

Supplementary Information

‘Click’ based fluorescent probe mimicking IMPLICATION logic gate for Cu(II) and Pb(II) sensing: DFT and Molecular Docking studies

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Table S2: Cartesian co-ordinates of **GT**-metal complex

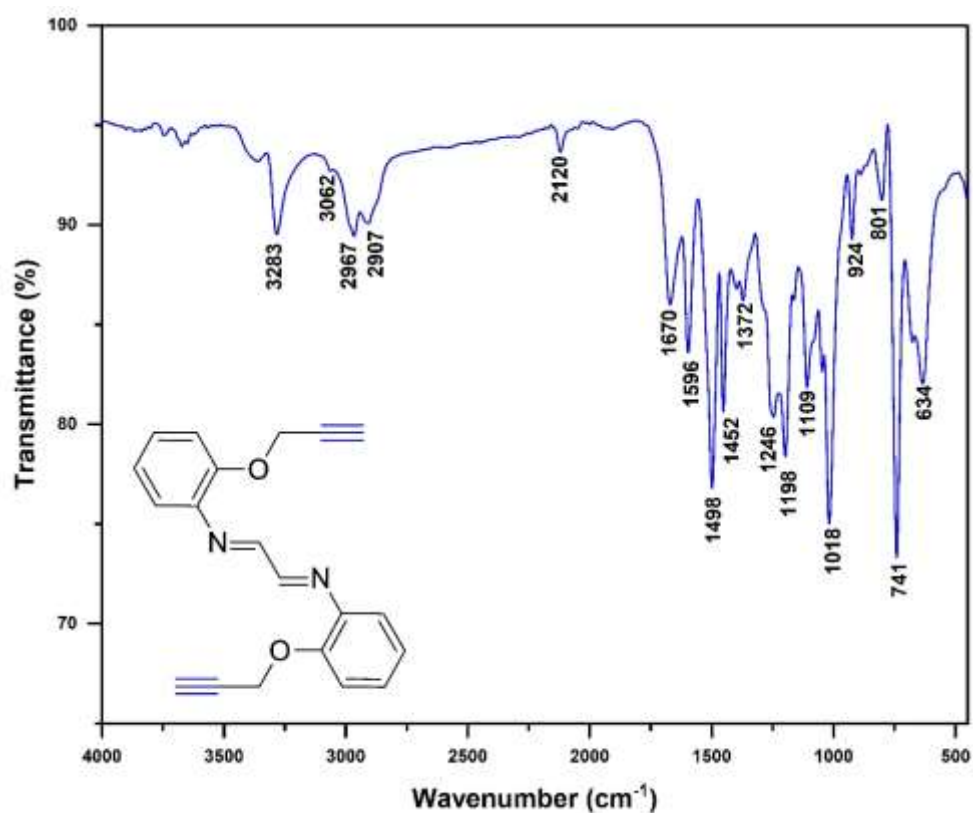


Figure S1. IR spectrum of alkyne 2

