Electronic supplementary information (ESI)

for

Development of near-infrared ratiometric fluorescent probe for glutathione under intramolecular charge transfer signaling mechanism and bioimaging application in living cells

Yong Zhou,[a] Li Zhang,[a] Xuan Zhang*[a,b] and Zhi-Jia Zhu[a]

[a] *Key Laboratory of Science and Technology of Eco-Textiles, Ministry of Education, College of Chemistry, Chemical Engineering & Biotechnology, Donghua University, Shanghai 201620, China;* [b] *State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian 116024, China.*

**E-mail address: xzhang@dhu.edu.cn*

Contents:

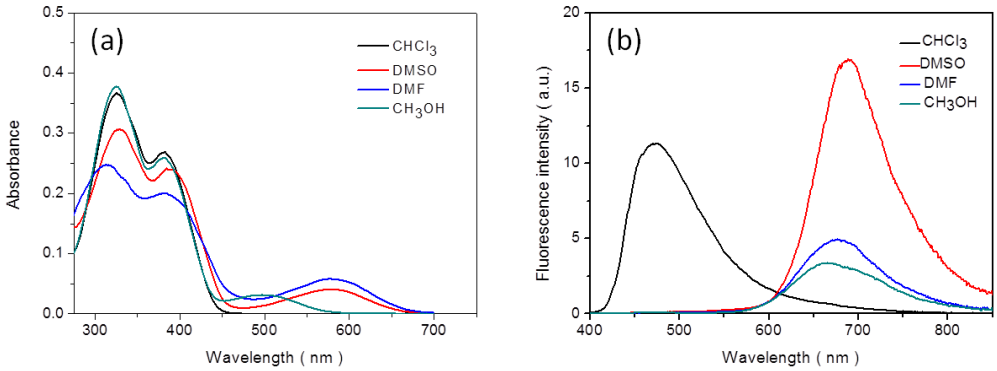

Fig.S1 The absorption and fluorescence spectra of compound **1** in various solvents with excitation wavelength at 330 nm.

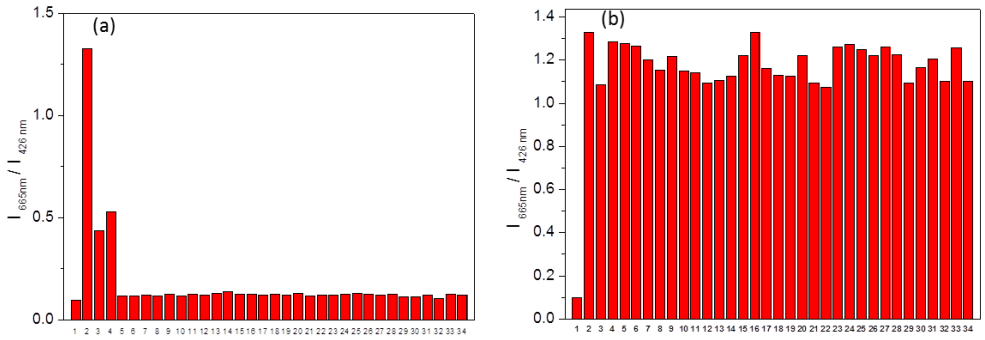

Fig. S2 The ratios of two fluorescence emission intensities ($I_{665\ nm}/I_{426\ nm}$) enhancement in the absence and presence of various species (a), and the change of ratios in the absence and presence of interference species. The numbers 1-34 represents the probe only, GSH, Cys, Hcy, Asp, Asn, Ser, Pro, Ala, Gly, Val, Leu, lle, Thr, Arg, Glu, Gln, Tyr, His, Met, Phe, Trp, Lys, Tau, Na^+, K^+, Ca^{2+}, Mg^{2+}, SO_4^{2-}, NO_3^-, CO_3^{2-}, Cl^-), Na_2S and glucose, respectively.

