202264435	**1a4w**
346	**A86**	**3**	0	5	5	508.6	0.00398	**1dwc**
352	**A92**	**3**	1	4	4	503.7	0.1	**1fpc**

group 1

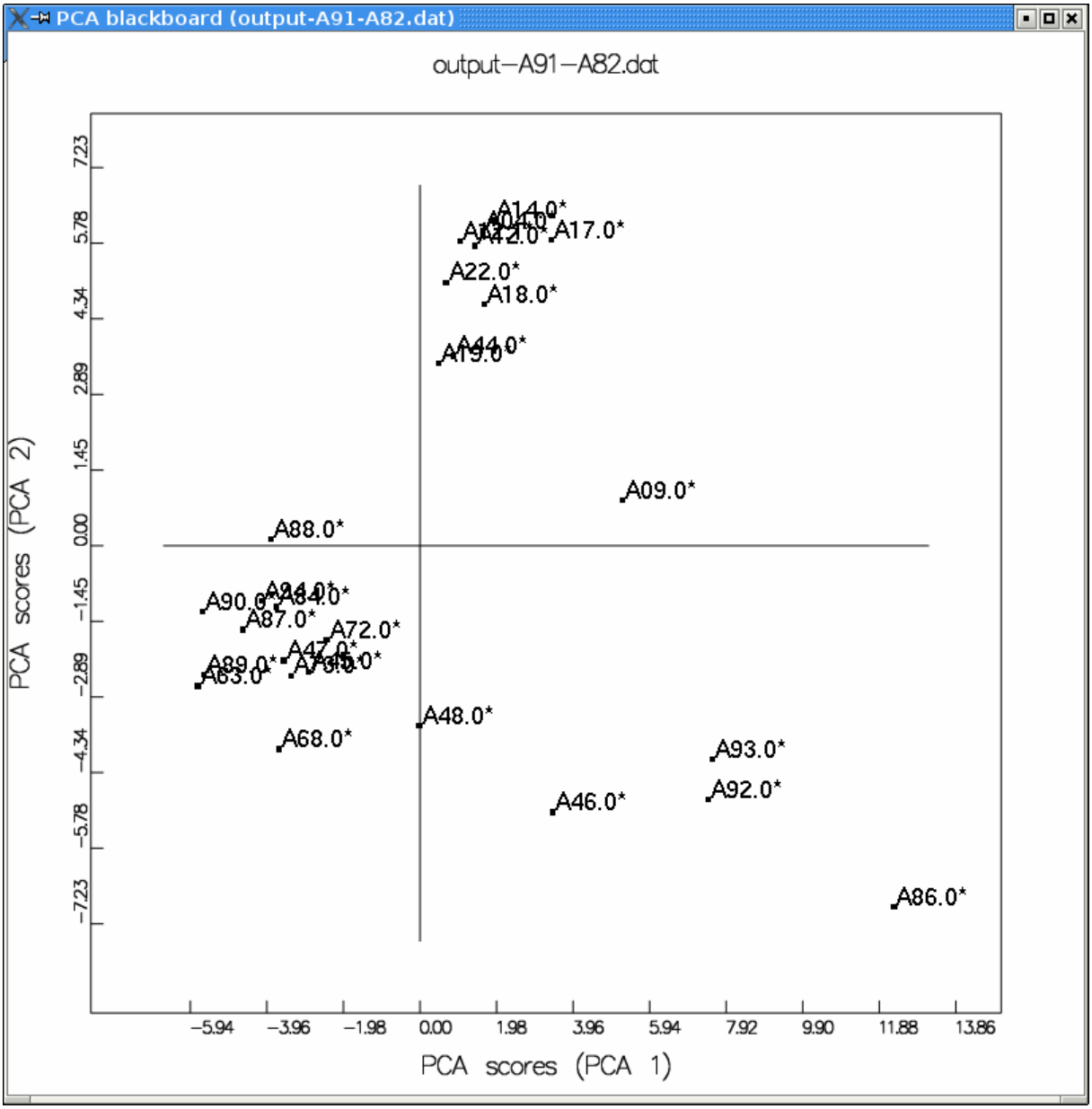


thrombin-model2_group1.png

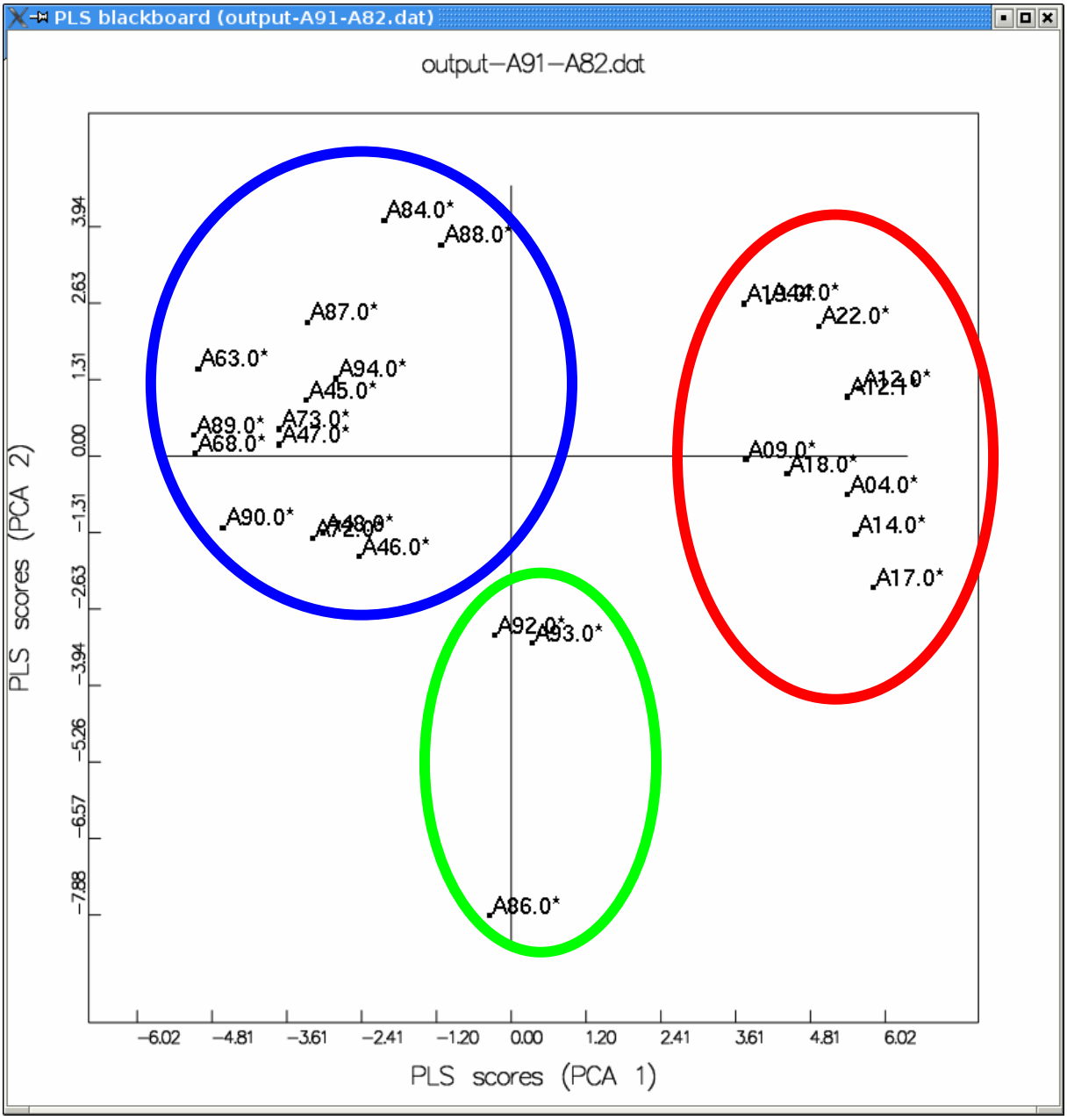
group 2



thrombin-model2_group2.png



PCA_output-A91-A82.png



PLS_output-A91-A82.png

Building different COMBINE models

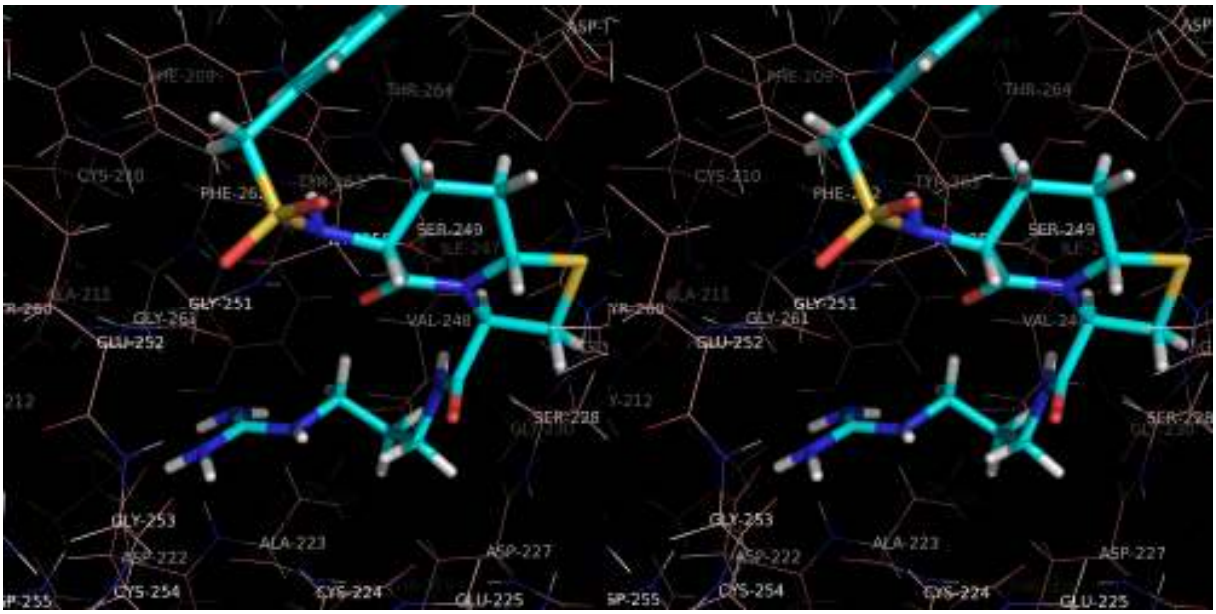
Problems with following ligands:
A82
A68
A48
A73
A94

checked_Xray.xls

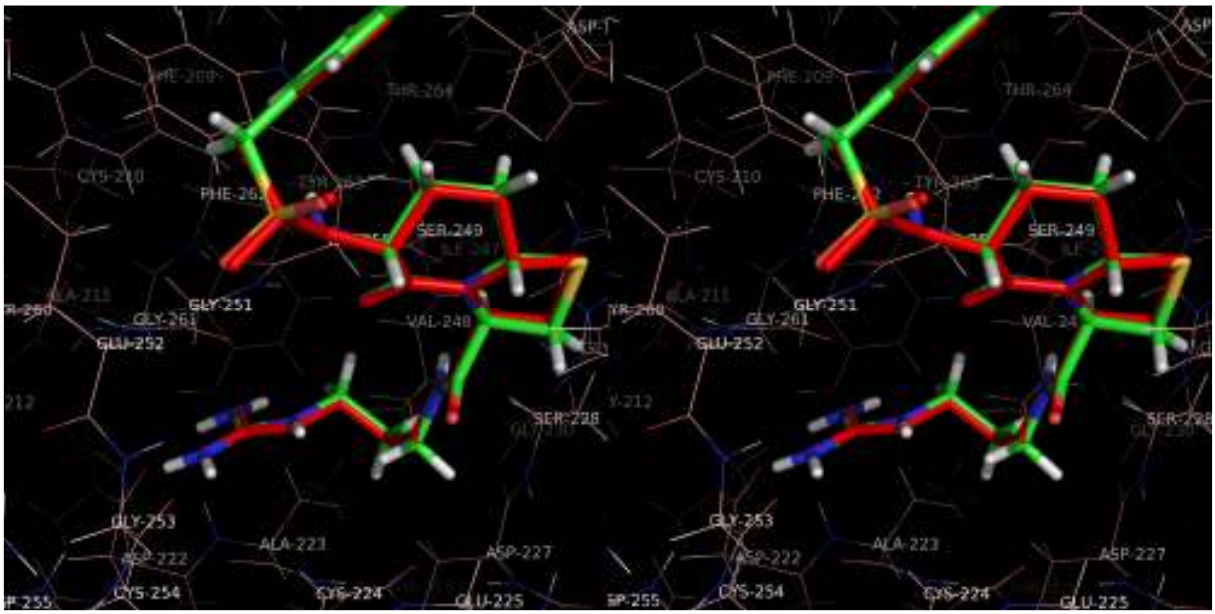
ID	residue	netcharge	thrombin	PDB_thrombin	
21	**A04**	1	0.76	**1o2g**	OK
13	**A09**	1	8.5	**1ghy**	Benzimidazole 5-ring end carbon not flat in minimized structure, should be flat acc. To CSD
10	**A12**	1	63	**1ghw_1ghx**	OK
20	**A14**	1	11	**1gj5**	OK
8	**A17**	1	11	**1o5g**	OK
2	**A18**	1	85	**1gj4**	OK
288	**A19**	1	20.4	**1c5n**	OK
289	**A20**	1	29	**1c5o**	not available
291	**A22**	1	45	**1ghv**	OK
312	**A44**	1	10	**1bcu**	OK
313	**A45**	1	0.14791	**1bhx**	sulphone amide and guanidine nitrogens not flat in minimized
314	**A46**	1	0.07943	**1bmm**	sulphone amide & guanidine nitrogens not flat
316	**A47**	1	0.00675	**1ets_1dwd**	not flat sulphone amide in minimized
315	**A48**	1	0.00372	**1bmn**	sulphone amide & guanidine nitrogens not flat
317	**A49**	1	2.3	**1c1u**	not available
318	**A58**	2	3.7	**1c1v**	not available
322	**A62**	1	1.122	**1d6w**	A62 not available
323	**A63**	1	0.0008	**1d9i**	X-ray not quite flat amide, minimized not flat 5-ring, look up!!
328	**A68**	1	0.003	**1ta2**	OK
329	**A69**	1	0.00074	**1ta6**	A69 nto available
332	**A72**	0	0.004	**1k21**	guanidino group not flat
333	**A73**	0	0.002	**1k22**	OK
342	**A82**	1	4.17	**1qbv**	OK
