Supplementary Material (ESI) for Dalton Transactions

Luminescence Properties of Heterodinuclear Pt-Eu complexes from Unusual Nonadentate Ligands

Pascal Kadjane,[a] Carlos Platas-Iglesias,[b] Raymond Ziessel*[a] and Loïc J. Charbonnière*[a,†]

Electronic Supplementary Information (8 pages)

Figure S1. Minimum energy conformation for the $[(tpy)Pt\mathbf{L_1}]^+$ system obtained from B3LYP/6-31G(d)/LanL2DZ calculations in vacuo.

Figure S2. Calculated UV-Vis absorption spectra of the species formed upon titration of $Na_3[(tpy)Pt\mathbf{L_1}]$ by $Eu(ClO_4)_3$ in CH_2Cl_2/TFA.

Figure S3. Evolution of the concentrations of the species formed during the titration of $Na_3[(tpy)Pt\mathbf{L_1}]$ by $Eu(ClO_4)_3$ in CH_2Cl_2/TFA.

Figure S4. UV-Vis spectrophotometric titration of $Na_3[(tpy)Pt\mathbf{L_2}]$ by $La(OTf)_3$ in CH_2Cl_2/TFA.

Figure S5. Spectrofluorimetric titration of $Na_3[(tpy)Pt\mathbf{L_2}]$ by $La(OTf)_3$ in CH_2Cl_2/TFA.

Table S1. Cartesian coordinates (Å) of the optimized structure of $[(tpy)Pt\mathbf{L_1}]^+$.

Table S2. Cartesian coordinates (Å) of the optimized structure of the lowest-energy triplet state of $[(tpy)Pt\mathbf{L_1}]^+$.

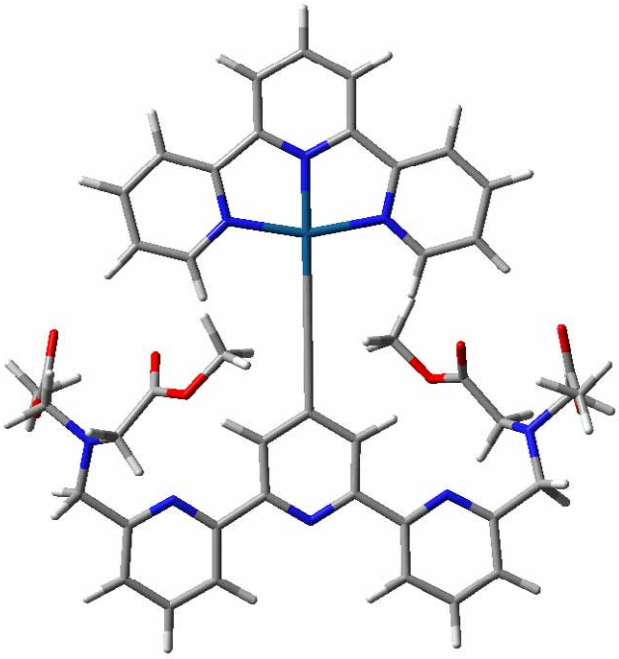

Figure S1. Minimum energy conformation for the $[(tpy)Pt\mathbf{L_1}]^+$ system obtained from B3LYP/6-31G(d)/LanL2DZ calculations in vacuo.

