Electronic Supporting Information

Influence of anchoring moieties on new benzimidazole-based Schiff base copper(II) complexes towards estrogen dependent breast cancer cells

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Table S2. Selected bond distances (Å) and angles (°) for compound **1**.

Table S3. Hydrogen bond geometry (Å, °) in compound **1**.

Table S4. Cartesian atomic coordinates of the equilibrium structures.

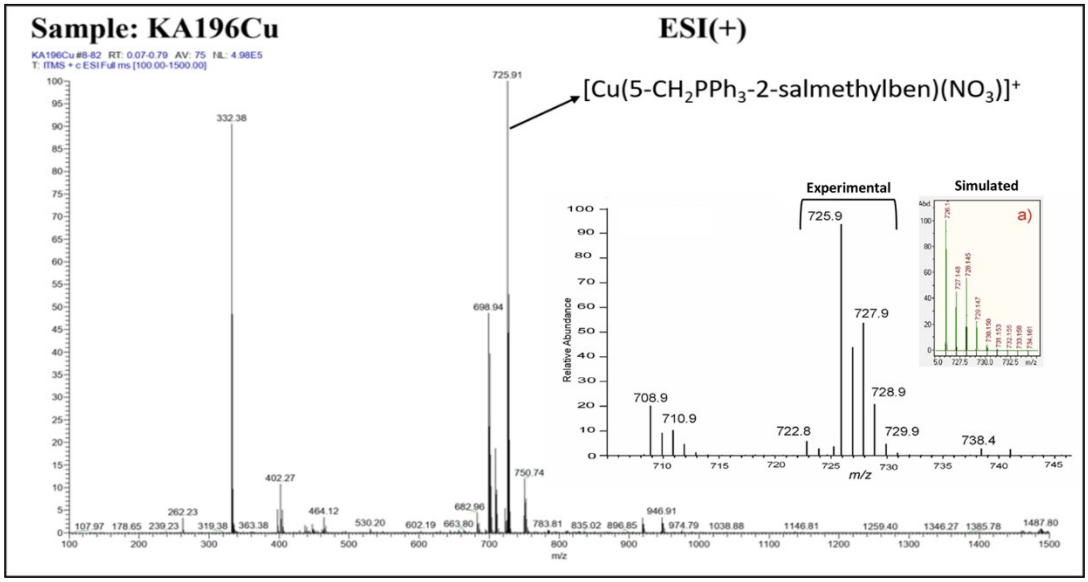

Figure S1. ESI-MS spectrum of **1** in MeOH. Inset showing the experimental and simulated isotopic mass distribution pattern of the parent ion peak.

