Supporting Information

Zinc Oxide Calotropis procera Flower Extracts: A Green Approach to Pineapple Nano Leaves for Biological Applications

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I. Satistical Analysis

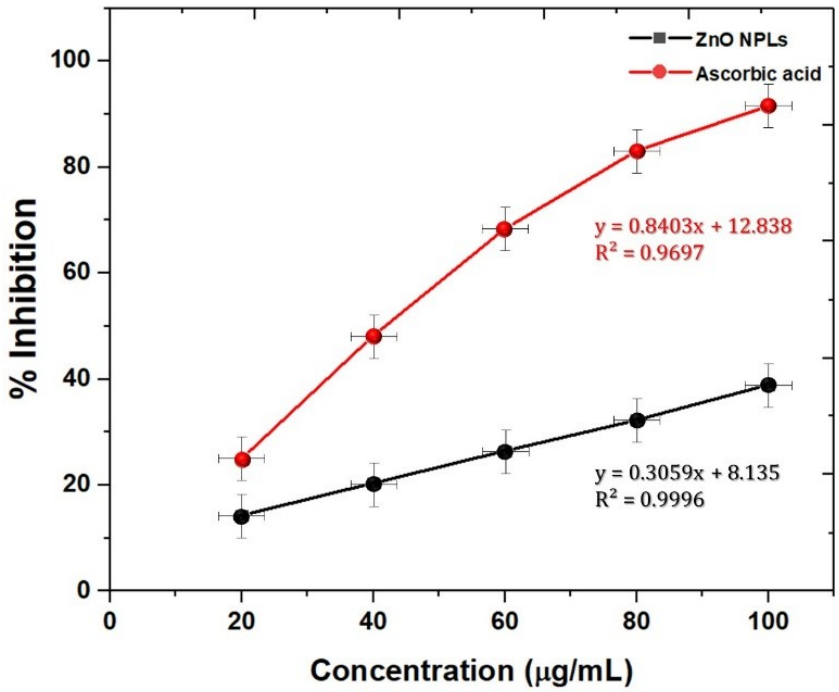


Fig. SI-1. DPPH radical scavenging activity in a dose-dependent manner of green synthesized ZnO NPLs using *C. procera* flower extract. Ascorbic acid is treated as a positive control. Experiments performed in triplicates and using one-way ANOVA indicate that all values are significant ($p < 0.05$).

Table SI-1. Statistical evaluation of DPPH radical scavenging activity.

Concentration of ZnO PNLs (µg/mL)	Mean OD @ 517 nm ± SD (ZnO NPLs)	Mean OD @ 517 nm ± SD (Ascorbic Acid)	t-value	p-value	Significance
20	0.144 ± 0.0008	0.285 ± 0.0003	25.72	1.36×10^{-5}	***
40	0.134 ± 0.0008	0.228 ± 0.0003	37.97	2.87×10^{-6}	***
60	0.116 ± 0.0008	0.171 ± 0.0003	48.99	1.04×10^{-6}	***
80	0.125 ± 0.0008	0.114 ± 0.0003	60.01	4.62×10^{-7}	***
100	0.105 ± 0.0008	0.078 ± 0.0003	73.48	2.06×10^{-7}	***

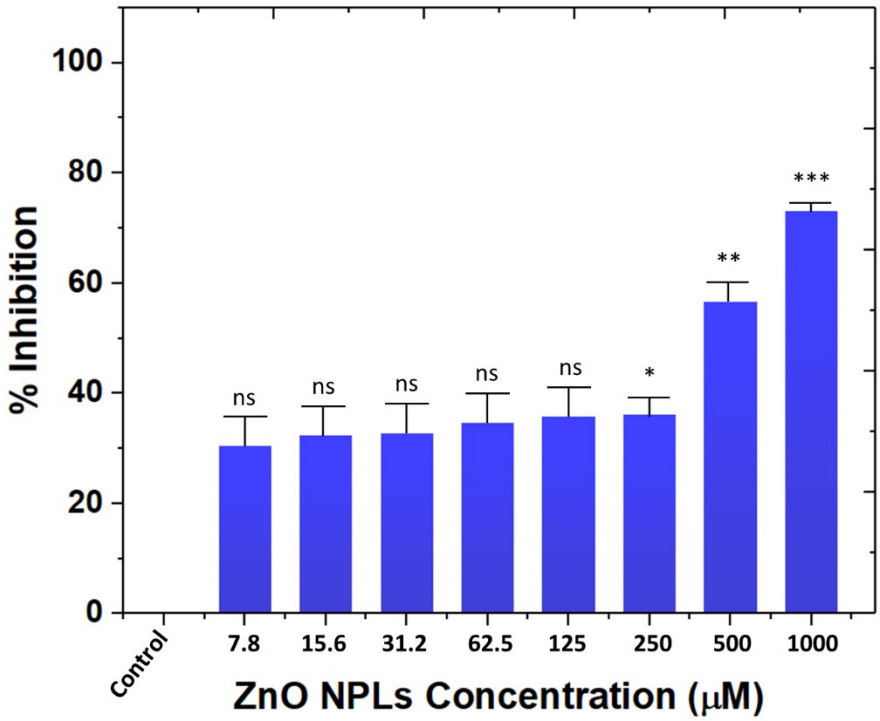
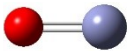
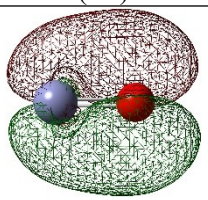
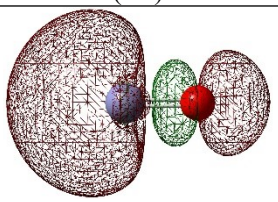
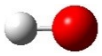
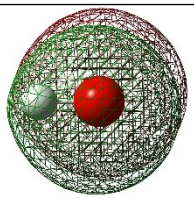
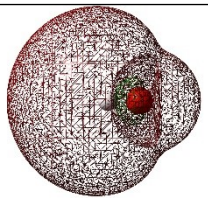
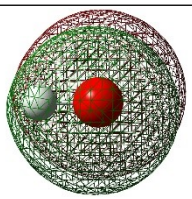
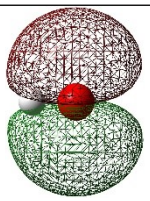
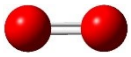
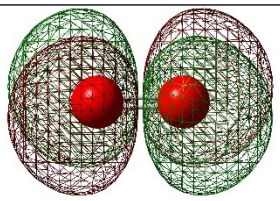
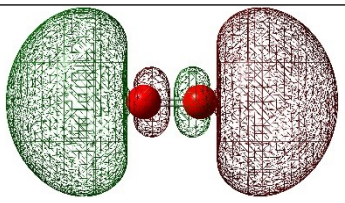
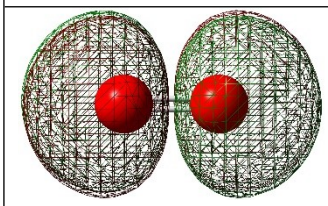
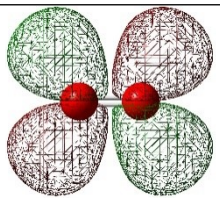


Fig. SI-2. Determination of Minimum Inhibitory Concentration (MIC) for ZnO NPLs, where all values represent mean (n = 3) ± Standard Error of the Mean. One way ANOVA was applied to compare treatments with control where P value vs control: *< 0.05, **< 0.01, ***< 0.001, ns = not significant.

II. Density Function Studies

Table *SI-2*. The Optimized molecular structure of zinc oxide, hydroxyl radical & superoxide radical using B3LYP/6-31G level of theory in Gaussian 09 program. The corresponding frontier highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) diagrams and band gap energies.

Compound	**Optimized Structure**	**HOMO** (eV)	**LUMO** (eV)	**Bang Gap** (eV)
Zinc oxide		 -6.99	 -4.59	2.40
Hytdroxyl radical		 Alpha MOs -9.67	 Alpha MOs -0.53	9.14
		 Beta MOs -8.93	 Beta MOs -5.05	3.88
Superoxide radical		 Alpha MOs 1.72	 Alpha 7.62	-5.9
		 Beta MOs 2.16	 Beta 4.94	-2.78

III. Docking studies

Table *SI-3*. The calculated binding affinity and the corresponding RMSD values of different poses of zinc oxide , hydroxyl radical and superoxide radical against (i) PI3K (Phosphoinositide 3-kinase, Pdb: 8SO9), (ii) c-Kit receptor (Pdb: 6GQJ), (iii) MEK1 (Mitogen-Activated Protein Kinase Kinase, Pdb: 4U7Z), (iv) PIP5K1α (Phosphatidylinositol-4-phosphate 5-kinase type 1alpha, Pdb: 4TZ7), (v) MAPK (Mitogen-Activated Protein Kinase, pdb: 3RP9), (vi) c-Met/MET receptor (mesenchymal-epithelial transition factor, pdb: 3DKF), (vii) mTOR (mammalian target of rapamycin, pdb: 2NPU), (viii) CDK2 (Cyclin dependent kinase 2, pdb: 2M1L), (ix) VEGFR (Vascular Endothelial Growth Factor Receptor, Pdb: 1QTY), (x) EGFR (Epidermal Growth Factor Receptor, Pdb: 1M17), and (xi) FGFR (Fibroblast Growth Factor Receptor, Pdb: 1AGW) protease by using Auto Dock Vina program.

Mode	**Zinc oxide – 8so9 A chain**			Mode	**Zinc oxide – 8so9 B chain**		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.3	0.000	0.000	1	-2.2	0.000	0.000
2	-2.1	4.878	4.878	2	-2.2	23.735	23.735
3	-2.1	2.243	2.243	3	-2.2	10.899	10.899
4	-2.1	15.848	15.848	4	-2.1	27.900	27.900
5	-2.0	6.551	6.551	5	-2.1	15.629	15.629
6	-2.0	6.949	6.949	6	-2.1	22.977	22.977
7	-2.0	4.433	4.433	7	-2.0	12.977	12.977
8	-1.9	8.043	8.043	8	-1.9	14.179	14.179
9	-1.9	18.274	18.274	9	-1.8	27.989	27.989
Inhibition Constant: 20.52 mM				**Inhibition Constant: 24.30 mM**			

Mode	**Zinc oxide – 6gqj A chain**			Mode	**Zinc oxide – 6gqj B chain**		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.2	0.000	0.000	1	-2.3	0.000	0.000
2	-2.2	10.500	10.500	2	-2.1	12.698	12.698
3	-2.1	4.035	4.035	3	-2.1	2.798	2.798
4	-2.0	3.924	3.924	4	-2.0	23.717	23.717
5	-2.0	2.747	2.747	5	-1.9	24.320	24.320
6	-2.0	10.320	10.320	6	-1.9	25.503	25.503
7	-1.9	24.320	24.320	7	-1.9	27.869	27.869
8	-1.8	17.115	17.115	8	-1.8	22.793	22.793
9	-1.8	9.971	9.971	9	-1.8	20.724	20.724
Inhibition Constant: 24.30 mM				**Inhibition Constant: 20.52 mM**			

Mode	**Zinc oxide – 4u7z**			Mode	**Zinc oxide – 4tz7 A chain**		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.4	0.000	0.000	1	-1.9	0.000	0.000
2	-2.3	1.887	1.887	2	-1.9	17.365	17.365
3	-2.0	3.281	3.281	3	-1.9	2.399	2.399
4	-2.0	23.240	23.240	4	-1.9	18.531	18.531
5	-2.0	29.047	29.047	5	-1.9	4.943	4.943
6	-1.9	12.698	12.698	6	-1.8	2.742	2.742
7	-1.9	16.634	16.634	7	-1.8	20.136	20.136
8	-1.8	15.806	15.806	8	-1.8	10.683	10.683
9	-1.8	11.531	11.531	9	-1.7	13.015	13.015
Inhibition Constant: 17.33 mM				**Inhibition Constant: 40.34 mM**			

Mode	Zinc oxide – 3rp9 A chain			Mode	Zinc oxide – 3dkf		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.4	0.000	0.000	1	-2.3	0.000	0.000
2	-2.3	11.189	11.189	2	-2.2	23.254	23.254
3	-2.1	15.127	15.127	3	-2.1	23.586	23.586
4	-2.1	8.496	8.496	4	-2.1	4.276	4.276
5	-2.0	9.548	9.548	5	-2.0	3.882	3.882
6	-2.0	18.318	18.318	6	-2.0	24.435	24.435
7	-1.9	2.002	2.002	7	-1.9	2.032	2.032
8	-1.9	8.647	8.647	8	-1.9	36.121	36.121
9	-1.9	14.920	14.920	9	-1.9	2.419	2.419
Inhibition Constant: 17.33 mM				**Inhibition Constant: 20.52 mM**			

Mode	Zinc oxide – 2npu A chain			Mode	Zinc oxide – 2m1l A chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.4	0.000	0.000	1	-1.7	0.000	0.000
2	-2.3	11.163	11.163	2	-1.6	15.528	15.528
3	-2.1	15.134	15.134	3	-1.5	4.463	4.463
4	-2.0	14.916	14.916	4	-1.5	2.137	2.137
5	-1.9	13.329	13.329	5	-1.4	15.701	15.701
6	-1.9	8.672	8.672	6	-1.4	17.870	17.870
7	-1.9	14.995	14.995	7	-1.4	5.289	5.289
8	-1.9	15.875	15.875	8	-1.4	7.101	7.101
9	-1.8	16.421	16.421	9	-1.4	8.736	8.736
Inhibition Constant: 17.33 mM				**Inhibition Constant: 56.56 mM**			

Mode	Zinc oxide – 2m1l B chain			Mode	Zinc oxide – 1qty R chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-1.8	0.000	0.000	1	-1.8	0.000	0.000
2	-1.7	19.346	19.346	2	-1.8	9.545	9.545
3	-1.6	12.056	12.056	3	-1.6	13.904	13.904
4	-1.6	3.883	3.883	4	-1.5	21.496	21.496
5	-1.5	4.699	4.699	5	-1.5	26.565	26.565
6	-1.5	19.257	19.257	6	-1.4	3.409	3.409
7	-1.5	30.721	30.721	7	-1.4	14.964	14.964
8	-1.4	11.066	11.066	8	-1.4	2.292	2.292
9	-1.4	23.427	23.427	9	-1.4	24.893	24.893
Inhibition Constant: 47.77 mM				**Inhibition Constant: 47.77 mM**			

Mode	Zinc oxide – 1qty S chain			Mode	Zinc oxide – 1qty T chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-1.9	0.000	0.000	1	-2.1	0.000	0.000
2	-1.6	23.527	23.527	2	-1.9	14.150	14.150
3	-1.6	26.983	26.983	3	-1.8	12.294	12.294
4	-1.5	2.462	2.462	4	-1.7	13.280	13.280
5	-1.5	13.816	13.816	5	-1.7	6.416	6.416
6	-1.4	3.409	3.409	6	-1.6	15.323	15.323
7	-1.4	23.502	23.502	7	-1.6	14.916	14.916
8	-1.4	12.750	12.750	8	-1.6	13.660	13.660
9	-1.3	19.758	19.758	9	-1.6	17.972	17.972
Inhibition Constant: 40.34 mM				**Inhibition Constant: 28.77 mM**			

Mode	Zinc oxide – 1qty U chain			Mode	Zinc oxide – 1qty V chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.2	0.000	0.000	1	-1.9	0.000	0.000
2	-1.9	6.560	6.560	2	-1.9	9.250	9.250
3	-1.9	12.221	12.221	3	-1.8	23.126	23.126
4	-1.9	6.267	6.267	4	-1.6	30.351	30.351
5	-1.9	6.423	6.423	5	-1.6	13.933	13.933
6	-1.9	8.114	8.114	6	-1.6	29.210	29.210
7	-1.7	22.182	22.182	7	-1.5	28.792	28.792
8	-1.6	23.542	23.542	8	-1.5	3.252	3.252
9	-1.6	10.773	10.773	9	-1.5	4.132	4.132
Inhibition Constant: 24.30 mM				**Inhibition Constant: 40.34 mM**			