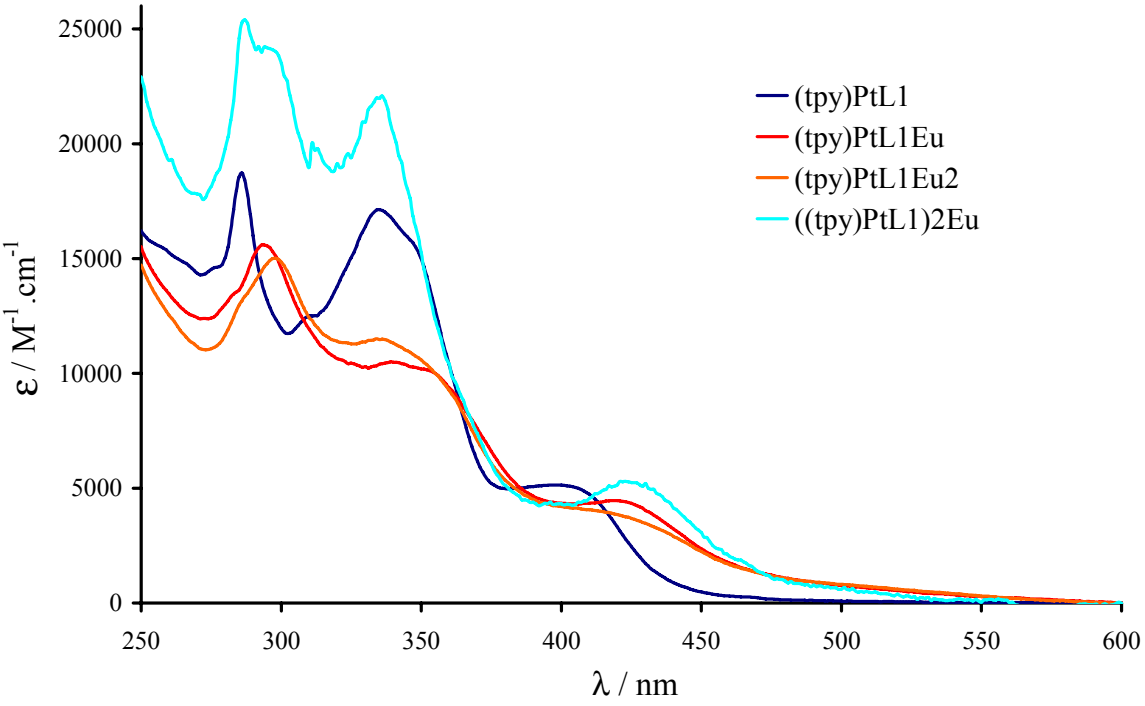

Figure S2. Calculated UV-Vis absorption spectra of the species formed upon titration of $Na_3[(tpy)Pt\mathbf{L_1}]$ by $Eu(ClO_4)_3$ in CH_2Cl_2/TFA.

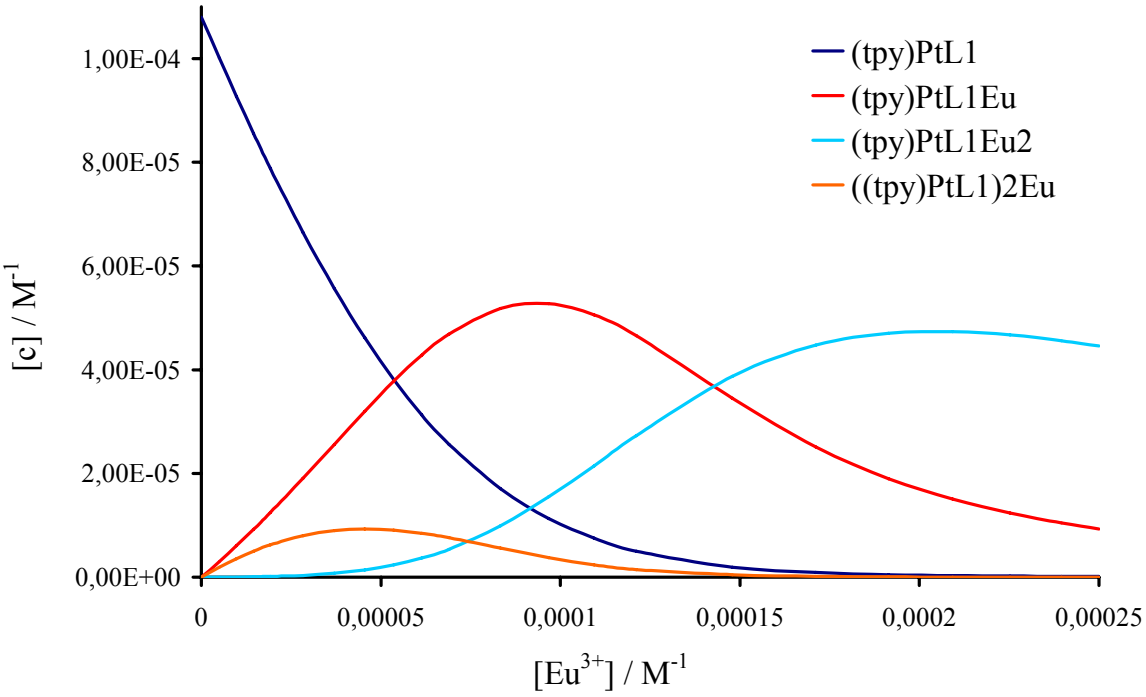

Figure S3. Evolution of the concentrations of the species formed during the titration of $Na_3[(tpy)Pt\mathbf{L_1}]$ by $Eu(ClO_4)_3$ in CH_2Cl_2/TFA.

