

## Electronic Supplementary Information for:

### A benzo[1,2-*b*:4,5-*b'*]dithiophene core $\pi$ -system that bears alkyl, alkylthio and alkoxy groups at 3,7-positions

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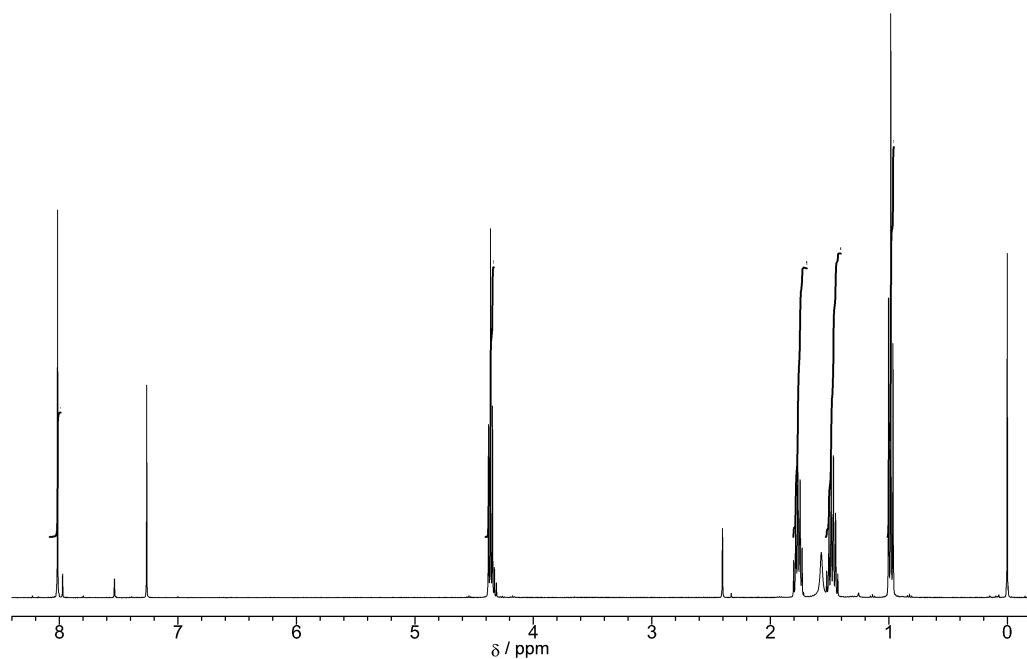
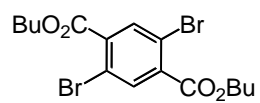
<sup>b</sup> The Institute of Scientific and Industrial Research, Osaka University, 8-1 Mihogaoka, Ibaraki, Osaka 567-0047, Japan

#### Contents

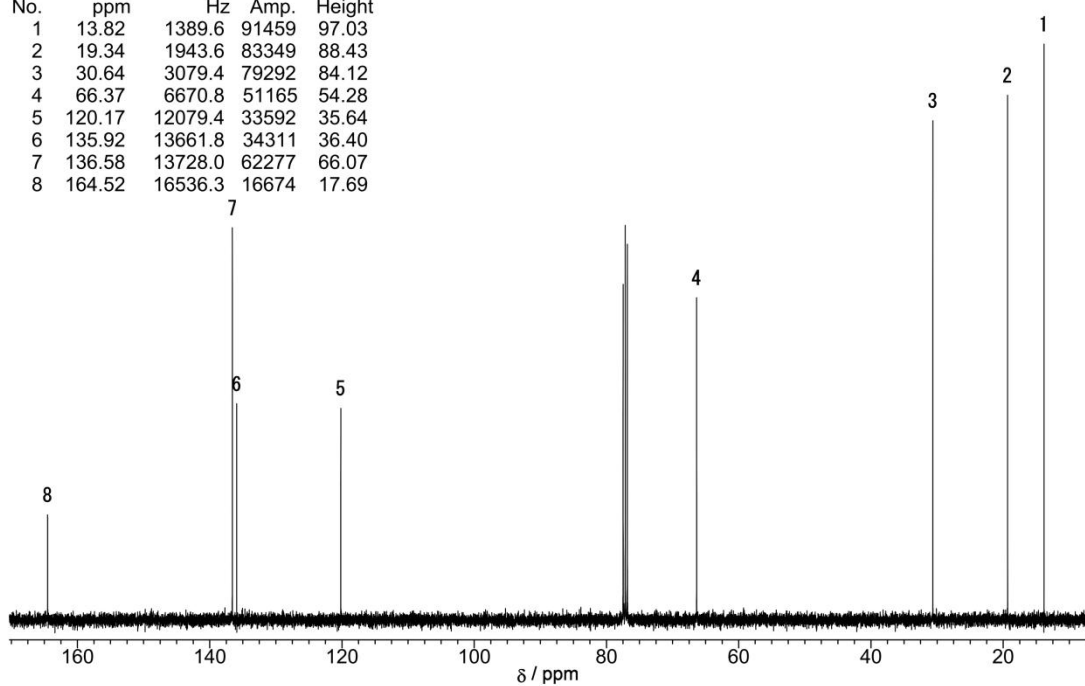
<sup>1</sup>H and <sup>13</sup>C NMR Spectra

S2–S22

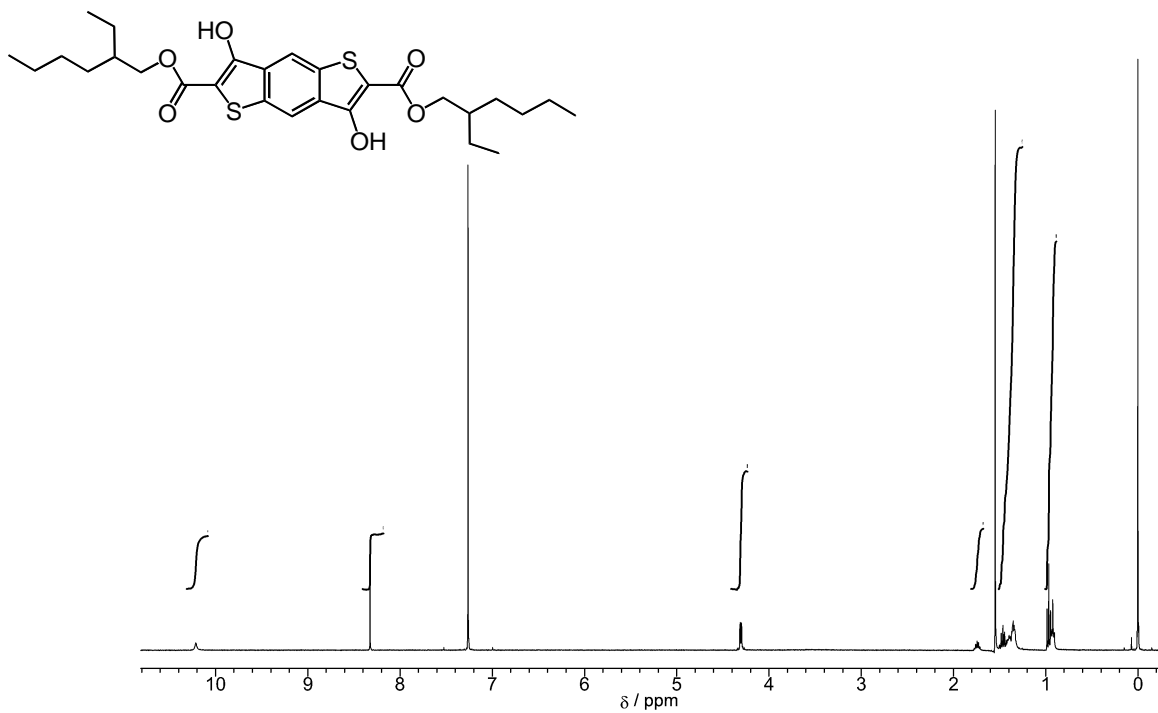
[  $^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra of **5** ]



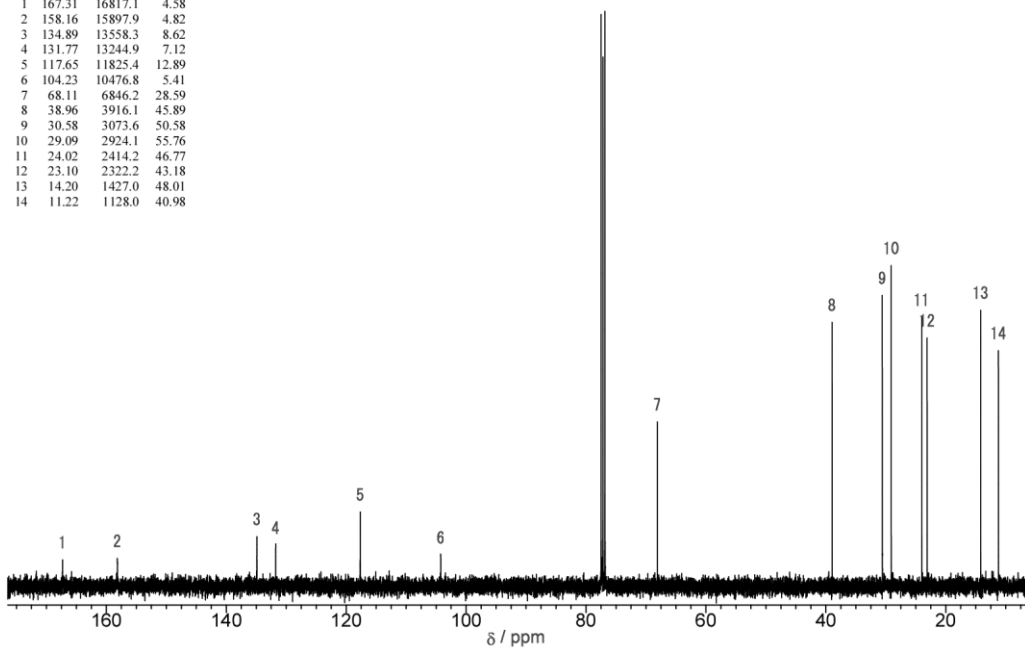
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3	30.64	3079.4	79292	84.12
4	66.37	6670.8	51165	54.28
5	120.17	12079.4	33592	35.64
6	135.92	13661.8	34311	36.40
7	136.58	13728.0	62277	66.07
8	164.52	16536.3	16674	17.69



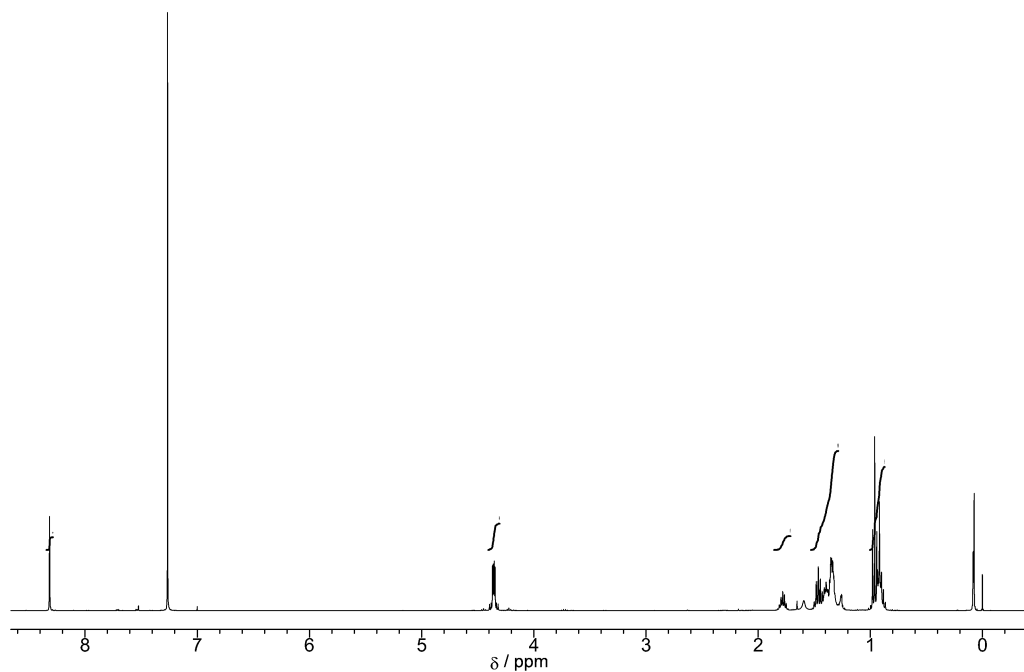
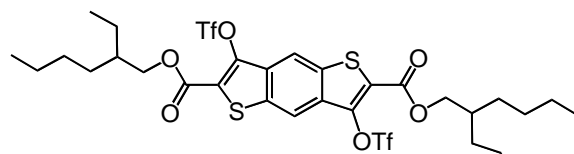
[<sup>1</sup>H and <sup>13</sup>C NMR Spectra of **6**]



