

Supporting Information

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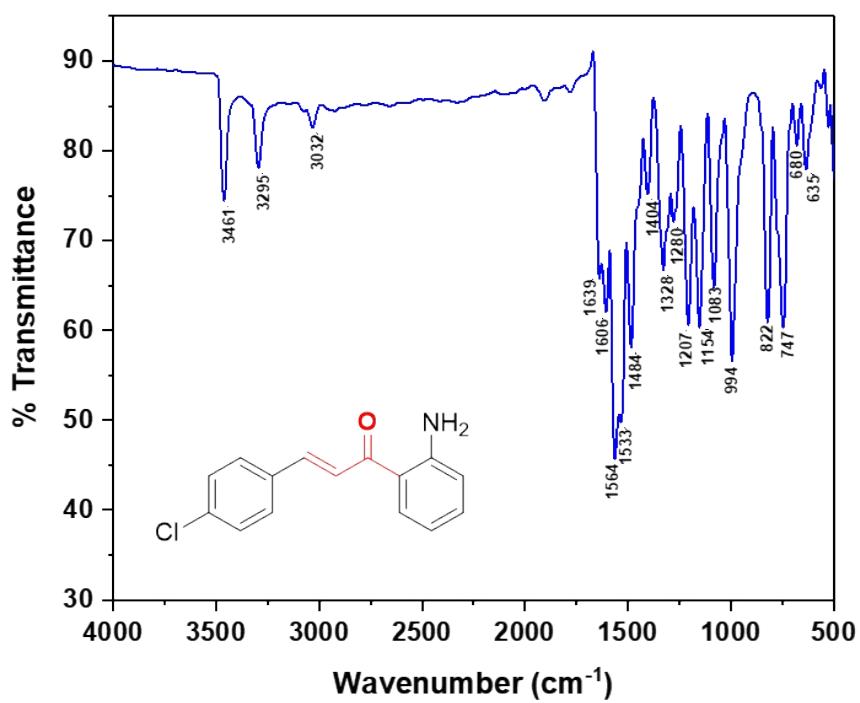


Figure S1: IR spectrum of chalcone 3a

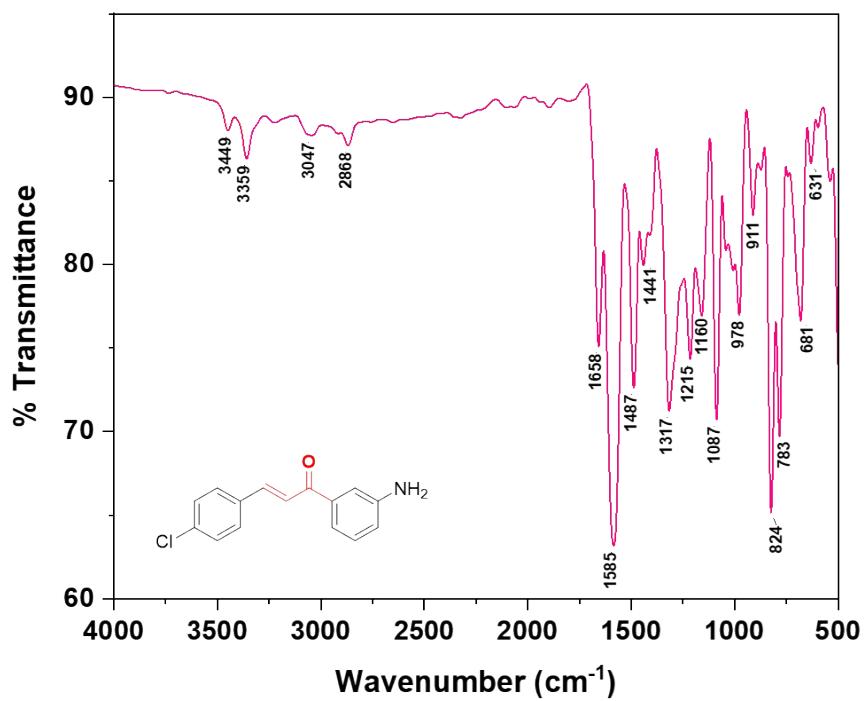


Figure S2: IR spectrum of chalcone 3b

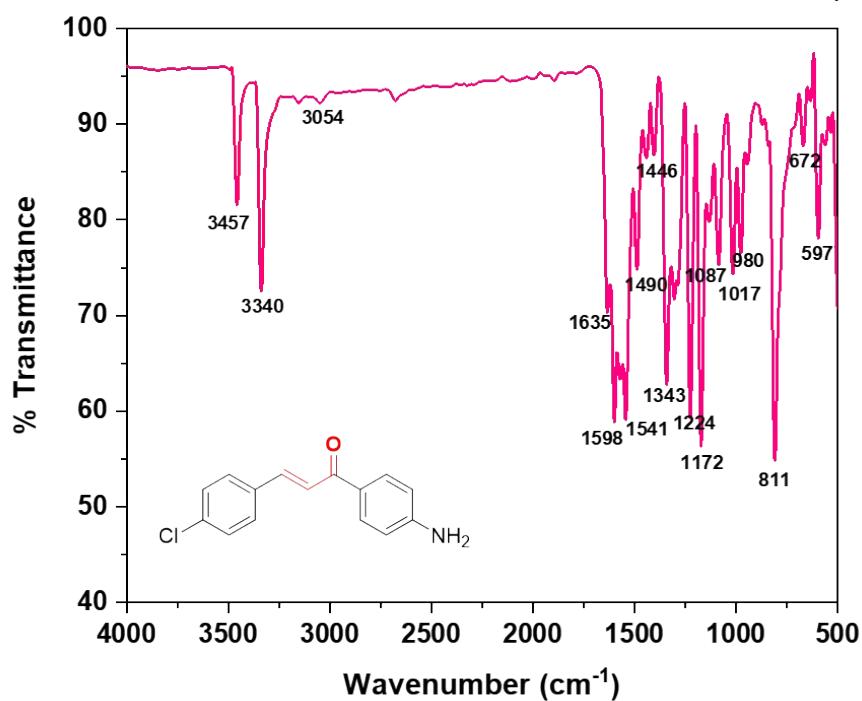


Figure S3: IR spectrum of chalcone 3c

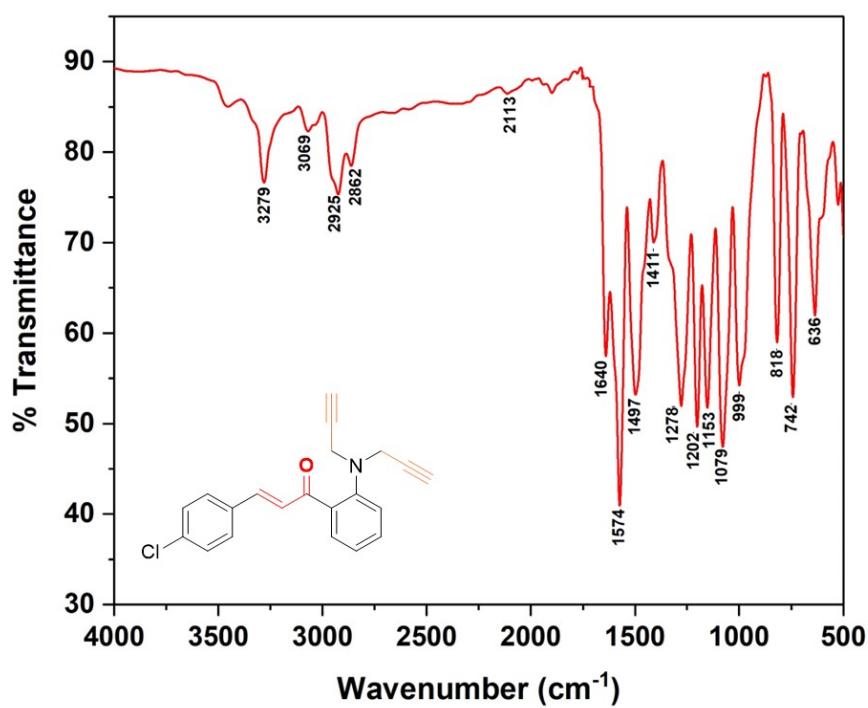


Figure S4: IR spectrum of alkyne 4a

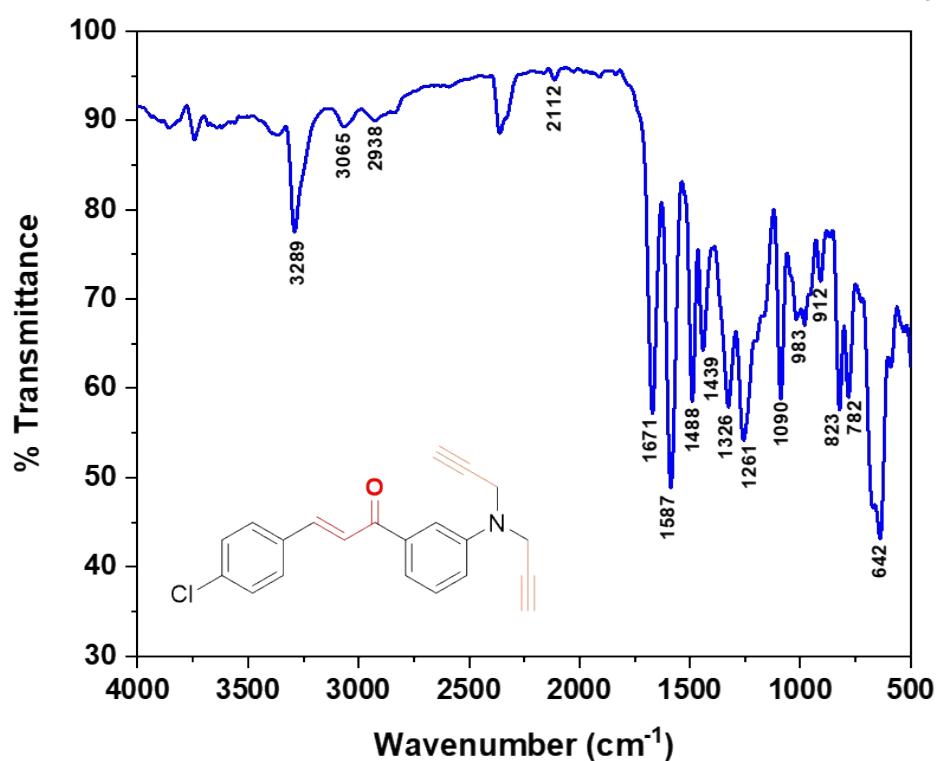
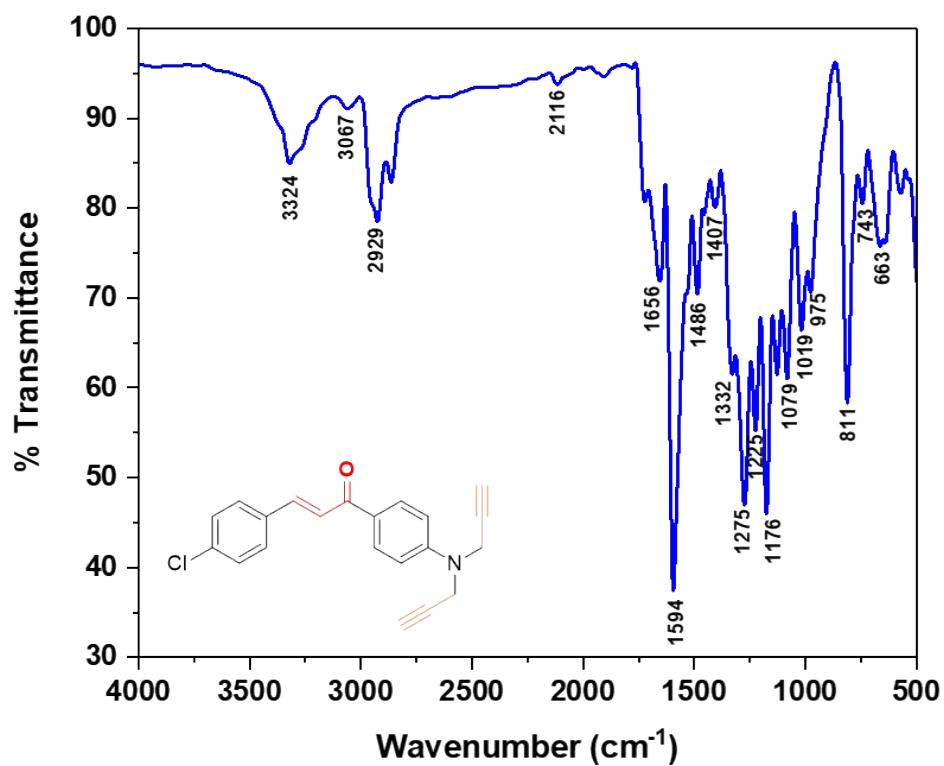