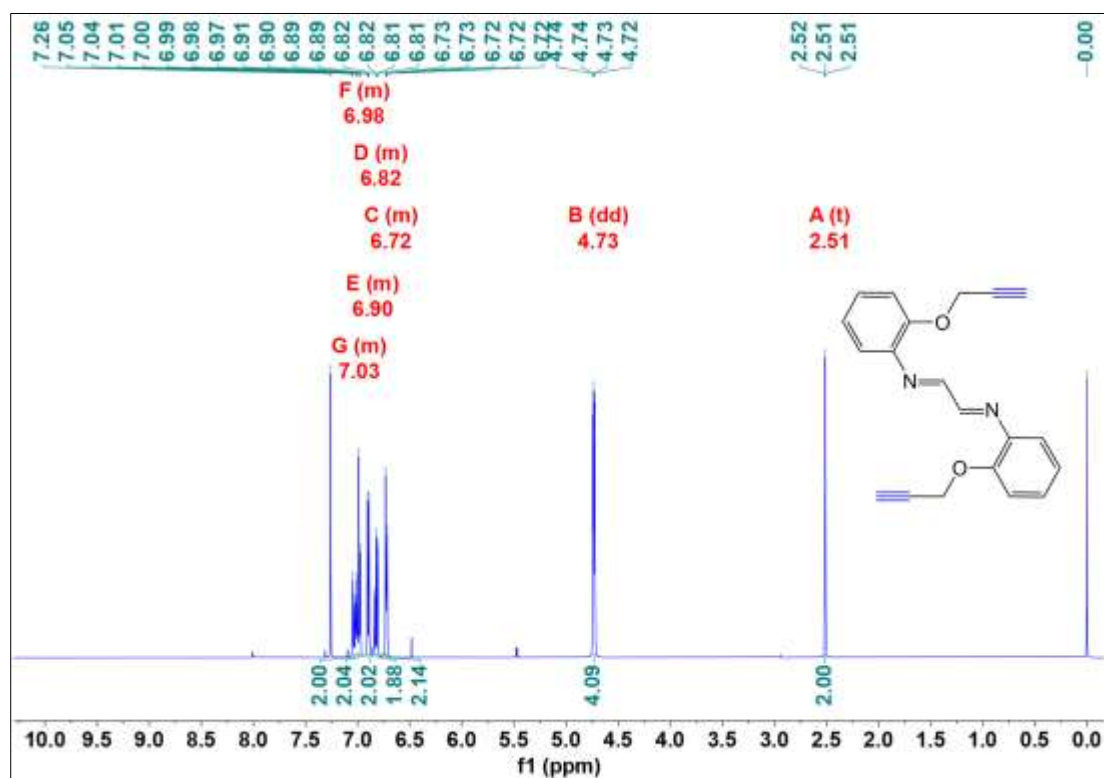


Figure S2. ^1H NMR spectrum of alkyne 2

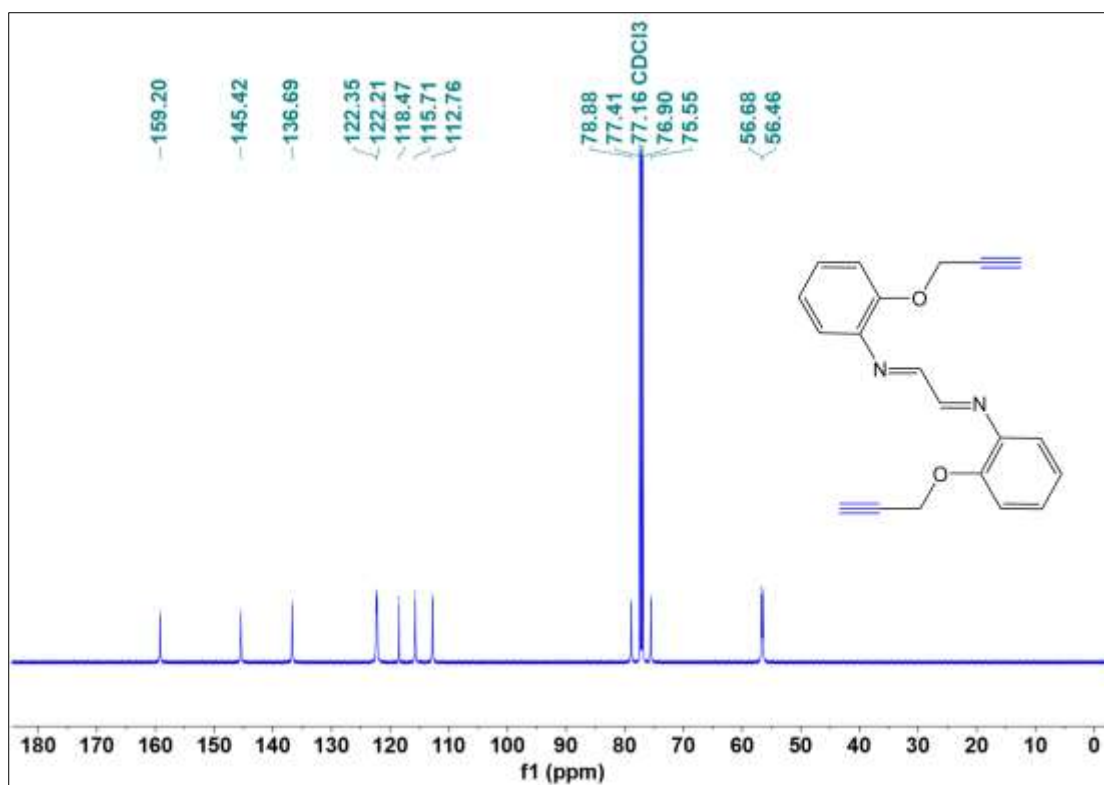


Figure S3. ¹³C NMR spectrum of alkyne 2

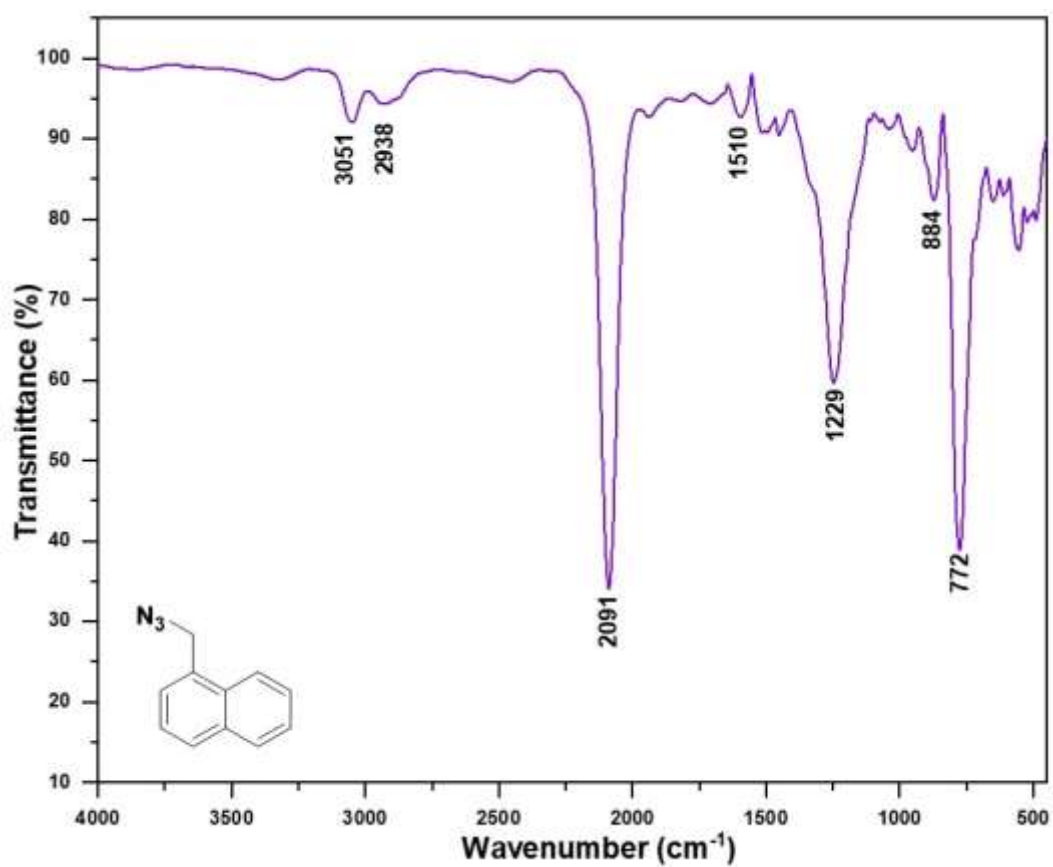


Figure S4. IR spectrum of 1-(azidomethyl)naphthalene

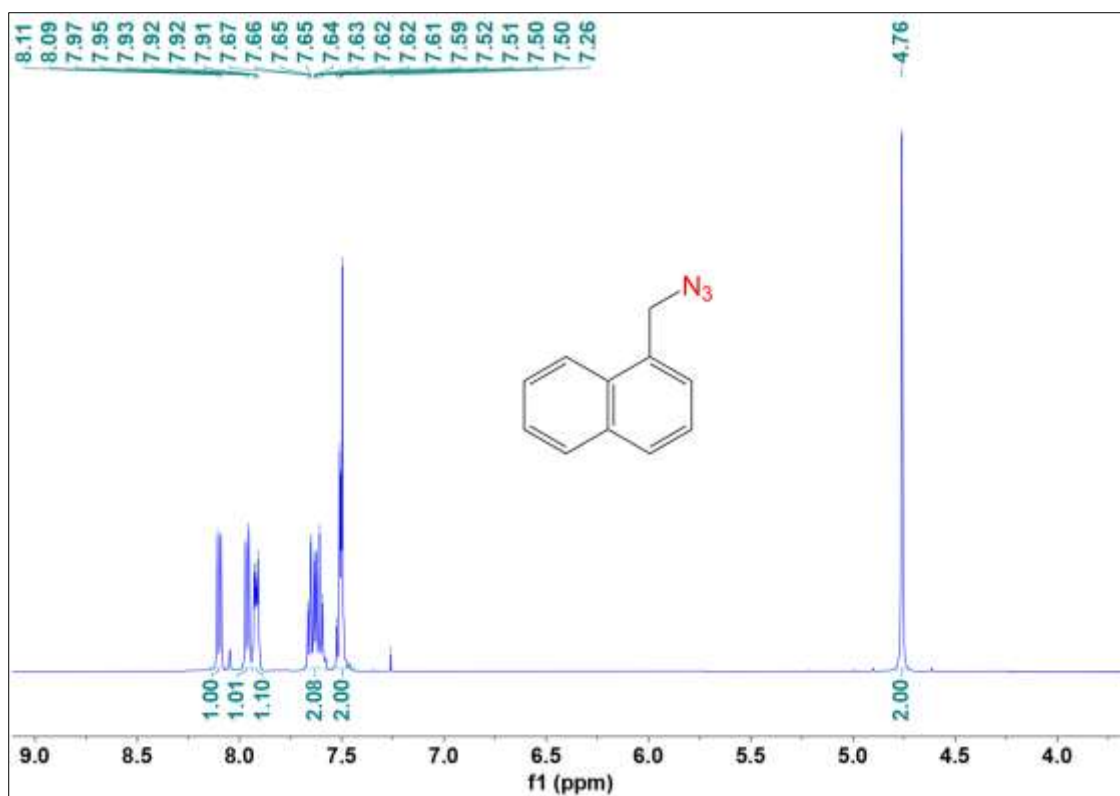


Figure S5. ^1H NMR spectrum of 1-(azidomethyl)naphthalene