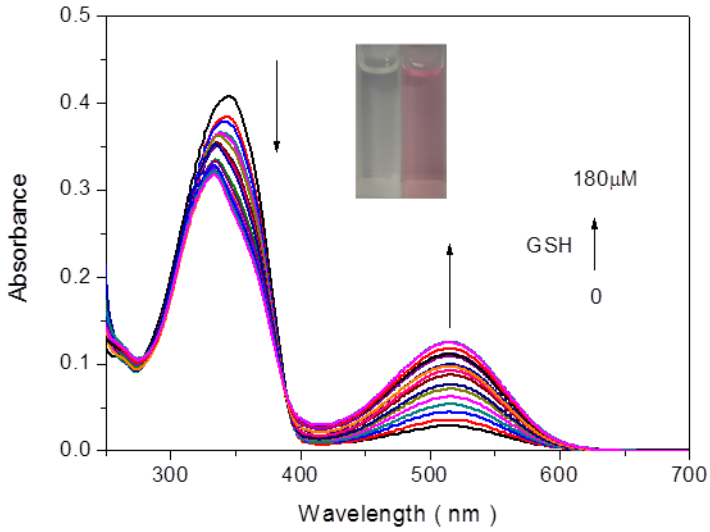

Fig. S3 Change of absorption spectra of **HBT-GSH** (10 μM) with addition of various amounts of GSH (0–180 μM). Insets are color change before and after addition of GSH.

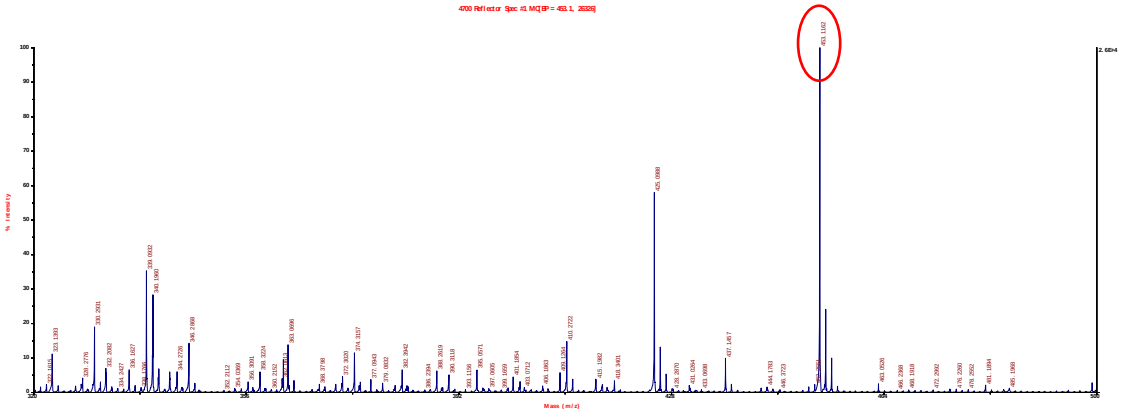

Fig. S4 Mass spectra of the probe **HBT-GSH** in the presence of GSH.

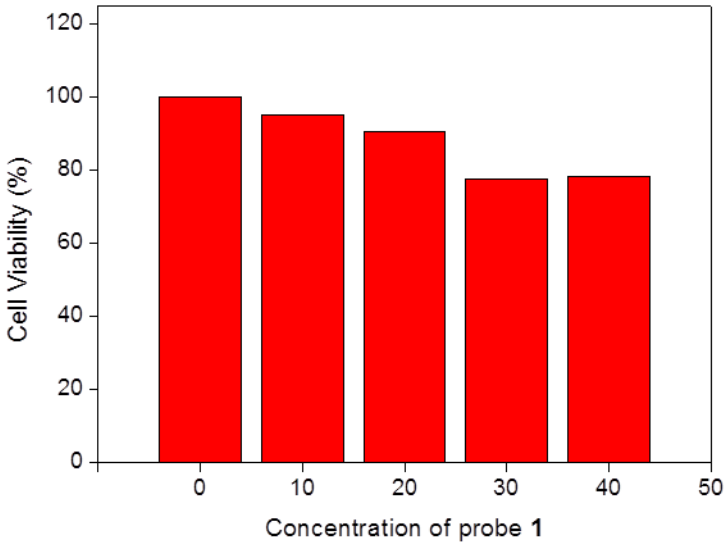

Fig. S5 Cell viability of HeLa cells treated with different concentrations of probe **HBT-GSH**.

