

Supporting Information

N-Amino-thieno[3,2-c]pyridin-4-ones: A new class of Pd²⁺chemosensor and Aggregation Induced Emission

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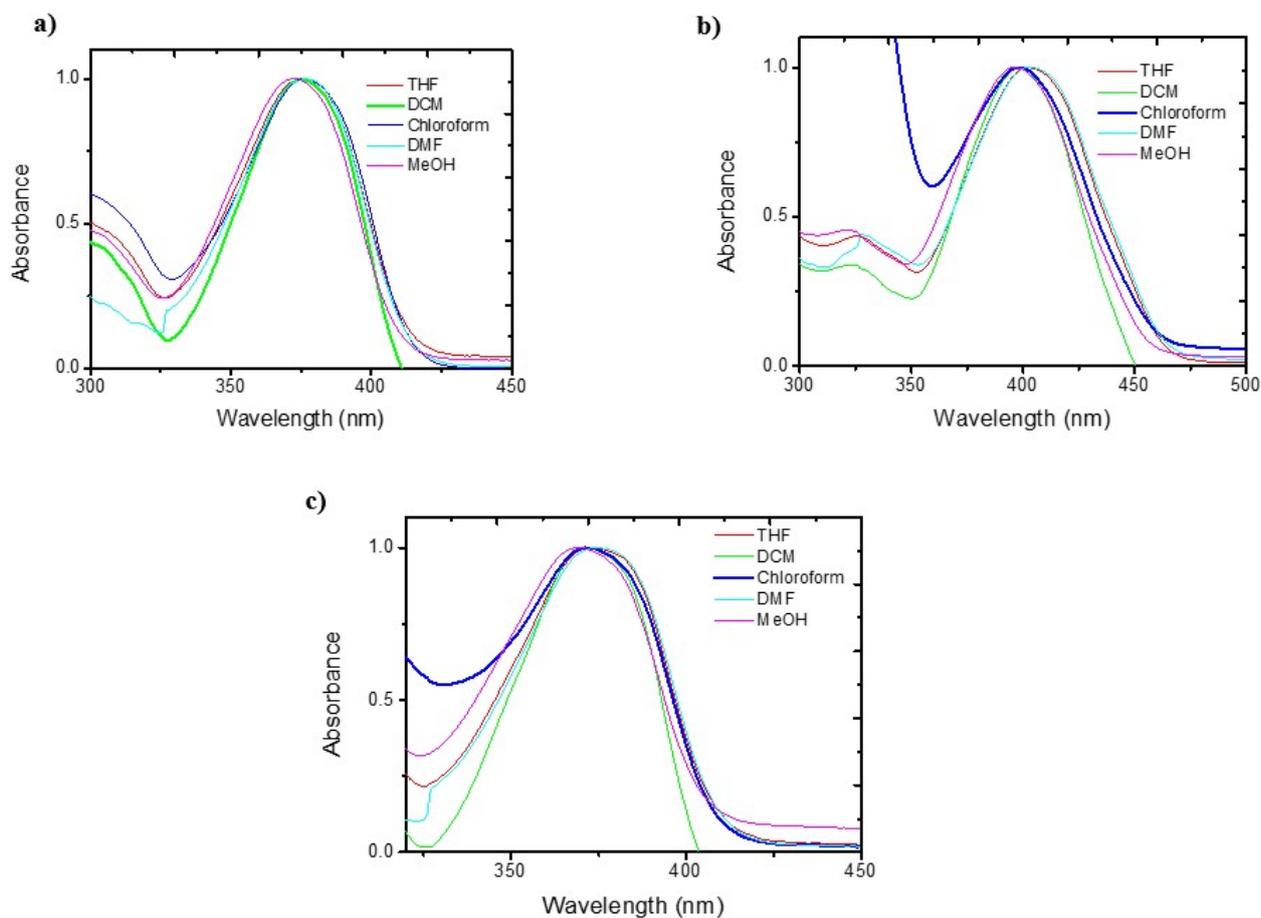


Fig. S1 Normalized absorption spectra of (a) **5a**, (b) **5b**, and (c) **5c** in solvents of different polarity.

Table S1 Photophysical properties of compounds **5a**, **5b** and **5c**.

Compounds	Solvent	$\lambda_{ab}(nm)^a$	$\lambda_{em}(nm)^b$	Stokes's shift (cm^{-1})
5a	THF	376	444	4072
	Dichloromethane	376	459	4806
	Chloroform	376	459	4806
	DMF	377	467	5112
	methanol	373	444	4286
	THF	403	507	5090
	Dichloromethane	399	507	5339

5b	Chloroform	398	506	5363
	DMF	403	510	5206
	methanol	396	492	4928
5c	THF	374	441	4062
	Dichloromethane	372	442	4258
	Chloroform	372	439	4103
	DMF	375	460	4245
	methanol	371	436	4018

^a absorption and ^b emission maxima were recorded in different polarity solvents for **5a**, **5b** and **5c**.