344	**A84**	2	40.738	**7kme**	OK
346	**A86**	0	0.00398	**1dwc**	X-ray not flat carboxylate!! Minimized not flat guanidine, sulphone amide, P3 nitrogen
347	**A87**	1	0.28184	**1ae8**	OK
348	**A88**	1	16.2181	**1afe**	5-ring flat in X-ray structure, not in minimized
349	**A89**	1	4.4E-05	**1c4u**	OK
350	**A90**	1	1.6E-05	**1c4v**	5-ring flat in X-ray, not in minimized. Amidine nitrogen
351	**A91**	1	0.01202	**1c4y**	5-ring flat in X-ray, not in minimized. end nitrogen
352	**A92**	1	0.1	**1fpc**	P2 amide nitrogen in sp2 in minimized, not flat in X-ray but X-ray is probably wrong
353	**A93**	1	1.20226	**1a4w**	OK
354	**A94**	1	0.00501	**1tom**	positive amine nitrogen, giving total charge +2??; pKa -9.47

The minimization for some of the ligands resulted in wrong geometries even with supplying bond information by SD file. The reason for this is the different ways of generating ligand.pdb and ligand.sdf. The pdb-file was retrieved from ProteinDataBase and the SDF was sketched in ChemDraw and subsequently hydrogens and 3D coordinates were generated in CORINA. This leads to different atom names and a different order of the atoms in the file.
For example, A45 (1bhx) showed a non planar guanidine group (A45_min-unsort.png), but if the atoms of the PDB and SDF file were ordered in the same way, the minimization gave a planar guanidine group very similar to the X-ray structure (A45_xray_min-sort.png).

The question is now: **How to sort the atoms of the PDB in the same way like in the SD file?** This is also necessary for calculating RMSD between X-ray structure and the docking solutions.



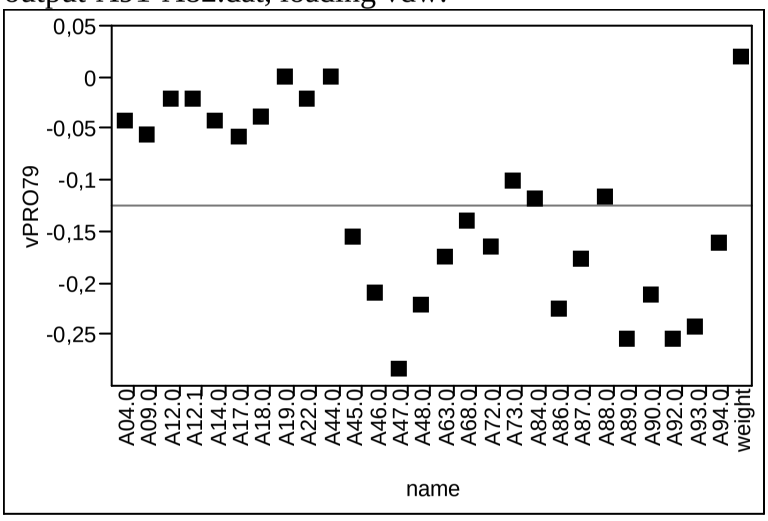
A45_min-unsort.png
Minimized A45 without sorting atoms.