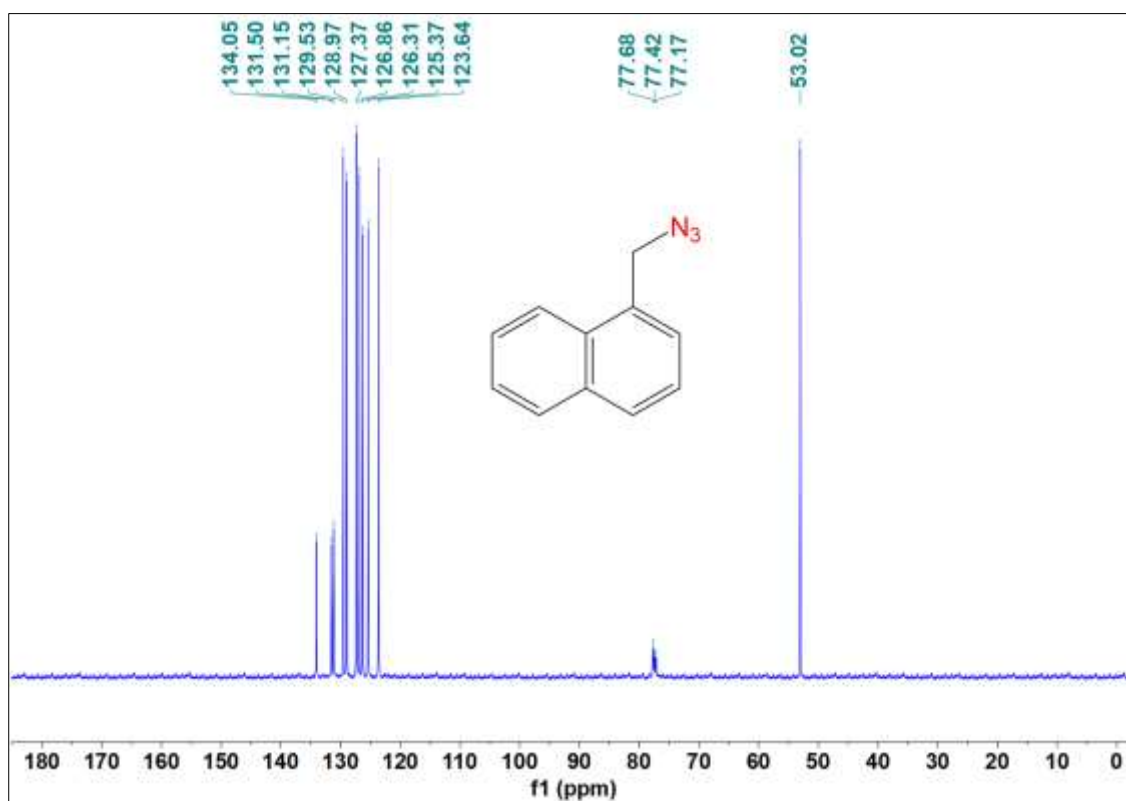


Figure S6. ^{13}C NMR spectrum of 1-(azidomethyl)naphthalene

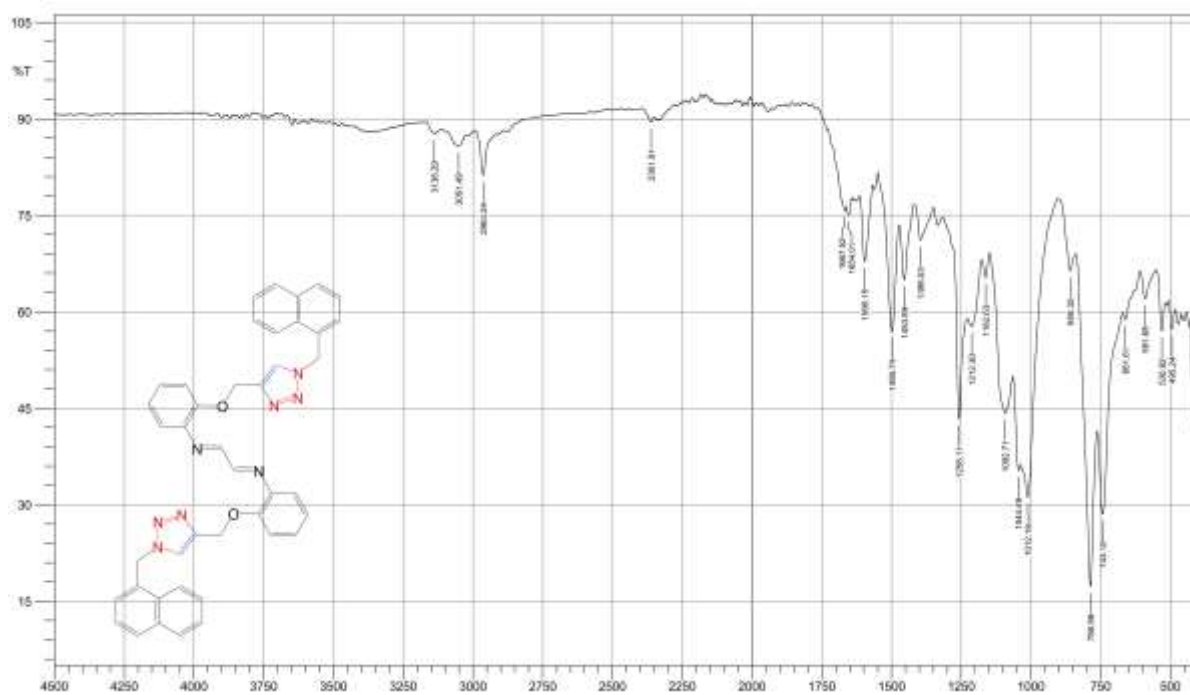


Figure S7. IR spectrum of probe **GT**

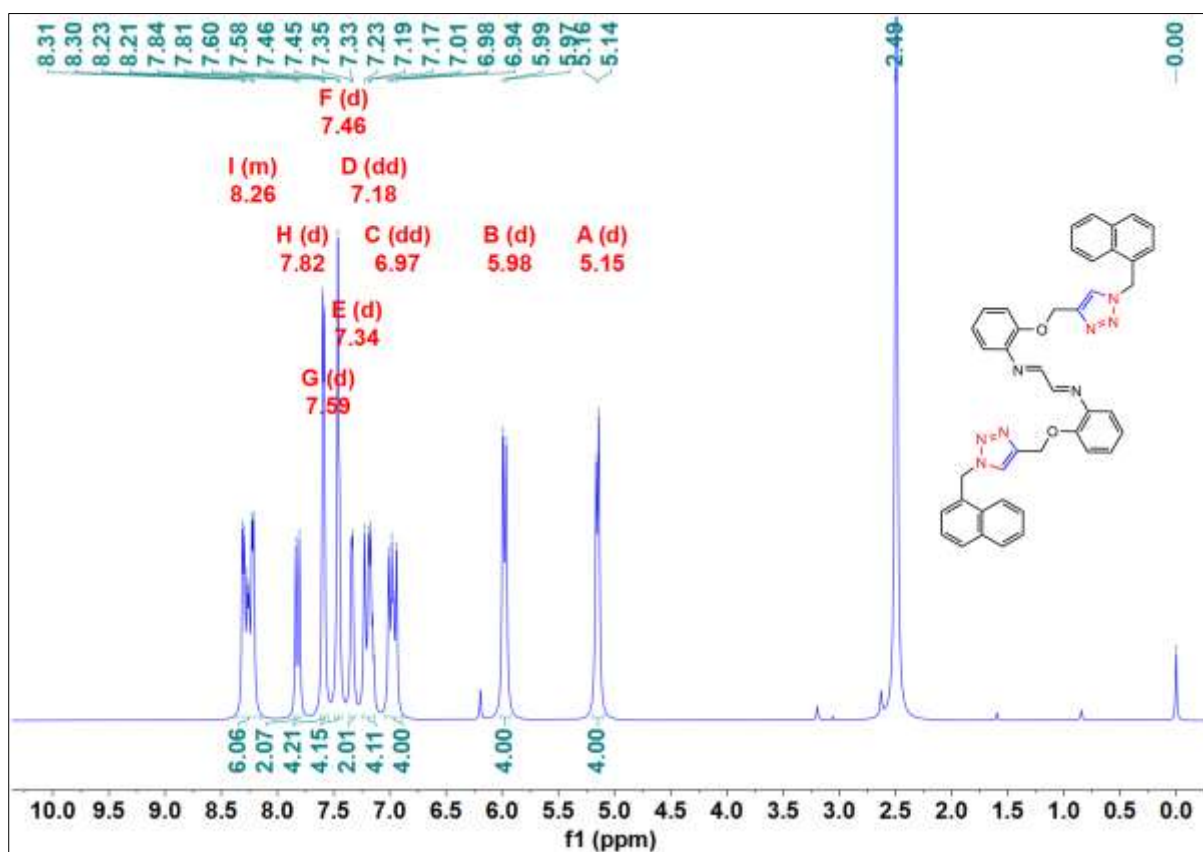


Figure S8. ^1H NMR spectrum of probe **GT**

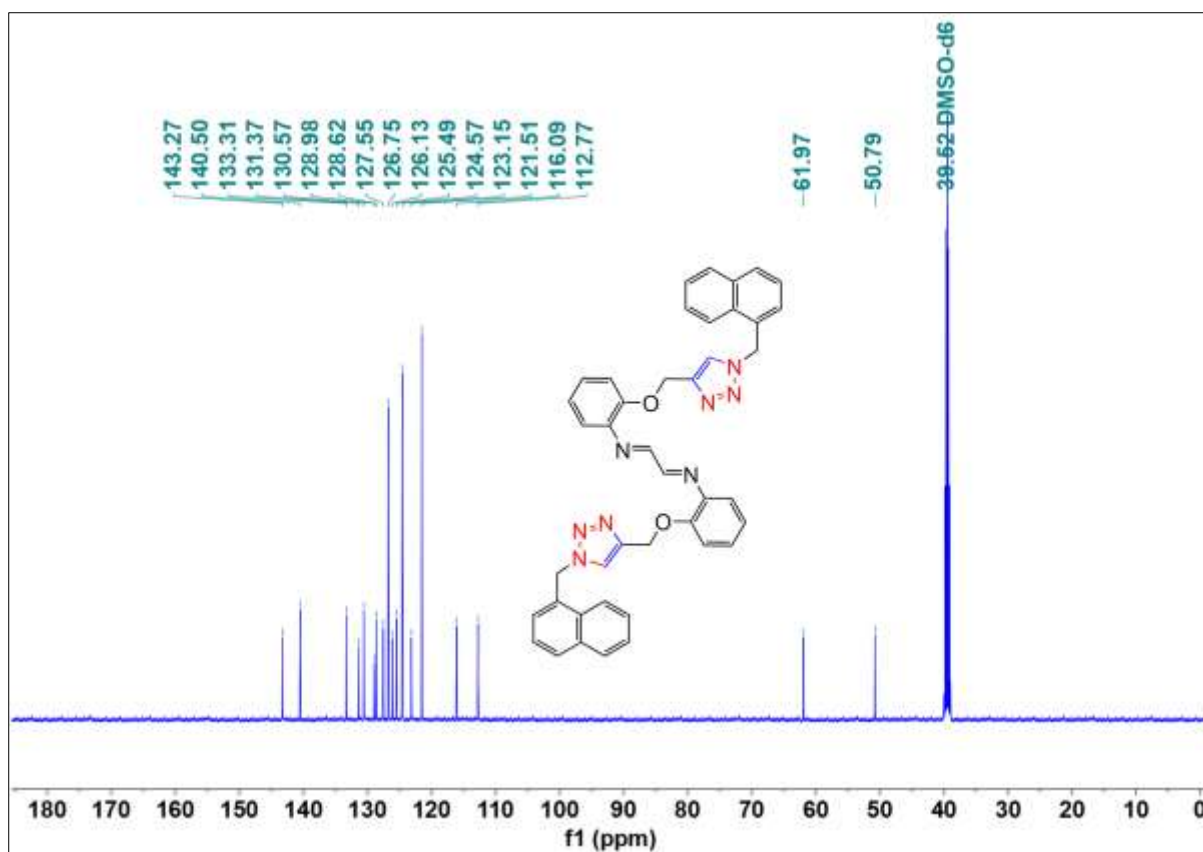