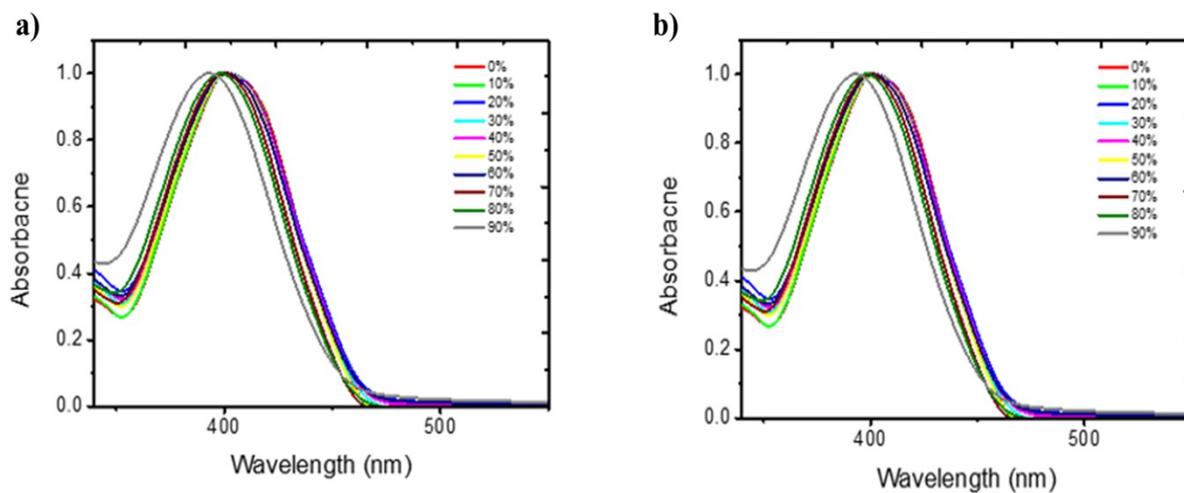


Fig. S2 Absorption spectra of (a) **5a** (b) **5b** and (c) **5c** in THF–water mixtures with different water fractions.

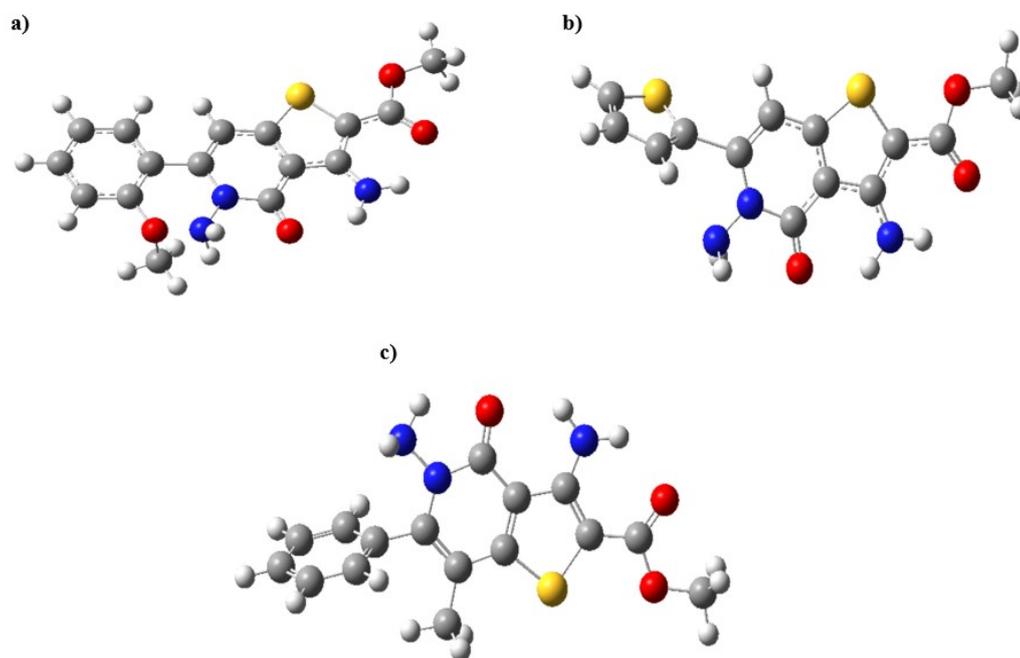


Fig. S3 DFT optimized structure of a) **5a**, b) **5b** and c) **5c**.