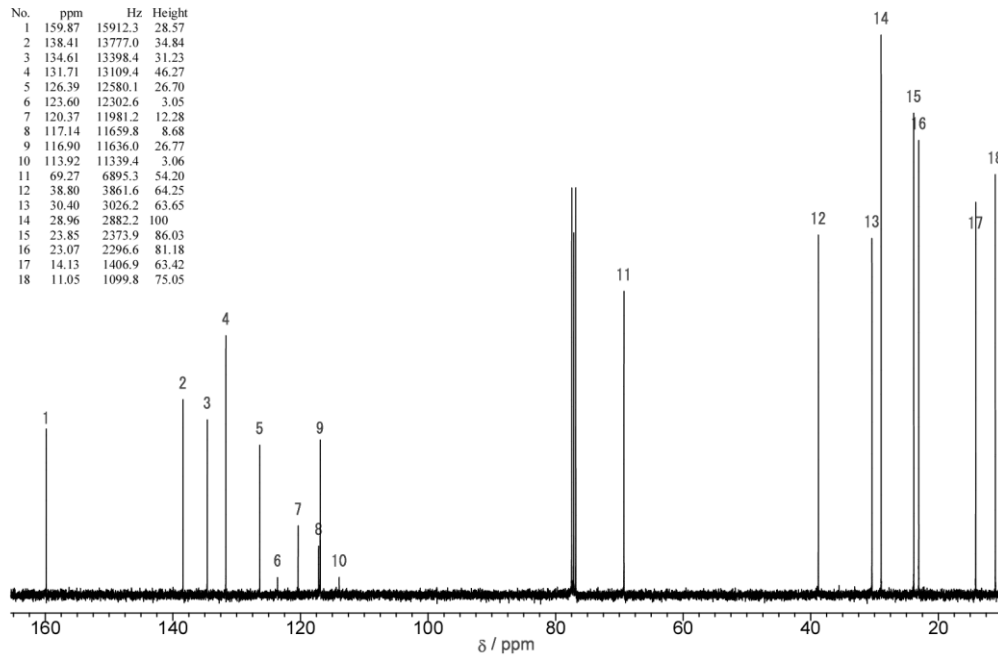
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4	131.77	13244.9	7.12
5	117.65	11825.4	12.89
6	104.23	10476.8	5.41
7	68.11	6846.2	28.59
8	38.96	3916.1	45.89
9	30.58	3073.6	50.58
10	29.09	2924.1	55.76
11	24.02	2414.2	46.77
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13	14.20	1427.0	48.01
14	11.22	1128.0	40.98



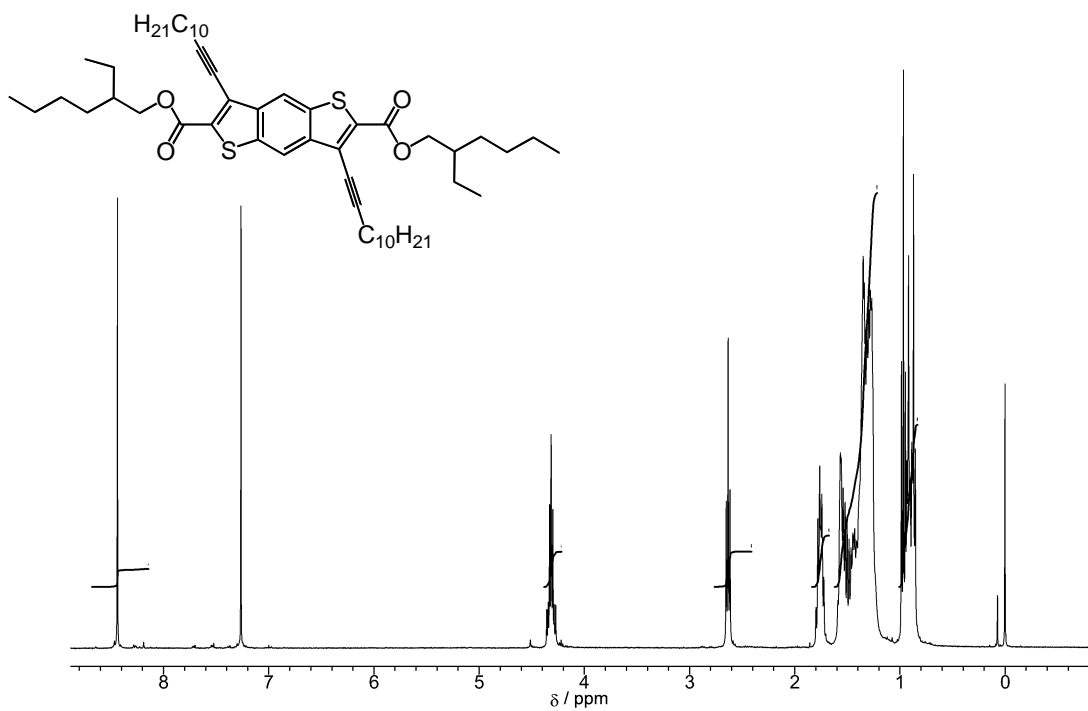
[<sup>1</sup>H and <sup>13</sup>C NMR Spectra of 7]



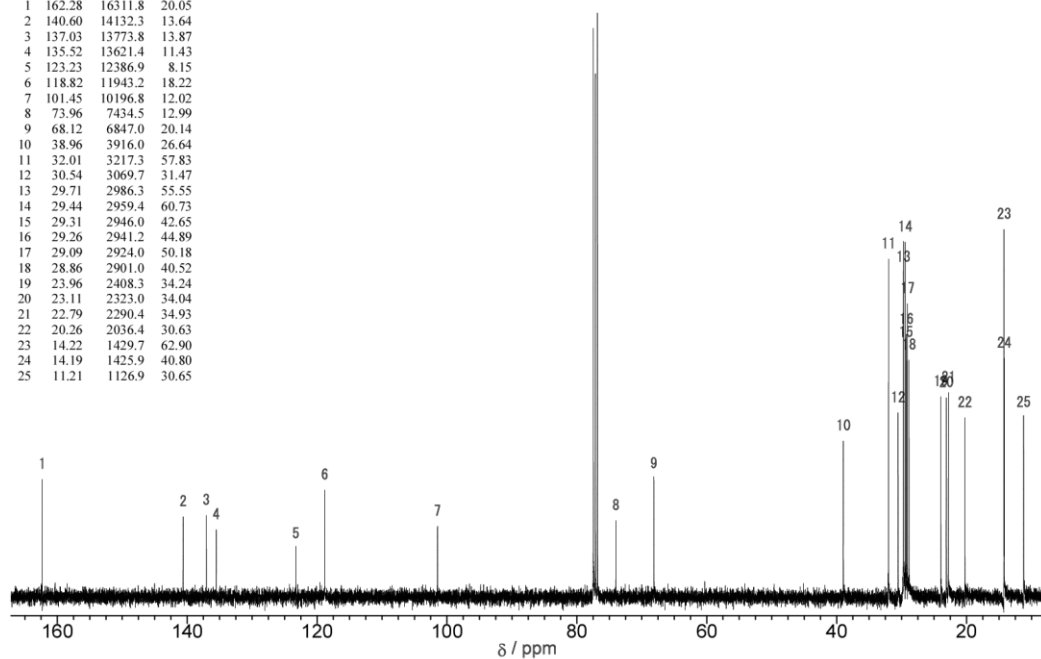
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4	131.71	13109.4	46.27
5	126.39	12580.1	26.70
6	123.60	12302.6	3.05
7	120.37	11981.2	12.28
8	117.14	11659.8	8.68
9	116.90	11636.0	26.77
10	113.92	11339.4	3.06
11	69.27	6895.3	54.20
12	38.80	3861.6	64.25
13	30.40	3026.2	63.65
14	28.96	2882.2	100
15	23.85	2373.9	86.03
16	23.07	2296.6	81.18
17	14.13	1406.9	63.42
18	11.05	1099.8	75.05



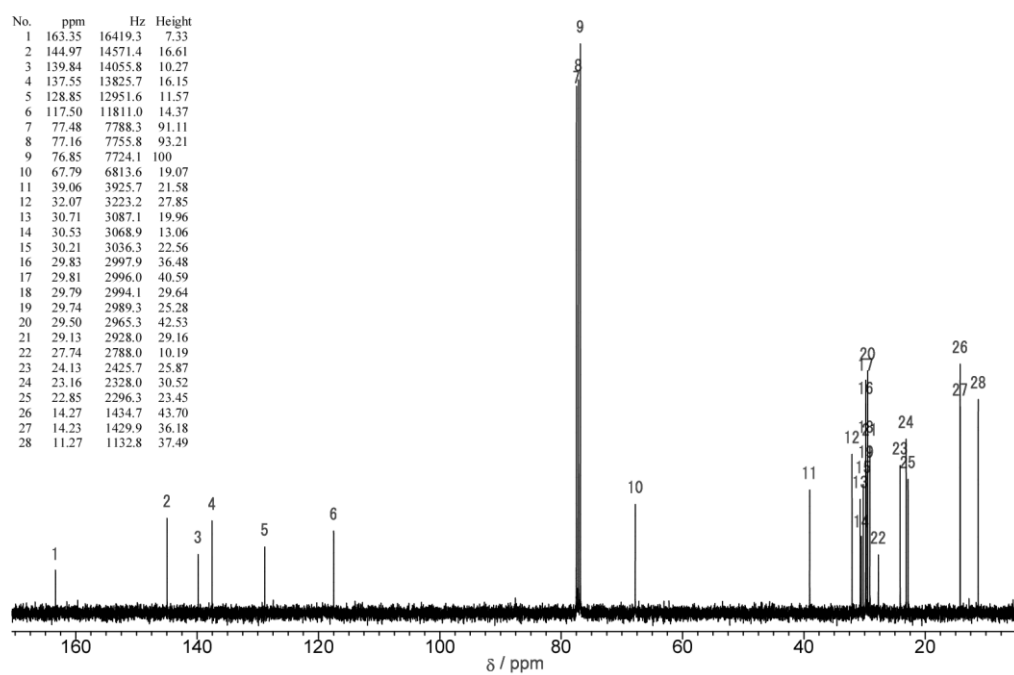
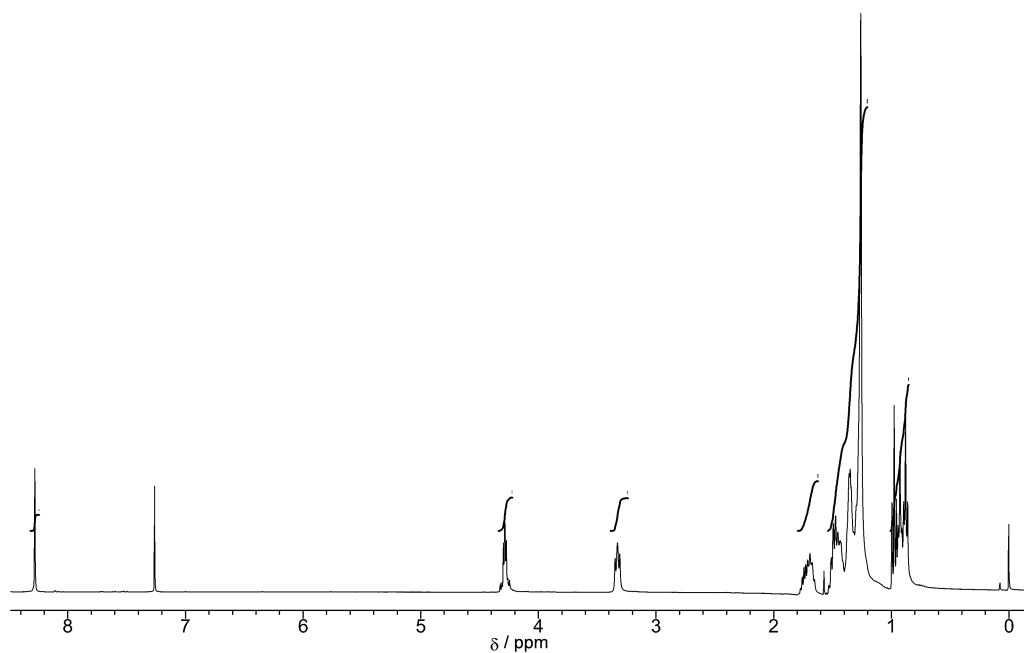
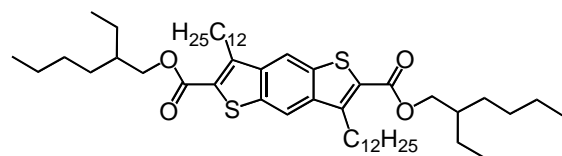
[<sup>1</sup>H and <sup>13</sup>C NMR Spectra of **8**]