Figure S9. ¹³C NMR spectrum of probe GT

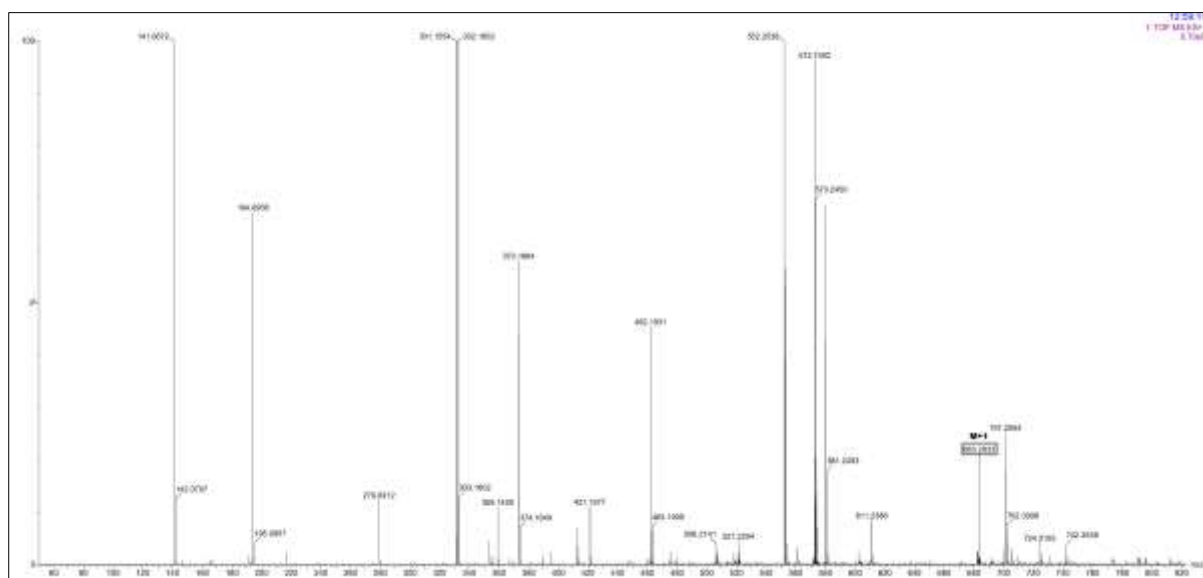


Figure S10. Mass spectrum of probe GT

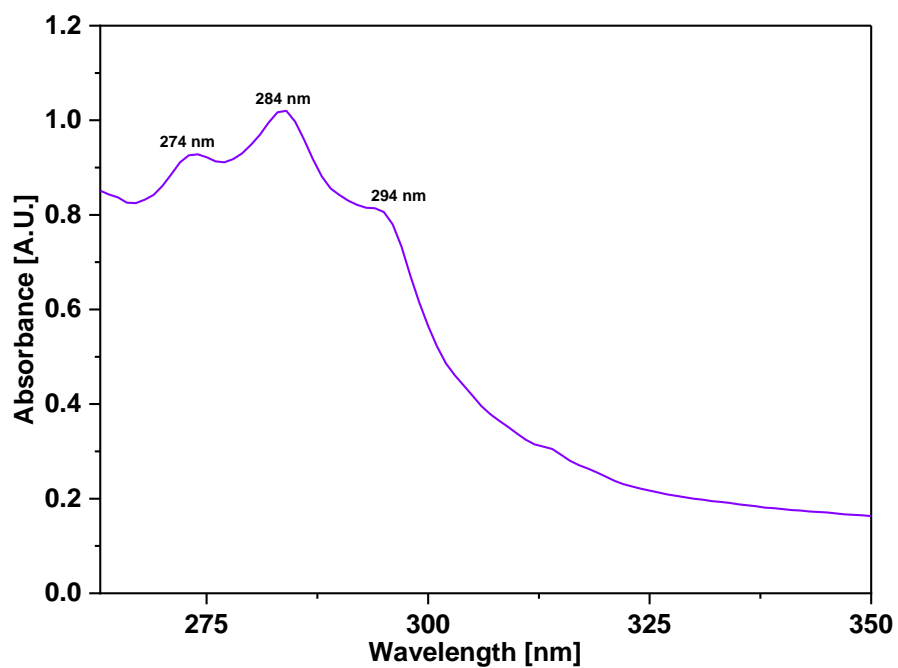


Figure S11. UV-Vis spectrum of probe **GT** (0.05 mM) in DMSO depicting absorption maxima at $\lambda_{\text{max}} = 274 \text{ nm}$, 284 nm, and 294 nm

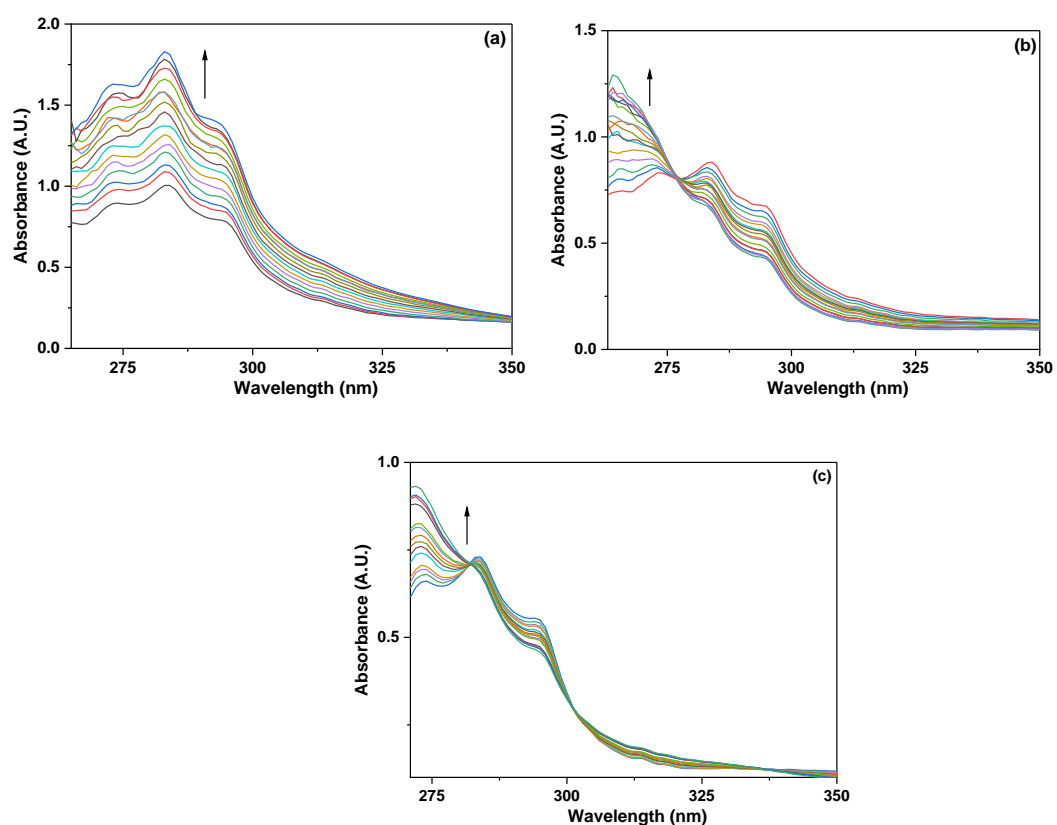


Figure S12. UV-Vis spectra of probe **GT** (0.05 mM) in DMSO signifying the recognition of (a) Cu(II) among various metal ions in the absence of Pb(II); (b) Pb(II) among various metal

ions in the absence of Cu(II); and (c) recognition of Pb(II) among various metal ions present in equimolar concentration including Cu(II)