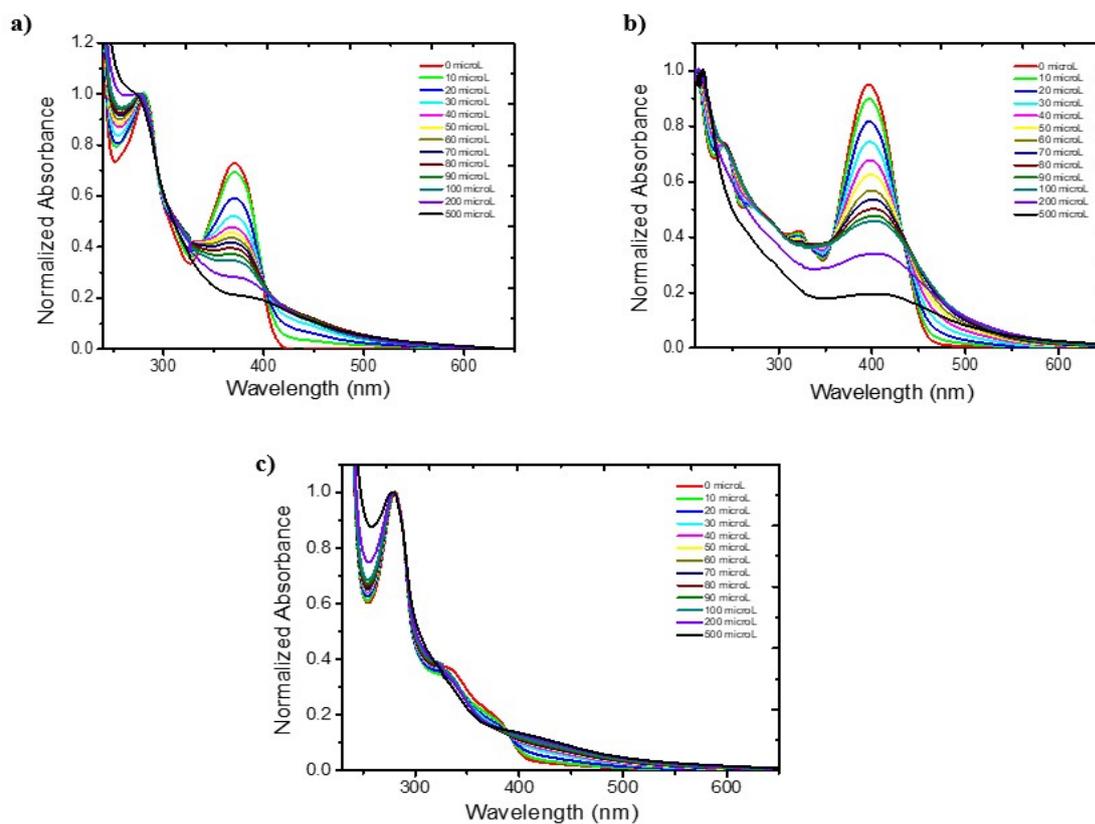


Fig. S4 Normalized absorption spectra of A) **5a**, B) **5b** and C) **5c** on exposure to increasing conc. of $\text{Pd}(\text{OAc})_2$.

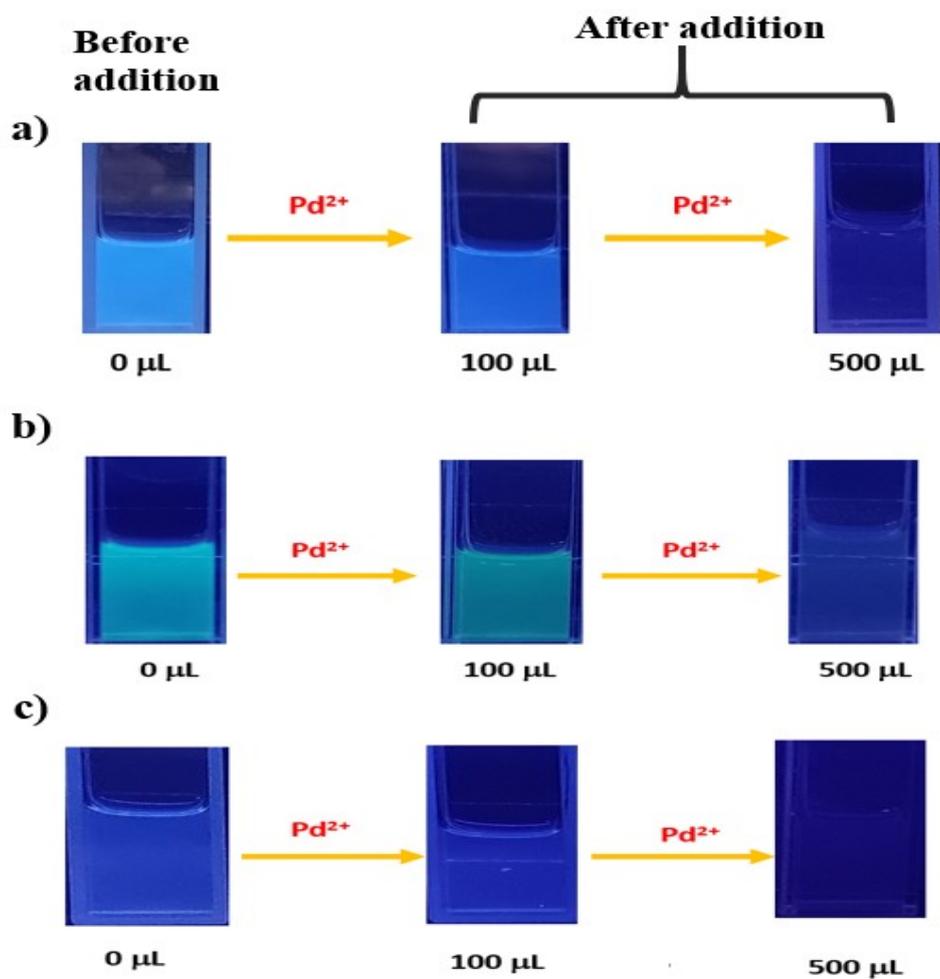


Fig. S5 Fluorescence images of the compounds a) **5a**, b) **5b** and c) **5c** before and after addition of Pd^{2+} metal ions taken under 365 nm irradiation.

