A Fluorescent Cy7-Mercaptopyridine for the Selective Detection of Glutathione over Homocysteine and Cysteine

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† These authors contributed equally.

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1. Supplementary data
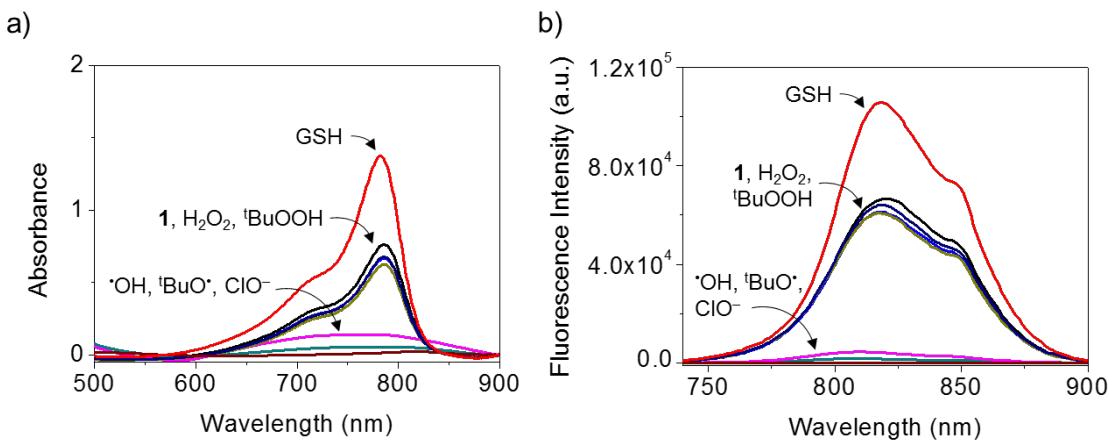
Figure S1. (a) UV-Vis absorption and (b) fluorescence spectra of **1** (10 μM) in presence of reactive oxygen species such as $^{\bullet}O_2^-$, $^{\bullet}OH$, t-BuO$^{\bullet}$, H_2O_2, t-BuOOH, and ClO$^-$ (1 mM, respectively). All data was obtained in HEPES buffer (10 mM, pH 7.4) containing 1% (v/v) of DMSO after incubation of 1 h at room temperature. The excitation wavelength was affected at 720 nm.
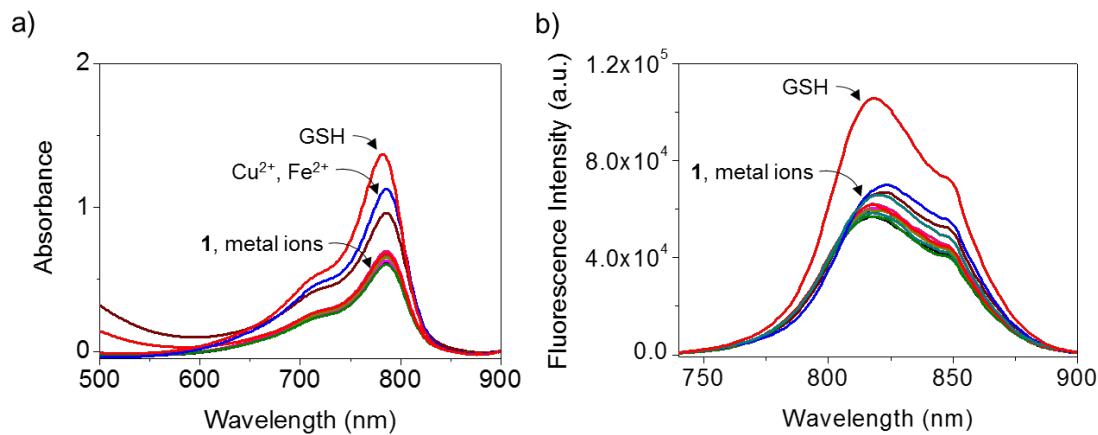
Figure S2. (a) UV-Vis absorption and (b) fluorescence spectra of **1** (10 μM) in presence of various anions such as various metal ions Na$^+$, K$^+$, Mg^{2+}, Ca^{2+}, Fe^{2+}, Co^{2+}, Zn^{2+}, Fe^{3+}, Cu^{2+}, and Cu$^+$ (1 mM, respectively). All data was obtained in HEPES buffer (10 mM, pH 7.4) containing 1% (v/v) of DMSO after incubation of 1 h at room temperature. The excitation wavelength was affected at 720 nm.
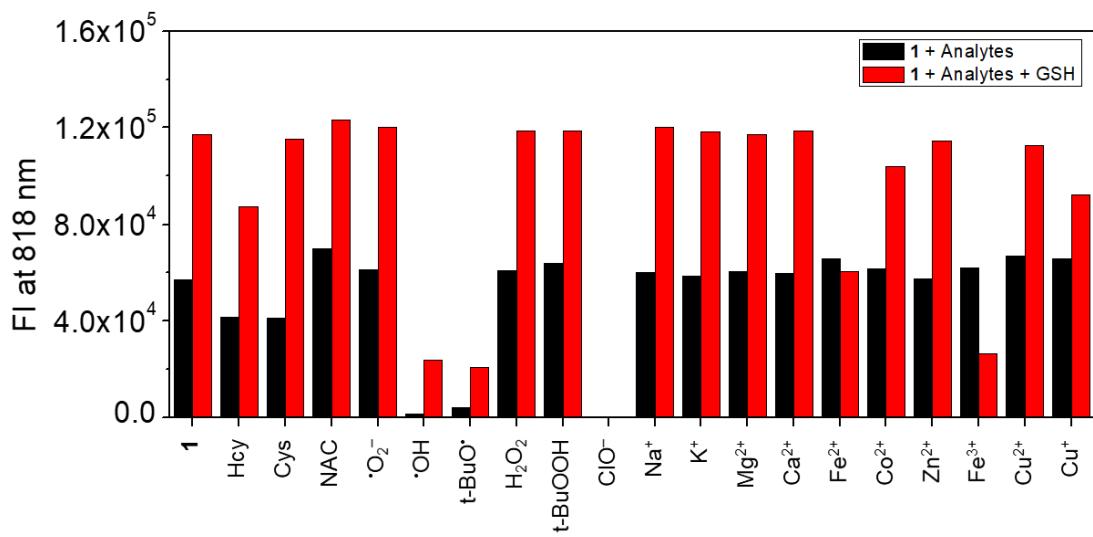
Figure S3. Relative fluorescence intensity at 818 nm of **1** (10 μM) in the absence and presence of GSH with other analytes such as thiols (10 mM), ROS (1 mM), and metals (1 mM). Black bars indicate fluorescence intensity of **1** in the absence and presence of various analytes. Red bars indicate fluorescence intensity of **1** towards GSH in the presence of other analytes. All data were obtained in HEPES buffer (10 mM, pH 7.4) containing 1% (*v/v*) of DMSO after incubation of 1 h at room temperature. The excitation wavelength was affected at 720 nm.

