Table 13. Docking of protein (ERK+ pentetic acid) and Chromium chelators using *i*Gemdock.

	S. No.	Chromium Compound & Chelators	Energy	VDW	H bond
Interaction with ERK complex (1ERK+pentetic acid)		Ammonium dichromate	-78.82	-51.97	-26.85
		Calcium Chromate	-9.8	3.18	-6.62
		Chromium trioxide	-46.24	-20.2	-26.04
		Lead Chromate	-59.99	-45.99	-14
		Potassium chromate	-62.27	-31.89	-30.39
		Potasium dichromate	-10.22	-12.44	2.22
		Sodium Chromate	-62.27	-31.89	-30.39
		Sodium dichromate	-28.14	-20.98	-76.16
		Strontium dichromate	-56.49	-25.54	-30.95
		Zinc chromate	-59.96	-46.24	-13.72
		NAC	-82.26	-68.16	-14.59
		EDTA	-14.56	1.09	-10.27
		$CaNa_2$ EDTA	-200.05	-181.89	-18.16
		Ascorbic acid	-27.64	-20.64	-7
		Dimercaprol	-44.95	-36.5	-8.5
		DMSA	-72.37	-58.1	-13.91
		DMPS	-76.51	-60.45	-16.06
		Pentetic acid	-115.5	-74.61	-30.18
		Citric acid	-24.84	-11.57	-4.47
		Oxalic Acid	-61.34	-35.89	-25.45

Table 14.Docking of protein (ERK+ ascorbic acid) and Chromium chelators using *i*Gemdock

	S. No.	Chromium Compound & Chelators	Energy	VDW	H bond
Interaction with ERK complex (1erk+ASCORBIC ACID)		Ammonium dichromate	-78.83	-52.18	-26.65
		Calcium Chromate	11.43	22.82	-11.39
		Chromium trioxide	-44.35	-34.03	-10.32
		Lead Chromate	-60.06	-46.06	-14
		Potassium chromate	-59.62	-46.13	-13.49
		Potasium dichromate	-28.55	-28.55	0
		Sodium Chromate	-62.24	-32.11	-30.14
		Sodium dichromate	-40.66	-35.34	-5.32
		Strontium dichromate	-59.56	-43.51	-16.05
		Zinc chromate	-59.56	-43.51	-16.05
		NAC	-79.35	-63.34	-16
		EDTA	161.57	153.46	13.06
		$CaNa_2$ EDTA	-199.28	-173.78	-25.5
		Ascorbic acid	-5.54	3.39	-8.94
		Dimercaprol	-43.31	-36.31	-7

		DMSA	-74.89	-62.34	-12.5
		DMPS	-74.84	-62.34	-12.5
		Pentetic acid	-124	-80.82	-34.91
		Citric acid	-31.56	-28.76	-1.62

Table 15. Docking of protein (ERK+ oxalic acid) and Chromium chelators using *i*Gemdock.

	S. No.	Chromium Compound & Chelators	Energy	VDW	H bond
Interaction with ERK complex (1erk+oxalic acid)		Ammonium dichromate	-4.03	0.98	3.05
		Calcium Chromate	15.33	-10.1	-5.23
		Chromium trioxide	-41.74	-30.55	-11.19
		Lead Chromate	-59.97	-46.15	-13.83
		Potassium chromate	-62.08	-31.76	-30.32
		Potassium dichromate	-21.64	-11.8	-9.83
		Sodium Chromate	-60.23	-44.73	-15.5
		Sodium dichromate	-3.7	11.09	-14.78
		Strontium dichromate	-60.28	-46.29	13.99
		Zinc chromate	60.25	-46.26	-13.99
		NAC	-68.52	-48.31	-20.2
		EDTA	-22.06	-12.2	-11.1
		$CaNa_2$ EDTA	-205.73	-181.41	-24.32
		Ascorbic acid	-4.09	0.98	-3.05
		Dimercaprol	-44.06	-36.19	-7.87
		DMSA	-47.02	-59.49	-14.48
		DMPS	-74.85	-62.44	-12.4
		Pentetic acid	-123.86	-81.01	-34.62
		Citric acid	16.11	24.11	-9.51
		Oxalic Acid	-63.74	-25.14	-38.6