Figure S5: IR spectrum of alkyne 4b



FigureS6: IR spectrum of alkyne 4c

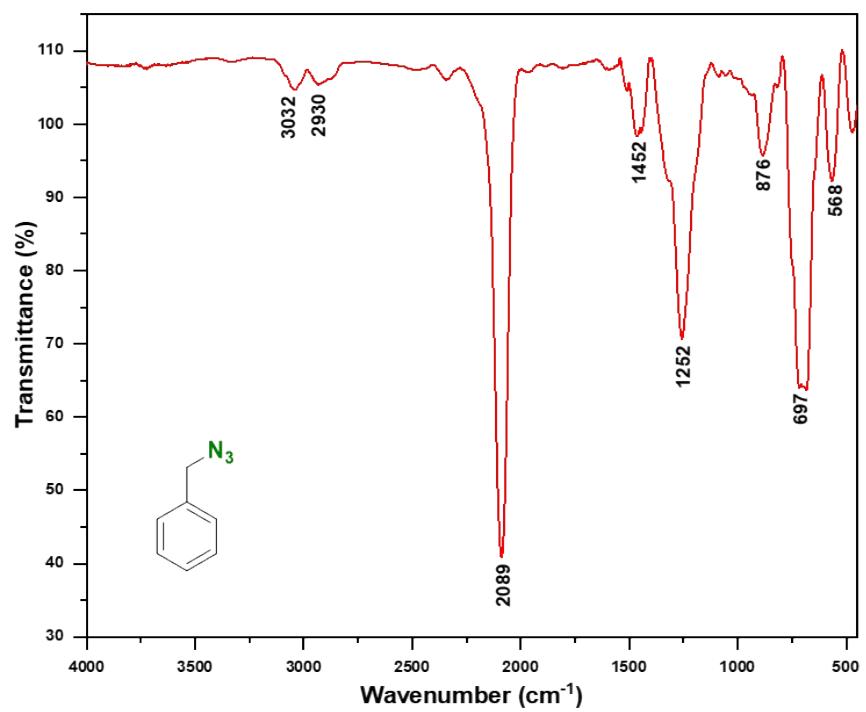


Figure S7: IR spectrum of benzyl azide 5

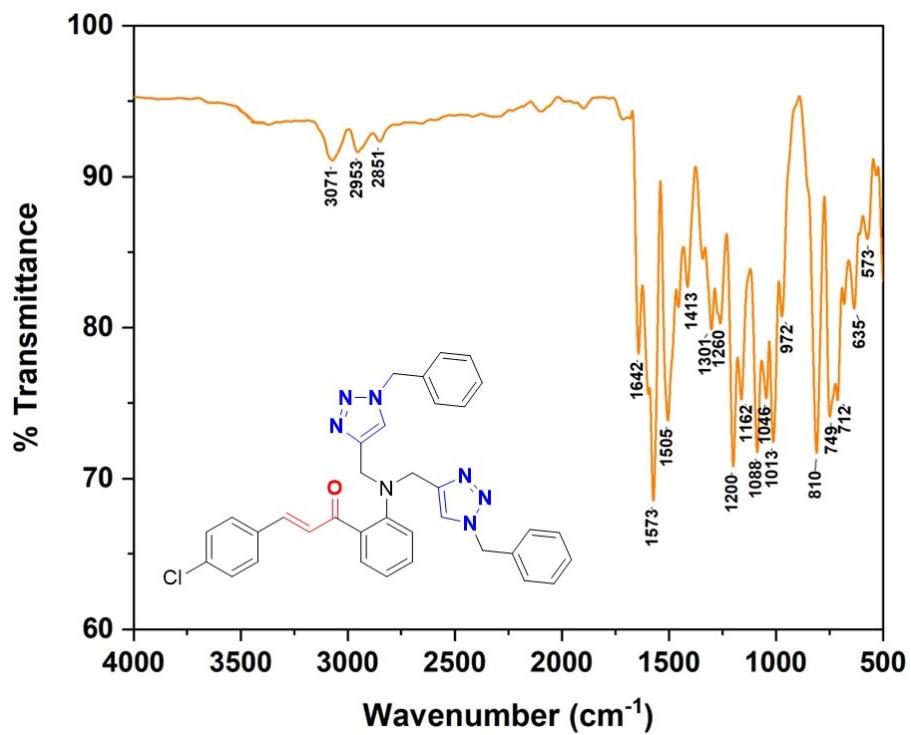


Figure S8: IR spectrum of probe 6a

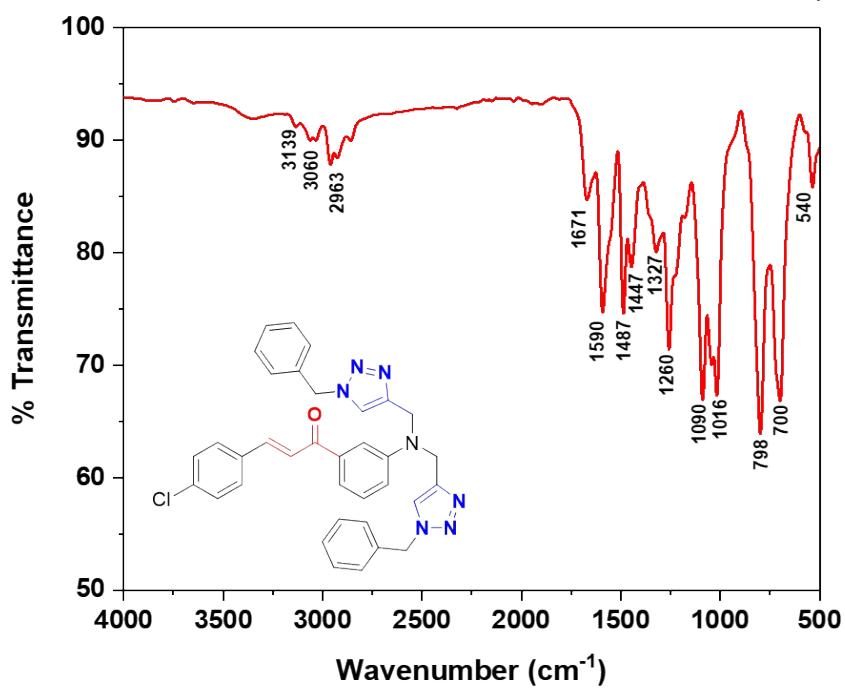


Figure S9: IR spectrum of probe 6b

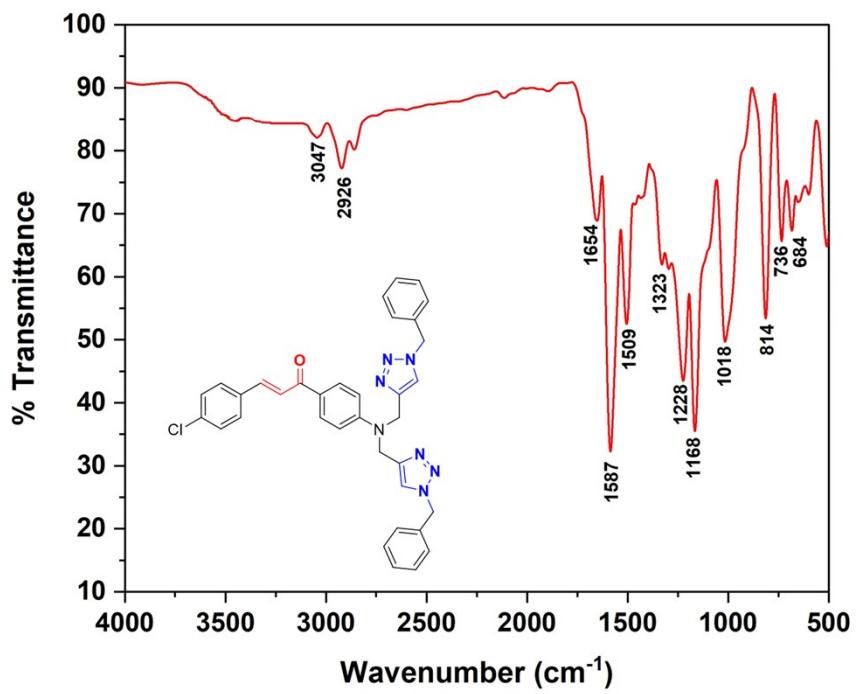


Figure S10: IR spectrum of probe 6c

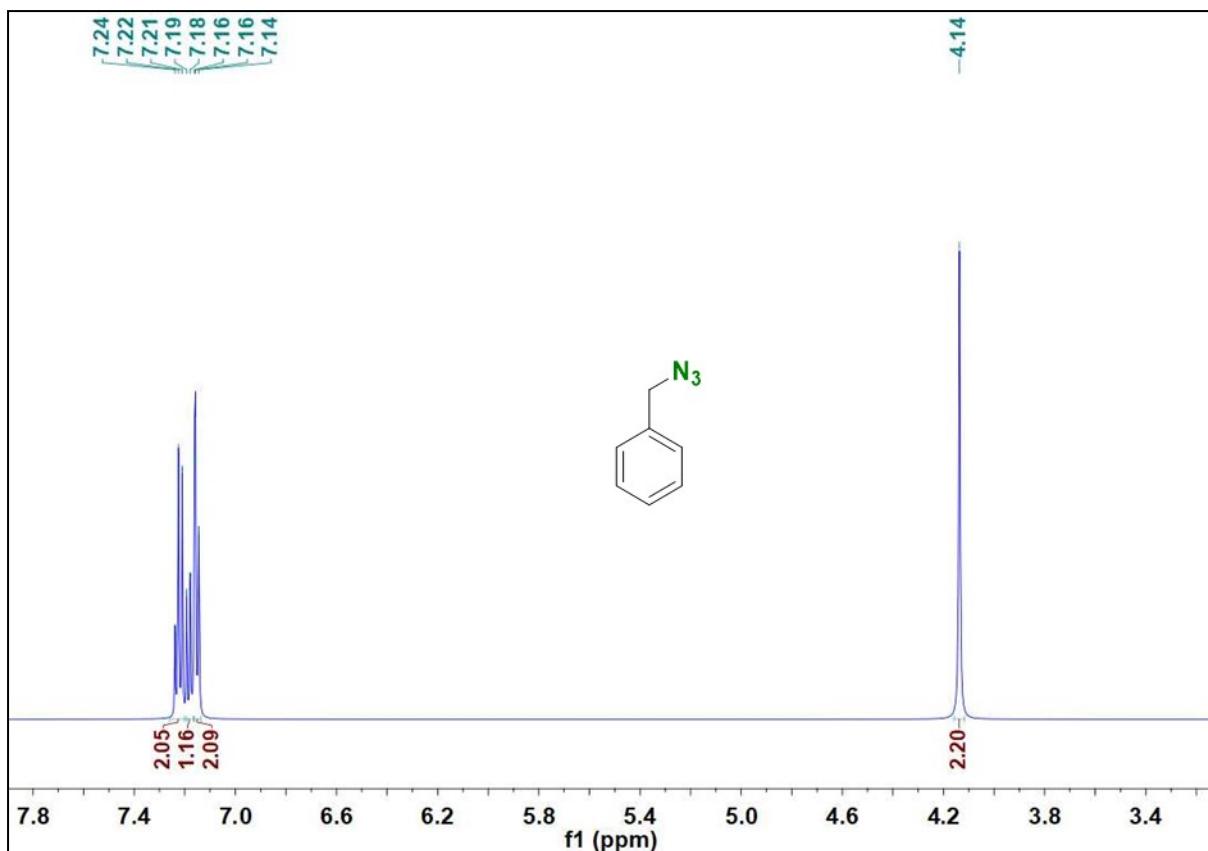


Figure S17: ¹H NMR spectrum of benzyl azide 5

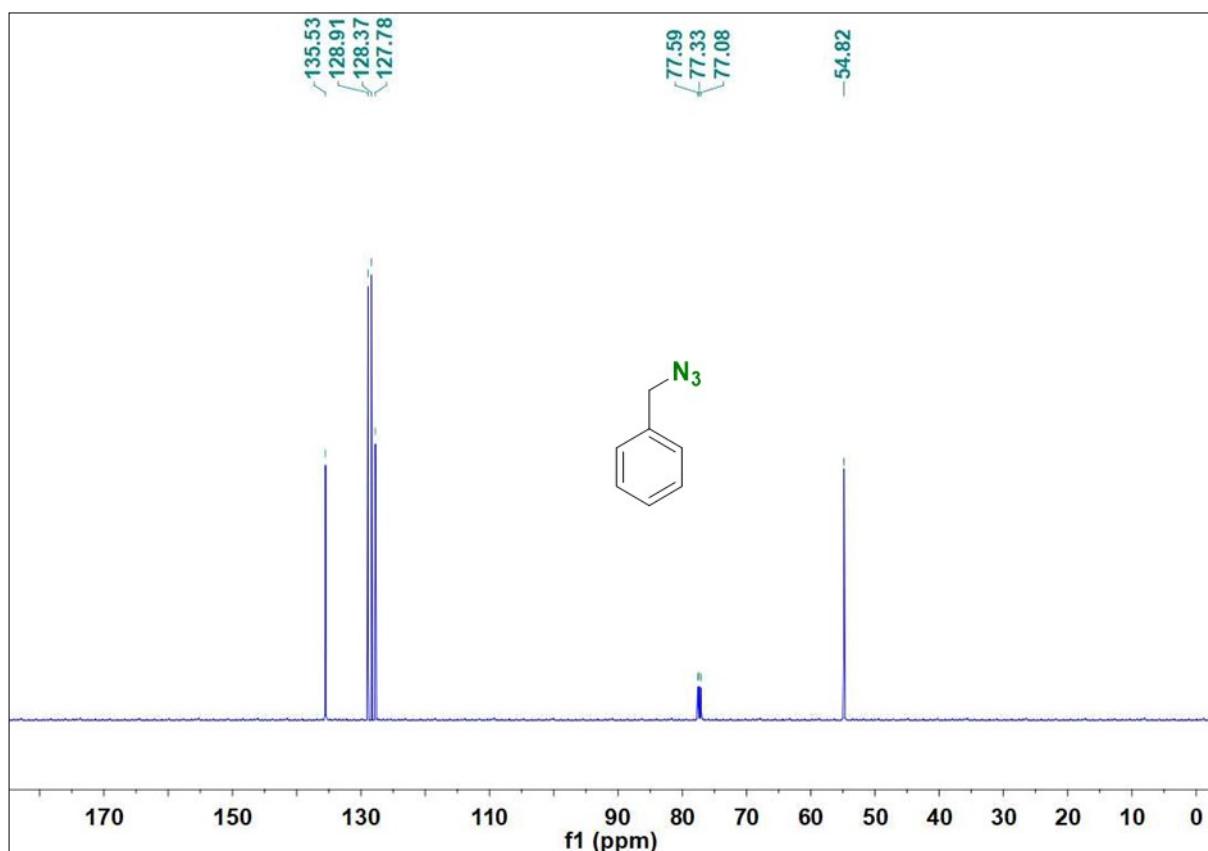


Figure S18: ¹³C NMR spectrum of benzyl azide 5

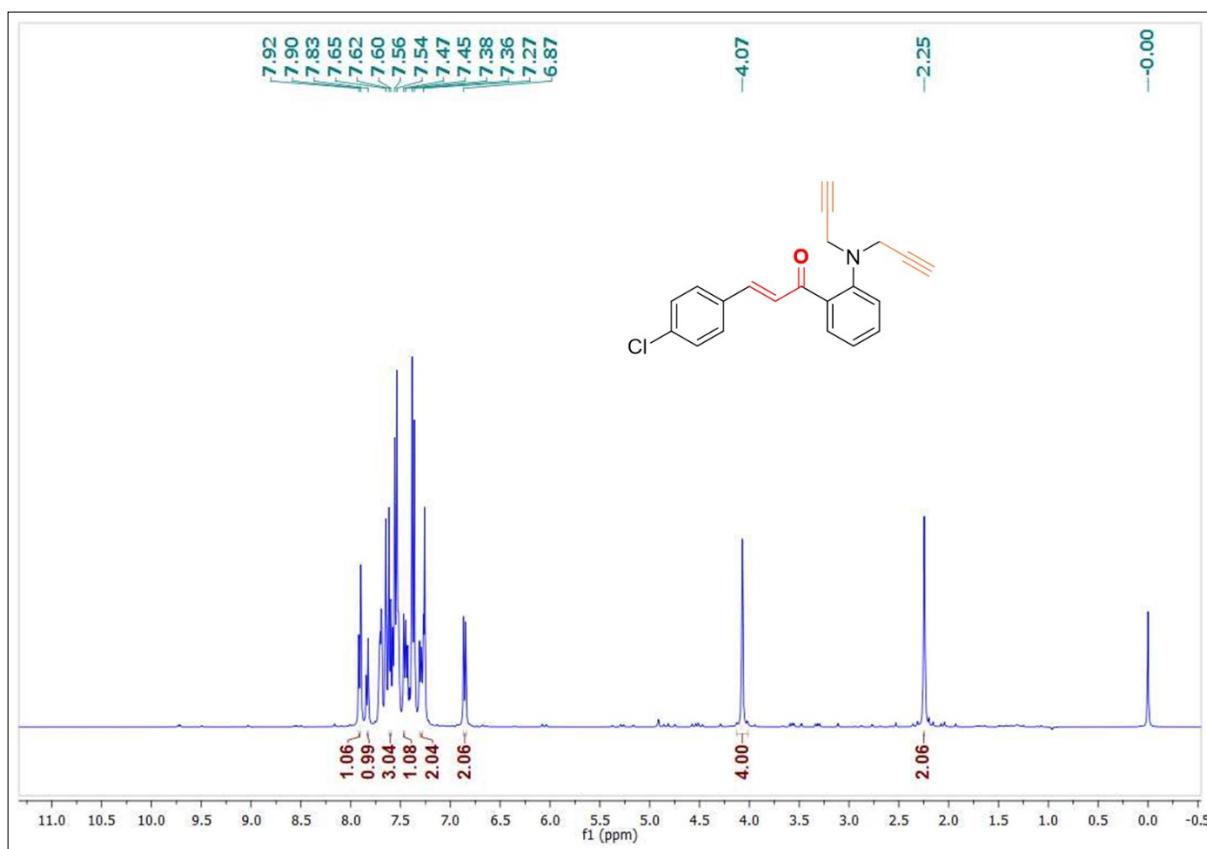


Figure S11: ¹H NMR spectrum of alkyne 4a

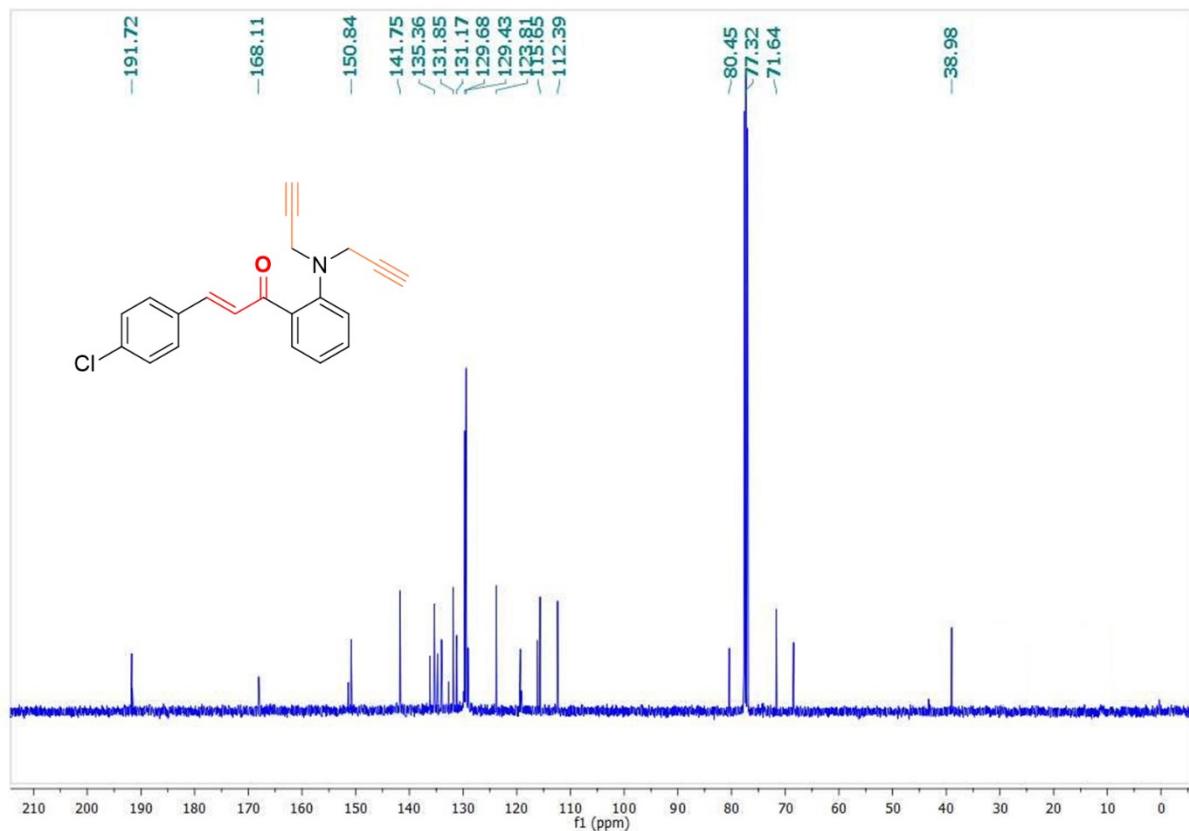


Figure S12: ¹³C NMR spectrum of alkyne 4a