Equation	y = a + b		
Adj. R-Squa	0.99364		
		Value	Standard Err
B	Intercept	61121.219	301.00797
B	Slope	26.13473	0.93451
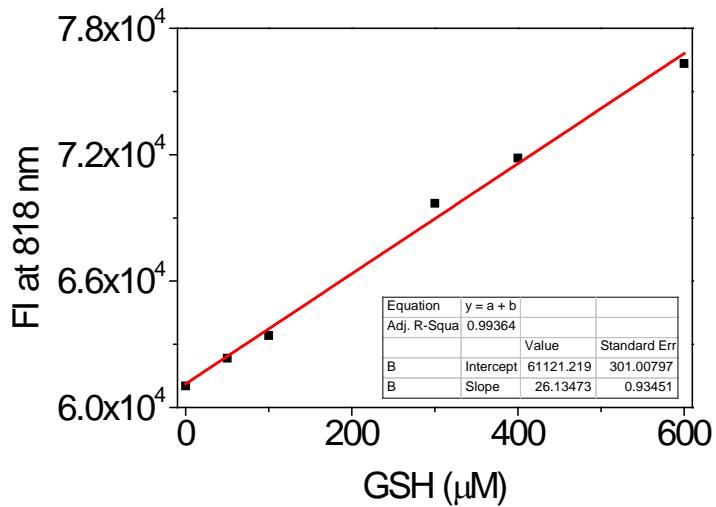
Figure S4. Plot of fluorescence intensity at 818 nm of **1** *vs.* [GSH] in the range of 0-600 μM.
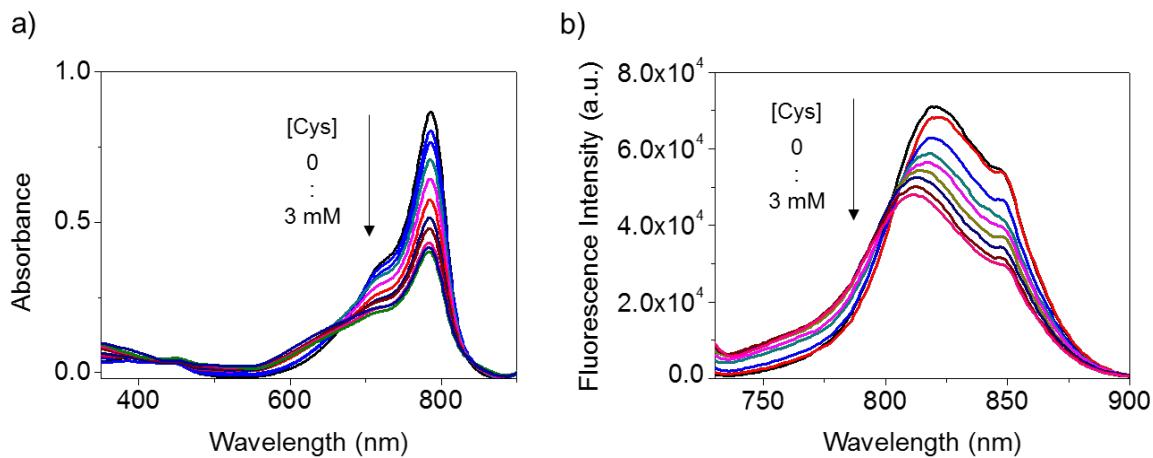
Figure S5. (a) Absorption and (b) fluorescence spectra of **1** (10 μM) in presence of different concentrations of Cys (0-3 mM). All data was obtained in HEPES buffer (10 mM, pH 7.4) containing 1% (*v/v*) of DMSO after incubation of 1 h at room temperature. The excitation wavelength was affected at 720 nm.
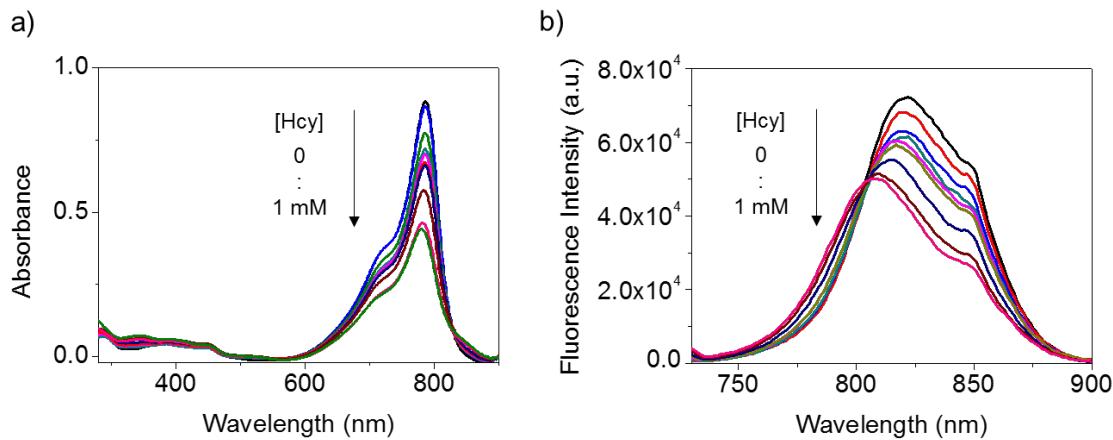

