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Supporting Information

Synthesis, Characterization, and Biological Applications of Zinc(II)

Complexes of Methylthiosalicylate Ligand

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Figure S4 -¹³C NMR spectrum of complex 2





Figure S6- ¹³C NMR spectrum of Complex 3



Figure S7 - ¹H NMR spectrum of Complex 4



Figure S8-¹³C NMR spectrum of Complex 4

Time dependent ¹H-NMR spectrum





Figure10- Time dependent ¹H NMR spectra of Complex 2



Figure 11 Time dependent ¹H NMR spectra of Complex 3





Figure S13. IR spectrum of Complex 1



Figure S14. IR spectrum of Complex 2



Figure S15. IR spectrum of Complex 3



Figure S16. IR spectra of Complex-4

The conformation to existence of complexes 1-4 in both solid and liquid



Figure S17 Solid and solution phase IR Spectra of complex 1

phase via Solid and Liquid IR spectrum



Figure S18 Solid and solution phase IR Spectra of complex 2







Figure S20 Solid and solution phase IR Spectra of complex 4



Figure S21. Packing diagram of **1** showing $(sp^3)C-H\cdots O(H_2O)$, $(sp^2)C-H\cdots O(H_2O)$



Figure S22. Packing diagram of **3** showing $(sp^3)C-H\cdots O$, $(sp^2)C-H\cdots O$, and $(sp^2)C-H\cdots S$ interactions (blue dotted line)



Figure S23. Packing diagram of **3** showing (sp³) C-H···O, (sp²) C-H···O, and (sp²) C-H···S interactions (green dotted line).

Figure 24 Packing diagram of 4 showing (sp^3) C-H···O, (sp^2) C-H···O, and (sp^2) C-H···S interactions.

Calculated (DFT) and Experimental (Single Crystal X-ray Diffraction) Bond Lengths and Bond Angles

Table S1. For complex 1

Bond distance (Å)	Experimental	Calculated (DFT)
	(X-ray)	
Zn(1)-S(2)	2.289(3)	2.318
Zn(1)-S(1)	2.287(3)	2.316
Bond Argle)-Nangle/°)	Experimental	Cakeulated
Zn(1)-N(2)	2. 1(X3(Pay)	2.2(4) (FT)
S(1)-Zn(1)-S(2)	123.14(11)	127.50
N(1)-Zn(1)-S(2)	115.0(3)	120.17
N(1)-Zn(1)-S(1)	112.4(3)	100.06
N(1)-Zn(1)-N(2)	84.4(4)	84.40
N(2)-Zn(1)-S(2)	103.3(3)	106.49
N(2)-Zn(1)-S(1)	110.9(3)	109.86

Table S2- For complex 2

Bond distance (Å)	Experimental	Calculated (DFT)
	(X-ray)	
Zn(1)-S(2)	2.3140(15)	2.333
Zn(1)-S(1)	2.278(14)	2.322

Zn(1)-O(1)	2.389(3)	2.322
Zn(1)-N(1)	2.115(4)	2.179
Zn(1)-N(2)	2.137(4)	2.222

Bond Angle (Angle/°)	Experimental (X-ray)	Calculated (DFT)
S(2)-Zn(1)-O(1)	87.01(10)	88.85
S(1)-Zn(1)-S(2)	124.30(5)	132.56
S(1)-Zn(1)-O(1)	82.48(9)	84.14
N(1)-Zn(1)-S(2)	110.43(10)	108.75
N(1)-Zn(1)-S(1)	122.89(10)	117.75
N(1)-Zn(1)-O(1)	85.50(13)	87.98
N(1)-Zn(1)-N(2)	76.62(15)	74.61
N(2)-Zn(1)-S(2)	109.46(11)	105.70
N(2)-Zn(1)-S(1)	97.86(11)	95.27
N(2)-Zn(1)-O(1)	158.95(14)	160.07

 Table S3- For complex 3

Bond distance	Experimental (X-ray)	Calculated (DFT)
Zn(1)-S(2)	2.299(3)	2.322
Zn(1)-S(1)	2.280(3)	2.319
Zn(1)-O(1)	2.302(6)	2.331
Zn(1)-N(2)	2.142(7)	2.180
Bond AZgld)-N(1)	Expermental	Calculated
(Angle/°)	(X-ray)	(DFT)
S(2)-Zn(1)-O(1)	102.54(2)	92.48
S(1)-Zn(1)-S(2)	131.04(12)	138.48
S(1)-Zn(1)-O(1)	84.2(2)	84.99
N(2)-Zn(1)-S(2)	95.2(2)	101.38
N(2)-Zn(1)-S(1)	133.7(2)	114.07
N(2)-Zn(1)-O(1)	85.1(3)	85.06
N(2)-Zn(1)-N(1)	76.73(3)	74.96
N(1)-Zn(1)-S(2)	104.89(2)	106.67
N(1)-Zn(1)-S(1)	89.73(2)	94.51
N(1)-Zn(1)-O(1)	148.3(3)	158.98

Table S4-For complex 4

Bond distance (Å)	Experimental	Calculated (DFT)
	(A-ray)	
Zn(1)-S(1)	2.280(5)	2.260
Zn(1)-S(2)	2.274(5)	2.260
Zn(1)-N(2)	2.095(15)	1.946
$Zn(1)-N(1)^{1}$	2.112(15)	1.958

Bond Angle (Angle/°)	Experimental (X-ray)	Calculated (DFT)
S(2)-Zn(1)-S(1)	126.78(2)	113.36
N(2)-Z(1)-S(1)	104.17(5)	104.59
N(2)-Zn(1)-S(2)	111.54(5)	112.16
N(2)-Zn(1)-N(1)1	93.48(6)	107.20
N(1)1-Zn(1)-S(1)	107.38(5)	107.67
N(1)1-Zn(1)-S(2)	108.38(4)	111.72

