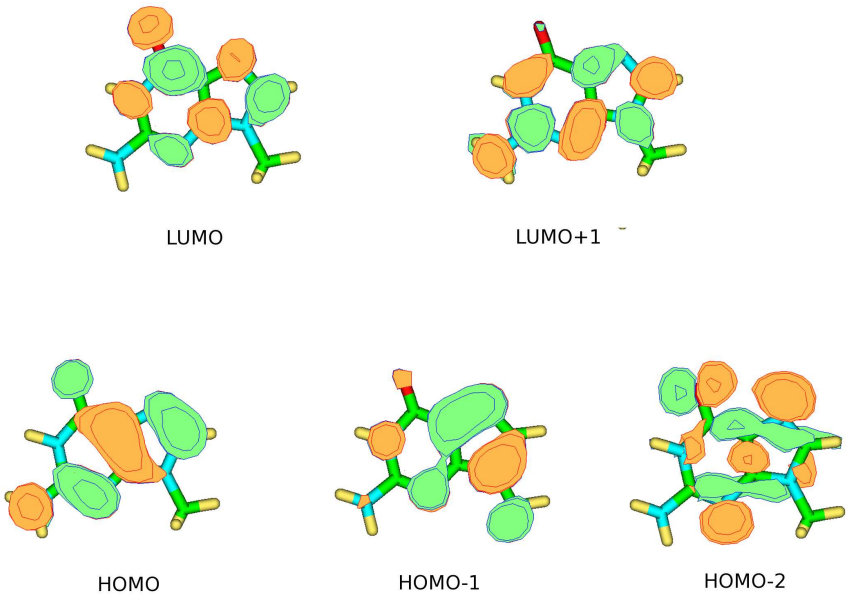

Figure 1: Schematic drawing of the frontier orbitals of 9Me-Gua as predicted by PCM/M052X/6-31+G(d,p) calculations

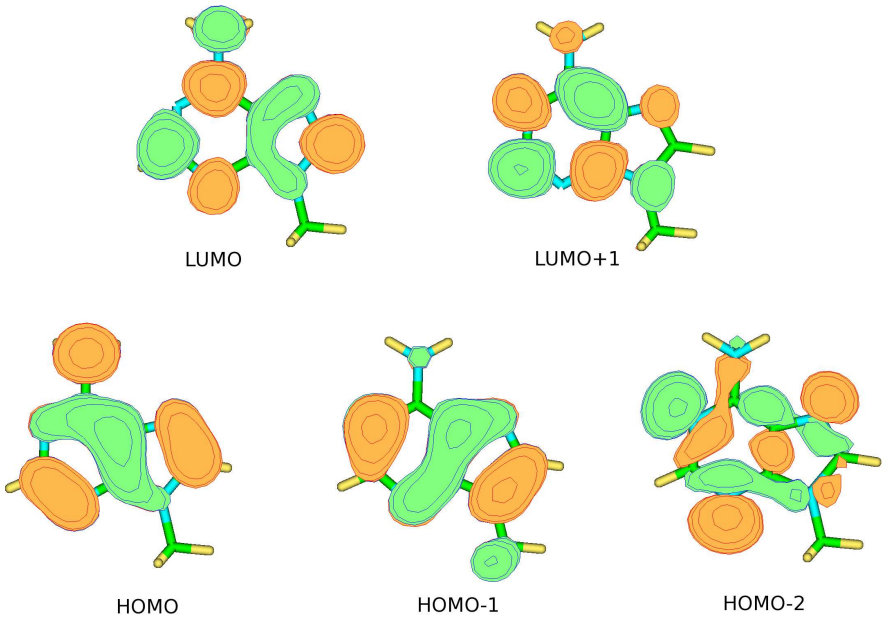

Figure 2: Schematic drawing of the frontier orbitals of 9Me-Ade as predicted by PCM/M052X/6-31+G(d,p) calculations

