

Supplementary Data

Discovery of novel 4-propoxy-2-arylquinolines as dual EGFR and FAK inhibitors with *in vitro* antitumor activity

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ⁱ Moores Comprehensive Cancer Center, University of California San Diego, La Jolla, CA, USA

^j Veterans Affairs Medical Center, La Jolla, CA, USA

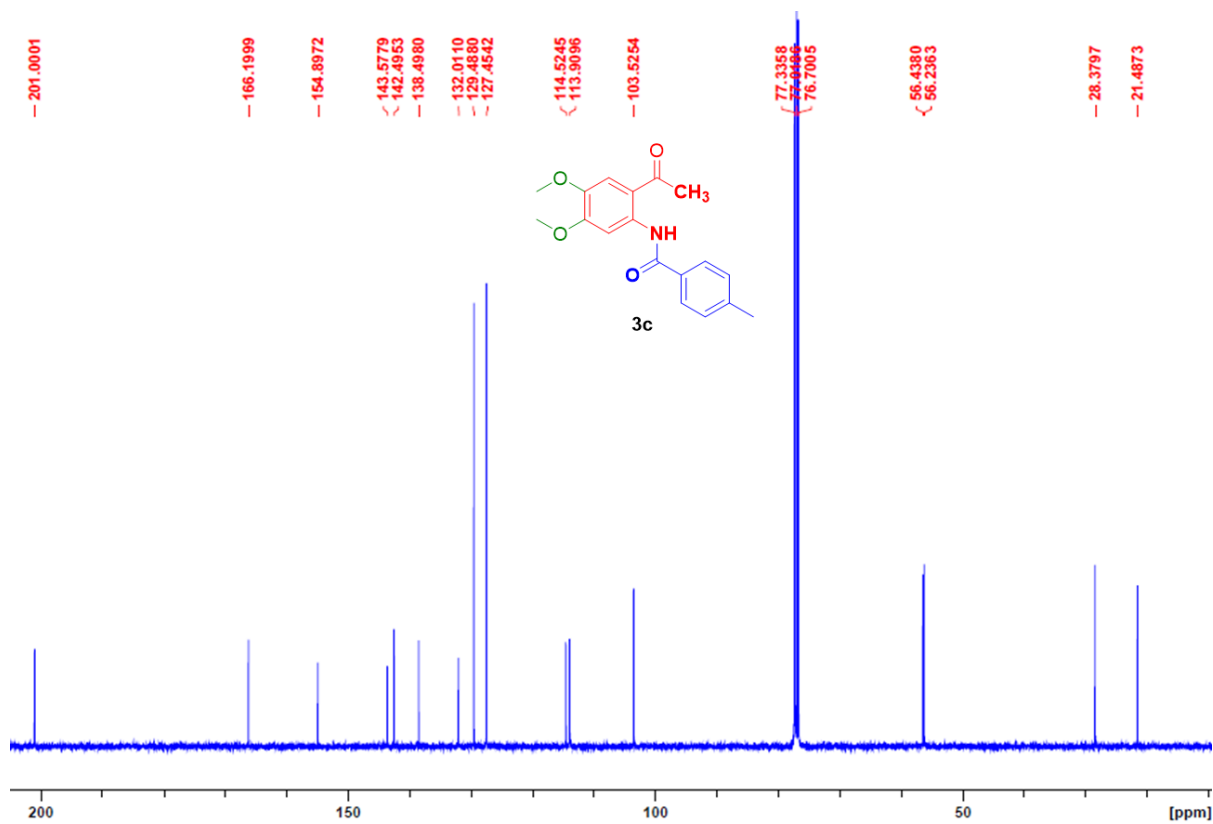
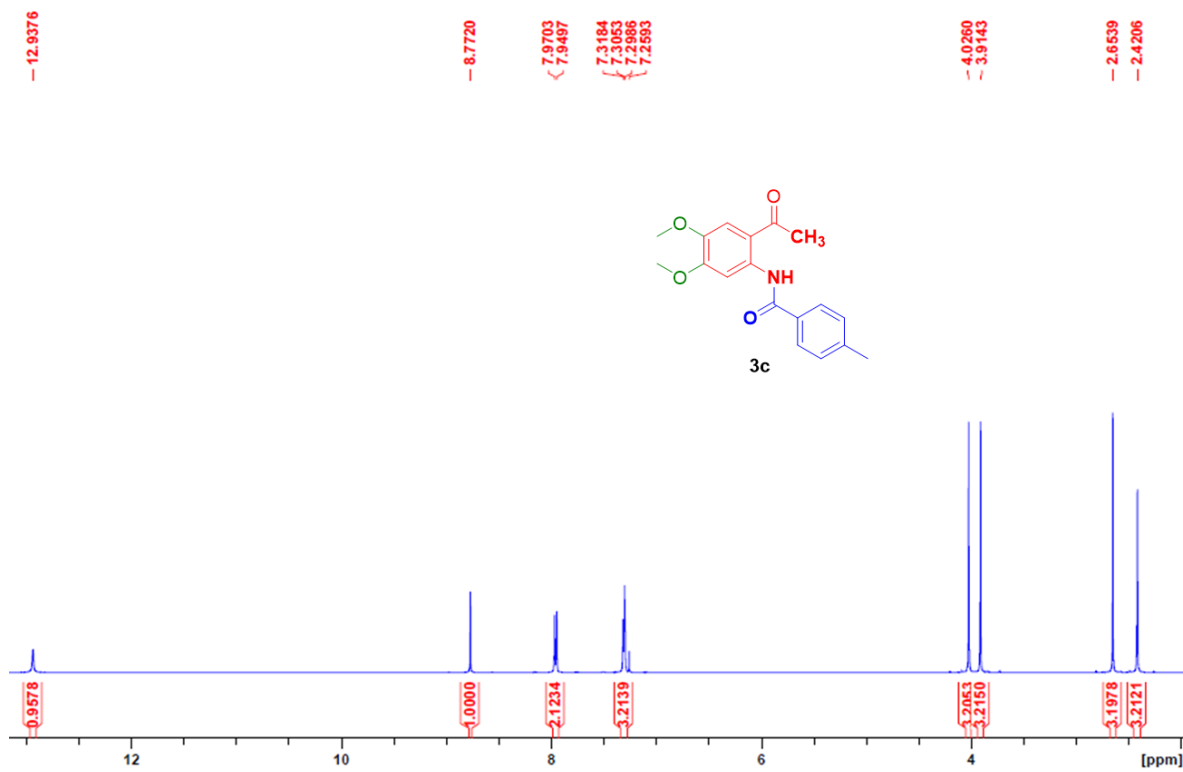
* Corresponding author: mostafa_elbadawi@pharm.kfs.edu.eg

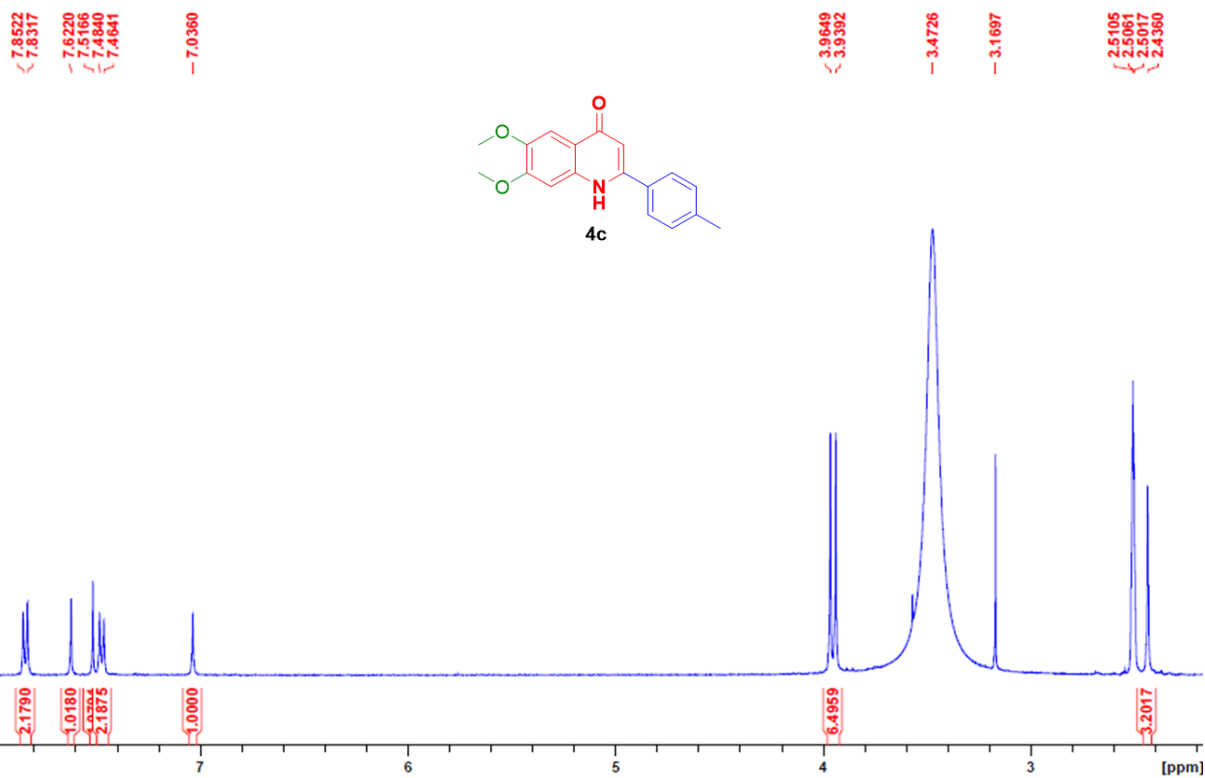
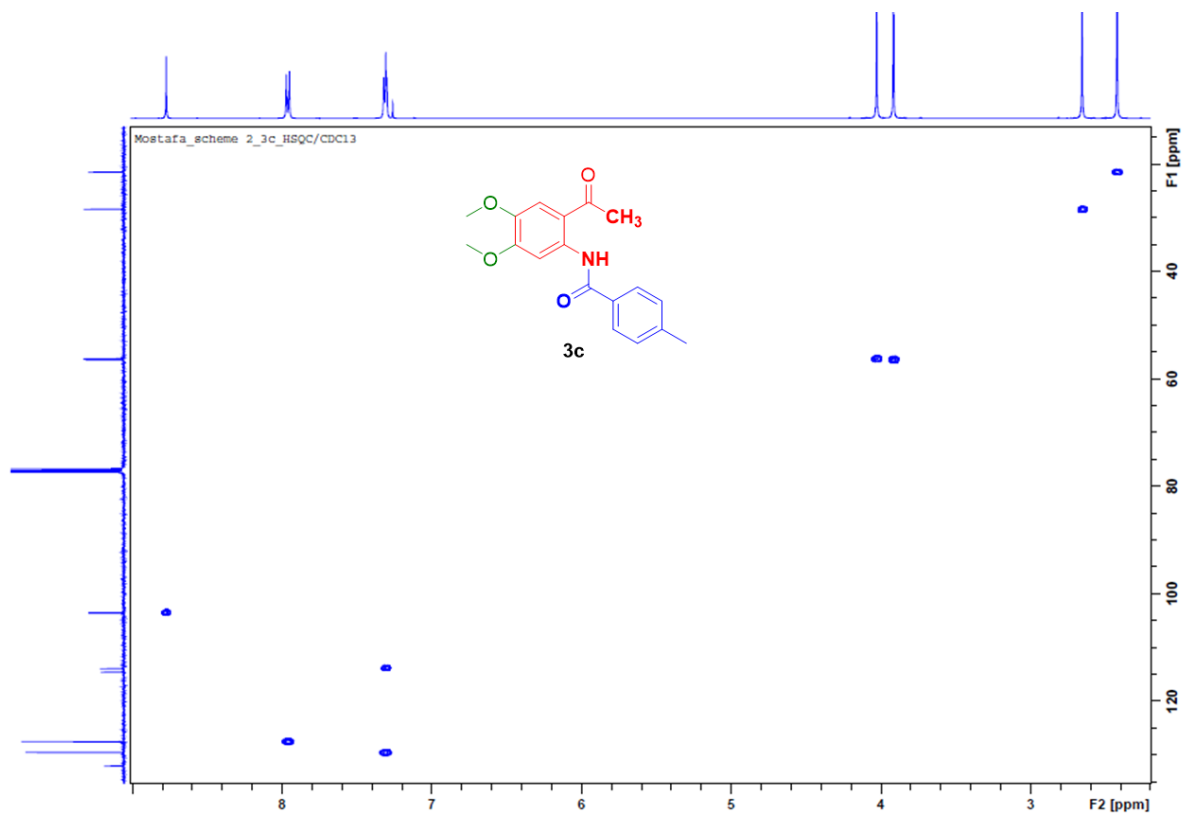
** Corresponding author: mabe@hiroshima-u.ac.jp

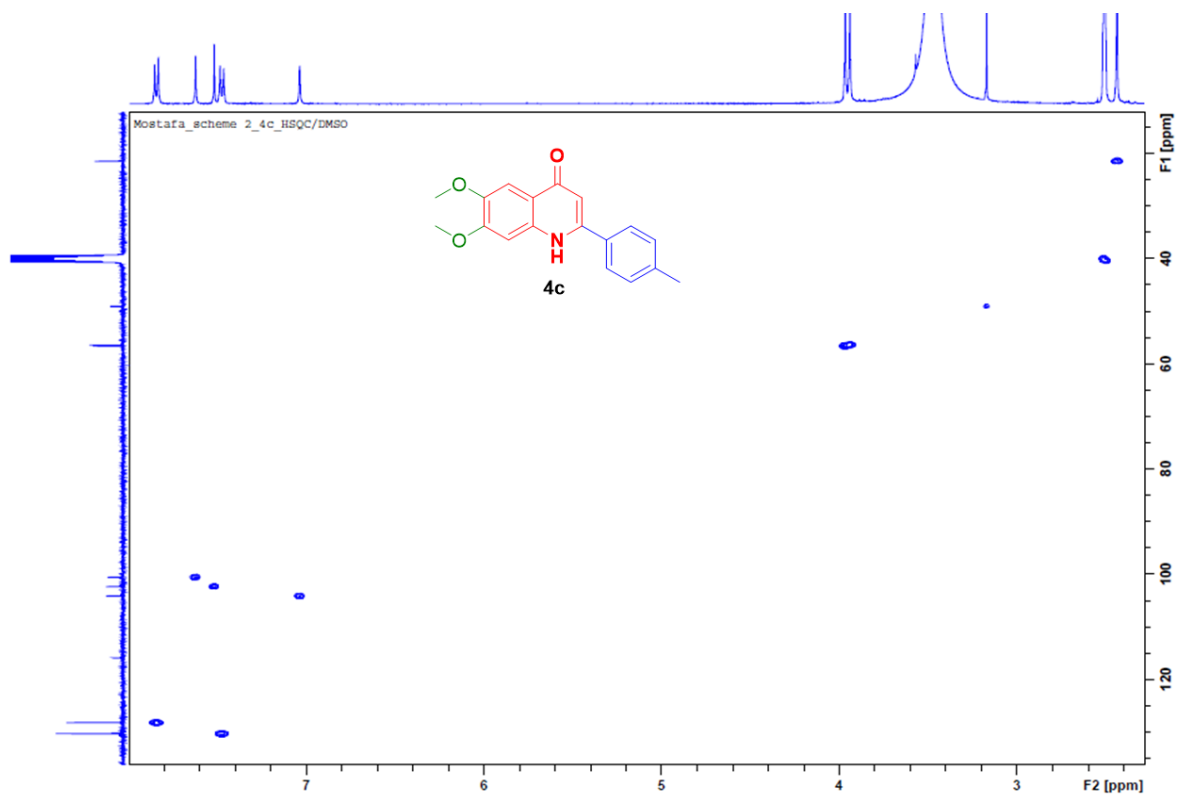
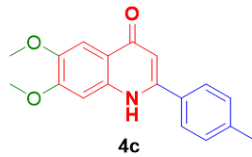
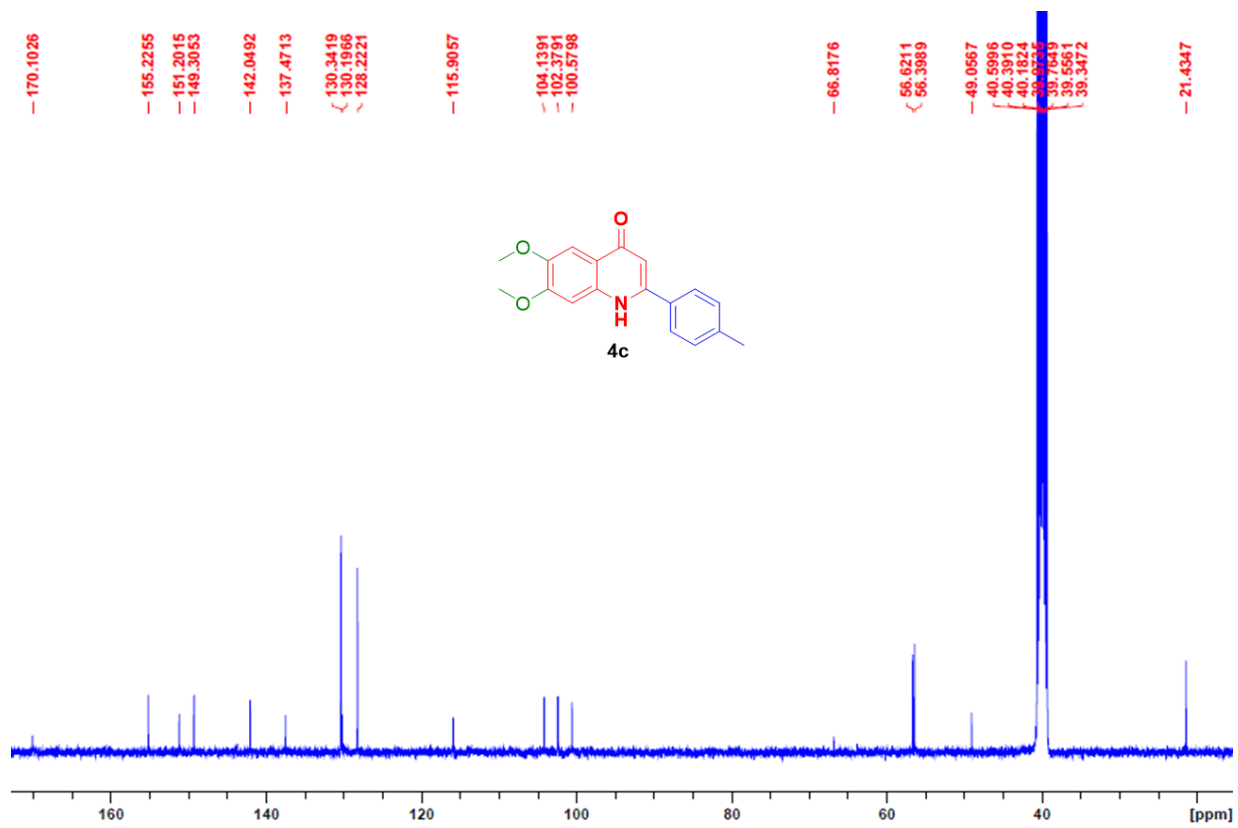
Table of contents

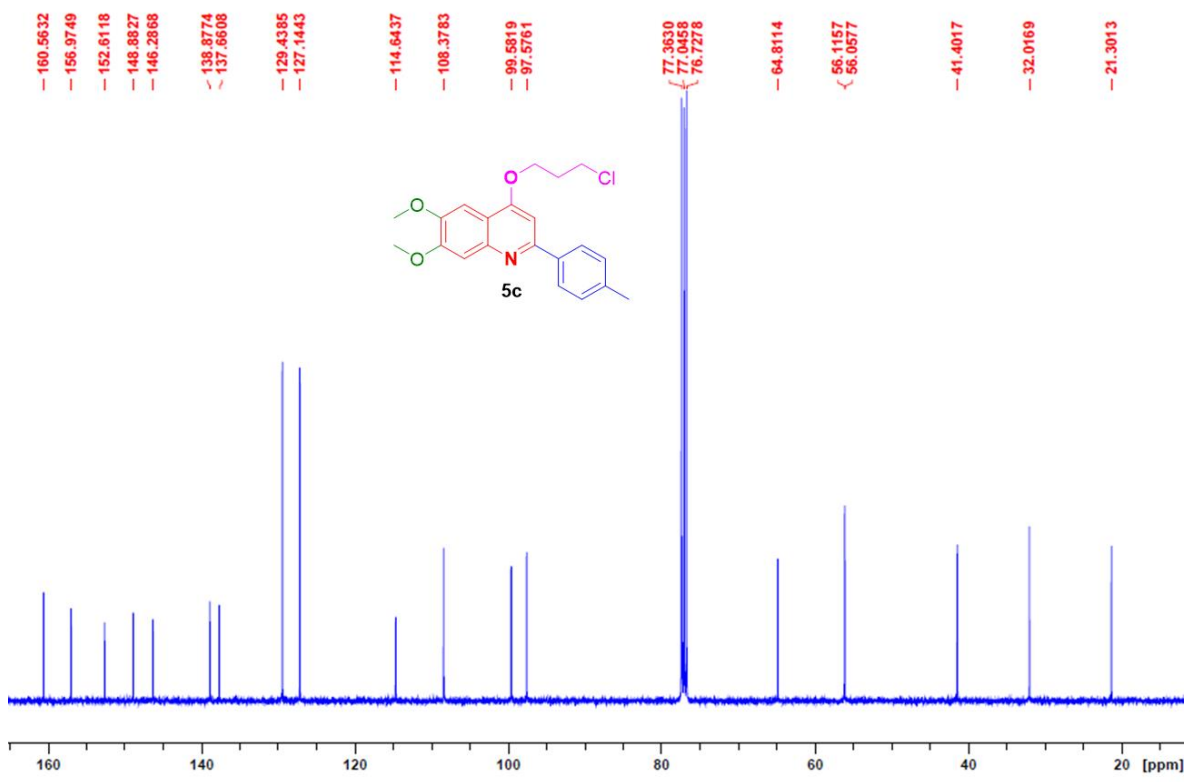
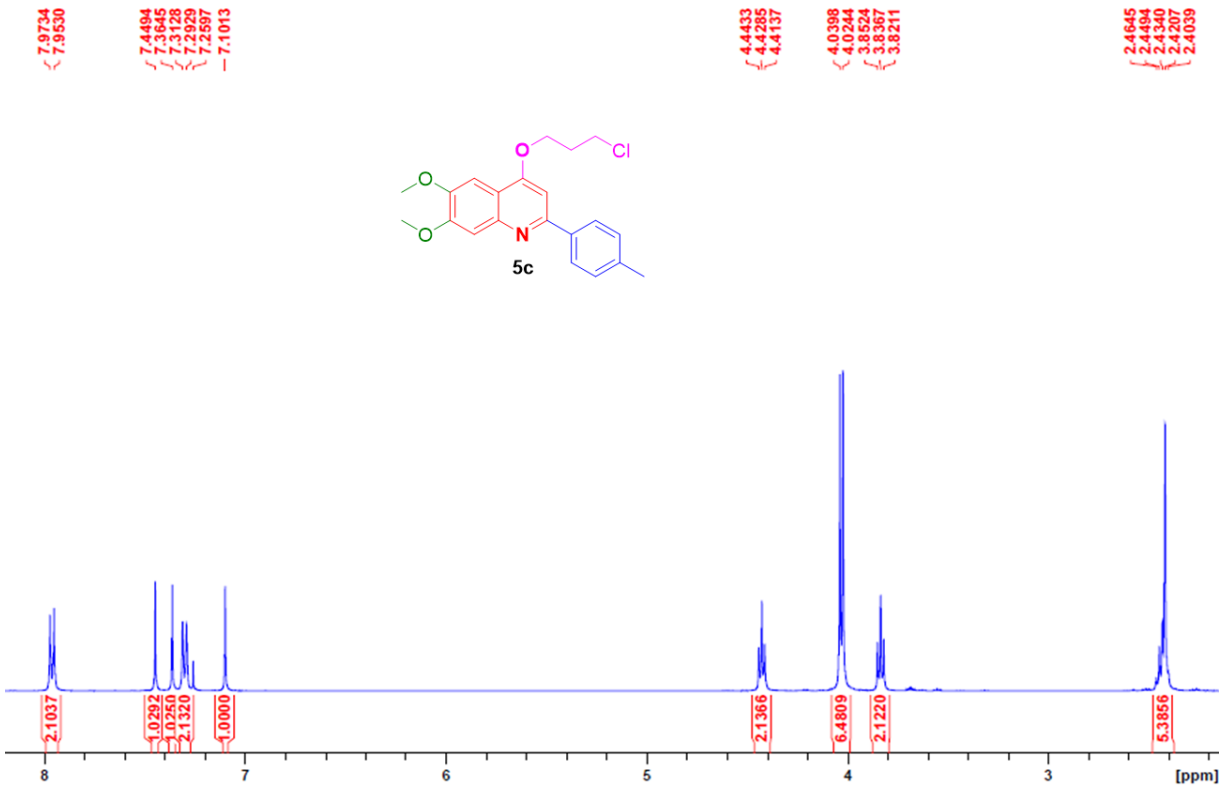
Content	Page
NMR data.....	S2
Topoisomerase I-mediated DNA cleavage assay.....	S114
Table S1. Kinase profiling.....	S118
Representative HPLC traces.....	S119

NMR data

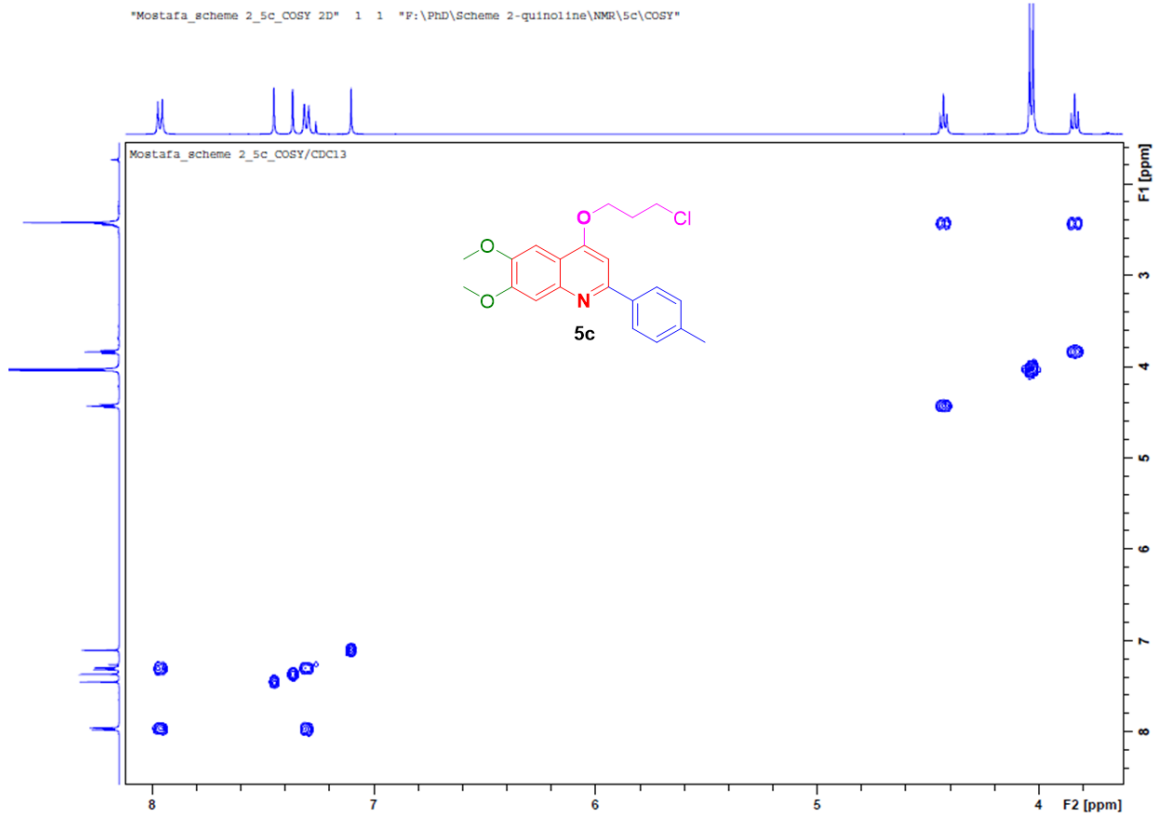








Mostafa_scheme 2_5c_COSY 2D 1 1 *F:\PhD\Scheme 2-quinoline\NMR\5c\COSY*



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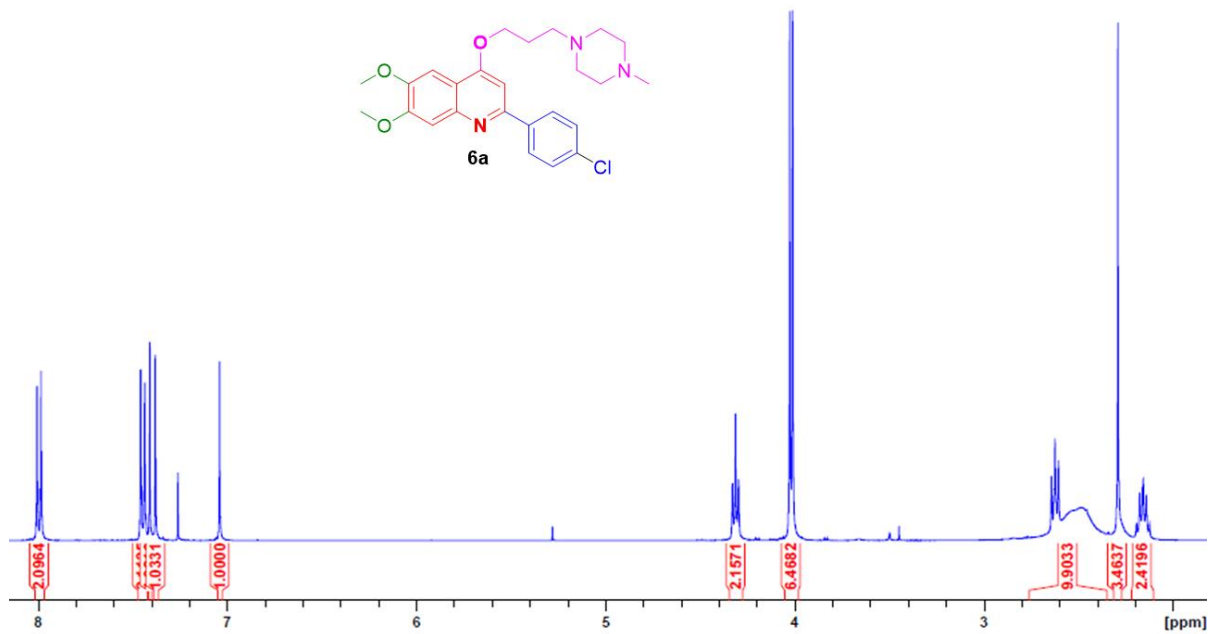
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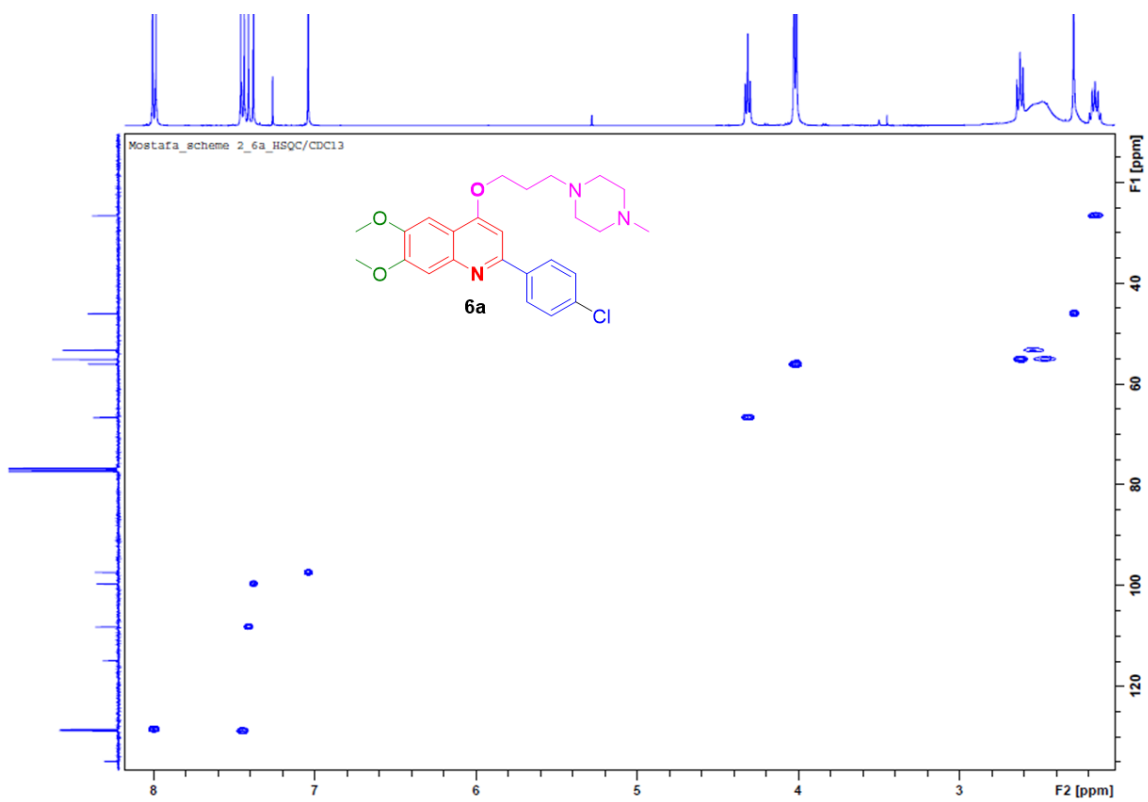
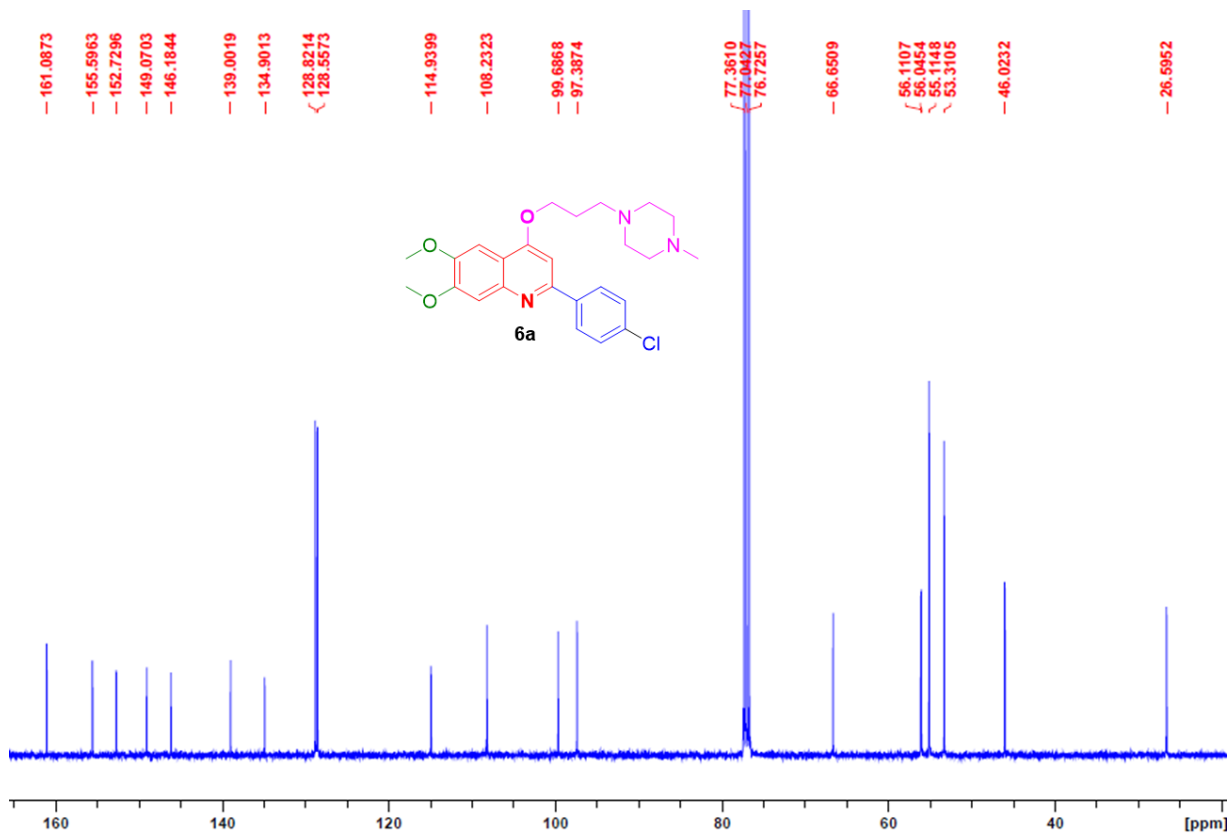
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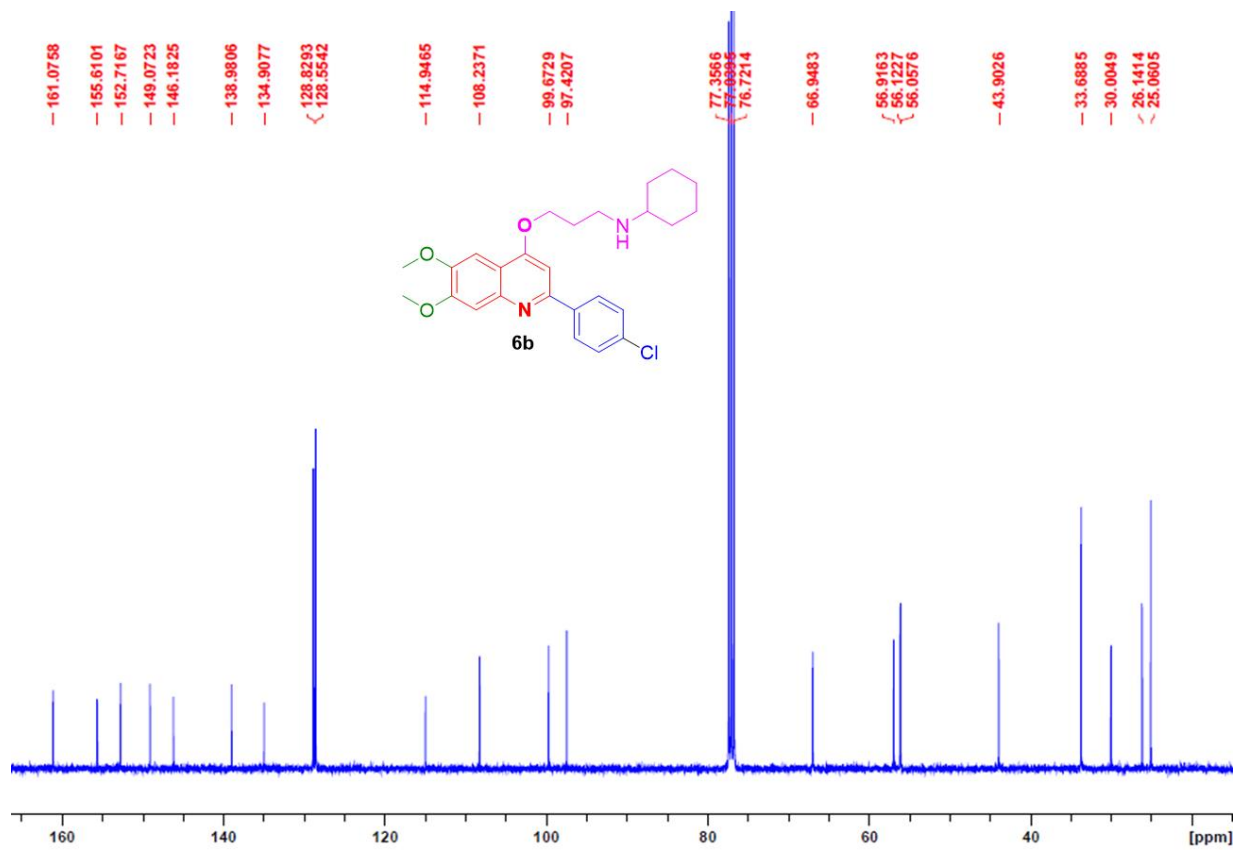
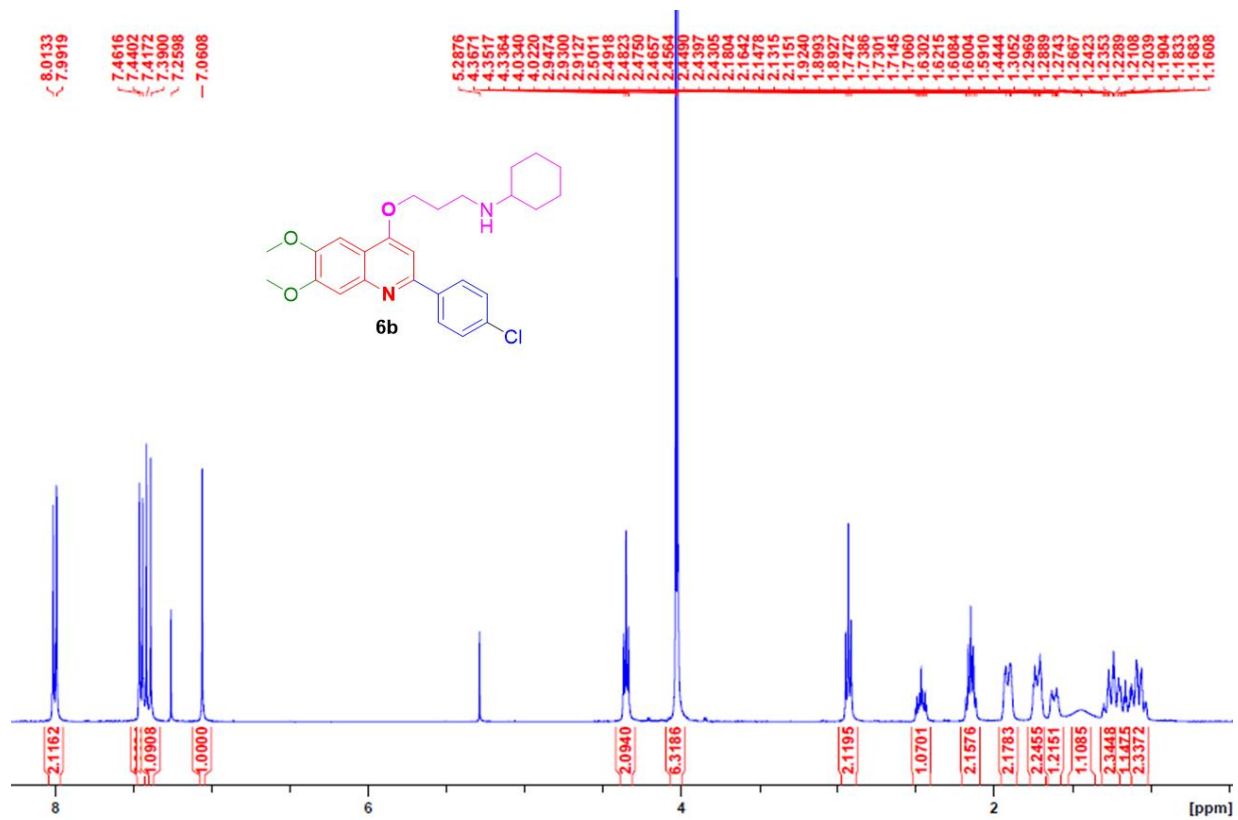
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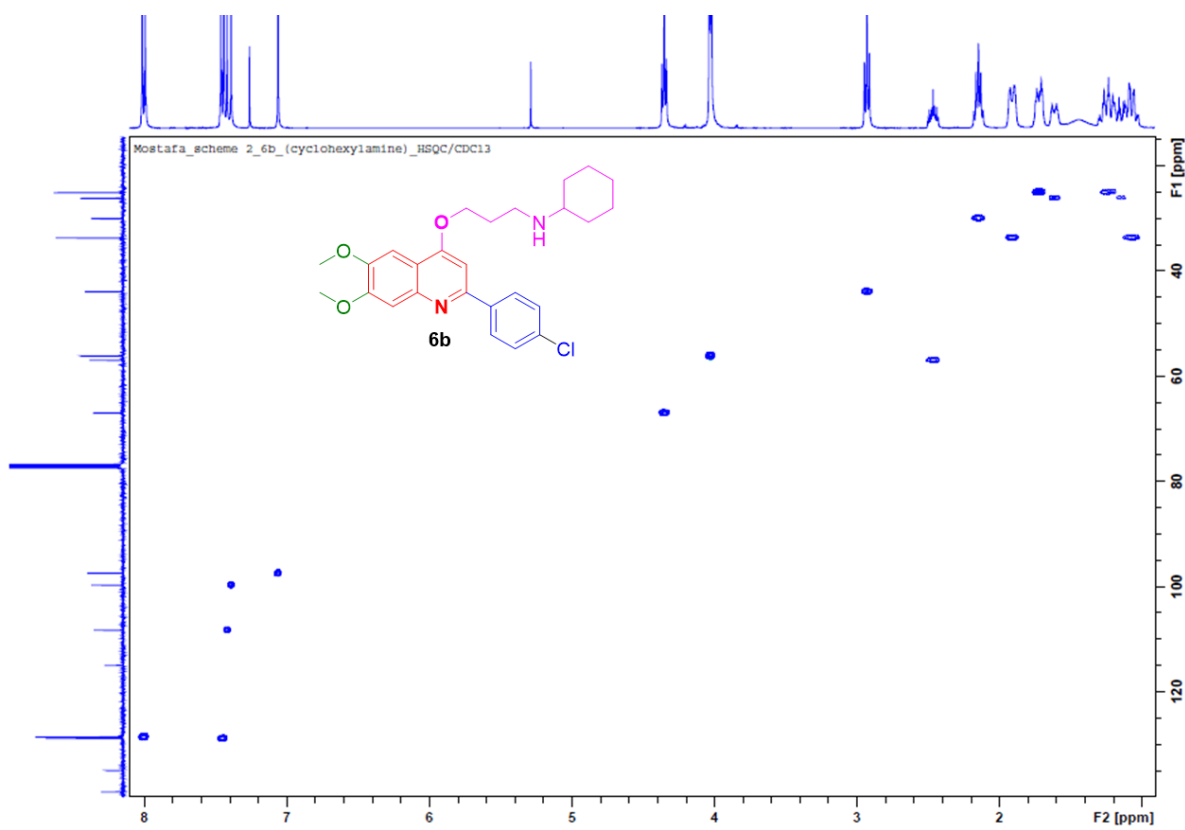
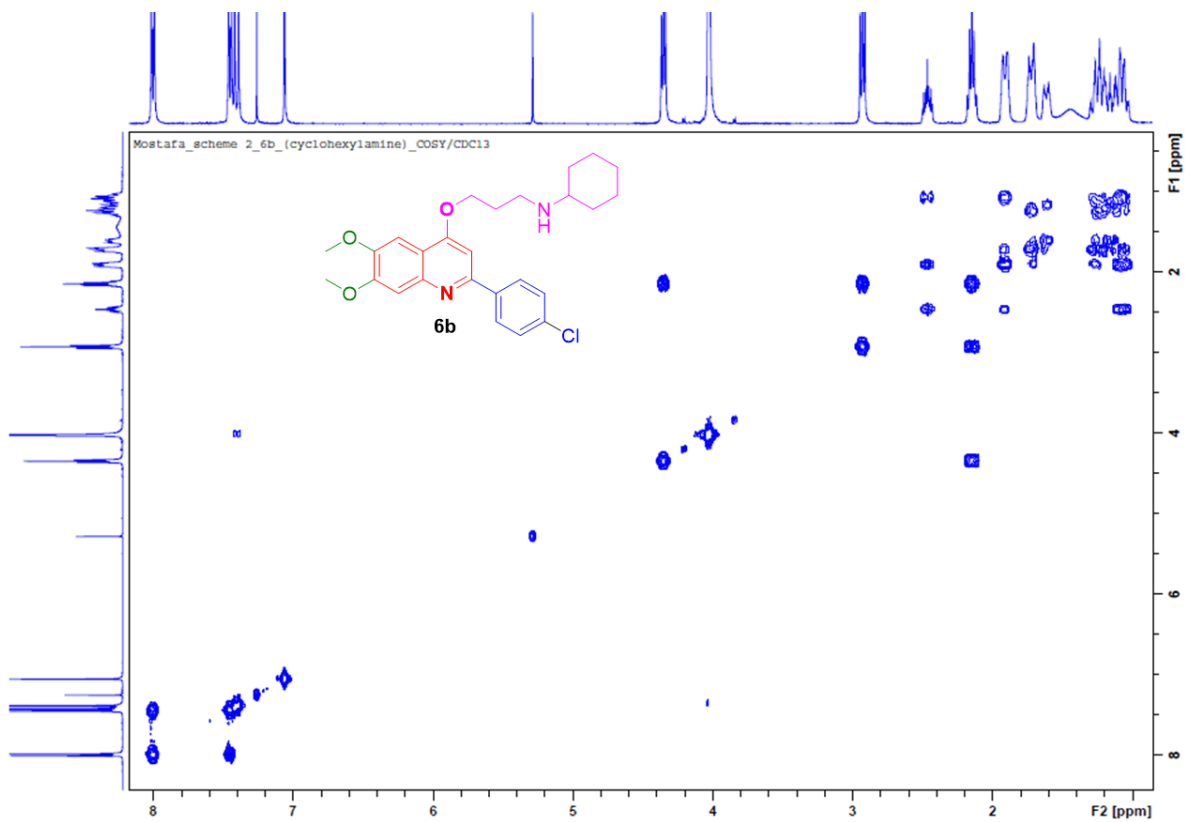
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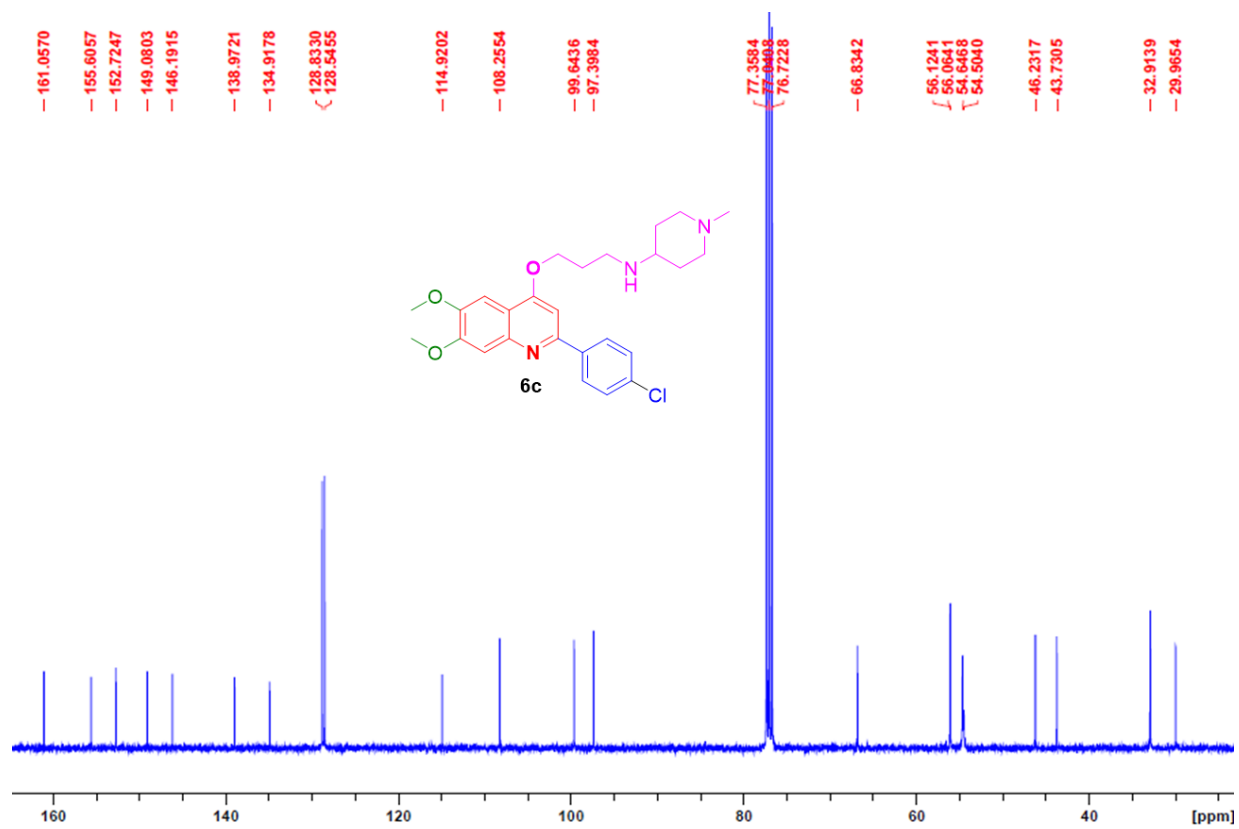
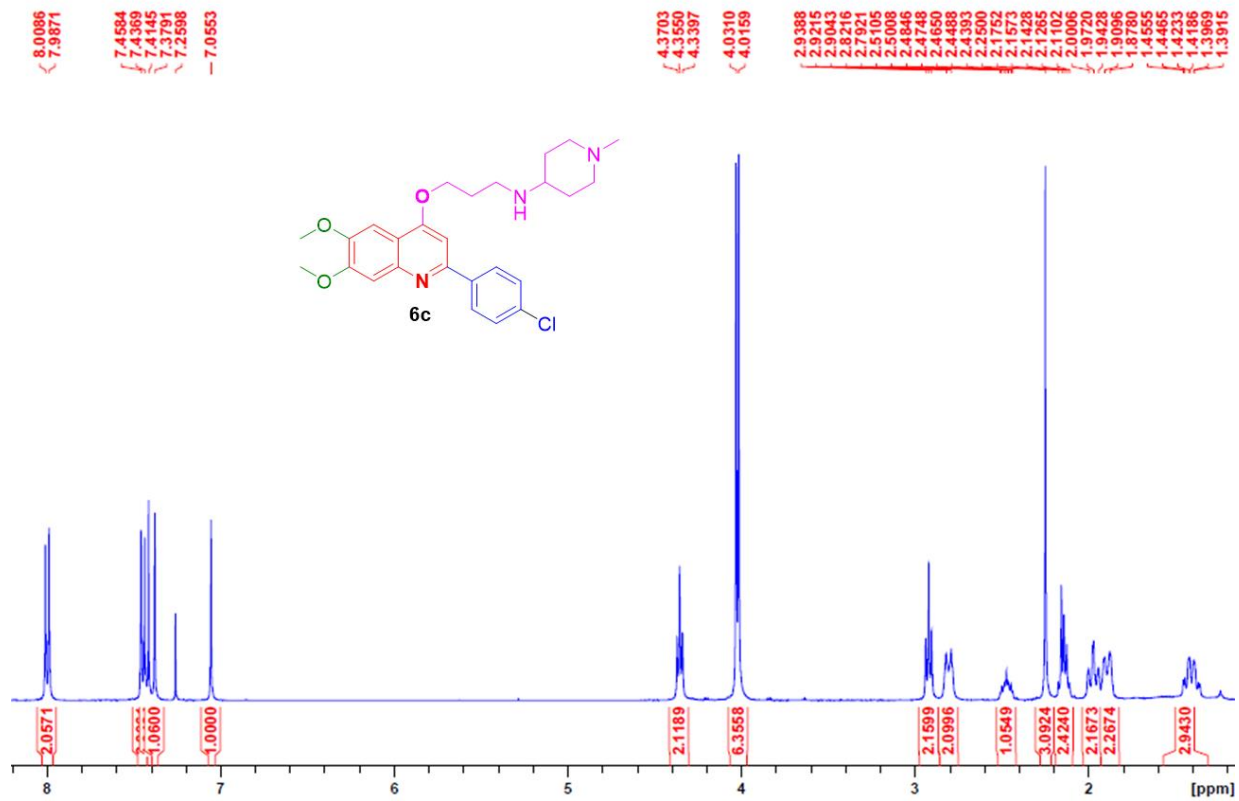
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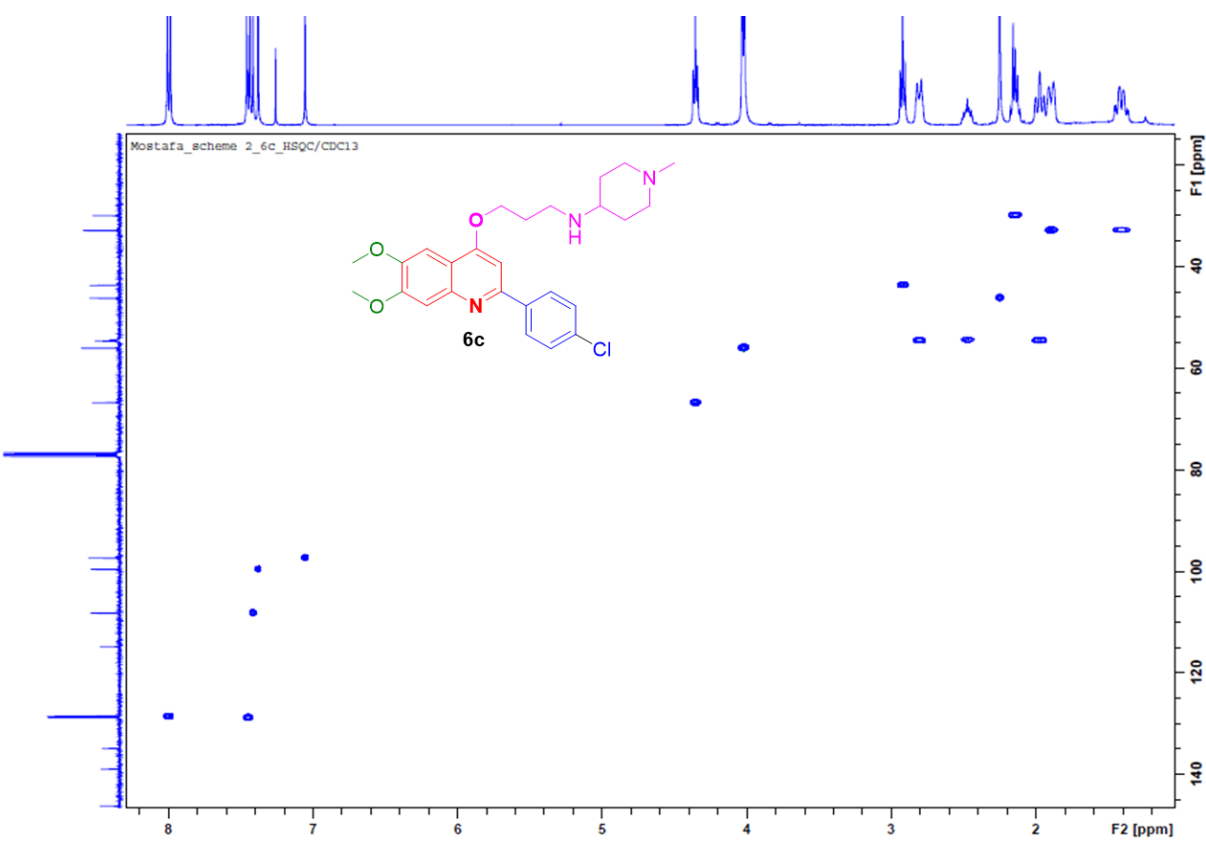
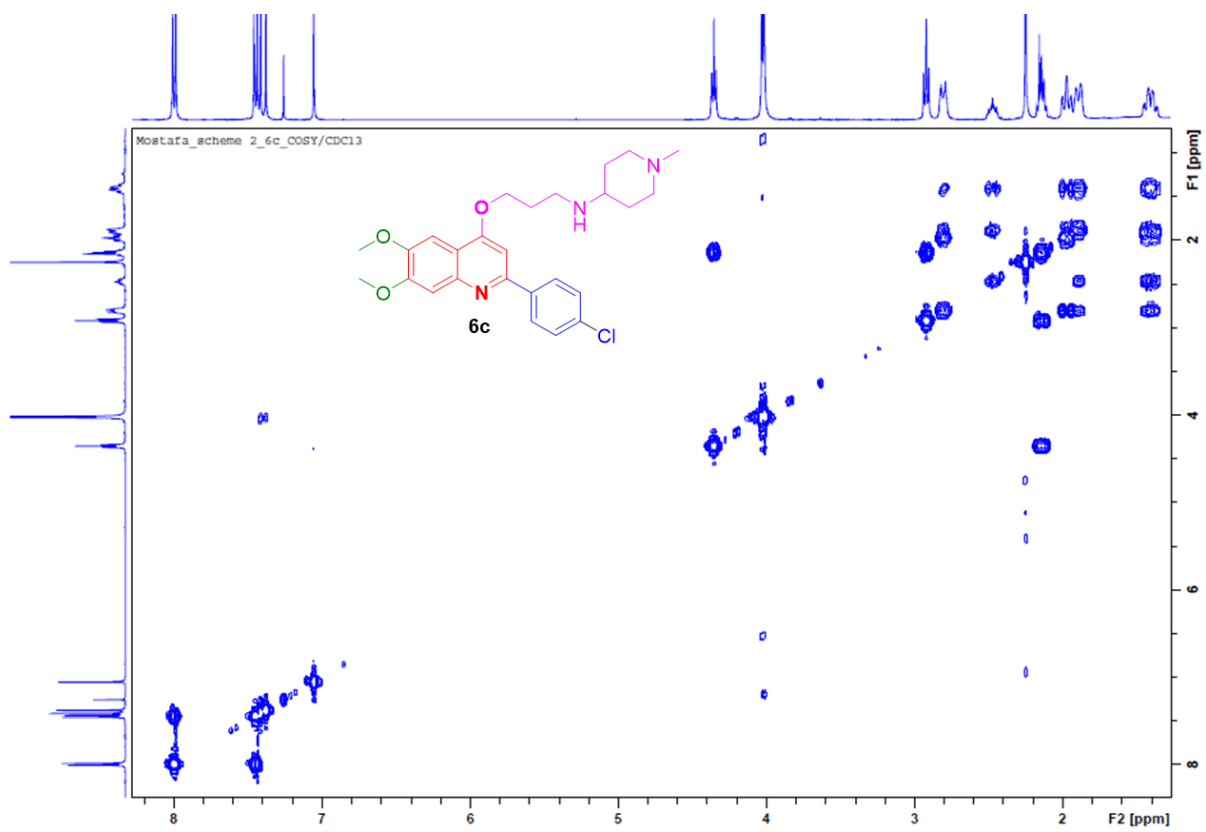
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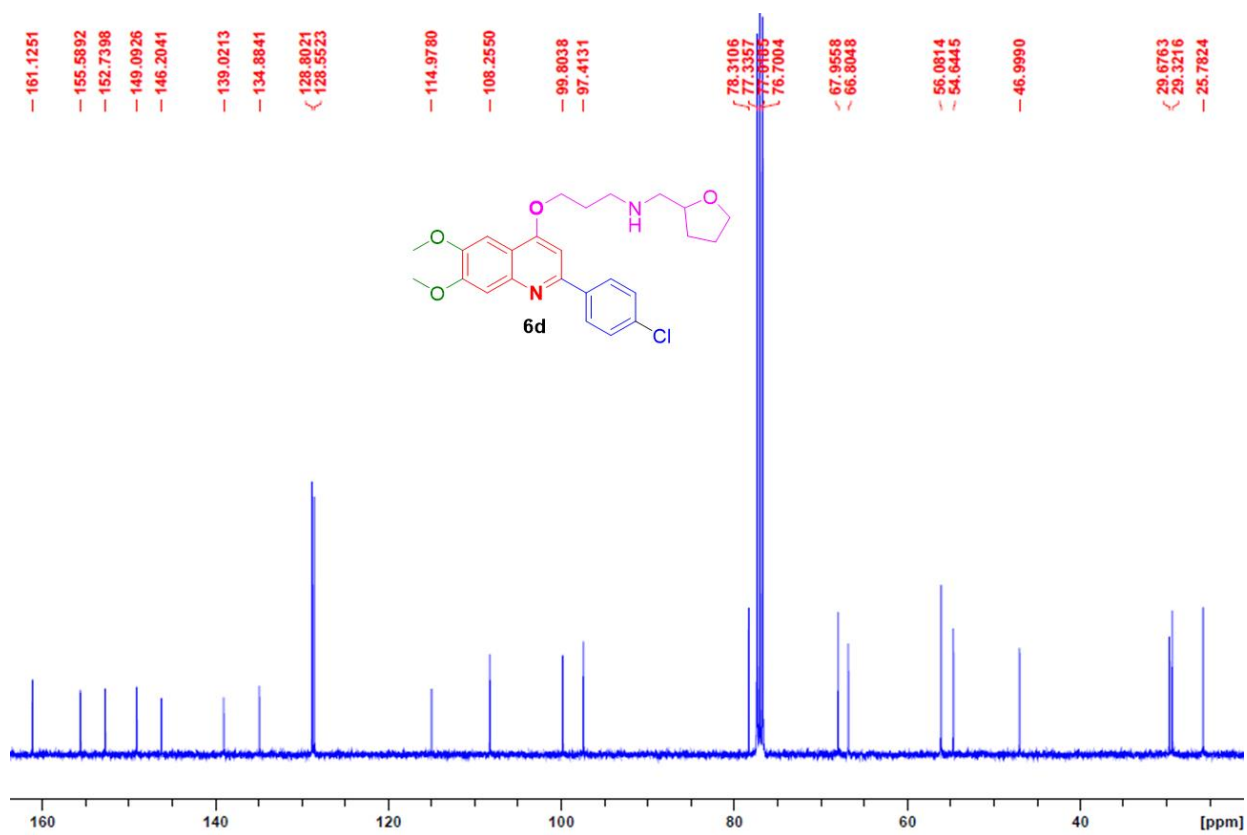
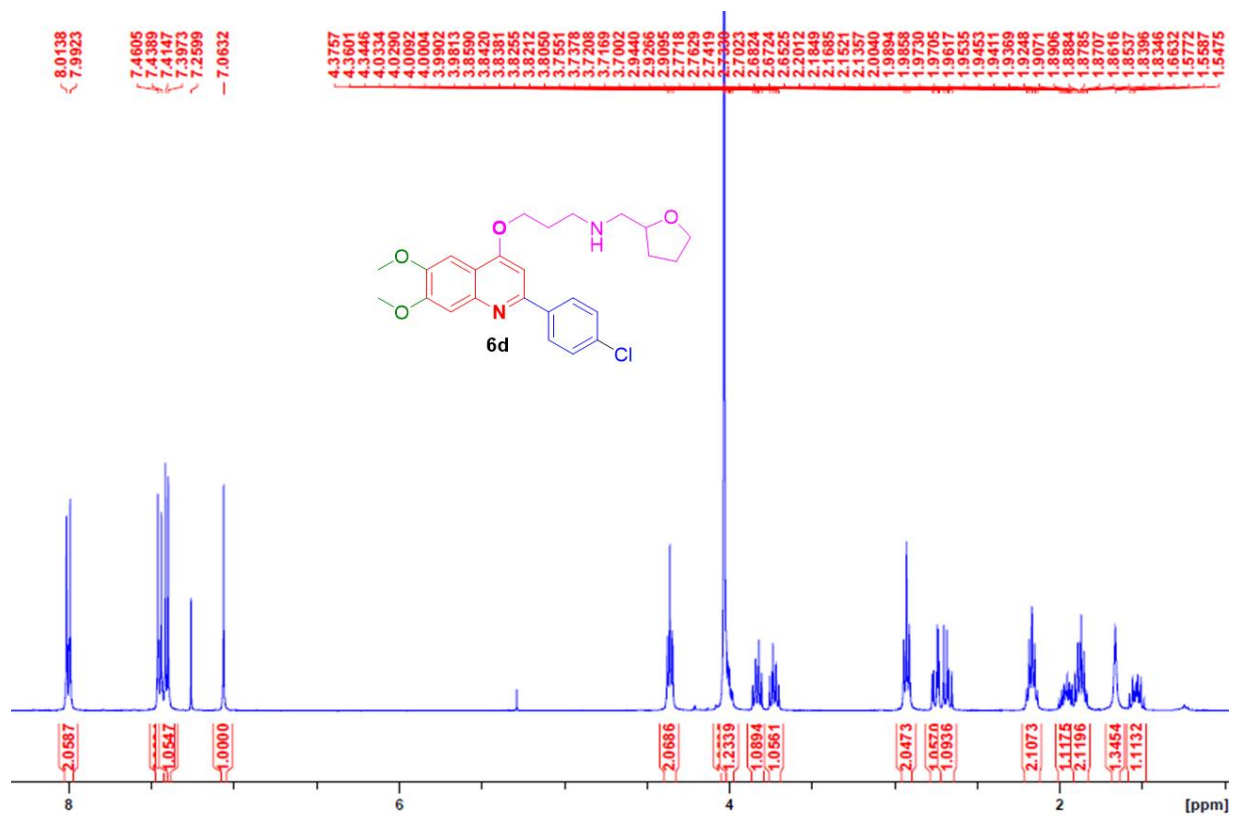


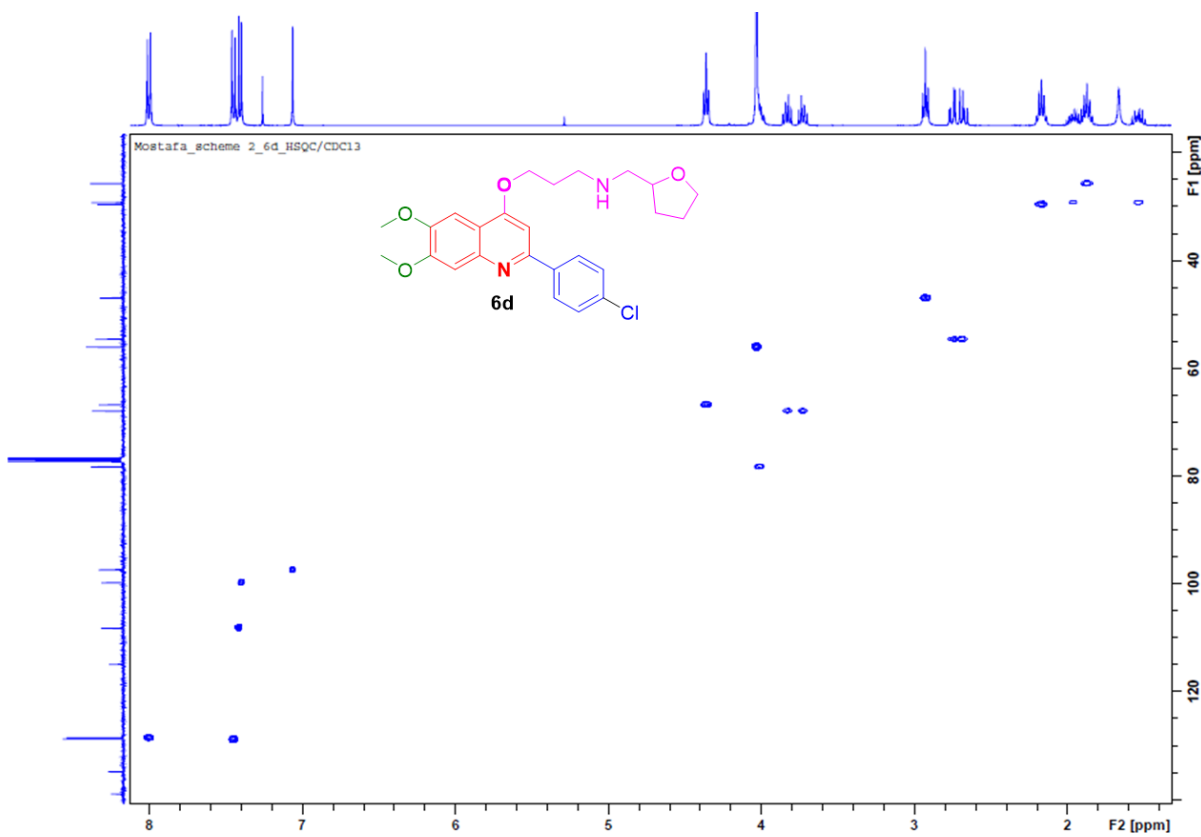
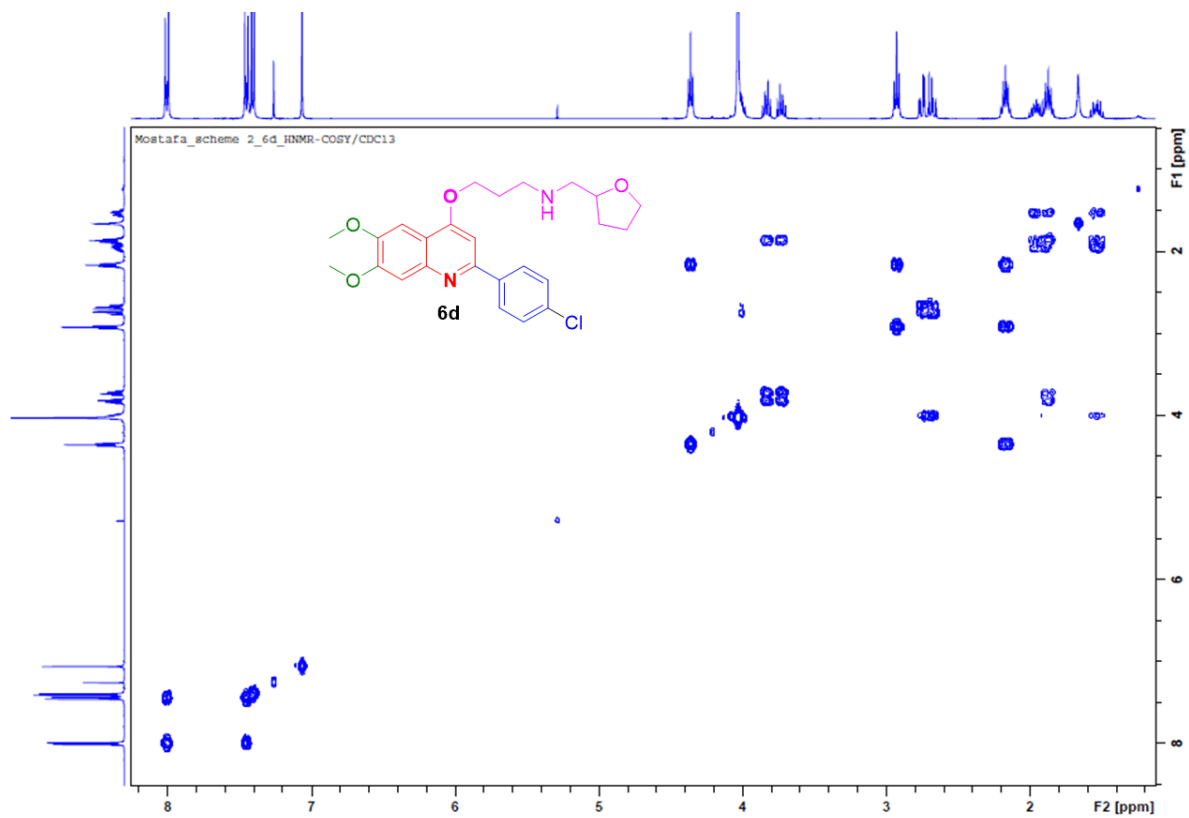


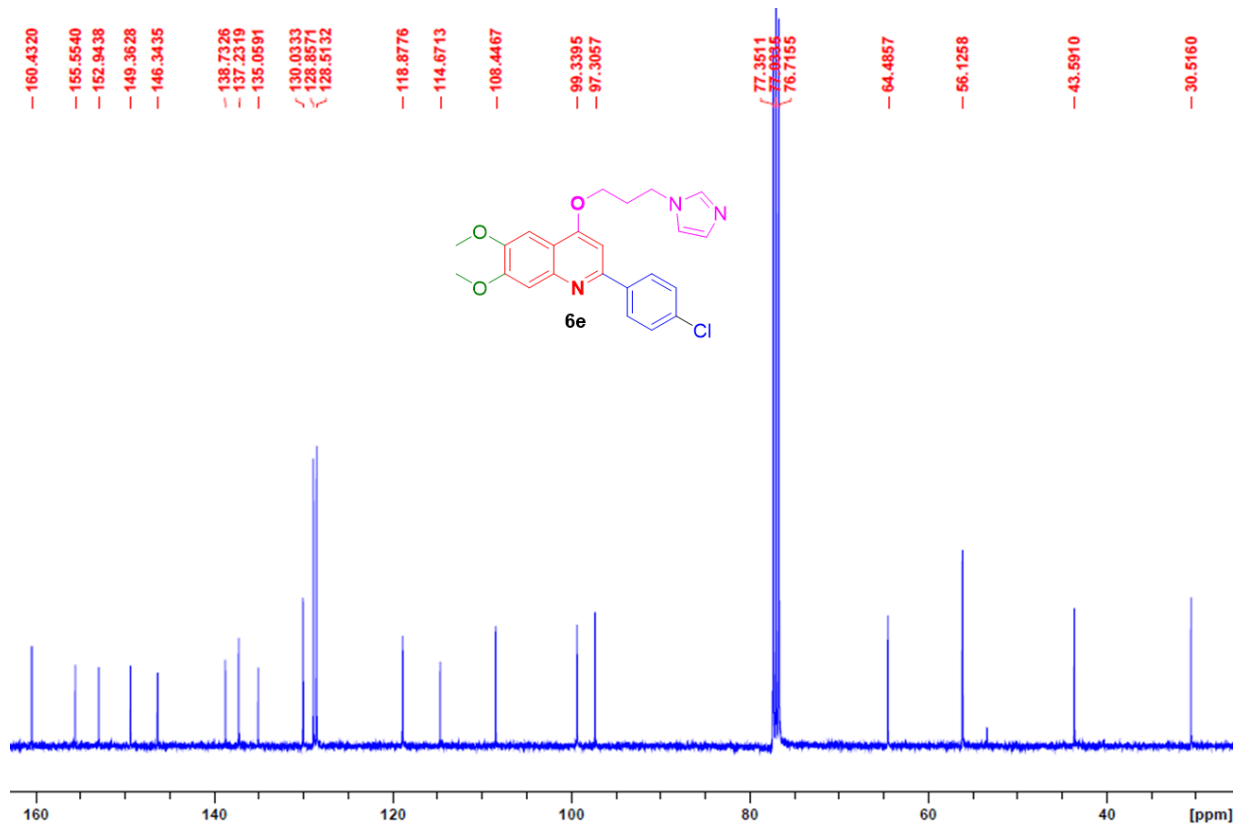
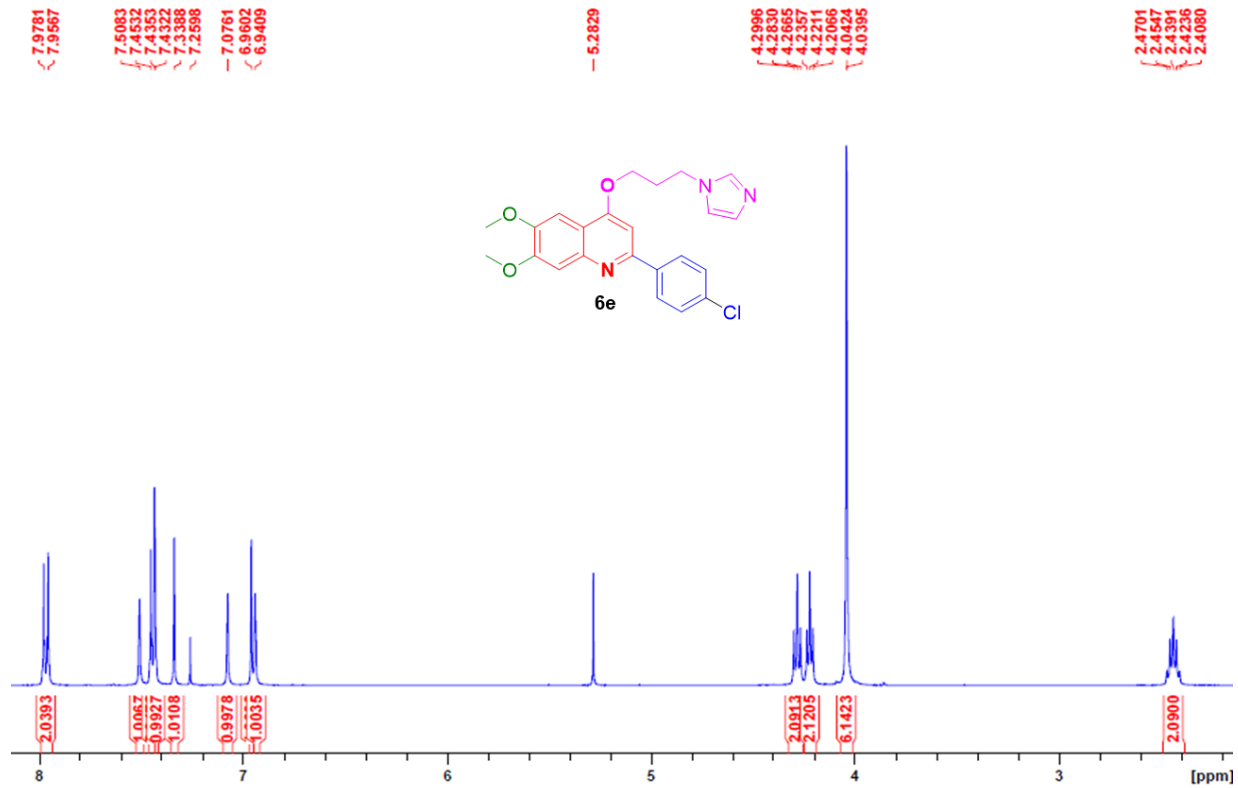


