

Supporting Information

Total Synthesis and Antimalarial Activity of 2-(p-Hydroxybenzyl)-prodigiosins, Isoheptylprodigiosin and Geometric Isomers of Tambjamine MYP1, Isolated from Marine Bacteria

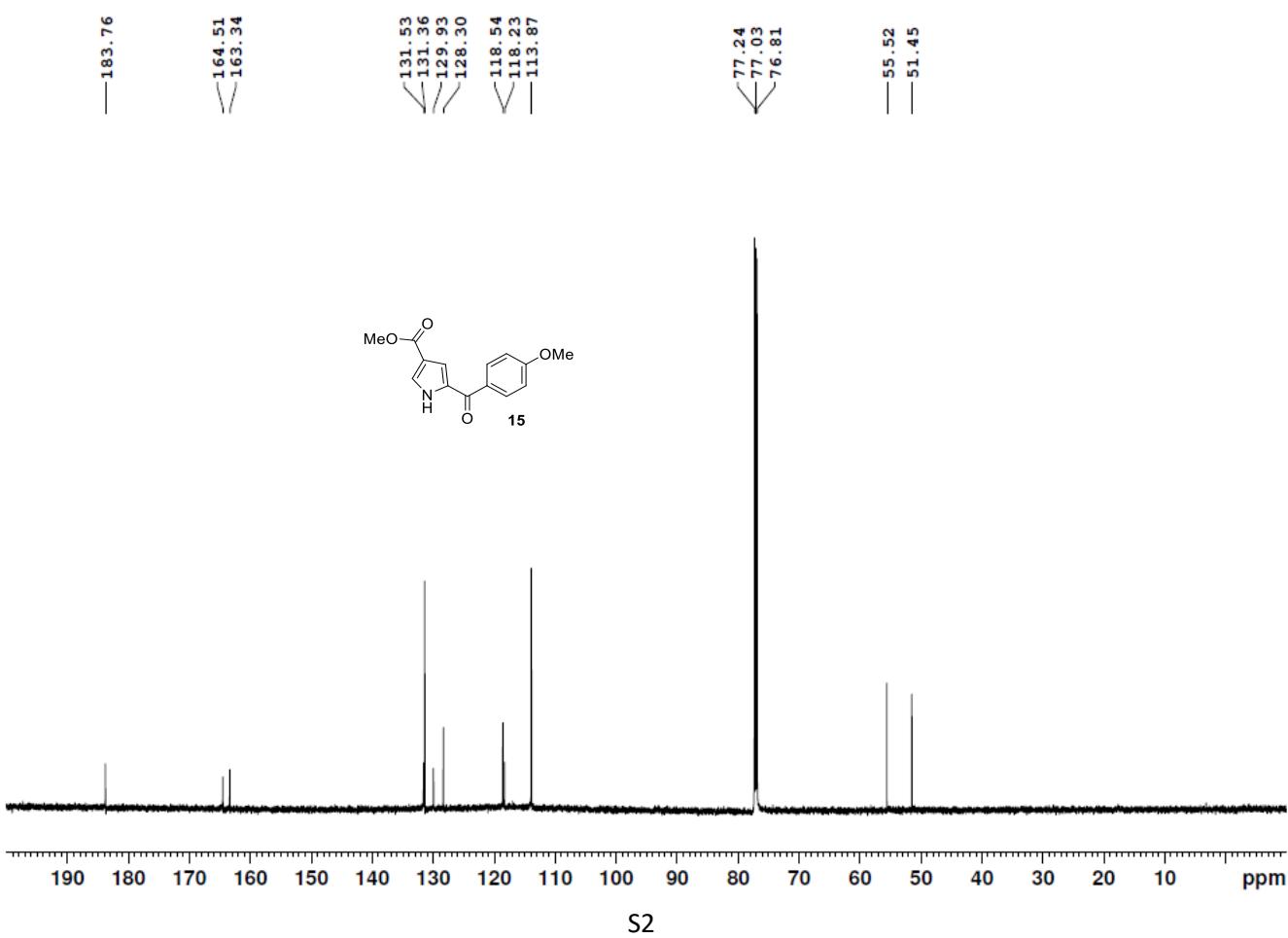
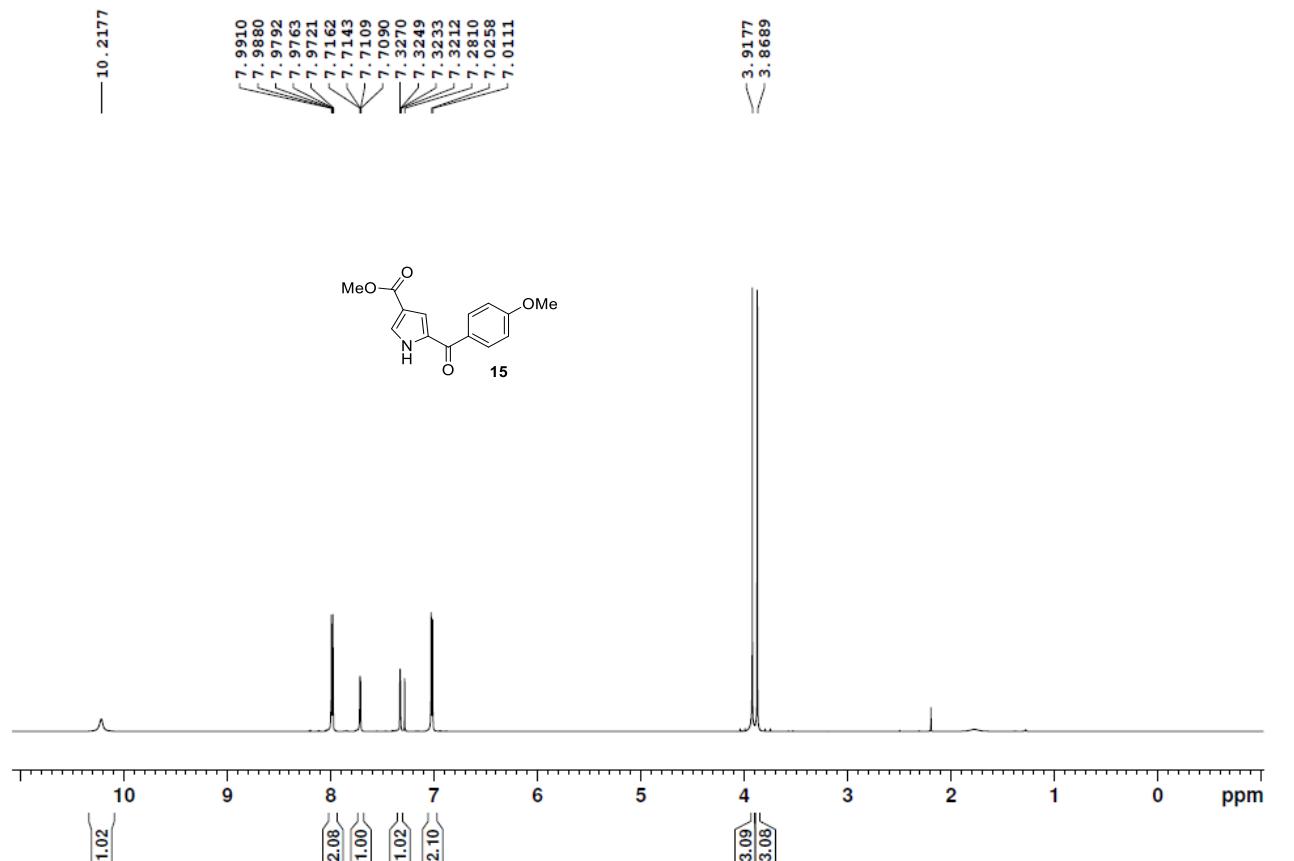
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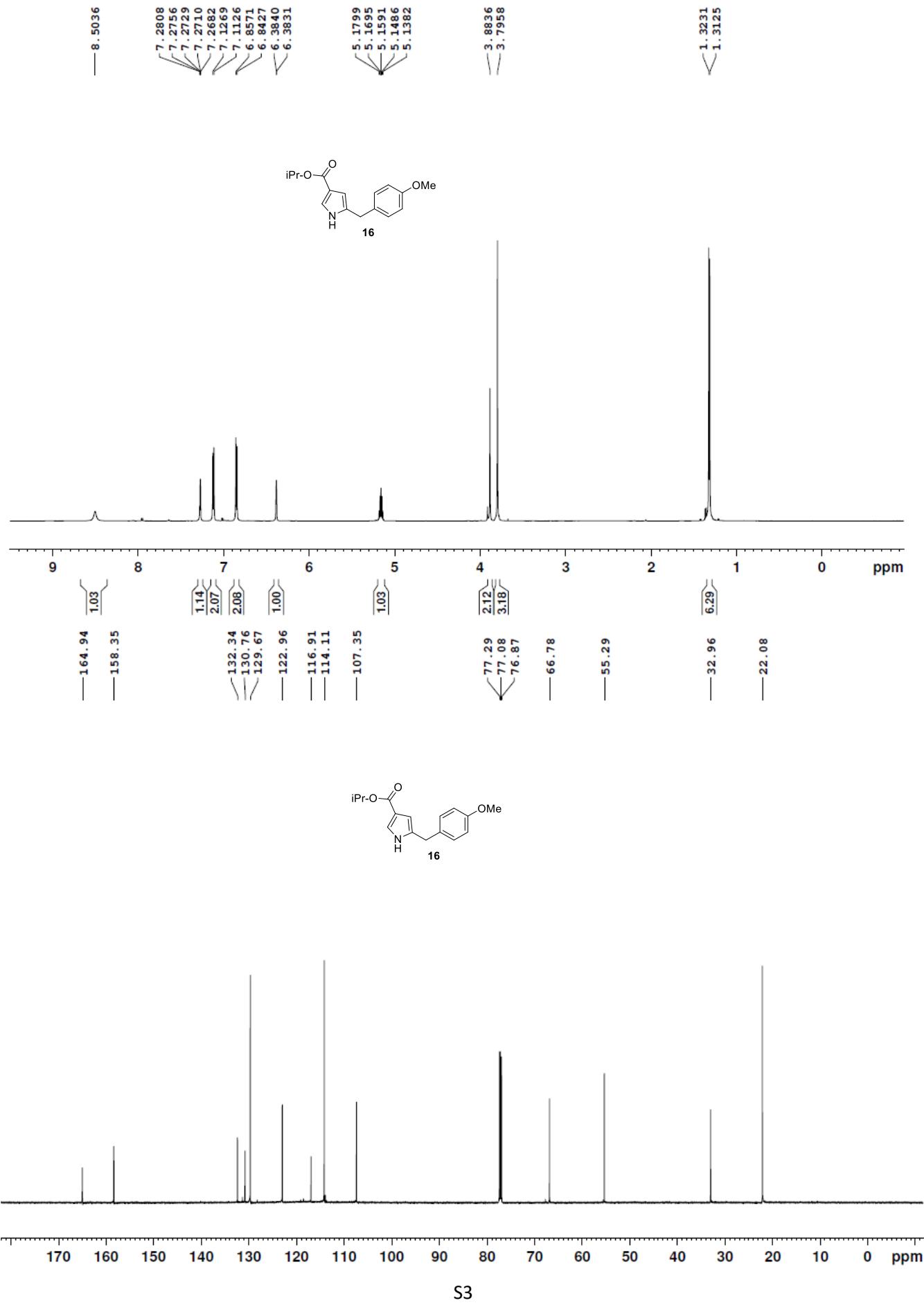
[†]Department of Chemistry, Portland State University, Portland, Oregon 97201, United States

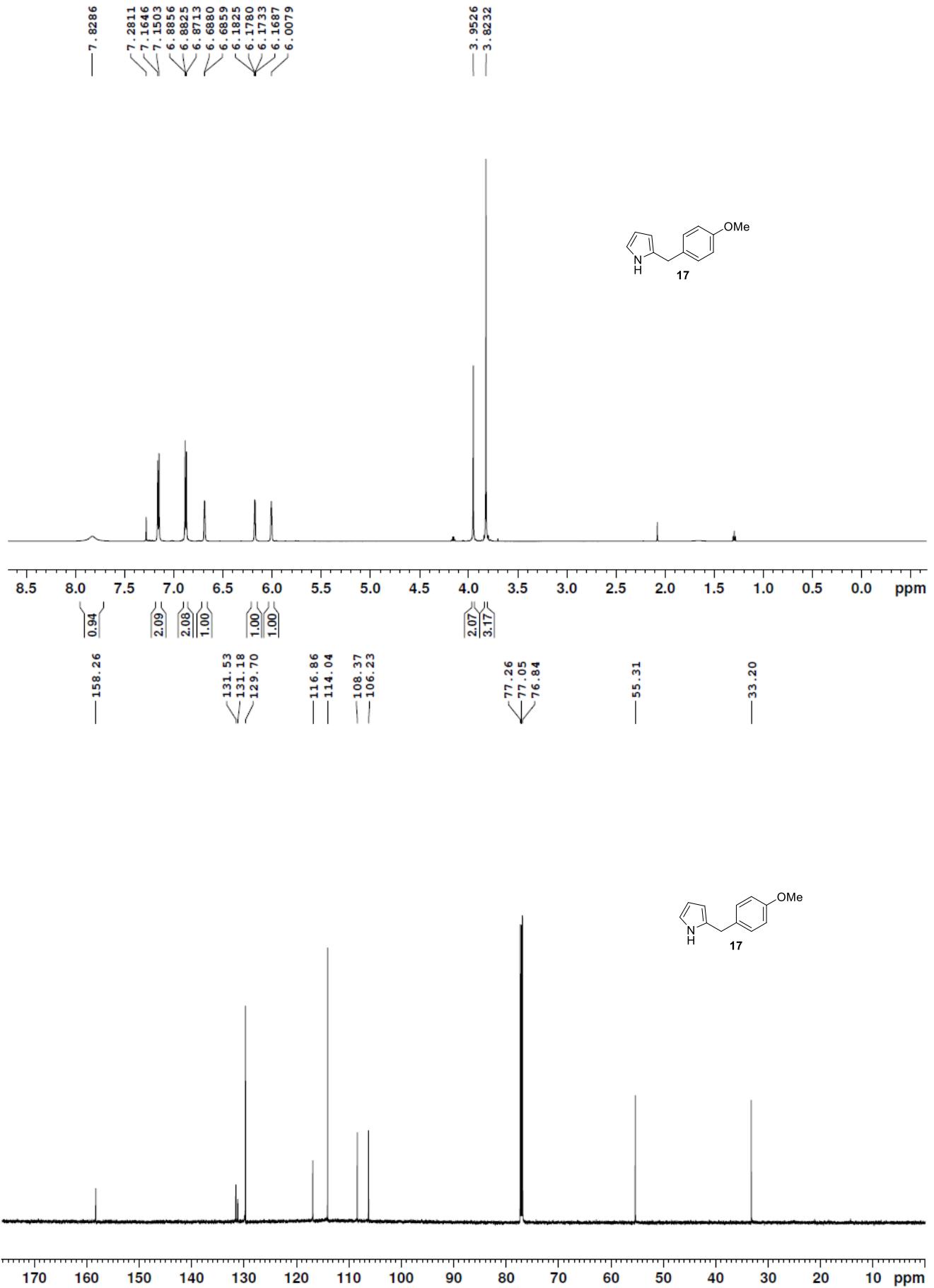
[‡]Department of Veterans Affairs Medical Center, Portland, Oregon 97239, United States

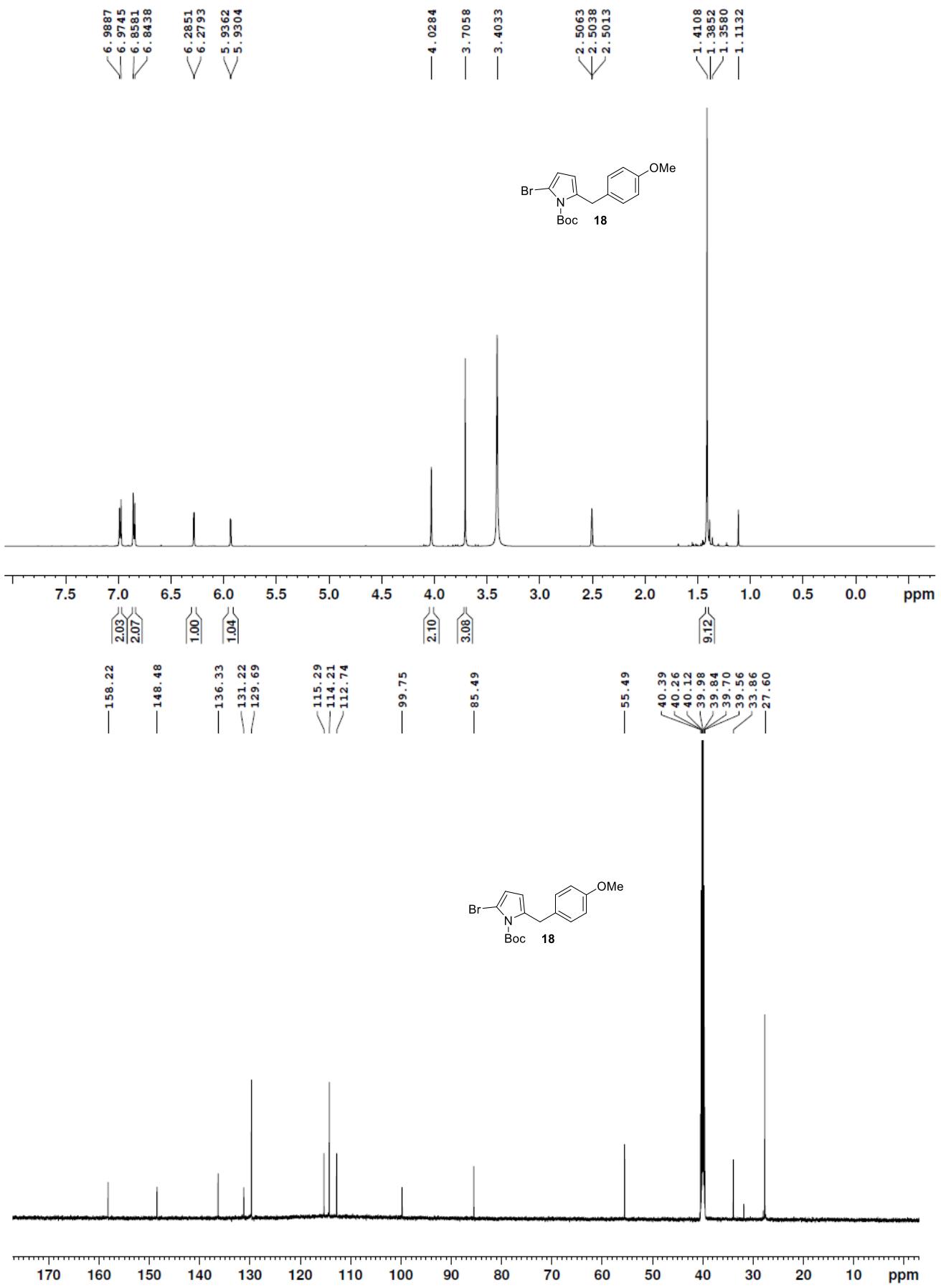
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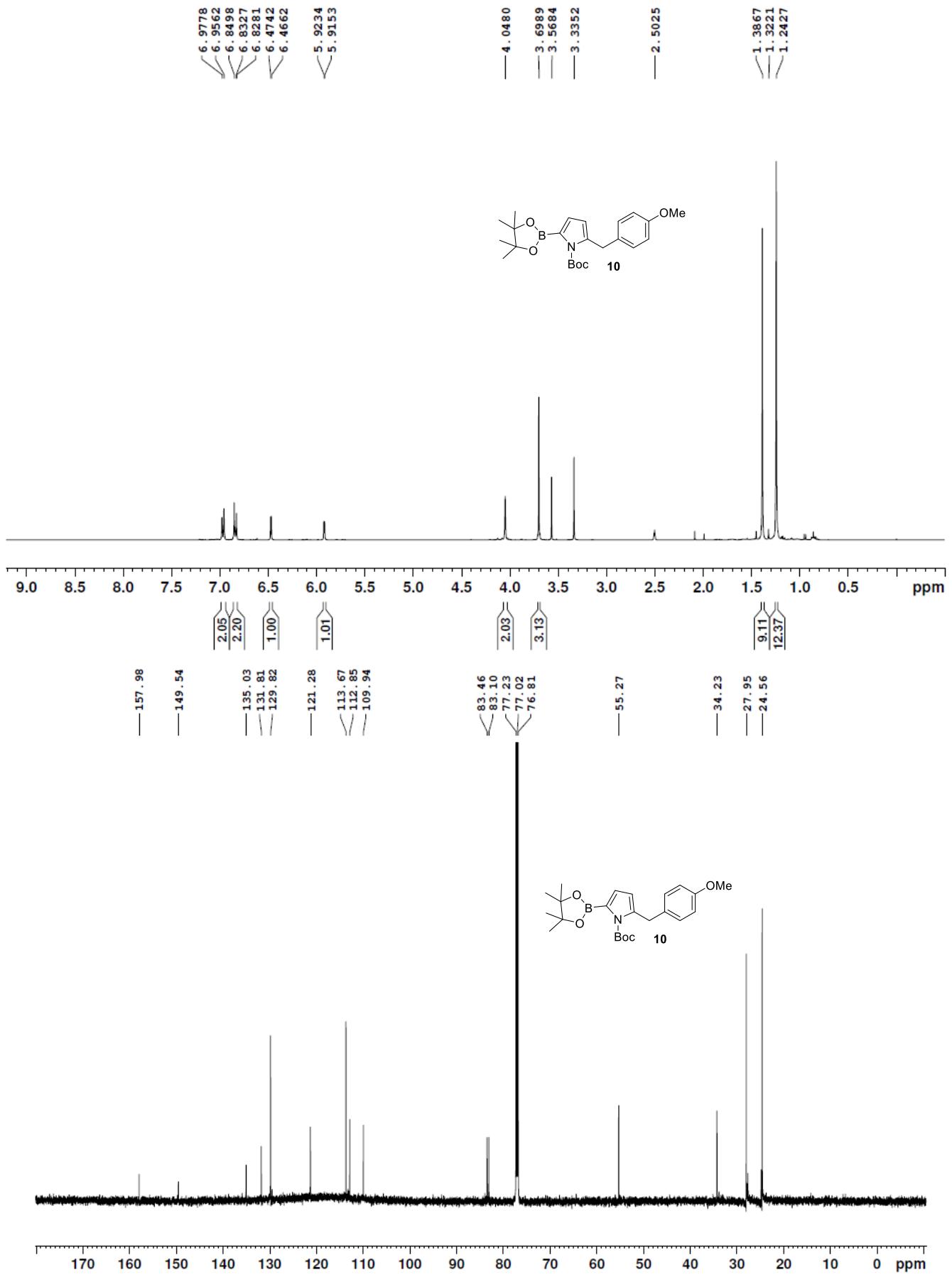
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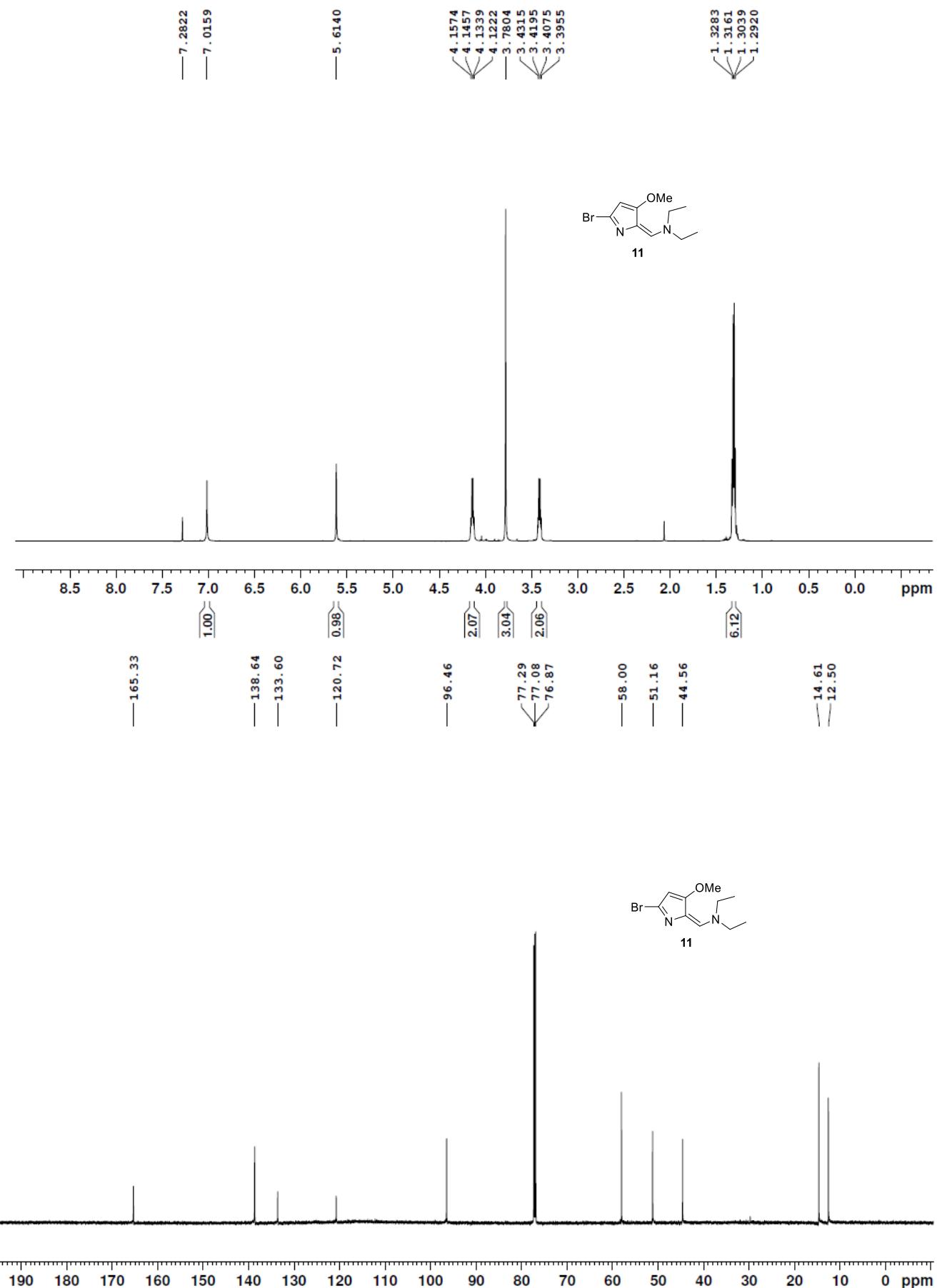