Figure S6. (a) Absorption and (b) fluorescence spectra of **1** (10 μM) in presence of different concentrations of Hcy (0-1 mM). All data was obtained in HEPES buffer (10 mM, pH 7.4) containing 1% (*v/v*) of DMSO after incubation of 1 h at room temperature. The excitation wavelength was affected at 720 nm.
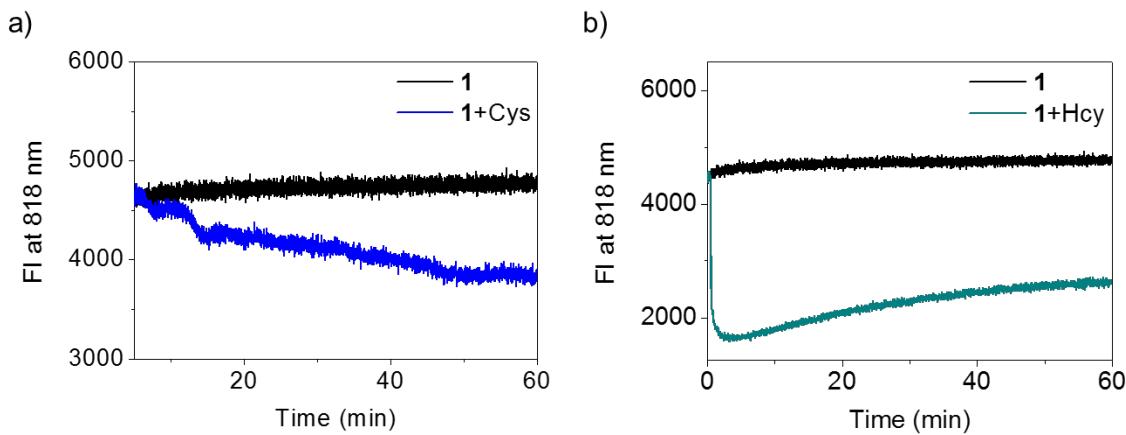
Figure S7. Time-dependent fluorescence responses of **1** (10 μM) toward (a) Cys and (b) Hcy (10 mM) in HEPES buffer (0.01 M, pH 7.4) containing 1% (*v/v*) of DMSO.
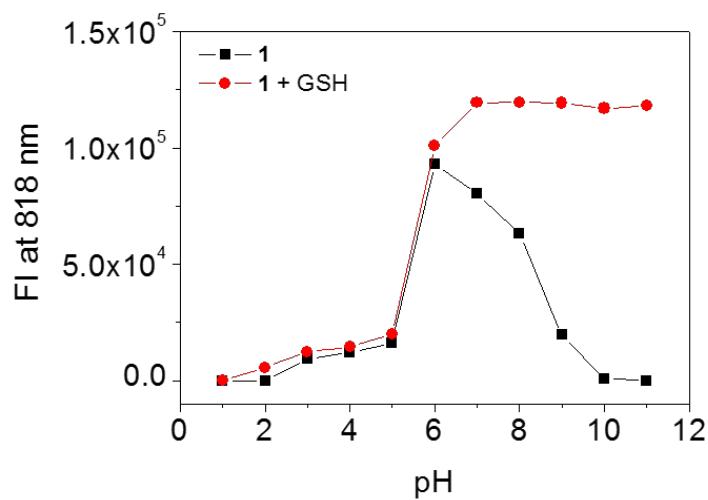
Figure S8. The pH effect on fluorescence change of **1** (10 μM) in absence (black line) and presence (red line) of GSH (10 mM). All data was obtained in HEPES buffer (10 mM, pH 7.4) containing 1% (*v/v*) of DMSO after incubation of 1 h at room temperature. The excitation wavelength was affected at 720 nm.
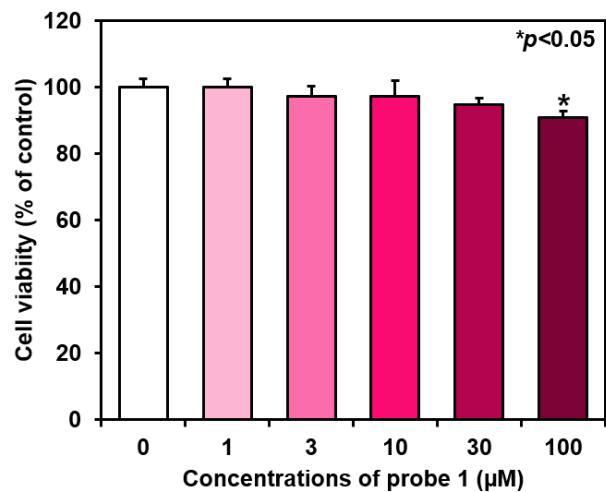
Figure S9. Cell viability of probe **1**. Cells were incubated with 0, 1, 3,10, 30 and 100 μM of probe **1** for 6 h in MDA-MB-231 cells. The values represent mean ± SE of three independent experiments performed in triplicate