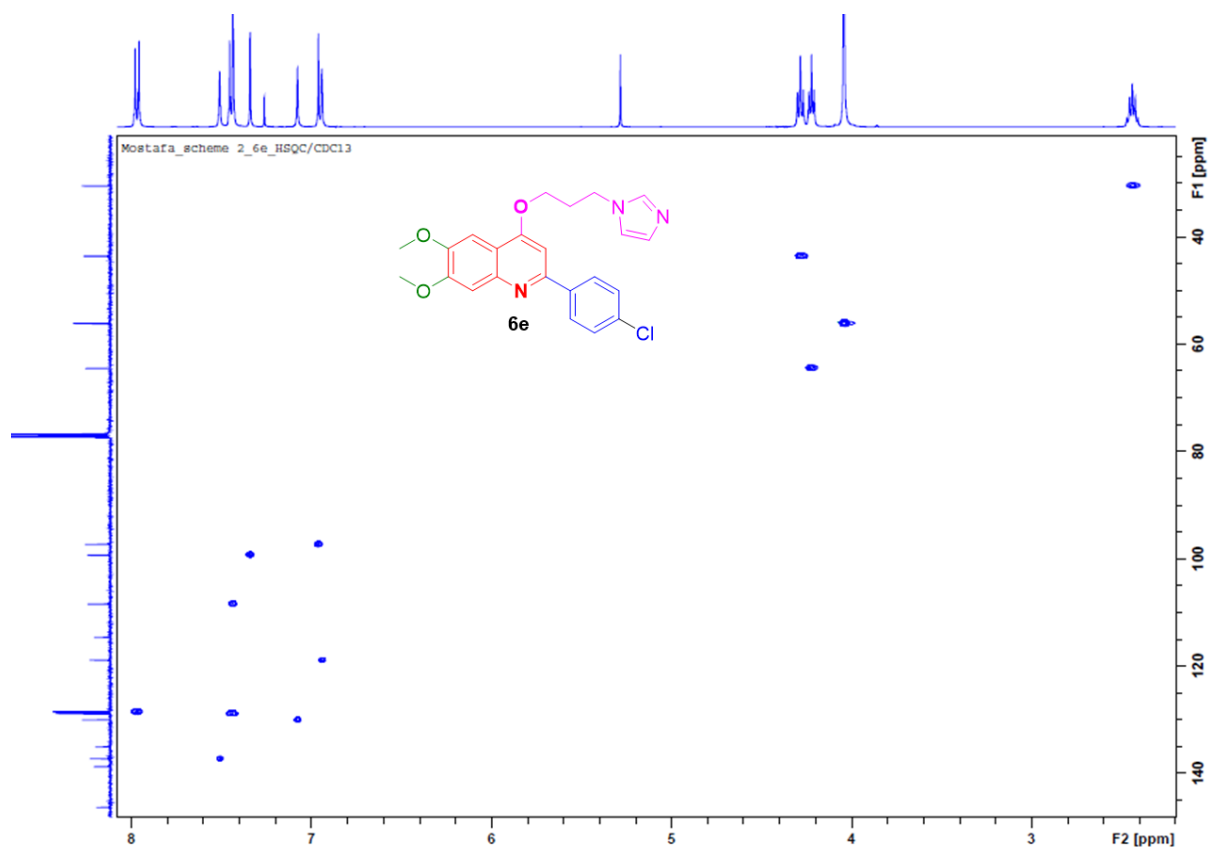
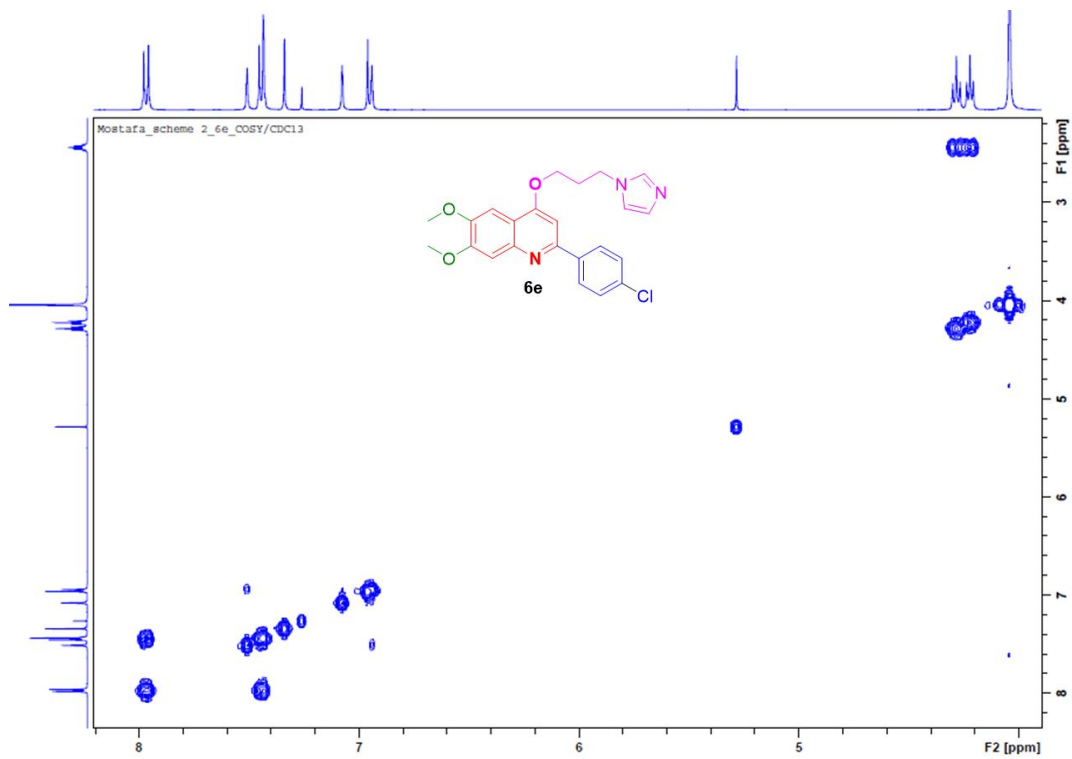


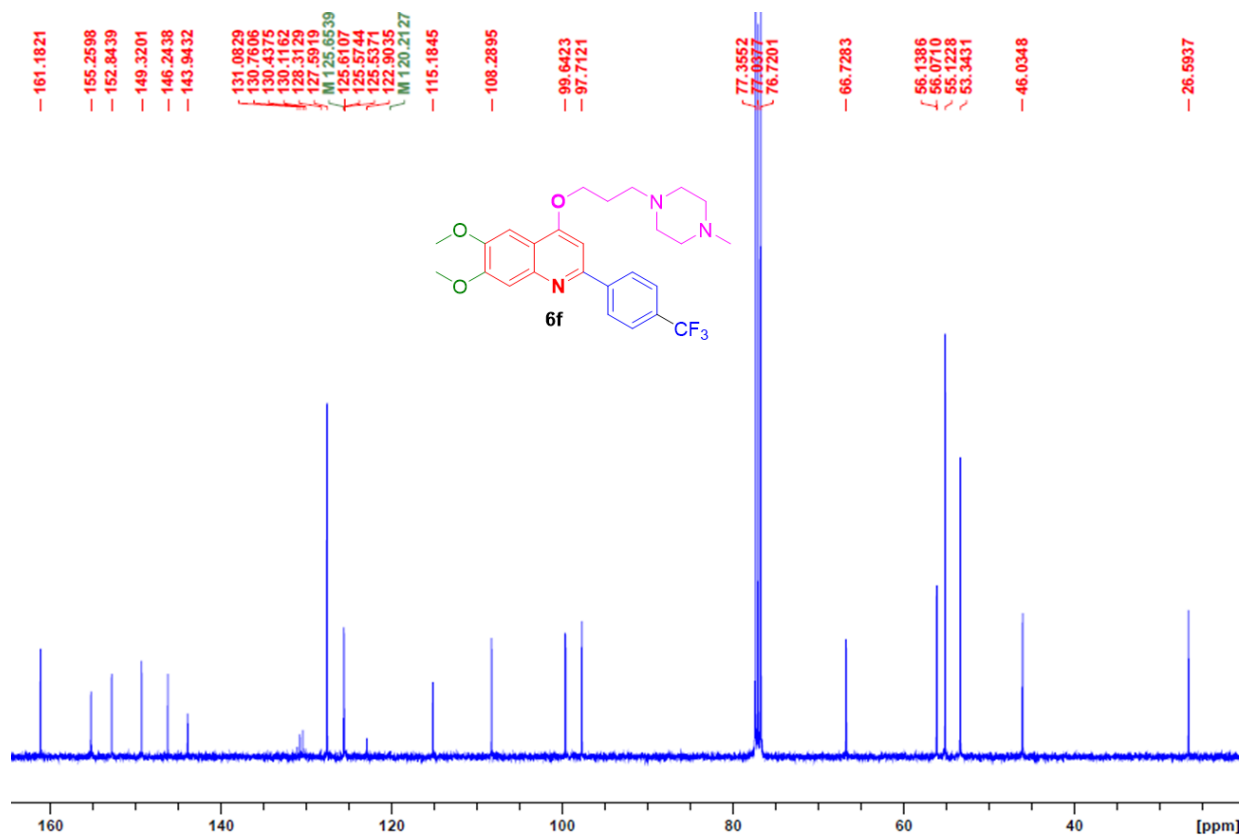
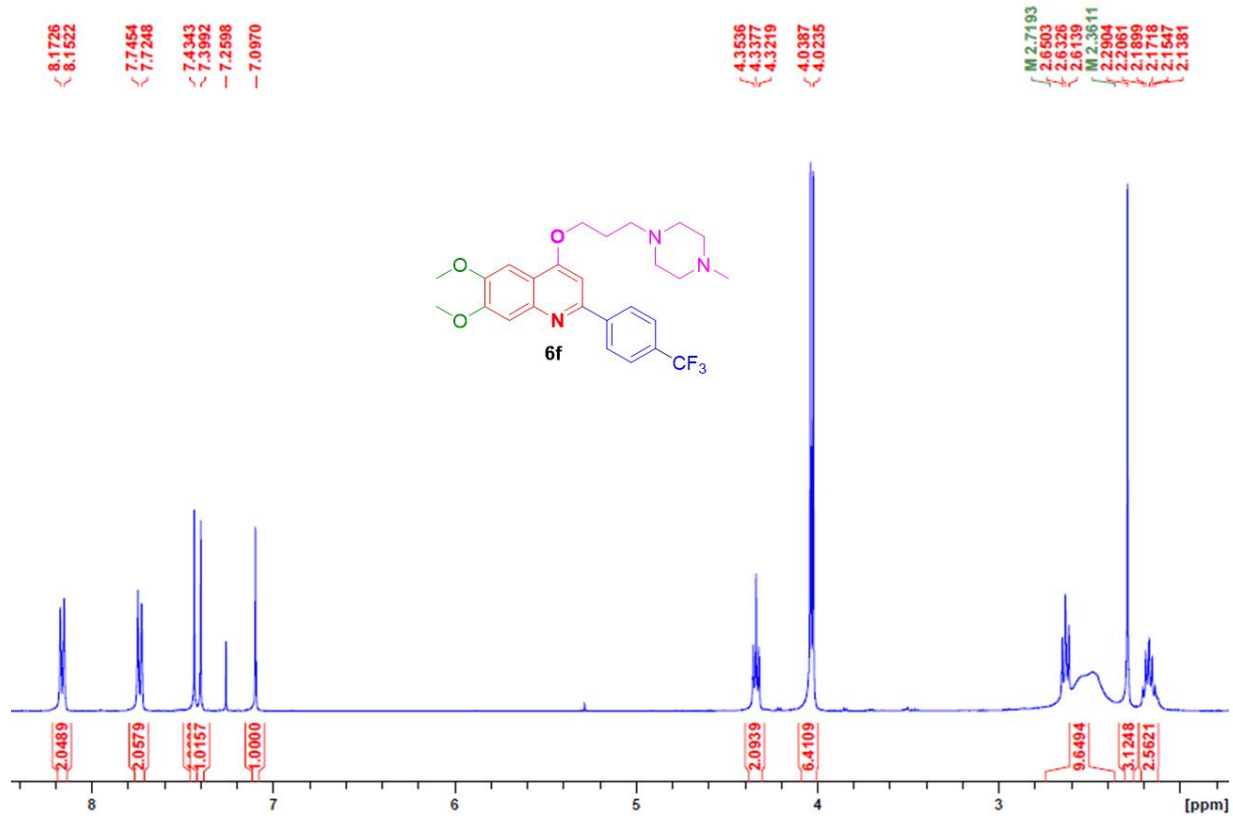




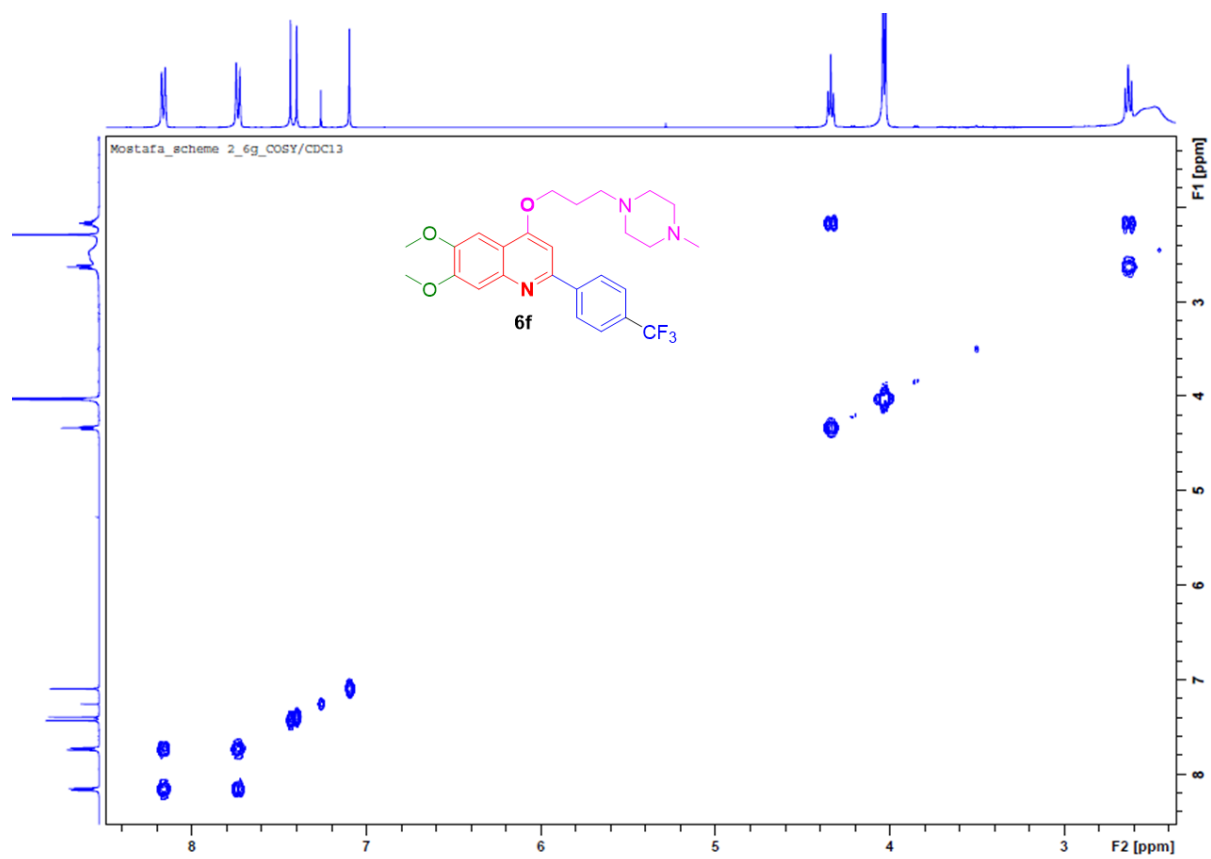
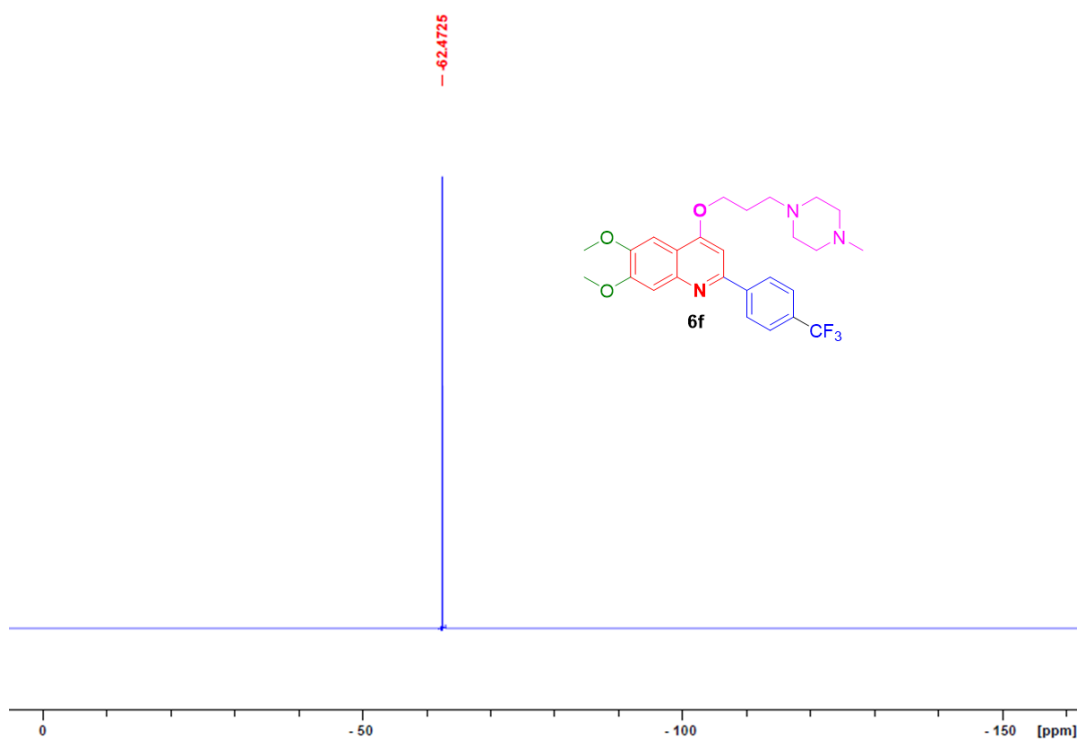


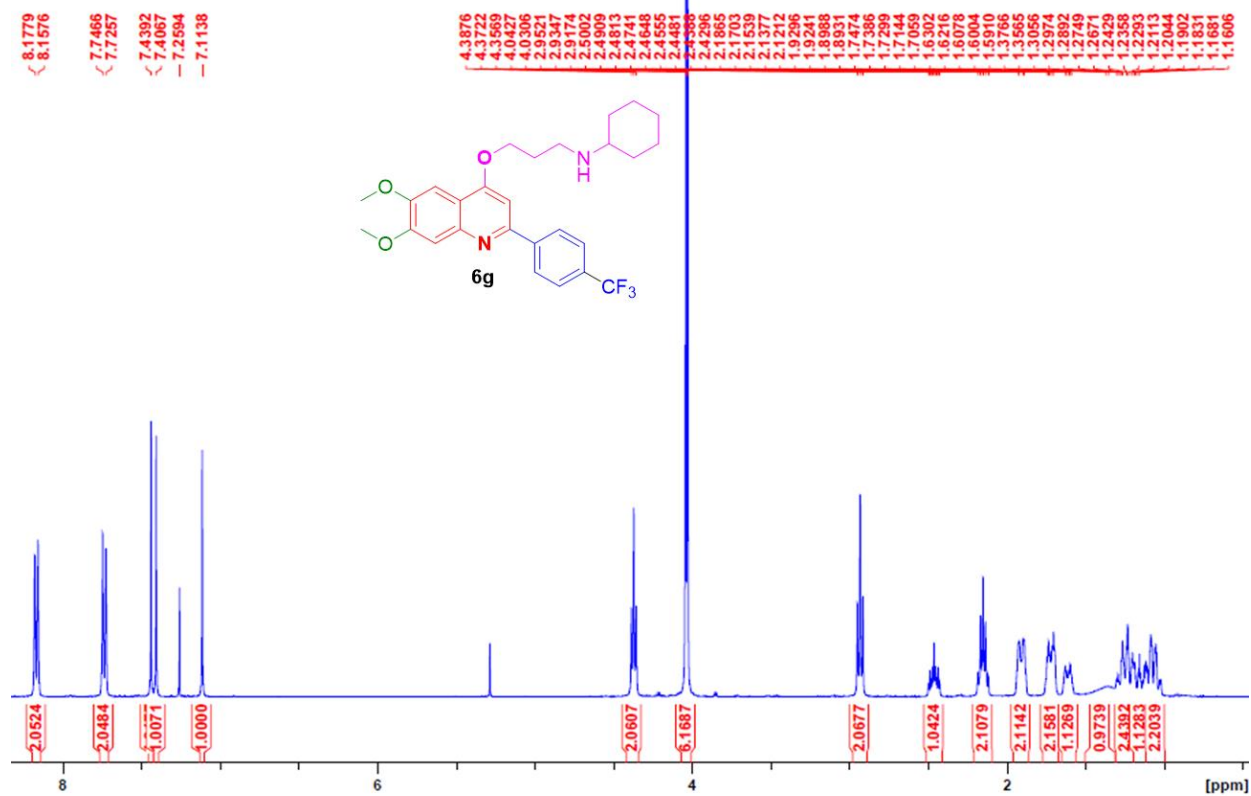
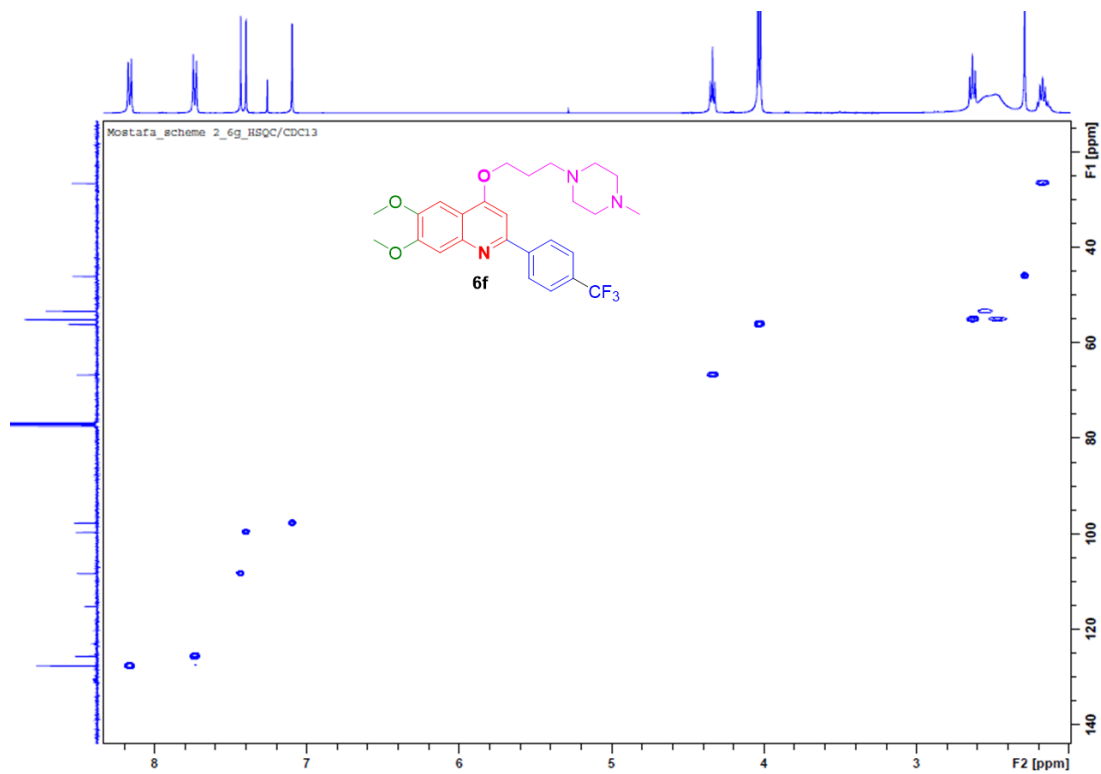


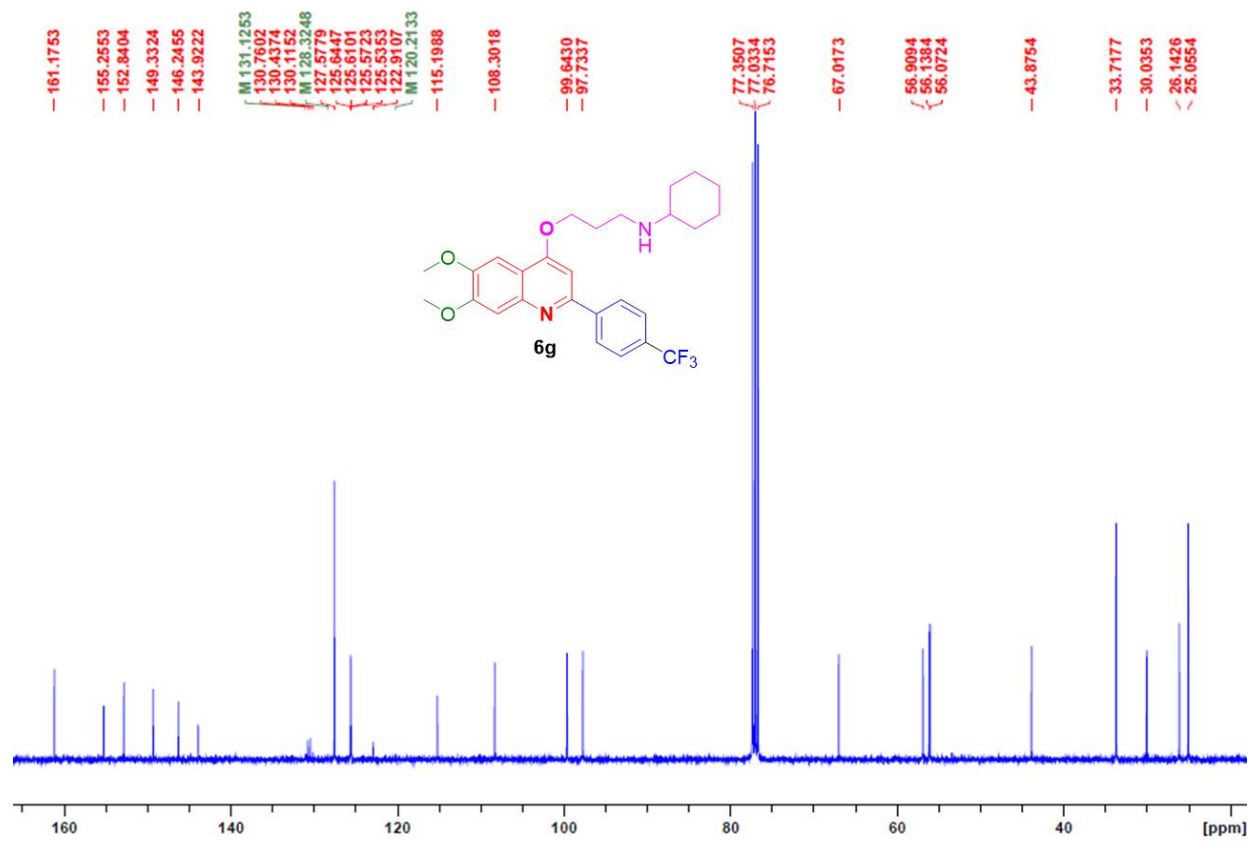




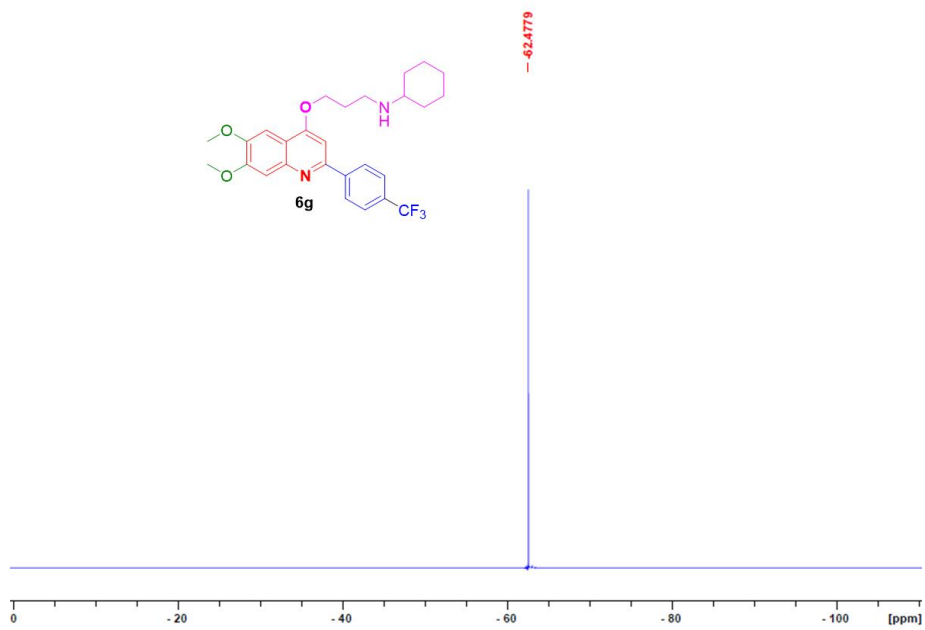
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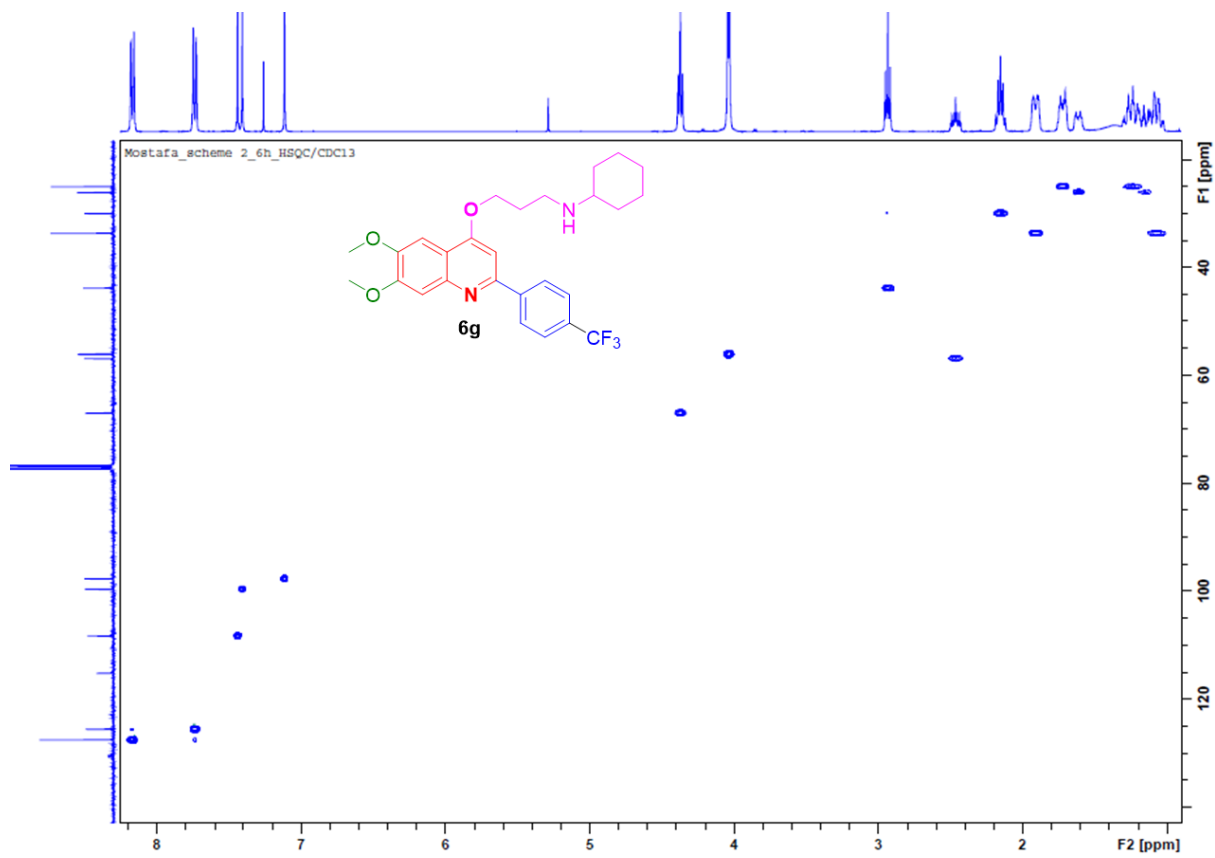
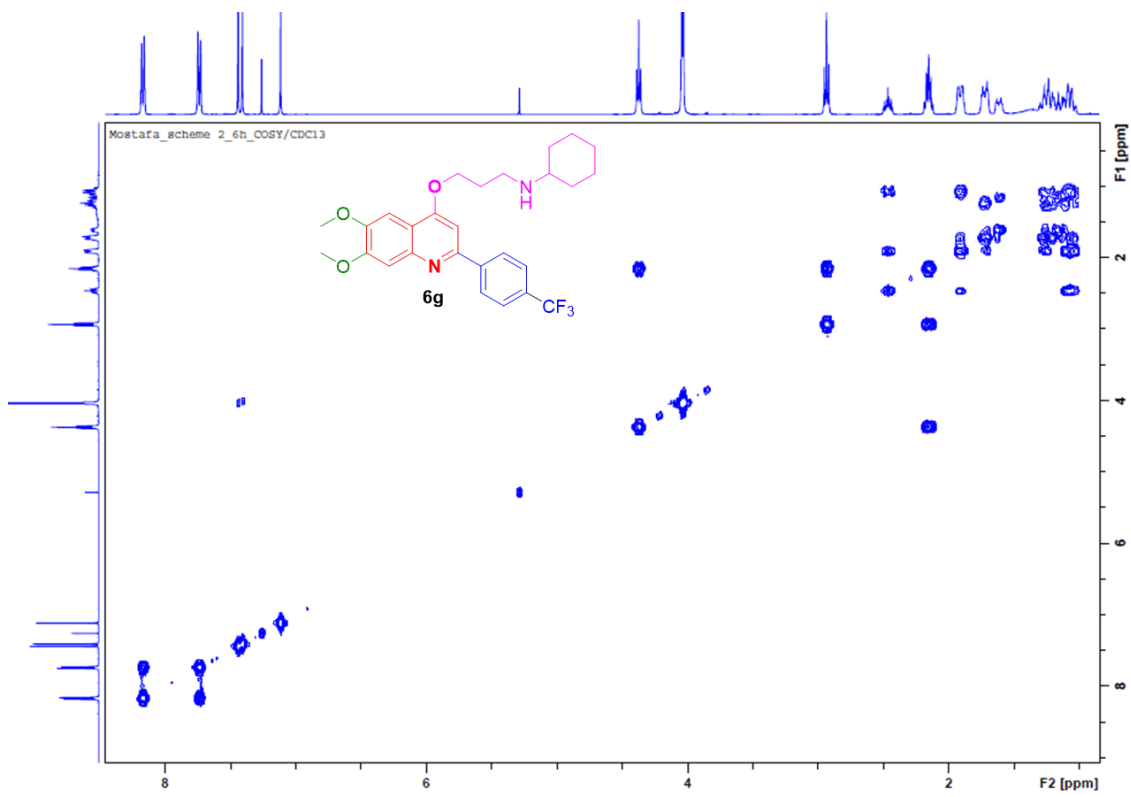


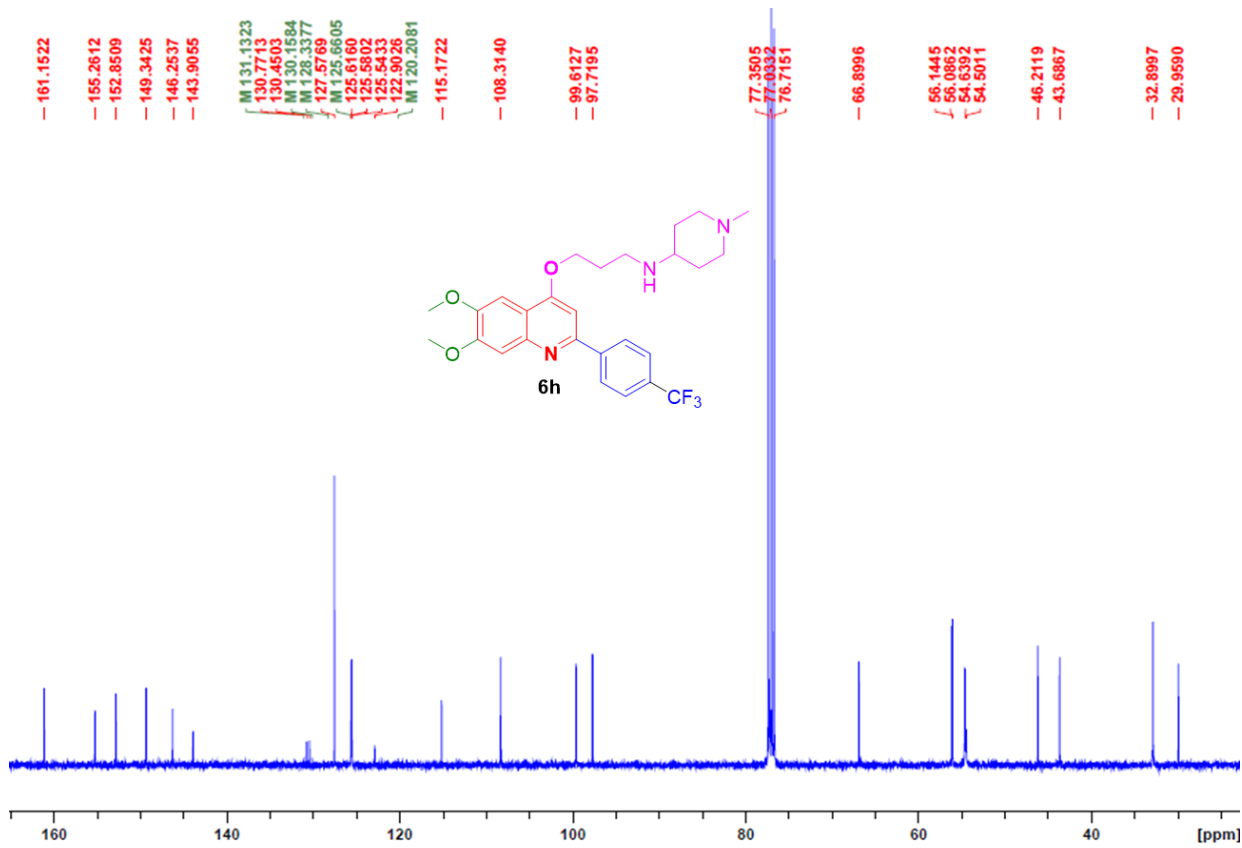
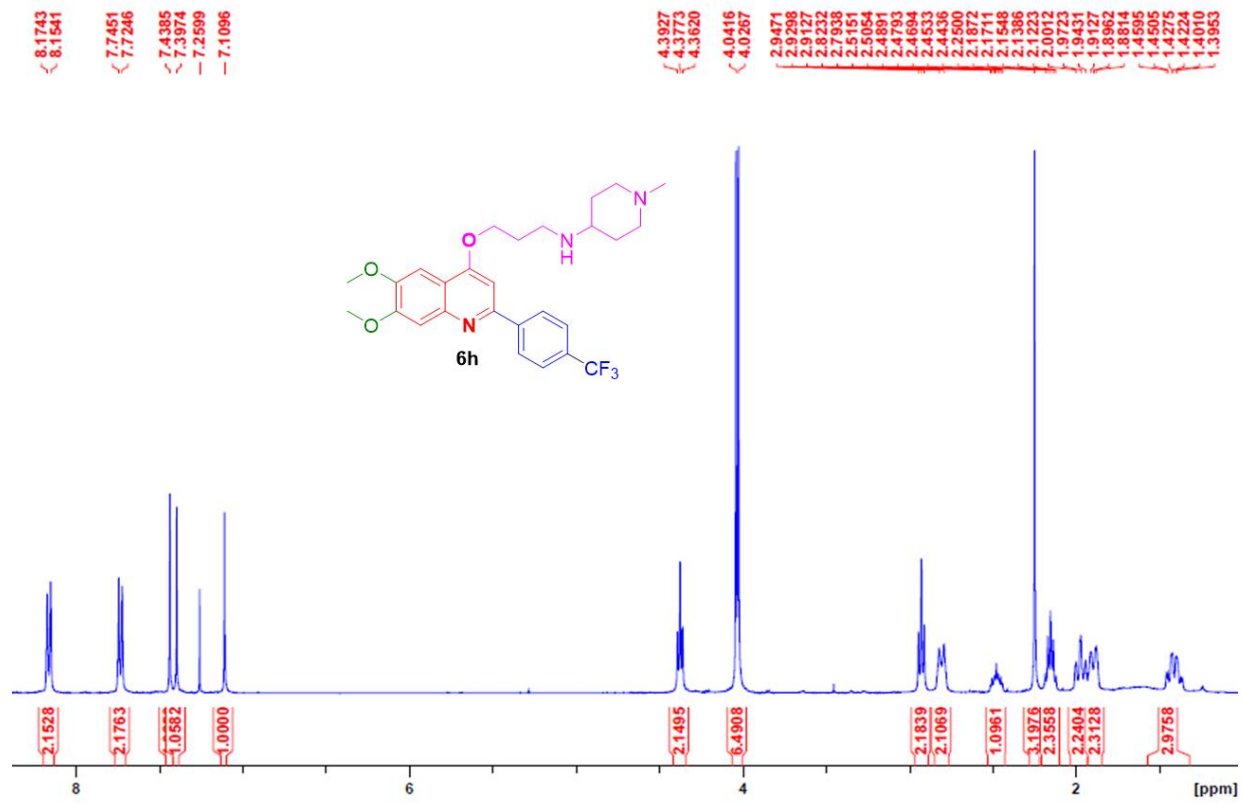




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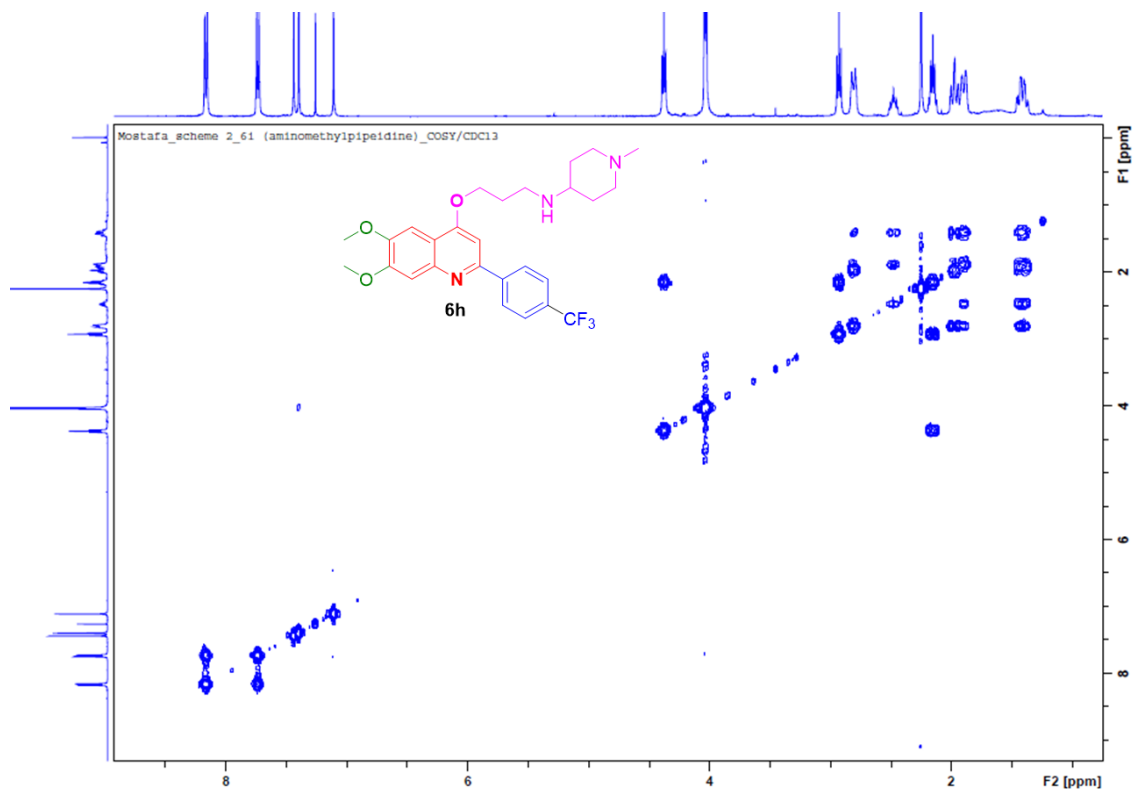
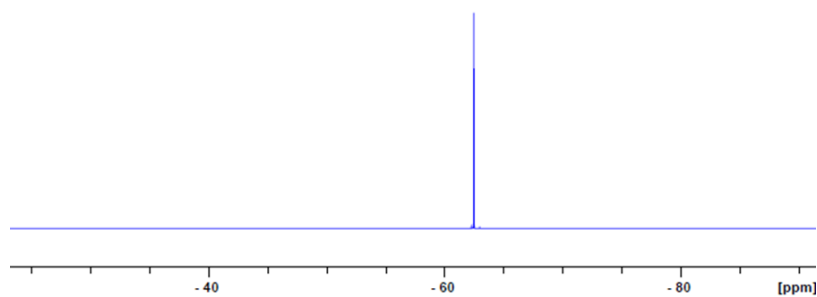
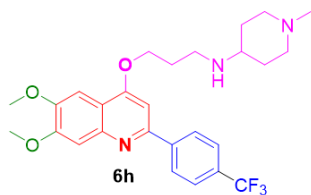


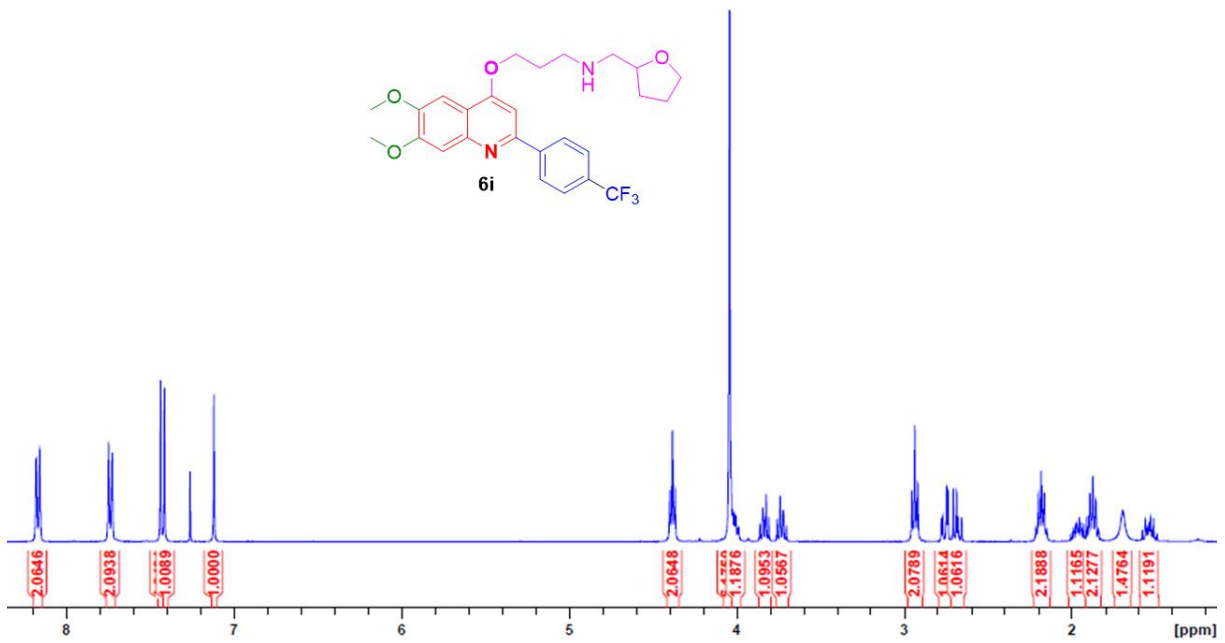
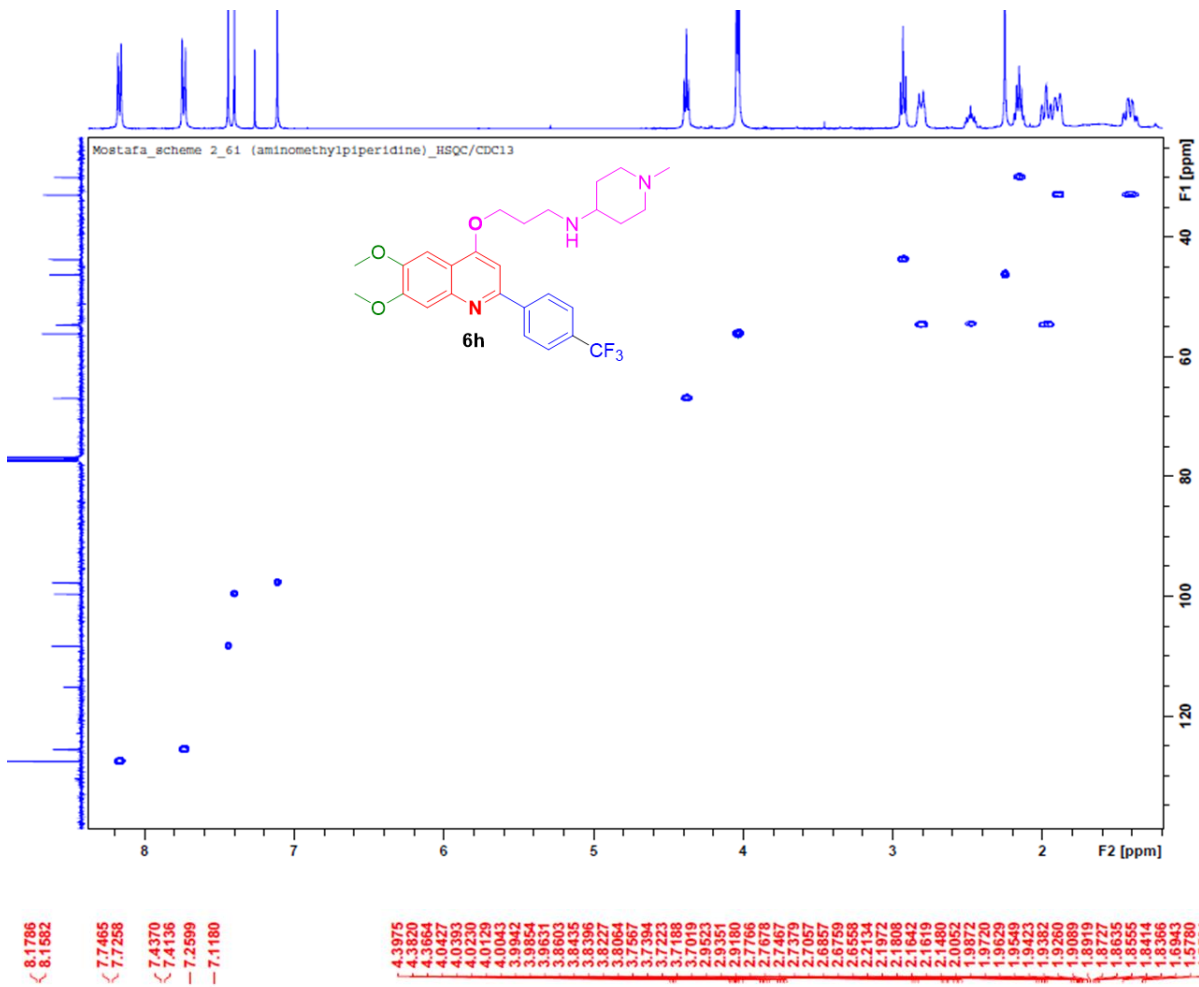


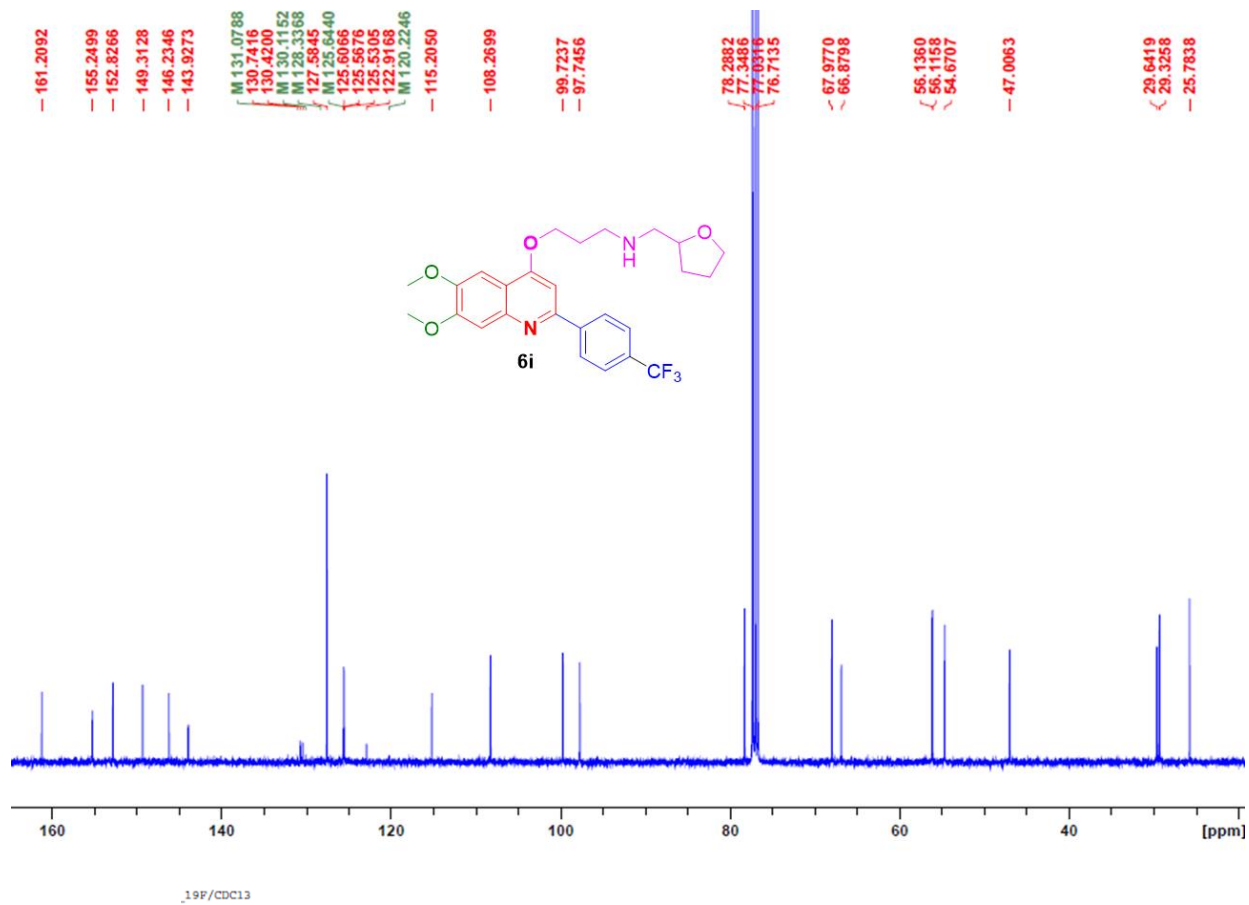


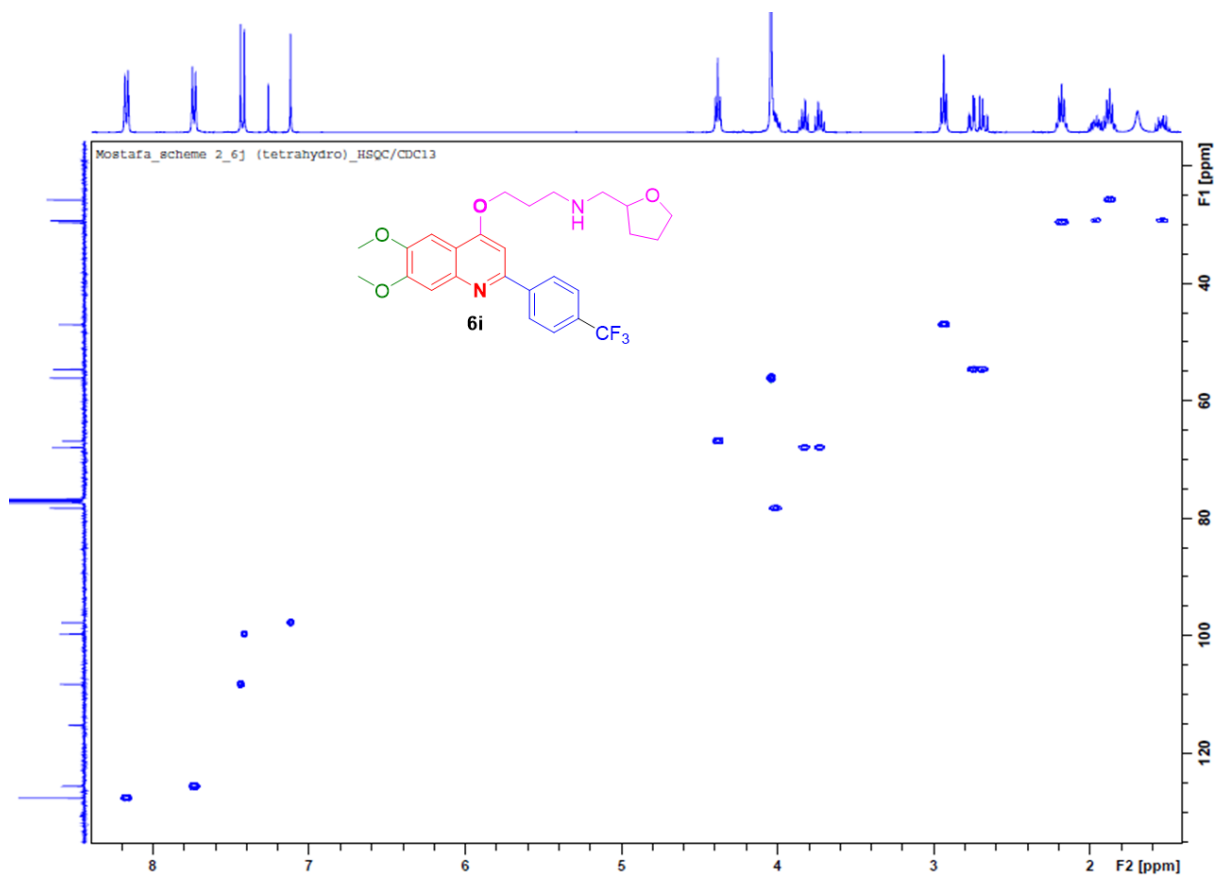
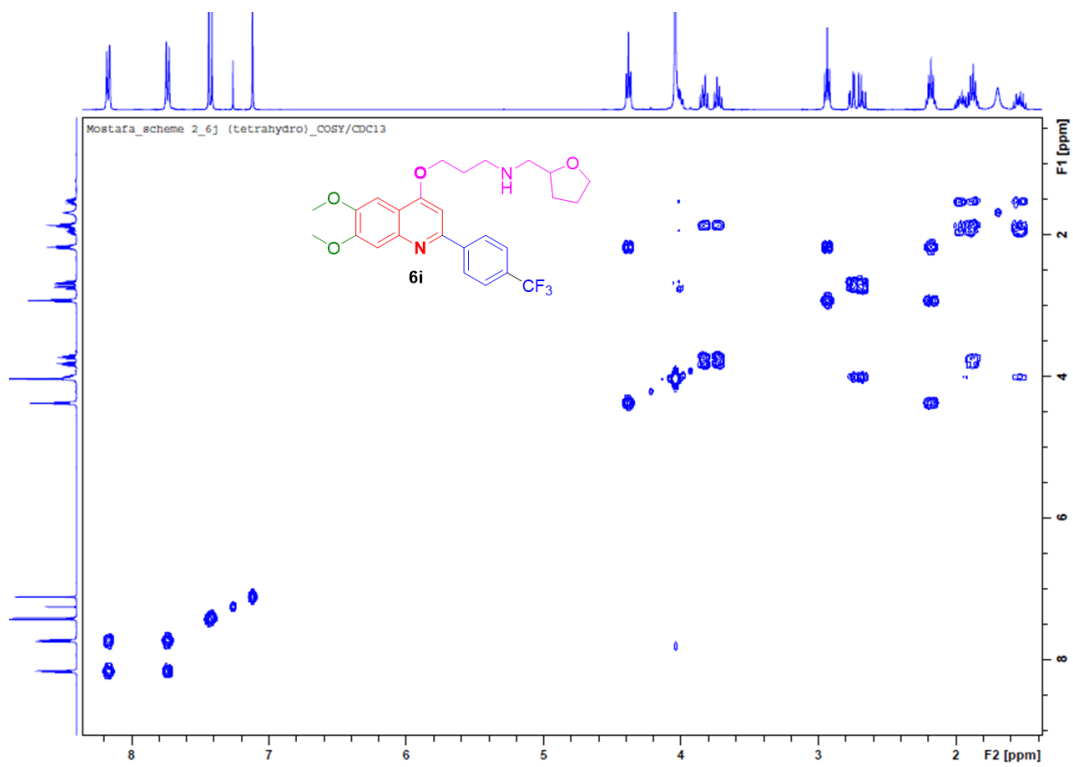
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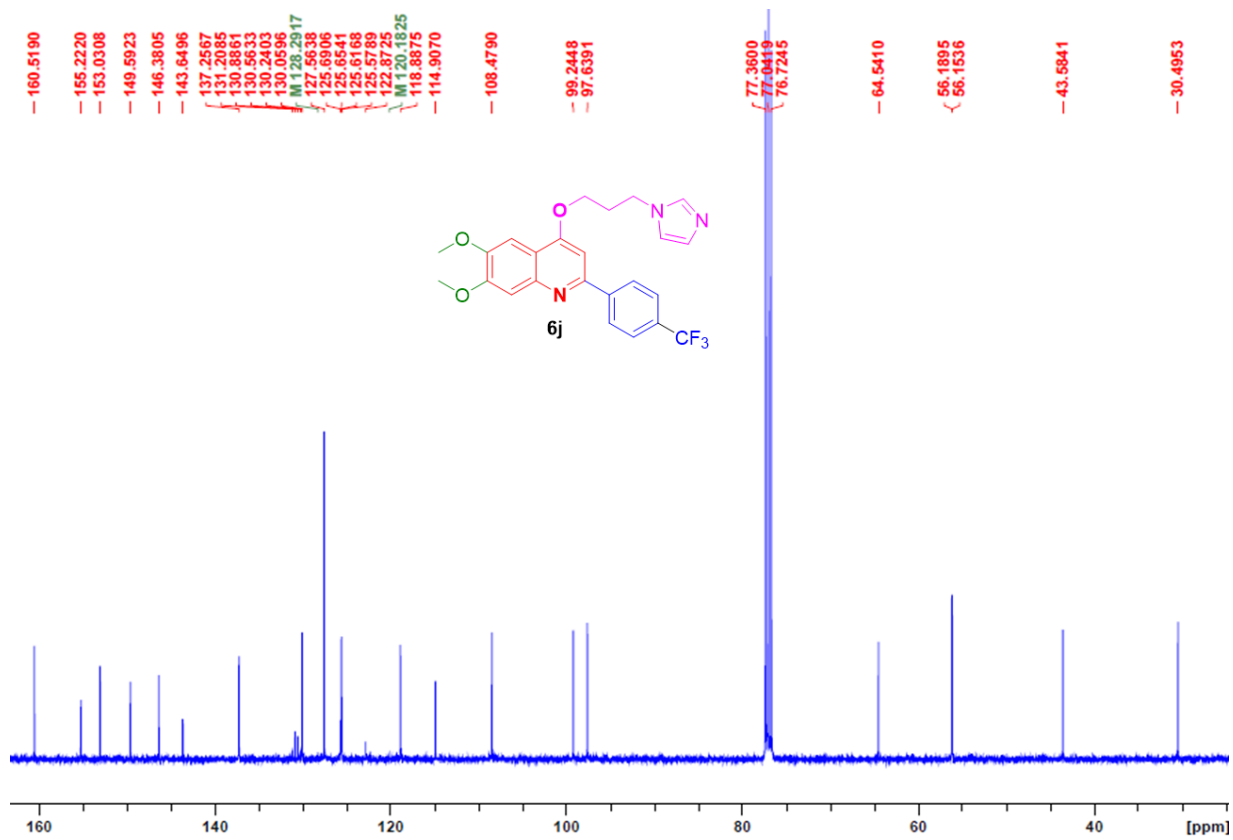
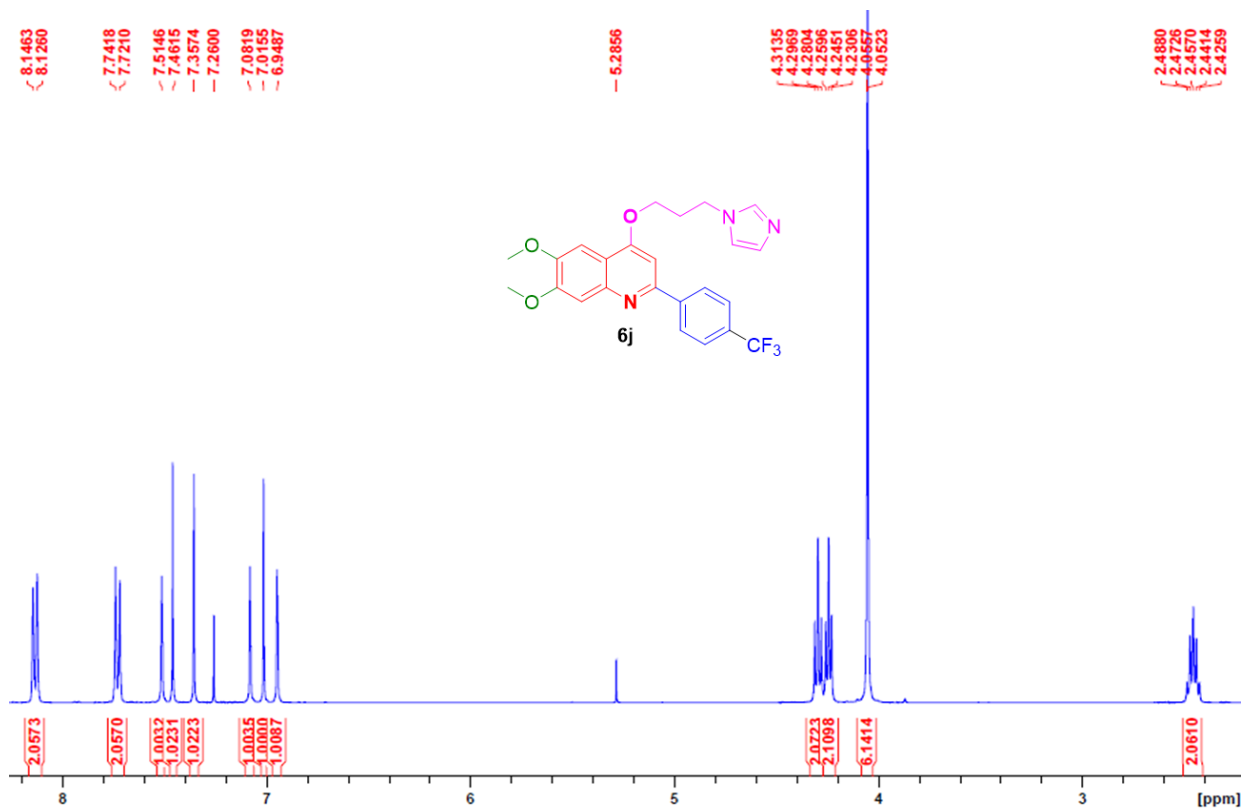
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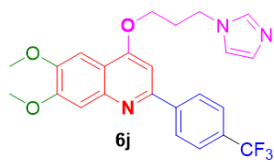




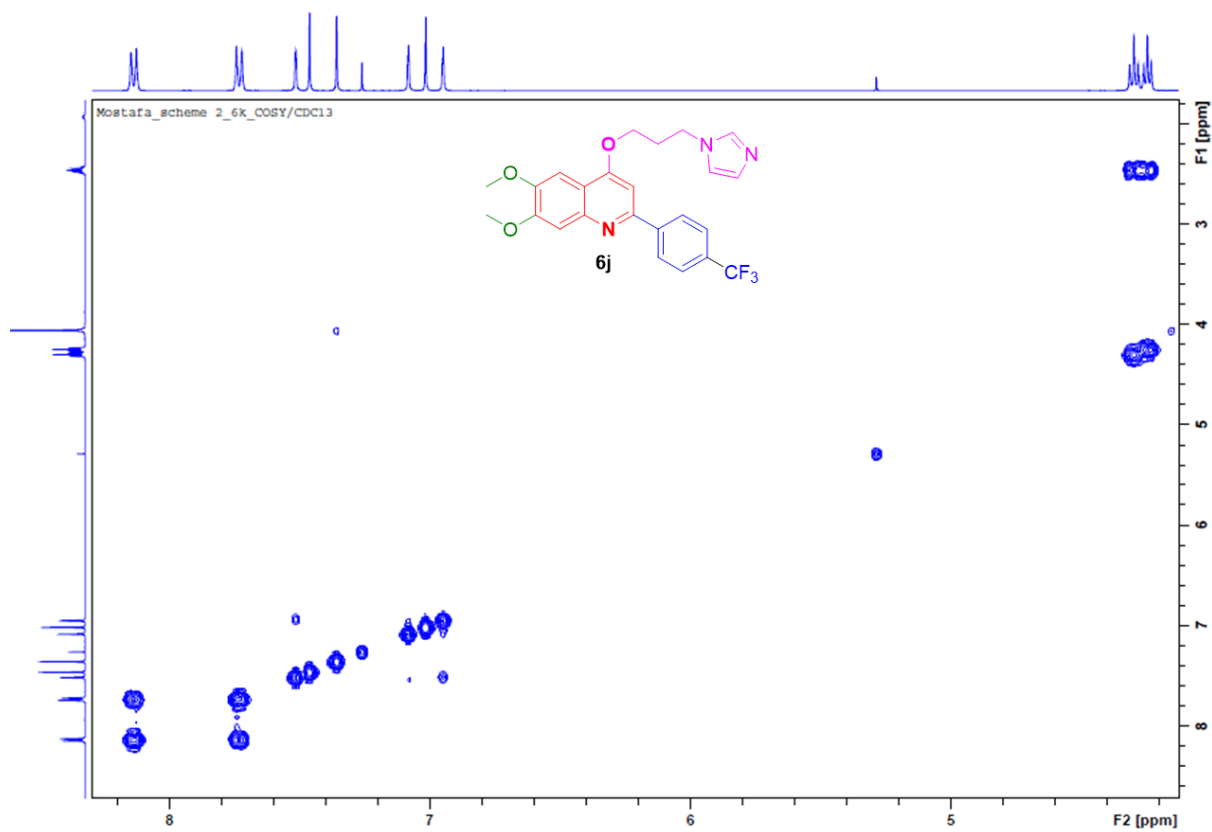


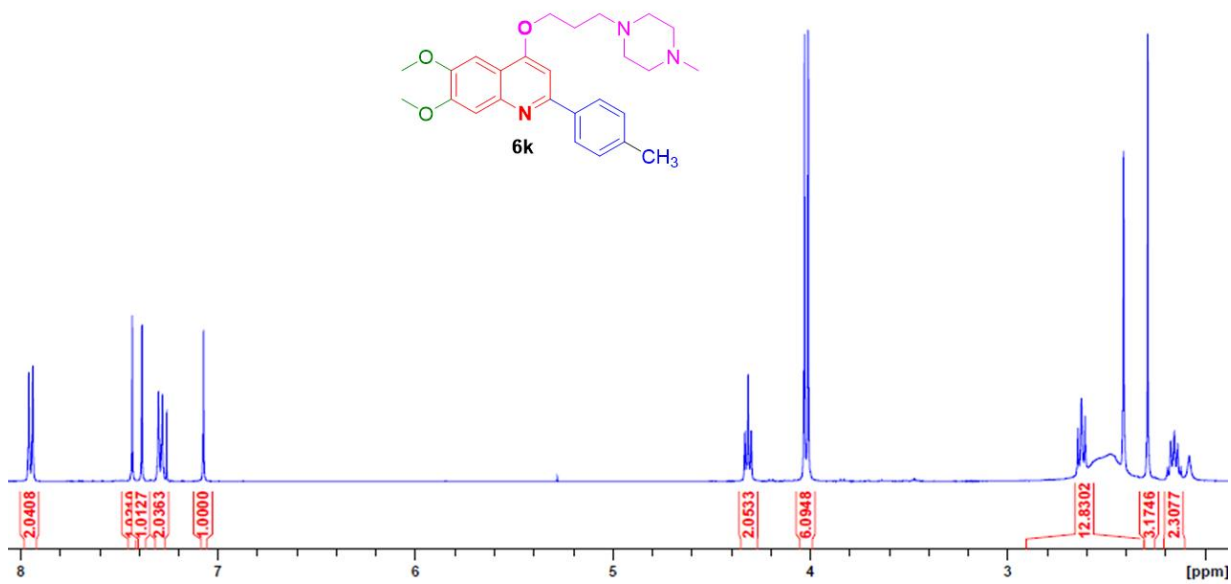
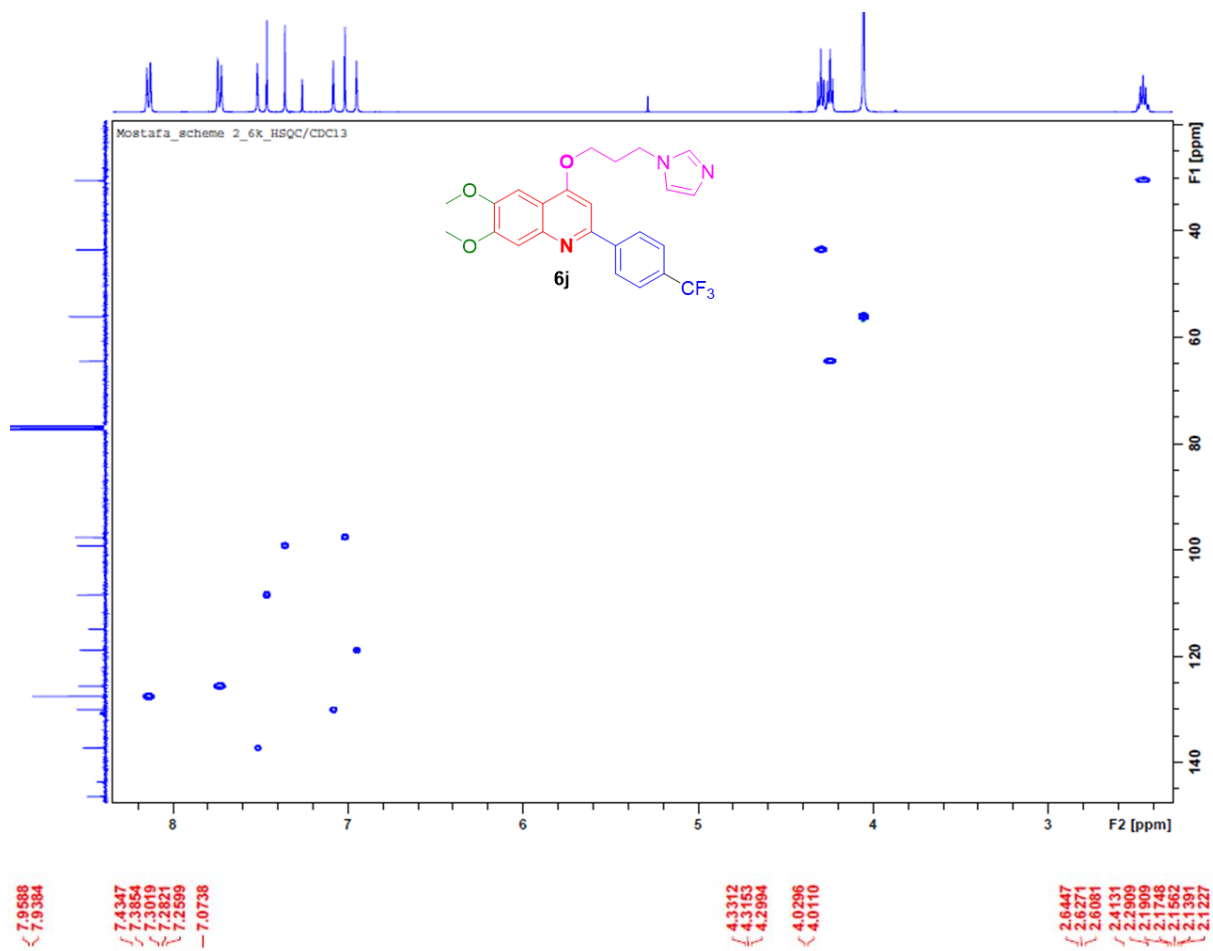
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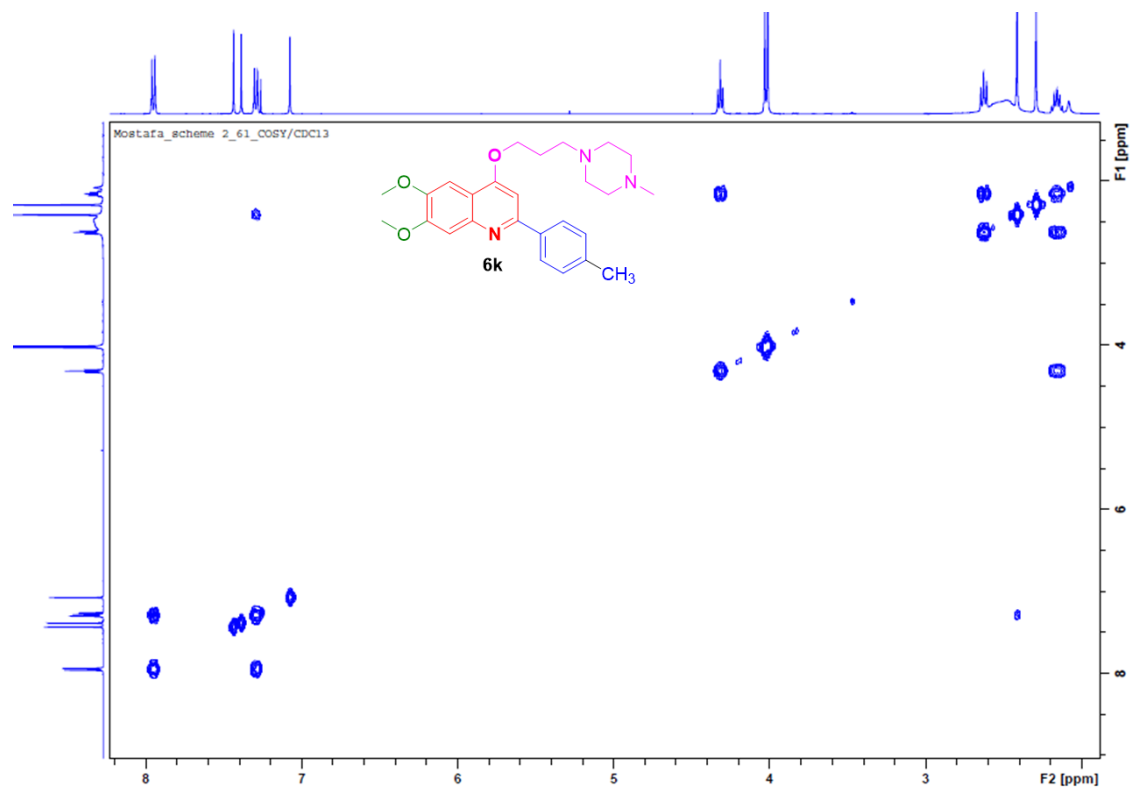
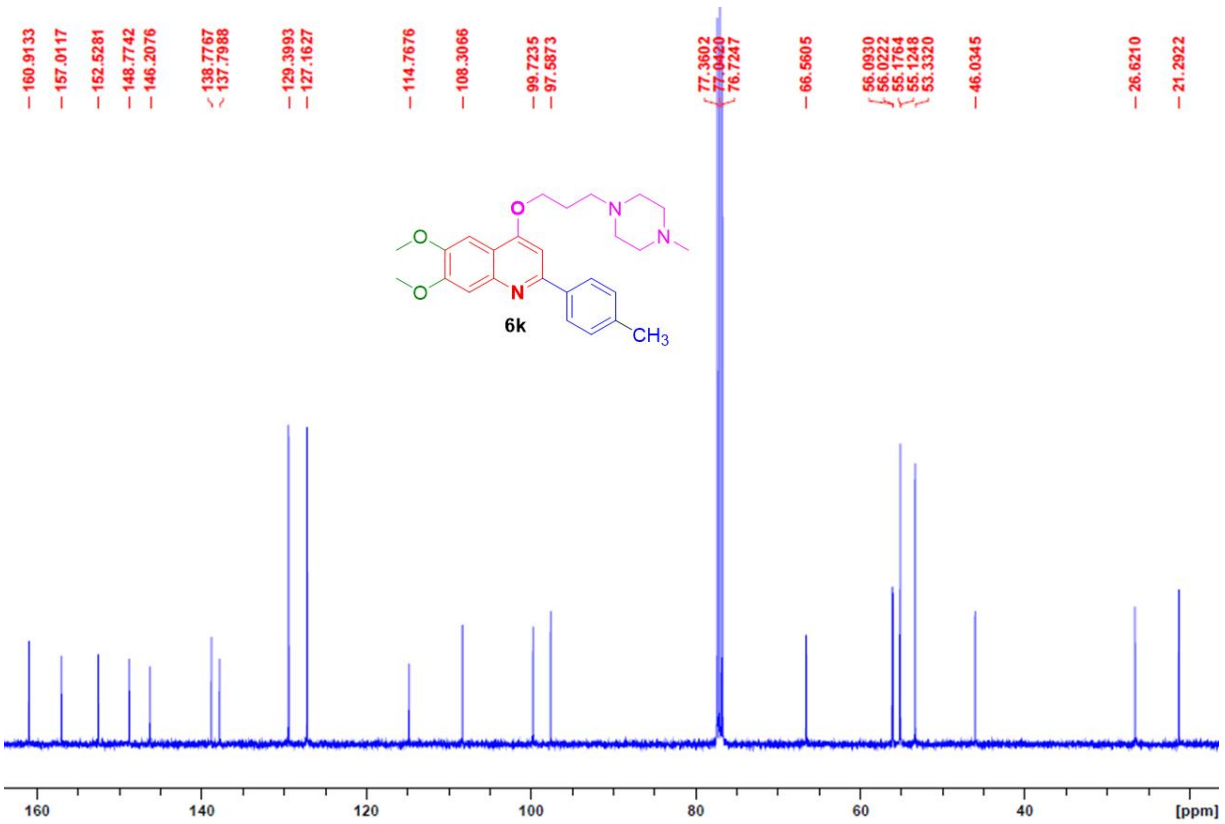
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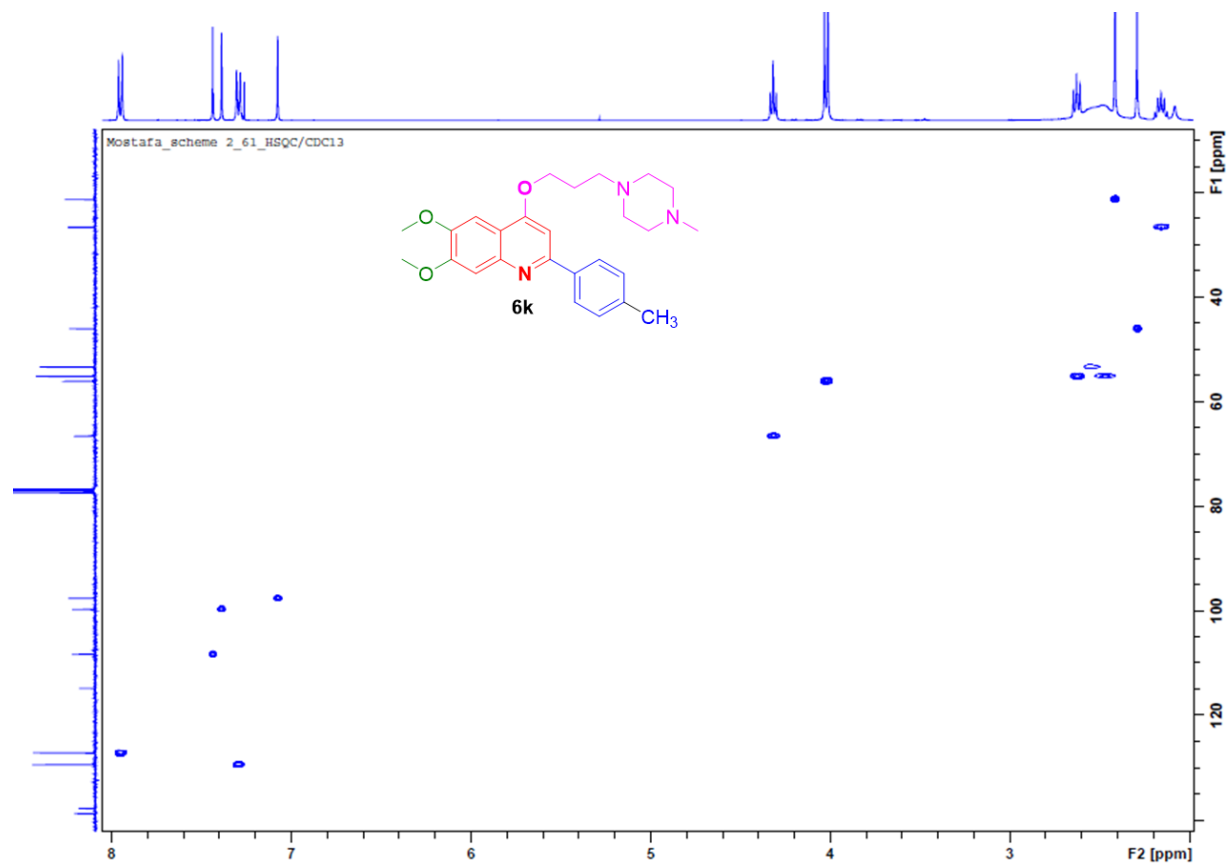


-50 -100 -150 [ppm]