Mode	Zinc oxide – 1qty W chain			Mode	Zinc oxide – 1qty X chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-1.7	0.000	0.000	1	-1.9	0.000	0.000
2	-1.7	12.550	12.550	2	-1.8	14.883	14.883
3	-1.7	23.772	23.772	3	-1.8	13.947	13.947
4	-1.7	30.360	30.360	4	-1.7	14.827	14.827
5	-1.6	13.984	13.984	5	-1.6	21.536	21.536
6	-1.5	23.439	23.439	6	-1.6	17.525	17.525
7	-1.5	27.361	27.361	7	-1.6	14.439	14.439
8	-1.5	21.732	21.732	8	-1.5	21.595	21.595
9	-1.4	2.973	2.973	9	-1.5	17.198	17.198
Inhibition Constant: 56.56 mM				**Inhibition Constant: 40.34 mM**			

Mode	Zinc oxide – 1qty Y chain			Mode	Zinc oxide – 1m17		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.2	0.000	0.000	1	-1.7	0.000	0.000
2	-1.8	14.337	14.337	2	-1.6	15.528	15.528
3	-1.7	12.199	12.199	3	-1.5	4.463	4.463
4	-1.7	10.689	10.689	4	-1.5	2.137	2.137
5	-1.6	22.417	22.417	5	-1.4	15.701	15.701
6	-1.6	12.880	12.880	6	-1.4	17.870	17.870
7	-1.5	13.845	13.845	7	-1.4	5.289	5.289
8	-1.5	17.545	17.545	8	-1.4	7.101	7.101
9	-1.4	17.514	17.514	9	-1.4	8.736	8.736
Inhibition Constant: 24.30 mM				**Inhibition Constant: 56.56 mM**			

Mode	Zinc oxide – 1agw A chain			Mode	Zinc oxide – 1agw B chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.3	0.000	0.000	1	-2.3	0.000	0.000
2	-2.1	1.735	1.735	2	-2.1	1.752	1.752
3	-2.0	17.744	17.744	3	-2.0	9.160	9.160
4	-1.9	3.322	3.322	4	-2.0	5.148	5.148
5	-1.8	22.923	22.923	5	-2.0	17.750	17.750
6	-1.7	33.151	33.151	6	-1.9	3.327	3.327
7	-1.7	32.340	32.340	7	-1.8	22.933	22.933
8	-1.7	12.781	12.781	8	-1.8	36.762	36.762
9	-1.6	10.902	10.902	9	-1.8	32.864	32.864
Inhibition Constant: 20.52 mM				**Inhibition Constant: 20.52 mM**			

Mode	Hydroxy radical – 8so9 A chain			Mode	Hydroxy radical – 8so9 B chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-1.8	0.000	0.000	1	-1.6	0.000	0.000
2	-1.8	32.801	32.801	2	-1.5	12.165	12.165
3	-1.6	23.527	23.527	3	-1.5	29.984	29.984
4	-1.6	18.342	18.342	4	-1.5	24.515	24.515
5	-1.6	30.326	30.326	5	-1.4	19.057	19.057
6	-1.5	10.137	10.137	6	-1.4	34.863	34.863
7	-1.5	26.906	26.906	7	-1.3	18.863	18.863
8	-1.5	14.333	14.333	8	-1.3	17.990	17.990
9	-1.4	17.210	17.210	9	-1.3	20.248	20.248
Inhibition Constant: 47.77 mM				**Inhibition Constant: 66.97 mM**			

Mode	Hydroxy radical – 6gqj A chain			Mode	Hydroxy radical – 6gqj B chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-1.8	0.000	0.000	1	-1.8	0.000	0.000
2	-1.5	14.577	14.577	2	-1.5	12.914	12.914
3	-1.5	9.179	9.179	3	-1.5	14.572	14.572
4	-1.5	12.989	12.989	4	-1.4	9.717	9.717
5	-1.5	13.151	13.151	5	-1.3	13.146	13.146
6	-1.4	15.538	15.538	6	-1.3	18.665	18.665
7	-1.4	9.417	9.417	7	-1.3	11.214	11.214
8	-1.4	12.661	12.661	8	-1.2	8.798	8.798
9	-1.4	15.385	15.385	9	-1.2	21.425	21.425
Inhibition Constant: 47.77 mM				**Inhibition Constant: 47.77 mM**			

Mode	Hydroxy radical – 4u7z			Mode	Hydroxy radical – 4tz7 A chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-1.5	0.000	0.000	1	-1.4	0.000	0.000
2	-1.4	15.016	15.016	2	-1.3	8.674	8.674
3	-1.3	21.754	21.754	3	-1.3	22.192	22.192
4	-1.3	23.188	23.188	4	-1.3	30.200	30.200
5	-1.3	20.378	20.378	5	-1.3	11.304	11.304
6	-1.3	3.993	3.993	6	-1.3	24.913	24.913
7	-1.3	21.707	21.707	7	-1.3	8.631	8.631
8	-1.2	13.358	13.358	8	-1.2	24.514	24.514
9	-1.2	19.634	19.634	9	-1.2	27.531	27.531
Inhibition Constant: 79.29 mM				**Inhibition Constant: 93.89 mM**			

Mode	Hydroxy radical – 3rp9 A chain			Mode	Hydroxy radical – 3dkf		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-1.9	0.000	0.000	1	-1.6	0.000	0.000
2	-1.9	16.742	16.742	2	-1.6	18.526	18.526
3	-1.8	2.690	2.690	3	-1.5	7.408	7.408
4	-1.6	14.695	14.695	4	-1.5	18.721	18.721
5	-1.6	15.346	15.346	5	-1.5	7.101	7.101
6	-1.5	7.097	7.097	6	-1.4	23.722	23.722
7	-1.5	8.020	8.020	7	-1.4	19.212	19.212
8	-1.5	16.717	16.717	8	-1.4	23.452	23.452
9	-1.5	9.928	9.928	9	-1.3	21.498	21.498
Inhibition Constant: 40.34 mM				**Inhibition Constant: 66.97 mM**			

Mode	Hydroxy radical – 2npu A chain			Mode	Hydroxy radical - 2m1l A chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-1.9	0.000	0.000	1	-1.3	0.000	0.000
2	-1.9	16.742	16.742	2	-1.3	4.109	4.109
3	-1.8	2.690	2.690	3	-1.1	4.375	4.375
4	-1.6	13.261	13.261	4	-1.1	2.538	2.538
5	-1.6	14.695	14.695	5	-1.1	18.751	18.751
6	-1.5	7.096	7.096	6	-1.0	22.009	22.009
7	-1.5	7.072	7.072	7	-1.0	15.155	15.155
8	-1.5	8.020	8.020	8	-1.0	23.555	23.555
9	-1.5	9.928	9.928	9	-1.0	32.169	32.169
Inhibition Constant: 40.34 mM				**Inhibition Constant: 111.18 µM**			

Mode	Hydroxy radical – 2m1l B chain			Mode	Hydroxy radical – 1qty R chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-1.3	0.000	0.000	1	-1.4	0.000	0.000
2	-1.2	22.789	22.789	2	-1.1	35.148	35.148
3	-1.1	9.410	9.410	3	-1.1	24.952	24.952
4	-1.1	12.454	12.454	4	-1.1	20.102	20.102
5	-1.0	17.458	17.458	5	-1.0	28.955	28.955
6	-1.0	20.939	20.939	6	-1.0	2.173	2.173
7	-1.0	8.333	8.333	7	-1.0	30.666	30.666
8	-1.0	9.325	9.325	8	-1.0	8.980	8.980
9	-1.0	12.330	12.330	9	-1.0	23.720	23.720
Inhibition Constant: 111.18 mM				**Inhibition Constant: 93.89 mM**			

Mode	Hydroxy radical – 1qty S chain			Mode	Hydroxy radical – 1qty T chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-1.5	0.000	0.000	1	-1.8	0.000	0.000
2	-1.2	15.102	15.102	2	-1.7	14.655	14.655
3	-1.1	8.685	8.685	3	-1.5	18.697	18.697
4	-1.1	35.205	35.205	4	-1.3	18.034	18.034
5	-1.1	37.246	37.246	5	-1.3	12.924	12.924
6	-1.1	22.450	22.450	6	-1.3	11.500	11.500
7	-1.0	10.981	10.981	7	-1.2	12.427	12.427
8	-1.0	28.744	28.744	8	-1.2	4.845	4.845
9	-1.0	29.074	29.074	9	-1.2	6.113	6.113
Inhibition Constant: 79.29 mM				**Inhibition Constant: 47.77 mM**			

Mode	Hydroxy radical – 1qty U chain			Mode	Hydroxy radical – 1qty V chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-1.7	0.000	0.000	1	-1.5	0.000	0.000
2	-1.6	14.800	14.800	2	-1.3	31.083	31.083
3	-1.4	9.070	9.070	3	-1.1	14.814	14.814
4	-1.4	6.153	6.153	4	-1.1	21.901	21.901
5	-1.4	18.904	18.904	5	-1.1	22.474	22.474
6	-1.3	20.725	20.725	6	-1.0	17.855	17.855
7	-1.3	11.583	11.583	7	-1.0	28.886	28.886
8	-1.2	9.232	9.232	8	-1.0	25.173	25.173
9	-1.2	4.111	4.111	9	-0.9	30.608	30.608
Inhibition Constant: 56.56 mM				**Inhibition Constant: 79.29 mM**			

Mode	**Hydroxy radical – 1qty W chain** Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b	Mode	**Hydroxy radical – 1qty X chain** Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-1.3	0.000	0.000	1	-1.8	0.000	0.000
2	-1.2	20.112	20.112	2	-1.6	18.386	18.386
3	-1.2	17.939	17.939	3	-1.5	14.562	14.562
4	-1.1	15.189	15.189	4	-1.4	11.330	11.330
5	-1.1	14.414	14.414	5	-1.2	18.949	18.949
6	-1.0	5.561	5.561	6	-1.2	12.724	12.724
7	-1.0	14.030	14.030	7	-1.2	12.221	12.221
8	-1.0	16.264	16.264	8	-1.2	12.791	12.791
9	-1.0	15.496	15.496	9	-1.1	12.424	12.424
Inhibition Constant: 111.18 mM				**Inhibition Constant: 47.77 mM**			

Mode	**Hydroxy radical – 1qty Y chain** Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b	Mode	**Hydroxy radical – 1m17** Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-1.9	0.000	0.000	1	-1.4	0.000	0.000
2	-1.6	14.748	14.748	2	-1.3	8.257	8.257
3	-1.4	18.408	18.408	3	-1.2	22.676	22.676
4	-1.3	11.765	11.765	4	-1.2	19.549	19.549
5	-1.3	13.179	13.179	5	-1.2	31.076	31.076
6	-1.3	12.749	12.749	6	-1.2	18.032	18.032
7	-1.2	18.311	18.311	7	-1.1	7.386	7.386
8	-1.1	20.020	20.020	8	-1.1	24.419	24.419
9	-1.1	12.279	12.279	9	-1.1	27.193	27.193
Inhibition Constant: 40.34 mM				**Inhibition Constant: 93.89 mM**			

Mode	**Hydroxy radical** – 1agw A chain Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b	Mode	**Hydroxy radical – 1agw B chain** Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-1.6	0.000	0.000	1	-1.4	0.000	0.000
2	-1.4	18.865	18.865	2	-1.4	32.249	32.249
3	-1.4	33.499	33.499	3	-1.4	36.585	36.585
4	-1.4	32.827	32.827	4	-1.4	29.335	29.335
5	-1.4	13.849	13.849	5	-1.4	25.239	25.239
6	-1.4	31.253	31.253	6	-1.4	32.607	32.607
7	-1.4	36.942	36.942	7	-1.4	32.720	32.720
8	-1.3	27.613	27.613	8	-1.3	39.083	39.083
9	-1.3	22.325	22.325	9	-1.3	20.937	20.937
Inhibition Constant: 66.97 mM				**Inhibition Constant: 93.89 mM**			

Mode	Superoxide radical– 8so9 A chain			Mode	Superoxide radical – 8so9 B chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.6	0.000	0.000	1	-2.6	0.000	0.000
2	-2.6	0.011	0.011	2	-2.4	32.885	32.885
3	-2.0	13.749	13.749	3	-2.1	30.879	30.879
4	-1.9	17.469	17.469	4	-2.1	21.491	21.491
5	-1.9	12.261	12.261	5	-1.8	19.511	19.511
6	-1.8	12.072	12.072	6	-1.8	13.631	13.631
7	-1.7	12.362	12.362	7	-1.8	37.384	37.384
8	-1.6	10.076	10.076	8	-1.7	14.481	14.481
9	-1.6	20.799	20.799	9	-1.7	17.884	17.884
Inhibition Constant: 12.36 mM				**Inhibition Constant: 12.36 mM**			

Mode	Superoxide radical – 6gqj A chain			Mode	Superoxide radical – 6gqj B chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.3	0.000	0.000	1	-2.2	0.000	0.000
2	-2.2	1.831	2.275	2	-2.2	13.148	13.148
3	-2.2	9.722	10.283	3	-1.9	11.810	11.810
4	-2.1	23.906	24.322	4	-1.9	12.653	12.653
5	-2.0	11.596	11.661	5	-1.8	8.488	8.488
6	-1.9	5.797	5.797	6	-1.7	11.949	11.949
7	-1.9	8.384	8.851	7	-1.7	19.513	19.513
8	-1.9	20.494	20.808	8	-1.7	6.910	6.910
9	-1.8	18.881	18.893	9	-1.6	13.462	13.462
Inhibition Constant: 20.52 mM				**Inhibition Constant: 24.30 mM**			

Mode	Superoxide radical – 4u7z			Mode	Superoxide radical – 4tz7 A chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.3	0.000	0.000	1	-2.1	0.000	0.000
2	-2.0	28.375	28.501	2	-1.9	17.543	18.053
3	-1.9	14.824	15.240	3	-1.9	13.164	13.744
4	-1.9	2.719	2.793	4	-1.9	22.318	22.533
5	-1.8	13.765	14.271	5	-1.8	20.167	20.643
6	-1.8	13.804	14.006	6	-1.8	26.753	26.803
7	-1.8	8.315	8.423	7	-1.8	16.055	16.495
8	-1.7	13.807	13.869	8	-1.8	13.177	13.495
9	-1.7	17.093	17.407	9	-1.8	13.502	14.640
Inhibition Constant: 20.52 mM				**Inhibition Constant: 28.77 mM**			

Mode	Superoxide radical – 3rp9 A chain			Mode	Superoxide radical – 3dkf		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.2	0.000	0.000	1	-2.1	0.000	0.000
2	-2.2	34.629	34.860	2	-2.1	23.546	23.801
3	-2.1	29.646	29.809	3	-2.0	20.889	21.205
4	-2.1	21.241	21.589	4	-2.0	0.993	1.718
5	-2.0	29.976	30.022	5	-1.9	3.798	4.405
6	-2.0	28.588	28.682	6	-1.8	25.969	26.059
7	-2.0	23.183	23.199	7	-1.7	26.735	27.190
8	-1.9	27.980	28.155	8	-1.7	9.706	10.202
9	-1.9	11.594	11.712	9	-1.6	15.791	16.013
Inhibition Constant: 24.30 mM				**Inhibition Constant: 28.77 mM**			