Table 16. Docking of protein (ERK+ $CaNa_2EDTA$) and Chromium chelators using *i*Gemdock

	S. No.	Chromium Compound & Chelators	Energy	VDW	H bond
Interaction with ERK complex (1ERK+$CaNa_2EDTA$)		Ammonium dichromate	-78.87	-51.91	-26.36
		Calcium Chromate	-5.22	-11.84	6.62
		Chromium trioxide	-44.86	-34.36	-10.5
		Lead Chromate	-60.16	-46.21	-13.95
		Potassium chromate	-62.23	-31.6	-30.63
		Potassium dichromate	-6.47	-3.67	-2.8
		Sodium Chromate	-62.31	-32.16	-30.15
		Sodium dichromate	-12.31	17.62	-29.93
		Strontium dichromate	-58.89	-28.89	-29.99
		Zinc chromate	-59.63	-45.63	-14
		NAC	-80.33	-65.05	-15.28
		EDTA	54.19	69.7	-12.49
		$CaNa_2$ EDTA	-202.16	-183.32	-18.84
		Ascorbic acid	-5.22	-11.84	6.62

		Dimercaprol	-46.34	-39.34	-7
		DMSA	-71.22	-44.15	-23.62
		DMPS	-74.83	-62.4	-12.43
		Pentetic acid	-119.66	-78.84	-32.02
		Citric acid	-47.52	-43.68	0
		Oxalic Acid	-61.88	-19.88	-42

Table 17. Docking of protein (p38) and Chromium chelators using *i*Gemdock

	S. No.	Chromium Compound & Chelators	Energy	VDW	H bond
Interaction with p38 (1CM8.PDB)		Ammonium dichromate	-87.77	-20.25	-67.52
		Calcium Chromate	-55.36	-10.36	-45
		Chromium trioxide	-49.77	-23.23	-26.54
		Lead Chromate	-21.62	-18.09	-3.53
		Potassium chromate	-22.95	-6.99	-15.96
		Potassium dichromate	-0.02	-2.15	-2.13
		Sodium Chromate	-60.05	-39.05	0
		Sodium dichromate	-30.52	-30.52	0
		Strontium dichromate	-58.48	-15.06	-43.42
		Zinc chromate	-58.02	-27.69	-30.33
		NAC	-24.81	-22.52	-2.61
		EDTA	7.17	9.92	-2.11
		$CaNa_2$ EDTA	-55.43	-55.43	0
		Ascorbic acid	-83.28	-55.54	-27.74
		Dimercaprol	-41.83	-30.8	-11.03
		DMSA	2.15	15.78	-13.06
		DMPS	21.79	10.63	11.161
		Pentetic acid	-135.94	-60.98	-54.87
		Citric acid	3.76	-15.56	-2.81
		Oxalic Acid	-86.9	1.23	-68.63

Table 18. Docking of protein (p38+pentetic acid) and Chromium chelators using *i*Gemdock

S. No.	Receptor	Ligands	Total Energy	VDW	HBond
	1cm8 + pentetic acid	$CaNa_2EDTA$	-107.785	-103.145	0
		Dimercaprol	-41.9529	-32.6948	-9.25811
		DMPS	-22.939	-22.939	0
		DMSA	-77.1224	-27.348	-35.0675
		Ascorbic Acid	-83.3929	-55.8692	-27.5237
		Ammonium Dichromate	-86.86	-30.7137	-56.1463
		Calcium Chromate	-55.4359	-24.5877	-30.8482
		Chromium Trioxide	-44.4463	-12.3024	-32.1439
		EDTA	47.6294	58.652	-4.24288
		Lead Chromate	-55.4777	-24.525	-30.9526
		NAC	-4.55641	2.2113	-8.51623
		Potassium Chromate	-60.4149	-39.4392	-20.9757
		Potassium Dichromate	-38.6133	-20.9309	-17.6824
		Sodium Chromate	-60.0969	-39.4303	-20.6667

		Sodium Dichromate	15.8287	15.8287	0
		Strontium Chromate	-58.0203	-15.3466	-42.6737
		Zinc Chromate	-58.7035	-14.9727	-43.7308
		Oxalic Acid	-84.3359	-29.9931	-54.3428
		Citric Acid	-27.7511	-13.0475	-8.87487
		Pentetic Acid	-127.15	-65.7513	-40.9508

Table 19. Docking of protein (p38+ascorbic acid) and Chromium chelators using *i*Gemdock.