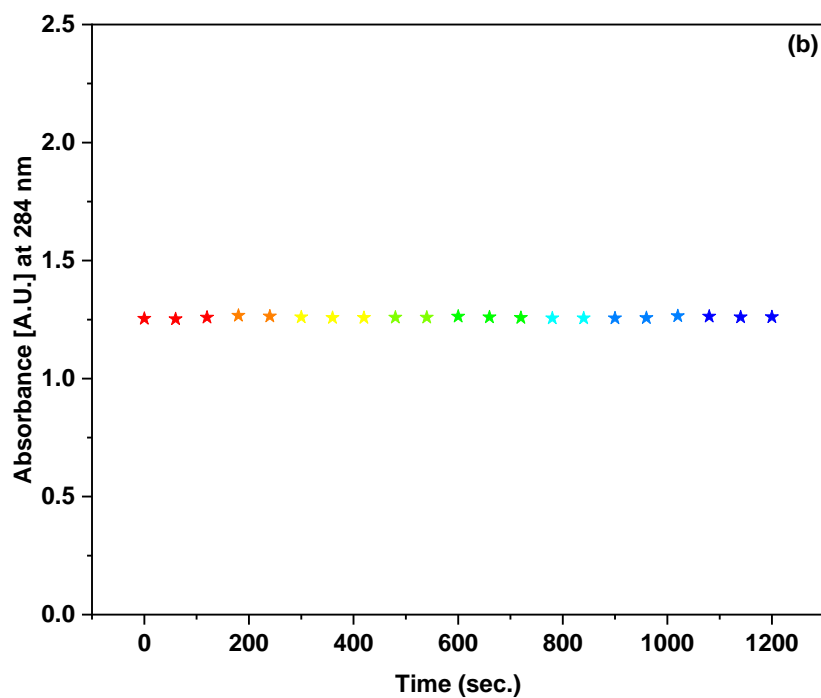
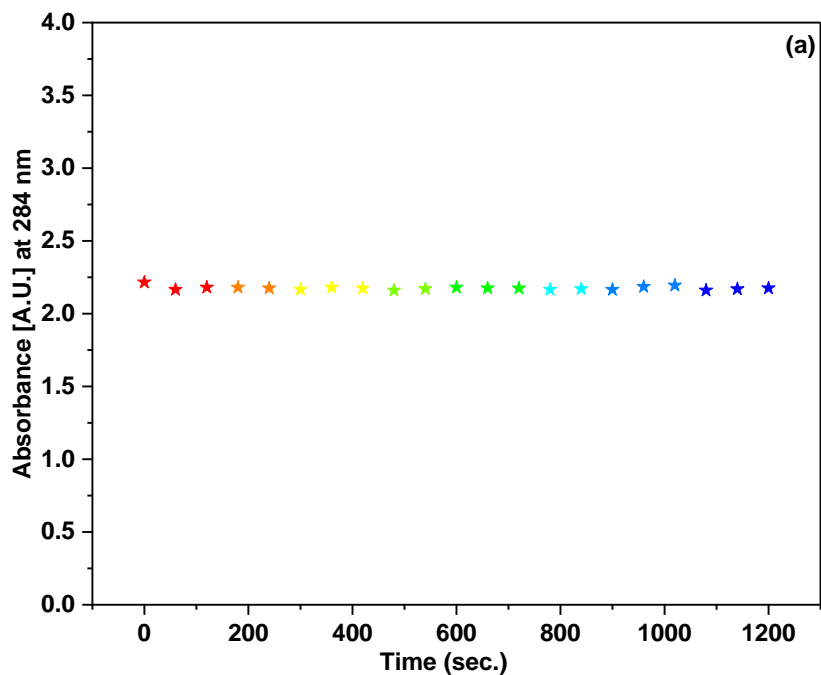


Figure S13. Time dependent absorption spectra of **GT**-metal complex solution displaying the trend in the absorption intensity with the passage of time: (a) **GT**-Cu(II) (b) **GT**-Pb(II)

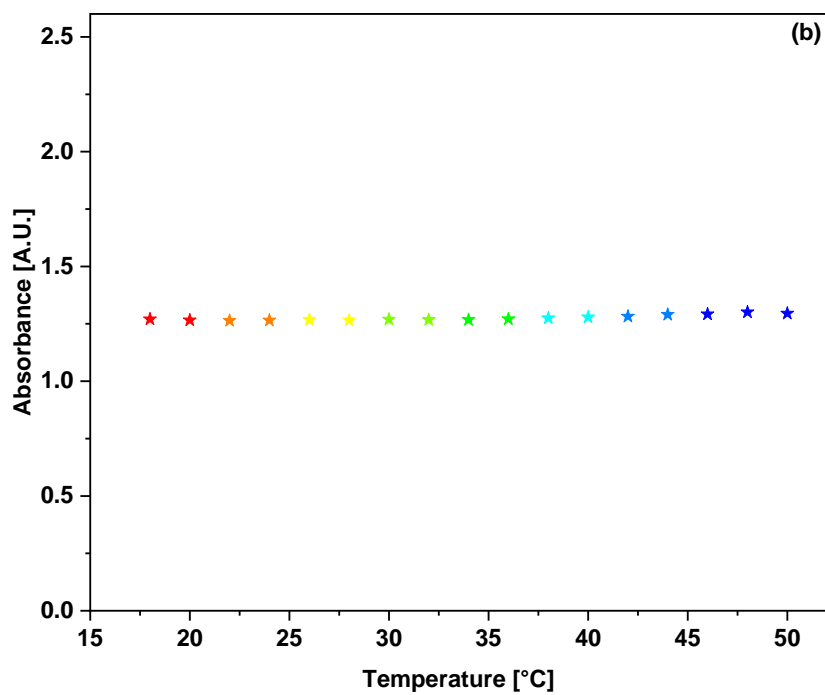
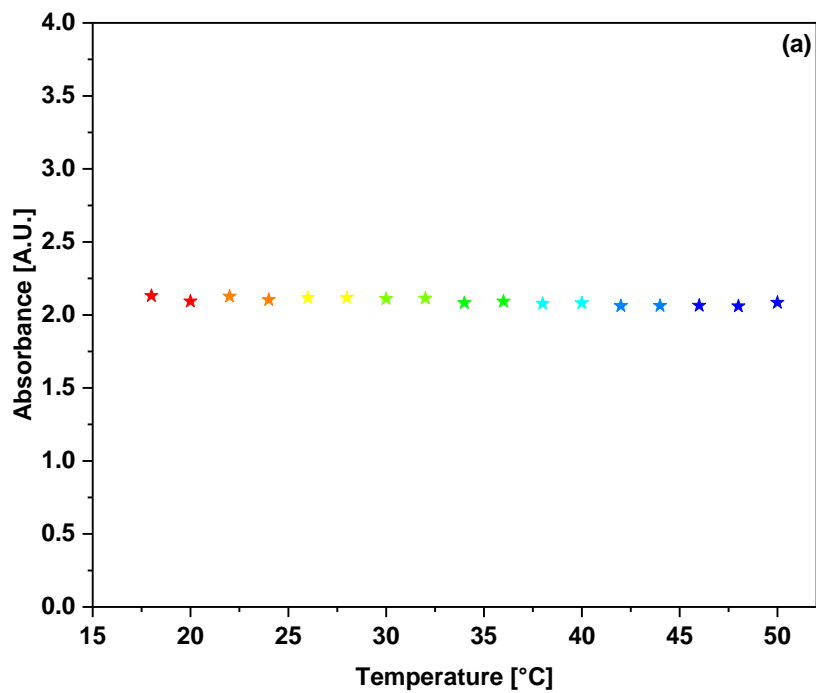


Figure S14. Temperature dependent absorption spectra of **GT**-metal complex solution demonstrating the trend in the absorption intensity over varying temperature range: (a) **GT**-Cu(II) (b) **GT**-Pb(II)