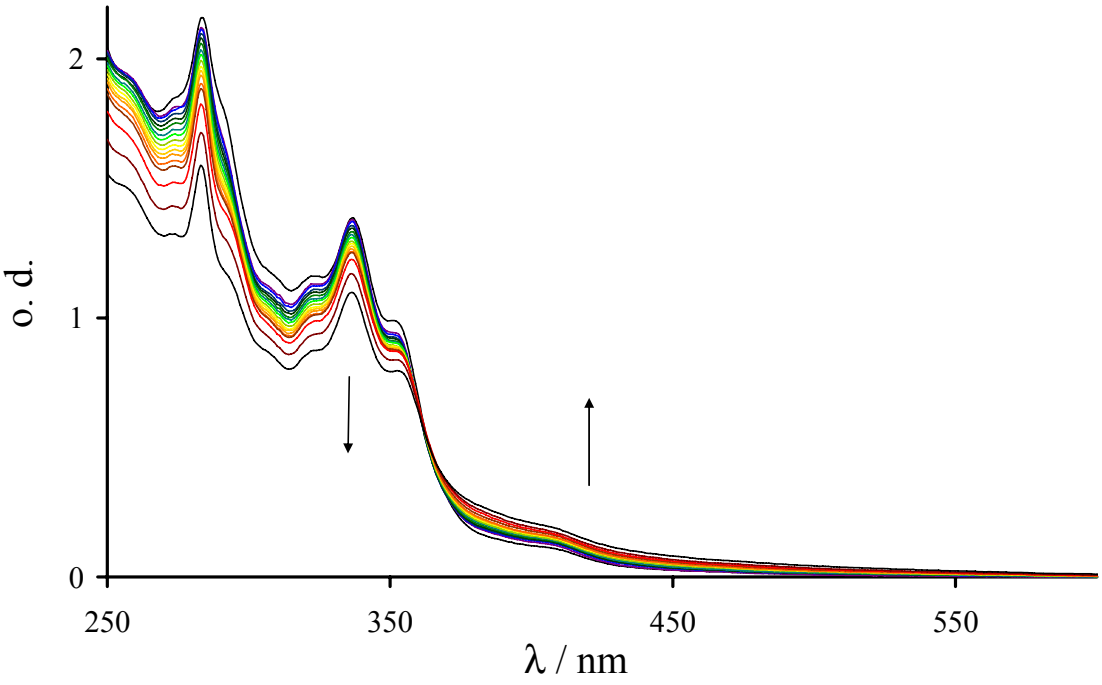

Figure S4. UV-Vis spectrophotometric titration of $Na_3[(tpy)Pt\mathbf{L_2}]$ ($c = 5.0\times10^{-5}$M) by $La(OTf)_3$ in CH_2Cl_2(5 mL)/TFA(8 µL) (uncorrected for dilution).