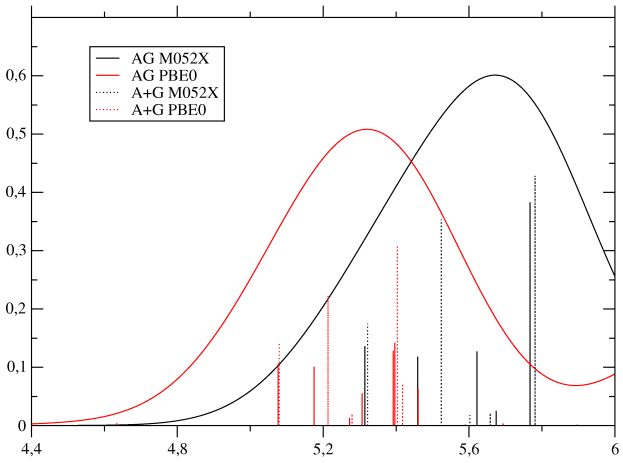

Figure 3: Comparison between the absorption spectra of AG computed by using LR-PCM/TD-PBE0/6-31G(d) or LR-PCM/TD-M052X/6-31G(d) calculations by using the geometry optimized at the PCM/PBE0/6-31G(d) level. The transitions of a mixture of the isolate monomers are also shown. The spectra are obtained by convoluting the stick spectra with a phenomenological gaussian with a HWMH of 0.20 eV.

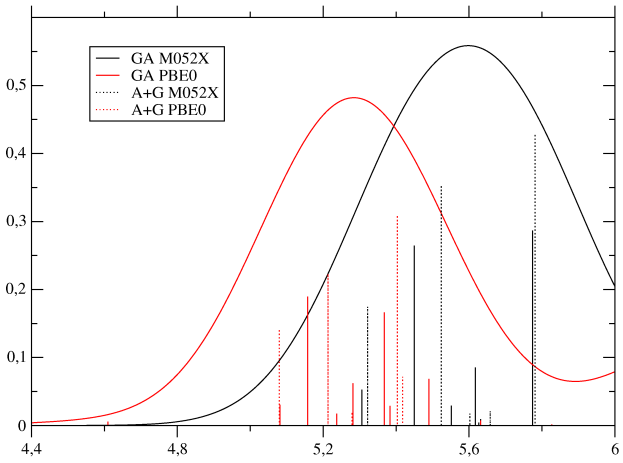

Figure 4: Comparison between the absorption spectra of GA computed by using LR-PCM/TD-PBE0/6-31G(d) or LR-PCM/TD-M052X/6-31G(d) calculations by using the geometry optimized at the PCM/PBE0/6-31G(d) level. The transitions of a mixture of the isolate monomers are also shown. The spectra are obtained by convoluting the stick spectra with a phenomenological gaussian with a HWMH of 0.20 eV.

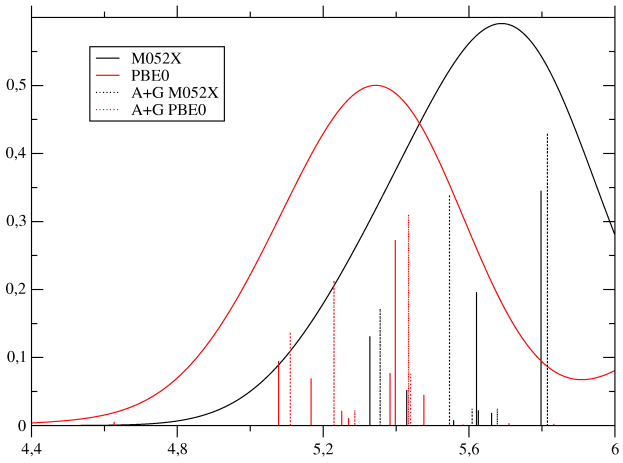

Figure 5: Comparison between the absorption spectra of AG computed by using LR-PCM/TD-PBE0/6-31G(d) or LR-PCM/TD-M052X/6-31G(d) calculations by using the geometry optimized at the PCM/M052X/6-31G(d) level. The transitions of a mixture of the isolate monomers are also shown. The spectra are obtained by convoluting the stick spectra with a phenomenological gaussian with a HWMH of 0.20 eV.