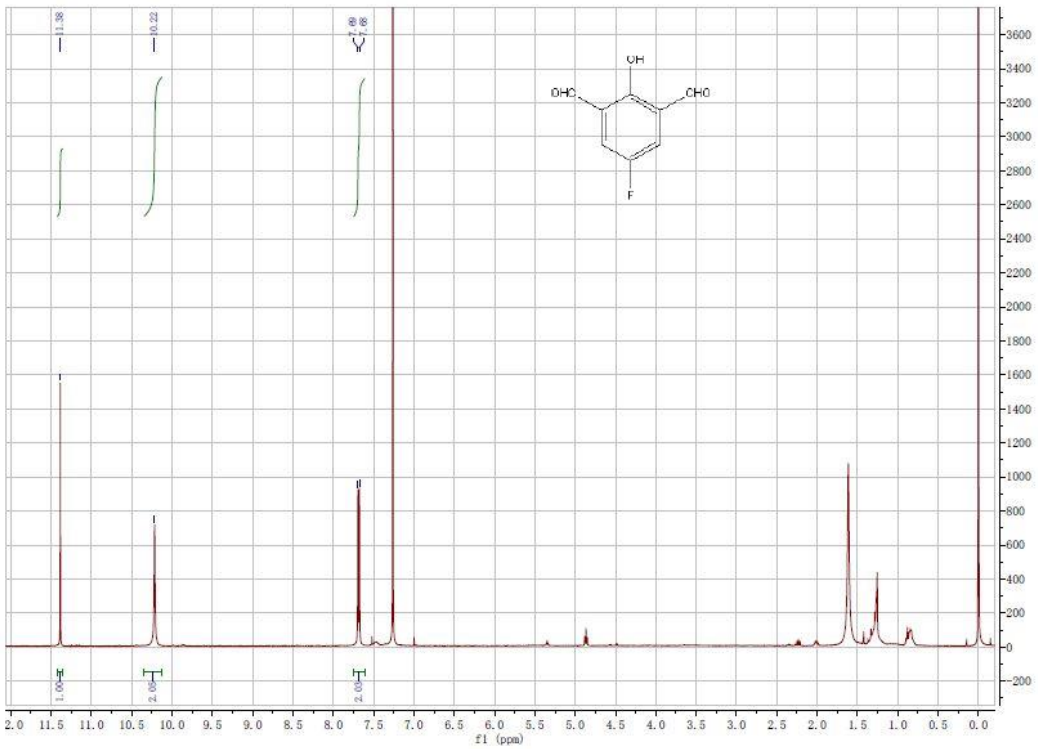

Fig. S6 ^{1}H NMR spectrum of 2,6-diformyl-4-fluorophenol.