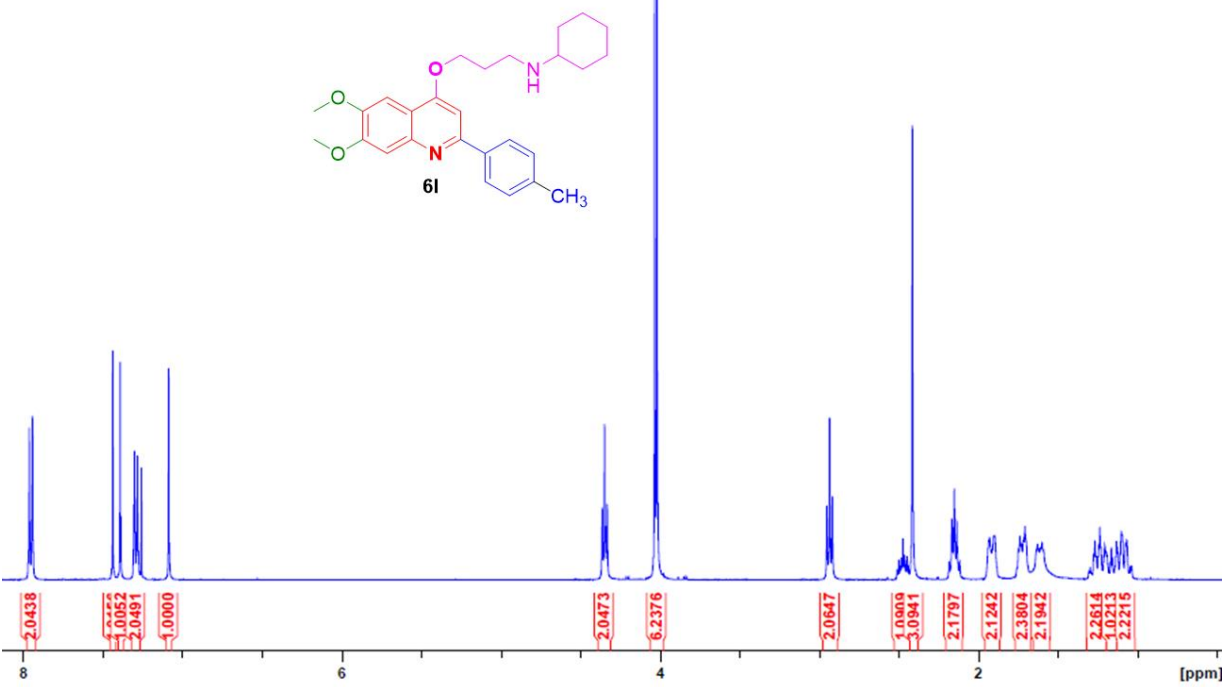


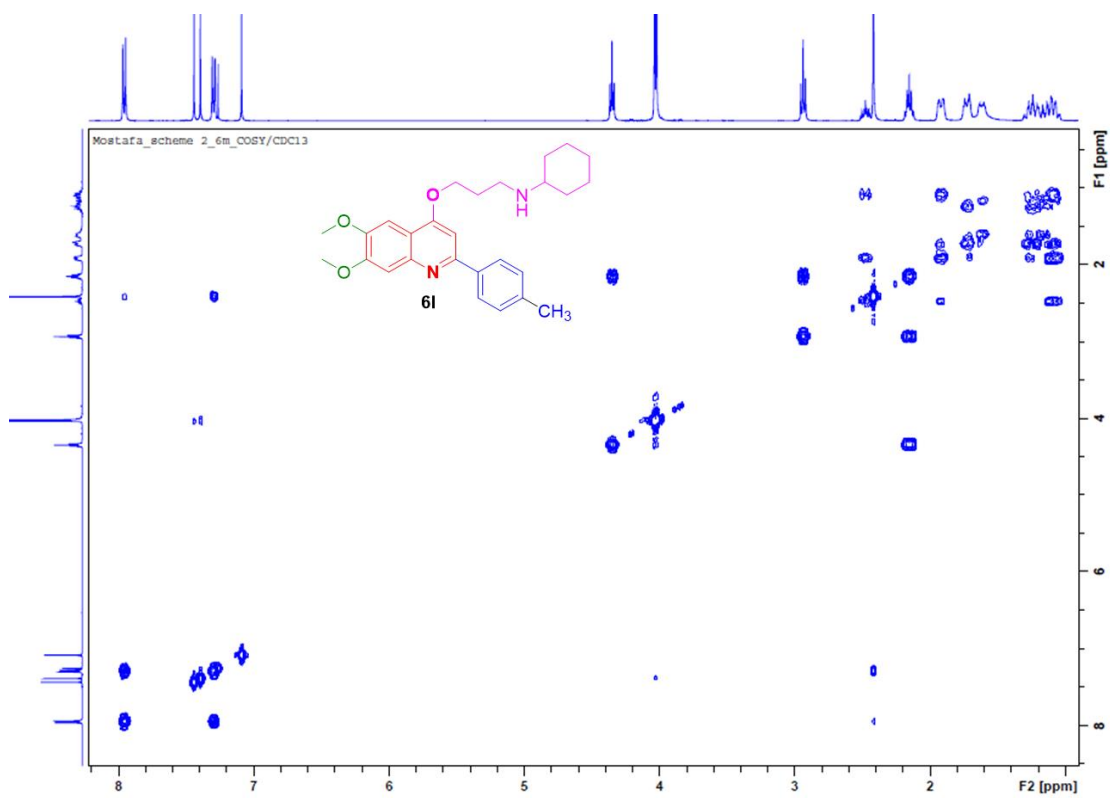
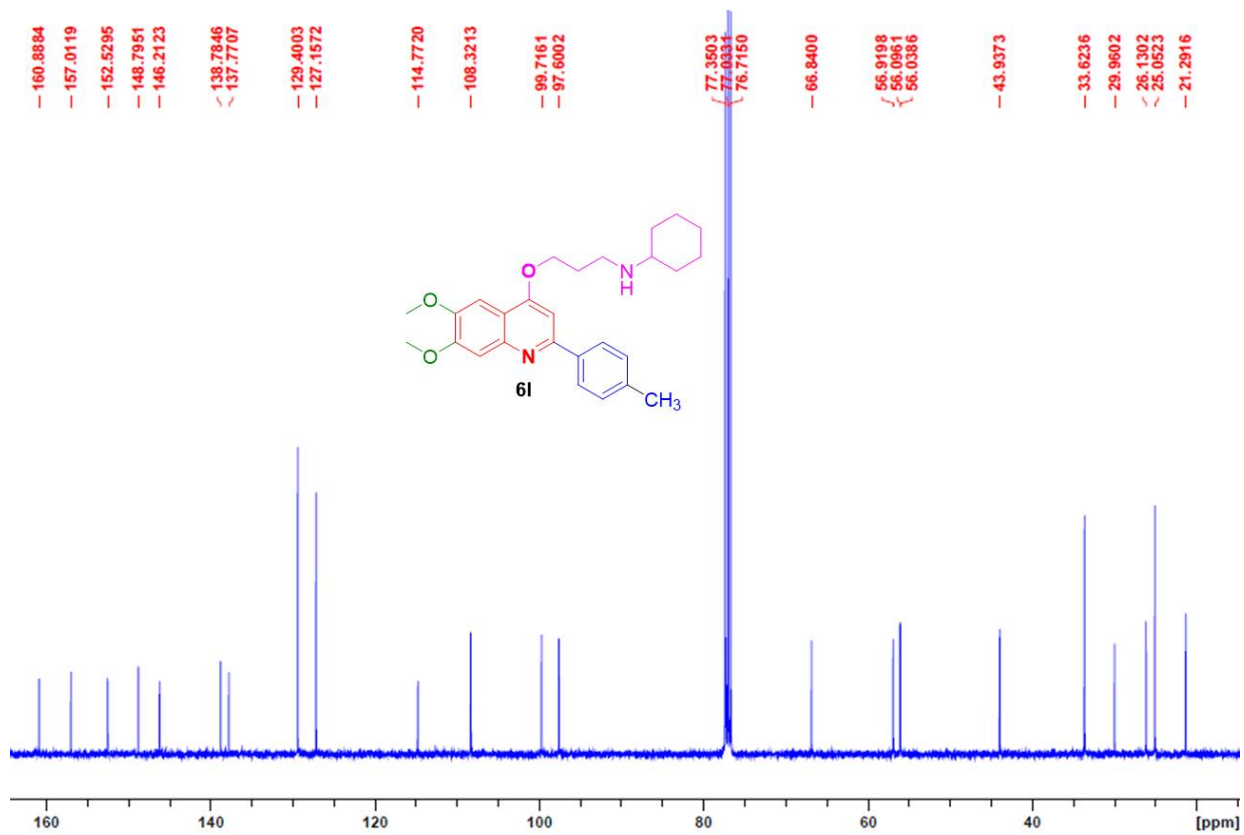


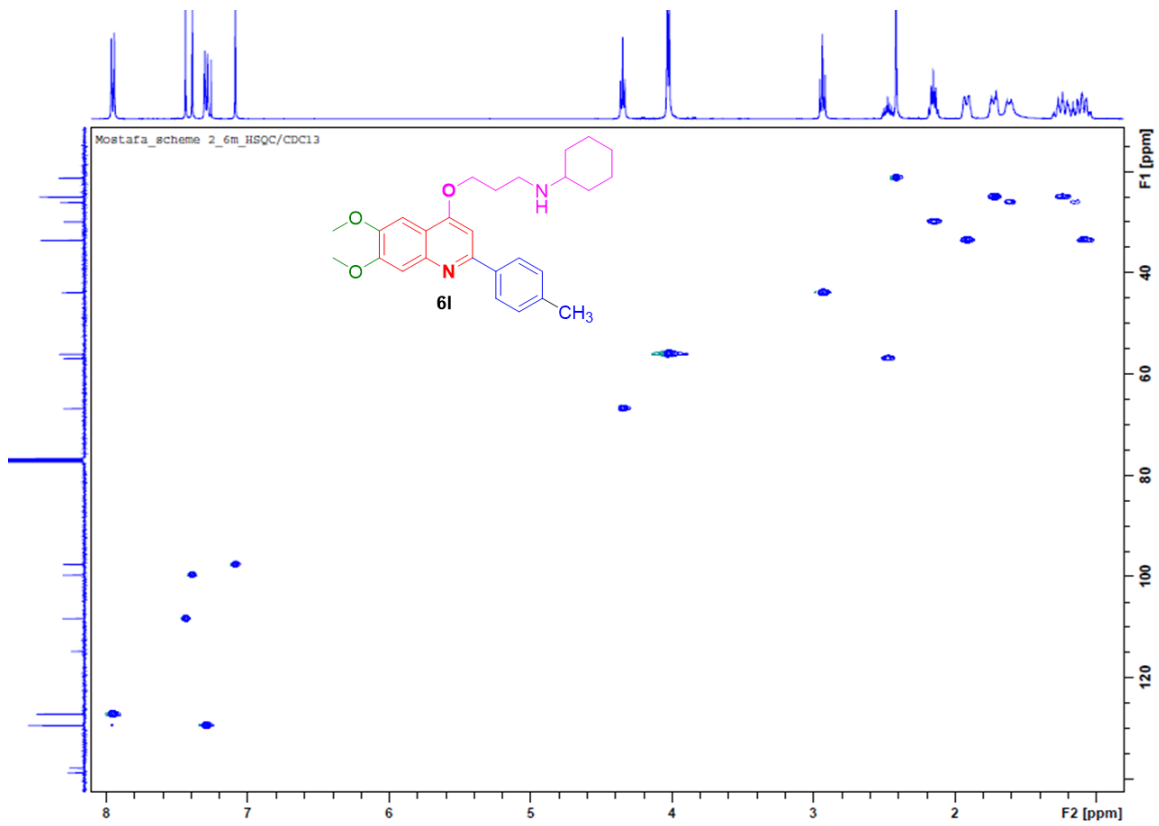
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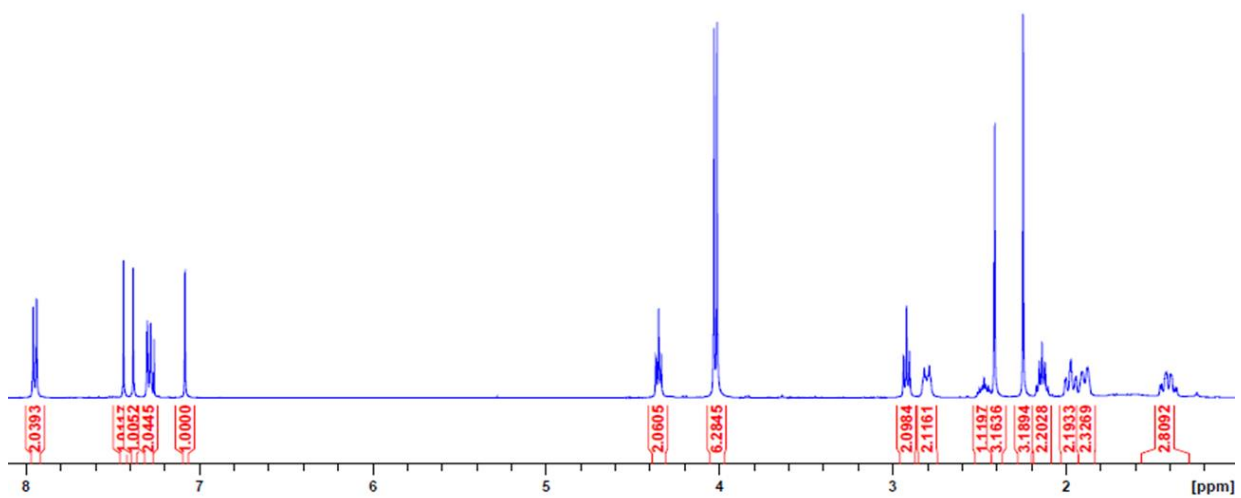
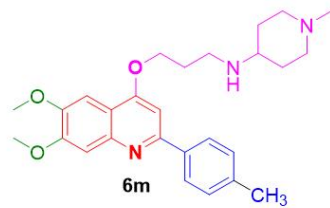


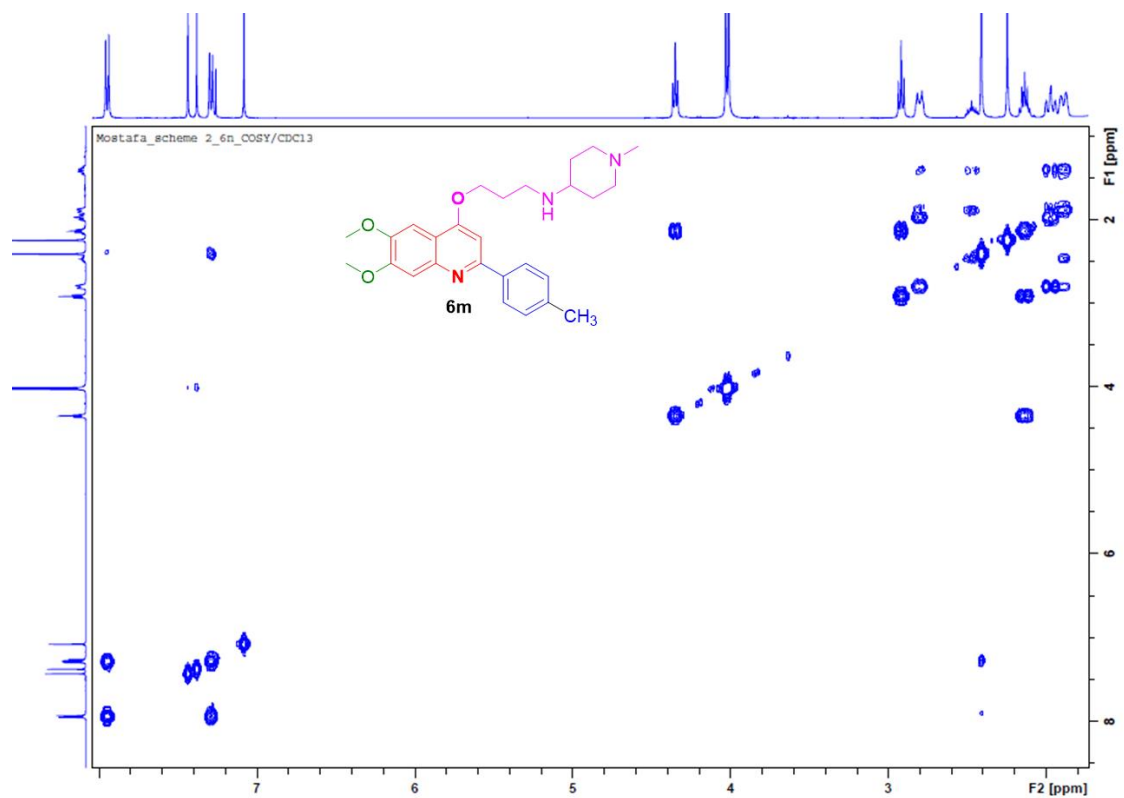
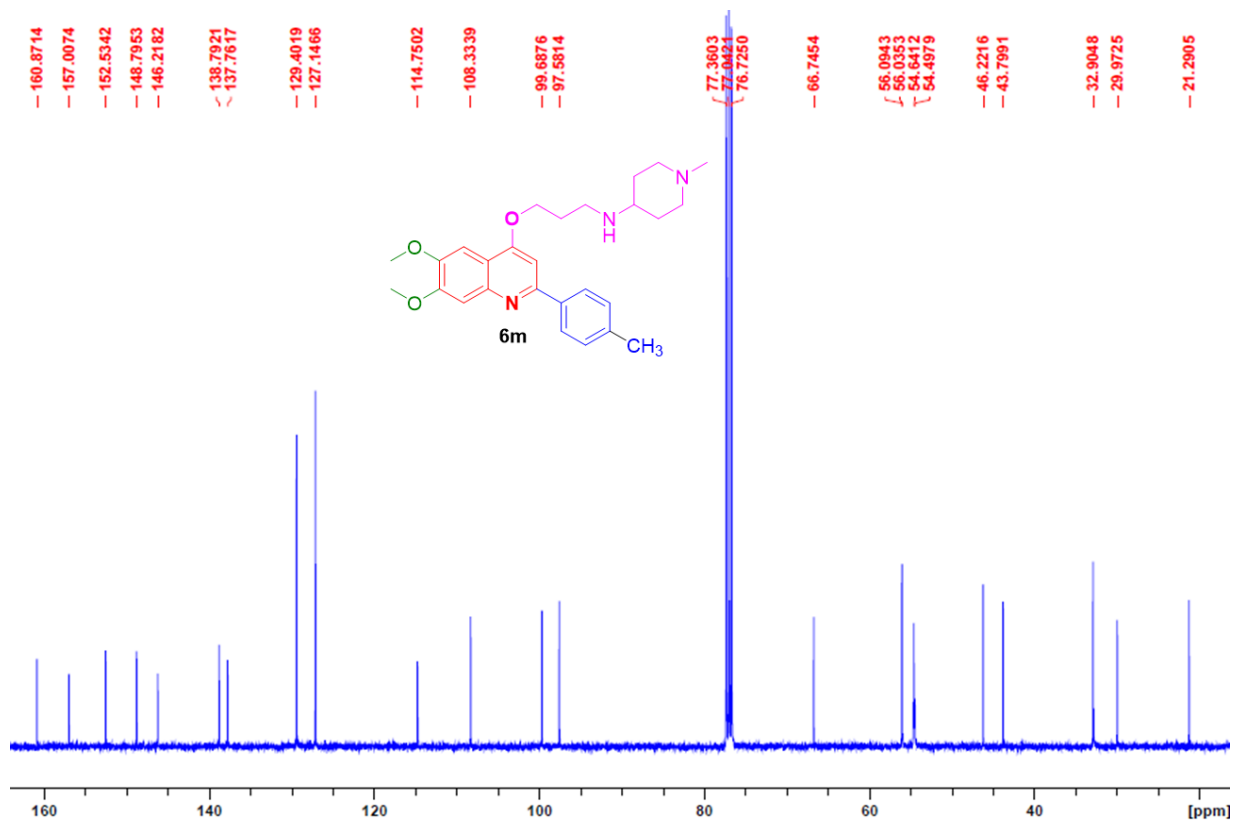
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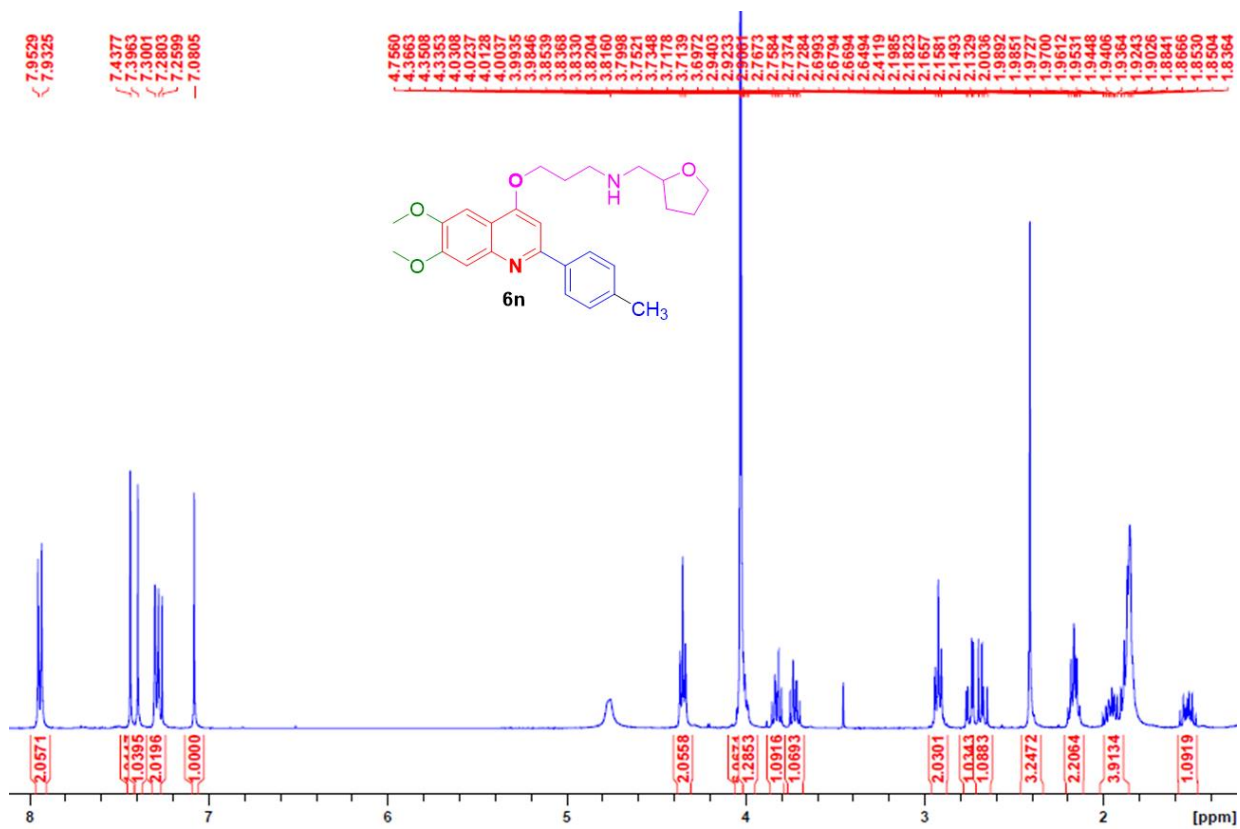
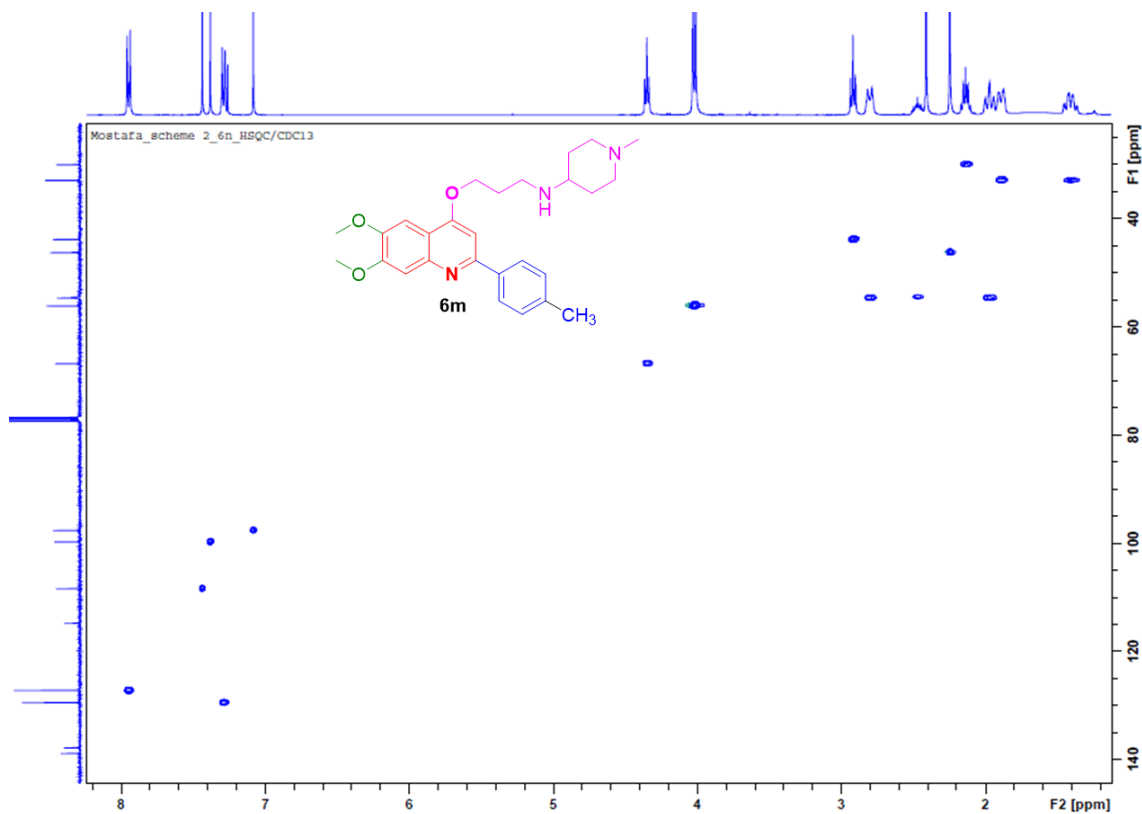
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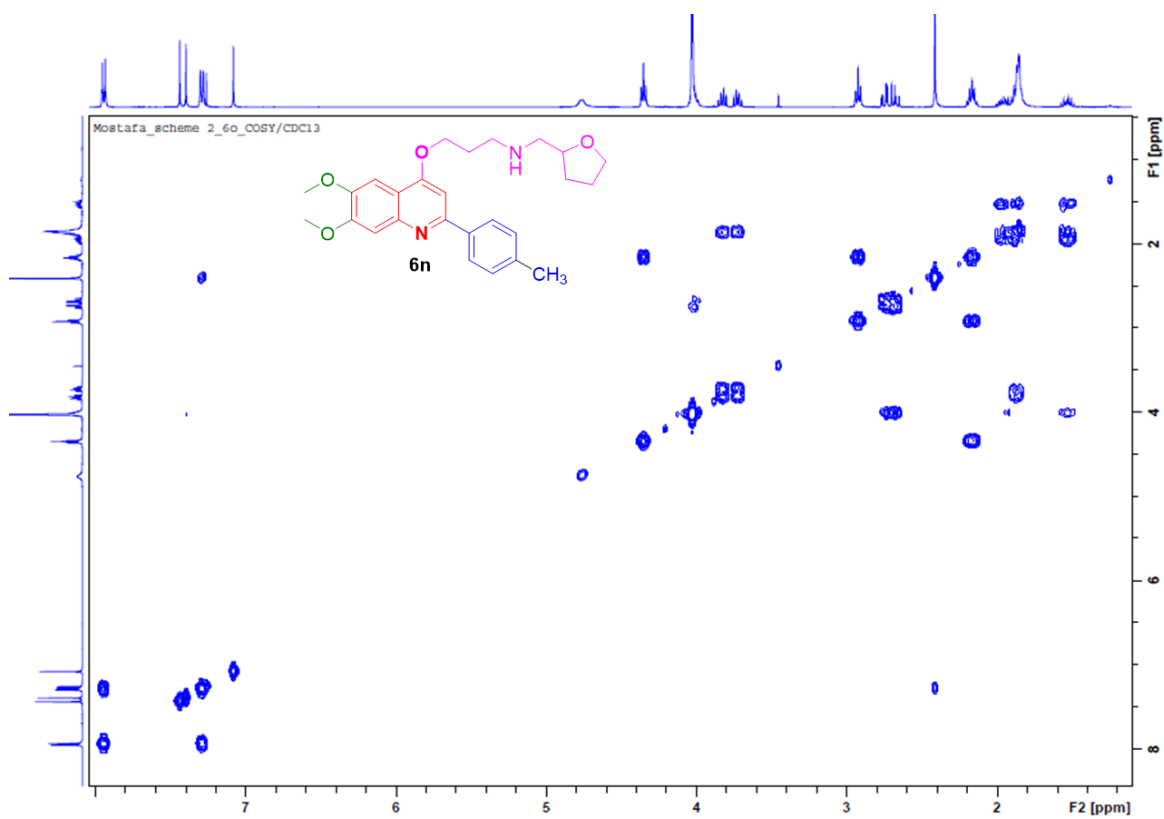
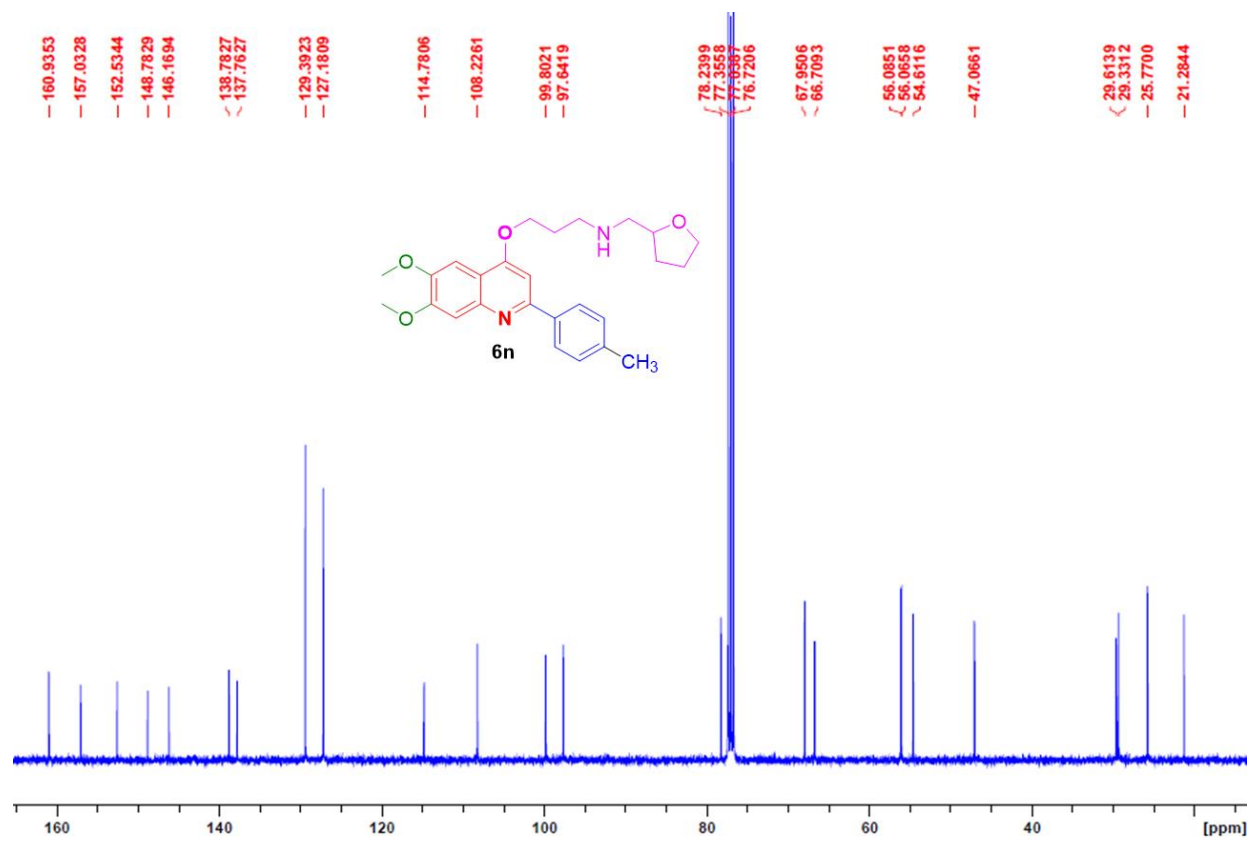
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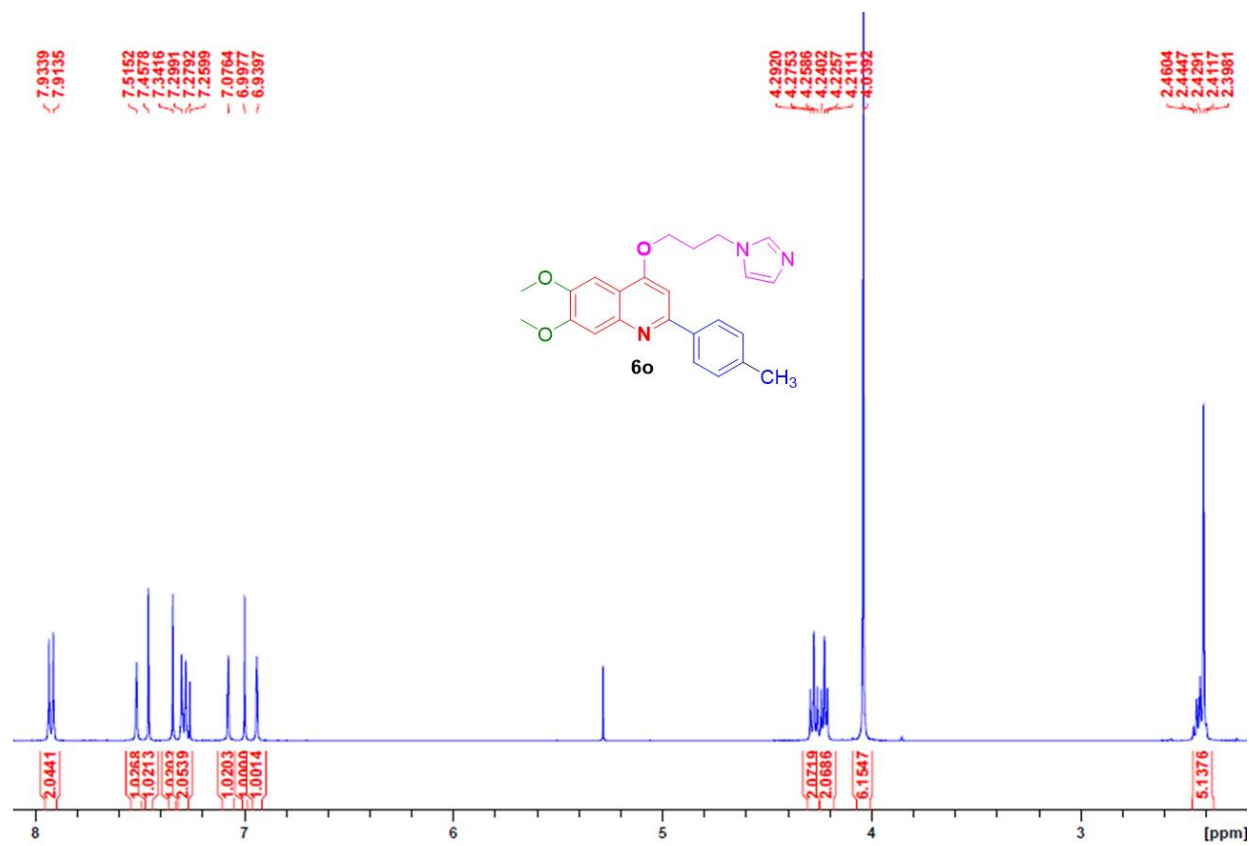
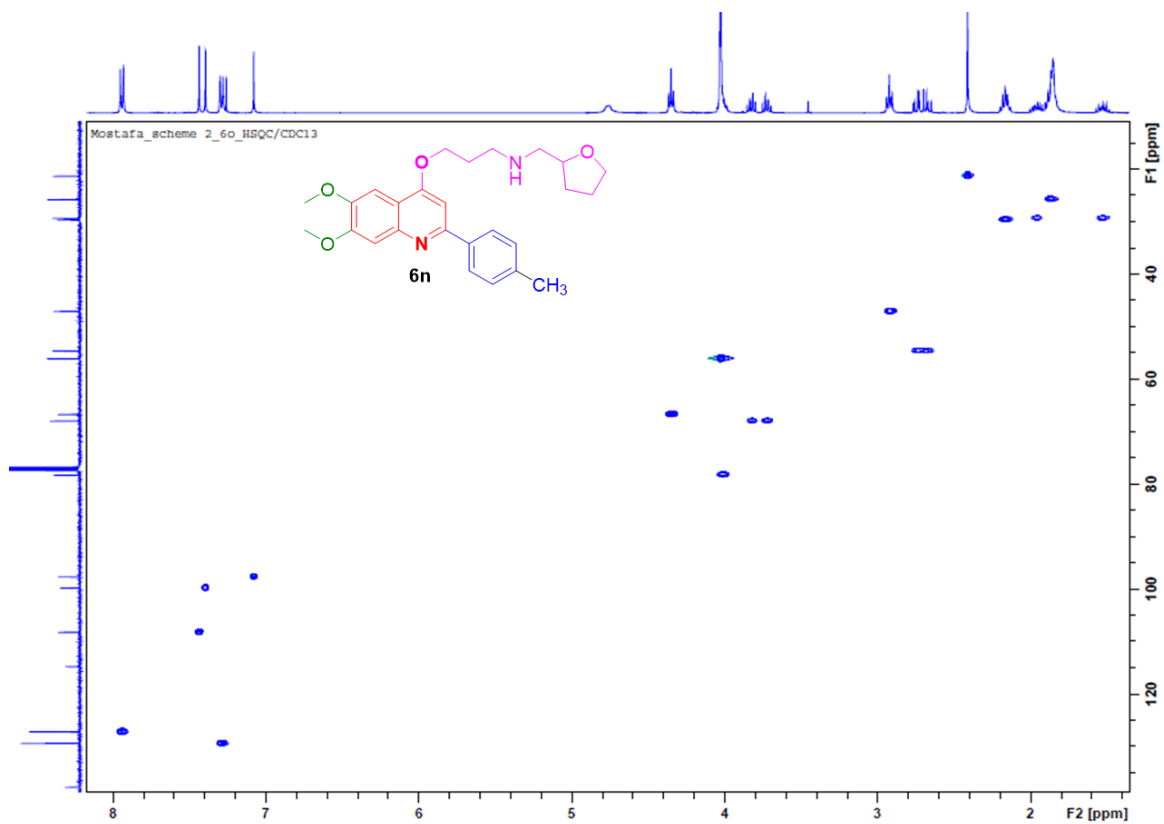
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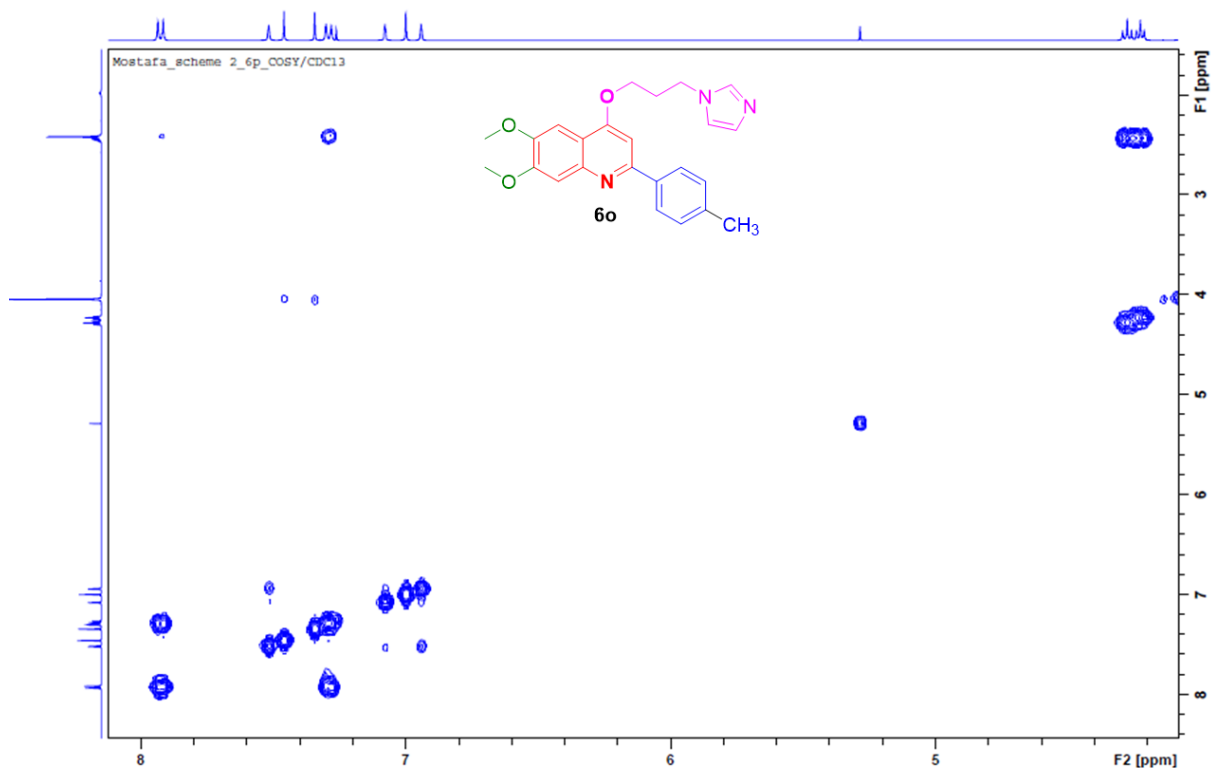
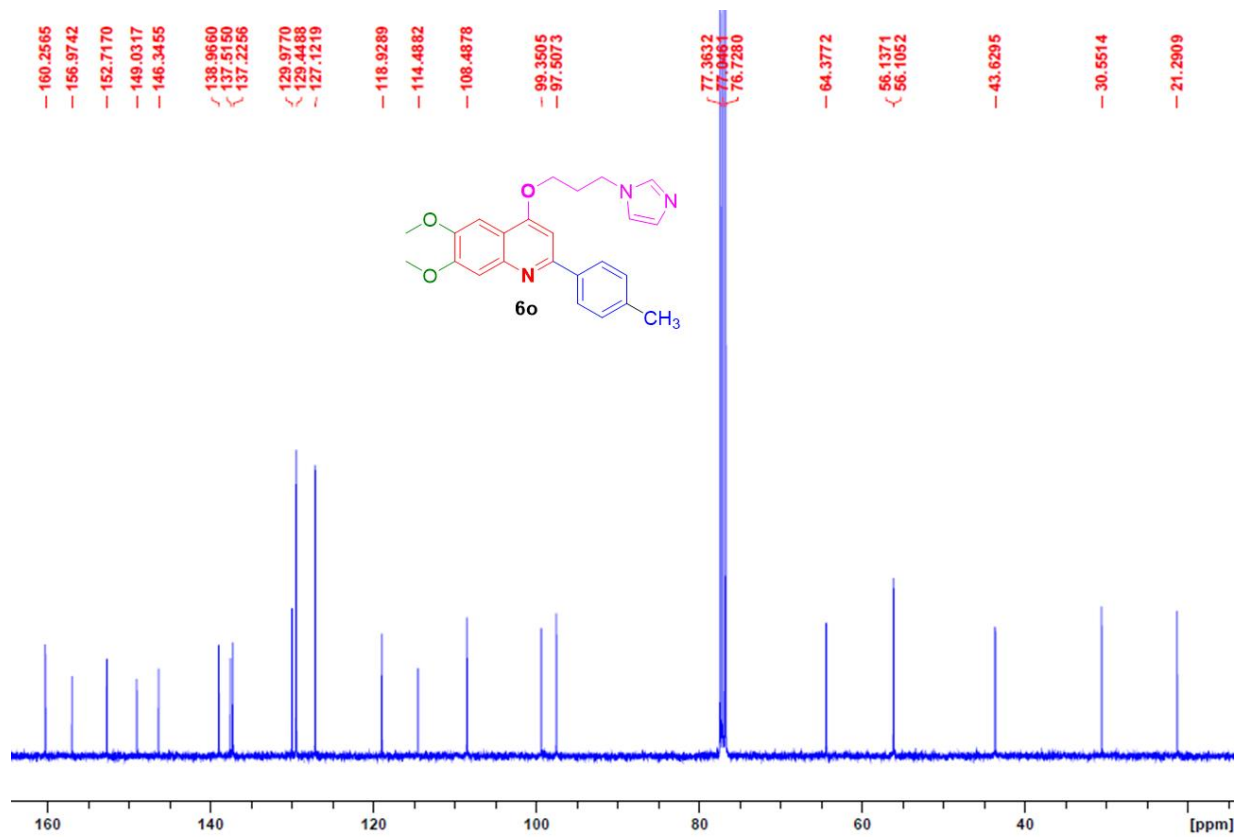


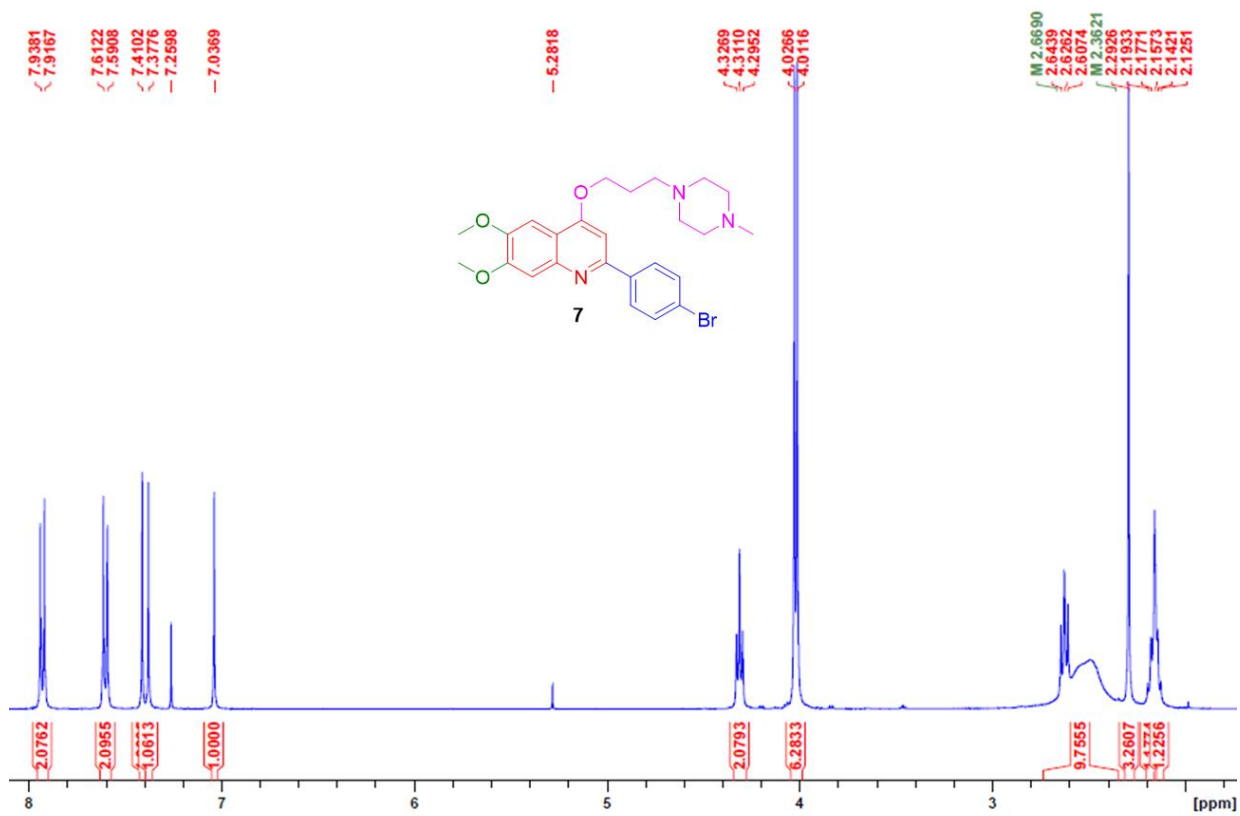
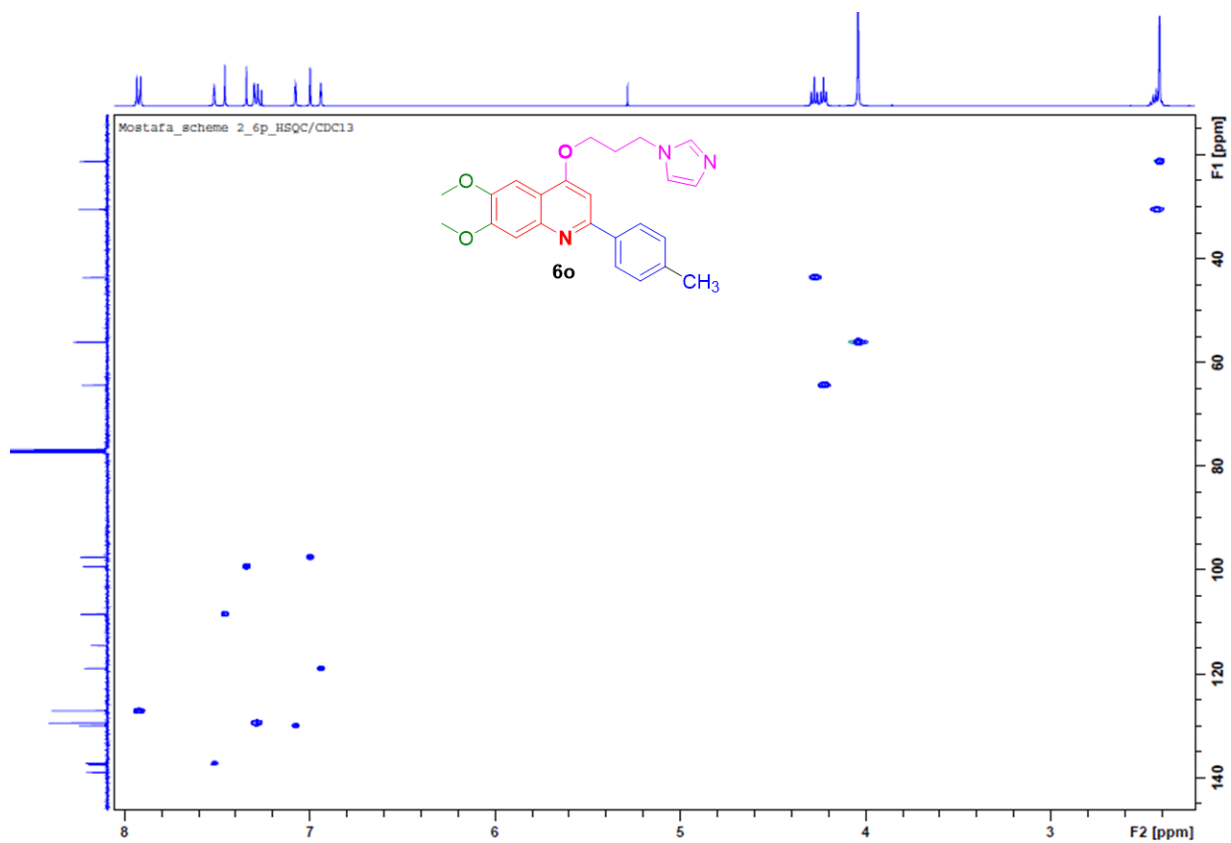


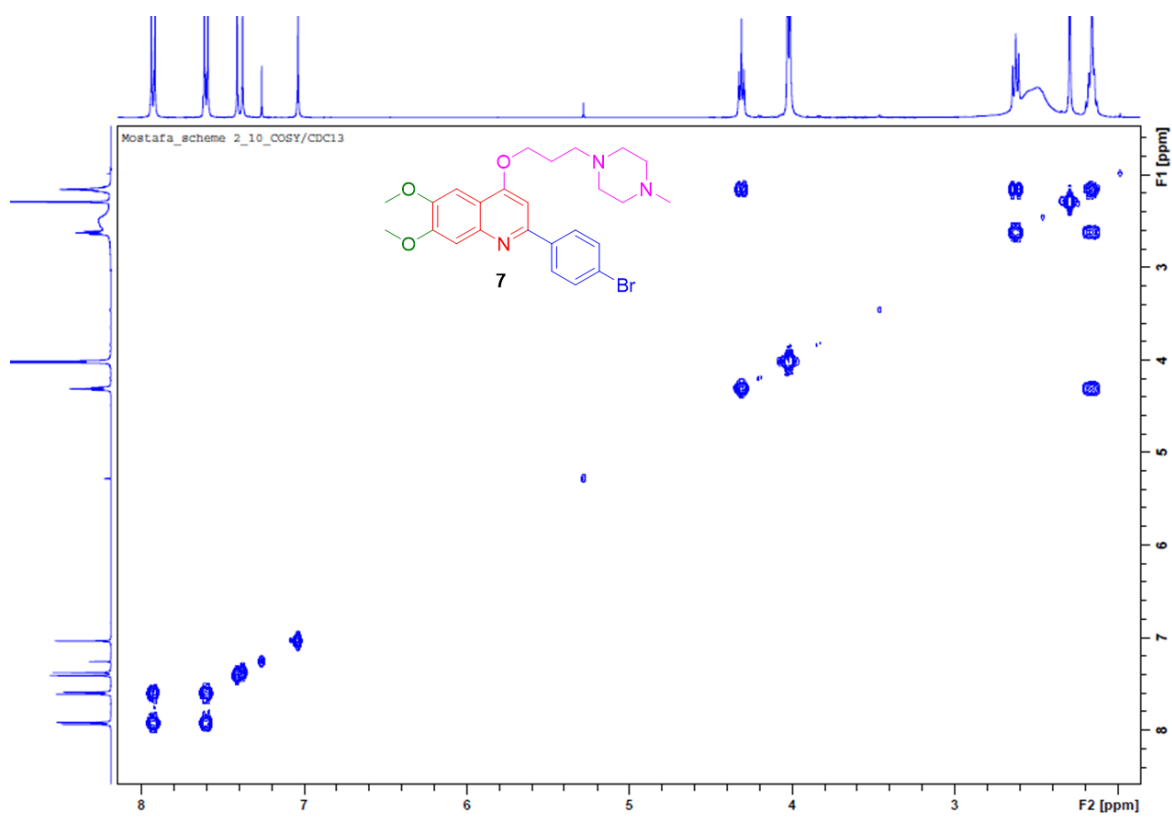
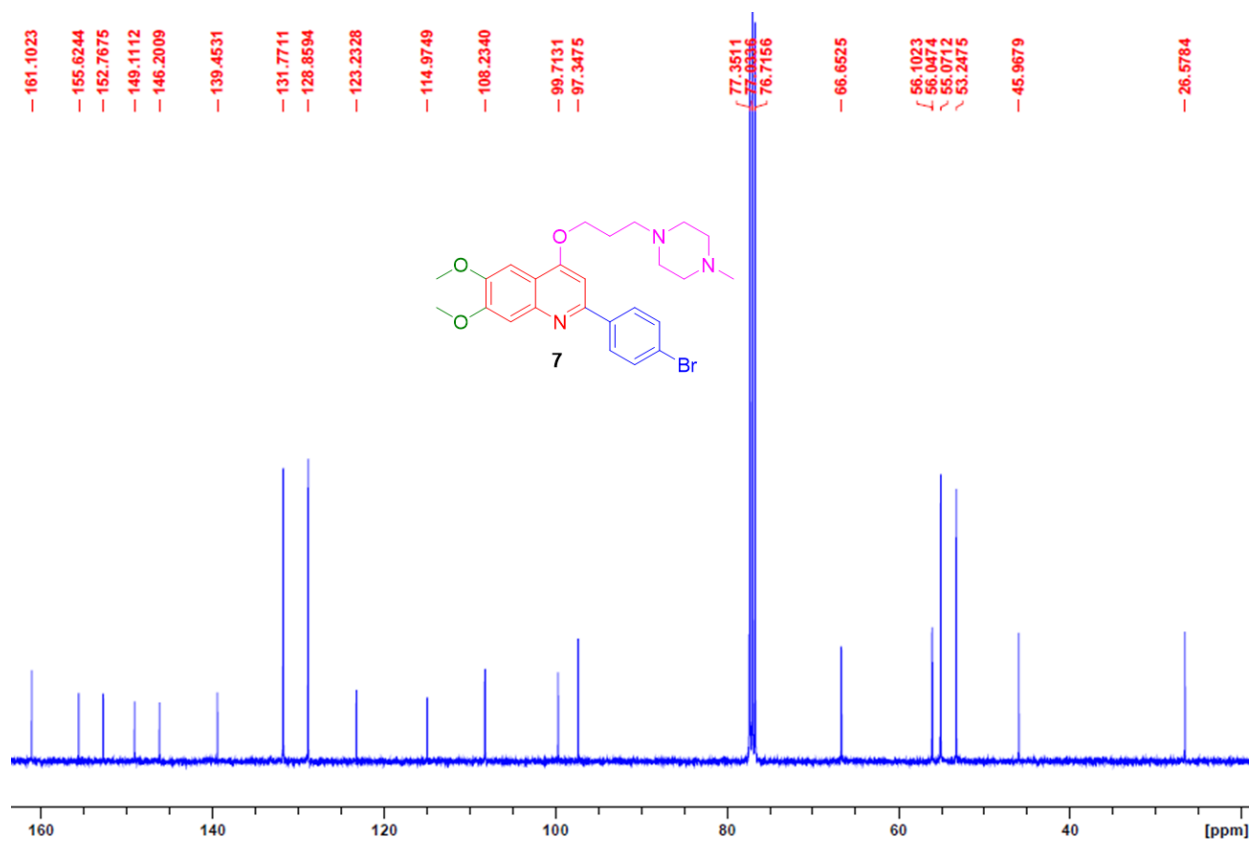


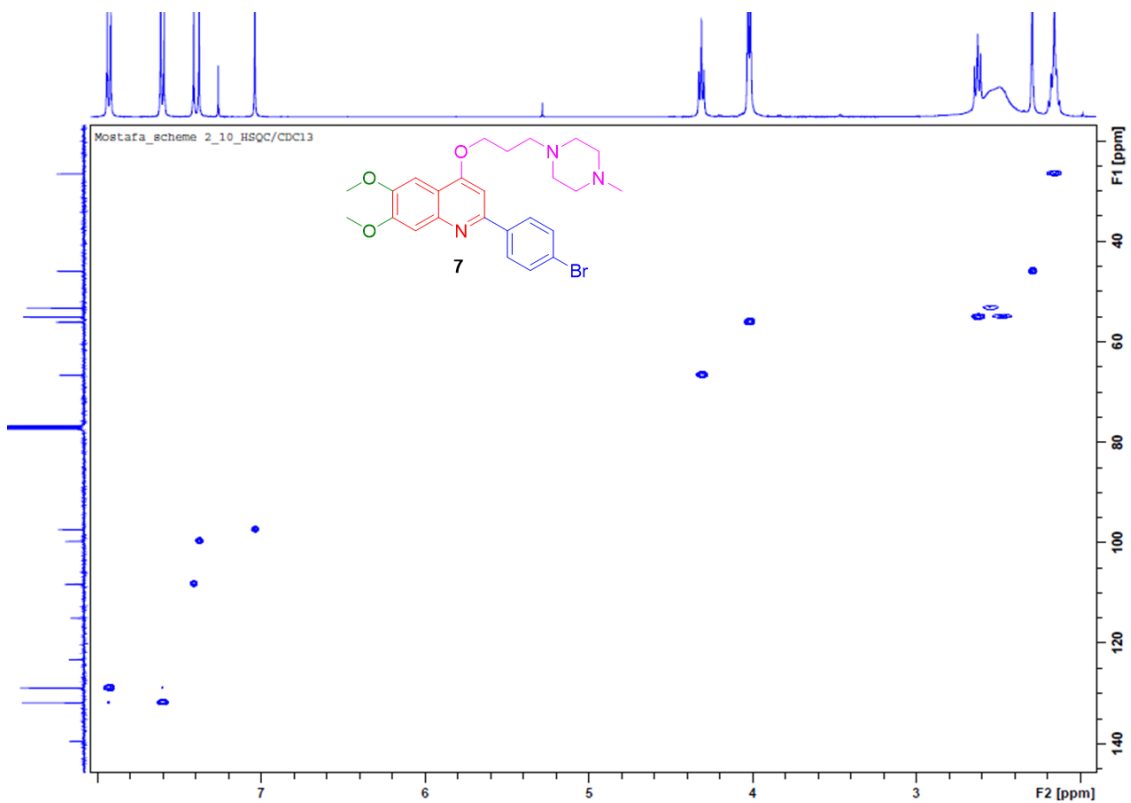




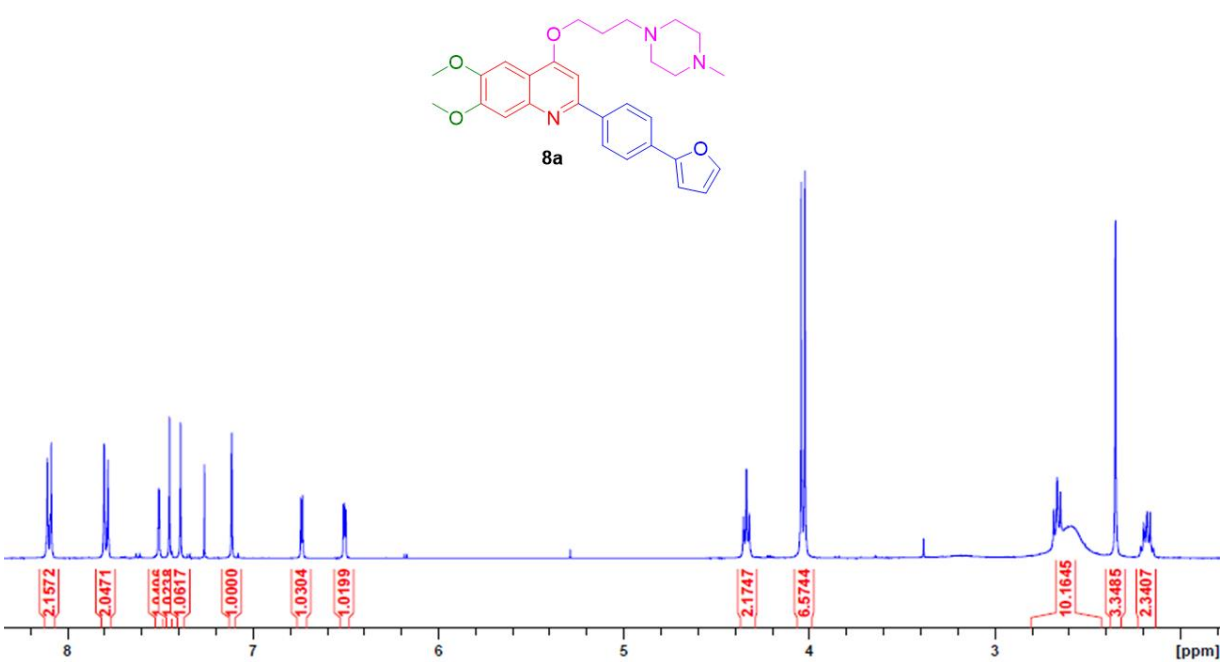


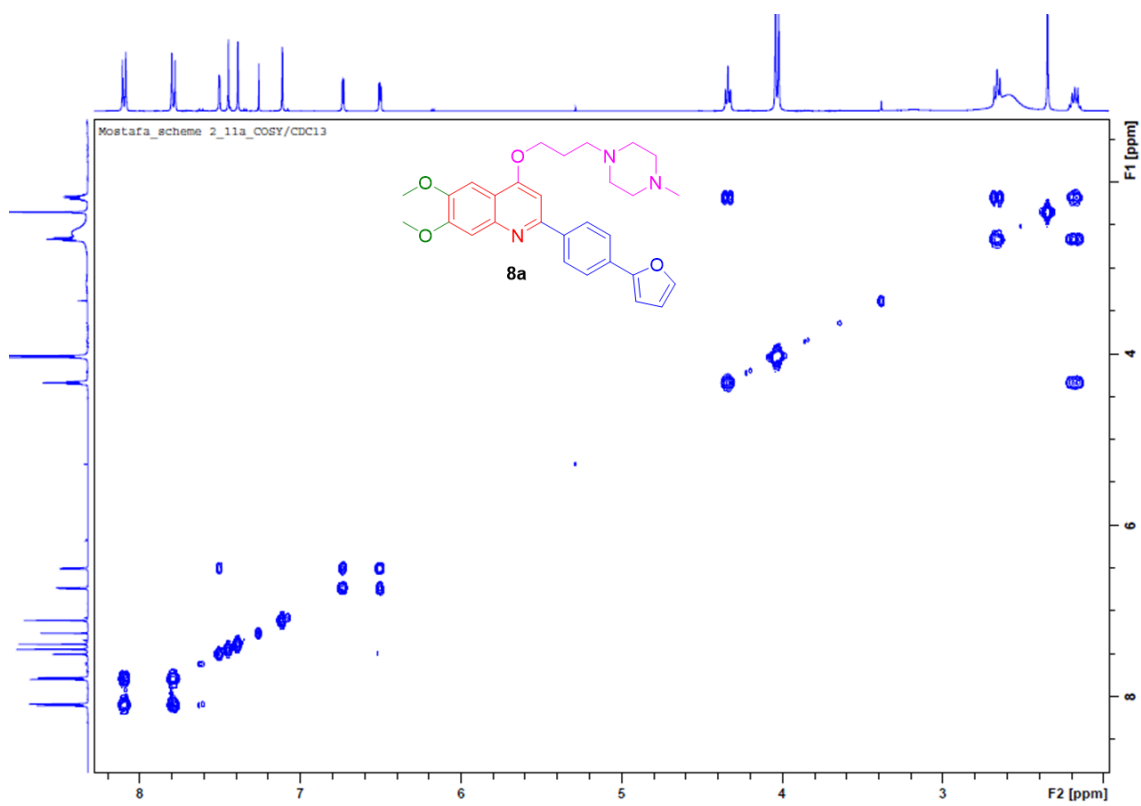
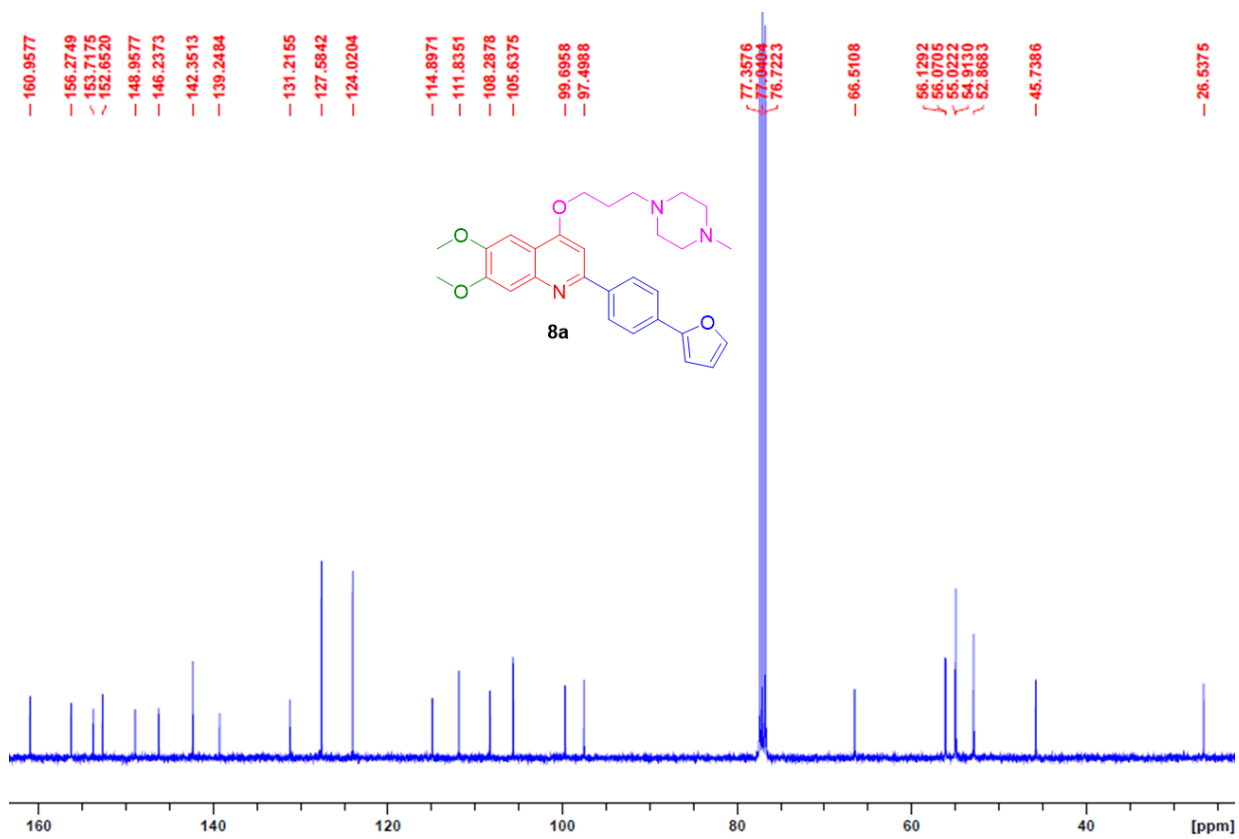


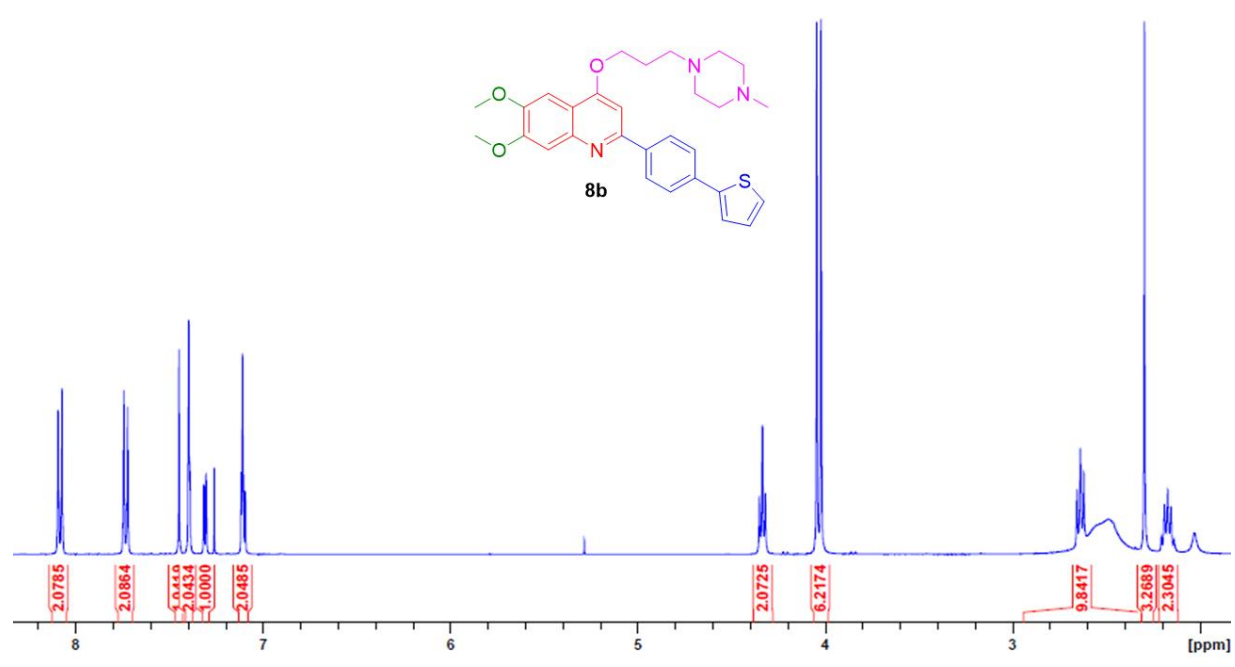
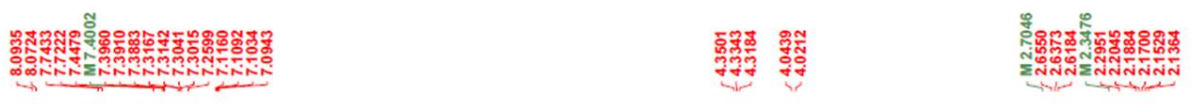
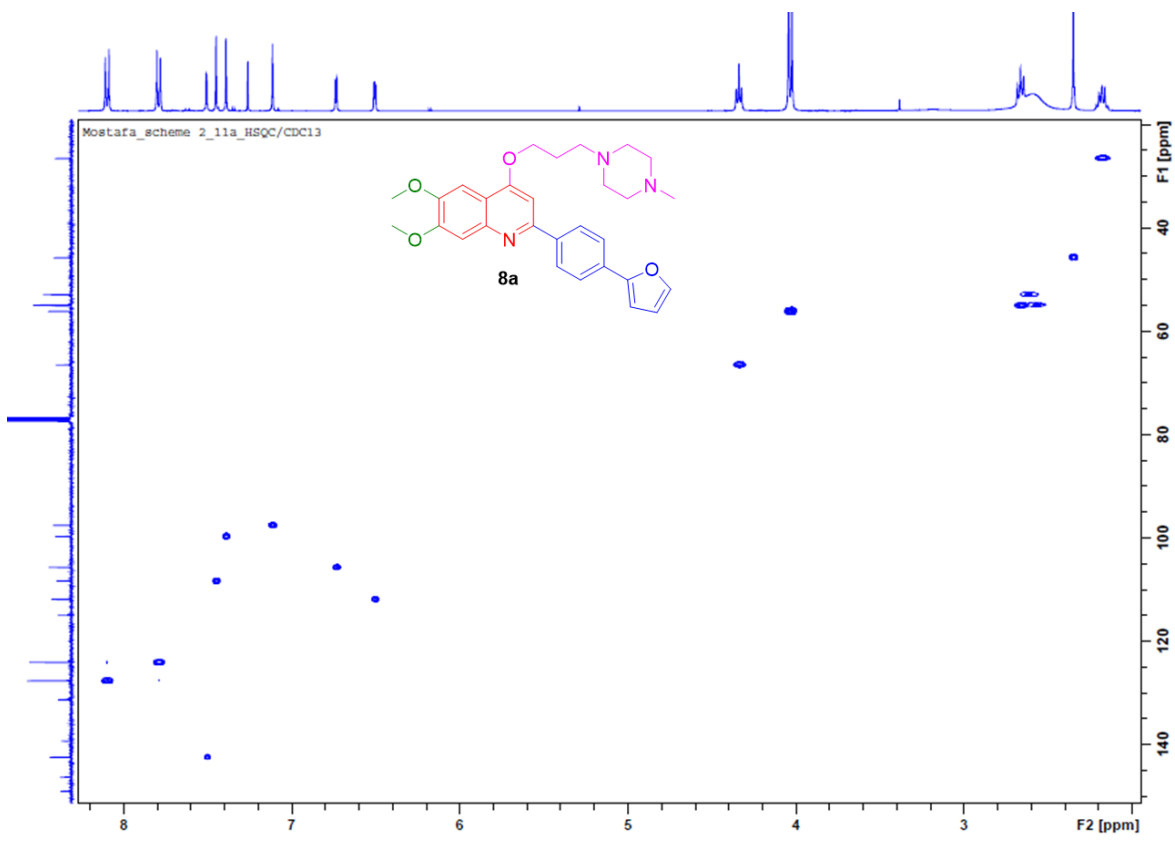


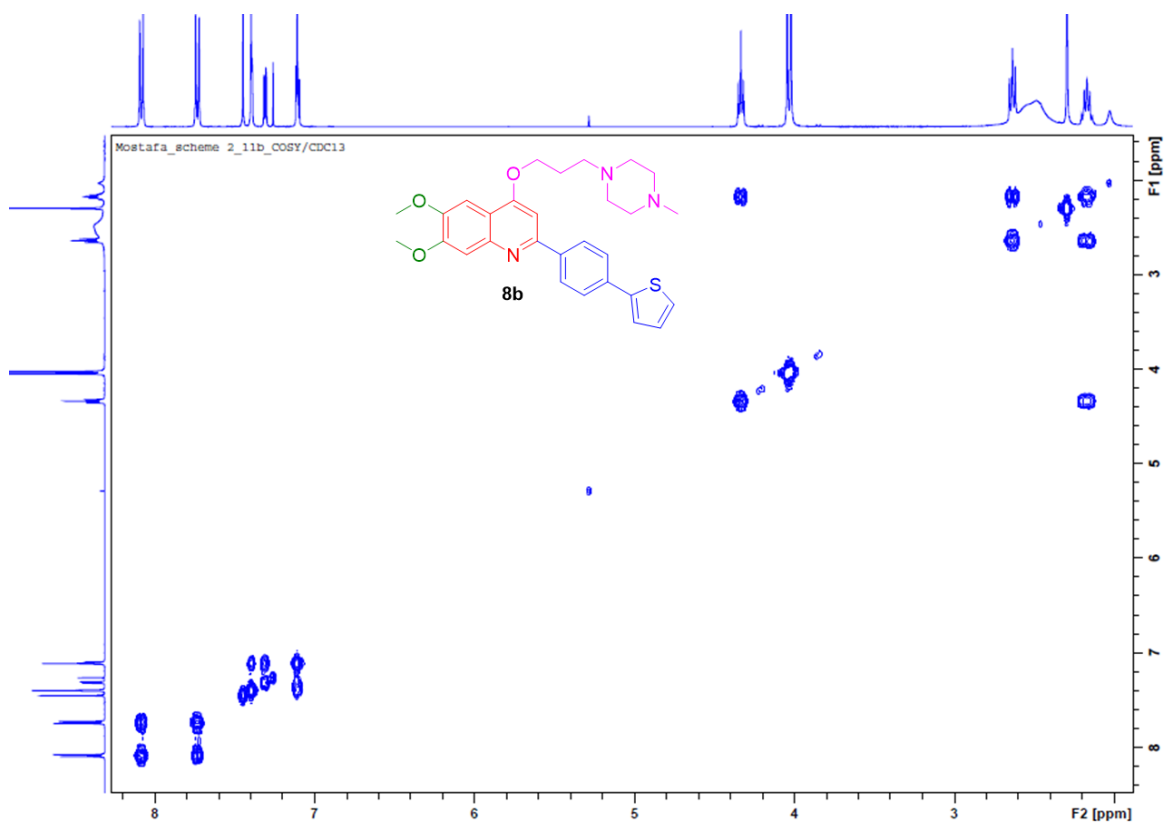
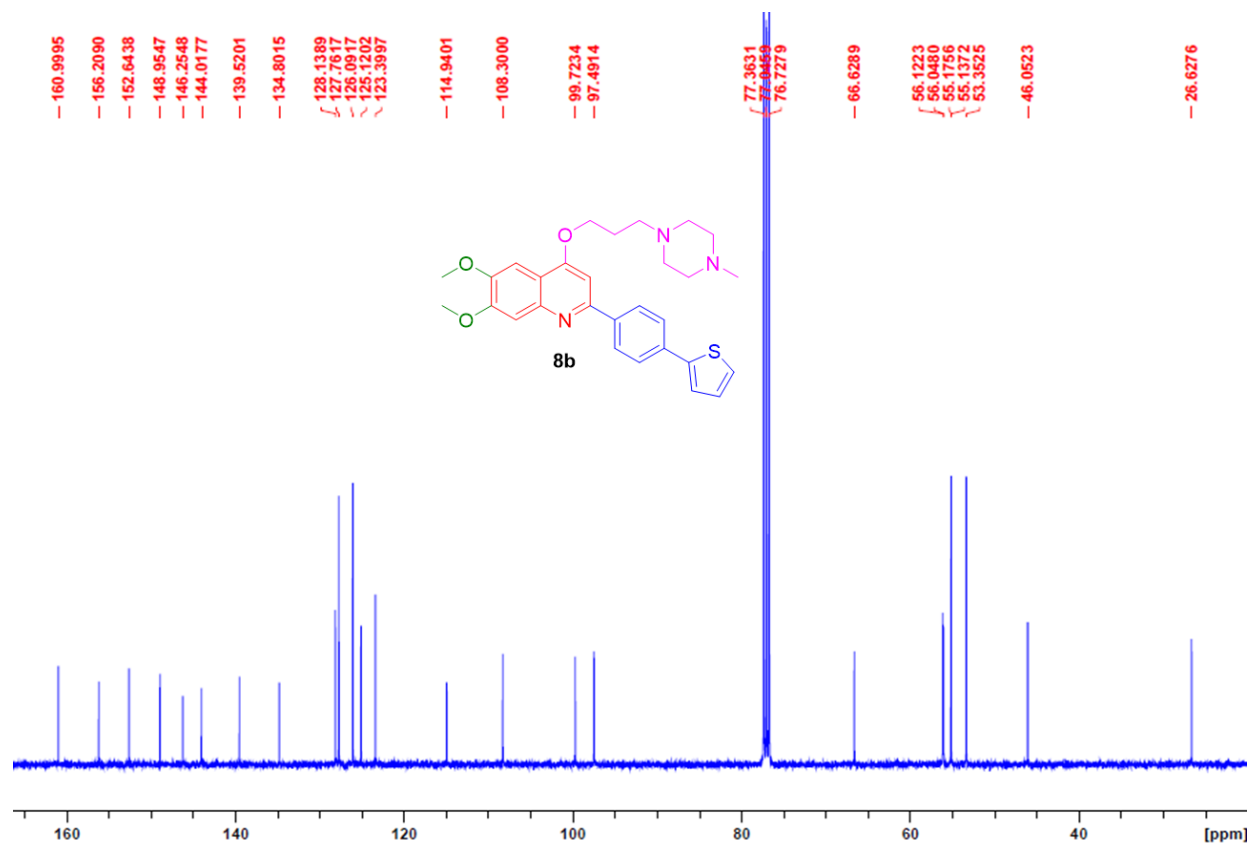


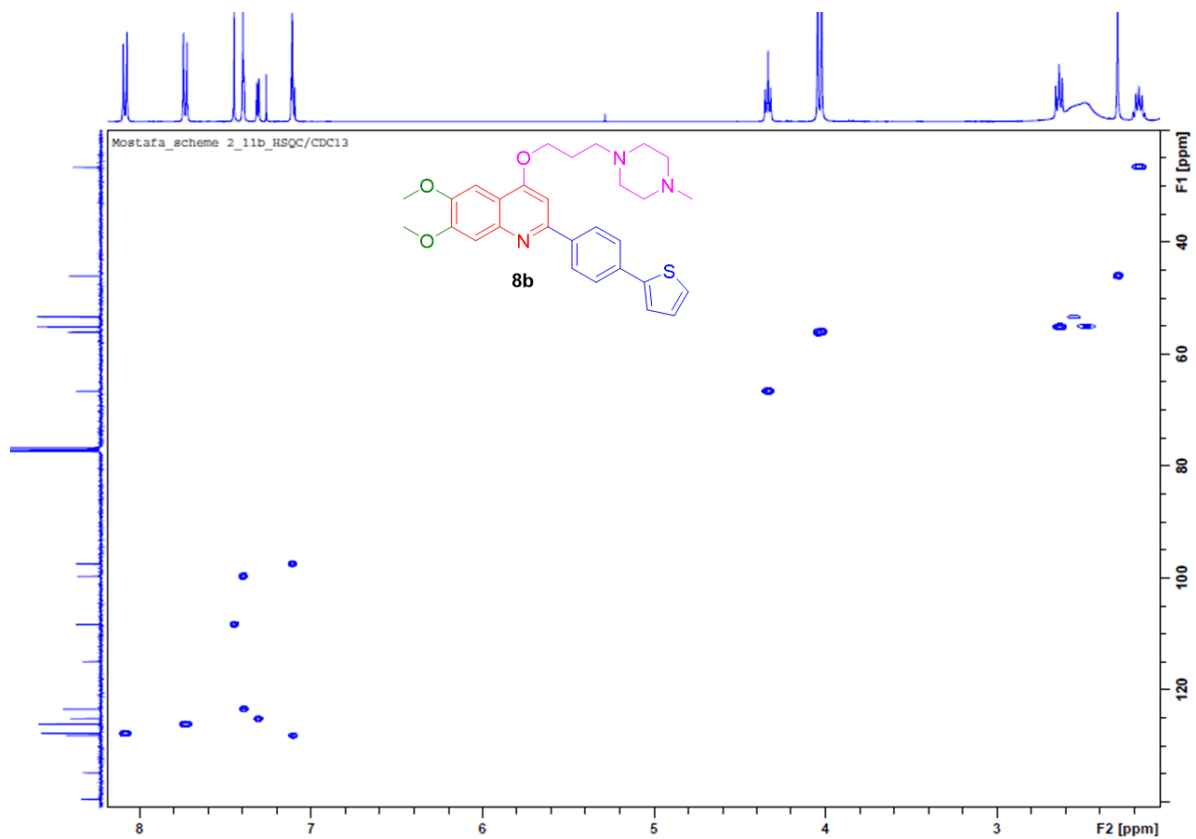
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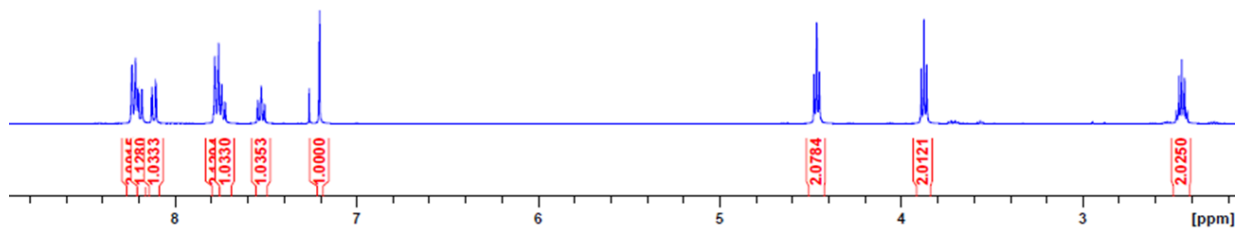
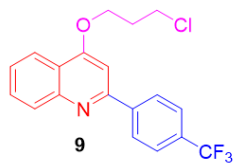