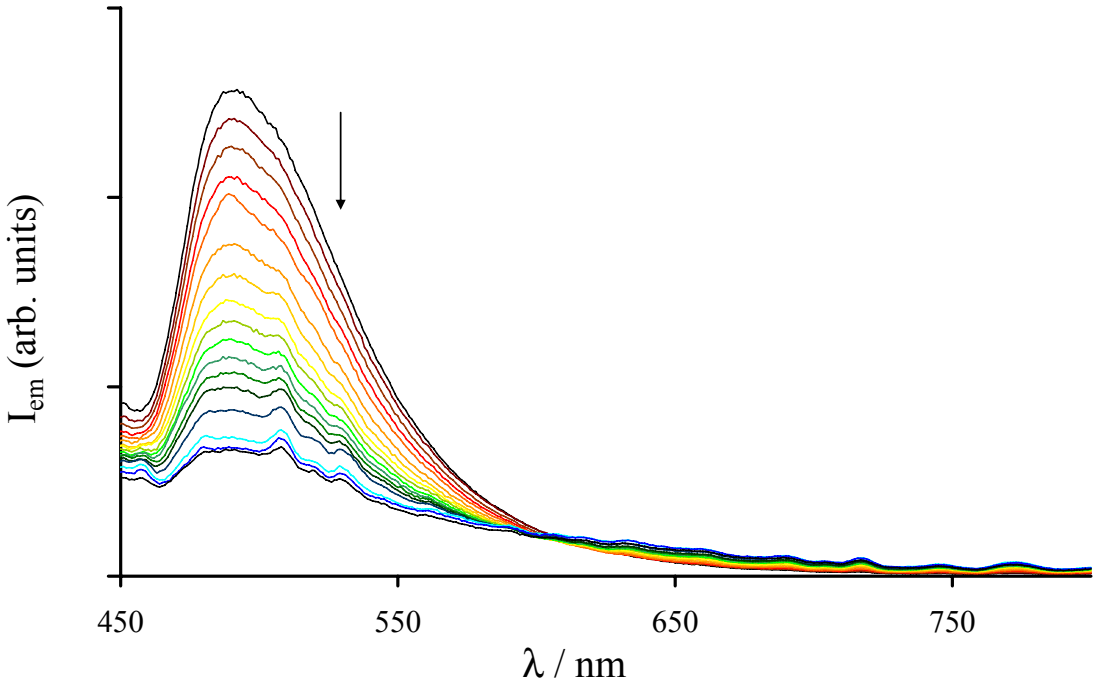

Figure S5. spectrofluorimetric titration of $Na_3[(tpy)Pt\mathbf{L_2}]$ ($c = 5.0\times10^{-5}$M) by $La(OTf)_3$ in CH_2Cl_2(5 mL)/TFA(8 μL) (uncorrected for dilution).

Table S1. Cartesian coordinates (Å) of the optimized structure of $[(tpy)Pt\mathbf{L_1}]^+$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6		-2.422711	4.618628	-0.025577
2	6		-2.432656	6.009406	0.122863
3	6		-3.661723	6.667201	0.092327
4	6		-4.828484	5.927745	-0.084354
5	6		-4.727137	4.534506	-0.212726
6	6		-5.990584	3.693210	-0.370942
7	6		-5.172078	2.151154	-2.081187
8	6		-6.820692	1.380546	-0.450767
9	1		-1.498614	6.542125	0.252962
10	1		-3.708107	7.747467	0.200179
11	1		-5.798837	6.415625	-0.122879
12	1		-6.503984	3.671449	0.595750
13	1		-6.675817	4.209650	-1.072541
14	1		-5.931134	1.996398	-2.871331
15	1		-6.779769	0.539824	-1.143825
16	1		-7.817424	1.847467	-0.539151
17	7		-3.552192	3.905293	-0.186733
18	7		-5.737294	2.312236	-0.756554
19	1		-4.623755	3.053158	-2.357082
20	6		-1.153436	3.835878	-0.012173
21	6		-1.202442	2.436971	-0.008203
22	6		1.153940	3.835577	0.011860