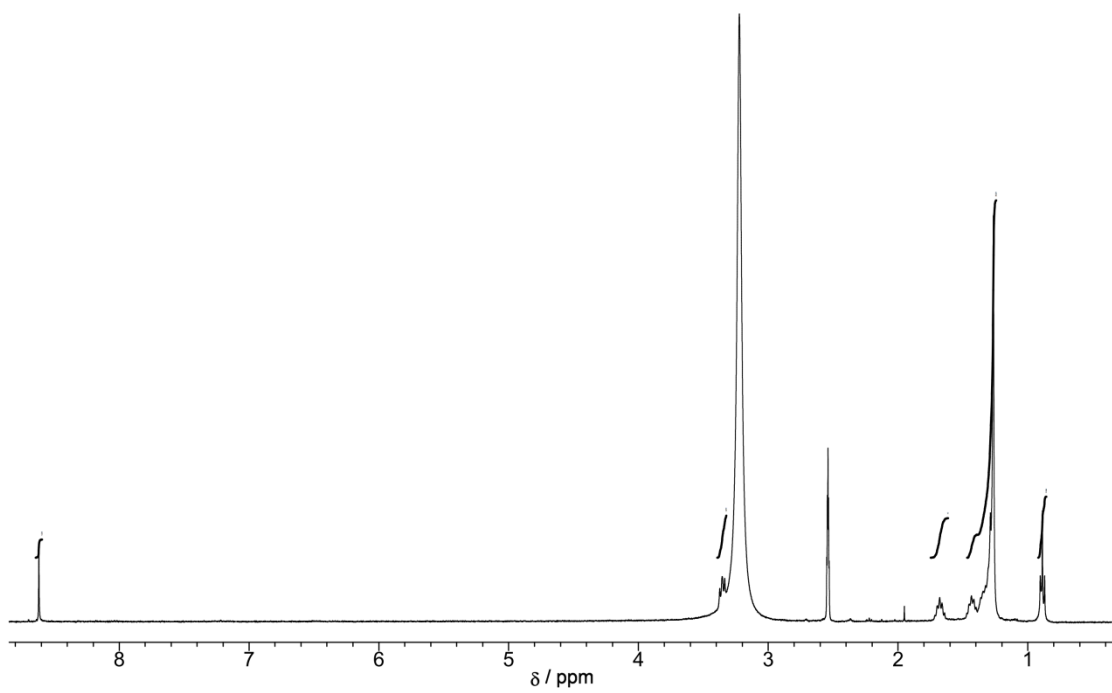
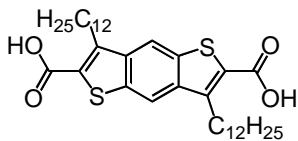
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4	135.52	13621.4	11.43
5	123.23	12386.9	8.15
6	118.82	11943.2	18.22
7	101.45	10196.8	12.02
8	73.96	7434.5	12.99
9	68.12	6847.0	20.14
10	38.96	3916.0	26.64
11	32.01	3217.3	38.77
12	30.54	3069.7	31.47
13	29.71	2986.3	55.55
14	29.44	2959.4	60.73
15	29.31	2946.0	42.65
16	29.26	2941.2	44.89
17	29.09	2924.0	50.18
18	28.86	2901.0	40.52
19	23.96	2408.3	34.24
20	23.11	2323.0	34.04
21	22.79	2290.4	34.93
22	20.26	2036.4	30.63
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25	11.21	1126.9	30.65



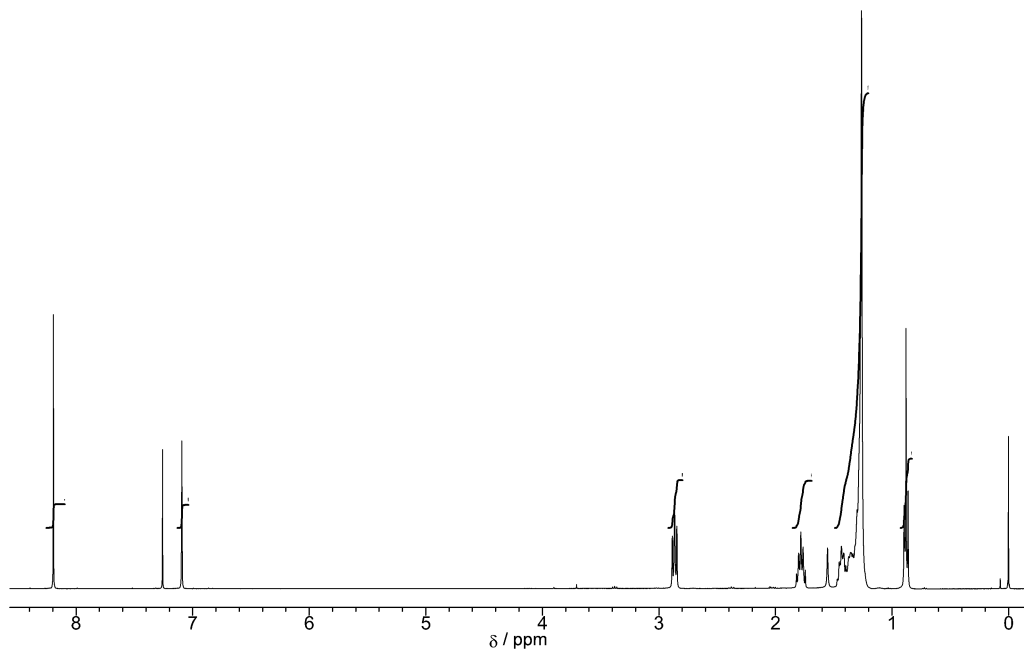
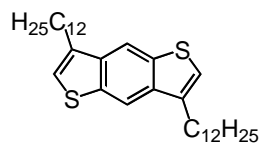
[  $^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra of **9** ]



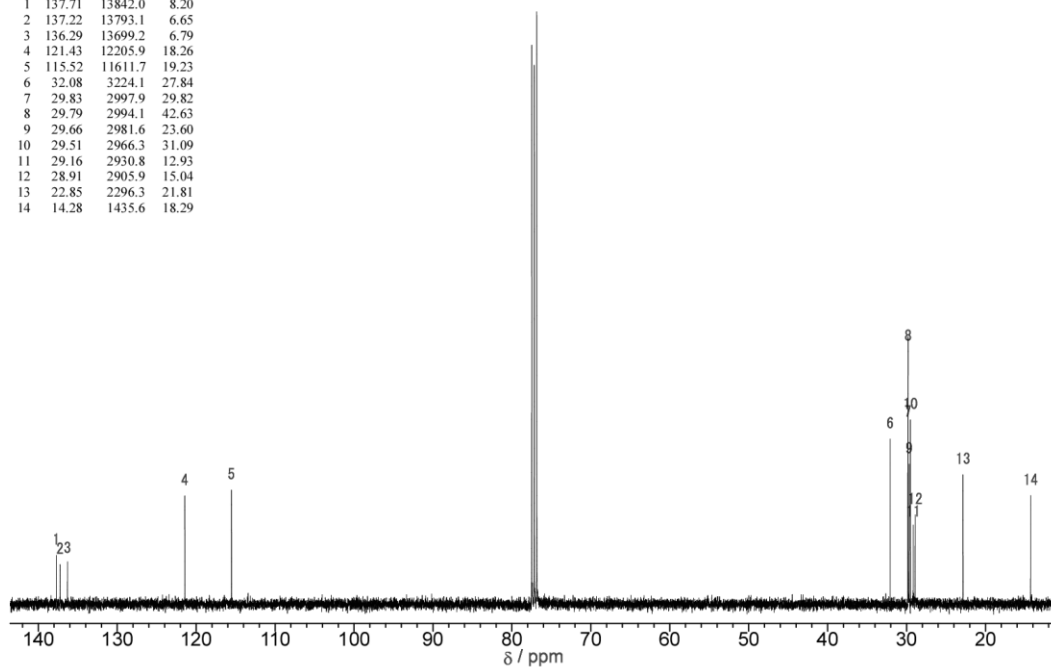
[  $^1\text{H}$  NMR Spectrum of **10** ]



[<sup>1</sup>H and <sup>13</sup>C NMR Spectra of **1a**]

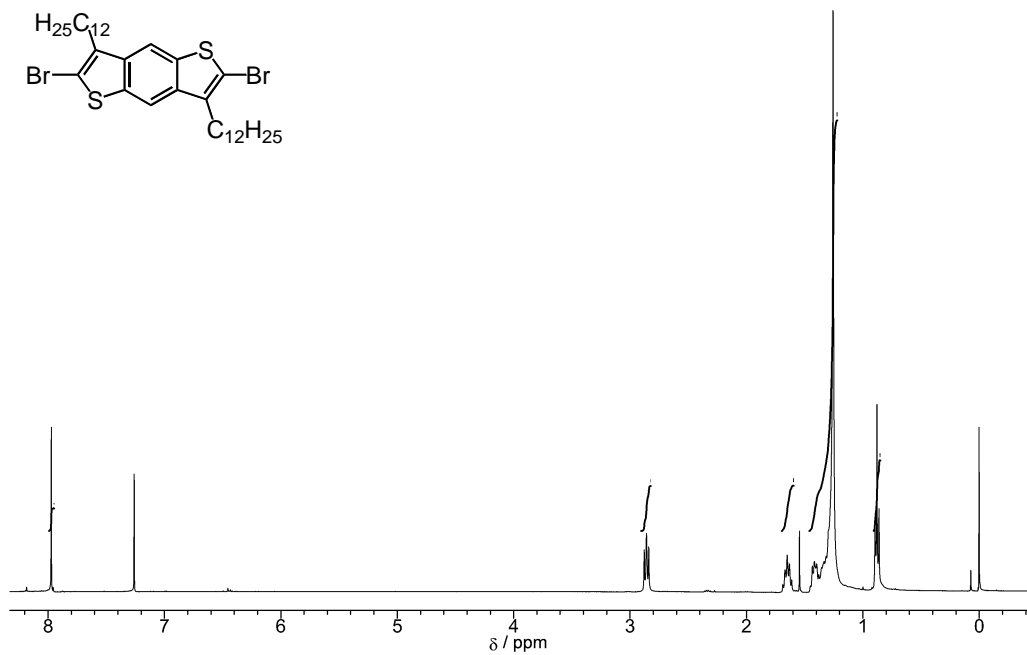
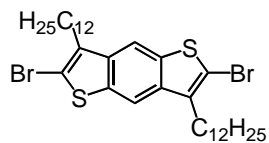


No.	ppm	Hz	Height
1	137.71	13842.0	8.20
2	137.22	13793.1	6.65
3	136.29	13699.2	6.79
4	121.43	12205.9	18.26
5	115.52	11611.7	19.23
6	32.08	3224.1	27.84
7	29.83	2997.9	29.82
8	29.79	2994.1	42.63
9	29.66	2981.6	23.60
10	29.51	2966.3	31.09
11	29.16	2930.8	12.93
12	28.91	2905.9	15.04
13	22.85	2296.3	21.81
14	14.28	1435.6	18.29