Mode	Superoxide radical – 2npu A chain			Mode	Superoxide radical - 2m1l A chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.2	0.000	0.000	1	-1.9	0.000	0.000
2	-2.2	34.719	34.937	2	-1.7	15.030	15.315
3	-2.1	29.707	29.843	3	-1.5	6.810	7.242
4	-2.1	21.239	21.622	4	-1.5	6.302	6.383
5	-2.0	30.004	30.048	5	-1.3	15.659	16.006
6	-2.0	28.619	28.666	6	-1.3	16.685	17.051
7	-1.9	31.536	31.554	7	-1.3	17.754	18.153
8	-1.9	27.998	28.155	8	-1.2	7.037	7.078
9	-1.9	23.226	23.226	9	-1.2	18.018	18.333
Inhibition Constant: 24.30 mM				**Inhibition Constant: 40.34 mM**			

Mode	Superoxide radical – 2m1l B chain			Mode	Superoxide radical – 1qty R chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.0	0.000	0.000	1	-1.9	0.000	0.000
2	-1.6	12.181	12.386	2	-1.9	8.097	8.177
3	-1.6	19.387	19.838	3	-1.7	10.437	10.757
4	-1.5	9.203	9.533	4	-1.7	22.468	23.102
5	-1.5	14.136	14.513	5	-1.6	29.699	29.977
6	-1.4	16.291	16.665	6	-1.5	20.745	21.237
7	-1.4	31.990	32.379	7	-1.5	1.291	1.745
8	-1.3	6.033	6.081	8	-1.4	21.096	21.598
9	-1.3	17.532	17.881	9	-1.4	8.554	8.652
Inhibition Constant: 34.06 mM				**Inhibition Constant: 40.34 mM**			

Mode	Superoxide radical – 1qty S chain			Mode	Superoxide radical – 1qty T chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.0	0.000	0.000	1	-2.0	0.000	0.000
2	-1.7	10.514	10.655	2	-2.0	11.577	11.578
3	-1.6	24.106	24.406	3	-1.9	11.571	11.784
4	-1.5	10.991	11.134	4	-1.7	15.109	15.471
5	-1.5	2.983	3.239	5	-1.7	14.169	14.269
6	-1.5	16.518	16.841	6	-1.7	21.340	21.463
7	-1.4	17.774	18.061	7	-1.6	6.805	6.911
8	-1.3	17.793	18.050	8	-1.6	13.001	13.129
9	-1.3	24.946	25.220	9	-1.6	21.870	22.193
Inhibition Constant: 34.06 mM				**Inhibition Constant: 34.06 mM**			

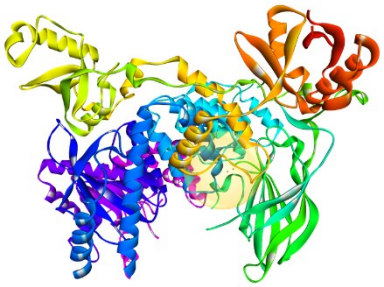
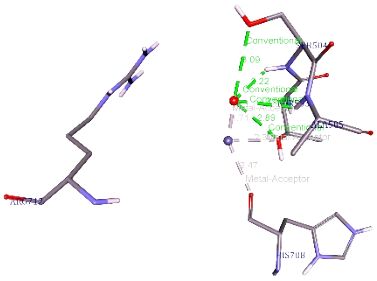
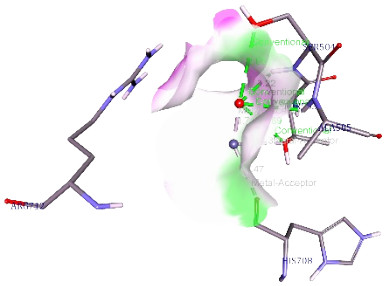
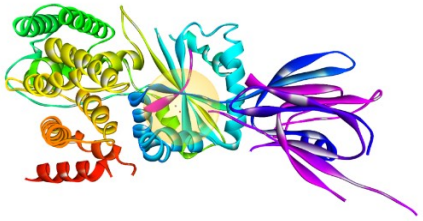
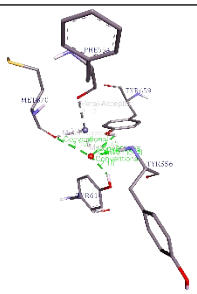
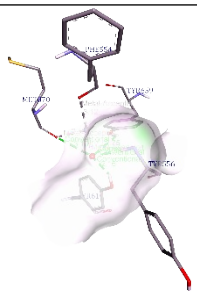
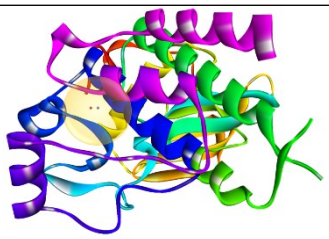
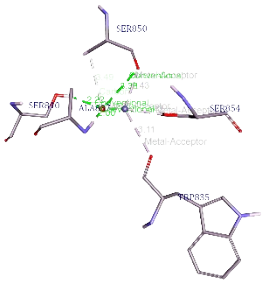
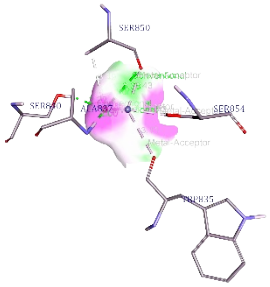
Mode	Superoxide radical – 1qty U chain			Mode	Superoxide radical – 1qty V chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.6	0.000	0.000	1	-2.6	0.000	0.000
2	-2.6	0.050	1.349	2	-2.6	0.050	1.349
3	-2.1	0.996	1.399	3	-2.1	0.996	1.399
4	-1.9	5.135	5.353	4	-1.9	5.135	5.353
5	-1.7	12.678	12.745	5	-1.7	12.678	12.745
6	-1.7	9.775	10.115	6	-1.7	9.775	10.115
7	-1.7	3.128	3.687	7	-1.7	3.128	3.687
8	-1.6	13.264	13.300	8	-1.6	13.264	13.300
9	-1.4	15.694	15.759	9	-1.4	15.694	15.759
Inhibition Constant: 12.36 mM				**Inhibition Constant: 12.36 mM**			

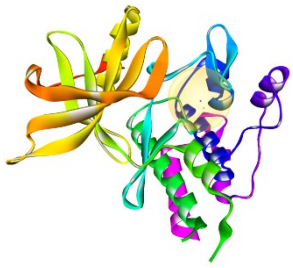
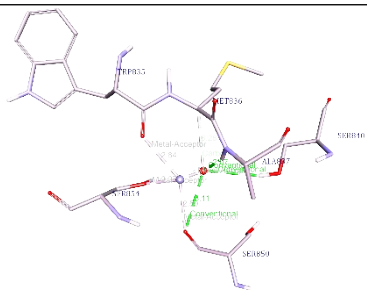
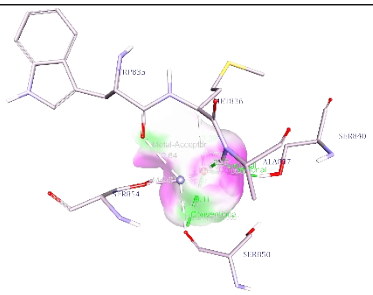
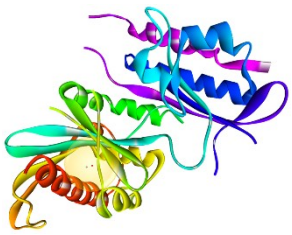
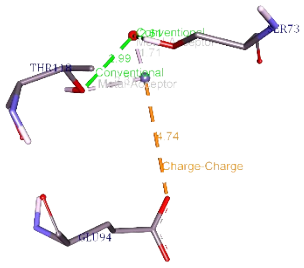
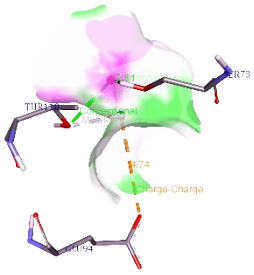
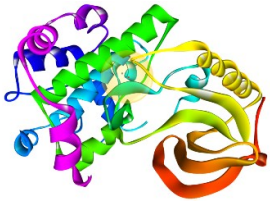
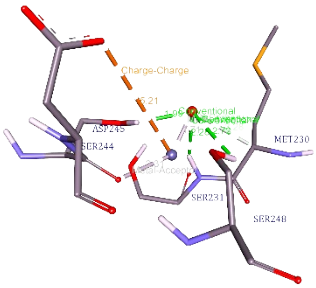
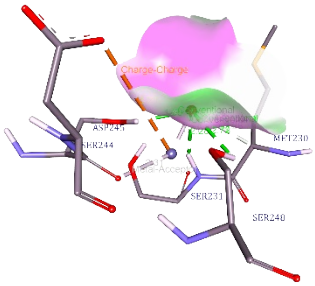
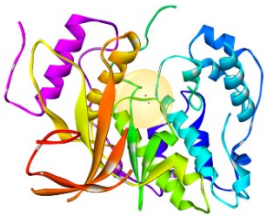
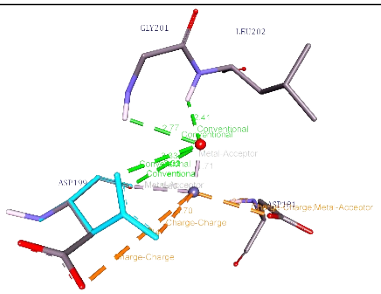
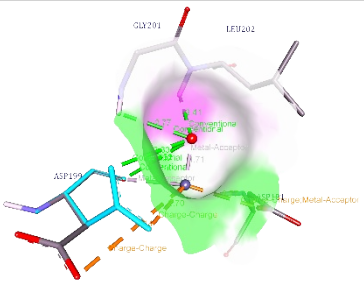
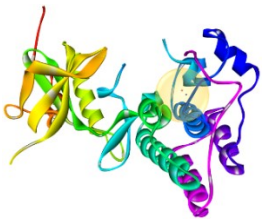
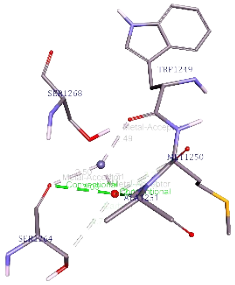
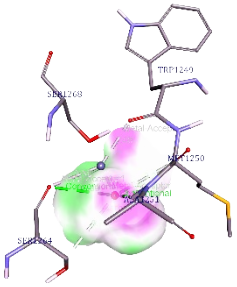
Mode	Superoxide radical – 1qty W chain			Mode	Superoxide radical – 1qty X chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-1.8	0.000	0.000	1	-2.0	0.000	0.000
2	-1.8	30.053	30.267	2	-1.8	16.910	17.212
3	-1.7	9.871	9.961	3	-1.7	18.722	18.862
4	-1.7	9.323	9.517	4	-1.6	13.468	13.794
5	-1.7	19.886	20.096	5	-1.5	15.429	15.305
6	-1.6	7.797	8.155	6	-1.5	14.180	14.305
7	-1.5	20.994	21.143	7	-1.5	14.523	14.636
8	-1.4	14.954	15.318	8	-1.5	20.305	20.583
9	-1.4	21.082	21.115	9	-1.4	21.078	21.317
Inhibition Constant: 47.77 mM				**Inhibition Constant: 34.06 mM**			

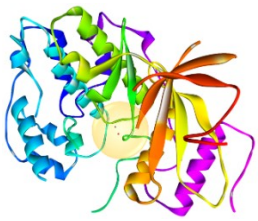
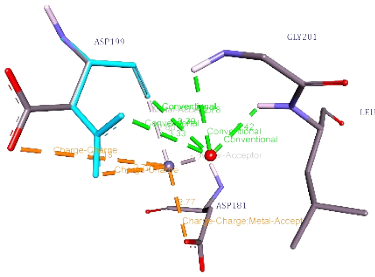
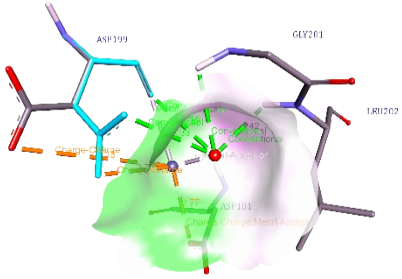
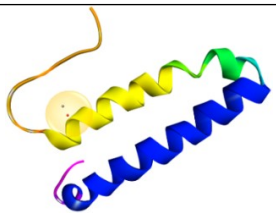
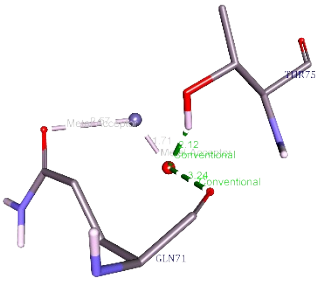
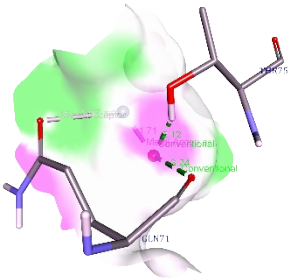
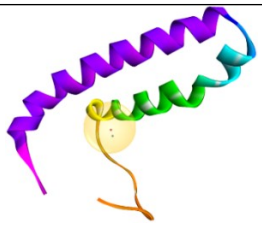
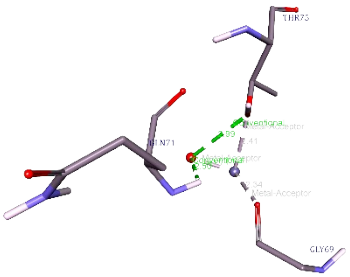
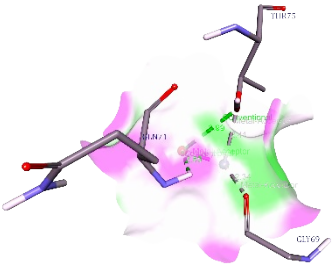
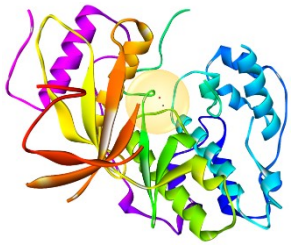
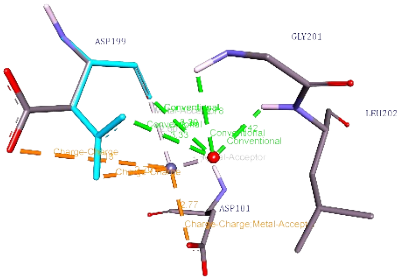
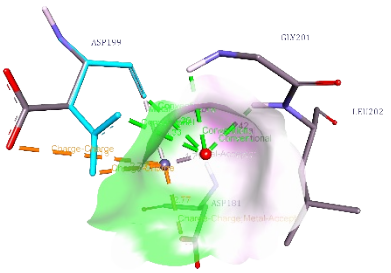
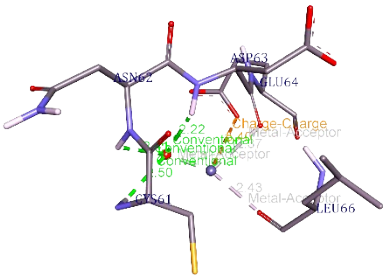
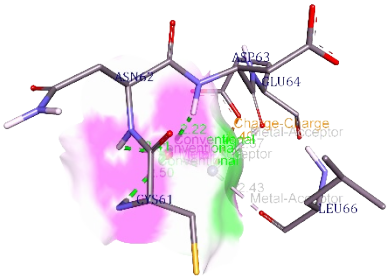
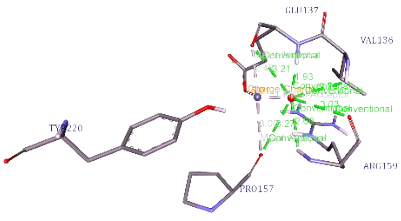
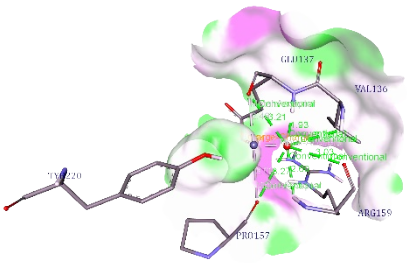
Mode	Superoxide radical – 1qty Y chain			Mode	Superoxide radical – 1m17		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.0	0.000	0.000	1	-2.0	0.000	0.000
2	-1.9	11.659	11.730	2	-1.8	7.062	7.561
3	-1.8	1.995	2.054	3	-1.6	25.650	25.994
4	-1.8	0.964	1.359	4	-1.5	13.859	13.944
5	-1.7	19.235	19.838	5	-1.5	23.327	23.352
6	-1.7	18.203	18.421	6	-1.5	21.724	22.338
7	-1.6	13.961	14.218	7	-1.5	11.784	12.178
8	-1.6	17.653	18.187	8	-1.5	15.655	15.717
9	-1.5	15.390	15.940	9	-1.4	12.293	12.541
Inhibition Constant: 34.06 mM				**Inhibition Constant: 34.06 mM**			