2. ^{1}H, ^{13}C NMR and ESI-MS spectra of 1
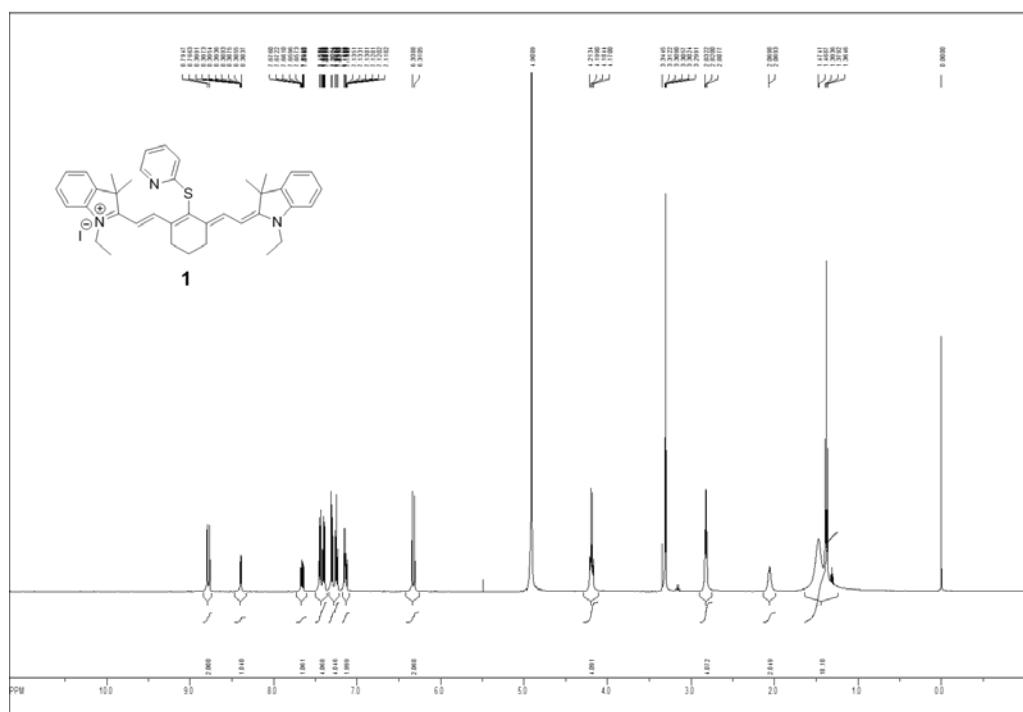
Figure S10. ^{1}H-NMR spectrum of **1** in DMSO-d_6.
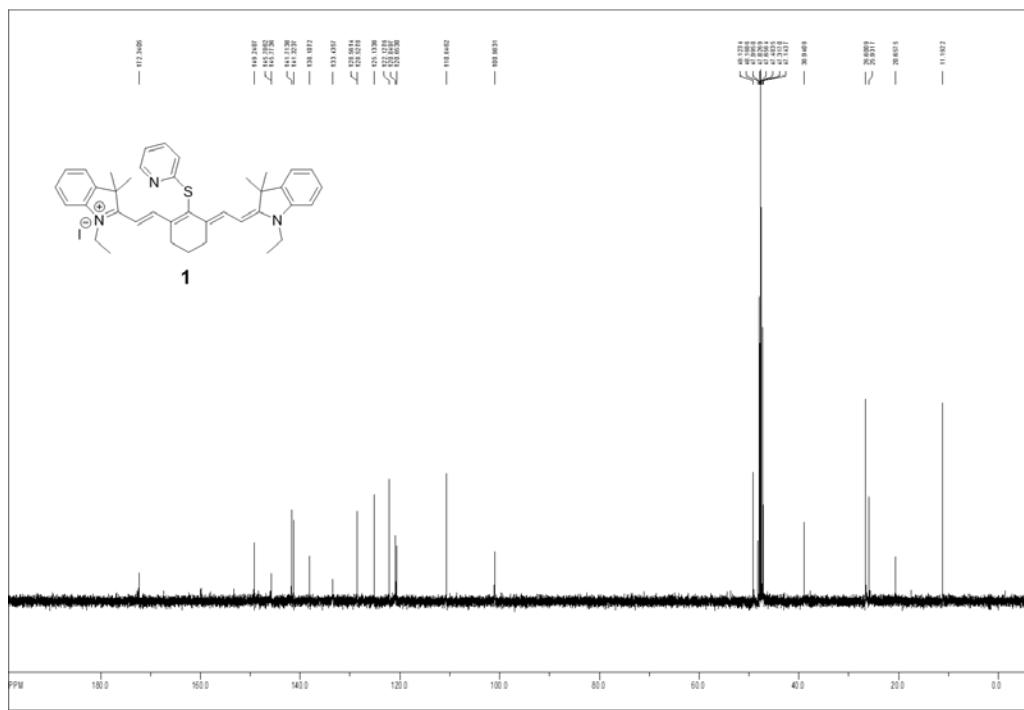
Figure S11. ^{13}C-NMR spectrum of **1** in DMSO-d_6.

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MassPeaks:687
RawMode:Single 0.780(157) BasePeak:586.30(4749984)
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Chemical Formula: $C_{39}H_{44}N_3S^+$
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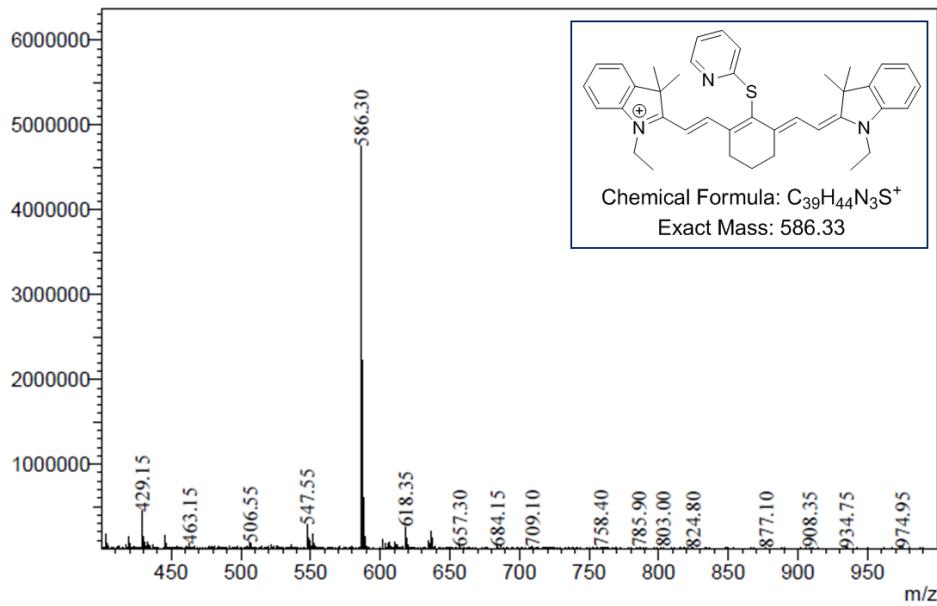
Figure S12. ESI-MS spectrum of **1**.

