

A concise approach for the synthesis of bitungolides: Total syntheses of (–)-bitungolide B & E

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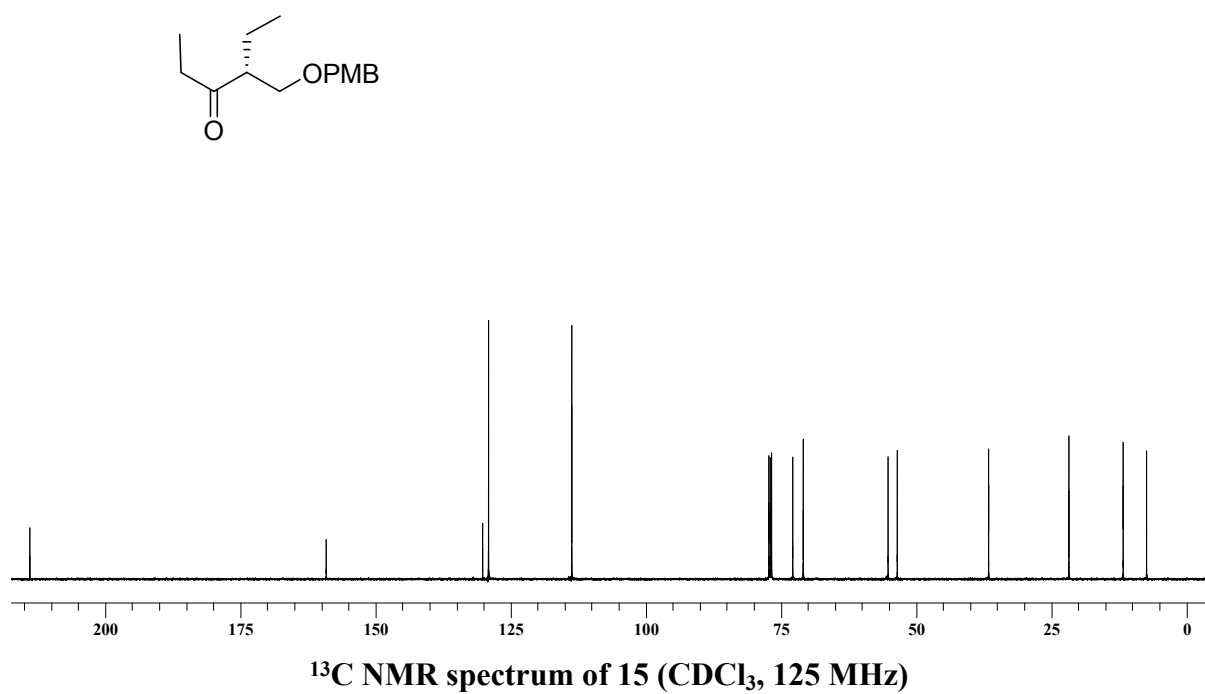
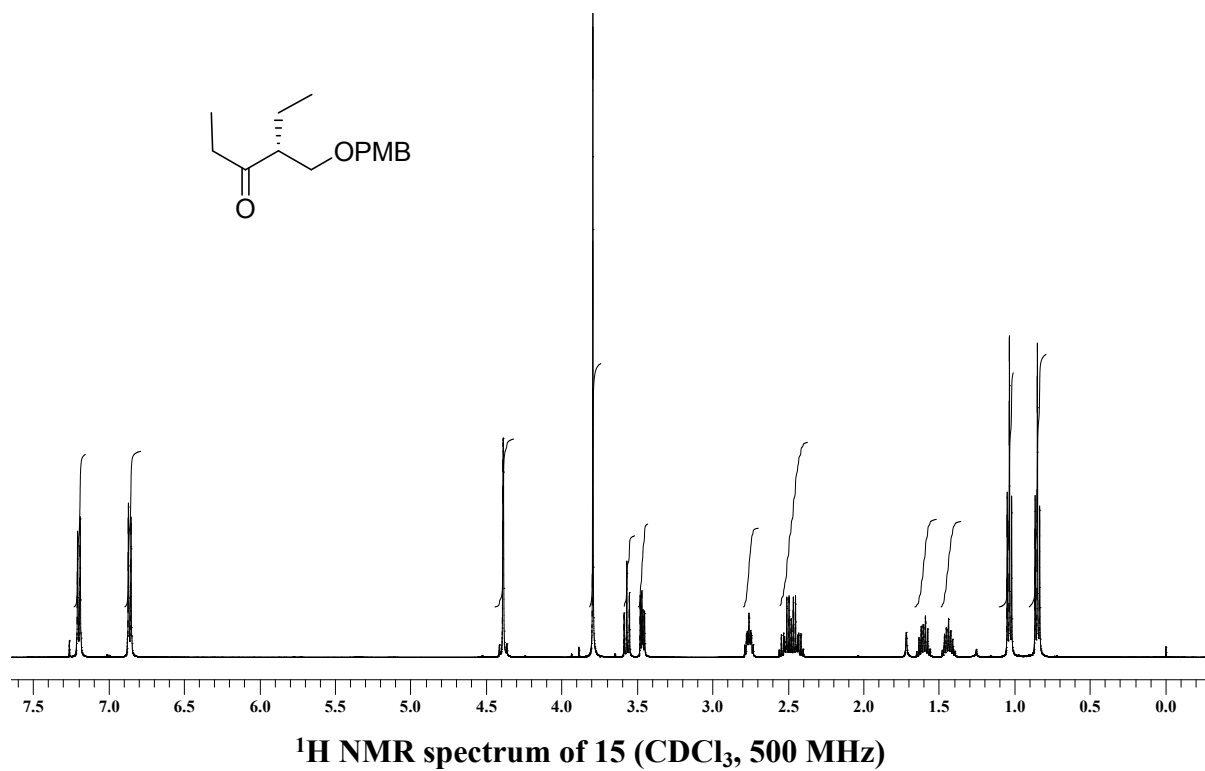
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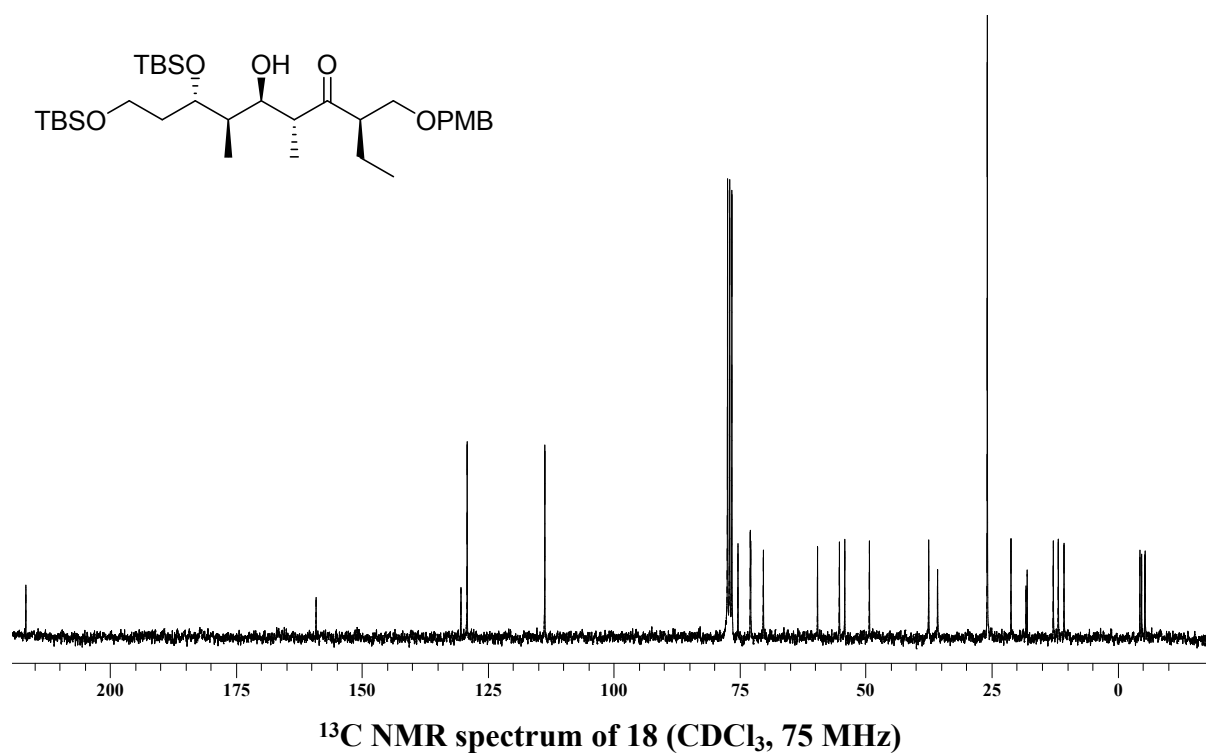
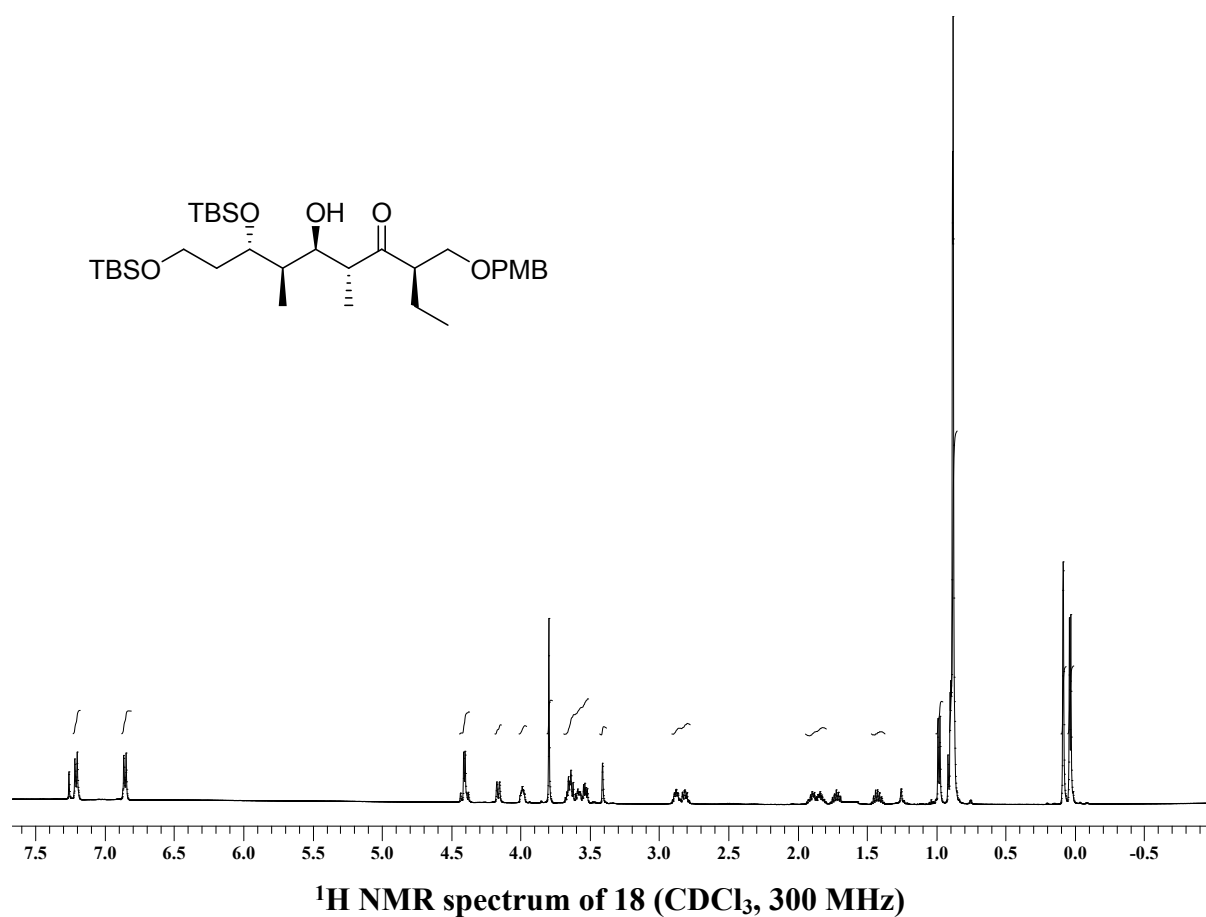
Supporting Information