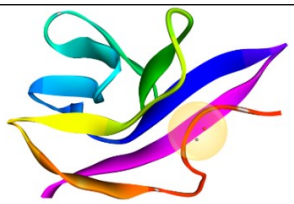
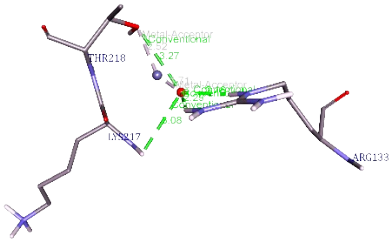
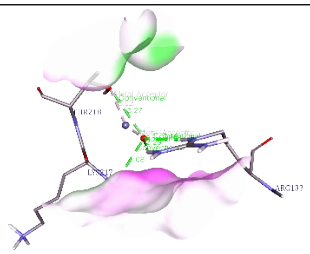
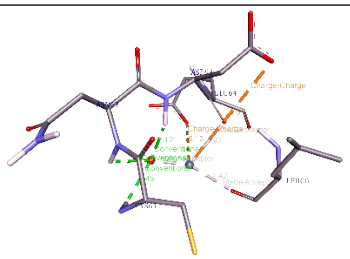
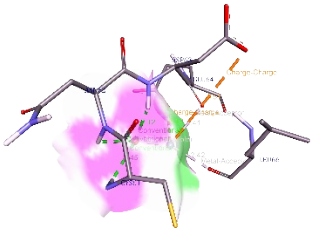
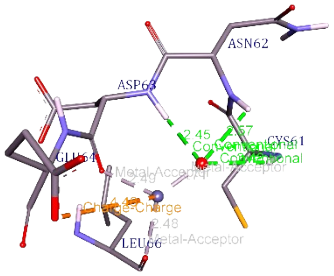
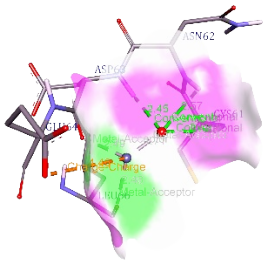
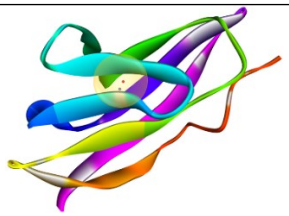
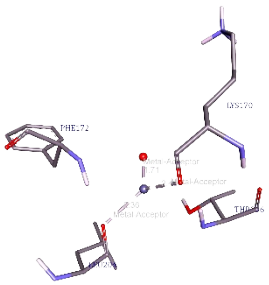
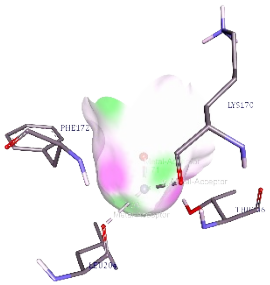
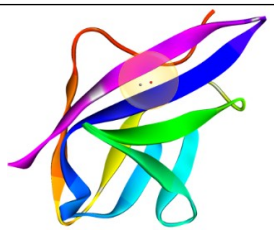
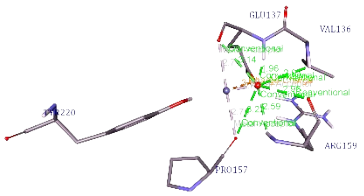
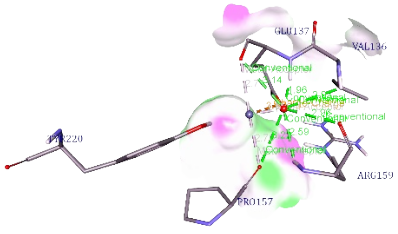
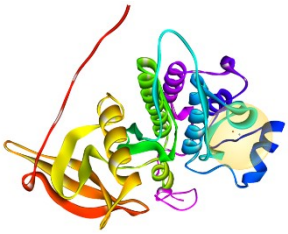
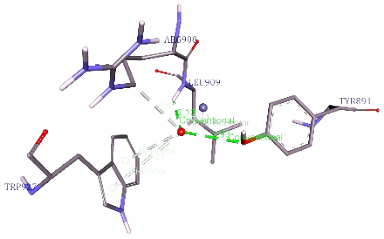
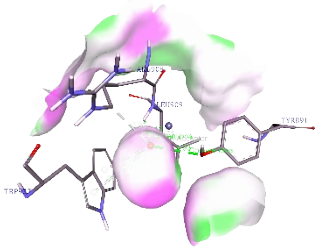
Mode	Superoxide radical – 1agw A chain			Mode	Superoxide radical – 1agw B chain		
	Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b		Affinity (Kcal mol^{-1})	rmsd l.b.	rmsd u.b
1	-2.1	0.000	0.000	1	-2.1	0.000	0.000
2	-2.0	23.536	23.592	2	-2.0	15.797	16.099
3	-2.0	25.859	26.134	3	-1.9	14.376	14.707
4	-1.9	16.108	16.505	4	-1.9	16.084	16.505
5	-1.9	17.518	17.522	5	-1.8	17.370	17.459
6	-1.8	18.058	18.173	6	-1.8	16.559	16.653
7	-1.7	16.549	16.970	7	-1.7	7.530	7.814
8	-1.6	14.134	14.350	8	-1.6	16.849	16.909
9	-1.6	16.849	16.885	9	-1.6	2.555	3.138
Inhibition Constant: 28.77 mM				**Inhibition Constant: 28.77 mM**			

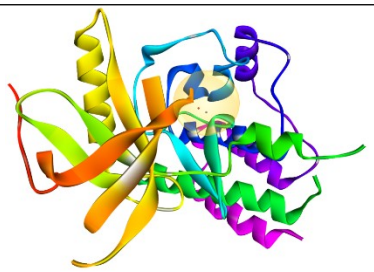
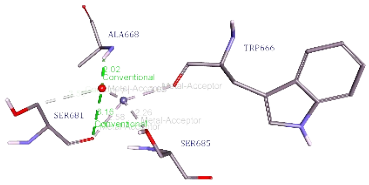
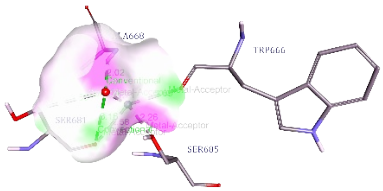
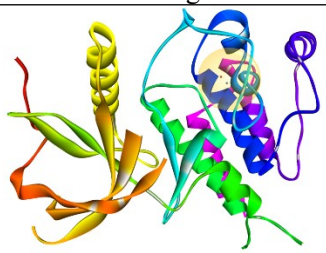
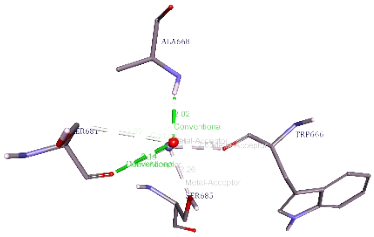
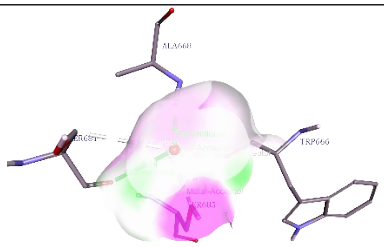
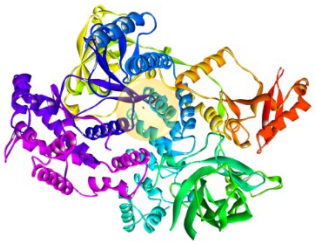
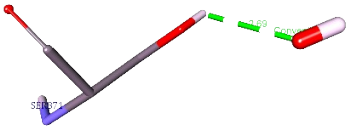
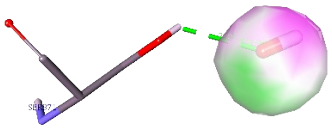
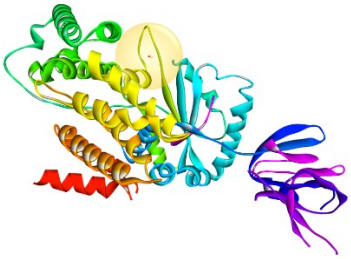
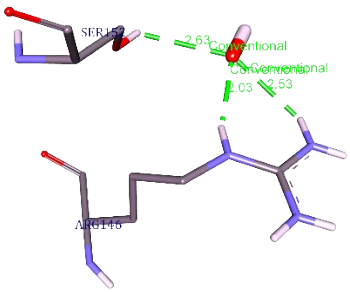
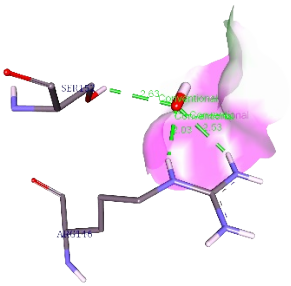
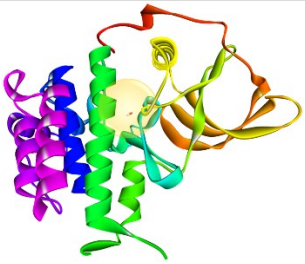
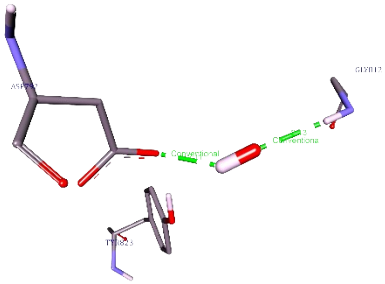
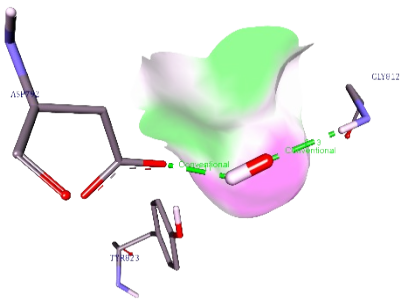
Table *SI-4*. The autodocked receptor-drug binding site for **Zinc oxide, hydroxyl radical & superoxide radical** against (i) PI3K (Phosphoinositide 3-kinase, Pdb: 8SO9), (ii) c-Kit receptor (Pdb: 6GQJ), (iii) MEK1 (Mitogen-Activated Protein Kinase Kinase, Pdb: 4U7Z), (iv) PIP5K1α (Phosphatidylinositol-4-phosphate 5-kinase type 1alpha, Pdb: 4TZ7), (v) MAPK (Mitogen-Activated Protein Kinase, pdb: 3RP9), (vi) c-Met/MET receptor (mesenchymal-epithelial transition factor, pdb: 3DKF), (vii) mTOR (mammalian target of rapamycin, pdb: 2NPU), (viii) CDK2 (Cyclin dependent kinase 2, pdb: 2M1L), (ix) VEGFR (Vascular Endothelial Growth Factor Receptor, Pdb: 1QTY), (x) EGFR (Epidermal Growth Factor Receptor, Pdb: 1M17), and (xi) FGFR (Fibroblast Growth Factor Receptor, Pdb: 1AGW) protease and their corresponding non-covalent interactions and H-bonding surface area.

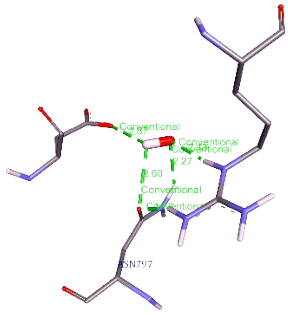
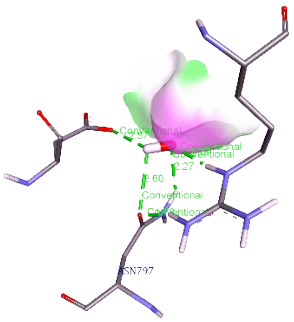
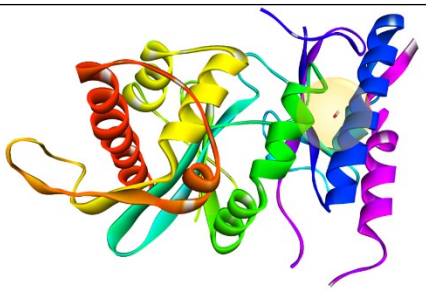
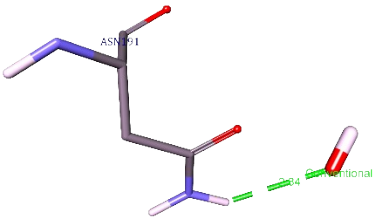
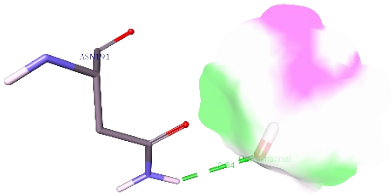
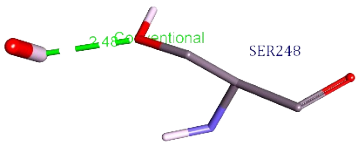
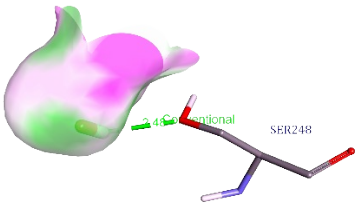
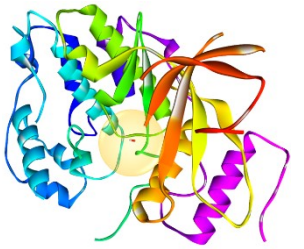
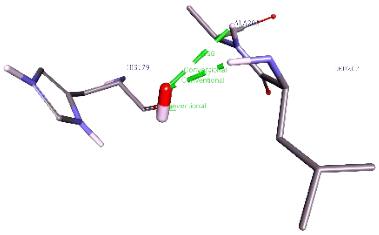
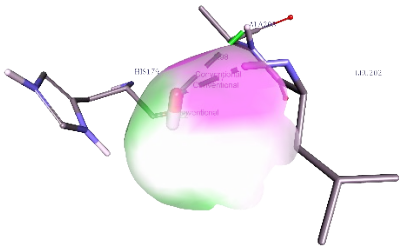
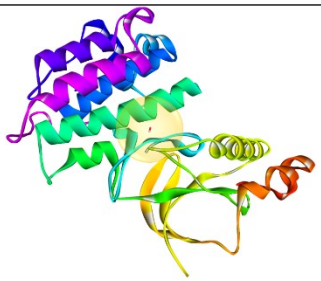
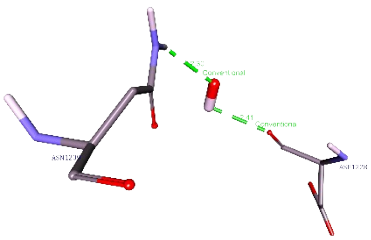
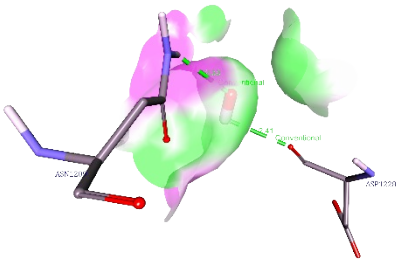
Receptor-Drug Binding Site	Receptor-Drug Interactions	Receptor-Drug H-bond Surface
 Zinc oxide – 8so9 A chain		
 Zinc oxide – 8so9 B chain		
 Zinc oxide – 6gqj A chain		