3. Computational data

HOMO   **LUMO**

A

(-5.32 eV)   (-2.62 eV)

B

(-5.31 eV)   (-3.03 eV)

C

(-5.48 eV)   (-3.32 eV)
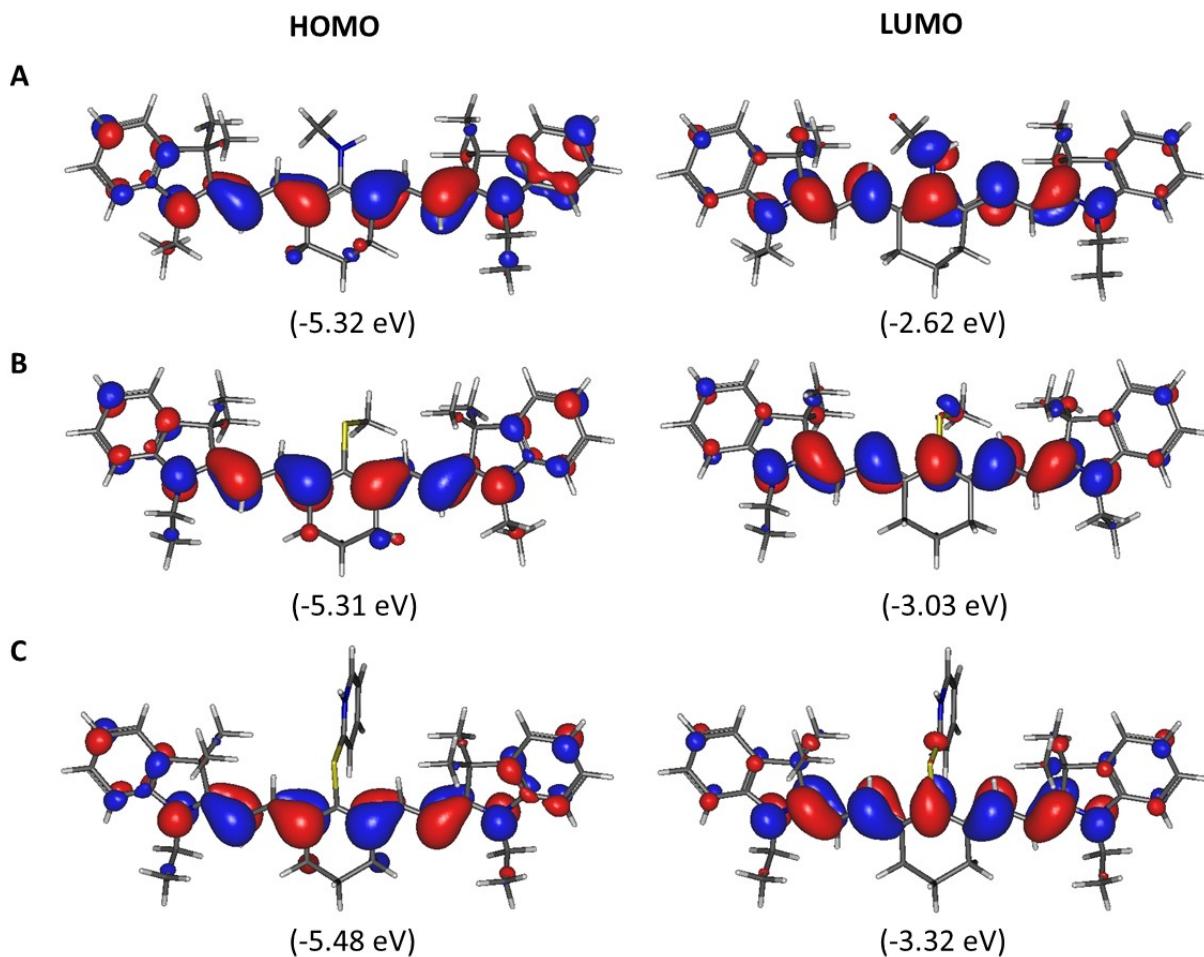
Figure S13. Isodensity surface (0.03 e.bohr^{-3}) of the HOMO (Left) and LUMO (Right) orbitals of a) **Cy7-NHMe**, b) **Cy7-SMe** and c) **1-H⁺** at the PCM-PBE0/6-311G(2d,p) level of theory. The associated orbital energies are shown between brackets in eV.

Table S1. Coordinates of optimized structures

1-GSH E(RωB97XD) = -3478.927477 Ha

Center Number	Atomic Number	X	Y	Z
		Coordinates (Angstroms)
1	1	0.483239	-0.429076	-3.761788
2	1	5.320828	-1.085730	-4.004515
3	1	6.979636	-1.716872	-3.971111
4	1	0.289969	1.205775	-4.406272
5	6	6.377155	-0.802676	-3.955926
6	1	4.448214	-3.452245	-0.620372
7	1	-1.810459	0.420070	-3.351126
8	6	0.329444	0.621040	-3.480535

9	6	-0.987529	0.763004	-2.721307
10	1	3.247457	-2.632360	0.392895
11	6	4.303444	-2.901286	0.314307
12	1	4.538522	-3.570515	1.148811
13	1	4.133871	0.375368	-2.338972
14	6	6.666832	0.010712	-2.695788
15	6	1.555090	0.348943	-1.302243
16	1	-1.165517	1.830344	-2.519123
17	6	4.008565	-0.171753	-1.411122
18	1	9.094300	-1.317632	-1.984280
19	6	2.692996	-0.187875	-0.811527
20	7	6.359734	-0.711779	-1.476469
21	6	0.233787	0.277426	-0.533533
22	6	5.103962	-0.788958	-0.892816
23	6	8.618053	-1.751411	-1.110722
24	1	7.722062	0.295476	-2.657847
25	6	7.282193	-1.511149	-0.803341
26	1	2.618609	-0.687805	0.145541
27	1	10.385267	-2.792005	-0.473664
28	6	9.340699	-2.589578	-0.254059
29	6	5.217853	-1.663767	0.370511
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31	16	0.320810	-0.738257	1.007043
32	6	8.745414	-3.168713	0.865696
33	6	7.395149	-2.919903	1.149785
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36	1	3.929675	-0.510049	1.727021
37	1	5.180372	-1.470673	2.531159
38	1	5.619324	0.029348	1.689745
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44	6	0.653831	-2.970214	-0.699926
45	1	-0.468936	-5.168838	2.236757
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74	6	-4.194840	-2.052052	1.260088
75	1	-3.206445	-1.617247	1.429603
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89	6	-2.262866	4.925390	1.550170
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106	1	-0.458339	0.267942	5.669747
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123	1	-1.126660	9.653517	-0.833367