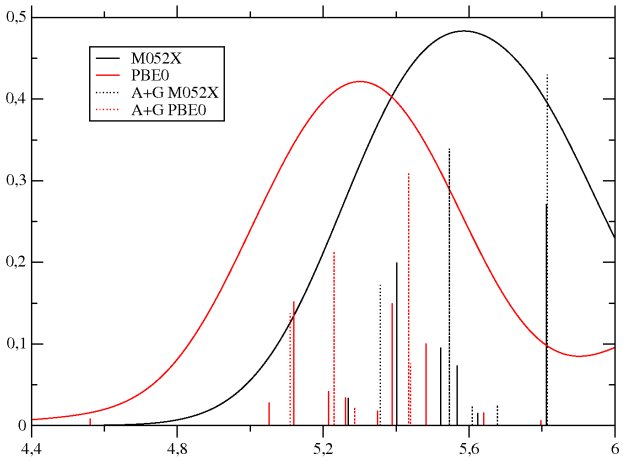

Figure 6: Comparison between the absorption spectra of AG computed by using LR-PCM/TD-PBE0/6-31G(d) or LR-PCM/TD-M052X/6-31G(d) calculations by using the geometry optimized at the PCM/M052X/6-31G(d) level. The transitions of a mixture of the isolate monomers are also shown. The spectra are obtained by convoluting the stick spectra with a phenomenological gaussian with a HWMH of 0.20 eV.

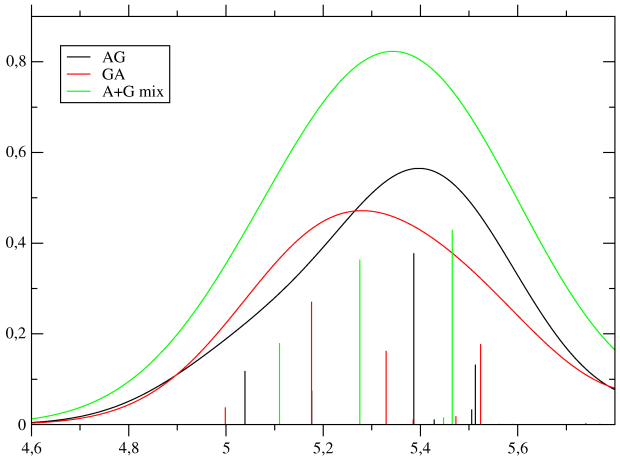

Figure 7: Comparison between the absorption spectra of AG (in black) and GA (in red) dimers with that of the isolated monomers. computed at the LR-PCM/CAM-B3LYP/6-31+G(d)//PCM/M052X/6-31G(d) level. The spectra are obtained by convoluting the stick spectra with a phenomenological gaussian with a HWMH of 0.20 eV.

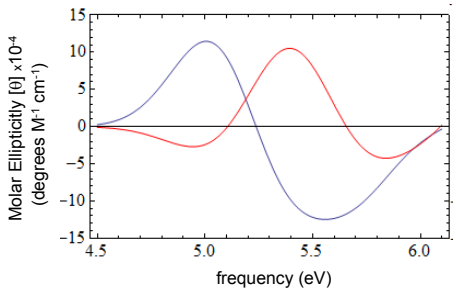

Figure 8: Comparison between the ECD spectra of AG (in red) and GA (in black) dimers, computed at the LR-PCM/M052X/6-31+G(d,p)//PCM/M052X/6-31G(d) level and convoluted by a phenomonological gaussian with HWMH of 0.20 eV

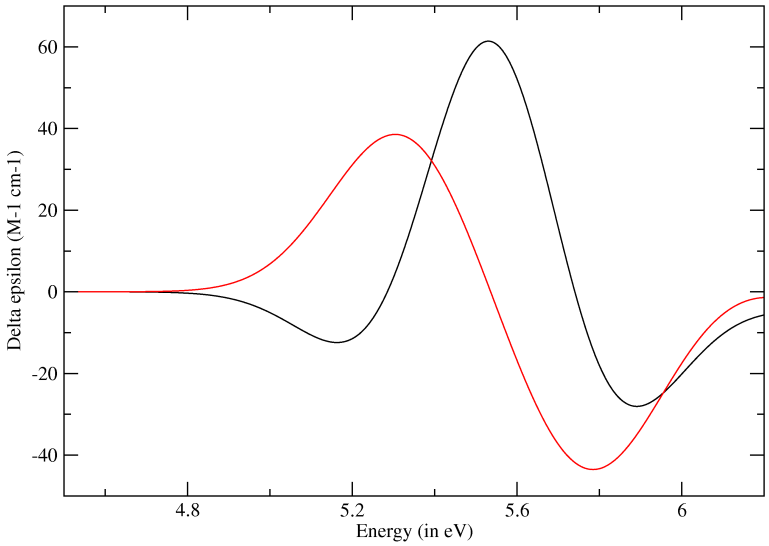

Figure 9: Comparison between the ECD spectra of AG (in red) and GA (in black) dimers, computed at the LR-PCM/PBE0/6-31+G(d,p)//PCM/M052X/6-31G(d) level and convoluted by a phenomenological gaussian with HWMH of 0.20 eV