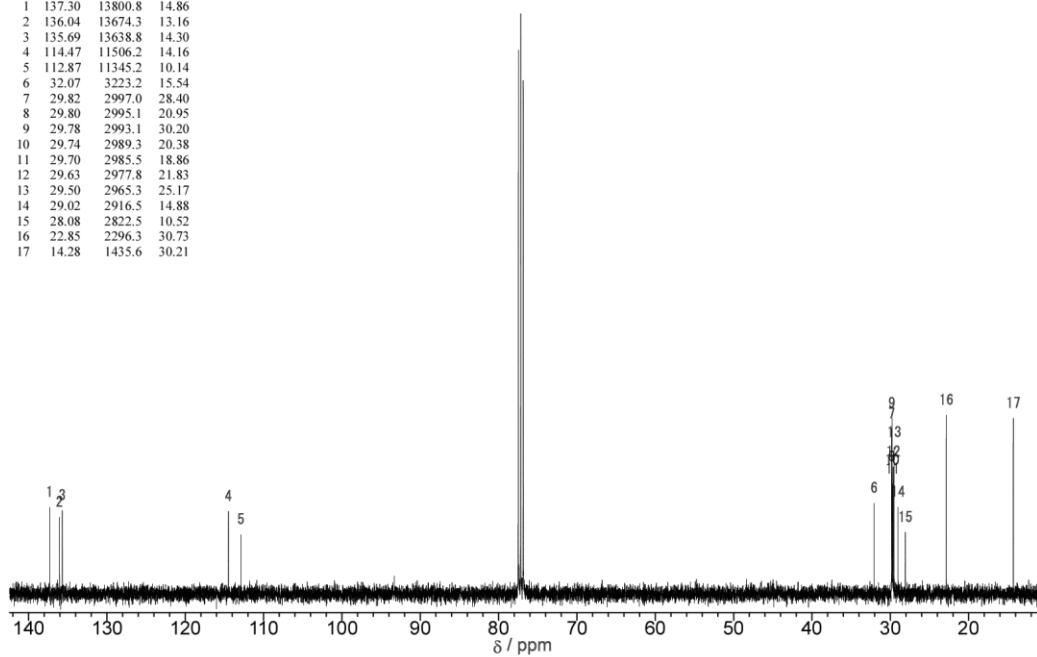




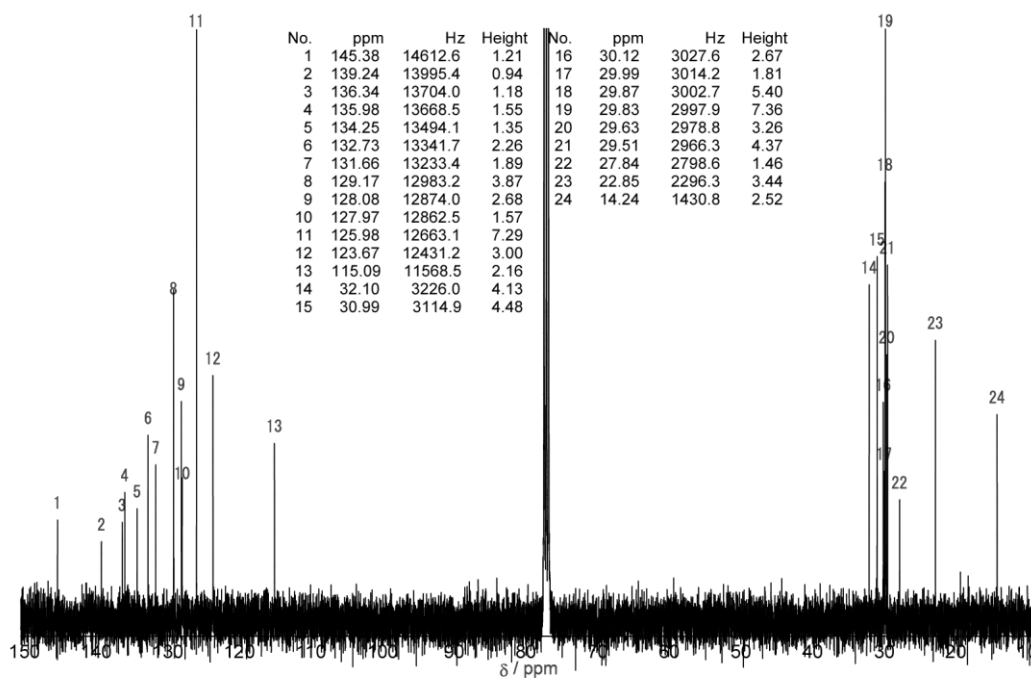
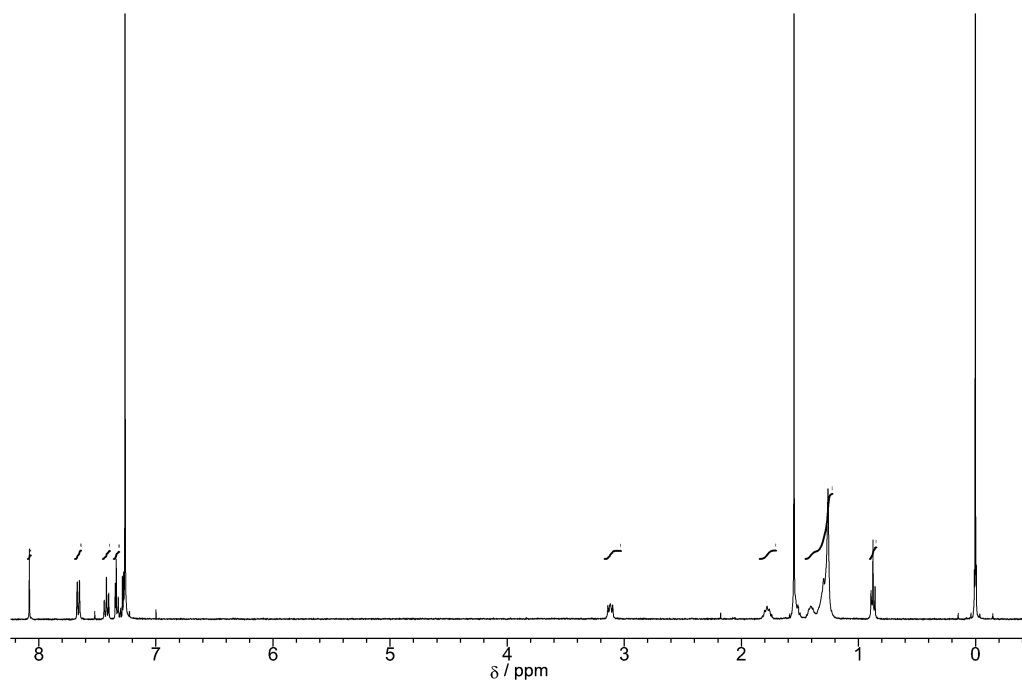
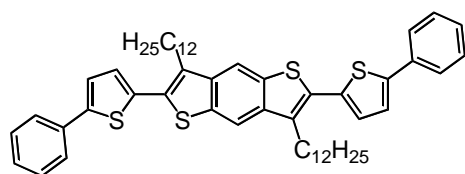
[<sup>1</sup>H and <sup>13</sup>C NMR Spectra of 11]



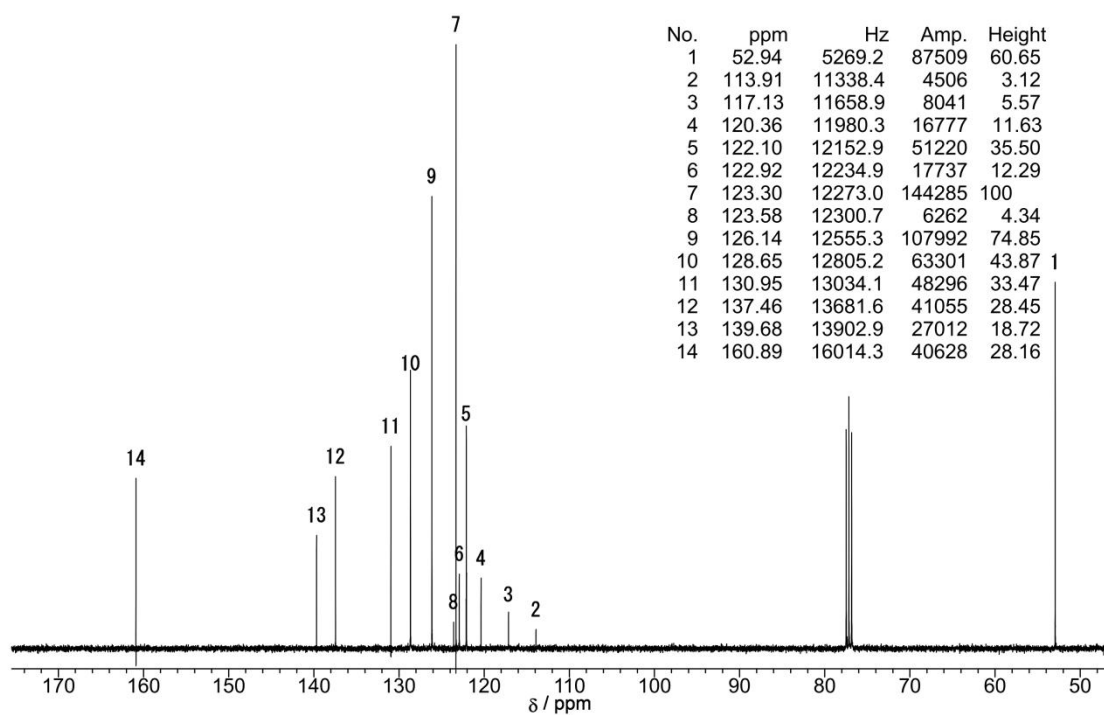
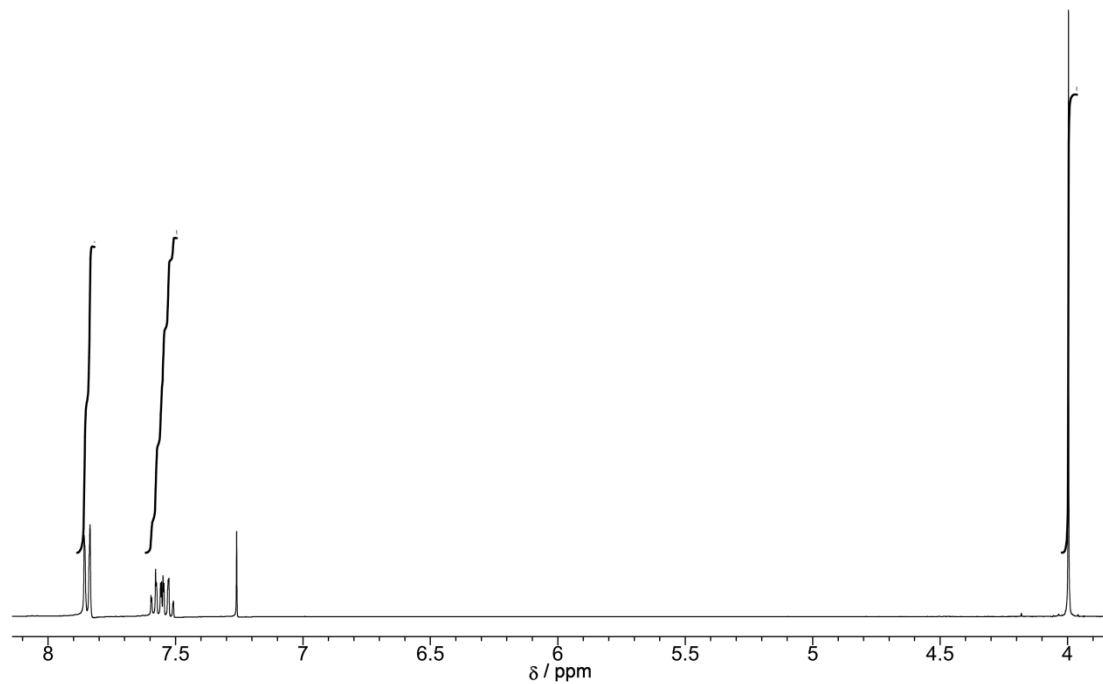
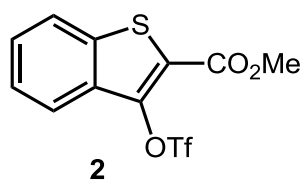
No.	ppm	Hz	Height
1	137.30	13800.8	14.86
2	136.04	13674.3	13.16
3	135.69	13638.8	14.30
4	114.47	11506.2	14.16
5	112.87	11345.2	10.14
6	32.07	3223.2	15.54
7	29.82	2997.0	28.40
8	29.80	2995.1	20.95
9	29.78	2993.1	30.20
10	29.74	2989.3	20.38
11	29.70	2985.5	18.86
12	29.63	2977.8	21.83
13	29.50	2965.3	25.17
14	29.02	2916.5	14.88
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16	22.85	2296.3	30.73
17	14.28	1435.6	30.21