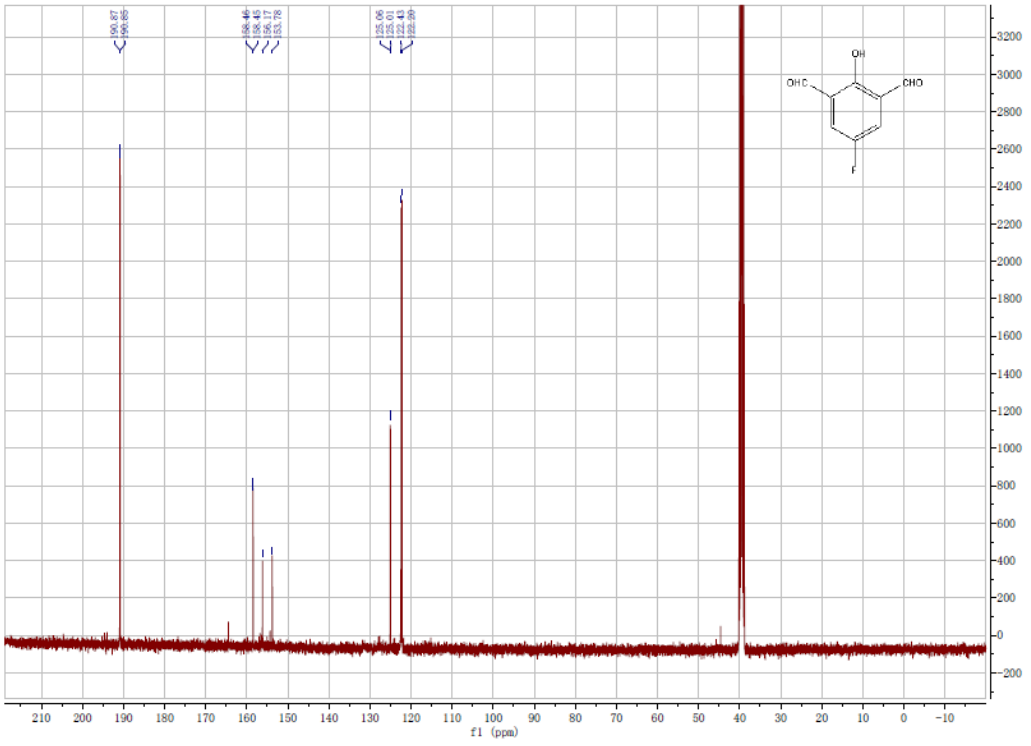

Fig. S7 ^{13}C NMR spectrum of 2,6-diformyl-4-fluorophenol.

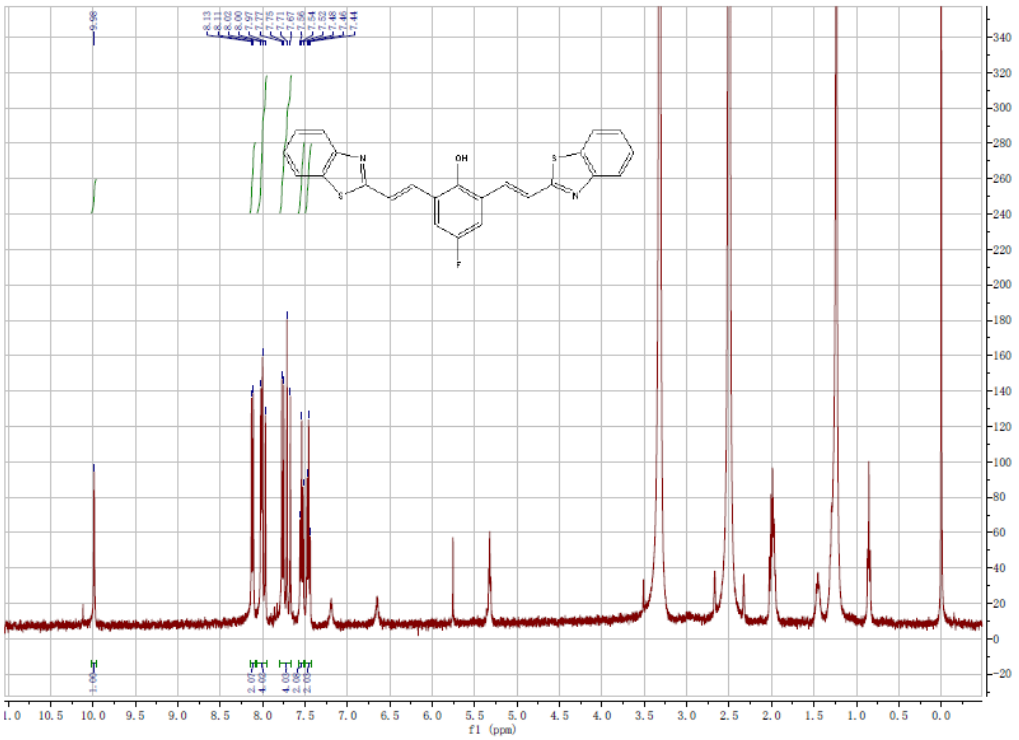

Fig. S8 ^{1}H NMR spectrum of **1**.