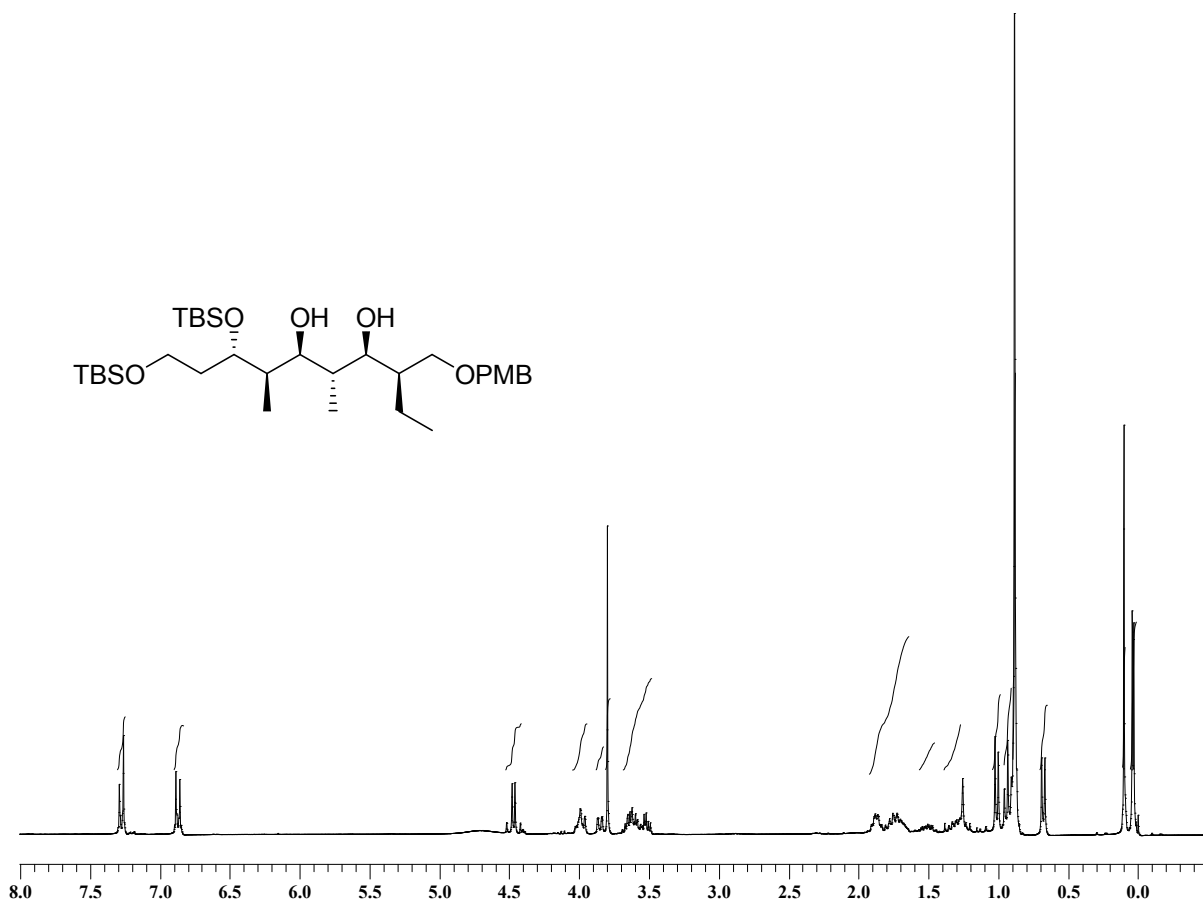
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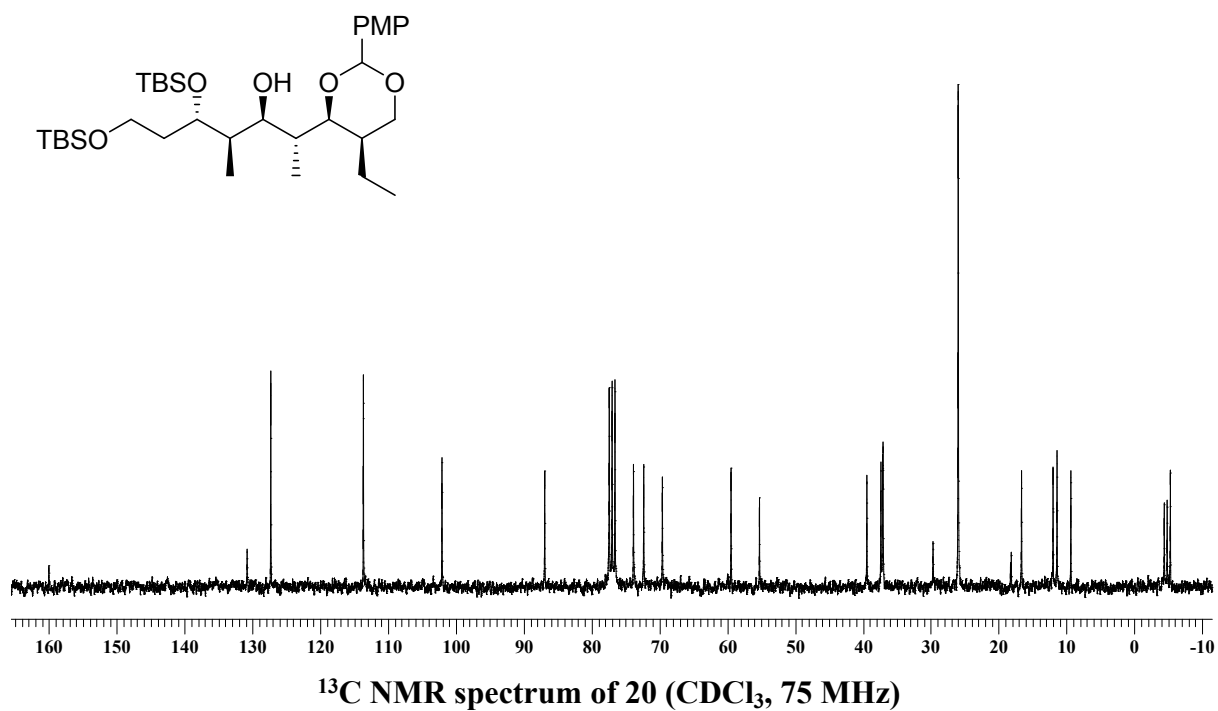
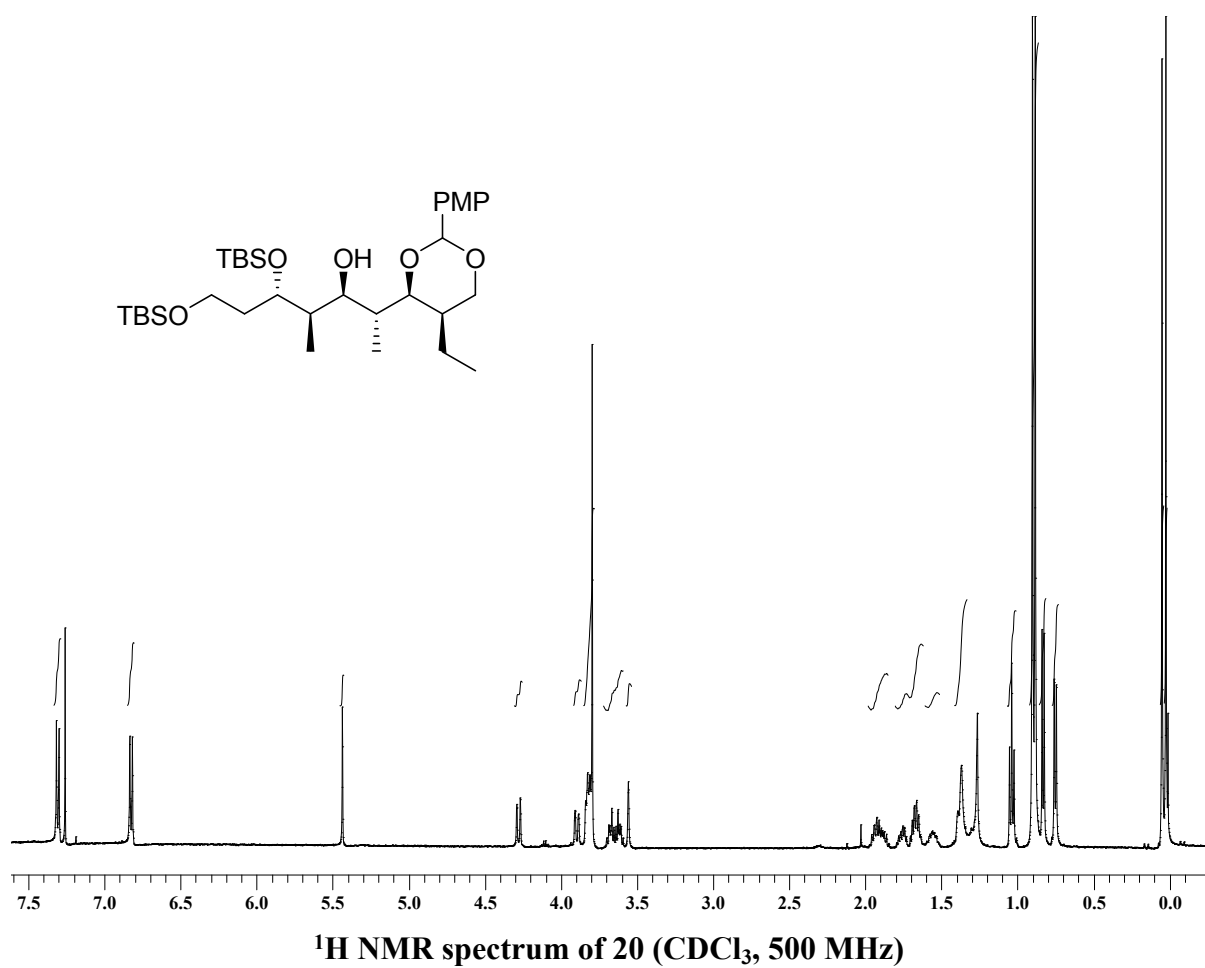
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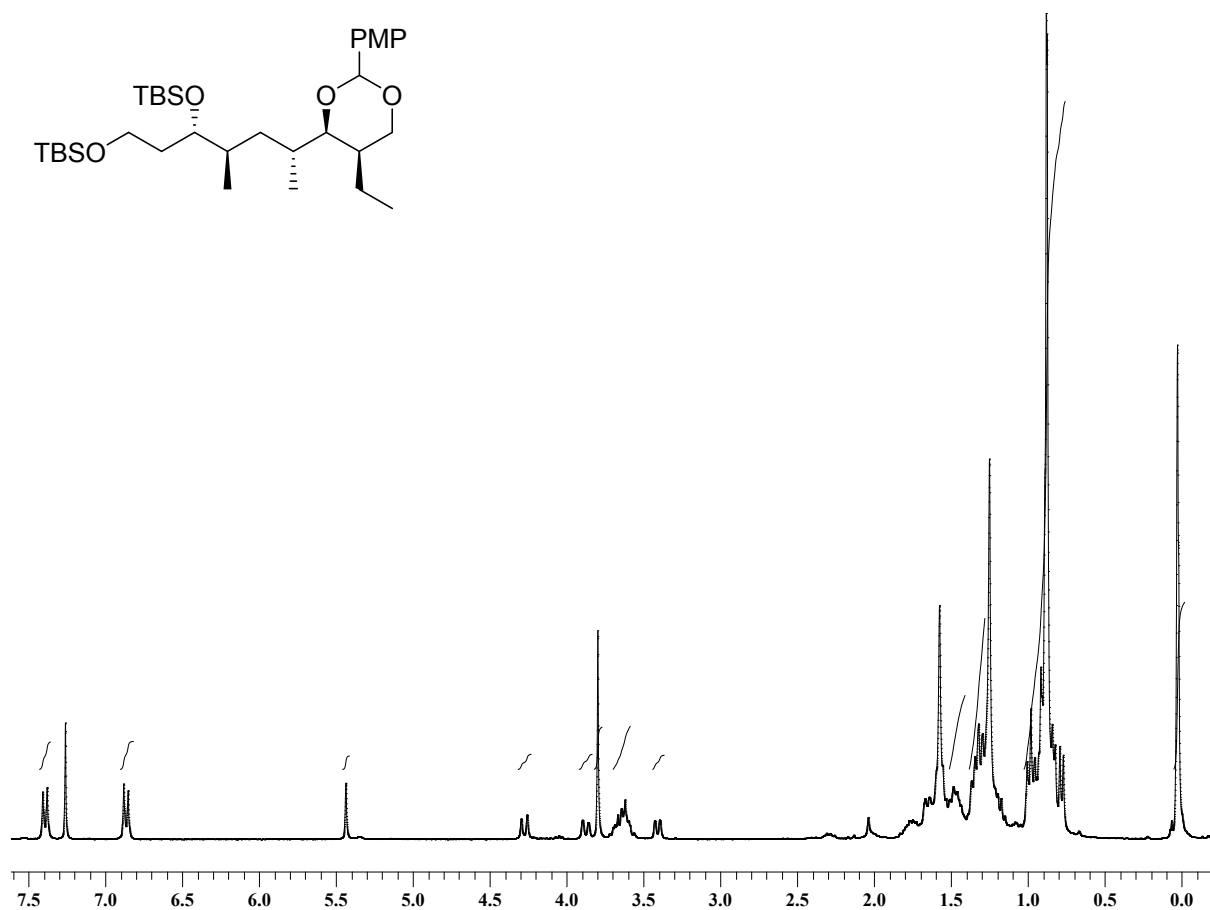
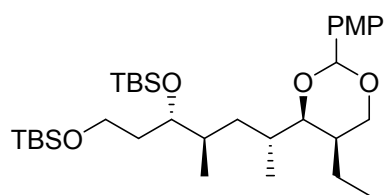