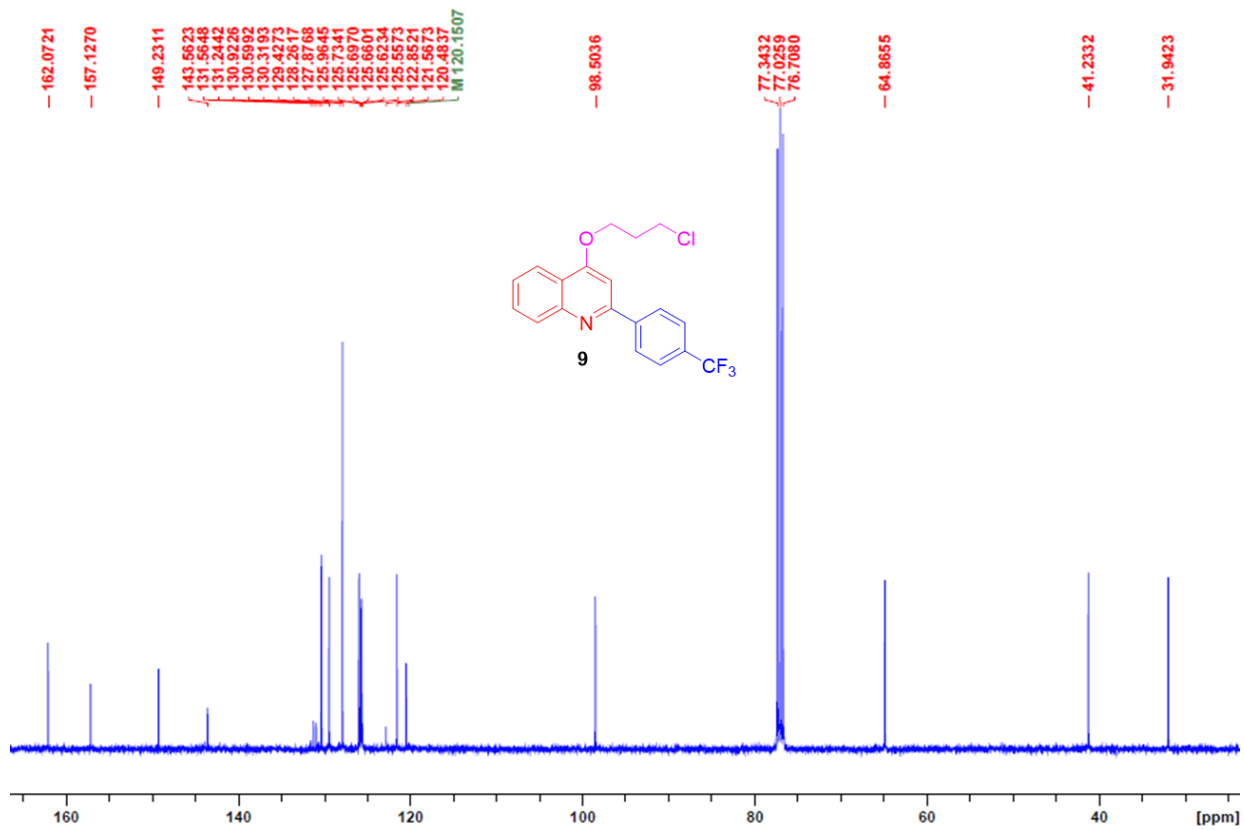
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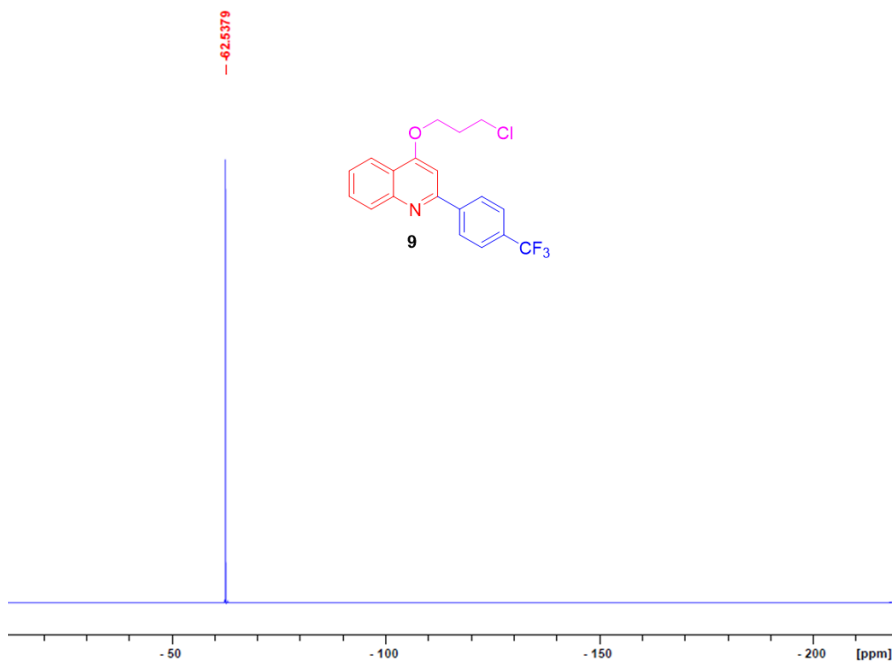
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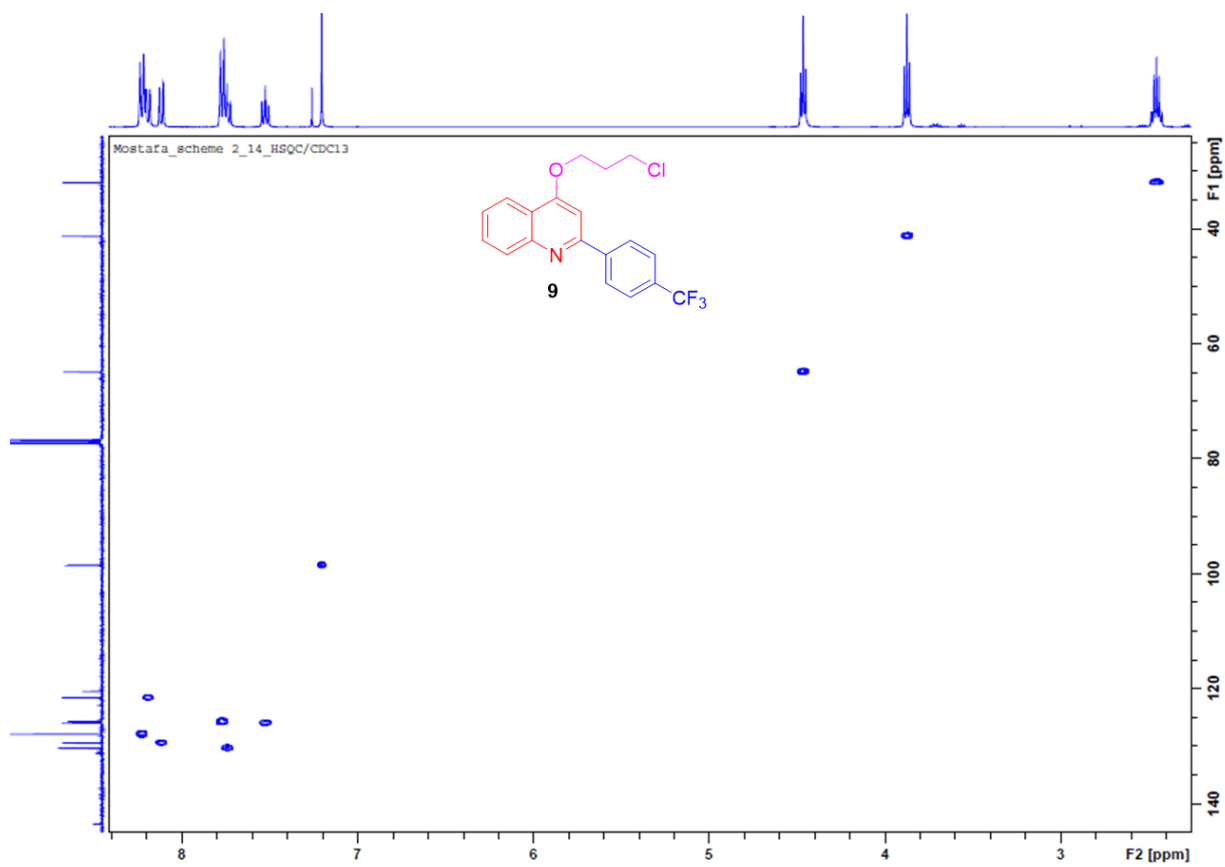
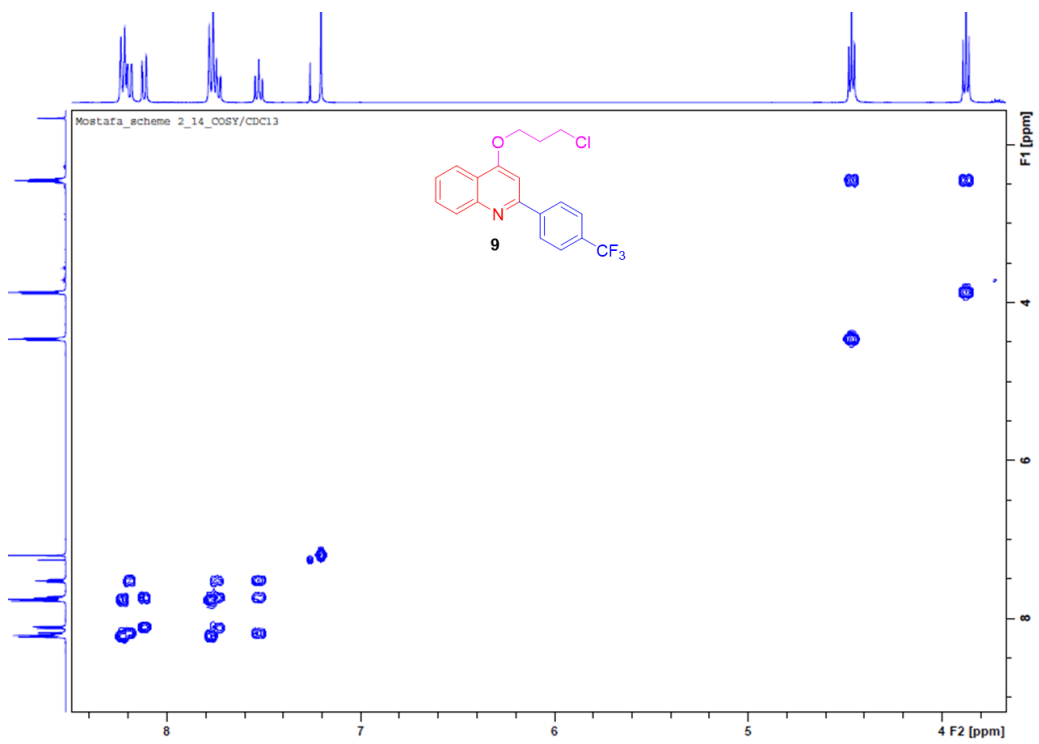
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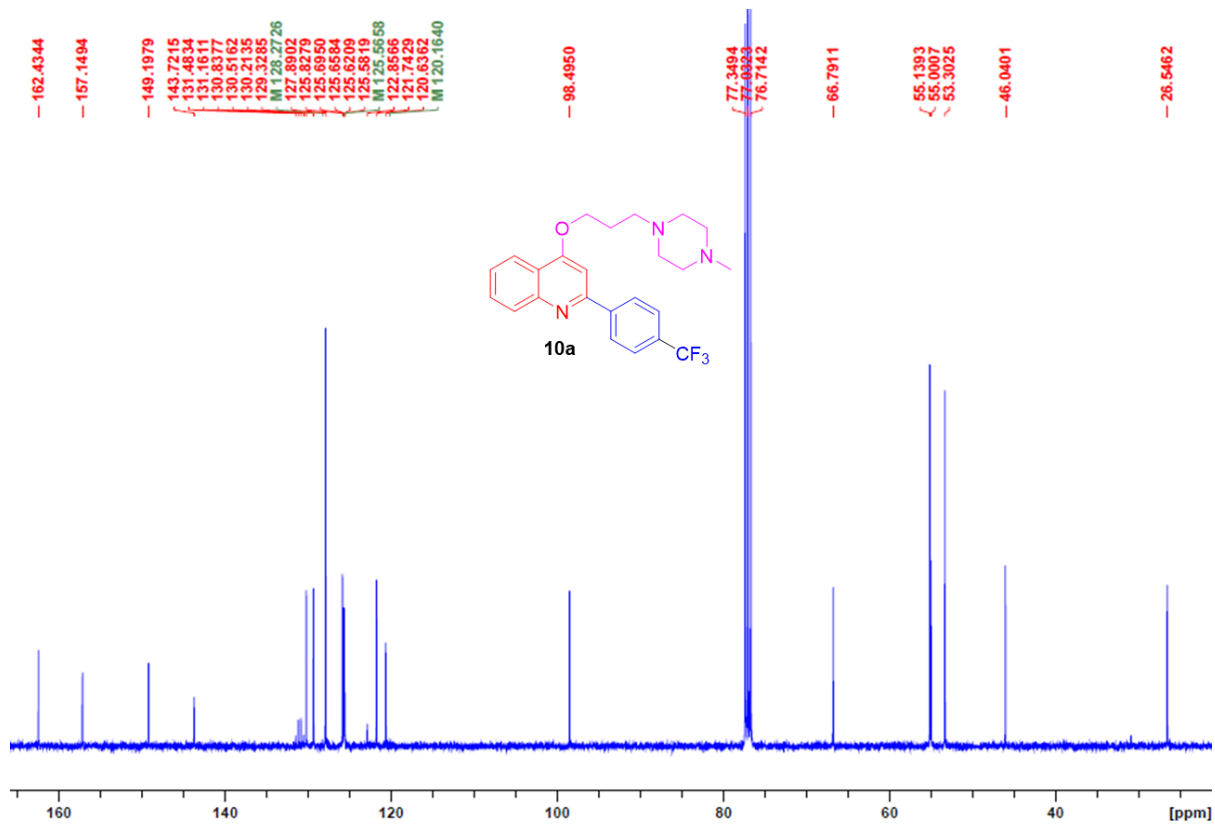
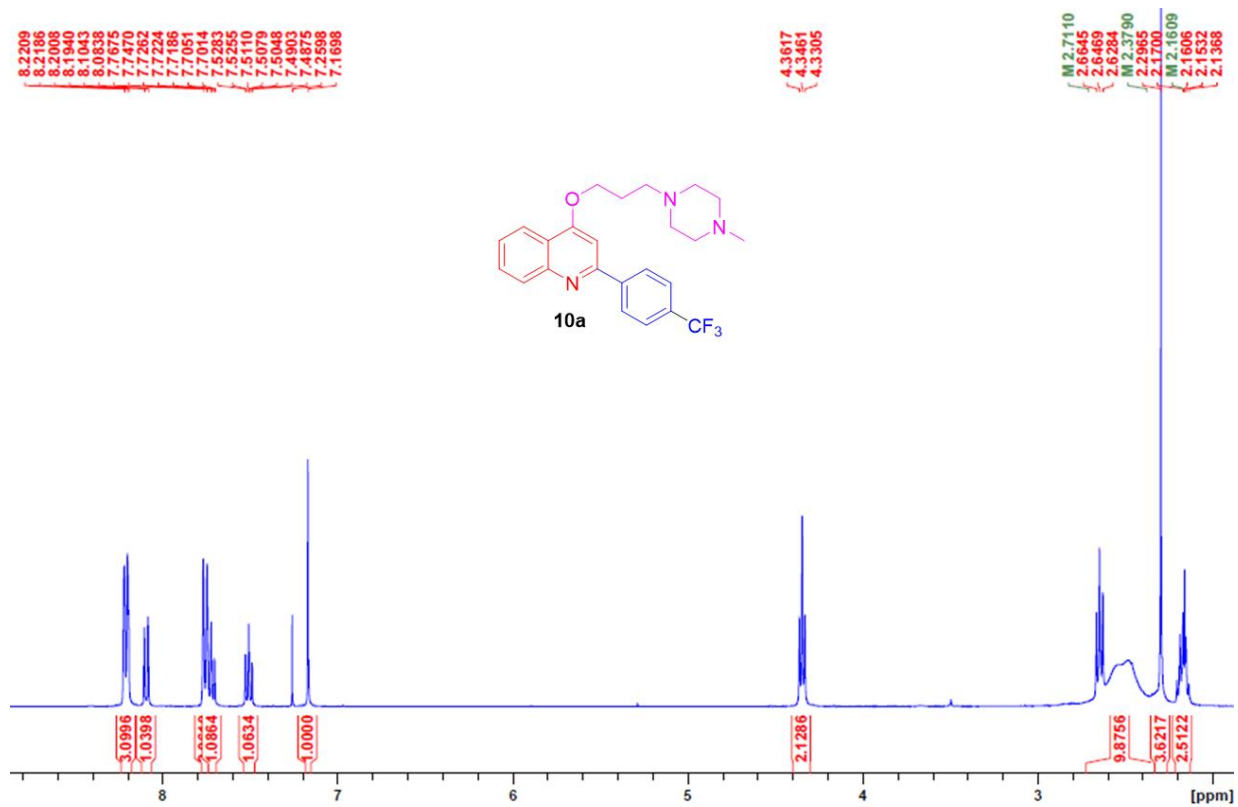




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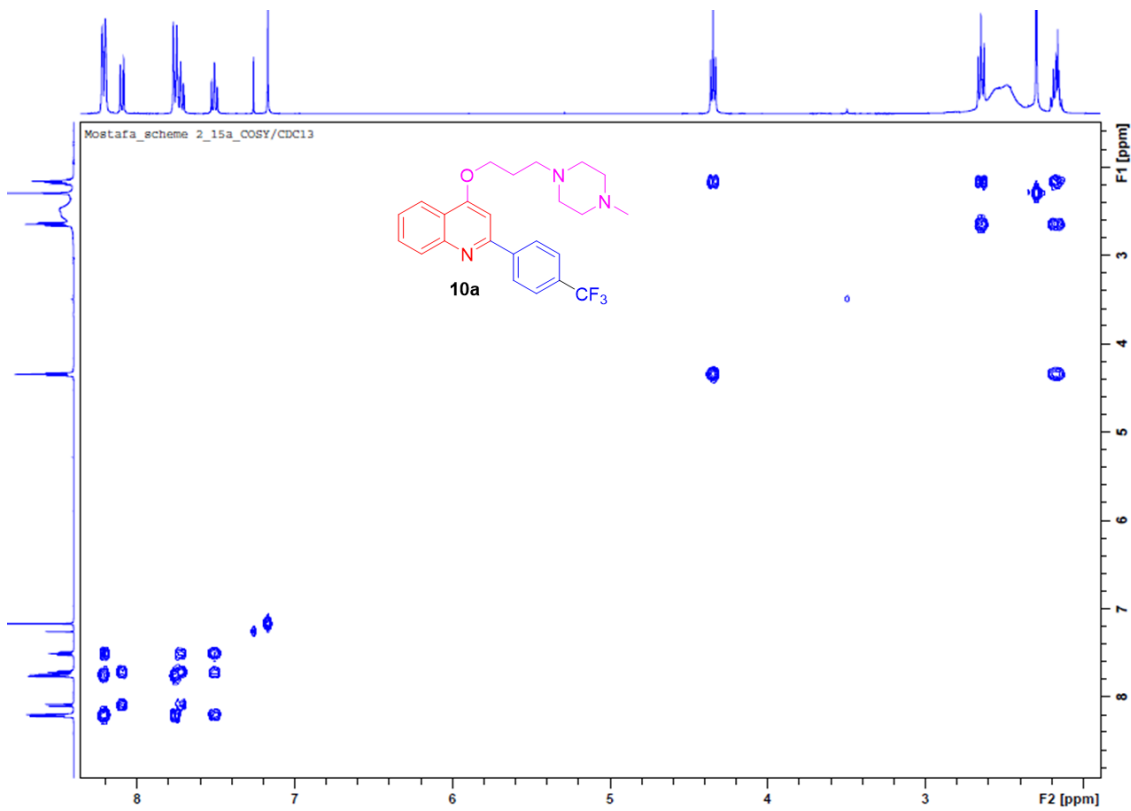
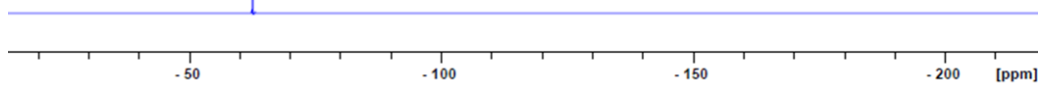
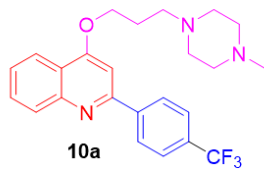


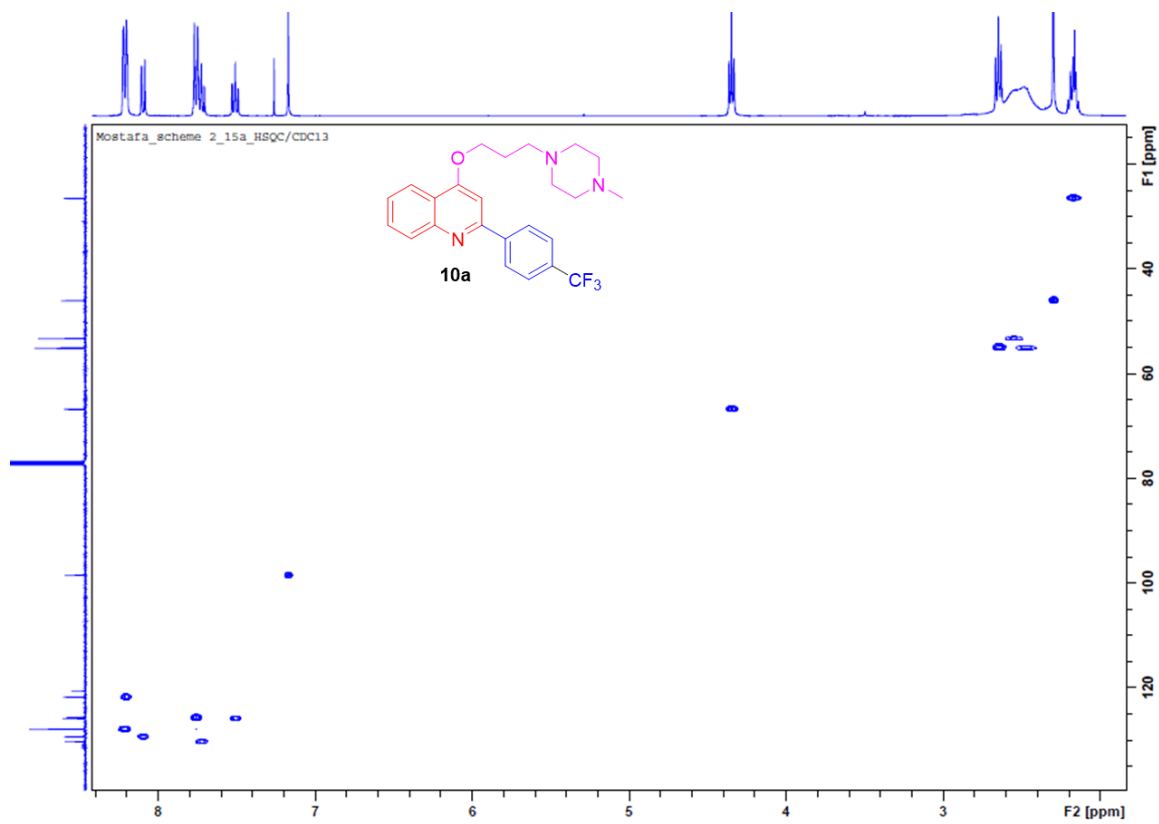




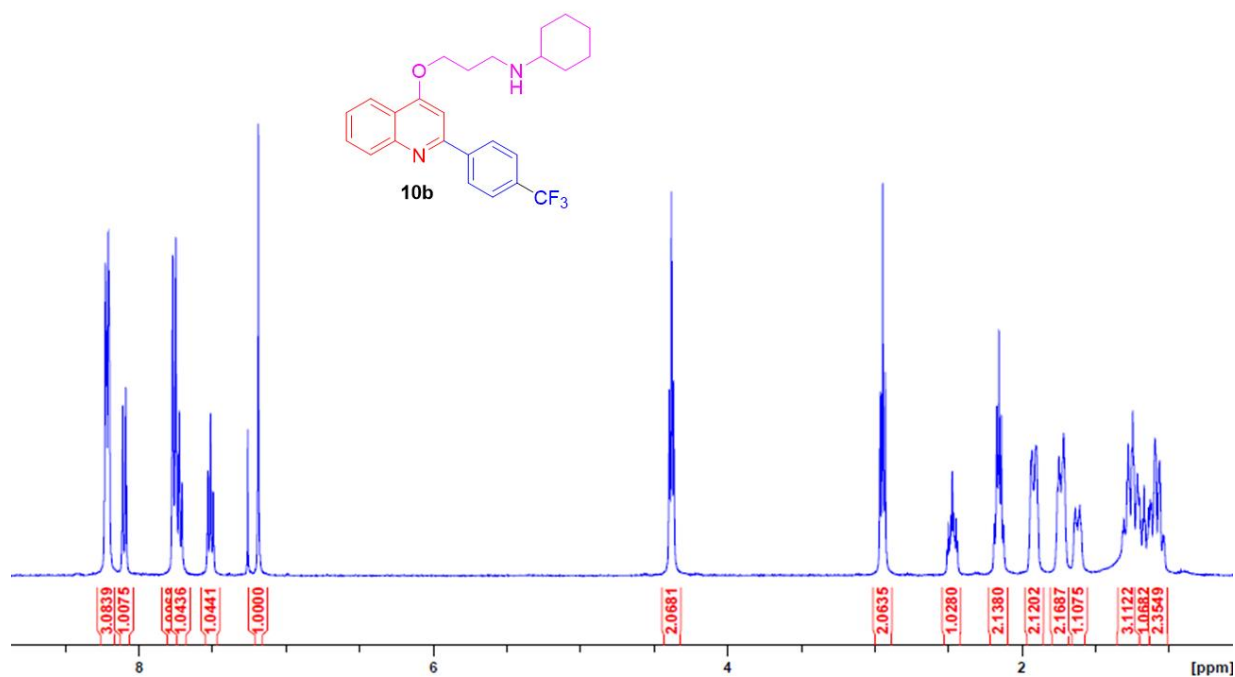
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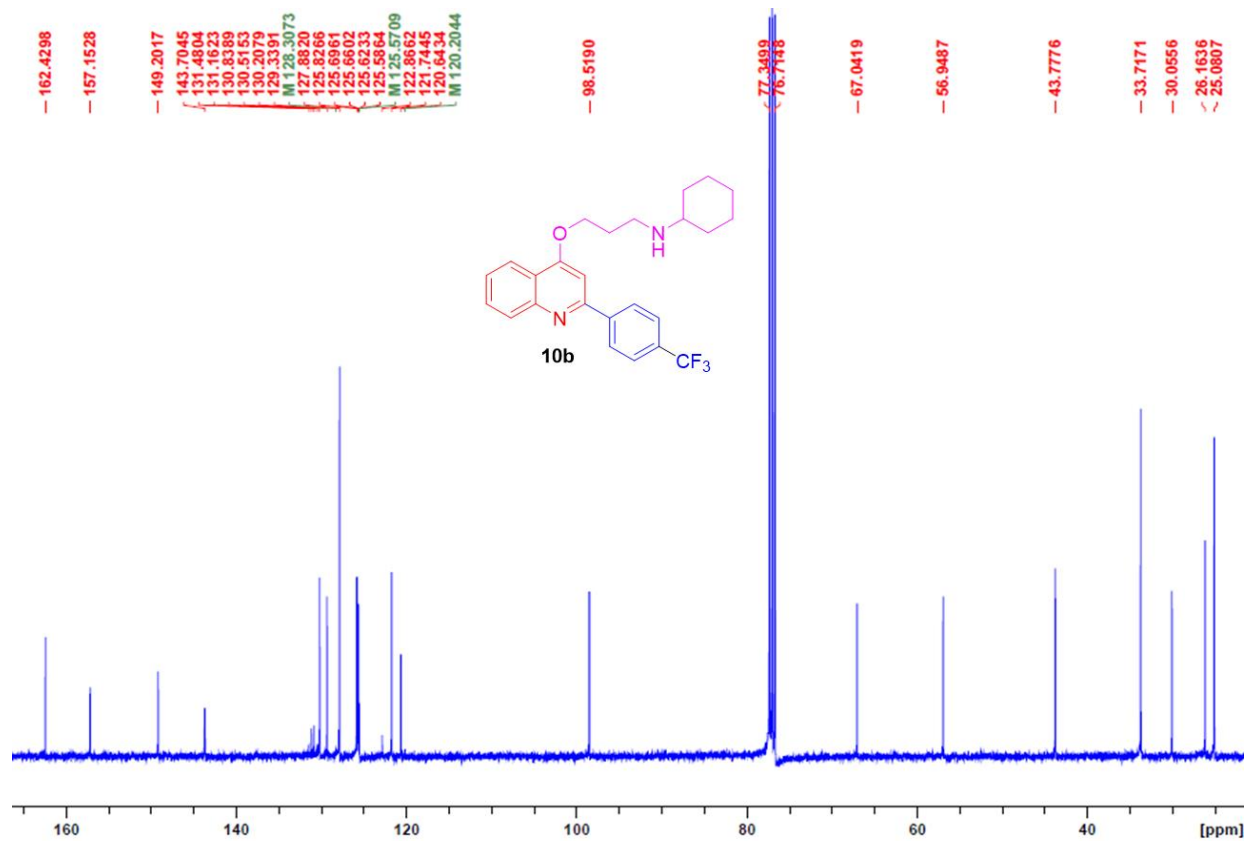




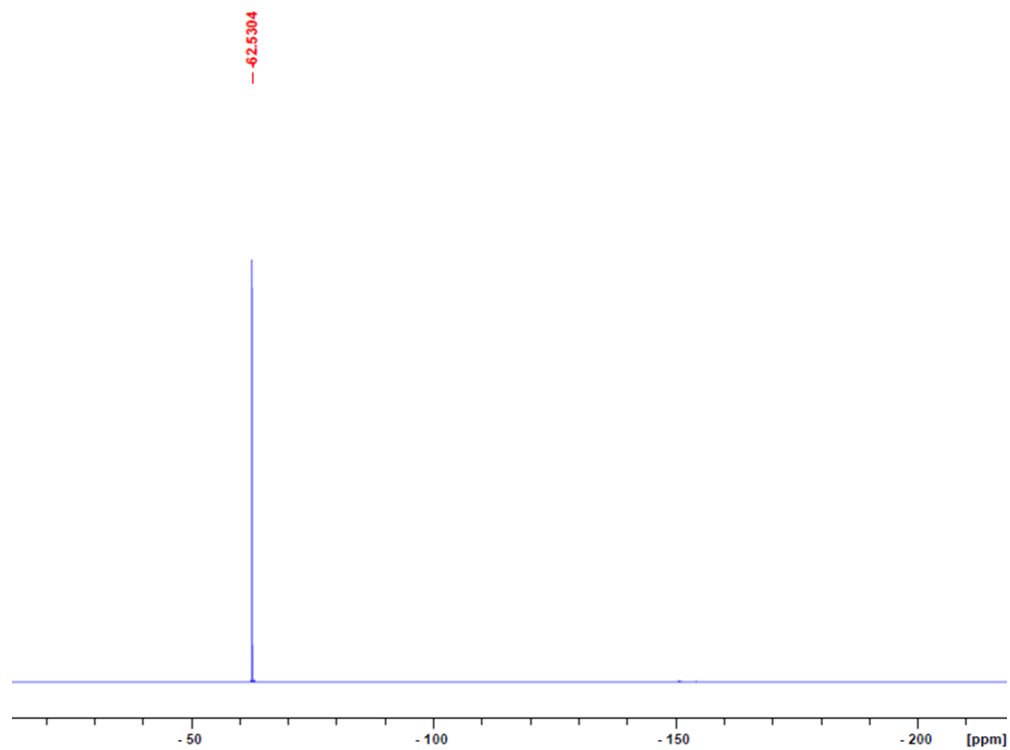
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| 7.7297 | 2.5075 |
| 7.7261 | 2.4882 |
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| 7.4951 | 2.1653 |
| 7.4951 | 2.1553 |
| 7.4926 | 2.1391 |
| 7.2599 | 2.1228 |
| 7.1880 | 1.9311 |
| | 1.9055 |
| | 1.7567 |
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| | 1.7080 |
| | 1.6985 |
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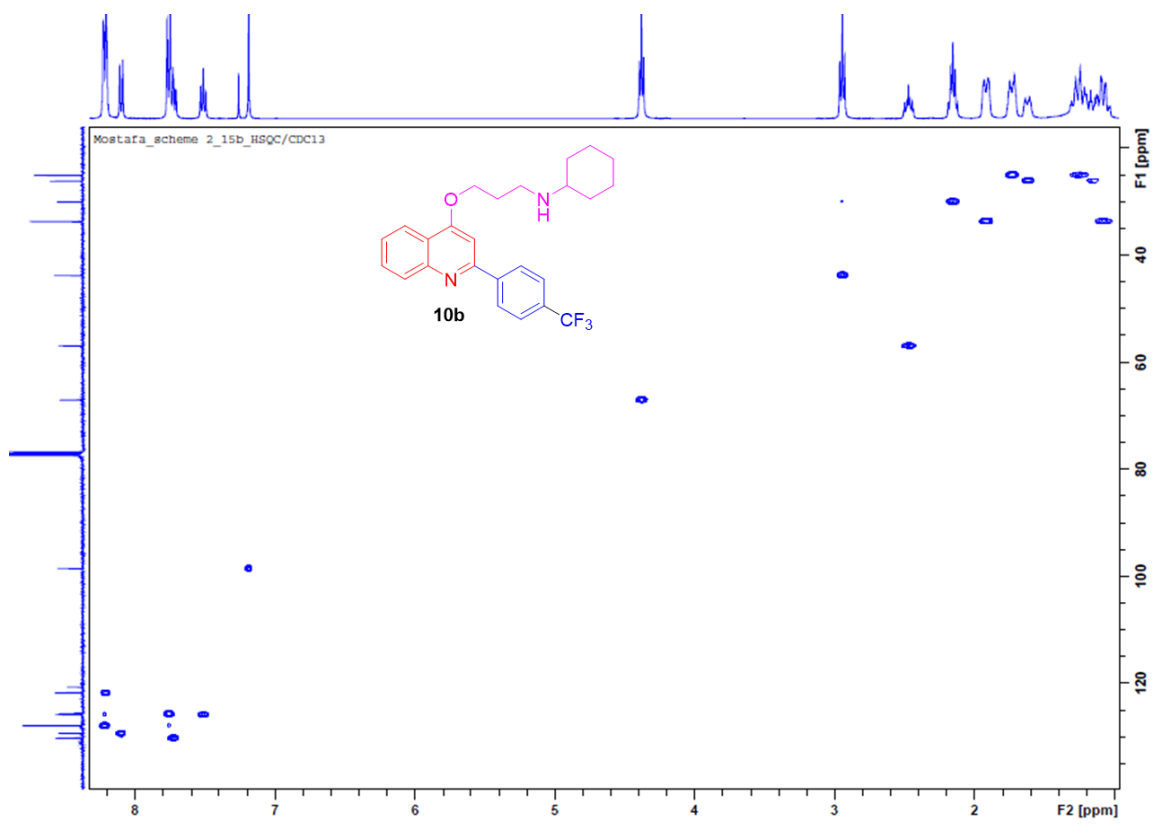
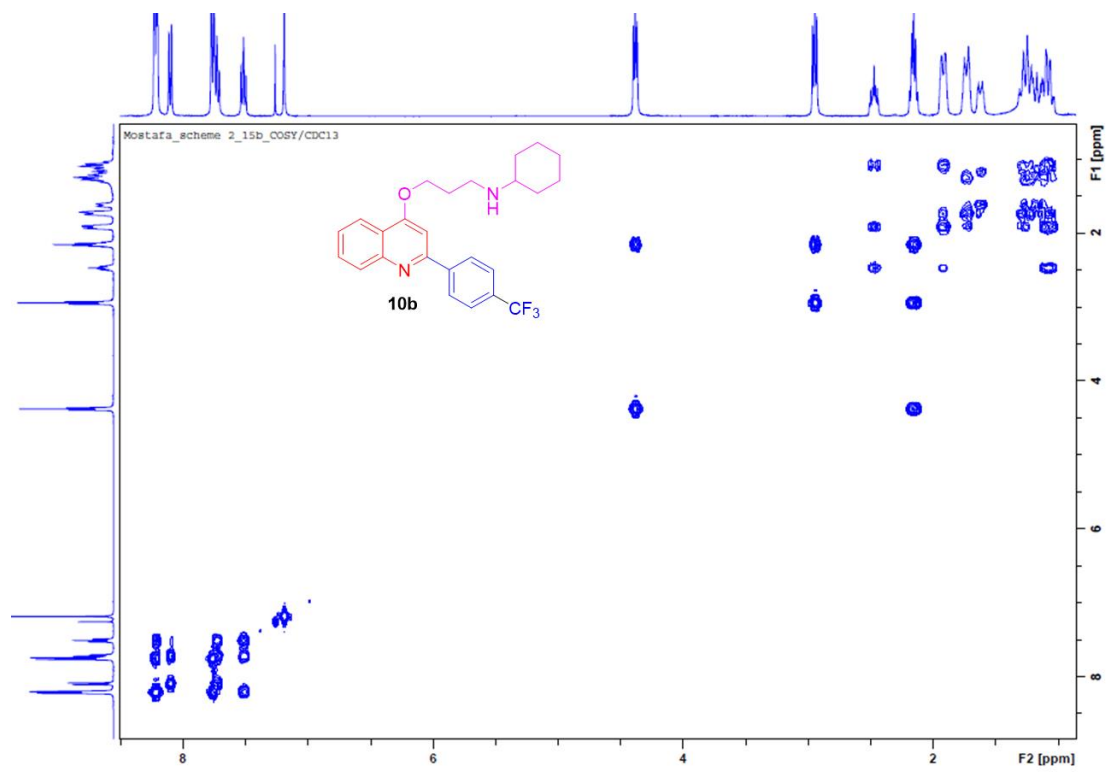


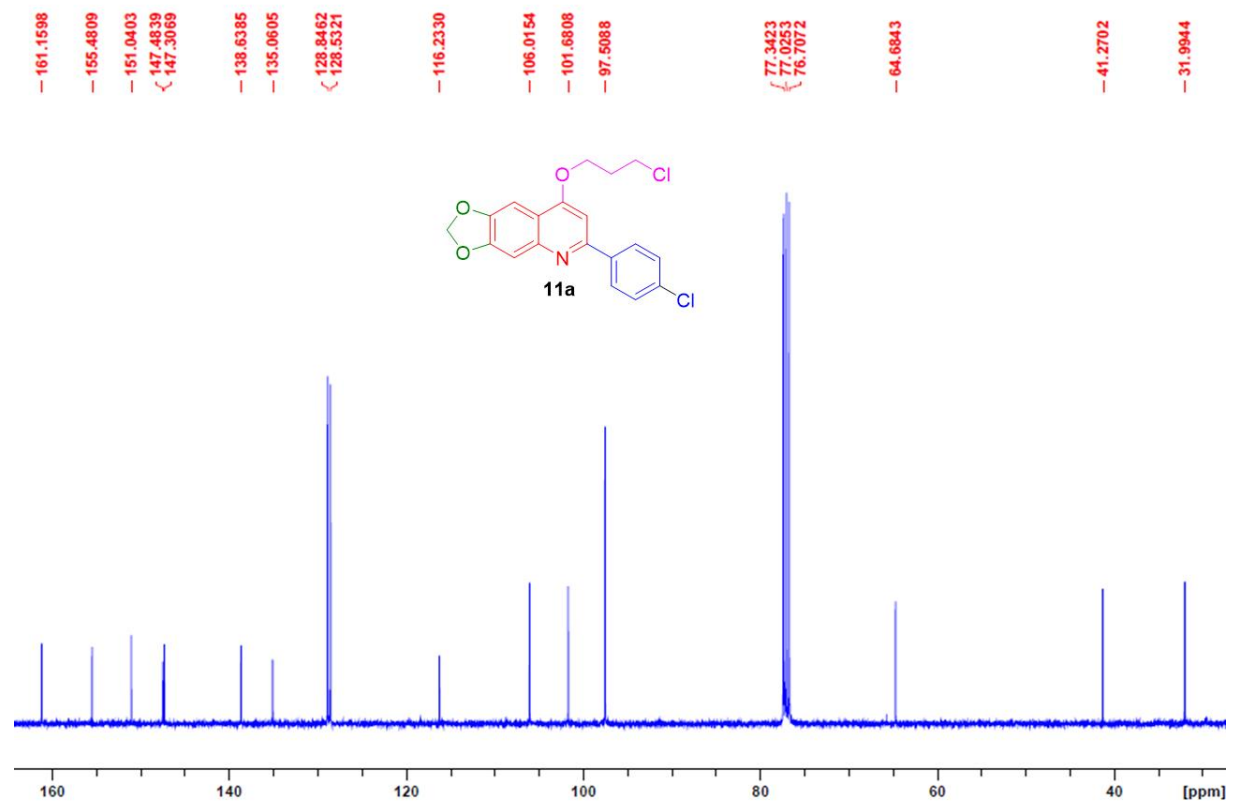
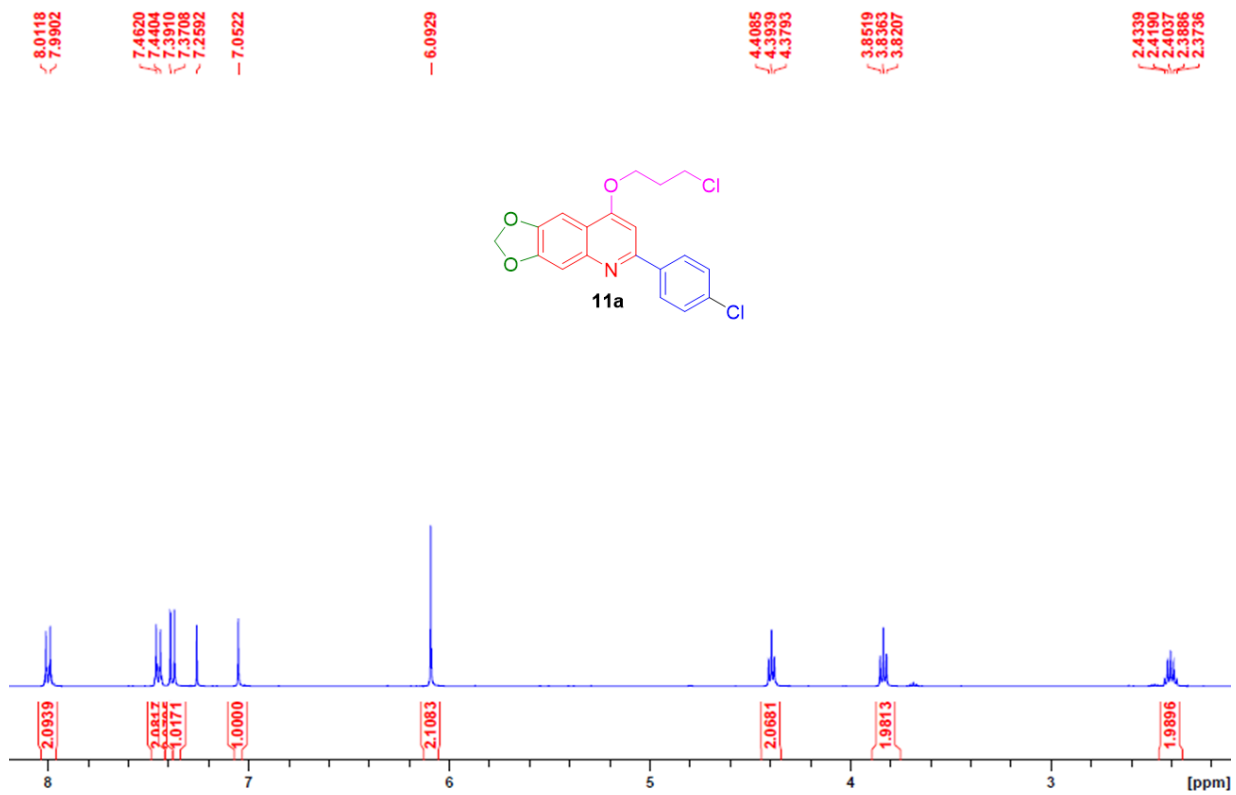
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| | 1.0280 |
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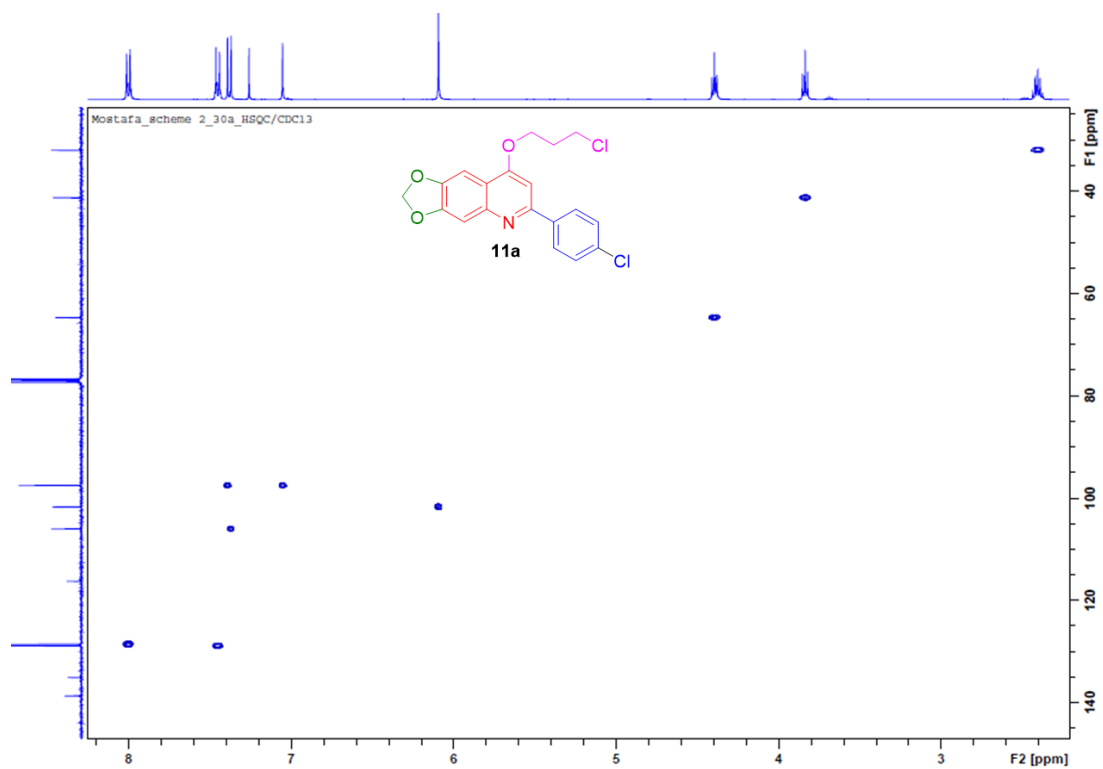
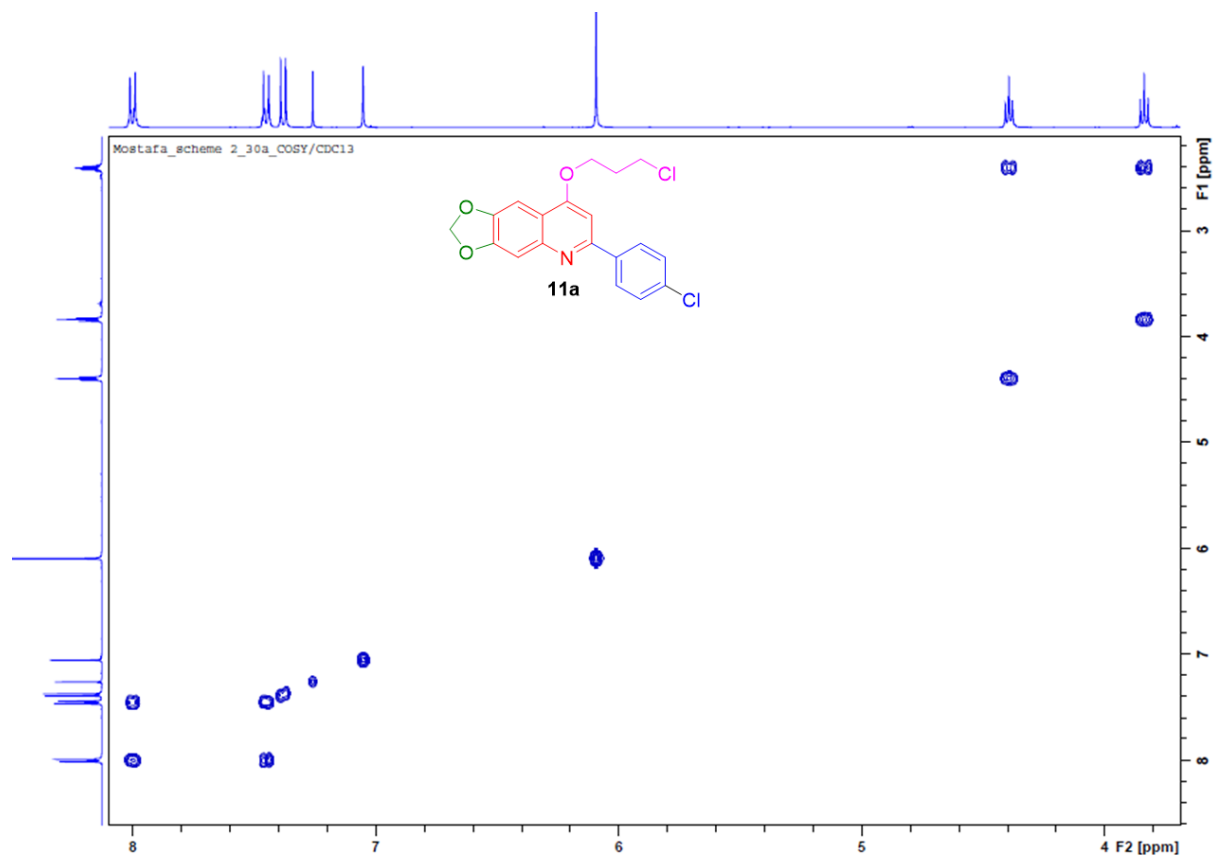


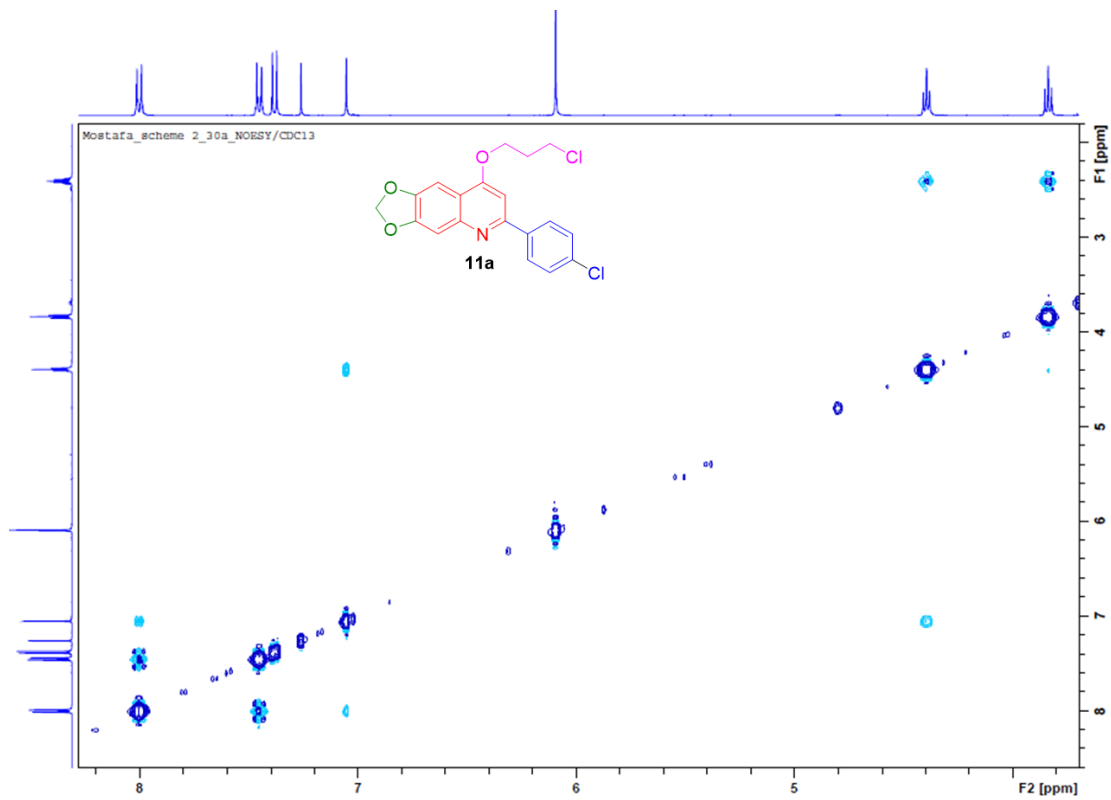
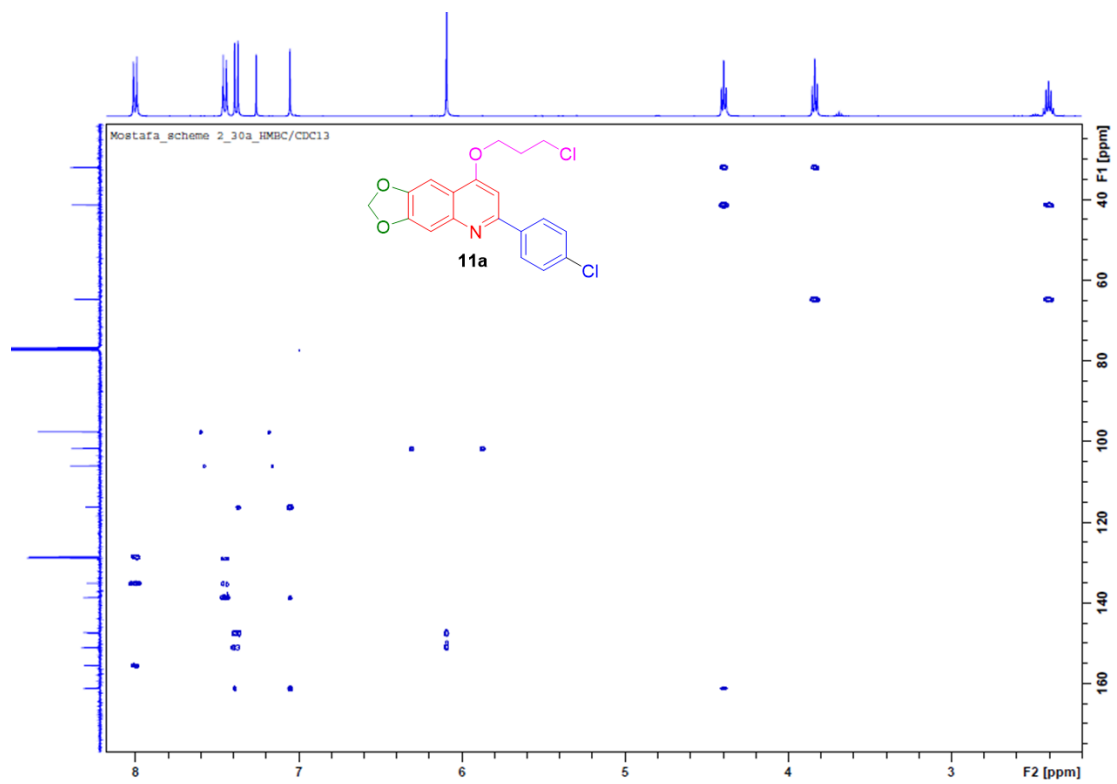
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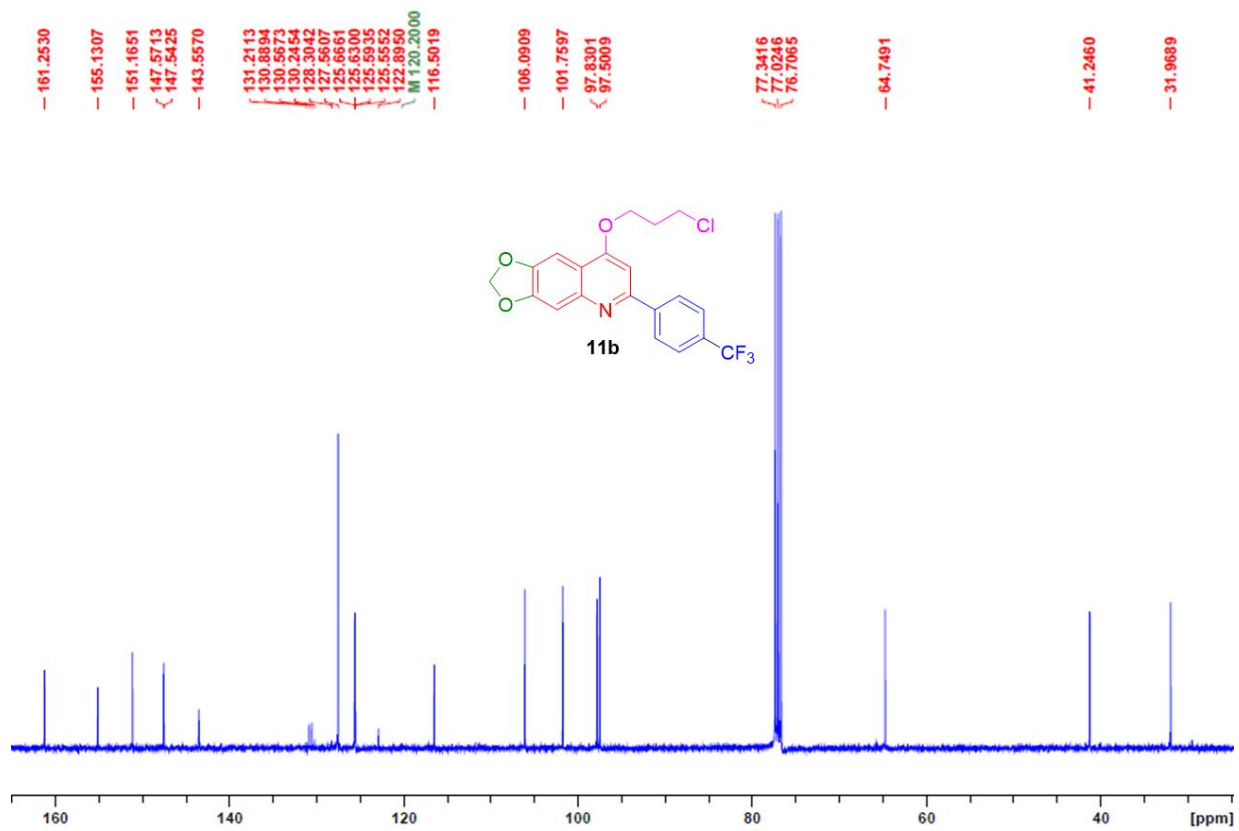
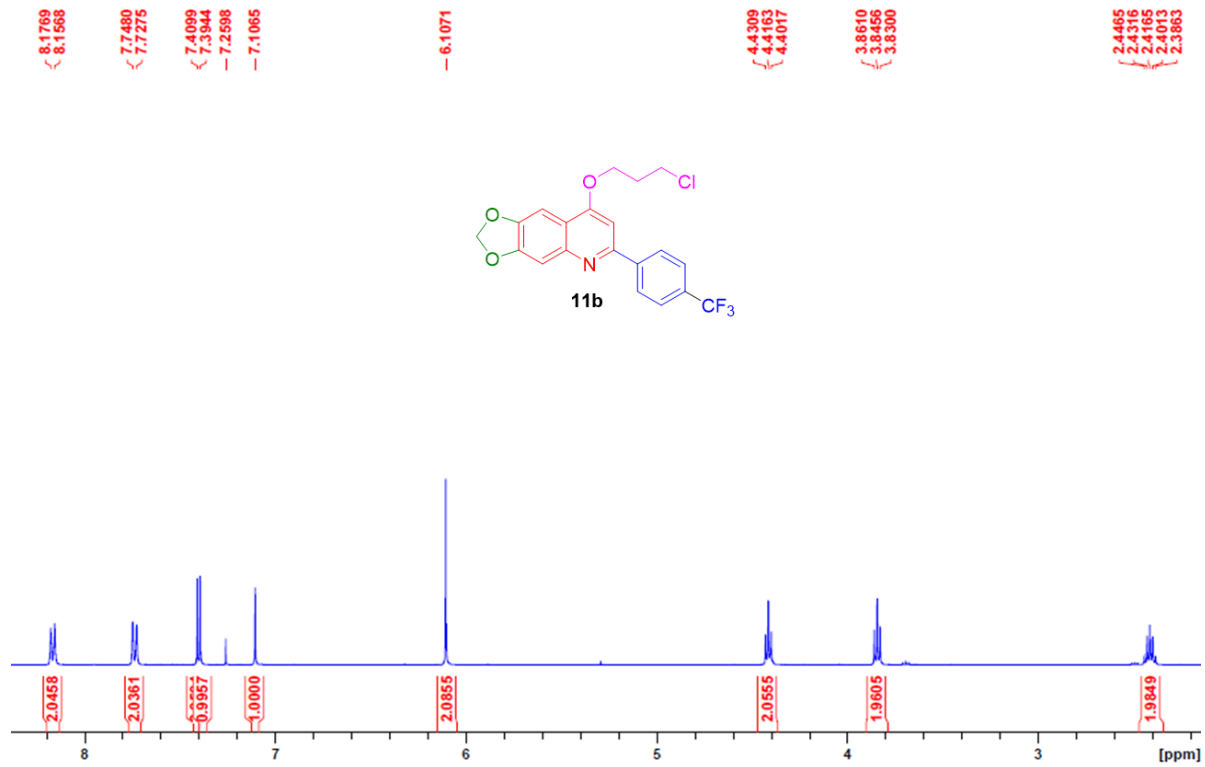


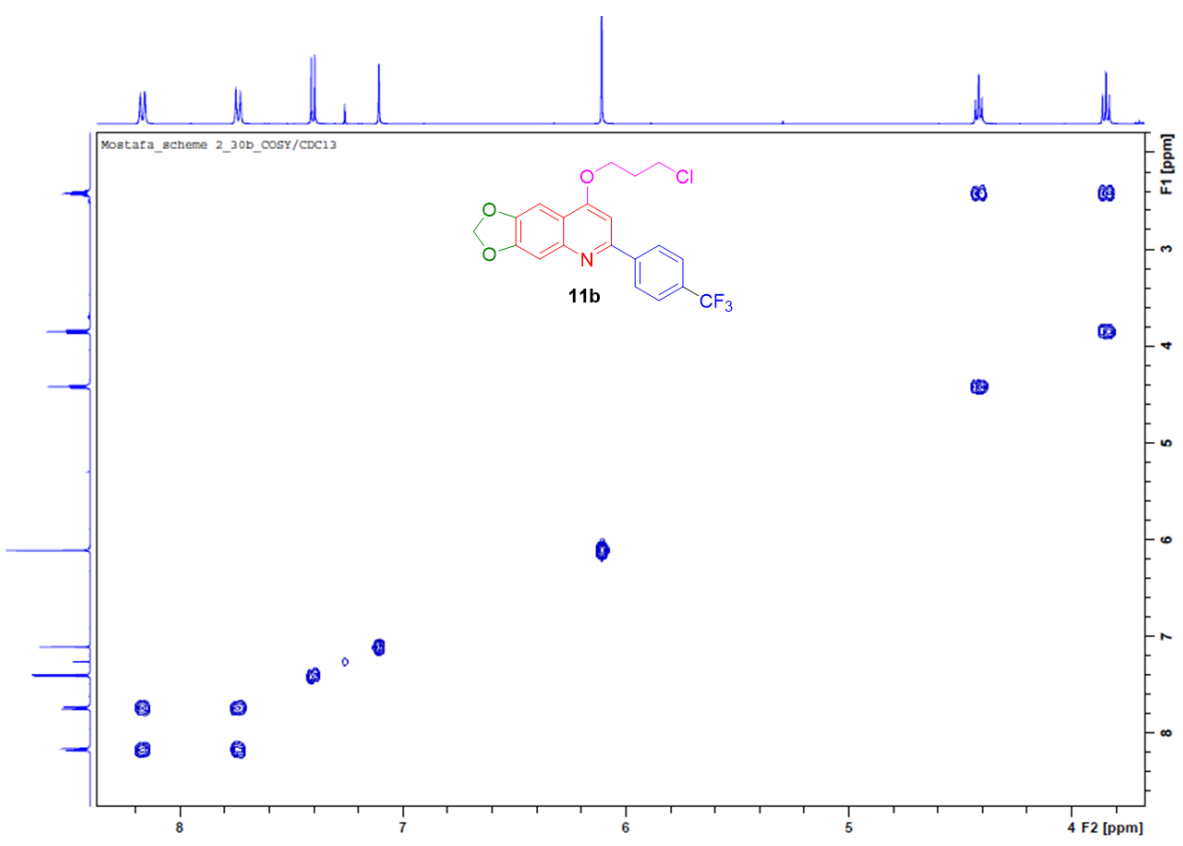
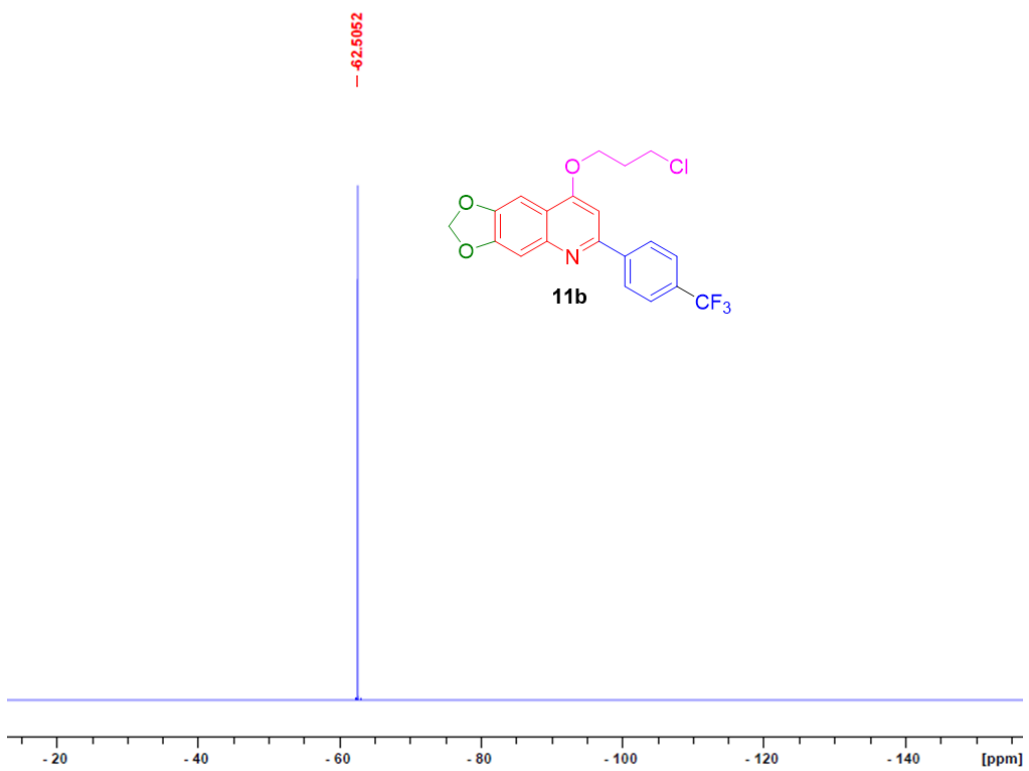


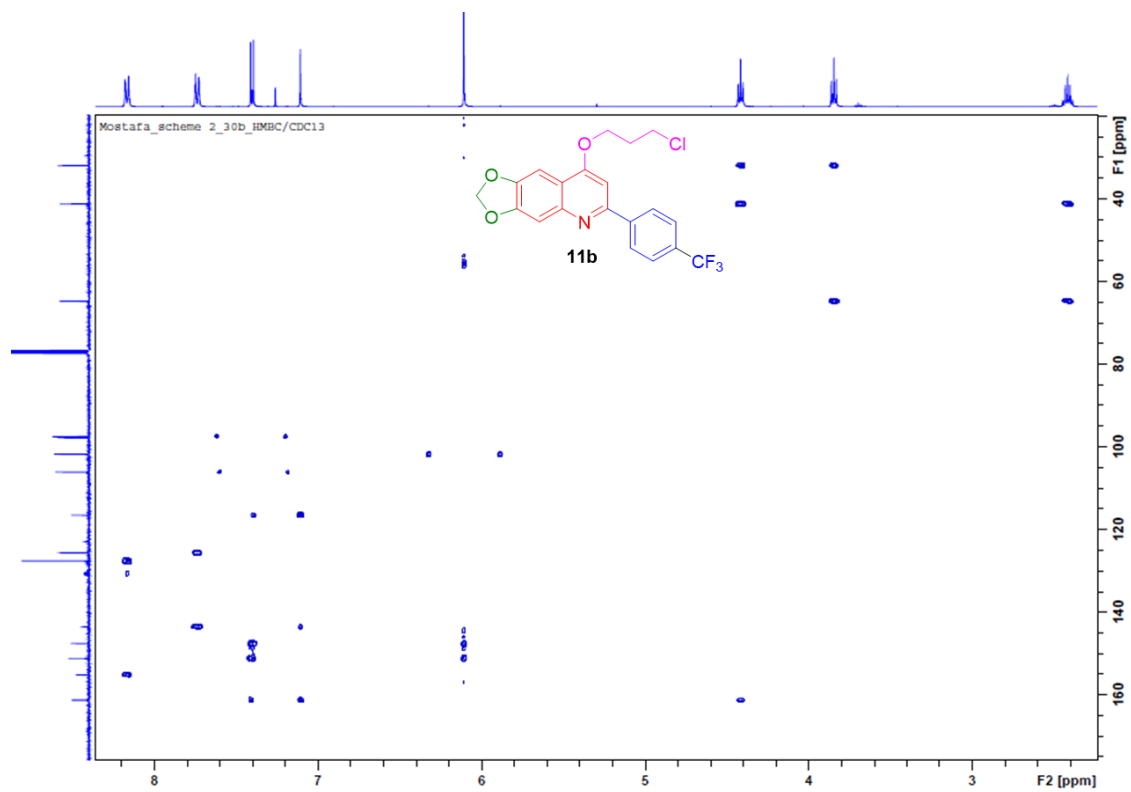
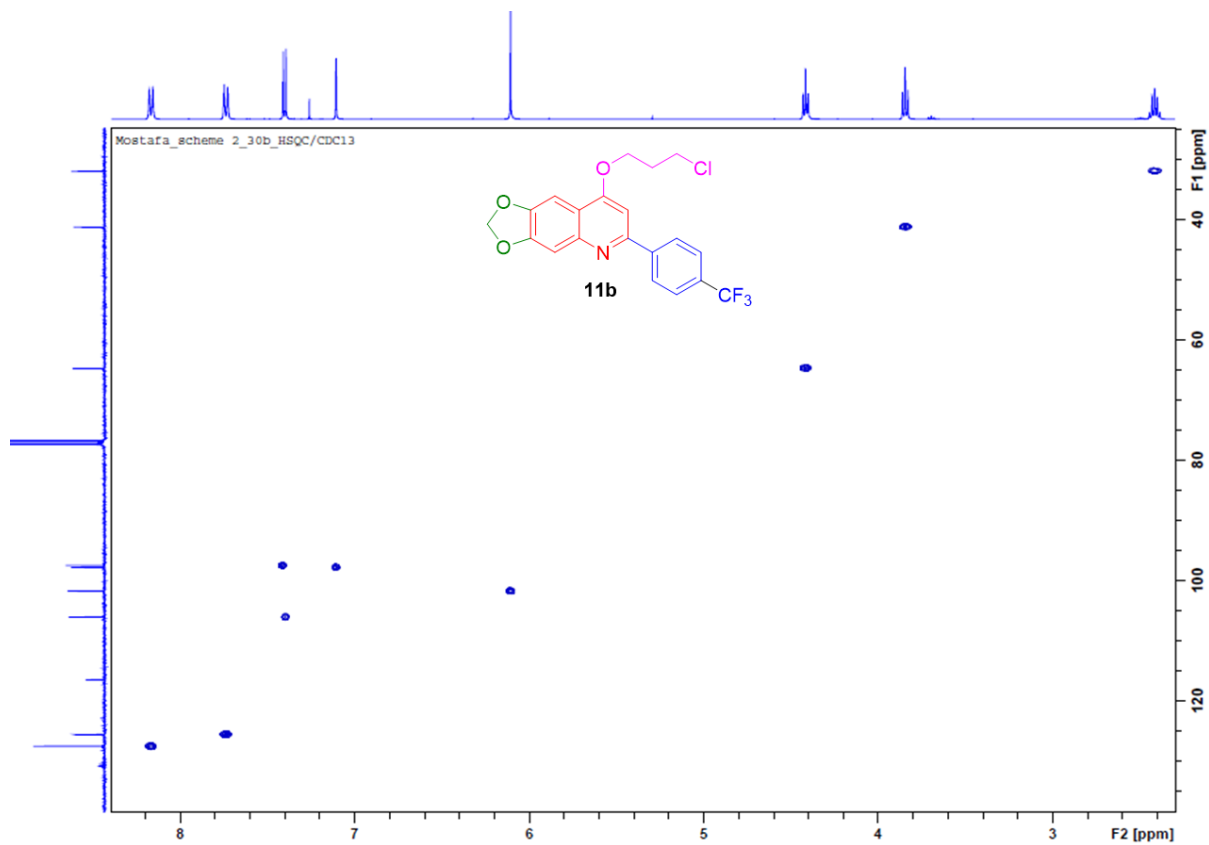