Donor NBO (i)	Acceptor NBO (j)	E(2)	E(j)-E(i)	F(i,j)
		kcal/mol	a.u.	a.u.
LP (1) O 4	LP*(6)Zn 1	6.51	0.74	0.068
LP (1) O 4	LP*(9)Zn 1	21.34	0.82	0.119
LP (3) S 3	LP*(6)Zn 1	67.92	0.35	0.142
LP (3) S 3	LP*(7)Zn 1	34.41	0.45	0.114
LP (3) S 3	LP*(8)Zn 1	1.70	0.39	0.024
LP (3) S 3	LP*(9)Zn 1	1.47	0.43	0.024
LP (3) S 2	LP*(6)Zn 1	89.34	0.34	0.161
LP (3) S 2	LP*(7)Zn 1	40.82	0.45	0.124
LP (3) S 2	LP*(8)Zn 1	3.63	0.39	0.035
LP (1) S 2	LP*(9)Zn 1	1.91	0.54	0.029
LP (1) N 5	LP*(6)Zn 1	14.35	0.47	0.080
LP (1) N 5	LP*(8)Zn 1	31.61	0.52	0.115
LP (1) N 7	LP*(6)Zn 1	15.77	0.47	0.083
LP(1)N 7	LP*(8)Zn 1	8.74	0.51	0.060
LP(1)N 7	LP*(9)Zn 1	21.72	0.55	0.098

Table S5 - Second Order Perturbation Theory Analysis ofcomplex 2

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
LP (1) N 6	LP*(6)Zn 1	12.86	0.47	0.076
LP (1) N 6	LP*(8)Zn 1	27.69	0.53	0.109
LP (1) N 6	LP*(9)Zn 1	7.05	0.55	0.056
LP(1)N 7	LP*(6)Zn 1	13.25	0.46	0.076
LP(1)N 7	LP*(8)Zn 1	15.97	0.52	0.082
LP(1)N 7	LP*(9)Zn 1	12.88	0.54	0.075
LP (3) S 2	LP*(6)Zn 1	87.75	0.35	0.162
LP (3) S 2	LP*(7)Zn 1	49.22	0.47	0.139
LP (2) S 2	LP*(8)Zn 1	9.62	0.34	0.051
LP (2) S 2	LP*(9)Zn 1	2.11	0.36	0.025
LP (3) S 3	LP*(6)Zn 1	69.96	0.36	0.148
LP (3) S 3	LP*(7)Zn 1	40.16	0.48	0.126
LP (3) S 3	LP*(8)Zn 1	1.75	0.42	0.025
LP (1) O 4	LP*(6)Zn 1	6.48	0.74	0.069
LP (1) O 4	LP*(9)Zn 1	21.44	0.81	0.120

Table S6- Second Order Perturbation Theory Analysis of
complex 3

UV-Vis absorption spectra (Experimental and Calculated)



Figure -S25-(a)UV spectrum of complex 1 (b) Selected molecular orbitals of complex 1 showing electronic transitions (orbital contour value = 0.02).



Fugure S26-(a) U V spectrum of complex 2 (b) Selected molecular orbitals of complex 2 showing electronic transitions (orbital contour value = 0.02).



Figure –S27 (a) U V spectrum of complex 3 (b) Selected molecular orbitals of complex 3 showing electronic transitions (orbital contour value = 0.02).



Figure –S28 (a) U V spectrum of complex 4 **(b)** Rrepresented Selected molecular orbitals of complex 4 showing electronic transitions (orbital contour value = 0.02).

Molecular docking results of Complex 1-4 with the targeted proteins expressed in cancer

Table S7. For complex 1				
Proteins	Pocket ID	Vina Score	Cavity volume (Å3)	Interacting amino acids
VEGF	C1			Chain E: TYR139 SER140 GLU141 PHE172
		-5.2	95	THR218 ASN219
	C2	0.2		Chain E: PRO163 ASN164 ILE165 THR166
				VAL167 PRO179 GLY181 ILE184 ILE185
		-4.9	84	TRP186 ASP187 PHE192
	C3			Chain E: ARG133 PRO134 THR161 SER162
				ASN164 ILE165 THR166 THR210 VAL211
		-4.8	83	ASN212
	C4			Chain E: THR166 VAL167 THR168 LEU169
		1.0		LYS170 THR176 LEU177 ILE178 PRO179
	05	-4.6	11	GLU208 ALA209 IHR210 LEU215
	05			Chain E: GLU144 ILE145 ILE146 HIS14/ MET148 THD140 ADC152 CLU152 LEU154
		5 5	73	MET148 THR149 ARG152 GLU155 LEU154 VAL 155 PPO157 GLN225
TGFR1	C1	-5.5	15	Chain $\mathbf{A} \cdot \mathbf{I}$ FU20 II F22 I FU28 TRP30 TYR39
10101				ALA41 ASN42 PHF43 CYS44 CYS78 PRO80
		-5.1	126	LEU83 ASN103 MET104 VAL106
	C2			Chain A: CYS7 PHE8 SER10 THR11 GLU12
				LYS13 CYS16 VAL17 ARG18 GLN19 PHE43
		-4.9	83	LEU45 GLY46
	C3			Chain A: PRO47 CYS48 PRO49 TYR50 ALA63
				ASN66 GLN67 PRO70 GLY71 ALA72 ALA75
		-5.3	56	PRO76
	C4			Chain A: THR4 PHE8 GLN19 PRO36 TYR39
		5 1	40	HIS40 ASN42 GLU84 LEU86 PRO87 ILE105
	<u>C5</u>	-5.1	49	VAL106 AKG10/ Chaire A. CNS7 DHE9 SED 10 THD 11 CLU12
	0.5			Chain A: $CYS/PHE8$ SERIO THRIT GLU12 I VS12 CVS16 VAL 17 ADC18 CL N10 DHE42
		-5	44	I FII45 GI V46
BRAF	C1	5		Chain A : ILF463 GLY464 VAL471 ALA481
DIVIN				LYS483 GLN530 TRP531 CYS532 GLY534
				SER535 SER536 HIS539 ASN580 PHE583
		-6.8	2436	ASP594 PHE595 LEU597
	C2			Chain B: SER467 ALA497 ASN500 GLU501
				VAL504 LEU505 THR508 LEU567 ILE572