S. No.	Receptor	Ligands	Total Energy	VDW	HBond
	1cm8 + ascorbic acid	$CaNa_2EDTA$	-55.2515	-55.2515	0
		Dimercaprol	-41.02	-34.037	-6.98302
		DMPS	-25.3021	-20.9491	-4.35298
		DMSA	-26.2783	-11.9413	-17.5942
		Ascorbic Acid	-80.2023	-62.09	-18.1124
		Ammonium Dichromate	-87.3531	-31.9626	-55.3905
		Calcium Chromate	-57.2307	-28.3614	-28.8694
		Chromium Trioxide	-48.0978	-18.7094	-29.3885
		EDTA	47.8337	45.1106	0.863976
		Lead Chromate	-57.0902	-24.9848	-32.1054
		NAC	-24.99	-22.4254	-3.20016
		Potassium Chromate	-60.4464	-39.5626	-20.8837
		Potassium Dichromate	-2.51016	-3.02943	0.519266
		Sodium Chromate	-60.4487	-39.4487	-21
		Sodium Dichromate	-31.9878	-26.4535	-5.53423
		Strontium Chromate	-56.5178	-29.6697	-26.8481
		Zinc Chromate	-56.384	-15.0357	-41.3482
		Oxalic Acid	-84.3349	-30.1709	-54.164
		Citric Acid	-52.2187	-24.5506	-14.4289
		Pentetic Acid	-115.815	-95.22	-17.6548

Table 20. Docking of protein (p38+oxalic acid) and Chromium chelators using *i*Gemdock.

S. No.	Receptor	Ligands	Total Energy	VDW	HBond
	1cm8 + oxalic acid	$CaNa_2EDTA$	-149.731	-153.167	0
		Dimercaprol	-41.9328	-30.9349	-10.9979
		DMPS	-18.7227	-12.1285	-6.59414
		DMSA	-39.1809	-26.4306	-9.86109
		Ascorbic Acid	-83.6065	-55.5787	-28.0279
		Ammonium Dichromate	-86.2373	-31.6897	-54.5477
		Calcium Chromate	-56.4483	-29.3374	-27.1109
		Chromium Trioxide	-48.6079	-21.5768	-27.0311
		EDTA	3.54497	9.37581	-5.95682
		Lead Chromate	-55.4161	-24.8147	-30.6014
		NAC	60.297	63.797	-3.5
		Potassium Chromate	-60.3304	-39.5487	-20.7817
		Potassium Dichromate	-8.42616	0.154439	-8.5806

		Sodium Chromate	-60.2941	-39.3577	-20.9365
		Sodium Dichromate	20.8355	33.9175	-13.082
		Strontium Chromate	-58.5022	-14.8232	-43.679
		Zinc Chromate	-55.2619	-17.5496	-37.7122
		Oxalic Acid	-83.5422	-29.0957	-54.4465
		Citric Acid	17.7157	7.54635	12.5058
		Pentetic Acid	-124.389	-71.5684	-40.2151

Table 21. Docking of Protein (1cm8+$CaNa_2EDTA$) and Chromium chelators using *i*Gemdock.