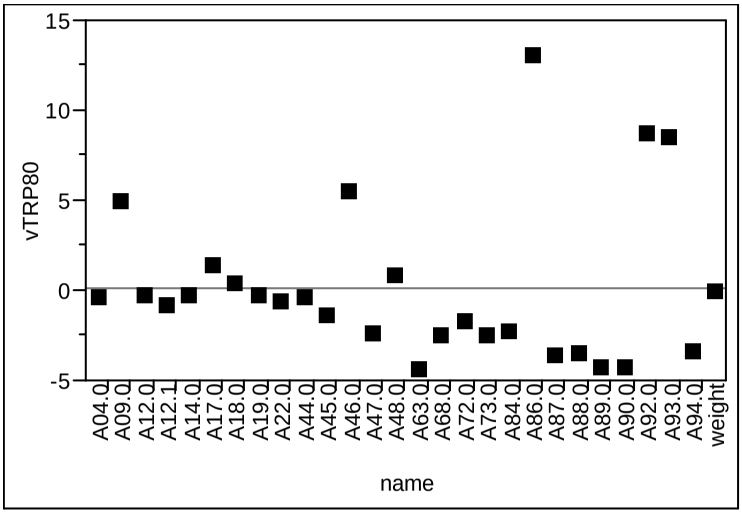
A45_xray_min-sort.png
red: X-ray structure of A45; green: Minimized A45 with sorting atoms.

See data in /scratch/mcm/henricsn/test-antechamber/ and in /zope/2006-05/ for images:
For some reasons it works even without supplying a SD file resulting in the same geometry like supplying bonds in the correct order. This is inconsistent to early results where no charges could be determined.
Model 3 is calculated without extra bond information from SD file.

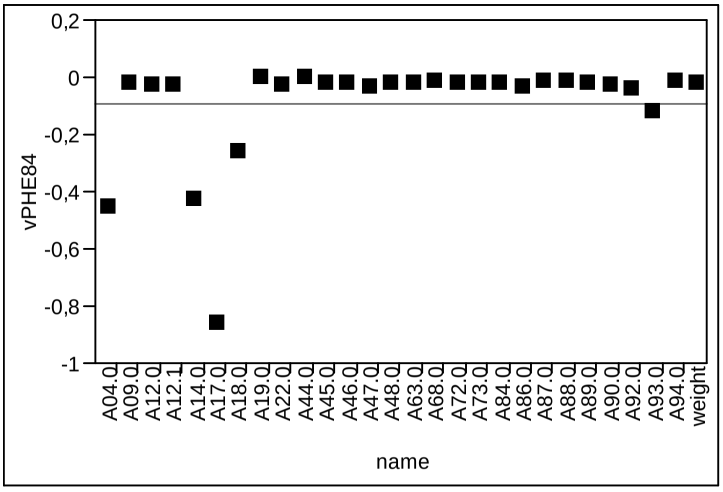
output-A91-A82.dat, loading vdw:



separated into two groups
partial weight: +0.01871

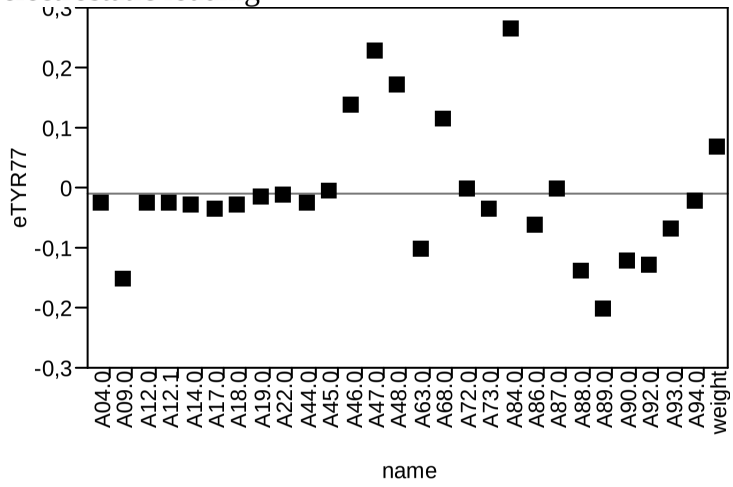


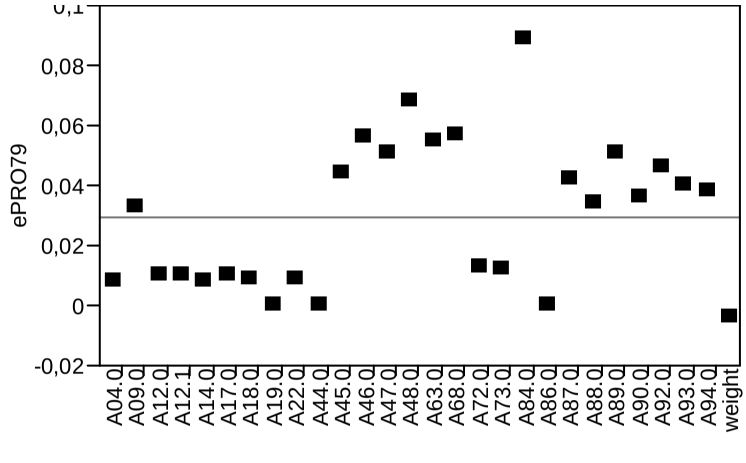
A86 strong positive
partial weight -0.07955

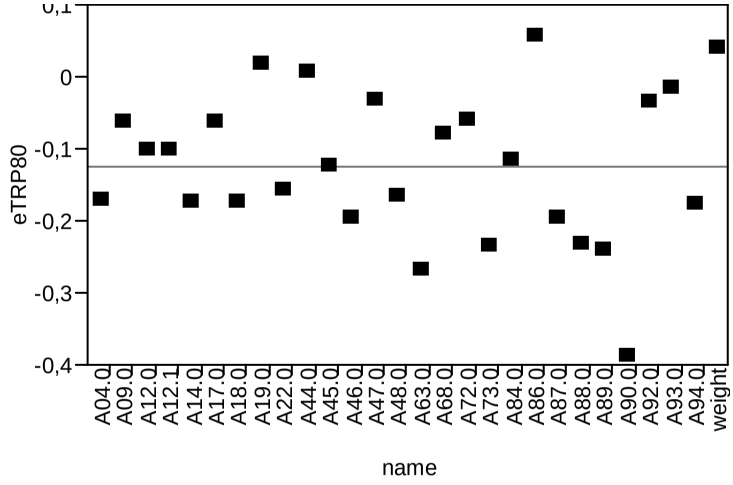


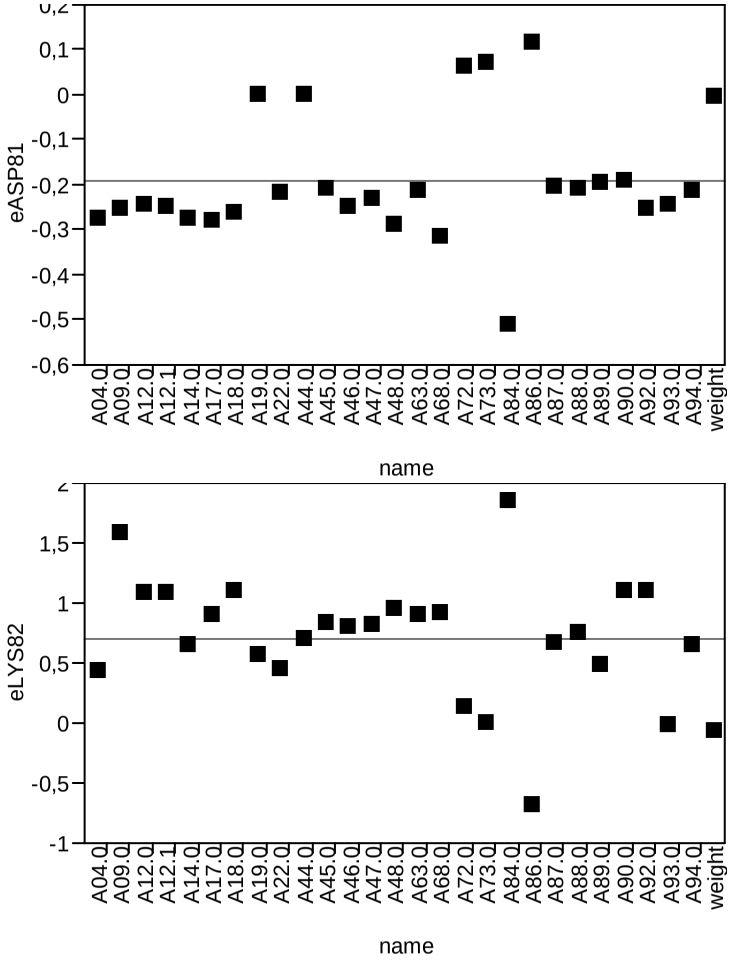
A17; A04, A14, A18 strong negative
partial weight 0