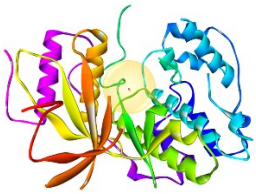
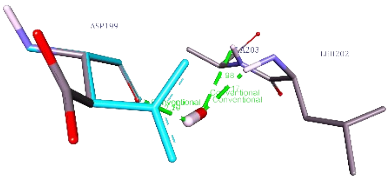
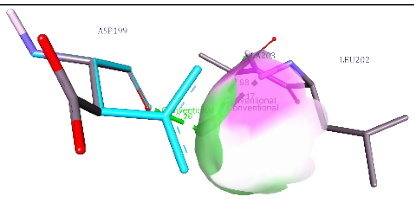
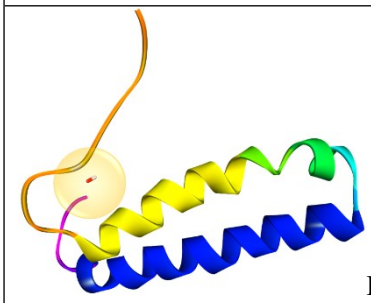
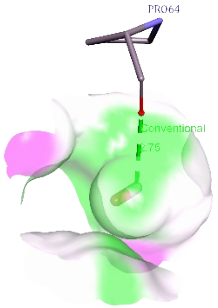
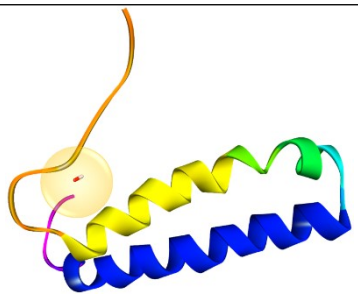
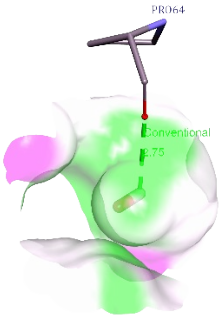
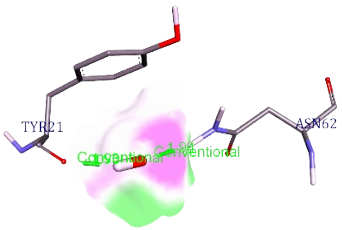
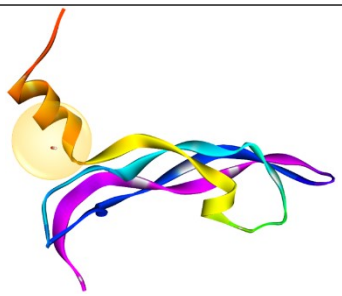
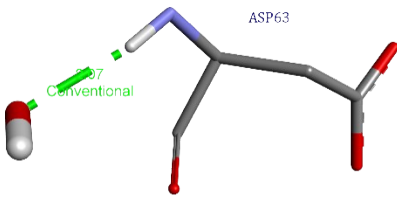
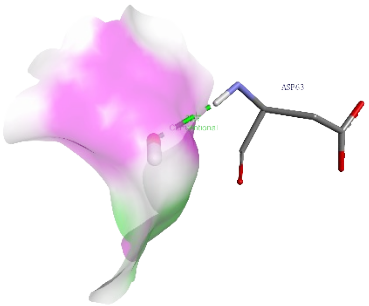
 Zinc oxide – 6gqj B chain		
 Zinc oxide – 4tz7 A chain		
 Zinc oxide – 4u7z		
 Zinc oxide – 3rp9 A chain		
 Zinc oxide – 3dkf		

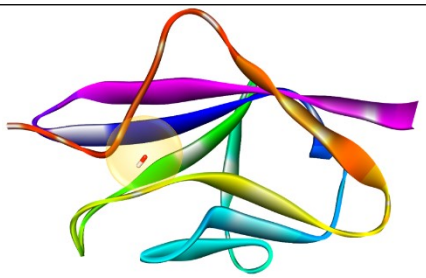
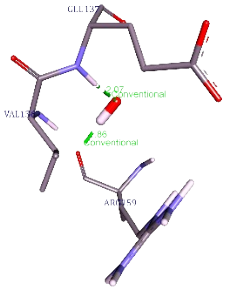
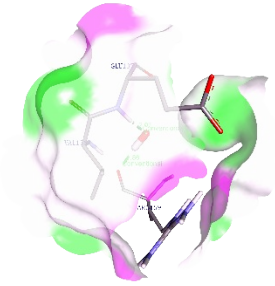
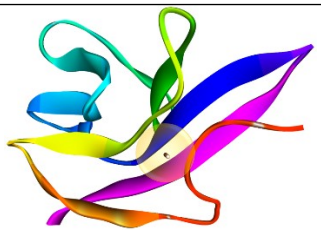
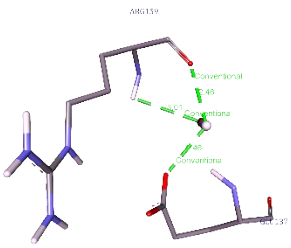
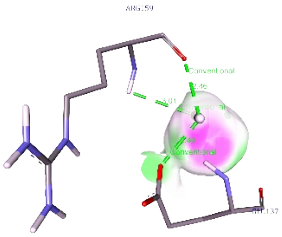
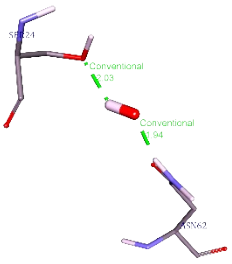
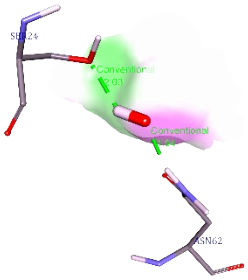
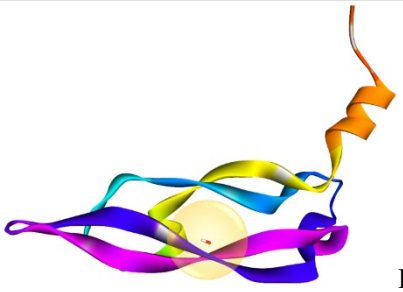
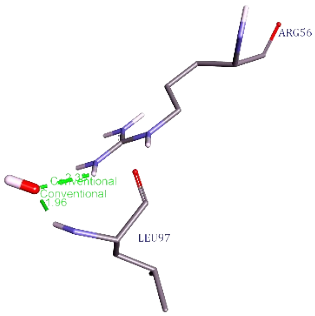
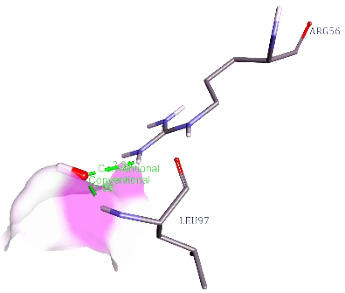
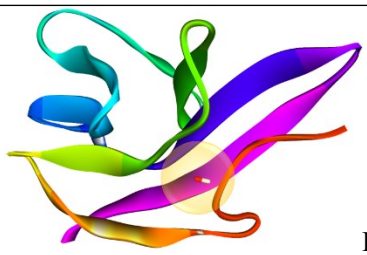
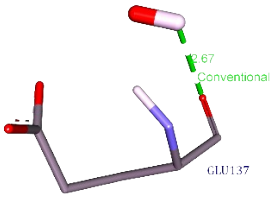
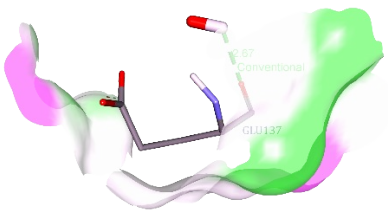
 Zinc oxide – 2npu A chain		
 Zinc oxide - 2m1l A chain		
 Zinc oxide – 2m1l B chain		
 Zinc oxide – 1qty R chain		
 Zinc oxide – 1qty S chain		
 Zinc oxide – 1qty T chain		

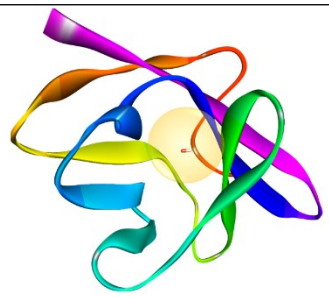
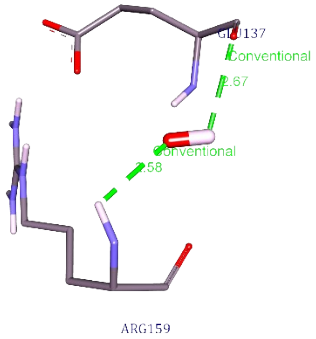
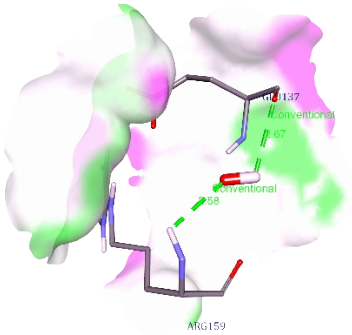
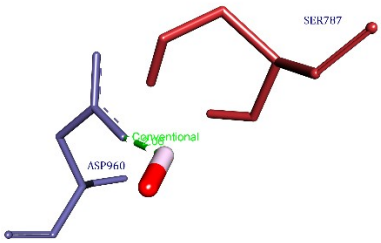
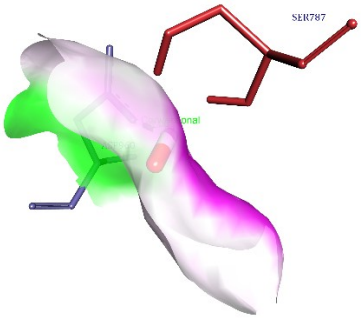
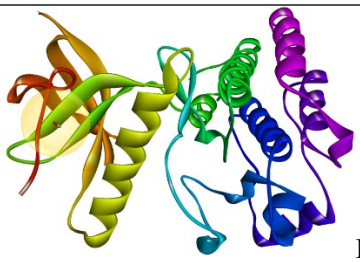
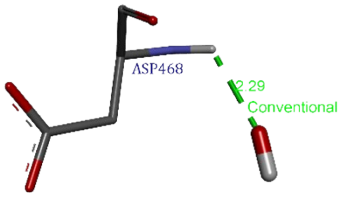
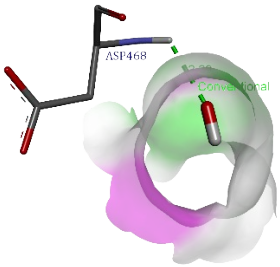
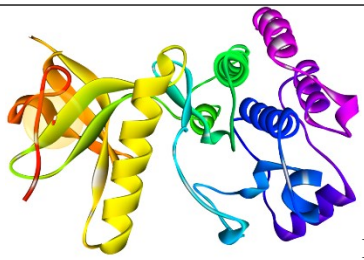
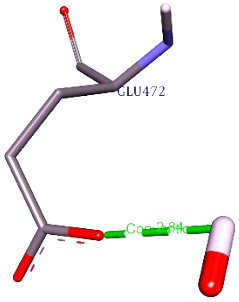
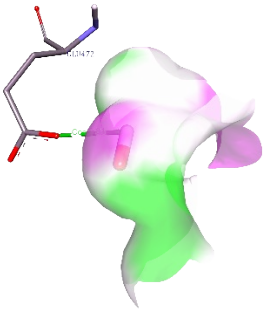
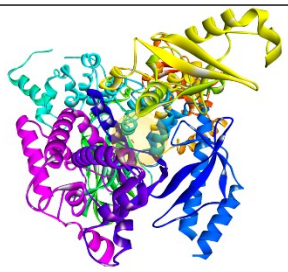
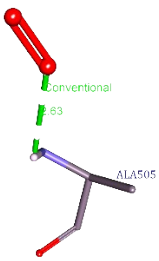
 Zinc oxide – 1qty U chain		
 Zinc oxide – 1qty V chain		
 Zinc oxide – 1qty W chain		
 Zinc oxide – 1qty X chain		
 Zinc oxide – 1qty Y chain		
 Zinc oxide – 1m17		

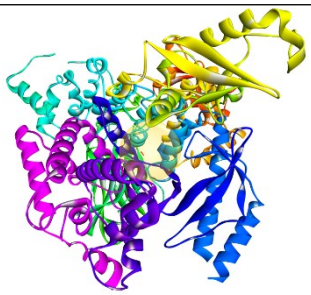
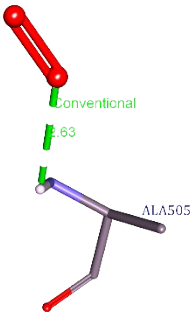
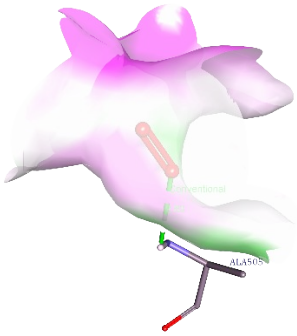
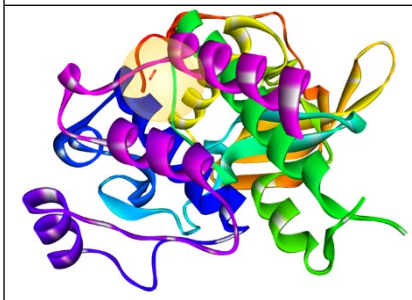
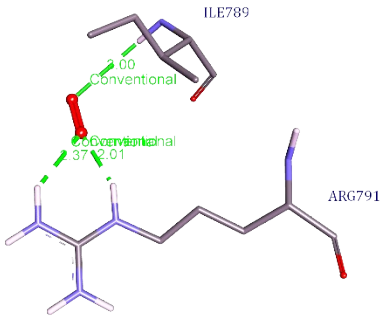
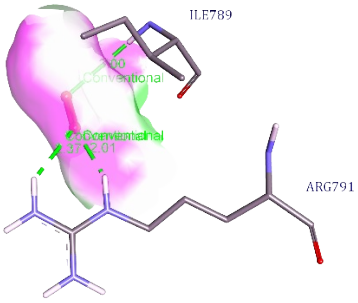
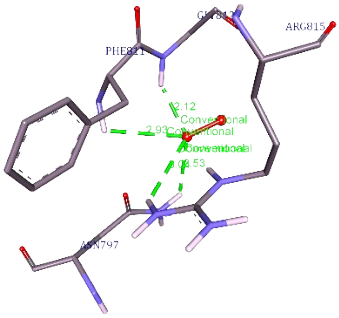
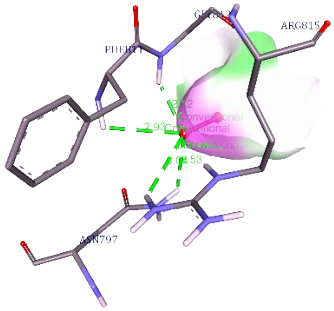
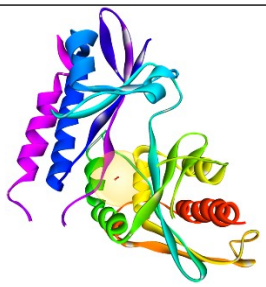
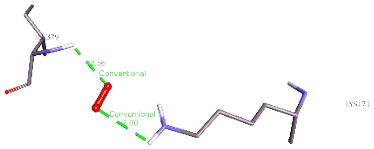
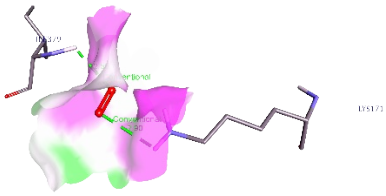
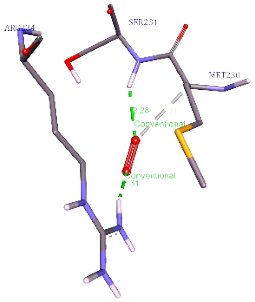
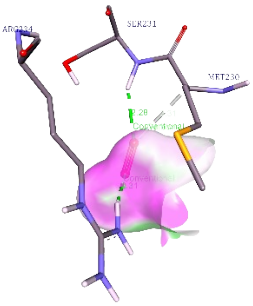
 Zinc oxide – 1agw A chain		
 Zinc oxide – 1agw B chain		
 Hydroxyl radical – 8so9 A chain		
 Hydroxyl radical – 8so9 B chain		
 Hydroxyl radical – 6gqj A chain		