S. No.	Receptor	Ligands	Total Energy	VDW	HBond
	1cm8 + $CaNa_2EDTA$	$CaNa_2EDTA$	-93.0812	-47.2089	-47.9911
		Dimercaprol	-39.394	-33.8471	-5.54695
		DMPS	26.6134	20.5531	6.06023
		DMSA	-9.2833	-3.53062	-6.89857
		Ascorbic Acid	-84.1032	-32.8199	-51.2833
		Ammonium Dichromate	-87.746	-19.9707	-67.7753
		Calcium Chromate	-57.682	-14.6278	-43.0542
		Chromium Trioxide	-48.3781	-20.5049	-27.8732
		EDTA	-31.7645	-19.4949	-13.3003
		Lead Chromate	-58.5776	-15.1438	-43.4338
		NAC	-31.914	-30.5862	-1.67132
		Potassium Chromate	-60.4323	-39.4323	-21
		Potassium Dichromate	27.9196	30.0283	-2.10865
		Sodium Chromate	-60.4404	-39.4996	-20.9408
		Sodium Dichromate	-22.8792	-12.2196	-10.6596
		Strontium Chromate	-57.6463	-15.4799	-42.1664
		Zinc Chromate	-58.0112	-15.419	-42.5921
		Oxalic Acid	-82.9793	-38.1892	-44.7901
		Citric Acid	0.268638	-6.09665	-4.81507
		Pentetic Acid	-132.066	-66.6871	-45.1708

Table 22. Docking of protein (1cm8+dimercaprol) and Chromium chelators using *i*Gemdock.

S. No.	Receptor	Ligands	Total Energy	VDW	HBond
	1cm8 + dimercaprol	$CaNa_2EDTA$	-88.1159	-92.5581	0
		Dimercaprol	-41.031	-32.0725	-8.95855
		DMPS	20.0459	26.3478	-6.30185
		DMSA	-22.4194	-22.7644	-4.05143
		Ascorbic Acid	-80.522	-62.1871	-18.3349
		Ammonium Dichromate	-78.9765	-52.9891	-25.9873
		Calcium Chromate	-57.6981	-14.0897	-43.6084
		Chromium Trioxide	-48.9732	-24.3709	-24.6023
		EDTA	64.6771	68.5532	-0.99332
		Lead Chromate	-57.0795	-25.2699	-31.8096
		NAC	-29.0655	-29.2751	0
		Potassium Chromate	-59.41	-30.2974	-29.1125

		Potassium Dichromate	-9.48656	-4.45751	-5.02905
		Sodium Chromate	-60.3918	-39.5351	-20.8567
		Sodium Dichromate	-9.12267	-8.38976	-0.7329
		Strontium Chromate	-55.3745	-24.8787	-30.4958
		Zinc Chromate	-55.295	-24.5971	-30.6979
		Oxalic Acid	-82.8796	-29.7951	-53.0845
		Citric Acid	-13.4875	-20.0122	-2.77063
		Pentetic Acid	-129.994	-64.9836	-44.5202

Table 23. Docking of protein (JNK) and Arsenic chelators using *i*Gemdock.

Receptor	Ligand	Total Energy	VDW	HBond
JNK	Arsenic pentaoxide	-40.83	-8.46	-32.37
	Trichloro arsenic	-18.9	-18.9	0
	Arsenite	-34.65	-11.47	-23.18
	DMPS	-41.84	-31.0	-10.73
	DMSA	4.24	9.14	-3.97
	$CaNa_2EDTA$	-189.99	-137.75	-39.32
	Dimercaprol	-31.26	-24.42	-6.84
	Pentetic Acid	-97.5	-62.2	-26.24

Table 24. Docking of Protein (JNK+ Pentetic acid) and Arsenic chelators using *i*Gemdock

Receptor	Ligand	Total Energy	VDW	HBond
JNK + Pentetic acid	Arsenic pentaoxide	-50.03	-33.03	-17.01
	$CaNa_2EDTA$	-123.12	-73.62	-60
	Trichloro arsenic	-24.12	-24.12	0
	Arsenite	-40.63	-14.22	-26.42
	DMPS	6.31	7.84	-1.53
	DMSA	-1.3	-1.79	-0.43
	Dimercaprol	-44.42	-30.46	-13.96

Table 25. Docking of protein (JNK+ CaNa2EDTA) and Arsenic chelators using *i*Gemdock

Receptor	Ligand	Total Energy	VDW	HBond
JNK+$CaNa_2EDTA$	Arsenic pentaoxide	-51.12	-27.9	-23.14
	Trichloro arsenic	-24.08	-24.08	0
	Arsenite	-39.21	-22.9	-16.31
	DMPS	-18.04	-18.04	0
	DMSA	-13.54	-12.25	-4.75
	Dimercaprol	-46.43	-33.79	-12.64

Table 26. Docking of protein (ERK) and Arsenic chelators using *i*Gemdock.