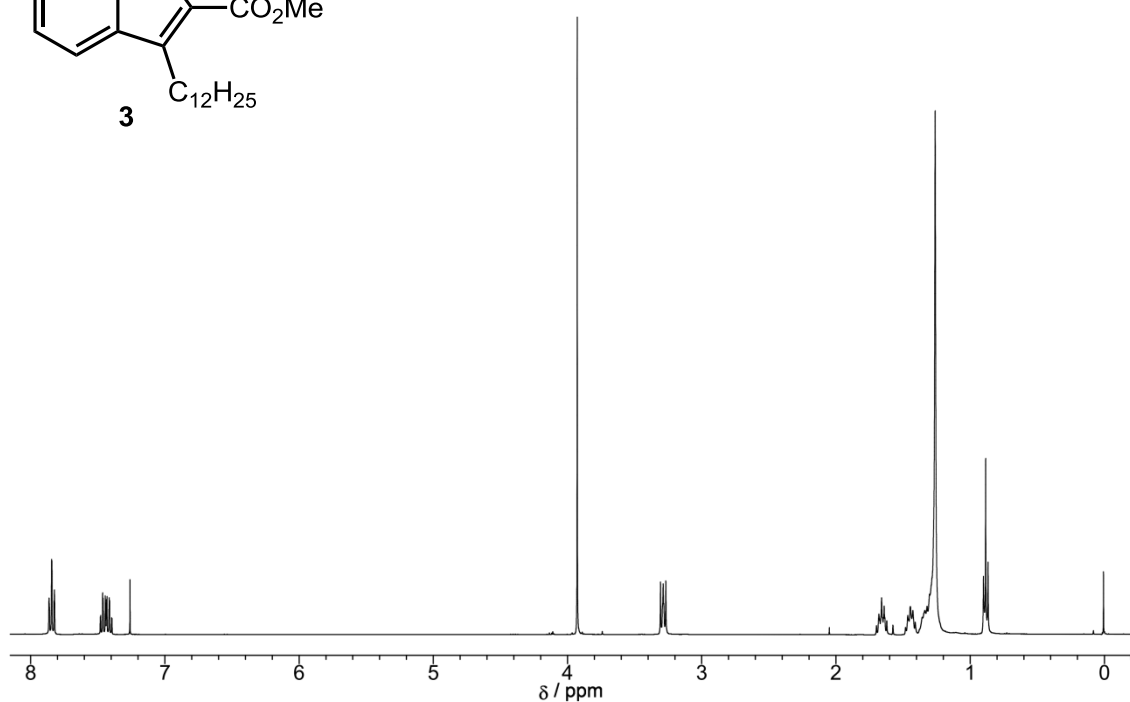
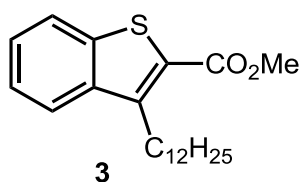
<sup>1</sup>H NMR Spectrum of **2a**]



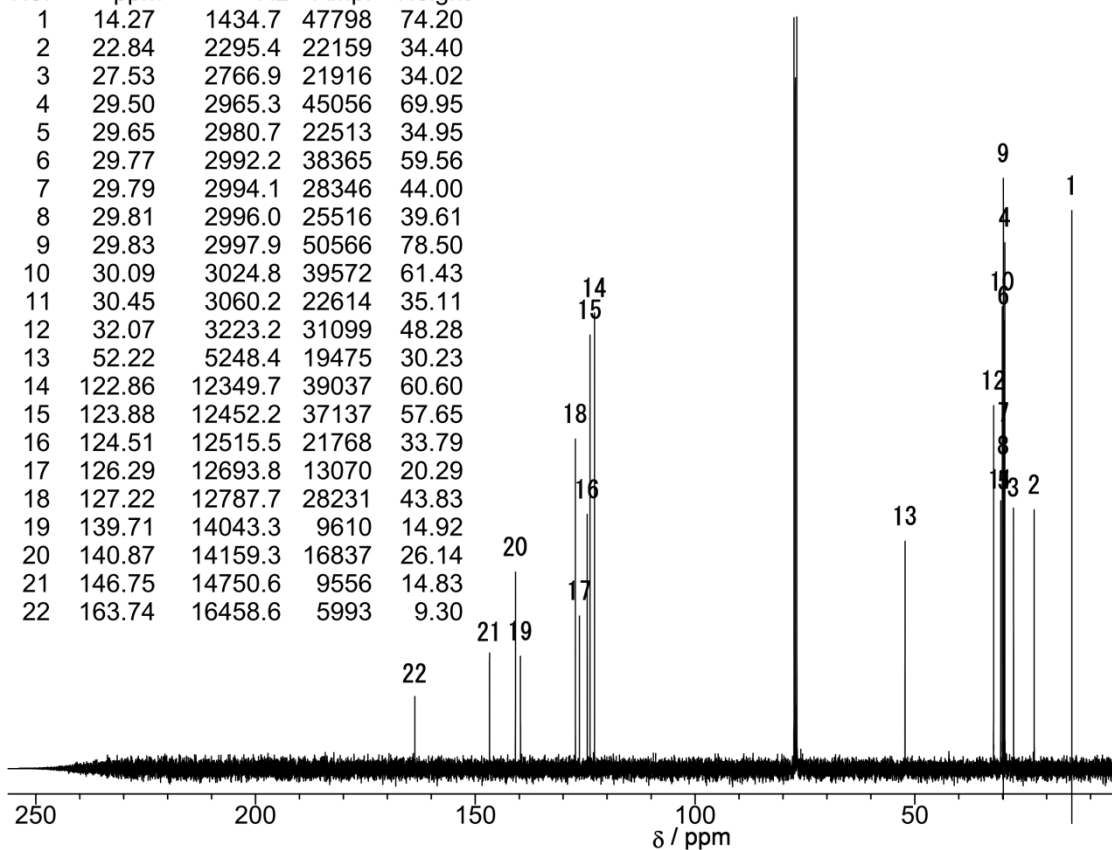
[<sup>1</sup>H and <sup>13</sup>C NMR Spectra of **12**]



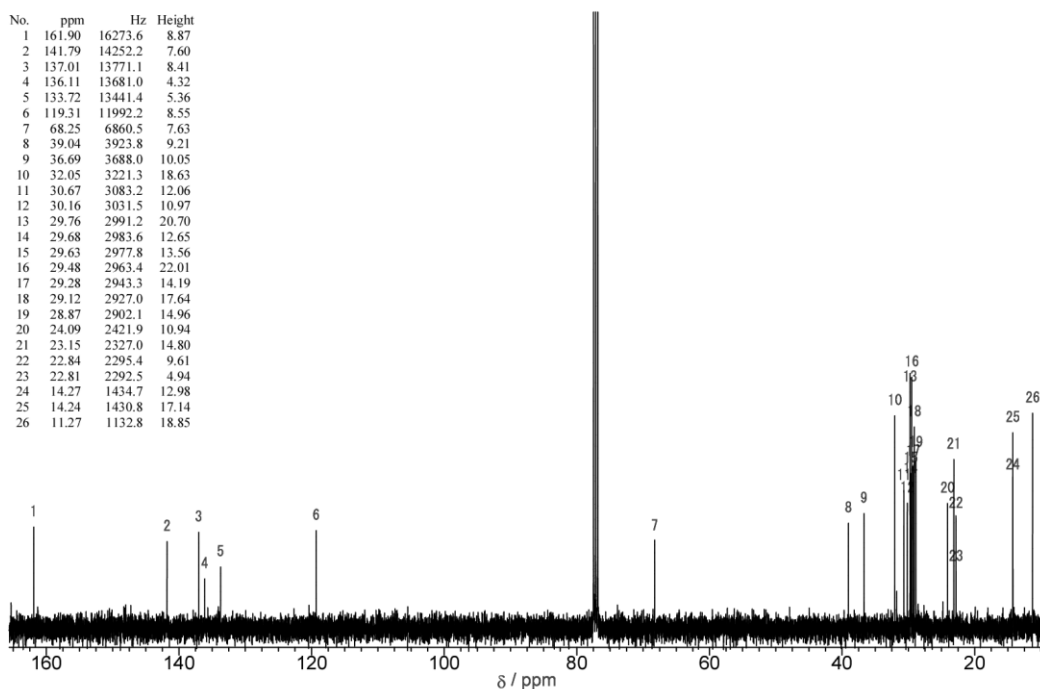
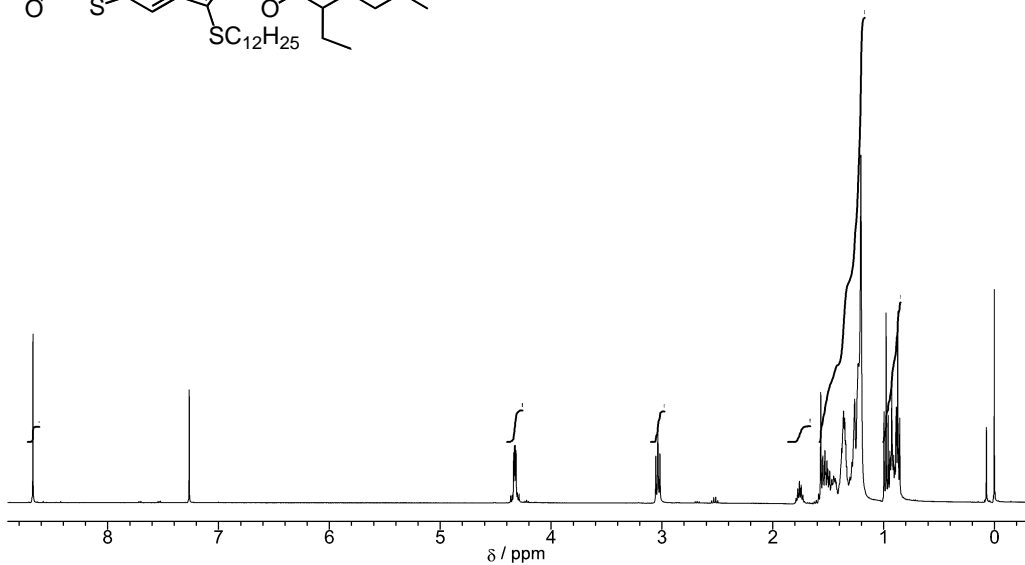
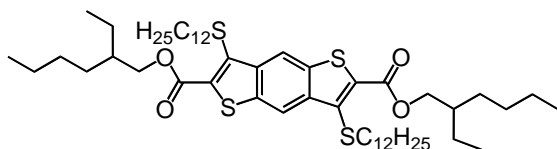
[<sup>1</sup>H and <sup>13</sup>C NMR Spectra of **13**]



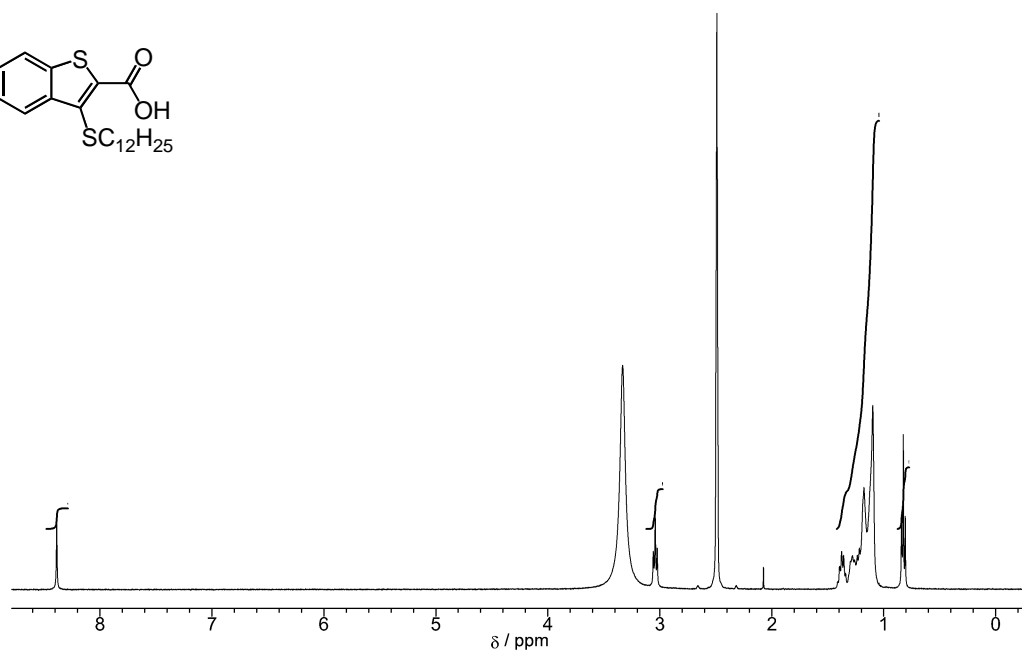
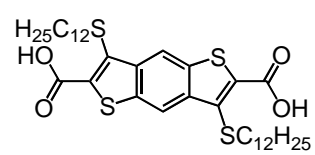
No.	ppm	Hz	Amp.	Height
1	14.27	1434.7	47798	74.20
2	22.84	2295.4	22159	34.40
3	27.53	2766.9	21916	34.02
4	29.50	2965.3	45056	69.95
5	29.65	2980.7	22513	34.95
6	29.77	2992.2	38365	59.56
7	29.79	2994.1	28346	44.00
8	29.81	2996.0	25516	39.61
9	29.83	2997.9	50566	78.50
10	30.09	3024.8	39572	61.43
11	30.45	3060.2	22614	35.11
12	32.07	3223.2	31099	48.28
13	52.22	5248.4	19475	30.23
14	122.86	12349.7	39037	60.60
15	123.88	12452.2	37137	57.65
16	124.51	12515.5	21768	33.79
17	126.29	12693.8	13070	20.29
18	127.22	12787.7	28231	43.83
19	139.71	14043.3	9610	14.92
20	140.87	14159.3	16837	26.14
21	146.75	14750.6	9556	14.83
22	163.74	16458.6	5993	9.30