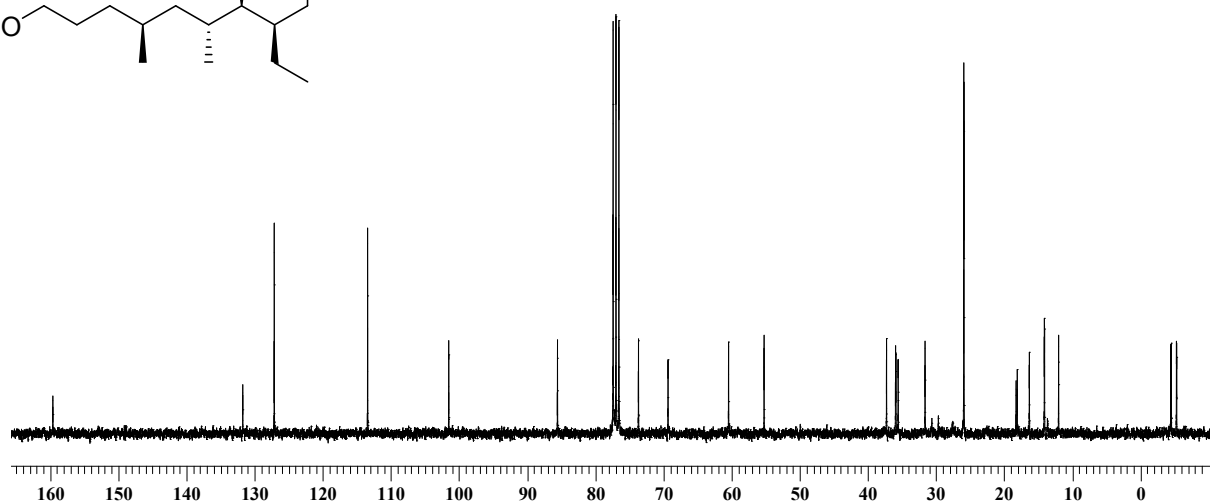
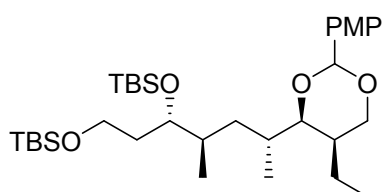
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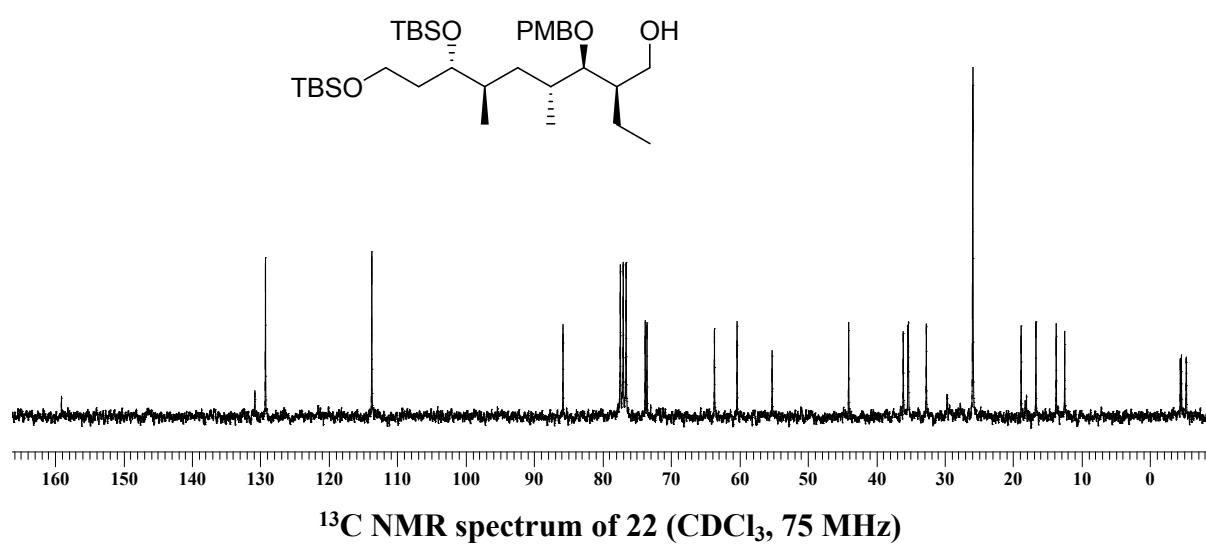
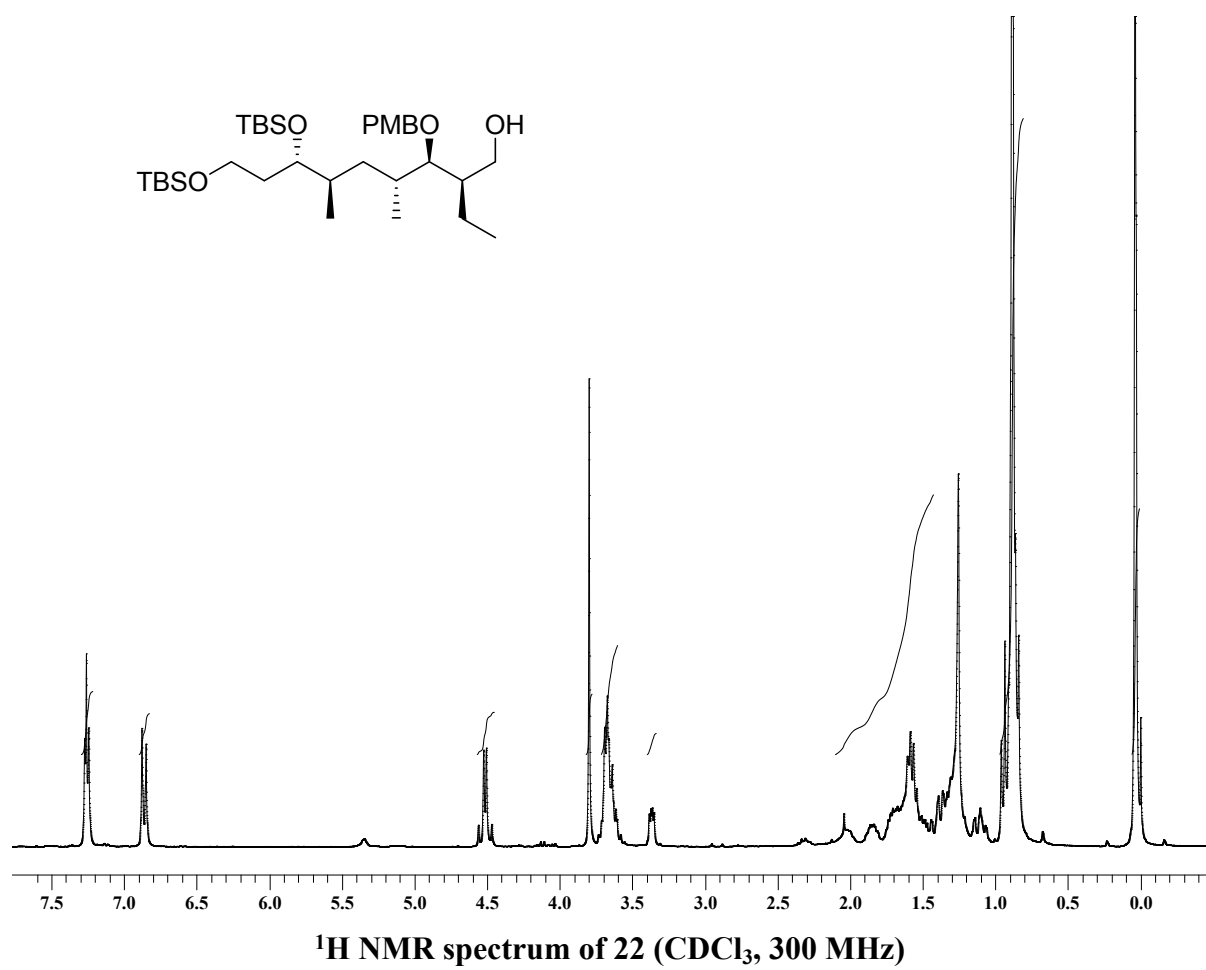