1-GSH *cyclic* E(RωB97XD) = -2796.2942764 Ha

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
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1-GSH *acyclic* E(RωB97XD) = -2796.2958988 Ha

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
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4	1	0.110877	1.353457	4.368990
5	6	-5.621809	-1.332065	3.679874
6	1	-3.596974	-3.116813	-0.080798
7	1	2.260309	1.142622	3.133189
8	6	0.121981	0.981194	3.338760
9	6	1.364926	1.495886	2.617905
10	1	-2.487963	-1.966519	-0.839604
11	6	-3.497912	-2.379845	-0.883735
12	1	-3.614246	-2.894918	-1.843135
13	1	-3.647775	0.408044	2.250802
14	6	-6.087145	-0.368225	2.590118
15	6	-1.153492	0.961764	1.173483
16	1	1.377445	2.593791	2.682758
17	6	-3.492859	0.059585	1.236085
18	1	-8.345383	-1.877968	1.699622
19	6	-2.223767	0.357776	0.611965
20	7	-5.739835	-0.818867	1.255695
21	6	0.106925	1.302214	0.386284
22	6	-4.516403	-0.610932	0.640342
23	6	-7.854704	-2.080963	0.753088
24	1	-7.172810	-0.243035	2.627483
25	6	-6.577623	-1.607981	0.467713
26	1	-2.142393	0.079544	-0.430647
27	1	-9.494885	-3.226723	-0.026603
28	6	-8.496984	-2.846679	-0.226454
29	6	-4.561388	-1.274819	-0.748999
30	6	-5.945214	-1.896358	-0.742676
31	16	0.145768	0.583057	-1.326734
32	6	-7.880328	-3.131658	-1.443981
33	6	-6.588787	-2.653173	-1.705001
34	1	-8.397816	-3.728819	-2.188641
35	6	-4.449458	-0.249795	-1.894024
36	1	-3.453928	0.199367	-1.951417
37	1	-4.644893	-0.746989	-2.850095
38	1	-5.182573	0.553119	-1.768510
39	6	0.116293	-1.162517	-1.120746
40	7	-0.036916	-1.870089	-2.266323
41	6	-0.068704	-3.219122	-2.320454
42	6	0.051849	-3.950855	-1.163734
43	6	0.210641	-3.262755	0.042503
44	6	0.246084	-1.876295	0.069260
45	1	-0.195790	-3.651280	-3.303867
46	1	0.022184	-5.031868	-1.204039
47	1	0.310329	-3.812743	0.971916
48	1	-5.900571	-0.948118	4.666286
49	1	4.055608	-2.689832	-0.264921
50	1	-2.022680	1.082810	3.134050
51	6	-1.136601	1.439068	2.606036

52	1	2.923980	-1.580405	-1.055321
53	6	3.954662	-1.942575	-1.058220
54	1	4.135352	-2.433393	-2.020343
55	1	3.959400	0.720063	2.198460
56	6	1.407813	1.077258	1.165075
57	1	-1.177088	2.538849	2.628028
58	6	3.821077	0.393833	1.173795
59	1	8.786386	-1.253511	1.554554
60	6	2.525993	0.608112	0.569242
61	7	6.120962	-0.335781	1.152256
62	6	4.882080	-0.187387	0.550492
63	1	-5.660245	0.628403	2.738691
64	6	8.302440	-1.458226	0.604916
65	6	6.998325	-1.052613	0.338666
66	1	10.001536	-2.484622	-0.214036
67	6	8.982159	-2.157555	-0.398770
68	6	4.961781	-0.794541	-0.863082
69	6	6.376346	-1.342824	-0.876748
70	6	8.375894	-2.443114	-1.621335
71	6	7.057426	-2.032743	-1.863225
72	1	8.922662	-2.987876	-2.384997
73	1	6.579961	-2.258197	-2.813898
74	6	4.804902	0.275776	-1.960814
75	1	3.796914	0.699612	-1.980193
76	1	4.999196	-0.173700	-2.940558
77	1	5.518219	1.092177	-1.810016
78	16	0.133278	3.142356	-0.030227
79	7	-0.977388	4.287178	-2.771447
80	6	-1.678605	4.631883	-1.496178
81	1	-0.591964	5.191354	-3.107565
82	1	-2.729819	4.795890	-1.746622
83	6	-1.602805	3.498601	-0.482220
84	1	-2.164401	3.794546	0.404768
85	1	-2.058825	2.593686	-0.892434
86	6	-1.100473	6.002680	-1.014529
87	8	-1.416926	6.351079	0.136923
88	8	-0.409671	6.612217	-1.871101
89	1	-0.141090	-1.365519	-3.143669
90	1	2.454250	0.366548	-0.483330
91	1	0.376631	-1.344799	1.001233
92	6	6.445223	0.083420	2.502616
93	6	6.054741	-0.953945	3.553640
94	1	7.519825	0.282393	2.541019
95	1	4.978775	-1.153542	3.525546
96	1	6.312620	-0.592145	4.554012
97	1	6.584509	-1.896337	3.379977
98	1	5.951001	1.040863	2.693254
99	1	-6.102447	-2.878958	-2.651061
100	1	-1.579384	3.860504	-3.476322
101	1	-0.181498	3.662513	-2.599824