Anion Reversibility:

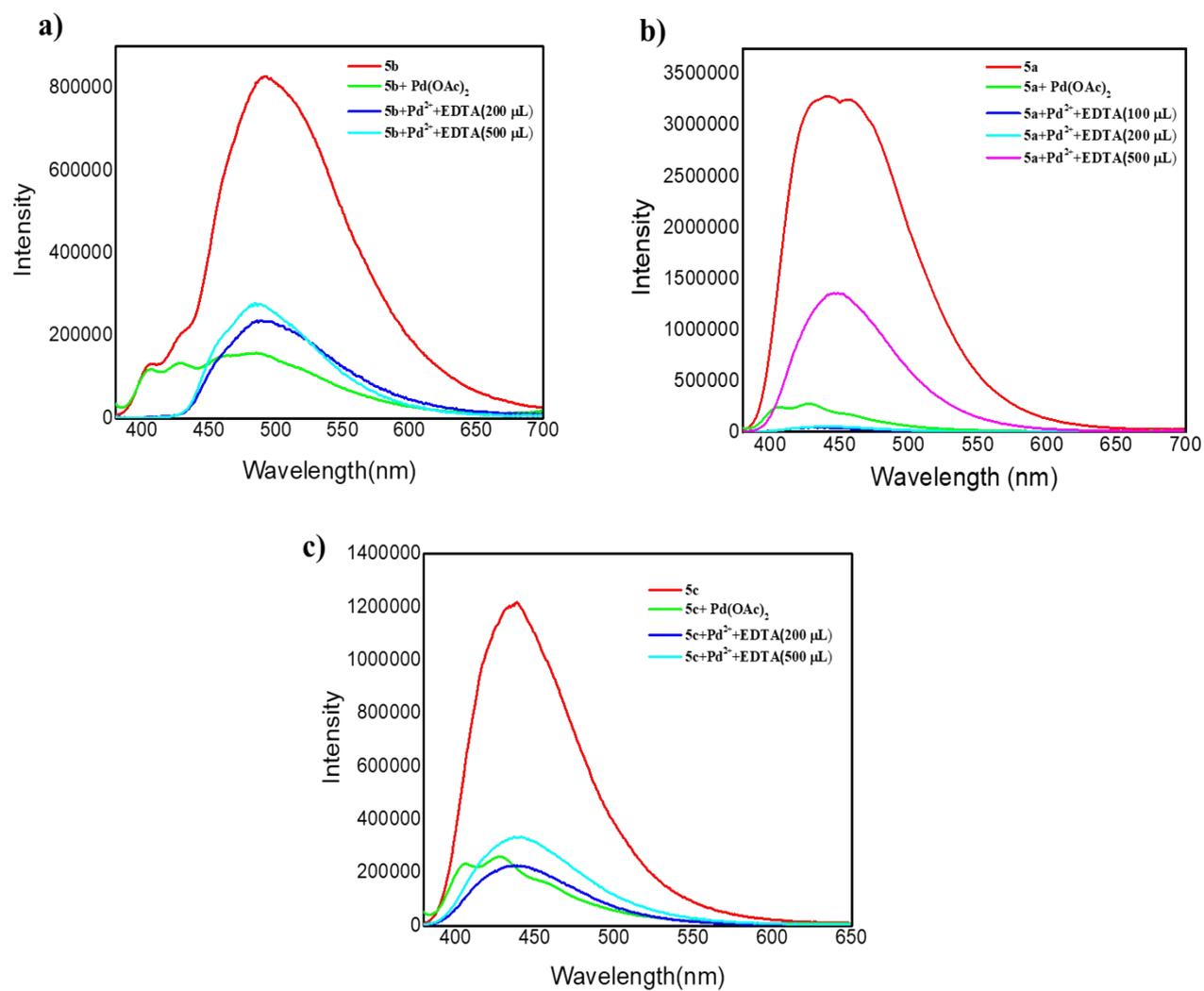


Fig. S6 Fluorescence spectra showing anion (EDTA) reversibility test of compound a) **5b**, b) **5a** and c) **5c** with Pd^{2+} in methanol ($\lambda_{\text{exc}} = 370 \text{ nm}$).