23	6	-0.000027	1.712611	0.000080
24	1	-2.161833	1.935428	-0.011353
25	6	1.202578	2.436659	0.008230
26	1	2.161837	1.934864	0.011507
27	7	0.000343	4.523083	-0.000253
28	6	2.423427	4.617984	0.025066
29	6	2.433801	6.008663	-0.124247
30	6	3.663062	6.666113	-0.093961
31	1	1.499936	6.541573	-0.254829
32	6	4.727800	4.533302	0.212622
33	6	4.829579	5.926427	0.083344
34	1	3.709782	7.746295	-0.202515
35	1	5.800073	6.414045	0.121673
36	7	3.552675	3.904422	0.186869
37	6	5.990986	3.691767	0.371662
38	1	6.505051	3.669916	-0.594671
39	1	6.675846	4.208073	1.073727
40	7	5.737179	2.310841	0.757169
41	6	-6.672666	0.780101	0.944905
42	8	-6.436351	-0.388352	1.182224
43	8	-6.847580	1.704729	1.905064
44	6	-4.183416	0.993467	-2.151681
45	8	-4.059036	0.113432	-1.323169
46	8	-3.468230	1.061699	-3.286484
47	6	6.820697	1.379015	0.452103
48	1	6.778842	0.538068	1.144827
49	1	7.817449	1.845677	0.541606
50	6	5.171567	2.150080	2.081699
51	1	5.930406	1.995544	2.872092
52	1	4.623151	3.052149	2.357190
53	6	4.182871	0.992430	2.152209
54	8	4.058604	0.112244	1.323844
55	8	3.467475	1.060907	3.286868
56	6	6.673772	0.779096	-0.943907
57	8	6.850872	1.703790	-1.903614
58	8	6.436448	-0.389025	-1.181833
59	1	-5.712317	-4.354698	0.452023
60	6	-4.676387	-4.045239	0.354779
61	6	-3.664347	-5.007186	0.287999
62	6	-4.345323	-2.695815	0.291082
63	6	-2.338478	-4.603980	0.172991
64	1	-3.907987	-6.063146	0.328495
65	6	-2.999169	-2.342178	0.174248
66	1	-5.094882	-1.911296	0.340248
67	7	-2.024579	-3.263516	0.126455
68	6	-1.191782	-5.538480	0.090351
69	1	-2.686909	-1.309002	0.100792
70	78	-0.000415	-2.911308	-0.000100
71	6	-1.214332	-6.935091	0.092104
72	7	-0.000507	-4.911786	-0.000259
73	7	2.023713	-3.263685	-0.126744
74	6	-0.000299	-0.939854	0.000059
75	6	-0.000631	-7.622334	-0.000445
76	1	-2.147735	-7.481235	0.162652
77	6	1.190711	-5.538576	-0.090959
78	6	2.337491	-4.604170	-0.173486
79	6	2.998380	-2.342426	-0.174444
80	6	-0.000200	0.285125	0.000166
81	6	1.213133	-6.935189	-0.092902
82	1	-0.000680	-8.707598	-0.000518
83	6	3.663321	-5.007474	-0.288601

84	6	4.344500	-2.696160	-0.291375
85	1	2.686203	-1.309237	-0.100833
86	1	2.146487	-7.481407	-0.163524
87	6	4.675441	-4.045604	-0.355278
88	1	3.906866	-6.063450	-0.329261
89	1	5.094127	-1.911697	-0.340435
90	1	5.711341	-4.355139	-0.452599
91	6	2.494521	0.020057	3.488511
92	1	2.015646	0.251481	4.439886
93	1	1.760890	0.018859	2.678094
94	1	2.985234	-0.956345	3.535668
95	6	6.674688	1.250946	-3.259257
96	1	7.390766	0.458897	-3.491513
97	1	5.659045	0.874368	-3.403929
98	1	6.852662	2.125950	-3.883887
99	6	-6.670230	1.251351	3.260370
100	1	-5.654872	0.873480	3.403662
101	1	-6.846318	2.126430	3.885430
102	1	-7.386996	0.460138	3.493361
103	6	-2.495361	0.020769	-3.488117
104	1	-1.761636	0.019620	-2.677784
105	1	-2.986138	-0.955609	-3.535105
106	1	-2.016581	0.252051	-4.439574

Table S2. Cartesian coordinates (Å) of the optimized structure of the lowest-energy triplet state of $[(tpy)Pt\mathbf{L_1}]^+$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6		2.421843	-4.609474	-0.063593
2	6		2.413964	-6.002354	0.051514
3	6		3.638389	-6.670341	0.011787
4	6		4.810914	-5.936075	-0.138195
5	6		4.725004	-4.537757	-0.233300
6	6		5.996612	-3.705276	-0.351577
7	6		5.278651	-2.124622	-2.062330
8	6		6.840467	-1.400105	-0.342622
9	1		1.476356	-6.532384	0.165052
10	1		3.674845	-7.753037	0.093191
11	1		5.777357	-6.430983	-0.180713
12	1		6.492576	-3.712214	0.624231
13	1		6.689668	-4.211420	-1.052761
14	1		6.081838	-2.030701	-2.814691
15	1		6.795532	-0.519216	-0.984533
16	1		7.839557	-1.854996	-0.460536
17	7		3.555120	-3.899976	-0.201739
18	7		5.758793	-2.314844	-0.709283
19	1		4.684372	-2.994448	-2.357382
20	6		1.164221	-3.810829	-0.033421
21	6		1.218965	-2.414000	-0.035180
22	6		-1.164061	-3.810854	0.033412
23	6		0.000056	-1.691519	-0.000042
24	1		2.175571	-1.906088	-0.070899
25	6		-1.218837	-2.414027	0.035125
26	1		-2.175455	-1.906135	0.070834
27	7		0.000088	-4.485711	0.000004
28	6		-2.421665	-4.609523	0.063609