				ILE573 HIS574 ARG575 ASP576 GLY593
				ASP594
	C3			Chain A: VAL511 ASP555 ARG558 GLN559
		-6.6	1855	ARG562 ASN588 THR589
				Chain B: ASP479 GLN530 TRP531 GLU533
				HIS585 GLU586
	C4			Chain A: ALA497 ASN500 GLU501 VAL504
				LEU505 LEU567 ILE572 ILE573 HIS574
				ARG575 ASP576 GLY593 ASP594 GLY596
		-7.2	1065	THR599
	C5			Chain B: LEU674 SER675 PRO676 ASP677
				LEU678 MET693 ALA694 LEU697 LYS698
		-4.1	309	LYS699
p53	C1			Chain B: SER1742 ASP1743 ALA1746
				HIS1809 ARG1811 TYR1852 LEU1854
		-5.7	413	GLU1945 GLN1949 LYS1964 TYR1969
	C2			Chain B: LEU1931 ALA1934 GLU1935
				GLN1938 LEU1939 PRO1940 VAL1941
				VAL1942 PHE1959 LYS1960 HIS1962
		-6.8	272	TYR1965 LYS1966 HIS1967 ASP1968
	C3			Chain B: PRO1769 PRO1770 PHE1771
				ASP1807 SER1827 HIS1828 VAL1829 HIS1832
		-4.7	265	ASP1833
	C4			Chain B: GLN1801 GLY1822 PRO1824
				TYR1843 ARG1844 LEU1847 TRP1862
		-5.1	187	PRO1864 ARG1865
	C5			Chain B: ARG1811 PHE1884 THR1922
				ASP1923 PRO1924 SER1943 GLN1944
				GLU1945 LYS1964 HIS1967 TYR1969
		-6	113	VAL1970
BSA	C1			Chain A: THR190 ARG194 ARG217 GLN220
				ALA290 GLU291 LYS294 GLU339 TYR340
				ALA341 VAL342 LYS439 GLU443 PRO446
		-6	8389	CYS447 ASP450 TYR451
	C2			Chain A: ASP108 SER109 PRO110 ASP111
				LEU112 PRO113 LYS114 ARG144 PRO420
		-6.3	3498	VAL423 GLU424 ARG458 ILE522
	C3			Chain A: GLU503 LYS504 PHE506 THR507
				PHE508 HIS509 ALA568 GLY571 PRO572
		-5.2	1508	VAL575
	C4			Chain A: GLU100 LEU103 SER104 ILE202
				GLN203 LYS204 LYS242 CYS245 HIS246
		-5.6	793	ASP248
	C5			Chain A: LEU386 GLN389 ASN390 GLN393

	VAL408 ARG409 ARG412 LYS413 SER488
	LEU490 THR491 PRO492

			Table S8	5. For complex 2
	Pocket	Vina	Cavity	Interacting amino acids
Proteins	ID	Score	volume	
			(Å3)	
VEGF	C1			Chain E: SER140 GLU141 LYS170 LYS171
				PHE172 PRO173 LEU174 LEU204 THR206
		-6	95	GLU208 LYS217 ASN219
	C2			Chain E: PRO163 ASN164 ILE165 THR166
				VAL167 PRO179 ASP180 GLY181 ILE184
		-5.3	84	ILE185 TRP186 SER188
	C3			Chain E: ARG133 PRO134 THR161 SER162
		-4.8	83	ASN164 ILE165 THR210 VAL211 ASN212
	C4			Chain E: ARG133 PRO134 THR161 SER162
		-4.7	77	ASN164 ILE165 THR210 VAL211 ASN212
	C5			Chain E: GLU137 GLU144 ILE145 ILE146
				HIS147 GLU153 LEU154 VAL155 PRO157
		-5.7	73	ARG159 ARG189 LYS190
TGFB1	C1			Chain A: LEU20 ILE22 LEU28 TYR39 ALA41
				ASN42 PHE43 CYS44 CYS78 VAL79 PRO80
		-5.6	126	LEU83 ASN103 MET104 ILE105 VAL106
	C2			Chain A: ASP23 PHE24 ARG25 TRP30 LYS31
		-5	83	TRP32 ILE33 HIS34 GLU35 PRO36 LYS37
	C3			Chain A: PRO47 CYS48 PRO49 TYR50 ALA63
				ASN66 GLN67 PRO70 GLY71 ALA72 ALA75
		-5.9	56	PRO76
	C4			Chain A: THR4 PHE8 GLN19 TYR21 PRO36
				GLY38 TYR39 HIS40 ASN42 GLU84 PRO85
		-5.9	49	LEU86 PRO87 ILE105 VAL106 ARG107
	C5			Chain A: CYS7 SER10 THR11 GLU12 LYS13
		-5.9	44	CYS16 ARG18 GLN19 PHE43 LEU45
BRAF	C1			Chain A: ILE463 GLY464 SER465 VAL471
				ALA481 LYS483 LEU514 TRP531 CYS532
				GLY534 SER535 SER536 HIS539 ASN580
		-8.2	2436	PHE583 ASP594 PHE595 LEU597
	C2			Chain B: ILE463 GLY464 SER465 GLY466
				SER467 VAL471 ALA481 VAL482 LYS483
				LEU514 ILE527 THR529 GLN530 TRP531
				CYS532 GLY534 SER535 SER536 PHE583
		-8.7	2121	ASP594 PHE595 GLY596
	C3			Chain A: VAL511 ASN512 ASP555 ARG558
				GLN559 ARG562 HIS585 ASN588 THR589
				Chain B: ASP479 TRP531 GLU533 HIS585