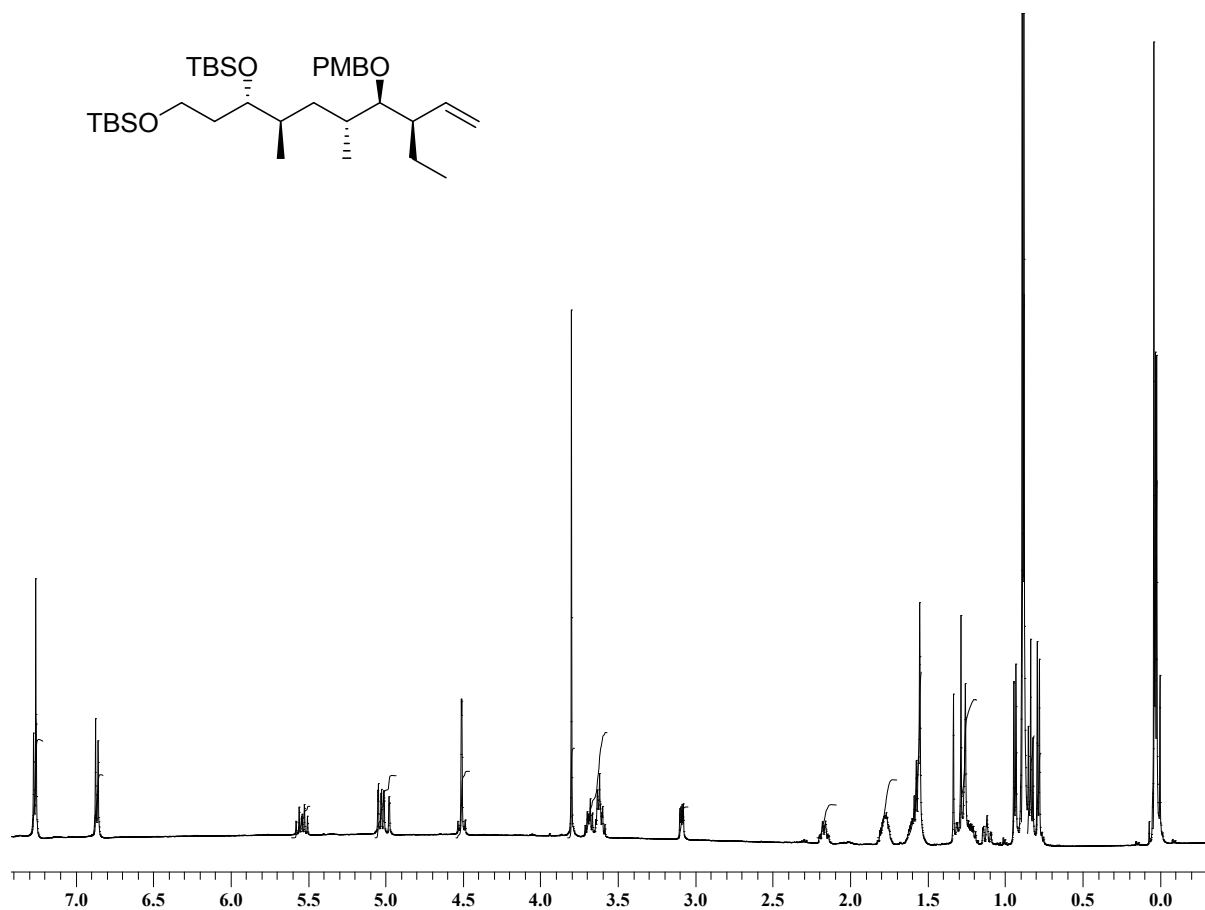
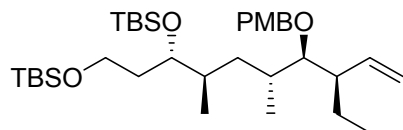


^1H NMR spectrum of 21 (CDCl_3 , 300 MHz)

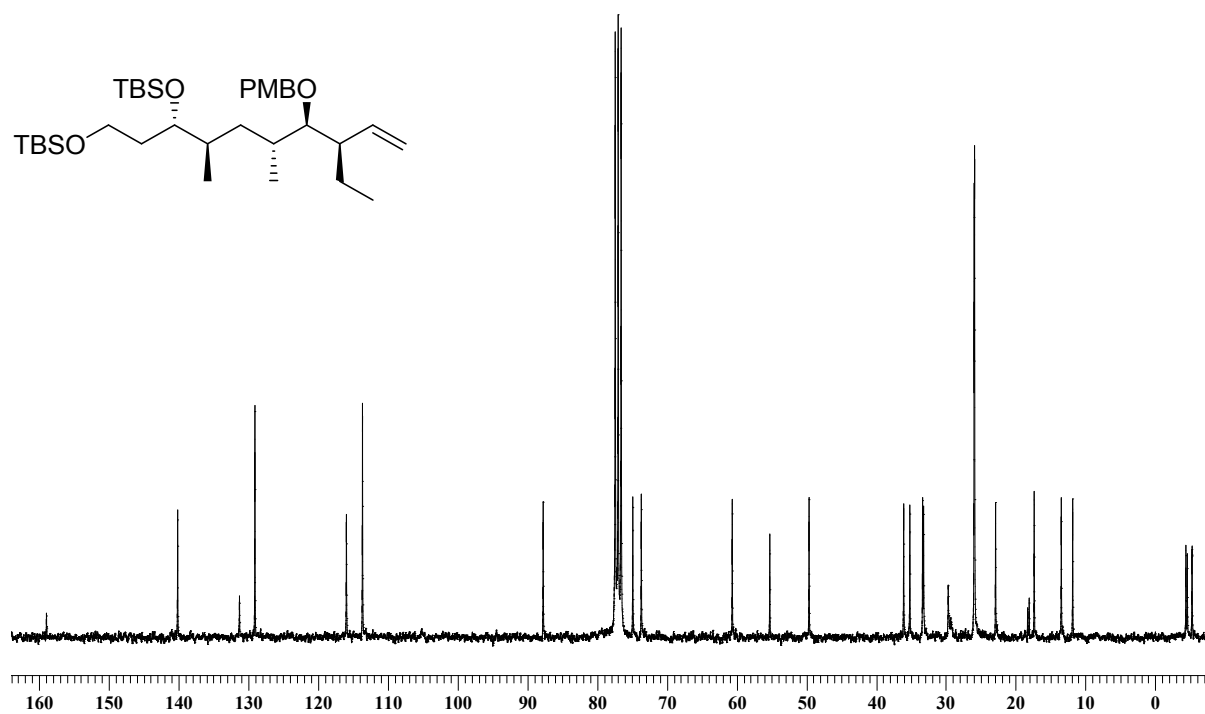


^{13}C NMR spectrum of 21 (CDCl_3 , 75 MHz)