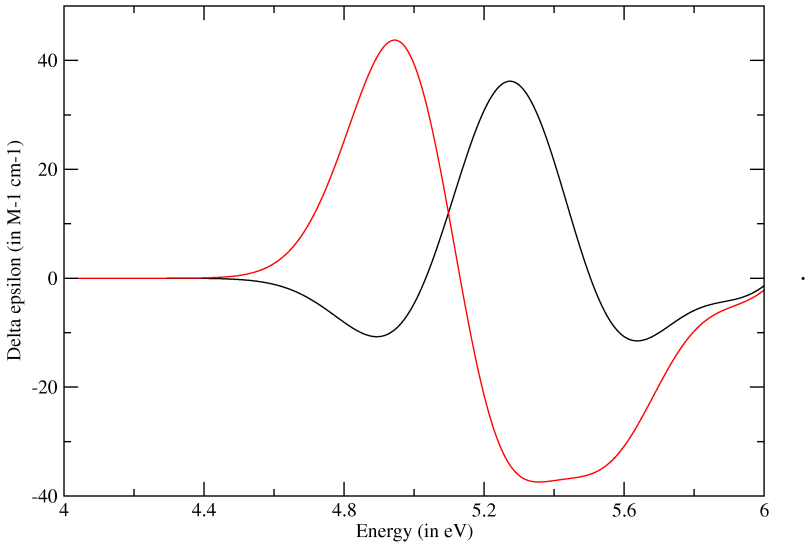

Figure 10: Comparison between the ECD spectra of AG (in red) and GA (in black) dimers, computed at the LR-PCM/CAM-B3LYP/6-31+G(d,p)//PCM/M052X/6-31G(d) level and convoluted by a phenomenological gaussian with HWMH of 0.20 eV

Table 1: Main features of the lowest energy excited states of AG related to the $\pi\pi^*$ transitions of the monomer, according tp PCM-TDM052X/6-31+G(d,p) calculations on the minimum provided by PCM/PBE0/6-31G(d) partial geometry optimizations of B-DNA like AG. NonEquilibrium Solvation

State	1	2	3	4
		LR Results		
VEE	5.14	5.29	5.51	5.60
O.St	0.13	0.13	0.38	0.14
	KS excitations involved in the transitions			
	0.57 G-H→G-L	0.61 A-H→A-L	0.43 G-H→A-L	0.43 G-H→A-L
	0.25 G-H→A-L	-0.23 G-H→G-L1	0.29 A-H→A-L	-0.33 G-H→G-L
	-0.26 G-H→G-L1		0.32 G-H→G-L1	0.34 G-H→G-L1
		$\mathbf{Q}_m$		
9Me-A	0.02	0.01	-0.32	-0.46
9Me-G	-0.02	-0.01	0.32	0.46
		$\mathbf{v}_m$		
9Me-A	0.10	0.46	0.51	0.65
9Me-G	0.42	0.28	0.49	0.92
		SS Results		
VEE	5.10	5.38	5.19	5.32
O.St	0.10	0.07	0.02	0.09
μ	9.20	8.20	13.3	12.8
	KS excitations involved in the transitions			
	0.57 G-H→G-L	0.58 A-H →A-L	0.50 G-H→A-L	0.54 A-H→A-L
	0.26 G-H→A-L	-0.26 G-H →G-L1	-0.28 G-H →G-L	0.40 G-H→H-L
	-0.24 G-H→G-L1	-0.27 G-H →G-L		
		$\mathbf{Q}_m$		
9Me-A	0.02	-0.01	-0.47	-0.37
9Me-G	-0.02	0.01	0.47	0.37
		$\mathbf{v}_m$		
9Me-A	0.09	0.41	0.54	0.53
9Me-G	0.38	0.29	0.56	0.57

Table 2: Main features of the lowest energy excited states of GA related to the $\pi\pi^*$ transitions of the monomer, according tp PCM-TDM052X/6-31+G(d,p) calculations on the minimum provided by PCM/PBE0/6-31G(d) partial geometry optimizations of B-DNA like AG. NonEquilibrium Solvation