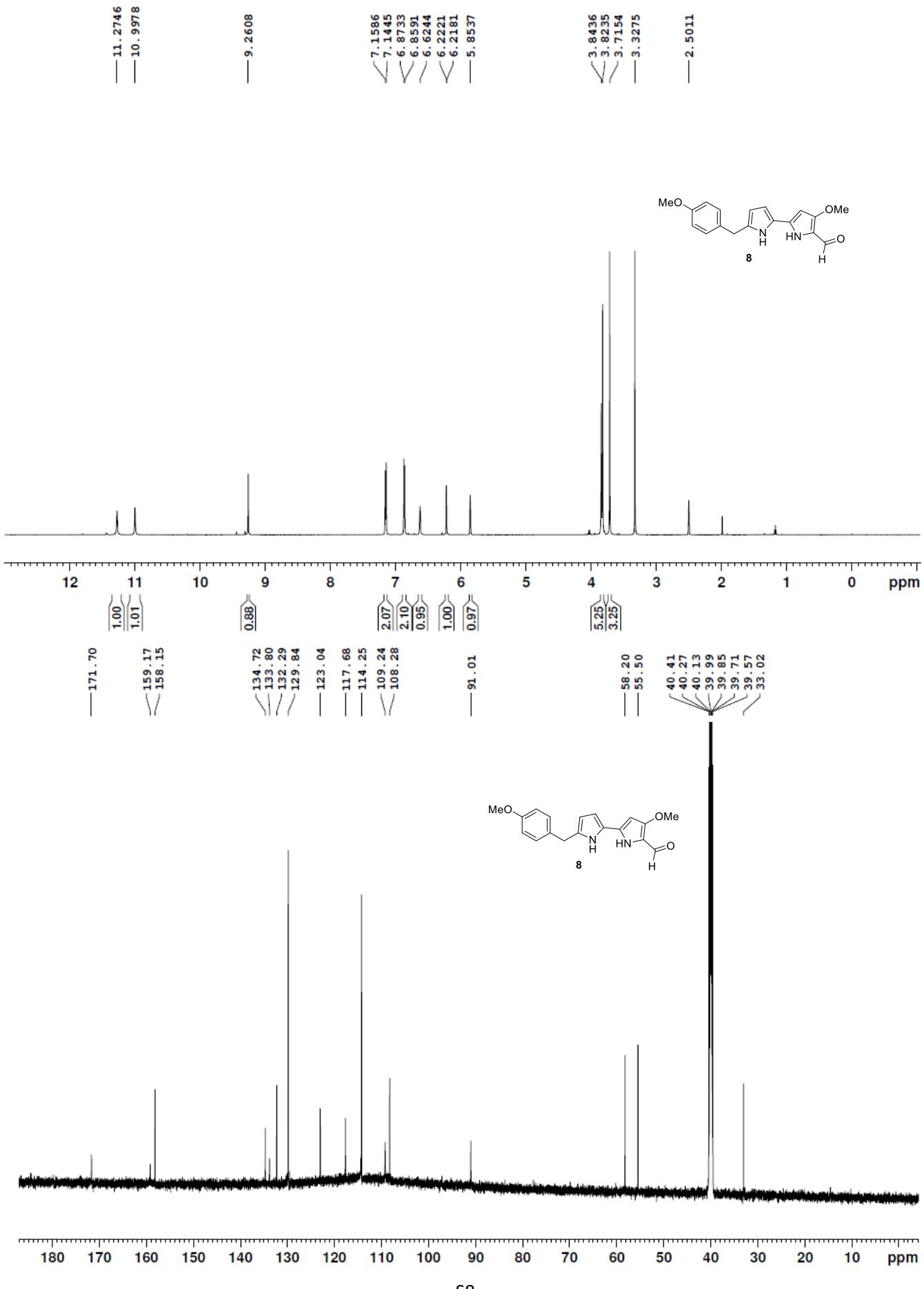


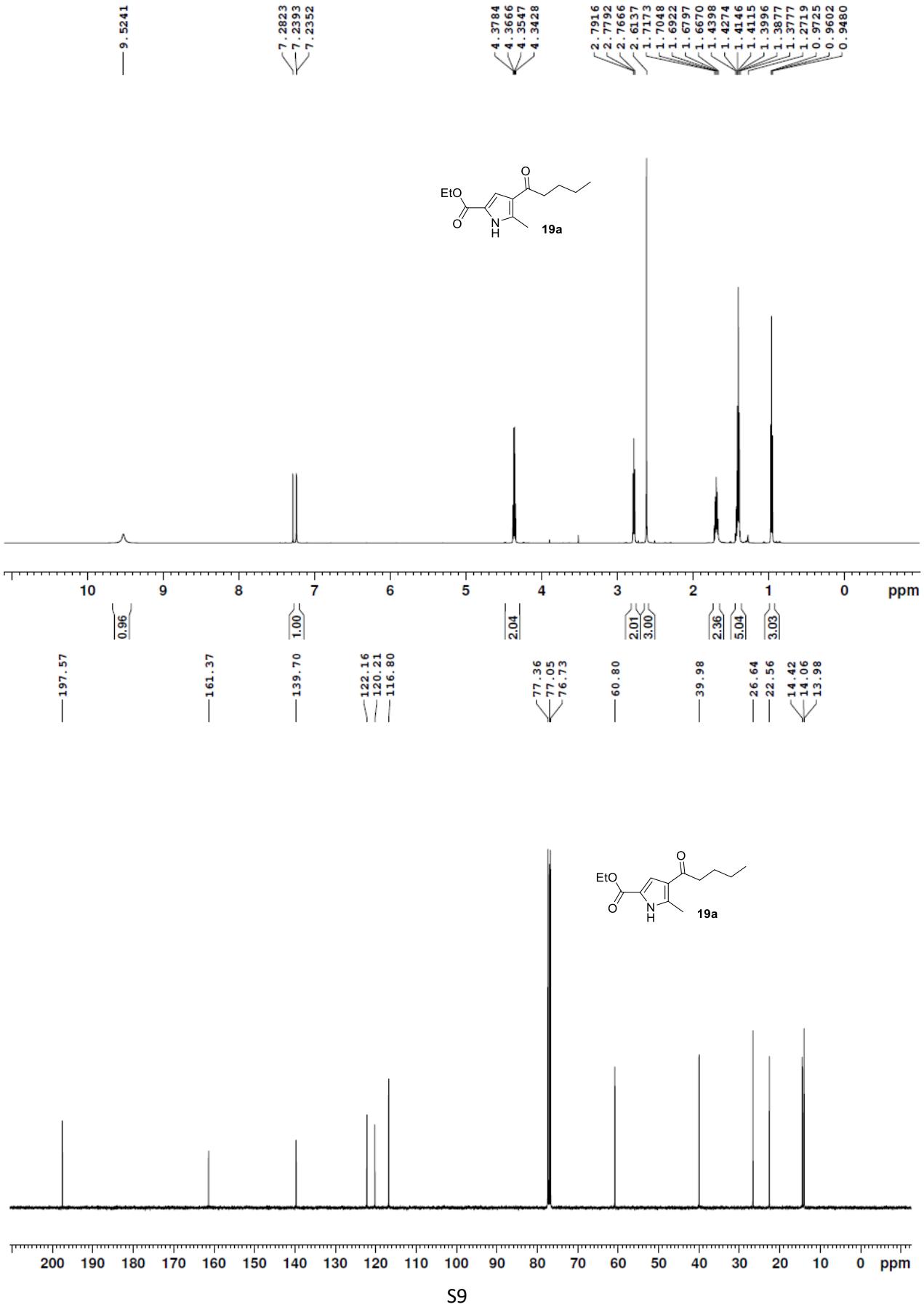


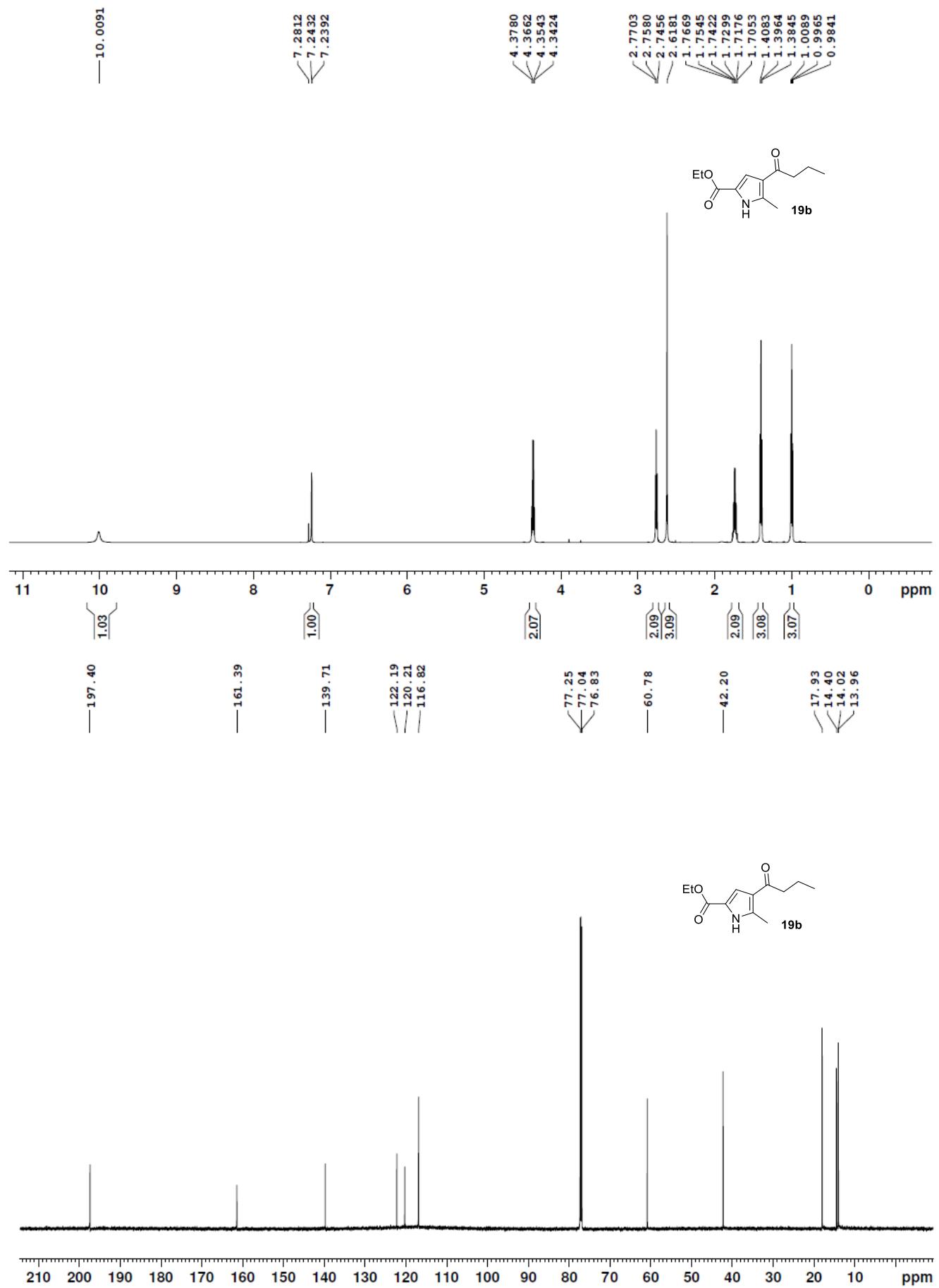


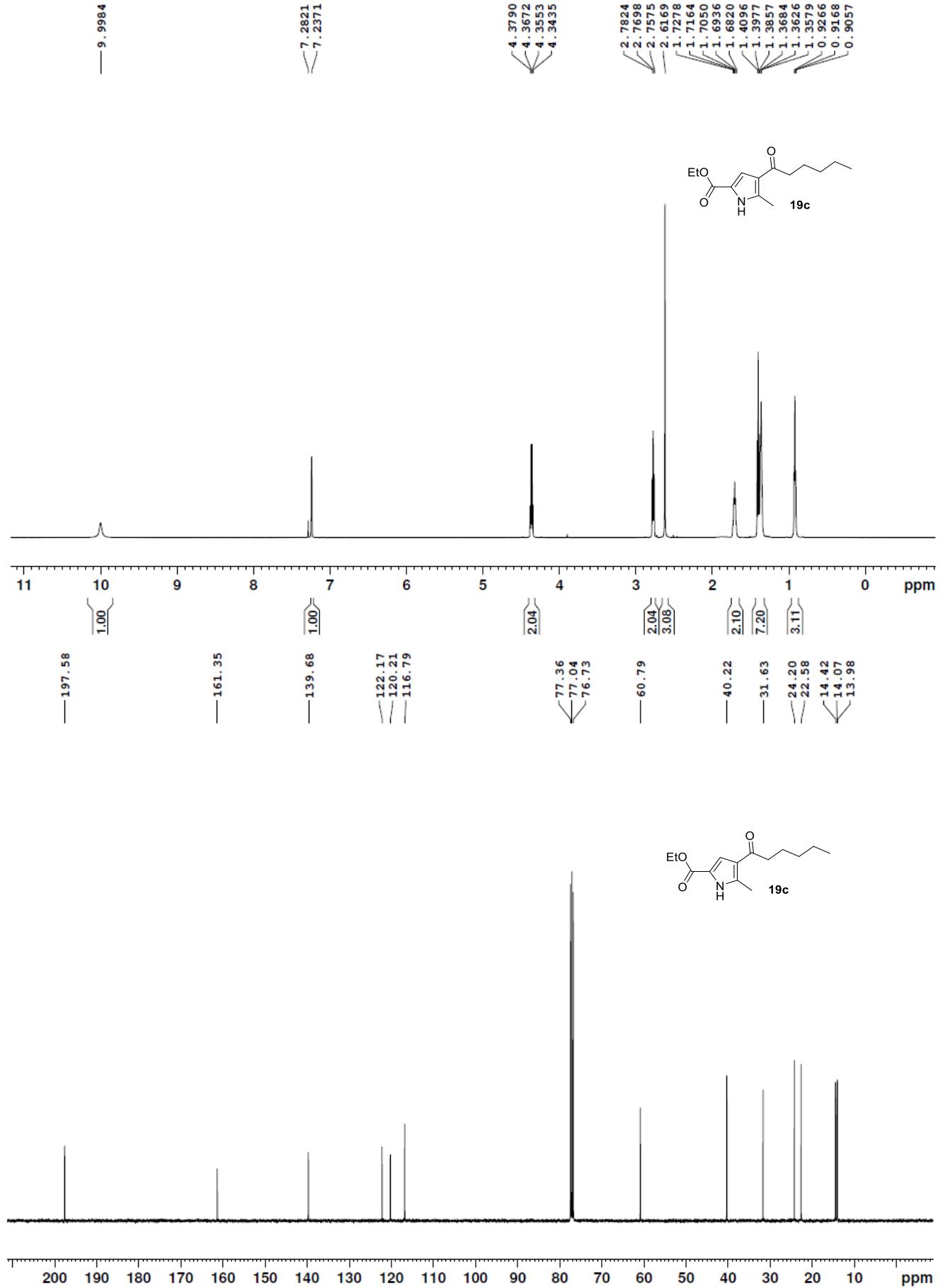


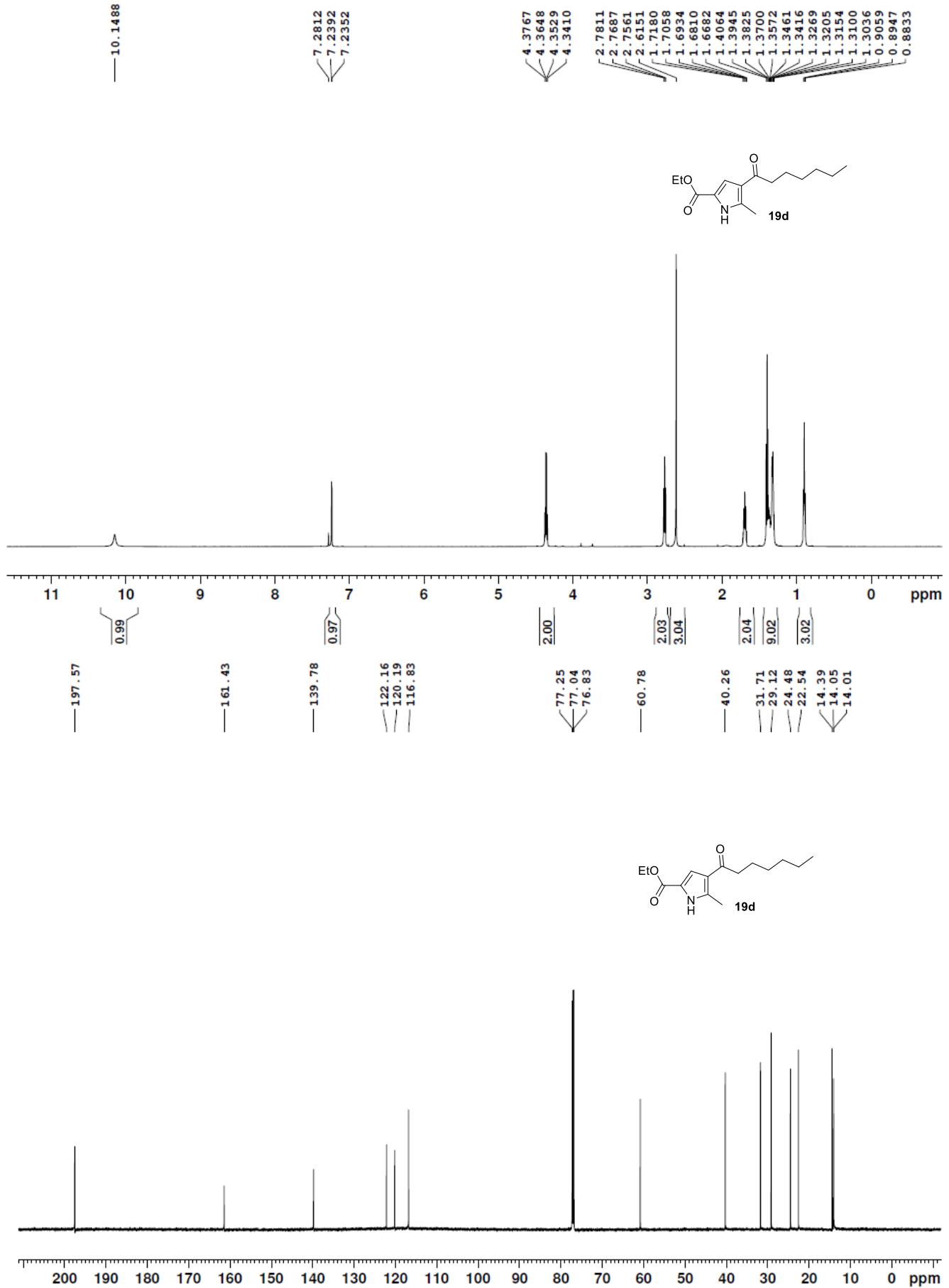


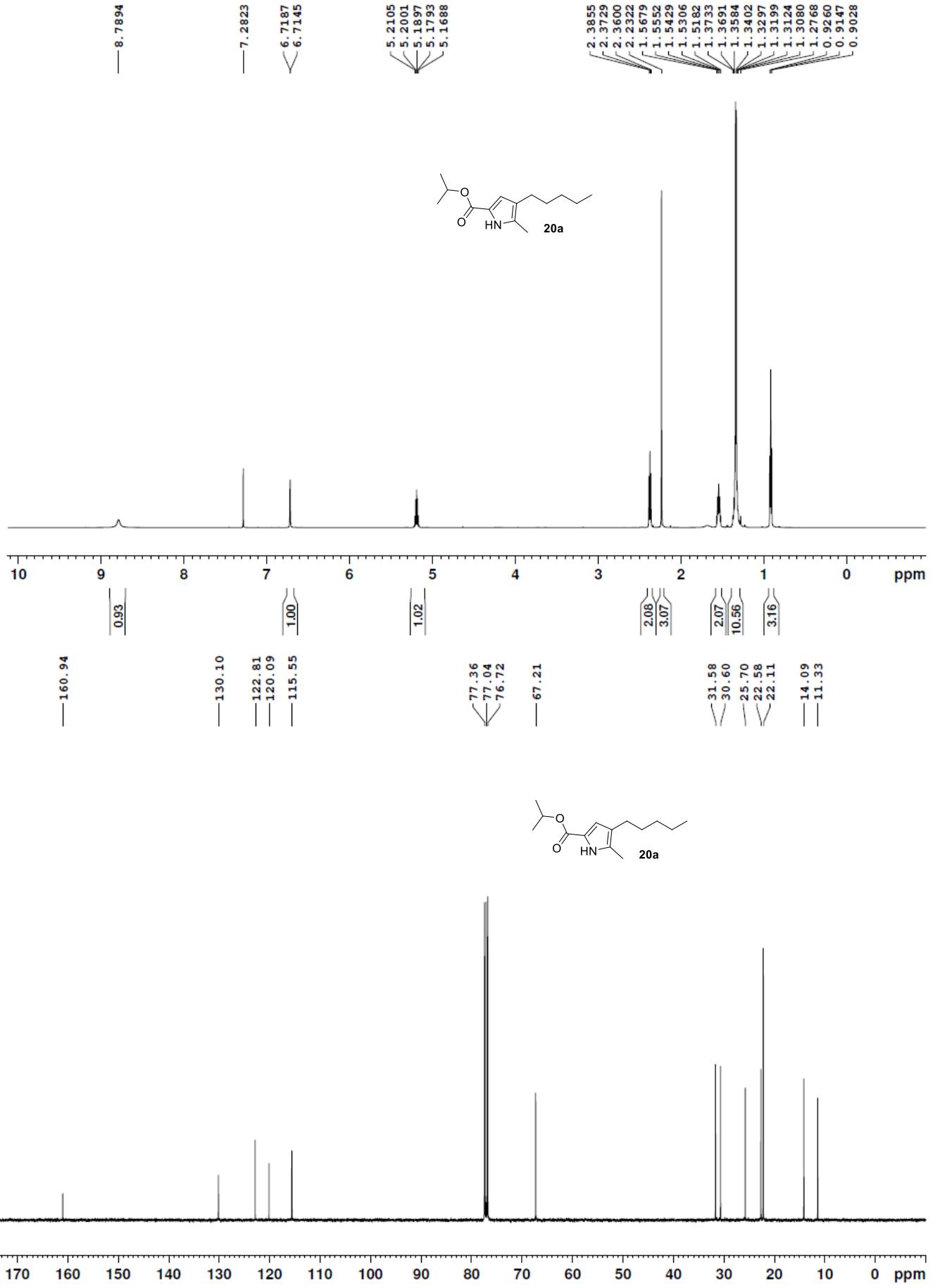


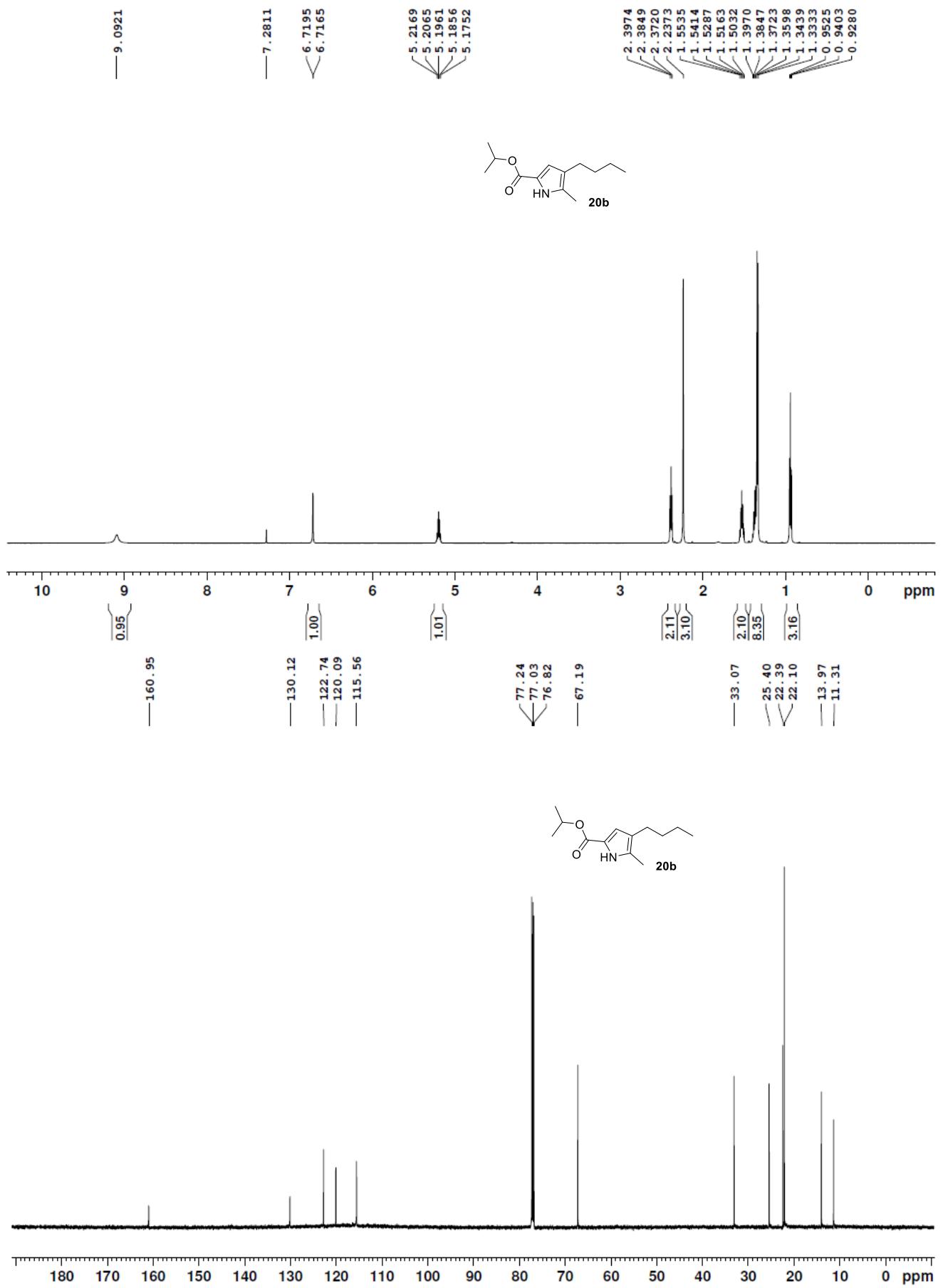


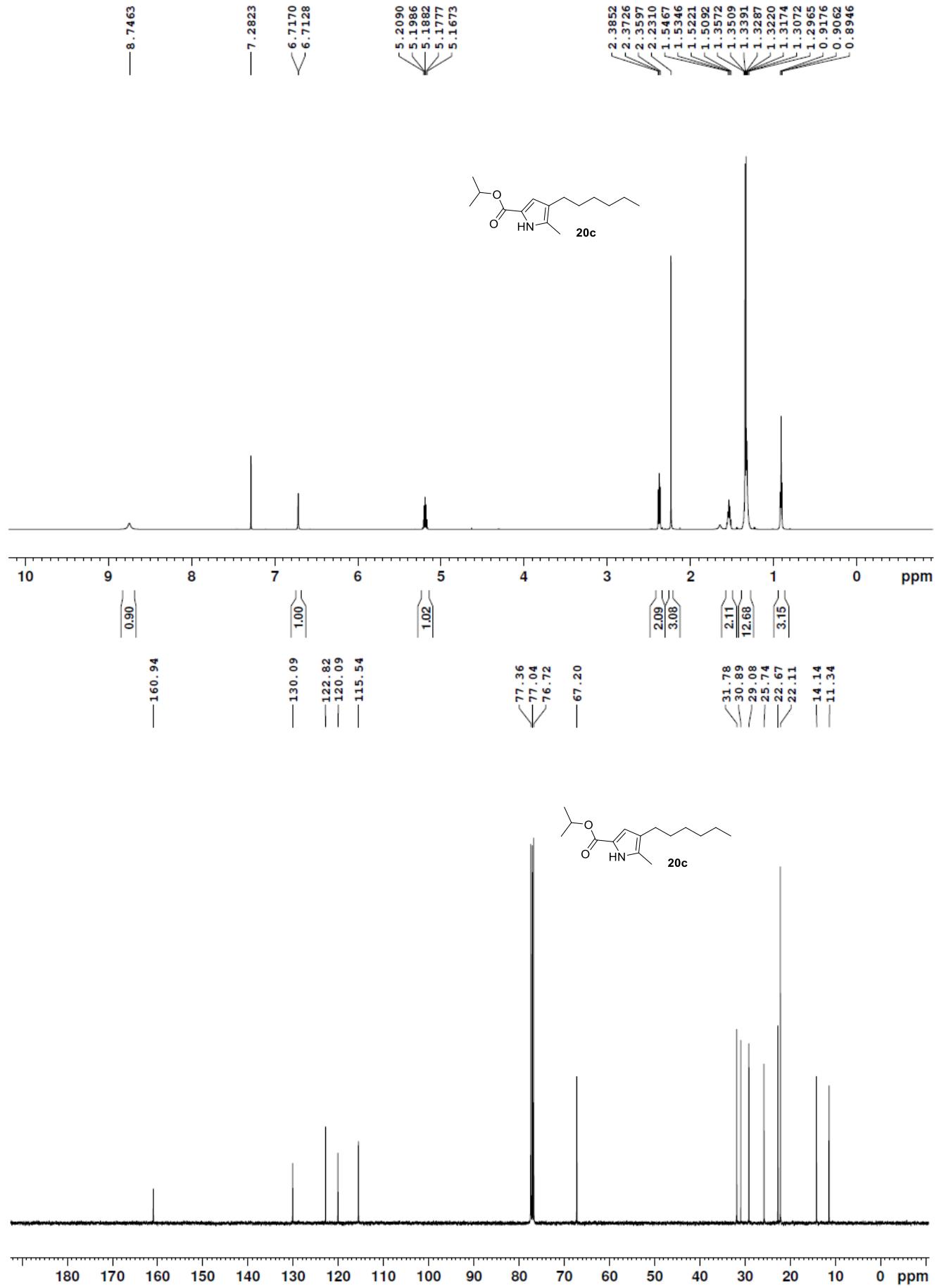


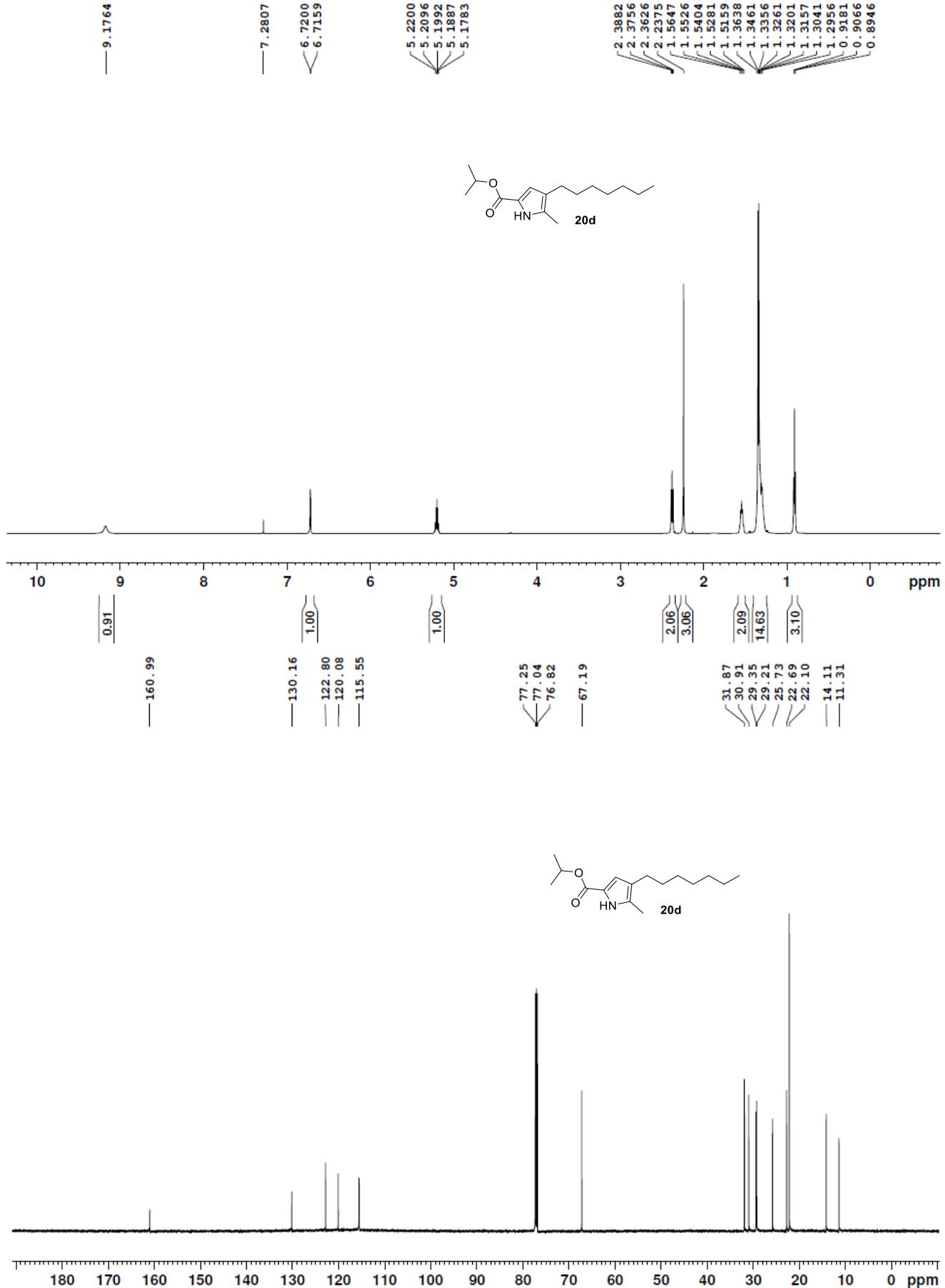


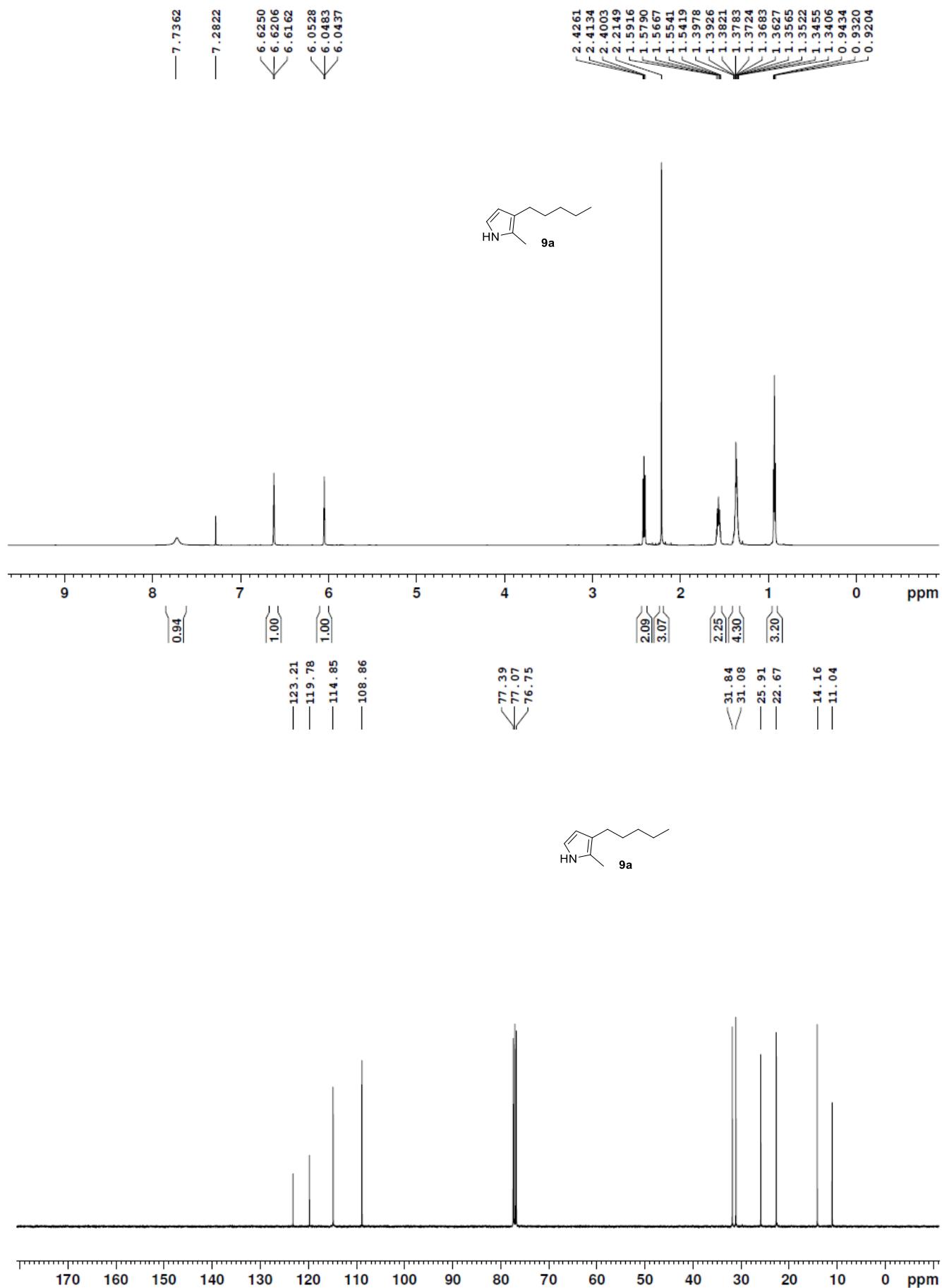


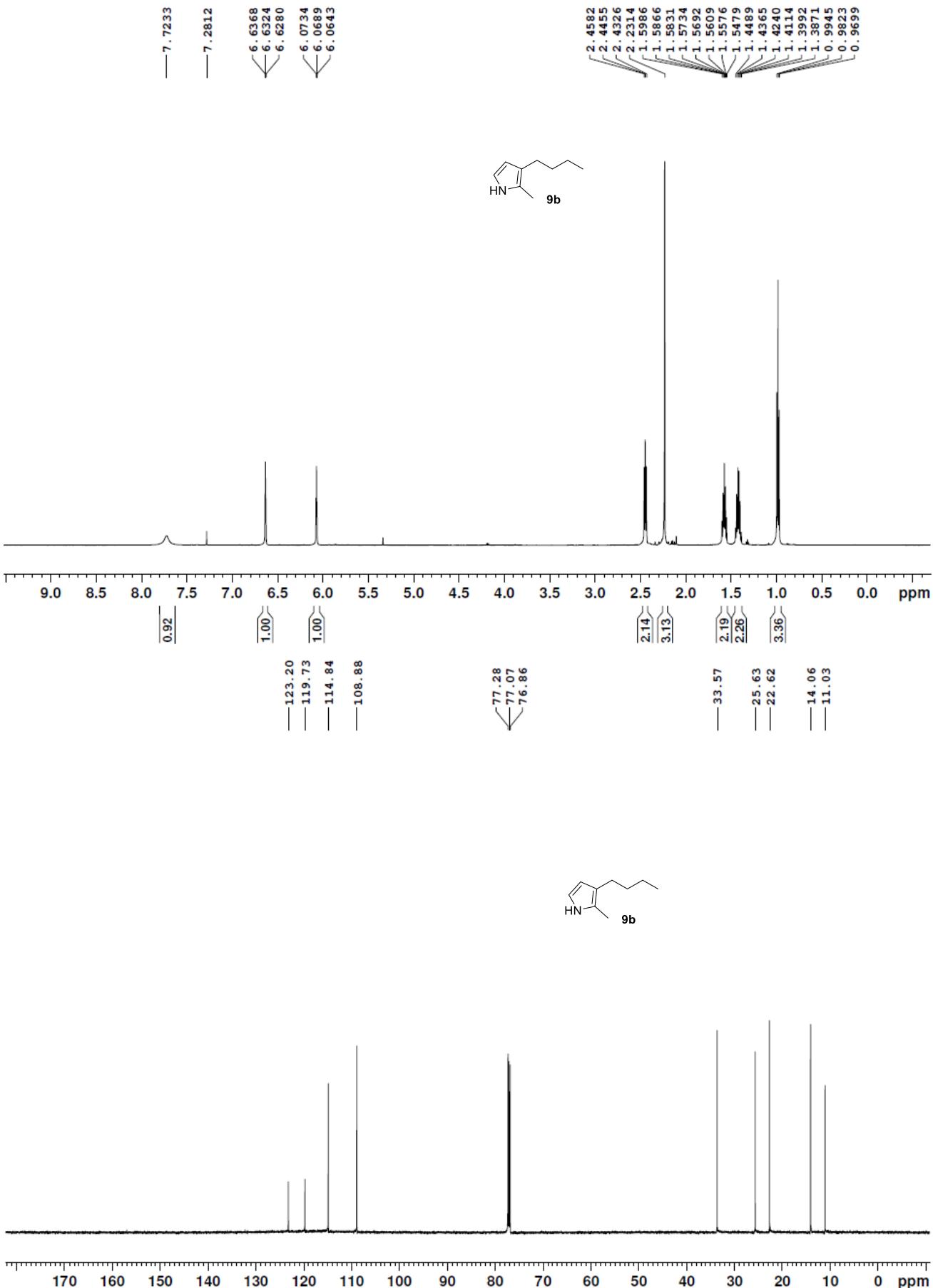