				· · · · · · · · · · · · · · · · · · ·
				GLU586 THR589
	C4			Chain A: PHE468 LYS483 ALA497 ASN500
				GLU501 VAL504 LEU505 LEU567 ILE572
				ILE573 HIS574 ARG575 GLY593 ASP594
		-8.3	1065	GLY596 LEU597 THR599 TYR633
	C5			Chain B: LEU674 SER675 LEU678 ALA694
		-5	309	LEU697 LYS698 LYS699
P53	C1			Chain A: THR102 GLN104 PHE109 ARG110
				LEU111 GLY112 PHE113 TYR126 PRO128
		-6.6	470	ALA129 ASN131 TRP146 ASN268 SER269
	C2			Chain A: VAL197 GLU198 GLY199 LEU201
				ARG202 VAL218 PRO219 GLU221 PRO222
				PRO223 CYS229 THR230 THR231 ILE232
		-6.3	215	HIS233
	C3			Chain A: LEU145 VAL157 VAL197 GLU198
				GLY199 LEU201 VAL218 PRO219 TYR220
				GLU221 PRO222 PRO223 CYS229 THR230
		-5.8	208	THR231 ILE232 HIS233
	C4			Chain A: SER96 PRO98 SER99 ARG156
				ARG158 MET160 LEU206 ASP208 THR211
				ARG213 SER215 ILE254 THR256 GLU258
		-6.8	127	SER261 GLY262 ASN263 LEU264 ARG267
	C5			Chain A: VAL147 ASP148 SER149 THR150
		-4.3	101	TYR220 PRO222 PRO223 GLU228
BSA	C1			Chain A: ARG194 ARG217 GLN220 LYS221
				ALA290 GLU291 VAL292 GLU293 LYS294
				PRO338 GLU339 TYR340 ALA341 VAL342
				ARG435 LYS439 GLU443 PRO446 CYS447
		-6.5	8389	ASP450 TYR451
	C2			Chain A: ASP108 SER109 PRO110 ASP111
				LEU112 LYS114 ARG144 PRO420 VAL423
				GLU424 ARG427 ARG458 THR518 GLU519
		-7.1	3498	ILE522
	C3			Chain A: PHE501 GLU503 LYS504 PHE506
				THR507 PHE508 HIS509 PHE567 ALA568
		-5.8	1508	GLY571 PRO572 VAL575
	C4			Chain A: GLU100 LEU103 SER104 TYR147
				CYS199 ILE202 GLN203 LYS204 LYS242
		-6	793	CYS245 HIS246
	C5			Chain A: LEU386 GLN389 ASN390 GLN393
				ALA405 VAL408 ARG409 ARG412 LYS413
		-6.6	356	SER488 ALA489 LEU490 THR491 PRO492

Table S9. For complex 3				
Proteins	Pocket ID	Vina Score	Cavity volume (Å3)	Interacting amino acids

VEGF	C1			Chain E: MET138 TYR139 SER140 GLU141 PRO143 PHE172 LEU204 THR206 LEU215
		-6.4	95	TYR216 LYS217 ASN219
	C2			Chain E: ILE165 THR166 VAL167 THR168
				LEU169 THR176 LEU177 ILE178 PRO179
		-5.5	84	ASP180 GLY181 TRP186
	C3			Chain E: ARG133 PRO134 THR161 SER162
				ASN164 ILE165 THR166 THR210 VAL211
		-5.7	83	ASN212 TYR216
	C4			Chain E: ARG133 PRO134 THR161 SER162
				ASN164 ILE165 THR166 THR210 VAL211
		-5.7	77	ASN212
	C5			Chain E: GLU144 ILE145 ILE146 HIS147
				MET148 THR149 ARG152 GLU153 VAL155
		-6.3	73	PRO157 GLN225
TGFB1	C1			Chain A: LEU20 TYR21 ILE22 ASP27 LEU28
				TYR39 ALA41 ASN42 PHE43 CYS44 PRO80
		-6.8	126	LEU83 ASN103 MET104 ILE105 VAL106
	C2			Chain A: PHE24 ARG25 TRP30 LYS31 TRP32
				ILE33 HIS34 GLU35 PRO36 LYS37 TYR91
		-5.9	83	VAL92 GLY93
	C3			Chain A: ASN14 GLY46 PRO47 CYS48 PRO49
				TYR50 ASN66 GLN67 PRO70 GLY71 ALA72
		-6.1	56	SER73 ALA74 ALA75 PRO76
	C4			Chain A: THR4 PHE8 GLN19 PRO36 GLY38
				TYR39 HIS40 ASN42 LEU86 PRO87 ILE105
		-5.7	49	ARG107
	C5			Chain A: CYS7 PHE8 SER10 THR11 GLU12
				LYS13 VAL17 ARG18 GLN19 PHE43 LEU45
		-6.4	44	GLY46
BRAF	C1			Chain A: ILE463 GLY464 VAL471 ALA481
				LYS483 LEU514 THR529 GLN530 TRP531
				CYS532 GLY534 SER535 SER536 HIS539
		-9.6	2436	ASN580 PHE583 PHE595 LEU597
	C2			Chain B: SER467 ALA497 ASN500 GLU501
				VAL504 LEU505 THR508 ILE513 LEU567
			0.1.0.1	ILE5/2 ILE5/3 HIS5/4 ARG5/5 ASP5/6 GLY593
		-8	2121	ASP594
	C3			Chain A: VAL511 ASN512 ASP555 GLN559
				ARG562 HIS585 GLU586 ASN588 THR589
			1055	Chain B: ASP479 GLN530 TRP531 GLU533
		-8.3	1855	HIS585 GLU586 ASN588 THR589
	C4			Chain A: GLN493 ALA497 ASN500 GLU501
				VAL504 LEU505 LEU567 ILE572 ILE573 HIS574
			1005	ARG575 GLY593 ASP594 GLY596 THR599
		-8.6	1065	
	05	5.0	200	Unain B: SEK6/5 PRO6/6 LEU6/8 ALA694
D52		-5.3	309	LEU09/LYS098LYS099LYS/00GLU/03
P55	CI			Unain B: SER1/42 ASP1/43 LEU1/45 ALA1/46
			410	SEK1/49 AKG1811 TYK1852 LEU1854 SER1943
		-/.8	413	GLN1944 GLU1945 GLN1949 LYS1964 TYR1969

	C2			Chain B: LEU1931 LYS1932 ALA1934 GLU1935
				GLN1938 LEU1939 PRO1940 VAL1941 PHE1959
		-7.4	272	LYS1960 TYR1965 LYS1966 HIS1967 ASP1968
	C3			Chain B: PRO1769 PRO1770 PHE1771 ASP1807
				SER1827 HIS1828 VAL1829 HIS1832 ASP1833
		-6	265	TYR1846 LEU1848 PRO1849
	C4			Chain B: GLN1801 SER1821 GLY1822 PRO1824
				TYR1843 ARG1844 LEU1847 TRP1862 PRO1864
		-6.3	187	ARG1865 GLU1866 ASN1867
	C5			Chain B: THR1740 SER1742 ARG1811 PHE1816
				PHE1884 THR1922 ASP1923 PRO1924 SER1943
				GLN1944 GLU1945 ILE1948 LYS1964 LYS1966
		-7.9	113	HIS1967 TYR1969 VAL1970 SER1971
BSA	C1			Chain A: TYR149 GLU152 TYR156 GLU186
				LYS187 THR190 SER191 ARG194 ARG198
				TRP213 ARG217 ARG256 HIS287 ALA290
		-8.1	8389	GLU291 TYR451
	C2			Chain A: LYS114 HIS145 ARG185 GLU186
				LEU189 THR190 SER192 ALA193 GLU424
				ARG427 SER428 LYS431 ARG435 TYR451
		-9.9	3498	LEU454 ILE455 ARG458 THR518 ILE522
	C3			Chain A: PHE501 GLU503 LYS504 PHE506
				THR507 PHE508 HIS509 PHE567 ALA568
		-6.8	1508	GLY571 PRO572 VAL575
	C4			Chain A: GLU100 LEU103 SER104 TYR147
				ARG196 ILE202 GLN203 LYS204 GLU207
		-6.7	793	LYS242 CYS245 HIS246
	C5			Chain A: ASN385 LEU386 GLN389 ASN390
				GLN393 LEU406 VAL408 ARG409 TYR410
				ARG412 LYS413 SER488 LEU490 THR491
		-7.7	356	PRO492