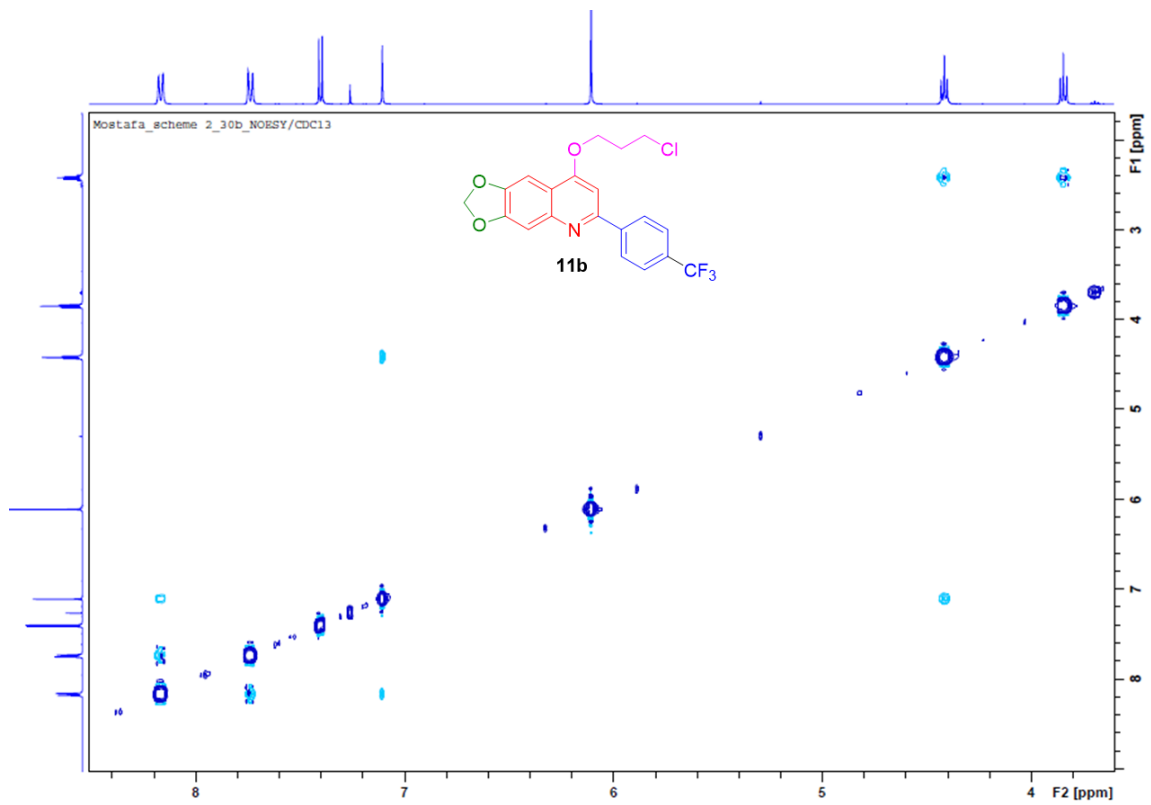












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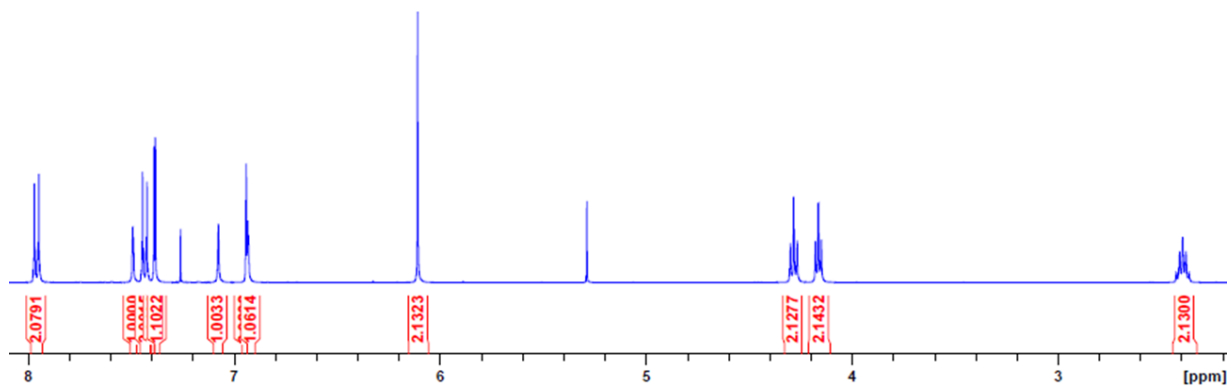
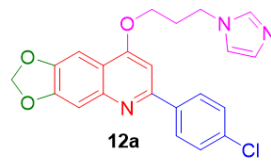
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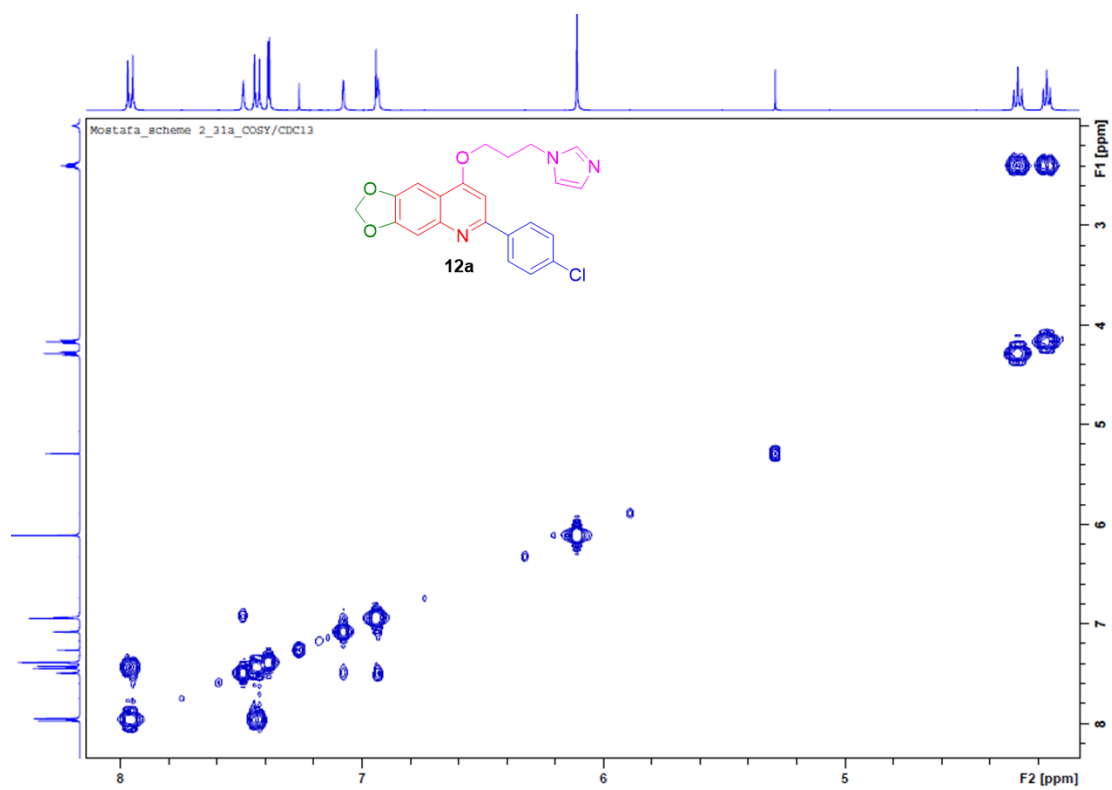
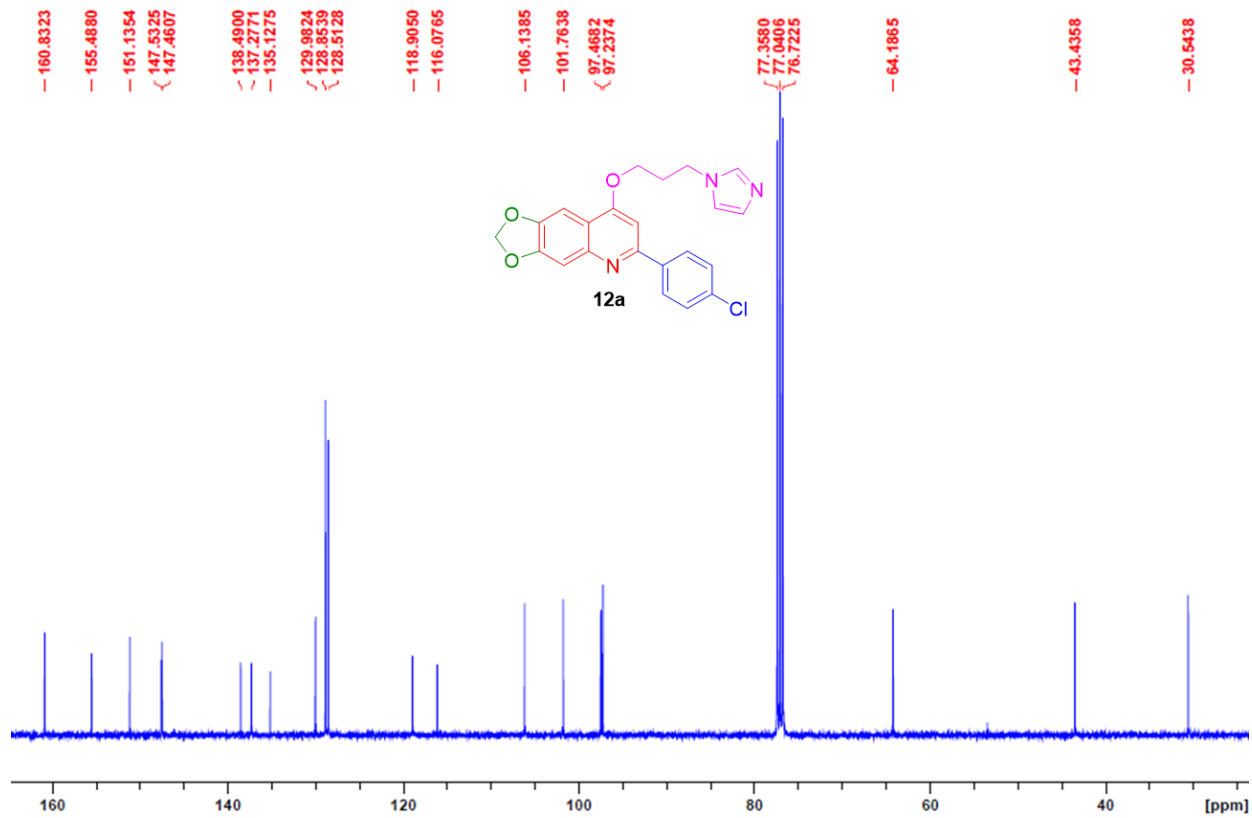
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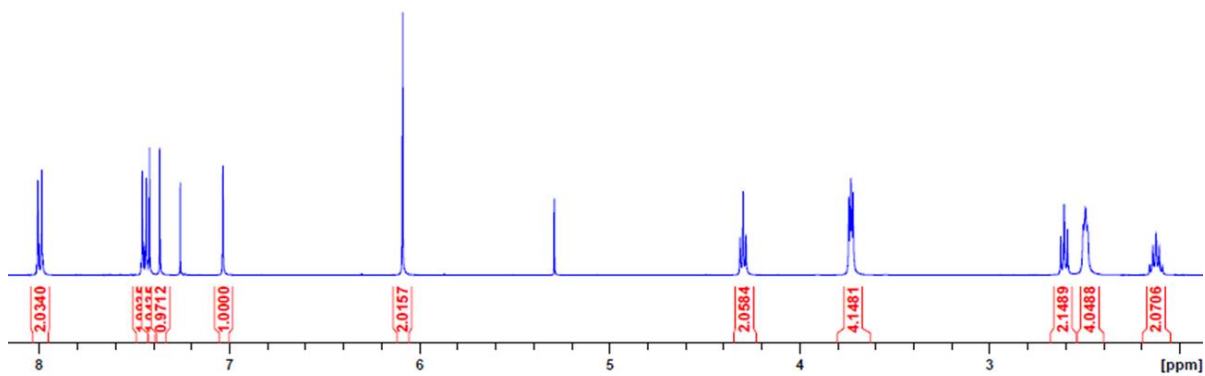
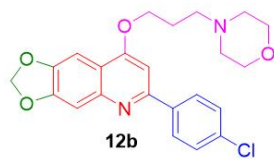
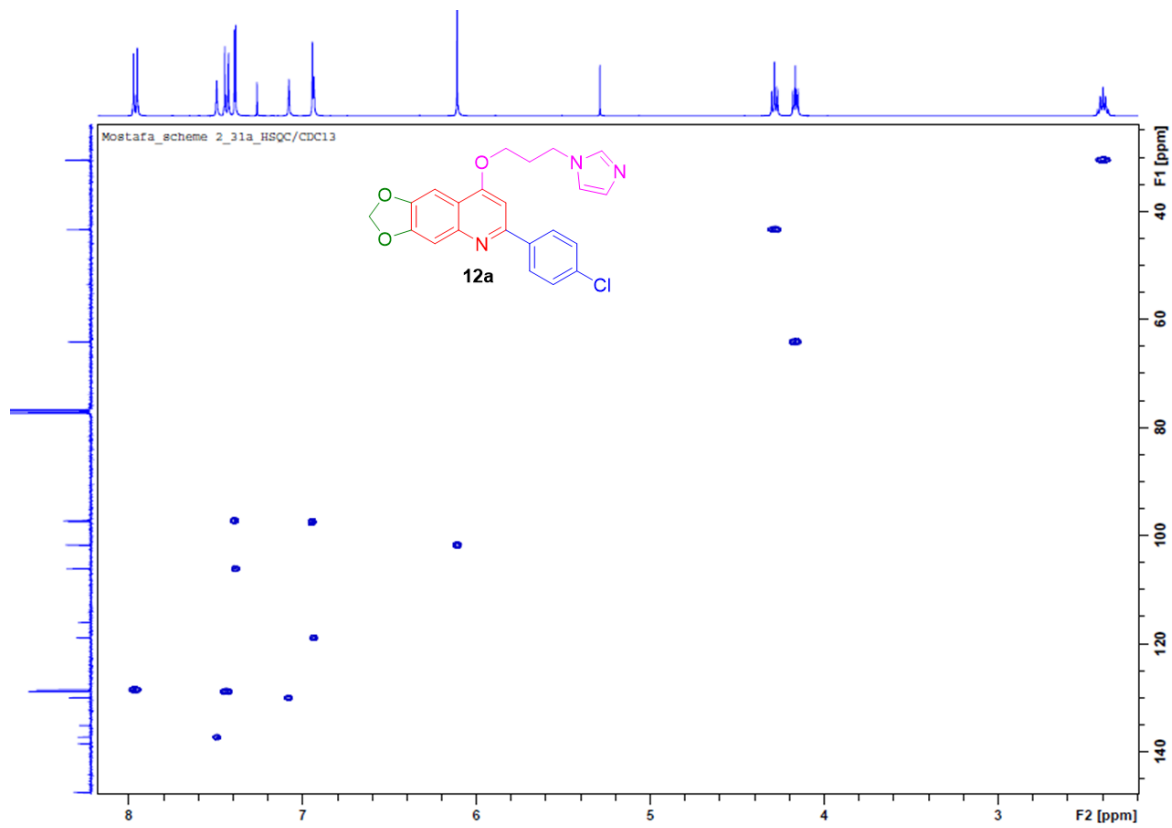
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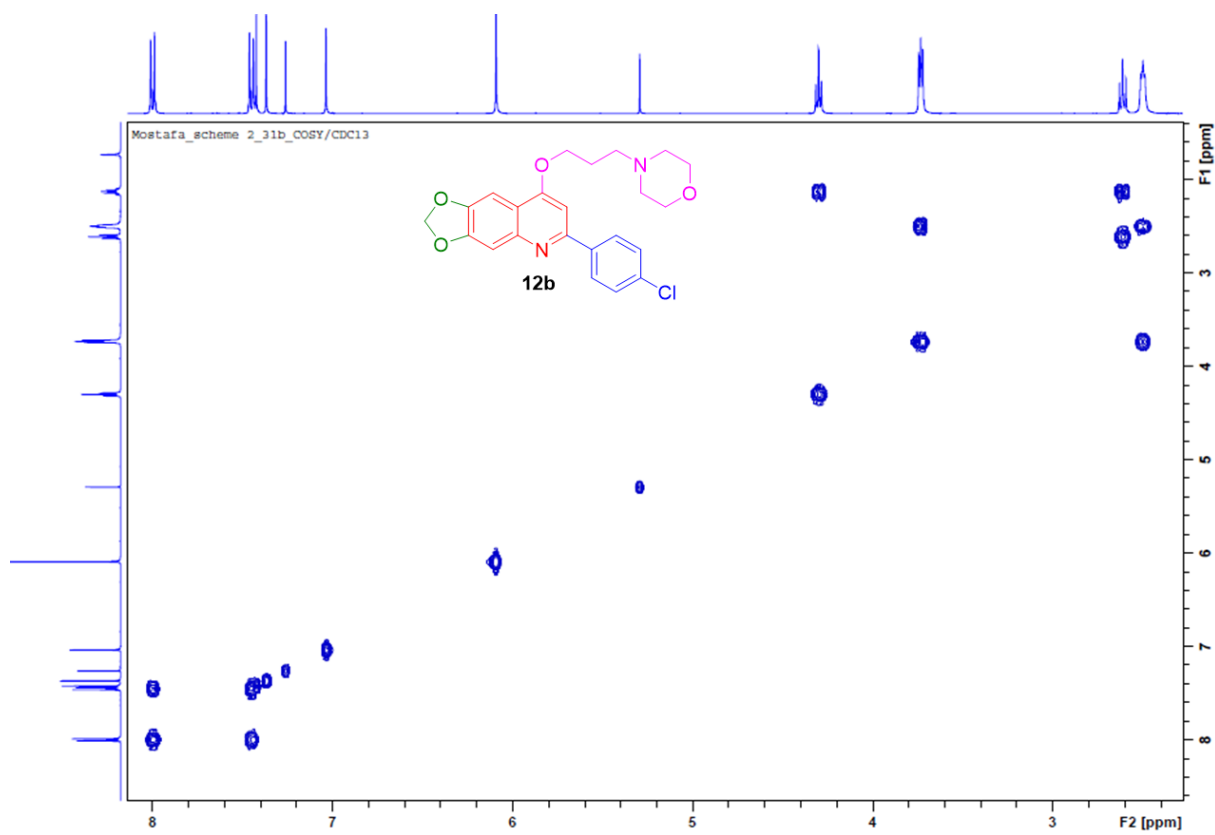
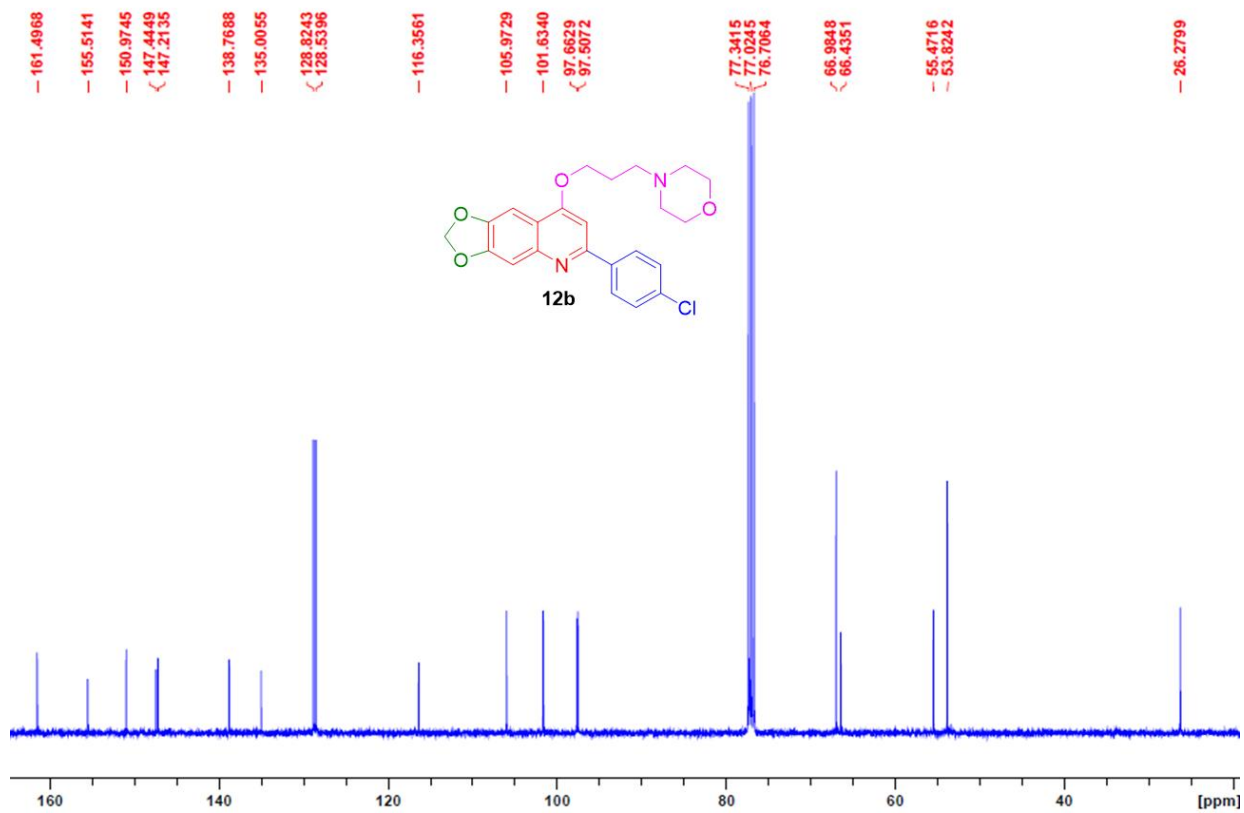
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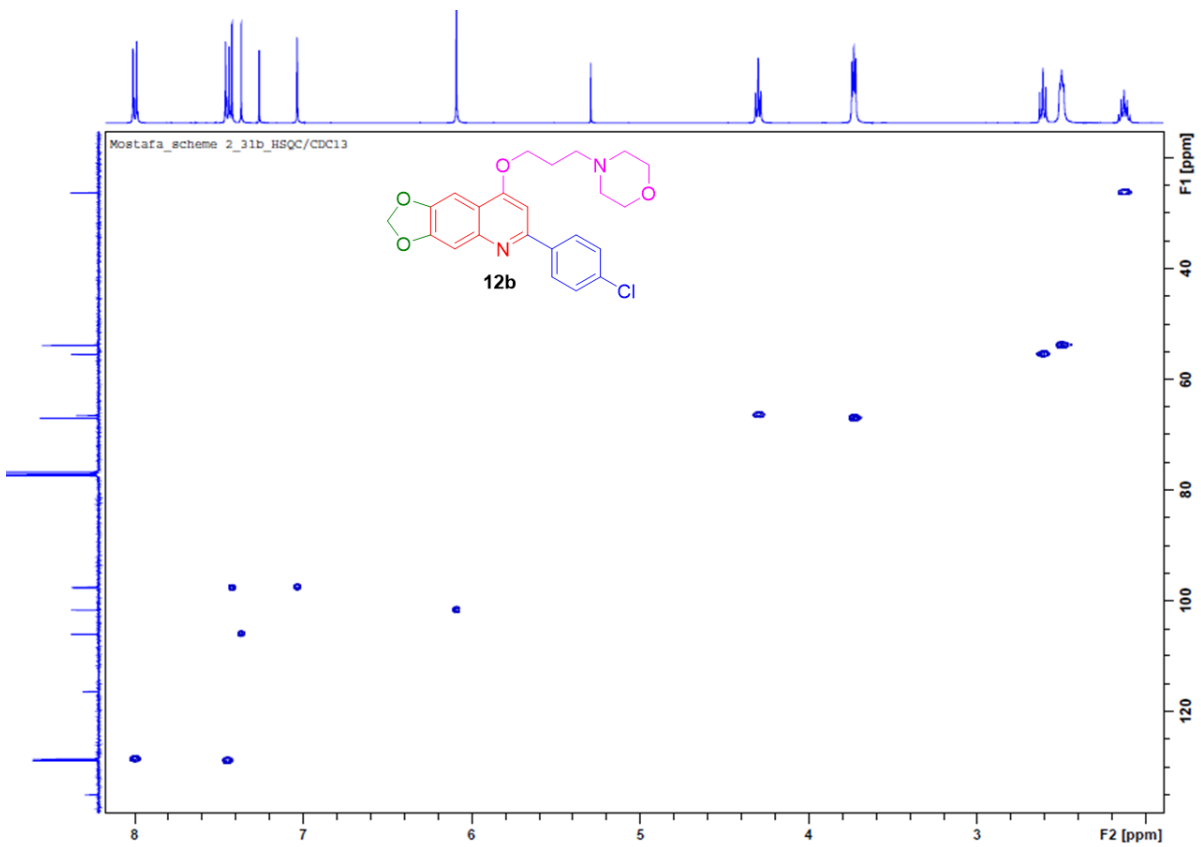
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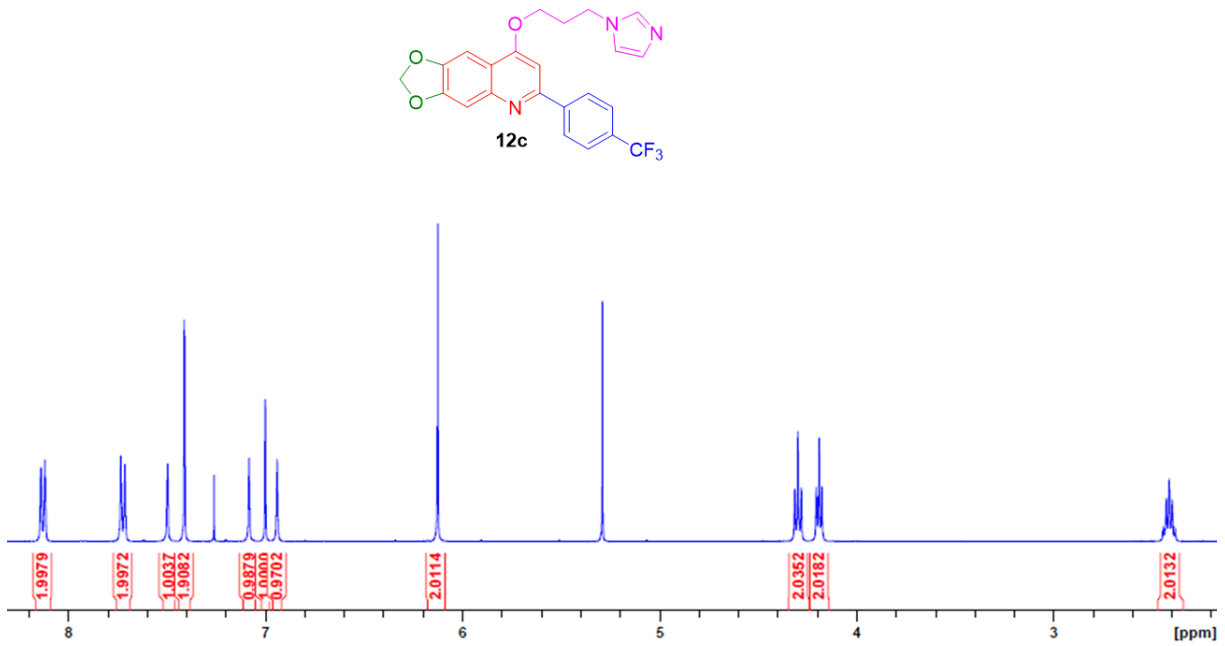


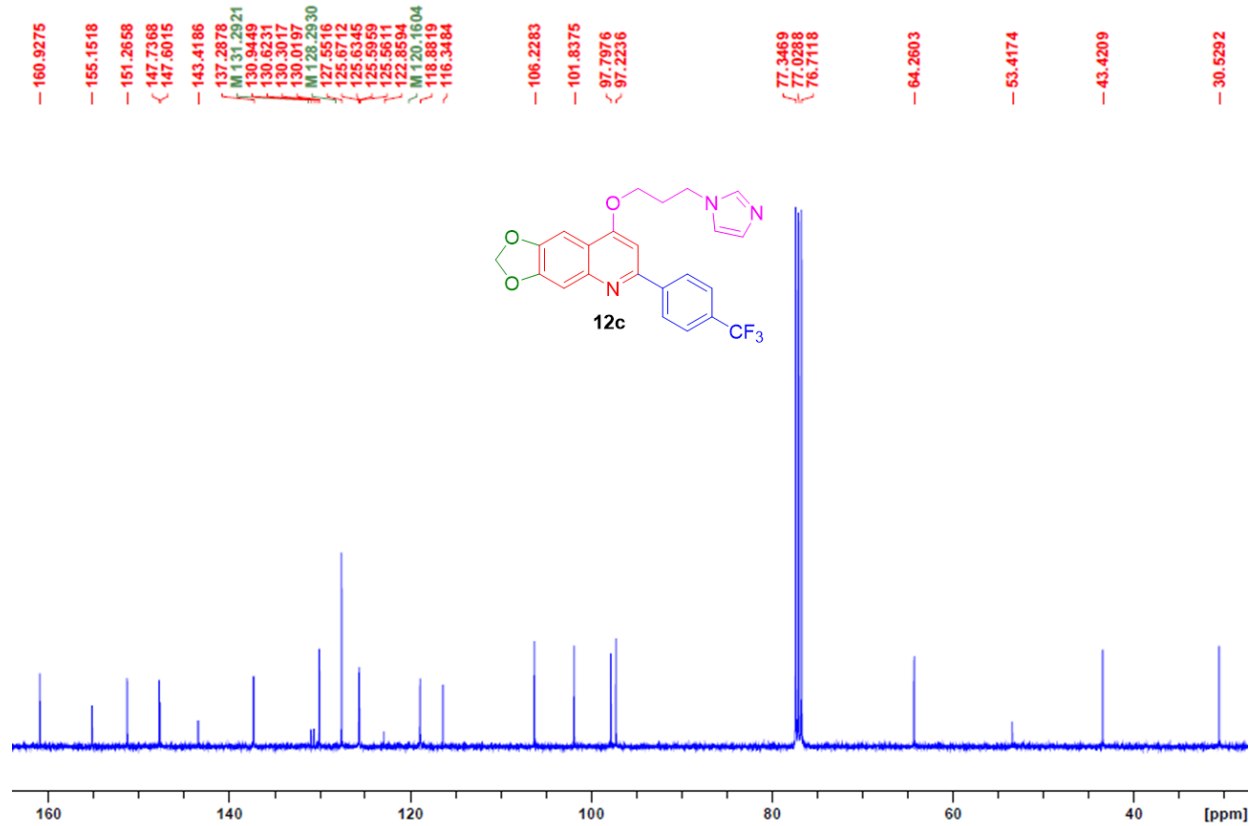




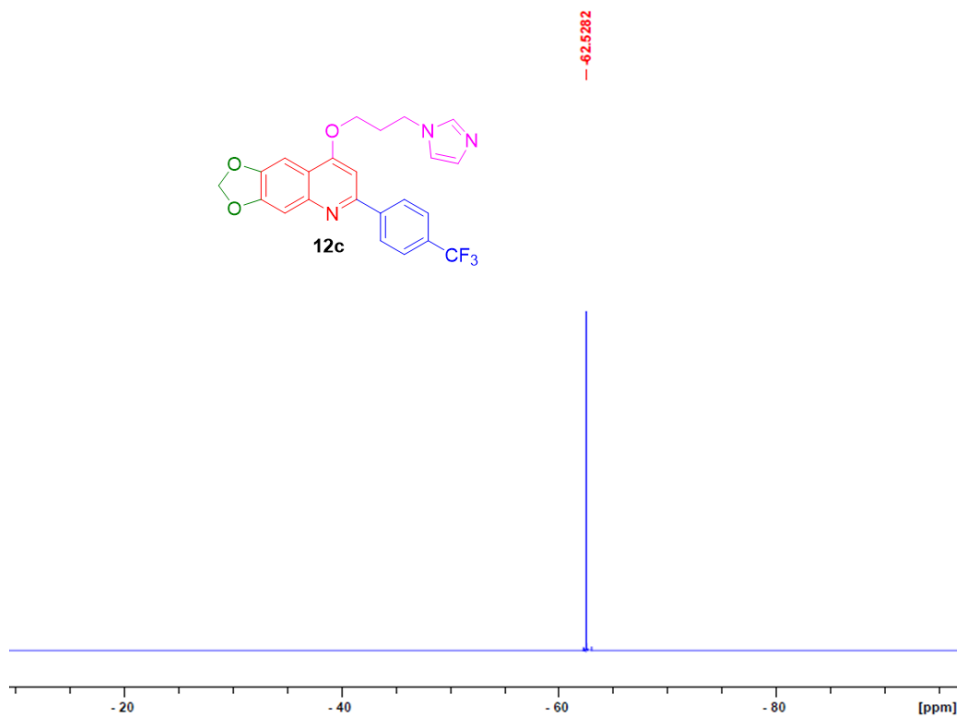


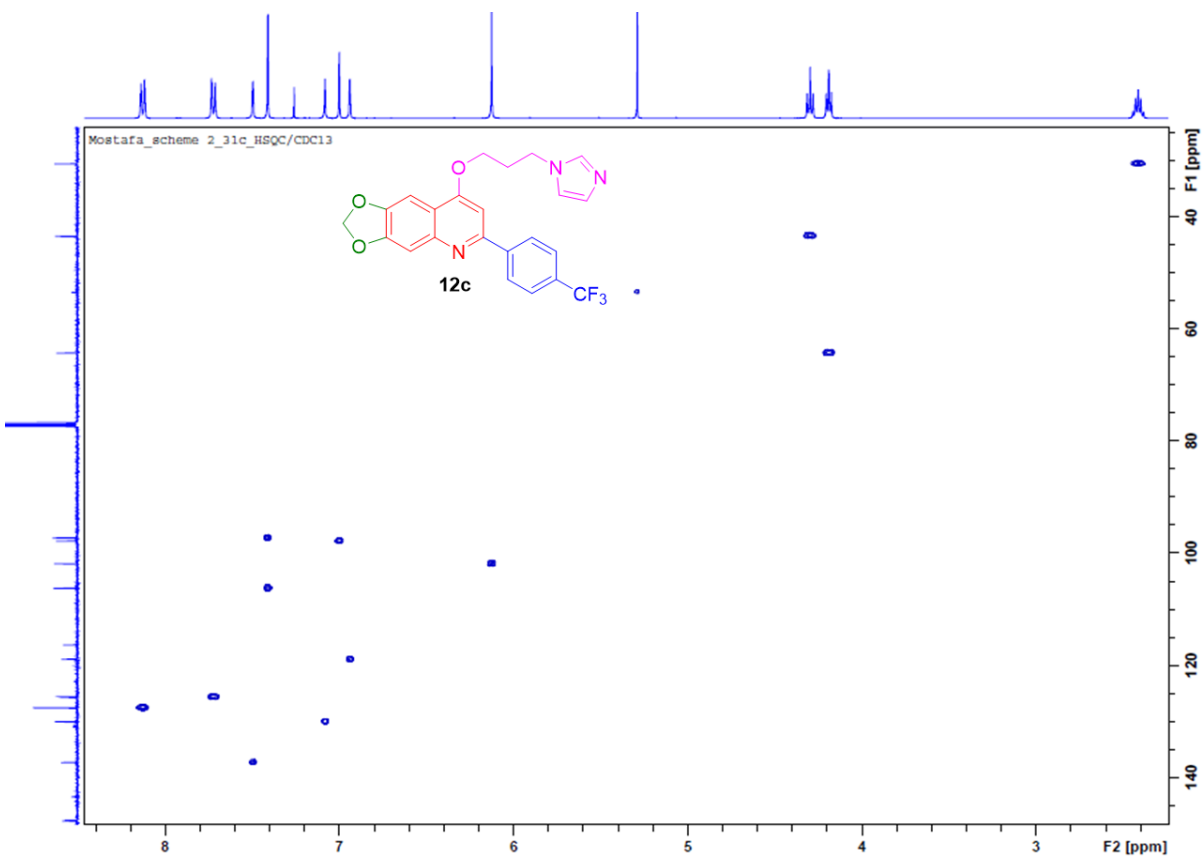
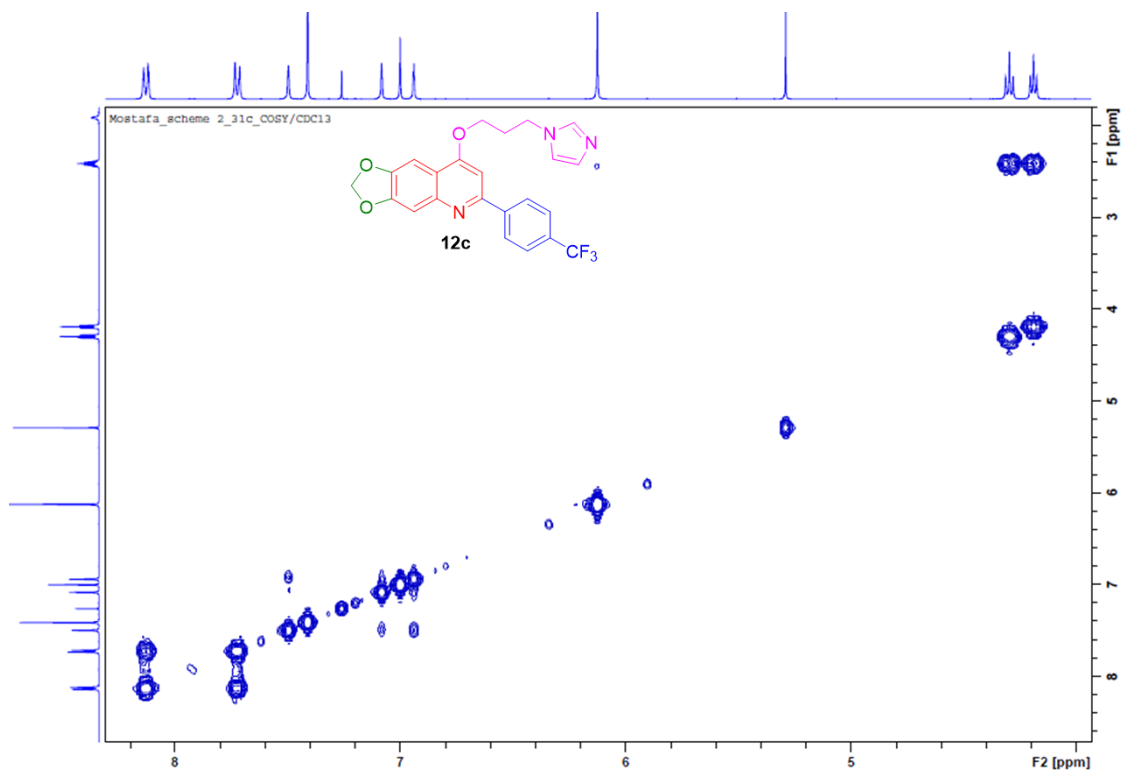
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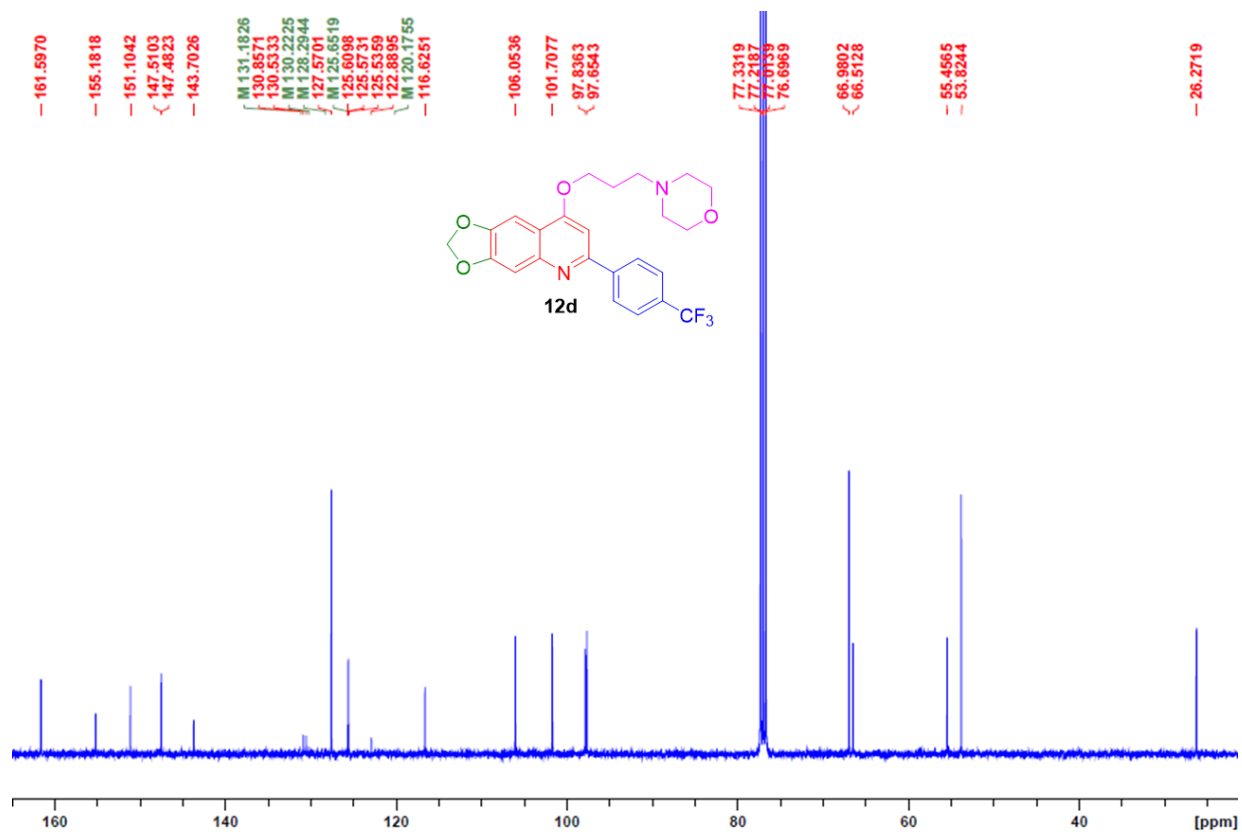
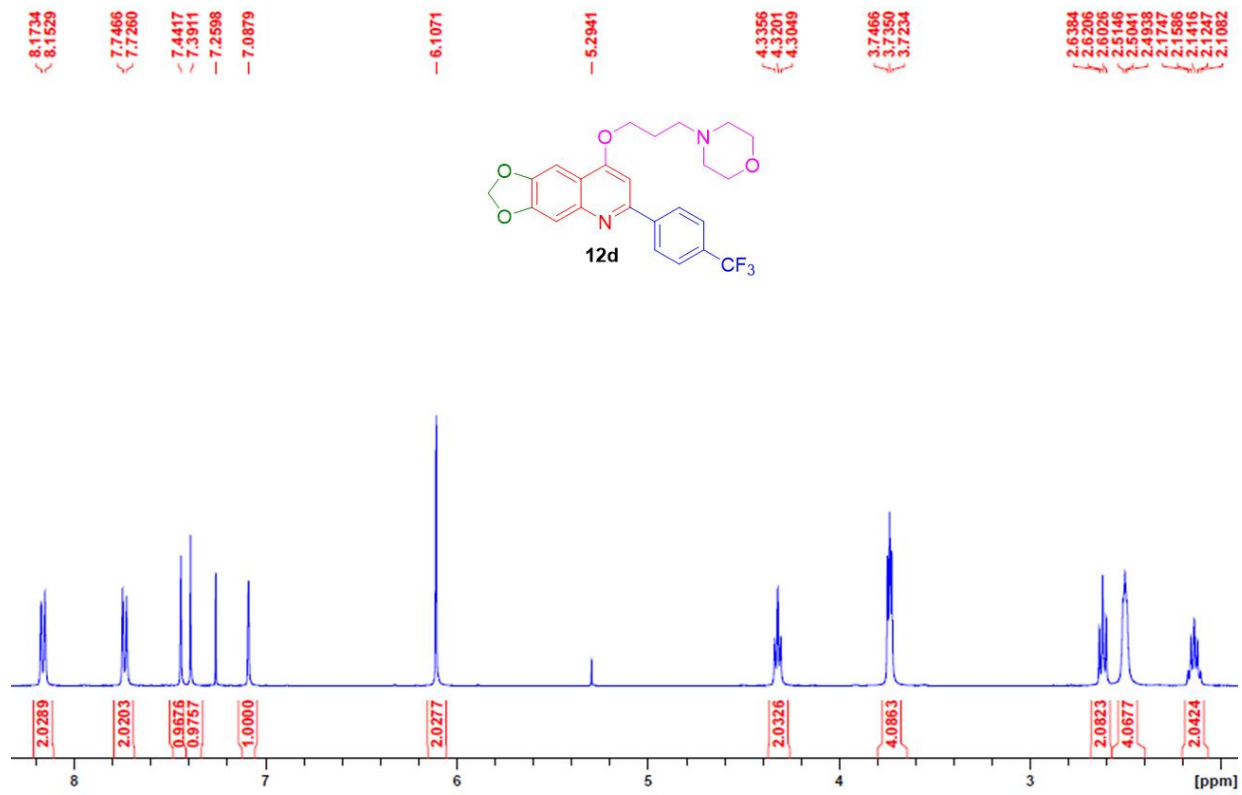




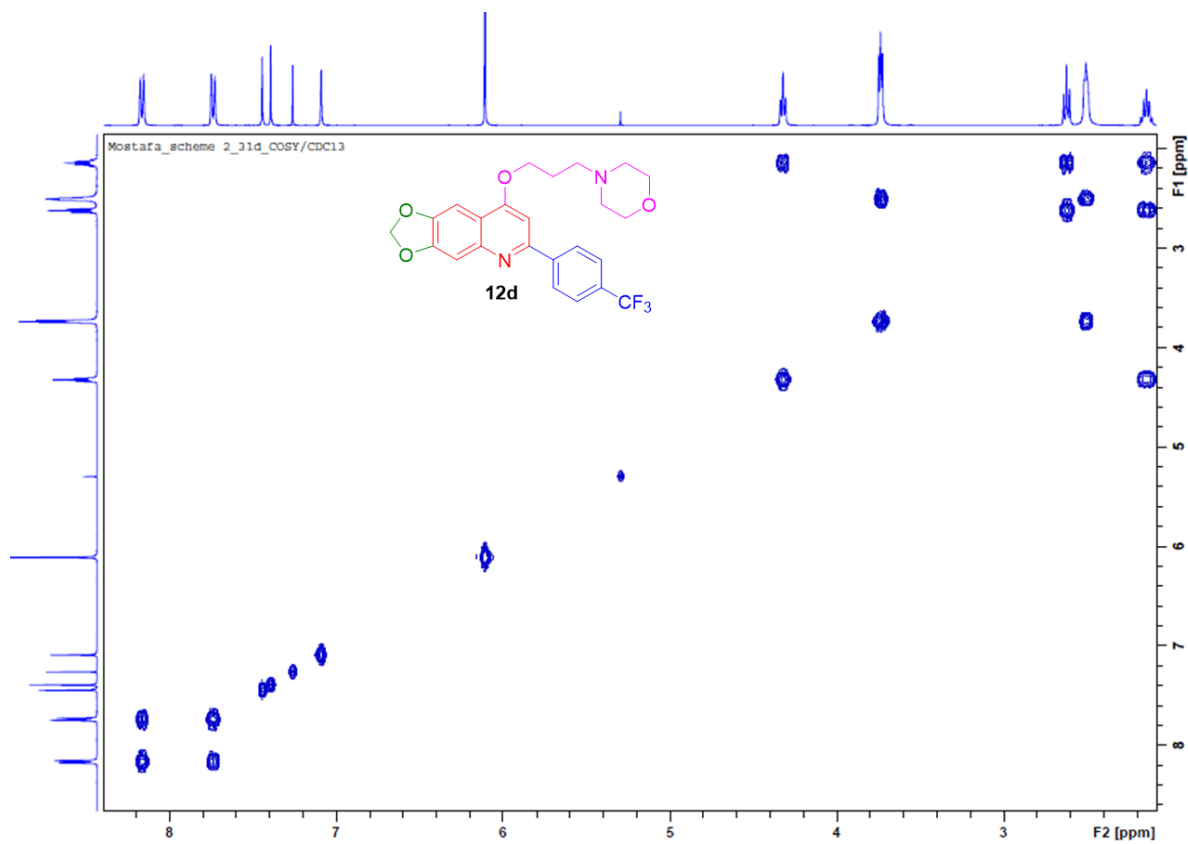
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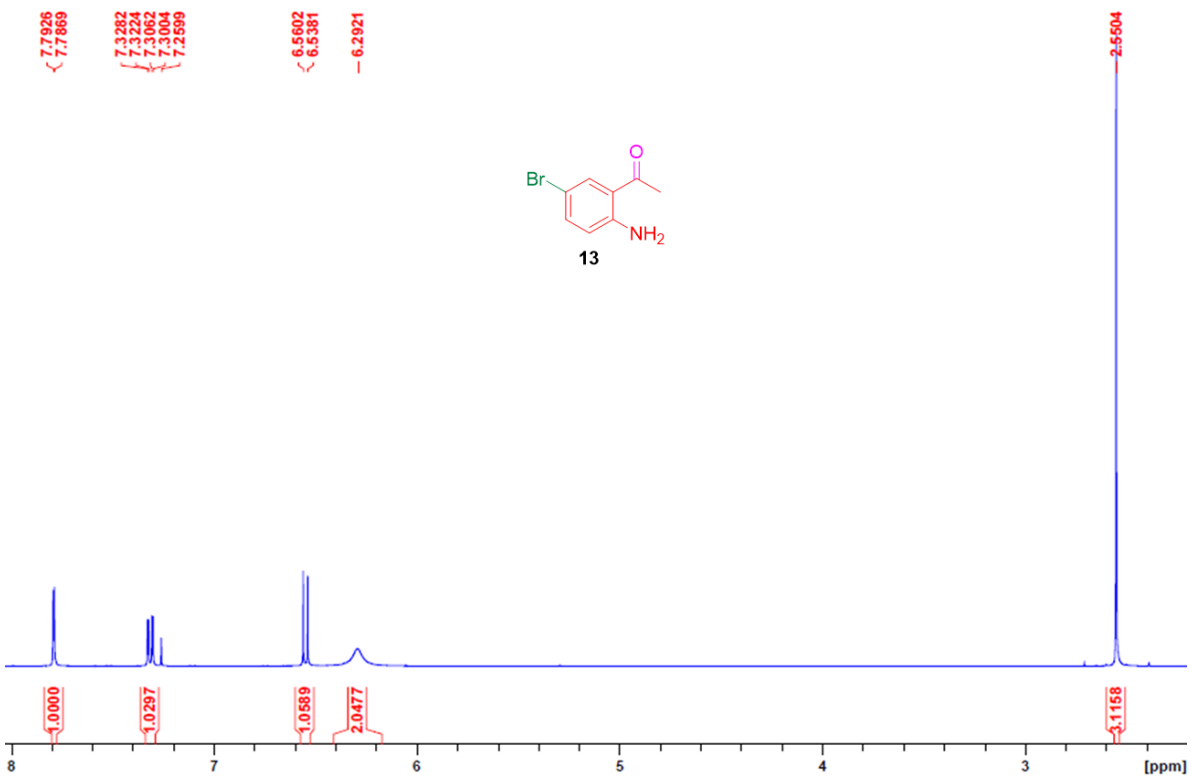
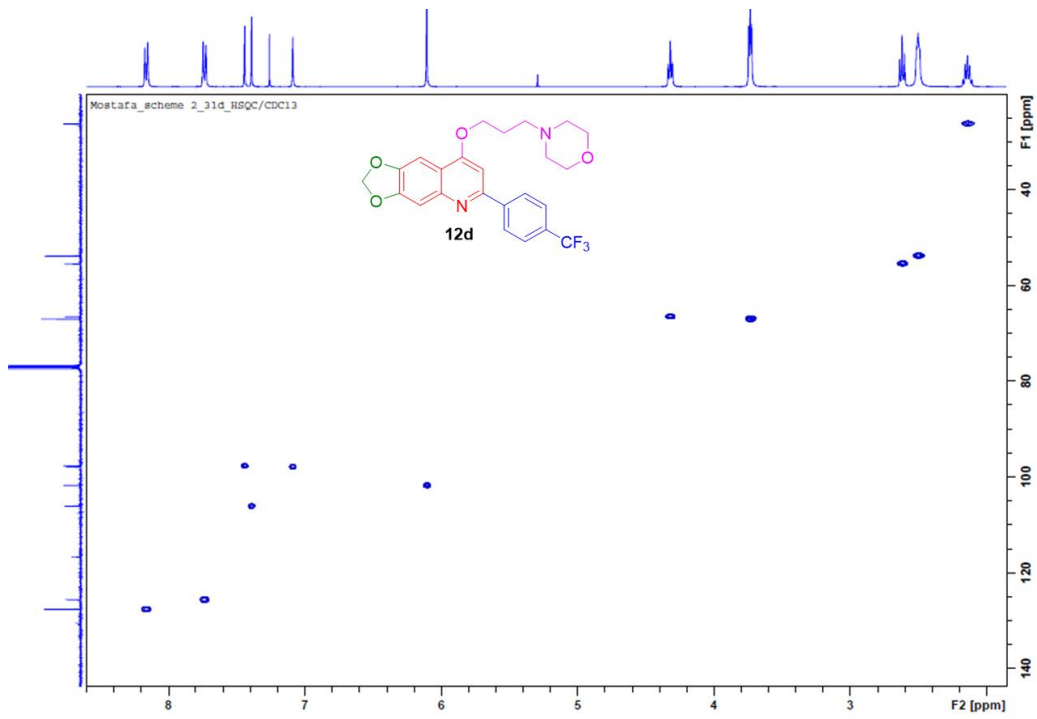


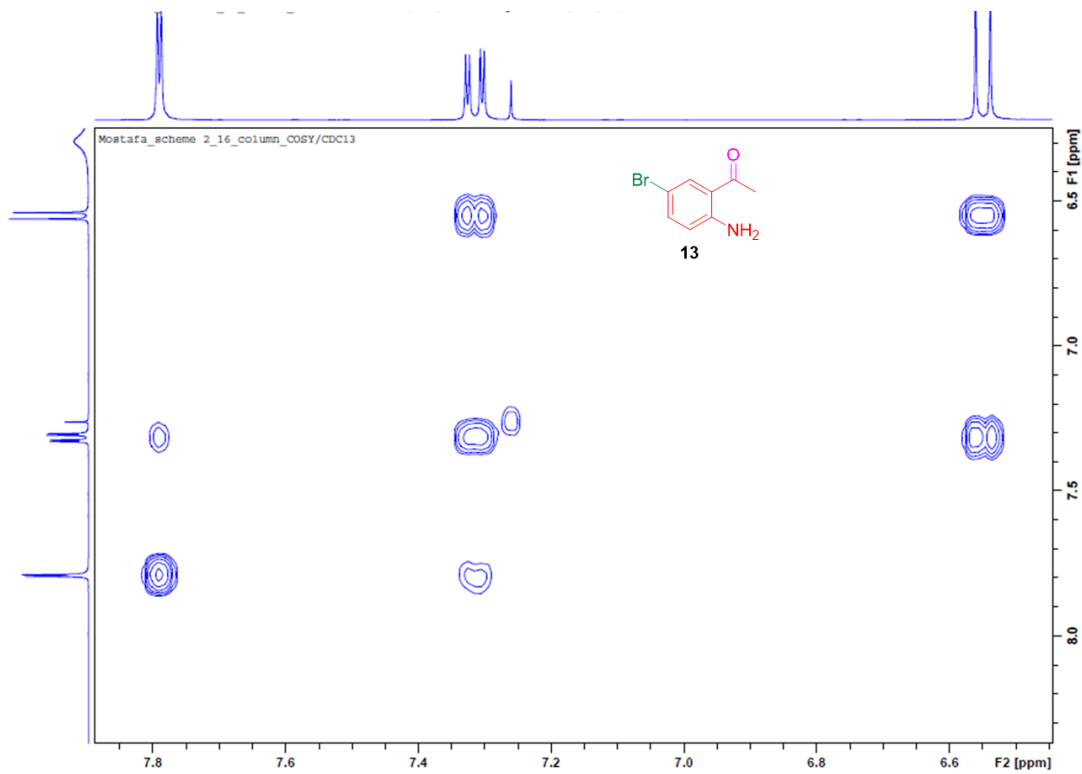
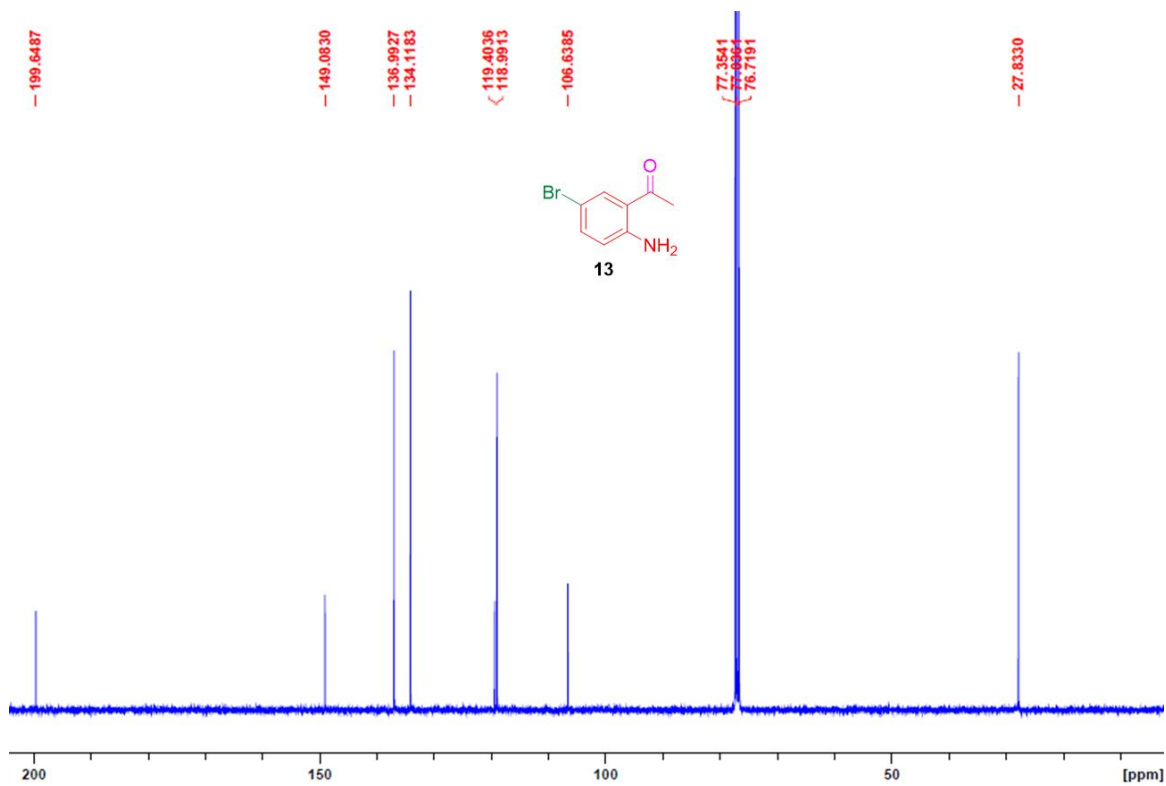


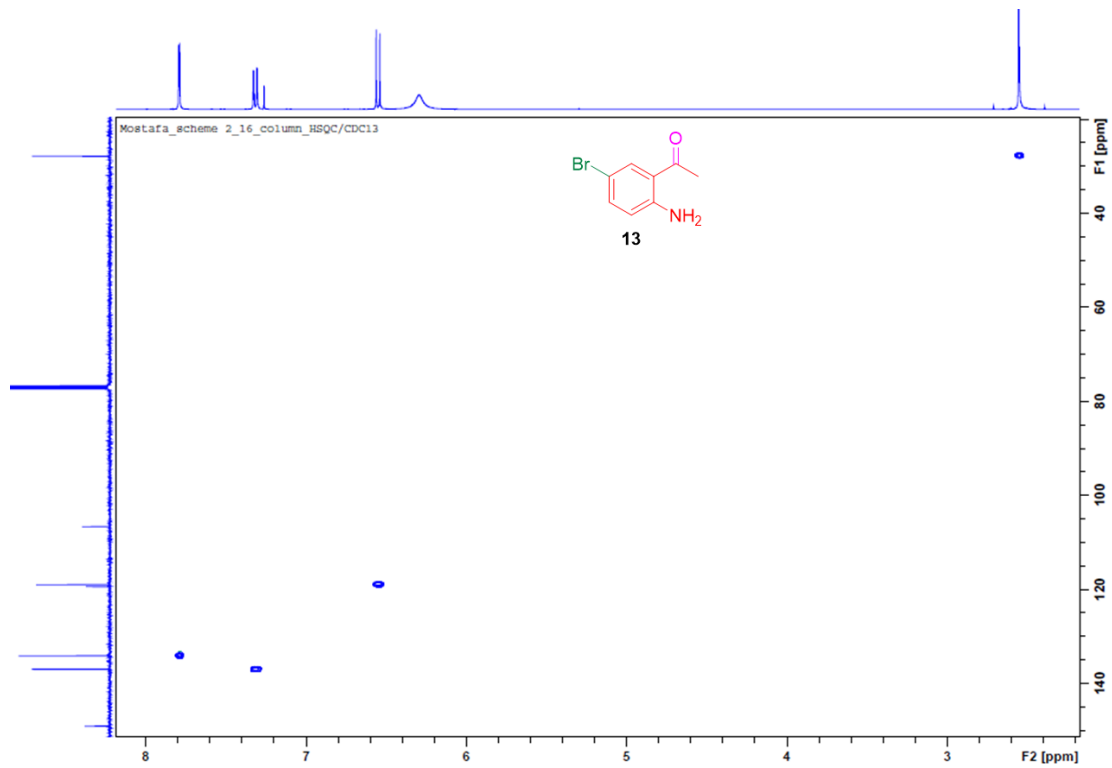


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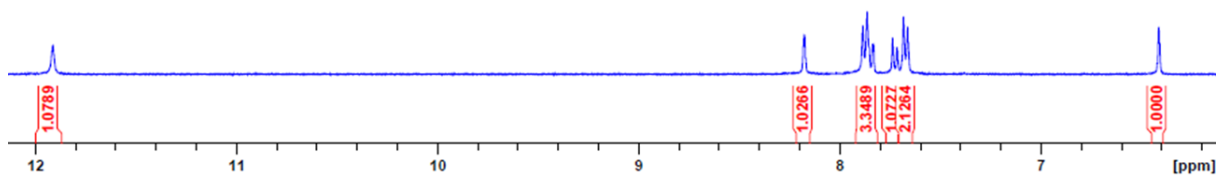
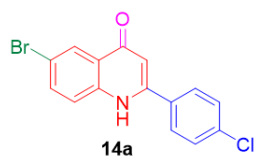


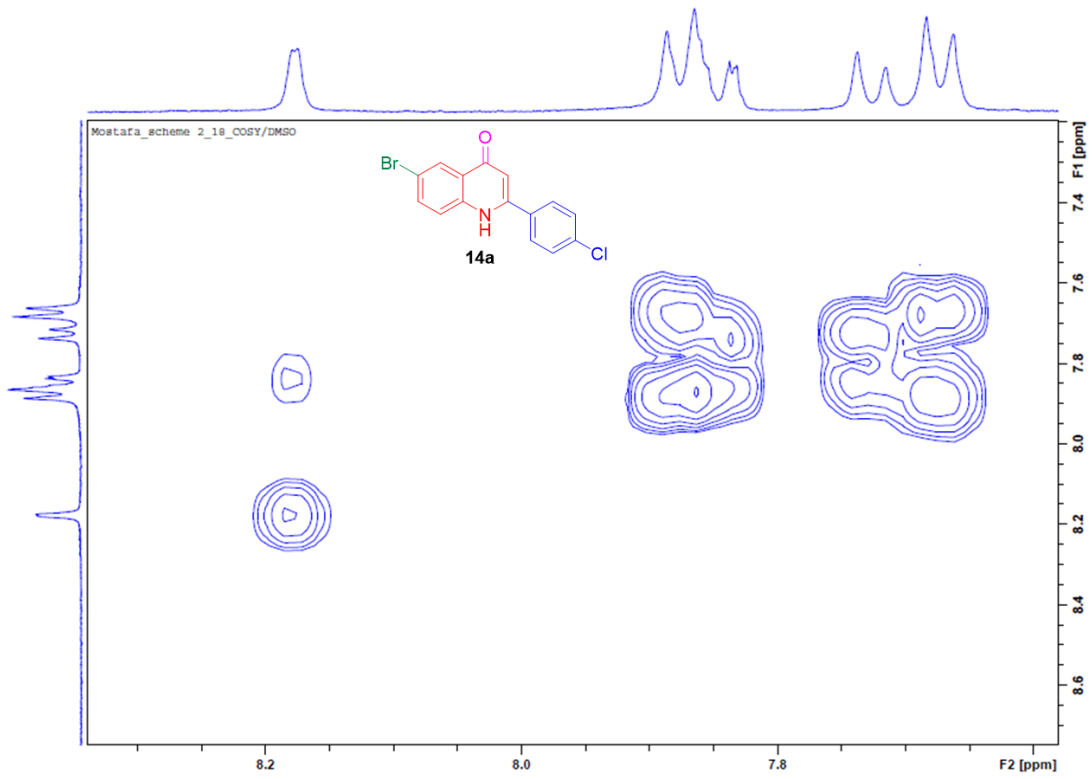
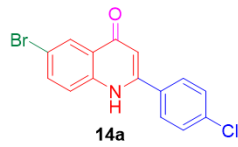
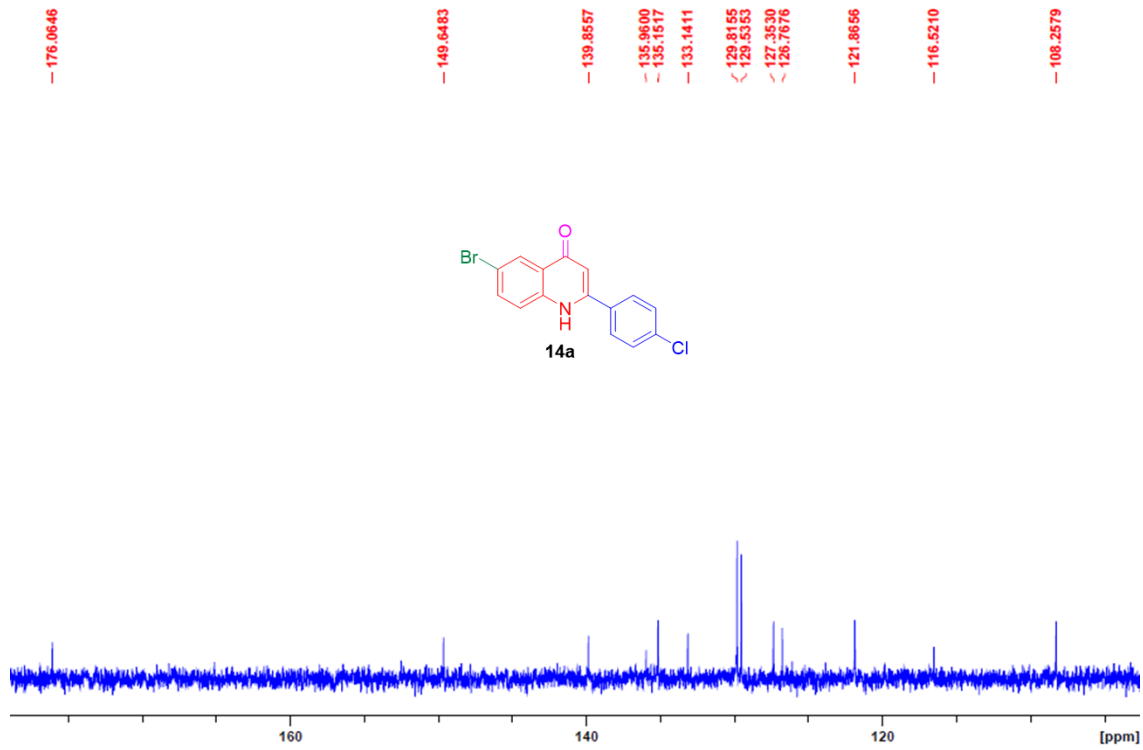


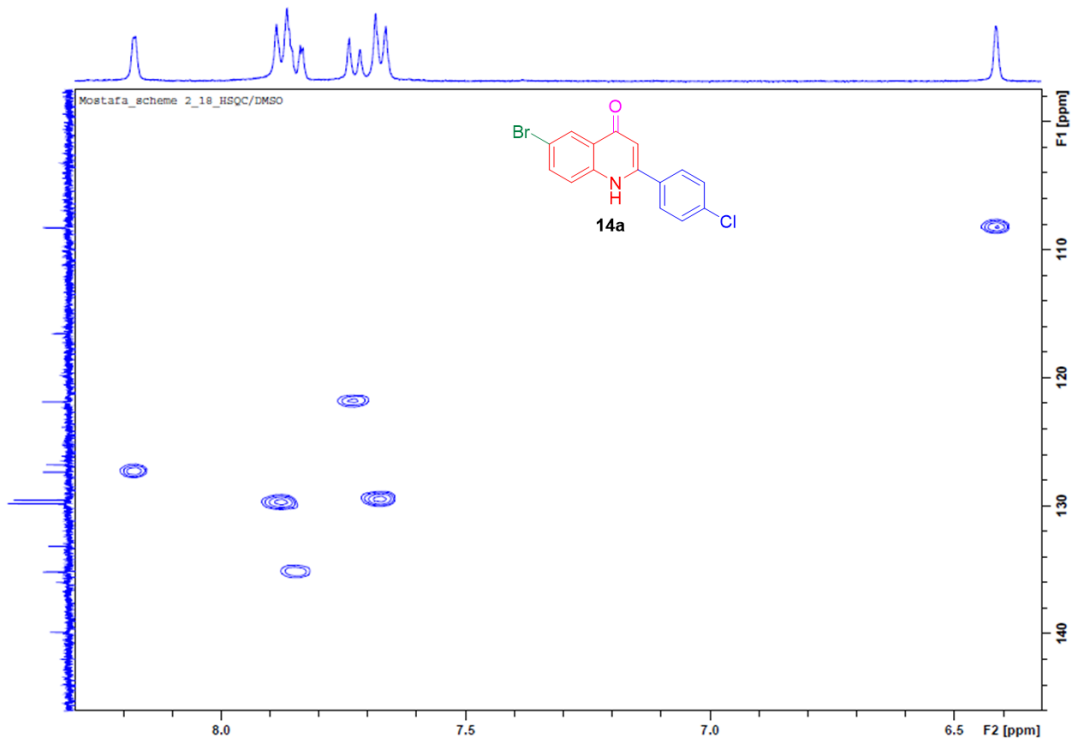
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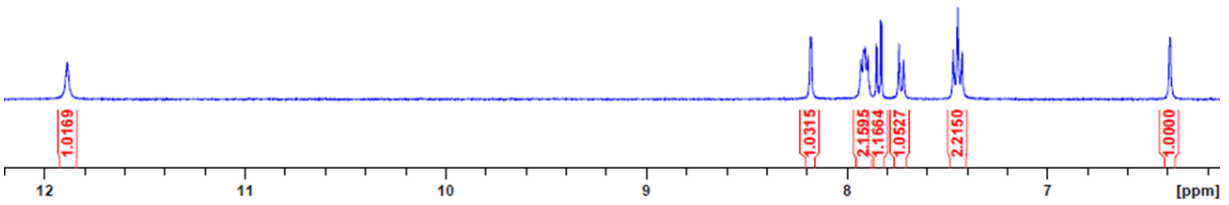
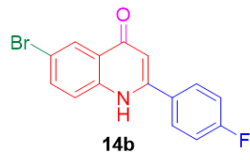


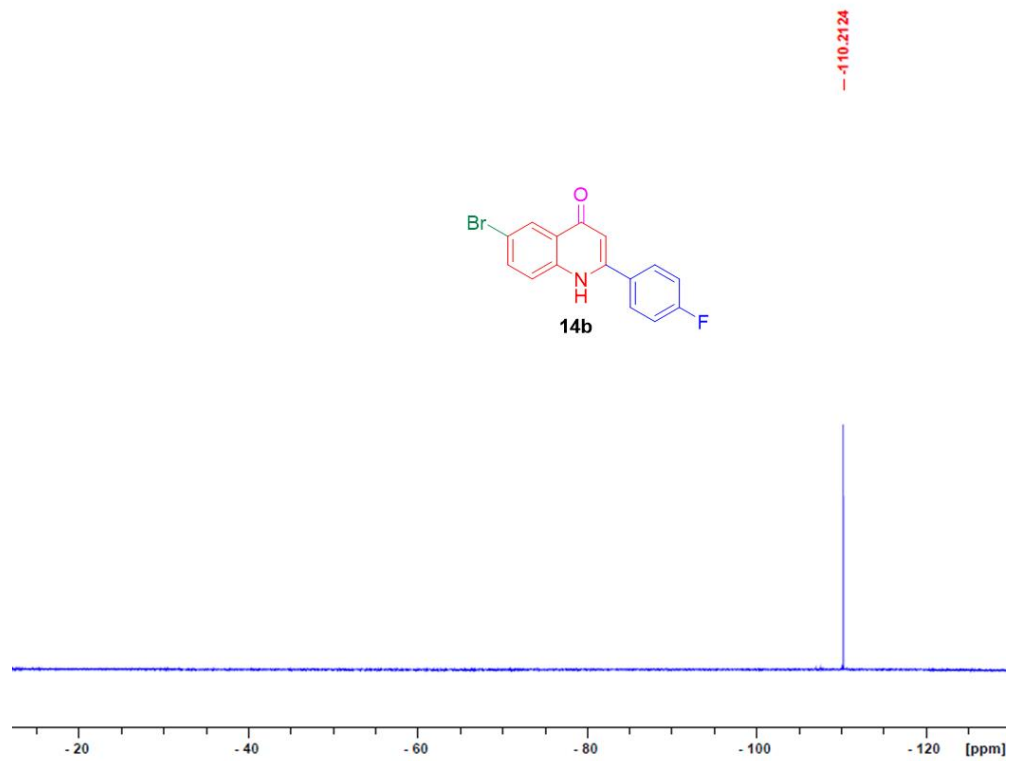
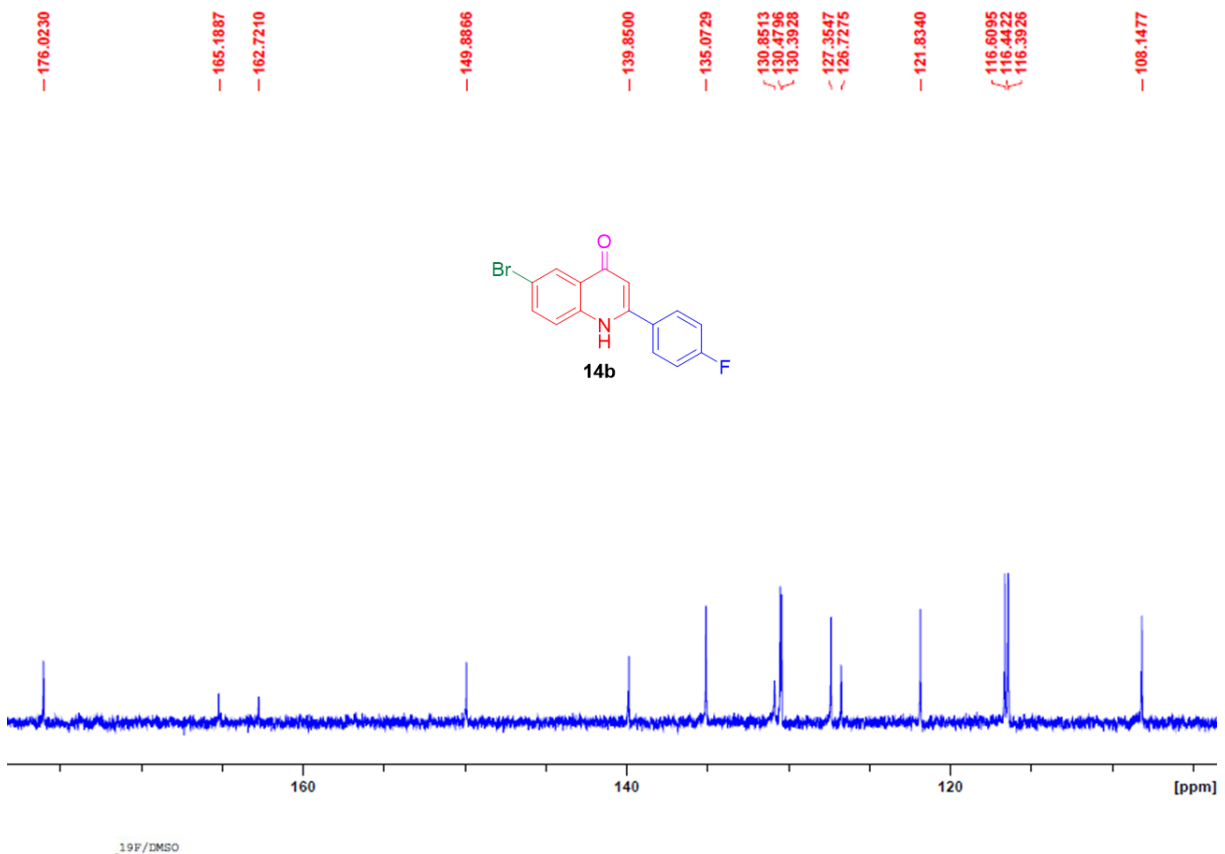


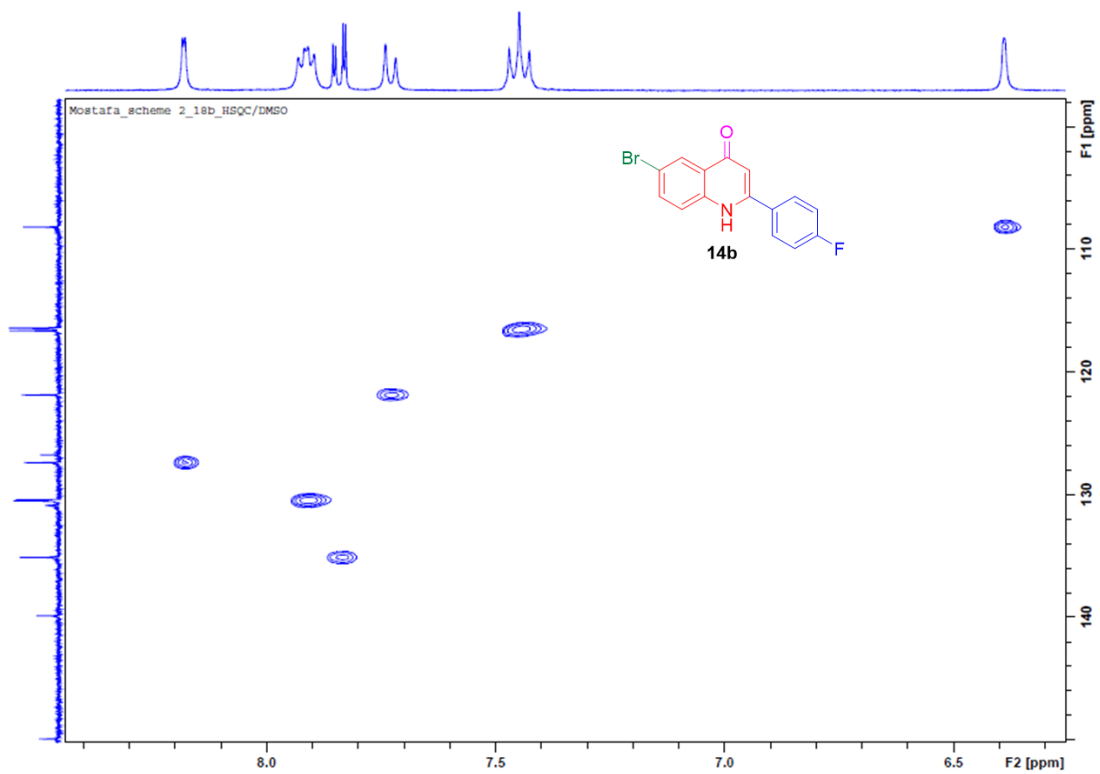
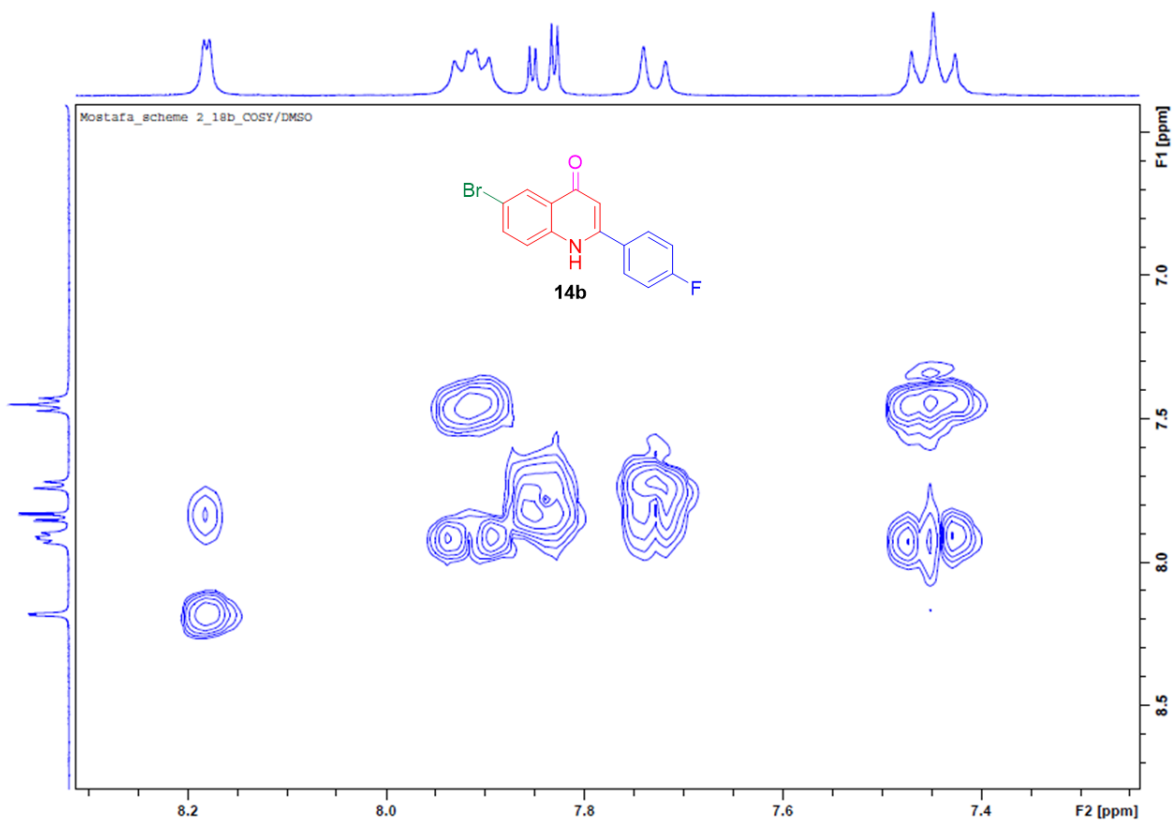
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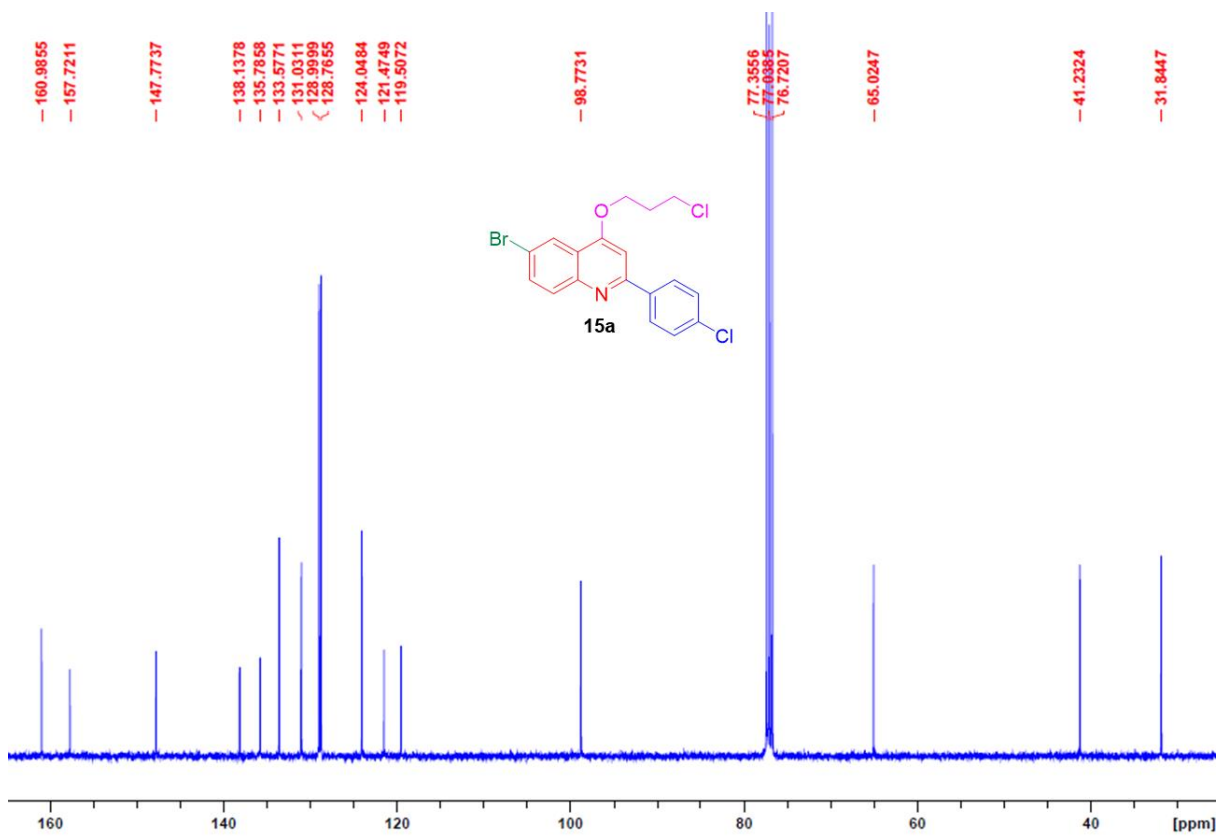
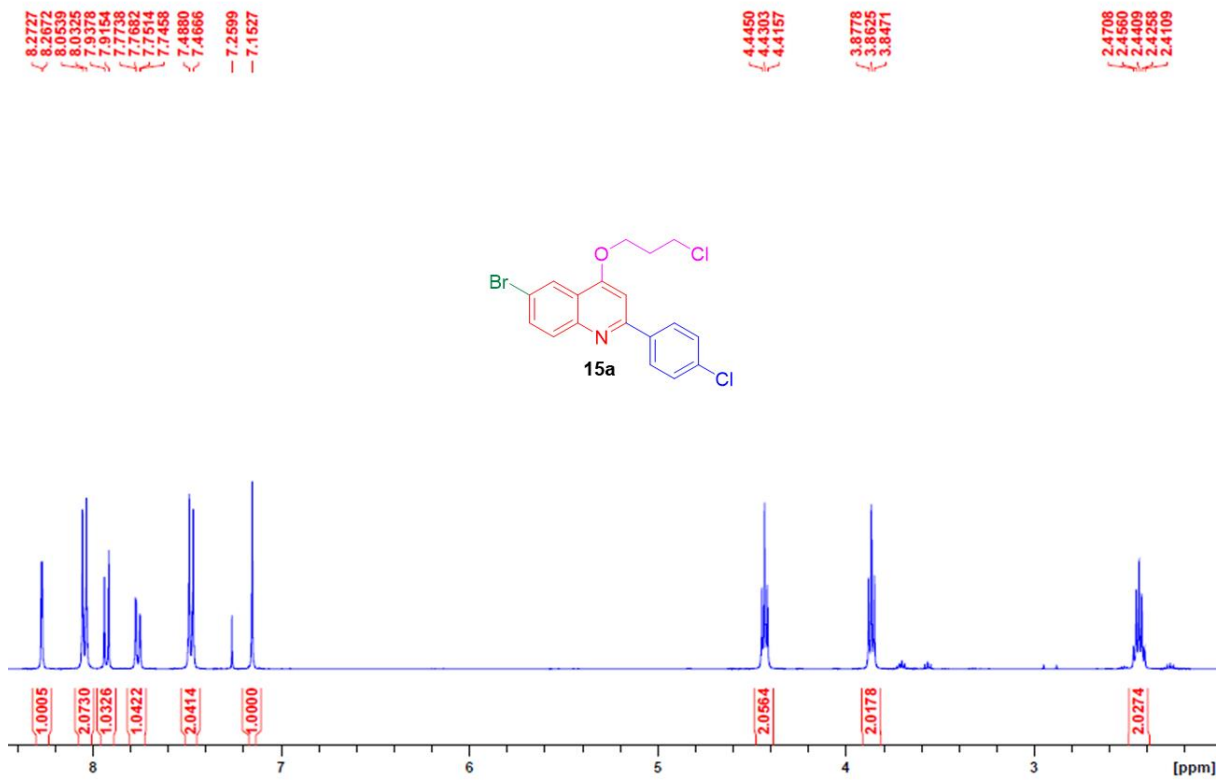
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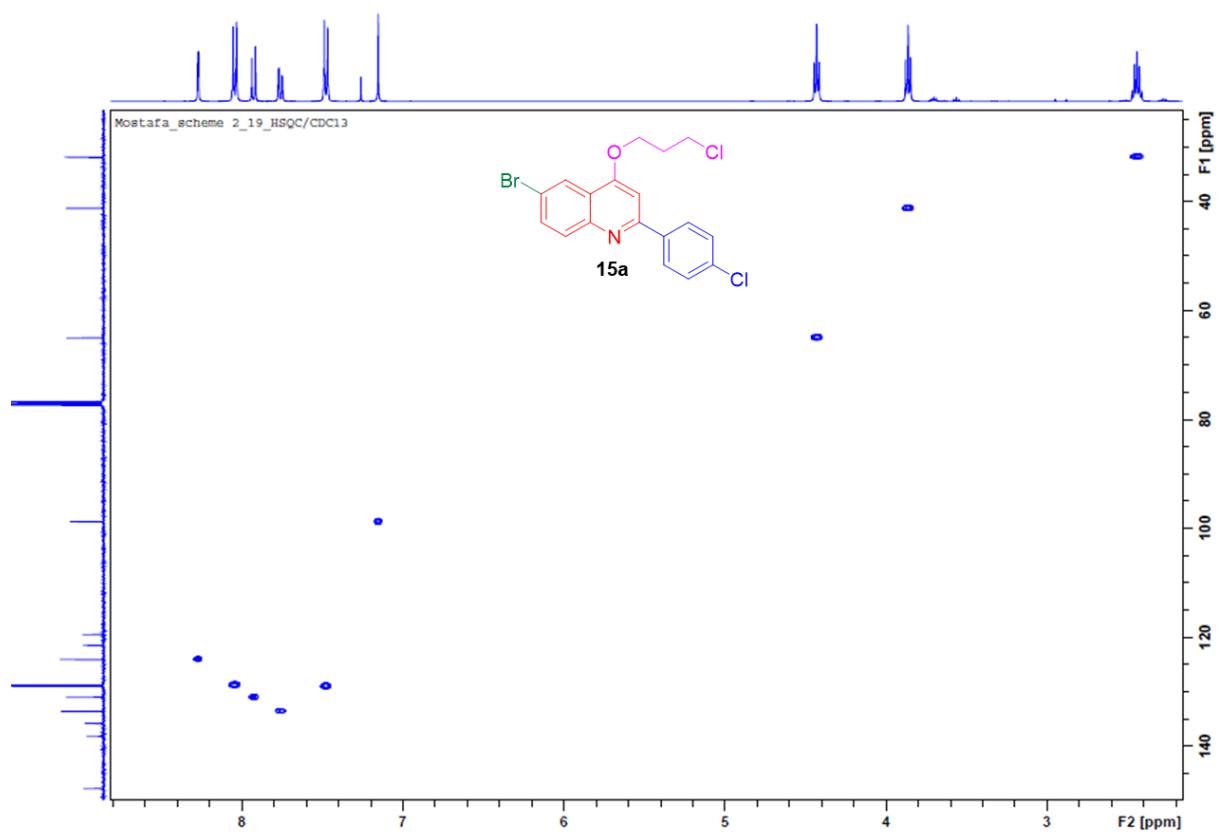
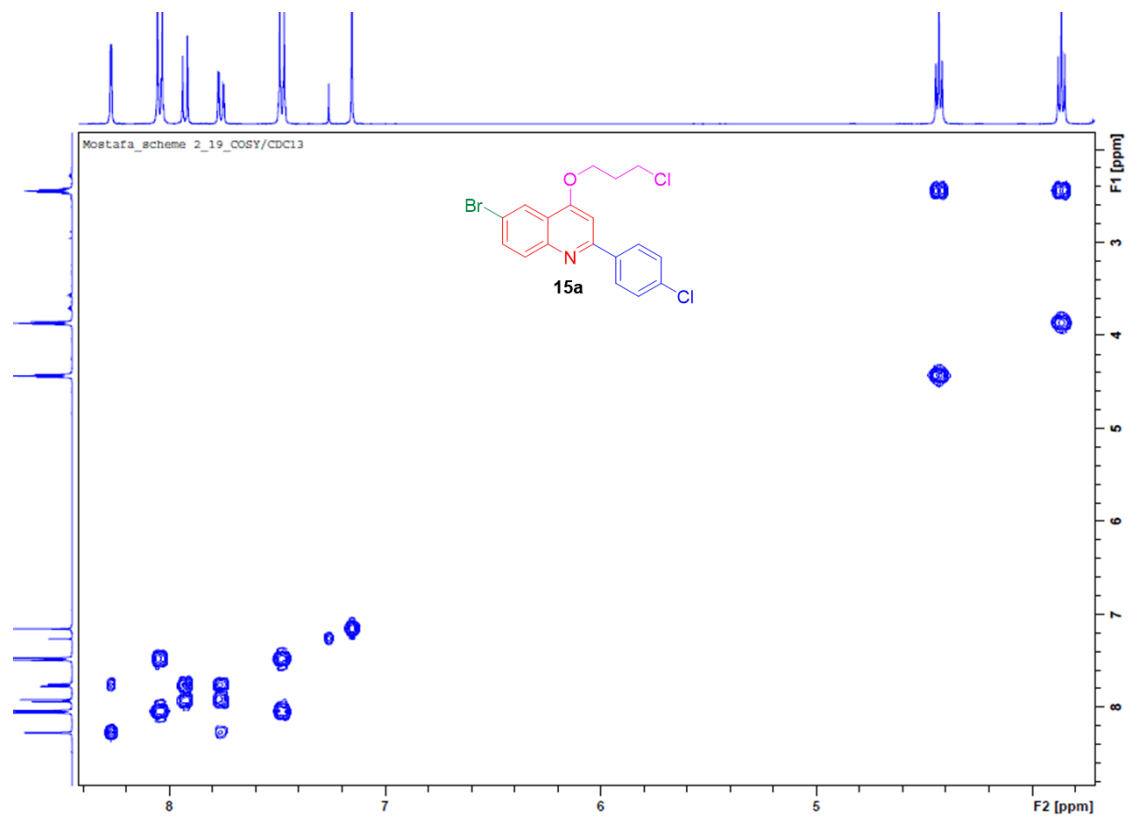
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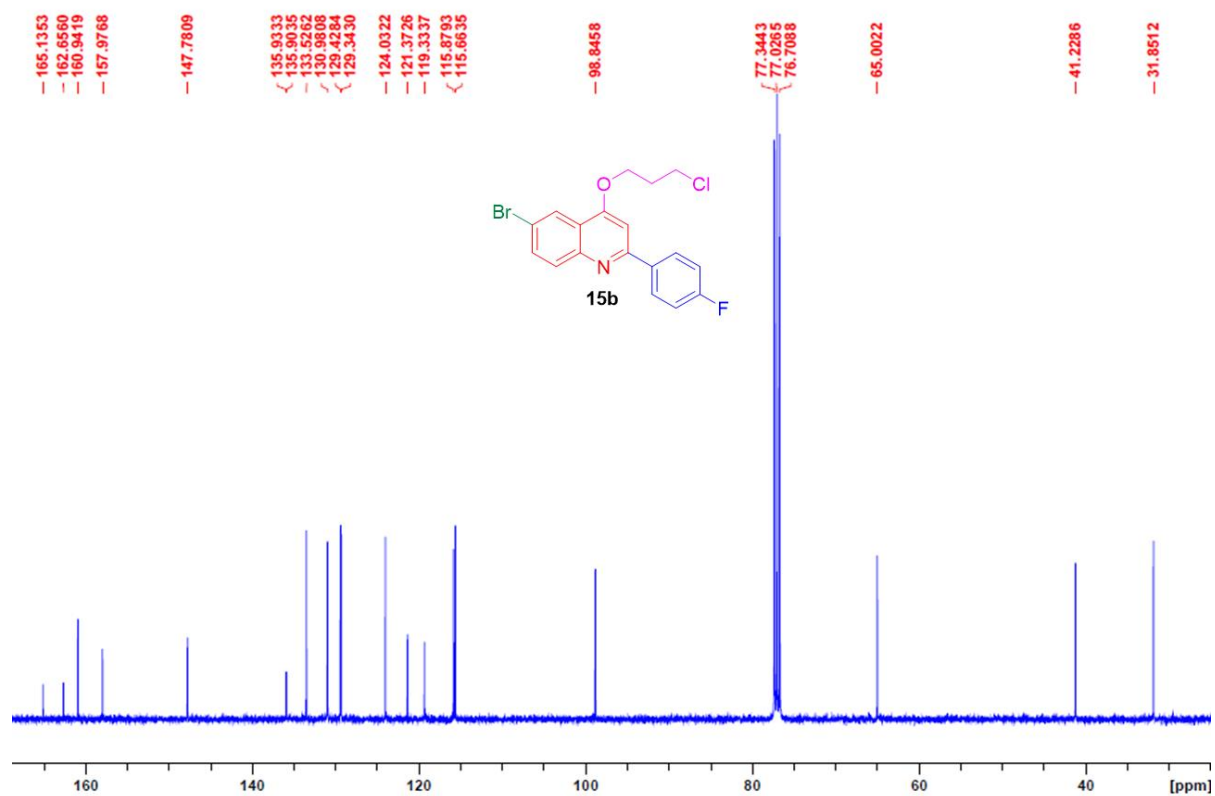
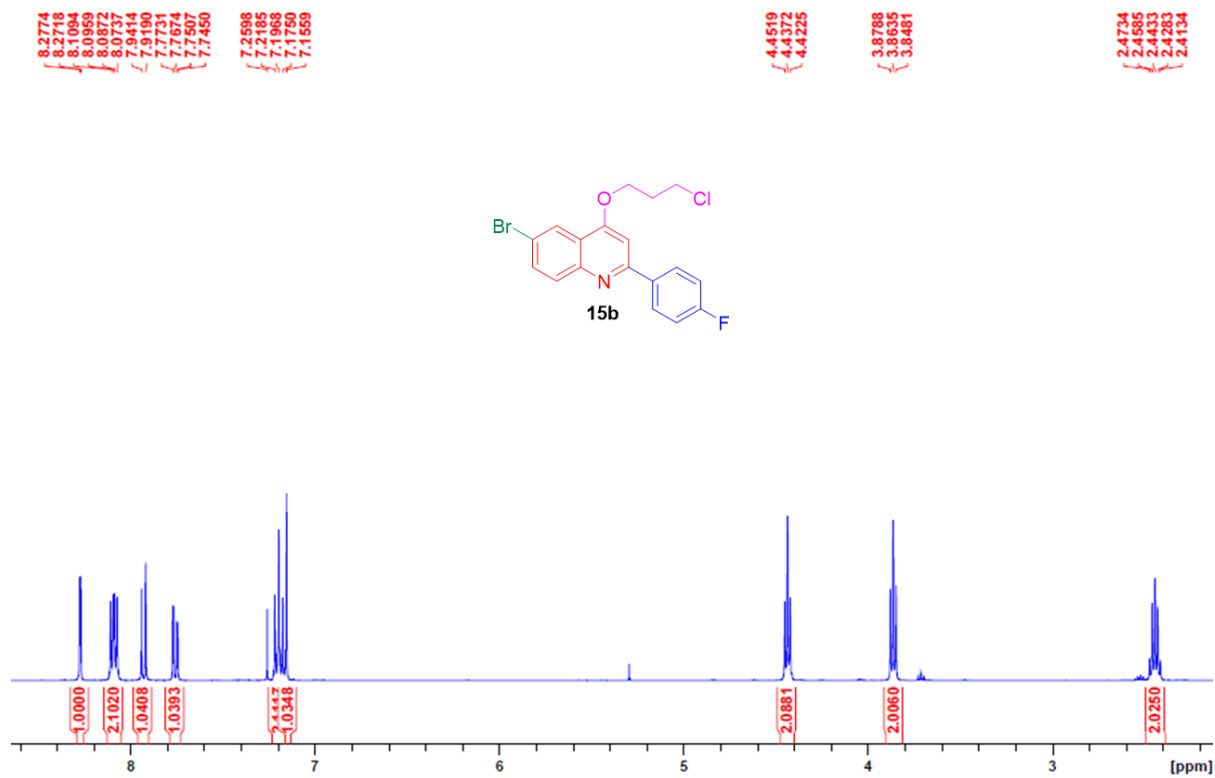