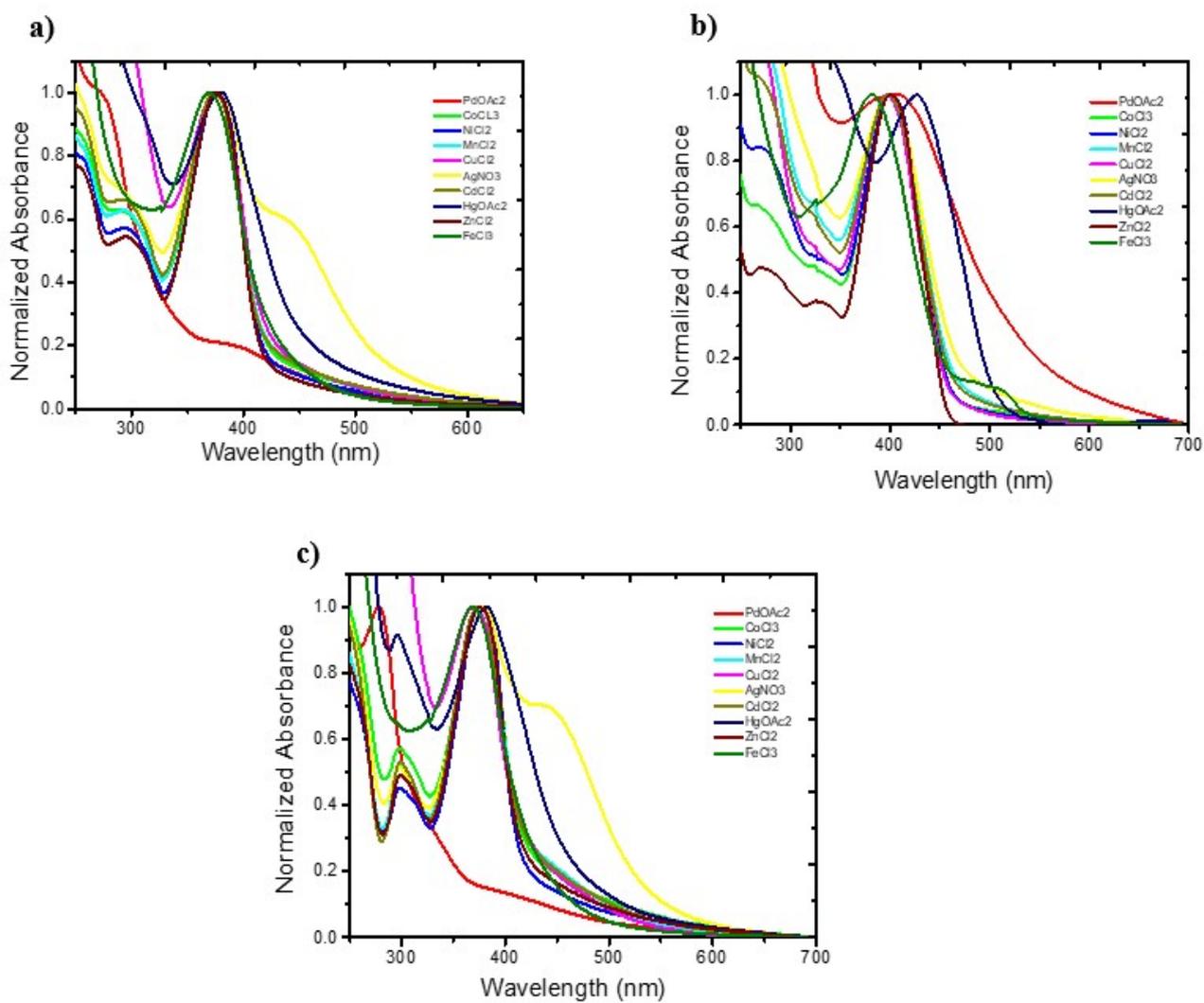


Fig. S7 Comparative normalized absorption spectra of the compounds a) **5a**, b) **5b** and c) **5c** with metal ions.

DFT Calculation data of 5a, 5b and 5c

Calculation method: B3LYP/6-31G (d,p) with Gaussian 09

5a:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.545241	-0.207428	-0.322636
2	6	0	0.067588	1.643733	-0.589311
3	6	0	1.102854	0.693419	-0.301527
4	6	0	0.801575	-0.645334	-0.038169
5	6	0	-0.535928	-1.103387	-0.044292
6	7	0	-1.240826	1.115381	-0.572757
7	7	0	-2.276773	2.002212	-0.950629
8	1	0	-1.784101	2.820220	-1.314759
9	1	0	-2.754053	2.286112	-0.094007
10	8	0	0.237572	2.846520	-0.864232
11	16	0	2.225828	-1.588842	0.281386
12	6	0	3.255810	-0.163499	0.055806
13	6	0	2.514877	0.982232	-0.250683
14	7	0	3.020275	2.213072	-0.472962
15	1	0	4.023291	2.335584	-0.433046
16	1	0	2.379592	2.959535	-0.708370
17	6	0	4.689612	-0.191425	0.171193
18	8	0	5.416329	0.791470	0.014211
19	8	0	5.179007	-1.423377	0.474122

20	6	0	6.607248	-1.518055	0.601641
21	1	0	7.096401	-1.231392	-0.332674
22	1	0	6.807193	-2.564048	0.834083
23	1	0	6.964930	-0.870531	1.406246
24	6	0	-5.240066	-0.639765	0.512102
25	6	0	-3.934092	-0.141048	0.530829
26	6	0	-2.962766	-0.652008	-0.358860
27	6	0	-3.338294	-1.665422	-1.248505
28	6	0	-4.642696	-2.164878	-1.274997
29	6	0	-5.588839	-1.647852	-0.392424
30	1	0	-2.593012	-2.053297	-1.936016
31	1	0	-4.912426	-2.944285	-1.980099
32	1	0	-6.607516	-2.024167	-0.398718
33	1	0	-5.987663	-0.254608	1.194735
34	1	0	-0.790025	-2.129934	0.185910
35	8	0	-3.506373	0.835445	1.391802
36	6	0	-4.386267	1.280558	2.423185
37	1	0	-3.810593	1.993909	3.013714
38	1	0	-5.270099	1.778775	2.007373
39	1	0	-4.698433	0.445439	3.060545

Rotational constants (GHZ): 0.5268363 0.1067848 0.0968536

5b:

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	0.261111	1.873449	-0.086183
2	6	0	-0.733468	0.844554	-0.022263
3	6	0	-0.367457	-0.500874	0.067887
4	6	0	0.989366	-0.884923	0.120324
5	1	0	1.274383	-1.922068	0.236967
6	7	0	1.597689	1.416261	-0.050635
7	7	0	2.585671	2.433606	-0.087582
8	1	0	2.041336	3.296921	-0.006274
9	1	0	2.998931	2.431435	-1.022132
10	8	0	0.041323	3.096316	-0.166442
11	16	0	-1.748499	-1.553238	0.128132
12	6	0	-2.846150	-0.166022	0.025240
13	6	0	-2.159780	1.050431	-0.049249
14	7	0	-2.725531	2.271696	-0.136762
15	1	0	-3.734824	2.334578	-0.148842
16	1	0	-2.120670	3.080659	-0.182286
17	6	0	-4.280929	-0.285980	0.019053
18	8	0	-5.053802	0.670769	-0.052423
19	8	0	-4.710369	-1.572387	0.100207
20	6	0	-6.135566	-1.761003	0.098567