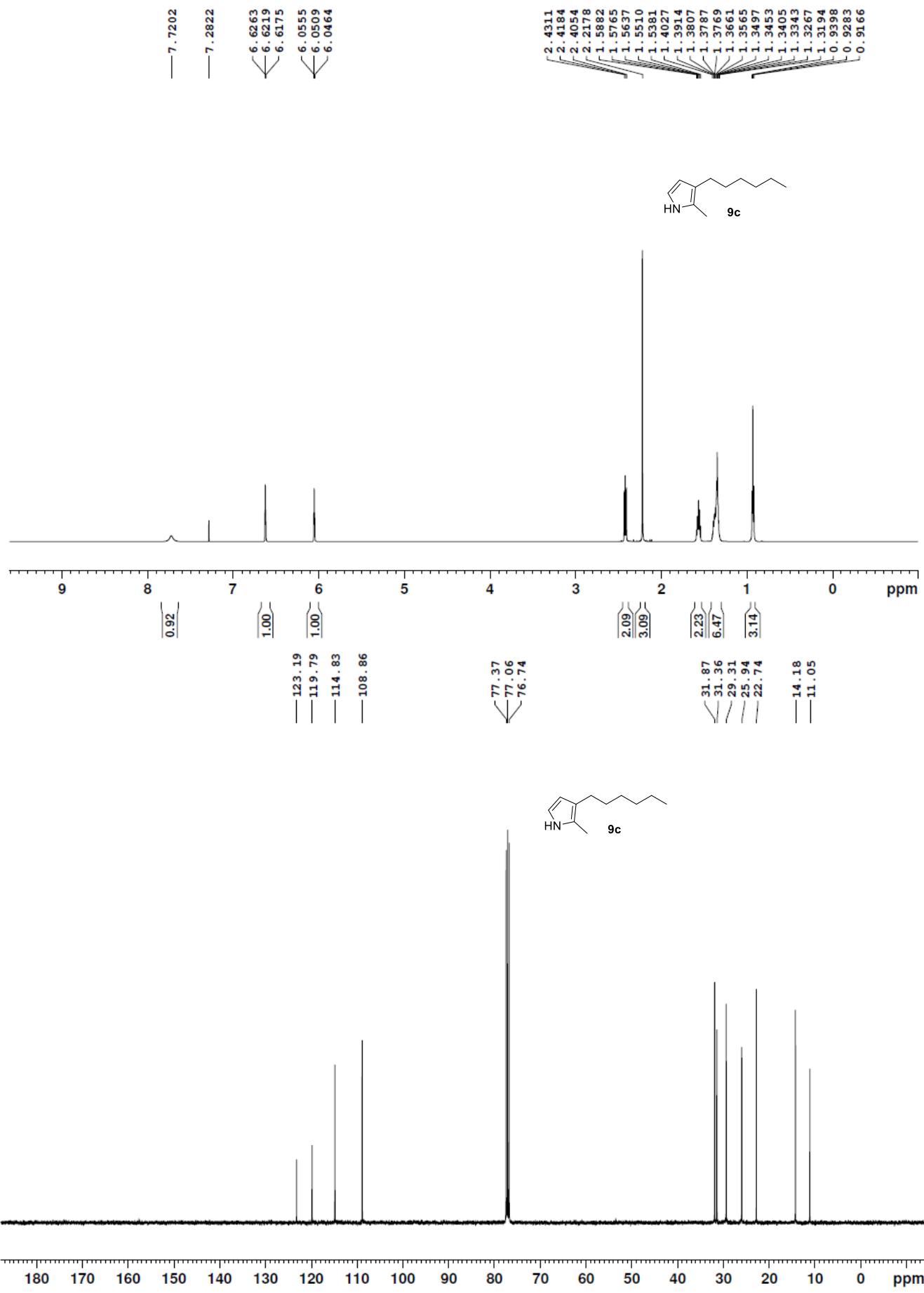


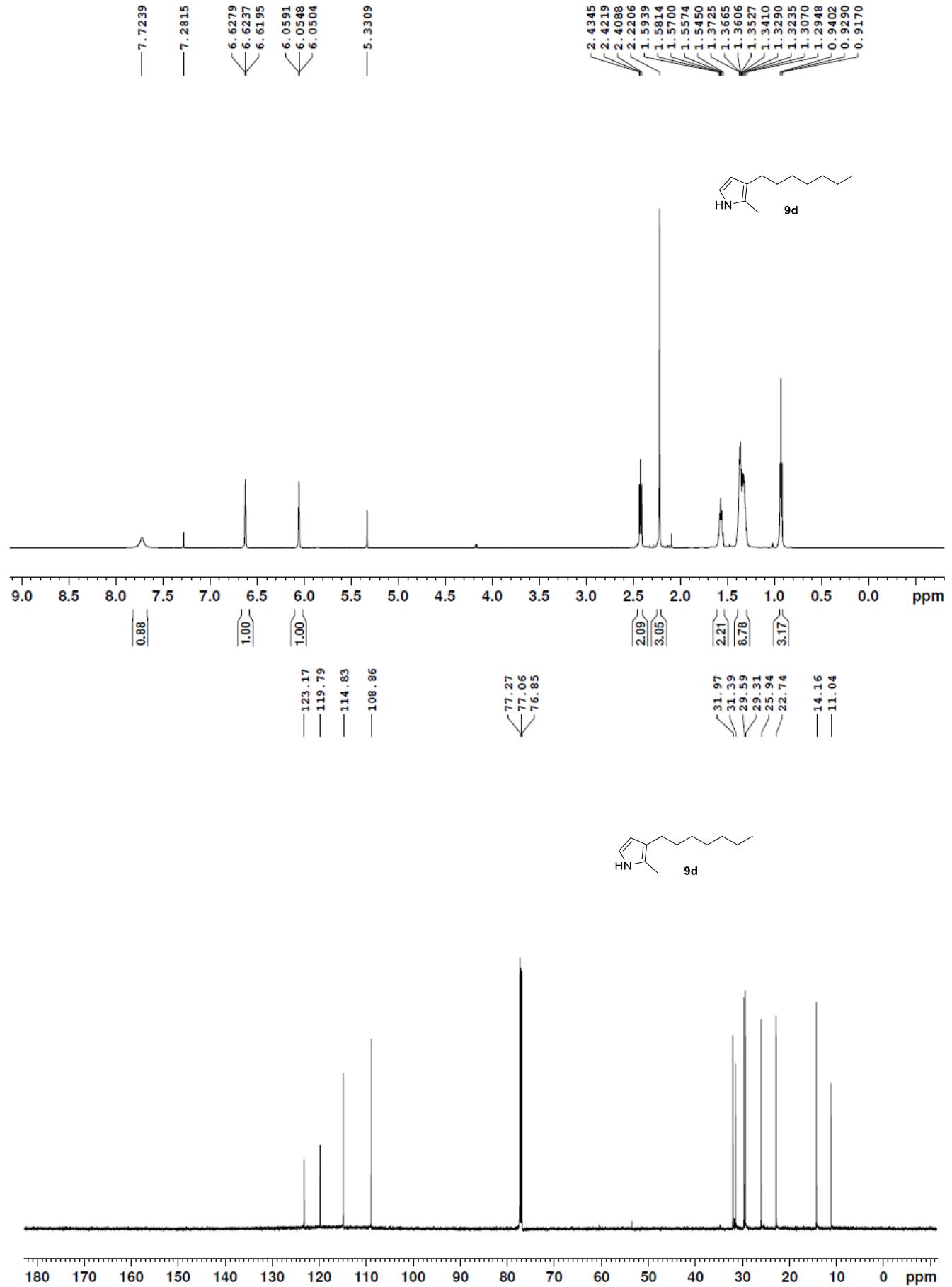


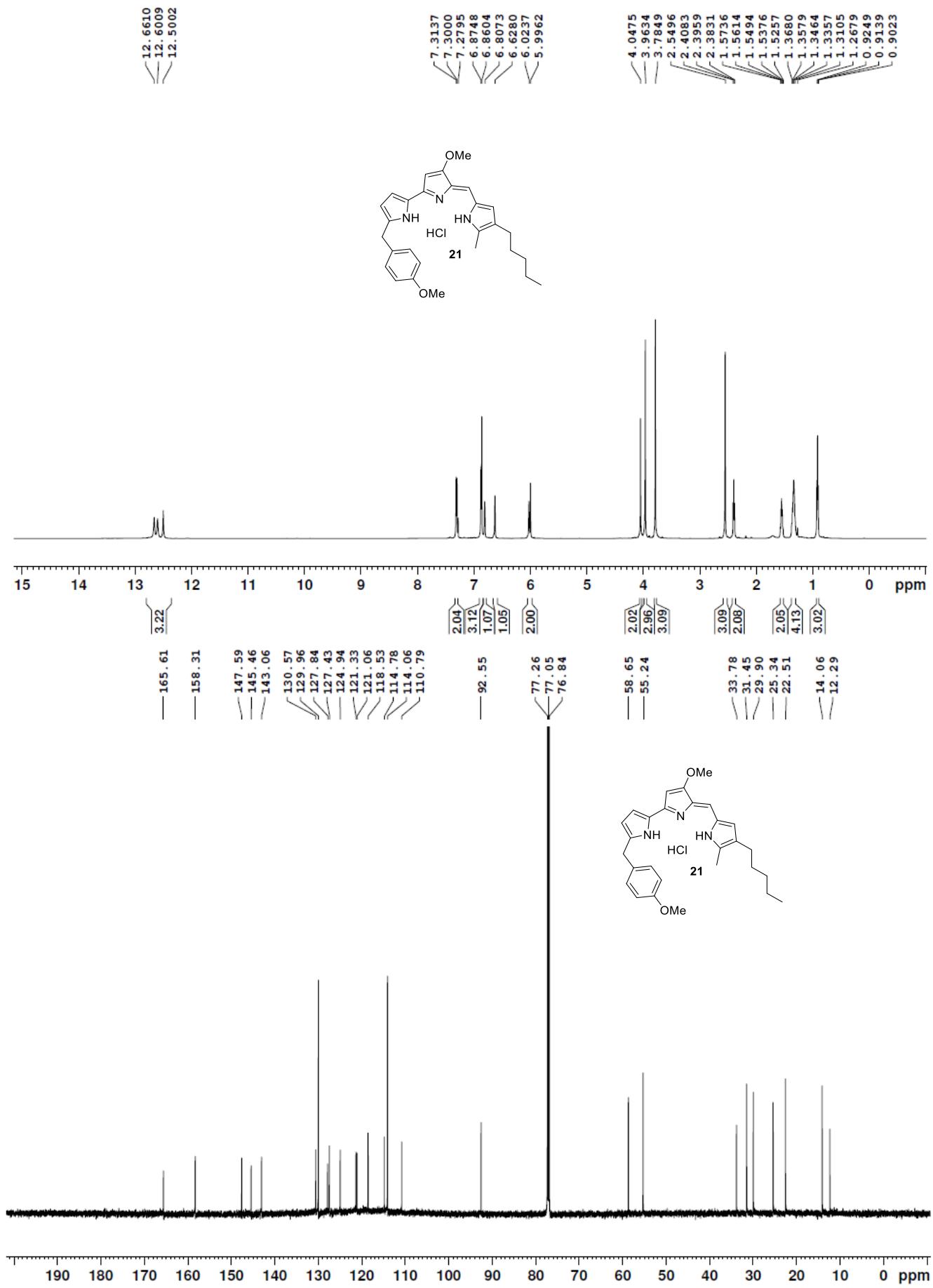


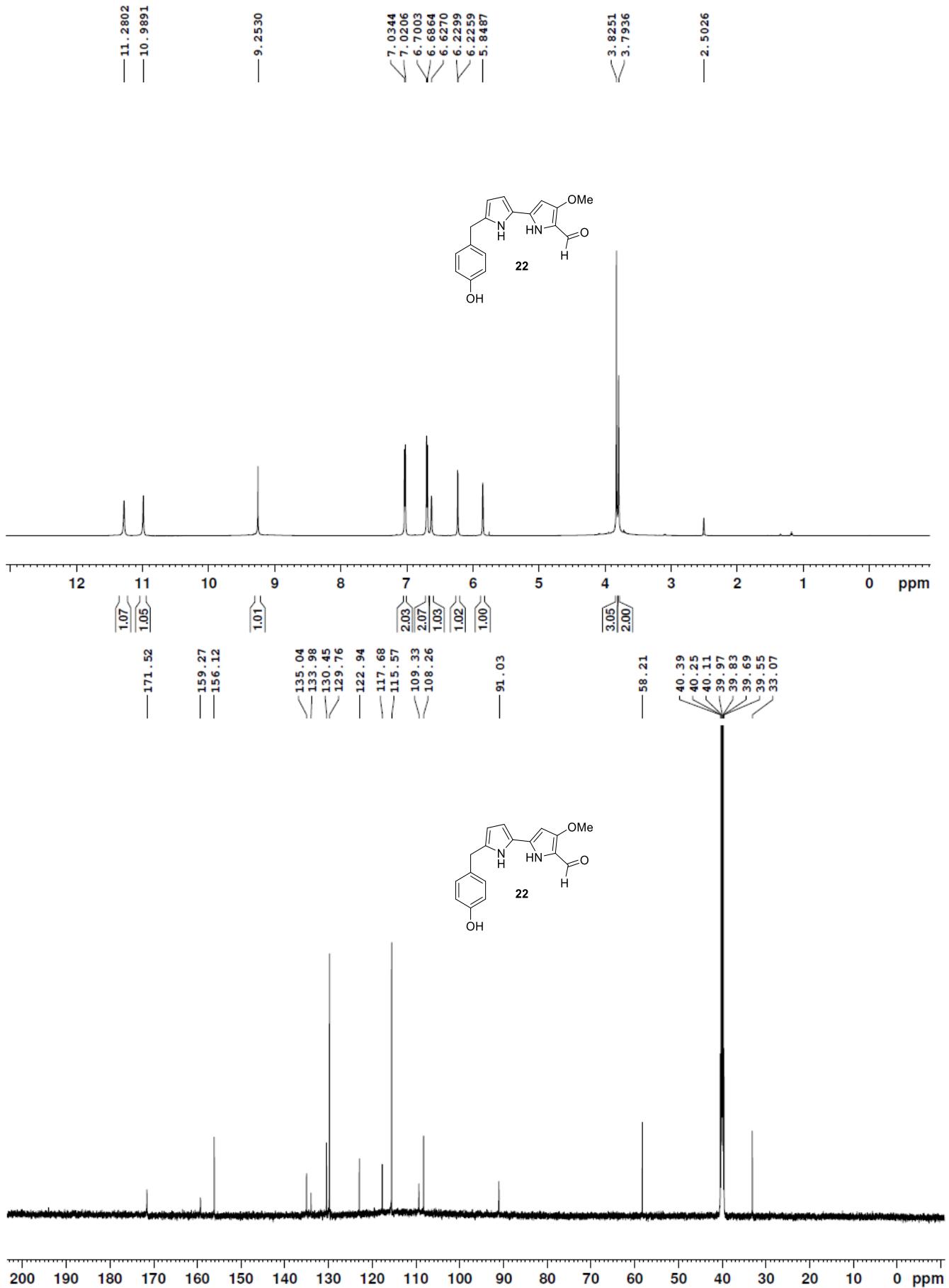




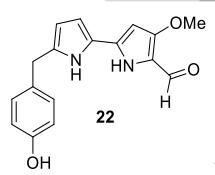








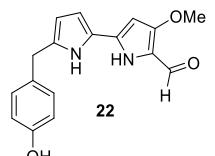
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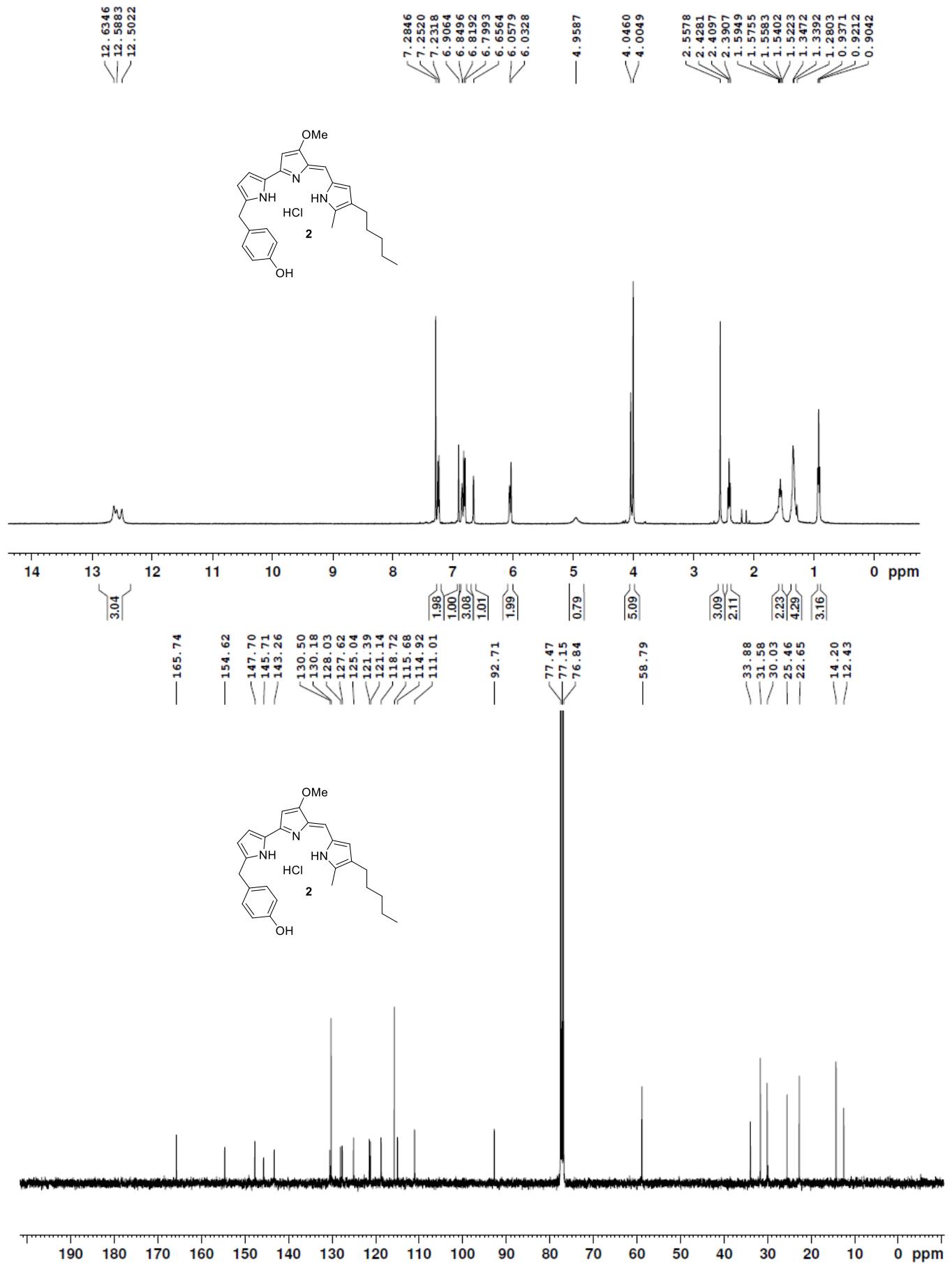


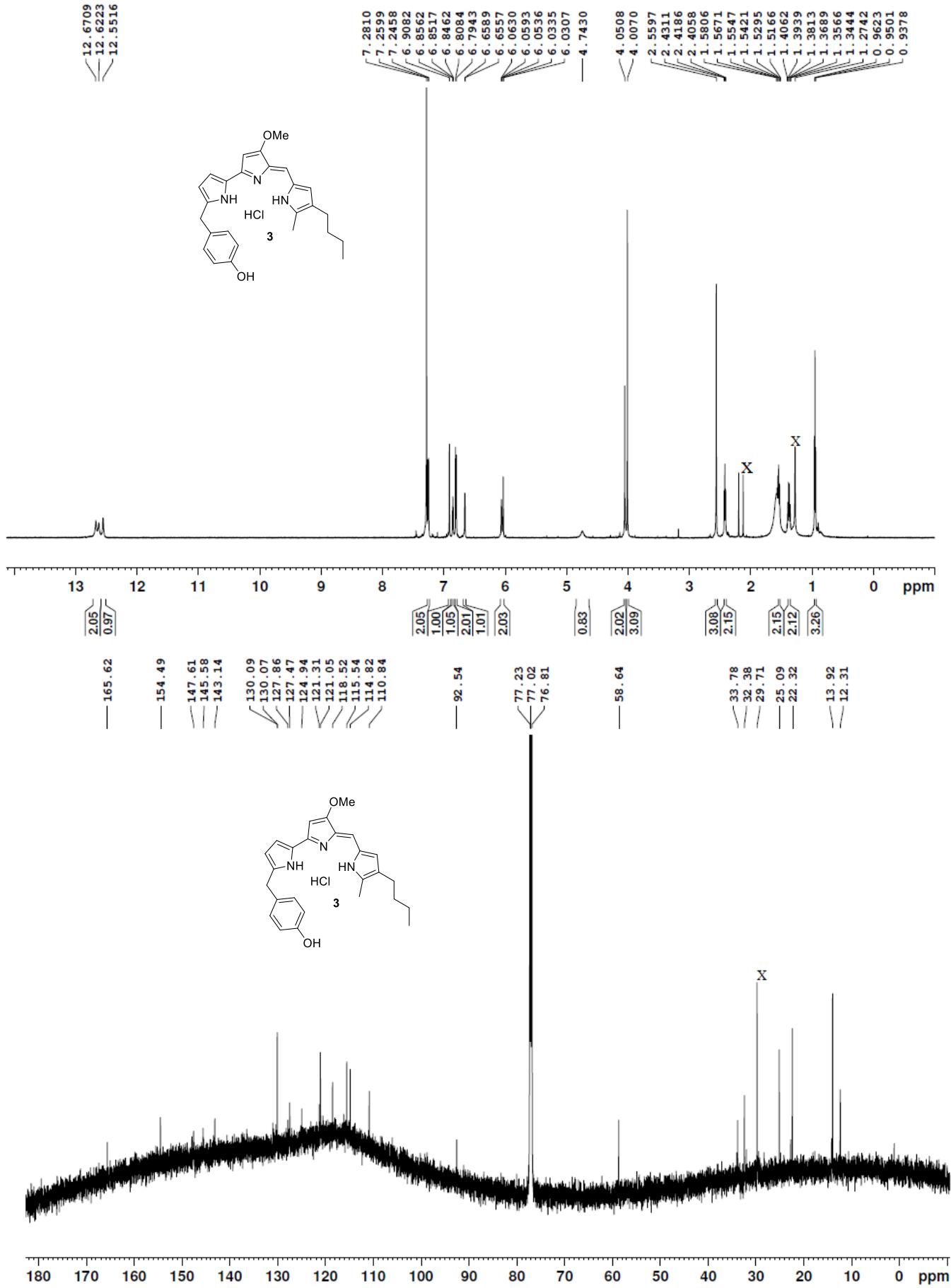
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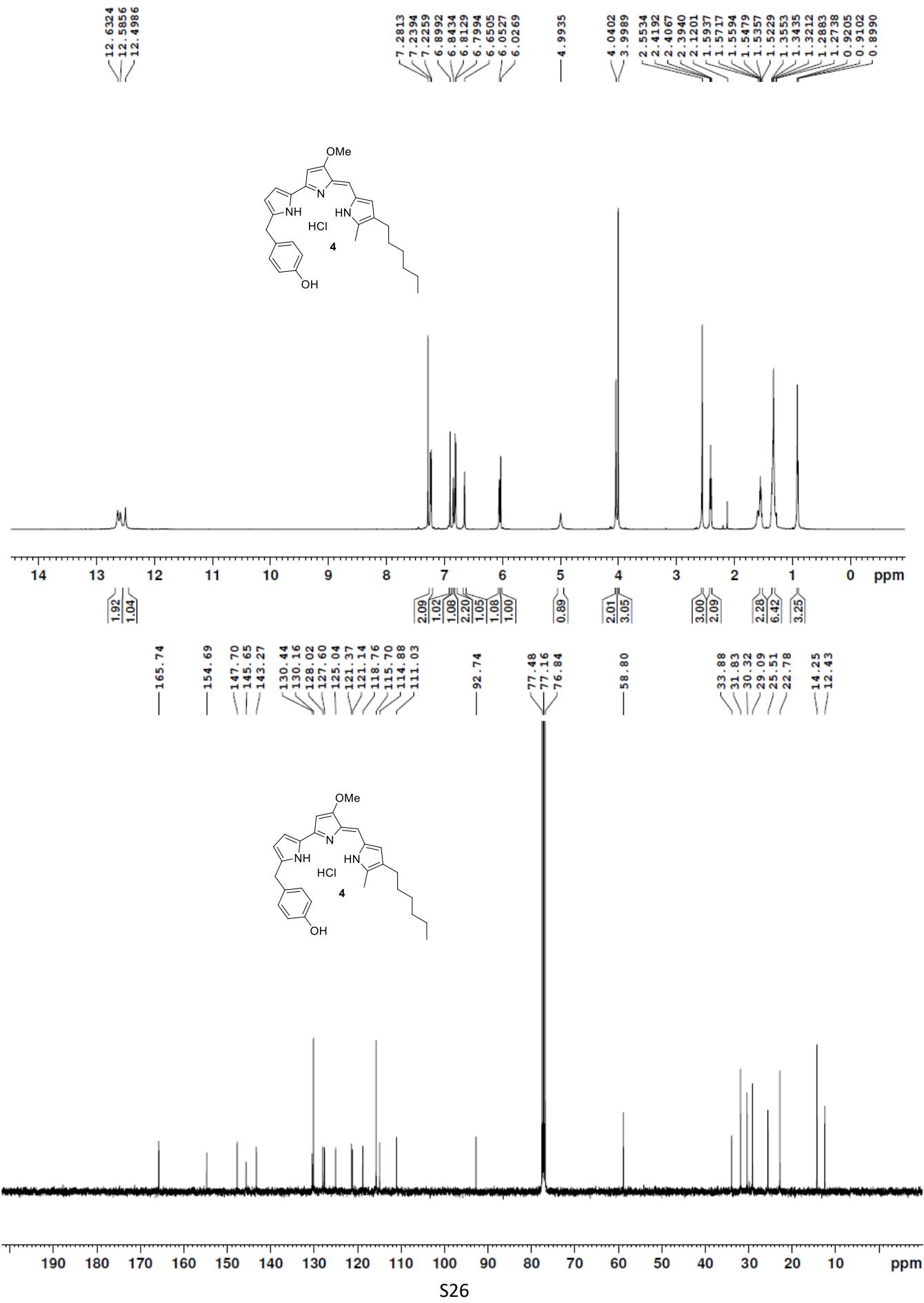