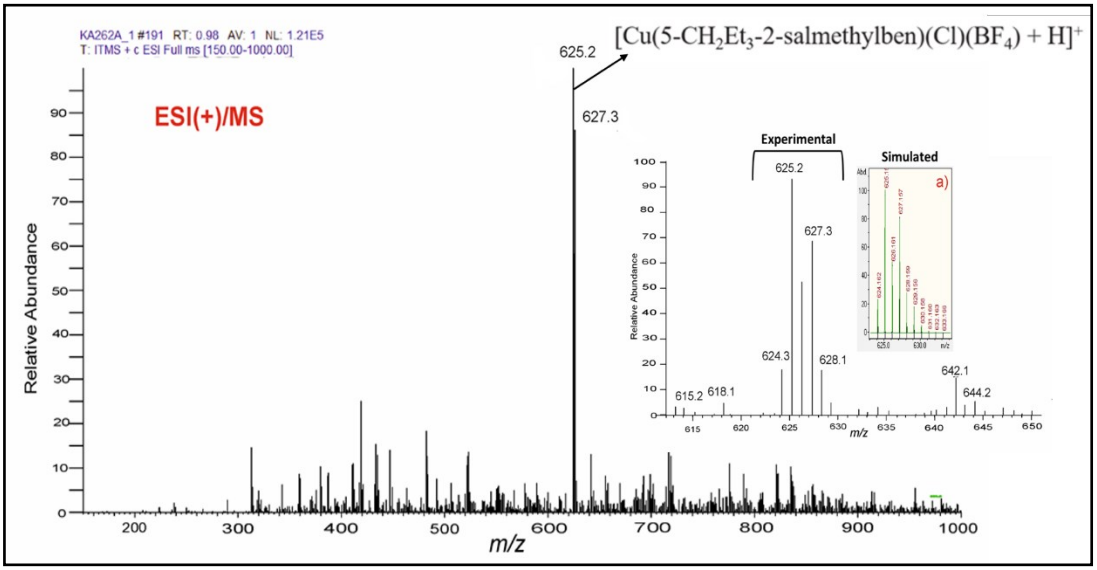

Figure S2. ESI-MS spectrum of **2** in MeOH. Inset showing the experimental and simulated isotopic mass distribution pattern of the parent ion peak.

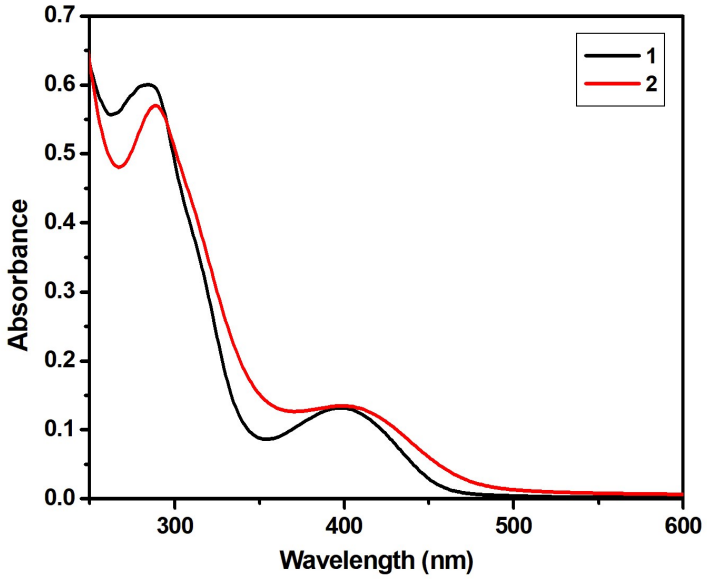

Figure S3. UV-vis spectra of **1** and **2** recorded in DMF solution.

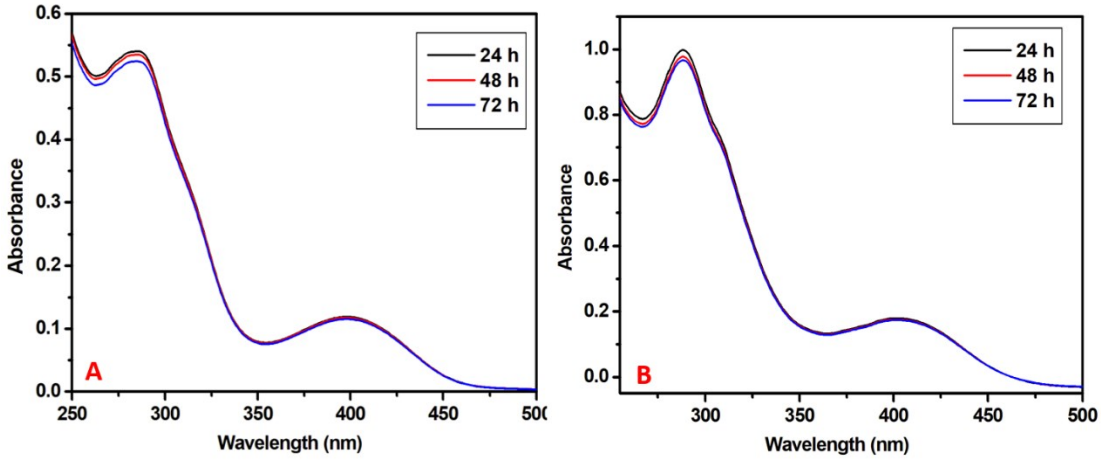

Figure S4. UV-vis spectra of **1** (A) and **2** (B) recorded in 1% DMF and DMSO solution with 5 mM Tris-HCl/50 mM NaCl buffer (pH 7.4).