Receptor	Ligand	Total Energy	VDW	HBond
ERK2	Arsenic pentaoxide	-59.98	-34.88	-25.1
	Trichloro arsenic	-26.09	-26.09	0
	Arsenite	-43.29	-16.85	-26.44
	DMPS	-65.53	-33.54	-29.99

	DMSA	-11.98	-12.79	0
	$CaNa_2EDTA$	-58.16	-58.16	0
	Dimercaprol	-44.16	-27.12	-17.04
	Pentetic Acid	-125.34	-71.55	-38.20

Table 27. Docking of protein (ERK + Pentetic acid) and Arsenic chelators using *i*Gemdock.

Receptor	Ligand	Total Energy	VDW	HBond
ERK2 + Pentetic acid	Arsenic pentaoxide	-59.89	-34.5	-25.31
	$CaNa_2EDTA$	-203.51	-183.7	-19.81
	Trichloro arsenic	-28.64	-28.64	0
	Arsenite	-44.0	-9.94	-34.26
	DMPS	-60.88	-34.79	-26.08
	DMSA	-17.43	-17.35	-1.34
	Dimercaprol	-44.54	-30.11	-14.43

Table 28. Docking ofprotein (ERK + $CaNa_2EDTA$) and Arsenic chelators using *i*Gemdock.

Receptor	Ligand	Total Energy	VDW	HBond
ERK2 + $CaNa_2EDTA$	Arsenic pentaoxide	-57.86	-31.8	-26.06
	Trichloro arsenic	-26.4	-26.4	0
	Arsenite	-45.53	-11.67	-33.86
	DMPS	-61.76	-38.95	-22.81
	DMSA	-19.28	-16.46	-6.36
	Dimercaprol	-43.77	-27.91	-15.86
	Pentetic Acid	-136.29	-83.83	-36.88

Table 29. Docking of protein (p38) and Arsenic chelators using *i*Gemdock.

Receptor	Ligands	Total Energy	VDW	HBond
1cm8	Arsenic pentaoxide	-57.74	-18.5	-39.25
	Trichloro arsenic	-18.79	-18.79	0
	Arsenite	-43.82	-14.05	-29.78
	DMPS	-60.79	-28.18	-36.61
	DMSA	-28.31	4.08	-16.25
	$CaNa_2EDTA$	-218.35	-117.1	-73.47
	Dimercaprol	-36.63	-19.15	-17.49
	Pentetic Acid	-135.88	-61.08	-54.7

Table 30. Docking of Protein (p38 + Pentetic acid) and Arsenic chelators using *i*Gemdock.

Receptor	Ligand	Total Energy	VDW	HBond
1cm8 + Pentetic acid	Arsenic pentaoxide	-56.39	-17.43	-38.96
	$CaNa_2EDTA$	-64.5	-64.5	0
	Trichloro arsenic	-25.43	-25.43	0
	Arsenite	-43.44	-13.61	-29.84
	DMPS	-31.28	-15.44	-15.84
	DMSA	-11.93	-7.34	-3.5
	Dimercaprol	-42.11	-32.86	-9.25

Table 31. Docking of protein (p38 + Pentetic acid) and Arsenic chelators using *i*Gemdock.

Receptor	Ligand	Total Energy	VDW	HBond
1cm8 + $CaNa_2EDTA$	Arsenic pentaoxide	-55.65	-26.6	-29.05
	Trichloro arsenic	-24.59	-24.59	0
	Arsenite	-42.02	-10.53	-31.49
	DMPS	-28.31	-26.53	-1.78
	DMSA	-31.78	-31.84	-0.67
	Dimercaprol	-41.35	-36.35	-5
	Pentetic acid	-131.65	-67.2	-44.32