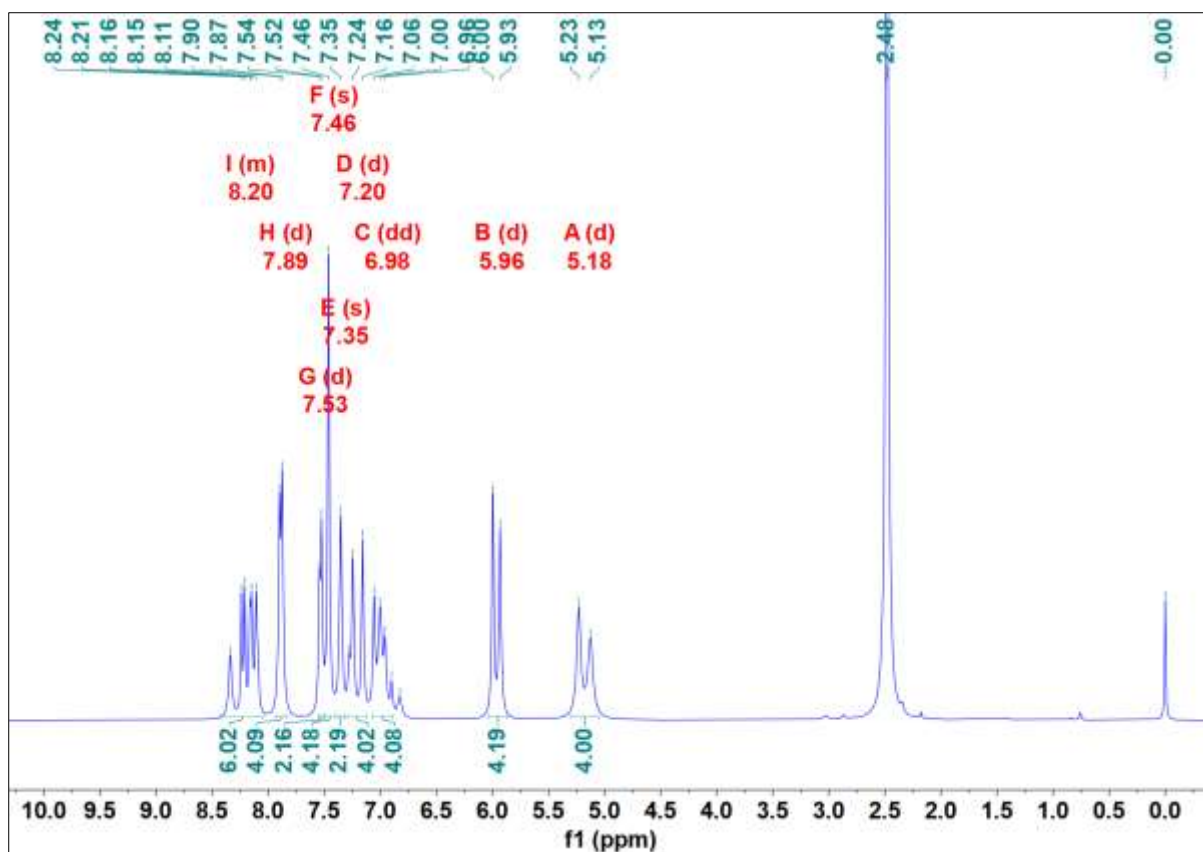


Figure S15. ^1H NMR spectrum of GT-metal complex

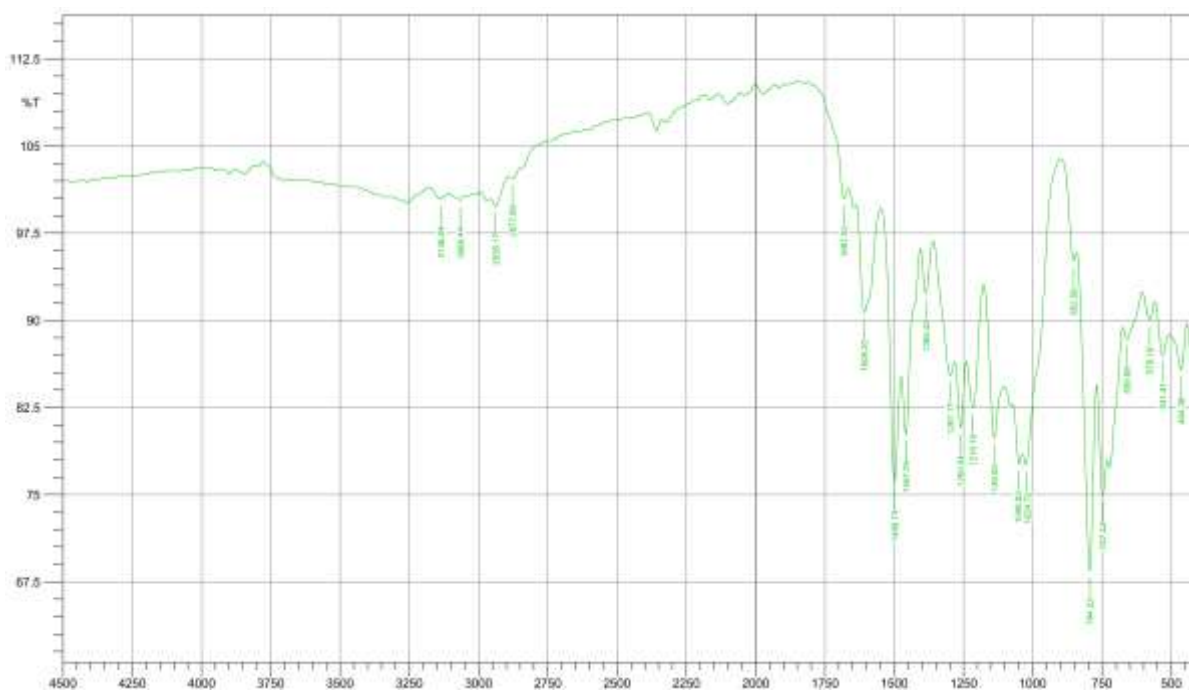


Figure S16. IR spectrum of GT-metal complex

Symbol	X	Y	Z
O	-0.27147	3.832481	-0.24321
O	0.693632	-1.49338	1.770921
N	-1.56982	2.428389	1.819619
N	1.476497	0.995838	2.820901
C	-2.11573	3.573179	1.219712
C	2.058398	-0.2159	3.223658
C	-1.49171	4.288605	0.163628
C	1.694236	-1.48379	2.697926
C	-3.39646	3.965526	1.624624
C	3.127117	-0.149	4.124242
C	-2.14973	5.371582	-0.42206
C	2.382002	-2.62631	3.109759
C	-4.03457	5.065719	1.060604
C	3.787694	-1.29389	4.556716
C	-3.40807	5.765715	0.034437
C	3.412676	-2.53223	4.045125
C	-0.32596	2.354683	2.11395
C	0.214365	1.103573	2.634318
H	-3.87025	3.386272	2.408621
H	3.416137	0.831518	4.484149
H	-1.68524	5.91947	-1.23094
H	2.117222	-3.59498	2.707918
H	-5.01563	5.363706	1.410643
H	4.597888	-1.2165	5.271707
H	-3.89454	6.618284	-0.42517
H	3.925763	-3.43365	4.359722
H	0.38426	3.172931	1.985087
H	-0.50474	0.305614	2.823317
C	0.342447	4.412461	-1.39301
H	-0.3237	4.353163	-2.26088
C	0.414224	-2.6971	1.050814
H	1.319141	-3.08414	0.57239