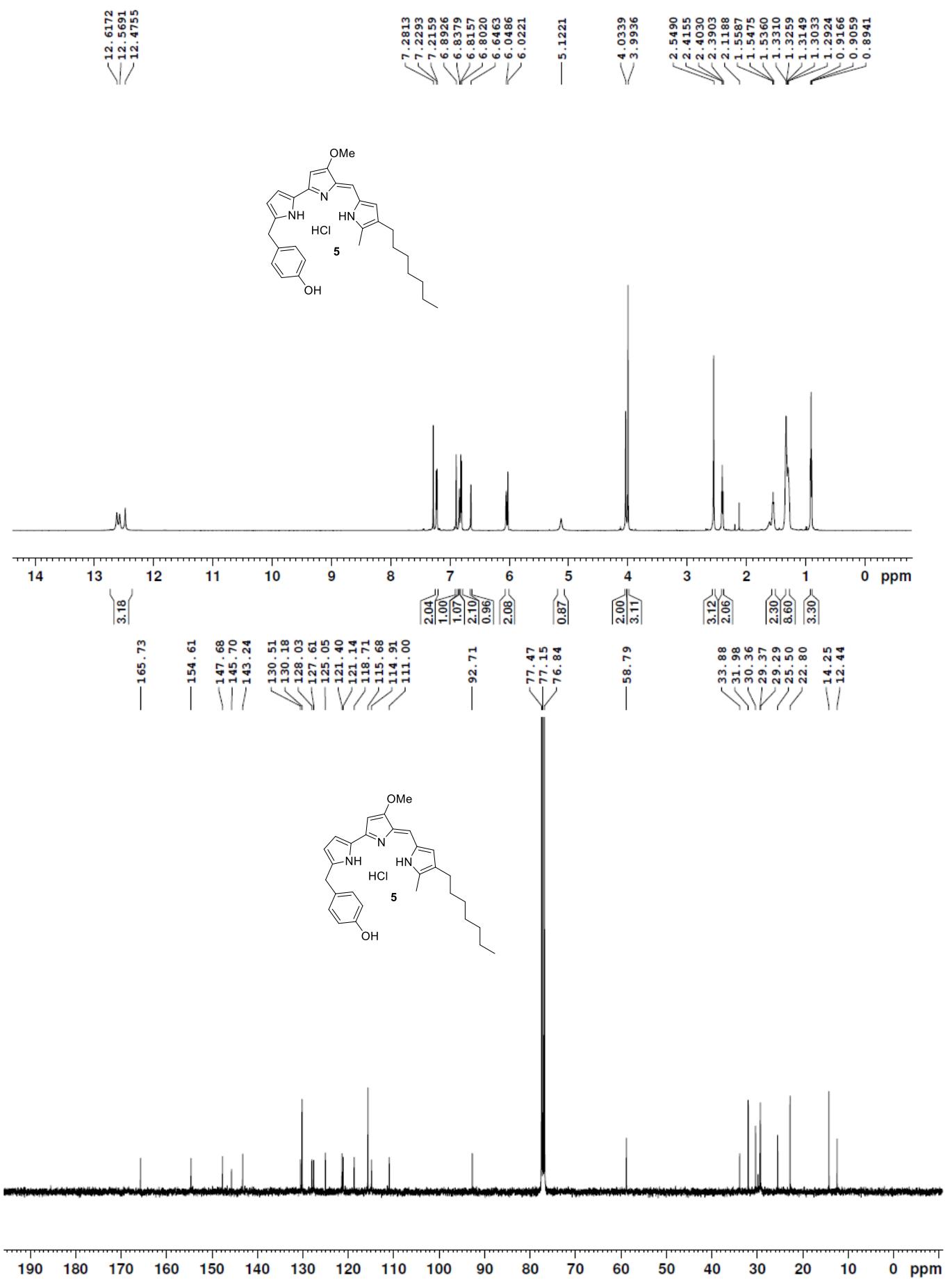
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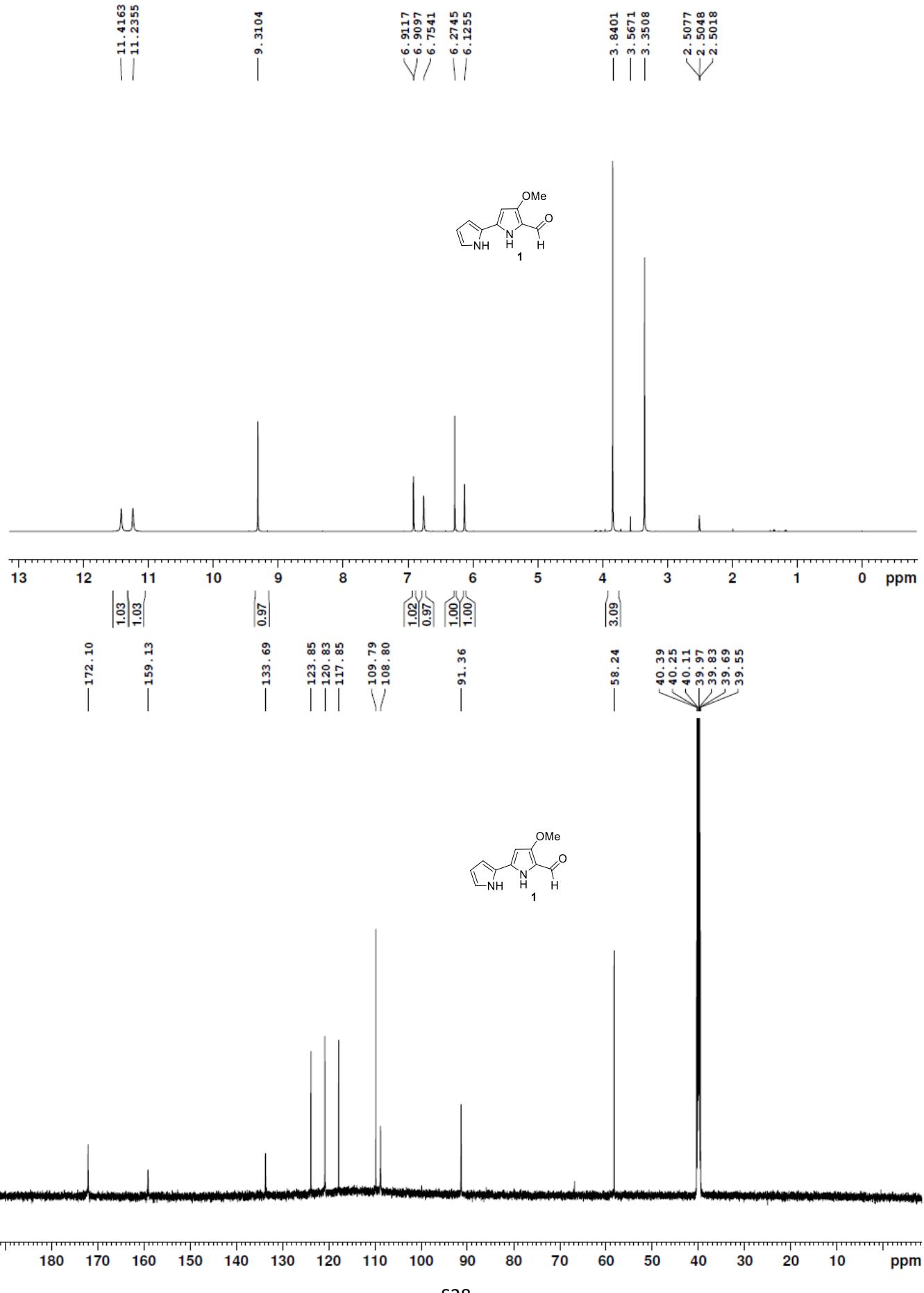


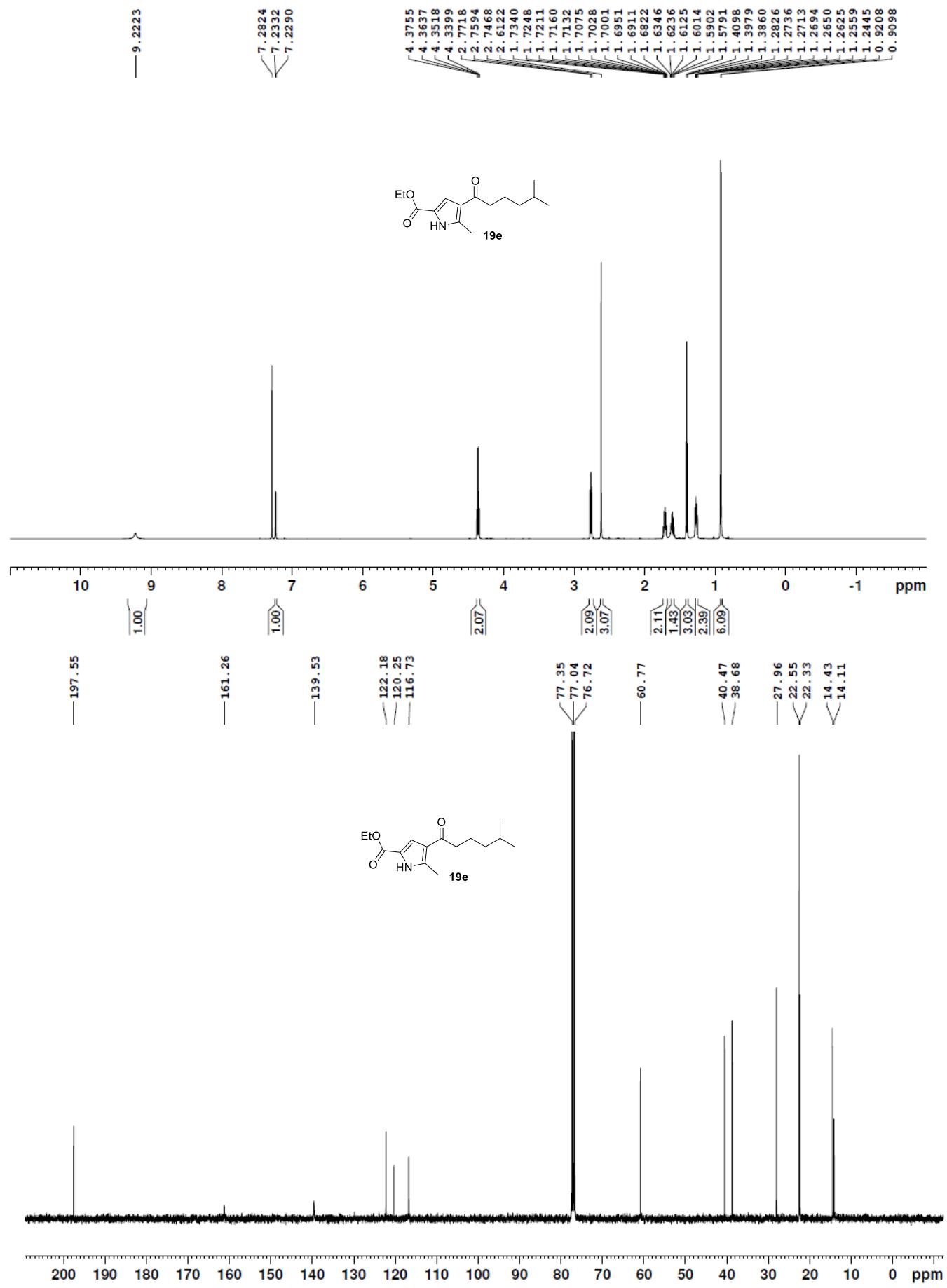


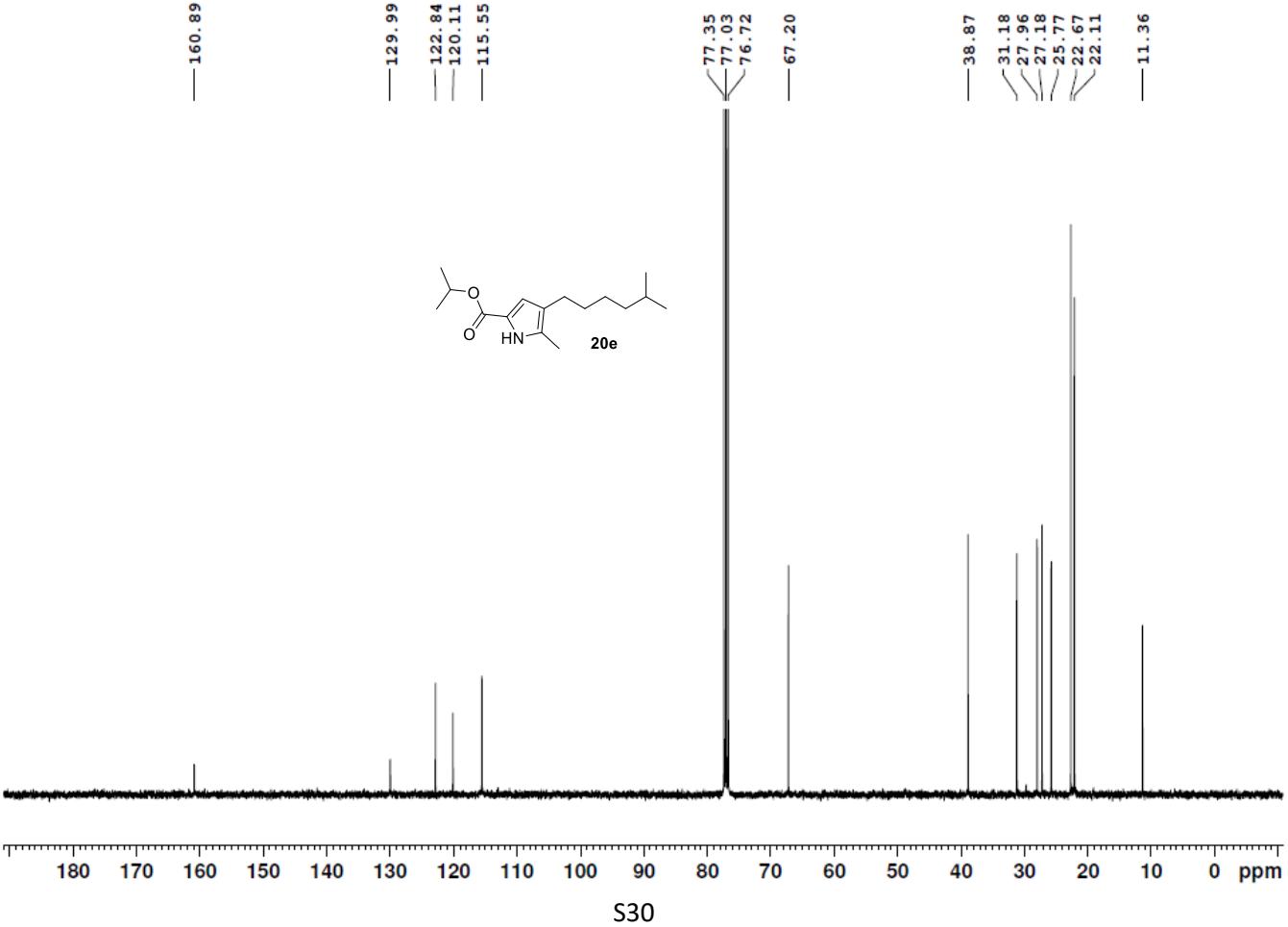
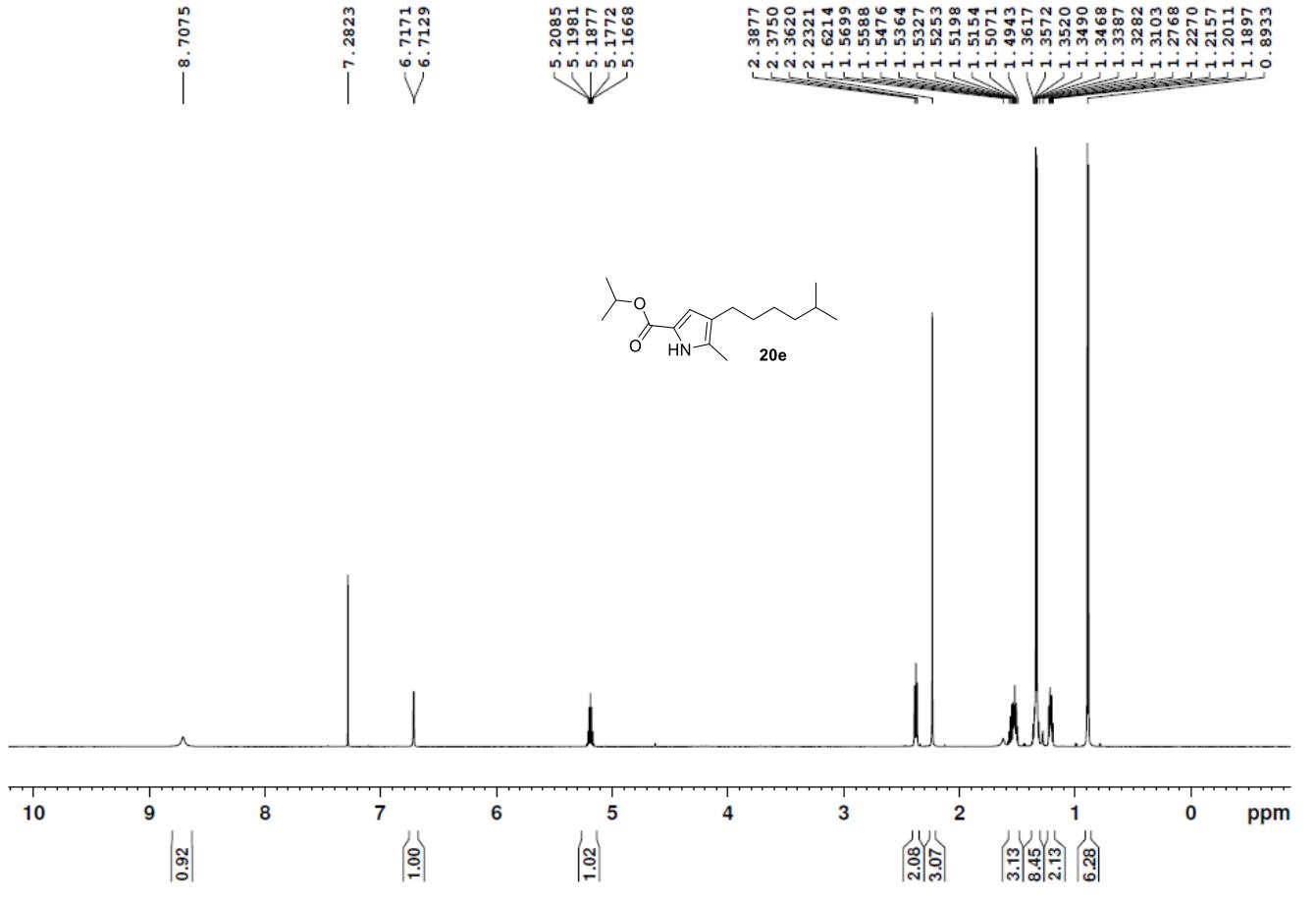