Table 32. Results of protein (JNK) and chromium compounds using HEX

Receptor	Ligands	Etotal	Eshape	Eforce	Eair	BMP	RMS
JNK	$CaNa_2EDTA$	-171.4	-171.4	0.0	0.0	-1	-1.0
	Dimercaprol	-128.2	-128.2	0.0	0.0	-1	-1.0
	DMPS	-152.1	-152.1	0.0	0.0	-1	-1.0
	DMSA	-143.8	-143.8	0.0	0.0	-1	-1.0
	Ascorbic Acid	-164.2	-164.2	0.0	0.0	-1	-1.0
	Ammonium Dichromate	-157.4	-157.4	0.0	0.0	-1	-1.0
	Calcium Chromate	-136.3	-136.3	0.0	0.0	-1	-1.0
	Chromium Trioxide	-92.0	-92.0	0.0	0.0	-1	-1.0
	EDTA	-200.5	-200.5	0.0	0.0	-1	-1.0
	Lead Chromate	-117.1	-117.1	0.0	0.0	-1	-1.0
	NAC	-146.7	-146.7	0.0	0.0	-1	-1.0
	Potassium Chromate	-132.4	-132.4	0.0	0.0	-1	-1.0
	Potassium Dichromate	-147.3	-147.3	0.0	0.0	-1	-1.0
	Sodium Chromate	-154.5	-154.5	0.0	0.0	-1	-1.0
	Sodium Dichromate	-169.1	-169.1	0.0	0.0	-1	-1.0
	Strontium Chromate	-111.6	-111.6	0.0	0.0	-1	-1.0
	Zinc Chromate	-99.5	-99.5	0.0	0.0	-1	-1.0
	Oxalic Acid	-108.9	-108.9	0.0	0.0	-1	-1.0
	Citric Acid	-152.8	-152.8	0.0	0.0	-1	-1.0
	Pentetic Acid	-262.7	-262.7	0.0	0.0	-1	-1.0

Table 33. Results of protein (1ERK) and chromium compounds using HEX

Receptor	Ligands	Etotal	Eshape	Eforce	Eair	BMP	RMS
1ERK	$CaNa_2EDTA$	-175.1	-175.1	0.0	0.0	-1	-1.0
	Dimercaprol	-124.4	-124.4	0.0	0.0	-1	-1.0
	DMPS	-154.9	-154.9	0.0	0.0	-1	-1.0
	DMSA	-171.0	-171.0	0.0	0.0	-1	-1.0
	Ascorbic Acid	-171.0	-171.0	0.0	0.0	-1	-1.0
	Ammonium Dichromate	-179.7	-179.7	0.0	0.0	-1	-1.0
	Calcium Chromate	-135.4	-135.4	0.0	0.0	-1	-1.0
	Chromium Trioxide	-102.4	-102.4	0.0	0.0	-1	-1.0
	Lead Chromate	-128.6	-128.6	0.0	0.0	-1	-1.0
	NAC	-154.4	-154.4	0.0	0.0	-1	-1.0

	Potassium Chromate	-124.0	-124.0	0.0	0.0	-1	-1.0
	Potassium Dichromate	-157.5	-157.5	0.0	0.0	-1	-1.0
	Sodium Chromate	-148.3	-148.3	0.0	0.0	-1	-1.0
	Sodium Dichromate	-183.7	-183.7	0.0	0.0	-1	-1.0
	Strontium Chromate	-125.9	-125.9	0.0	0.0	-1	-1.0
	Zinc Chromate	-106.4	-106.4	0.0	0.0	-1	-1.0
	Oxalic Acid	-112.5	-112.5	0.0	0.0	-1	-1.0
	Citric Acid	-166.6	-166.6	0.0	0.0	-1	-1.0
	Pentetic Acid	-164.4	-164.4	0.0	0.0	-1	-1.0