C	-0.5935	-2.37391	-0.00297
C	-1.62568	-1.46135	-0.00276
H	0.032659	-3.4577	1.743565
N	-0.59541	-3.0232	-1.19918
N	-1.5694	-2.56249	-1.93336
N	-2.20125	-1.61072	-1.21982
C	-3.32308	-0.86888	-1.81199
H	-3.01383	0.17024	-1.9408
H	-3.45502	-1.30262	-2.80412
H	-1.96836	-0.74058	0.719623
C	-4.59234	-0.92375	-0.99095
C	-5.35833	-2.12955	-0.88355
C	-5.02426	0.219882	-0.3545
C	-6.56199	-2.11095	-0.10609
C	-6.2121	0.233714	0.41132
H	-4.44222	1.131791	-0.43924
C	-6.9624	-0.90762	0.532863
H	-6.52216	1.150839	0.898472
H	-7.87579	-0.90695	1.118511
C	-4.98367	-3.34598	-1.51593
C	-7.33377	-3.29669	0.004612
C	-5.75718	-4.47666	-1.38861
C	-6.94312	-4.45531	-0.62186
H	-5.45167	-5.39379	-1.87943
H	-7.54162	-5.35453	-0.52948
H	-4.07273	-3.39433	-2.09892
H	-8.24361	-3.27132	0.595311
H	0.561497	5.470982	-1.20485
C	1.601698	3.658665	-1.6748
C	2.330688	2.794307	-0.89022
N	2.238593	3.798127	-2.87023
N	3.318876	3.071177	-2.86589
N	3.388935	2.45336	-1.67068

C	4.499013	1.556692	-1.37534
H	5.315685	1.877698	-2.02587
H	4.806129	1.745767	-0.3433
C	4.205128	0.079905	-1.57894
C	2.996019	-0.36104	-2.06443
C	5.231055	-0.86857	-1.2638
C	2.735886	-1.73935	-2.24903
H	2.221859	0.353115	-2.31616
C	4.965912	-2.26307	-1.4576
C	3.69847	-2.66907	-1.95165
H	1.767008	-2.05613	-2.61623
H	3.503395	-3.7269	-2.09313
C	6.51095	-0.49242	-0.77249
H	6.747297	0.55366	-0.62075
C	5.978702	-3.20896	-1.1525
C	7.471168	-1.43583	-0.48711
C	7.204839	-2.80926	-0.67815
H	5.766599	-4.26215	-1.3054
H	7.969629	-3.54348	-0.4516
H	8.440488	-1.12307	-0.11535
H	2.187707	2.404748	0.103539

Table S1. Cartesian co-ordinates of probe **GT**

Symbol	X	Y	Z
O	0.173741	-2.311697	1.050495
O	0.789778	3.502086	0.311111
N	1.523691	-0.439272	2.627751
N	-1.019438	1.971071	1.993307
C	1.610235	-1.834742	2.925784
C	-1.328734	3.24767	1.464275
C	0.910604	-2.80894	2.160759
C	-0.509795	3.995226	0.568027
C	2.461438	-2.283896	3.956504

C	-2.601022	3.781473	1.785264
C	1.014787	-4.178152	2.447651
C	-0.954245	5.201931	0.006952
C	2.556225	-3.653051	4.263613
C	-3.040727	5.001315	1.249645
C	1.829075	-4.59897	3.516034
C	-2.219523	5.711651	0.349708
C	0.349999	0.127357	2.604126
C	0.187177	1.529757	2.210142
H	3.012159	-1.544663	4.531018
H	-3.216089	3.223559	2.486077
H	0.483331	-4.914446	1.849928
H	-0.297429	5.760648	-0.655511
H	3.192315	-3.980132	5.080089
H	-4.010914	5.39994	1.530419
H	1.905777	-5.656623	3.750625
H	-2.551198	6.659134	-0.064209
H	-0.572491	-0.402559	2.863201
H	1.095392	2.122549	2.095129
C	-1.159651	-2.832797	0.754763
H	-1.094787	-3.670029	0.04582
C	1.213485	3.24307	-1.070404
H	0.368399	3.304734	-1.765723
C	1.803542	1.858192	-1.040021
C	2.974408	1.451303	-0.369393
H	1.971746	3.980371	-1.35843
N	1.211102	0.714961	-1.510058
N	1.964244	-0.362892	-1.137076
N	3.033152	0.091459	-0.44167
C	4.016664	-0.848854	0.230895
H	3.501599	-1.215797	1.122376
H	4.161414	-1.675582	-0.47083
H	3.722034	2.027157	0.151088

C	5.291192	-0.132644	0.601881
C	6.324673	0.113819	-0.372128
C	5.460888	0.27052	1.928246
C	7.529037	0.780469	0.062823
C	6.652132	0.925668	2.349065
H	4.671781	0.079452	2.653288
C	7.663463	1.173632	1.431425
H	6.765737	1.221908	3.387085
H	8.578348	1.670018	1.746415
C	6.221921	-0.269201	-1.74746
C	8.573816	1.032685	-0.880535
C	7.255073	-0.012235	-2.641524
C	8.443025	0.646448	-2.207132
H	7.166707	-0.318026	-3.680538
H	9.242397	0.836917	-2.917335
H	5.332955	-0.783562	-2.107885
H	9.478637	1.530023	-0.540338
H	-1.664595	-3.185484	1.661572
C	-1.891967	-1.662739	0.167747
C	-3.038606	-0.998079	0.594227
N	-1.431405	-0.955557	-0.928612
N	-2.235012	0.110088	-1.198153
N	-3.211185	0.06	-0.262598
C	-4.258604	1.149487	-0.202172
H	-3.805526	1.964728	0.370335
H	-4.394725	1.481004	-1.236048
C	-5.534364	0.667589	0.447854
C	-5.808861	1.059573	1.757687
C	-6.470392	-0.159766	-0.272506
C	-7.004727	0.653668	2.414054
H	-5.106307	1.697205	2.290889
C	-7.679486	-0.571335	0.400307
C	-7.918546	-0.148661	1.745713

H	-7.198958	0.980561	3.430787
H	-8.836434	-0.460059	2.238254
C	-6.267965	-0.587148	-1.623974
H	-5.378909	-0.278552	-2.169668
C	-8.628418	-1.386334	-0.292704
C	-7.21082	-1.375665	-2.273206
C	-8.401643	-1.783803	-1.602825
H	-9.538194	-1.684826	0.222276
H	-9.130082	-2.396163	-2.125093
H	-7.051742	-1.679302	-3.30462
H	-3.713204	-1.192677	1.410955
Pb	0.071562	-1.167396	-2.368409

Table S2: Cartesian co-ordinates of **GT**-metal complex