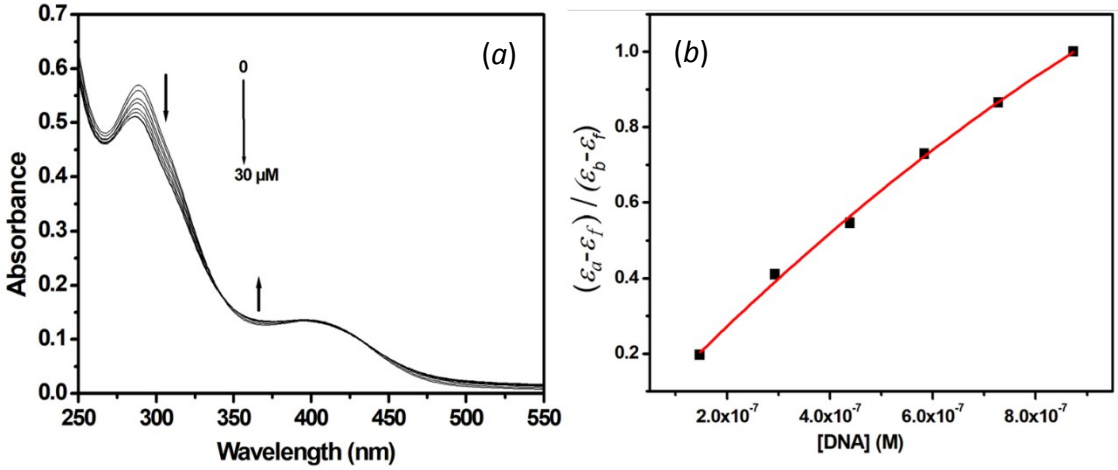

Figure S5. (a) Absorption spectra of complex **2** (2.01×10^{-5} M) in the absence and presence of increasing amounts of CT-DNA (0-8.7 X 10^{-7} M) at 25 °C in 5 mM Tris-HCl/50 mM NaCl buffer (pH 7.4). Arrow shows the absorbance changing upon increasing DNA concentrations. (b) The non-linear fit of $(\varepsilon_a - \varepsilon_f)/(\varepsilon_b - \varepsilon_f)$ *vs.* [DNA].