Table 34. Results of protein (1cm8) and chromium compounds using HEX

S.No.	Receptor	Ligands	Etotal	Eshape	Eforce	Eair	BMP	RMS
	1cm8	$CaNa_2EDTA$	-140.6	-140.6	0.0	0.0	-1	-1.0
		Dimercaprol	-129.4	-129.4	0.0	0.0	-1	-1.0
		DMPS	-156.9	-156.9	0.0	0.0	-1	-1.0
		DMSA	-163.0	-163.0	0.0	0.0	-1	-1.0
		Ascorbic Acid	-175.1	-175.1	0.0	0.0	-1	-1.0
		Ammonium Dichromate	-172.1	-172.1	0.0	0.0	-1	-1.0
		Calcium Chromate	-119.3	-119.3	0.0	0.0	-1	-1.0
		Chromium Trioxide	-83.3	-83.3	0.0	0.0	-1	-1.0
		Lead Chromate	-112.1	-112.1	0.0	0.0	-1	-1.0
		NAC	-138.6	-138.6	0.0	0.0	-1	-1.0
		Potassium Chromate	-142.8	-142.8	0.0	0.0	-1	-1.0
		Potassium Dichromate	-171.3	-171.3	0.0	0.0	-1	-1.0
		Sodium Chromate	-154.3	-154.3	0.0	0.0	-1	-1.0
		Sodium Dichromate	-191.3	-191.3	0.0	0.0	-1	-1.0
		Strontium Chromate	-111.1	-111.1	0.0	0.0	-1	-1.0
		Zinc Chromate	-90.5	-90.5	0.0	0.0	-1	-1.0
		Oxalic Acid	-104.1	-104.1	0.0	0.0	-1	-1.0
		Citric Acid	-169.7	-169.7	0.0	0.0	-1	-1.0
		Pentetic Acid	-229.7	-229.7	0.0	0.0	-1	-1.0

Table 35. Docking of protein (JNK) and Arsenic chelators and compounds using HEX

S. No.	Receptor	Ligands	Etotal	Eshape	Eforce	Eair	BMP	RMS
	JNK	Arsenic pentaoxide	-133.2	-133.2	0.0	0.0	-1	-1.0
		Trichloro arsenic	-122.7	-122.7	0.0	0.0	-1	-1.0
		Arsenite	-97.0	-97.0	0.0	0.0	-1	-1.0
		Dmps	-152.1	-152.1	0.0	0.0	-1	-1.0
		DMSA	-143.8	-143.8	0.0	0.0	-1	-1.0
		$CaNa_2EDTA$	-128.2	-128.2	0.0	0.0	-1	-1.0
		Dimercaprol	-262.7	-262.7	0.0	0.0	-1	-1.0
		Pentetic Acid	-171.4	-171.4	0.0	0.0	-1	-1.0

Table 36. Docking of protein (ERK) and Arsenic chelators and compounds using HEX

S. No.	Receptor	Ligands	Etotal	Eshape	Eforce	Eair	BMP	RMS
	ERK2	Arsenic pentaoxide	-139.4	-139.4	0.0	0.0	-1	-1.0
		Trichloro arsenic	-135.2	-135.2	0.0	0.0	-1	-1.0
		Arsenite	-112.4	-112.4	0.0	0.0	-1	-1.0
		Dmps	-158.3	-158.3	0.0	0.0	-1	-1.0
		DMSA	-138.3	-138.3	0.0	0.0	-1	-1.0
		$CaNa_2EDTA$	-170.3	-170.3	0.0	0.0	-1	-1.0
		Dimercaprol	-136.2	-136.2	0.0	0.0	-1	-1.0
		Pentetic Acid	-259.8	-259.8	0.0	0.0	-1	-1.0

Table 37. Docking of protein (1cm8) with Arsenic chelators and compounds using HEX

S. No.	Receptor	Ligands	Etotal	Eshape	Eforce	Eair	BMP	RMS
	1cm8	Arsenic Pentaoxide	-139.4	-139.4	0.0	0.0	-1	-1.0
		Trichloro Arsenic	-135.2	-135.2	0.0	0.0	-1	-1.0
		Arsenite	-112.4	-112.4	0.0	0.0	-1	-1.0
		DMPS	-158.3	-158.3	0.0	0.0	-1	-1.0
		DMSA	-138.3	-138.3	0.0	0.0	-1	-1.0
		Dimercaprol	-170.3	-170.3	0.0	0.0	-1	-1.0
		Pentetic acid	-136.2	-136.2	0.0	0.0	-1	-1.0
		$CaNa_2EDTA$	-259.8	-259.8	0.0	0.0	-1	-1.0