electrostatic loading

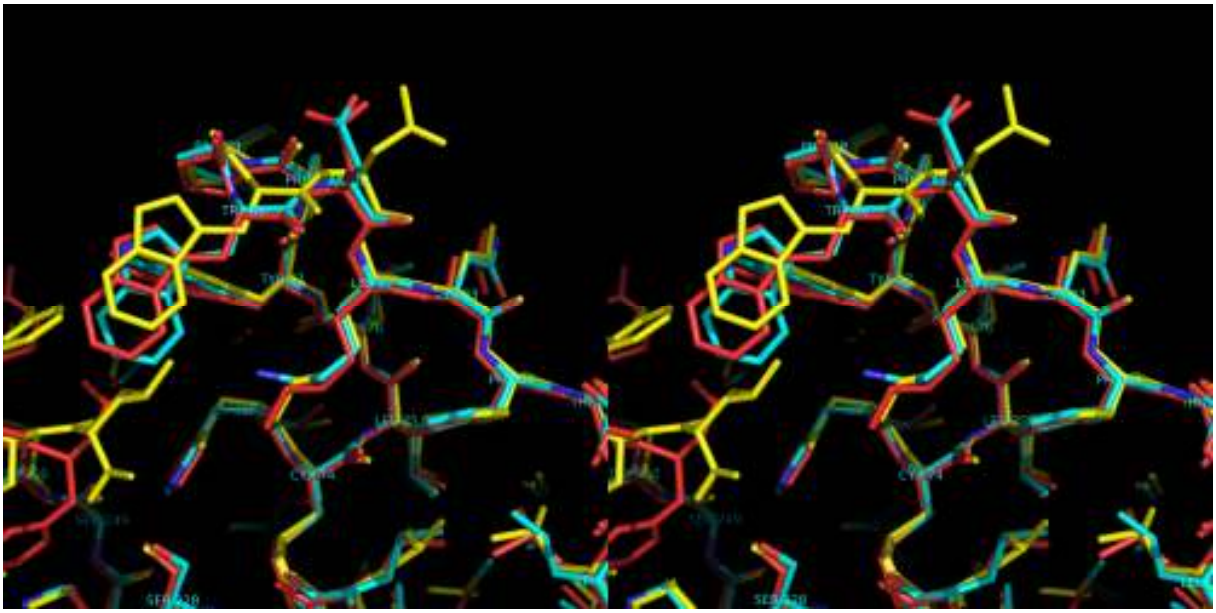




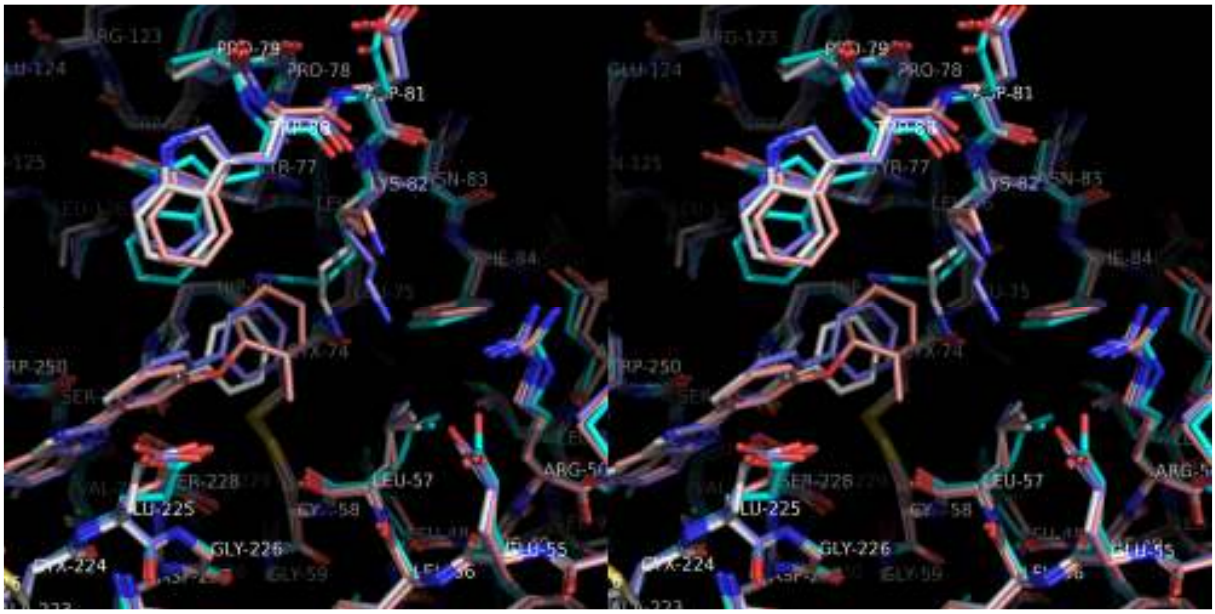



0,2
0,1
0
-0,1
-0,2
-0,3
-0,4
-0,5
-0,6
eASP81
A04.0
A09.0
A12.0
A12.1
A14.0
A17.0
A18.0
A19.0
A22.0
A44.0
A45.0
A46.0
A47.0
A48.0
A63.0
A68.0
A72.0
A73.0
A84.0
A86.0
A87.0
A88.0
A89.0
A90.0
A92.0
A93.0
A94.0
weight
name

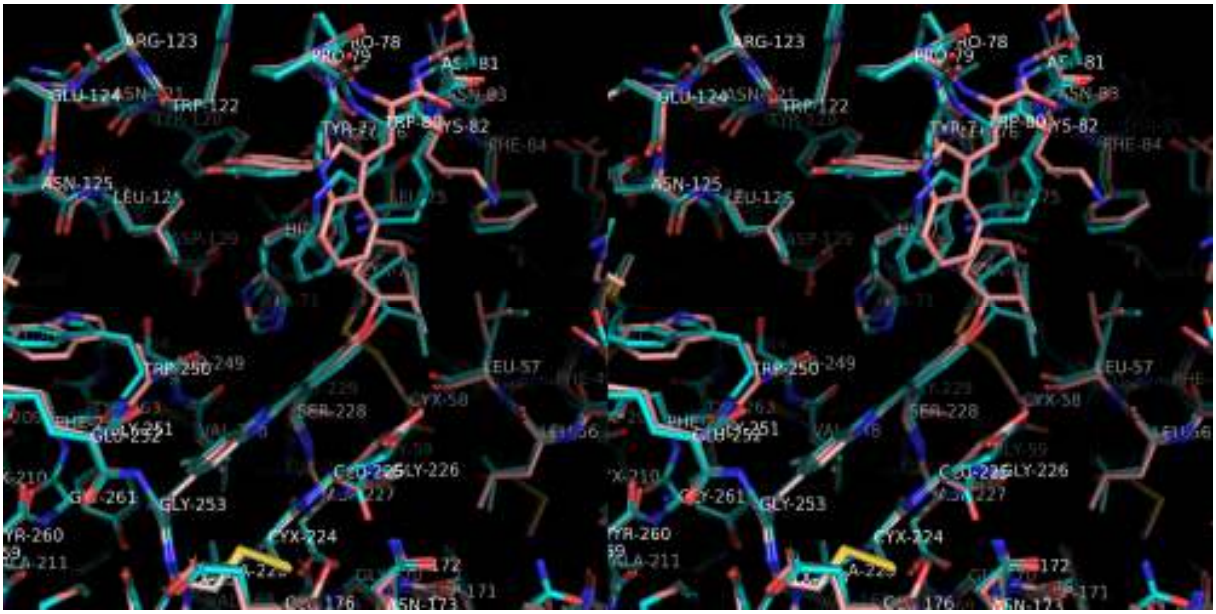
2
1,5
1
0,5
0
-0,5
-1
eLYS82
A04.0
A09.0
A12.0
A12.1
A14.0
A17.0
A18.0
A19.0
A22.0
A44.0
A45.0
A46.0
A47.0
A48.0
A63.0
A68.0
A72.0
A73.0
A84.0
A86.0
A87.0
A88.0
A89.0
A90.0
A92.0
A93.0
A94.0
weight
name