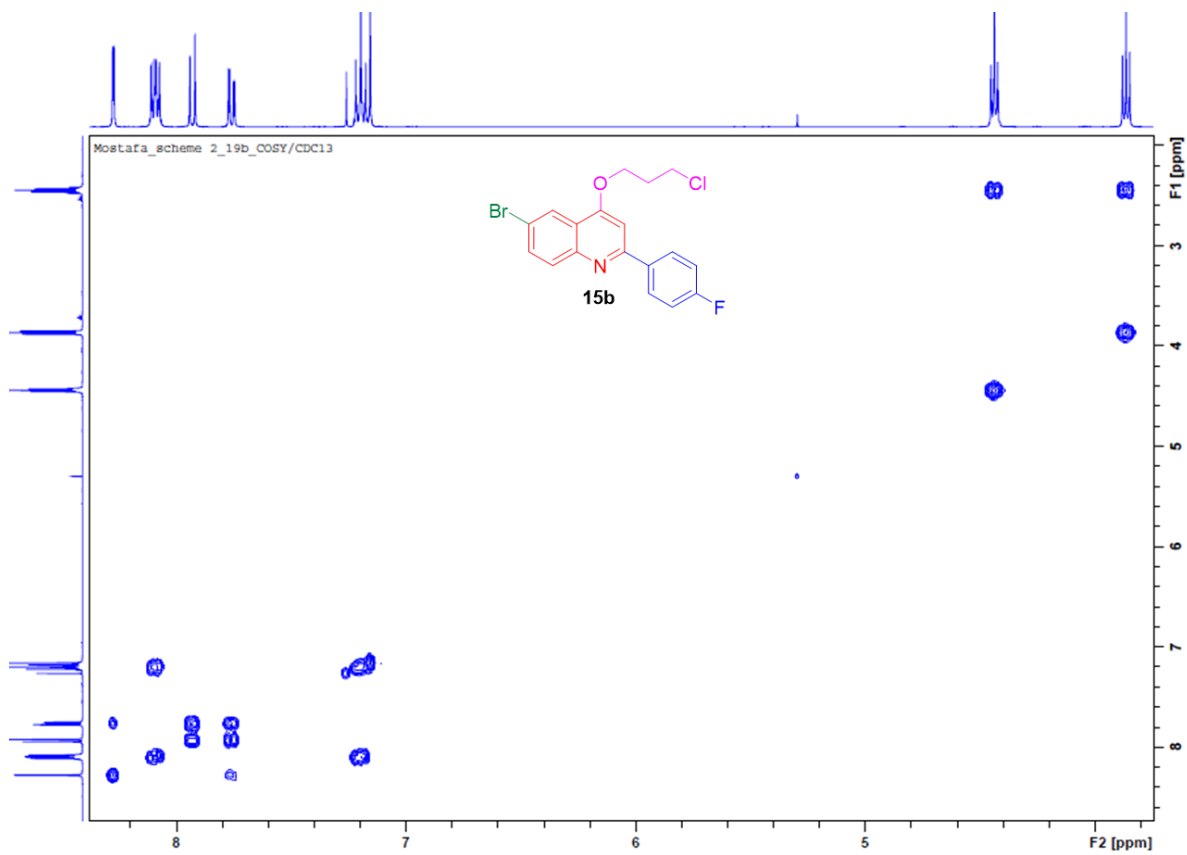
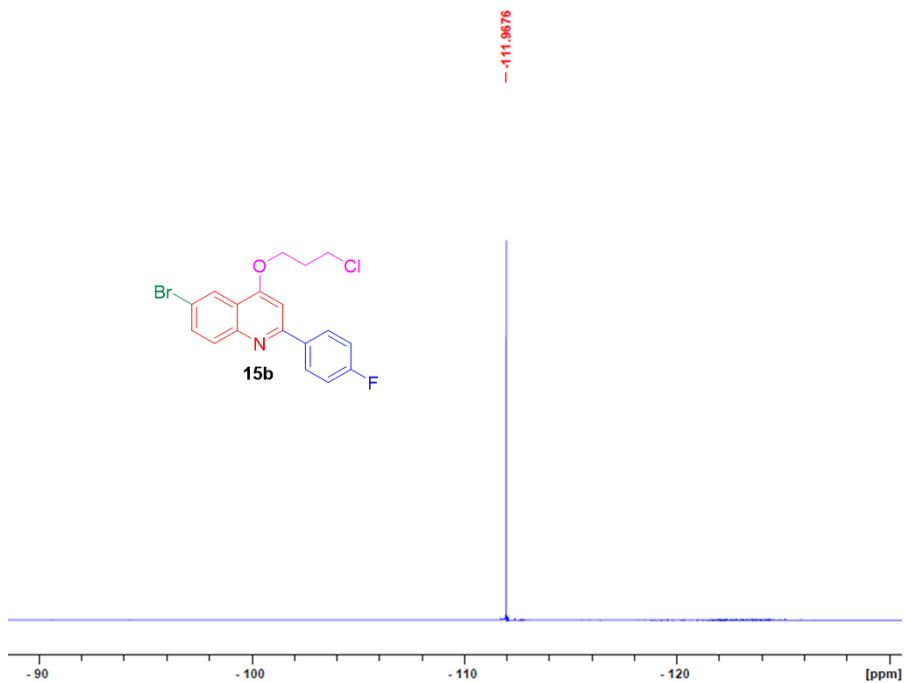


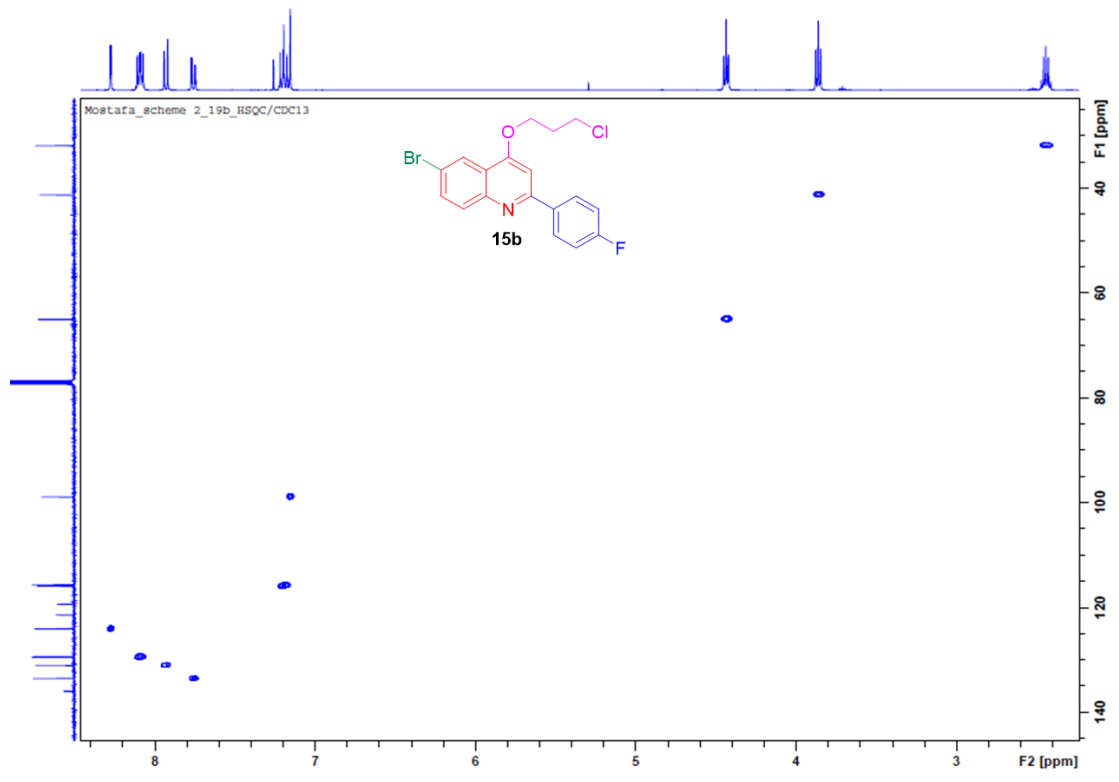






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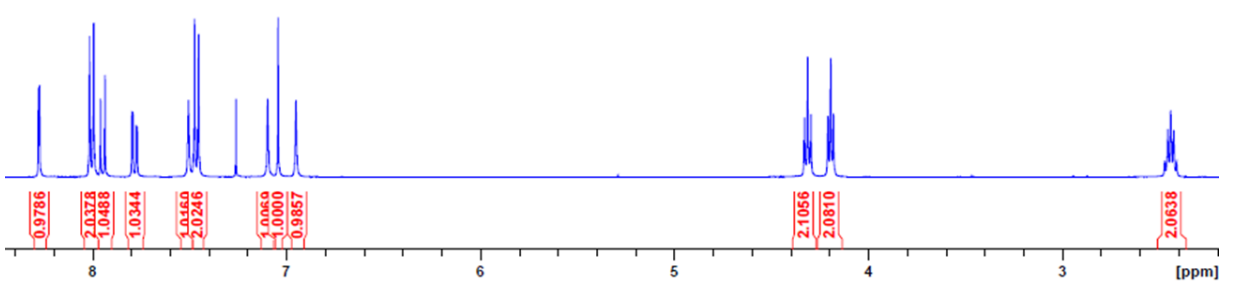
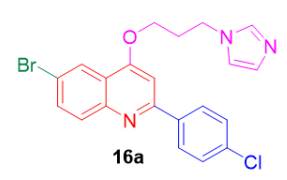


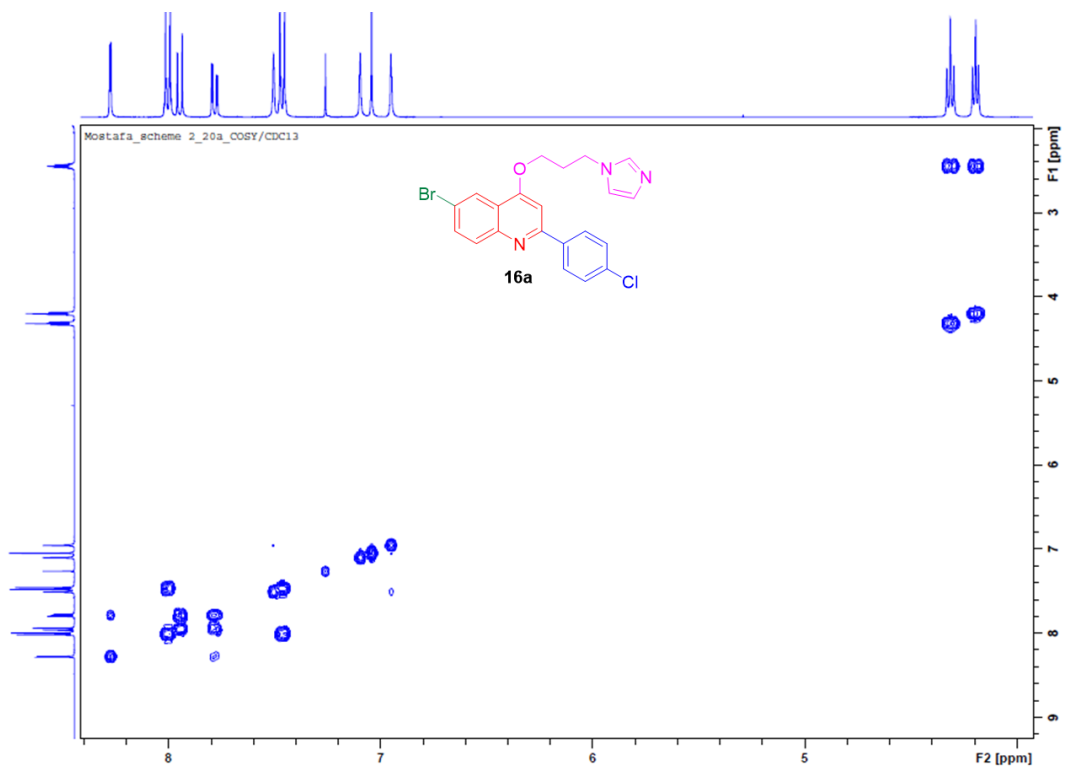
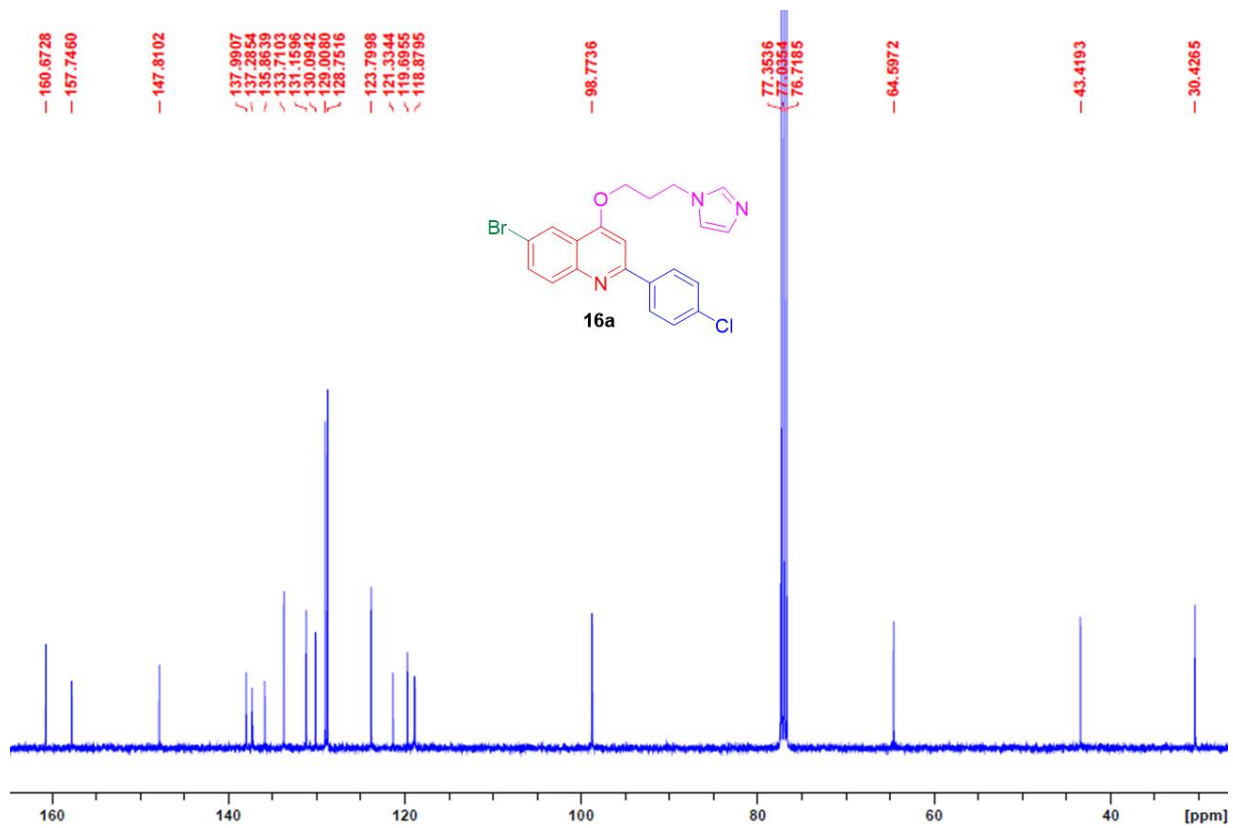


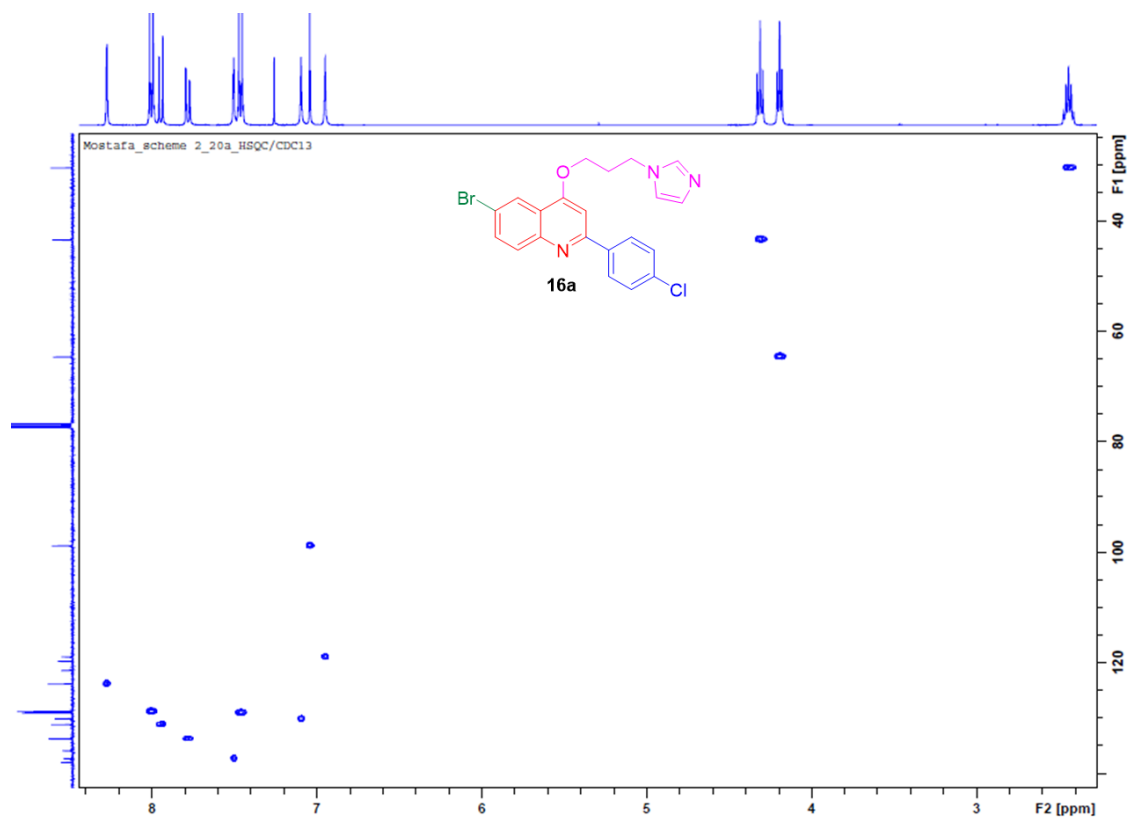
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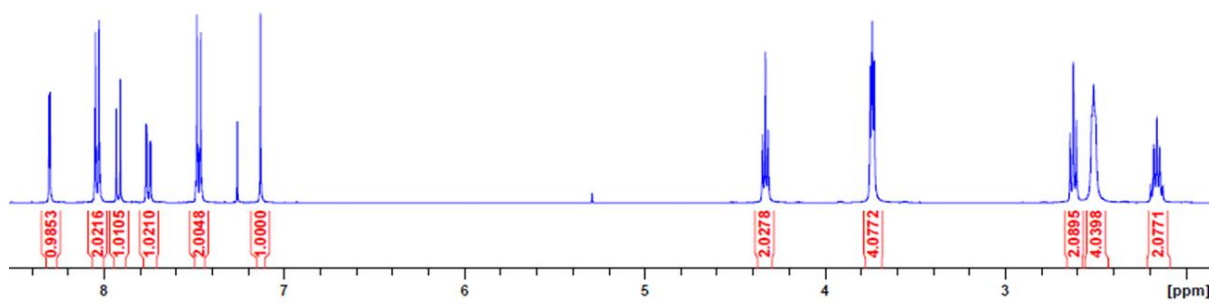
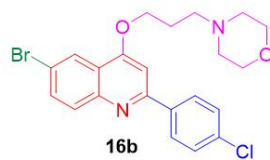


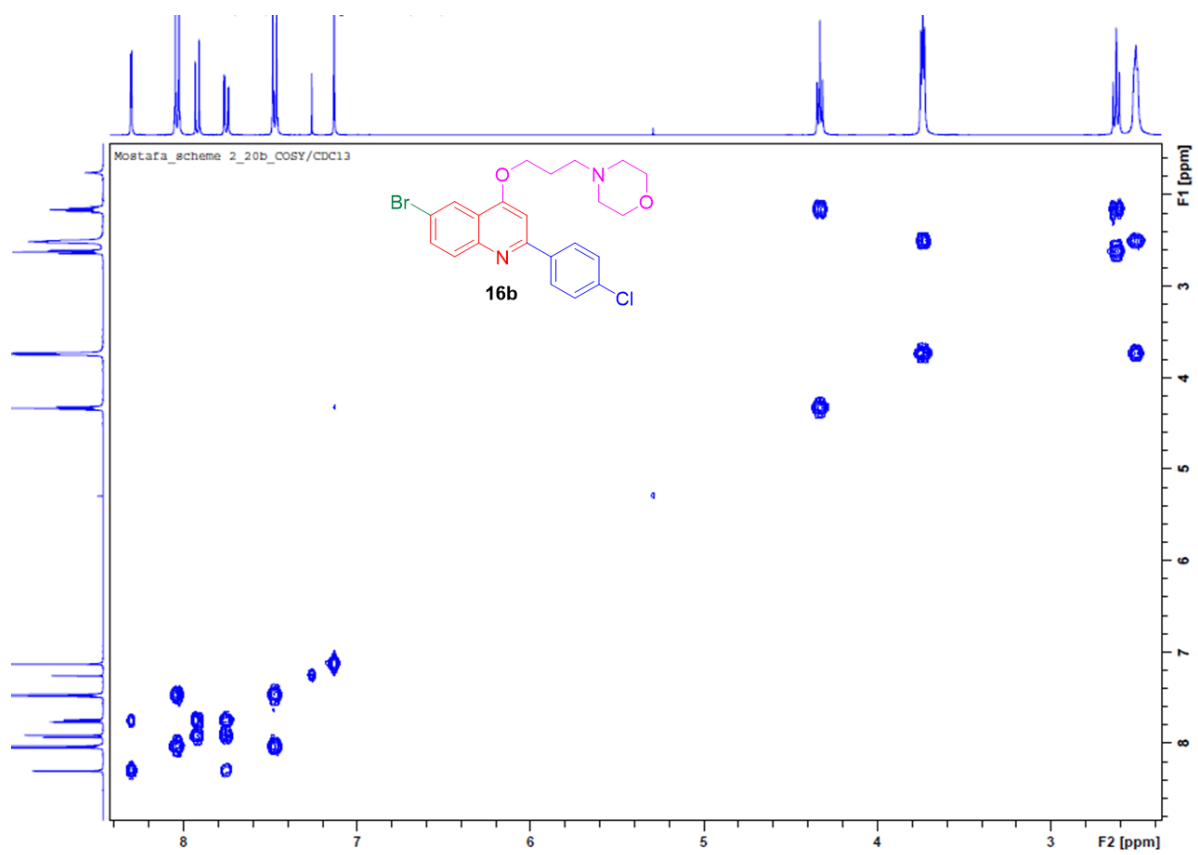
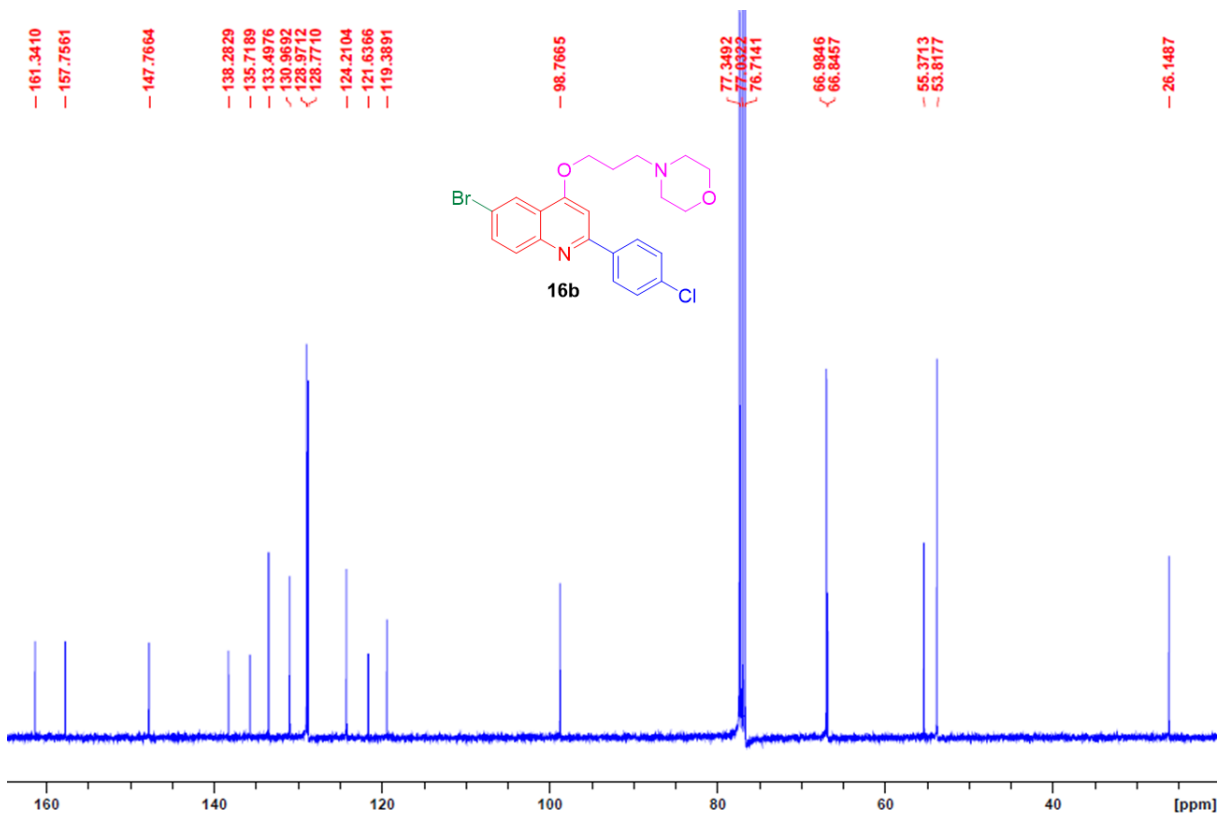
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- 7.2598
- 7.1314

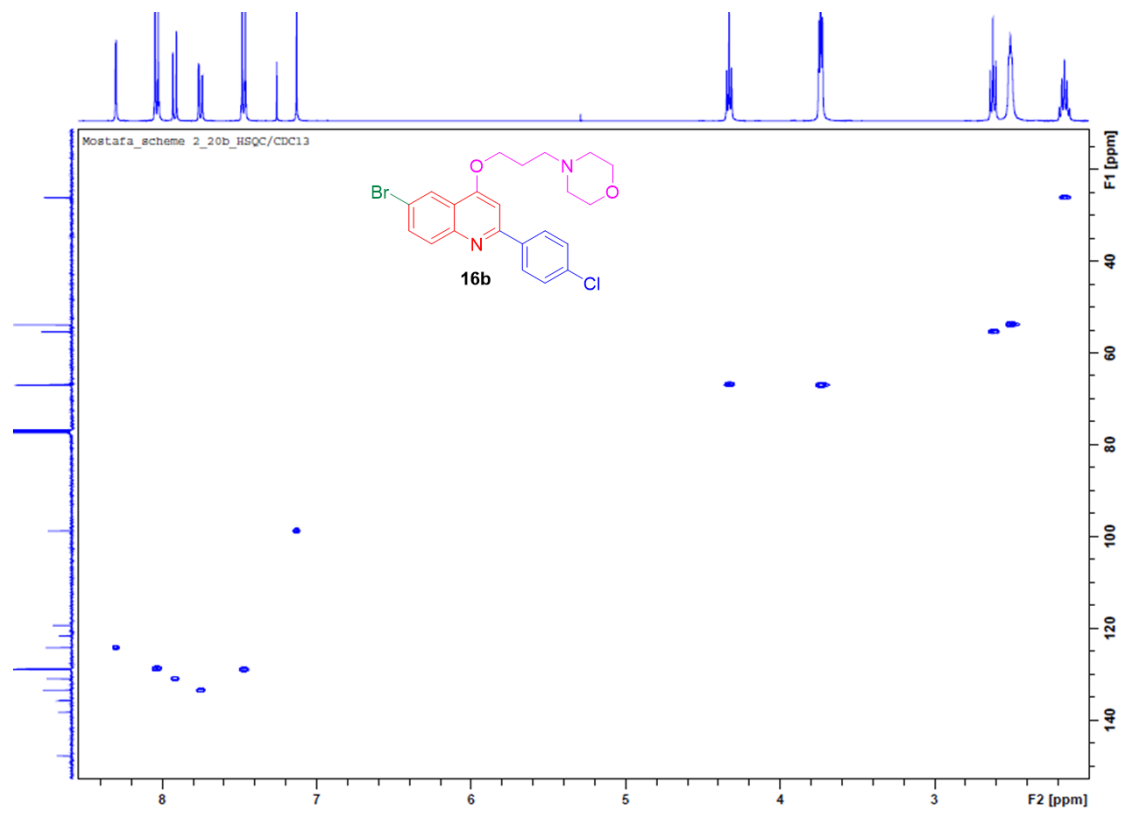
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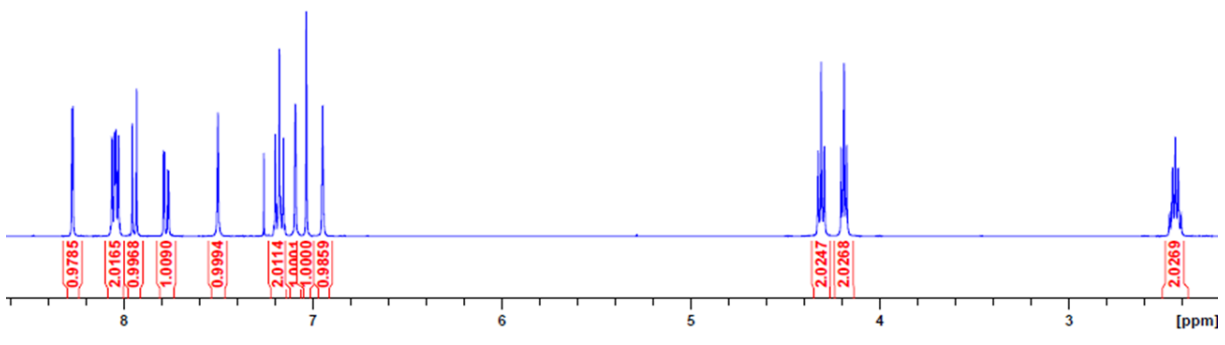
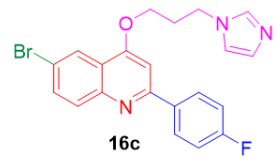


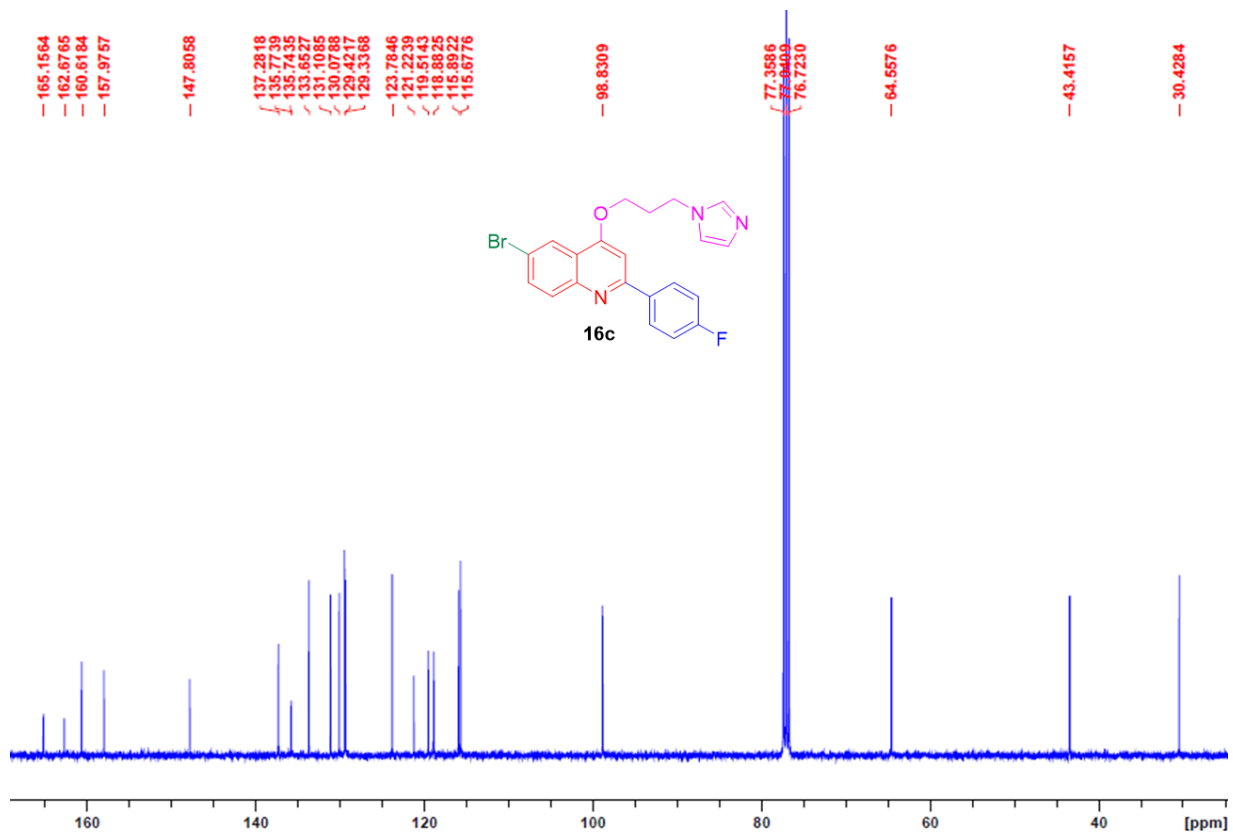


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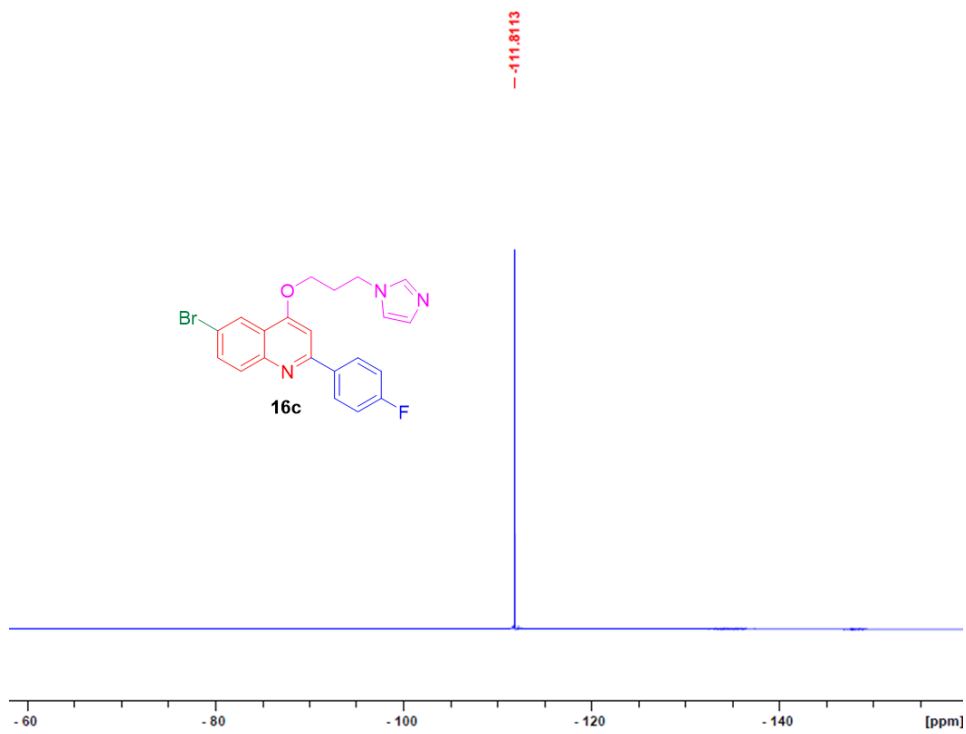
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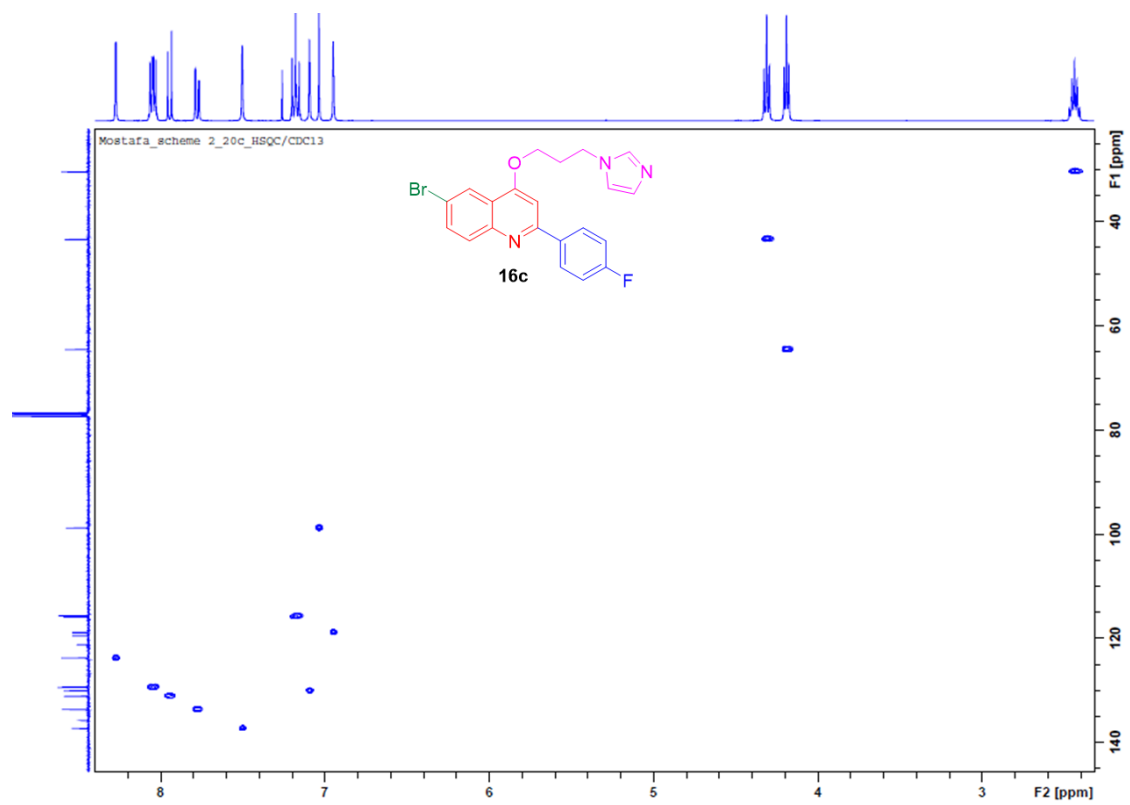
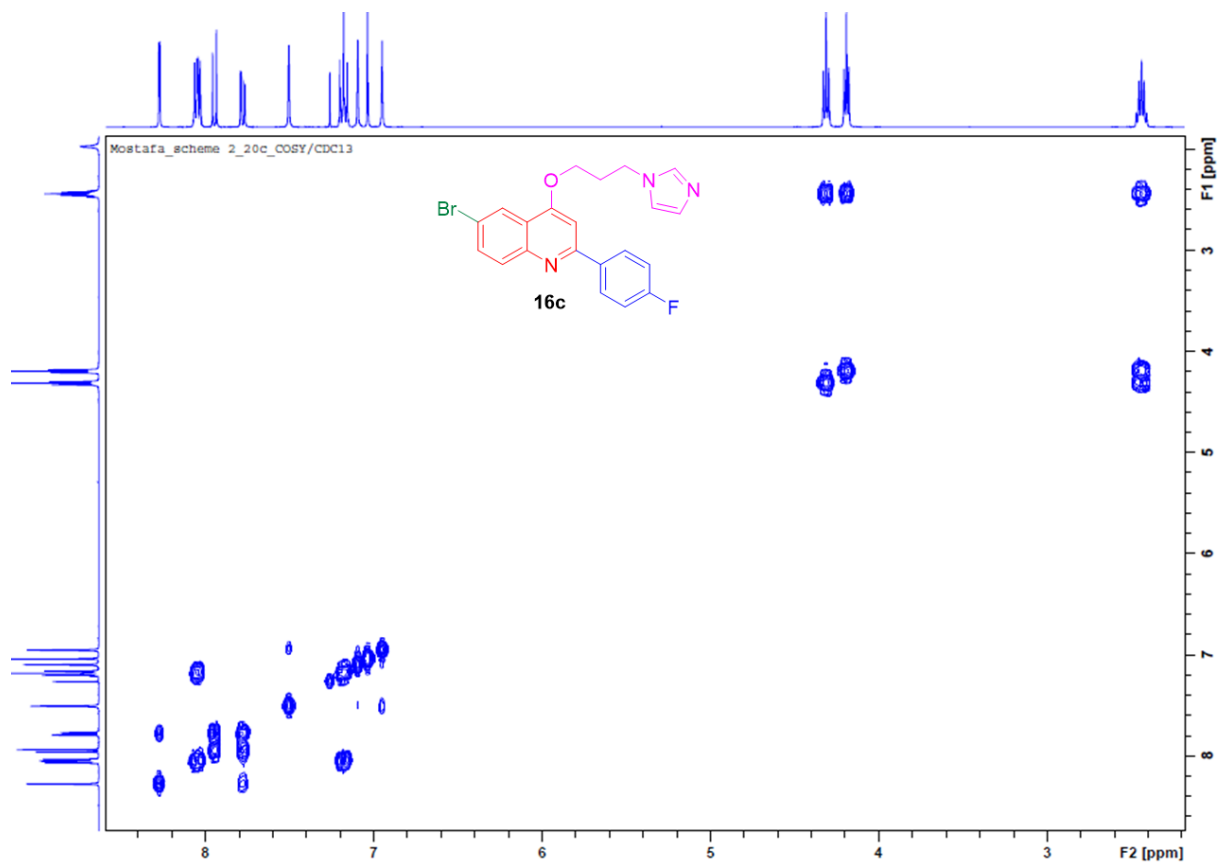
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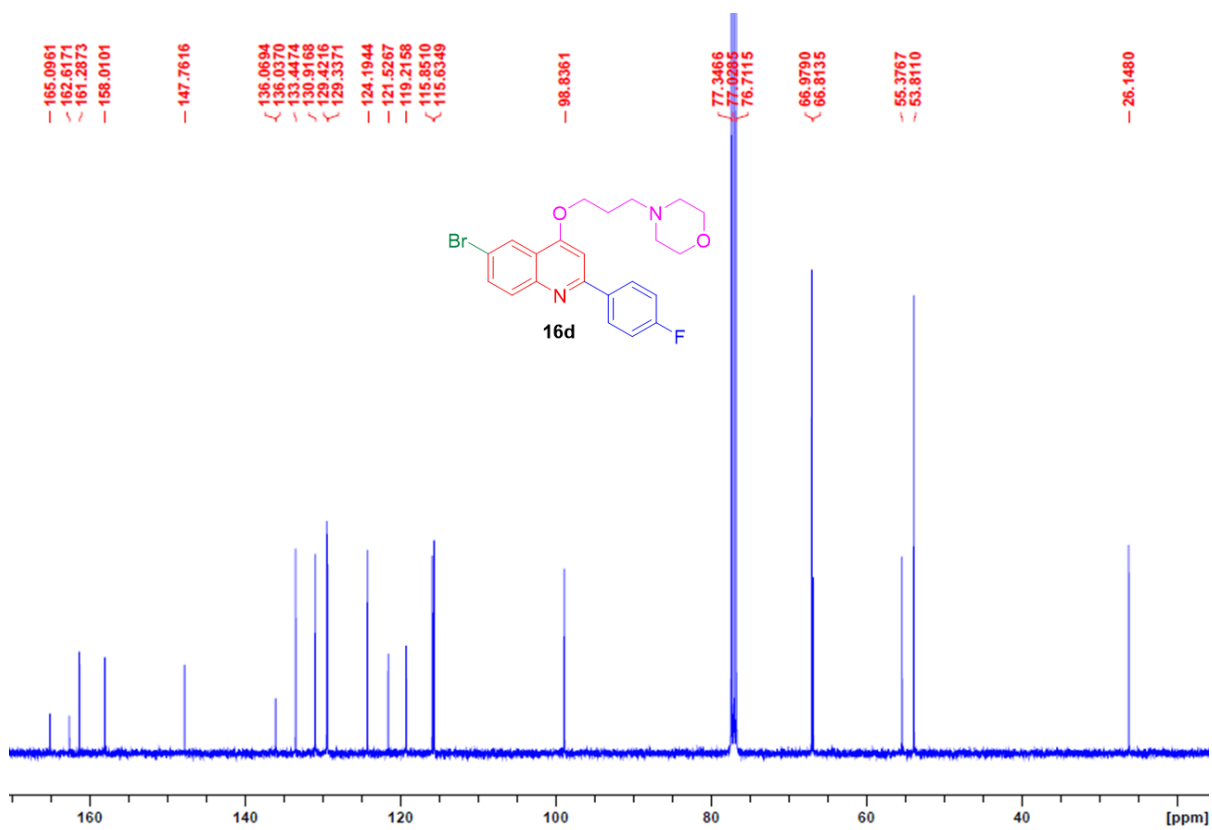
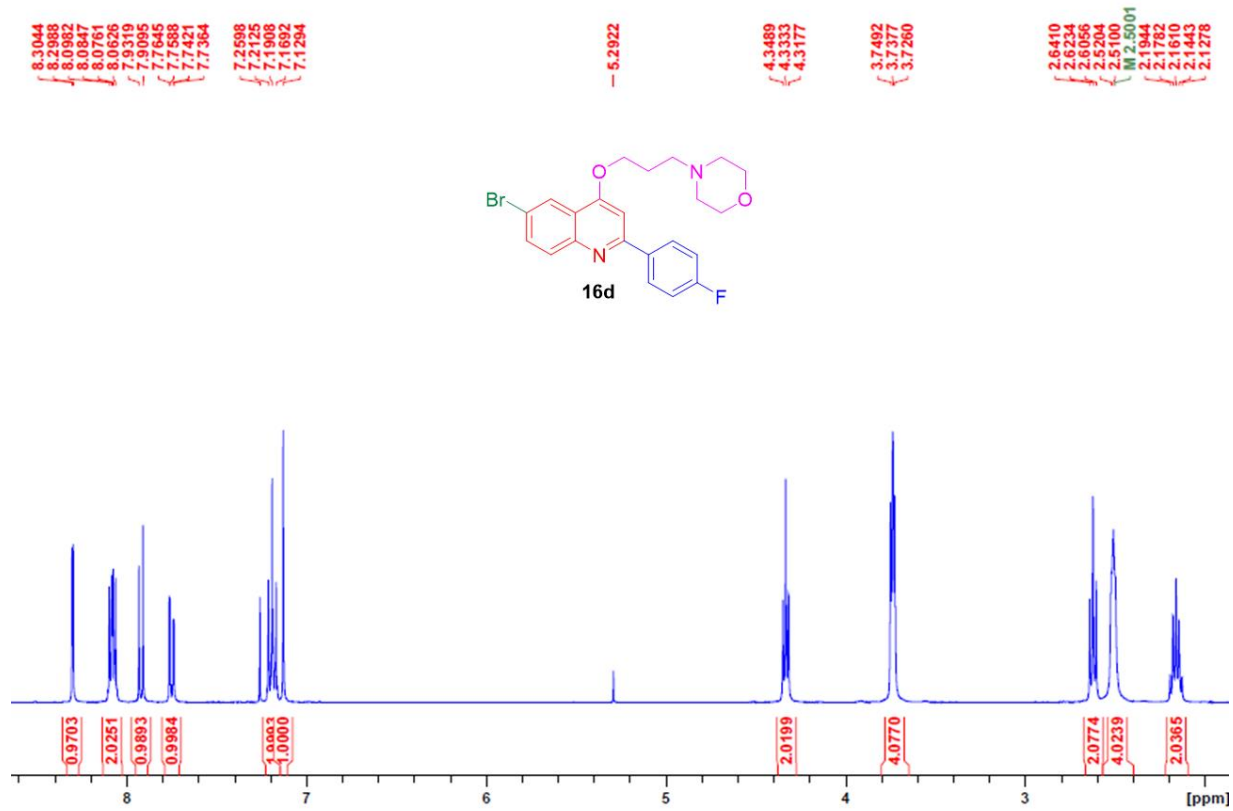




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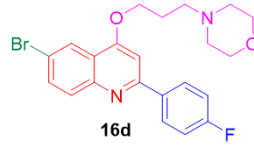




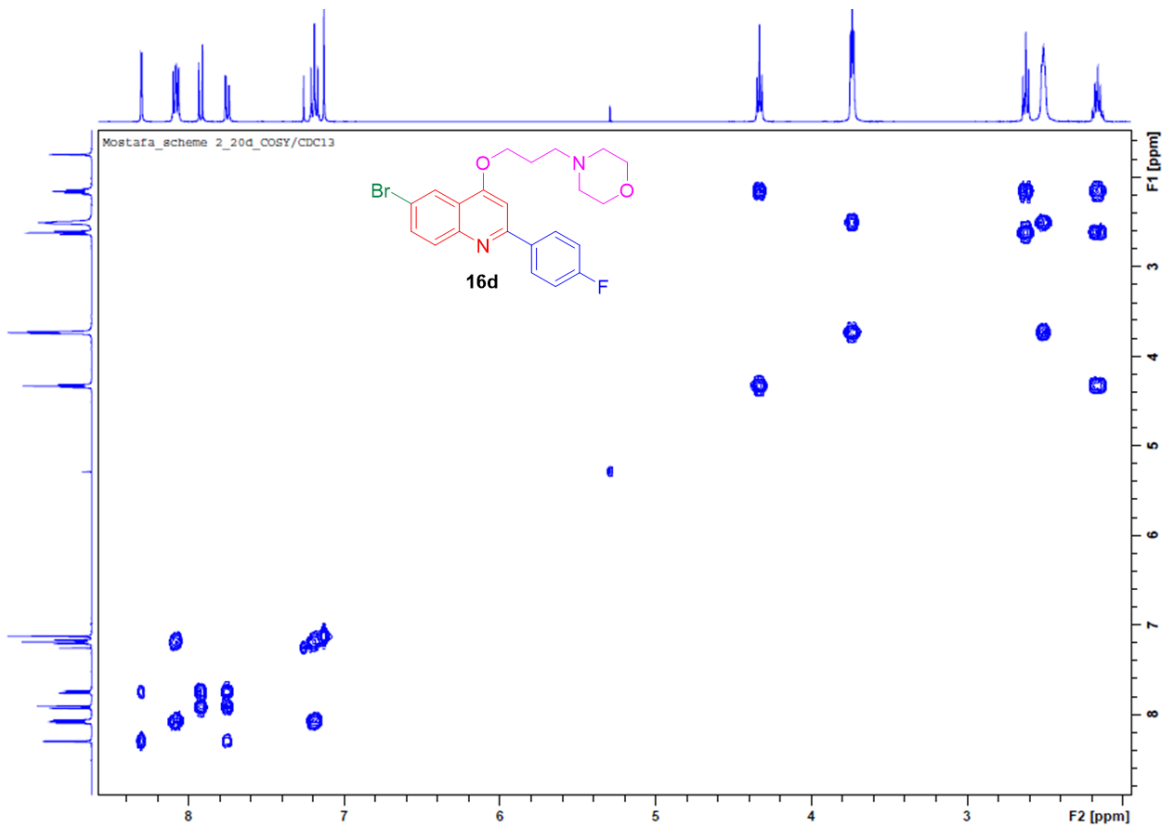


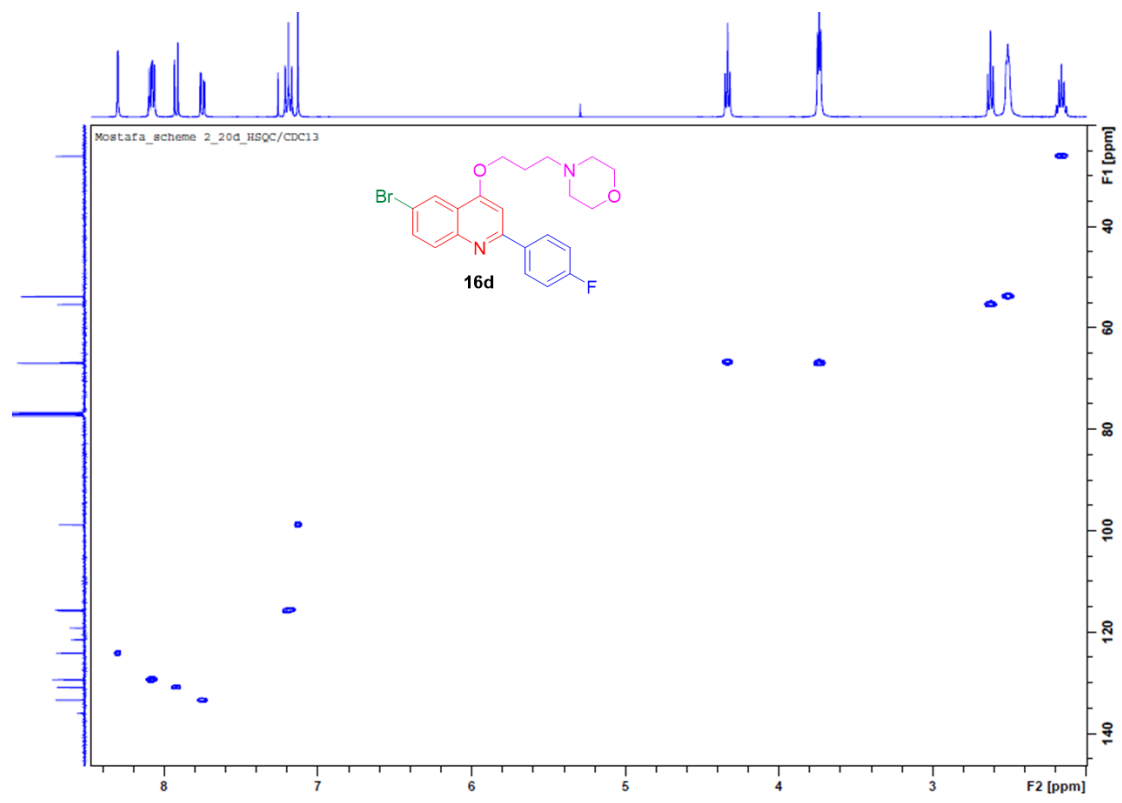
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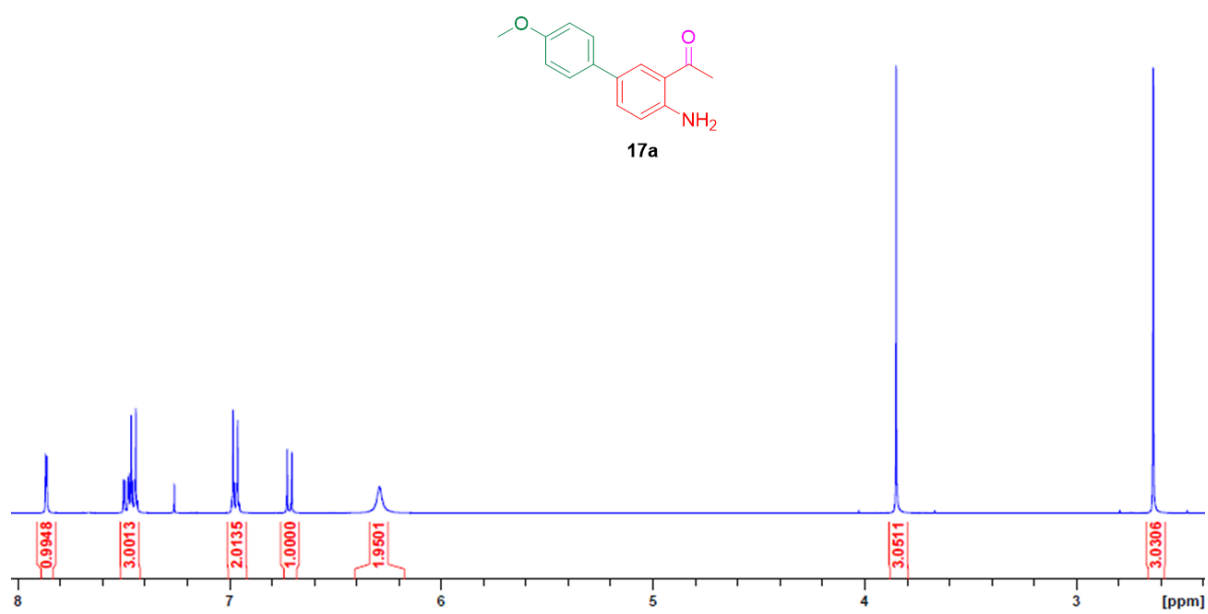


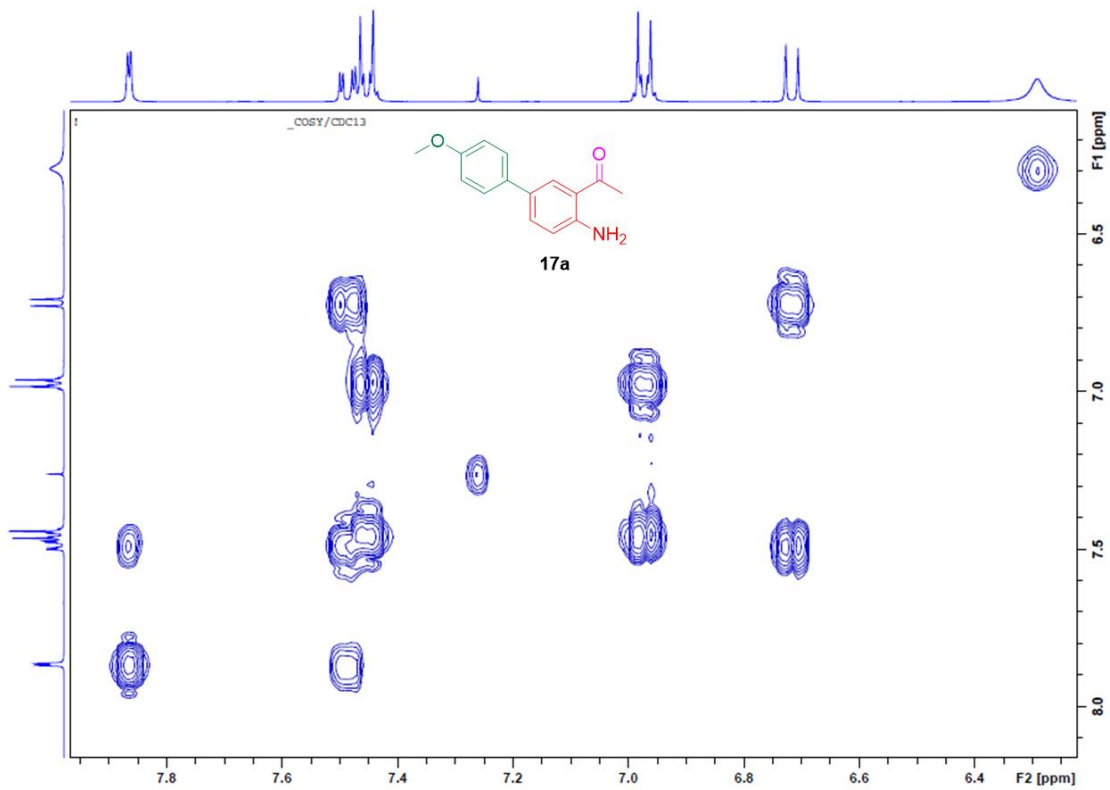
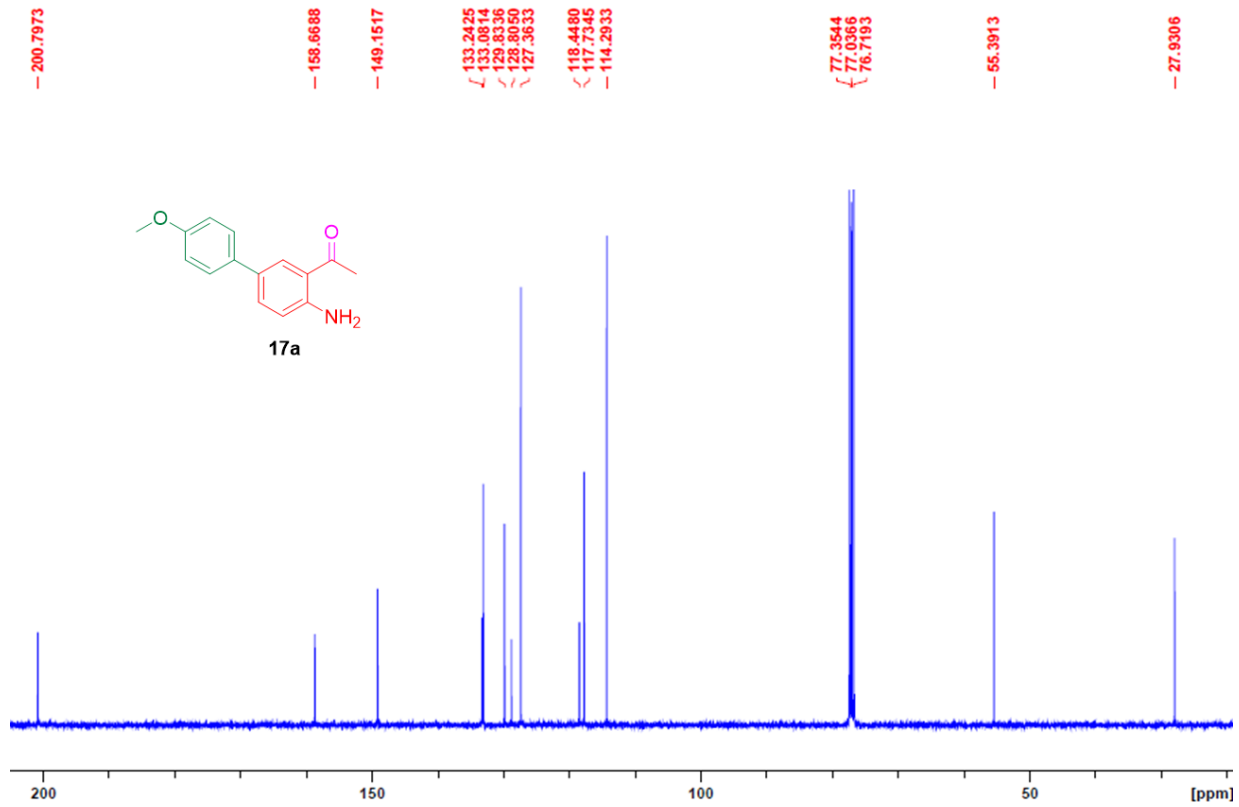
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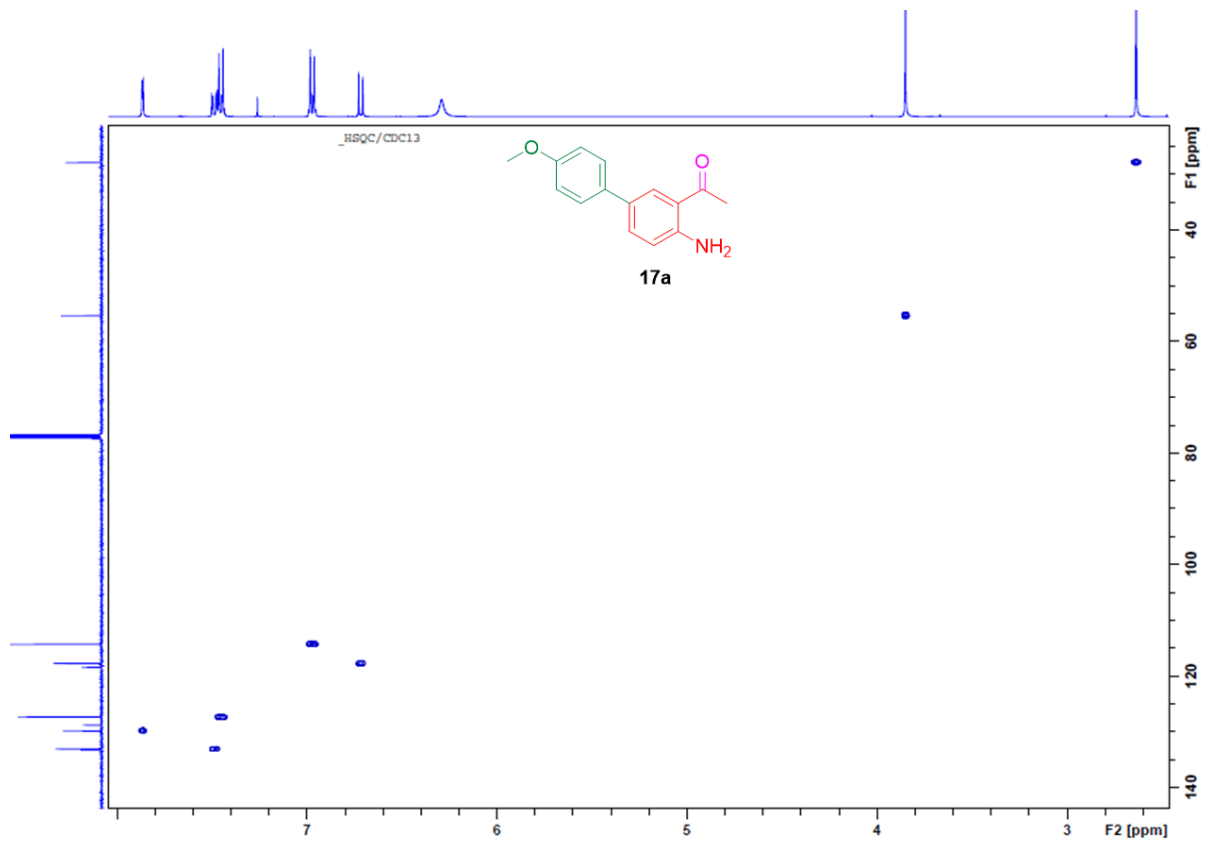




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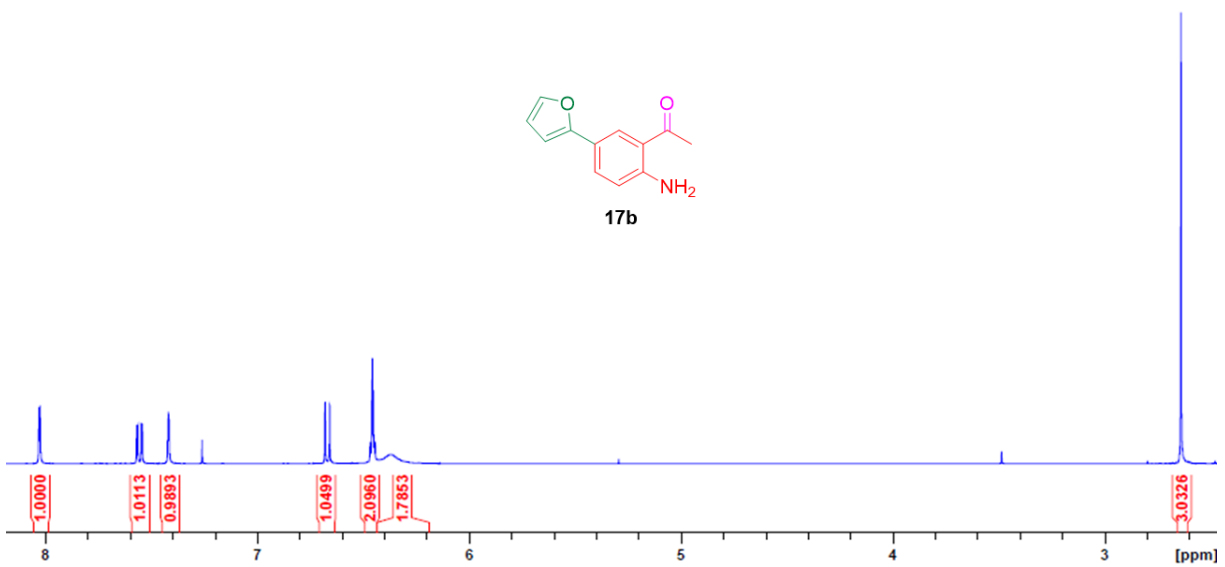


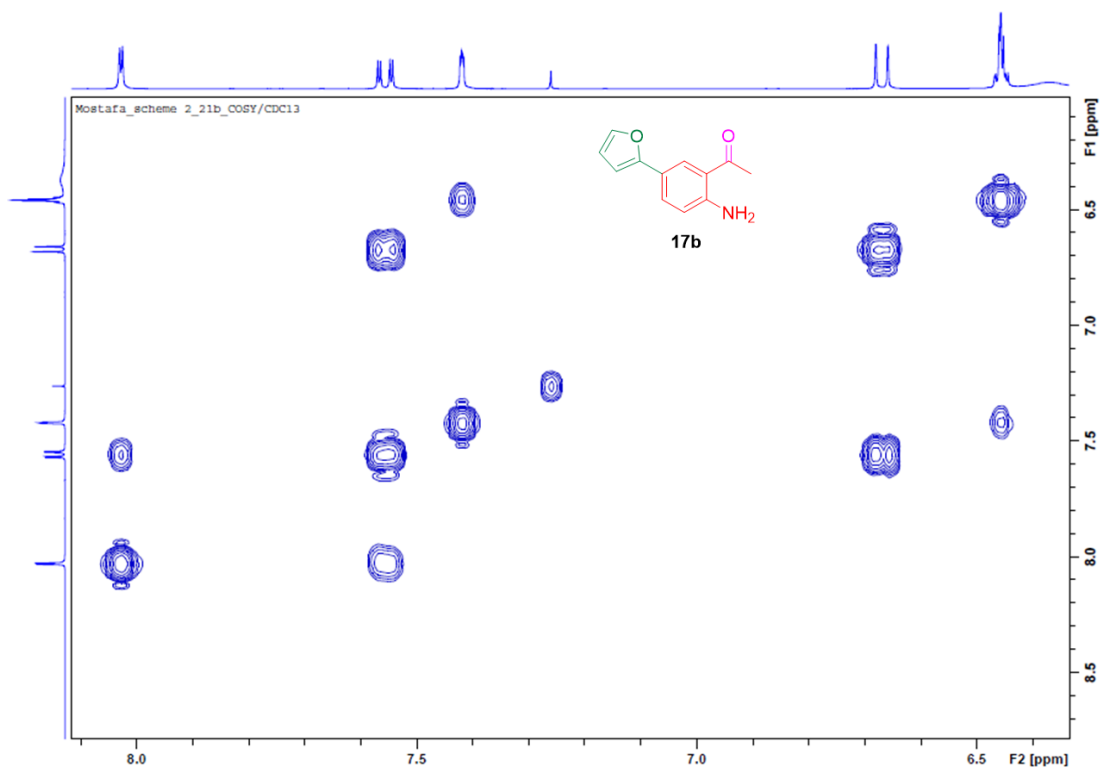
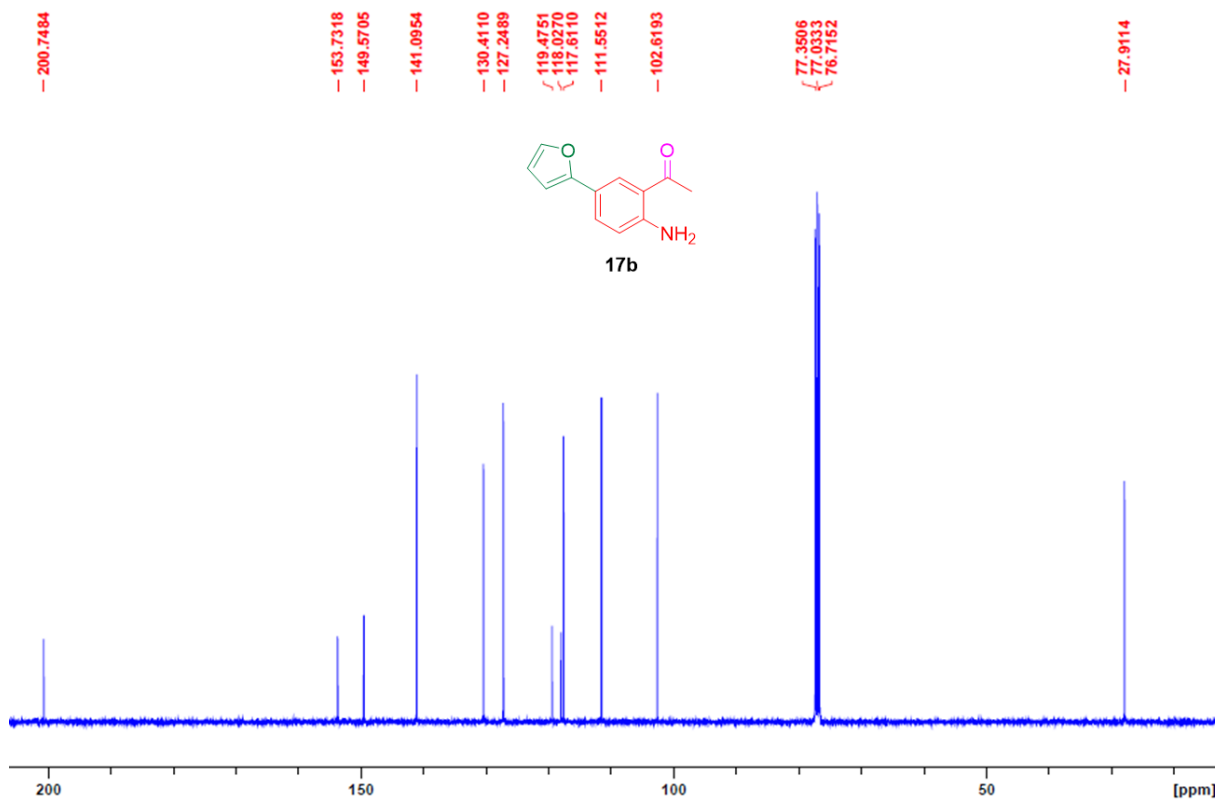