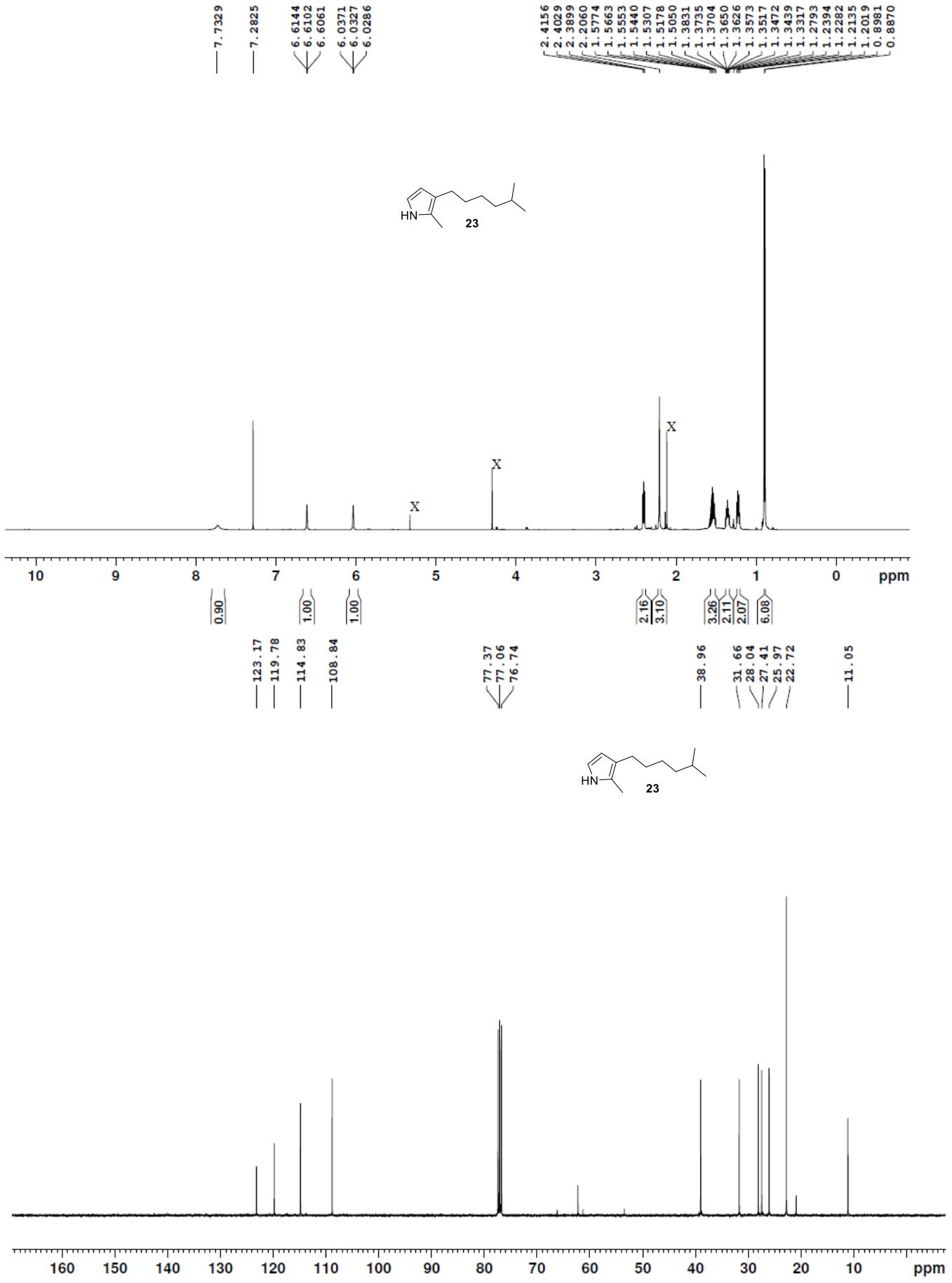


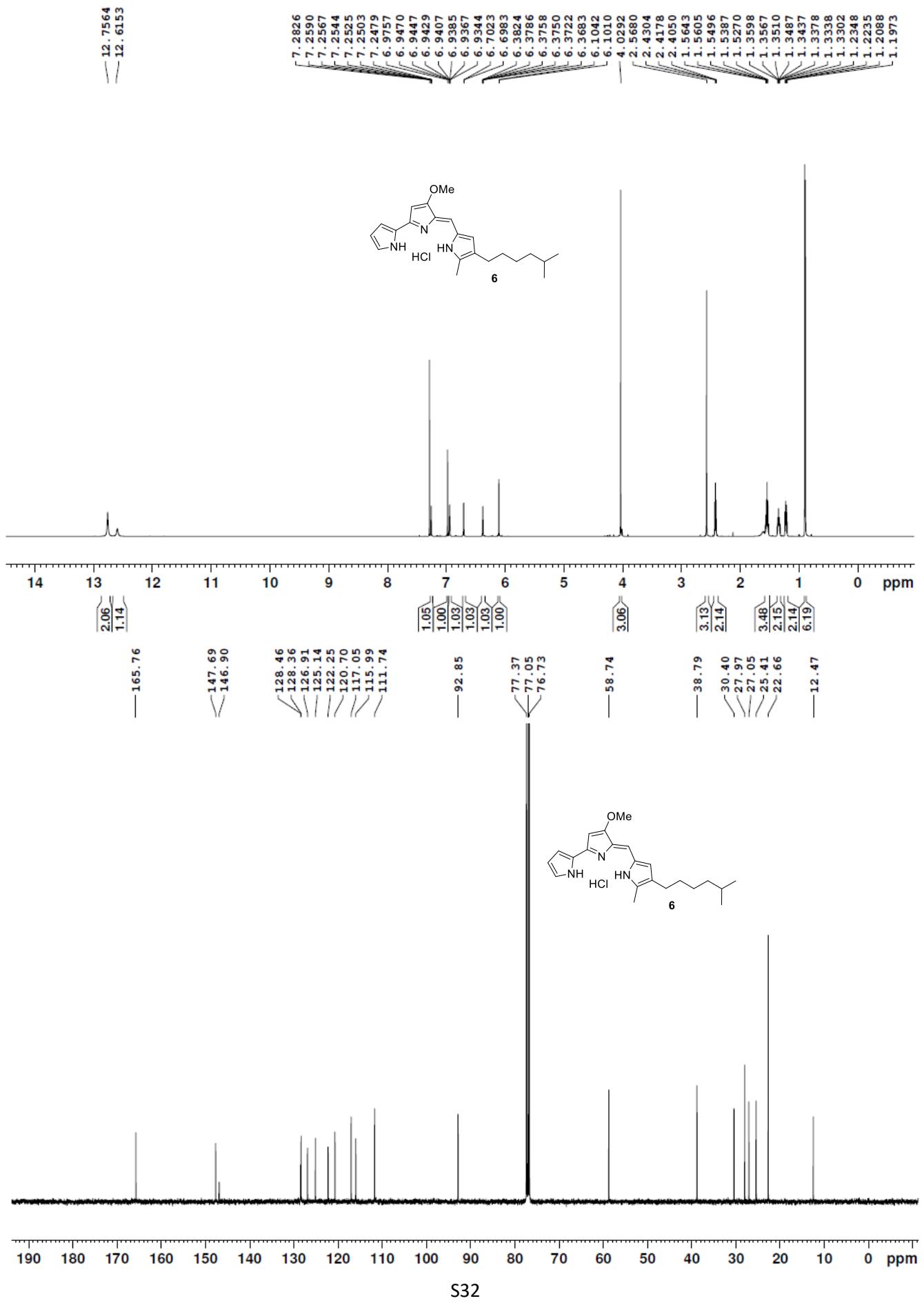


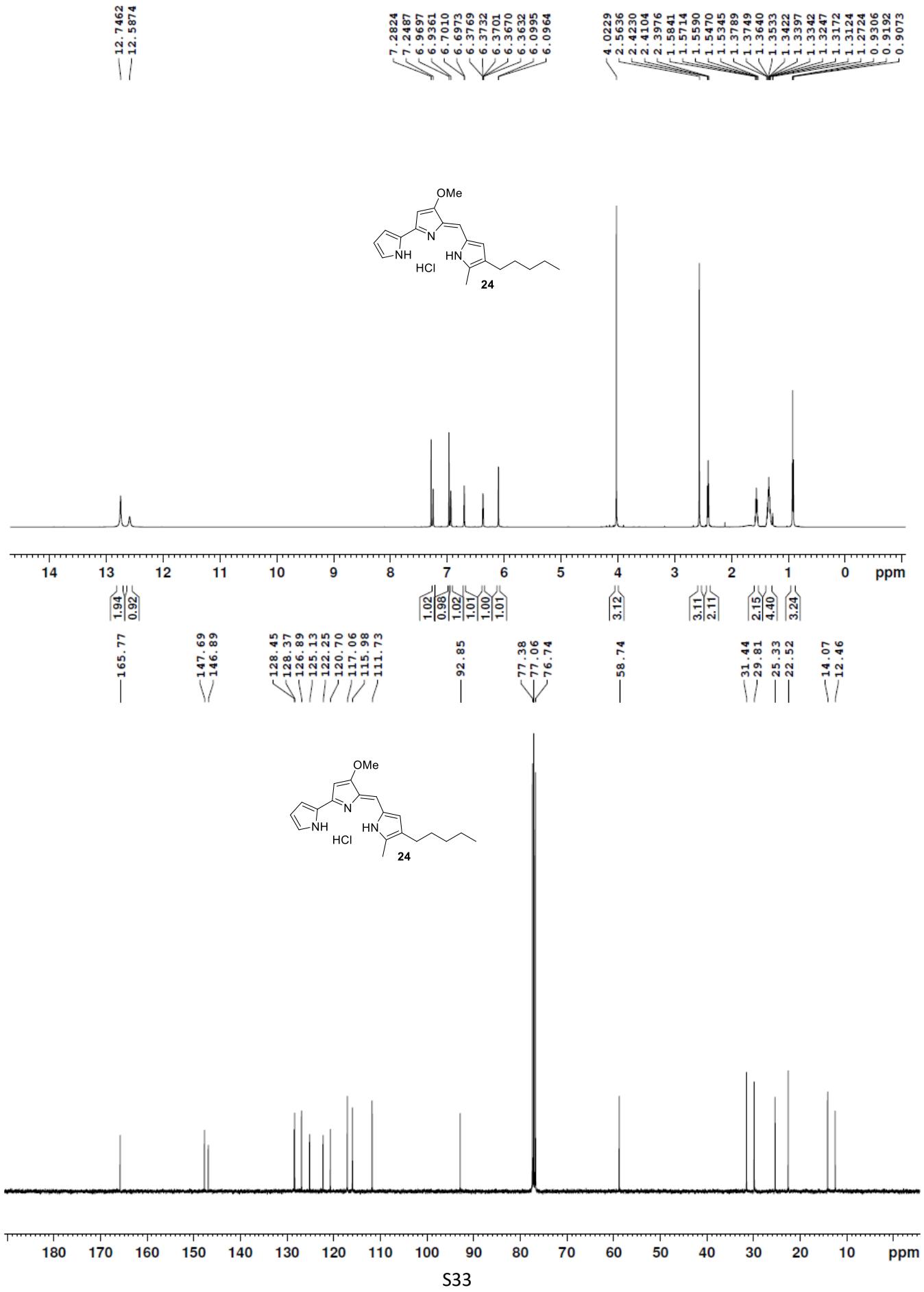


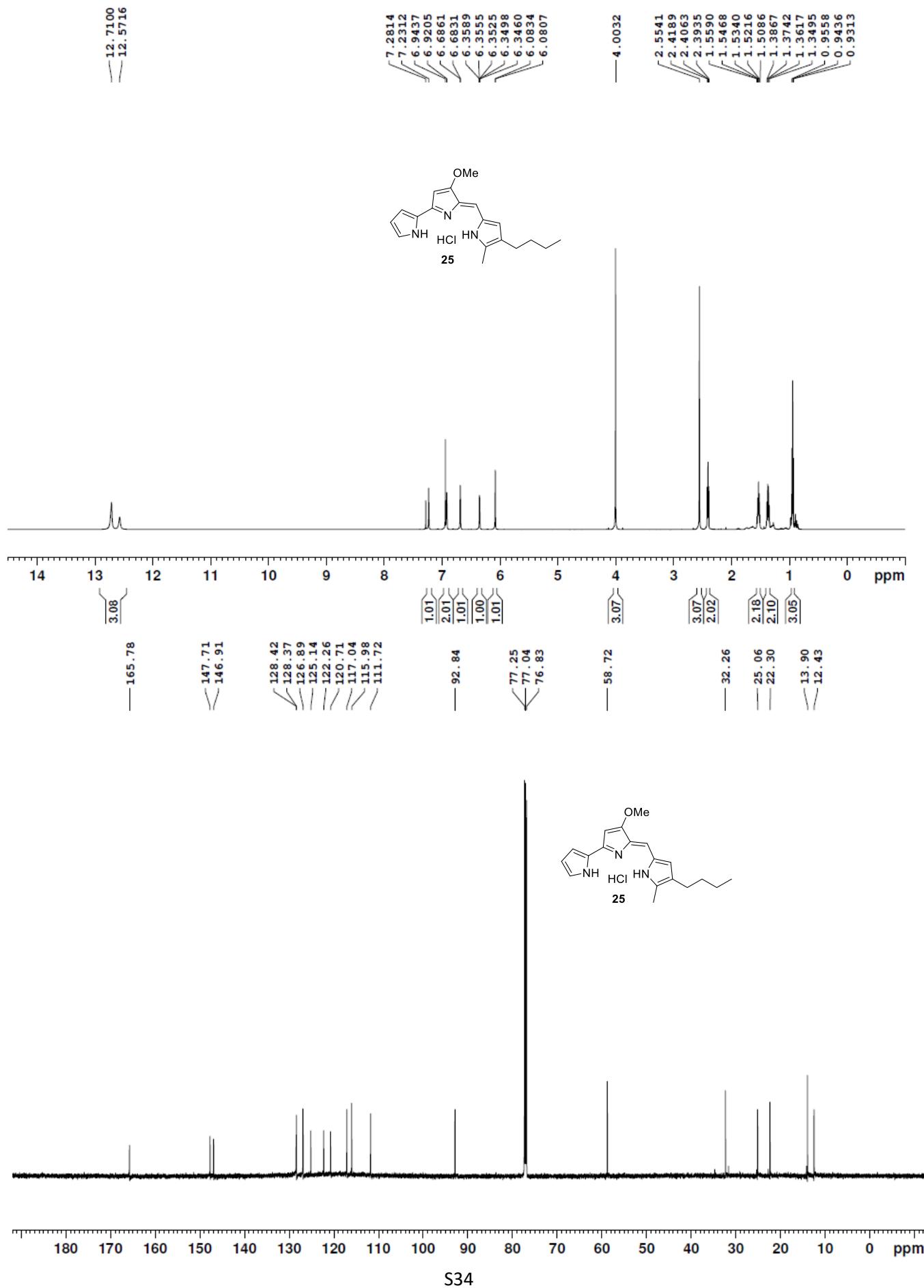


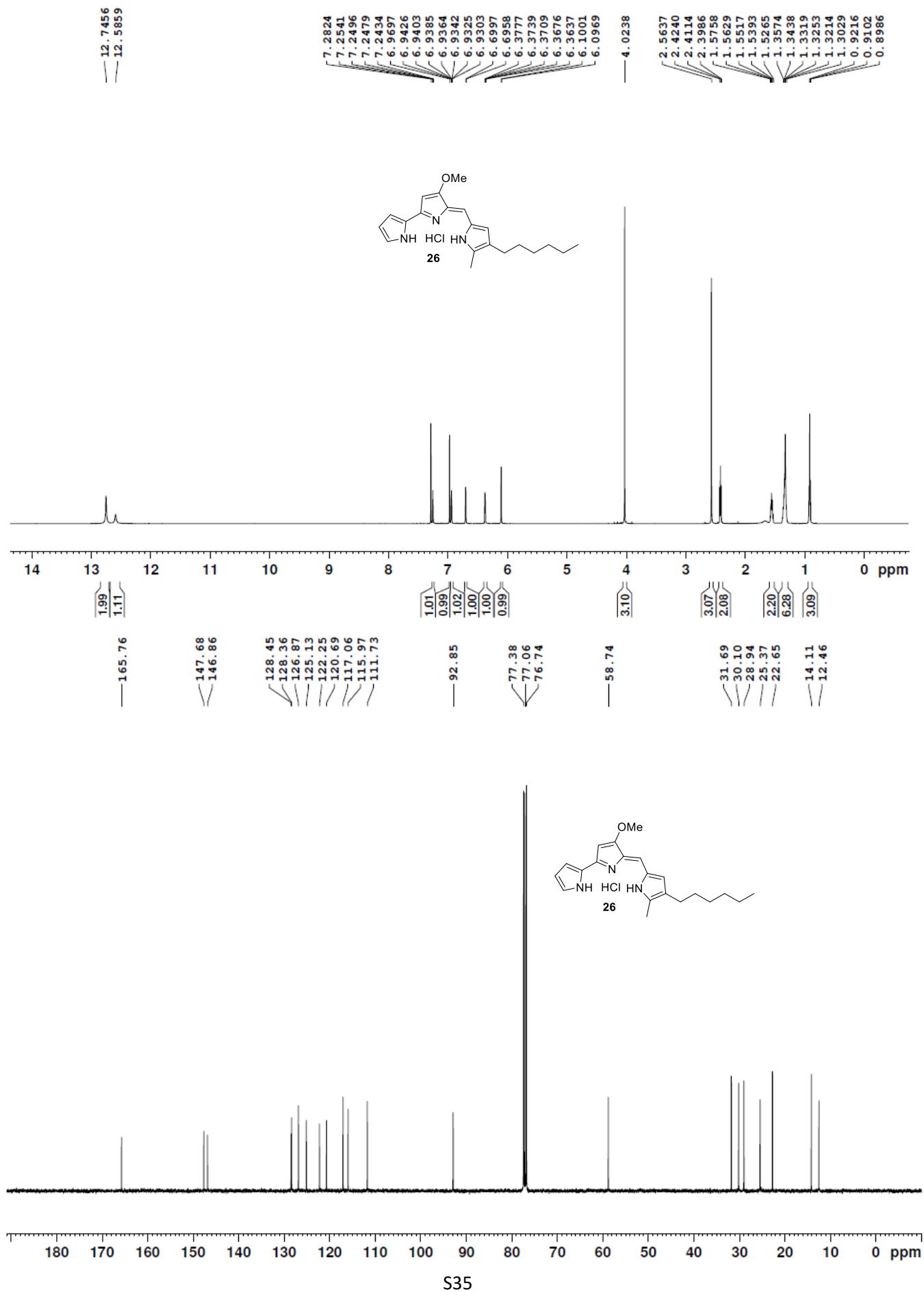


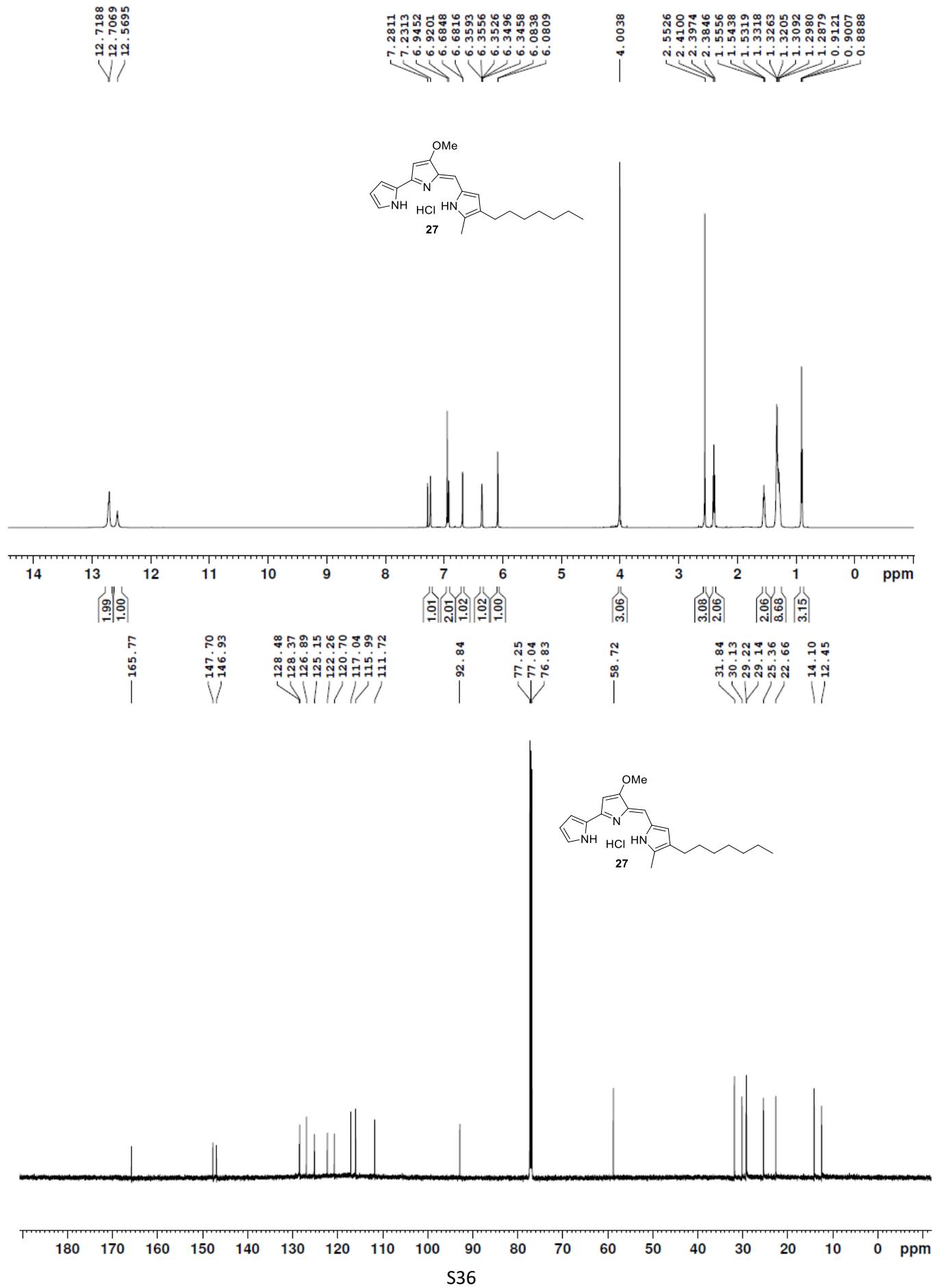


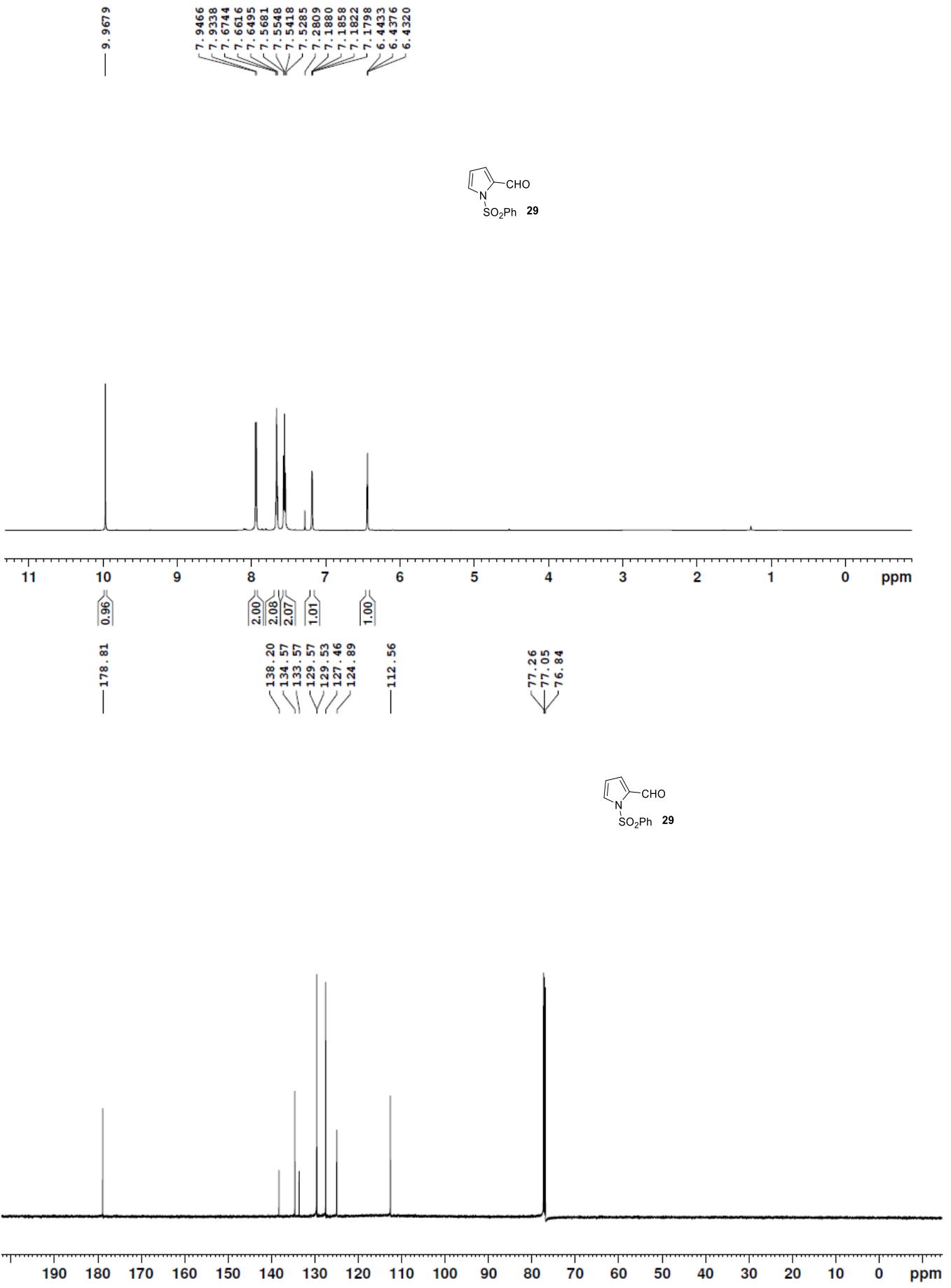


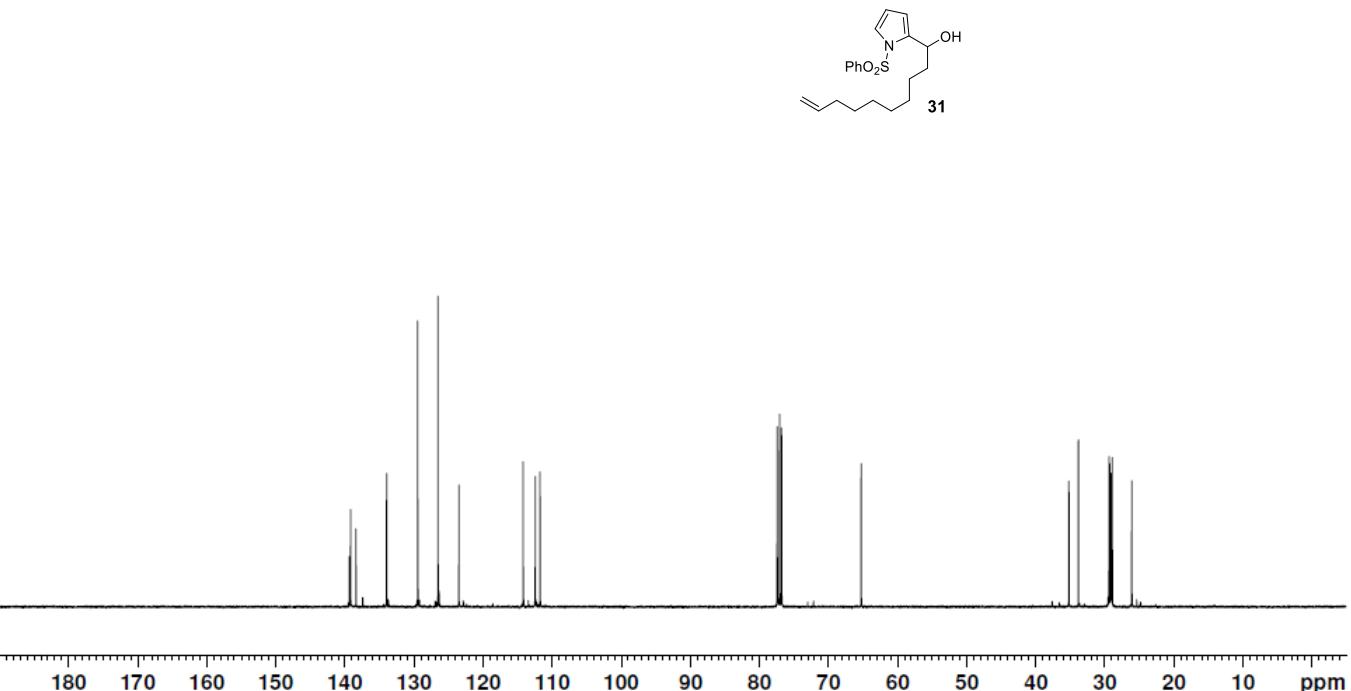
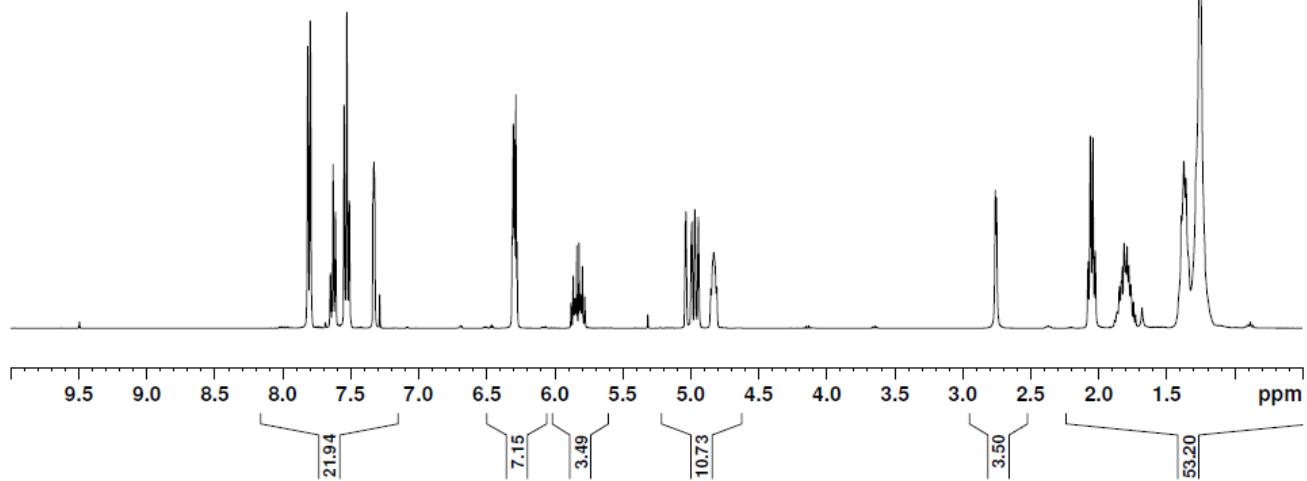
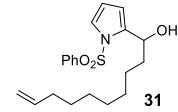