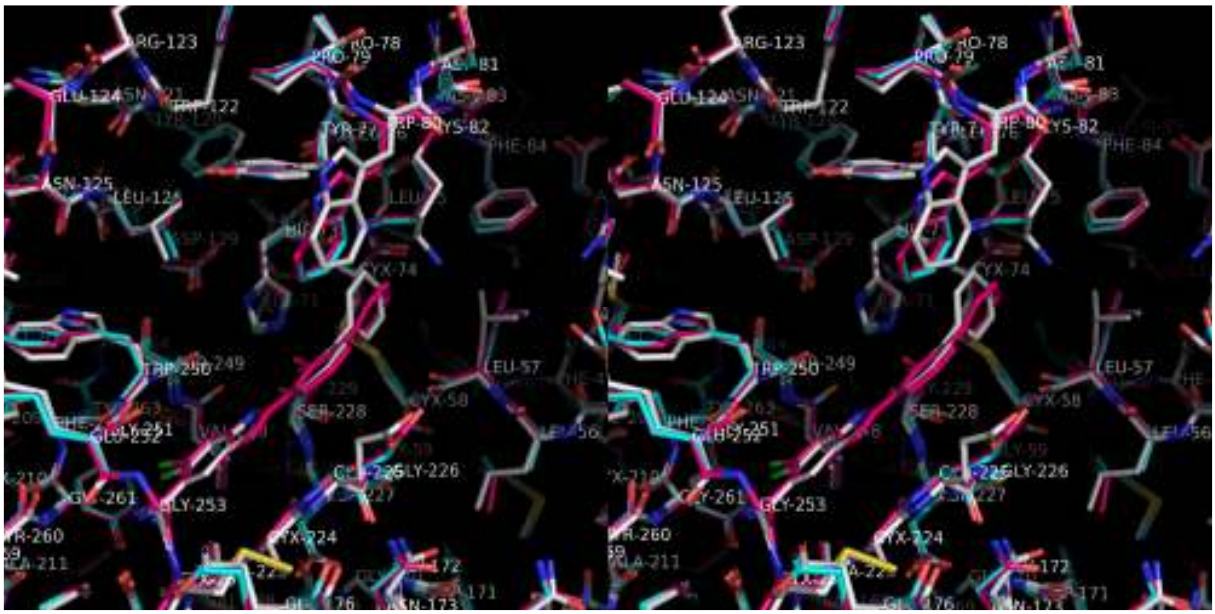
thrombin-model2_A86_A84.png
Trp80, Asp81 Lys82 are showing large differences between A86 and A84
cyan: thrombin-model2_260406 (1c4u)
red: 7kme (A84)
yellow: 1dwc (A86)
see vTRP80 and eLys82



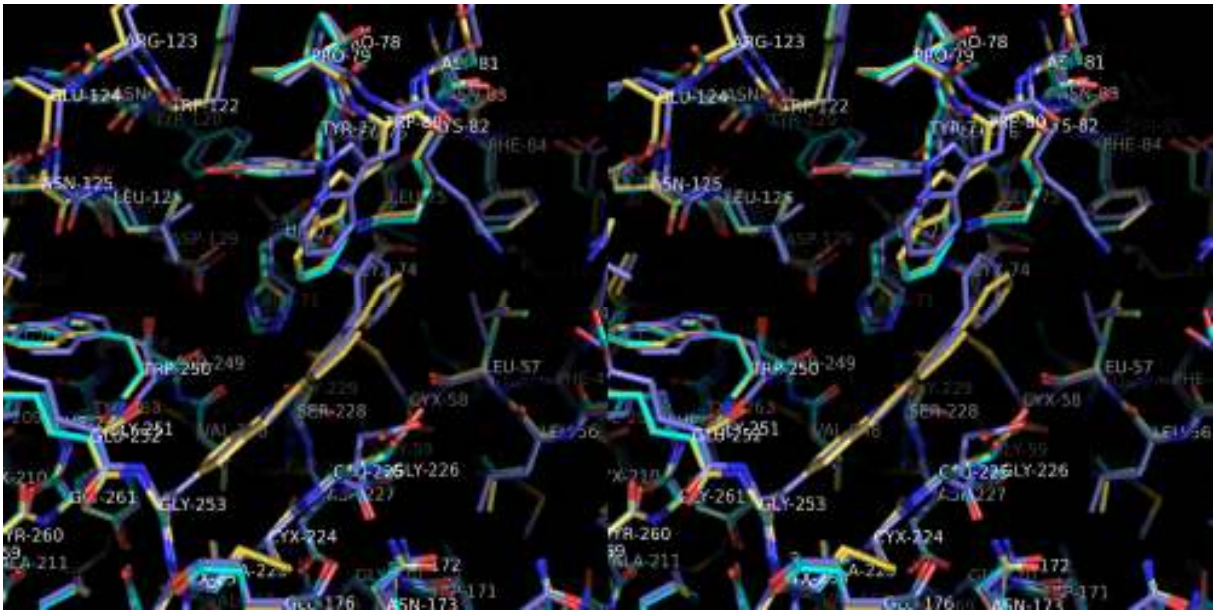
thrombin-model2_A17_A18_A04-group2.png
Lys82 and Trp80 are showing large differences to thrombin model2 (1c4u). These residues clashes with ligands A17 (1o5g, red), A18 (1gj4, white) and A04 (1o2g, blue) of group 2.
cyan: thrombin-model2_260406 (1c4u)
red: xray structure of A17 (1o5g, red)
white: xray structure of A18 (1gj4, white)
blue: xray structure of A04 (1o2g, blue)



thrombin-model2_A17-min-xray.png
The ligand, and Lys82 show movements during minimization.
cyan: thrombin-model2_260406 (1c4u)
green: minimized thrombin model
red: xray structure of A17 (1o5g, red)



thrombin-model2_A18-min-xray.png
The ligand shows movements during minimization.
cyan: thrombin-model2_260406 (1c4u)
red: minimized thrombin model
white: xray structure of A18 (1gj4, white)



thrombin-model2_A04-min-xray.png
The ligand, Trp80 and Lys82 show movements during minimization.
cyan: thrombin-model2_260406 (1c4u)
yellow: minimized thrombin model
blue: xray structure of A04 (1o2g, blue)

Conclusion

Lys82 should be moved

Inspection of docking solutions of model 2

The docking solutions of the ligands, which were used as a training set were manually inspected and compared to xray structures. The docking solutions were categorized into three groups:

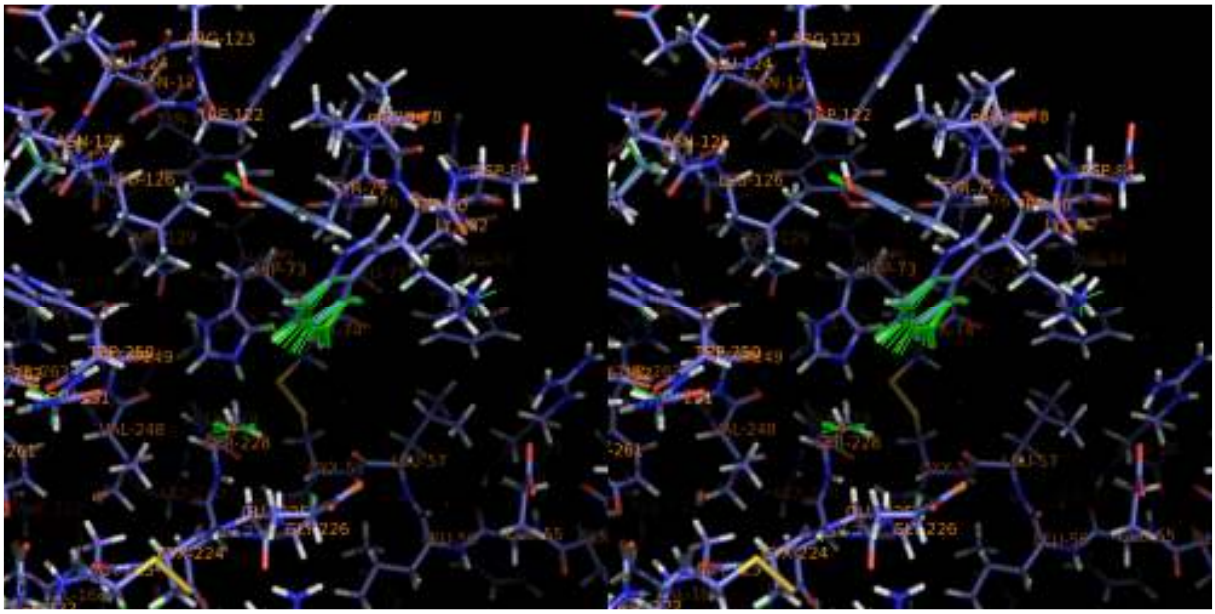
1. good docking pose
2. not correct binding mode, but the amidino/guanidine group shows more or less the correct orientation.
3. totally wrong docking solution