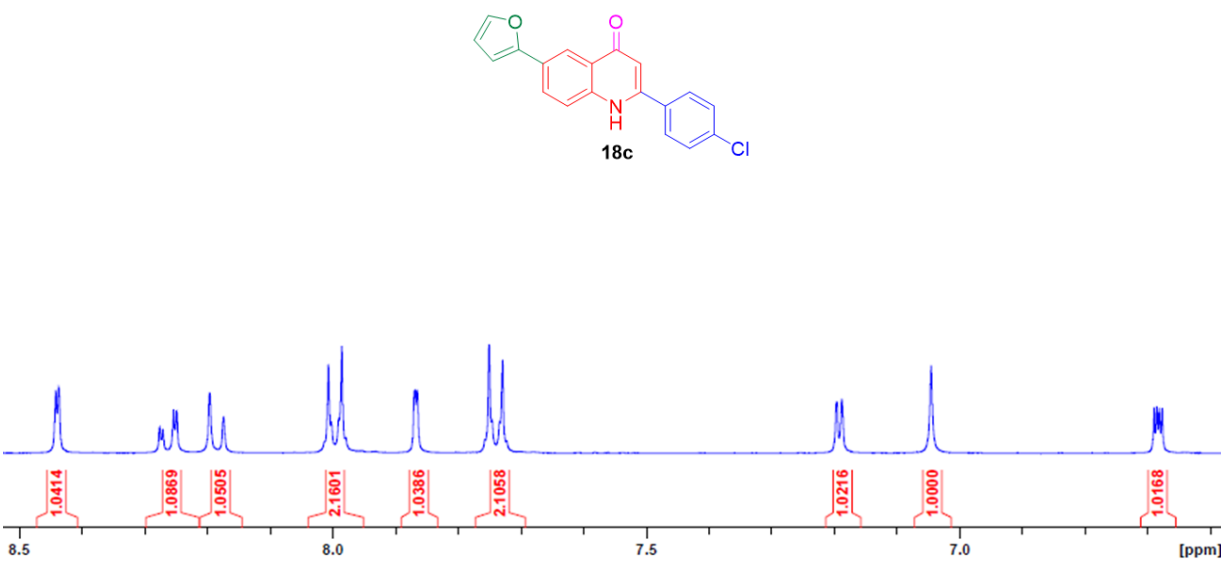
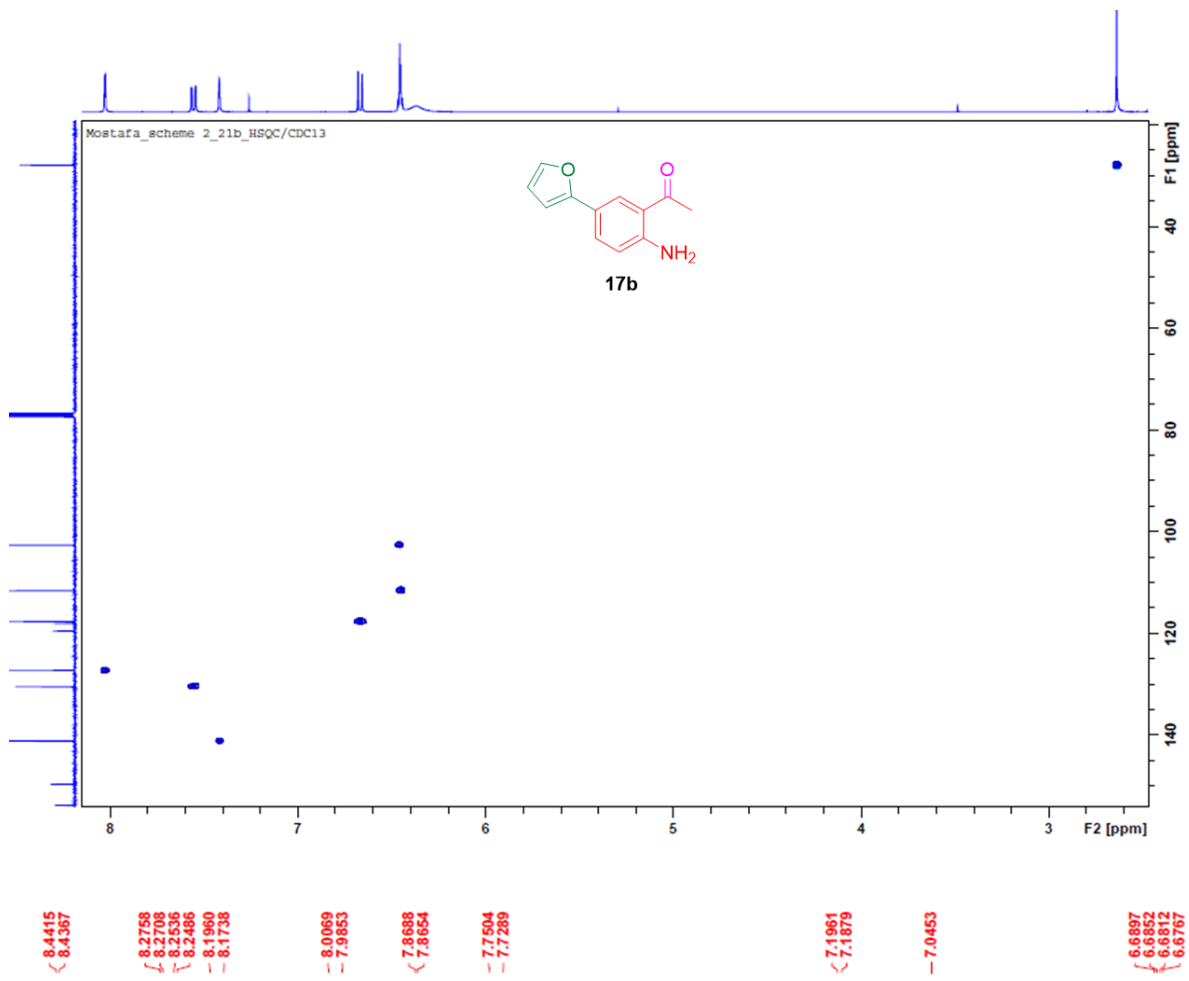


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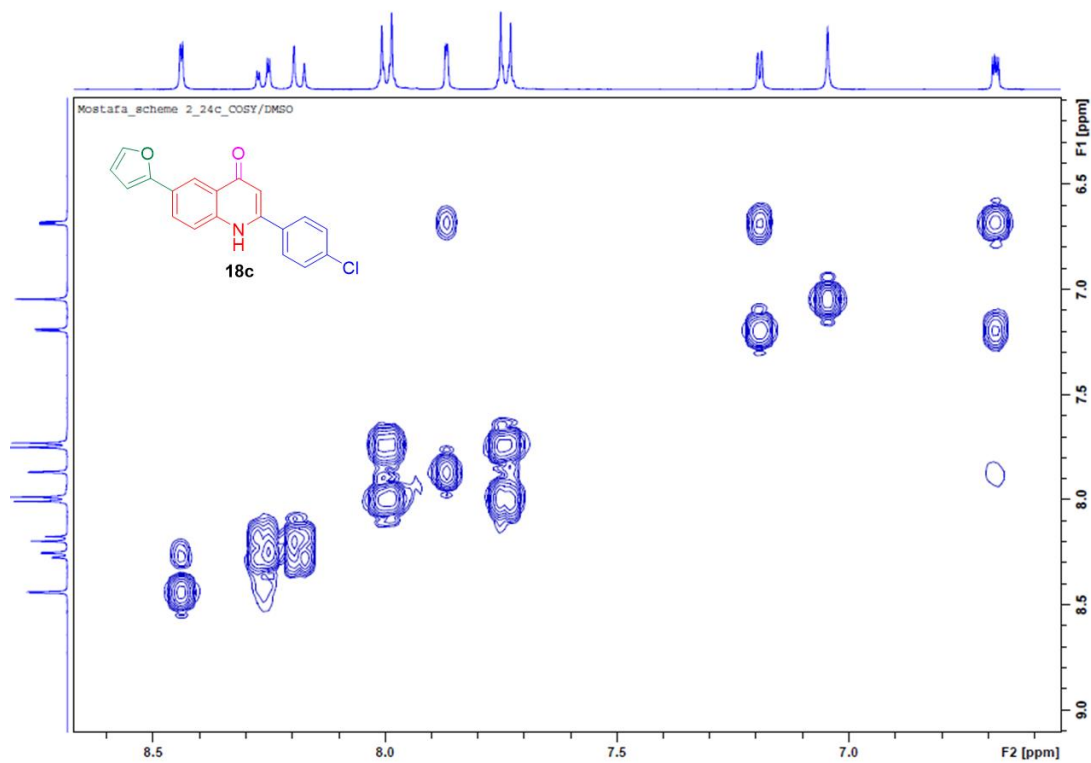
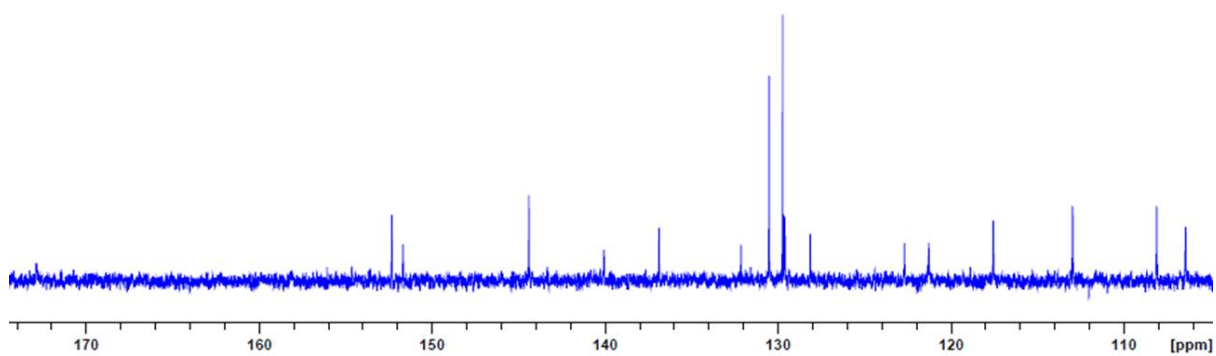
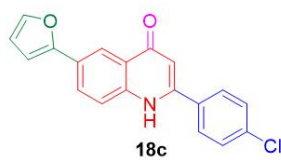


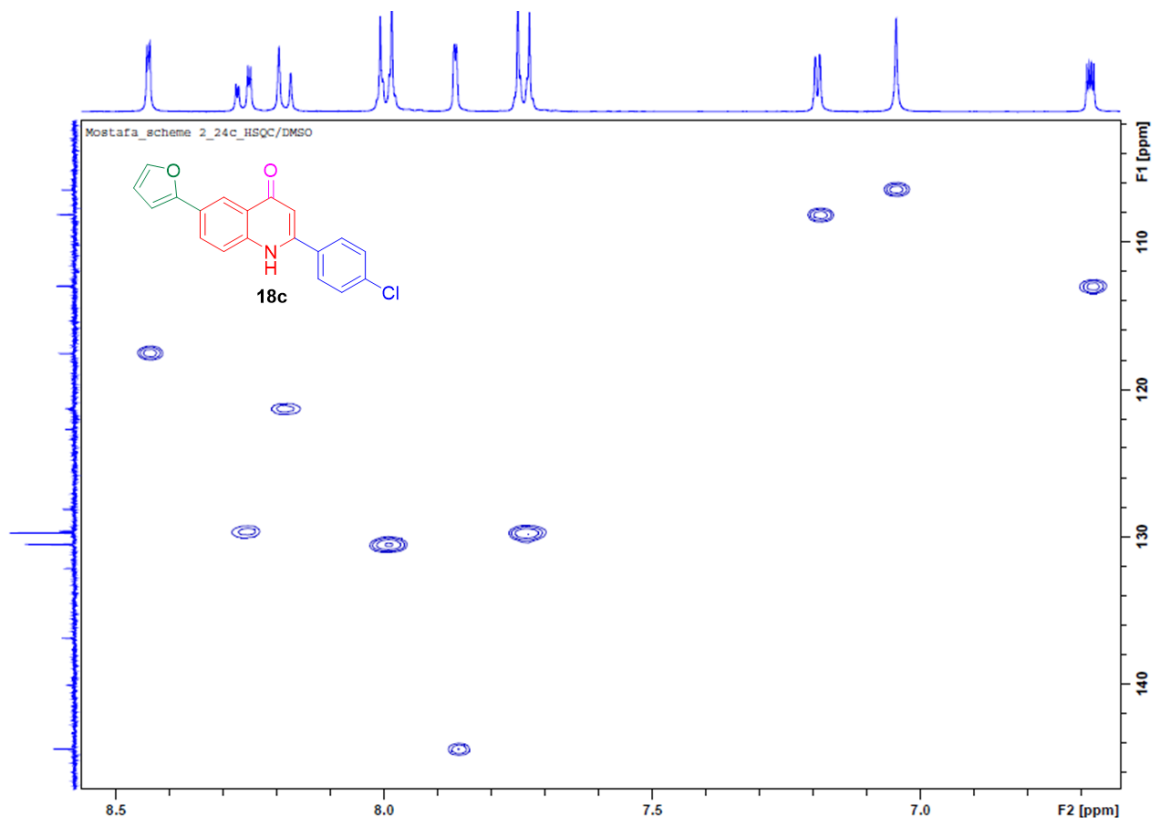




—M 172.8658

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- 144.3920
- 140.0695
- 136.8680
- 132.1259
- 130.4961
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- 106.4254



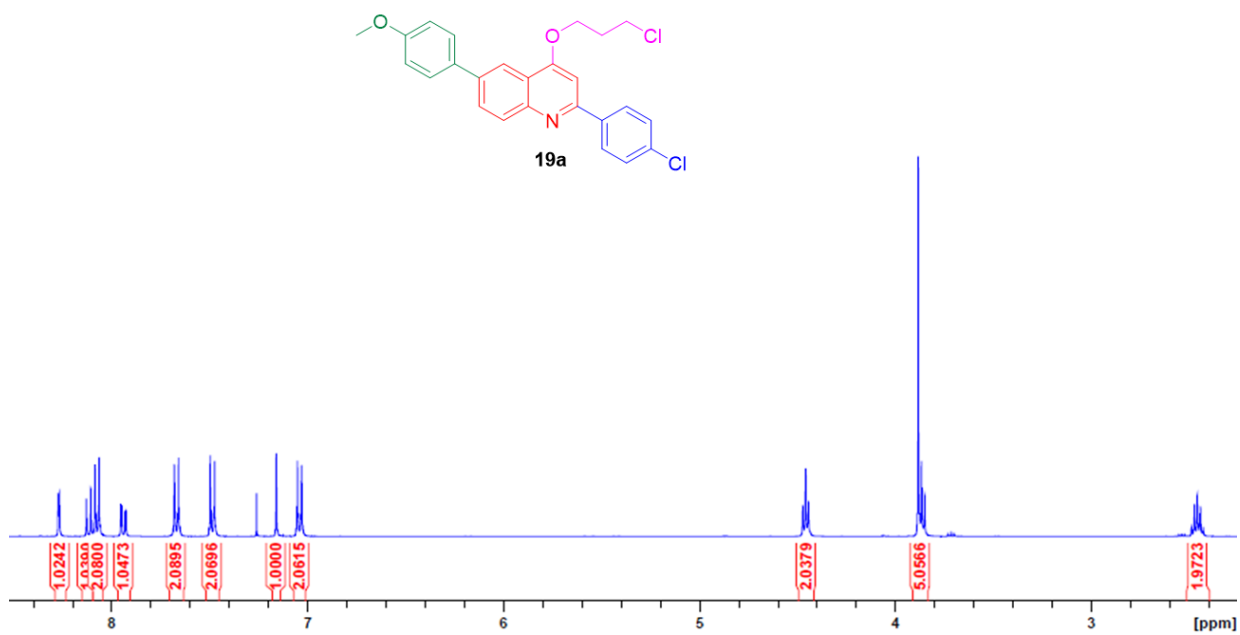


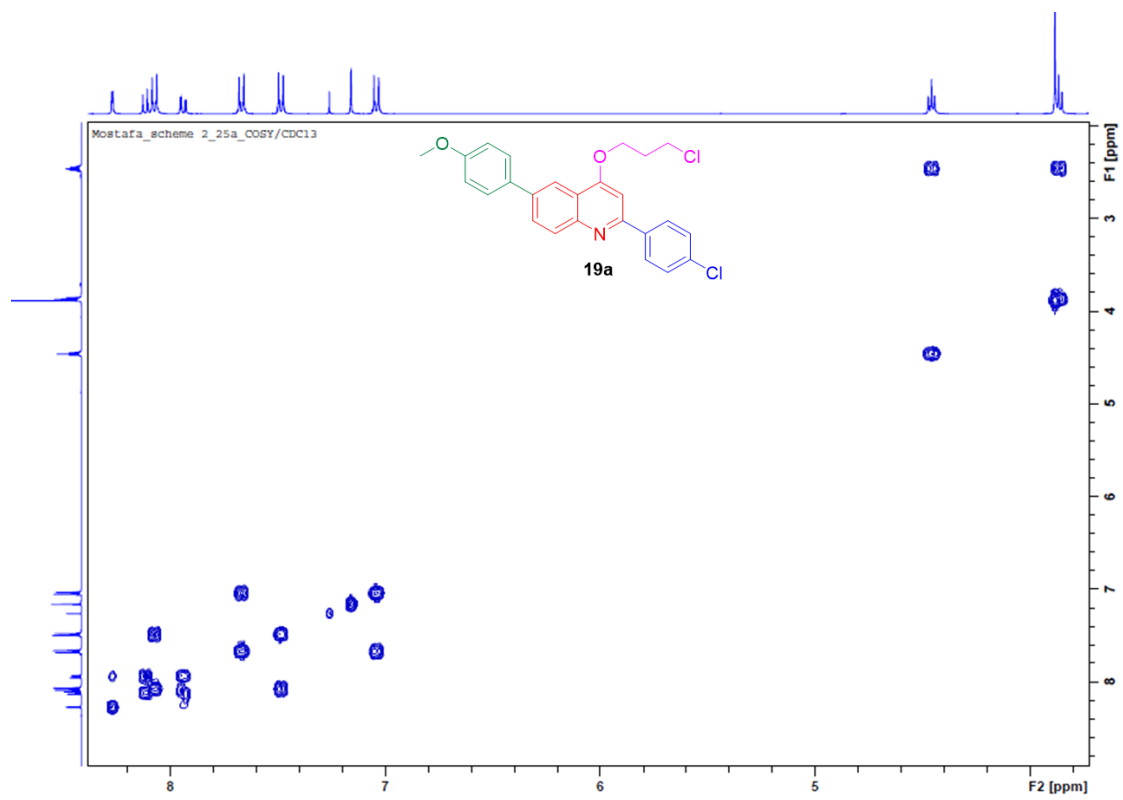
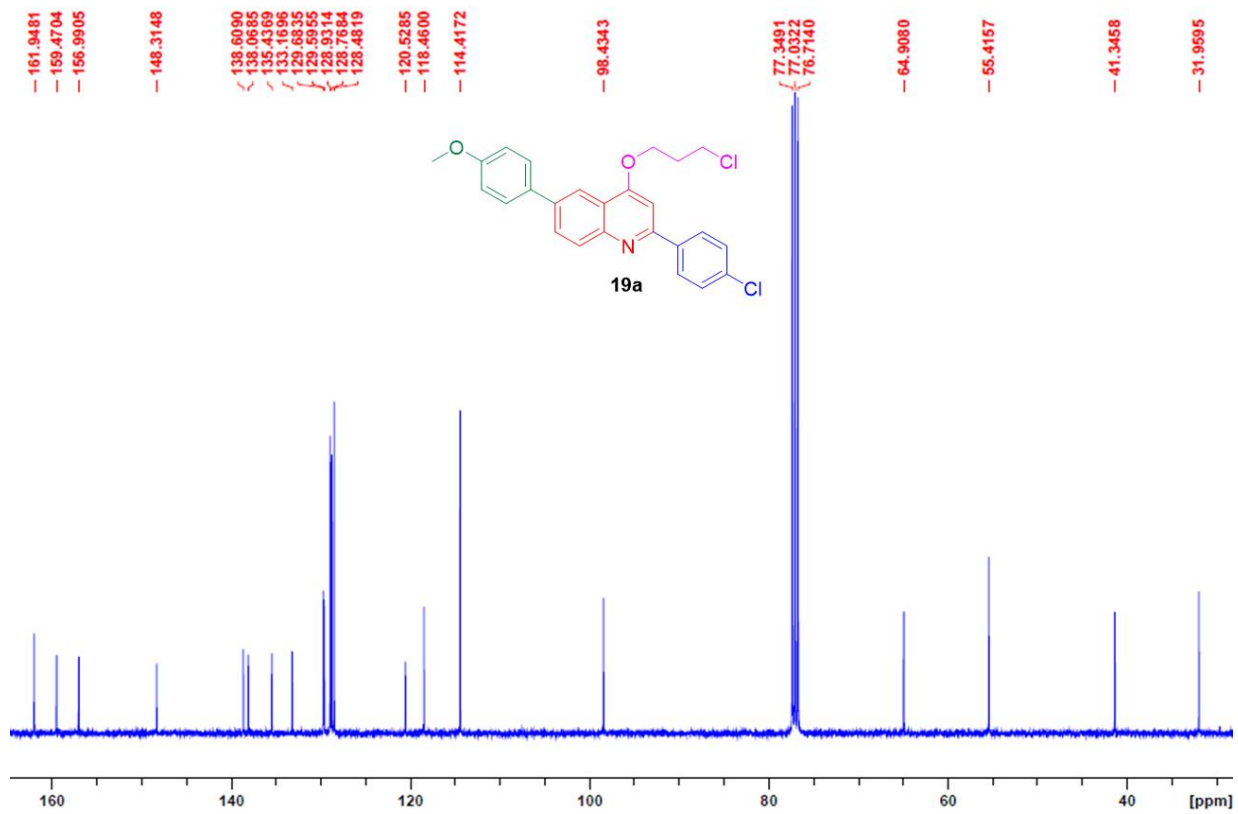
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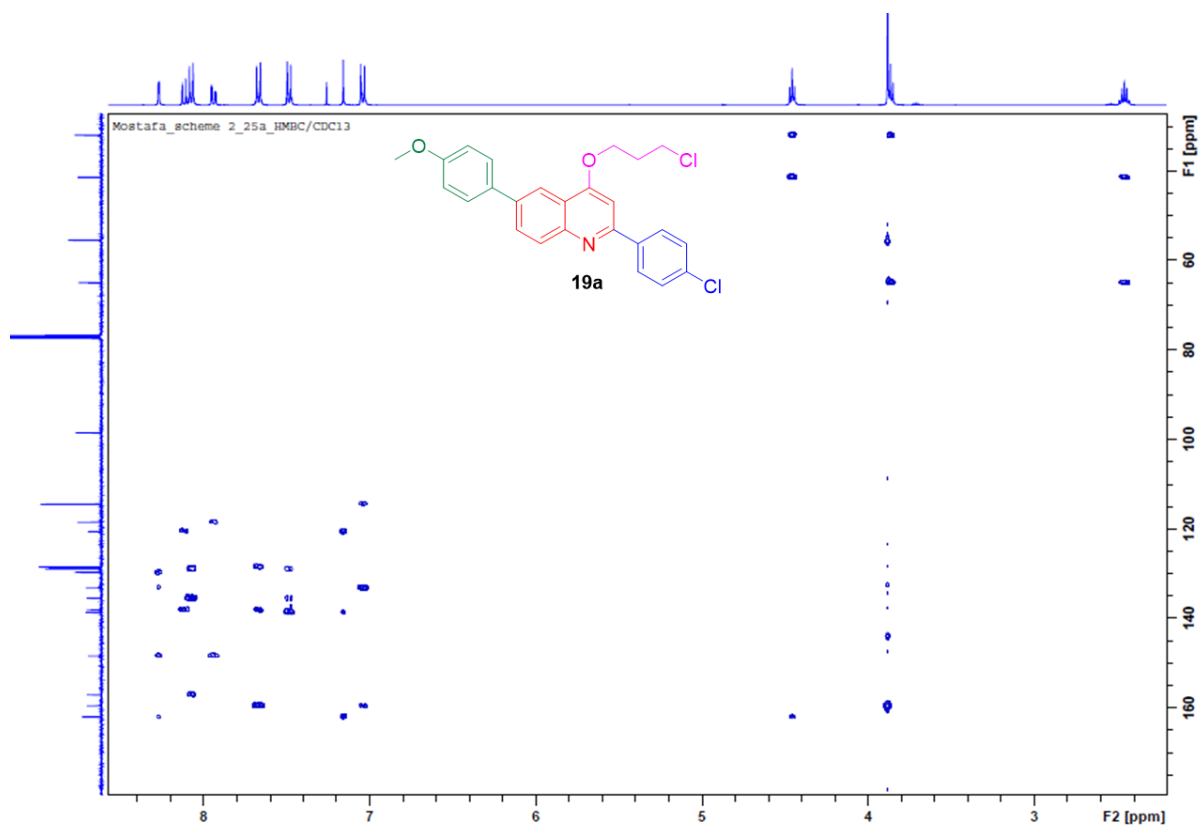
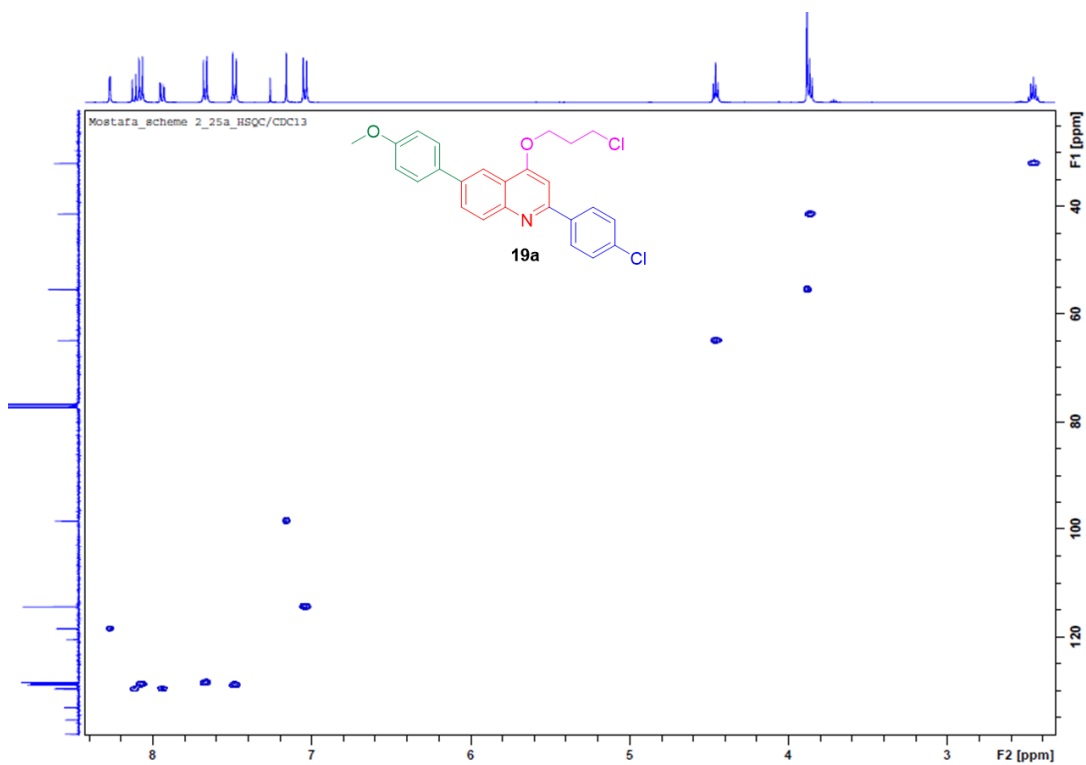
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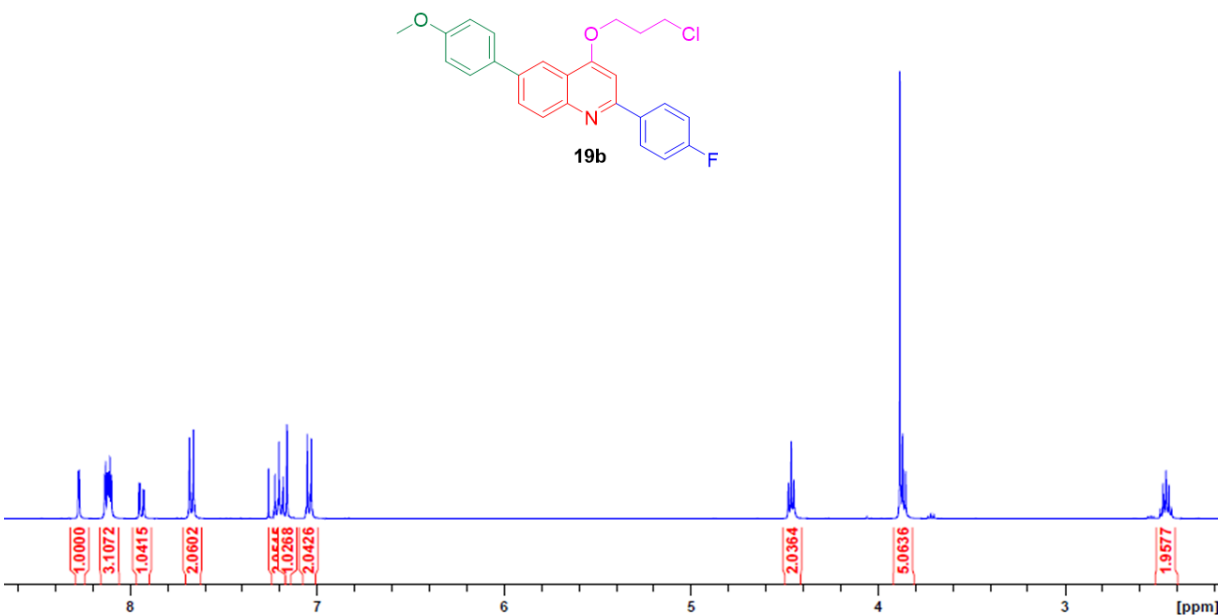
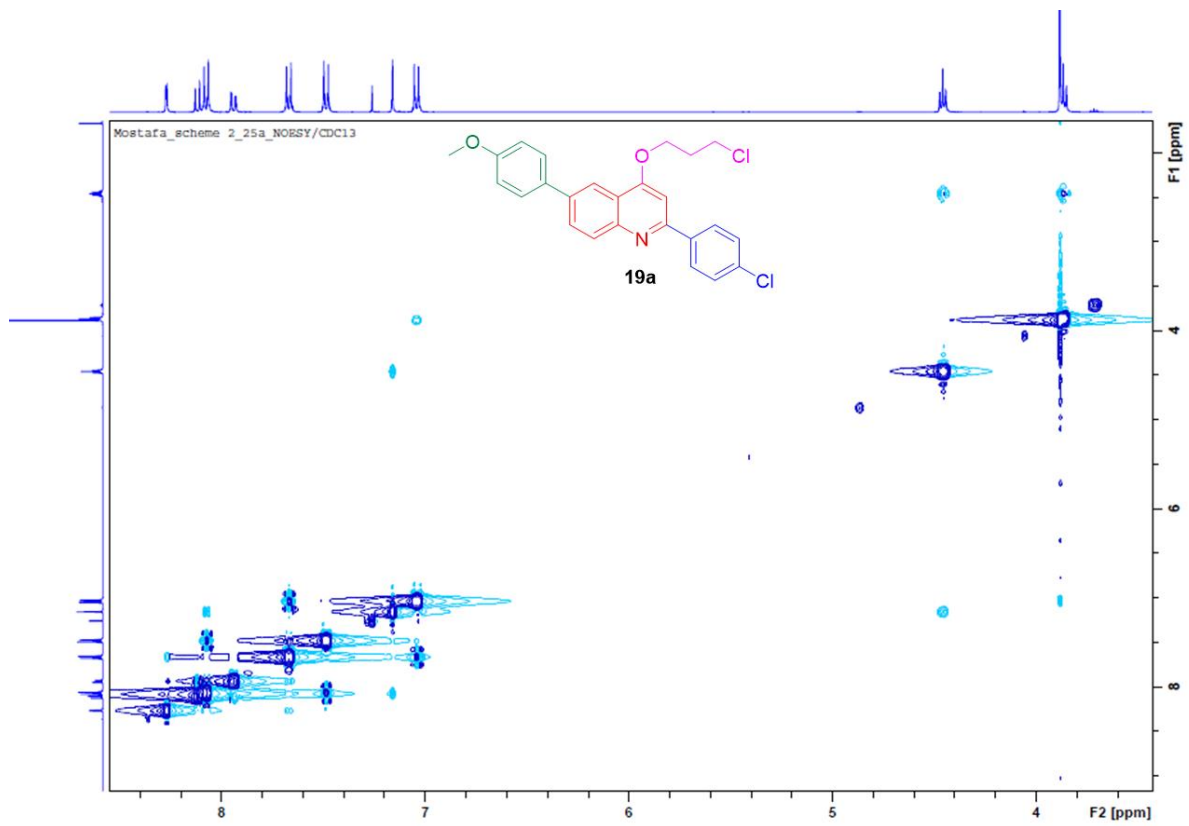
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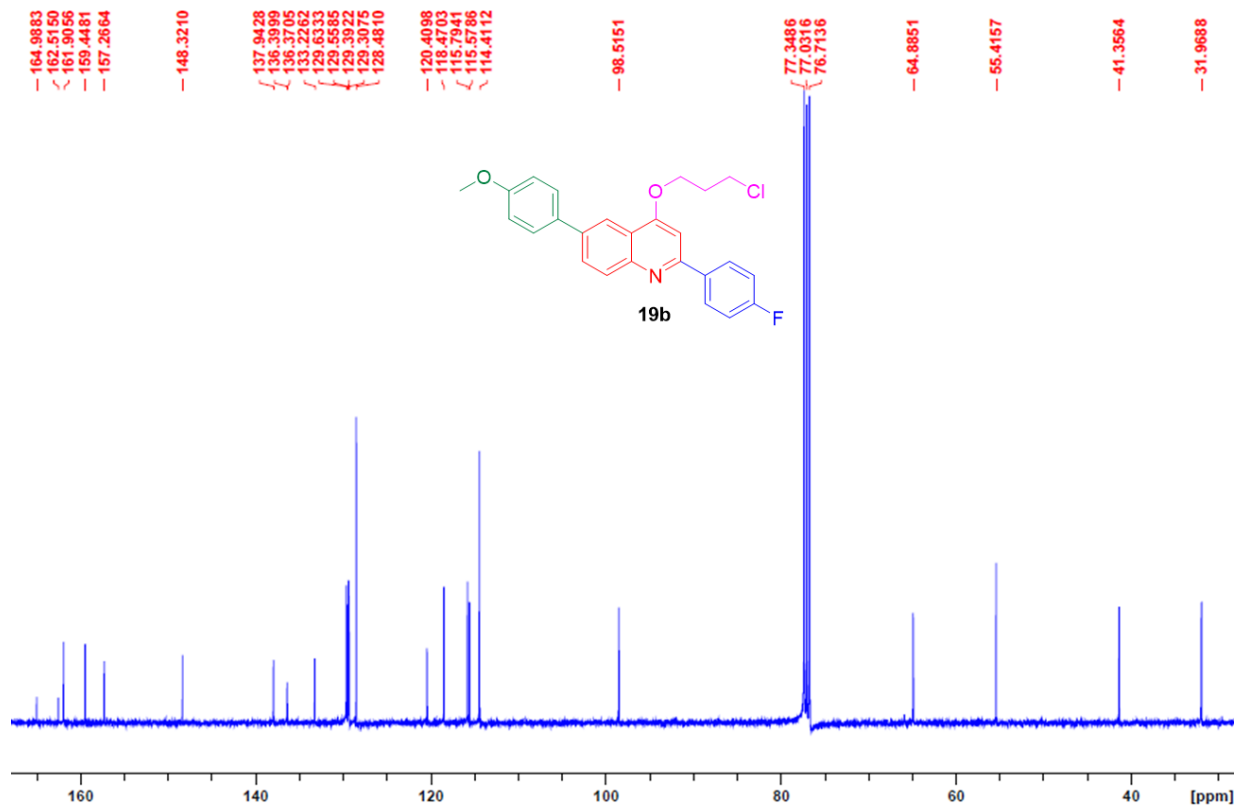
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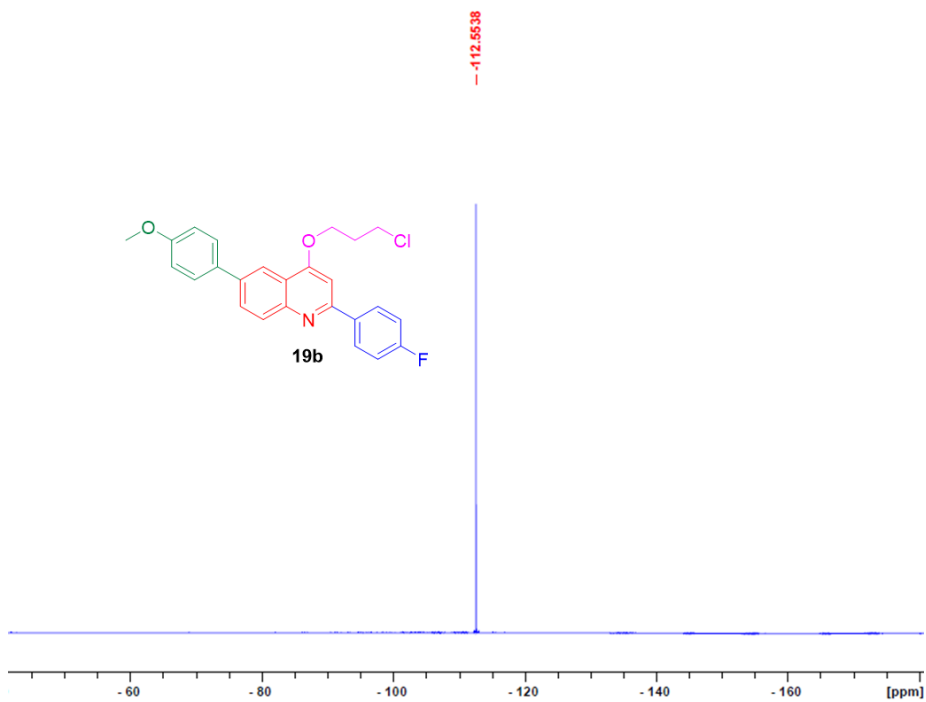


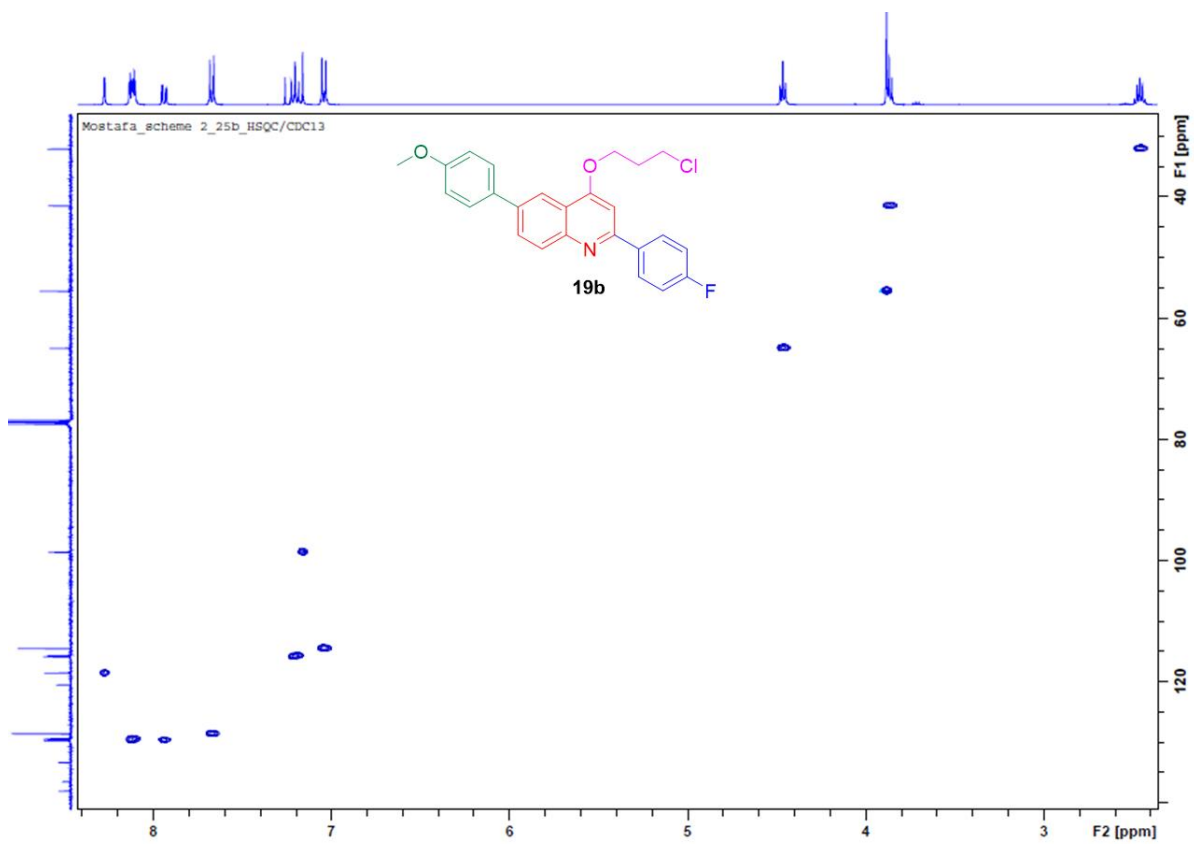
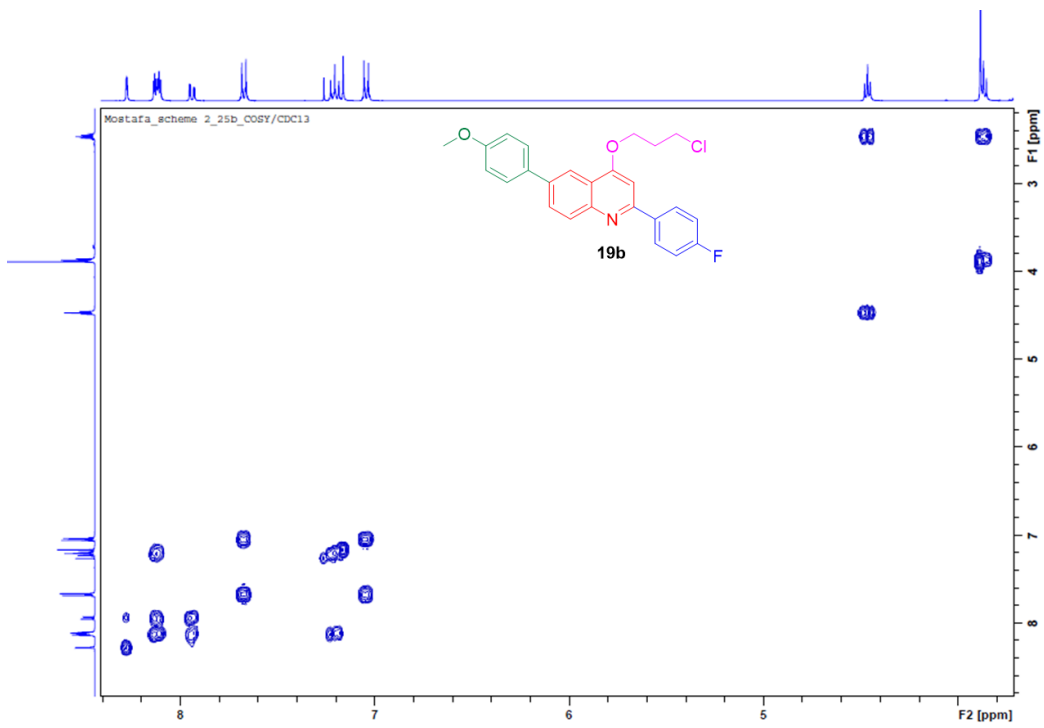


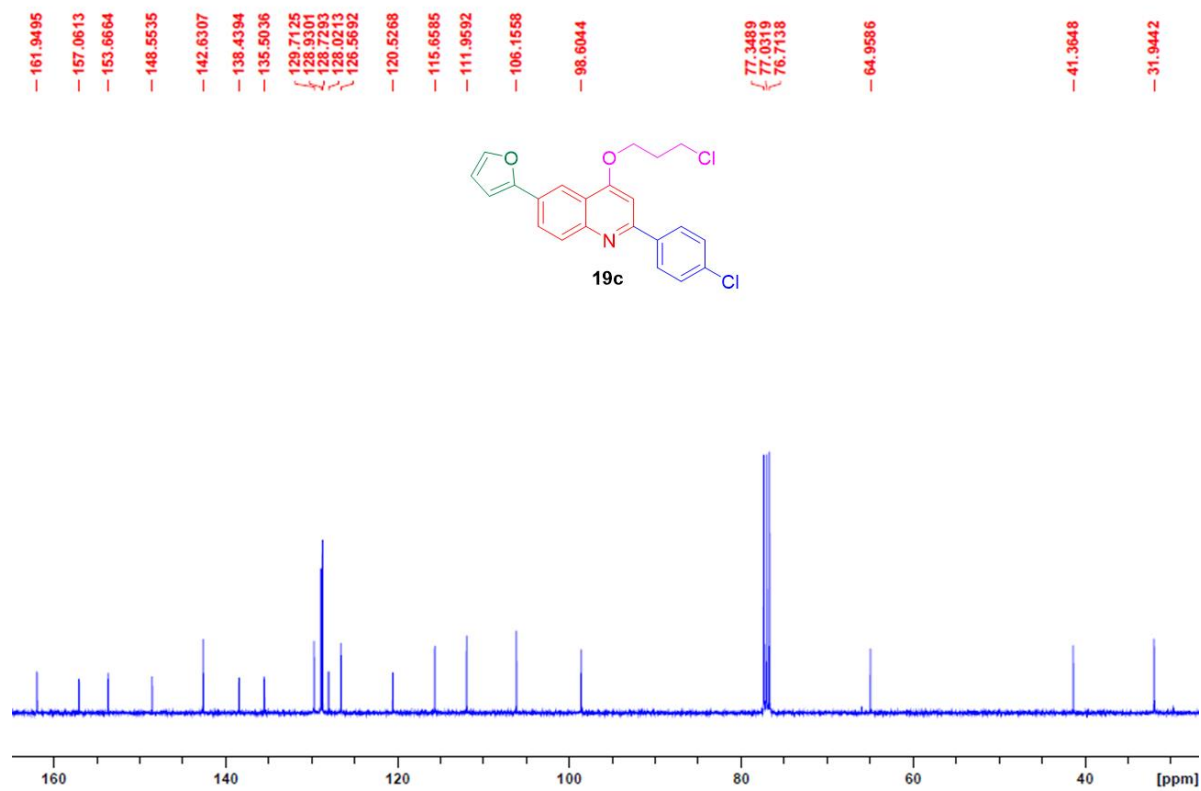
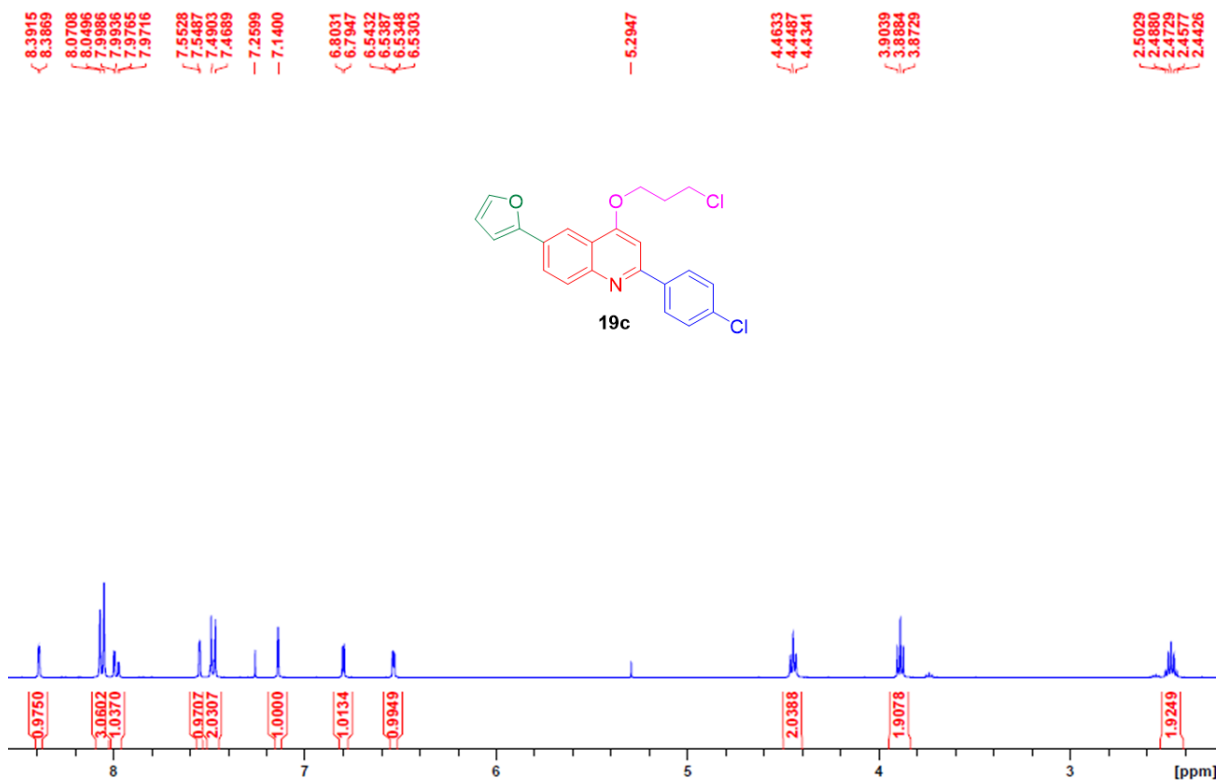


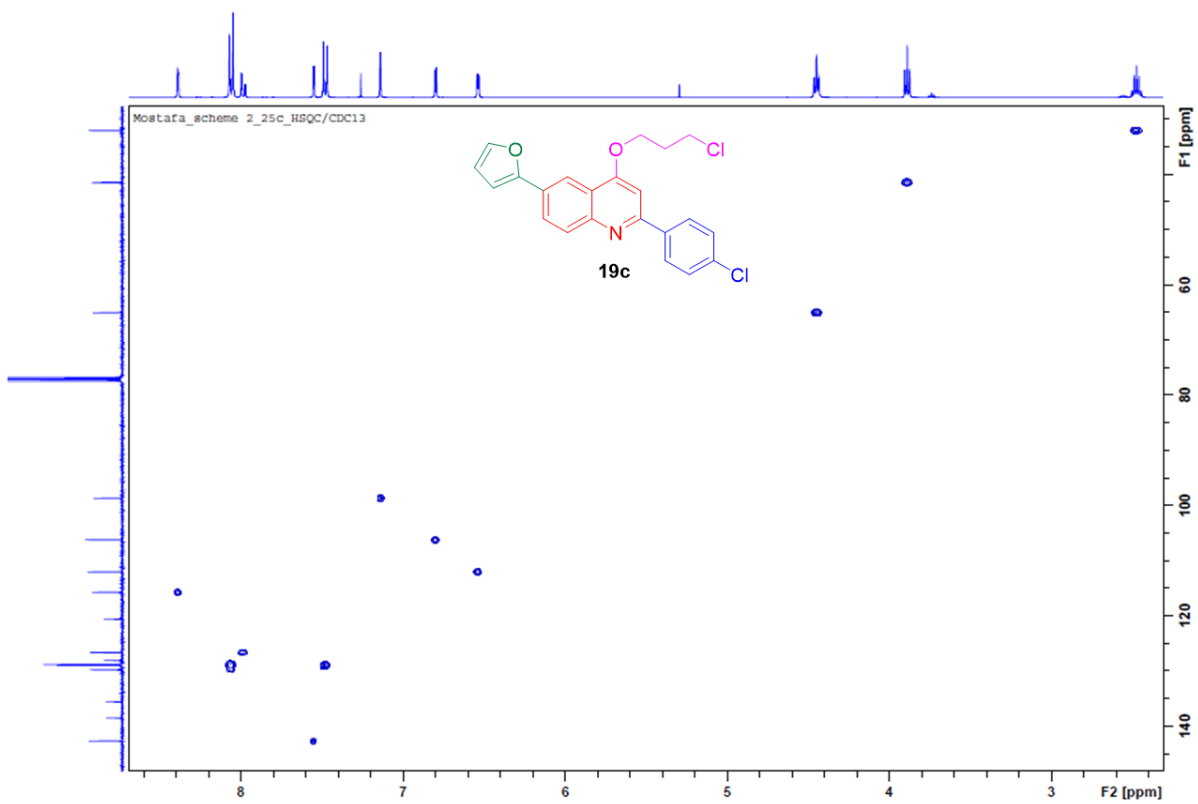
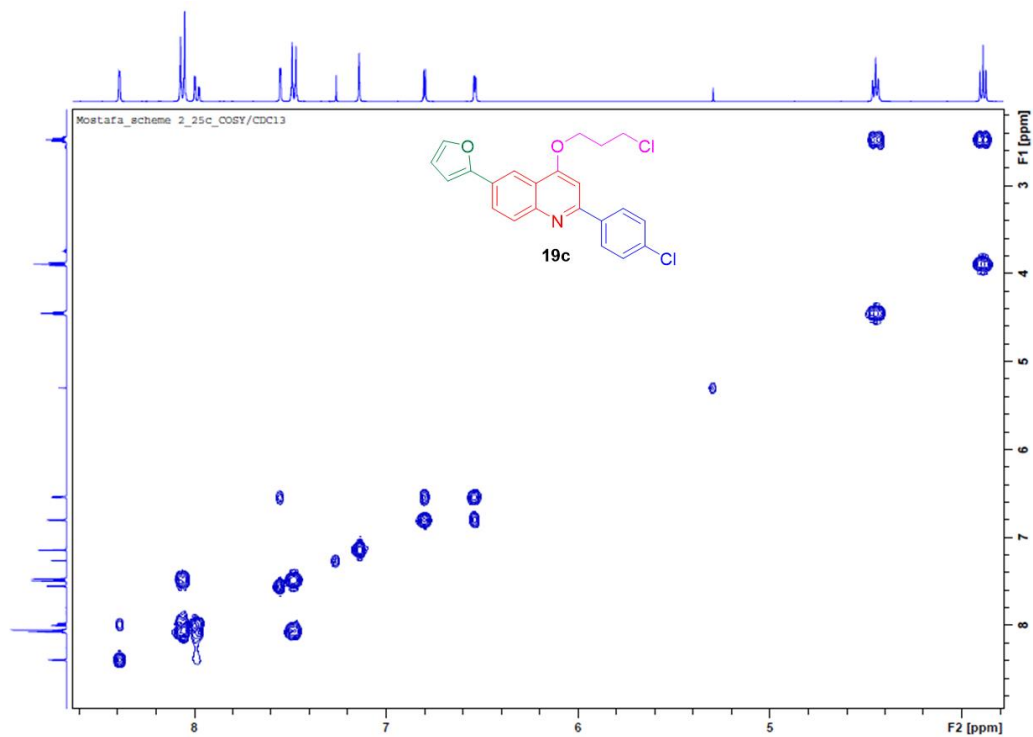


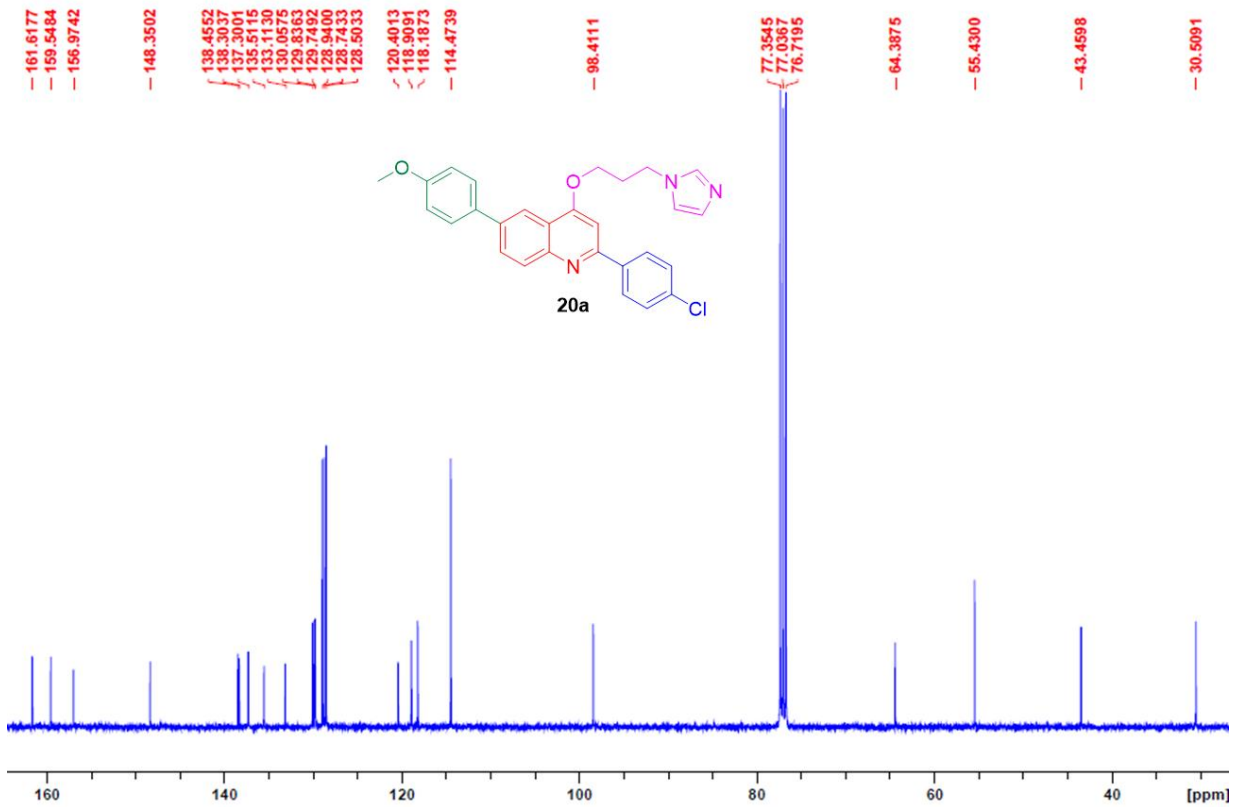
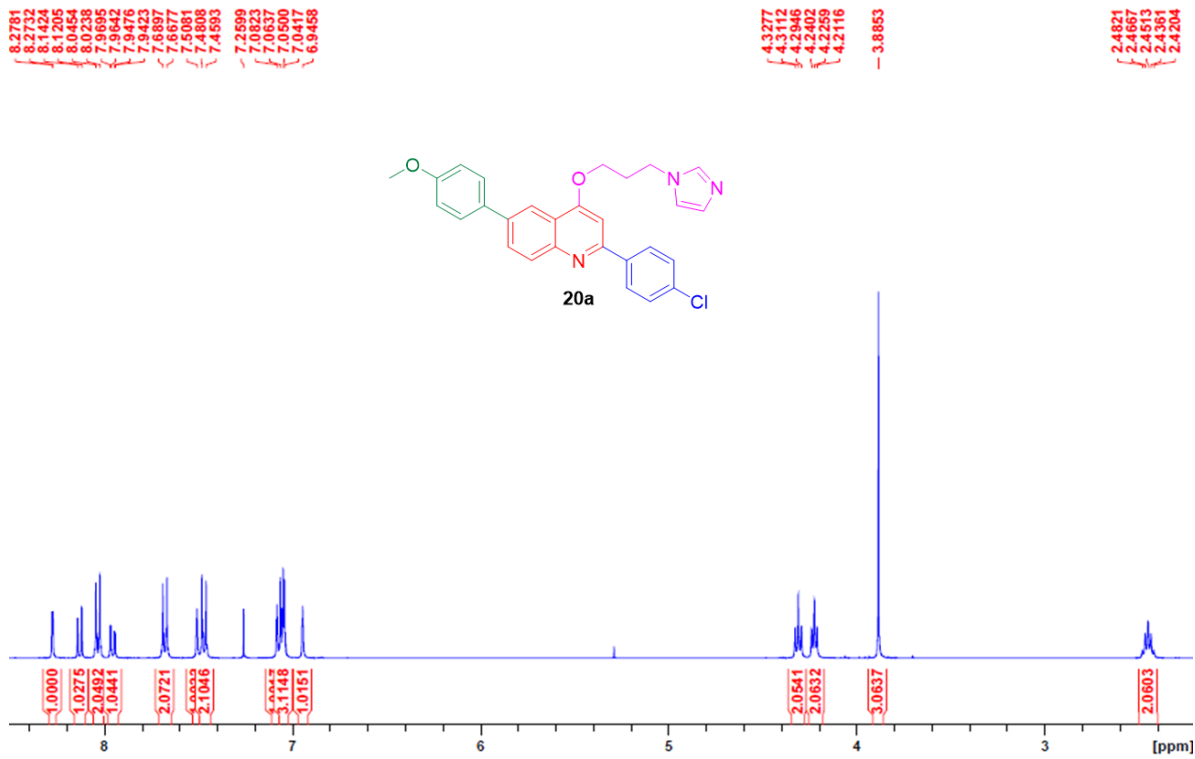
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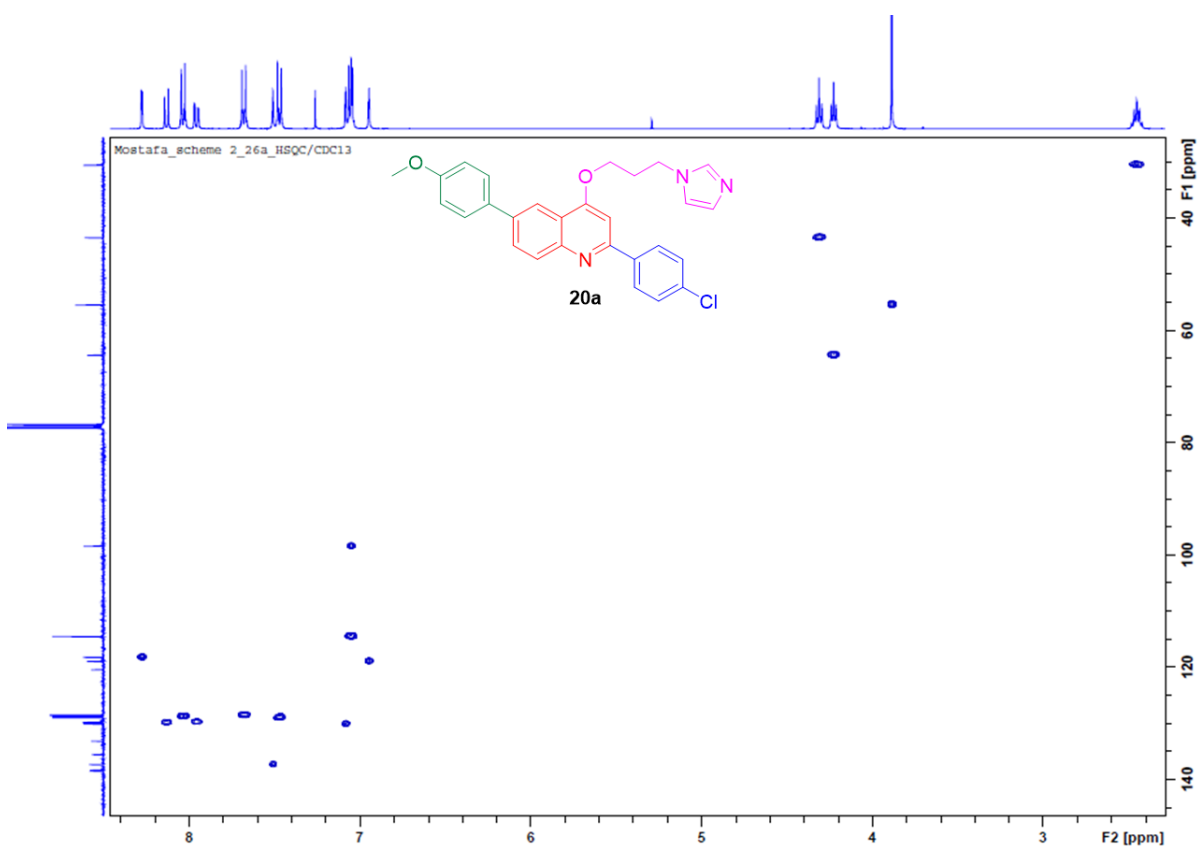
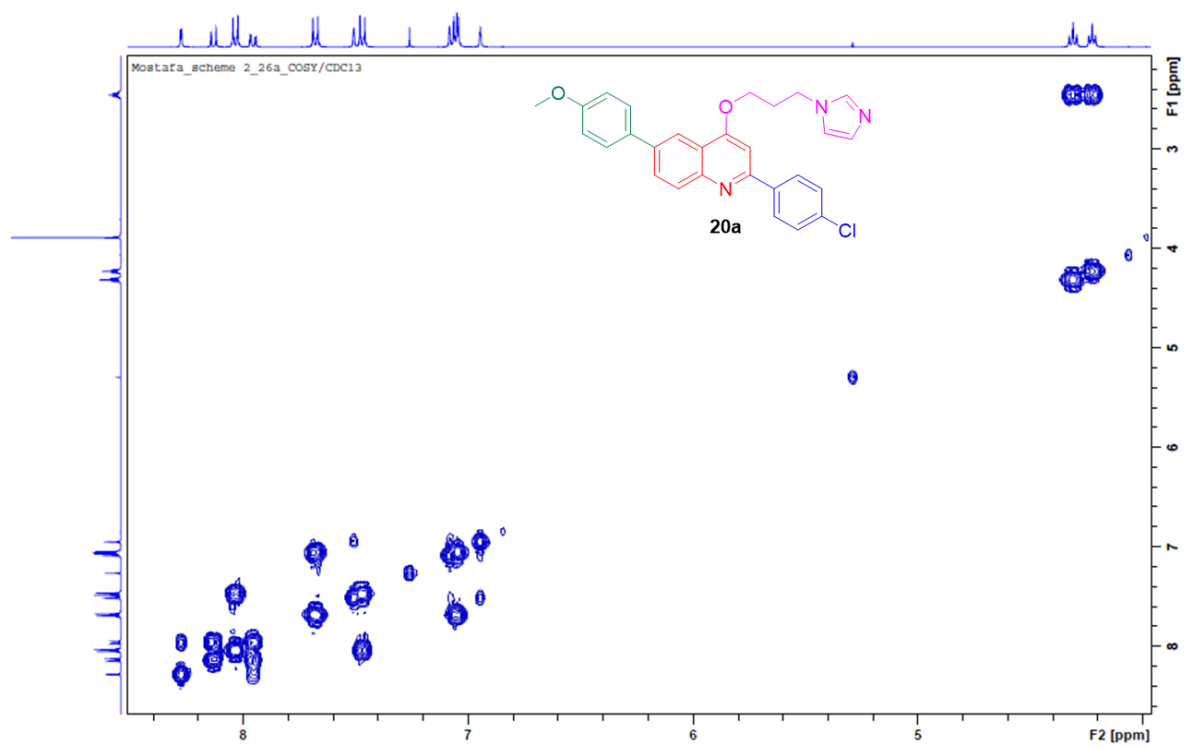


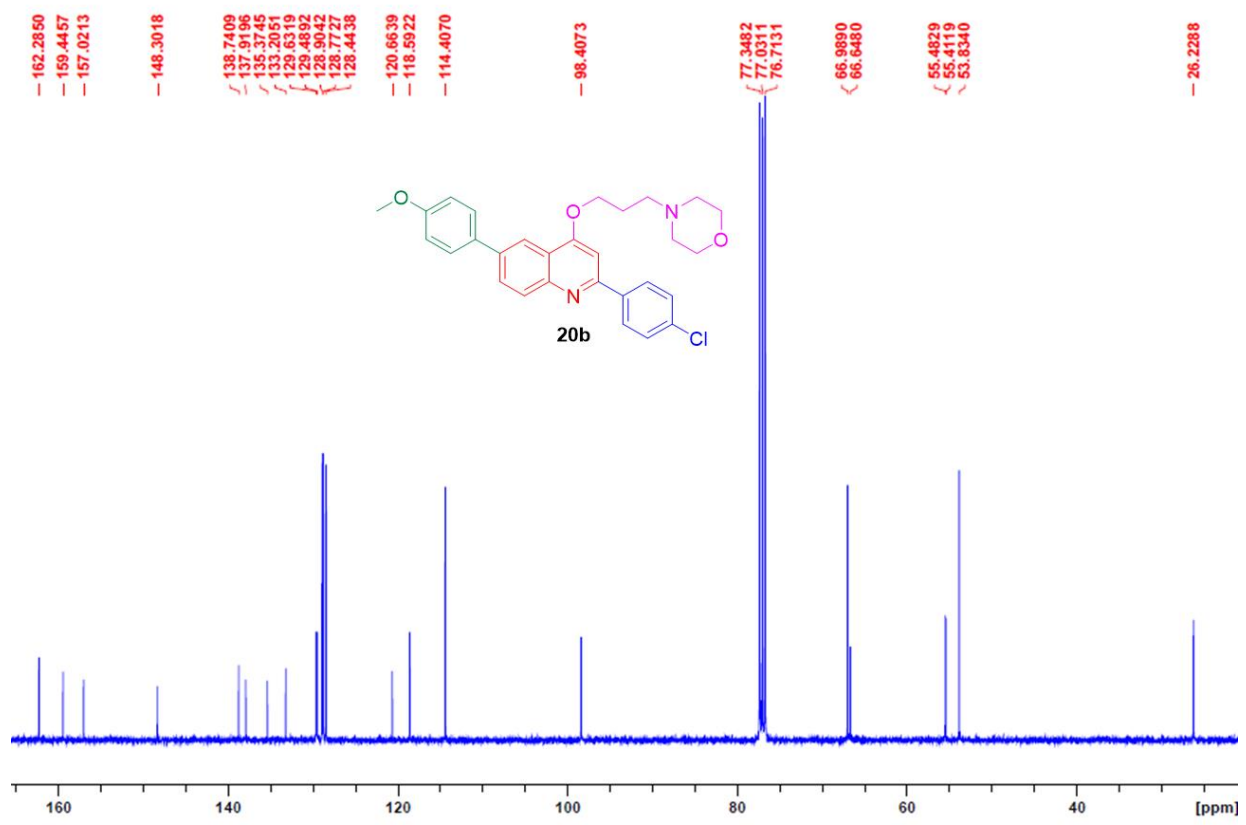
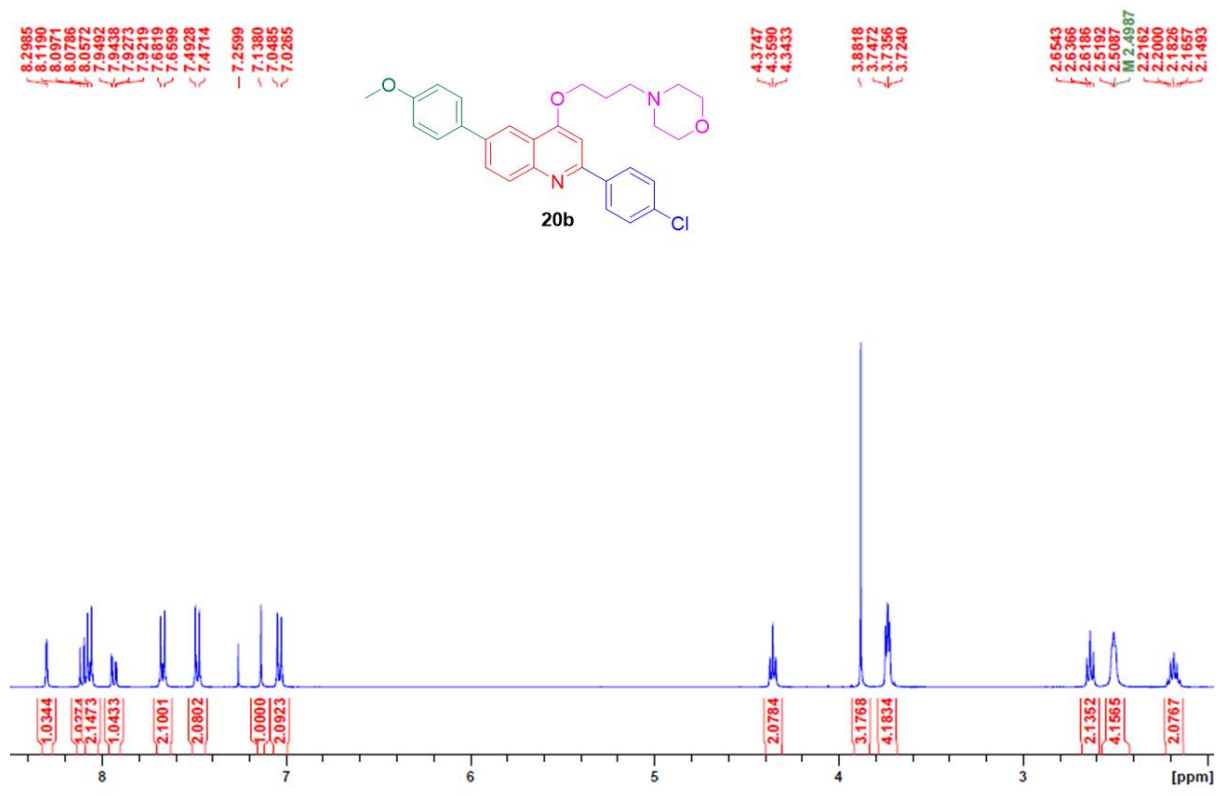


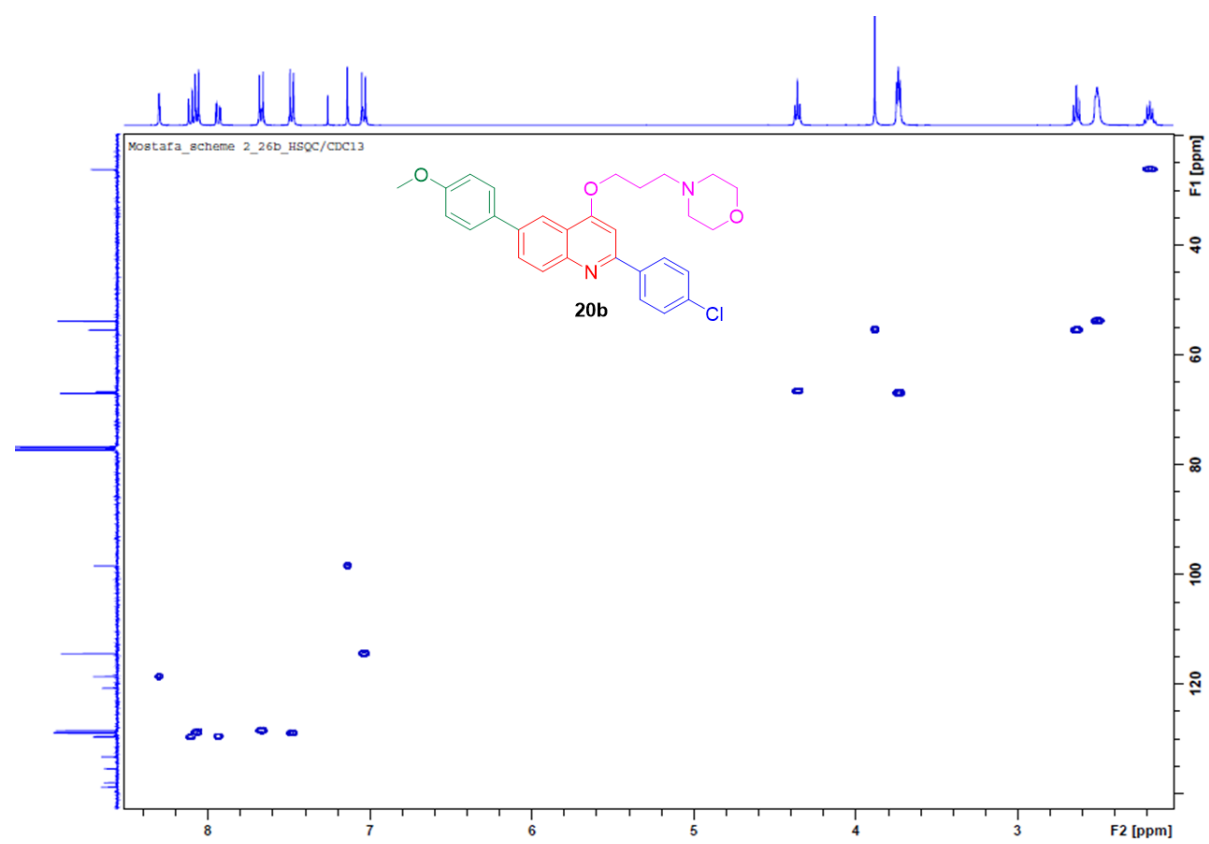
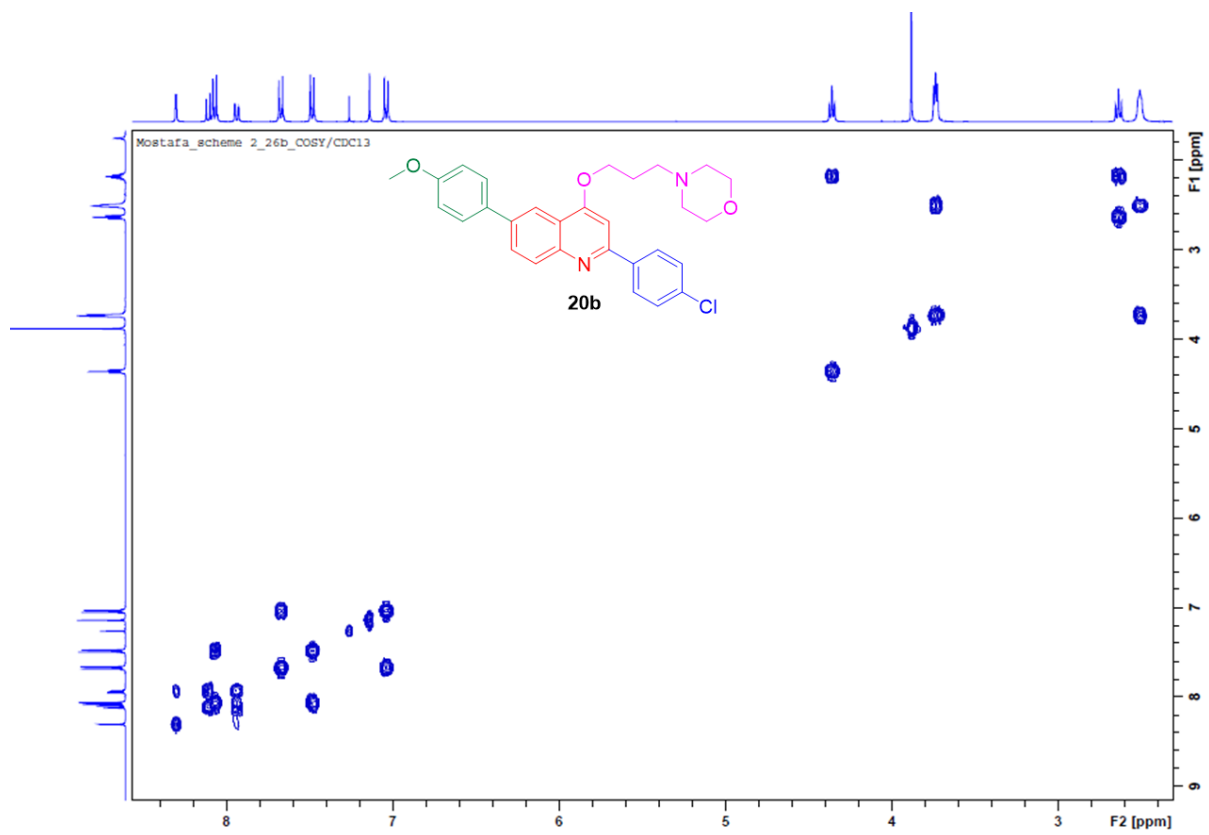


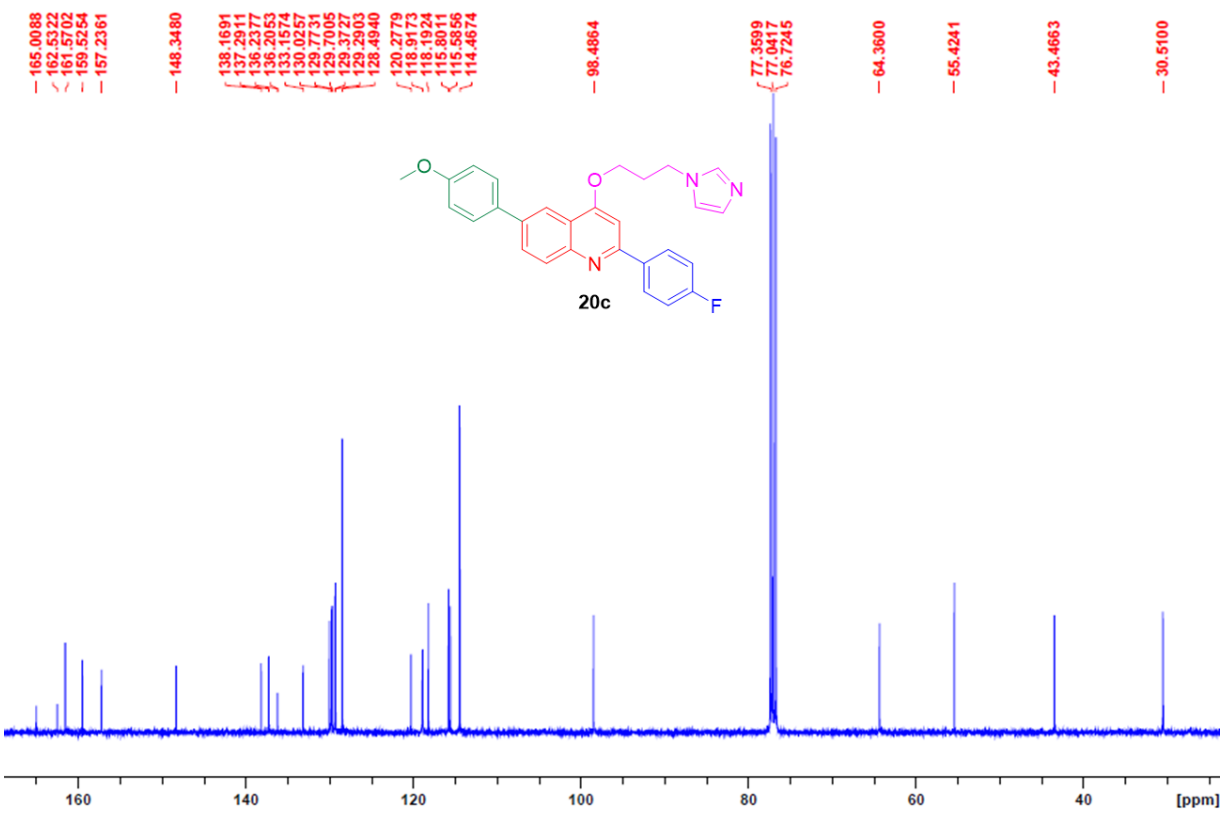
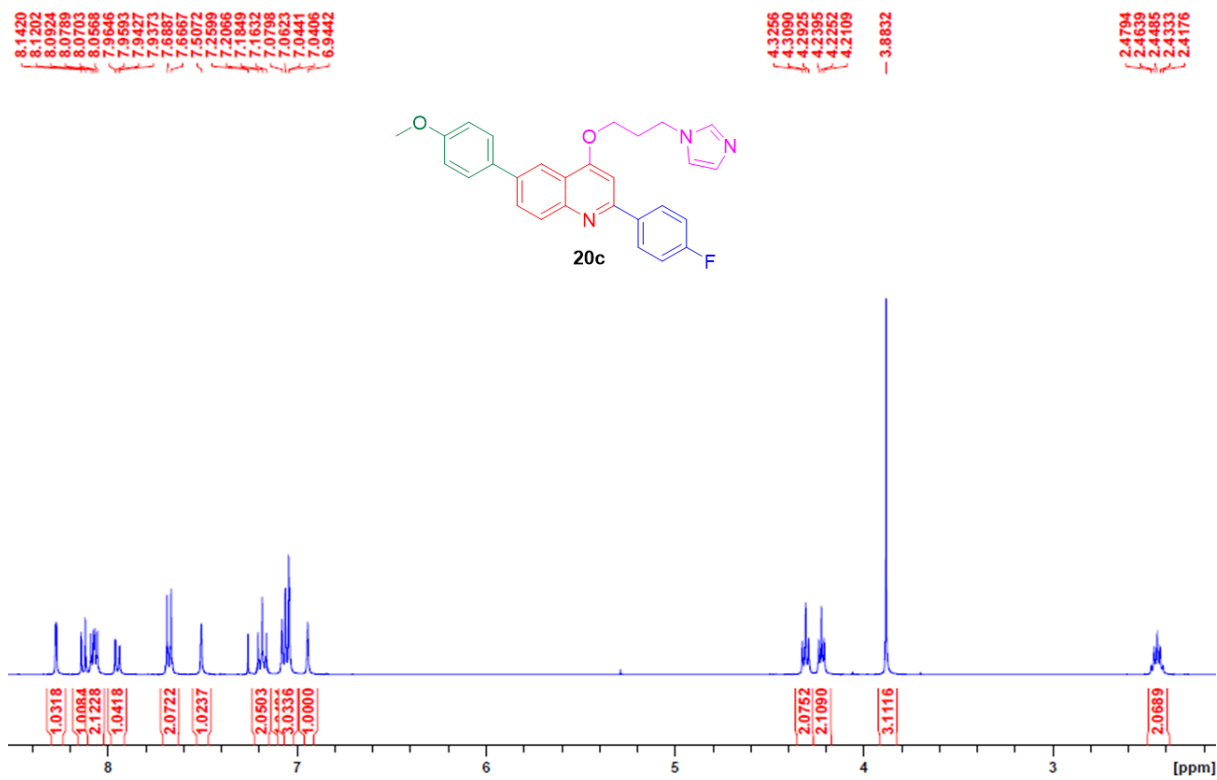