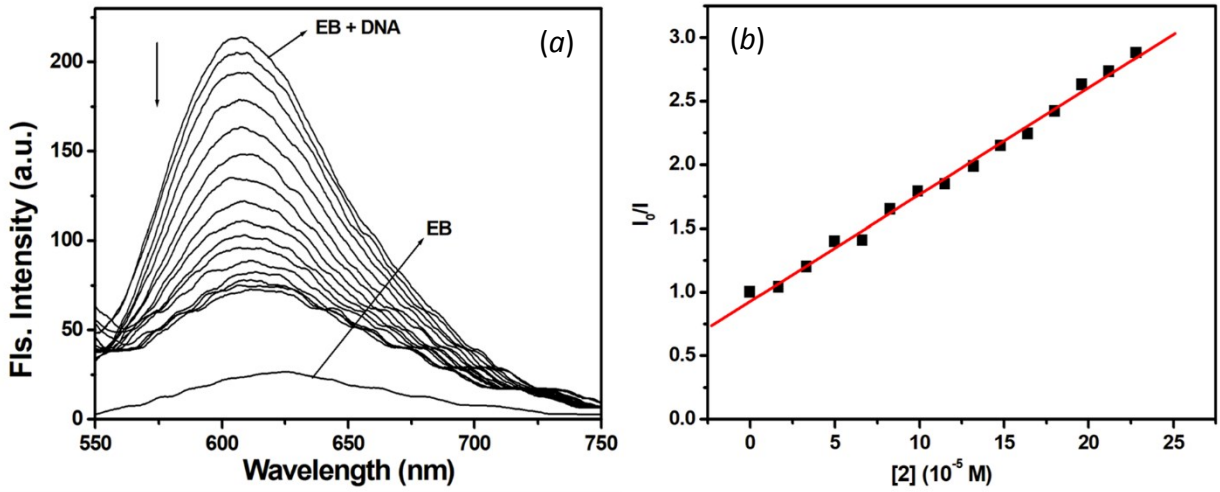

Figure S6. (a) Emission spectra from EB bound to the DNA in the absence and in the presence of **2** (a). [EB] = 3.3 μM, [DNA] = 3.3 μM, [**2**] = 0-25 μM. (b) Arrow shows changes in the emission intensity upon addition of increasing complex concentration. Stern-Volmer plots of the EB-DNA fluorescence titration for complex **2**.

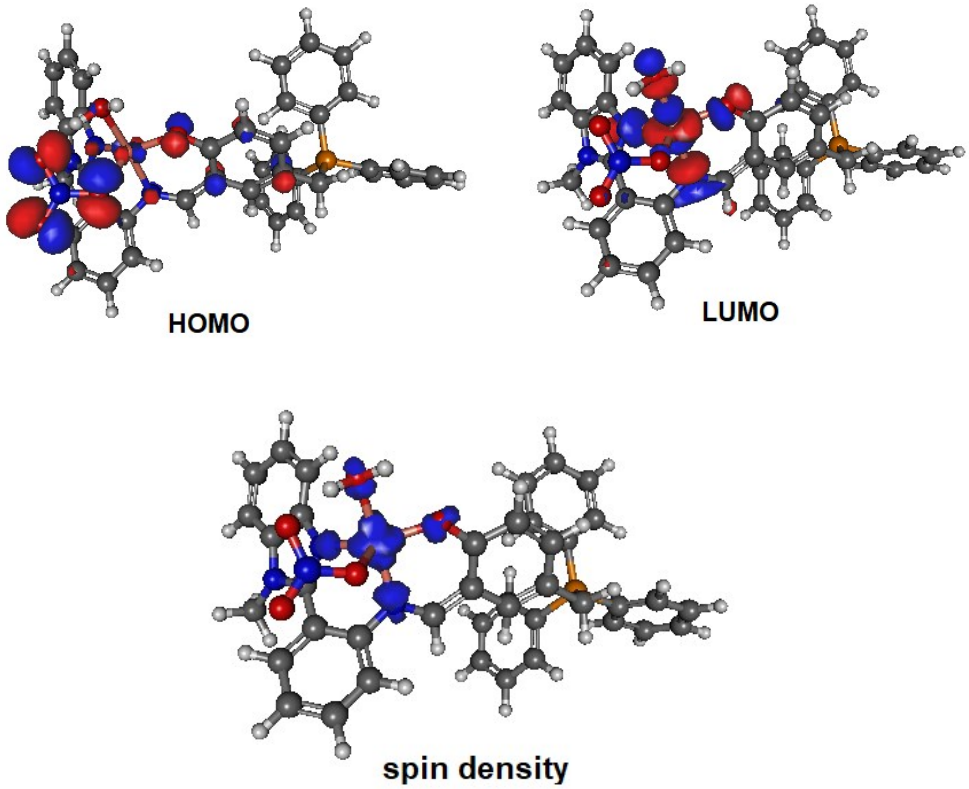

Figure S7. Plots of the HOMO, LUMO and spin density distribution in **1'**$^{+}$.