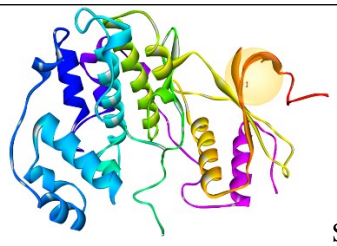
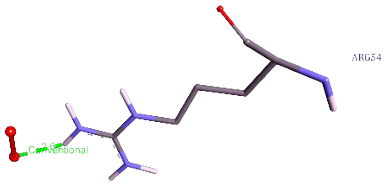
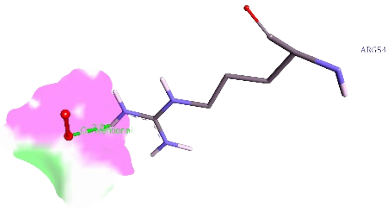
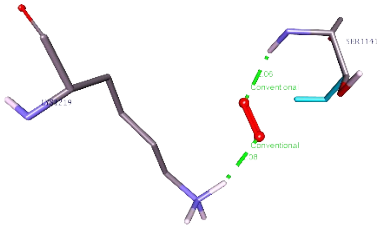
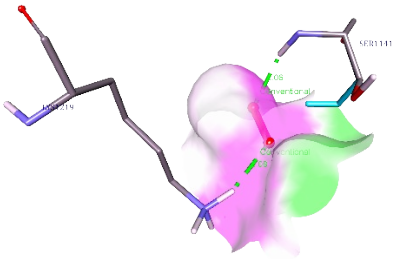
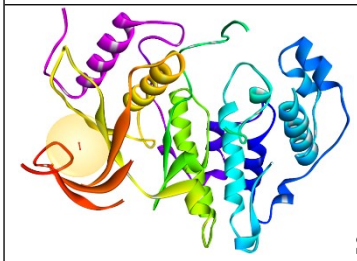
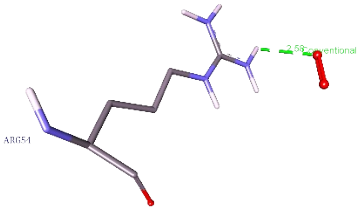
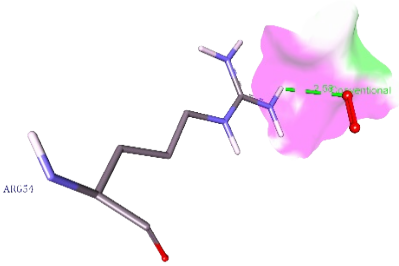
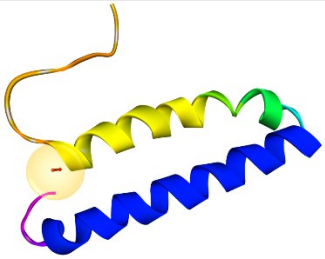
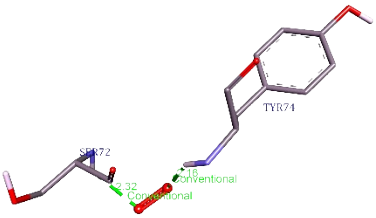
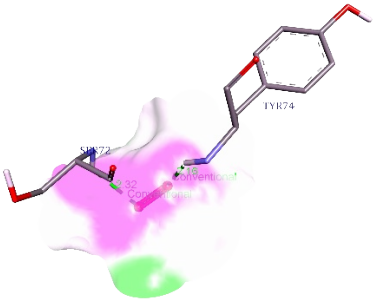
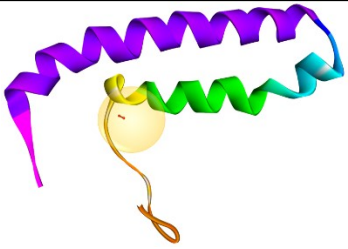
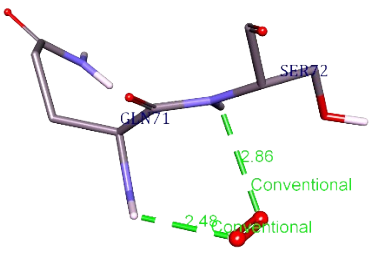
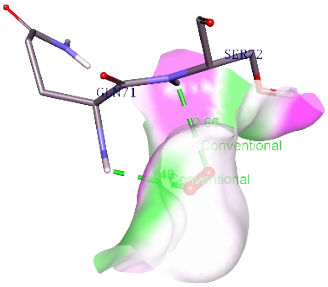
 Hydroxyl radical – 6gqj B chain		
 Hydroxyl radical – 4tz7 A chain		
 Hydroxyl radical – 4u7z		
 Hydroxyl radical – 3rp9 A chain		
 Hydroxyl radical – 3dkf		

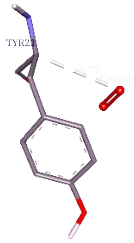
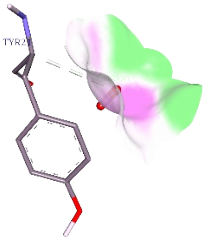
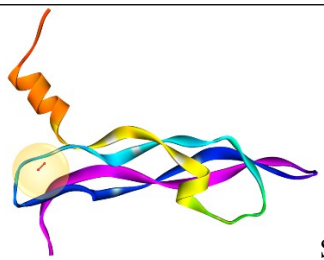
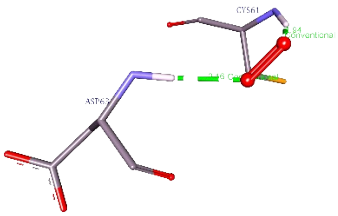
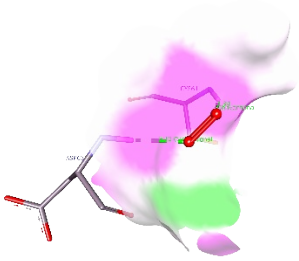
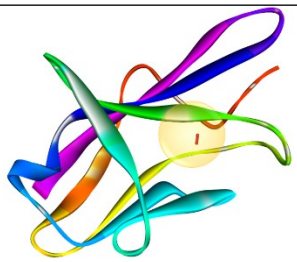
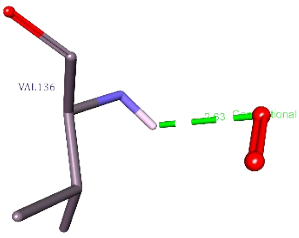
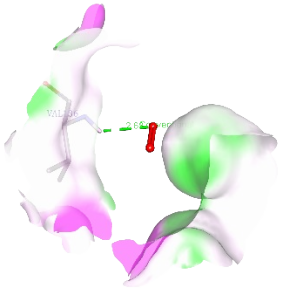
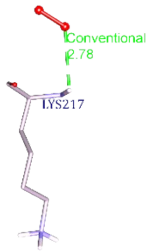
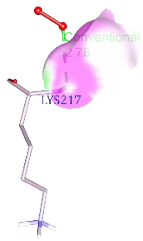
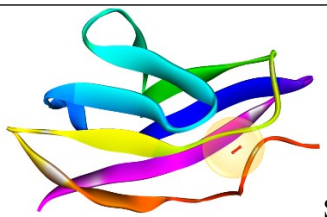
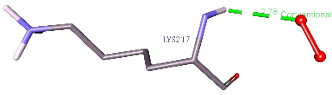
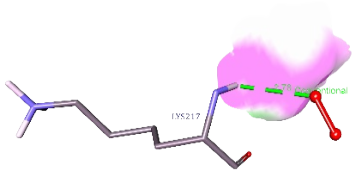
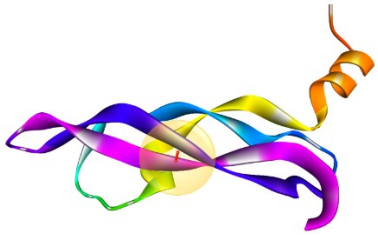
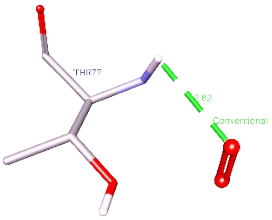
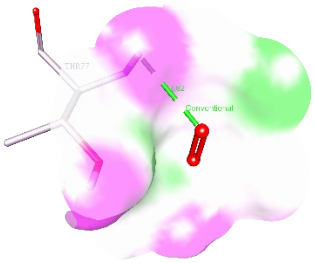
 Hydroxyl radical – 2npu A chain		
 Hydroxyl radical - 2m1l A chain		
 Hydroxyl radical – 2m1l B chain		
 Hydroxyl radical – 1qty R chain		
 Hydroxyl radical – 1qty S chain		

 Hydroxyl radical – 1qty T chain		
 Hydroxyl radical – 1qty U chain		
 Hydroxyl radical – 1qty V chain		
 Hydroxyl radical – 1qty W chain		
 Hydroxyl radical – 1qty X chain		

 Hydroxyl radical – 1qty Y chain		
 Hydroxy l radical – 1m17		
 Hydro xyl radical – 1agw A chain		
 Hydro xyl radical e – 1agw B chain		
 Superoxide radical – 8so9 A chain		

 Superoxide radical – 8so9 B chain		
 Superoxide radical – 6gqj A chain		
 Superoxide radical – 6gqj B chain		
 Superoxide radical – 4tz7 A chain		
 Superoxide radical – 4u7z		

 Superoxide radical – 3rp9 A chain		
 Superoxide radical – 3dkf		
 Superoxide radical – 2npu A chain		
 Superoxide radical - 2m11 A chain		
 Superoxide radical – 2m11 B chain		

 Supero xide radical – 1qty R chain		
 Superoxid e radical – 1qty S chain		
 Superoxide radical – 1qty T chain		
 Superoxide radical – 1qty U chain		
 Superoxid e radical – 1qty V chain		
 Supe		

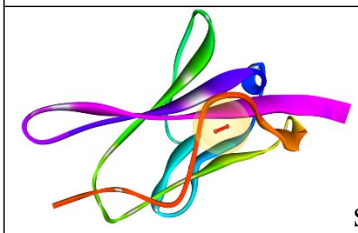
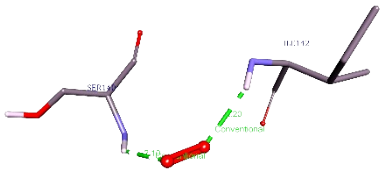
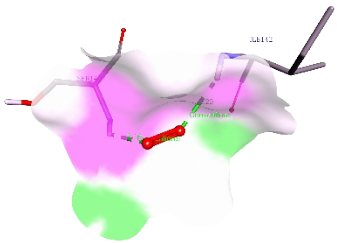
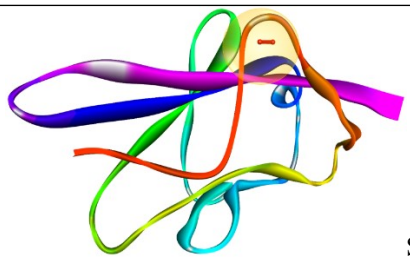
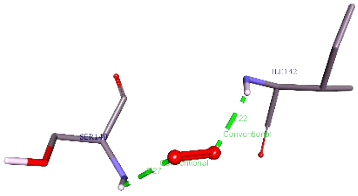
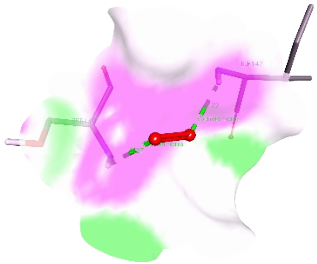
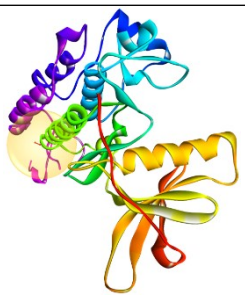
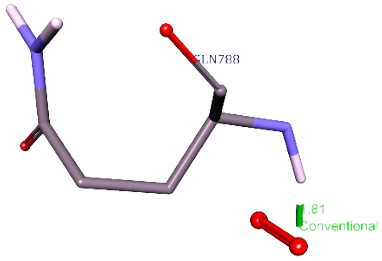
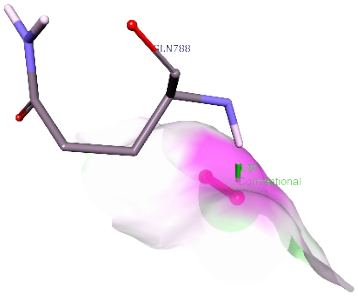
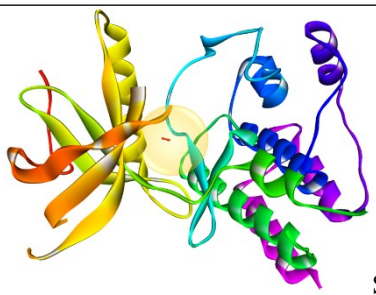
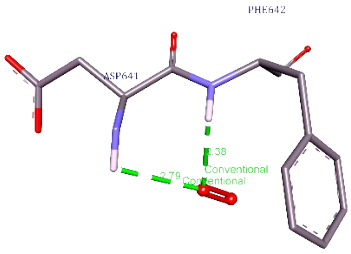
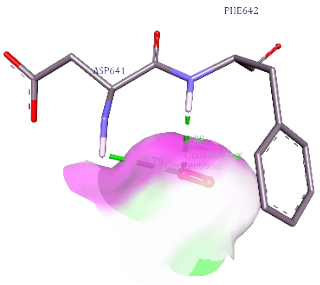
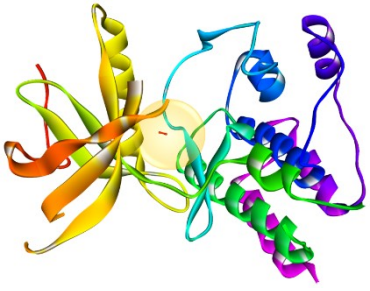
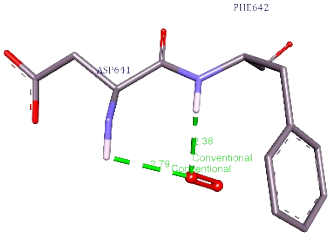
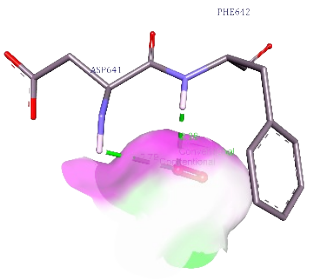
roxide radical – 1qty W chain		
 Superoxide radical – 1qty X chain		
 Superoxide radical – 1qty Y chain		
 Superoxide radical – 1m17		
 Superoxide radical – 1agw A chain		
 Superoxide radical – 1agw B chain		

Table *SI-5*. The non-covalent aminoacid residue interactions of Zinc oxide, hydroxyl radical & superoxide radical against (i) PI3K (Phosphoinositide 3-kinase, Pdb: 8SO9), (ii) c-Kit receptor (Pdb: 6GQJ), (iii) MEK1 (Mitogen-Activated Protein Kinase Kinase, Pdb: 4U7Z), (iv) PIP5K1α (Phosphatidylinositol-4-phosphate 5-kinase type 1alpha, Pdb: 4TZ7), (v) MAPK (Mitogen-Activated Protein Kinase, pdb: 3RP9), (vi) c-Met/MET receptor (mesenchymal-epithelial transition factor, pdb: 3DKF), (vii) mTOR (mammalian target of rapamycin, pdb: 2NPU), (viii) CDK2 (Cyclin dependent kinase 2, pdb: 2M1L), (ix) VEGFR (Vascular Endothelial Growth Factor Receptor, Pdb: 1QTY), (x) EGFR (Epidermal Growth Factor Receptor, Pdb: 1M17), and (xi) FGFR (Fibroblast Growth Factor Receptor, Pdb: 1AGW) protease.