State	1	2	3	4
		LR Results		
VEE	5.13	5.30	5.46	5.64
O.St	0.04	0.33	0.19	0.18
	KS excitations involved in the transitions			
	0.50 G-H→G-L	0.61 A-H→A-L	0.50 G-H→G-L1	0.41 G-H→G-L
	-0.30 G-H→G-L1	0.25 G-H→A-L	0.41 G-H→G-L	-0.40 G-H→A-L
	0.26 G-H→A-L			0.23 G-H→G-L1
	0.23 A-H→A-L			
		$\mathbf{Q}_m$		
9Me-A	-0.10	-0.08	-0.30	-0.56
9Me-G	0.10	0.08	0.30	0.56
		$\mathbf{v}_m$		
9Me-A	0.16	0.54	0.45	0.70
9Me-G	0.54	0.17	0.58	0.87
		SS Results		
VEE	5.12	5.38	a	a
O.St	0.03	0.22		
μ	13.3	12.2		
	KS excitations involved in the transitions			
	0.50 G-H→G-L	0.59 A-H →A-L		
	0.28 G-H→A-L	0.31 G-H →A-L		
	-0.28 G-H→G-L1			
	-0.22 A-H→A-L			
		$\mathbf{Q}_m$		
9Me-A	-0.12	-0.14		
9Me-G	0.12	0.14		
		$\mathbf{v}_m$		
9Me-A	0.20	0.55		
9Me-G	0.47	0.23		

Notes: a: convergence to S_2

Cartesian coordinates of the B-DNA like AG minima. PBE0/6-31G(d) partial geometry optimizations.

Atomic Number	X	Y	Z
7	2.971542	0.592119	-0.186165
6	3.497513	-0.278475	0.730638
7	2.884252	-1.436599	0.784856
6	1.888018	-1.318537	-0.157822
6	1.923973	-0.066051	-0.773317
6	0.883460	-2.196845	-0.605396
7	0.043382	-1.778525	-1.566544
6	0.192652	-0.538363	-2.048675
7	1.089185	0.386395	-1.715161
6	3.427045	1.930998	-0.494016
1	2.645489	2.429869	-1.068546
1	3.606433	2.486070	0.429067
1	4.345439	1.902877	-1.086937
1	4.348100	0.004612	1.338410
7	0.759756	-3.459181	-0.136260
1	-0.107863	-3.937475	-0.331773
1	1.205128	-3.682493	0.741460
1	-0.525504	-0.250163	-2.814220
7	-0.826188	2.426898	0.281065
6	0.072002	2.314633	1.313734
7	0.035473	1.155276	1.919292
6	-0.972366	0.476176	1.272326
6	-1.515880	1.250427	0.250614
6	-1.513537	-0.826951	1.504405
7	-2.570645	-1.084901	0.602994
6	-3.018295	-0.249776	-0.384442
7	-2.520784	0.947827	-0.598124
6	-0.981539	3.534371	-0.635307
1	-2.042595	3.748179	-0.778643
1	-0.490456	4.413389	-0.215362
1	-0.528677	3.292772	-1.601174
1	0.745898	3.128275	1.551618
8	-1.196231	-1.676304	2.329986
1	-2.976049	-2.009496	0.690874
7	-3.993963	-0.726496	-1.201009
1	-4.616752	-1.440831	-0.852200
1	-4.441088	-0.024494	-1.773518

Cartesian coordinates of the B-DNA like GA minima. PBE0/6-31G(d) partial geometry optimizations.

Atomic Number	X	Y	Z
7	-2.563881	1.170165	-0.096158
6	-3.225342	0.441528	-1.053521
7	-2.908803	-0.828439	-1.058614
6	-1.984528	-0.943994	-0.045497
6	-1.759298	0.287797	0.564026
6	-1.277349	-2.087818	0.439909
7	-0.441747	-1.722197	1.519300
6	-0.270096	-0.462044	2.025446
7	-0.900581	0.592345	1.559866
6	-2.696092	2.584788	0.179643
1	-1.824074	2.904816	0.751506
1	-2.737151	3.141348	-0.758739
1	-3.600008	2.785645	0.761708
1	-3.934768	0.915553	-1.720006
8	-1.312487	-3.254308	0.063882
1	0.071388	-2.494140	1.928150
7	0.553832	-0.335854	3.100653
7	1.527985	2.104457	-0.347351
6	0.695725	2.144982	-1.433945
7	0.513746	0.985065	-2.017748
6	1.307547	0.130625	-1.287006
6	1.951337	0.806418	-0.247971
6	1.571192	-1.248649	-1.383629
7	2.431751	-1.801878	-0.513168
6	2.990434	-1.017575	0.417266
7	2.807718	0.282547	0.637285
6	1.875519	3.192557	0.539453
1	2.946880	3.166571	0.747967
1	1.625515	4.138474	0.056977
1	1.322147	3.107620	1.479081
1	0.230483	3.074956	-1.737412
7	1.017947	-2.028507	-2.340965
1	1.044541	-3.025982	-2.183628
1	0.194527	-1.678439	-2.809002
1	3.684985	-1.519887	1.089311
1	1.312906	-0.996062	3.198304
1	0.822466	0.618359	3.297989