21	1	0	-6.591248	-1.249819	0.950208
22	1	0	-6.283633	-2.838190	0.173359
23	1	0	-6.572316	-1.375956	-0.826293
24	6	0	3.395617	-0.275051	0.111434
25	6	0	4.466179	0.348871	0.721136
26	16	0	3.911363	-1.785899	-0.622734
27	6	0	5.680499	-0.386256	0.616076
28	1	0	4.371172	1.299741	1.226690
29	6	0	5.537074	-1.558197	-0.081638
30	1	0	6.621438	-0.056013	1.040791
31	1	0	6.293072	-2.293617	-0.321378
32	6	0	1.972588	0.086001	0.070773

Rotational constants (GHZ): 0.6349994 0.1294557 0.1089721

5c:

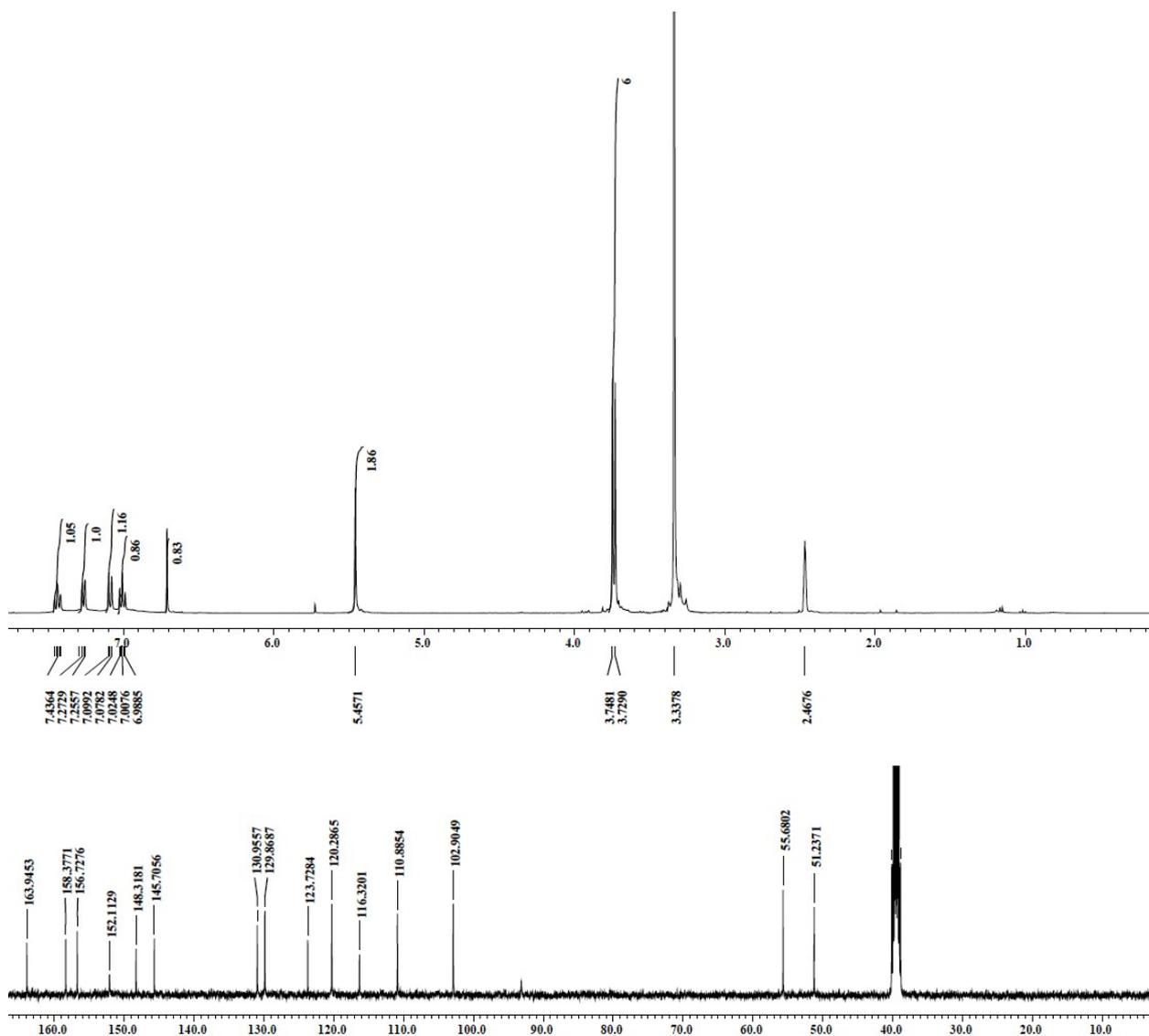
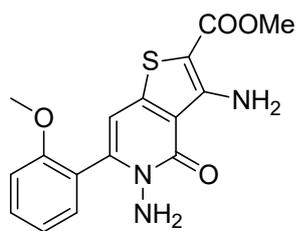
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.865933	0.037378	-0.013863
2	6	0	-0.210487	1.880733	0.062840
3	6	0	0.802044	0.868778	0.026463
4	6	0	0.465721	-0.485408	-0.018650