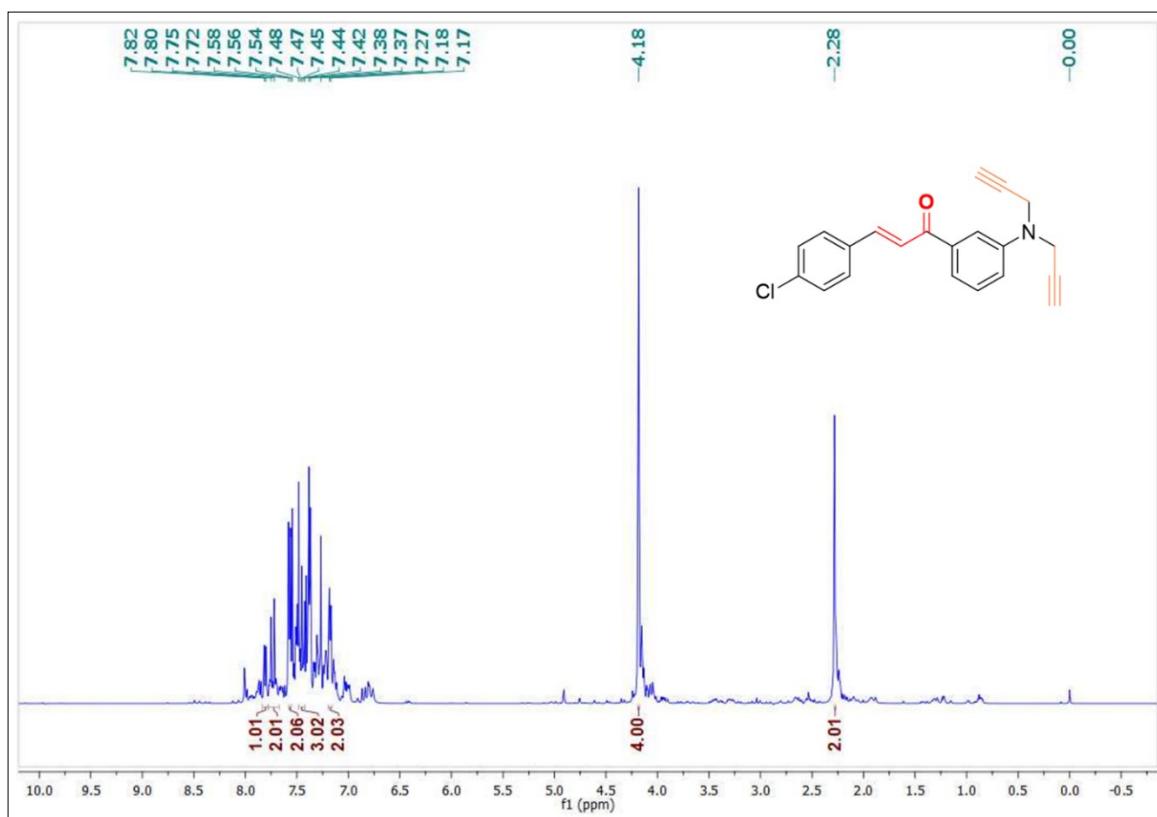


Figure S13: ¹H NMR spectrum of alkyne 4b

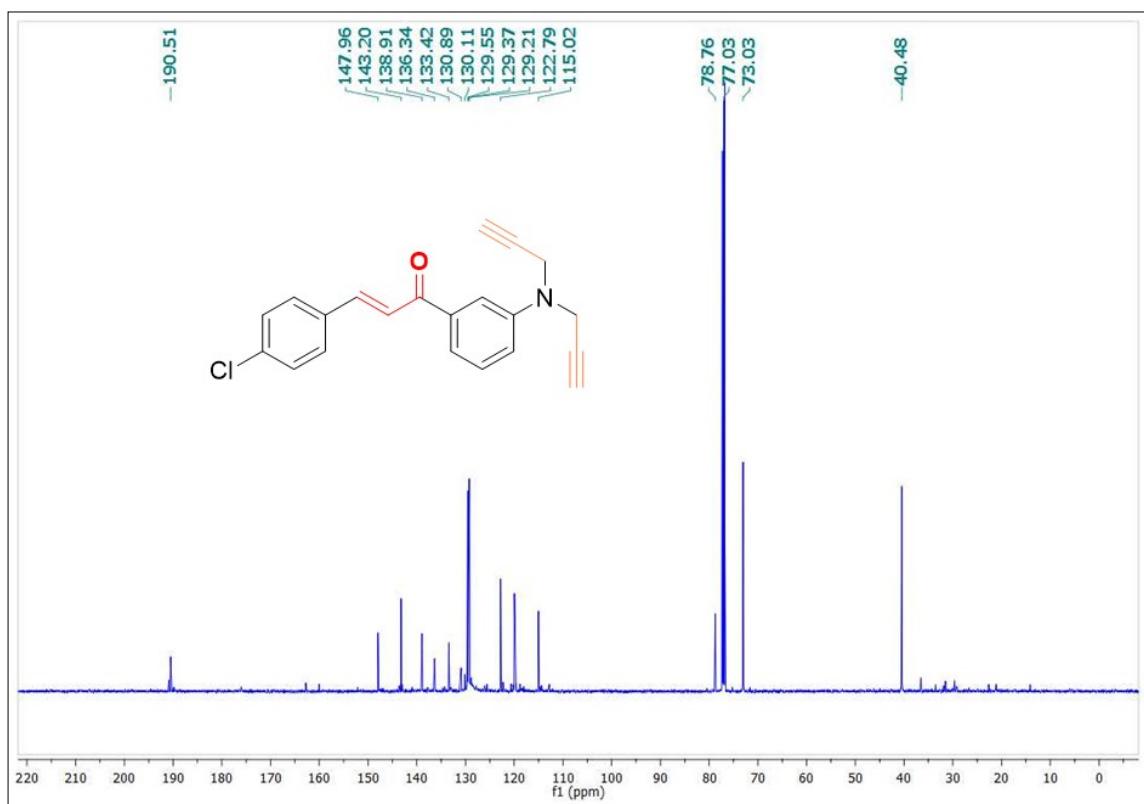


Figure S14: ¹³C NMR spectrum of alkyne 4b

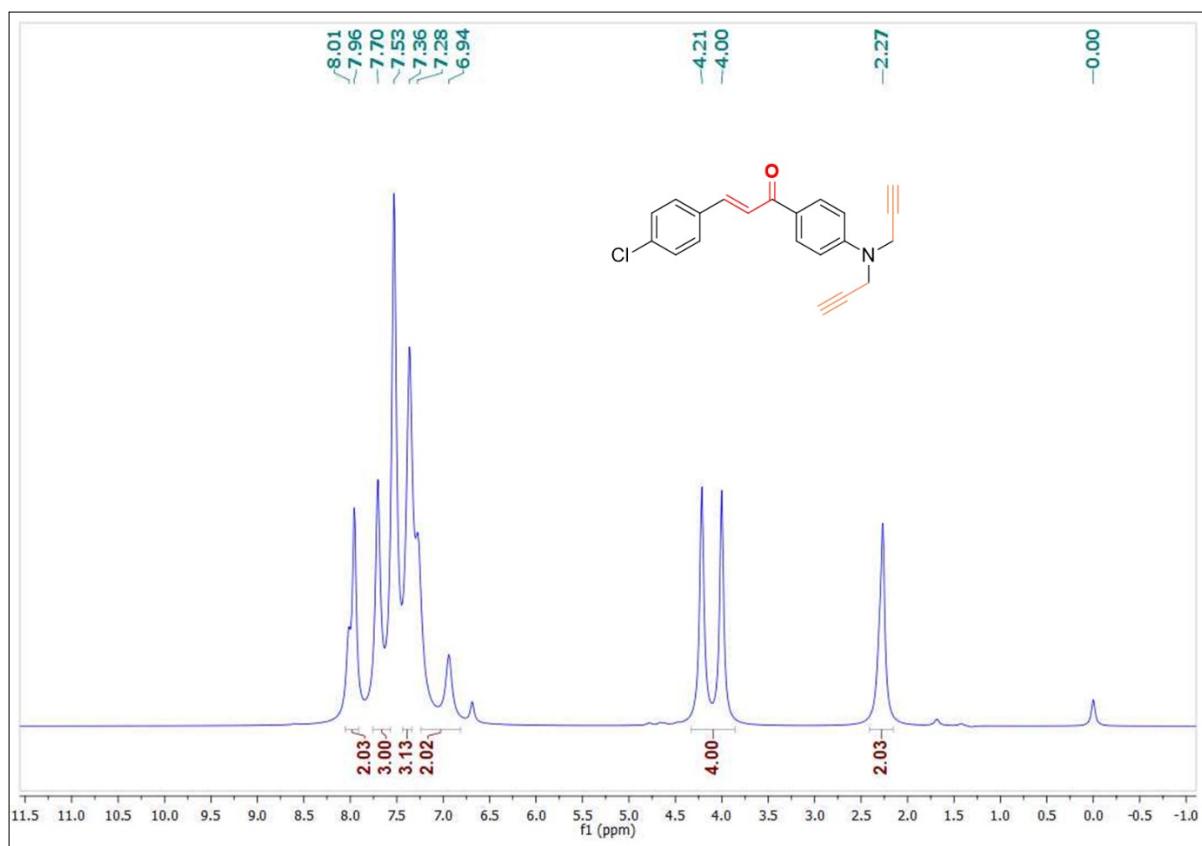


Figure S15: ¹H NMR spectrum of alkyne 4c

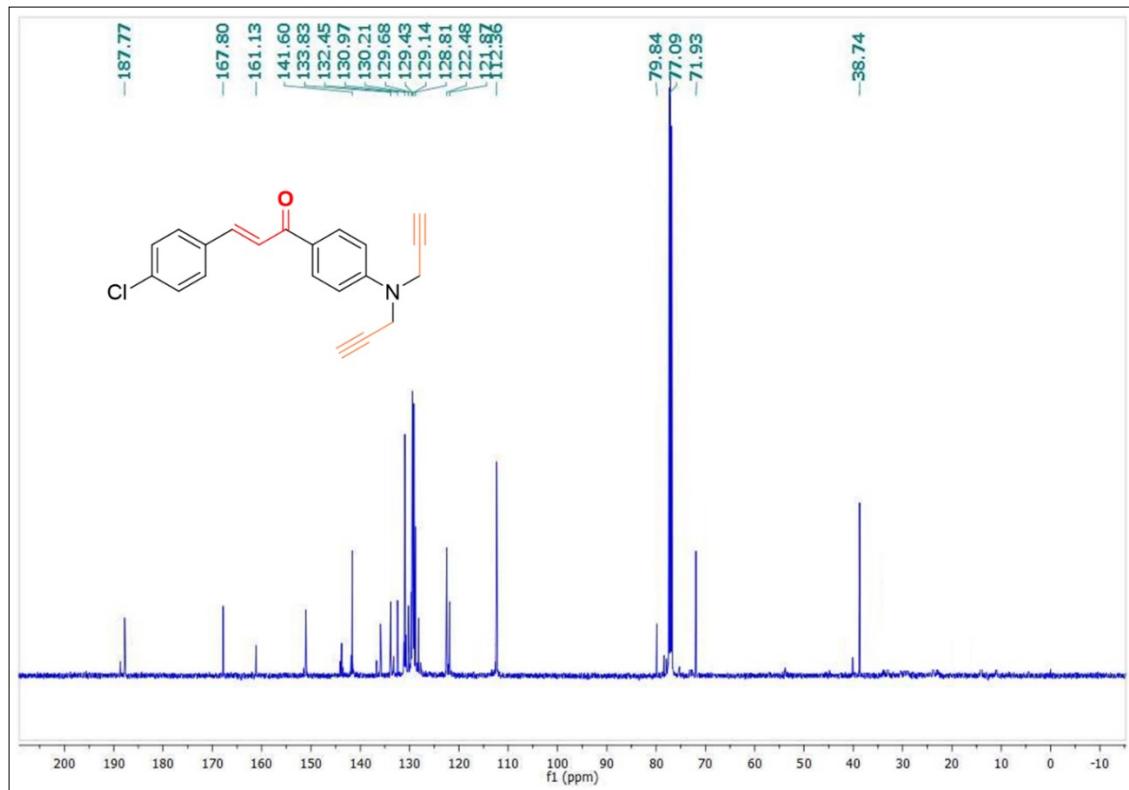


Figure S16: ¹³C NMR spectrum of alkyne 4c

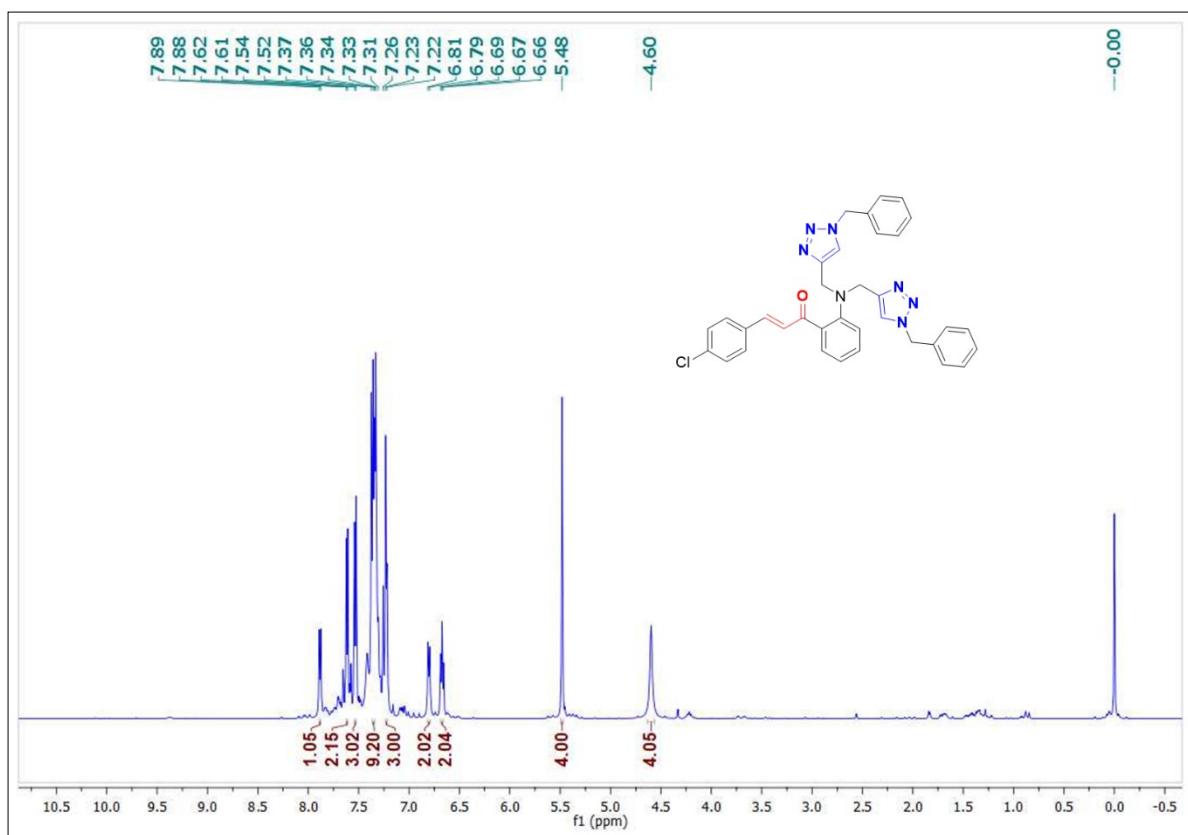


Figure S19: ¹H NMR spectrum of probe 6a

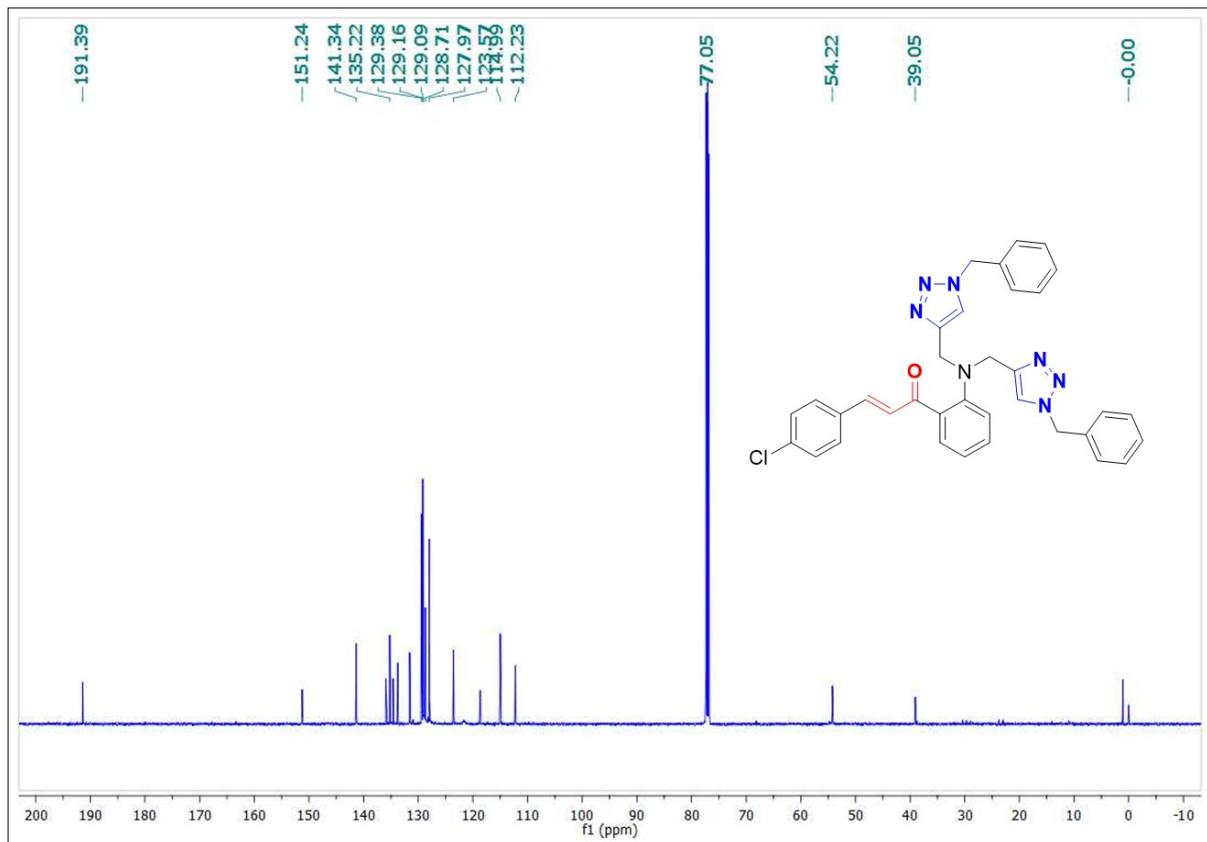


Figure S20: ¹³C NMR spectrum of probe 6a

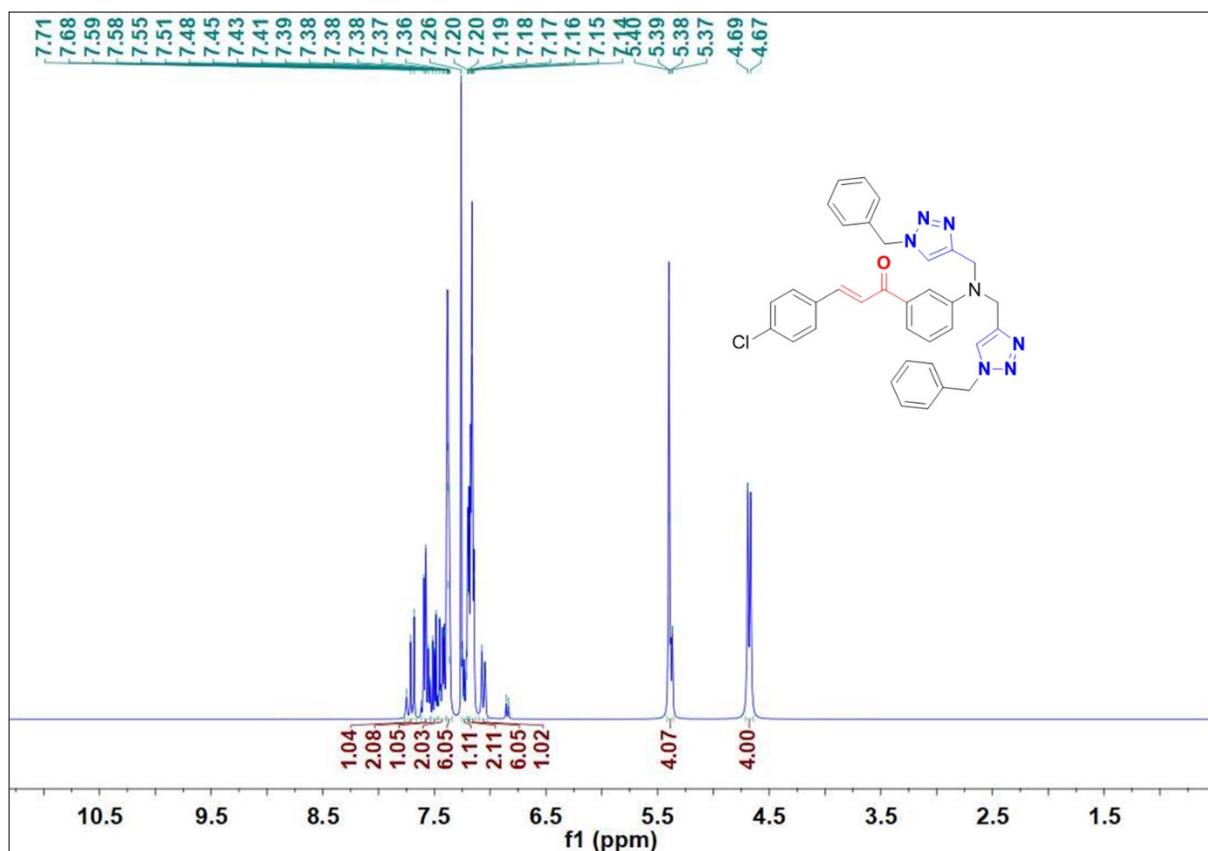


Figure S21: ¹H NMR spectrum of probe 6b

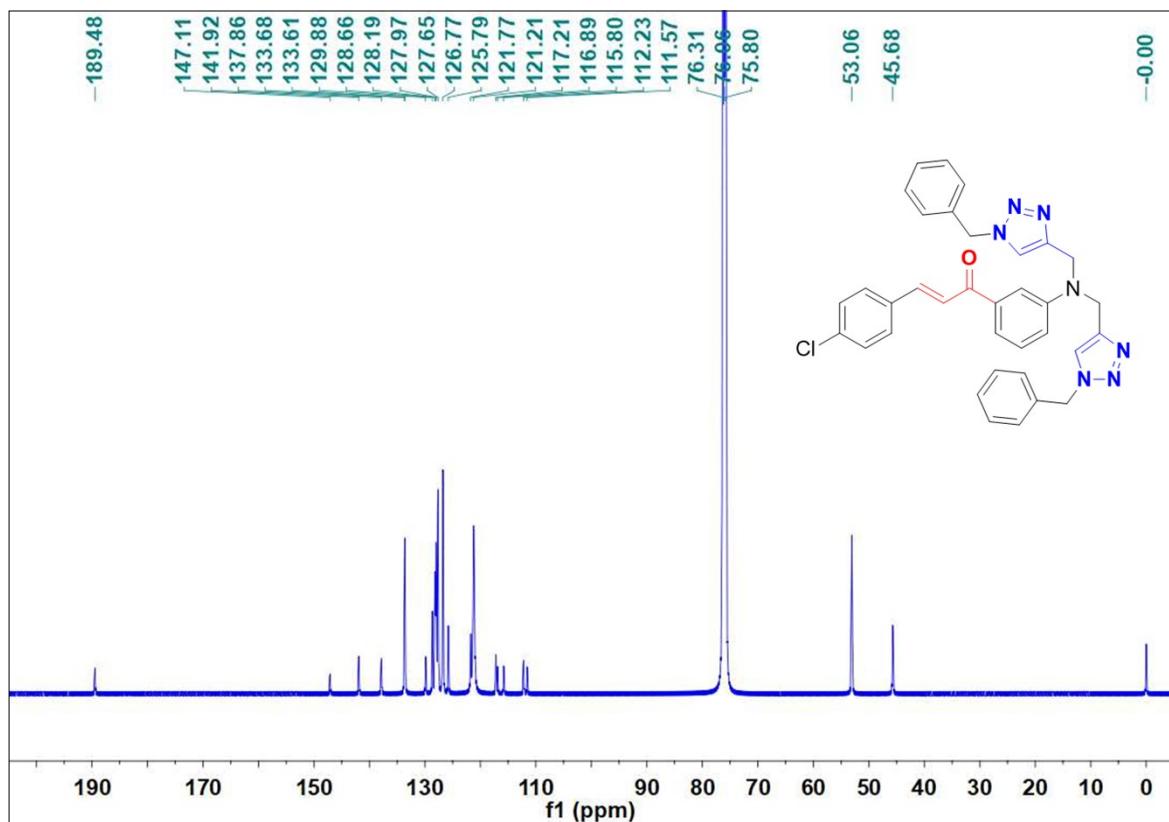


Figure S22: ¹³C NMR spectrum of probe 6b

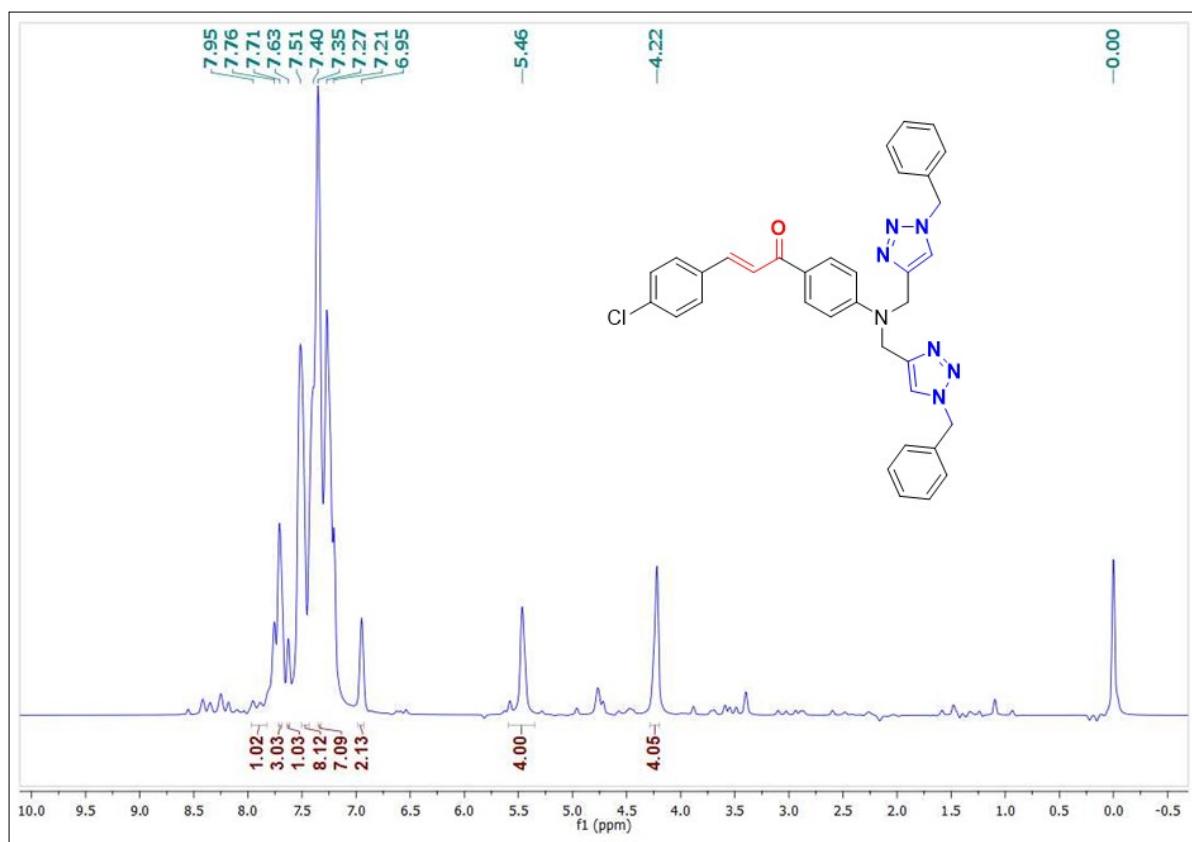