Table S10. For complex 4							
Proteins	Pocket ID	Vina Score	Cavity volume (Å3)	Interacting amino acids			
VEGF	C1	(7	05	Chain E: TYR139 SER140 GLU141 PR0143 LYS171 PHE172 PR0173 LEU174 ILE202 GLY203 LEU204 THR206 LYS217 ASN219 LEU221			
	C2	-0./	95	THR222 Chain E: PRO163 ILE165 THR166 VAL167 THR168 LEU169 THR176 LEU177 ILE178 PRO179 ASP180 GLY181 ILE184 ILE185 TRP186			
	C3	-5.5	84	ASP187 SER188 Chain E: ARG133 THR161 SER162 ASN164 ILE165 THR166 THR210 VAL 211 ASN212 GL X213			
	C4	-3.7	0.5	Chain E: PRO163 ASN164 ILE165 THR166 VAL167 THR168 LYS170 THR176 ILE178 PRO179 TRP186 SER188 PHE192 GLU208 ALA209			
	C5	-5.9	77	THR210 LEU215 Chain E: GLU137 GLU144 ILE145 ILE146 HIS147 MET148 THR149 ARG152 GLU153 LEU154 VAL155 PP0157 APG159 APG189 LVS190			
TGFB1	C1	-5.6	73	GLN225 Chain A: LEU20 TYR21 ILE22 LYS26 ASP27 LEU28 TYR39 ALA41 ASN42 PHE43 CYS44 CYS78 VAL79 PRO80			
		-6.2	126	LEU83 ASN103 MET104 ILE105 VAL106			
	C2	-5.2	83	Chain A: PHE24 ARG25 TRP30 LYS31 TRP32 ILE33 HIS34 GLU35 PRO36 LYS37 TYR91 GLY93			
	C3			Chain A: LYS13 ASN14 GLY46 PRO47 CYS48 PRO49 TYR50 ALA63 ASN66 GLN67 ASN69 PRO70 GLY71 ALA72 SER73 ALA74 ALA75 PRO76 CYS77			
	C4	-6.9	56	CYS78 Chain A: THR4 ASN5 PHE8 GLN19 PRO36 GLY38 TYR39 HIS40 ASN42 GLU84 LEU86 PRO87 ILE105 ARG107			
	C5	5		Chain A: CYS7 PHE8 SER10 THR11 GLU12 LYS13 VAL17 ARG18 GLN19 LEU20 TYR21 PHE43 LEU45 GLY46			
BRAF	C1	-5.1	44	PK047 Chain A: ILE463 GLY464 SER465 VAL471 ALA481 VAL482 LYS483 GLU501 LEU514 ILE527 THR529 GLN530 TRP531 CYS532 GLU533 GLY534 SER535 SER536 TYR538			