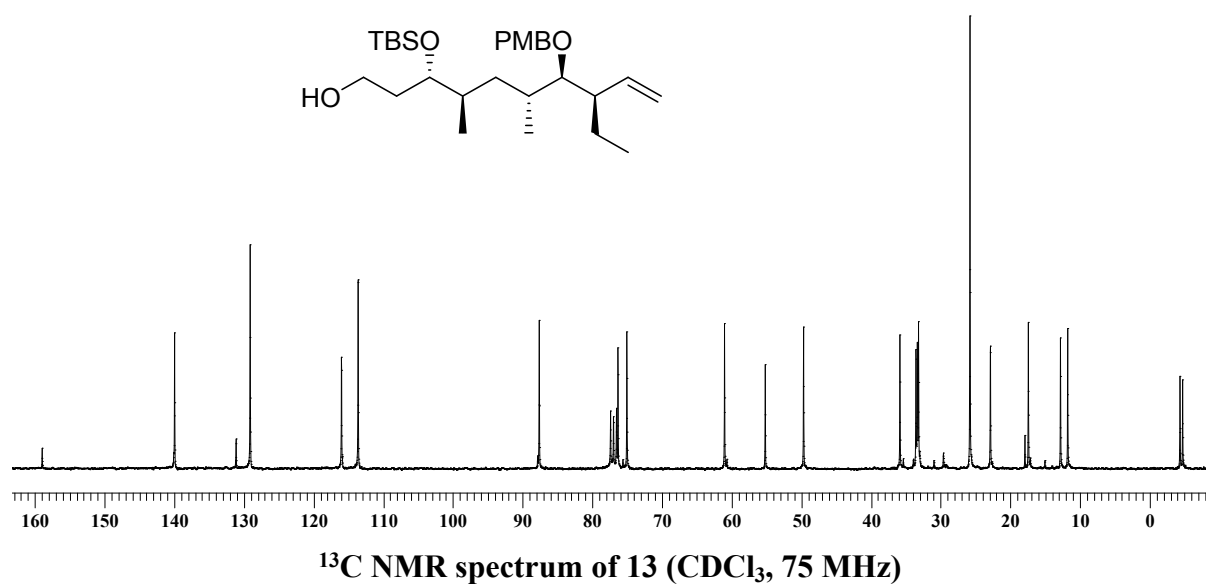
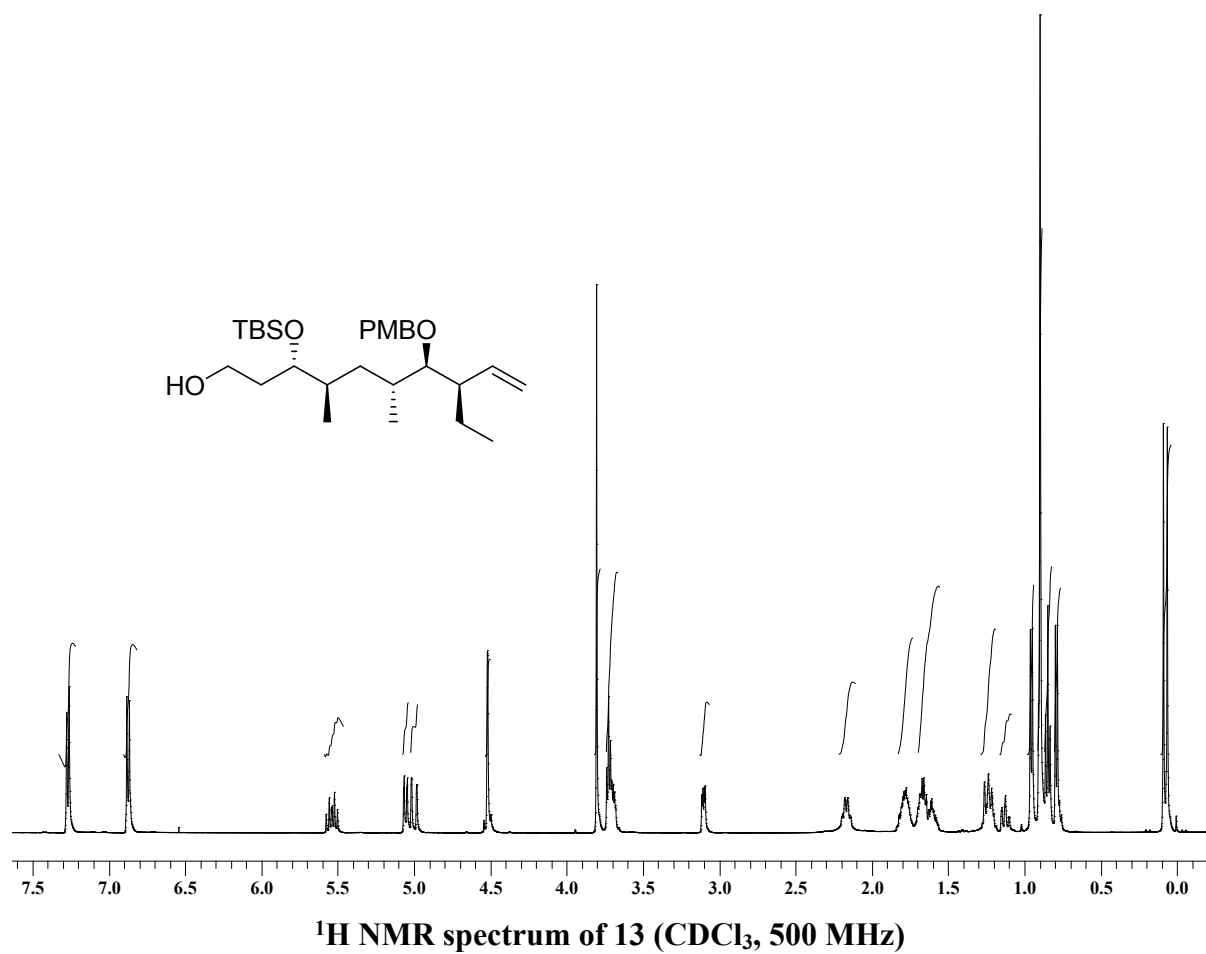


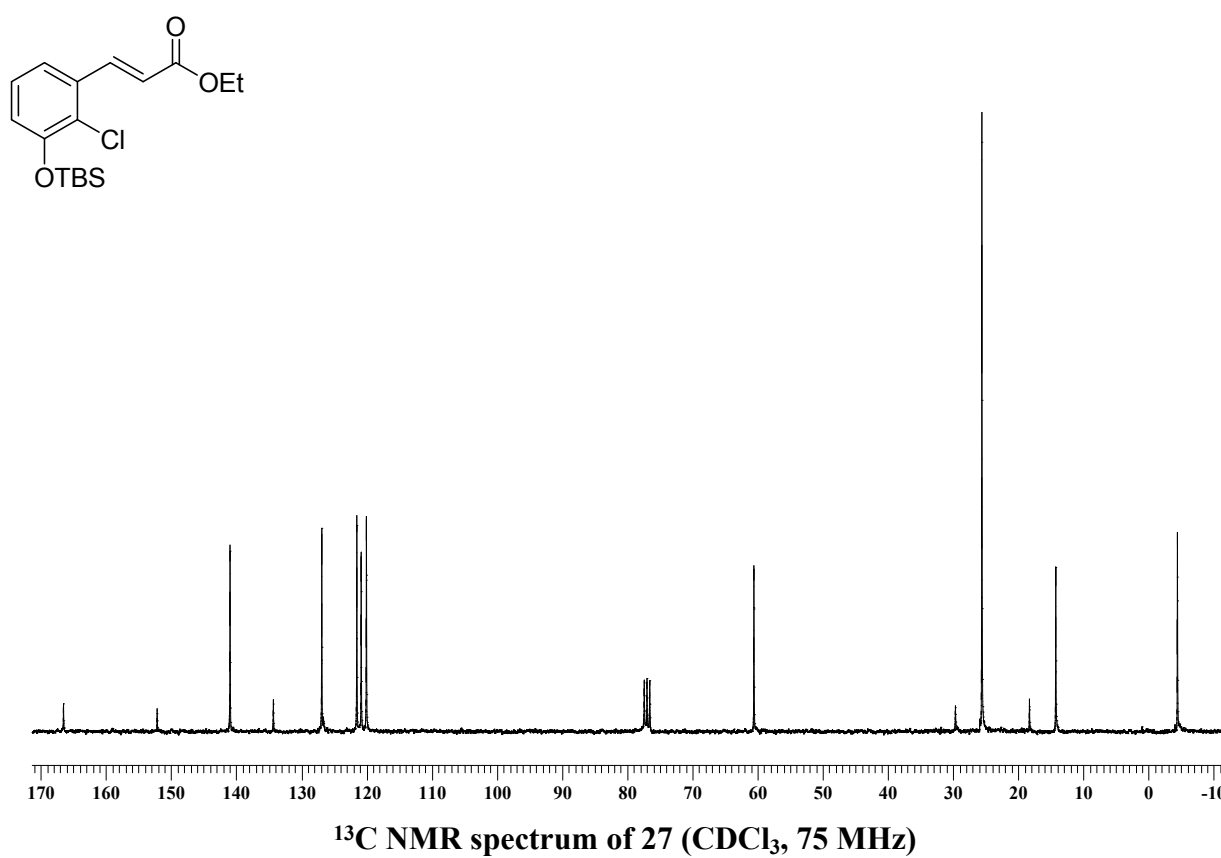
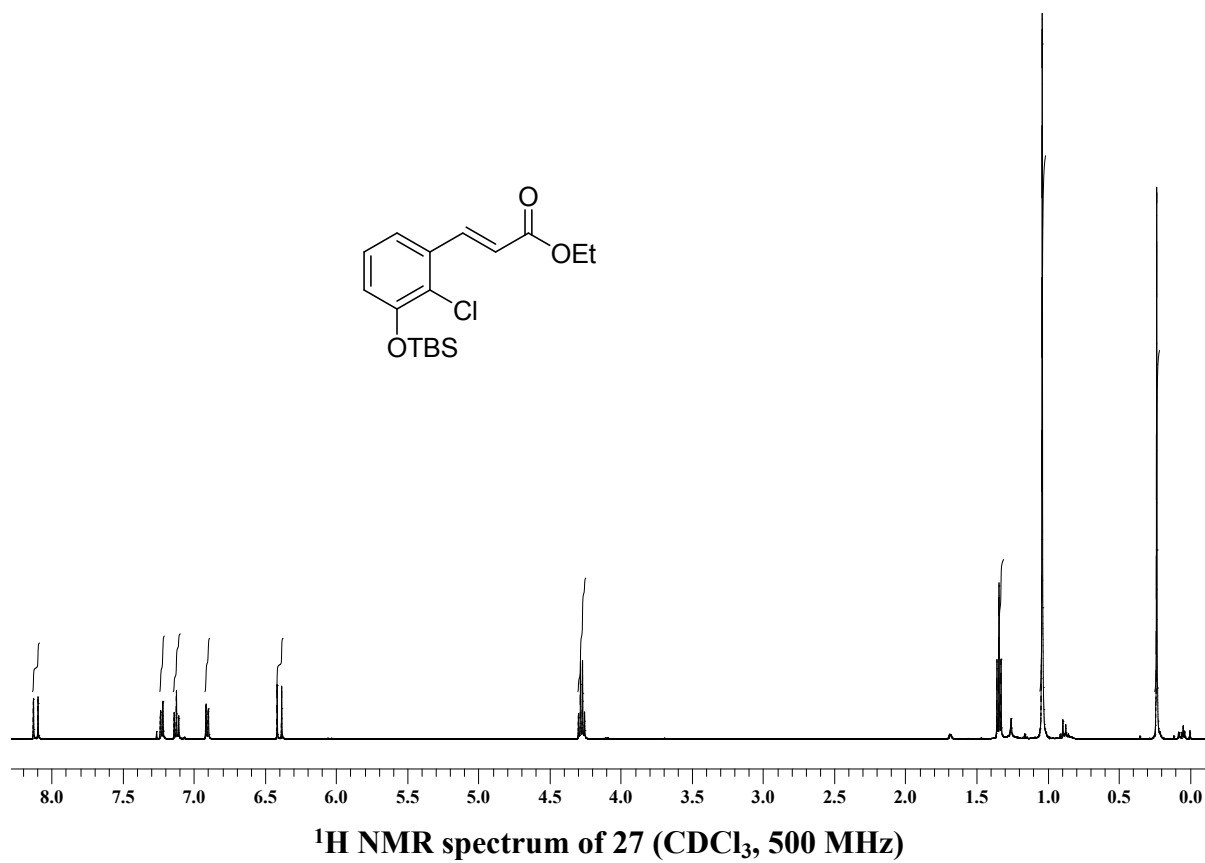