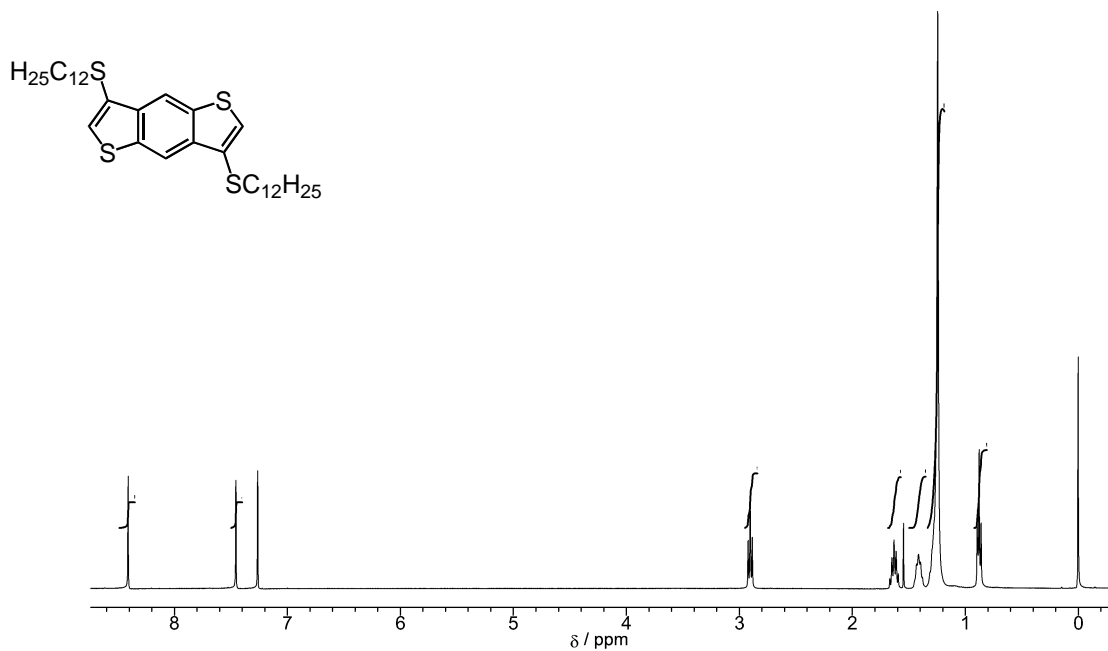
[<sup>1</sup>H and <sup>13</sup>C NMR Spectra of **14**]



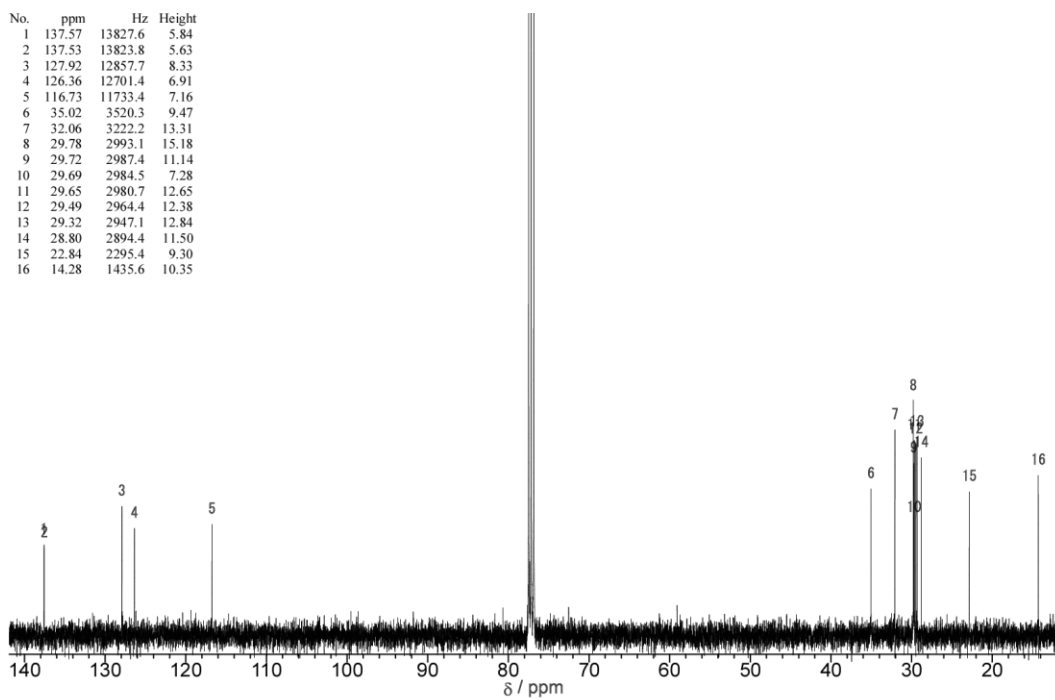
[  $^1\text{H}$  NMR Spectrum of **16** ]



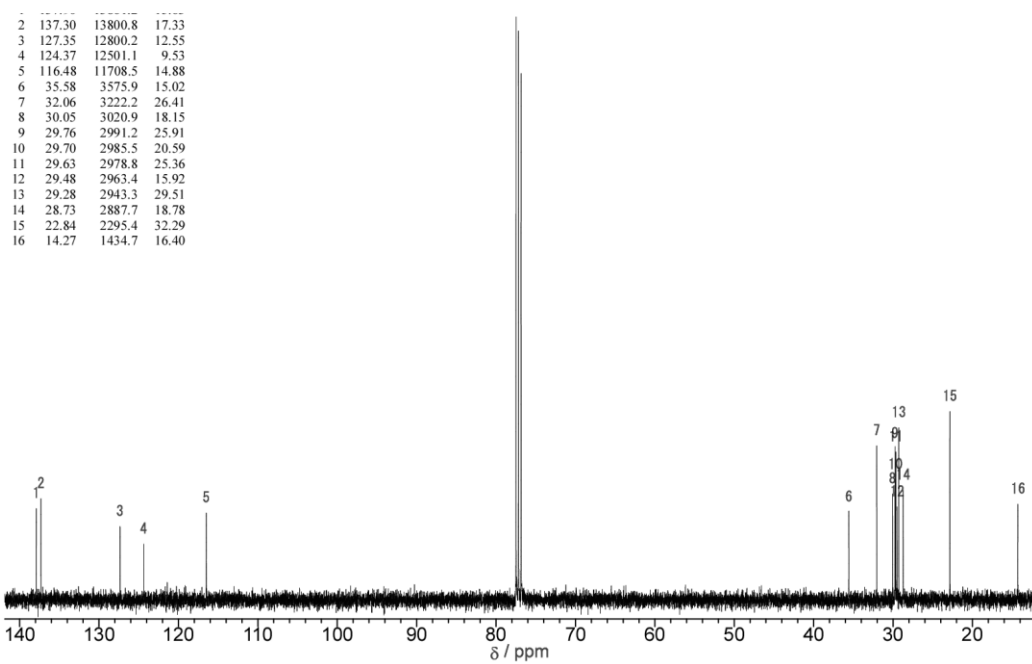
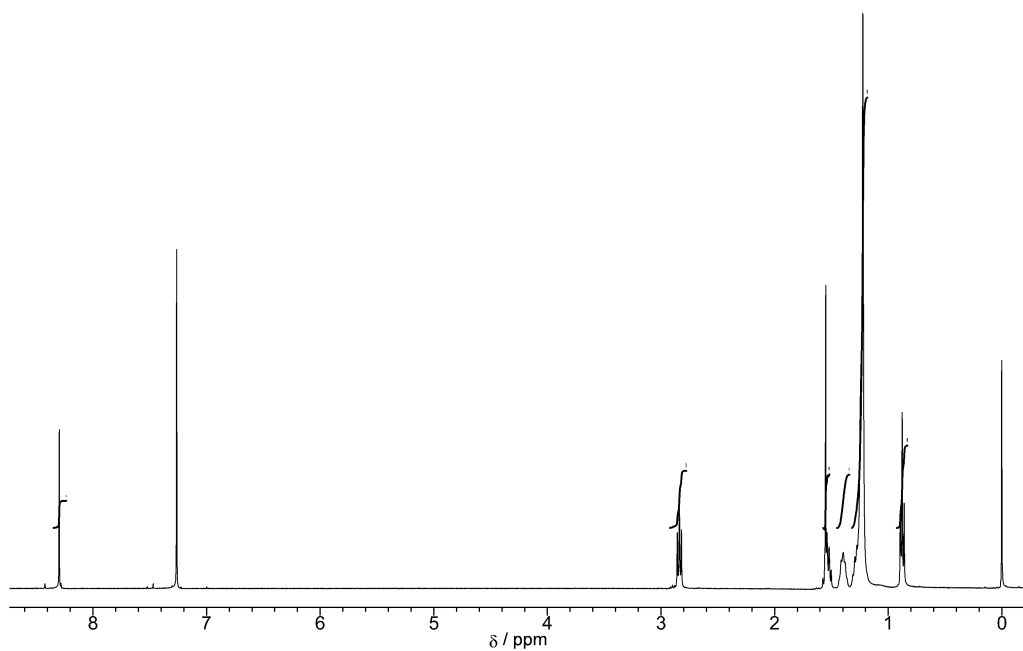
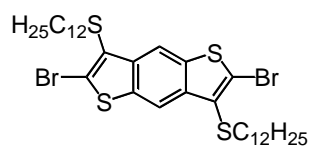
[<sup>1</sup>H and <sup>13</sup>C NMR Spectra of **1b**]



No.	ppm	Hz	Height
1	137.57	13827.6	5.84
2	137.53	13823.8	5.63
3	127.92	12857.7	8.33
4	126.36	12701.4	6.91
5	116.73	11733.4	7.16
6	35.02	3520.3	9.47
7	32.06	3222.2	13.31
8	29.78	2993.1	15.18
9	29.72	2987.4	11.14
10	29.69	2984.5	7.28
11	29.65	2980.7	12.65
12	29.49	2964.4	12.38
13	29.32	2947.1	12.84
14	28.80	2894.4	11.50
15	22.84	2295.4	9.30
16	14.28	1435.6	10.35

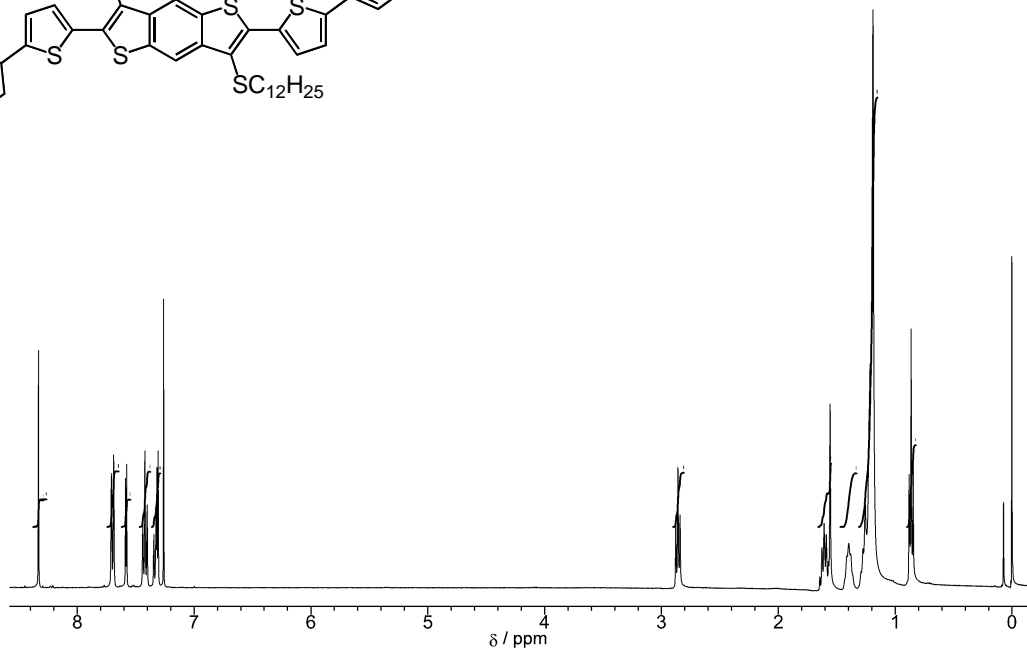
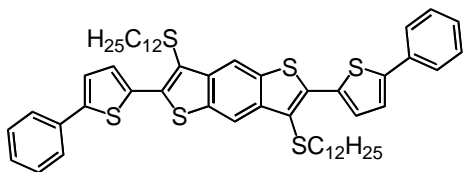