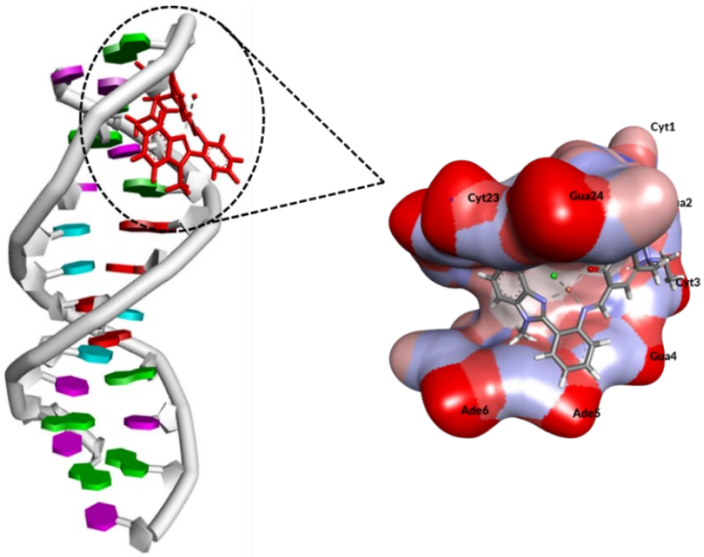

Figure S8. Molecular docked model of compound **2** with DNA (PDB ID: 1BNA).

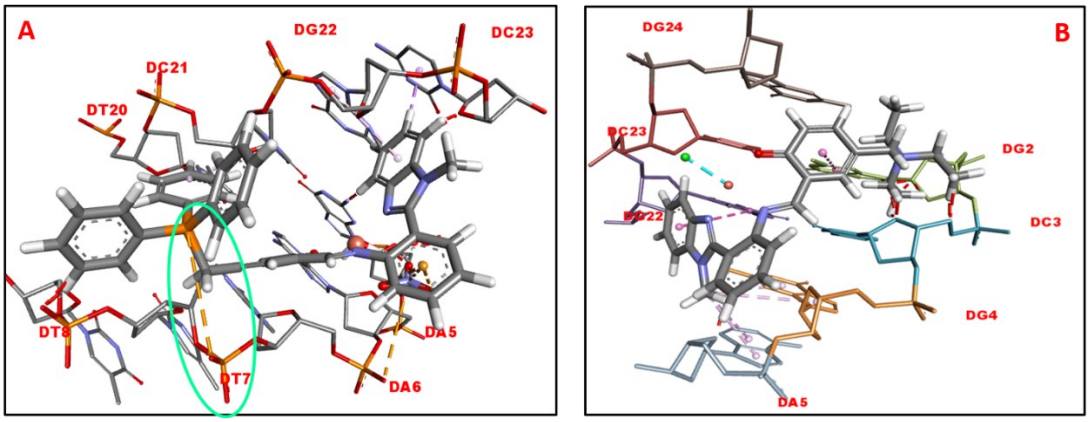

Figure S9. Close view of the molecular docked model of compounds **1** (A) and **2** (B) with DNA (PDB ID: 1BNA).

Table S1: Crystal data and structure refinement detail for compound **1**.

Identification name	**1**

Formula	$C_{40.33}H_{36.67}BCuF_4N_4O_6P$
Mol. wt.	854.786
Crystal system	Triclinic
Space group	P-1
Temperature /K	296
Wavelength /Å	0.71073
a /Å	9.9720(14)
b /Å	11.9734(18)
c /Å	16.945(3)
α/°	93.098(5)
β/°	98.044(5)
γ/°	109.200(5)
V/ Å^3	1881.0(5)
Z	2
Density/Mgm^{-3}	1.509
Abs. Coeff. /mm^{-1}	0.698
F(000)	880.758
Refl. collected	18407
Refl. unique	6615
Max. 2θ/°	25.00
Ranges (h, k, l)	-11<= h <=11 -14 <= k <=14 -20<= l <= 0
Complete to 2θ (%)	99.86
Refl. with I > 2σ(I)	4693
Data/Restraints/Parameters	6615/73/583
Goof (F^2)	1.0591
R1 [I > 2s(I)]	0.0439
wR2 [I > 2s(I)]	0.0790
R1 [all data]	0.0869
wR2 [all data]	0.1000

Table S2: Selected bond distances (Å) and angles (°) for compound **1**.

1	Cu1-O2 1.965(2); Cu1-O6 1.908(2); Cu1-O3 2.598(2); Cu1-N1 1.971(2); Cu1-N3 1.956(2). <O6-Cu1-O2 88.40(9); <O3-Cu1-O2 82.94(8); <O3-Cu1-O6 114.09(8); <N1-Cu1-O2 92.60(9); <N1-Cu1-O6 156.40(10); <N1-Cu1-O3 89.41(9); <N3-Cu1-

	O2 170.63(10); <N3-Cu1-O6 93.11(10); <N3-Cu1-O3 88.00(9); <N3-Cu1-N1 89.71(10).