Lead compounds & Reactive Oxygen Species	**Pub chem. Id**	**Protein chain**	**Residue Interaction**	**Nature of bond**				**Distance (Å)**
ZnO	8so9	A chain	:UNK0:O - A:SER504:OG	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	3.08
						:UNK0:O	A:SER504:OG	
			A:SER504:HN - :UNK0:O			A:SER504:HN	:UNK0:O	2.22
			A:ALA505:HN - :UNK0:O			A:ALA505:HN	:UNK0:O	2.54
			:UNK0:O - A:THR503:OG1			:UNK0:O	A:THR503:OG1	2.89
			:UNK0:Zn - :UNK0:O	Miscellaneous	Metal H-Acceptors Interactions	***Metal***	***H-Acceptor***	1.71
						:UNK0:Zn	:UNK0:O	
			:UNK0:Zn - A:THR503:OG1			:UNK0:Zn	A:THR503:OG1	2.37
			:UNK0:Zn - A:HIS708:O			:UNK0:Zn	A:HIS708:O	2.47
ZnO	8so9	B chain	:UNK0:O - B:MET870:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	3.09
						:UNK0:O	B:MET870:O	
			B:TYR616:HH - :UNK0:O			B:TYR616:HH	:UNK0:O	2.16
			B:TYR556:HN - :UNK0:O			B:TYR556:HN	:UNK0:O	1.96
			B:TYR659:HH - :UNK0:O			B:TYR659:HH	:UNK0:O	2.75
			:UNK0:Zn - :UNK0:O	Miscellaneous	Metal H-Acceptors Interactions	***Metal***	***H-Acceptor***	1.71
						:UNK0:Zn	:UNK0:O	
			:UNK0:Zn - B:MET870:O			:UNK0:Zn	B:MET870:O	2.40
			:UNK0:Zn - B:PHE554:O			:UNK0:Zn	B:PHE554:O	3.12
			A:ALA837:HN - :UNK0:O		Classical	***H-Donor***	***H-Acceptor***	2.00
						A:ALA837:HN	:UNK0:O	

ZnO	6gqj	A chain	A:SER840:HG - :UNK0:O	H-Bonding Interactions	H-Bonding Interactions	A:SER840:HG	:UNK0:O	2.22
			A:ALA837:HN - :UNK0:O			A:ALA837:HN	:UNK0:O	2.00
			A:SER850:CB - :UNK0:O		Non-Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	3.49
						A:SER850:CB	:UNK0:O	
			:UNK0:Zn - A:SER850:O	Miscellaneous	Metal H-Acceptors interactions	***Metal***	***H-Acceptor***	2.43
						:UNK0:Zn	A:SER850:O	
			:UNK0:Zn - A:SER854:OG			:UNK0:Zn	A:SER854:OG	2.41
			:UNK0:Zn - A:TRP835:O			:UNK0:Zn	A:TRP835:O	3.11
ZnO	6gqj	B chain	:UNK0:O - B:SER850:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	3.11
						:UNK0:O	B:SER850:O	
			B:SER840:HG - :UNK0:O			B:SER840:HG	:UNK0:O	2.91
			B:ALA837:HN - :UNK0:O			B:ALA837:HN	:UNK0:O	2.07
			:UNK0:Zn - B:SER850:O	Miscellaneous	Metal H-Acceptors interactions	***Metal***	***H-Acceptor***	2.59
						:UNK0:Zn	B:SER850:O	
			:UNK0:Zn - B:TRP835:O			:UNK0:Zn	B:TRP835:O	2.64
			B:MET836:CA - :UNK0:O			B:MET836:CA	:UNK0:O	3.28
ZnO	4tz7	A chain	:UNK0:O - A:THR118:OG1	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.99
						:UNK0:O	A:THR118:OG1	
			:UNK0:Zn - A:GLU94:OE1	Electrostatic Interactions	Atractive charges	***Positive***	***Negative***	4.74
						:UNK0:Zn	A:GLU94:OE1	
			:UNK0:Zn - A:THR118:OG1	Miscellaneous	Metal H-Acceptors interactions	***Metal***	***H-Acceptor***	2.37
						:UNK0:Zn	A:THR118:OG1	
			:UNK0:Zn - :UNK0:O			:UNK0:Zn	:UNK0:O	1.71
ZnO	4u7z	-	A:SER244:HG - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	1.99
						A:SER244:HG	:UNK0:O	
			A:SER231:HN - :UNK0:O			A:SER231:HN	:UNK0:O	2.28
			A:SER248:HG - :UNK0:O			A:SER248:HG	:UNK0:O	2.72
			A:MET230:CA - :UNK0:O		Non-Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	3.28
						A:MET230:CA	:UNK0:O	
			:UNK0:Zn - A:ASP245:OD1	Electrostatic Interactions	Attractive charges	***Positive***	***Negative***	5.21
						:UNK0:Zn	A:ASP245:OD1	
			:UNK0:Zn - A:SER244:O	Miscellaneous	Metal H-Acceptors interactions	***Metal***	***H-Acceptor***	2.31
						:UNK0:Zn	A:SER244:O	
						H-Donor	***H-Acceptor***	

ZnO	3rp9	A chain	:UNK0:O - A:ASP199:O	H-Bonding Interactions	Classical H-Bonding Interactions	:UNK0:O	A:ASP199:O	3.32
			:UNK0:O - A:ASP199:OD1:B			:UNK0:O	A:ASP199:OD1:B	3.33
			A:GLY201:HN - :UNK0:O			A:GLY201:HN	:UNK0:O	2.77
			A:LEU202:HN - :UNK0:O			A:LEU202:HN	:UNK0:O	2.40
						Positive	***Negative***	
			:UNK0:Zn - A:ASP199:OD2	Electrostatic Interactions	Attractive charges	:UNK0:Zn	A:ASP199:OD2	5.14
			:UNK0:Zn - A:ASP199:OD2:B			:UNK0:Zn	:ASP199:OD2:B	2.70
			:UNK0:Zn - A:ASP181:OD2			:UNK0:Zn	A:ASP181:OD2	2.77
						Metal	***H-Acceptor***	
			:UNK0:Zn - A:ASP199:O:B	Miscellaneous	Metal H-Acceptors interactions	:UNK0:Zn	A:ASP199:O:B	2.60
			:UNK0:Zn - A:ASP181:OD2			:UNK0:Zn	A:ASP181:OD2	2.77
ZnO	3dkf	-				***H-Donor***	***H-Acceptor***	
			:UNK0:O - A:SER1264:O	H-Bonding Interactions	Classical H-Bonding Interactions	:UNK0:O	A:SER1264:O	3.09
			A:ALA1251:HN - :UNK0:O			A:ALA1251:HN	:UNK0:O	2.17
					Non-Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
			A:SER1264:CB - :UNK0:O			A:SER1264:CB	:UNK0:O	3.71
			A:MET1250:CA - :UNK0:O			A:MET1250:CA	:UNK0:O	3.23
						Metal	***H-Acceptor***	
			:UNK0:Zn - A:SER1264:O	Miscellaneous	Metal H-Acceptors interactions	:UNK0:Zn	A:SER1264:O	2.50
			:UNK0:Zn - A:TRP1249:O			:UNK0:Zn	A:TRP1249:O	2.49
ZnO	2npu	A chain				***H-Donor***	***H-Acceptor***	
			:UNK0:O - A:ASP199:OD1:B	H-Bonding Interactions	Classical H-Bonding Interactions	:UNK0:O	A:ASP199:OD1:B	3.32
			:UNK0:O - A:ASP199:O:B			:UNK0:O	A:ASP199:O:B	3.29
			A:GLY201:HN - :UNK0:O			A:GLY201:HN	:UNK0:O	2.78
			A:LEU202:HN - :UNK0:O			A:LEU202:HN	:UNK0:O	2.41
						Positive	***Negative***	
			:UNK0:Zn - A:ASP181:OD2	Electrostatic Interactions	Attaractive charges	:UNK0:Zn	A:ASP181:OD2	2.77
			:UNK0:Zn - A:ASP199:OD2:B			:UNK0:Zn	A:ASP199:OD2:B	2.70
			:UNK0:Zn - A:ASP199:OD2			:UNK0:Zn	A:ASP199:OD2	5.13
						Metal	***H-Acceptor***	
			:UNK0:Zn - A:ASP181:OD2	Miscellaneous	Metal H-Acceptors interactions	:UNK0:Zn	A:ASP181:OD2	2.77
			:UNK0:Zn - A:ASP199:O:B			:UNK0:Zn	A:ASP199:O:B	2.60
ZnO	2m1l	A chain				***H-Donor***	***H-Acceptor***	
			:UNK0:O - A:GLN71:O	H-Bonding Interactions	Classical H-Bonding Interactions	:UNK0:O	A:GLN71:O	3.24
			A:THR75:HG1 - :UNK0:O			A:THR75:HG1	:UNK0:O	2.12

			:UNK0:Zn - A:GLN71:OE1	Miscellaneous	Metal H-Acceptors interactions	***Metal***	***H-Acceptor***	2.57
						:UNK0:Zn	A:GLN71:OE1	
ZnO	2m1l	B chain	B:GLN71:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.50
						B:GLN71:HN	:UNK0:O	
			:UNK0:O - B:THR75:OG1			:UNK0:O	B:THR75:OG1	2.99
			:UNK0:Zn - B:THR75:OG1	Miscellaneous	Metal H-Acceptors interactions	***Metal***	***H-Acceptor***	2.41
						:UNK0:Zn	B:THR75:OG1	
			:UNK0:Zn - B:GLY69:O			:UNK0:Zn	B:GLY69:O	2.34
ZnO	1qty	R chain	R:CYS61:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.51
						R:CYS61:HN-	:UNK0:O	
			R:ASN62:HN - :UNK0:O			R:ASN62:HN	:UNK0:O	2.34
			R:ASP63:HN - :UNK0:O			R:ASP63:HN	:UNK0:O	2.11
			:UNK0:Zn - R:GLU64:OE1	Electrostatic Interactions	Attractive charges	***Positive***	***Negative***	5.35
						:UNK0:Zn	R:GLU64:OE1	
			:UNK0:Zn - R:ASP63:OD1			:UNK0:Zn	R:ASP63:OD1	5.39
			:UNK0:Zn - R:LEU66:O	Miscellaneous	Metal H-Acceptors interactions	***Metal***	***H-Acceptor***	2.45
						:UNK0:Zn	R:LEU66:O	
			:UNK0:Zn - R:ASP63:O			:UNK0:Zn	R:ASP63:O	2.46
ZnO	1qty	S chain	S:ASP63:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.22
						S:ASP63:HN	:UNK0:O	
			S:ASN62:HN - :UNK0:O			S:ASN62:HN	:UNK0:O	2.41
			S:CYS61:HN - :UNK0:O			S:CYS61:HN	:UNK0:O	2.50
			:UNK0:Zn - S:GLU64:OE1	Electrostatic Interactions	Attractive charges	***Positive***	***Negative***	5.39
						:UNK0:Zn	S:GLU64:OE1	
			:UNK0:Zn - S:LEU66:O	Miscellaneous	Metal H-Acceptors interactions	***Metal***	***H-Acceptor***	2.43
						:UNK0:Zn	S:LEU66:O	
			:UNK0:Zn - S:ASP63:O			:UNK0:Zn	S:ASP63:O	2.37
ZnO	1qty	T chain	:UNK0:O - T:PRO157:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	3.27
						:UNK0:O	T:PRO157:O	
			T:ARG159:HN - :UNK0:O			T:ARG159:HN	:UNK0:O	2.60
			:UNK0:O - T:ARG159:O			:UNK0:O	T:ARG159:O	3.03
			T:VAL136:HN - :UNK0:O			T:VAL136:HN	:UNK0:O	2.79
			T:GLU137:HN - :UNK0:O			T:GLU137:HN	:UNK0:O	1.93
			:UNK0:O - T:GLU137:O			:UNK0:O	T:GLU137:O	3.21
			:UNK0:Zn - T:GLU137:OE2	Electrostatic Interactions	Attractive charges	***Positive***	***Negative***	5.01
						:UNK0:Zn	T:GLU137:OE2	

ZnO	1qty	U chain				***H-Donor***	***H-Acceptor***	
			U:LYS217:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	U:LYS217:HN	:UNK0:O	3.08
			U:ARG133:HH22 - :UNK0:O			U:ARG133:HH22	:UNK0:O	2.29
			U:ARG133:HE - :UNK0:O			U:ARG133:HE	:UNK0:O	2.16
			:UNK0:O - U:THR218:OG1			:UNK0:O	U:THR218:OG1	3.27
				Miscellaneous	Metal H-Acceptors interactions	***Metal***	***H-Acceptor***	
			:UNK0:Zn - U:THR218:OG1			:UNK0:Zn	U:THR218:OG1	2.52
ZnO	1qty	V chain				***H-Donor***	***H-Acceptor***	
			V:CYS61:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	V:CYS61:HN	:UNK0:O	2.45
			V:ASN62:HN - :UNK0:O			V:ASN62:HN	:UNK0:O	2.40
			V:ASP63:HN - :UNK0:O			V:ASP63:HN	:UNK0:O	2.12
ZnO	1qty	W chain		Electrostatic Interactions	Attractive charges	***Positive***	***Negative***	
			:UNK0:Zn - V:ASP63:OD1			:UNK0:Zn	V:ASP63:OD1	5.51
			:UNK0:Zn - V:GLU64:OE1			:UNK0:Zn	V:GLU64:OE1	5.12
				Miscellaneous	Metal H-Acceptors interactions	***Metal***	***H-Acceptor***	
			:UNK0:Zn - V:LEU66:O			:UNK0:Zn	V:LEU66:O	2.42
			:UNK0:Zn - V:ASP63:O			:UNK0:Zn	V:ASP63:O	2.41
ZnO	1qty	X chain				***H-Donor***	***H-Acceptor***	2.48
			W:CYS61:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	W:CYS61:HN	:UNK0:O	
			W:ASN62:HN - :UNK0:O			W:ASN62:HN	:UNK0:O	2.57
			W:ASP63:HN - :UNK0:O			W:ASP63:HN	:UNK0:O	2.45
				Electrostatic Interactions	Attractive charges	***Positive***	***Negative***	
			:UNK0:Zn - W:GLU64:OE1			:UNK0:Zn	W:GLU64:OE1	4.45
				Miscellaneous	Metal H-Acceptors interactions	***Metal***	***H-Acceptor***	
			:UNK0:Zn - W:ASP63:O			:UNK0:Zn	W:ASP63:O	2.49
			:UNK0:Zn - W:LEU66:O			:UNK0:Zn	W:LEU66:O	2.48
ZnO	1qty	Y chain				***H-Donor***	***H-Acceptor***	
			:UNK0:O - Y:PRO157:O	H-Bonding Interactions	Classical H-Bonding Interactions	:UNK0:O	Y:PRO157:O	3.22
			Y:ARG159:HN - :UNK0:O			Y:ARG159:HN	:UNK0:O	2.59
			:UNK0:O - Y:ARG159:O			:UNK0:O	Y:ARG159:O	2.96
			Y:VAL136:HN - :UNK0:O			Y:VAL136:HN	:UNK0:O	2.93
			Y:GLU137:HN - :UNK0:O			Y:GLU137:HN	:UNK0:O	1.96
			:UNK0:O - Y:GLU137:O			:UNK0:O	Y:GLU137:O	3.14
				Electrostatic	Attractive charges	***Positive***	***Negative***	