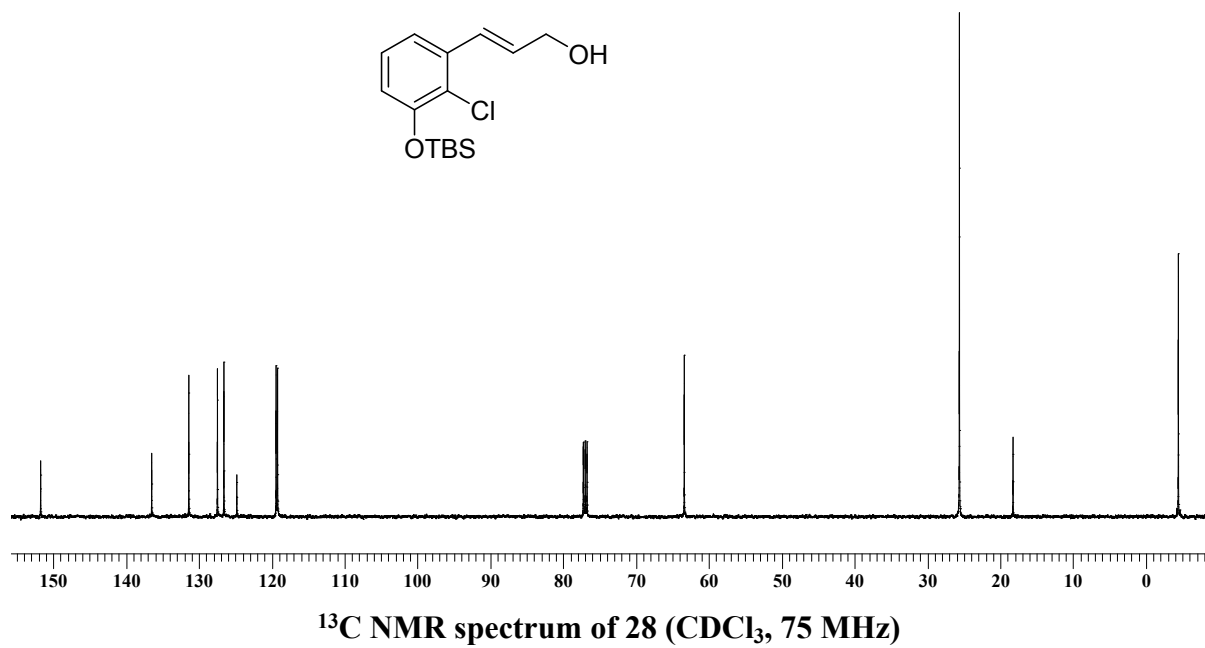
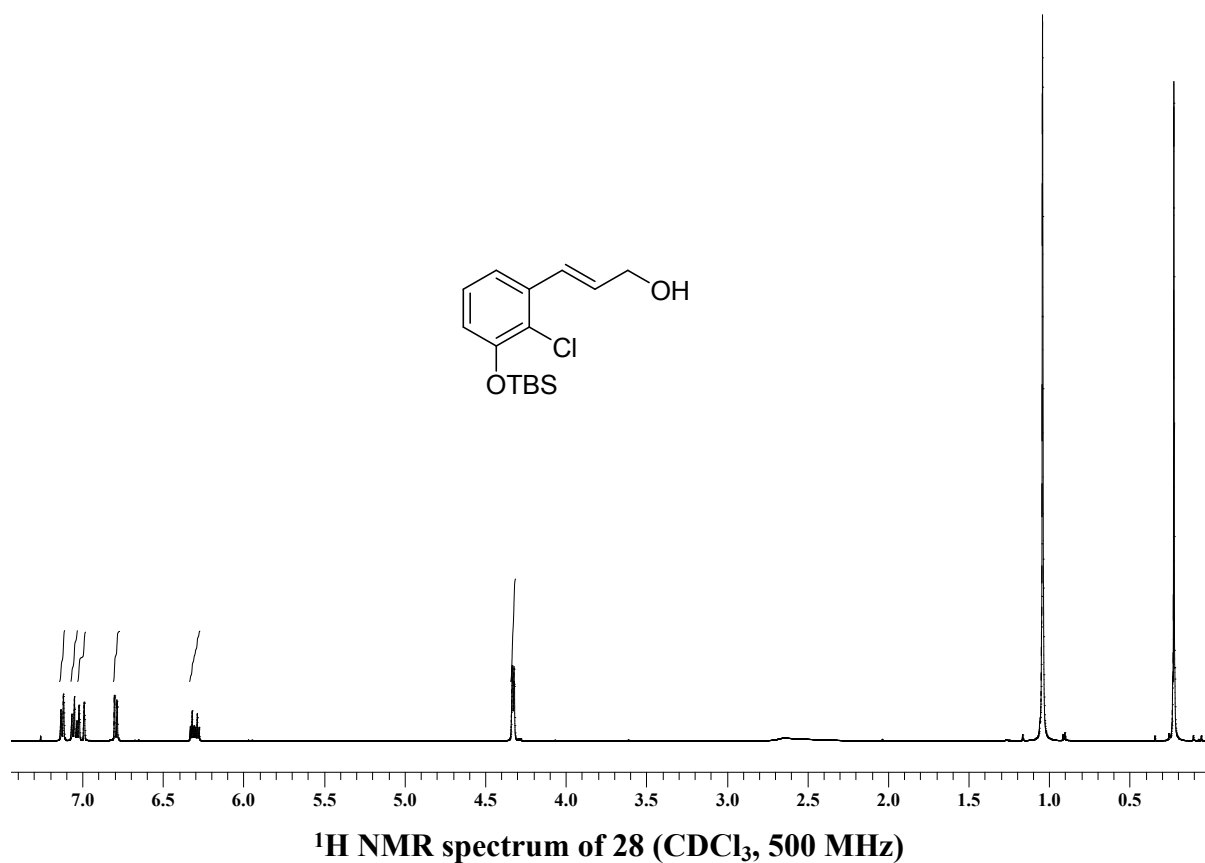
^1H NMR spectrum of 23 (CDCl_3 , 500 MHz)

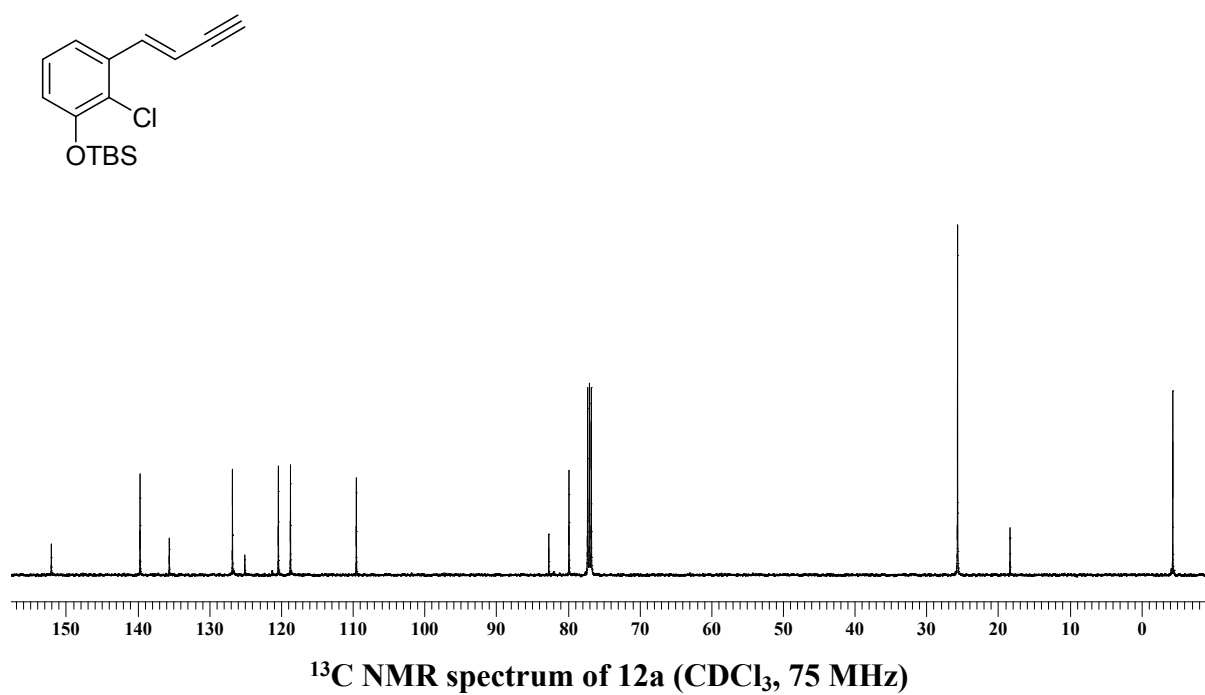
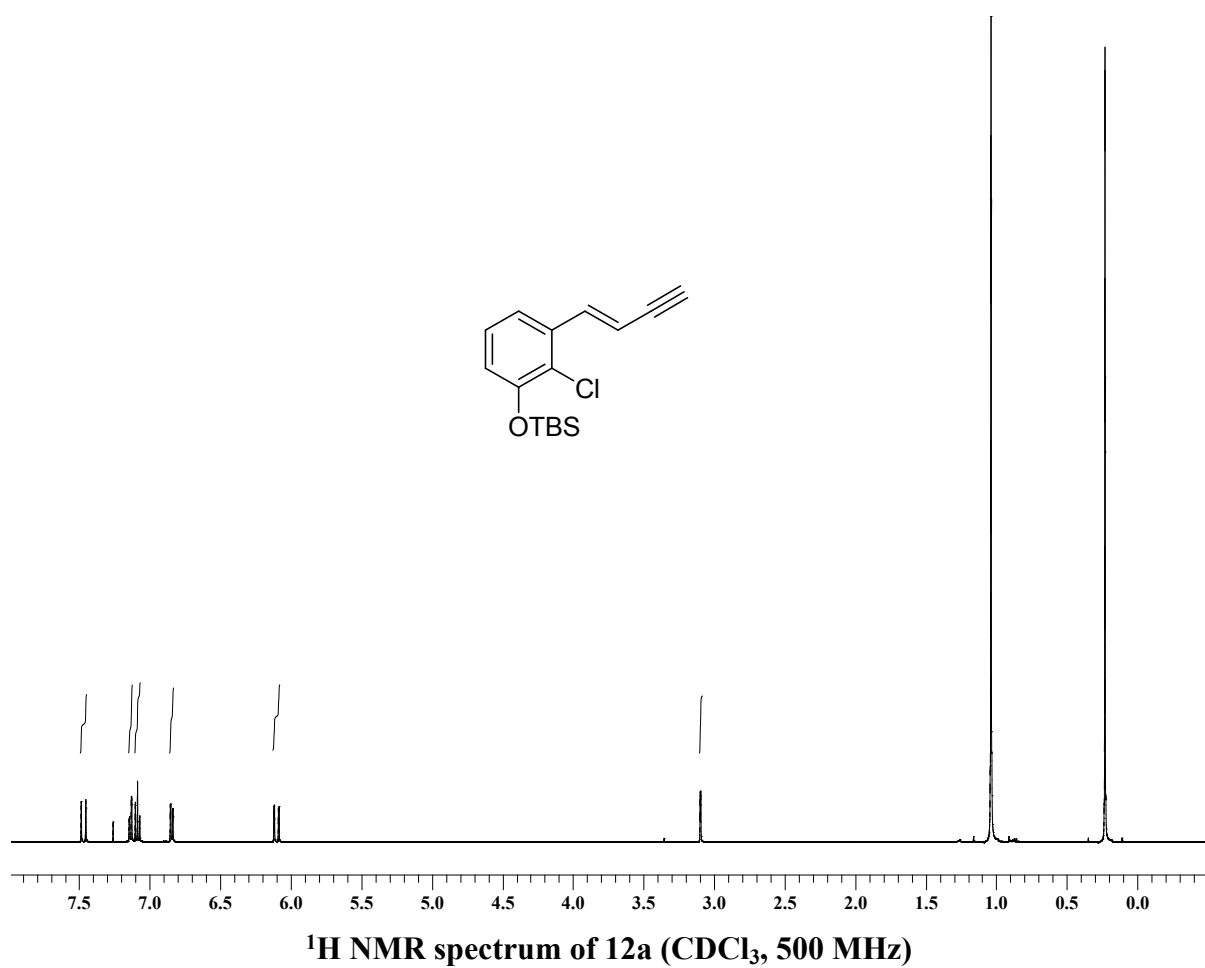