Table S3: Hydrogen bond geometry (Å, °) in compound **1**.

Compound	D-H···A	D···H (Å)	H···A (Å)	D···A (Å)	<D−H···A(°)
1	O2-H2A···O5	0.90	1.76	2.666(3)	179.9
	O2-H2B···O1B	0.90	1.79	2.687(2)	178.0
	O1B-H1Ba···O4	0.84	2.05	2.890(2)	170.6
	O1B-H1Bb···F1A	0.85	2.09	2.908(3)	159.6
	C22-H22A···F1A	0.97	2.52	3.410(5)	152.9
	C22-H22A···F2A	0.97	2.93	3.850(1)	157.7
	C5-H5···O4	0.93	2.55	3.476(5)	172.7
	C38-H38···O5	0.93	2.70	3.452(5)	137.5

Table S4. Cartesian atomic coordinates of the equilibrium structures (nuclear charges are indicated in the first column).

1'$^{+}$

29	2.884140	0.654309	-1.192611
15	-4.816959	-0.147879	-0.072163
8	3.808188	2.288058	-1.906179
1	4.662897	1.817965	-2.172668
1	3.328992	2.466506	-2.731296
8	1.240973	1.315732	-2.005607
8	5.829341	0.643109	-2.303742
8	3.998716	-0.491145	-2.646113
8	5.887624	-1.516462	-2.403582
7	4.033903	0.609977	0.459233
7	2.060462	-1.052436	-0.641212
7	5.265235	-0.472513	-2.451735
7	4.957274	-0.305979	2.261427
6	0.074204	0.801900	-1.914661
6	4.338280	-0.529277	1.061644
6	-0.219422	-0.447805	-1.264332
6	-6.573378	-0.539936	-0.154078
6	4.481970	1.633634	1.272753
6	-2.600513	-0.208516	-1.760361
6	-7.240941	-0.981151	0.994036
1	-6.696989	-1.122372	1.927191

6	4.424344	3.019188	1.115588
1	3.991998	3.455222	0.217950
6	-3.293932	2.128057	0.381179
1	-2.434879	1.460455	0.439633
6	4.099638	-1.845850	0.474040
6	2.979100	-2.085861	-0.350057
6	-2.305563	1.004153	-2.427383
1	-3.119809	1.566195	-2.889489
6	-1.027692	1.489273	-2.504797
1	-0.803823	2.417150	-3.026720
6	-4.019980	-0.673283	-1.642869
1	-4.122570	-1.767202	-1.694249
1	-4.635350	-0.260982	-2.454877
6	-4.584194	1.617380	0.170819
6	5.068901	1.067510	2.413358
6	0.796008	-1.310991	-0.744622
1	0.453620	-2.304451	-0.418233
6	2.834091	-3.328900	-0.964978
1	2.015804	-3.477215	-1.666955
6	-4.096094	-1.074760	1.293104
6	-1.549290	-0.911476	-1.207151
1	-1.736344	-1.868736	-0.712654
6	-3.112194	3.497108	0.514013
1	-2.112160	3.894704	0.671689
6	5.043199	-2.865596	0.634823
1	5.953897	-2.664632	1.194382
6	-8.603663	-1.244840	0.941829
1	-9.121233	-1.589033	1.834250
6	-8.643722	-0.627535	-1.392363
1	-9.191036	-0.490858	-2.322107
6	4.964445	3.793608	2.129140
1	4.946452	4.877503	2.037927
6	-7.282247	-0.358239	-1.348473
1	-6.783043	0.002904	-2.247165
6	3.767266	-4.336243	-0.765915
1	3.645263	-5.290732	-1.273051
6	-3.690858	-0.439175	2.469120
1	-3.756768	0.643646	2.561016
6	-5.486424	3.852577	0.239968
1	-6.338905	4.525930	0.190801
6	-4.205920	4.356845	0.441489
1	-4.057695	5.429611	0.545927
6	-4.027848	-2.470902	1.191717
1	-4.369978	-2.980655	0.290167
6	-5.681124	2.483349	0.103176
1	-6.684431	2.088597	-0.050439