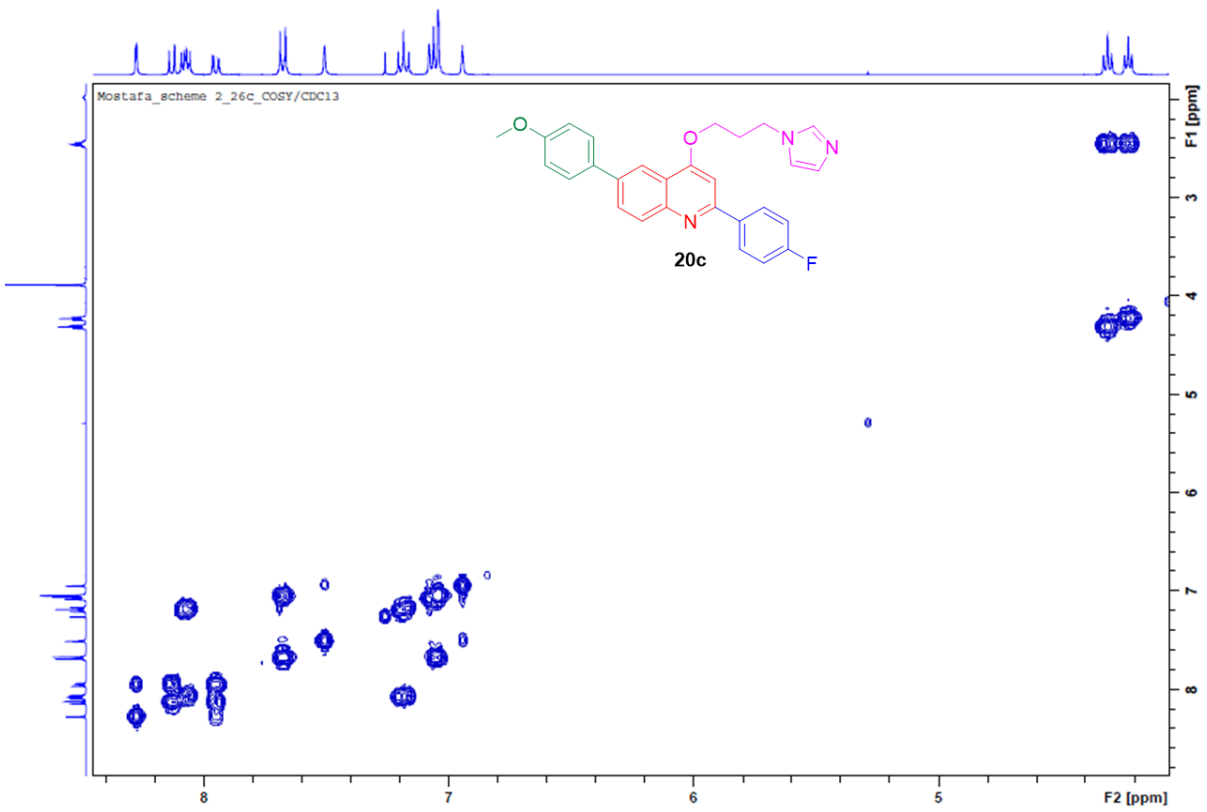
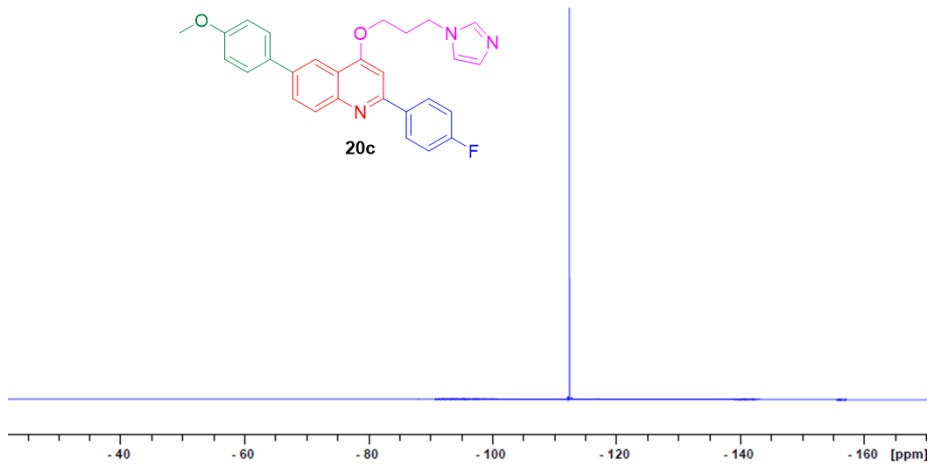


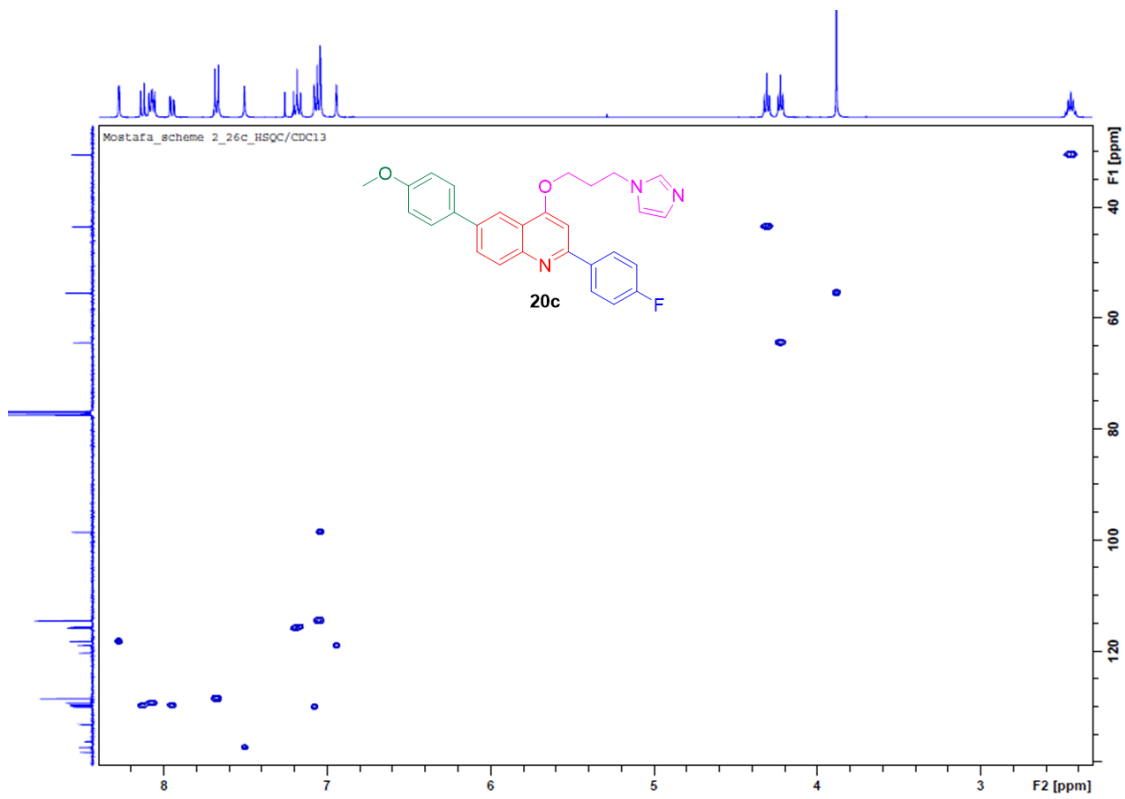




_19F/CDC13

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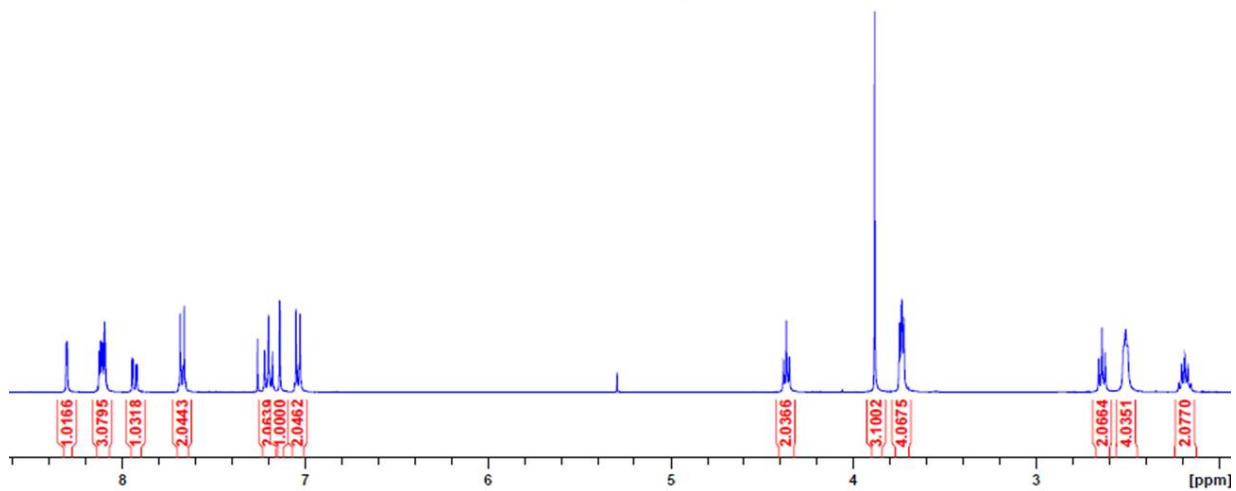
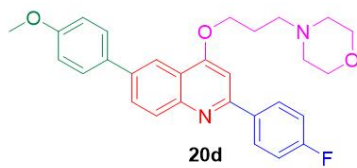


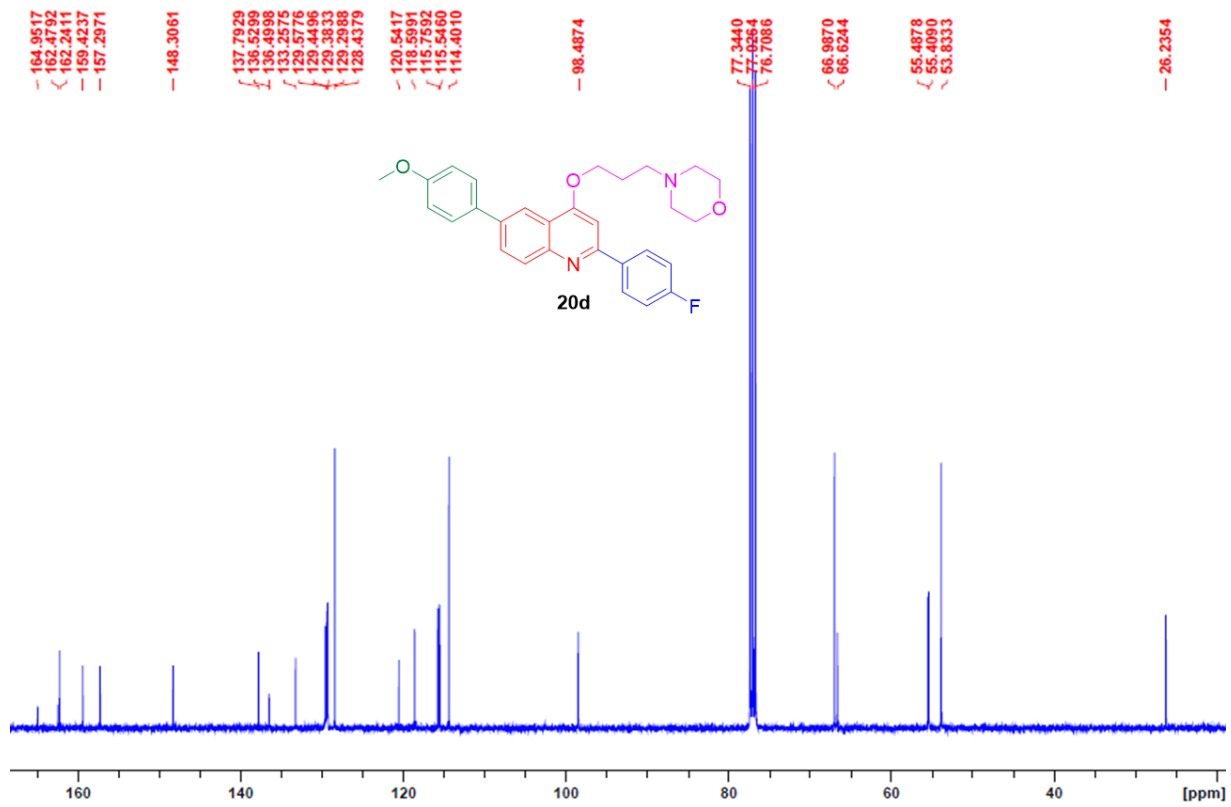


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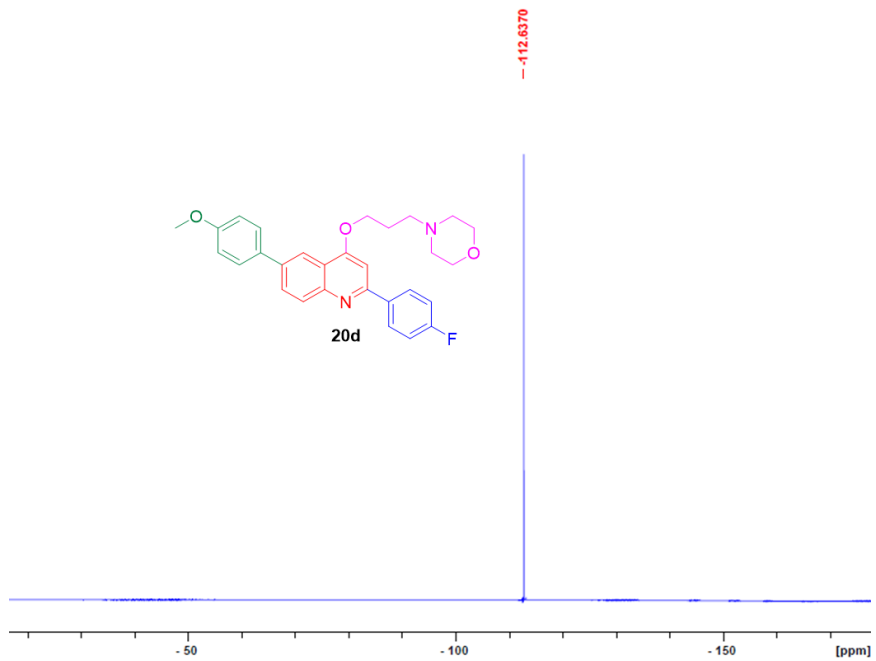
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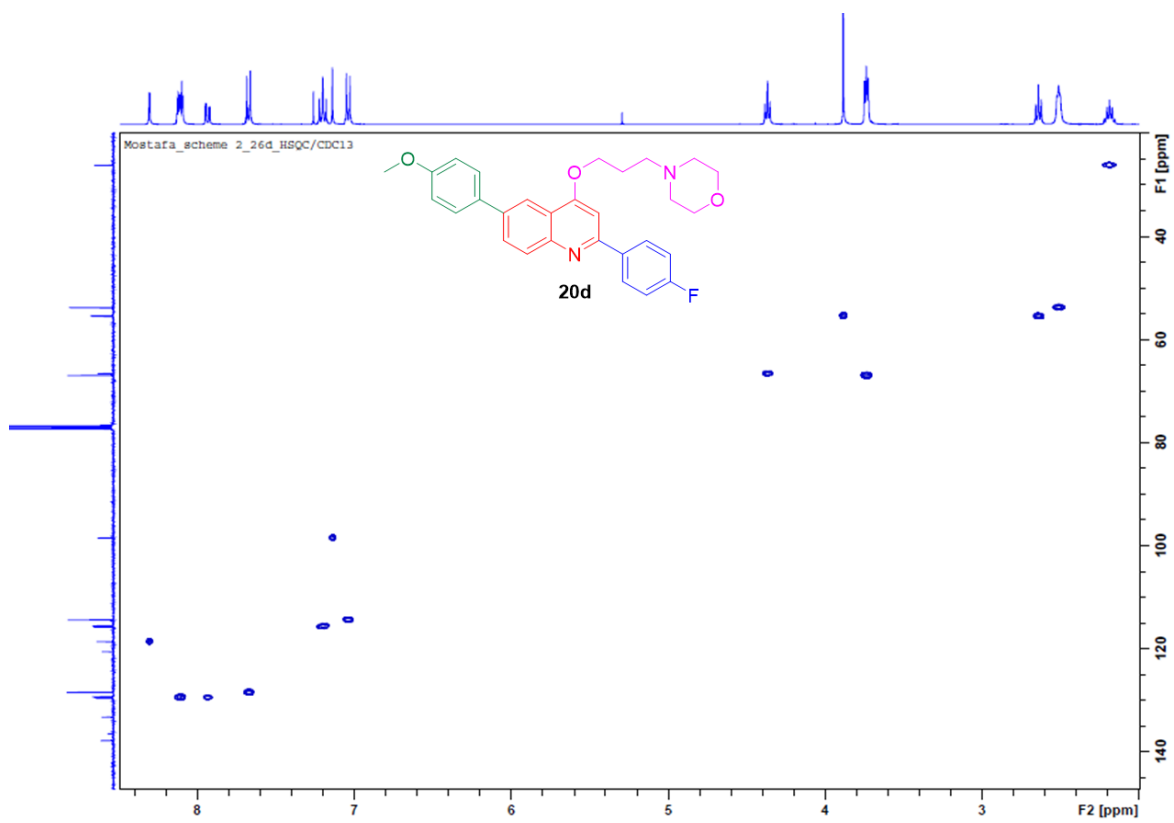
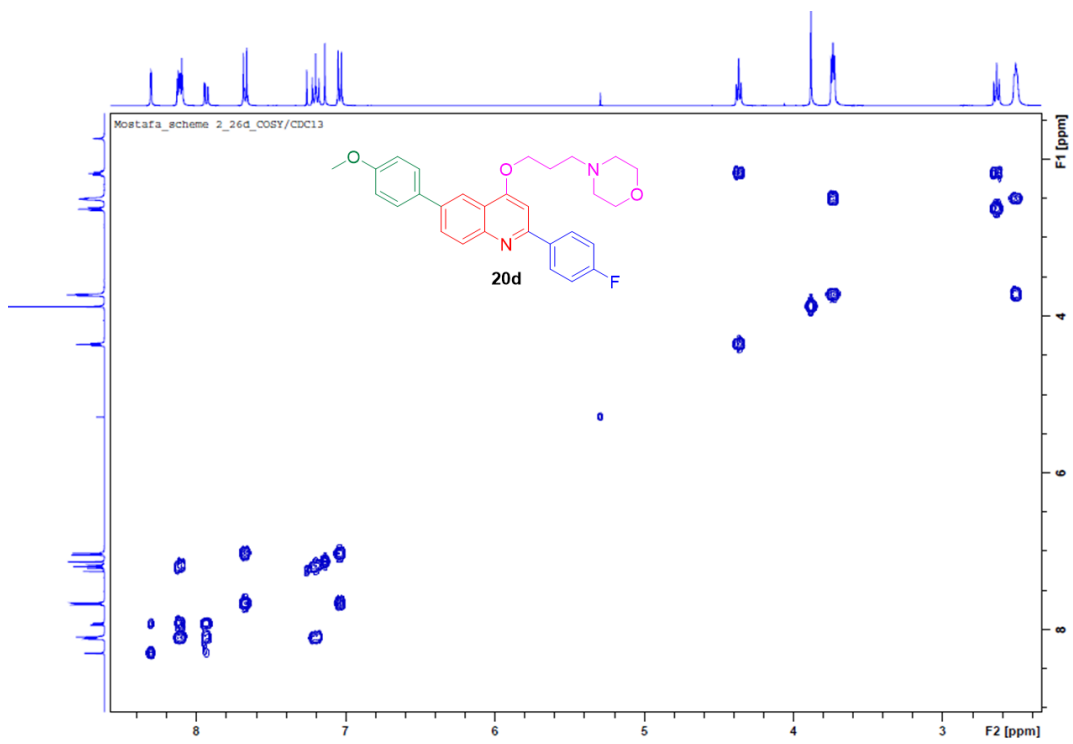
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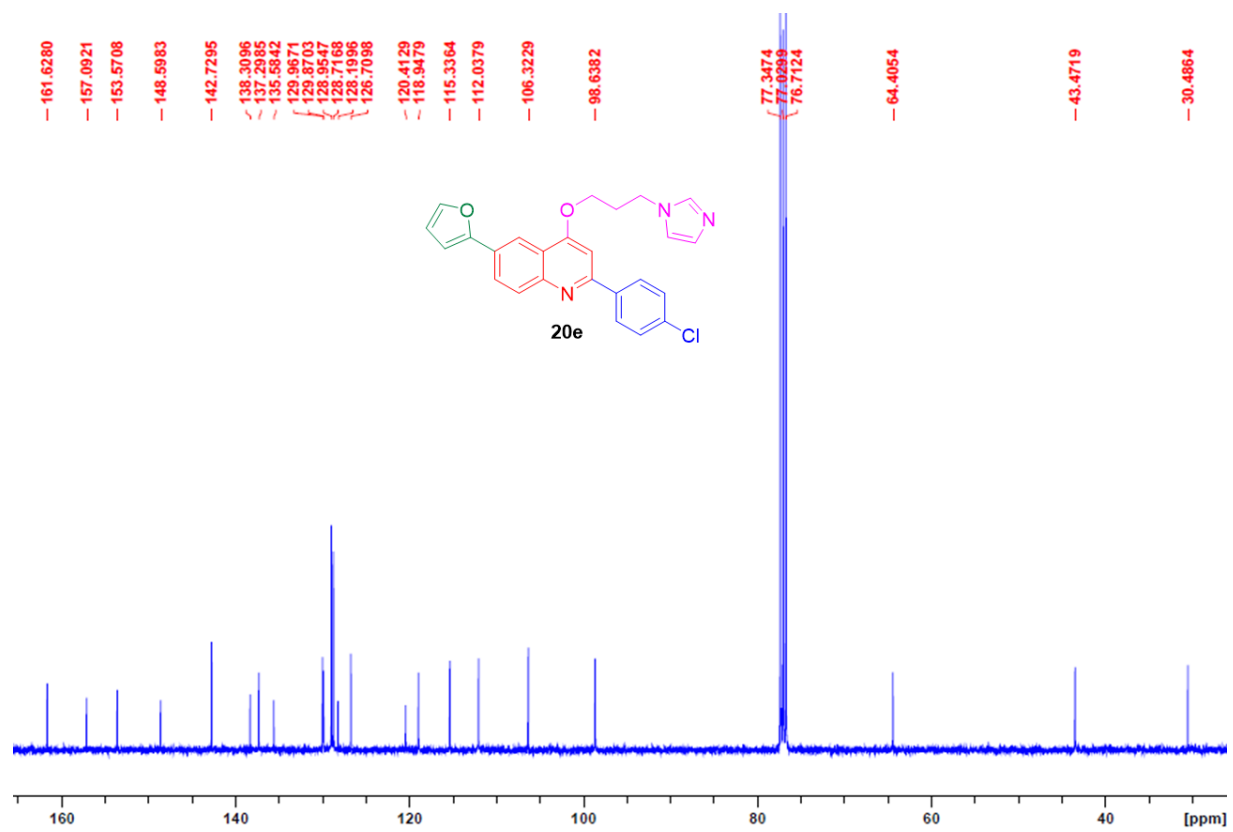
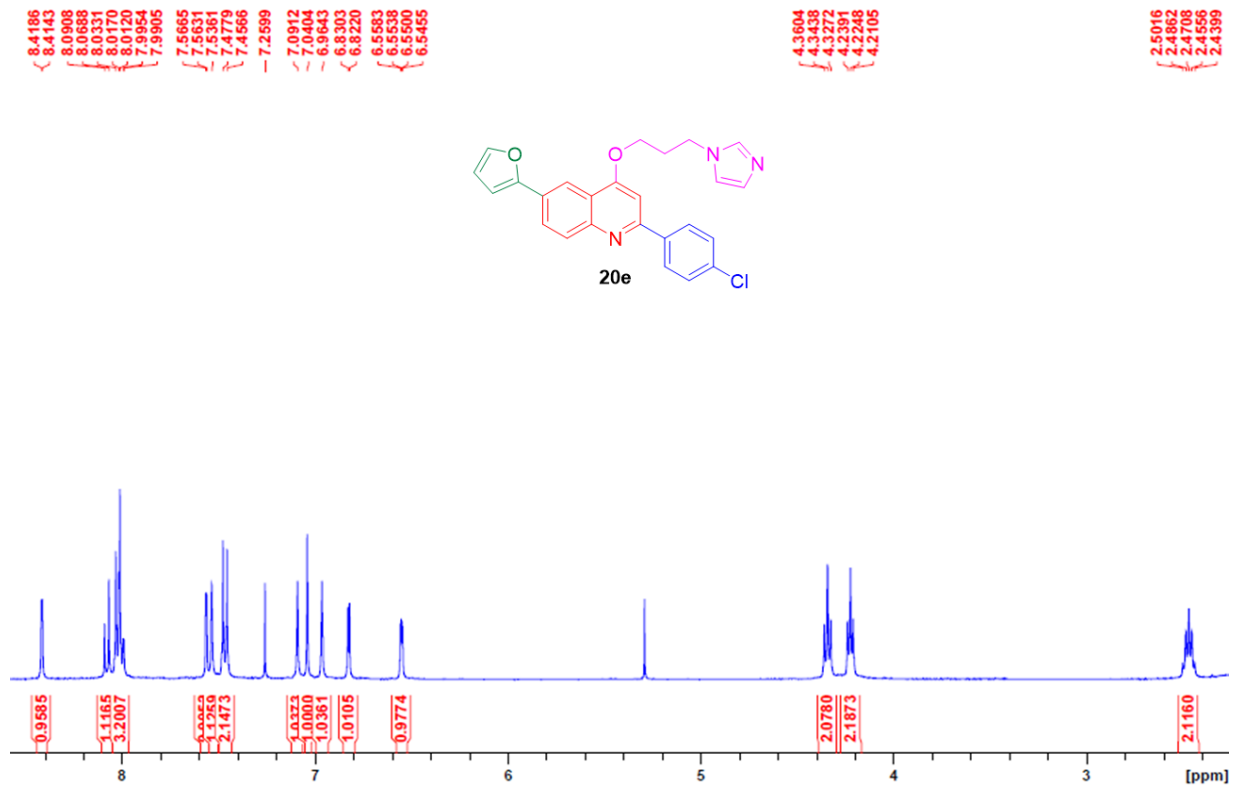


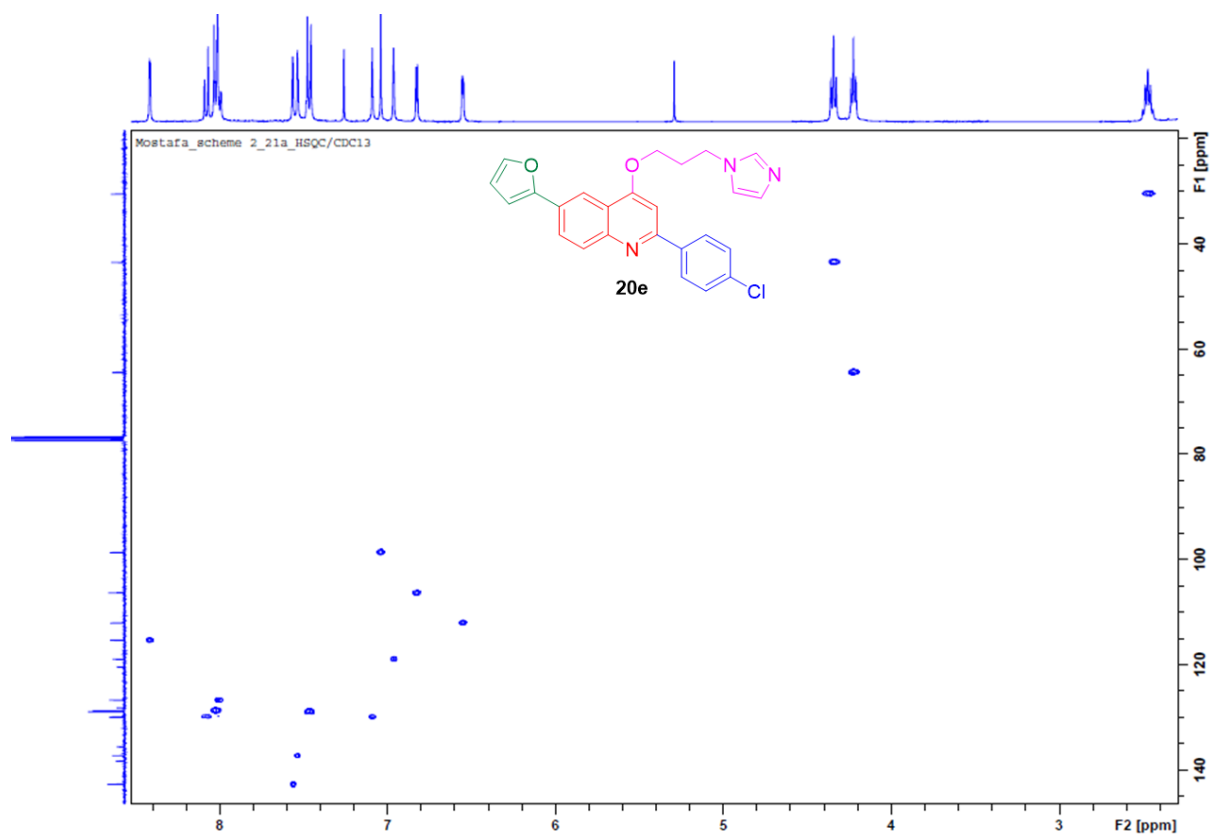
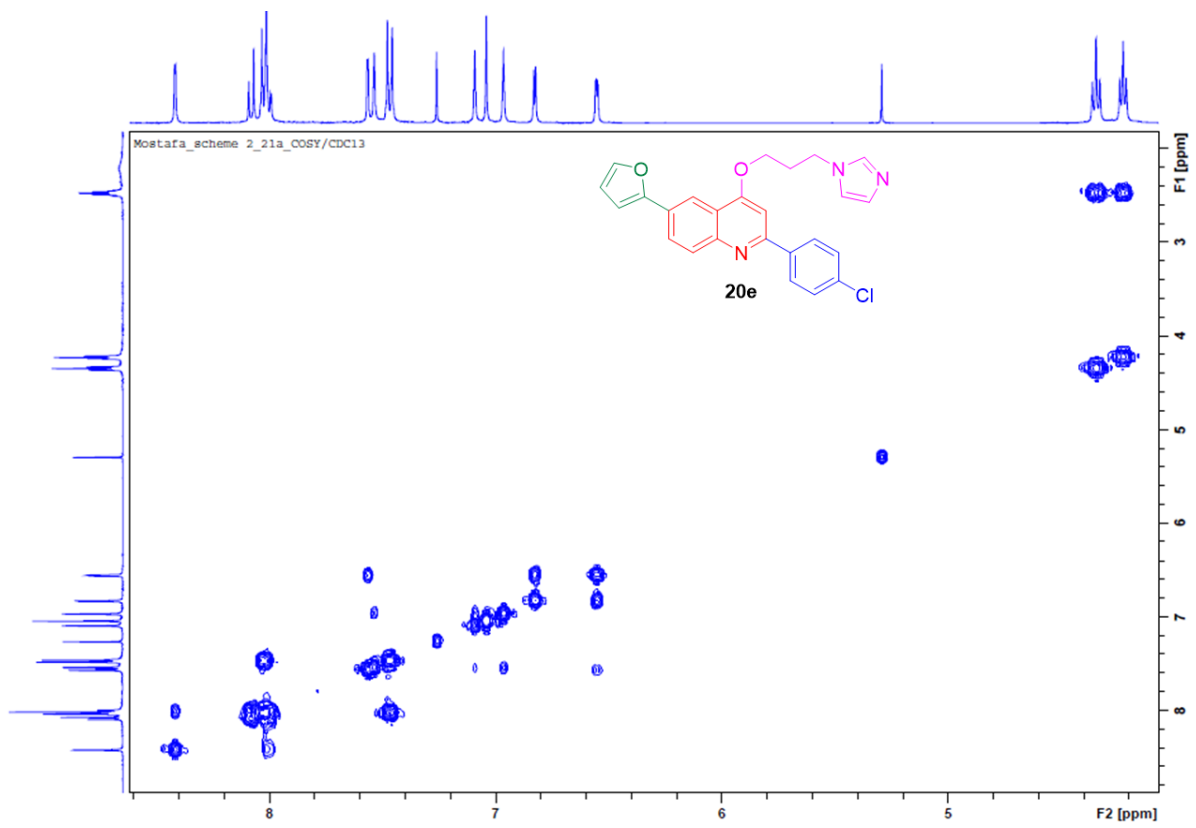


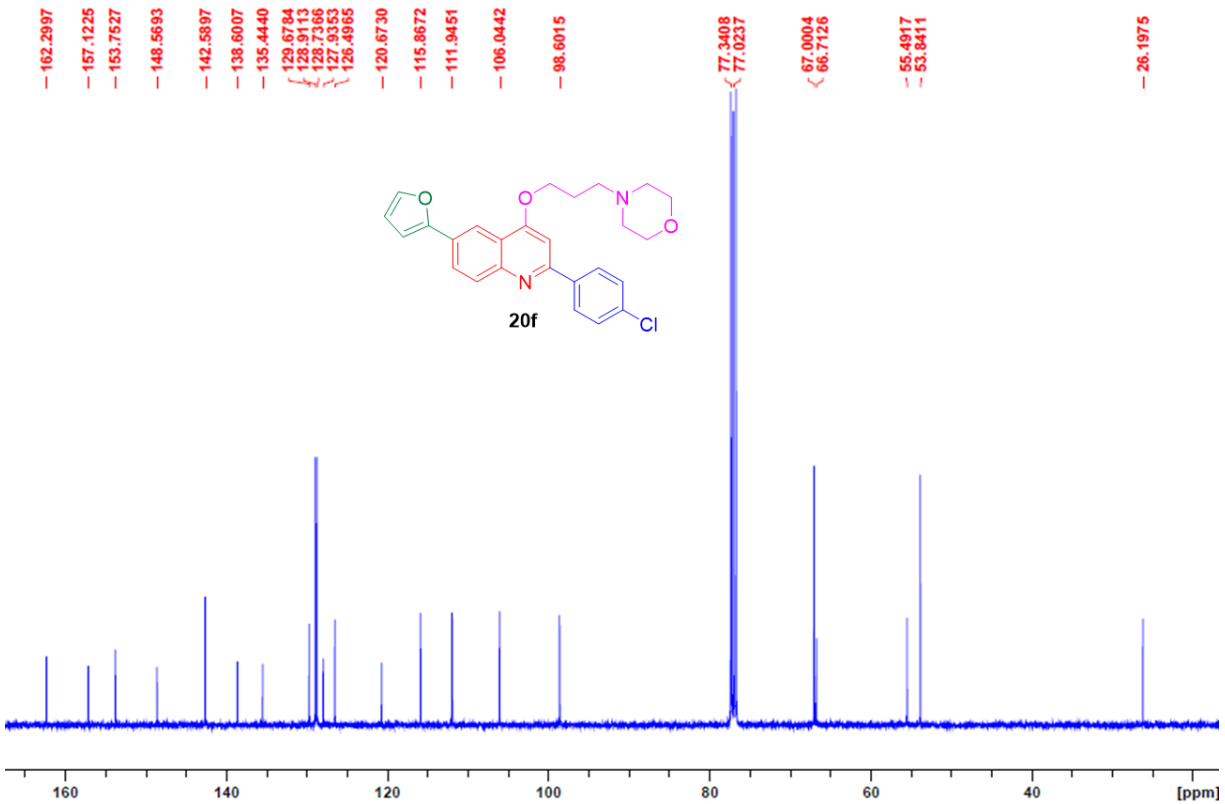
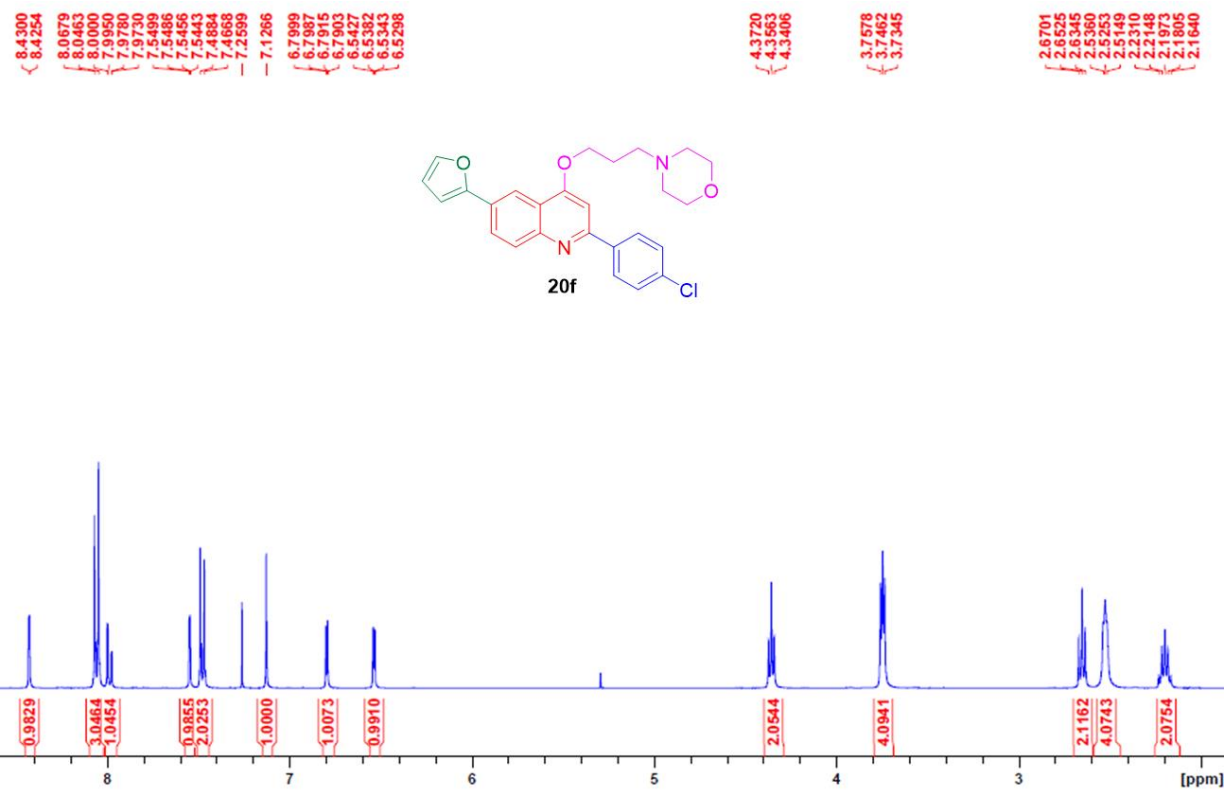
19F/CDCl₃



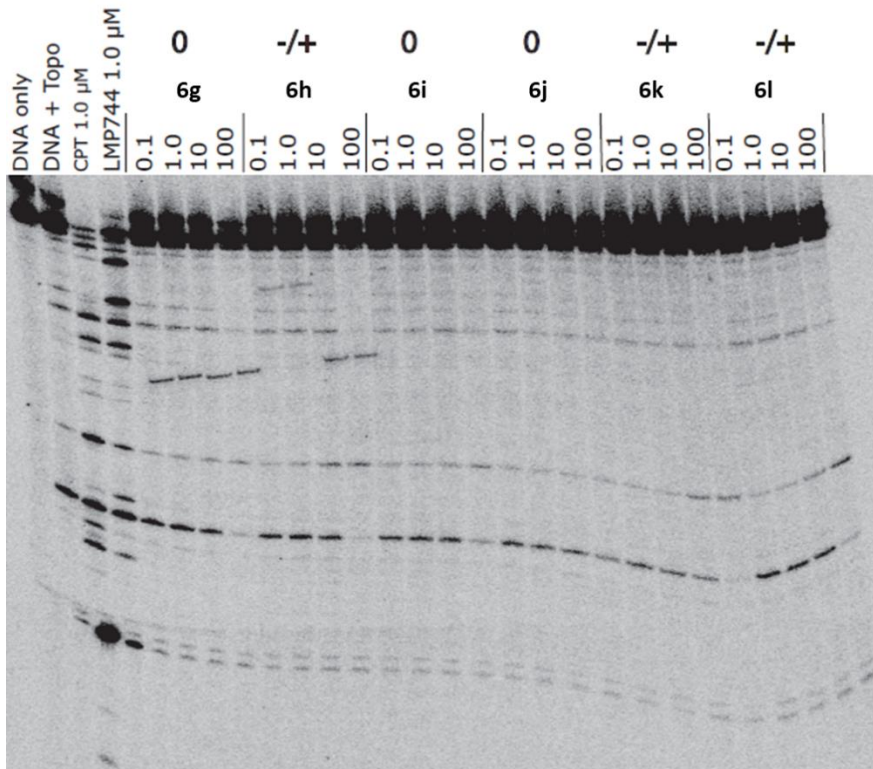
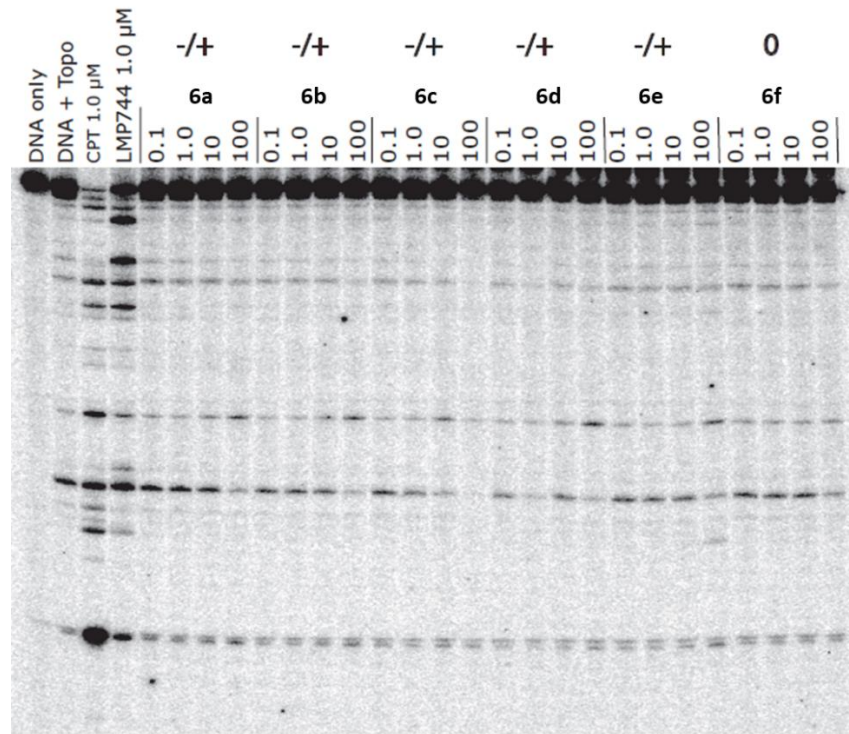


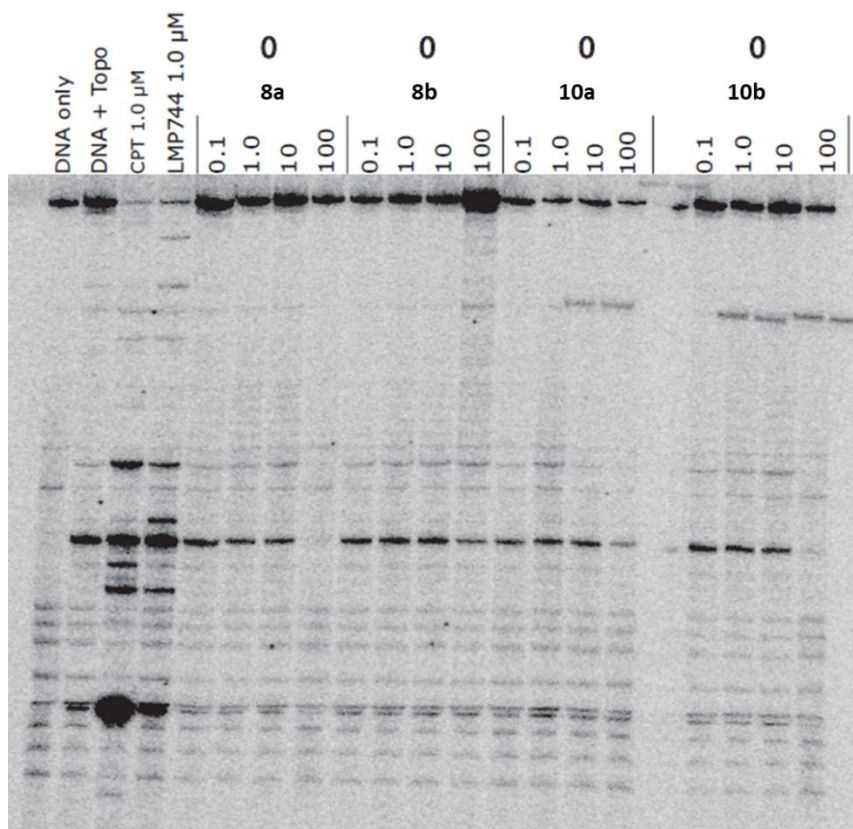
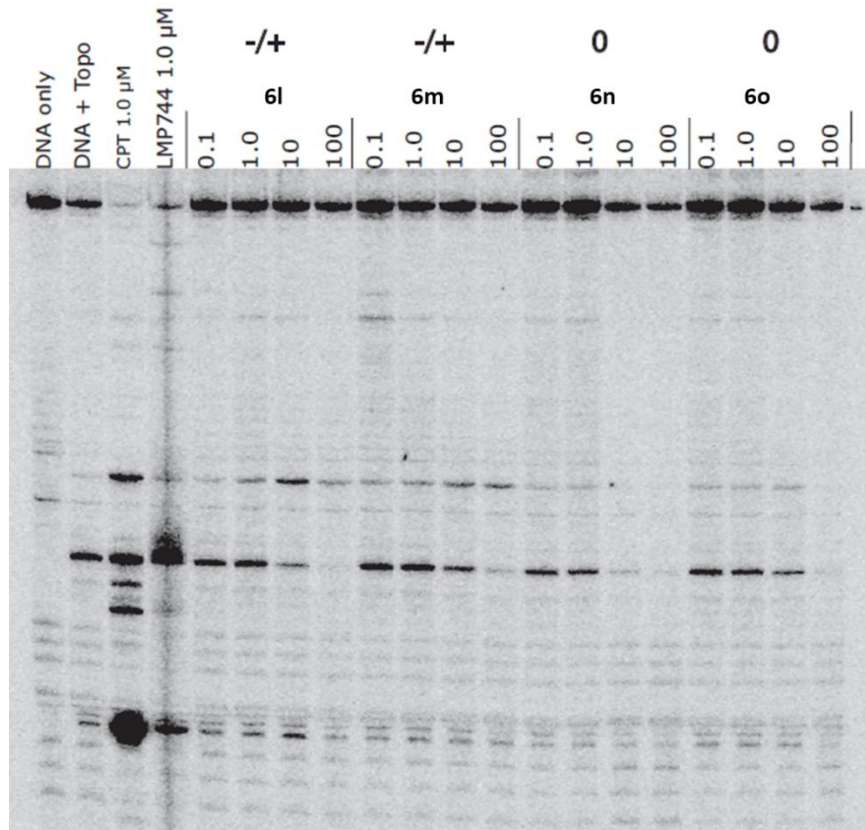


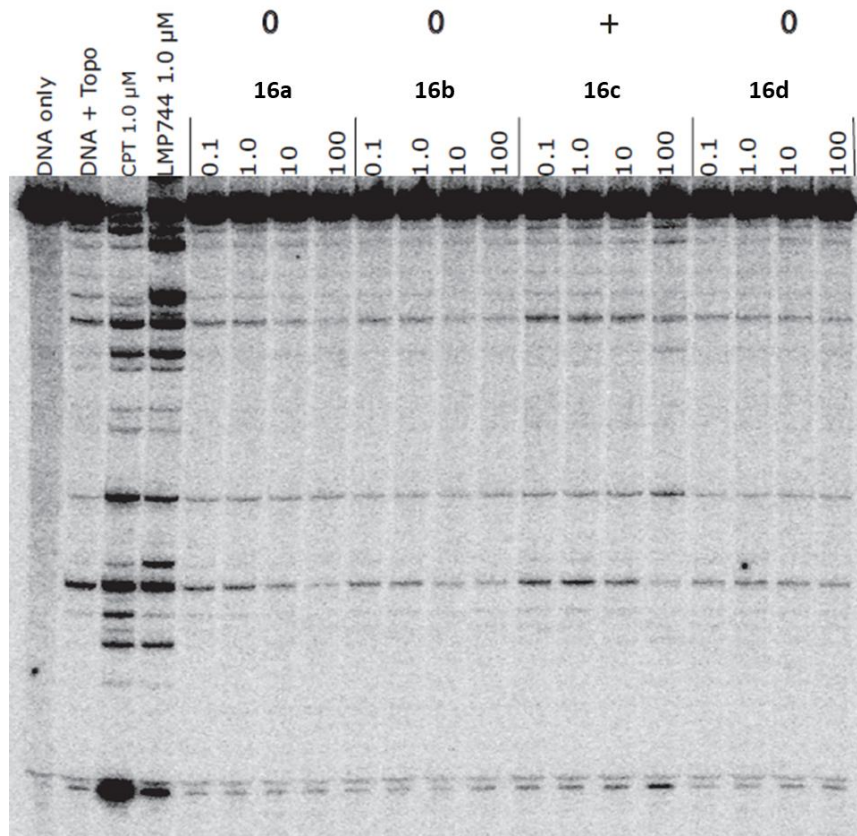
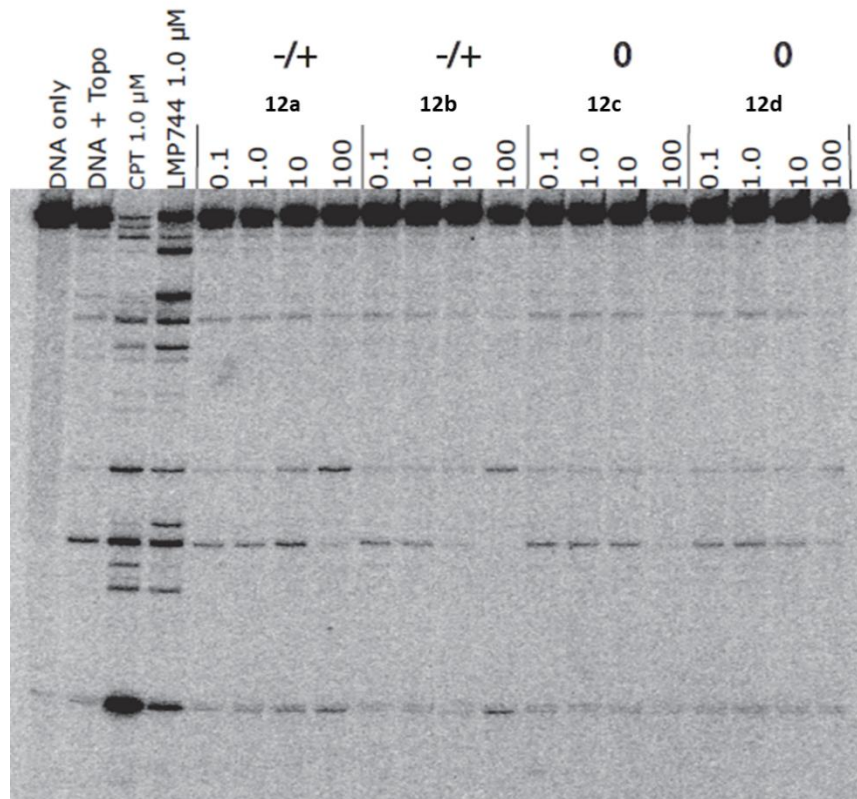




Topoisomerase I-mediated DNA cleavage assay







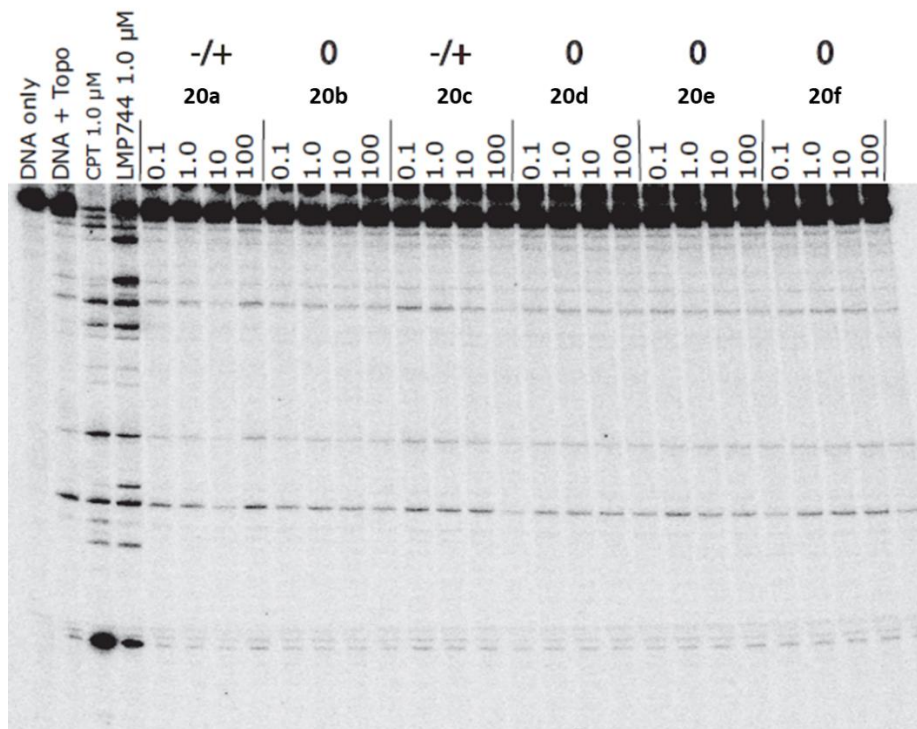


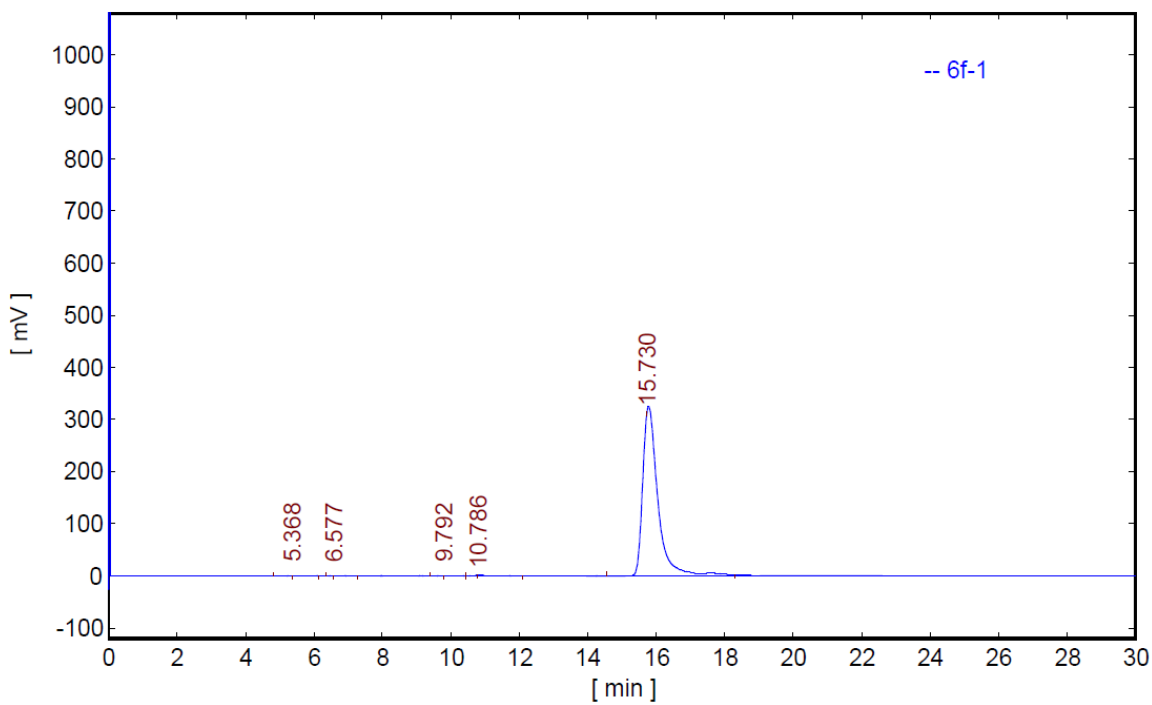
Figure S1. TOP1-mediated DNA cleavage induced by compounds **6a-o**, **8a,b**, **10a,b**, **12a-d**, **16a-d** and **20a-f**. From the left: lane 1, DNA only; lane 2, DNA + TOP1; lane 3, CPT (1 μ M); lane 4, LMP744 (1 μ M); lanes from 5, tested compounds at 0.1, 1, 10, 100 μ M.

Kinase profiling

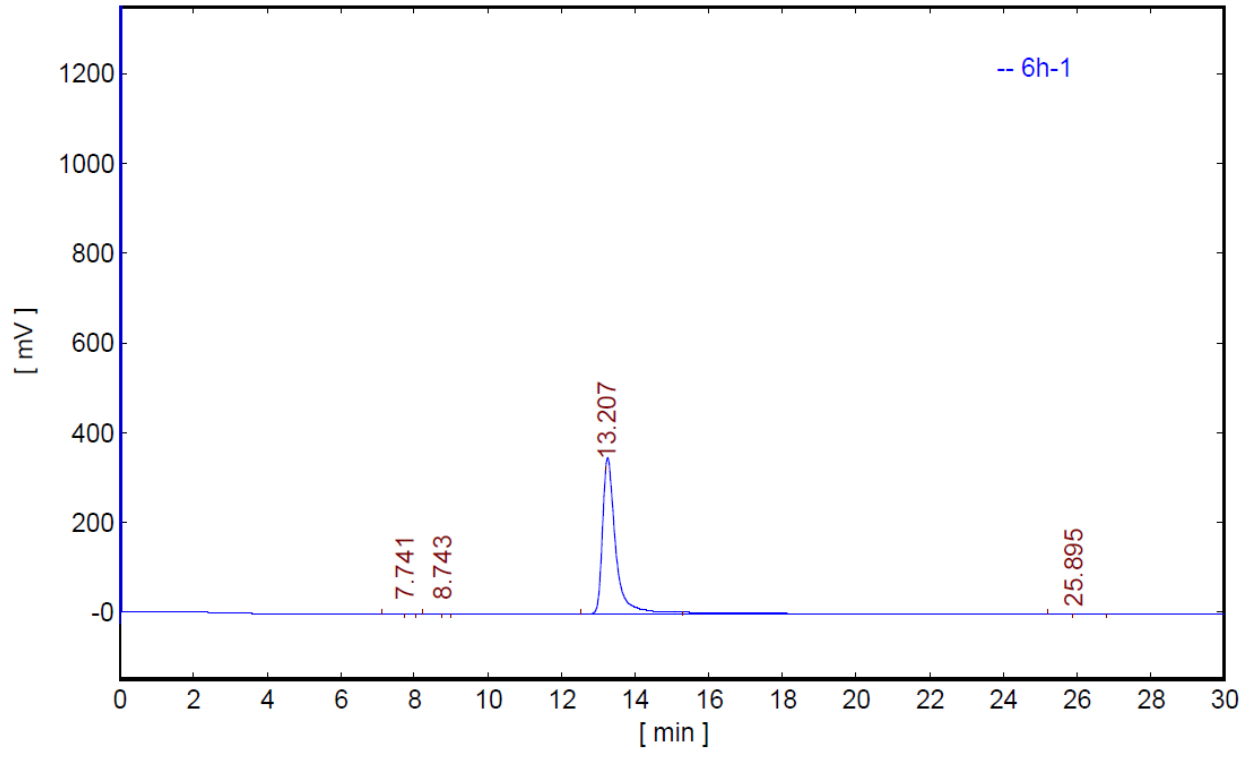
Table S1. IC₅₀ values of the target quinolines against different kinases.

Comp.	IC ₅₀ (nM)						
	FRK	IGF-1R	BTK	c- <i>Src</i>	VEGFR-1	VEGFR-2	HER-2
6a	825.45	1018.99	1585.09	783.22	95.30	268.29	1238.62
6b	9150.28	8062.93	8521.88	2497.77	3332.58	6740.59	123.00
6c	1559.15	2034.34	2250.63	1504.17	606.28	405.21	1380.30
6d	506.56	1592.03	1374.51	407.96	302.85	492.05	695.06
6e	8998.85	2163.20	4941.62	197.66	7329.54	3763.81	82.10
6f	5045.59	5345.29	8794.35	3940.04	1729.02	1940.12	638.82
6g	1279.54	1482.85	4756.76	2759.17	1109.74	997.07	454.75
6h	330.47	196.67	3477.02	3580.40	463.77	2454.98	1580.82
6i	1210.19	1711.01	7289.68	7013.46	800.64	8238.73	1380.98
6j	138.75	218.75	185.48	185.84	768.93	391.62	206.41
6k	3168.47	2395.70	2760.92	6448.99	5037.65	5959.68	1349.38
6l	743.12	1817.73	1608.41	1923.90	346.06	2397.87	756.48
6m	2763.16	2806.03	2458.95	980.12	864.57	2828.75	331.90
6n	2516.77	2808.17	819.15	82.69	555.65	1186.92	1391.69
6o	785.93	408.08	3828.83	3487.44	511.46	3618.59	1379.93
8a	845.56	1061.81	5597.33	4537.32	648.06	6367.57	989.01
8b	3921.86	3900.07	2916.17	7198.49	6959.50	8374.57	1068.67
10a	8910.00	197.92	4755.43	1025.83	4388.00	8547.43	1024.09
10b	4372.15	5742.42	2980.17	7775.37	8509.91	8683.43	597.68
12a	733.80	5366.45	195.55	55.26	1755.01	48.29	34.77
12b	1133.79	7156.88	213.36	42.30	5986.46	26.97	27.31
12c	4877.54	8995.21	99.53	118.70	7718.25	56.89	168.65
12d	6534.31	452.80	653.35	1452.31	2536.64	854.67	897.05
16a	6147.60	5232.65	4804.88	1347.51	1963.43	3408.44	2016.89
16b	3129.15	3491.20	2884.60	1324.72	1266.97	3231.53	2313.75
16c	6668.22	6690.88	5624.98	1733.09	2556.44	5095.37	1610.40
16d	1732.93	2229.33	2097.21	3897.24	1768.49	4692.09	357.58
20a	2616.37	2859.51	8668.64	2903.25	1351.78	1251.85	1012.65
20b	8713.05	8905.71	8976.83	4212.78	4737.61	2301.72	1650.64
20c	1436.19	1882.31	8667.93	9054.63	1751.70	8969.80	1231.21
20d	133.32	41.23	1776.06	250.84	711.77	294.23	1768.17
20e	216.42	3014.15	271.20	137.68	720.44	242.54	98.78
20f	631.98	3528.39	23.47	92.14	870.40	89.35	250.64
TAE226	321.76	125.79	133.94	864.05	224.58	246.37	390.08

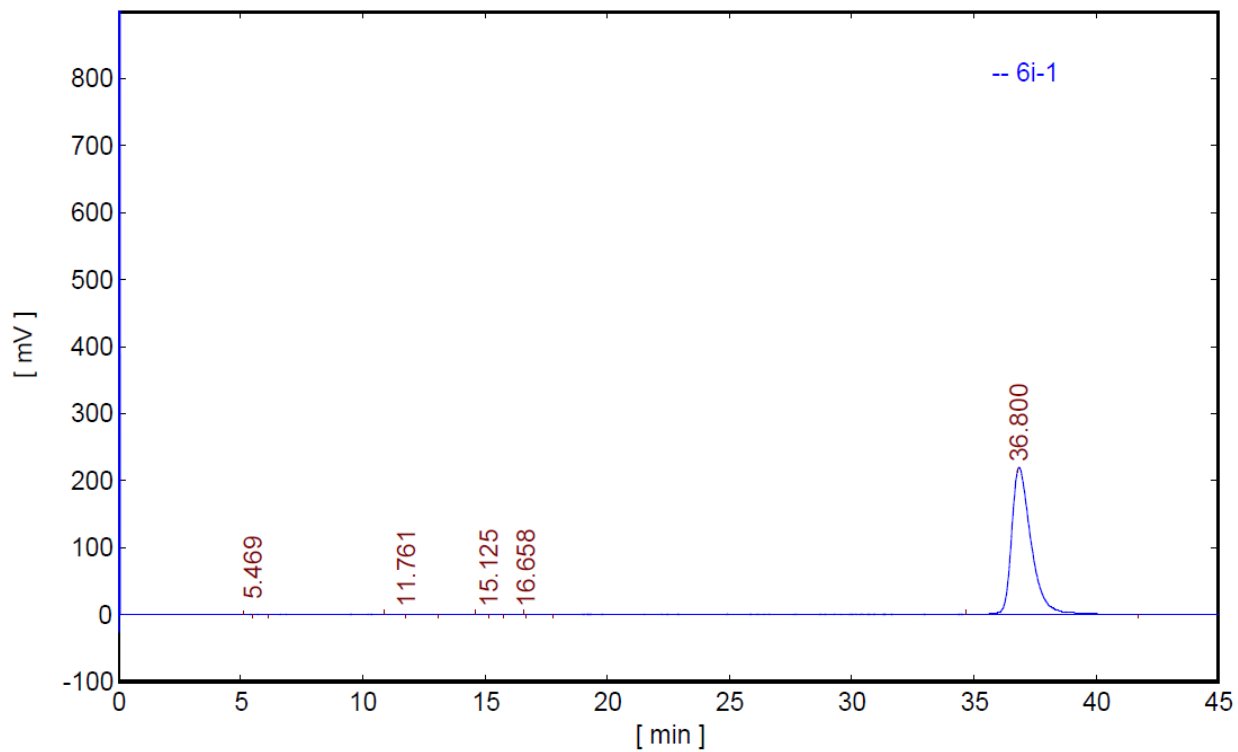
Representative HPLC traces



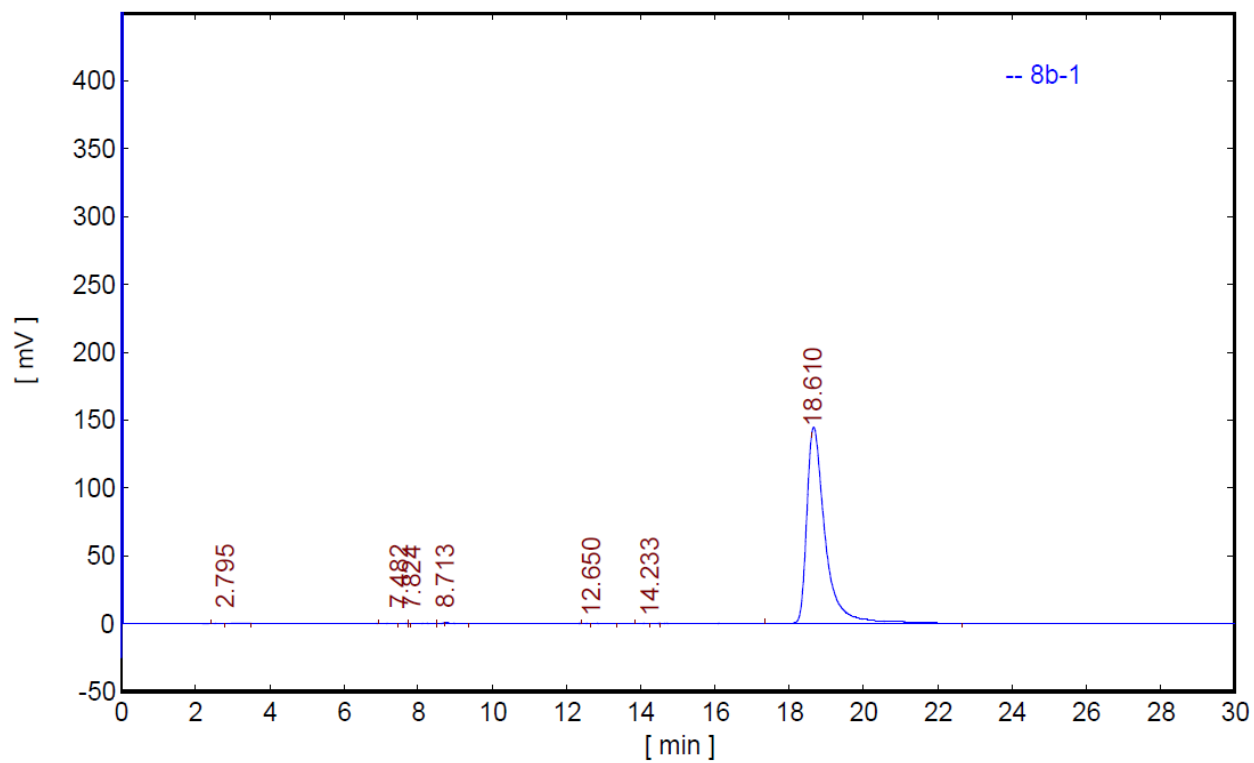
No.	Time	Area	Hight	% Conc.
1	5.36830	17078.85	669.71	0.17
2	6.57709	17783.21	791.42	0.18
3	9.79209	23857.56	1010.08	0.24
4	10.7856	49604.19	1990.82	0.49
5	15.7298	0025772.2	326459.65	98.93



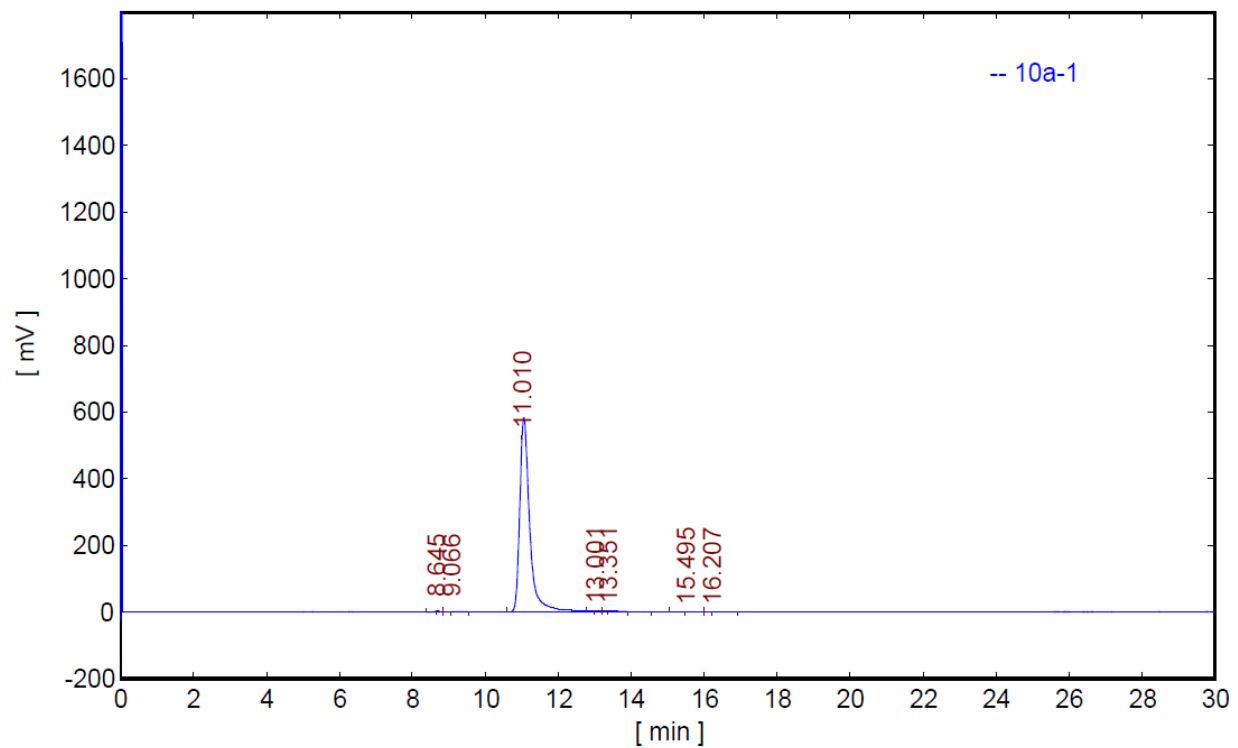
No.	Time	Area	Hight	% Conc.
1	7.74127	5586.25	154.61	0.07
2	8.74340	5377.98	254.05	0.06
3	13.2067	8523139.41	347128.01	99.75
4	25.8947	10550.28	238.14	0.12



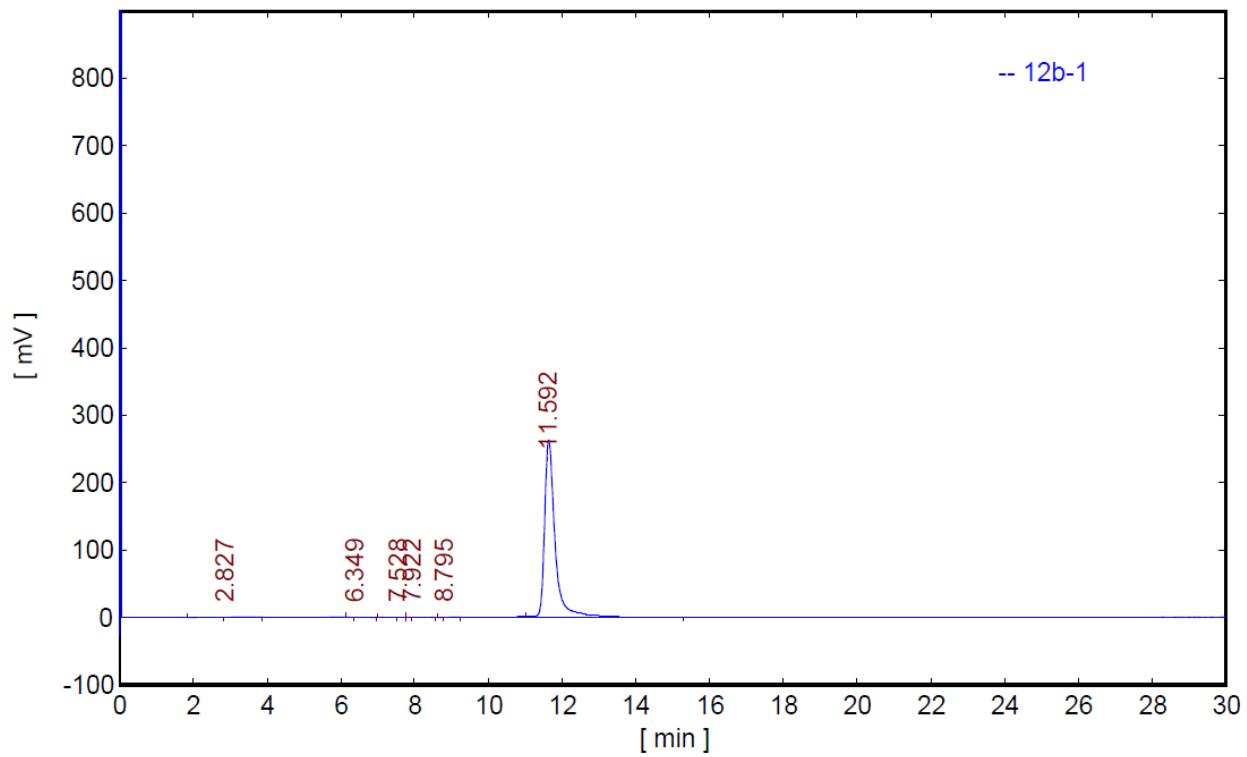
No.	Time	Area	Hight	% Conc.
1	5.46920	5196.88	200.89	0.04
2	11.7606	22951.78	390.46	0.19
3	15.1251	10567.63	460.29	0.09
4	16.6583	5907.20	45.29	0.05
5	36.8001	12063367.6	219255.17	99.63



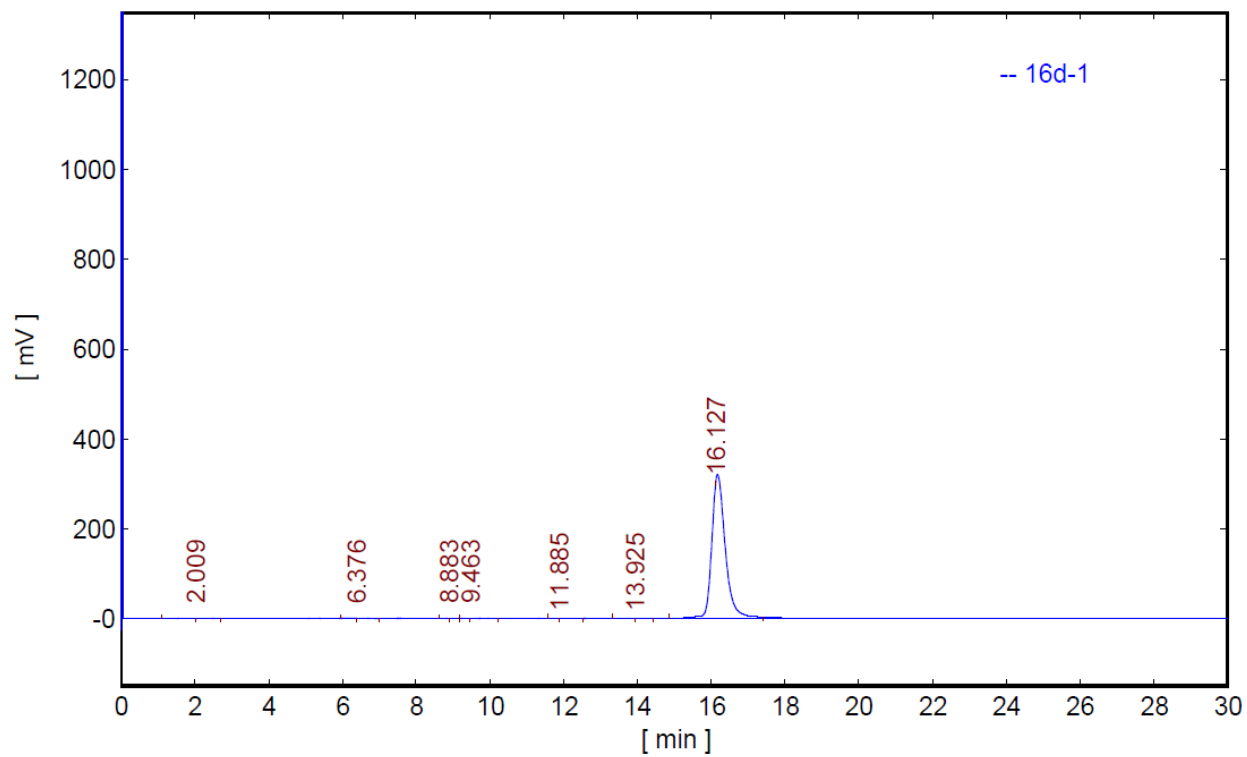
No.	Time	Area	Hight	% Conc.
1	2.79482	5410.71	229.53	0.11
2	7.48237	10709.48	369.94	0.22
3	7.82366	6247.08	151.18	0.13
4	8.71322	12992.29	1050.26	0.26
5	12.6497	9180.99	340.63	0.18
6	14.2325	7281.03	289.16	0.15
7	18.6099	4921757.34	144978.32	98.96



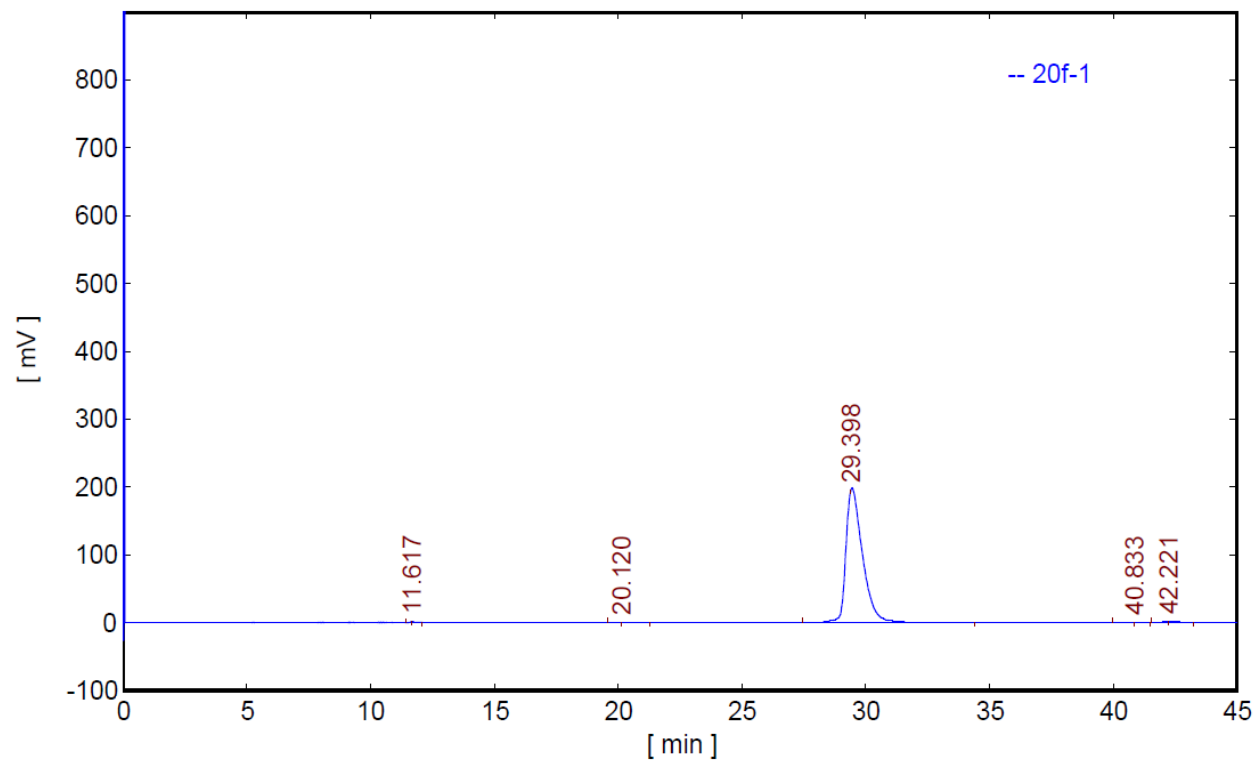
No.	Time	Area	Hight	% Conc.
1	8.64536	30346.51	3974.23	0.27
2	9.06580	17570.42	1073.60	0.16
3	11.0103	11136381.7	591386.75	98.63
4	13.0008	12307.09	743.23	0.11
5	13.3508	33758.24	1563.75	0.30
6	15.4949	43342.38	1189.39	0.38
7	16.2072	17803.62	686.46	0.16



No.	Time	Area	Hight	% Conc.
1	2.82687	15783.72	275.01	0.30
2	6.34896	14799.62	380.91	0.28
3	7.52754	9120.26	322.91	0.17
4	7.92236	9995.42	217.15	0.19
5	8.79526	5692.54	443.95	0.11
6	11.5919	5177474.76	266303.41	98.94



No.	Time	Area	Hight	% Conc.
1	2.00876	16147.84	382.58	0.20
2	6.37583	13388.29	433.04	0.16
3	8.88264	7523.51	480.73	0.09
4	9.46339	8706.04	267.45	0.11
5	11.8850	12436.89	503.58	0.15
6	13.9251	11058.41	345.71	0.14
7	16.1265	8114469.22	322679.85	99.15



No.	Time	Area	Hight	% Conc.
1	11.6165	19836.34	1648.32	0.21
2	20.1197	15111.46	331.22	0.16
3	29.3984	9177196.25	198282.67	98.79
4	40.8329	17747.66	456.74	0.19
5	42.2212	59459.82	1529.21	0.64