Figure S23: ¹H NMR spectrum of probe 6c

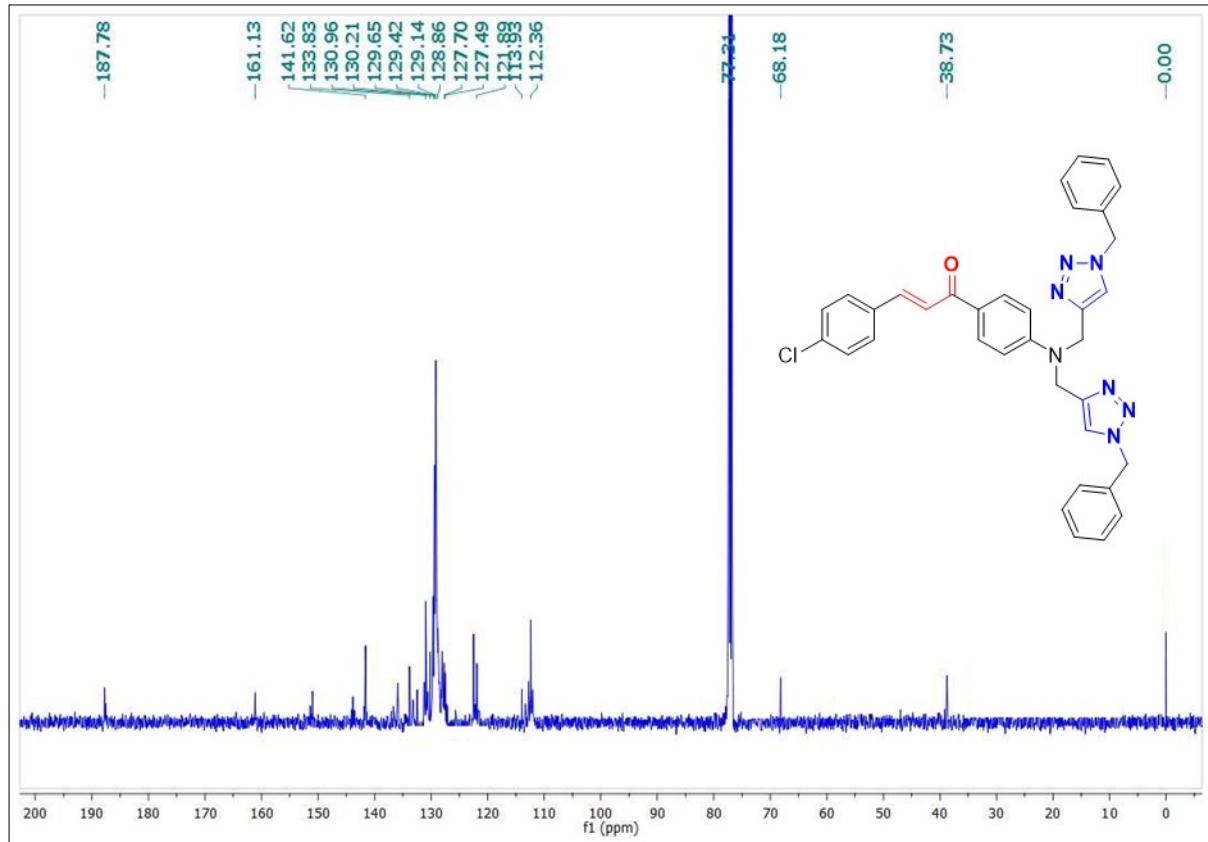


Figure S24: ¹³C NMR spectrum of probe 6b

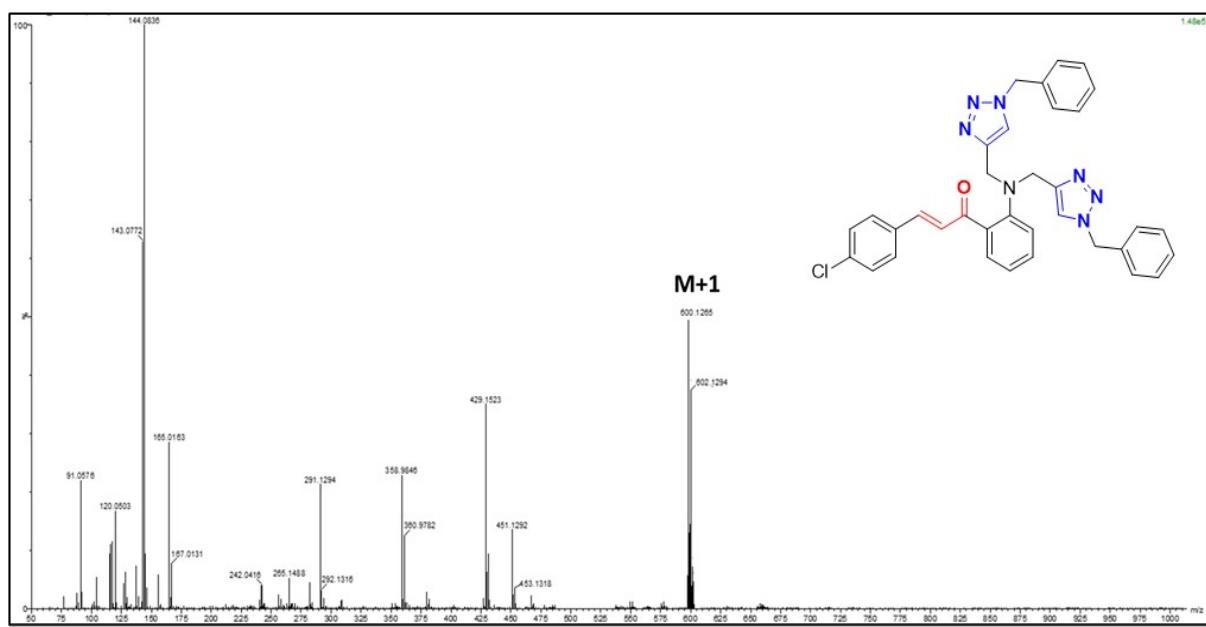


Figure S25: Mass spectrum of probe 6a

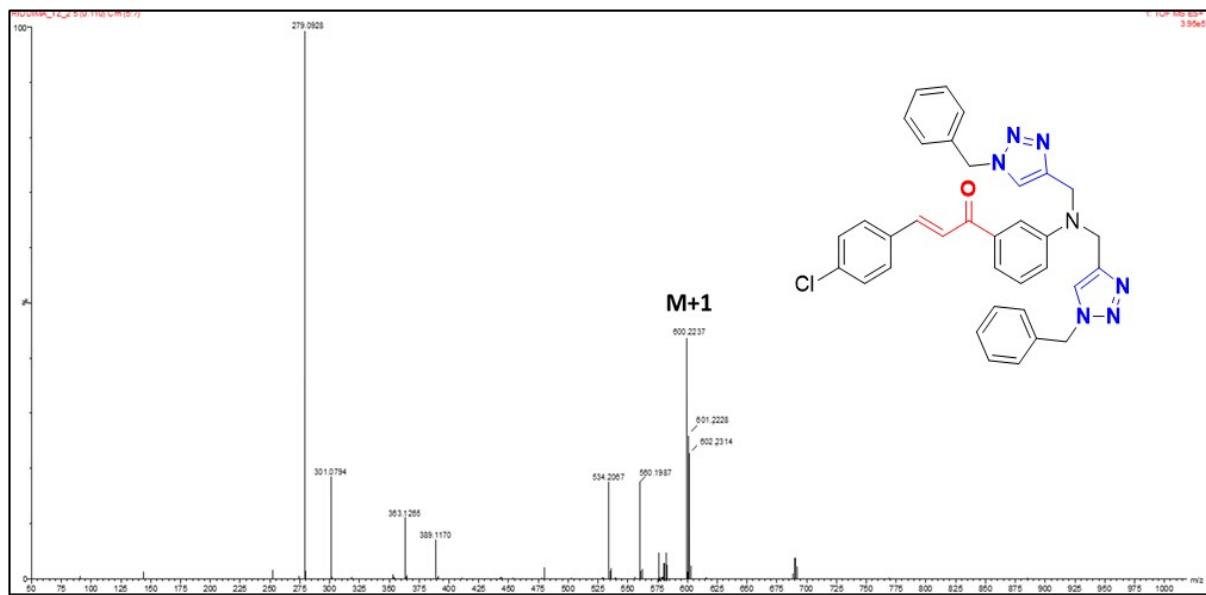


Figure S26: Mass spectrum of probe 6b

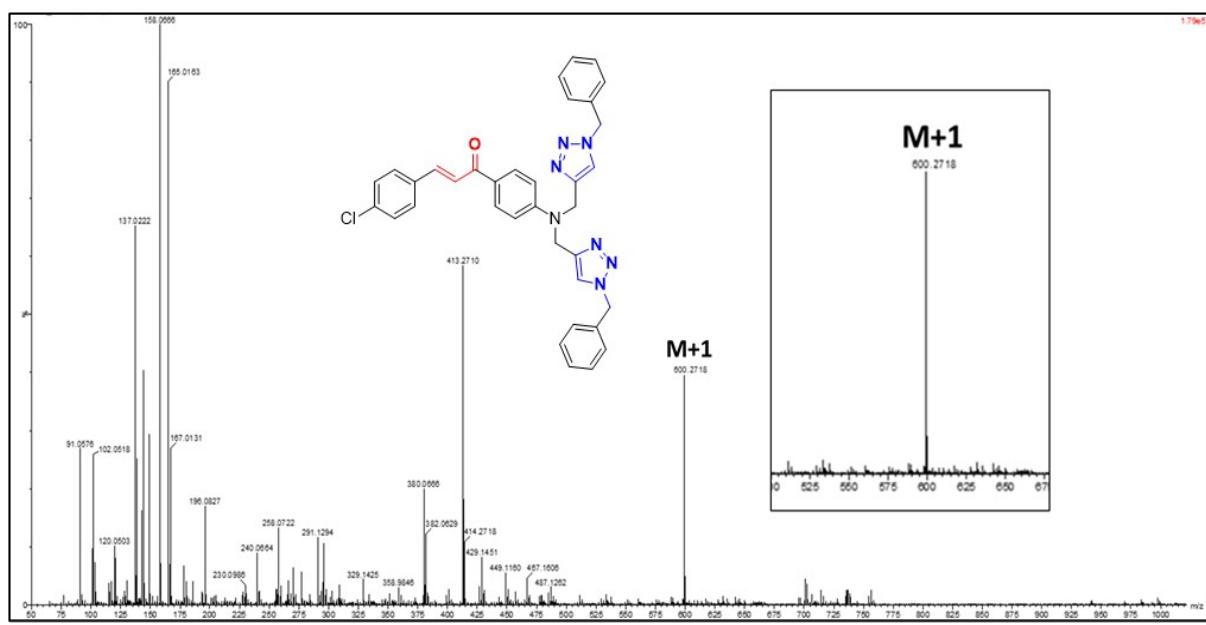


Figure S27: Mass spectrum of probe 6c

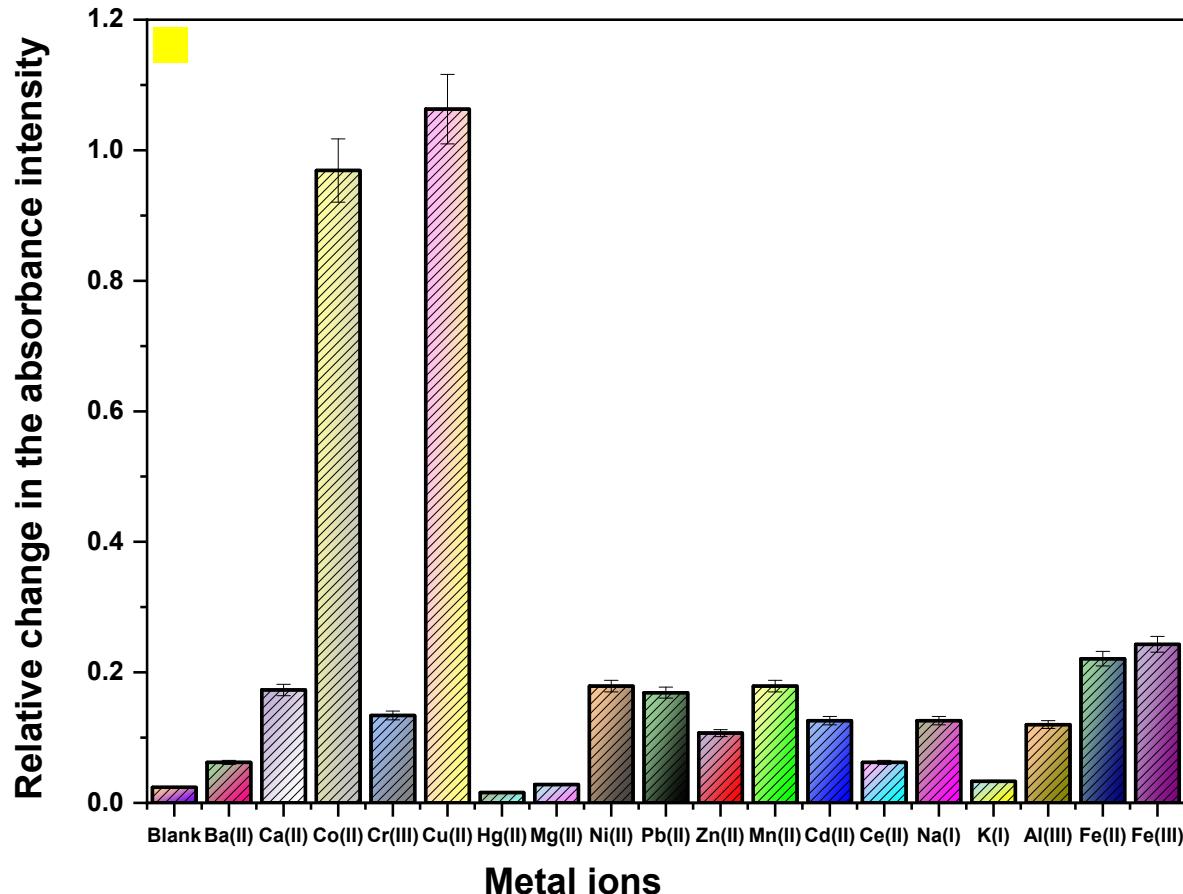


Figure S28: Graphical representation of relative absorption changes of probe 6a on addition of 15 equivalents of various metal ions.

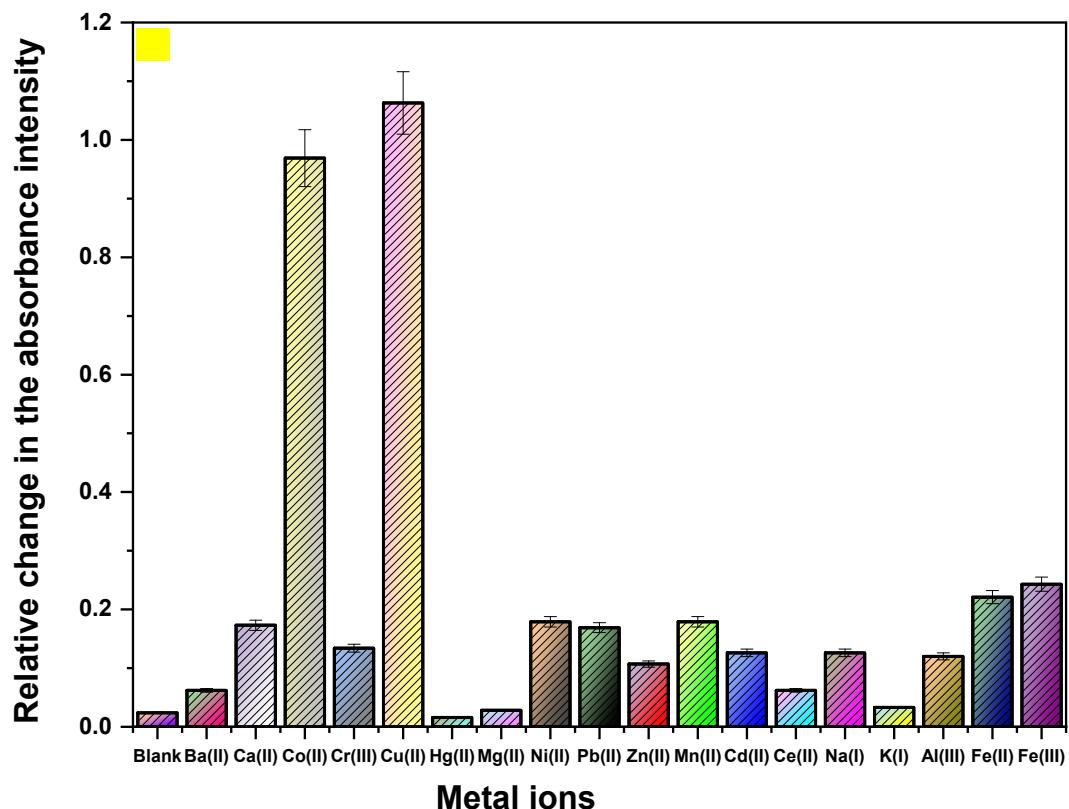


Figure S29: Graphical representation of relative absorption changes of probe 6a on addition of 15 equivalents of various metal ions.