C2 Call Chain B: GLY466 V THR529 C GLY534 S HIS539 A HIS539 A Chain A: GLY596 Chain B: I GLN559 A HIS585 G THR589 Chain B: I GLN559 A HIS585 G THR589 Chain A: GLN494 A VAL504 I ASP576 L LEU597 A VAL504 I ASP677 L ARG691 A HIS53 C5 C4 Chain A: GLN494 A VAL504 I ASP576 L LEU597 A HIS53 C4 Chain A: GLN494 A VAL504 I ASP677 L ASP677 L ARG691 A HIS538 L C5 C5 Chain B: ASP677 L ARG691 A HIS53 L C1 F53 C1 C2 Chain A: HIS52 P C3 C3 Chain A: PR0152 P	LA543 ASN580 PHE583 HE595 GLY596 LEU597 LE463 GLY464 SER465 AL471 ALA481 LEU514 LN530 TRP531 CYS532 ER535 SER536 TYR538 SN580 PHE583 PHE595 ASP479 TRP531 GLU533 JU586 ASP587 ASN588 YS551 ASP555 ARG558 RG562 GLU586 ASN588 PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
C2 Chain B: GLY466 V THR529 C GLY345 V GLY534 S HIS539 A GLY534 S HIS539 A GLY534 S HIS539 A GLY594 P -6.4 2121 GLY596 GLY596 S THR589 Chain A: GLN559 A HIS585 G THR589 C3 Chain A: HIS585 G THR589 C4 Chain A: HIS55 C4 Chain A: HIS55 C4 Chain A: GLN494 A VAL504 I ASP576 L LEU597 A VAL504 I ASP677 L ASP677 L ASP677 L ARG691 A SP677 L ARG691 A LEU114 H ALA129 A ARG101 I LEU114 H ALA129 A ASP68 S P53 C1 Chain A: ASP67 L ARG601 A LEU201 A TYR220 C C2 C2 Chain A: ASP675 P C3 Chain A: ASP675 P C3	HE595 GLY596 LEU597 LE463 GLY464 SER465 YAL471 ALA481 LEU514 LN530 TRP531 CYS532 ER535 SER536 TYR538 SN580 PHE583 PHE595 ASP479 TRP531 GLU533 LU586 ASP587 ASN588 YS551 ASP555 ARG558 RG562 GLU586 ASN588 PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
C2 Chain B: GLY466 V THR529 C GLY534 S HIS539 A HIS539 A HIS539 A HIS539 A HIS539 A HIS539 A HIS539 A C3 C3 -6.4 2121 GLY534 S GLY534 S HIS539 A Chain A: HIS585 G THR589 Chain B: I GLN559 A HIS587 G THR589 Chain B: I GLN559 A HIS587 G THR589 Chain B: I GLN559 A HIS587 A HIS587 A HIS587 A HIS587 A HIS587 A HIS589 A Chain A: GLN59 A Chain A: ASP576 L LEU597 A VAL504 I VAL504 I VAL504 I ASP577 L ASP677 L ARG691 A LEU597 A ASP677 L ARG691 A LEU114 H ALA129 A ARG110 I LEU114 H ALA129 A ASN268 S C2 P53 C1 Chain A: ARG110 I LEU114 H ALA129 A ASN268 S C2 C2 Chain A: ARG110 I LEU201 A TYR220 C C3 C3 Chain A: PRO152 P	LE463 GLY464 SER465 (AL471 ALA481 LEU514 LN530 TRP531 CYS532 ER535 SER536 TYR538 SN580 PHE583 PHE595 ASP479 TRP531 GLU533 LU586 ASP587 ASN588 YS551 ASP555 ARG558 RG562 GLU586 ASN588 PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
C2 Chain B: (GLY466 V) (GLY534 S) (GLY534 S) (GLY534 S) (GLY534 S) (GLY536 C) (GLY596 C) (GLY596 C) (GLY596 C) (GLY596 C) (THR589 C) (Chain A: (GLN559 A) (Chain B: I) (GLN559 A) (Chain B: I) (GLN559 A) (Chain B: I) (GLN559 A) (Chain A: (GLN56 A) (Chain A: (GLN494 A) (VAL504 I) (GLN494 A) (VAL504 I) (GLN494 A) (VAL504 I) (GLN494 A) (VAL504 I) (GLN494 A) (VAL504 I) (GLN494 A) (VAL504 I) (GLN494 A) (C1)(C1)(C1)(C1)(C1) (GLN494 A) (C2)(C1)(C1)(C1)(C1)(C1)(C1) (GLN494 A) (C1)(C1)(C1)(C1)(C1)(C1)(C1)(C1)(C1) (GLN494 A) (C1)(C1)(C1)(C1)(C1)(C1)(C1)(C1)(C1)(C1)	LE463 GLY464 SER465 AL471 ALA481 LEU514 LN530 TRP531 CYS532 ER535 SER536 TYR538 SN580 PHE583 PHE595 ASP479 TRP531 GLU533 LU586 ASP587 ASN588 YS551 ASP555 ARG558 RG562 GLU586 ASN588 PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
-6.4 2121 GLY466 V -6.4 2121 GLY534 S HIS539 A HIS539 A C3 Chain A: HIS585 G THR589 Chain B: I GLN559 A C4 Chain B: I GLN559 A GLN559 A C4 Chain A: GLN559 A GLN559 A VAL504 I ASP576 L LEU597 A S C5 Chain B: I ASP677 L ASP677 L ARG691 A LEU144 F ALA129 A ARG110 I LEU114 F ALA129 A C2 C1 Chain A: C2 C1 Chain A: C3 C1 Chain A:	AL471 ALA481 LEU514 LN530 TRP531 CYS532 ER535 SER536 TYR538 SN580 PHE583 PHE595 ASP479 TRP531 GLU533 LU586 ASP587 ASN588 YS551 ASP555 ARG558 .RG562 GLU586 ASN588 PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
-6.4 2121 GLY534 S GLY534 S HIS539 A GLY596 C3 -6.4 2121 GLY596 C3 Chain A: HIS585 G THR589 -6.4 2121 GLN559 A GLN559 A -5.1 1855 THR589 C4 Chain A: GLN494 A -5.1 1855 THR589 C4 Chain A: GLN494 A -6.9 1065 TYR633 C5 C5 Chain B: ASP677 L ARG691 A -6.9 1065 TYR633 C5 C1 Chain A: ARG6110 I LEU114 F -5 309 LYS698 L C2 -7.1 470 ASN268 S -7.1 C2 C1 Chain A: ARG110 I LEU201 A -7.1 C3 C1 Chain A: PR0152 P -5.3	LN530 TRP531 CYS532 ER535 SER536 TYR538 SN580 PHE583 PHE595 ASP479 TRP531 GLU533 JU586 ASP587 ASN588 YS551 ASP555 ARG558 RG562 GLU586 ASN588 PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
-6.4 2121 GLY534 S HIS539 A GLY596 C3 -6.4 2121 GLY596 C3 Chain A: HIS585 G THR589 - Chain B: I GLN559 A -5.1 1855 THR589 C4 Chain A: GLN494 A - ASP576 L -6.9 1065 TYR633 C5 Chain B: ASP677 L - ARG691 A -5 309 LYS698 L P53 C1 Chain A: ARG110 I LEU114 H -7.1 470 ASN268 S C2 Chain A: LEU201 A - TYR220 C -5.3 215 CYS229 T C3 Chain A: PR0152 P - PR0152 P	ER535 SER536 TYR538 SN580 PHE583 PHE595 ASP479 TRP531 GLU533 LU586 ASP587 ASN588 YS551 ASP555 ARG558 RG562 GLU586 ASN588 PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
-6.4 2121 HIS539 A: GLY596 C3 Chain A: HIS585 G: THR589 HIS585 G: THR589 -5.1 1855 THR589 C4 Chain A: GLN597 A GLN559 A C4 Chain A: GLN494 A VAL504 I ASP576 L LEU597 A LEU597 A C5 Chain B: I ASP677 L ASP677 L ASP677 L ASP671 L -5 309 LYS698 L P53 C1 Chain A: ARG110 I C2 Chain A: ARC601 A ARG110 I -7.1 470 ASN268 S C2 Chain A: ARC10 I TYR220 C -5.3 215 CYS29 T C3 Chain A: PR0152 P PR0152 P	SN580 PHE583 PHE595 ASP479 TRP531 GLU533 LU586 ASP587 ASN588 YS551 ASP555 ARG558 RG562 GLU586 ASN588 PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
-6.4 2121 GLY596 C3 Chain A: HIS585 G THR589 HIS585 G THR589 -5.1 1855 THR589 C4 Chain A: GLN559 A GLN559 A C4 Chain A: GLN559 A GLN559 A -5.1 1855 THR589 C4 Chain A: GLN494 A VAL504 I ASP576 L LEU597 A -6.9 1065 TYR633 C5 Chain B: I ASP677 L ASP677 L ASP677 L ARG691 A -5 309 LYS698 L P53 C1 Chain A: ARG110 I LEU114 F ALA129 A -7.1 470 ASN268 S C2 Chain A: LEU201 A -5.3 215 CYS29 T C3 Chain A: PR0152 P PR0152 P	ASP479 TRP531 GLU533 LU586 ASP587 ASN588 YS551 ASP555 ARG558 RG562 GLU586 ASN588 PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