29	6	-2.413761	-6.002407	-0.051455
30	6	-3.638173	-6.670414	-0.011706
31	1	-1.476144	-6.532424	-0.164979
32	6	-4.724826	-4.537842	0.233323
33	6	-4.810712	-5.936165	0.138258
34	1	-3.674610	-7.753113	-0.093078
35	1	-5.777145	-6.431089	0.180790
36	7	-3.554955	-3.900042	0.201735
37	6	-5.996449	-3.705379	0.351578
38	1	-6.492405	-3.712333	-0.624234
39	1	-6.689506	-4.211526	1.052758
40	7	-5.758658	-2.314937	0.709277
41	6	6.684614	-0.882034	1.084555
42	8	6.398098	0.259458	1.381124
43	8	6.913634	-1.846916	1.994326
44	6	4.353007	-0.919176	-2.194991
45	8	3.903541	-0.254897	-1.284506
46	8	4.079253	-0.697476	-3.493486
47	6	-6.840387	-1.400246	0.342648
48	1	-6.795429	-0.519328	0.984518
49	1	-7.839455	-1.855161	0.460649
50	6	-5.278539	-2.124717	2.062336
51	1	-6.081739	-2.030875	2.814692
52	1	-4.684199	-2.994509	2.357364
53	6	-4.352974	-0.919214	2.195038
54	8	-3.903459	-0.254942	1.284574
55	8	-4.079343	-0.697463	3.493551
56	6	-6.684636	-0.882232	-1.084561
57	8	-6.913786	-1.847132	-1.994281
58	8	-6.398087	0.259236	-1.381193
59	1	5.701164	4.350678	0.682418
60	6	4.669488	4.043135	0.543017
61	6	3.668983	4.996645	0.433811
62	6	4.337932	2.681605	0.469107
63	6	2.334114	4.602223	0.264188
64	1	3.907233	6.053617	0.482914
65	6	3.008619	2.330397	0.298373
66	1	5.086358	1.900711	0.554081
67	7	2.023206	3.250771	0.207047
68	6	1.209870	5.512294	0.138783
69	1	2.708047	1.295410	0.213533
70	78	-0.000027	2.895344	-0.000021
71	6	1.213651	6.900524	0.140536
72	7	-0.000072	4.861528	-0.000005
73	7	-2.023275	3.250681	-0.207086
74	6	0.000016	0.962096	-0.000050
75	6	-0.000136	7.594213	0.000033
76	1	2.141890	7.450725	0.247950
77	6	-1.210045	5.512241	-0.138775
78	6	-2.334246	4.602120	-0.264203
79	6	-3.008644	2.330263	-0.298437
80	6	0.000037	-0.290554	-0.000077
81	6	-1.213891	6.900471	-0.140489
82	1	-0.000162	8.678688	0.000048
83	6	-3.669132	4.996483	-0.433827
84	6	-4.337972	2.681412	-0.469172
85	1	-2.708023	1.295290	-0.213615
86	1	-2.142156	7.450630	-0.247888
87	6	-4.669591	4.042928	-0.543058
88	1	-3.907431	6.053445	-0.482912
89	1	-5.086362	1.900485	-0.554165

90	1	-5.701281	4.350426	-0.682459
91	6	-3.178343	0.387615	3.774907
92	1	-3.084161	0.414609	4.860314
93	1	-2.205380	0.208413	3.309243
94	1	-3.586753	1.329996	3.400804
95	6	-6.746285	-1.464159	-3.373552
96	1	-7.438131	-0.658257	-3.629552
97	1	-5.721314	-1.130265	-3.552465
98	1	-6.967261	-2.360041	-3.953231
99	6	6.746026	-1.463893	3.373570
100	1	5.721059	-1.129931	3.552376
101	1	6.966892	-2.359771	3.953296
102	1	7.437897	-0.658025	3.629613
103	6	3.178194	0.387565	-3.774798
104	1	2.205284	0.208358	-3.309028
105	1	3.586617	1.329974	-3.400777
106	1	3.083903	0.414509	-4.860196