Unfortunately, I couldn't find any tool for calculating reliable RMSD between the ligand.pdb-file of xray structure and the corresponding sketched SD file. In both files the atom names the order of the atoms in the file were arbitrary chosen, so the atoms couldn't matched onto each other.

thrombin model 3

19.05.2006

Model 3 based on the minimized structure of model 2 and Lys82 was rotated by Pymol to create a more open active site. A minimization together with ligand A89 (1c4u) was done and the ligand was removed afterwards.
The minimization of the 29 structures of the training set showed almost no shift in Lys82 but large shifts in Tyr80. May be Tyr80 should be moved, too. Because of the high side and main chain flexibility of Tyr80 and Lys82 it could be interesting not to use the corresponding X values in COMBINE model.



thrombin_model3_min_shift_Y80_K82.png
blue: thrombin model 3
green: 29 receptor conformations of minimization with different ligands.
It can be seen that Lys82 shows just minor shifts but Tyr80 moves a lot.

file	command	#	var0	var	LV	r2	q2 (LOO)	D/FFD	var	LV	r2	q2 (LOO)	SDEP
output.dat		29	590	232	2	0.68	0.40	2	109	1	0.62	0.53	1.82
output-A68-A82-A91.dat	w/o A68, A82, A91	26	590	228	5	0.92	0.62	5	104	5	0.93	0.76	
output-A68-A82-A91.dat	w/o A68, A82, A91; remove vTYR80, vLYS82	26	590	226	4	0.90	0.54	4	98	3	0.89	0.72	
output-A68-A82-A91.dat	w/o A68, A82, A91; remove eLYS82	26	590	227	5	0.92	0.62	5	105	5	0.92	0.73	
output-A68-A82-A91.dat	w/o A68, A82, A91; remove solvation	26	590	226	5	0.93	0.65	5	108	5	0.92	0.74	1.40
output-A68-A82-A91_buw.dat	w/o A68, A82, A91; BUW	26	590	228	7	0.94	0.56	7	100	5	0.94	0.79	1.25
output-set1.dat	A04, A12, A90, A48, A84, A73, A47, A45, A88, A19, A12.1, A17, A18	13	590	226			<0.05						
output-set2.dat	A72, A93, A14, A89, A46, A94, A92, A86, A44, A87, A22, A09, A63	13	590	216	2	0.77	0.47	2		1	0.76	0.65	
output-set3.dat	A04, A72, A93, A12, A14, A90, A89, A48, A46, A84, A94, A73, A92, A47	13	590	222	4	0.95	0.23						
output-set4.dat	A86, A45, A44, A88, A87, A19, A22, A12.1, A09,A17, A63, A18	13	590	222	3	0.92	0.54	3		2	0.93	0.70	
output-A68-A82-A91-A12-1.dat	**w/o A68, A82, A91, A12.1**	**25**	**590**	**228**	**5**	**0.93**	**0.64**	**5**	**106**	**5**	**0.93**	**0.75 (LOO) 0.74 (LTO) 0.64 (3 groups @20)**	**1.36 (LOO) 1.38 (LTO) 1.63 (3 groups @20)**
output-A68-A82-A91-A12-1.dat	**w/o A68, A82, A91, A12.1; remove vTYR80**	**25**	**590**	**227**	**4**	**0.91**	**0.53**	**4**	**102**	**4**	**0.91**	**0.70**	**1.47**

model 3	command	LV	prediction xray	#	SDEP	prediction docking	#	SDEP
output-A68-A82-A91.dat	w/o A68, A82, A91	5	output.dat	29	1.57 (1.34@LV3)	PDB_thrombin 120406_3D	510	2.38

						active.dat		
output-A68-A82-A91.dat	w/o A68, A82, A91; remove vTYR80, vLYS82	3	output.dat	29	1.21	PDB_thrombin 120406_3D active.dat	510	2.51
output-A68-A82-A91.dat	w/o A68, A82, A91; remove eLYS82	5	output.dat	29	1.52 (1.32@LV3)	PDB_thrombin 120406_3D active.dat	510	2.40
output-A68-A82-A91.dat	w/o A68, A82, A91; remove solvation	5	output.dat	29	1.59 (1.31@LV3)	PDB_thrombin 120406_3D active.dat	510	2.42
output-A68-A82-A91_buw.dat	w/o A68, A82, A91; BUW	5	output.dat	29	3.80 (2.45@LV1)	PDB_thrombin 120406_3D active.dat	510	3.51
output.dat		1	output.dat	29	1.65	PDB_thrombin 120406_3D active.dat	510	2.51 (2.30@LV2)
output-A68-A82-A91-A12-1.dat	**w/o A68, A82, A91, A12.1**	5	output.dat	29	1.66 (1.30@LV3)	PDB_thrombin 120406_3D active.dat	510	2.46
output-A68-A82-A91-A12-1.dat	**w/o A68, A82, A91, A12.1; remove vTYR80**	4	output.dat	29	1.52	PDB_thrombin 120406_3D active.dat	510	2.50

output-A68-A82-A91-A12-1.dat

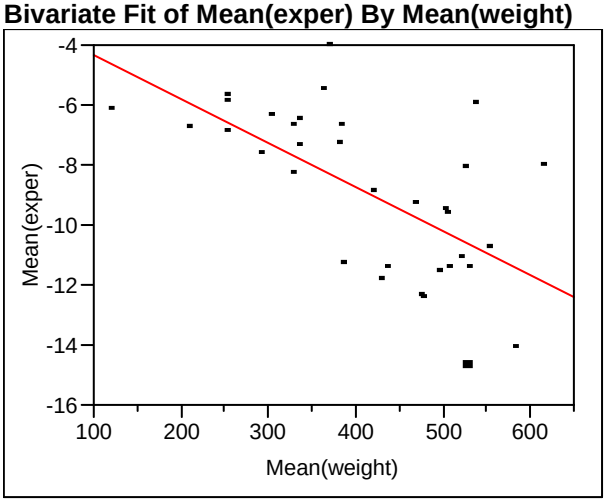
output.dat without the outlier structures A68, A82 and A91, and without the double structure A12.1 (output-A68-A82-A91-A12-1.dat, LV5, r2=0.93, q2=0.75, SDEP=1.36).

Conclusion of model 3

High correlation between weight and Ki (R2=0.41). The correlation for the minimum of ten docking solutions of predicted deltaG is just a little bit higher (R2=0.42).

Fit Y by X Group

Bivariate Fit of Mean(exper) By Mean(weight)



Linear Fit

Linear Fit

Mean(exper) = -2,846451 - 0,0146955 Mean(weight)

Summary of Fit

RSquare	0,410733
RSquare Adj	0,392318
Root Mean Square Error	2,119124
Mean of Response	-8,90802
Observations (or Sum Wgts)	34

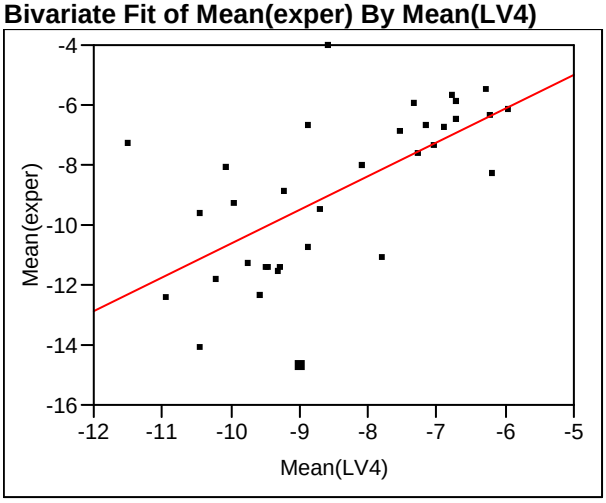
Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	1	100,16356	100,164	22,3047
Error	32	143,70195	4,491	Prob > F
C. Total	33	243,86551		<,0001