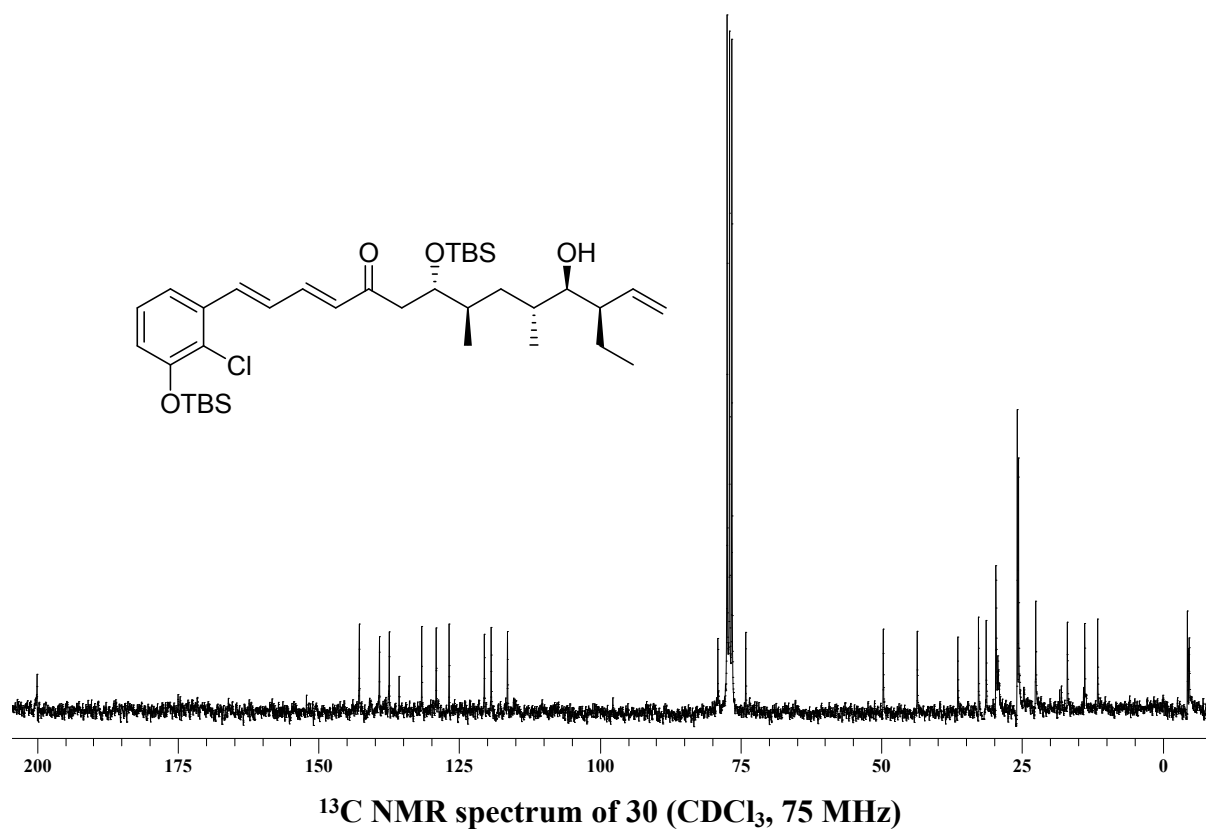
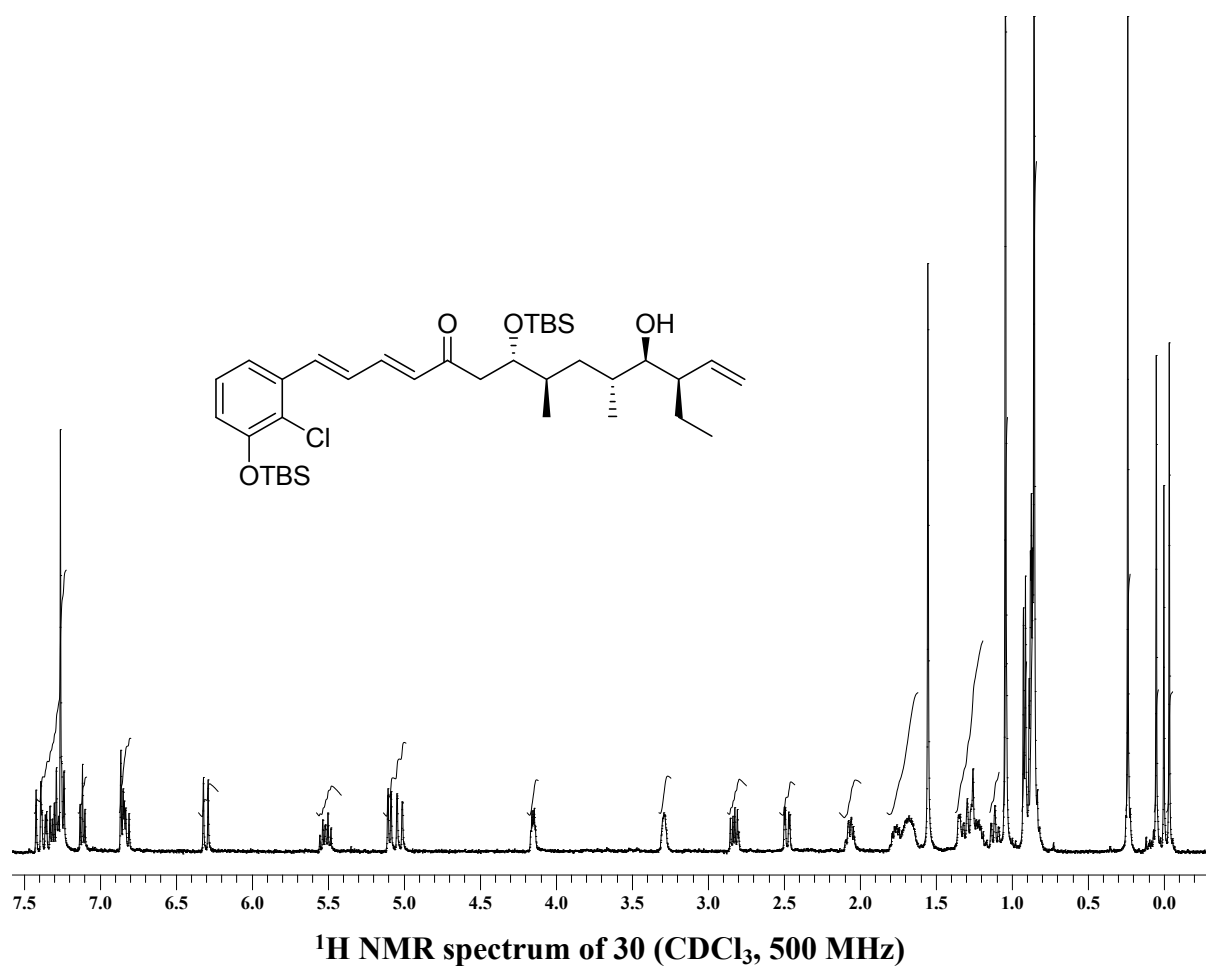
^{13}C NMR spectrum of 23 (CDCl_3 , 75 MHz)