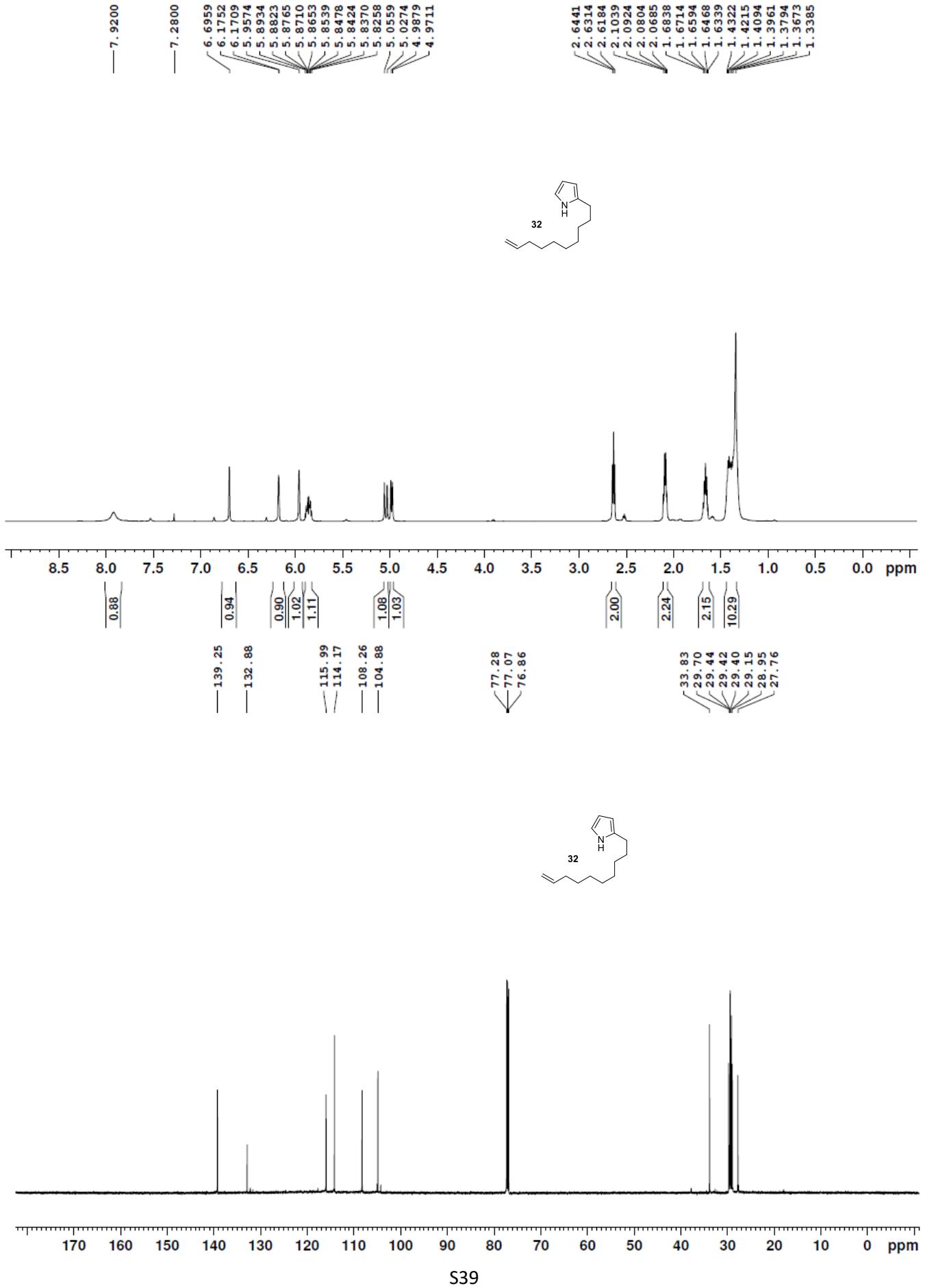


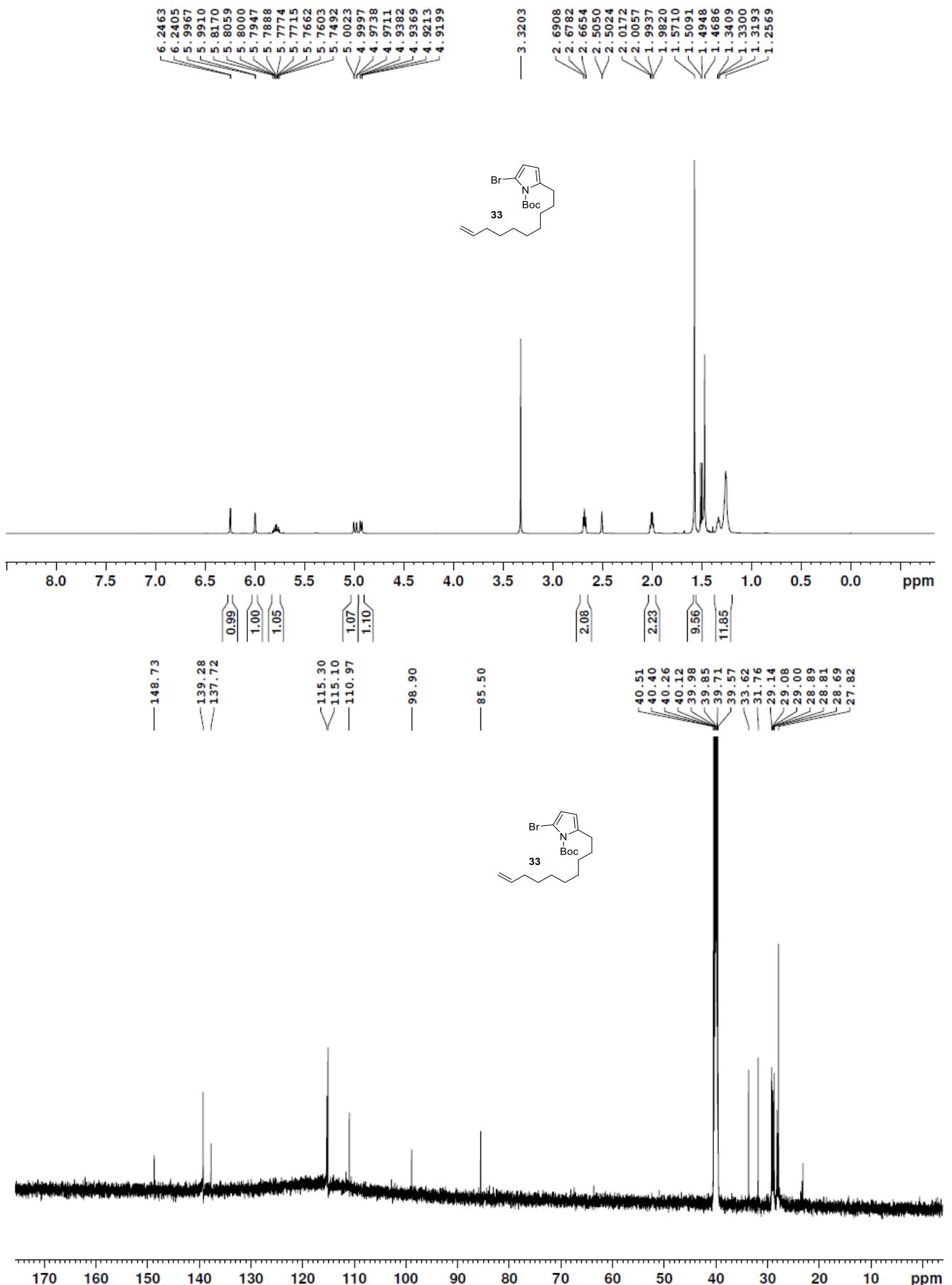


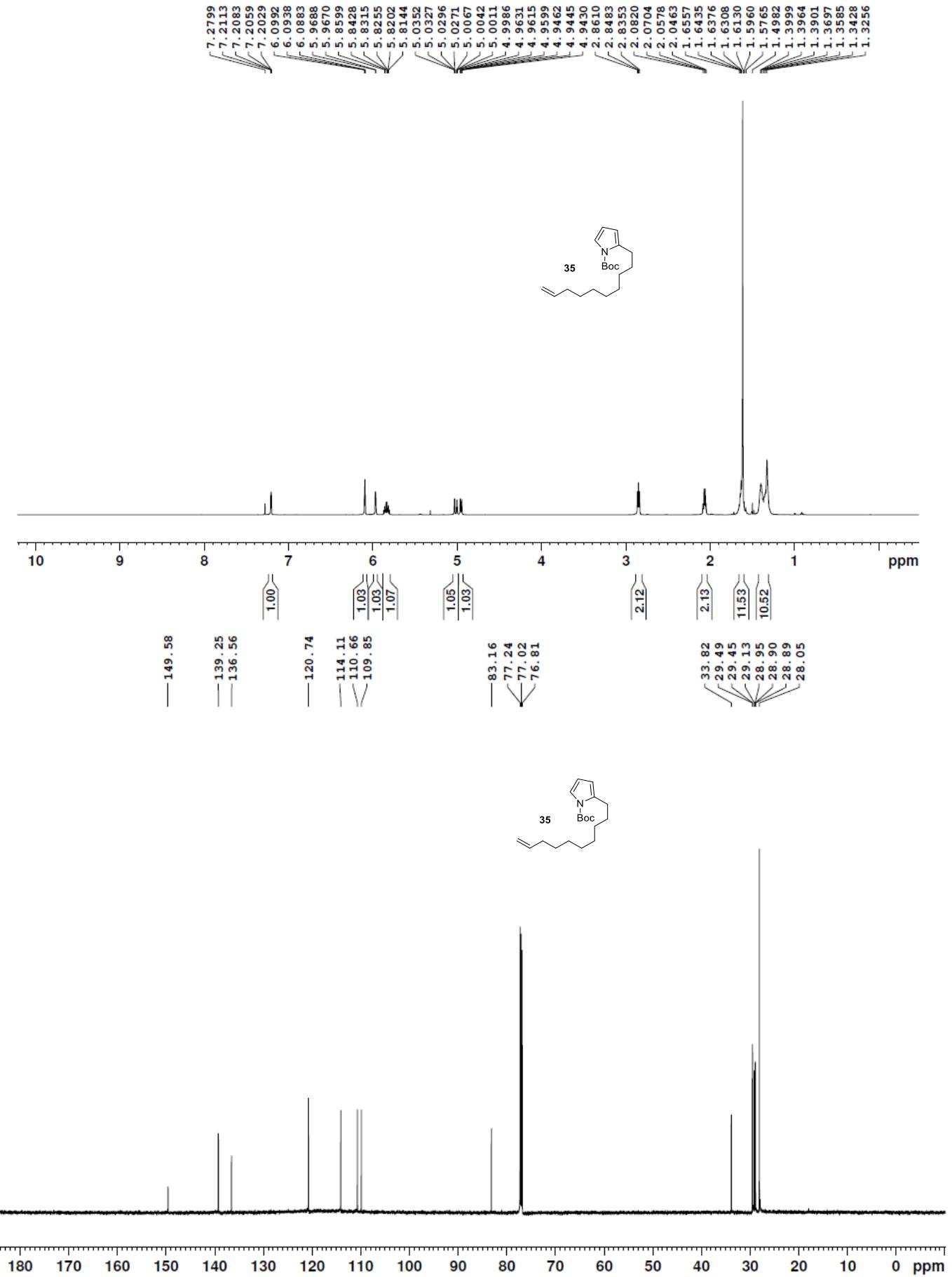


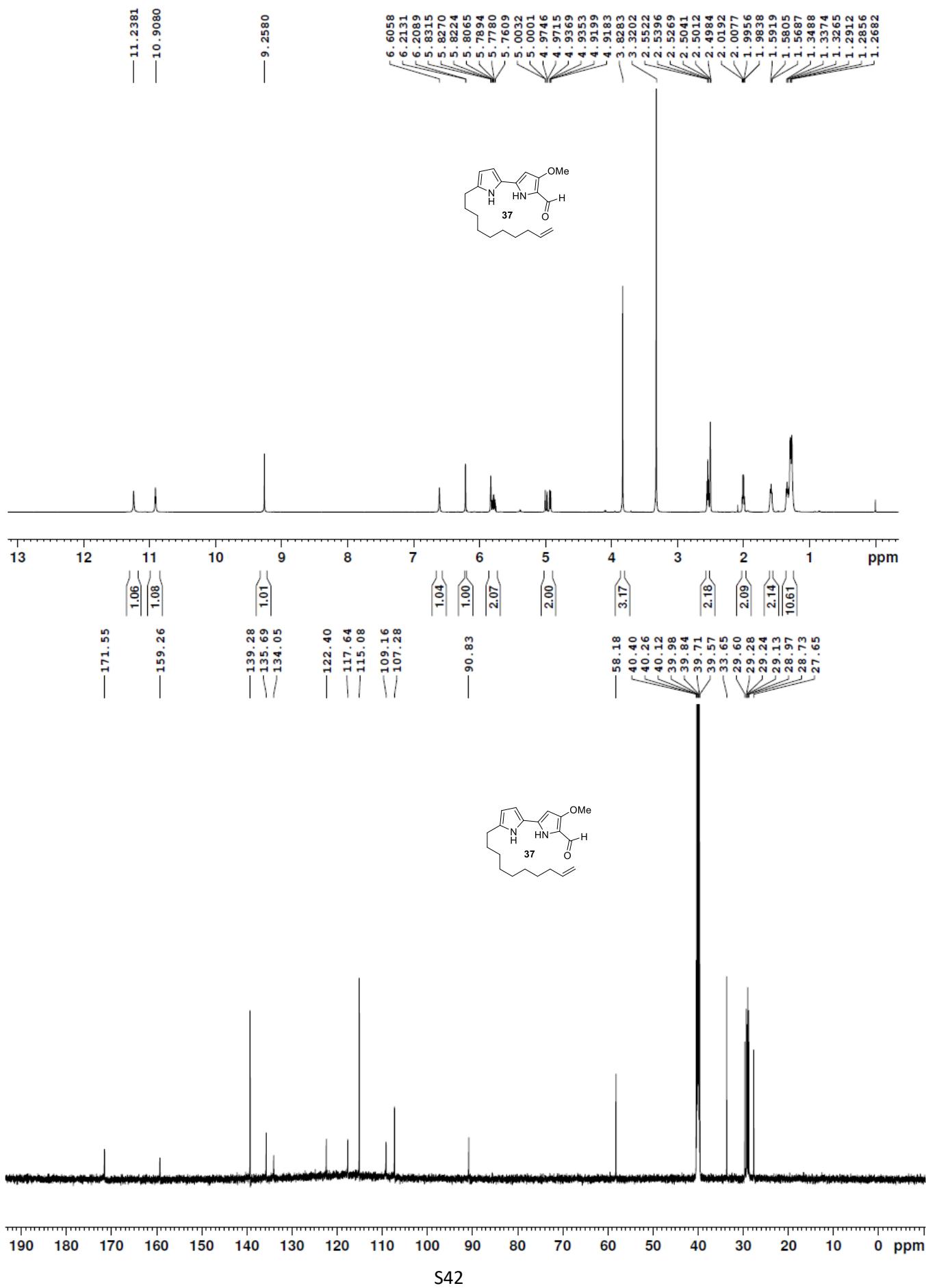


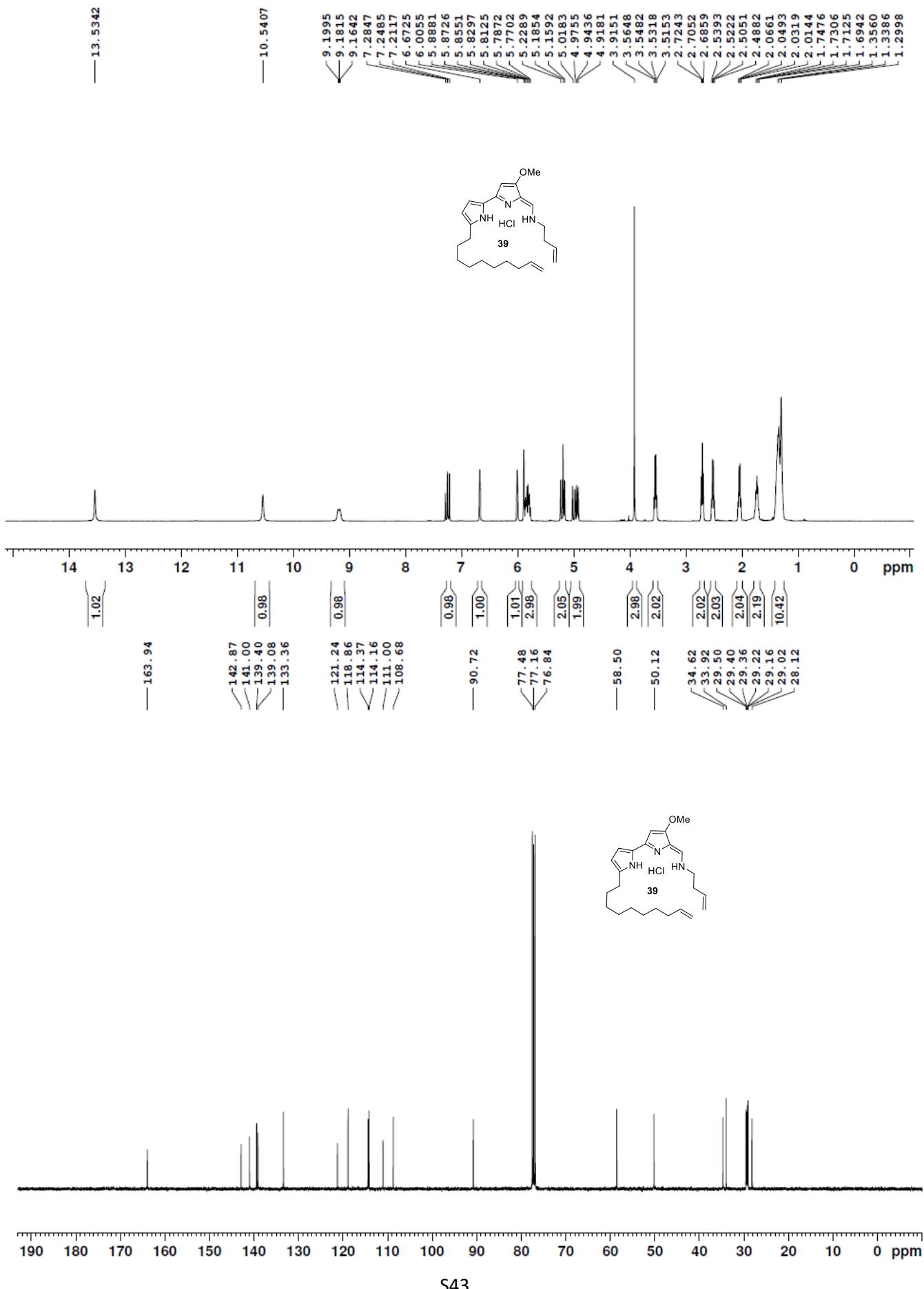


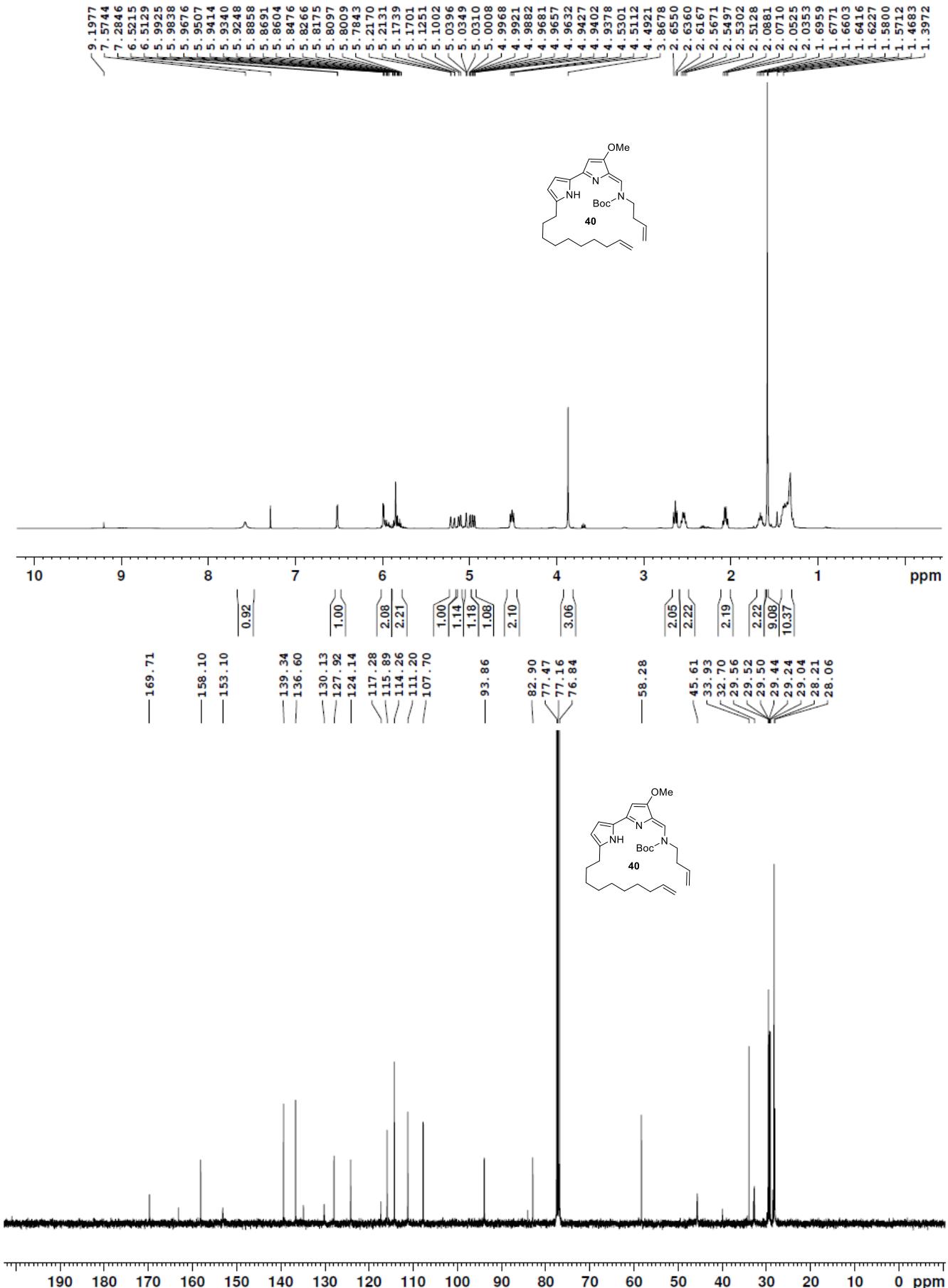


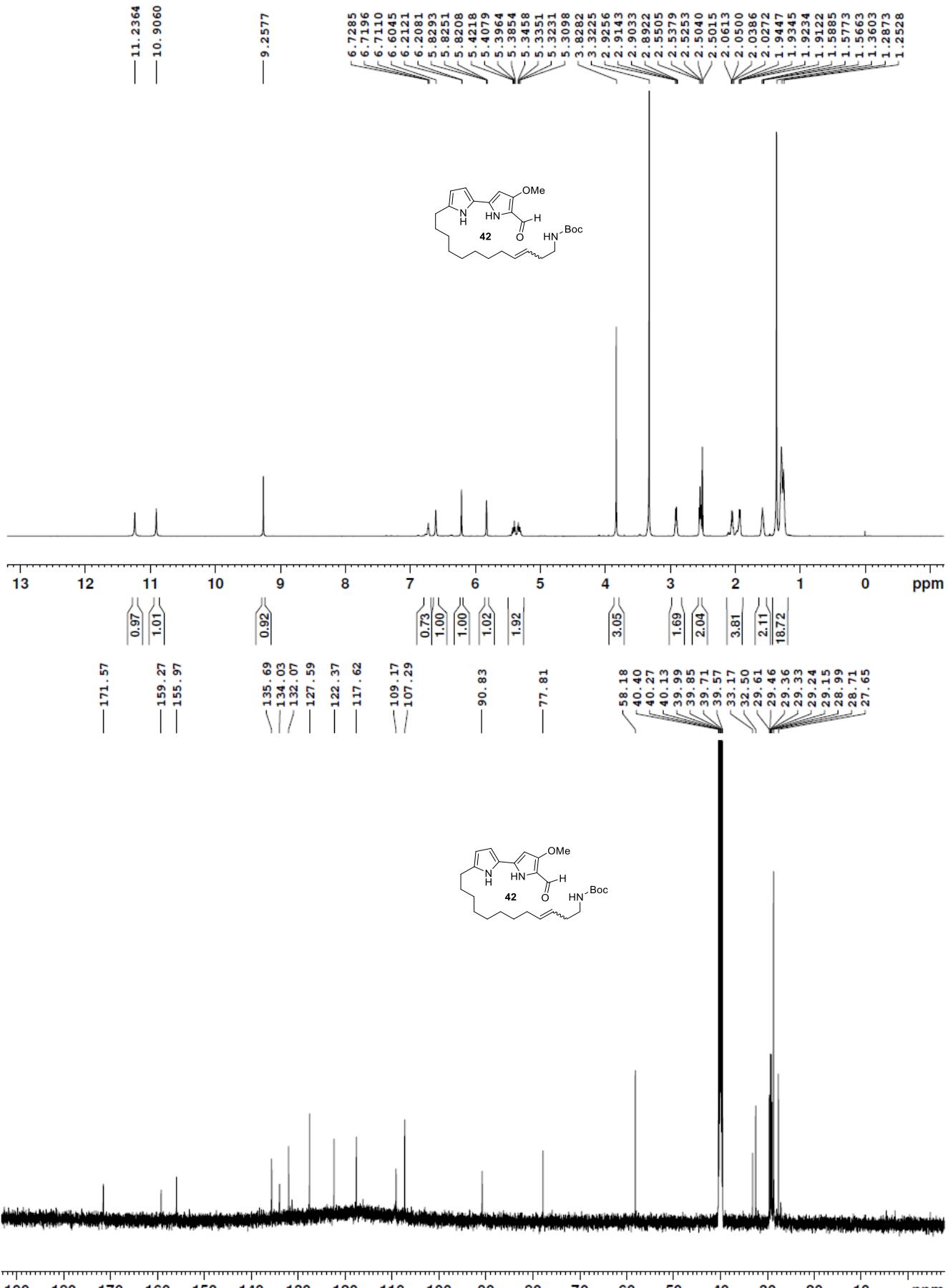


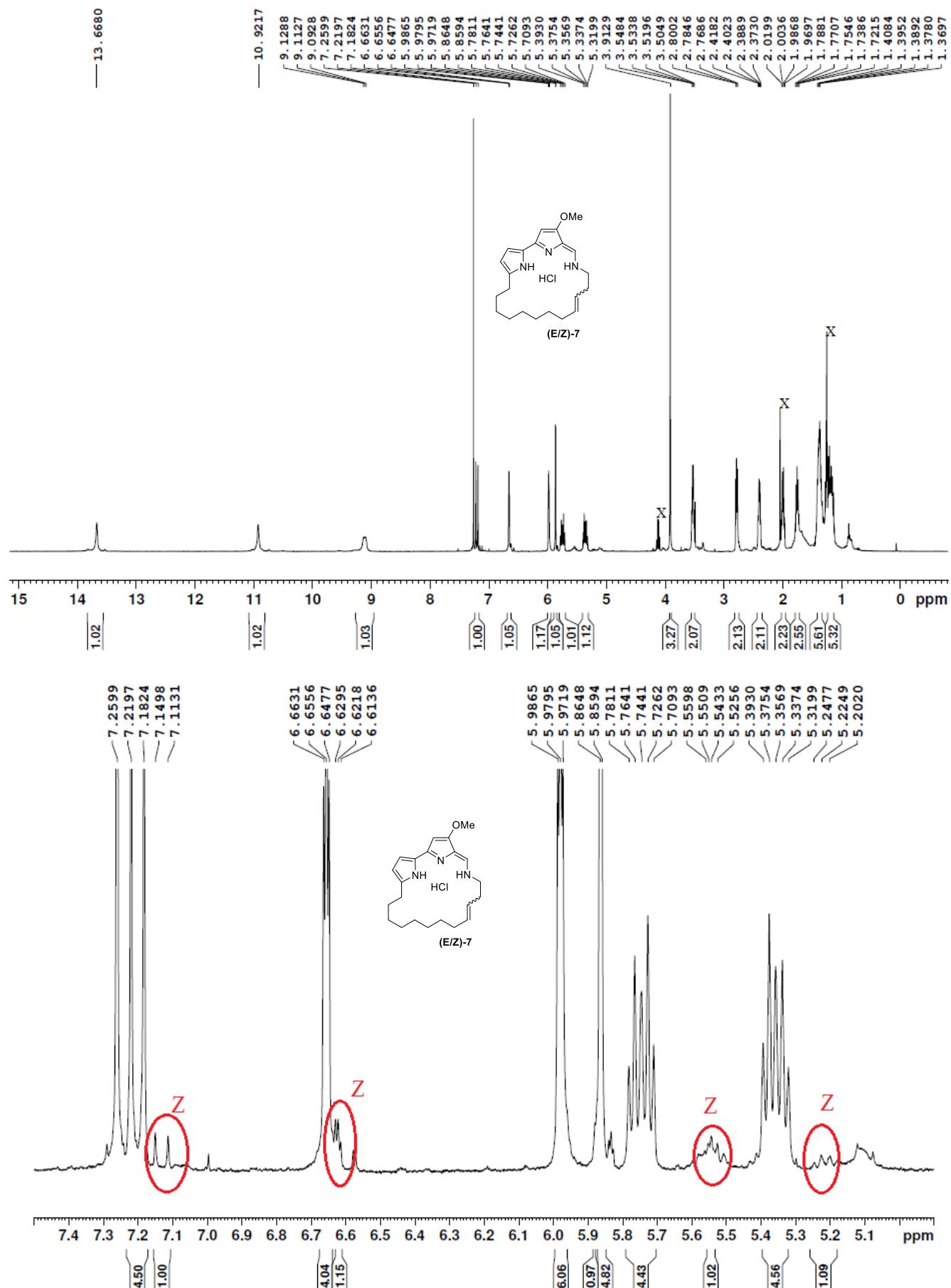


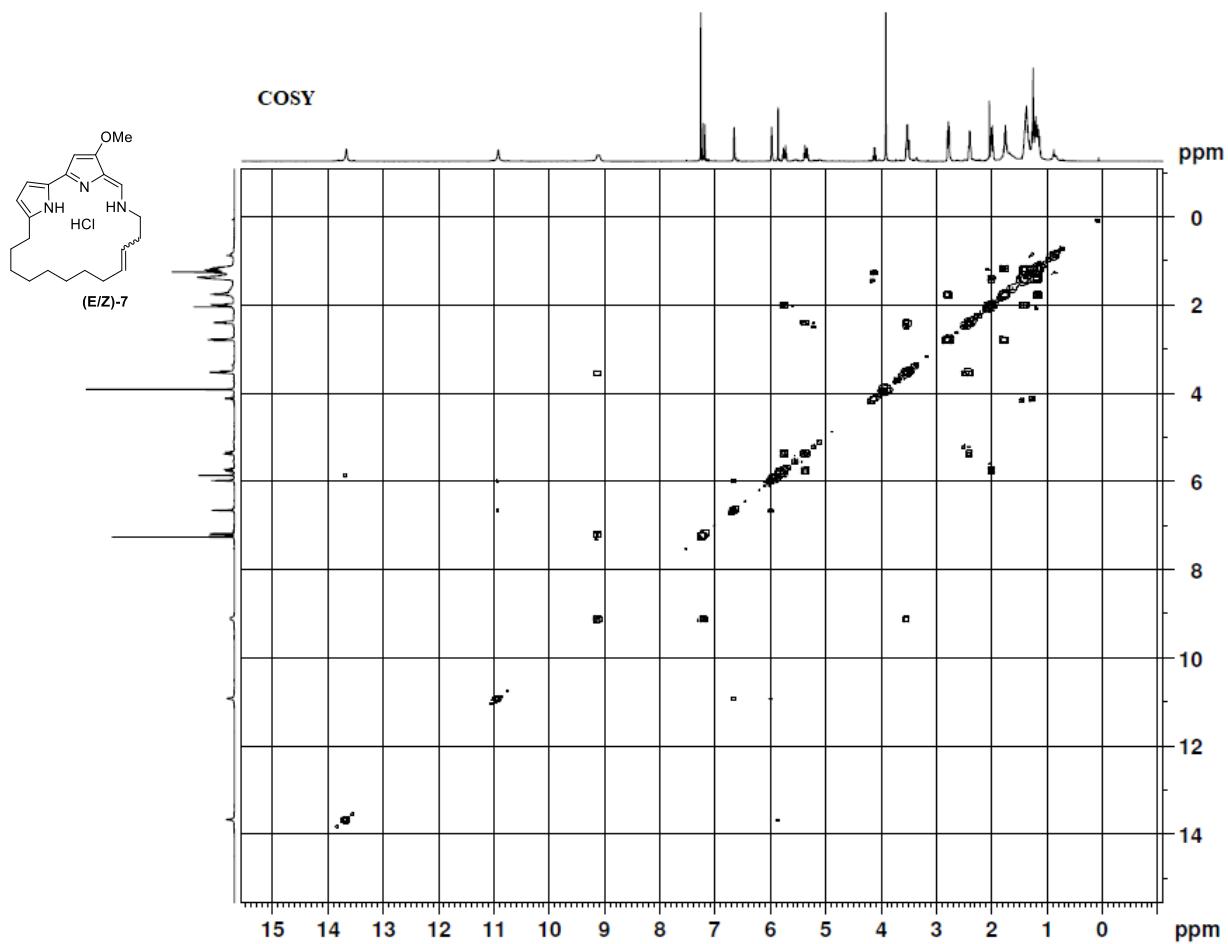
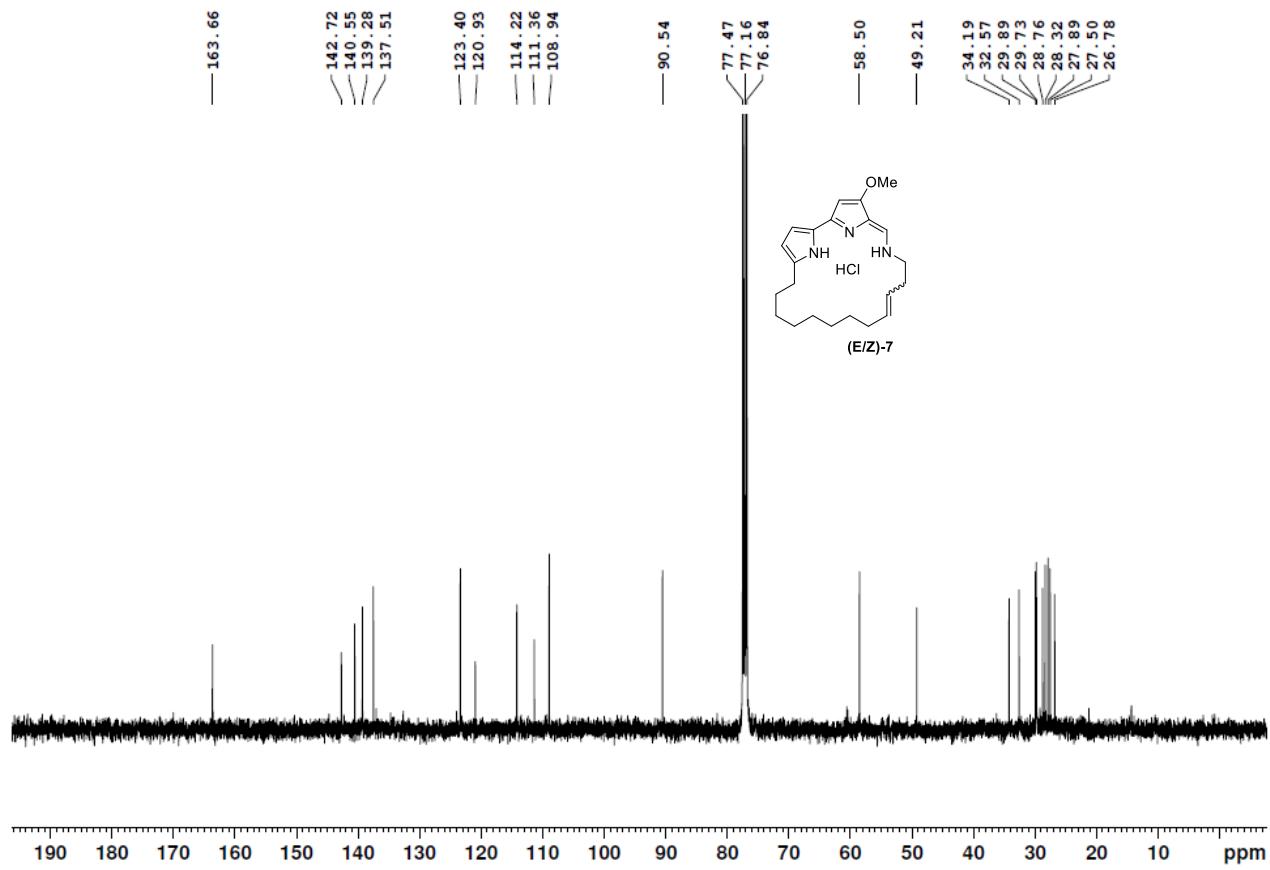