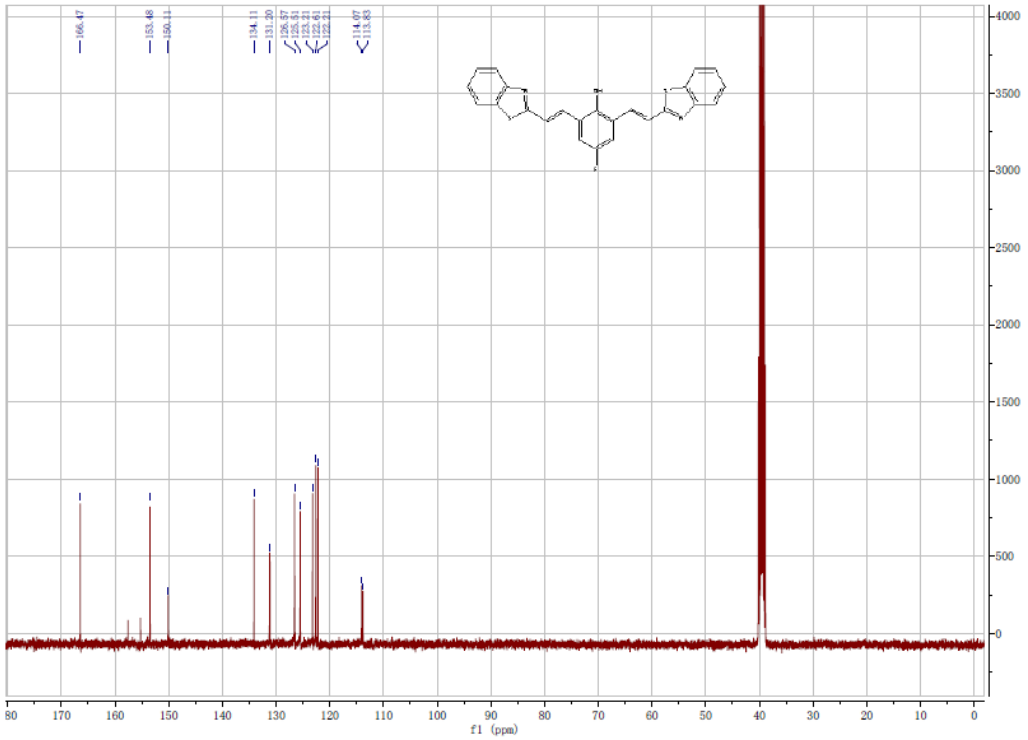

Fig. S9 ^{13}C NMR spectrum of **1**.