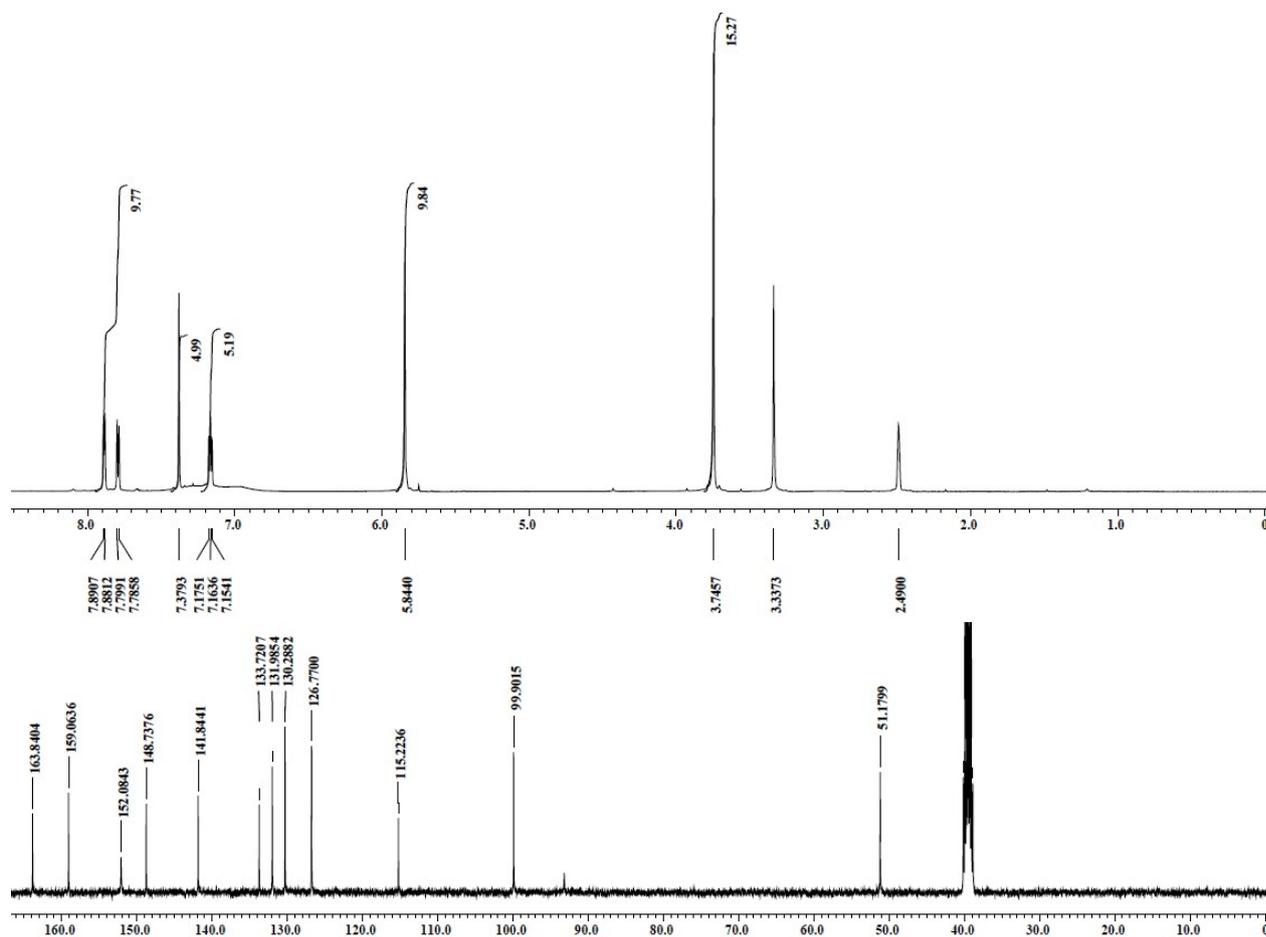
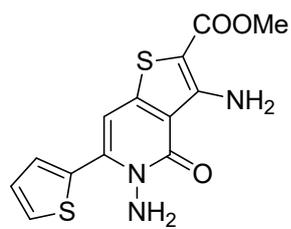
5	6	0	-0.885367	-0.936348	-0.040323
6	7	0	-1.523595	1.380628	0.051860
7	7	0	-2.553516	2.356721	0.025222
8	1	0	-2.045794	3.239833	-0.074635
9	1	0	-3.000455	2.369359	0.942979
10	8	0	-0.019406	3.112674	0.094155
11	16	0	1.876324	-1.504443	-0.052988
12	6	0	2.940327	-0.089836	-0.002846
13	6	0	2.223938	1.109829	0.036751
14	7	0	2.756474	2.348355	0.080035
15	1	0	3.763588	2.439527	0.078422
16	1	0	2.128099	3.140878	0.096844
17	6	0	4.377448	-0.172978	-0.006918
18	8	0	5.126432	0.804751	0.025855
19	8	0	4.840542	-1.450172	-0.050831
20	6	0	6.270045	-1.600028	-0.058630
21	1	0	6.703158	-1.106554	-0.932274
22	1	0	6.446942	-2.674796	-0.098181
23	1	0	6.705988	-1.171612	0.847369
24	6	0	-5.297087	-1.098929	1.148599
25	6	0	-3.935797	-0.779815	1.145513
26	6	0	-3.325659	-0.281629	-0.014724
27	6	0	-4.098309	-0.103888	-1.172192
28	6	0	-5.454934	-0.428447	-1.169347
29	6	0	-6.058123	-0.925458	-0.009180
30	1	0	-3.342130	-0.922610	2.044356
31	1	0	-3.634844	0.294925	-2.068795