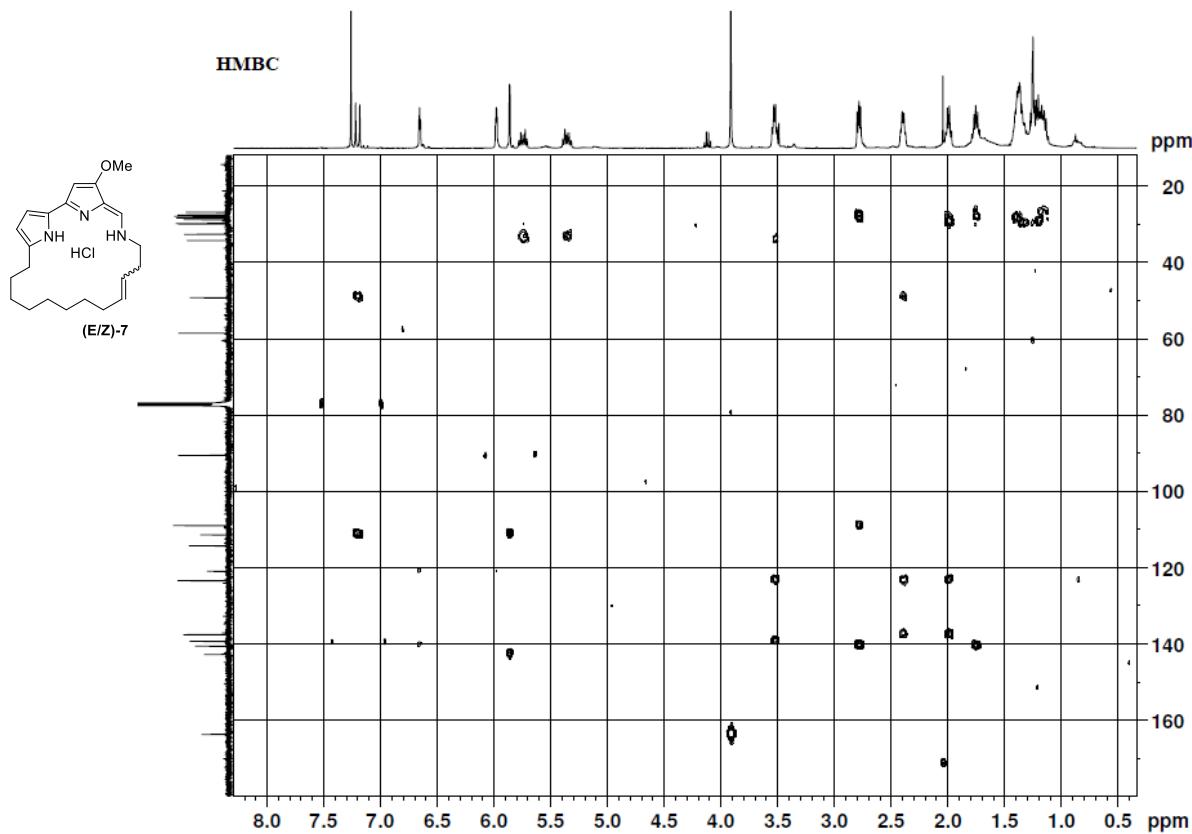
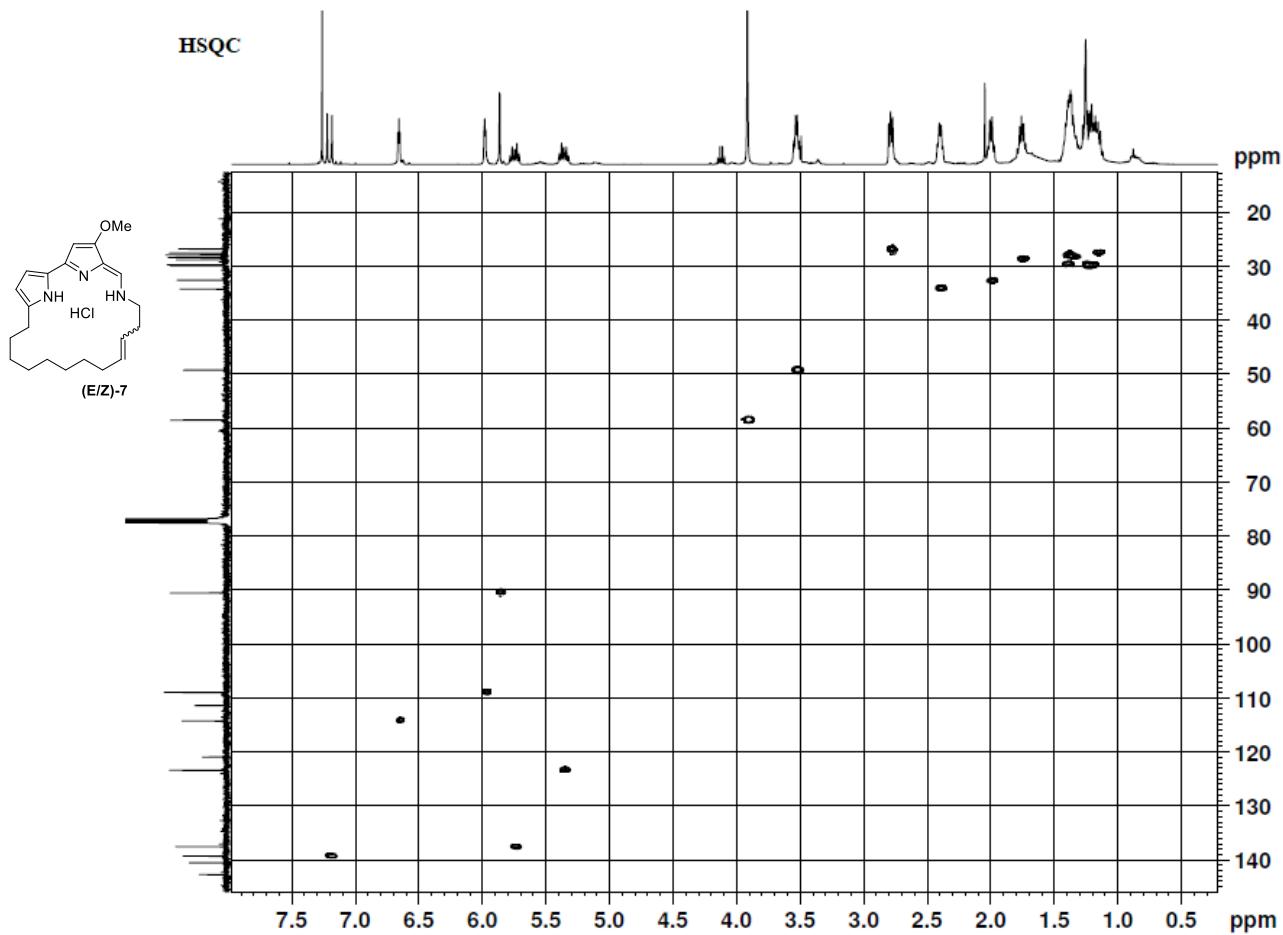
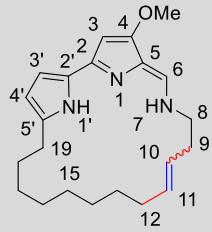
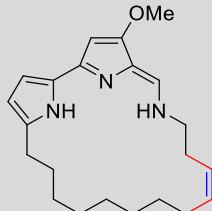


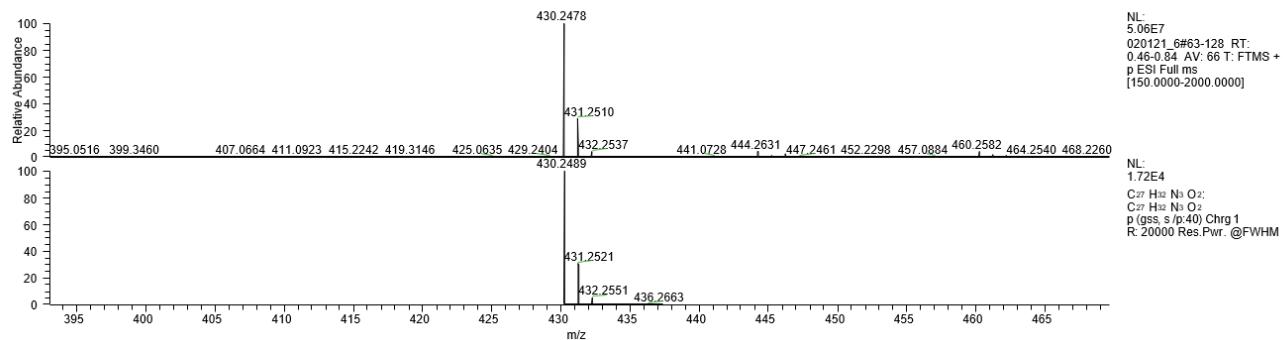
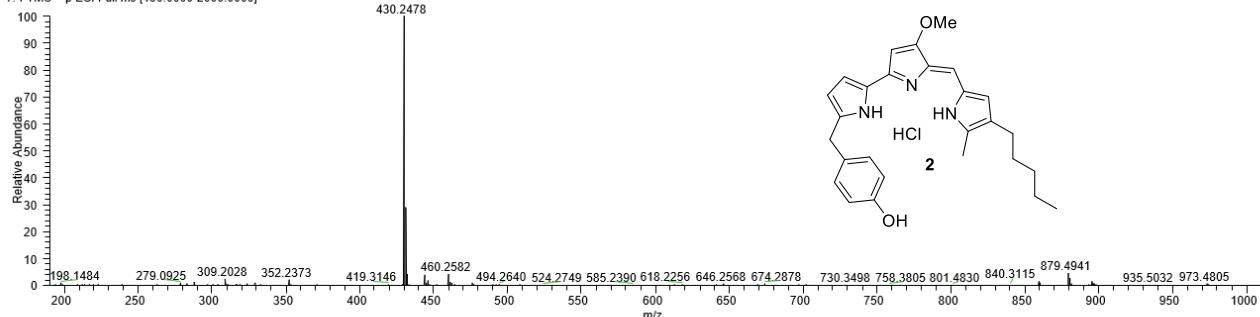
Table S1. Comparison of ^1H and ^{13}C NMR between major isomer of synthetic compound (*E/Z*)-7 and natural product 7*

Position	 Tambjamine-MYP1 ((<i>E/Z</i>)-7) (Synthetic compound)		 Tambjamine-MYP1 (Natural compound)	
	Major isomer (<i>E</i> or <i>trans</i>)		<i>Z</i> or <i>cis</i> -isomer	
	δ_{H} (<i>J</i> in Hz)	δ_{C}	δ_{H} (<i>J</i> in Hz)	δ_{C}
1' (NH)	10.92, s	-	10.74	-
2'	-	120.9	-	
3'	6.65, t (3.0)	114.2	6.63, s	113.5
4'	5.97, t (3.0)	108.9	5.99, s	109.7
5'	-	140.5	-	
1 (NH)	13.66, s	-		-
2	-	142.7	-	142.1
3	5.85, d (2.2)	90.5	5.87	90.4
4	-	163.7	-	163.0
5	-	111.4	-	110.1
6	7.20, d (14.9)	139.3	7.14, d (14.8)	140.1
7 (NH)	9.11, m	-	9.29, br d	-
8	3.53, q (5.8)	49.2	3.54, br	51.4
9	2.39, q, (6.3)	34.2	2.50, m	27.8
10	5.35, dt (15.2, 6.8)	123.4	5.22, dt (10.9, 7.7)	123.2
11	5.74, dt (15.2, 7.0)	137.5	5.55, dt (10.9, 7.2)	137.1
12	1.99, q (6.8)	32.6	2.06, m	27.4
13-17	1.40-1.11, m	29.9-27.6	1.29-0.85	28.6-31.8
18	1.75, m	28.8	1.82, m	27.7
19	2.78, t, (6.2)	26.8	2.75, br t (6.1)	27.2
OMe	3.91, s	58.5	3.92, s	58.5

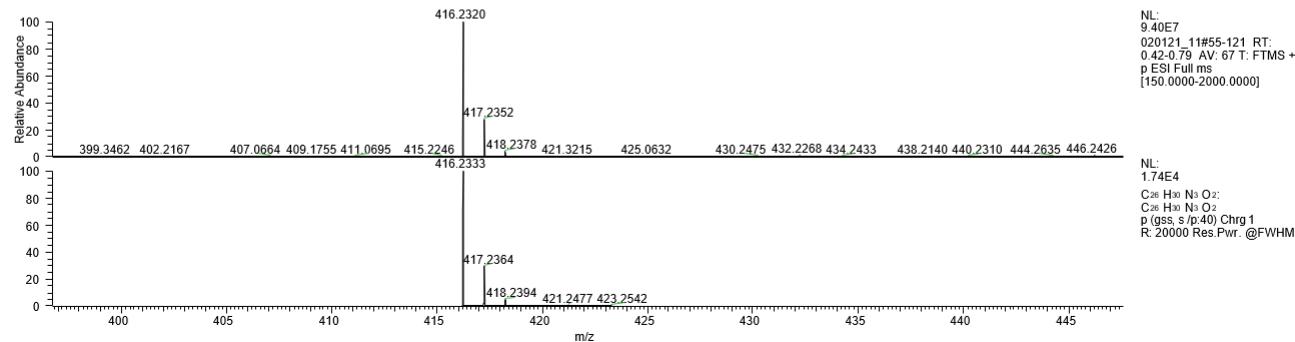
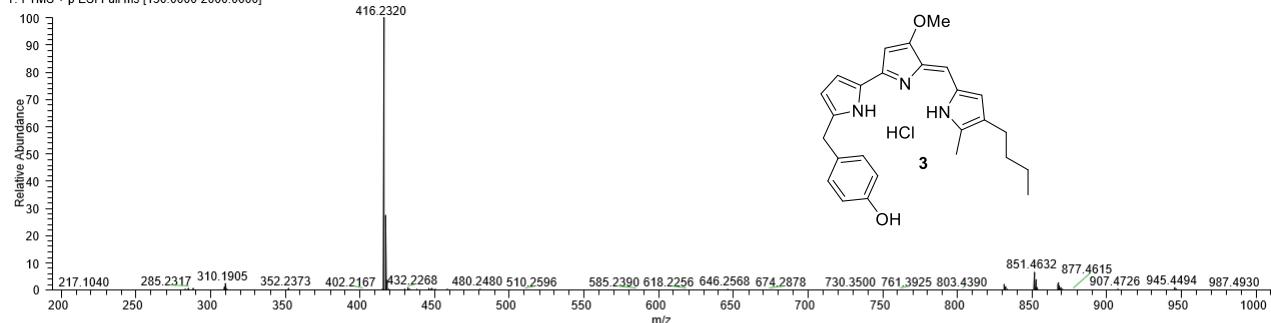
* Picott, K. J.; Deichert, J. A.; deKemp, E. M.; Schatte, G.; Sauriol, F.; Ross, A. C. Isolation and characterization of tambjamine MYP1, a macrocyclic tambjamine analogue from marine bacterium *Pseudoalteromonas citrea*. *Medchemcomm.* **2019**, *10*, 478–483.

HRMS of final compounds

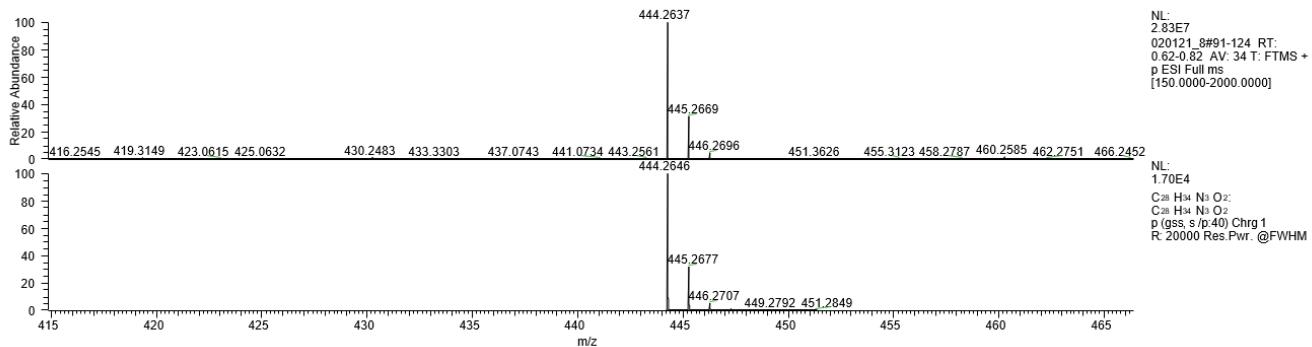
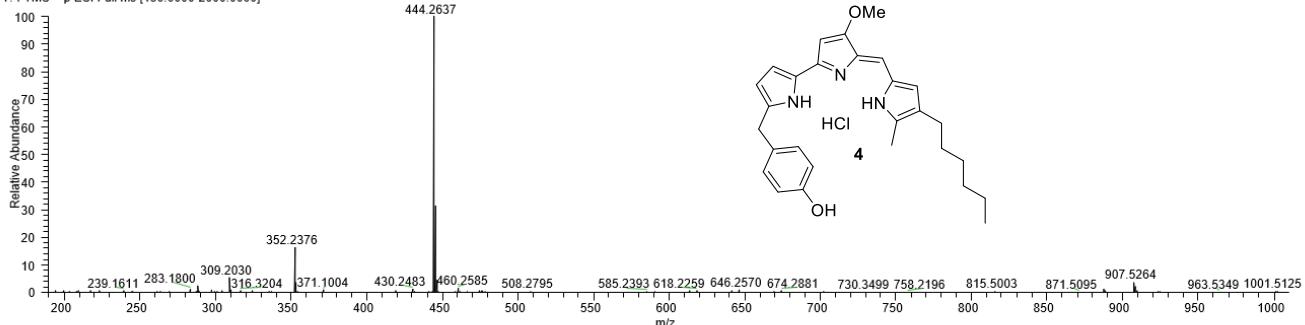
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T: FTMS + p ESI Full ms [150.0000-2000.0000]



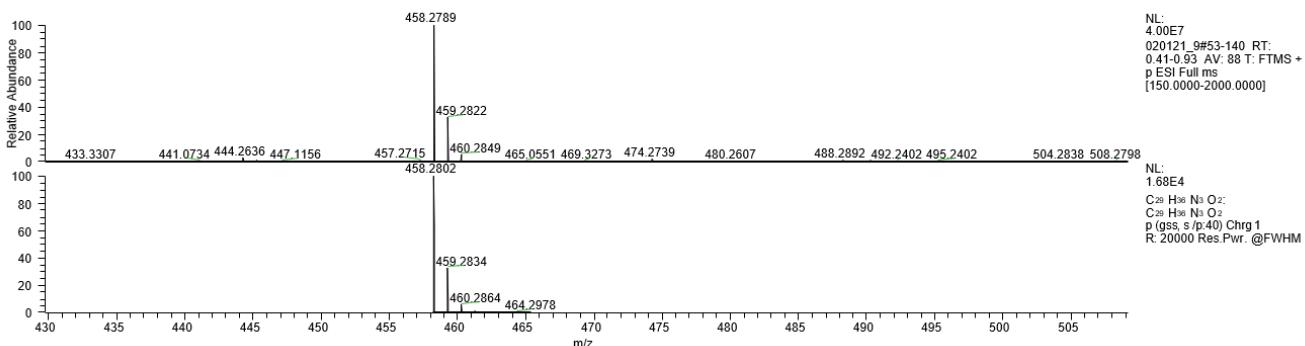
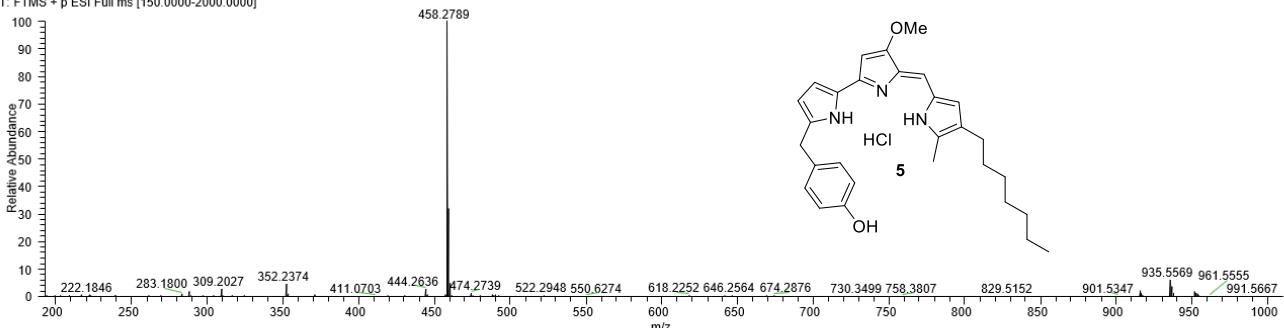
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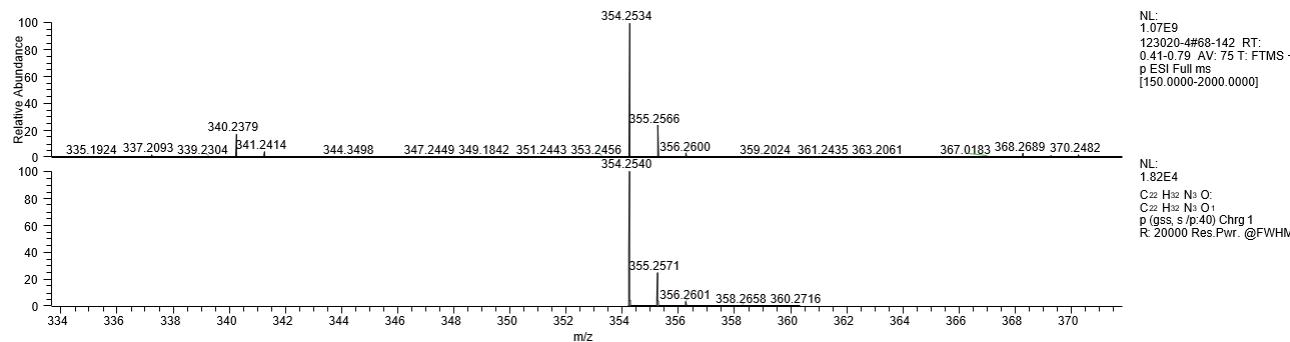
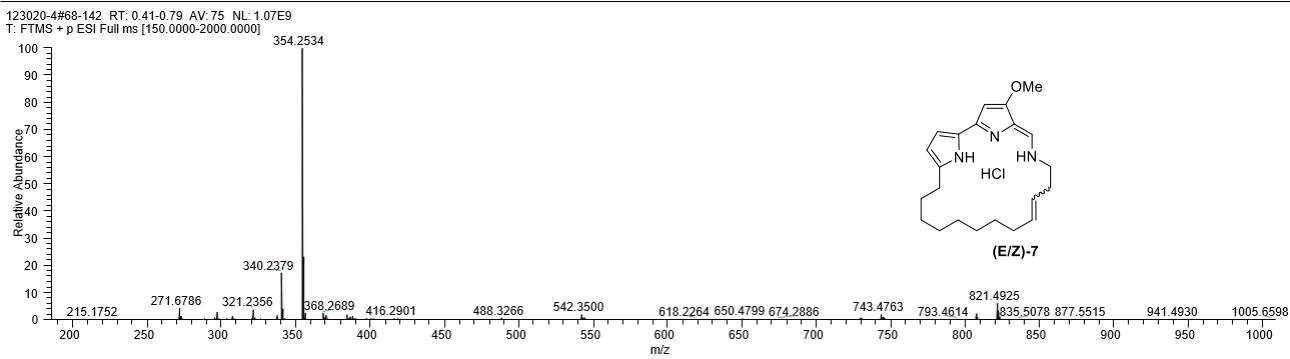
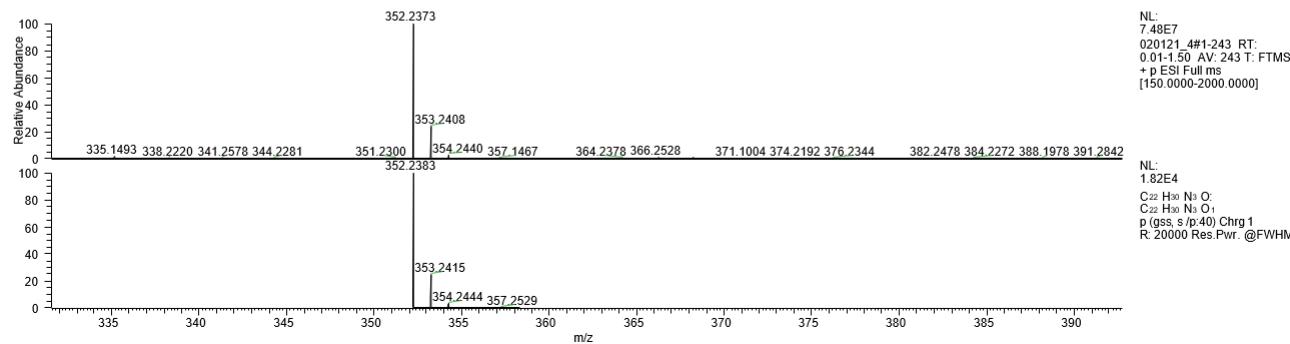
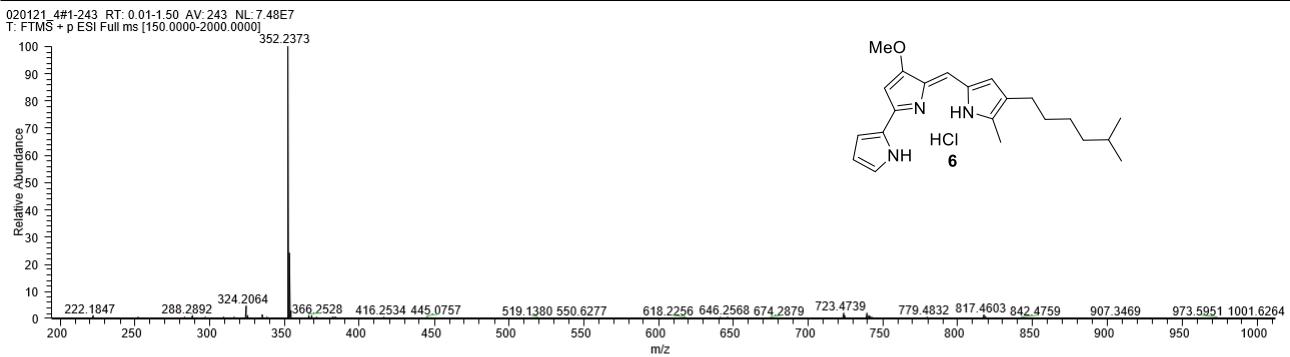


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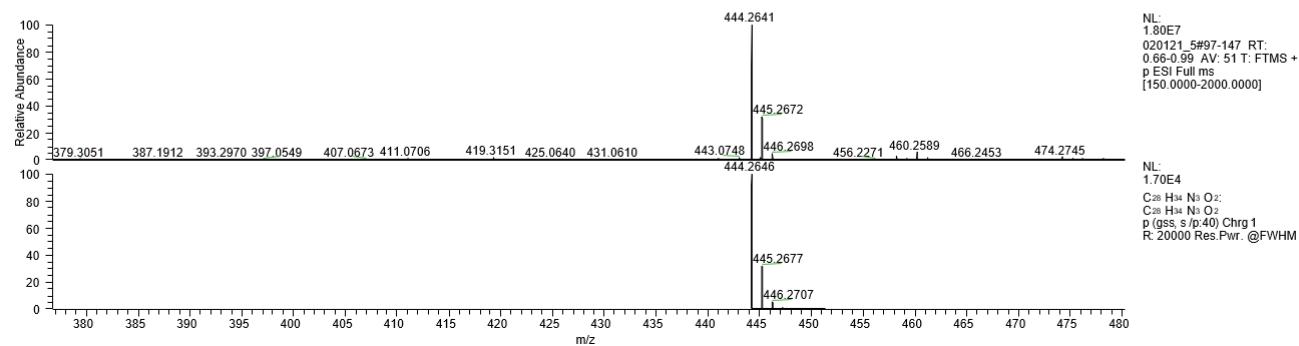
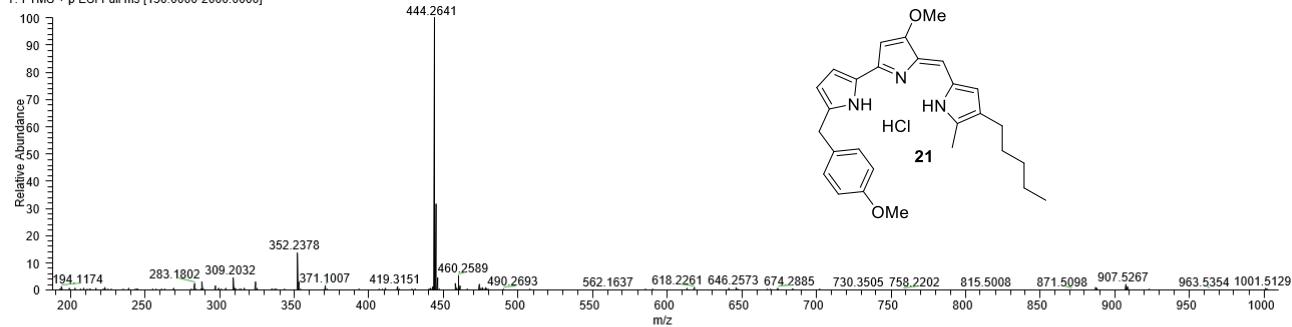


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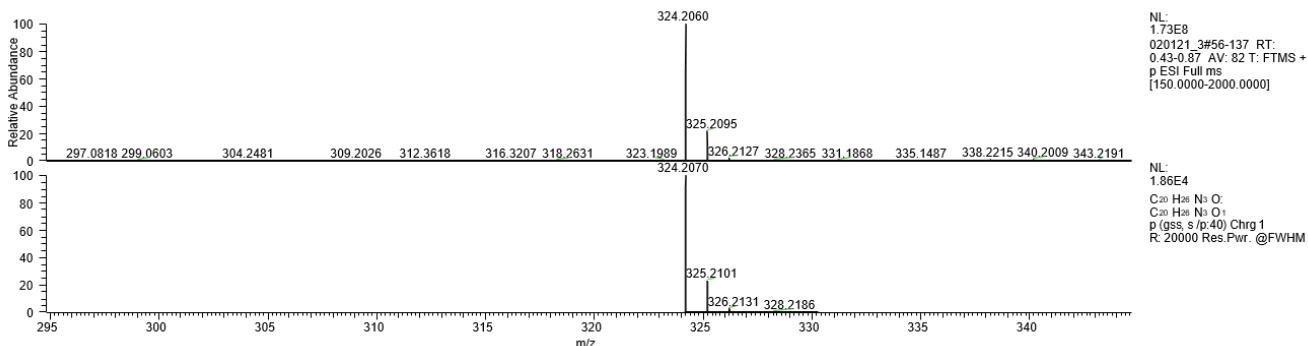
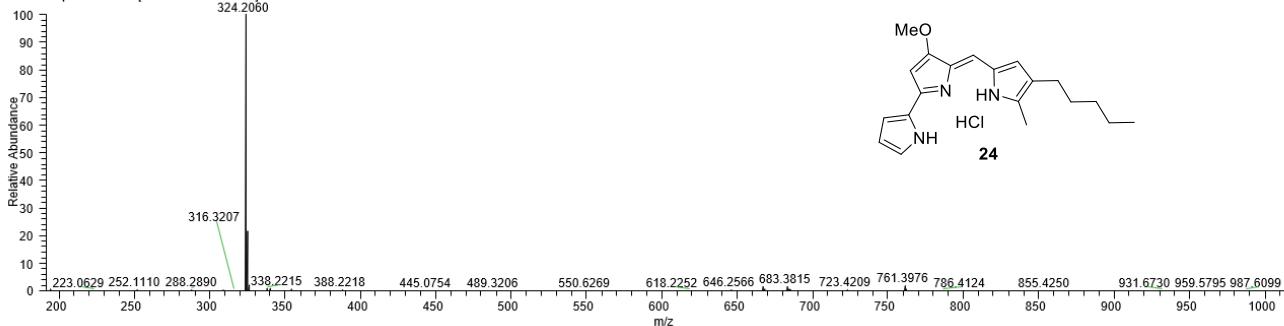