			:UNK0:Zn - Y:GLU137:OE1	Interactions		:UNK0:Zn	Y:GLU137:OE1	3.99
				Miscellaneous	Metal H-Acceptors interactions	***Metal***	***H-Acceptor***	
			:UNK0:Zn - Y:GLU137:O			:UNK0:Zn	Y:GLU137:O	2.71
			:UNK0:Zn - Y:PRO157:O			:UNK0:Zn	Y:PRO157:O	2.70
ZnO	1m17	-		H-Bonding Interactions		***H-Donor***	***H-Acceptor***	
			A:LEU909:HN - :UNK0:O		Classical H-Bonding Interactions	A:LEU909:HN	:UNK0:O	2.12
			:UNK0:O - A:TYR891:OH			:UNK0:O	A:TYR891:OH	2.92
					Non Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
			:UNK0:O - A:TRP927			:UNK0:O	A:TRP927	4.04
			:UNK0:O - A:TRP927			:UNK0:O	A:TRP927	3.57
			A:ARG908:CD - :UNK0:O			A:ARG908:CD	:UNK0:O	3.53
			:UNK0:Zn - :UNK0:O	Miscellaneous	Metal H-Acceptors interactions	***Metal***	***H-Acceptor***	1.71
						:UNK0:Zn	:UNK0:O	
ZnO	1agw	A chain		H-Bonding Interactions		***H-Donor***	***H-Acceptor***	
			:UNK0:O - A:SER681:O		Classical H-Bonding Interactions	:UNK0:O	A:SER681:O	3.16
			A:ALA668:HN - :UNK0:O			A:ALA668:HN	:UNK0:O	2.02
			A:SER681:CB - :UNK0:O		Non Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	3.59
						A:SER681:CB	:UNK0:O	
			:UNK0:Zn - A:SER681:O	Miscellaneous	Metal H-Acceptors interactions	***Metal***	***H-Acceptor***	
						:UNK0:Zn	A:SER681:O	2.58
			:UNK0:Zn - A:SER685:OG			:UNK0:Zn	A:SER685:OG	2.26
			:UNK0:Zn - A:TRP666:O			:UNK0:Zn	A:TRP666:O	2.65
ZnO	1agw	B chain		H-Bonding Interactions		***H-Donor***	***H-Acceptor***	
			:UNK0:O - A:SER681:O		Classical H-Bonding Interactions	:UNK0:O	A:SER681:O	3.14
			A:ALA668:HN - :UNK0:O			A:ALA668:HN	:UNK0:O	2.02
			A:SER681:CB - :UNK0:O		Non Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	3.58
						A:SER681:CB	:UNK0:O	
			:UNK0:Zn - A:SER681:O	Miscellaneous	Metal H-Acceptors interactions	***Metal***	***H-Acceptor***	
						:UNK0:Zn	A:SER681:O	2.58
			:UNK0:Zn - A:SER685:OG			:UNK0:Zn	A:SER685:OG	2.26
			:UNK0:Zn - A:TRP666:O			:UNK0:Zn	A:TRP666:O	2.65

OH•	8so9	A chain	A:SER871:HG - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.69
						A:SER871:HG - O	:UNK0:O	
OH•	8so9	B chain	B:ARG146:HH21 - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.53
						B:ARG146:HH21	:UNK0:O	
			B:ARG146:HE - :UNK0:O			B:ARG146:HE	:UNK0:O	2.03
			B:SER152:HG - :UNK0:O			B:SER152:HG	:UNK0:O	2.63
OH•	6gqj	A chain	:UNK0:H - A:ASP792:OD2	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						:UNK0:H	A:ASP792:OD2	2.11
			A:GLY812:HN - :UNK0:O			A:GLY812:HN	:UNK0:O	2.13
OH•	6gqj	B chain	B:ARG815:HE - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						B:ARG815:HE	:UNK0:O	2.13
			B:ASN797:HD22 - :UNK0:O			B:ASN797:HD22	:UNK0:O	2.27
			:UNK0:H - B:ASP810:OD1			:UNK0:H	B:ASP810:OD1	2.57
			:UNK0:H - B:ASN797:OD1			:UNK0:H	B:ASN797:OD1	2.60
OH•	4tz7	A chain	A:ASN191:HD21 - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.84
						A:ASN191:HD21	:UNK0:O	
OH•	4u7z	-	:UNK0:H - A:SER248:OG	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.48
						:UNK0:H	A:SER248:OG	
OH•	3rp9	A chain	A:LEU202:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.19
						A:LEU202:HN	:UNK0:O	
			A:ALA203:HN - :UNK0:O			A:ALA203:HN	:UNK0:O	2.98
			:UNK0:H - A:HIS179:O			:UNK0:H	A:HIS179:O	2.22
OH•	3dkf	-	A:ASN1209:HD22 - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.30
						A:ASN1209:HD22	:UNK0:O	
			:UNK0:H - A:ASP1228:O			:UNK0:H	A:ASP1228:O	2.41
OH•	2npu	A chain	:UNK0:H - A:ASP199:O	H-Bonding Interactions	Classical H-Bonding Interactions	**H-Donor**	**H-Acceptor**	2.20
						:UNK0:H	A:ASP199:O	
			A:LEU202:HN - :UNK0:O			A:LEU202:HN	:UNK0:O	2.17
			A:ALA203:HN - :UNK0:O			A:ALA203:HN	:UNK0:O	2.98
OH•	2m1l	A chain	:UNK0:H - A:PRO64:O	H-Bonding Interactions	Classical H-Bonding	***H-Donor***	***H-Acceptor***	2.75
						:UNK0:H	A:PRO64:O	

					Interactions			
OH•	2m1l	B chain	B:SER79:HG - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						B:SER79:HG	:UNK0:O	2.13
			:UNK0:H - B:GLU83:OE2			:UNK0:H	B:GLU83:OE2	2.06
OH•	1qty	R chain	:UNK0:H - R:TYR21:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						:UNK0:H	R:TYR21:O	1.93
			R:ASN62:HD22 - :UNK0:O			R:ASN62:HD22	:UNK0:O	1.93
OH•	1qty	S chain	S:ASP63:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.07
						S:ASP63:HN	:UNK0:O	
OH•	1qty	T chain	:UNK0:H - T:ARG159:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						:UNK0:H	T:ARG159:O	1.86
			T:GLU137:HN - :UNK0:O			T:GLU137:HN	:UNK0:O	2.07
OH•	1qty	U chain	:UNK0:H - U:ARG159:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						:UNK0:H	U:ARG159:O	2.46
			U:ARG159:HN - :UNK0:O			U:ARG159:HN	:UNK0:O	3.01
			:UNK0:H - U:GLU137:OE1			:UNK0:H	U:GLU137:OE1	2.45
OH•	1qty	V chain	:UNK0:H - V:SER24:OG	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						:UNK0:H	V:SER24:OG	2.03
			V:ASN62:HD22 - :UNK0:O			V:ASN62:HD22	:UNK0:O	1.94
OH•	1qty	W chain	W:LEU97:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						W:LEU97:HN	:UNK0:O	1.96
			W:ARG56:HH21 - :UNK0:O			W:ARG56:HH21	:UNK0:O	2.38
OH•	1qty	X chain	:UNK0:H - X:GLU137:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.67
						:UNK0:H	X:GLU137:O	
OH•	1qty	Y chain	Y:ARG159:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						Y:ARG159:HN	:UNK0:O	2.57
			:UNK0:H - Y:GLU137:O			:UNK0:H	Y:GLU137:O	2.67
OH•	1m17	1m17	:UNK0:H - A:ASP960:OD2	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.06
						:UNK0:H	A:ASP960:OD2	
OH•	1agw	A chain	A:ASP468:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.29
						A:ASP468:HN	:UNK0:O	

$OH^{\bullet}$	1agw	B chain	:UNK0:H - A:GLU472:OE1	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.84
						:UNK0:H	A:GLU472:OE1	
$O^{2-\bullet}$	8so9	A chain	A:ALA505:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.63
						A:ALA505:HN	:HN - :UNK0:O	
$O^{2-\bullet}$	8so9	B chain	B:SER606:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						B:SER606:HN	:UNK0:O	2.10
			B:ILE605:HN - :UNK0:O			B:ILE605:HN	:UNK0:O	2.67
			B:ASP604:HN1 - :UNK0:O			B:ASP604:HN1	:UNK0:O	1.97
$O^{2-\bullet}$	6gqj	A chain	A:ARG791:HE - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						A:ARG791:HE	:UNK0:O	2.00
			A:ARG791:HH21 - :UNK0:O			A:ARG791:HH21	:UNK0:O	2.37
			A:ILE789:HN - :UNK0:O			A:ILE789:HN	:UNK0:O	3.00
$O^{2-\bullet}$	6gqj	B chain	B:GLY812:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						B:GLY812:HN	:UNK0:O	2.12
			B:PHE811:HN - :UNK0:O			B:PHE811:HN	:UNK0:O	2.93
			B:ARG815:HH22 - :UNK0:O			B:ARG815:HH22	:UNK0:O	3.03
			B:ASN797:HD22 - :UNK0:O			B:ASN797:HD22	:UNK0:O	2.52
$O^{2-\bullet}$	4tz7	A chain	A:LYS171:HZ1 - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						A:LYS171:HZ1	:UNK0:O	2.90
			A:ILE379:HN - :UNK0:O			A:ILE379:HN	:UNK0:O	2.56
$O^{2-\bullet}$	4u7z	-	A:ARG234:HH11 - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						A:ARG234:HH11	:UNK0:O	2.31
			A:SER231:HN - :UNK0:O			A:SER231:HN	:UNK0:O	2.28
			A:MET230:CA - :UNK0:O		Non-Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						A:MET230:CA	:UNK0:O	3.31
$O^{2-\bullet}$	3rp9	A chain	A:ARG54:HH22 - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						A:ARG54:HH22	:UNK0:O	2.61
				H-Bonding	Classical	***H-Donor***	***H-Acceptor***	

$O^{2-\bullet}$	3dkf		A:LYS1219:HZ3 - :UNK0:O	Interactions	H-Bonding Interactions	A:LYS1219:HZ3	:UNK0:O	2.08
			A:SER1141:HN - :UNK0:O			A:SER1141:HN	:UNK0:O	2.06
$O^{2-\bullet}$	2npu	A chain	A:ARG54:HH22 - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.58
						A:ARG54:HH22	:UNK0:O	
$O^{2-\bullet}$	2m1l	A chain	A:TYR74:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						A:TYR74:HN	:UNK0:O	2.16
			A:SER72:HN - :UNK0:O			A:SER72:HN	:UNK0:O	2.32
$O^{2-\bullet}$	2m1l	B chain	B:GLN71:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						B:GLN71:HN	:UNK0:O	2.48
			B:SER72:HN - :UNK0:O			B:SER72:HN	:UNK0:O	2.86
$O^{2-\bullet}$	1qty	R chain	R:TYR21:CA - :UNK0:O	H-Bonding Interactions	Non-Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	3.79
						R:TYR21:CA	:UNK0:O	
$O^{2-\bullet}$	1qty	S chain	S:ASP63:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						S:ASP63:HN	:UNK0:O	2.16
			S:CYS61:HN - :UNK0:O			S:CYS61:HN	:UNK0:O	1.94
$O^{2-\bullet}$	1qty	T chain	T:VAL136:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.63
						T:VAL136:HN	:UNK0:O	
$O^{2-\bullet}$	1qty	U chain	U:LYS217:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.78
						U:LYS217:HN	:UNK0:O	
$O^{2-\bullet}$	1qty	V chain	U:LYS217:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.78
						U:LYS217:HN	:UNK0:O	
$O^{2-\bullet}$	1qty	W chain	W:THR77:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	2.82
						W:THR77:HN	:UNK0:O	
$O^{2-\bullet}$	1qty	X chain	X:SER140:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						X:SER140:HN	:UNK0:O	2.10
			X:ILE142:HN - :UNK0:O			X:ILE142:HN	:UNK0:O	2.20
$O^{2-\bullet}$	1qty	Y chain	Y:SER140:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						Y:SER140:HN	:UNK0:O	2.27
			Y:ILE142:HN - :UNK0:O			Y:ILE142:HN	:UNK0:O	2.2
				H-Bonding	Classical	***H-Donor***	***H-Acceptor***	

$O^{2-\bullet}$	1m17	-	A:GLN788:HN - :UNK0:O	Interactions	H-Bonding Interactions	A:GLN788:HN	:UNK0:O	1.81
$O^{2-\bullet}$	1agw	A chain	A:ASP641:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						A:ASP641:HN	:UNK0:O	2.79
			A:PHE642:HN - :UNK0:O			A:PHE642:HN	:UNK0:O	2.38
$O^{2-\bullet}$	1agw	B chain	A:ASP641:HN - :UNK0:O	H-Bonding Interactions	Classical H-Bonding Interactions	***H-Donor***	***H-Acceptor***	
						A:ASP641:HN	:UNK0:O	2.79
			A:PHE642:HN - :UNK0:O			A:PHE642:HN	:UNK0:O	2.38

Table *SI-6*. The Receptor grid boxes and corresponding grid box centre valuses for melanoma skin cancer 11 proteins such as (i) PI3K (Phosphoinositide 3-kinase, Pdb: 8SO9), (ii) c-Kit receptor (Pdb: 6GQJ), (iii) MEK1 (Mitogen-Activated Protein Kinase Kinase, Pdb: 4U7Z), (iv) PIP5K1α (Phosphatidylinositol-4-phosphate 5-kinase type 1alpha, Pdb: 4TZ7), (v) MAPK (Mitogen-Activated Protein Kinase, pdb: 3RP9), (vi) c-Met/MET receptor (mesenchymal-epithelial transition factor, pdb: 3DKF), (vii) mTOR (mammalian target of rapamycin, pdb: 2NPU), (viii) CDK2 (Cyclin dependent kinase 2, pdb: 2M1L), (ix) VEGFR (Vascular Endothelial Growth Factor Receptor, Pdb: 1QTY), (x) EGFR (Epidermal Growth Factor Receptor, Pdb: 1M17), and (xi) FGFR (Fibroblast Growth Factor Receptor, Pdb: 1AGW) protease.

Protein pdb id		Receptor grid box sizes			Receptor grid box centre		
		X	Y	Z	x	y	z
1agw	chain A	40	40	40	7.262	1.57	11.826
	chain B	40	40	40	7.262	1.57	11.826
1m17		40	40	40	4.999	13.192	60.169
1qty	chain R	40	40	40	-38.232	42.957	90.541
	chain S	40	40	40	-24.343	29.152	85.905
	chain T	40	40	40	-9.385	38.355	64.201
	chain U	40	40	40	-37.391	38.719	120.453
	chain V	40	40	40	2.221	-5.419	33.424
	chain W	40	40	40	-7.497	11.412	24.311
	chain X	40	40	40	-7.999	8.781	65.431
	chain Y	40	40	40	16.366	2.473	12.889
2m11	chain A	40	40	40	-5.218	-2.182	5.546
	chain B	40	40	40	1.870	0.125	-2.62
pu	chain A	40	40	40	-3.199	-7.892	2.019
3dkf		40	40	40	20.5	17.255	130.081
3rp9	chain A	40	40	40	-3.199	-7.892	2.019
4tz7	chain A	40	40	40	17.397	106.742	20.434
4u7z		40	40	40	-25.971	14.644	5.932
6gqi	chain A	40	40	40	26.11	101.197	5.667
	chain B	40	40	40	56.65	101.833	23.806
8so9	chain A	40	40	40	172.196	165.901	182.833
	chain B	40	40	40	174.502	170.428	127.944