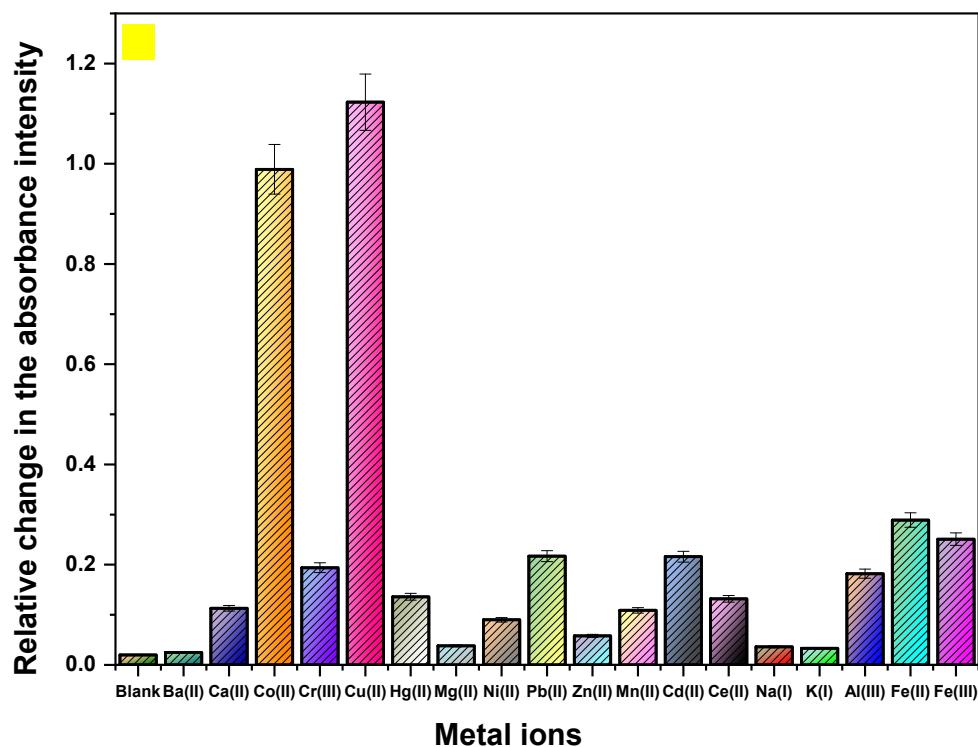


Figure S30: Graphical representation of relative absorption changes of probe 6a on addition of 15 equivalents of various metal ions.

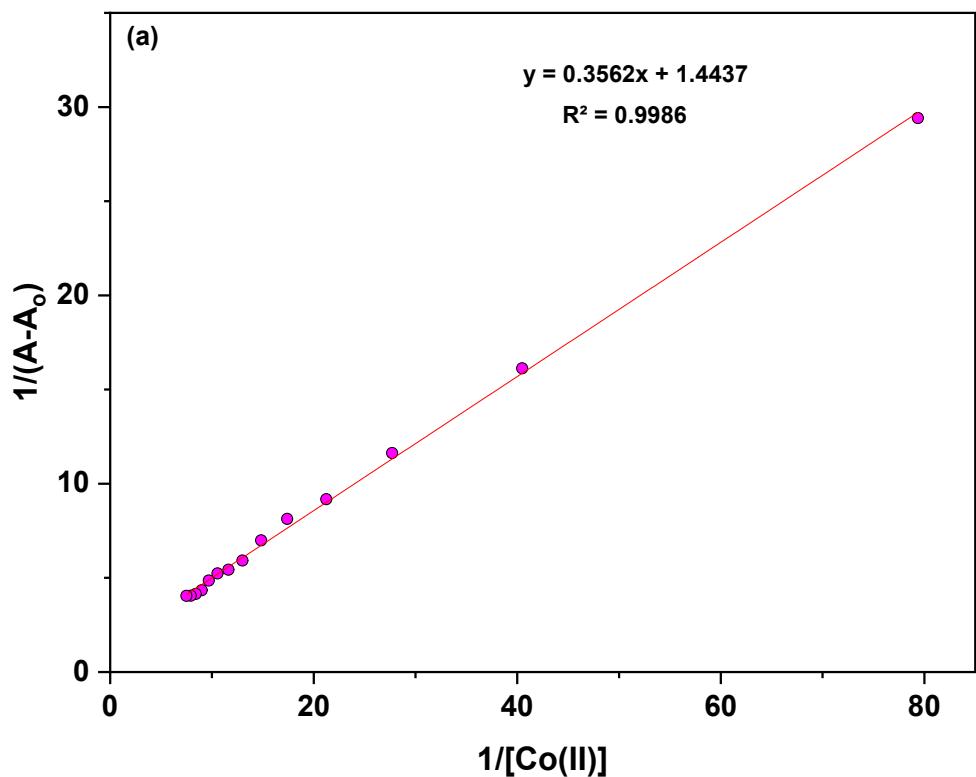


Figure S31: B-H plot for the metal complexation with probe 6a with Co(II)

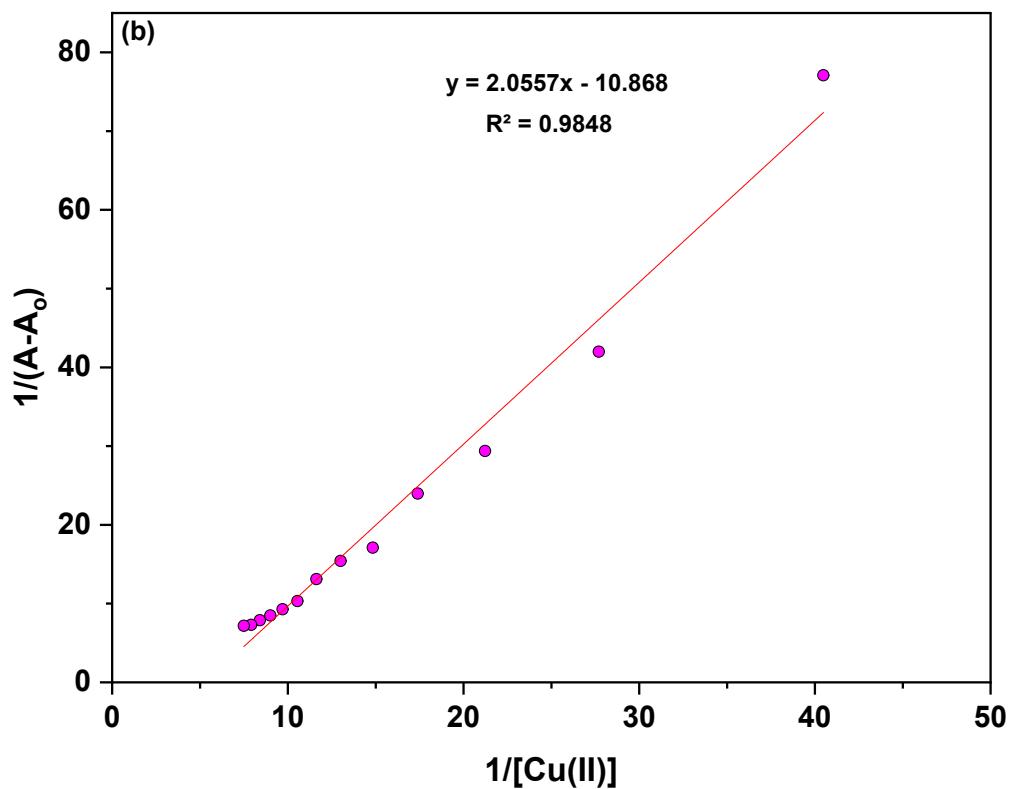


Figure S32: B-H plot for the metal complexation with probe 6a with Cu(II)

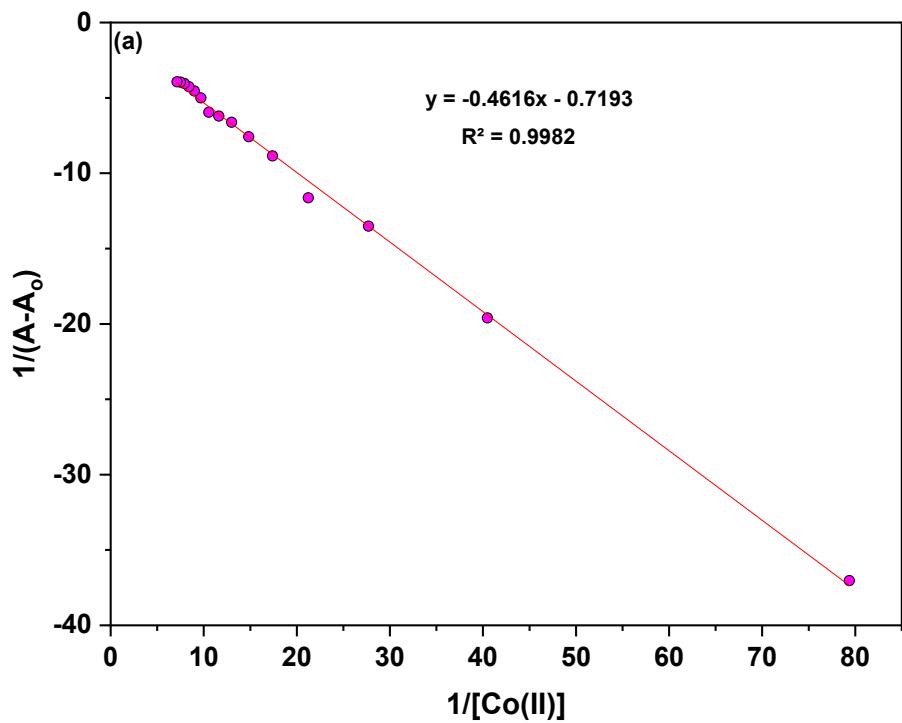


Figure S33: B-H plot for the metal complexation with probe 6b with Co(II)

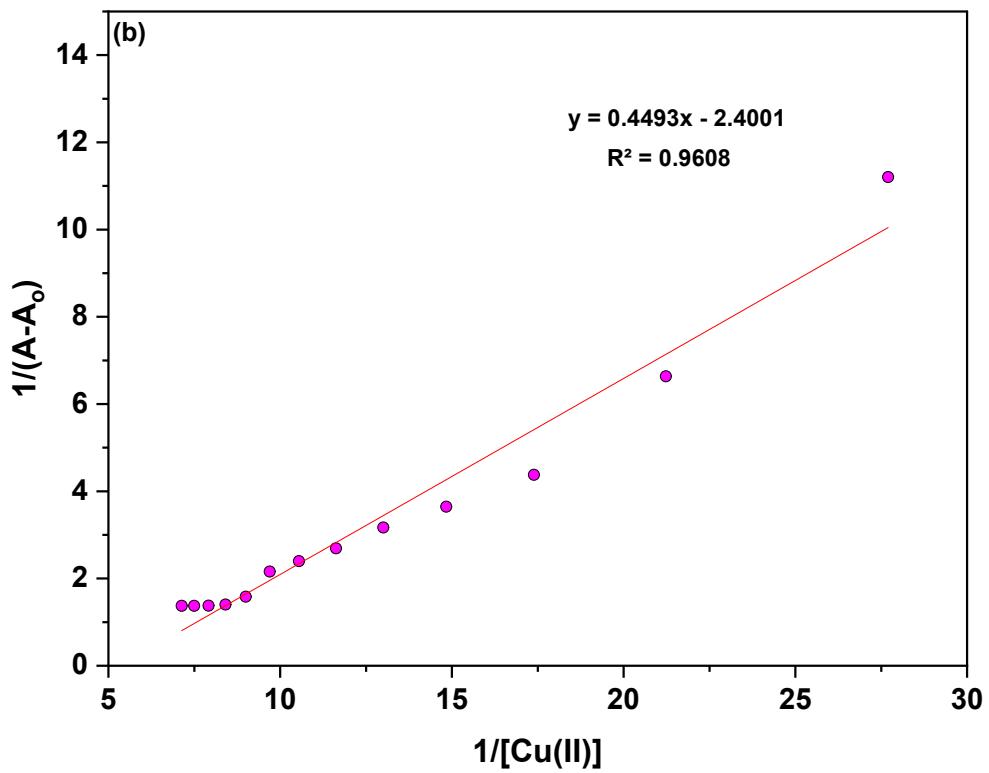


Figure S34: B-H plot for the metal complexation with probe 6b with Cu(II)

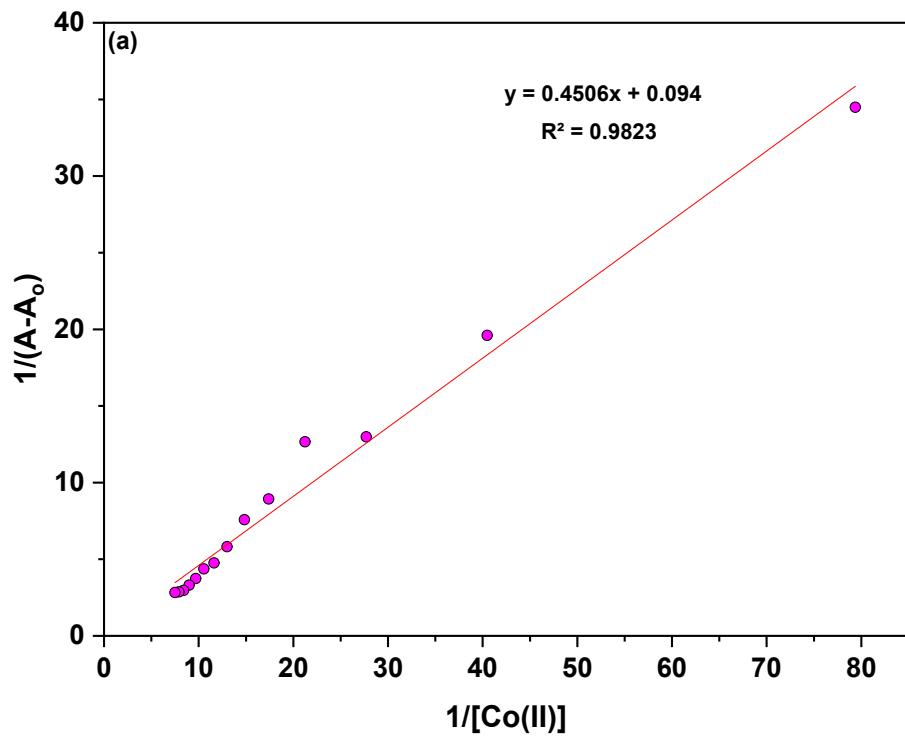


Figure S35: B-H plot for the metal complexation with probe 6c with Co(II)

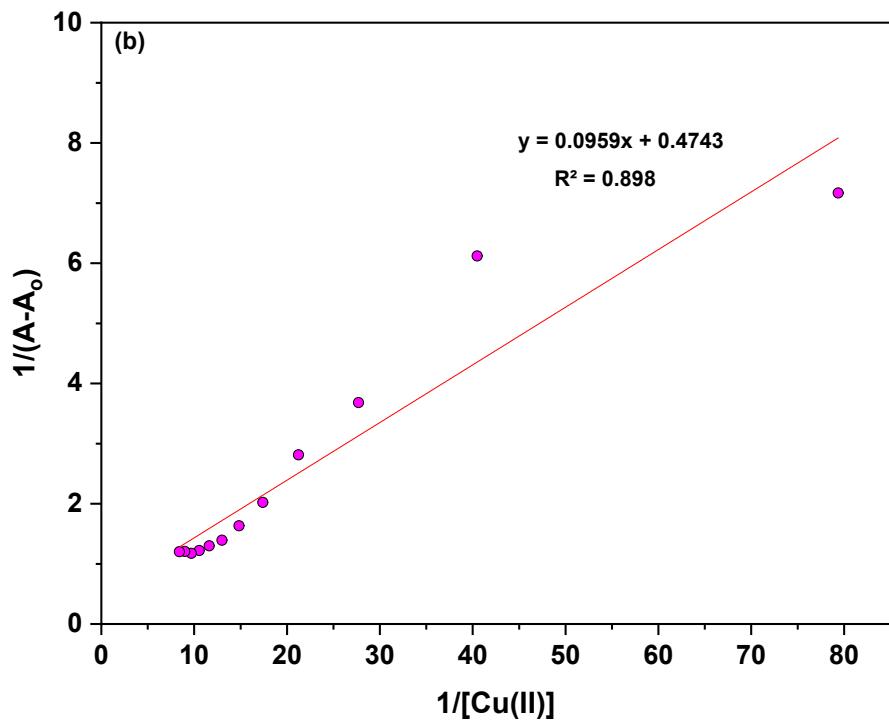


Figure S36: B-H plot for the metal complexation with probe 6c with Cu(II)

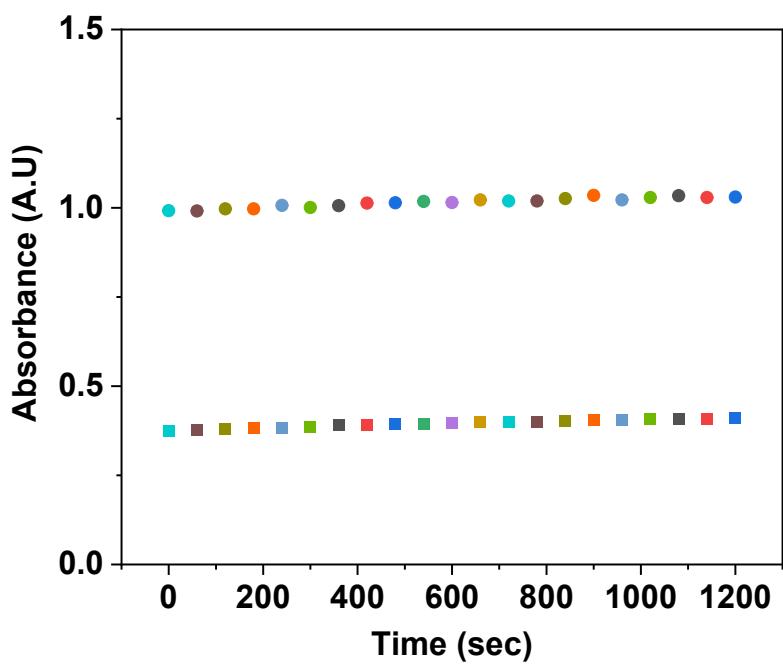


Figure S37: Time dependent spectra of probe 6a-Co(II) complex displaying the trend in the absorption.