C3 Chain A: HIS585 G C3 -5.1 1855 THR589 Chain B: I GLN559 A -5.1 1855 THR589 C4 Chain A: GLN494 A VAL504 I ASP576 L LEU597 A LEU597 A -6.9 1065 TYR633 C5 Chain B: I ASP677 L ASP677 L ASP677 L ARG691 A -5 309 LYS698 L P53 C1 Chain A: ARG110 I LEU114 H ALA129 A ARG110 I LEU201 A TYR220 C C -5.3 215 CYS29 T C3 C1 Chain A: PR0152 P	ASP479 TRP531 GLU533 LU586 ASP587 ASN588 YS551 ASP555 ARG558 RG562 GLU586 ASN588 PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
C3 -5.1 1855 Chain A HIS585 G. THR589 Chain B: I. GLN559 A GLN559 A C4 Chain A: GLN494 A VAL504 I ASP576 L LEU597 A -6.9 1065 TYR633 C5 Chain B: I ASP677 L ASP677 L ARG691 A ARG691 A -5 309 LYS698 L P53 C1 Chain A: -7.1 470 ASN268 S C2 Chain A: LEU201 A -7.1 470 ASN268 S C2 -5.3 215 C3 Chain A: PR0152 P	ASP479 TKP551 GLU555 LU586 ASP587 ASN588 YS551 ASP555 ARG558 RG562 GLU586 ASN588 PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
-5.1 1855 THR589 -5.1 1855 THR589 C4 Chain B: I GLN559 A C4 Chain A: GLN494 A VAL504 I ASP576 L LEU597 A -6.9 1065 TYR633 C5 Chain B: I ASP576 L -6.9 1065 TYR633 C5 Chain B: I ASP677 L ASP677 L ASP677 L ARG691 A -5 309 LYS698 L P53 C1 Chain A: ARG110 I LEU114 H ALA129 A -7.1 470 ASN268 S C2 Chain A: D LEU201 A TYR220 C -5.3 215 C3 Chain A: D PR0152 P	YS551 ASP587 ASN588 YS551 ASP555 ARG558 RG562 GLU586 ASN588 PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
-5.1 1855 111111111111111111111111111111111111	YS551 ASP555 ARG558 RG562 GLU586 ASN588 PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
-5.1 1855 Chain B: I GLN559 A GLN559 A C4 Chain A: A GLN494 A VAL504 I VAL504 I ASP576 L LEU597 A LEU597 A -6.9 1065 TYR633 C5 Chain B: I ASP677 L ASP677 L ASP677 L ARG691 A -5 309 LYS698 L P53 C1 Chain A: A -7.1 470 ASN268 S C2 Chain A: A LEU201 A TYR220 C -5.3 215 C3 Chain A: PR0152 P PR0152 P	YS551 ASP555 ARG558 RG562 GLU586 ASN588 PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
-5.1 1855 THR589 C4 Chain A:: GLN494 A VAL504 I ASP576 L LEU597 A LEU597 A -6.9 1065 TYR633 C5 Chain B: ASP677 L ARG691 A ASP677 L ARG691 A -5 309 LYS698 L -5 309 LYS698 L -7.1 470 ASN268 S C2 Chain A: LEU201 A -5.3 215 CYS229 T C3 C1 Chain A:	RG562 GLU586 ASN588 PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
-5.1 1855 THR589 C4 GLN494 A VAL504 I ASP576 L LEU597 A LEU597 A -6.9 1065 TYR633 C5 Chain B: I ASP677 L ASP677 L ASP677 L ARG691 A -5 309 LYS698 L P53 C1 Chain A: 1 ARG110 I LEU114 F ALA129 A ASN268 S C2 Chain A: 1 -5.3 215 CYS229 T C3 C1 PR0152 P	PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
C4 Chain A: GLN494 A VAL504 I ASP576 L LEU597 A -6.9 1065 TYR633 C5 Chain B: LEU597 A -5 309 LYS698 L -5 309 LYS698 L -5 309 LYS698 L -7.1 470 ASN268 S C2 Chain A: LEU201 A LEU201 A C3 C1 Chain A: PR0152 P	PHE468 THR491 GLN493 LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
-6.9 1065 GLN494 A VAL504 I ASP576 L LEU597 A LEU597 A C5 Chain B: I -5 309 P53 C1 -7.1 470 ASN268 S C2 Chain A: I -5.3 215 CYS229 T C3 C1	LA497 ASN500 GLU501 LE573 HIS574 ARG575 YS578 ASP594 GLY596
-6.9 1065 VAL504 I ASP576 L LEU597 A LEU597 A LEU597 A C5 Chain B: I -5 309 LYS698 L ARG691 A -5 309 P53 C1 -7.1 470 ARG110 I LEU114 F ALA129 A -7.1 470 ASN268 S C2 Chain A: 1 LEU201 A TYR220 C -5.3 215 CYS229 T C3 Chain A: 1	LE573 HIS574 ARG575 YS578 ASP594 GLY596
-6.9 1065 TYR633 C5 Chain B: 1 ASP677 L ASP677 L ARG691 A -5 309 LEU114 F ALA129 A -7.1 470 ASN268 S C2 Chain A: 1 -5.3 215 C3 C1	YS578 ASP594 GLY596
-6.9 1065 LEU597 A C5 Chain B: 1 ASP677 L ARG691 A -5 309 LYS698 L P53 C1 C2 Chain A: 1 ARG110 I LEU114 H ALA129 A C2 Chain A: 1 C3 C1	
-6.9 1065 TYR633 C5 Chain B: 1 ASP677 L ARG691 A -5 309 LYS698 L ARG110 I LEU114 H ALA129 A -7.1 470 ASN268 S C2 Chain A: 1 LEU201 A TYR220 C -5.3 215 CYS229 T C3 Chain A: 1	
-6.9 1065 14 R633 C5 Chain B: 1 ASP677 L ARG691 A ARG691 A -5 309 LYS698 L P53 C1 Chain A: 1 ARG110 I LEU114 F ALA129 A -7.1 470 ASN268 S C2 Chain A: 1 -5.3 215 CYS229 T C3 Chain A: 1	LA398 111K399 SER014
C5 Chain B: 1 ASP677 L ARG691 A -5 309 LYS698 L P53 C1 C1 Chain A: 1 ARG110 L LEU114 H ALA129 A C2 Chain A: 1 LEU201 A TYR220 C -5.3 215 C3 Chain A: 1 PR0152 P	
-5 309 ASP677 L -5 309 LYS698 L P53 C1 Chain A: ARG110 L LEU114 H ALA129 A -7.1 470 ASN268 S C2 Chain A: LEU201 A -5.3 215 CYS229 T C3 Chain A: PR0152 P	LEU674 SER675 PRO676
-5 309 ARG691 A LYS698 L P53 C1 Chain A: ARG110 I LEU114 H ALA129 A -7.1 470 ASN268 S C2 Chain A: LEU201 A TYR220 C Chain A: LEU201 A TYR220 C -5.3 215 CYS229 T C3 Chain A: PRO152 P	EU678 LYS687 LYS690
-5 309 LYS698 L P53 C1 Chain A: ARG110 I LEU114 H ALA129 A -7.1 470 ASN268 S C2 Chain A: LEU201 A TYR220 C -5.3 215 CYS229 T C3 Chain A: LEU201 A CYS22 C	LA694 GLU695 LEU697
P53 C1 Chain A: 1 ARG110 I LEU114 H ALA129 A -7.1 470 ASN268 S C2 Chain A: 1 ALA129 A -7.1 470 ASN268 S C2 Chain A: 1 LEU201 A -5.3 215 CYS229 T C3 Chain A: 1 PR0152 P	YS699
-7.1 470 ARG110 I -7.1 470 ASN268 S C2 Chain A: LEU201 A -5.3 215 CYS229 T C3 Chain A: PR0152 P	THR102 GLN104 PHE109
-7.1 470 LEU114 H ALA129 A ASN268 S C2 Chain A: LEU201 A TYR220 C -5.3 215 C3 Chain A: PRO152 P	EU111 GLY112 PHE113
-7.1 470 ALA129 A -7.1 470 ASN268 S C2 Chain A: LEU201 A -5.3 215 CYS229 T C3 Chain A: PR0152 P	IS115 TYR126 PRO128
-7.1 470 ASN268 S C2 Chain A: LEU201 A -5.3 215 CYS229 T C3 Chain A: PR0152 P	SN131 GI N144 TRP146
C2 Chain A: LEU201 A TYR220 C -5.3 215 C3 Chain A: PRO152 P	FR 269
C2 CHain A. LEU201 A TYR220 C -5.3 215 CYS229 T C3 Chain A: PRO152 P	EU145 VAL 157 CL V100
-5.3 215 CYS229 T C3 Chain A: PRO152 P	$\frac{1}{2} = \frac{1}{2} = \frac{1}$
-5.3 215 CYS229 T C3 CA PRO152 P	KG202 VAL218 PRO219
C3 -5.3 215 CYS229 1 C3 Chain A: PRO152 P	LU221 PRO222 PRO223
C3 Chain A: PRO152 P	HR230 THR231 ILE232
PRO152 P	LEU145 THR150 PRO151
	RO153 VAL157 VAL197
GLU198 C	LY199 LEU201 ARG202
VAL218 F	RO219 TYR220 GLU221
PRO222 P	RO223 CYS229 THR230
-6 208 THR231 I	E232 HIS233
C4 Chain A:	SER95 SER96 VAL 97 PRO98
	S101 TVD 102 ADC 159
	$\frac{1}{1} \frac{1}{1} \frac{1}$
ARG213 S	EK215 1HK256 GLU258
SER261 G	· · · · · · · · · · · · · · · · · · ·
-6.1 127 ARG267	LY 262 ASN263 LEU264
C5 Chain A:	LY 262 ASN263 LEU264
	LY 262 ASN263 LEU264 [RP146 VAL147 ASP148
SER149 T	LY 262 ASN263 LEU264 [RP146 VAL147 ASP148 HR150 PRO151 PRO152
SER149 T PRO153 T	LY 262 ASN263 LEU264 [RP146 VAL147 ASP148 HR150 PRO151 PRO152 YR220 GLU221 PRO222
-6.1 127 ARG267 C5 C5 CARCELLS SER261 G C5 C5 Chain A: 127	