[  $^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra of **18** ]

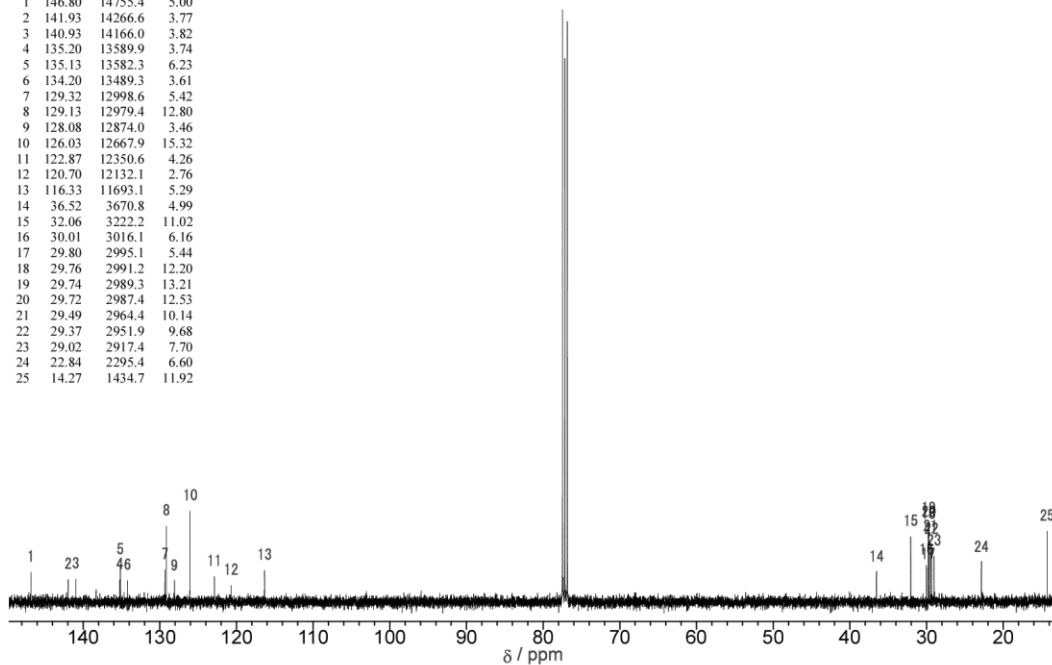




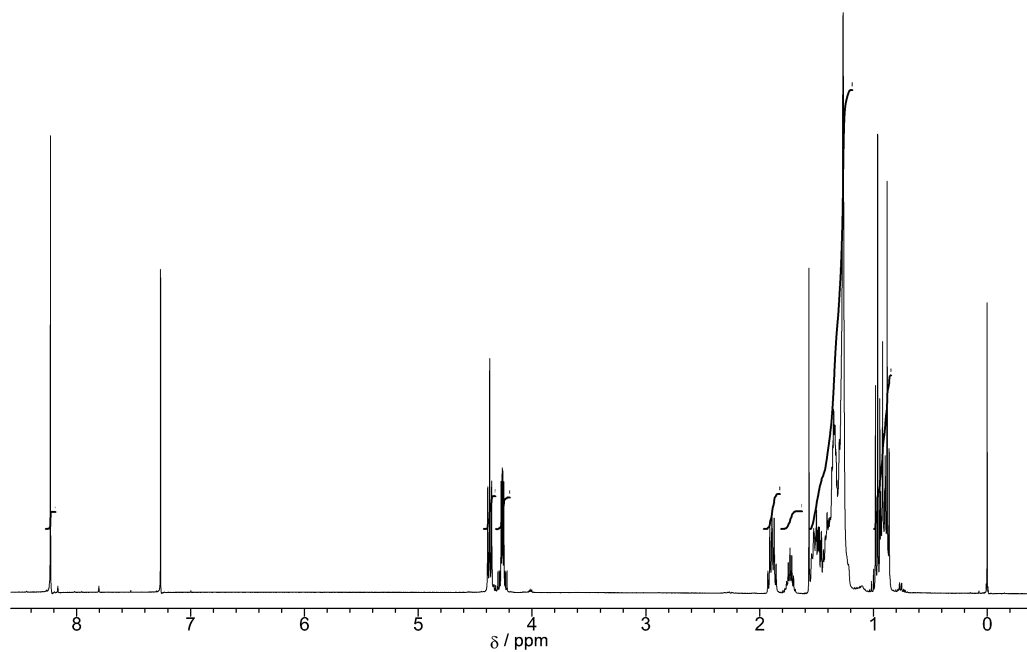
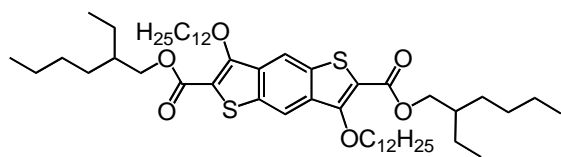
[<sup>1</sup>H and <sup>13</sup>C NMR Spectra of **2b**]



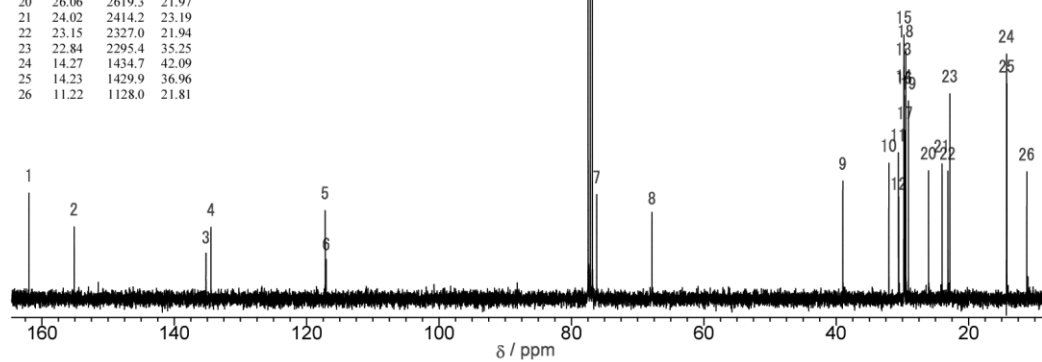
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1	146.80	14755.4	5.00
2	141.93	14266.6	3.77
3	140.93	14166.0	3.82
4	135.20	13589.9	3.74
5	135.13	13582.3	6.23
6	134.20	13489.3	3.61
7	129.32	12998.6	5.42
8	129.13	12979.4	12.80
9	128.08	12874.0	3.46
10	126.03	12667.9	15.32
11	122.87	12350.6	4.26
12	120.70	12132.1	2.76
13	116.33	11693.1	5.29
14	36.52	3670.8	4.99
15	32.06	3222.2	11.02
16	30.01	3016.1	6.16
17	29.80	2995.1	5.44
18	29.76	2991.2	12.20
19	29.74	2989.3	13.21
20	29.72	2987.4	12.53
21	29.49	2964.4	10.14
22	29.37	2951.9	9.68
23	29.02	2917.4	7.70
24	22.84	2295.4	6.60
25	14.27	1434.7	11.92



[<sup>1</sup>H and <sup>13</sup>C NMR Spectra of **15**]

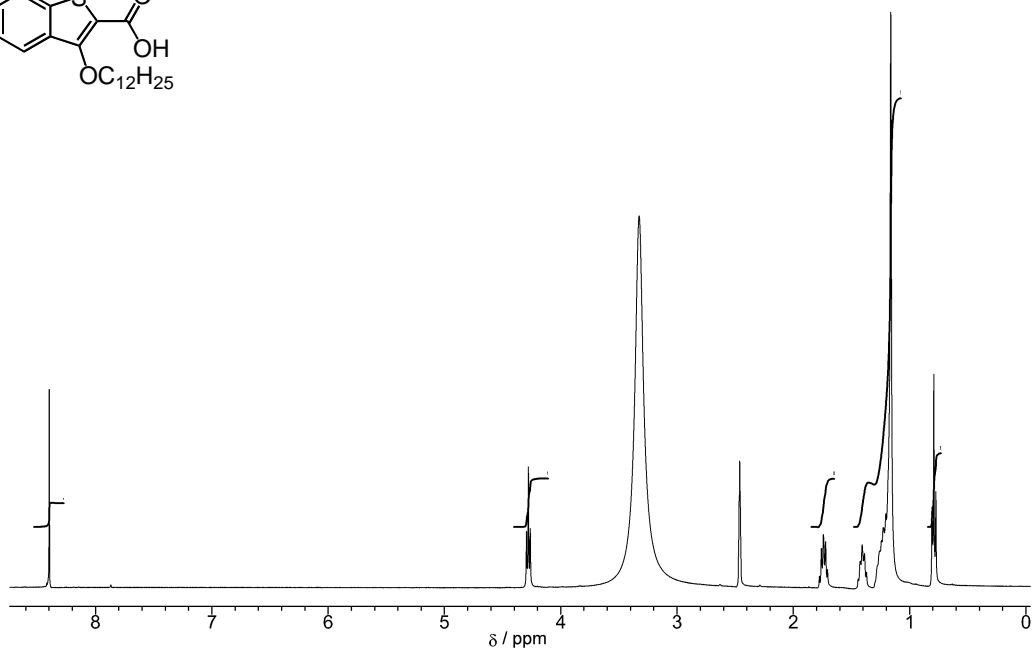
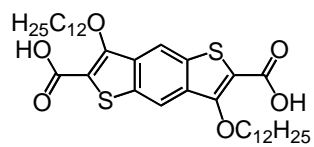


No.	ppm	Hz	Height
1	161.93	16276.5	18.13
2	155.12	15592.2	12.33
3	135.19	13589.0	7.47
4	134.45	13514.2	12.25
5	117.19	11779.4	15.12
6	117.03	11763.1	6.32
7	76.19	7658.0	17.87
8	67.82	6816.5	14.21
9	39.01	3920.9	20.19
10	32.06	3222.2	23.28
11	30.61	3076.5	25.09
12	30.56	3071.7	16.74
13	29.81	2996.0	39.93
14	29.78	2993.1	35.30
15	29.76	2991.2	45.38
16	29.74	2989.3	34.97
17	29.61	2975.9	28.93
18	29.50	2965.3	42.99
19	29.09	2924.1	34.02
20	26.06	2619.3	21.97
21	24.02	2414.2	23.19
22	23.15	2327.0	21.94
23	22.84	2295.4	35.25
24	14.27	1434.7	42.09
25	14.23	1429.9	36.96
26	11.22	1128.0	21.81

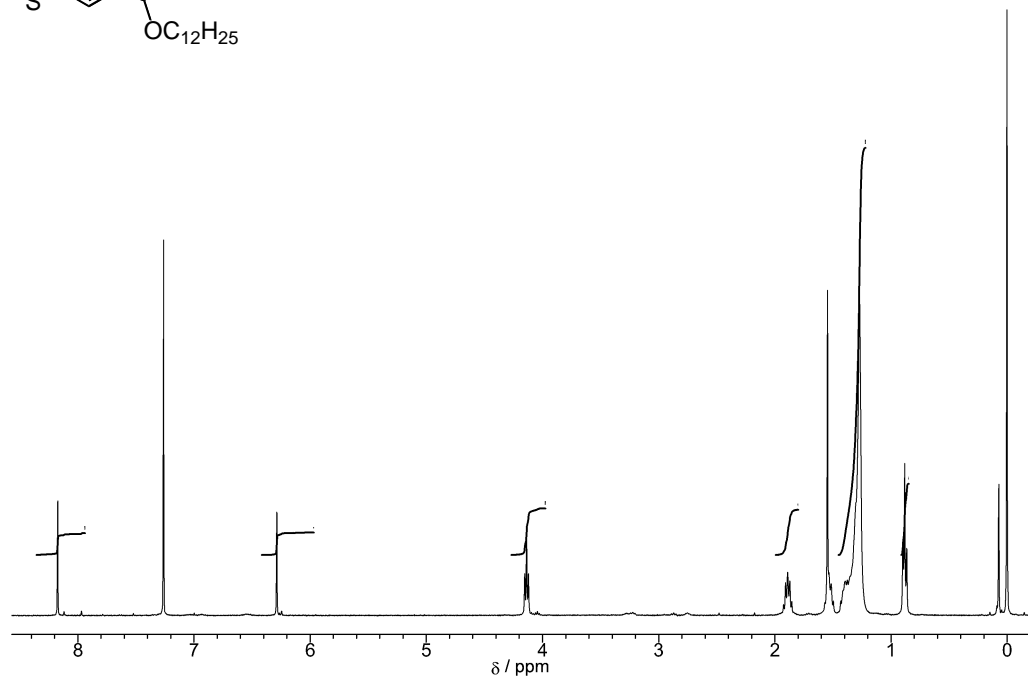
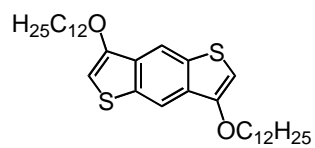