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	-2,846451	1,333933	-2,13	0,0406
Mean(weight)	-0,014696	0,003112	-4,72	<,0001

Bivariate Fit of Mean(exper) By Mean(LV4)



Linear Fit

Linear Fit

Mean(exper) = 0,5853775 + 1,1215659 Mean(LV4)

Summary of Fit

RSquare	0,408957
RSquare Adj	0,390487
Root Mean Square Error	2,122314
Mean of Response	-8,90802
Observations (or Sum Wgts)	34

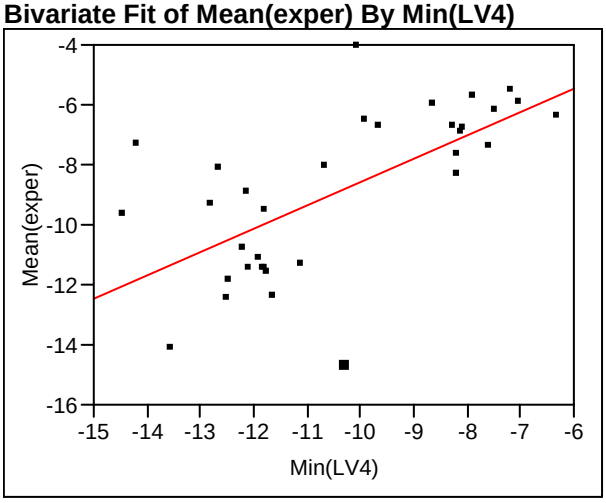
Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	1	99,73060	99,7306	22,1416
Error	32	144,13492	4,5042	Prob > F
C. Total	33	243,86551		<,0001

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	0,5853775	2,050084	0,29	0,7771
Mean(LV4)	1,1215659	0,238353	4,71	<,0001

Bivariate Fit of Mean(exper) By Min(LV4)



Linear Fit

Linear Fit

Mean(exper) = -0,788729 + 0,7772714 Min(LV4)

Summary of Fit

RSquare	0,424954
RSquare Adj	0,406984
Root Mean Square Error	2,093396
Mean of Response	-8,90802
Observations (or Sum Wgts)	34

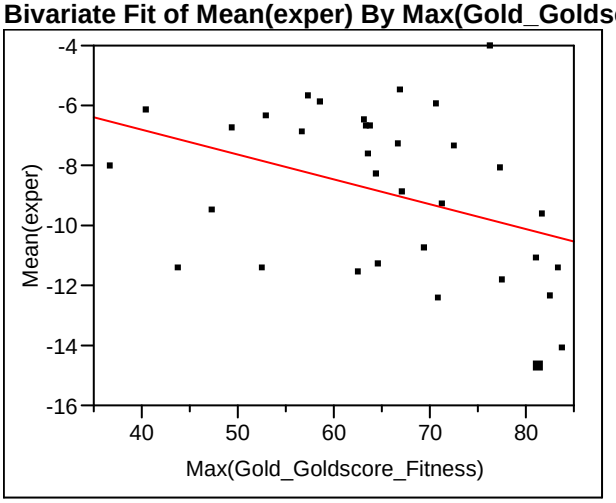
Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	1	103,63163	103,632	23,6477
Error	32	140,23388	4,382	Prob > F
C. Total	33	243,86551		<,0001

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	-0,788729	1,707804	-0,46	0,6473
Min(LV4)	0,7772714	0,159837	4,86	<,0001

Bivariate Fit of Mean(exper) By Max(Gold_Goldscore_Fitness)



Linear Fit

Linear Fit

Mean(exper) = -3,513706 - 0,0825801 Max(Gold_Goldscore_Fitness)

Summary of Fit

RSquare	0,148819
RSquare Adj	0,12222
Root Mean Square Error	2,546895
Mean of Response	-8,90802
Observations (or Sum Wgts)	34

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	1	36,29186	36,2919	5,5948
Error	32	207,57365	6,4867	Prob > F
C. Total	33	243,86551		0,0242

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	-3,513706	2,322017	-1,51	0,1400
Max(Gold_Goldscore_Fitness)	-0,08258	0,034913	-2,37	0,0242

Loaded Original Data
Active X-variables (SS > 1.0E-7)   = 228
Data file :
/home/henricsn/combine2go/data/thrombin/model3_180506/anal/output-A68-A82-A91_buw.dat
Comment : Pretreated file extracted from
/home/henricsn/combine2go/data/thrombin/model3_180506/anal/output-A68-A82-A91.dat

Number of variables = 590
Number of experiments = 26
Number of X-variables = 582 , Y-variables = 1
Active X-variables (SS > 1.0E-7)   = 228
Active Y-variables (SS > 1.0E-7)   = 1
Active X-variables after PRETREATMENT = 228
Active Y-variables after PRETREATMENT = 1

Principal Component Analysis (PCA)   26 objects   228 X-var

components	XVarExp	XAccum
1	35.4067	35.4067
2	27.2352	62.6419
3	12.8856	75.5275
4	6.5175	82.0450
5	4.9364	86.9814
6	3.1925	90.1739
7	**1.6088**	**91.7827**
8	1.0609	92.8435

PCA Rank Validation - using 4 random groups

components	PRESS	Seps	R
1	2.4897e+03	1.9055e+03	1.3066
2	2.1736e+03	1.1796e+03	1.8427
3	6.7148e+02	6.5267e+02	1.0288
4	3.7125e+02	4.0826e+02	0.9093
5	2.7553e+02	2.8542e+02	0.9653
6	1.8432e+02	1.9675e+02	0.9368
7	**1.5686e+02**	**1.4084e+02**	**1.1138**
8	1.4676e+02	1.1138e+02	1.3176

Partial Least Squares   (PLS)   26 objects   228 X-var   1 Y-var

Y1 components	XVarExp	XAccum	SDEC	r2
0	0.0000	0.0000	2.7234	0.0000
1	33.3195	33.3195	1.8435	0.5418
2	14.1450	47.4644	1.4760	0.7063
3	20.6448	68.1092	1.3076	0.7695
4	11.0355	79.1447	1.1157	0.8322
5	2.0505	81.1953	0.7973	0.9143
6	5.6482	86.8435	0.7167	0.9308
7	**2.9022**	**89.7457**	**0.6511**	**0.9428**
8	1.7144	91.4601	0.5898	0.9531

PLS Model Validation - LOO

Y1 components	SDEP	SDEV(sdep)	q2
0	2.8323	-	-0.0816
1	2.1458	-	0.3792
2	2.0721	-	0.4211
3	2.0058	-	0.4575
4	1.9694	-	0.4771
5	1.9171	-	0.5045
6	1.9263	-	0.4997

7	1.7978	-	0.5643
8	1.8528	-	0.5372

Deleted unselected vars. (D-Optimal)
2 : 228 -> 114 Comp.=7 , Mon May 22 17:16:24 2006
Active X-variables after VAR. SELECT. = 114

*** FFD Variable Selection Started ***
Max. dimensionality : 7
Validation Mode : LOO
Recalculate weights : yes
Comb./Var. ratio : 2.0
Use groups :
Uncertains : Retain
Fold-over design : no
perc. of dummies : 20

Deleted unselected vars. (F.Factorial)
2 : 114 -> 100 Comp.=7 , Mon May 22 17:16:40 2006
Active X-variables after VAR. SELECT. = 100

Principal Component Analysis (PCA) 26 objects 100 X-var

components	XVarExp	XAccum
1	38.2888	38.2888
2	29.2067	67.4955
3	10.3048	77.8003
4	5.1348	82.9350
5	**3.2605**	**86.1955**
6	2.2759	88.4715

PCA Rank Validation - using 4 random groups

components	PRESS	Seps	R
1	9.4901e+02	6.1163e+02	1.5516
2	2.3071e+02	3.6173e+02	0.6378
3	1.9760e+02	1.8228e+02	1.0841
4	3.9903e+02	1.1887e+02	3.3569
5	**1.0481e+02**	**8.7072e+01**	**1.2037**
6	8.5202e+01	6.6966e+01	1.2723