32	1	0	-6.042373	-0.290531	-2.072263
33	1	0	-7.114781	-1.176312	-0.009252
34	1	0	-5.757742	-1.485585	2.052940
35	6	0	-1.183943	-2.413153	-0.114562
36	1	0	-2.248927	-2.609176	-0.238498
37	1	0	-0.654972	-2.868596	-0.960314
38	1	0	-0.846321	-2.930403	0.792279

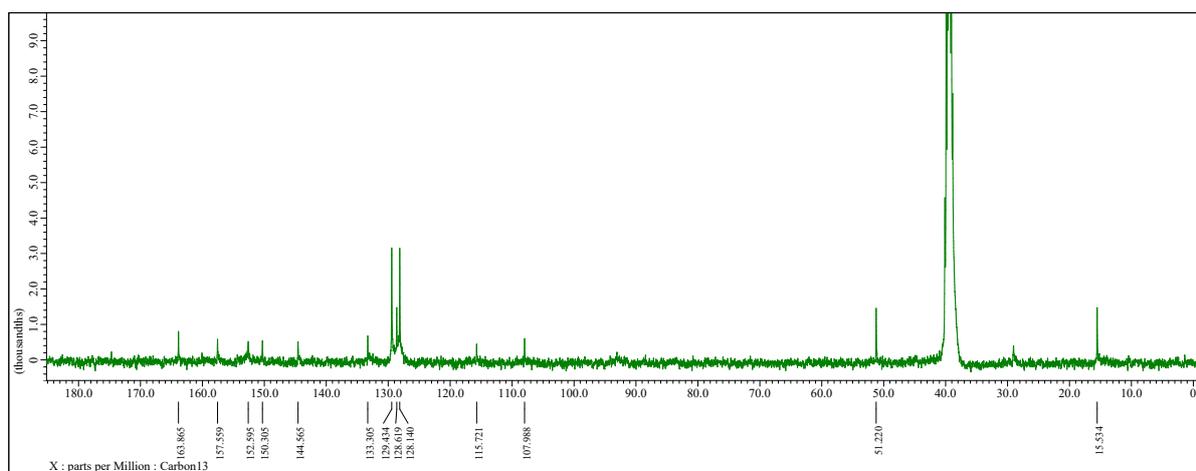
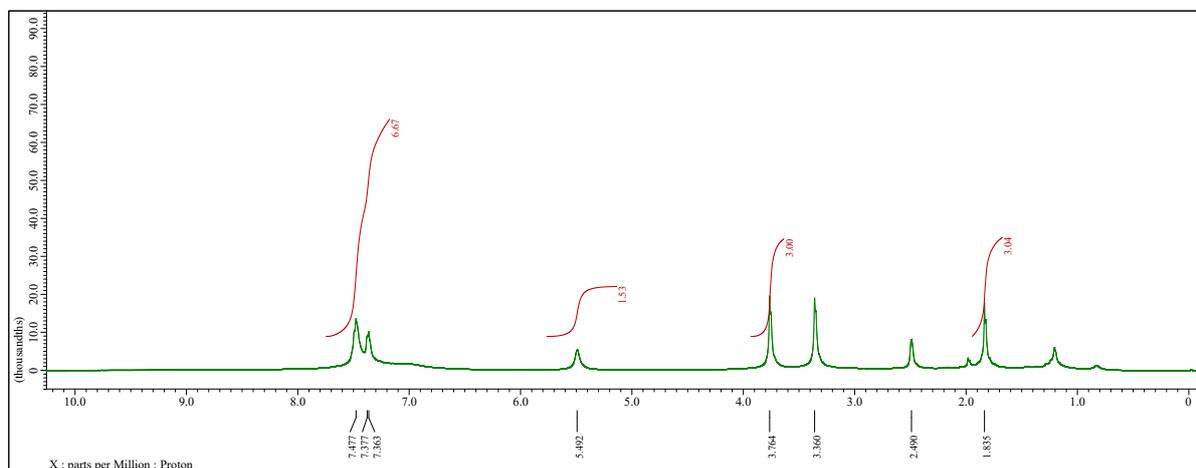
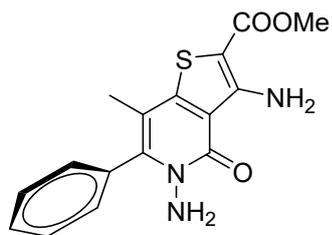
Rotational constants (GHZ): 0.6119271 0.1221076 0.1054674



¹H and ¹³C spectra of methyl 3,5-diamino-6-(2-methoxyphenyl)-4-oxo-4,5-dihydrothieno[3,2-c]pyridine-2-carboxylate (**5a**)



¹H and ¹³C spectra of methyl 3,5-diamino-4-oxo-6-(thiophen-2-yl)-4,5-dihydrothieno[3,2-*c*]pyridine-2-carboxylate (**5b**)



^1H and ^{13}C spectra of methyl 3,5-diamino-7-methyl-4-oxo-6-phenyl-4,5-dihydrothieno[3,2-c]pyridine-2-carboxylate (5c)