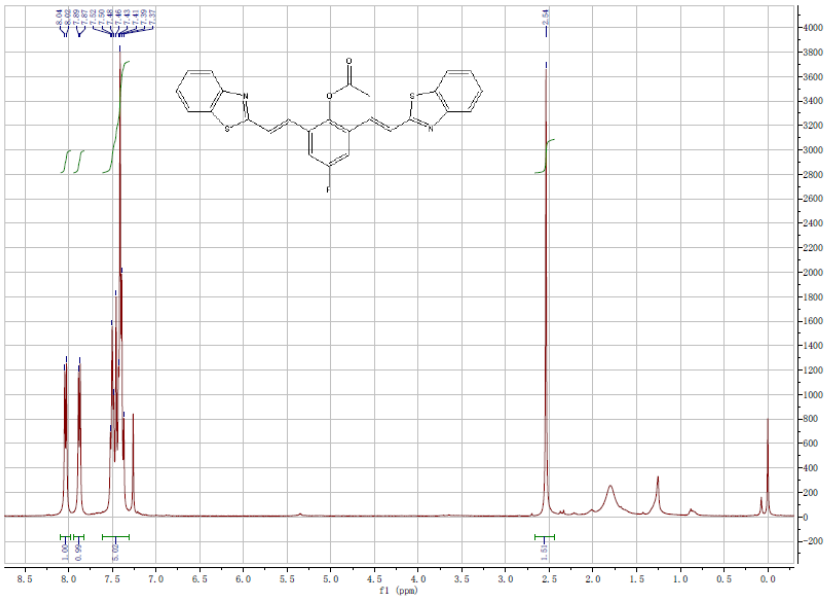

Fig. S10. ^{1}H NMR spectrum of the probe **HBT-GSH**.

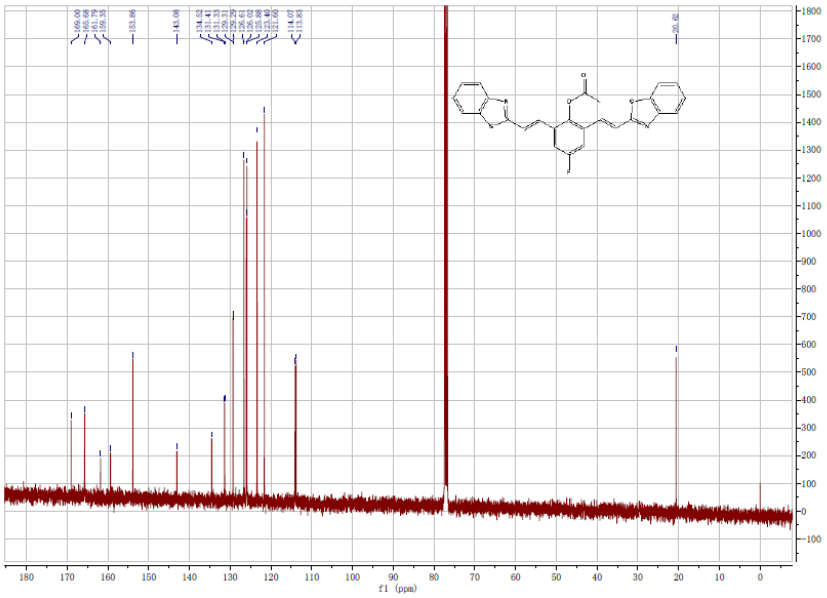

Fig. S11 ^{13}C NMR spectrum of the probe **HBT-GSH**.

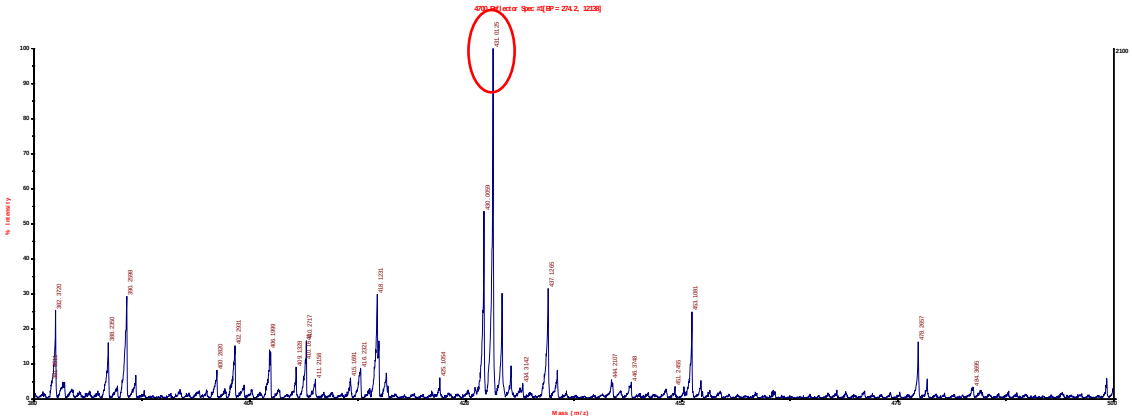

Fig. S12 Mass spectrum of **1**.