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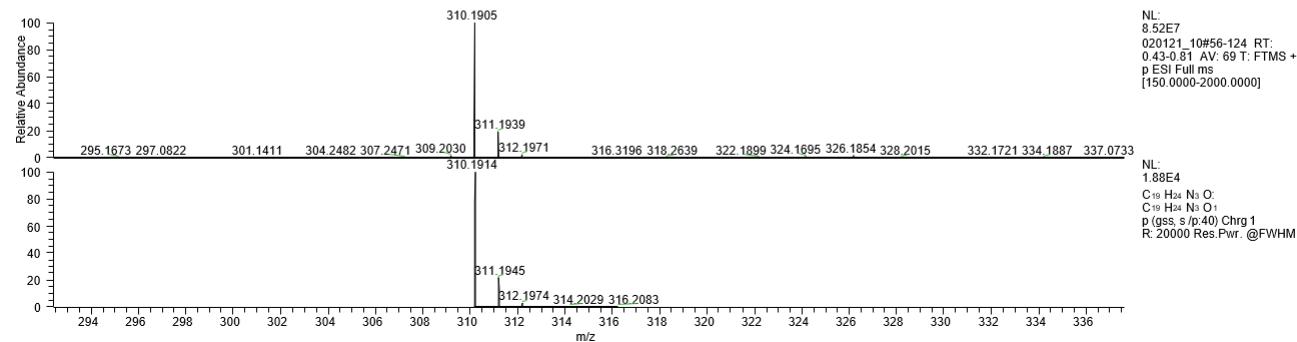
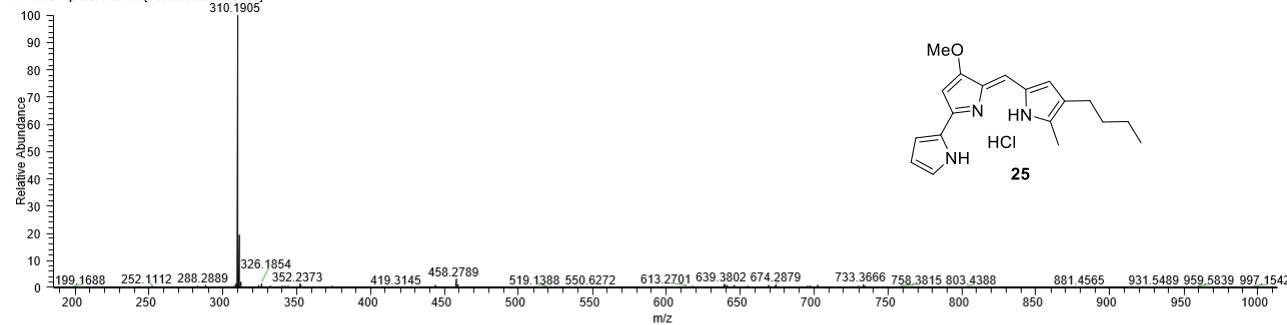


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324.2060



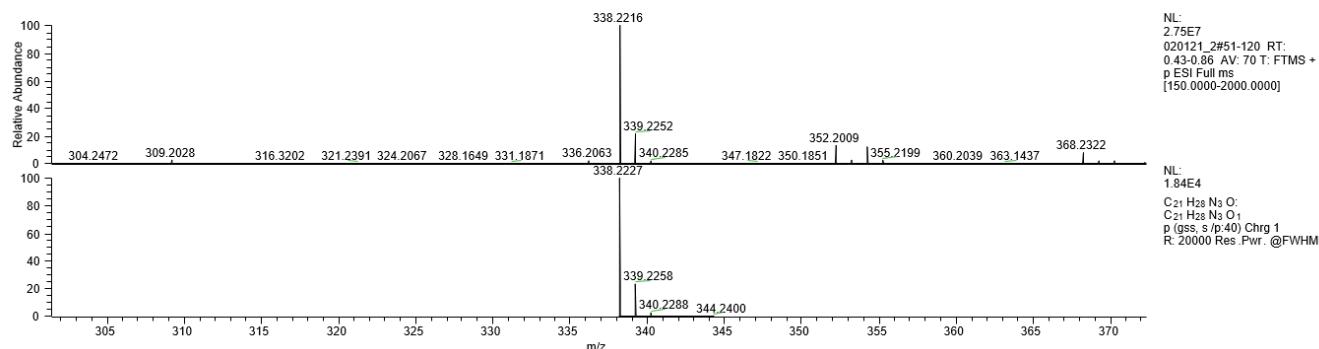
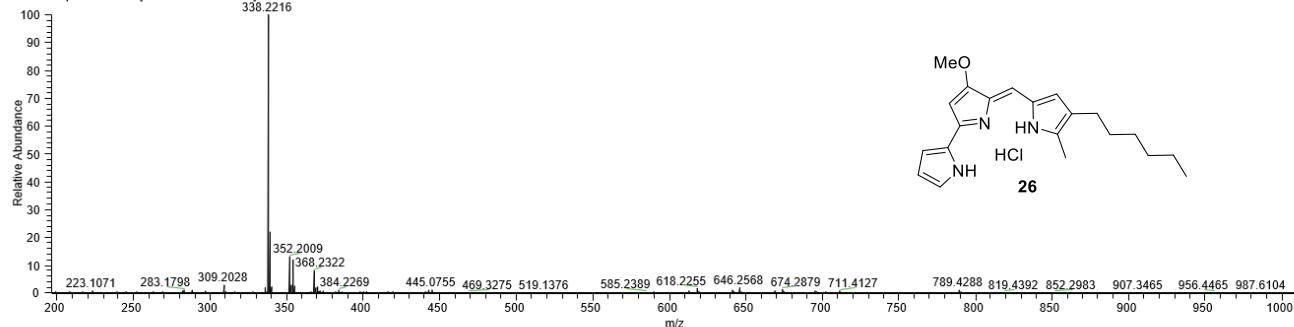
020121_1#56-124 RT: 0.43-0.81 AV: 69 NL: 8.52E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]

310.1905



020121_2 #51-120 RT: 0.43-0.86 AV: 70 NL: 2.75E7
T: FTMS + p ESI Full ms [150.0000-2000.0000]

338.2216



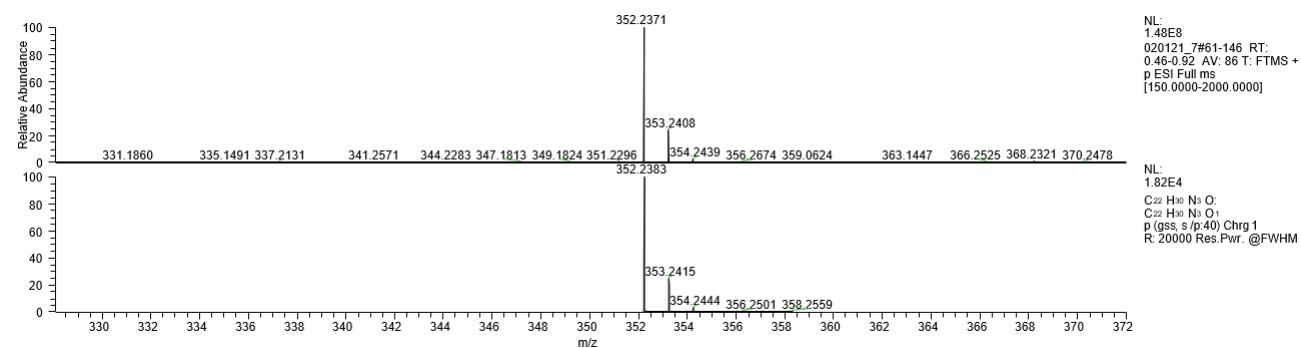
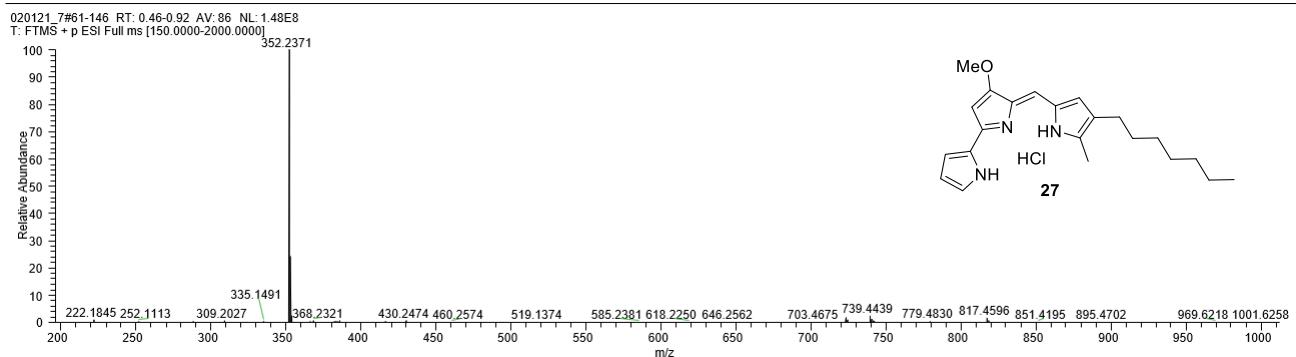
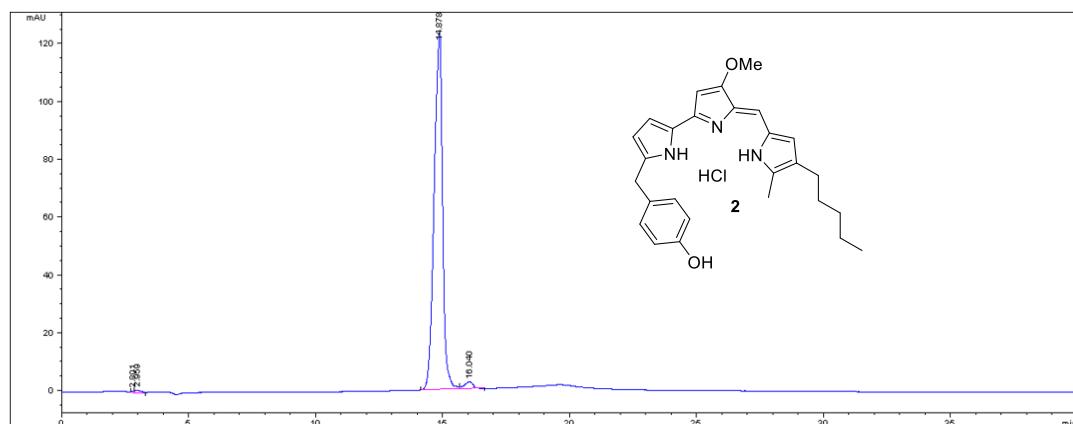


Table S2. HPLC gradient used for final compounds

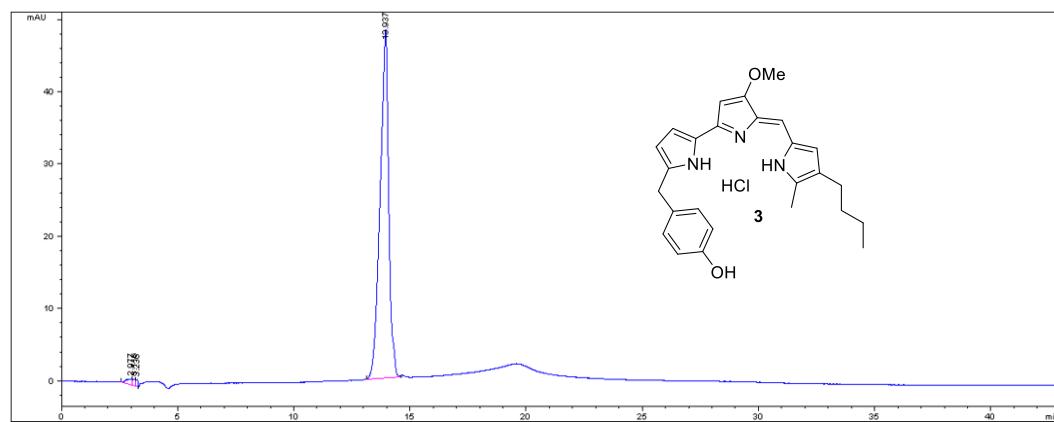
Time (min)	Flow rate (mL/min)	% A ^a	% B ^b
0	0.9	100	0
10	0.9	25	75
15	0.9	0	100
20	0.9	15	85
25	0.9	25	75
40	0.9	100	0

^aBuffer A: water/acetonitrile/methanol/TFA (50:10:40:0.15)

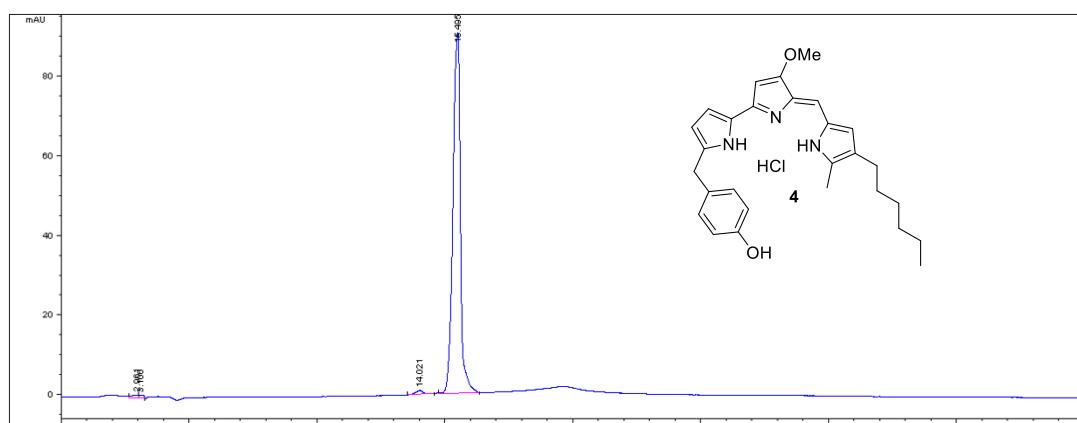
^bBuffer B: 100% methanol/0.15% TFA



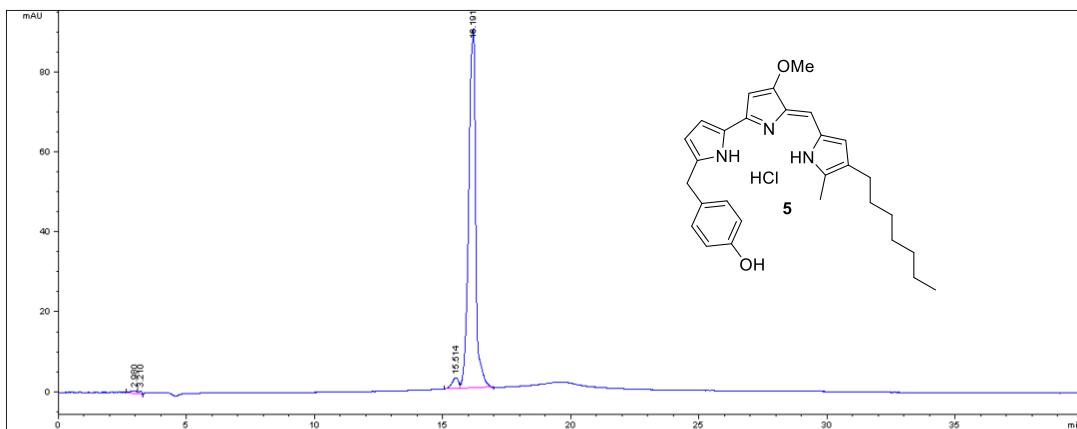
#	Time	Area	Height	Width	Area%	Symmetry
1	2.801	4.8	7.1E-1	0.097	0.165	1.644
2	2.959	17.9	9.8E-1	0.2269	0.611	0.431
3	14.878	2839.8	124.2	0.36	97.168	1.667
4	16.04	60.1	2.4	0.383	2.056	1.194



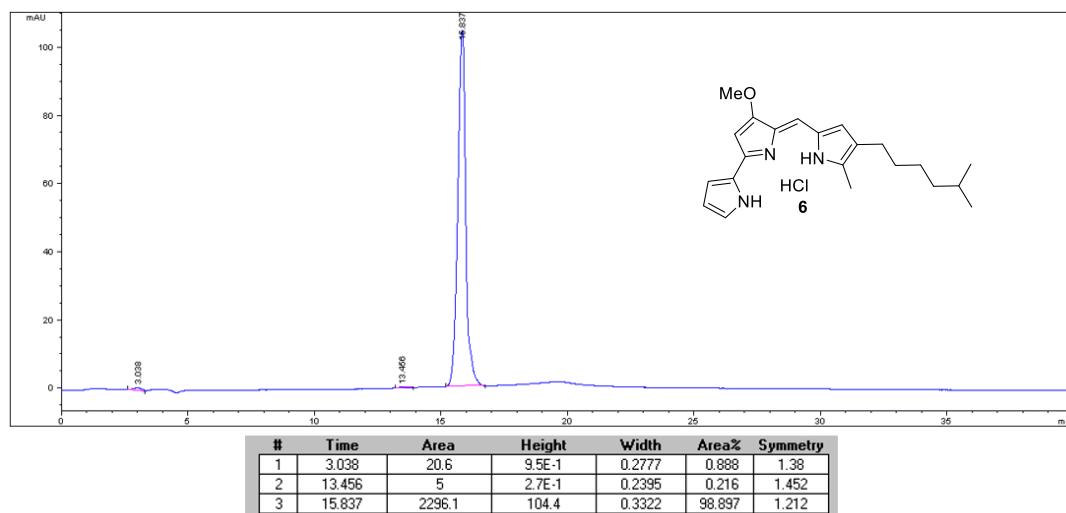
#	Time	Area	Height	Width	Area%	Symmetry
1	2.977	14.8	8.2E-1	0.2351	1.167	3.708
2	3.116	7.9	9.3E-1	0.1273	0.618	0.747
3	3.236	4	9.7E-1	0.0661	0.317	0.772
4	13.937	1244.6	48.2	0.3478	97.898	1.663



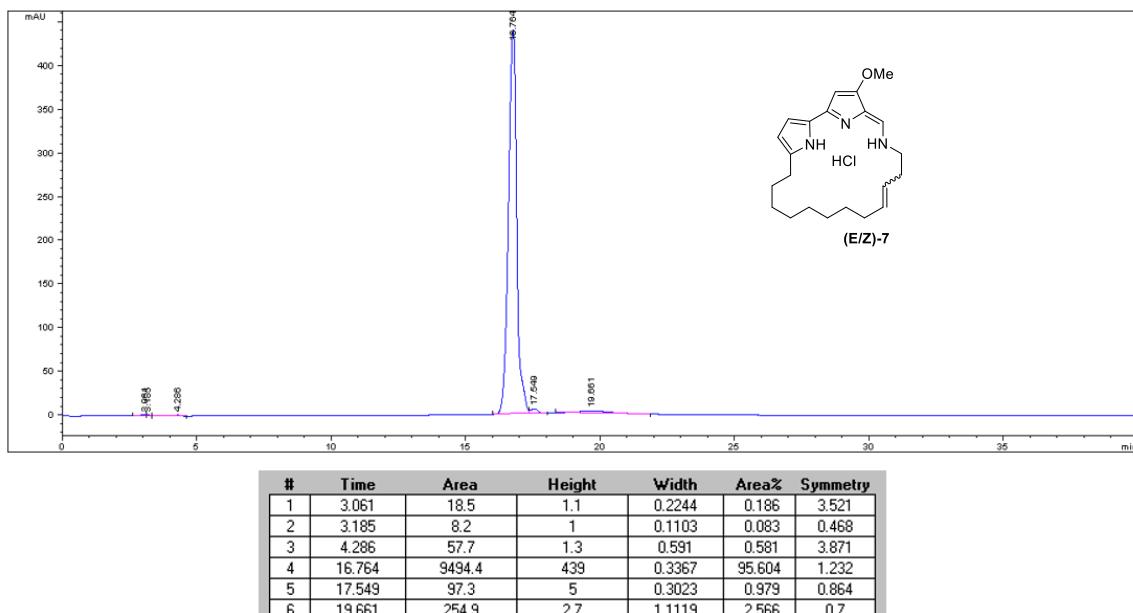
#	Time	Area	Height	Width	Area%	Symmetry
1	2.961	16.4	8.9E-1	0.2327	0.860	4.054
2	3.106	10	8E-1	0.1579	0.526	0.461
3	14.021	24	1	0.3411	1.259	1.046
4	15.495	1855.2	90.6	0.3176	97.355	1.604



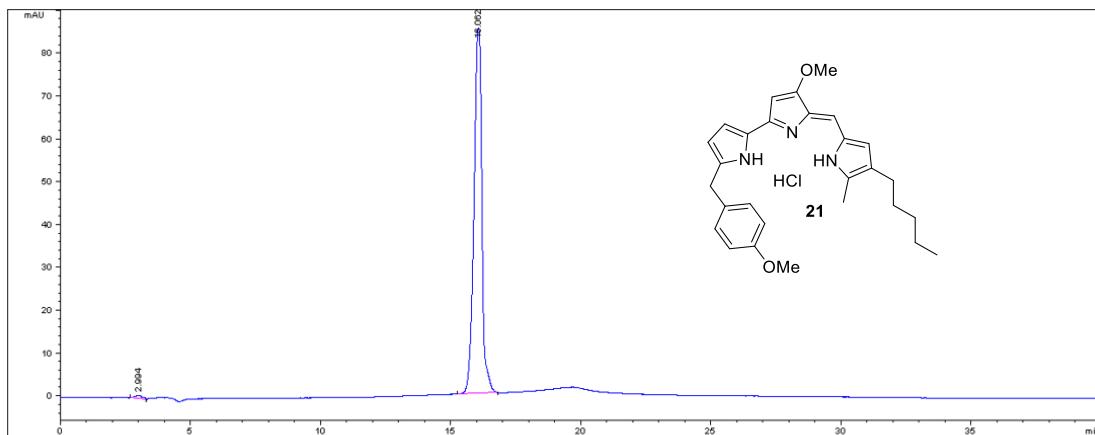
#	Time	Area	Height	Width	Area%	Symmetry
1	2.98	11.8	6.9E-1	0.2194	0.659	1.722
2	3.21	6.6	8.4E-1	0.1097	0.370	2.17
3	15.514	48.8	2.8	0.2687	2.734	1.799
4	16.191	1719	89.9	0.2551	96.236	1.767



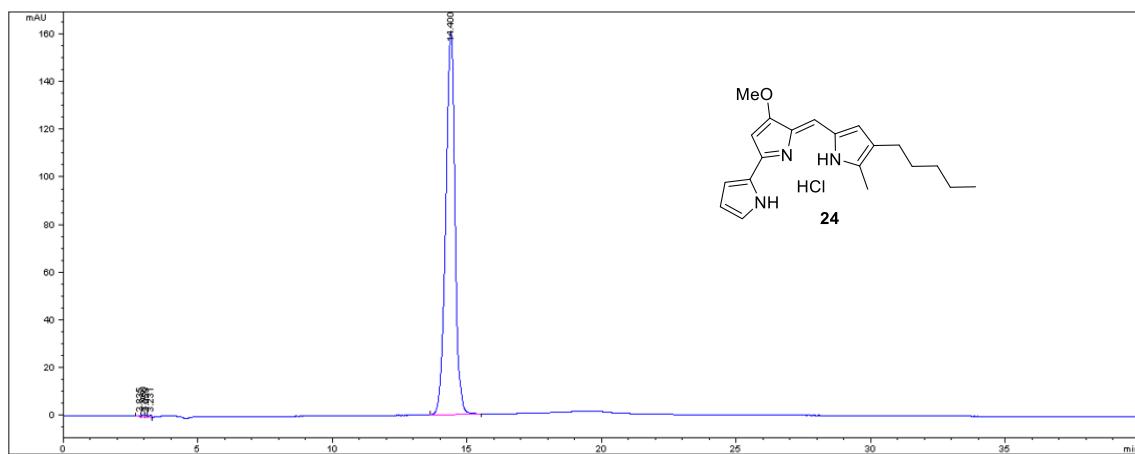
#	Time	Area	Height	Width	Area%	Symmetry
1	3.038	20.6	9.5E-1	0.2777	0.888	1.38
2	13.456	5	2.7E-1	0.2395	0.216	1.452
3	15.837	2296.1	104.4	0.3322	98.897	1.212



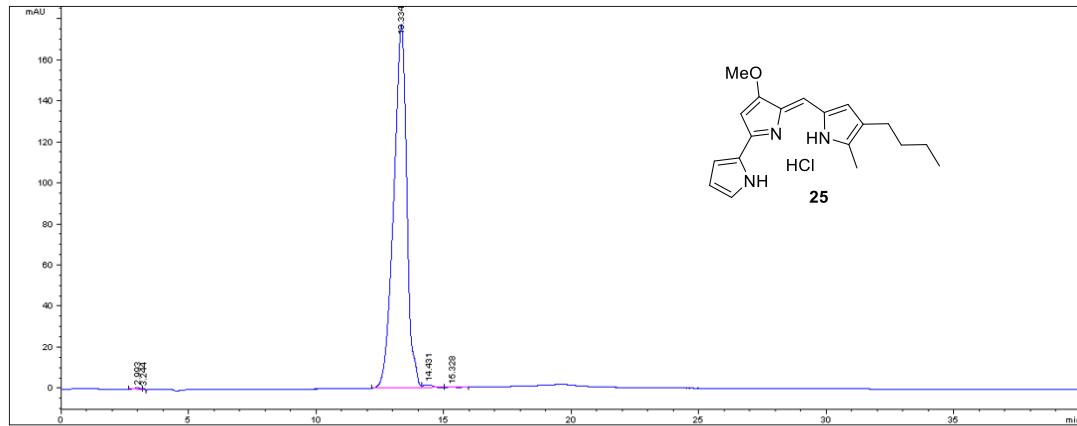
#	Time	Area	Height	Width	Area%	Symmetry
1	3.061	18.5	1.1	0.2244	0.186	3.521
2	3.185	8.2	1	0.1103	0.083	0.468
3	4.286	57.7	1.3	0.591	0.581	3.871
4	16.764	9494.4	439	0.3367	95.604	1.232
5	17.249	97.3	5	0.3023	0.979	0.864
6	19.661	254.9	2.7	1.1119	2.566	0.7



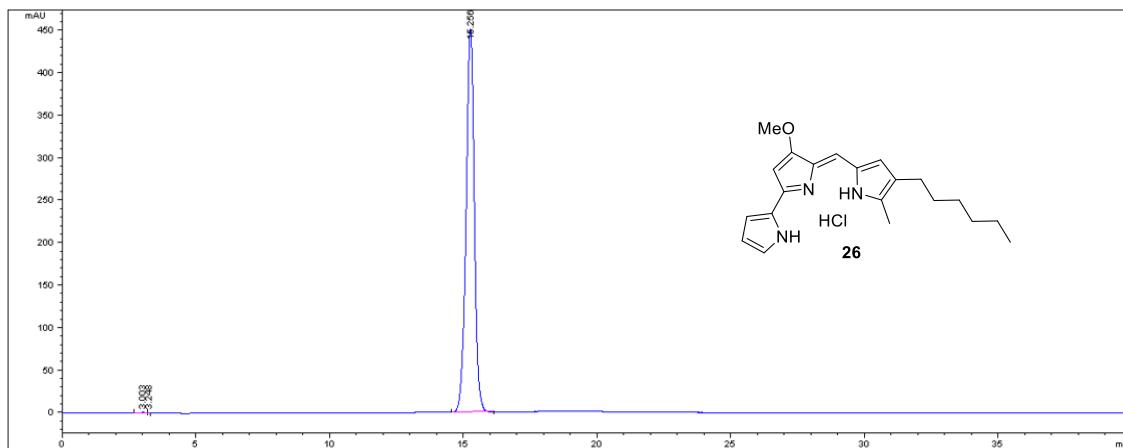
#	Time	Area	Height	Width	Area%	Symmetry
1	2.994	17.9	8.6E-1	0.2732	0.975	0.821
2	16.062	1817.3	85.2	0.3245	99.025	1.245



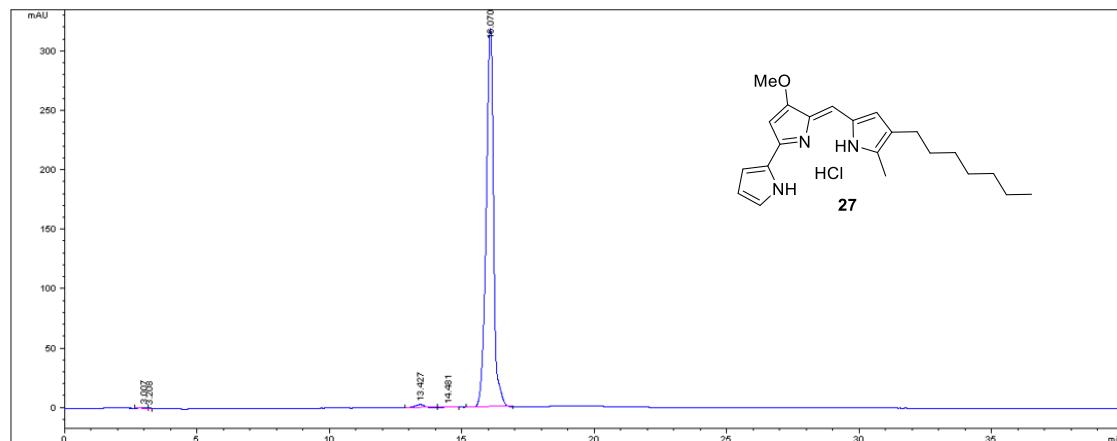
#	Time	Area	Height	Width	Area%	Symmetry
1	2.835	4.4	5.3E-1	0.1254	0.112	2.1
2	2.96	6.3	1E0	0.0907	0.161	1.165
3	3.059	5.6	8.8E-1	0.0923	0.145	0.561
4	3.231	6.8	9.2E-1	0.1062	0.174	1.823
5	14.4	3869.1	161	0.3678	99.408	1.255



#	Time	Area	Height	Width	Area%	Symmetry
1	2.993	20.7	1	0.2591	0.326	1.136
2	3.244	4	7.6E-1	0.0795	0.063	0.963
3	13.334	6294.4	177	0.5371	99.030	1.357
4	14.431	33.9	1.3	0.3508	0.533	1.506
5	15.328	3	2.2E-1	0.1699	0.047	1.697



#	Time	Area	Height	Width	Area%	Symmetry
1	3.003	16.9	9.5E-1	0.2261	0.174	1.176
2	3.248	2.9	6.2E-1	0.0722	0.030	0.972
3	15.256	9706.5	450.7	0.3299	99.796	1.08



#	Time	Area	Height	Width	Area%	Symmetry
1	3.007	16.1	9.3E-1	0.2397	0.255	1.339
2	3.208	3.3	6.8E-1	0.0805	0.053	0.606
3	13.427	69.7	2.7	0.3698	1.101	1.297
4	14.481	9.5	3.7E-1	0.332	0.150	0.849
5	16.07	6233	318.2	0.2984	98.442	1.272