BSA	C1			Chain A: TYR156 LYS187 THR190
				SER191 ARG194 ARG198 TRP213
				ARG217 GLN220 LYS221 HIS287
				ALA290 GLU291 VAL292 GLU293
				LYS294 PRO338 GLU339 TYR340
				ALA341 VAL342 ARG435 LYS439
				GLU443 PRO446 CYS447 ASP450
		-7.5	8389	TYR451
	C2			Chain A: ASP108 SER109 PRO110
				ASP111 LEU112 PRO113 LYS114
				ARG144 HIS145 PRO146 ARG185
				GLU186 LEU189 THR190 SER192
				ALA193 ARG196 PRO420 GLU424
				SER428 LYS431 ARG435 TYR451
				LEU454 ILE455 ARG458 GLU519
		-10.2	3498	ILE522
	C3			Chain A: PHE501 GLU503 LYS504
				PHE506 THR507 HIS509 GLU564
				PHE567 ALA568 GLY571 PRO572
		-5.2	1508	VAL575 VAL576 GLN579
	C4			Chain A: PRO96 GLU100 SER104
				HIS105 LYS106 ASP108 TYR147
				ARG196 ILE202 GLN203 LYS204
				LYS242 CYS245 HIS246 GLU464
		-6.2	793	LYS465
	C5			Chain A: GLU382 PRO383 ASN385
				LEU386 GLN389 ASN390 GLN393
				VAL408 ARG409 ARG412 LYS413
				ARG484 PRO485 PHE487 SER488
				ALA489 LEU490 THR491 PRO492
		-6.8	356	GLU540