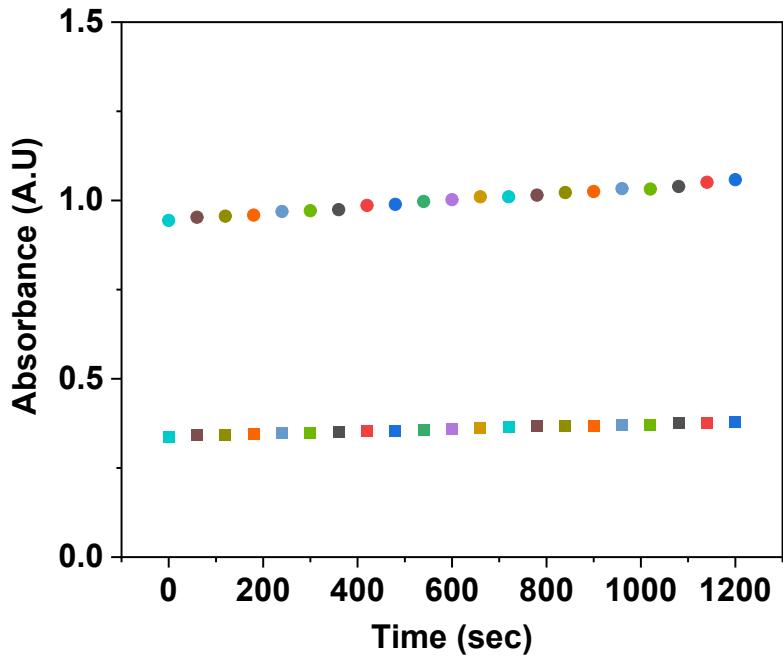


Figure S38: Time dependent spectra of probe 6a-Cu(II) complex displaying the trend in the absorption.

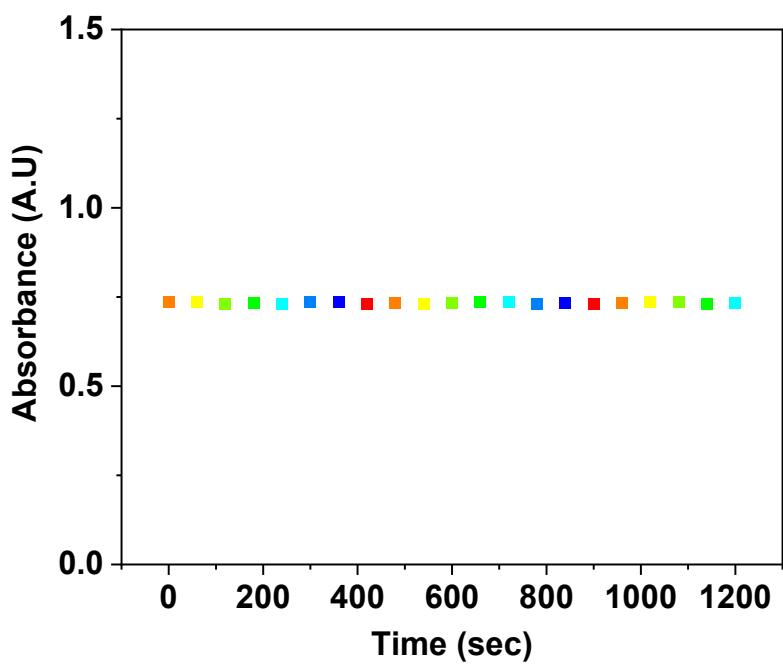


Figure S39: Time dependent spectra of probe 6b-Co(II) complex displaying the trend in the absorption.

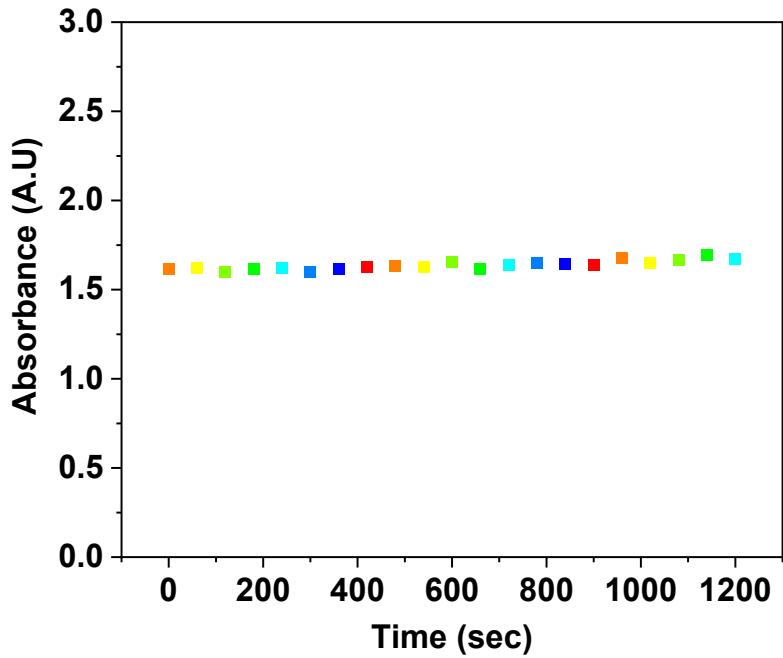


Figure S40: Time dependent spectra of probe 6b-Cu(II) complex displaying the trend in the absorption.

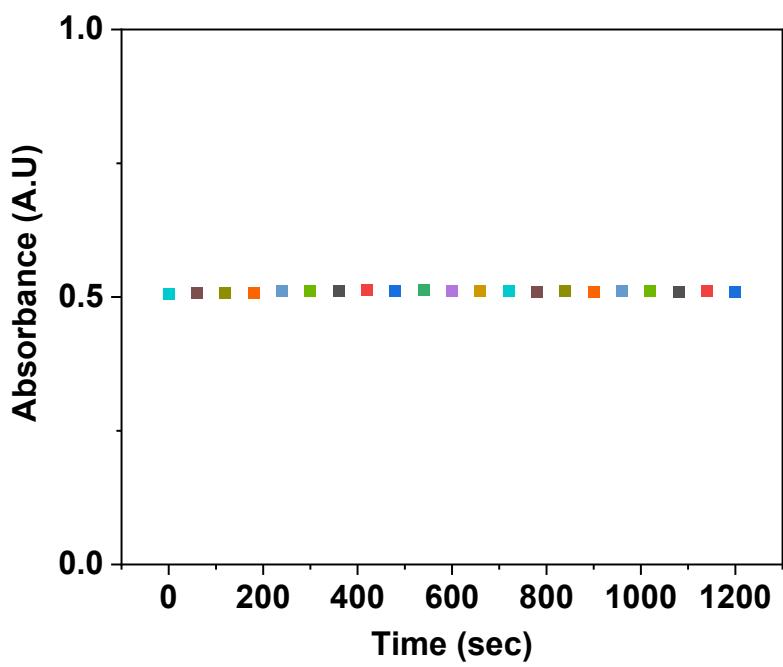


Figure S41: Time dependent spectra of probe 6c-Co(II) complex displaying the trend in the absorption.

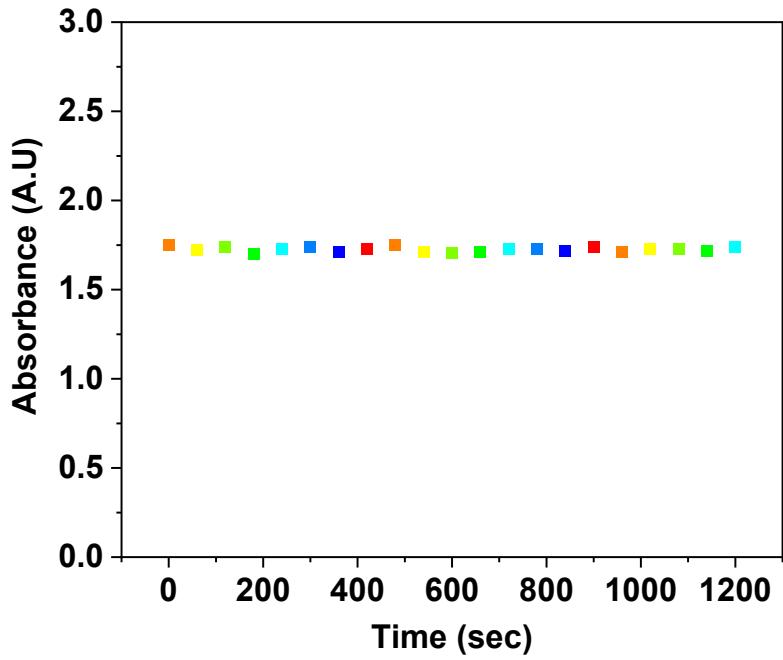


Figure S42: Time dependent spectra of probe 6c-Cu(II) complex displaying the trend in the absorption.

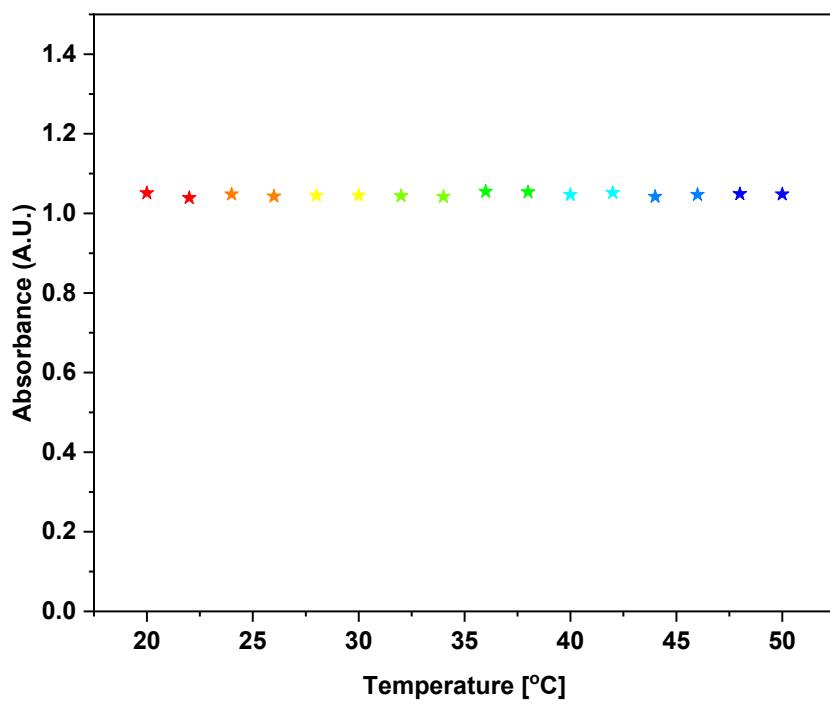


Figure S43: Temperature dependent spectra of probe 6a-Co(II) complex displaying the trend in the absorption.

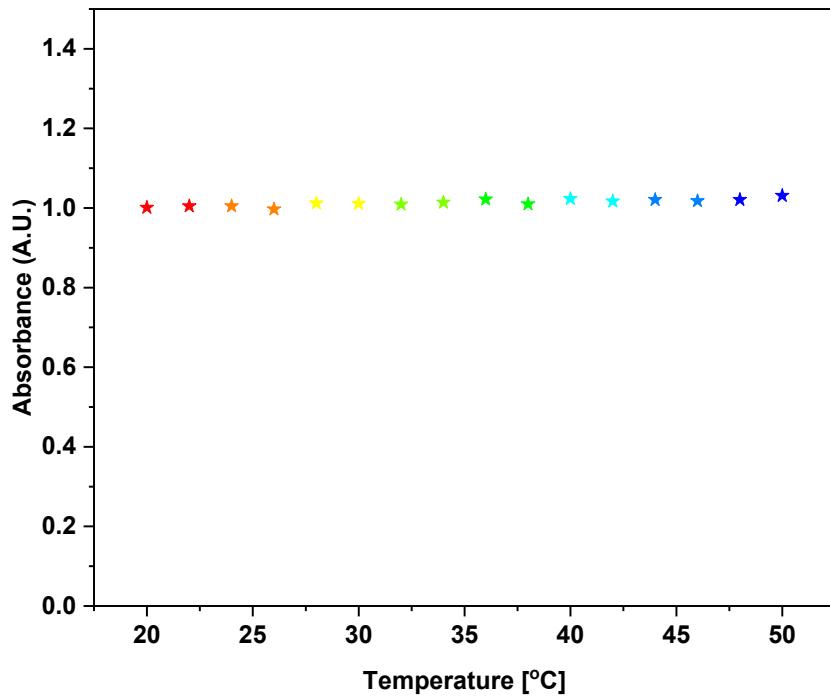


Figure S44: Temperature dependent spectra of probe 6a-Cu(II) complex displaying the trend in the absorption.

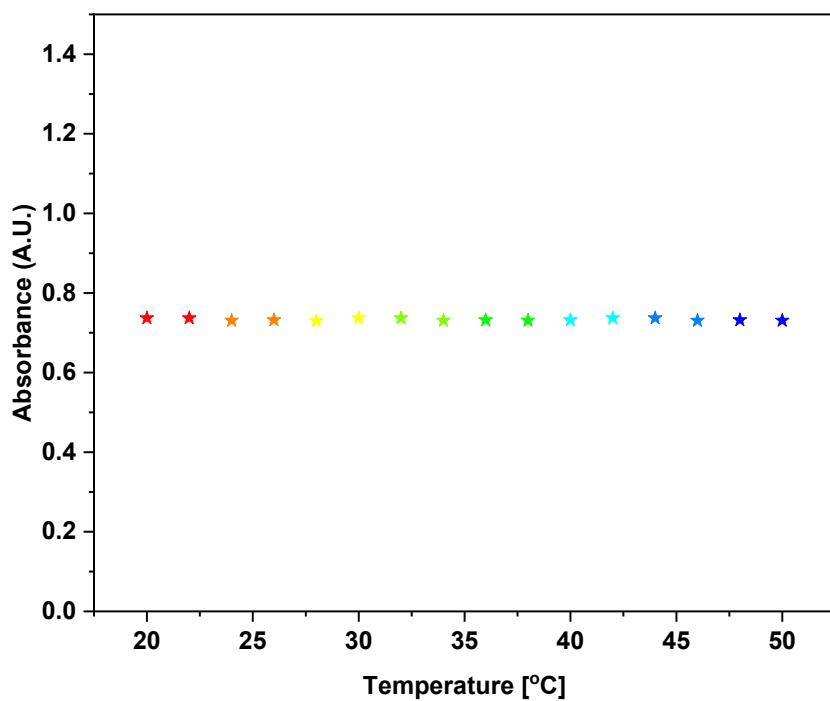


Figure S45: Temperature dependent spectra of probe 6b-Co(II) complex displaying the trend in the absorption.

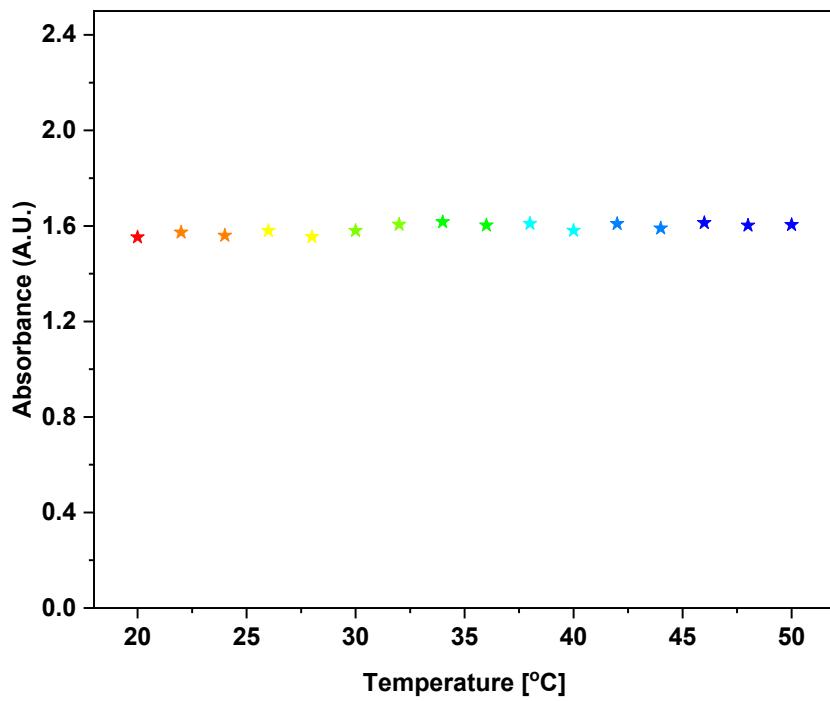


Figure S46: Temperature dependent spectra of probe 6b-Cu(II) complex displaying the trend in the absorption.

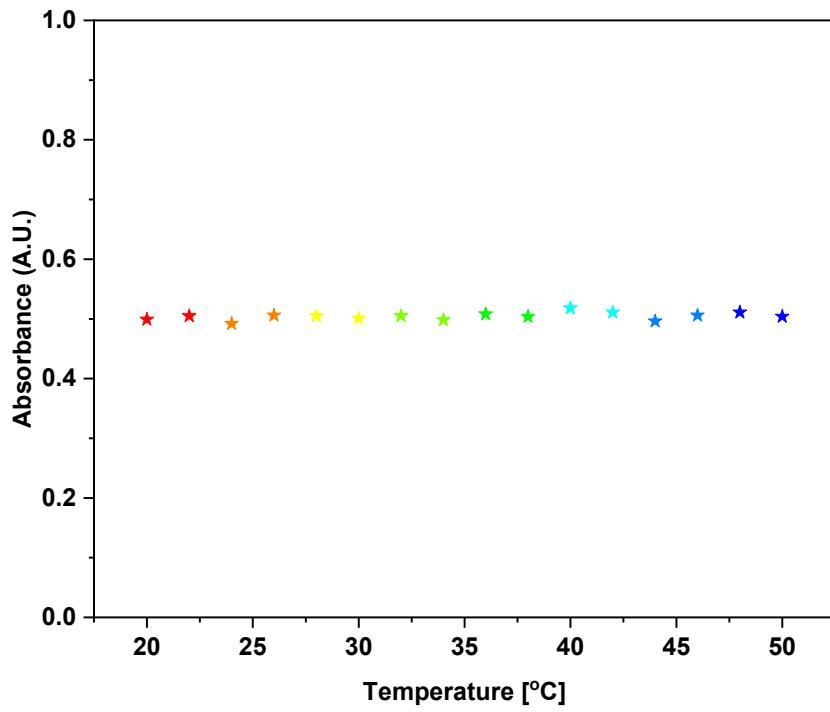


Figure S47: Temperature dependent spectra of probe 6c-Co(II) complex displaying the trend in the absorption.

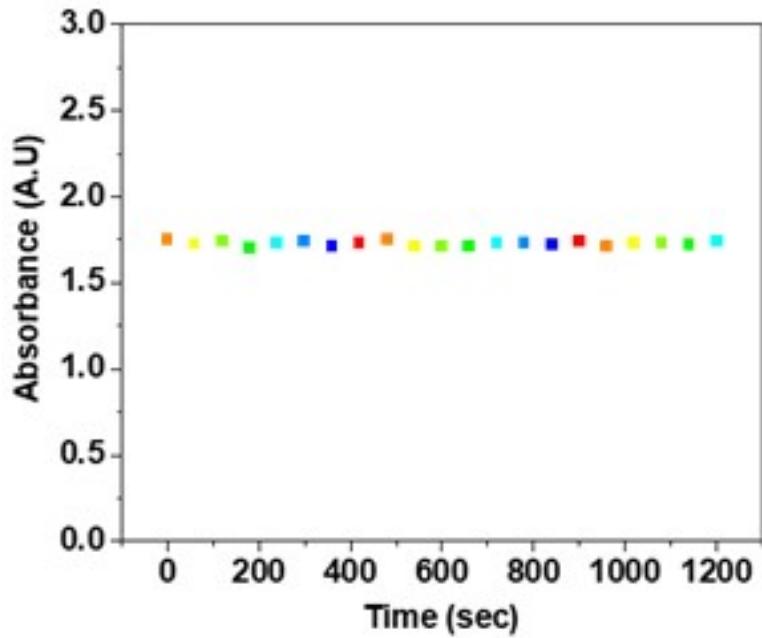


Figure S48: Temperature dependent spectra of probe 6c-Cu(II) complex displaying the trend in the absorption.