Cartesian coordinates of the B-DNA like AG minima. M052X/6-31G(d) partial geometry optimizations.

Atomic Number	X	Y	Z
7	2.951722	0.476790	-0.258803
6	3.467250	-0.416541	0.642481
7	2.806519	-1.545483	0.713079
6	1.788500	-1.383402	-0.202778
6	1.860083	-0.132696	-0.812103
6	0.702718	-2.193169	-0.585591
7	-0.153501	-1.730539	-1.508801
6	0.048722	-0.503443	-2.010519
7	1.012354	0.363160	-1.721651
6	3.444365	1.804504	-0.580921
1	2.617932	2.511762	-0.547132
1	4.193866	2.084782	0.154650
1	3.886736	1.812416	-1.575693
1	4.344148	-0.170028	1.221823
7	0.513408	-3.433921	-0.079487
1	-0.403327	-3.832301	-0.209766
1	0.968217	-3.649177	0.793244
1	-0.683443	-0.177536	-2.740935
7	-0.733759	2.477191	0.351796
6	0.196264	2.318033	1.351325
7	0.127569	1.158963	1.951269
6	-0.901069	0.510185	1.303798
6	-1.438623	1.311431	0.304145
6	-1.440554	-0.801653	1.494697
7	-2.504009	-1.029901	0.597740
6	-2.936991	-0.171727	-0.378115
7	-2.442955	1.030081	-0.558790
6	-0.845940	3.579188	-0.587195
1	-1.895658	3.822194	-0.733432
1	-0.326281	4.440708	-0.175439
1	-0.398112	3.298948	-1.540128
1	0.888247	3.110845	1.592140
8	-1.107600	-1.677324	2.283912
1	-2.891944	-1.962610	0.640050
7	-3.899521	-0.637298	-1.215801
1	-4.514058	-1.368825	-0.896054
1	-4.338658	0.069861	-1.783817

Cartesian coordinates of the B-DNA like GA minima. M052X/6-31G(d) partial geometry optimizations.

Atomic Number	X	Y	Z
7	-2.458715	1.293529	0.058523
6	-3.201497	0.629267	-0.886355
7	-2.955634	-0.654027	-0.934617
6	-1.997621	-0.846838	0.037018
6	-1.677202	0.354275	0.659202
6	-1.291746	-2.028315	0.427665
7	-0.380446	-1.734625	1.463161
6	-0.126224	-0.498071	1.995179
7	-0.740785	0.592905	1.606101
6	-2.480105	2.712632	0.369344
1	-1.459481	3.052444	0.531799
1	-2.912647	3.247042	-0.472622
1	-3.070090	2.898886	1.265384
1	-3.909118	1.158482	-1.505770
8	-1.377741	-3.172469	-0.003023
1	0.148490	-2.532043	1.789833
7	0.771537	-0.443730	3.015811
7	1.628273	2.046045	-0.418223
6	0.730269	2.153951	-1.447292
7	0.457815	1.021156	-2.045205
6	1.214982	0.102064	-1.352374
6	1.955251	0.719423	-0.345273
6	1.309268	-1.299644	-1.417871
7	2.153714	-1.927915	-0.587263
6	2.844611	-1.191633	0.296146
7	2.797560	0.119610	0.506974
6	2.064593	3.088543	0.493988
1	3.140385	3.015082	0.635217
1	1.818816	4.054609	0.060471
1	1.559954	2.976084	1.452887
1	0.318152	3.114792	-1.717939
7	0.581923	-2.027262	-2.300285
1	0.445123	-2.996278	-2.054583
1	-0.227095	-1.569704	-2.692373
1	3.519794	-1.751708	0.934639
1	1.491196	-1.149278	3.052616
1	1.104279	0.487612	3.213528