Cy7-PyrH E(RPBE0) = -2073.7125673 Ha

Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z

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  1      1       0.025392    3.752891   -0.890946
  2      1       5.498401    3.649590   -0.626876
  3      1       7.246647    3.378413   -0.707882
  4      1      -6.643093    4.486491    0.176176
  5      1      -0.021422    4.600776    0.649515
  6      6       6.406625    3.543341   -0.030422
  7      1       5.029661    0.000833   -2.709181
  8      1      -2.145877    3.381436    0.131579
  9      6      -0.014799    3.608243    0.193848
 10      6      -1.283514    2.861607    0.555688
 11      1       3.520247   -0.752317   -2.172577
 12      6       4.607634   -0.816704   -2.121510
 13      1       4.911578   -1.760075   -2.580066
 14      1       3.749726    2.238937    0.645573
 15      6       6.278112    2.404848    0.966185
 16      6       1.217717    1.431545    0.095953
 17      1      -1.424165    2.867282    1.644295
 18      6       3.683758    1.256394    0.196471
 19      1       8.891918    1.393304    0.562012
 20      6       2.425486    0.759901   -0.109926
 21      7       6.071321    1.117606    0.320000
 22      6      -0.025058    0.825188   -0.163834
 23      6       4.885136    0.589521   -0.026886
 24      1      -5.520435    2.686416    1.488645
 25      6       8.494584    0.494363    0.106900
 26      1       7.179056    2.315423    1.574274
 27      6       7.135474    0.285195   -0.054284
 28      1       2.358643   -0.231216   -0.538047
 29      1      10.417852   -0.375265   -0.241634
 30      6       9.347082   -0.504948   -0.350048
 31      6       5.116717   -0.773612   -0.674227
 32      6       6.623010   -0.859274   -0.648947
 33     16      -0.026226   -0.812602   -0.896310
 34      6       8.850464   -1.660031   -0.942481
 35      6       7.477876   -1.845013   -1.096549
 36      1       9.537649   -2.422752   -1.290055
 37      1       7.096556   -2.748167   -1.561407
 38      6       4.514385   -1.906364    0.170441
 39      1       3.425219   -1.863552    0.187711
 40      1       4.808469   -2.867347   -0.256664
 41      1       4.877195   -1.862966    1.199104
 42      6       0.071052   -1.853654    0.500327
 43      7       0.150706   -3.174532    0.240461
 44      6       0.228021   -4.119113    1.194875
 45      6       0.230969   -3.756528    2.513454
 46      6       0.149763   -2.400203    2.825838
 47      6       0.069186   -1.449361    1.828662
 48      1       0.287348   -5.140541    0.846208
 49      1       0.294704   -4.515396    3.280187
 50      1       0.148039   -2.082966    3.861873
 51      1       0.003409   -0.396051    2.062243
 52      1      -5.556335    3.571310   -0.879684
 53      1      -7.303467    3.288320   -0.945753
 54      1       6.577318    4.478792    0.505231
 55      6      -6.467002    3.511059   -0.280499
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56	1	-5.076875	-0.200620	-2.665367
57	1	2.111943	3.359802	0.313367
58	6	1.211610	2.835983	0.640660
59	1	-3.558469	-0.894146	-2.076795
60	6	-4.644902	-0.969255	-2.021692
61	1	-4.936755	-1.946463	-2.412145
62	1	-3.805953	2.273393	0.530406
63	6	-6.339247	2.458226	0.806260
64	6	-1.269628	1.436343	0.066697
65	1	1.252939	2.800923	1.737078
66	6	-3.734734	1.262128	0.151149
67	1	-8.946162	1.403052	0.476353
68	6	-2.474821	0.749589	-0.113943
69	7	-6.122933	1.124236	0.266296
70	6	-4.933522	0.576587	-0.032339
71	1	5.454493	2.573498	1.660231
72	6	-8.542628	0.474421	0.091860
73	1	-7.243359	2.413506	1.414406
74	6	-7.181975	0.260479	-0.048013
75	1	-2.401191	-0.265668	-0.479696
76	1	-10.460063	-0.429024	-0.197613
77	6	-9.388235	-0.560797	-0.291958
78	6	-5.155750	-0.830417	-0.580783
79	6	-6.661361	-0.922712	-0.552736
80	6	-8.883451	-1.754470	-0.794320
81	6	-7.509441	-1.943577	-0.928863
82	1	-9.565548	-2.544586	-1.086259
83	1	-7.121483	-2.876807	-1.323515
84	6	-4.547259	-1.899042	0.339332
85	1	-3.458124	-1.852460	0.350236
86	1	-4.839771	-2.888082	-0.019342
87	1	-4.907996	-1.785610	1.363409
88	1	0.154111	-3.481172	-0.726996

Cy7-SMe E(RPBE0) = -1865.6770065 Ha

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	1	-0.323483	3.116373	1.571349
2	1	-5.616632	3.175849	0.677237
3	1	-7.360721	2.876910	0.609147
4	1	6.642765	3.860416	1.360342
5	1	-0.066747	4.320283	0.314000
6	6	-6.483343	3.138458	0.014310
7	1	-5.198634	-0.696882	2.295719
8	1	1.995774	2.966456	0.918990
9	6	-0.094914	3.245428	0.507898
10	6	1.251464	2.624873	0.192258
11	1	-3.635973	-1.343087	1.771398
12	6	-4.715533	-1.423414	1.639396
13	1	-5.021764	-2.423872	1.952909
14	1	-3.754935	1.975618	-0.651475
15	6	-6.270191	2.140421	-1.110547
16	6	-1.239715	1.106676	-0.027965

17	1	1.600666	2.977576	-0.786983
18	6	-3.698951	0.944442	-0.325669
19	1	-8.878124	1.031106	-1.017627
20	6	-2.452132	0.420249	-0.002398
21	7	-6.072143	0.784053	-0.626343
22	6	-0.018777	0.440798	0.202349
23	6	-4.892326	0.237824	-0.271084
24	1	5.472653	2.834225	-0.588156
25	6	-8.484279	0.088049	-0.658785
26	1	-7.131023	2.119674	-1.780173
27	6	-7.132248	-0.111346	-0.436053
28	1	-2.387449	-0.619916	0.288185
29	1	-10.400358	-0.858791	-0.557109
30	6	-9.335375	-0.980330	-0.394591
31	6	-5.128041	-1.203633	0.177526
32	6	-6.626857	-1.314491	0.037699
33	16	-0.039856	-1.330795	0.448227
34	6	-8.845179	-2.192990	0.074386
35	6	-7.479860	-2.367391	0.294697
36	1	-9.530541	-3.008943	0.272764
37	1	-7.101865	-3.315544	0.662894
38	6	-4.437848	-2.207844	-0.757655
39	1	-3.351187	-2.147607	-0.686991
40	1	-4.739341	-3.220656	-0.481460
41	1	-4.727048	-2.036865	-1.796488
42	6	0.495323	-1.457224	2.177101
43	1	5.562232	2.577469	1.925614
44	1	7.305870	2.285789	1.820560
45	1	-6.638434	4.134397	-0.404535
46	6	6.460984	2.784302	1.341280
47	1	5.069643	-1.592415	1.866024
48	1	-2.150263	3.044298	-0.088596
49	6	-1.187154	2.583642	-0.314563
50	1	3.528525	-1.968131	1.078314
51	6	4.612138	-1.999409	0.962208
52	1	4.909701	-3.046198	0.869667
53	1	3.763723	2.052636	0.143142
54	6	6.298819	2.320101	-0.095706
55	6	1.220615	1.116362	0.184445
56	1	-1.000271	2.752937	-1.383098
57	6	3.685446	0.977122	0.042407
58	1	8.890506	1.200806	-0.369242
59	6	2.415518	0.408994	0.091647
60	7	6.068845	0.888613	-0.199231
61	6	4.869230	0.275687	-0.133822
62	1	-5.410278	2.411401	-1.724026
63	6	8.473147	0.203188	-0.430588
64	1	7.192203	2.545130	-0.679633
65	6	7.111297	-0.034259	-0.349026
66	1	2.319071	-0.666529	0.009700
67	1	10.373902	-0.752773	-0.656879
68	6	9.302237	-0.902611	-0.590032
69	6	5.074239	-1.231038	-0.283448
70	6	6.575805	-1.313544	-0.412989
71	6	8.781761	-2.188945	-0.661992
72	6	7.407162	-2.402378	-0.572529