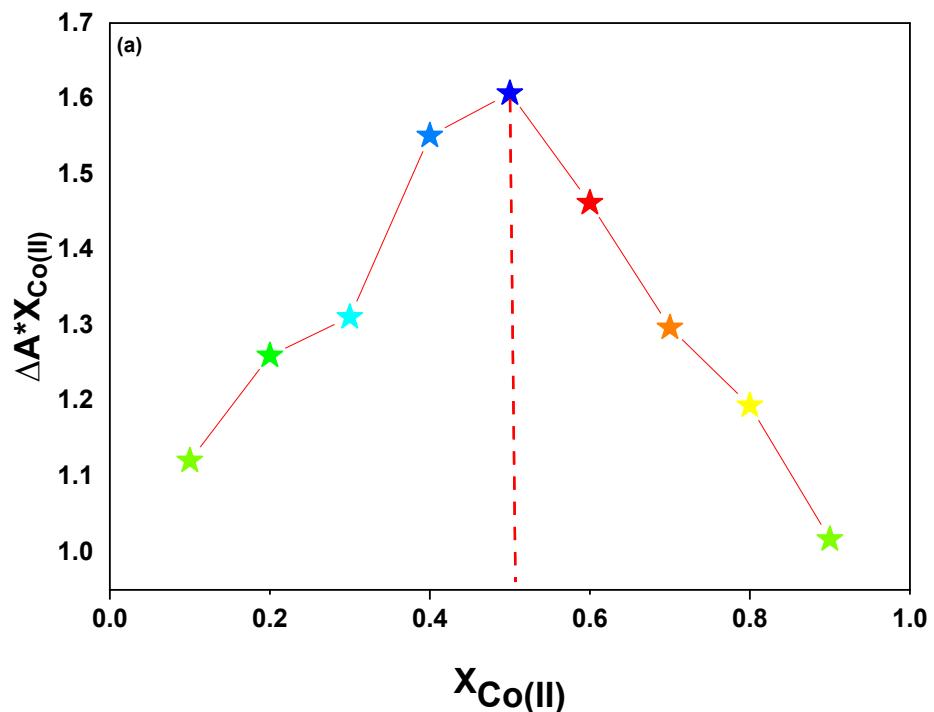


Figure S49: Job's plot analysis of probe 6a on interaction with Co(II) ions.

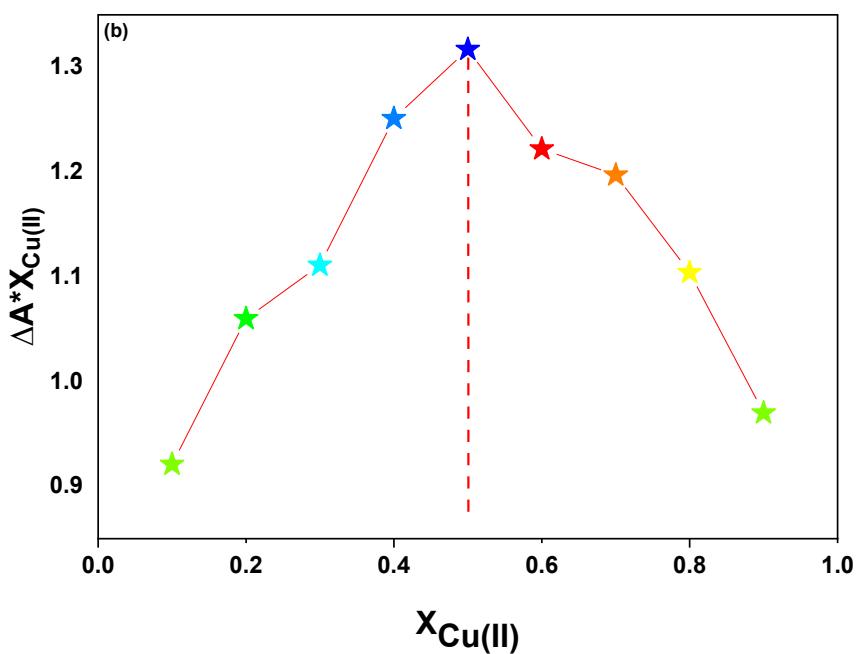


Figure S50: Job's plot analysis of probe 6a on interaction with Cu(II) ions.

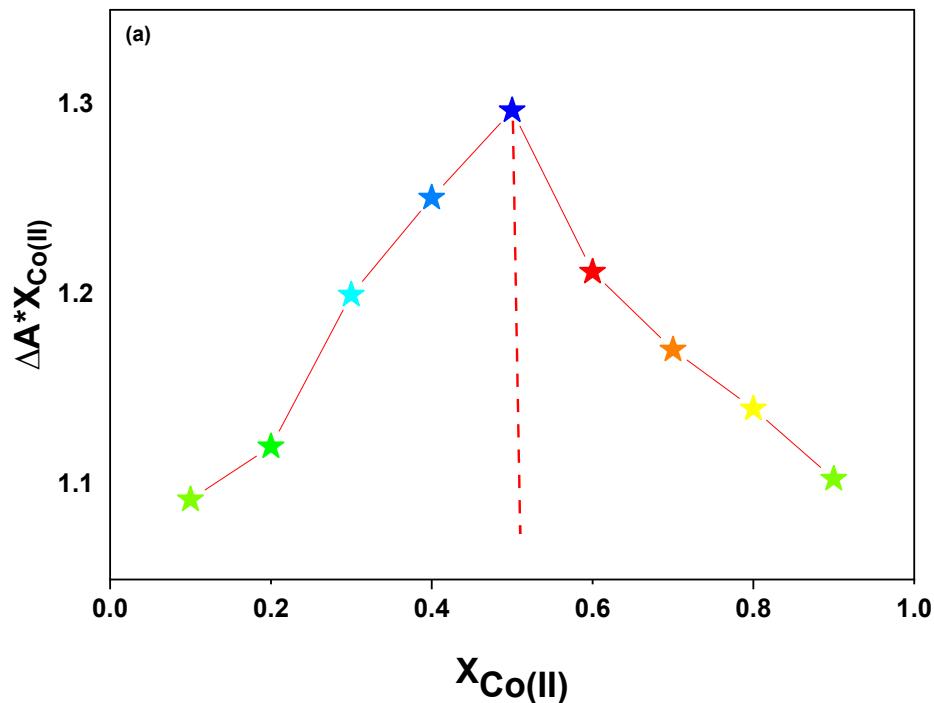


Figure S51: Job's plot analysis of probe 6b on interaction with Co(II) ions.

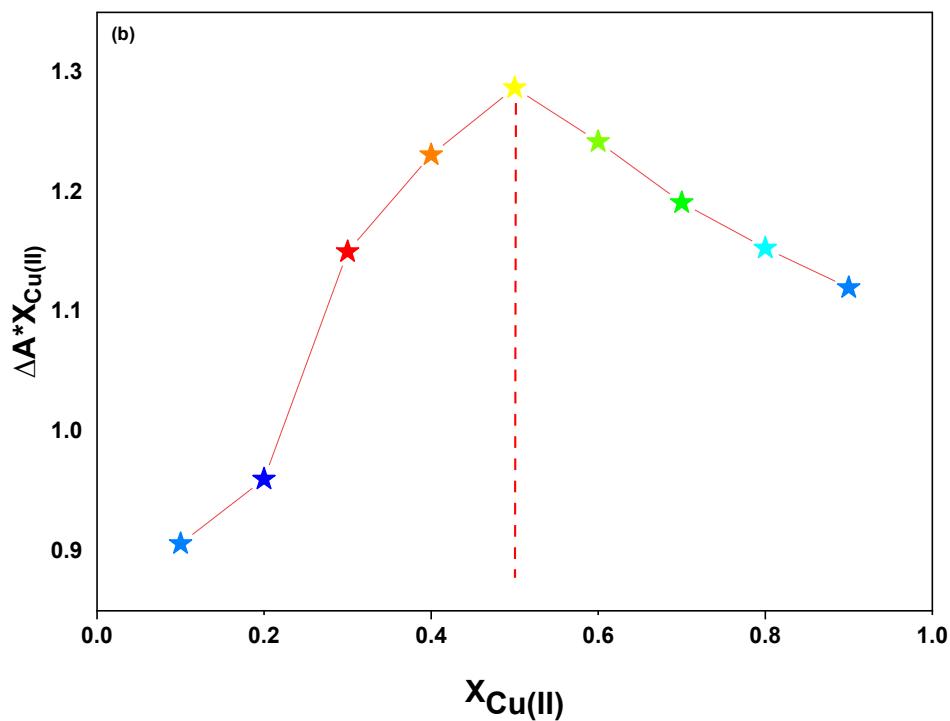


Figure S52: Job's plot analysis of probe 6b on interaction with Cu(II) ions.

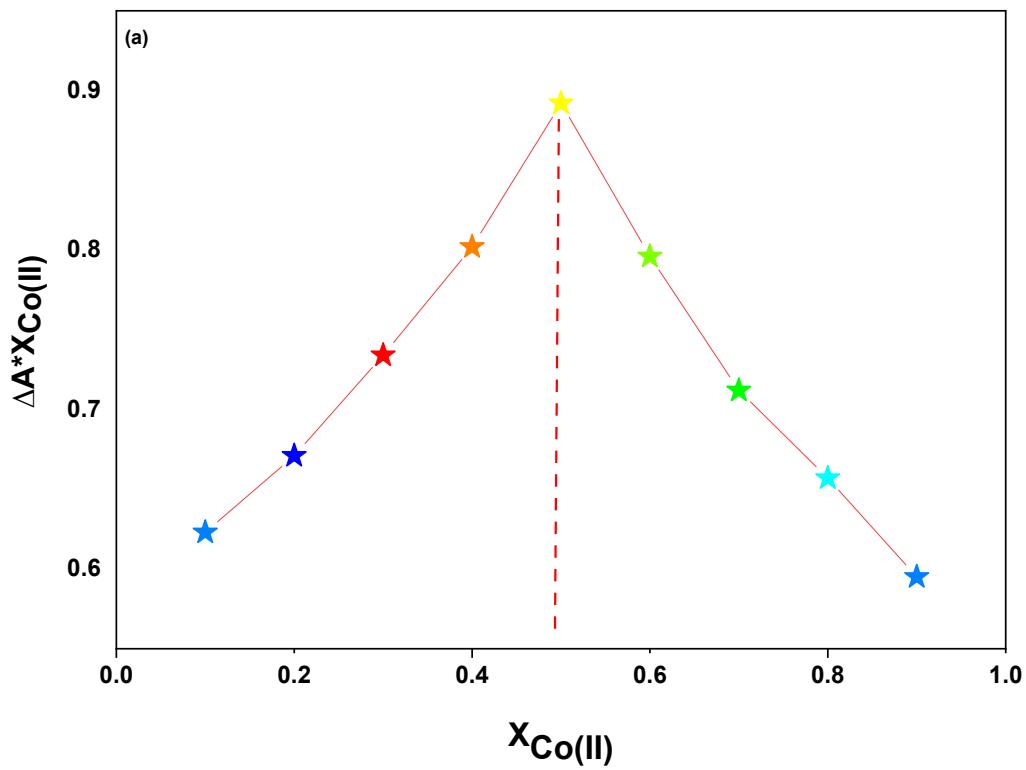


Figure S53: Job's plot analysis of probe 6c on interaction with Co(II) ions.

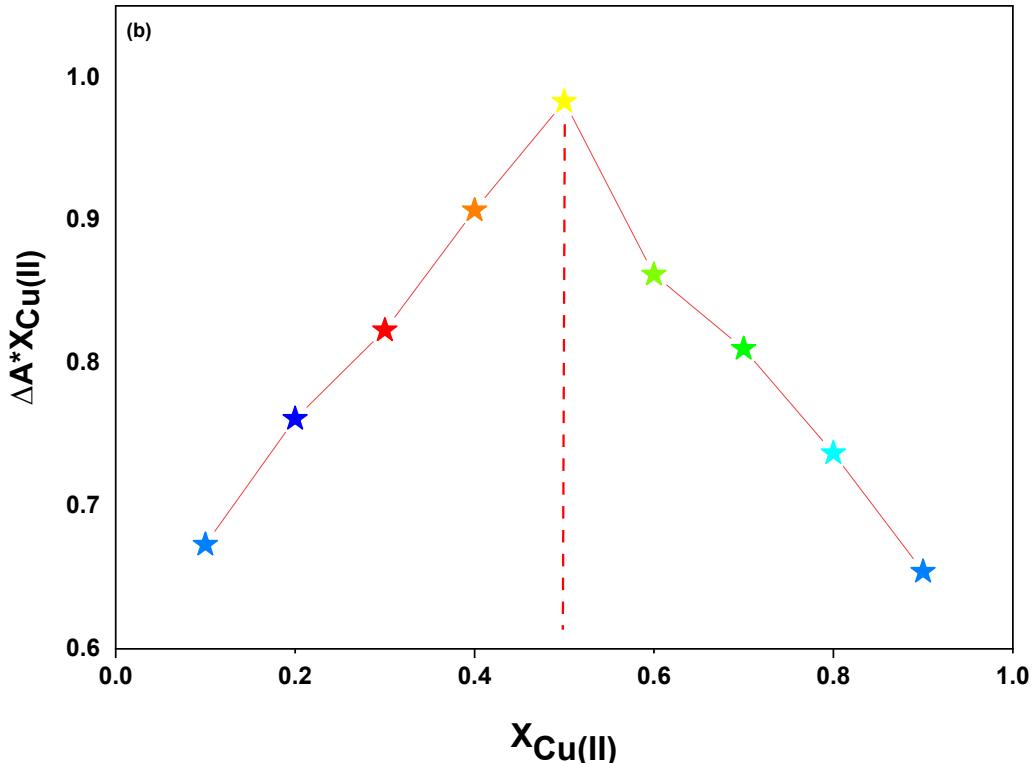


Figure S54: Job's plot analysis of probe 6c on interaction with Cu(II) ions.

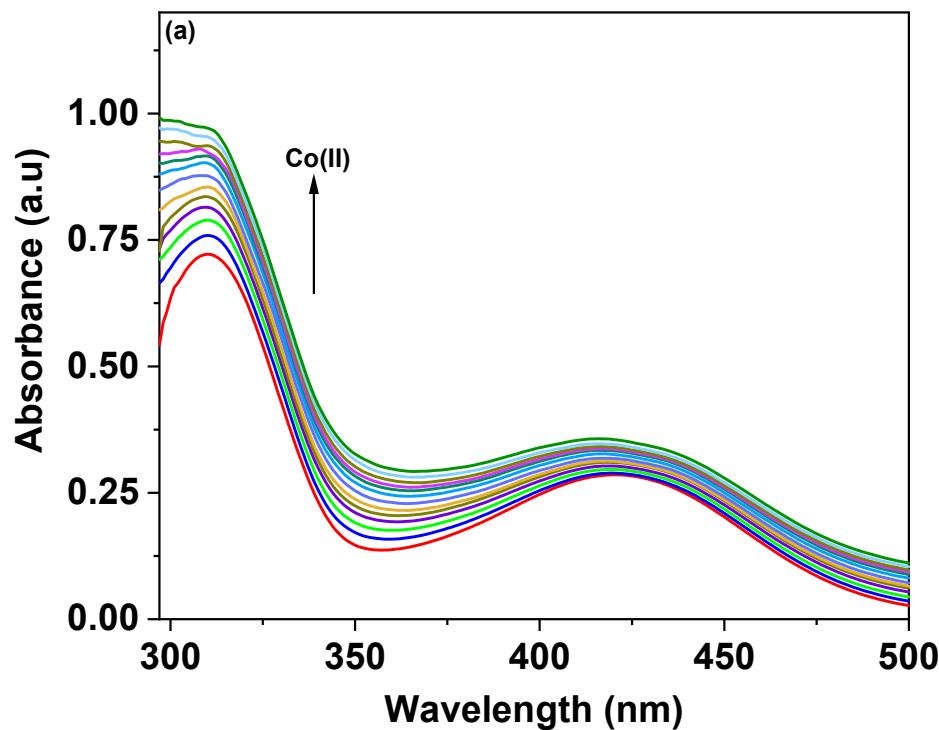


Figure S55: UV-Vis spectrum of probe **6a** in THF: H₂O (4:1), highlighting the selective detection of Co(II) among various metal ions at equimolar concentrations

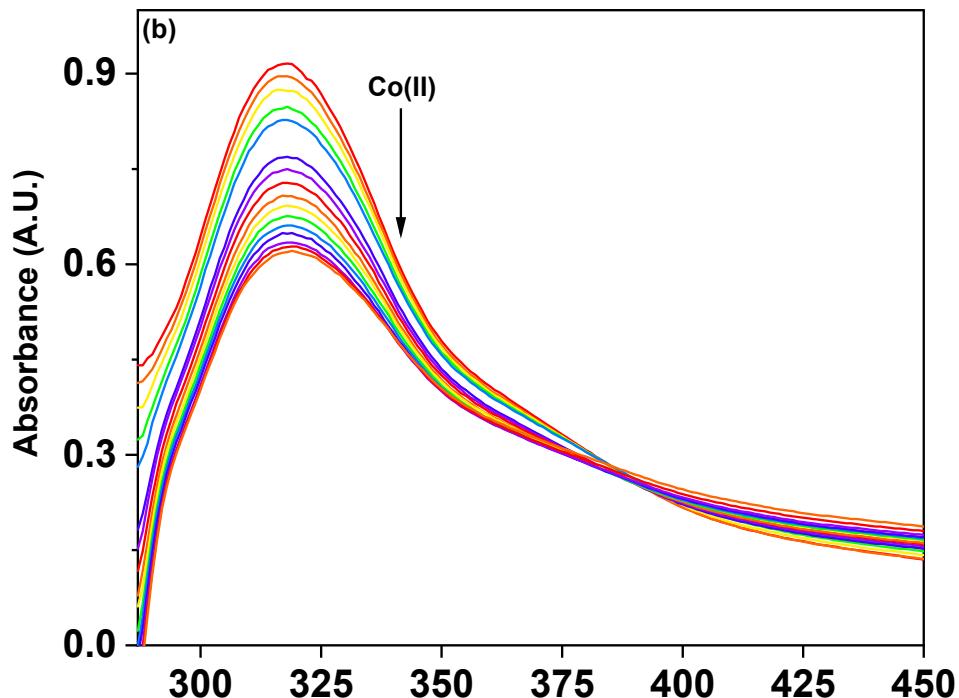


Figure S56: UV-Vis spectrum of probe **6b** in THF: H₂O (4:1), highlighting the selective detection of Co(II) among various metal ions at equimolar concentrations

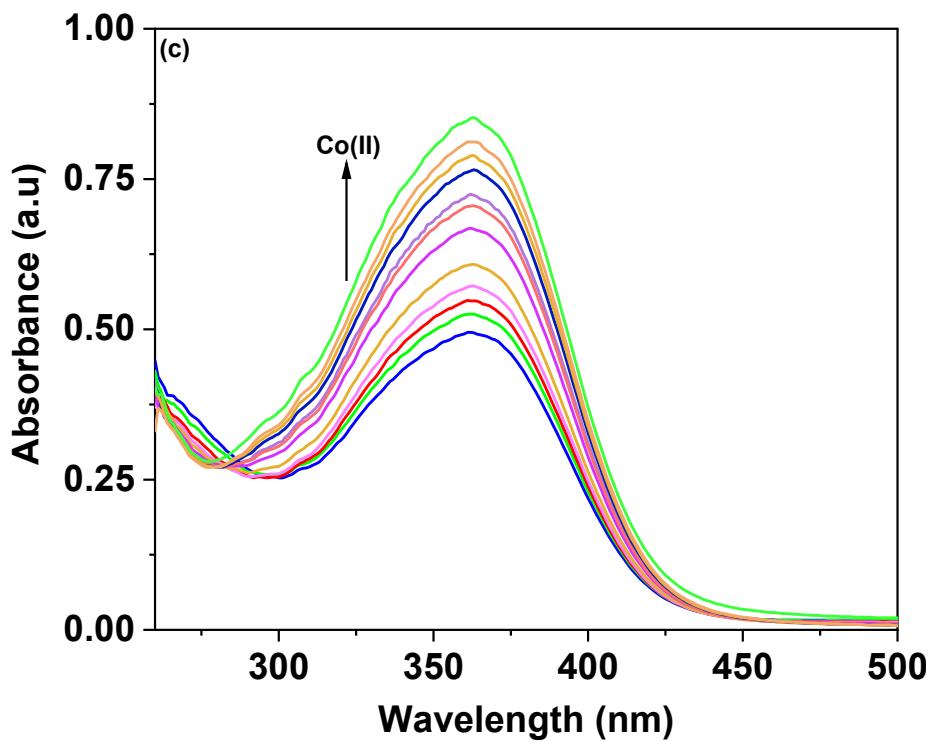


Figure S57: UV-Vis spectrum of probe **6c** in THF: H₂O (4:1), highlighting the selective detection of Co(II) among various metal ions at equimolar concentrations