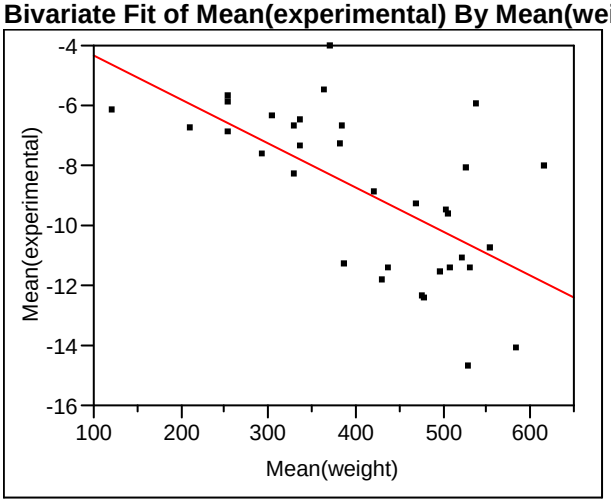
Partial Least Squares (PLS) 26 objects 100 X-var 1 Y-var

Y1 components	XVarExp	XAccum	SDEC	r2
0	0.0000	0.0000	2.7234	0.0000
1	33.6275	33.6275	1.6486	0.6336
2	24.5026	58.1301	1.3401	0.7579
3	16.6823	74.8124	1.0461	0.8524
4	5.8562	80.6687	0.7868	0.9165
5	**3.7559**	**84.4245**	**0.6742**	**0.9387**
6	2.1165	86.5410	0.6147	0.9491

PLS Model Validation - LOO

Y1 components	SDEP	SDEV(sdep)	q2
0	2.8323	-	-0.0816
1	1.9867	-	0.4678
2	1.7411	-	0.5913
3	1.5228	-	0.6874
4	1.3671	-	0.7480
5	**1.2520**	**-**	**0.7886**
6	1.4514	-	0.7160

Bivariate Fit of Mean(experimental) By Mean(weight)



Linear Fit

Mean(experimental) = -2,846451 - 0,0146955 Mean(weight)

Summary of Fit

RSquare	0,410733
RSquare Adj	0,392318
Root Mean Square Error	2,119124
Mean of Response	-8,90802
Observations (or Sum Wgts)	34

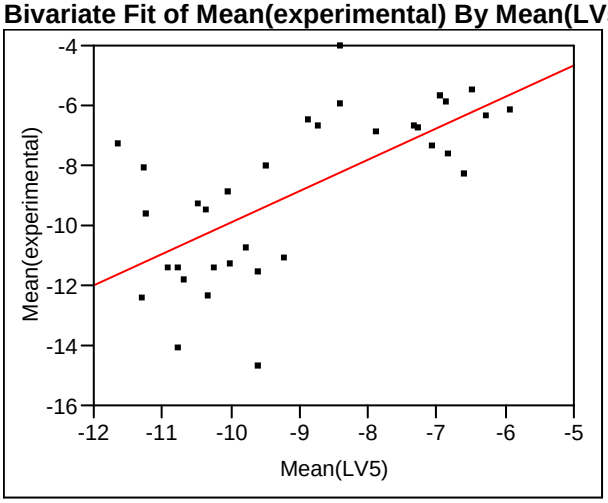
Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	1	100,16356	100,164	22,3047
Error	32	143,70195	4,491	Prob > F
C. Total	33	243,86551		<,0001

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	-2,846451	1,333933	-2,13	0,0406
Mean(weight)	-0,014696	0,003112	-4,72	<,0001

Bivariate Fit of Mean(experimental) By Mean(LV5)



Linear Fit

Mean(experimental) = 0,5247846 + 1,0418285 Mean(LV5)

Summary of Fit

RSquare	0,445602
RSquare Adj	0,428277
Root Mean Square Error	2,05547
Mean of Response	-8,90802
Observations (or Sum Wgts)	34

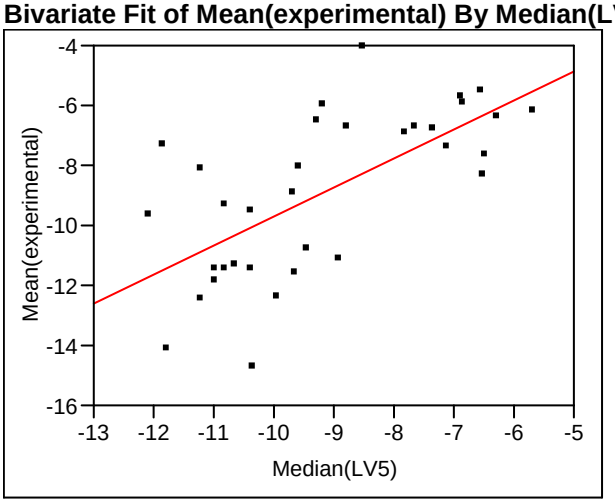
Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	1	108,66689	108,667	25,7202
Error	32	135,19862	4,225	Prob > F
C. Total	33	243,86551		<,0001

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	0,5247846	1,893069	0,28	0,7834
Mean(LV5)	1,0418285	0,205428	5,07	<,0001

Bivariate Fit of Mean(experimental) By Median(LV5)



Linear Fit

Linear Fit

Mean(experimental) = -0,041728 + 0,9651961 Median(LV5)

Summary of Fit

RSquare	0,439274
RSquare Adj	0,421752
Root Mean Square Error	2,067166
Mean of Response	-8,90802
Observations (or Sum Wgts)	34

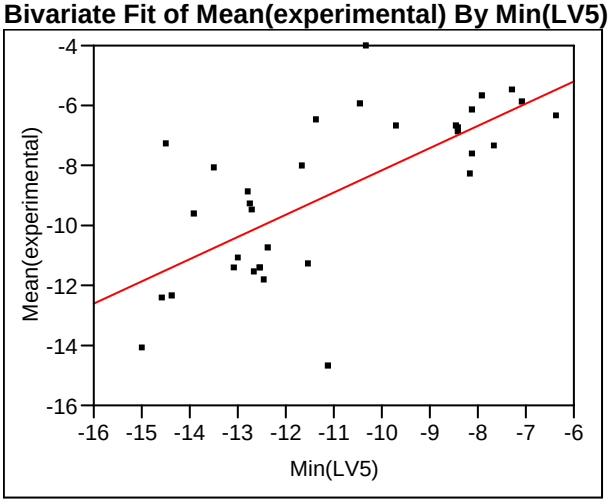
Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	1	107,12389	107,124	25,0689
Error	32	136,74162	4,273	Prob > F
C. Total	33	243,86551		<,0001

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	-0,041728	1,805957	-0,02	0,9817
Median(LV5)	0,9651961	0,192774	5,01	<,0001

Bivariate Fit of Mean(experimental) By Min(LV5)



Linear Fit

Linear Fit

Mean(experimental) = -0,754377 + 0,7391825 Min(LV5)

Summary of Fit

RSquare	0,480246
RSquare Adj	0,464004
Root Mean Square Error	1,99021
Mean of Response	-8,90802
Observations (or Sum Wgts)	34

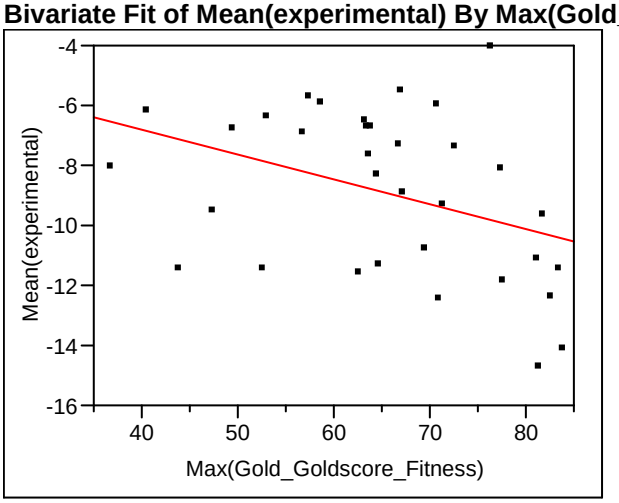
Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	1	117,11551	117,116	29,5676
Error	32	126,75000	3,961	Prob > F
C. Total	33	243,86551		<,0001

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	-0,754377	1,537845	-0,49	0,6271
Min(LV5)	0,7391825	0,135939	5,44	<,0001

Bivariate Fit of Mean(experimental) By Max(Gold_Goldscore_Fitness)



Linear Fit

Linear Fit

Mean(experimental) = -3,513706 - 0,0825801 Max(Gold_Goldscore_Fitness)

Summary of Fit

RSquare	0,148819
RSquare Adj	0,12222
Root Mean Square Error	2,546895
Mean of Response	-8,90802
Observations (or Sum Wgts)	34

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Ratio
Model	1	36,29186	36,2919	5,5948
Error	32	207,57365	6,4867	Prob > F
C. Total	33	243,86551		0,0242

Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Intercept	-3,513706	2,322017	-1,51	0,1400
Max(Gold_Goldscore_Fitness)	-0,08258	0,034913	-2,37	0,0242