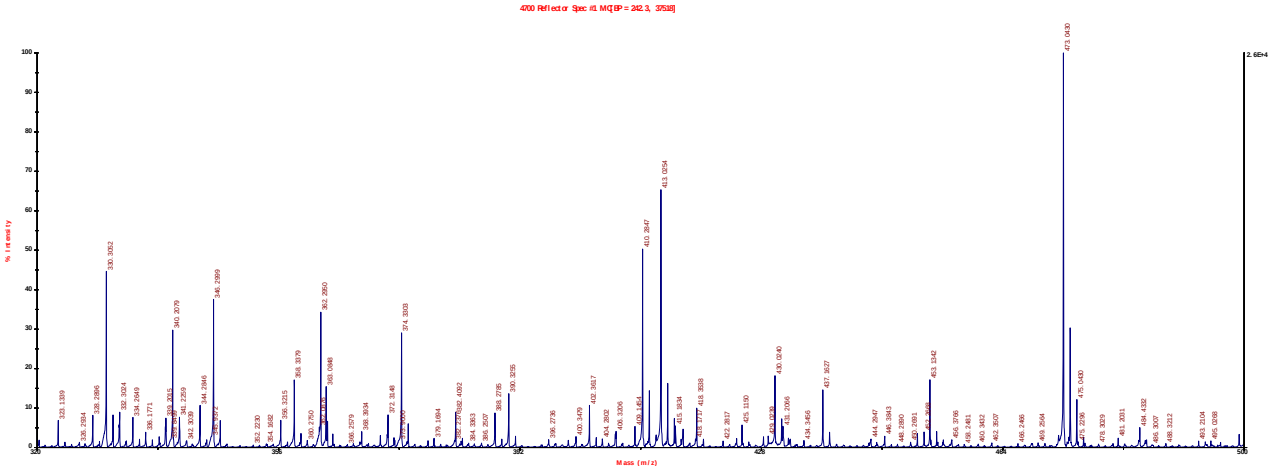

Fig. S13 Mass spectrum of the probe **HBT-GSH**.

Table S1 Theoretically calculated excitation energy (nm, eV), oscillator strength (*f*) and corresponding Cartesia coordinates for **HBT-GSH** and **1** anion, respectively.

	nm	eV	f
HBT-GSH	422.96	2.93	0.9051
1 anion	670.27	1.85	1.0405

Cartesia coordinates for HBT-GSH:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.175129	2.799001	-0.024229
2	6	0	-0.030997	3.491187	-0.003806
3	6	0	-1.272171	2.887737	0.001899
4	6	0	-1.287497	1.460588	0.007640
5	6	0	1.217889	1.375264	-0.029665
6	1	0	2.091078	3.376374	-0.060965
7	1	0	-2.173317	3.484336	-0.024179
8	6	0	2.422534	0.607067	-0.084461
9	6	0	3.707422	1.134426	-0.044623
10	1	0	2.306623	-0.465770	-0.197779
11	1	0	3.866974	2.202554	0.072659
12	6	0	-2.508478	0.714689	-0.046528
13	6	0	-3.791245	1.234129	-0.025903
14	1	0	-2.393400	-0.363130	-0.129483
15	1	0	-3.971550	2.299794	0.063301
16	6	0	-4.962081	0.444181	-0.113608
17	6	0	-7.136414	0.005818	-0.183838
18	6	0	-6.653070	-1.348142	-0.302170
19	6	0	-8.532801	0.250961	-0.179946
20	6	0	-7.536008	-2.423136	-0.414290
21	6	0	-9.394568	-0.820434	-0.291286
22	1	0	-8.887620	1.271533	-0.090376
23	6	0	-8.901307	-2.148260	-0.407811
24	1	0	-7.175292	-3.441919	-0.503924
25	1	0	-10.466822	-0.655158	-0.290908
26	1	0	-9.606712	-2.968545	-0.493937
27	6	0	4.916245	0.403293	-0.132973
28	6	0	7.115823	0.022429	-0.182047
29	6	0	6.693544	-1.330975	-0.334807