[ <sup>1</sup>H

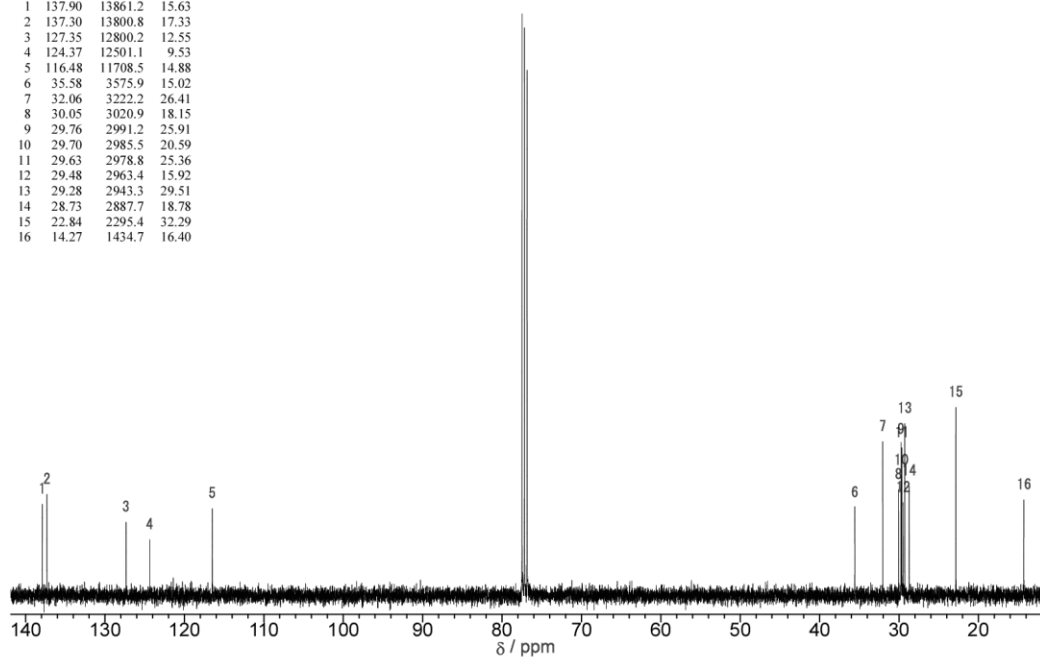
### NMR Spectrum of 17]



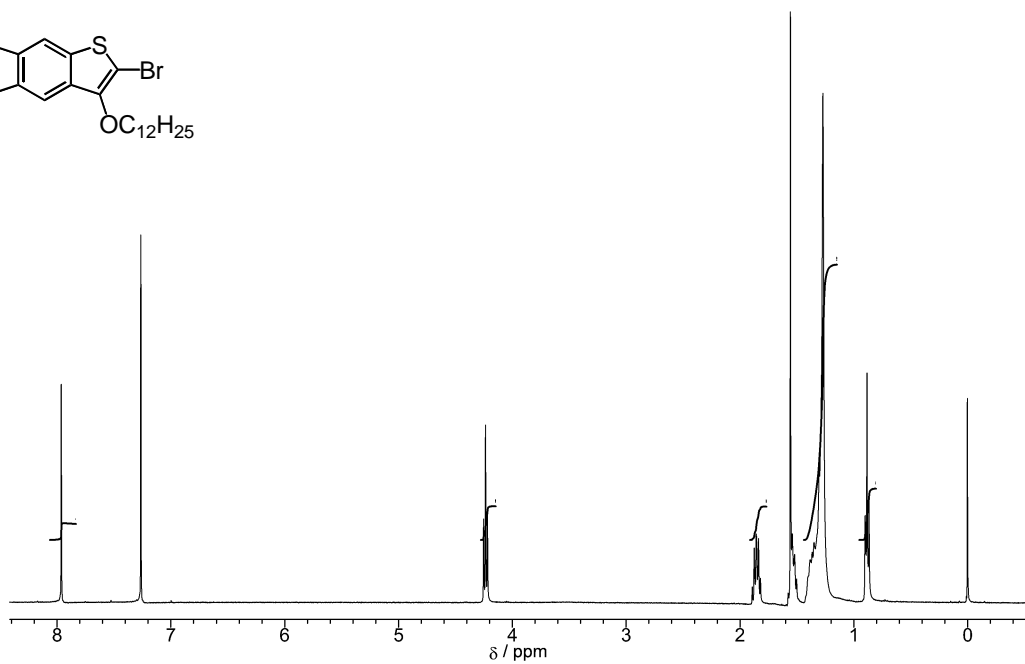
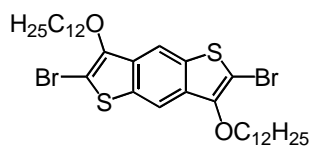
[  $^1\text{H}$  and  $^{13}\text{C}$  NMR Spectra of **1c** ]



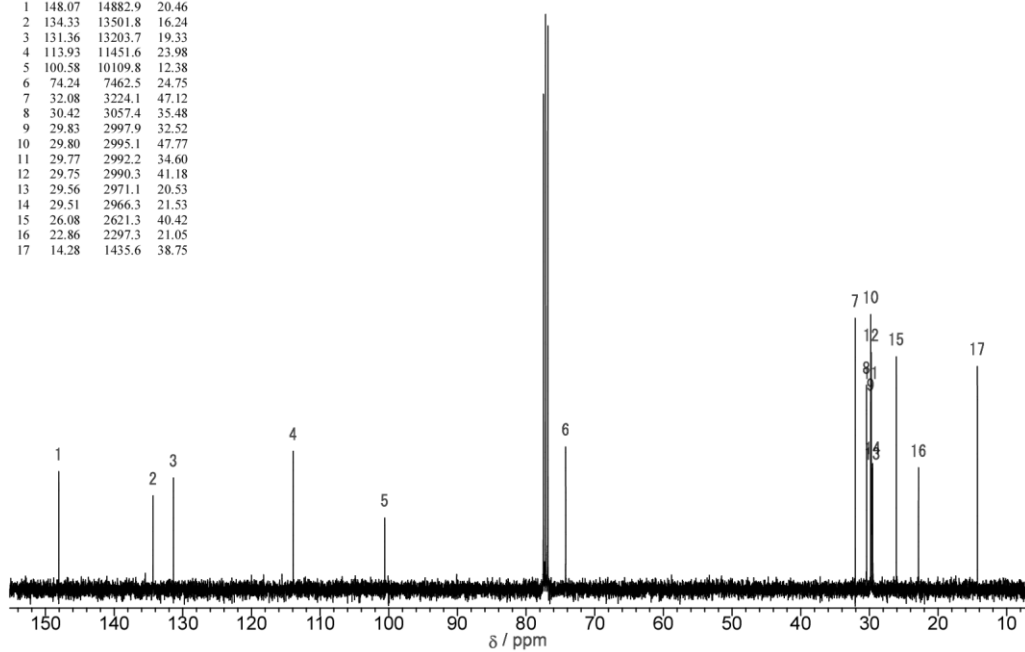
No.	ppm	Hz	Height
1	137.90	13861.2	15.63
2	137.30	13800.8	17.33
3	127.35	12800.2	12.55
4	124.37	12501.1	9.53
5	116.48	11708.5	14.88
6	35.58	3575.9	15.02
7	32.06	3222.2	26.41
8	30.05	3020.9	18.15
9	29.76	2991.2	25.91
10	29.70	2985.5	20.59
11	29.63	2978.8	25.36
12	29.48	2963.4	15.92
13	29.28	2943.3	29.51
14	28.73	2887.7	18.78
15	22.84	2295.4	32.29
16	14.27	1434.7	16.40



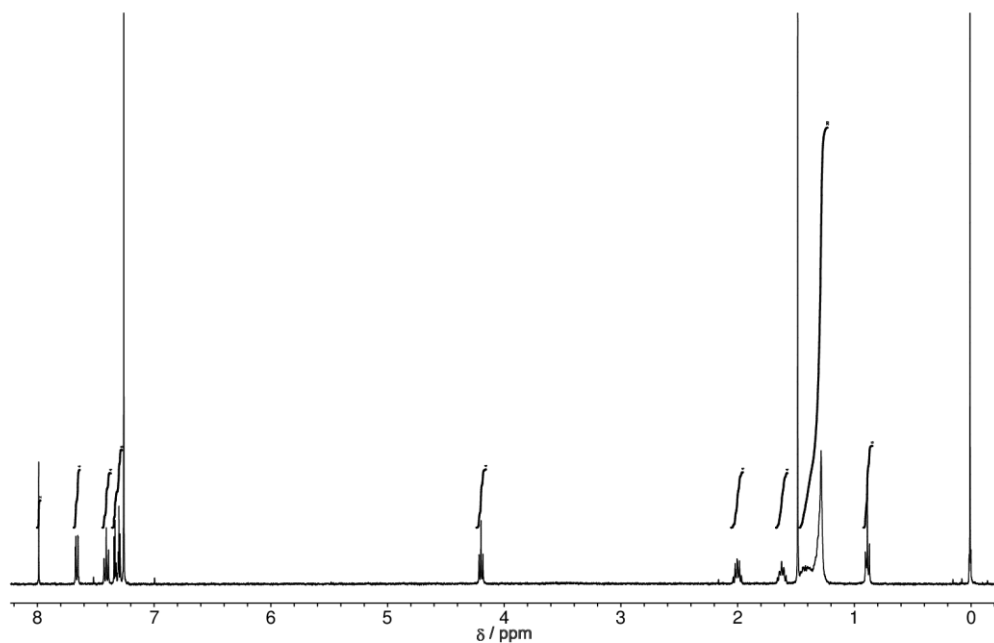
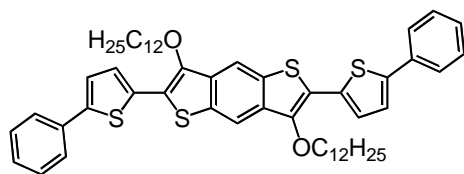
[<sup>1</sup>H and <sup>13</sup>C NMR Spectra of **19**]



No.	ppm	Hz	Height
1	148.07	14882.9	20.46
2	134.33	13501.8	16.24
3	131.36	13203.7	19.33
4	113.93	11451.6	23.98
5	100.58	10109.8	12.38
6	74.24	7462.5	24.75
7	32.08	3224.1	47.12
8	30.42	3057.4	35.48
9	29.83	2997.9	32.52
10	29.80	2995.1	47.77
11	29.77	2992.2	34.60
12	29.75	2990.3	41.18
13	29.56	2971.1	20.53
14	29.51	2966.3	21.53
15	26.08	2621.3	40.42
16	22.86	2297.3	21.05
17	14.28	1435.6	38.75



[<sup>1</sup>H NMR Spectrum of **2c**]



No.	ppm	Hz	Height	No.	ppm	Hz	Height
1	145.23	14597.4	0.34	16	29.69	2984.7	0.86
2	144.95	14569.7	0.30	17	29.61	2976.0	0.53
3	134.47	13516.3	0.22	18	29.39	2954.0	0.34
4	134.32	13501.0	0.30	19	26.22	2635.8	0.37
5	132.82	13350.5	0.32	20	22.71	2283.1	0.72
6	129.02	12968.1	0.76	21	14.10	1417.6	0.49
7	127.75	12840.6	0.34				
8	126.37	12702.6	0.30				
9	125.82	12647.0	0.79				
10	117.42	11802.6	0.22				
11	73.87	7425.2	0.40				
12	31.96	3212.8	0.37				
13	30.60	3075.7	0.43				
14	29.74	2989.5	0.80				
15	29.72	2987.5	0.51				