6	-9.302319	-1.072016	-0.249103
1	-10.368503	-1.284396	-0.287290
6	4.879956	-4.103675	0.031950
1	5.641961	-4.869364	0.153642
6	-3.203495	-1.196085	3.529655
1	-2.887882	-0.699874	4.444535
6	5.613160	1.840928	3.434119
1	6.081319	1.396572	4.310363
6	-3.539984	-3.218329	2.253733
1	-3.488388	-4.301777	2.174387
6	5.548152	3.216050	3.269314
1	5.968554	3.863374	4.035918
6	-3.125063	-2.579792	3.420932
1	-2.746060	-3.168468	4.253573
6	5.312386	-1.253188	3.299048
1	4.778886	-2.193973	3.144269
1	5.016192	-0.838810	4.269165
1	6.392061	-1.446084	3.309942

2'⁺

29	-1.715031	-0.720394	-1.273544
7	5.869153	-0.032932	0.764408
17	-2.805343	-2.125882	-2.545337
8	0.040436	-1.474680	-1.665088
7	-3.151192	-0.385192	0.050050
7	-0.891526	1.061605	-0.782938
7	-4.295166	0.700507	1.613928
6	1.186657	-0.998268	-1.408206
6	-3.457028	0.806855	0.537072
6	1.428061	0.309014	-0.851056
6	7.257273	0.565127	0.858568
6	-3.825504	-1.325185	0.807993
6	3.844387	-0.085067	-0.834064
6	-3.864175	-2.717196	0.715630
1	-3.329347	-3.230526	-0.080980
6	-3.015397	2.064820	-0.059257
6	-1.758804	2.174071	-0.694295
6	3.605426	-1.350897	-1.437089
1	4.451868	-1.981665	-1.715330
6	2.342321	-1.791600	-1.706808
1	2.159741	-2.756606	-2.174005
6	5.221546	0.409930	-0.579974
1	5.242537	1.503958	-0.543295
1	5.932206	0.086089	-1.349117
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6	-4.548770	-0.650592	1.801146

6	0.383046	1.253984	-0.627334
1	0.711025	2.252215	-0.297751
6	-1.401775	3.382741	-1.296908
1	-0.463421	3.440649	-1.845780
6	4.980579	0.445318	1.894013
6	2.746271	0.717448	-0.580786
1	2.896979	1.720668	-0.170582
6	-3.868460	3.173910	-0.067686
1	-4.865616	3.078616	0.356311
6	-4.636431	-3.387428	1.648487
1	-4.700719	-4.472278	1.603909
6	-2.252225	4.479560	-1.265716
1	-1.955648	5.404992	-1.754414
6	-3.494242	4.375031	-0.652645
1	-4.184287	5.215108	-0.655579
6	-5.325993	-1.320565	2.742060
1	-5.895862	-0.793580	3.504684
6	-5.353780	-2.702858	2.645213
1	-5.954644	-3.271957	3.351303
6	-4.731943	1.725418	2.541616
1	-4.089176	2.604951	2.458073
1	-4.652327	1.330807	3.560485
1	-5.773150	2.015950	2.354927
1	4.016709	-0.051237	1.736685
1	4.819101	1.515206	1.716623
6	5.499609	0.204142	3.294018
1	7.758936	0.050571	1.687713
6	7.320843	2.065567	1.040405
1	7.773569	0.275149	-0.062837
1	4.940556	-1.909285	0.706944
1	6.290644	-1.785402	1.846693
6	6.901305	-2.192026	-0.169741
1	6.776476	-3.277209	-0.081990
1	7.956573	-1.978204	0.029092
1	6.681501	-1.931536	-1.211236
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1	6.861944	2.620519	0.215072
1	8.378068	2.352329	1.061868
1	5.562605	-0.856955	3.556393
1	4.787624	0.655868	3.993801
1	6.473217	0.669841	3.483624