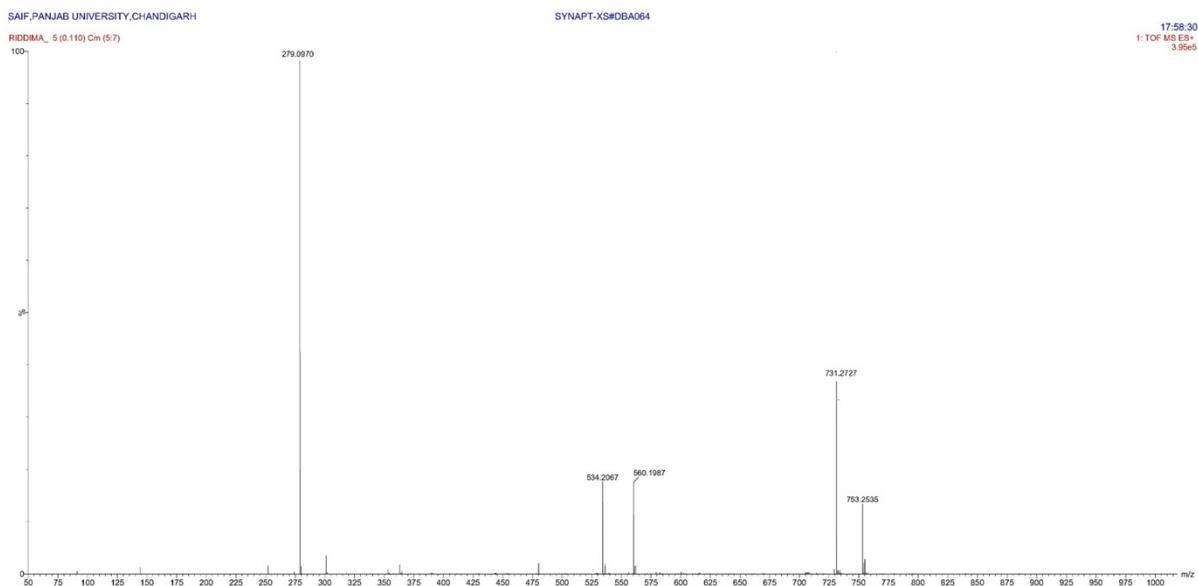


Figure S58: LCMS spectra of Co(II)-6a probe.

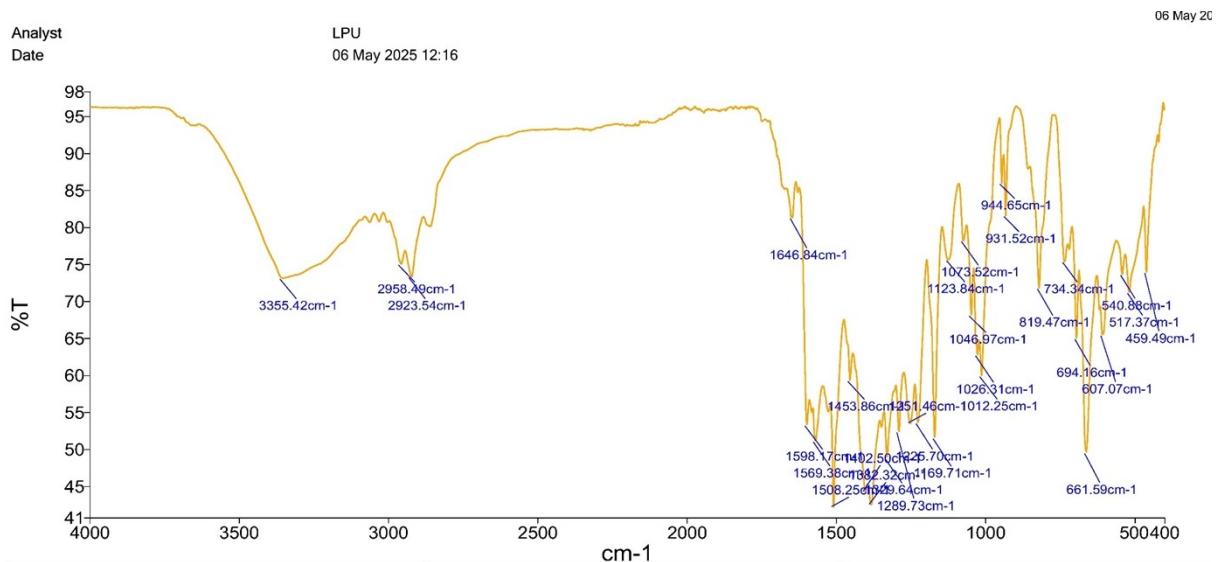


Figure S59: IR spectra of Co(II)-6a probe.

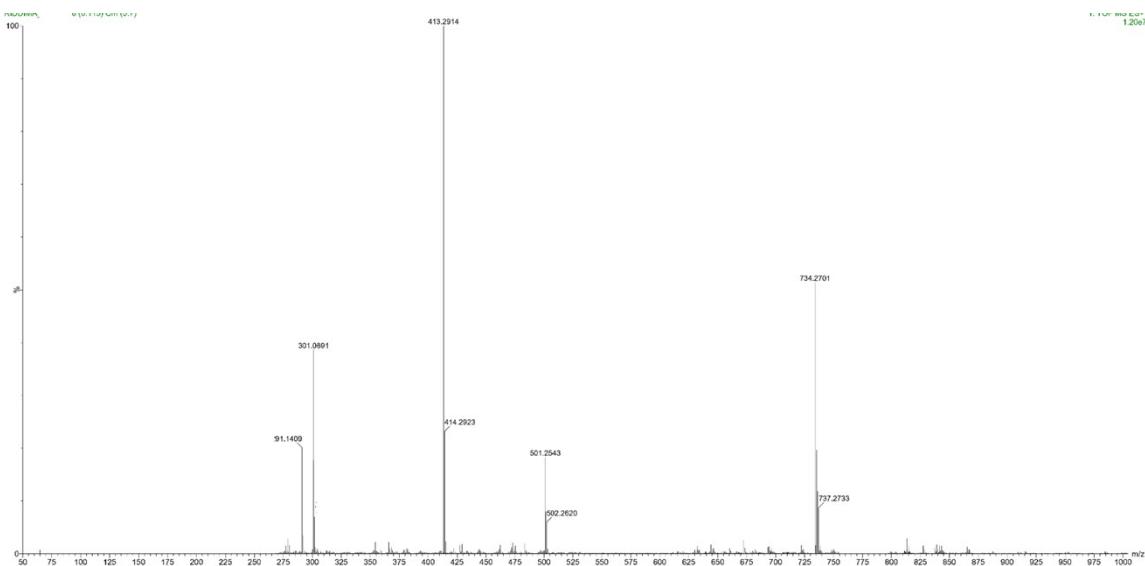


Figure S60: LCMS spectra of Cu(II)-6a probe.

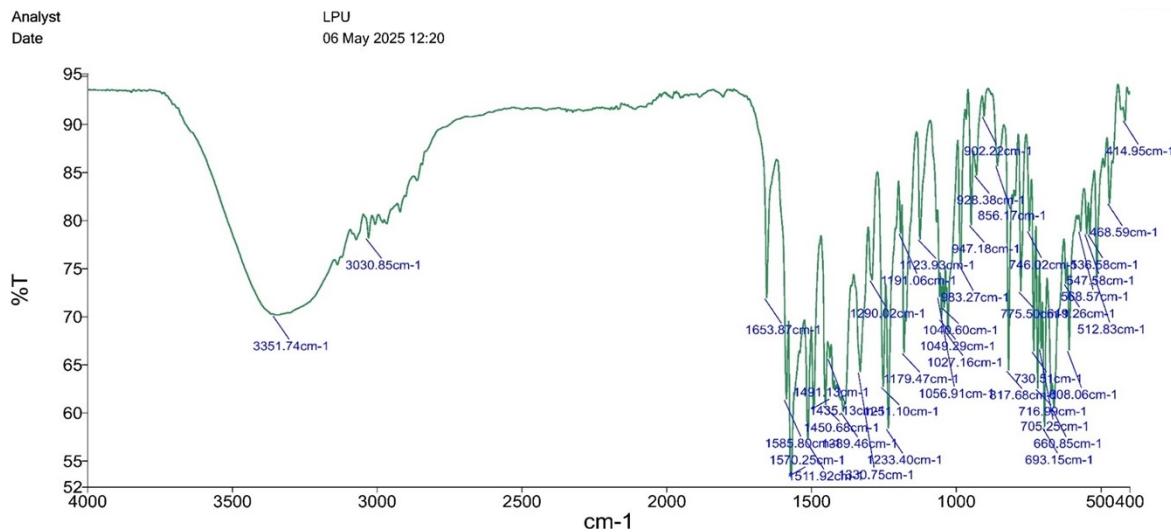


Figure S61: IR spectra of Cu(II)-6a probe.

C	-7.95789	-2.92461	-1.40511
C	-8.59469	-2.40591	-0.27719
C	-7.85124	-1.87773	0.78437
C	-6.46294	-1.87359	0.71226
C	-5.78779	-2.39255	-0.41129
C	-6.56563	-2.91274	-1.46332
Cl	-10.3466	-2.41236	-0.18622
C	-4.33158	-2.41603	-0.53749
C	-3.41462	-2.01544	0.36836
C	-1.9631	-2.08285	0.05387
O	-1.56193	-2.42052	-1.06075
C	-1.00048	-1.73852	1.15447
C	-1.26791	-2.21698	2.44917
C	-0.35652	-2.0507	3.49086
C	0.83406	-1.36153	3.25256
C	1.09544	-0.84522	1.98263
C	0.20215	-1.02159	0.91568
N	0.55739	-0.44743	-0.33886
C	1.36201	-1.30464	-1.2373
C	-0.40973	0.4526	-0.99899
C	0.16156	1.8267	-1.16641

C	2.81787	-1.34639	-0.90315
N	1.42081	2.01278	-1.85895
N	1.53232	3.43098	-2.05506
N	0.71255	4.01585	-0.98502
C	-0.25725	3.01445	-0.70066
C	3.59822	-2.36886	-0.52025
N	4.96116	-1.97428	-0.50396
N	4.91559	-0.50607	-0.47856
N	3.65859	-0.17464	-1.08702
C	0.27221	5.35612	-1.35154
C	5.83478	-2.50694	0.52831
C	-0.43255	6.06987	-0.21583
C	7.31352	-2.29236	0.25727
C	-1.64397	6.73623	-0.43987
C	-2.27836	7.43395	0.59265
C	-1.70949	7.46517	1.86766
C	-0.50352	6.7961	2.10193
C	0.1311	6.1054	1.06811
C	8.20797	-2.2373	1.33417
C	9.58131	-2.1029	1.11626
C	10.07619	-2.01291	-0.18742
C	9.18804	-2.05799	-1.26572
C	7.81584	-2.19856	-1.04561
H	-8.5431	-3.32971	-2.22308
H	-8.36001	-1.47439	1.65285
H	-5.90056	-1.45644	1.54117
H	-6.069	-3.31592	-2.3414
H	-3.94133	-2.80572	-1.47687
H	-3.70579	-1.61274	1.33319
H	-2.18523	-2.76968	2.63152
H	-0.57775	-2.45075	4.47556
H	1.54734	-1.20415	4.05645

H	1.99248	-0.26673	1.79312
H	1.24651	-0.89075	-2.24632
H	0.96125	-2.32617	-1.26962
H	-1.31509	0.53375	-0.39131
H	-0.71468	0.04046	-1.97048
H	-1.12534	3.24335	-0.09914
H	3.3191	-3.39634	-0.33184
H	1.1767	5.90761	-1.63665
H	-0.38798	5.33222	-2.2409
H	5.57635	-2.08121	1.5196
H	5.62737	-3.58219	0.59142
H	-2.09604	6.7083	-1.42832
H	-3.21672	7.94631	0.40054
H	-2.20137	8.00319	2.6728
H	-0.05529	6.81363	3.09133
H	1.06488	5.58186	1.24946
H	7.82858	-2.29638	2.35214
H	10.26065	-2.06098	1.96282
H	11.14253	-1.90161	-0.36097
H	9.5631	-1.97893	-2.28219
H	7.12304	-2.22221	-1.88004

Table S1: Cartesian co-ordinates of probe 6a

C	-7.65201	0.92038	0.59338
C	-9.02739	0.84285	0.78393
C	-9.63797	-0.4064	0.78311
C	-8.89224	-1.5702	0.59525
C	-7.52139	-1.47606	0.40567
C	-6.86918	-0.22974	0.39926
Cl	-11.37248	-0.52409	1.02317
C	-5.42953	-0.07531	0.20588
C	-4.51864	-1.03963	-0.0168
C	-3.08001	-0.70194	-0.15994

C -2.11547 -1.81141 -0.46484
O -2.67776 0.44705 -0.01805
C -0.76871 -1.58289 -0.17763
C 0.22598 -2.53306 -0.47451
C -0.19399 -3.73919 -1.07856
C -1.53449 -3.95815 -1.37683
C -2.50827 -3.01275 -1.07023
N 1.56146 -2.26439 -0.18865
C 1.90103 -1.32879 0.88161
C 2.62817 -3.14532 -0.67081
C 3.90017 -2.41525 -0.98276
C 2.17151 0.0792 0.42739
N 4.03542 -1.65563 -2.10866
N 5.21997 -1.12154 -2.12736
N 5.87178 -1.52829 -1.01709
C 5.08168 -2.34446 -0.27858
N 2.87381 0.9554 1.19845
N 2.93541 2.11041 0.5932
N 2.27928 1.98838 -0.57545
C 1.78735 0.73353 -0.7202
C 2.11451 3.14097 -1.45788
C 0.94077 4.03494 -1.09757
C -0.31628 3.50654 -0.78799
C -1.384 4.35287 -0.49926
C -1.21136 5.73634 -0.52313
C 0.03807 6.26963 -0.83134
C 1.10823 5.42153 -1.11236
C 7.25145 -1.10056 -0.77724
C 7.48098 -0.56252 0.61997
C 8.59385 -0.98421 1.35168
C 8.84461 -0.4663 2.62228
C 7.97562 0.47111 3.1757

C	6.85723	0.88961	2.45412
C	6.61346	0.38061	1.1817
H	-7.17227	1.89302	0.5949
H	-9.61787	1.73783	0.93191
H	-9.38445	-2.53433	0.59974
H	-6.95363	-2.38772	0.26421
H	-5.05064	0.94293	0.25072
H	-4.80505	-2.08214	-0.06843
H	-0.51265	-0.6263	0.25623
H	0.51772	-4.52164	-1.30349
H	-1.8203	-4.89188	-1.84857
H	-3.54118	-3.202	-1.3304
H	1.09223	-1.32751	1.61969
H	2.78683	-1.69298	1.40853
H	2.29035	-3.61297	-1.59492
H	2.83808	-3.94986	0.05064
H	5.40239	-2.77092	0.65669
H	1.25416	0.4102	-1.59687
H	2.0076	2.74882	-2.47275
H	3.0453	3.70706	-1.41708
H	-0.4758	2.43458	-0.75557
H	-2.34836	3.92324	-0.254
H	-2.04342	6.3938	-0.29724
H	0.1849	7.34388	-0.84345
H	2.08297	5.84285	-1.33696
H	7.92258	-1.9409	-0.97388
H	7.44325	-0.33896	-1.53603
H	9.26997	-1.72042	0.92787
H	9.71266	-0.80129	3.17891
H	8.16427	0.86965	4.16615
H	6.16762	1.61002	2.87818
H	5.73452	0.71106	0.64

Table S2: Cartesian co-ordinates of probe 6b

Cl	-10.43218	0.30096	0.48427
C	-8.83798	-0.44719	0.52025
C	-7.83632	0.05941	-0.30078
C	-6.58148	-0.53128	-0.26998
C	-6.30851	-1.62388	0.57103
C	-7.35071	-2.10514	1.37914
C	-8.61463	-1.52532	1.36287
C	-5.00456	-2.27932	0.64554
C	-3.87566	-1.94184	0.00006
C	-2.63119	-2.72765	0.19554
C	-1.3903	-2.31124	-0.49787
O	-2.63347	-3.71578	0.92651
C	-1.27393	-1.17356	-1.31032
C	-0.07989	-0.83195	-1.92179
C	1.07903	-1.62335	-1.75972
C	0.96196	-2.76692	-0.93181
C	-0.23452	-3.09254	-0.32835
N	2.26233	-1.29428	-2.3851
C	2.47899	0.01991	-2.99123
C	3.36112	-2.25625	-2.53466
C	4.57372	-1.97244	-1.69993
C	2.44343	1.17907	-2.03354
C	4.81911	-2.1291	-0.35563
N	6.06625	-1.64632	-0.17606
N	6.58589	-1.22945	-1.35355
N	5.68319	-1.42176	-2.26604
C	1.72895	2.35097	-2.11126
N	2.09615	3.05479	-1.0189
N	2.98935	2.34973	-0.2892
N	3.20071	1.22576	-0.90402
C	6.86629	-1.54768	1.04121

C	6.20878	-0.7664	2.16184
C	5.38664	0.33331	1.90782
C	4.84253	1.05886	2.96485
C	5.11758	0.69944	4.28184
C	5.93528	-0.39751	4.54029
C	6.47332	-1.12869	3.48453
C	1.64016	4.36338	-0.55389
C	0.17278	4.39035	-0.17766
C	-0.34857	3.45753	0.72387
C	-1.68983	3.50636	1.08754
C	-2.52502	4.49021	0.559
C	-2.01261	5.42215	-0.33772
C	-0.66905	5.36896	-0.70615
H	-8.039	0.89883	-0.95274
H	-5.80653	-0.13623	-0.9151
H	-7.16441	-2.94924	2.03353
H	-9.40934	-1.90427	1.9916
H	-4.93758	-3.14038	1.30515
H	-3.85613	-1.09355	-0.67144
H	-2.12465	-0.52671	-1.48141
H	-0.05268	0.05156	-2.54119
H	1.82199	-3.39389	-0.74074
H	-0.30334	-3.96534	0.3088
H	3.46761	-0.01615	-3.45104
H	1.76126	0.20077	-3.80145
H	2.97407	-3.25511	-2.34487
H	3.68288	-2.2418	-3.58017
H	4.21486	-2.49104	0.45902
H	1.01172	2.71907	-2.82616
H	7.11199	-2.55727	1.38106
H	7.79671	-1.07184	0.72389
H	5.14974	0.61936	0.88993

H	4.20007	1.90376	2.74722
H	4.69204	1.26545	5.10256
H	6.14794	-0.69031	5.56208
H	7.10308	-1.98802	3.69247
H	1.8489	5.10237	-1.33042
H	2.27343	4.59353	0.30479
H	0.29646	2.68993	1.13717
H	-2.08365	2.77832	1.78723
H	-3.56921	4.52872	0.8468
H	-2.65579	6.18907	-0.75358
H	-0.27423	6.09726	-1.40727

Table S3: Cartesian co-ordinates of probe 6c