73	1	9.450230	-3.033075	-0.786273
74	1	7.005155	-3.408780	-0.627472
75	6	4.403401	-1.770716	-1.554806
76	1	3.316052	-1.711078	-1.493750
77	1	4.678984	-2.819081	-1.689225
78	1	4.731073	-1.215202	-2.435729
79	1	0.506129	-2.522904	2.407927
80	1	-0.217578	-0.952348	2.827592
81	1	1.493383	-1.044935	2.316692

Cy7-SMe E(RPBE0) = -1522.922675 Ha

Center Number	Atomic Number	X	Y	Z
1	1	0.750292	2.794225	1.475483
2	1	-5.420815	2.132839	2.483537
3	1	-7.180686	1.982429	2.359895
4	1	6.312832	4.063760	-1.254670
5	1	0.152854	3.989810	0.331021
6	6	-6.306962	2.505597	1.965876
7	1	-5.235243	-1.975375	1.614614
8	1	2.005650	2.716692	-0.683257
9	6	0.227628	2.916043	0.521180
10	6	1.039242	2.226336	-0.568696
11	1	-3.698232	-2.255583	0.786716
12	6	-4.779558	-2.221416	0.653423
13	1	-5.117019	-3.217981	0.359817
14	1	-3.678732	1.838774	0.621561
15	6	-6.187203	2.308843	0.464316
16	6	-1.200221	0.818901	0.374770
17	1	0.517918	2.316886	-1.529951
18	6	-3.665259	0.805916	0.296314
19	1	-8.846798	1.418540	0.038904
20	6	-2.412604	0.181480	0.200781
21	7	-6.050600	0.913672	0.088007
22	6	0.017764	0.092114	0.207829
23	6	-4.884685	0.227393	0.009946
24	1	5.276397	2.001214	-2.195879
25	6	-8.492599	0.429692	-0.226178
26	1	-7.068967	2.696620	-0.048193
27	6	-7.146793	0.102160	-0.218456
28	1	-2.384020	-0.861407	-0.086682
29	1	-10.451123	-0.346870	-0.601254
30	6	-9.390428	-0.571381	-0.585215
31	6	-5.189036	-1.207443	-0.423004
32	6	-6.693993	-1.170224	-0.542599
33	7	0.056492	-1.249869	0.349417
34	6	-8.952551	-1.846859	-0.918288
35	6	-7.592595	-2.154381	-0.896915
36	1	-9.672846	-2.608567	-1.193785
37	1	-7.253783	-3.152738	-1.154559
38	6	-4.557402	-1.541281	-1.780997
39	1	-3.468382	-1.568247	-1.727159
40	1	-4.904154	-2.523638	-2.109751

41	1	-4.845846	-0.807081	-2.535857
42	1	5.367046	3.251741	0.001951
43	1	7.131751	3.111056	-0.008473
44	1	-6.414197	3.568392	2.191185
45	6	6.244051	3.162484	-0.642361
46	1	5.258319	-0.243461	2.380094
47	1	-1.632606	2.557358	1.556369
48	6	-1.166342	2.312293	0.594888
49	1	3.764238	-1.109544	1.996224
50	6	4.848897	-1.124285	1.881490
51	1	5.230386	-2.012888	2.389756
52	1	3.655241	1.664579	-1.027673
53	6	6.144239	1.938645	-1.537227
54	6	1.213635	0.786254	-0.179785
55	1	-1.795868	2.782803	-0.170352
56	6	3.676203	0.714729	-0.508225
57	1	8.836172	1.099864	-1.220285
58	6	2.444871	0.179319	-0.086871
59	7	6.056793	0.698398	-0.790027
60	6	4.910838	0.136547	-0.322530
61	1	-5.333012	2.855076	0.061003
62	6	8.516299	0.219061	-0.676760
63	1	7.017148	1.864359	-2.187950
64	6	7.180387	-0.043232	-0.419878
65	1	2.476681	-0.797729	0.382373
66	1	10.504164	-0.518063	-0.384889
67	6	9.450586	-0.696356	-0.200251
68	6	5.266480	-1.161807	0.406241
69	6	6.773008	-1.165064	0.291516
70	6	9.058031	-1.825632	0.506422
71	6	7.707132	-2.065969	0.757042
72	1	9.805627	-2.522499	0.867548
73	1	7.403044	-2.948410	1.310960
74	6	4.690206	-2.391762	-0.309038
75	1	3.601465	-2.421726	-0.256907
76	1	5.073771	-3.298372	0.164586
77	1	4.983972	-2.404951	-1.360418
78	6	-0.690676	-2.061931	1.287910
79	1	0.007244	-2.684746	1.851562
80	1	-1.402205	-2.723263	0.785813
81	1	-1.231700	-1.423872	1.984684
82	1	0.861674	-1.704127	-0.049516