30	6	0	8.497636	0.302152	-0.153643
31	6	0	7.609801	-2.374948	-0.456354
32	6	0	9.408918	-0.741433	-0.274926
33	1	0	8.824275	1.330624	-0.037713
34	6	0	8.974366	-2.071590	-0.425242
35	1	0	7.275278	-3.401360	-0.573007
36	1	0	10.473822	-0.527561	-0.253628
37	1	0	9.702705	-2.871552	-0.518642
38	16	0	-4.918030	-1.352941	-0.279883
39	16	0	4.940080	-1.391437	-0.340964
40	6	0	-0.063345	0.745255	0.030518
41	7	0	-6.184639	0.961634	-0.082714
42	7	0	6.121076	0.954474	-0.072557
43	9	0	0.024387	4.848763	-0.011924
44	8	0	-0.139322	-0.635959	0.025070
45	6	0	0.037518	-1.414465	1.169738
46	8	0	-0.125989	-2.600398	1.055681
47	6	0	0.400508	-0.697600	2.444588
48	1	0	1.388099	-0.237778	2.345630
49	1	0	-0.314476	0.100027	2.667179
50	1	0	0.411382	-1.426348	3.254167

Cartesia coordinates for **1** anion:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.230391	2.725289	0.000353
2	6	0	-0.000026	3.373432	0.000460
3	6	0	-1.230421	2.725324	0.000409
4	6	0	-1.265794	1.316640	0.000264
5	6	0	1.265776	1.316641	0.000205
6	1	0	2.136292	3.320931	0.000376
7	1	0	-2.136329	3.320951	0.000472
8	6	0	2.478334	0.544638	0.000055
9	6	0	3.757712	1.044862	0.000020
10	1	0	2.317464	-0.530471	-0.000041
11	1	0	3.940549	2.116465	0.000099
12	6	0	-2.478344	0.544666	0.000168
13	6	0	-3.757727	1.044890	0.000204
14	1	0	-2.317485	-0.530447	0.000062
15	1	0	-3.940569	2.116492	0.000313

16	6	0	-4.958095	0.272155	0.000109
17	6	0	-7.146013	-0.170825	0.000032
18	6	0	-6.687030	-1.520977	-0.000111
19	6	0	-8.535019	0.074019	0.000035
20	6	0	-7.576851	-2.595114	-0.000246
21	6	0	-9.419545	-1.000576	-0.000101
22	1	0	-8.888802	1.100437	0.000142
23	6	0	-8.950766	-2.327623	-0.000241
24	1	0	-7.214354	-3.619085	-0.000352
25	1	0	-10.490192	-0.812656	-0.000099
26	1	0	-9.657710	-3.152563	-0.000344
27	6	0	4.958090	0.272140	-0.000129
28	6	0	7.146014	-0.170816	-0.000279
29	6	0	6.687046	-1.520975	-0.000191
30	6	0	8.535021	0.074039	-0.000290
31	6	0	7.576877	-2.595102	-0.000121
32	6	0	9.419556	-1.000547	-0.000212
33	1	0	8.888795	1.100461	-0.000337
34	6	0	8.950792	-2.327600	-0.000128
35	1	0	7.214389	-3.619077	-0.000102
36	1	0	10.490202	-0.812616	-0.000220
37	1	0	9.657744	-3.152533	-0.000092
38	16	0	-4.933982	-1.533162	-0.000075
39	16	0	4.933996	-1.533177	-0.000353
40	6	0	-0.000015	0.567755	0.000218
41	8	0	-0.000003	-0.694635	-0.000059
42	7	0	-6.173025	0.791922	0.000151
43	7	0	6.173018	0.791919	-0.000257
44	9	0	0.000009	4.743035	0.000588