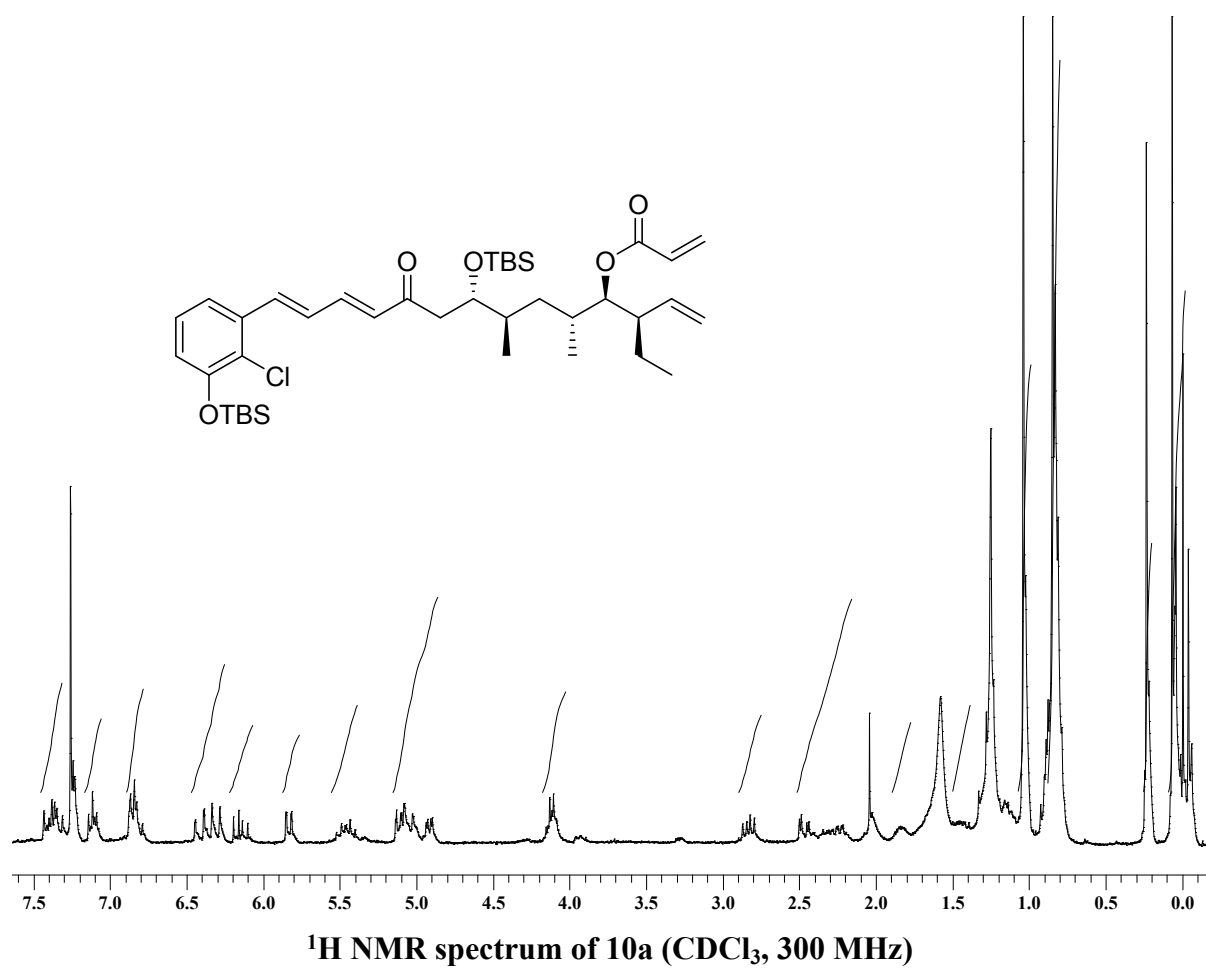


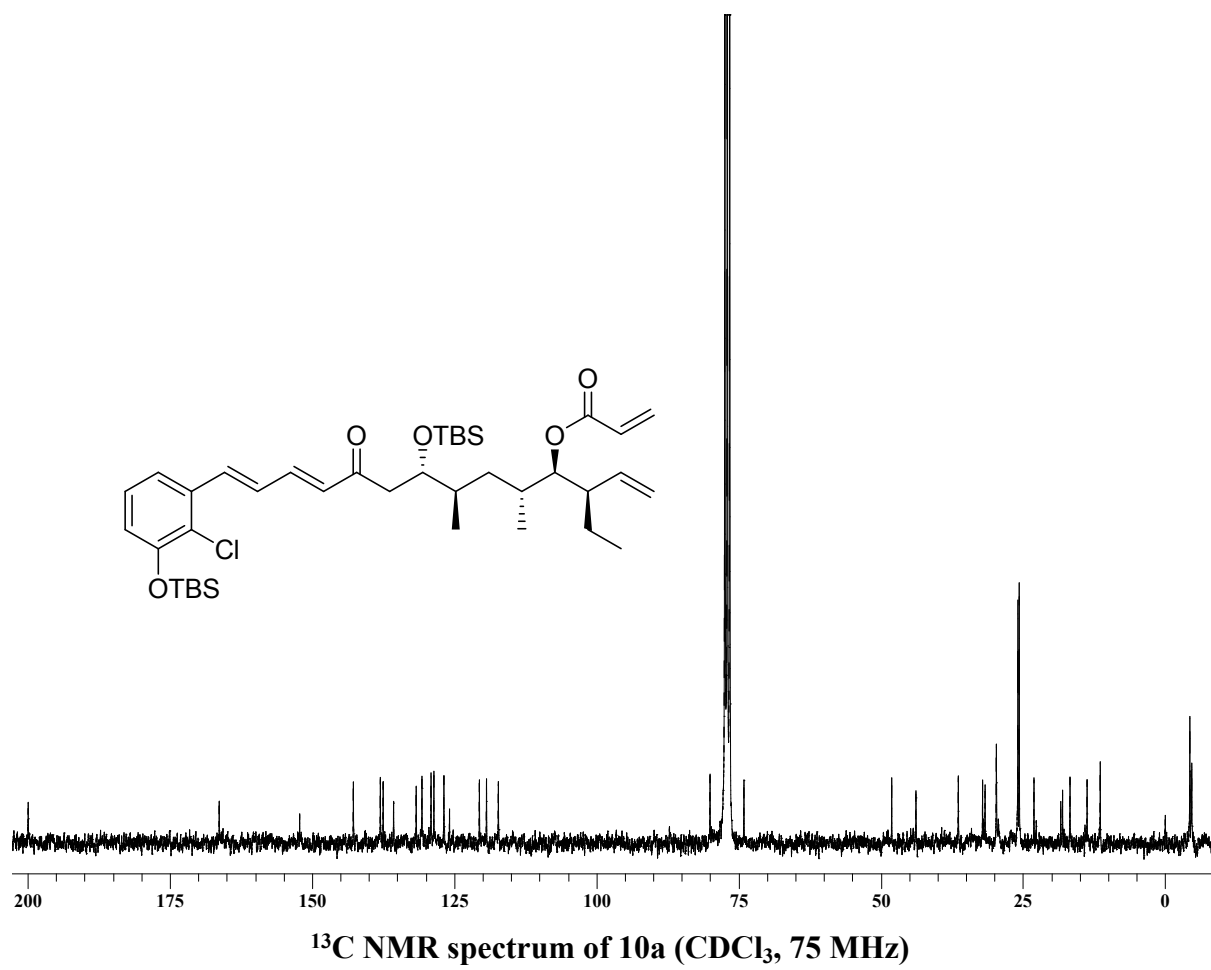


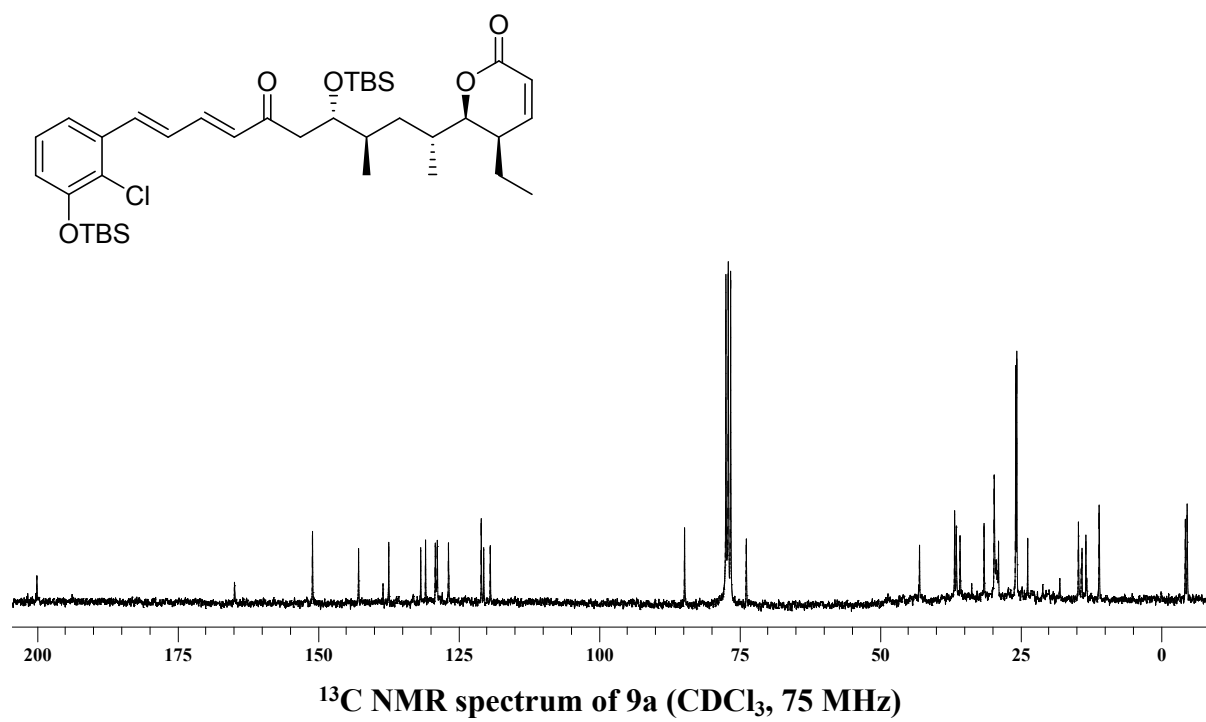
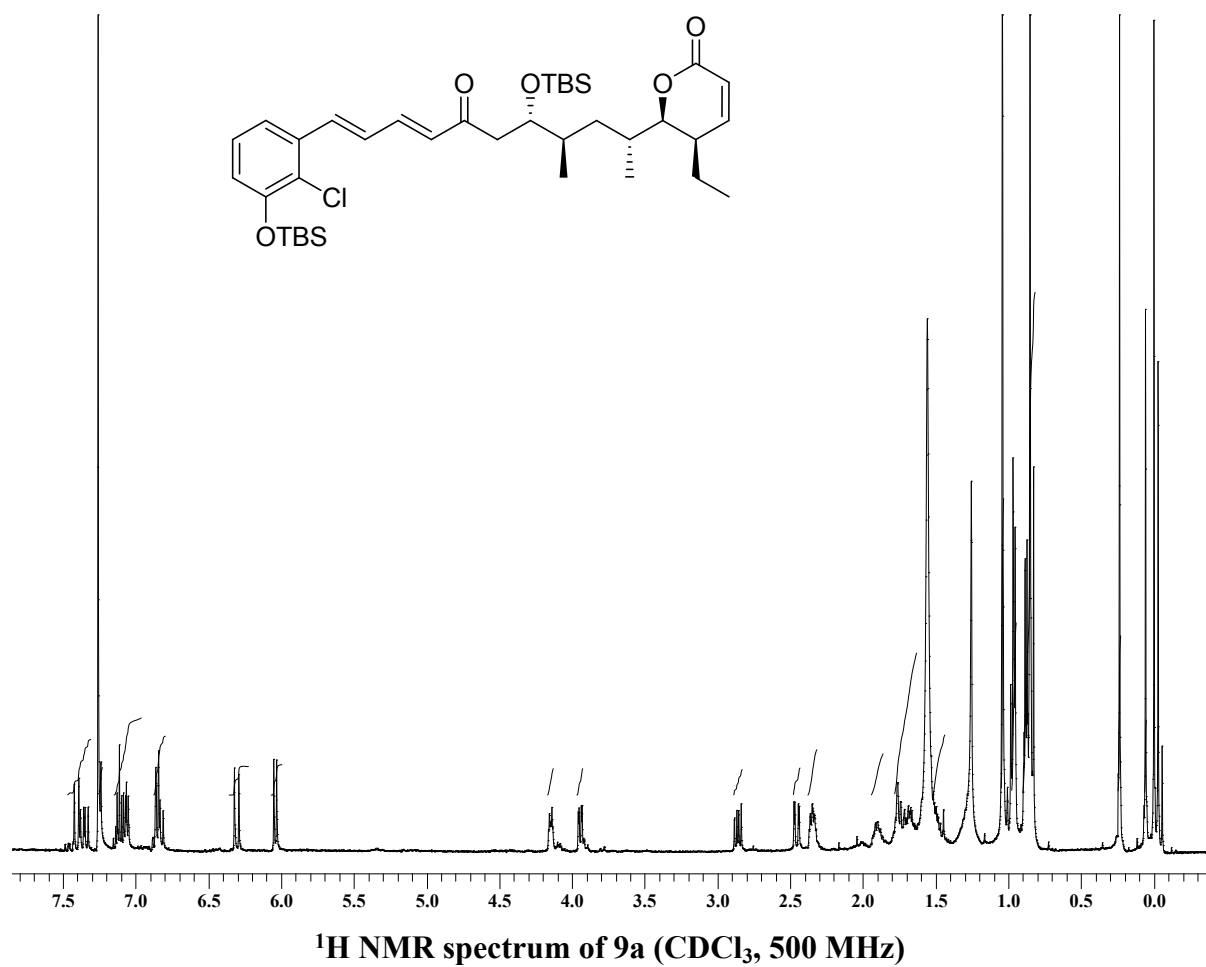


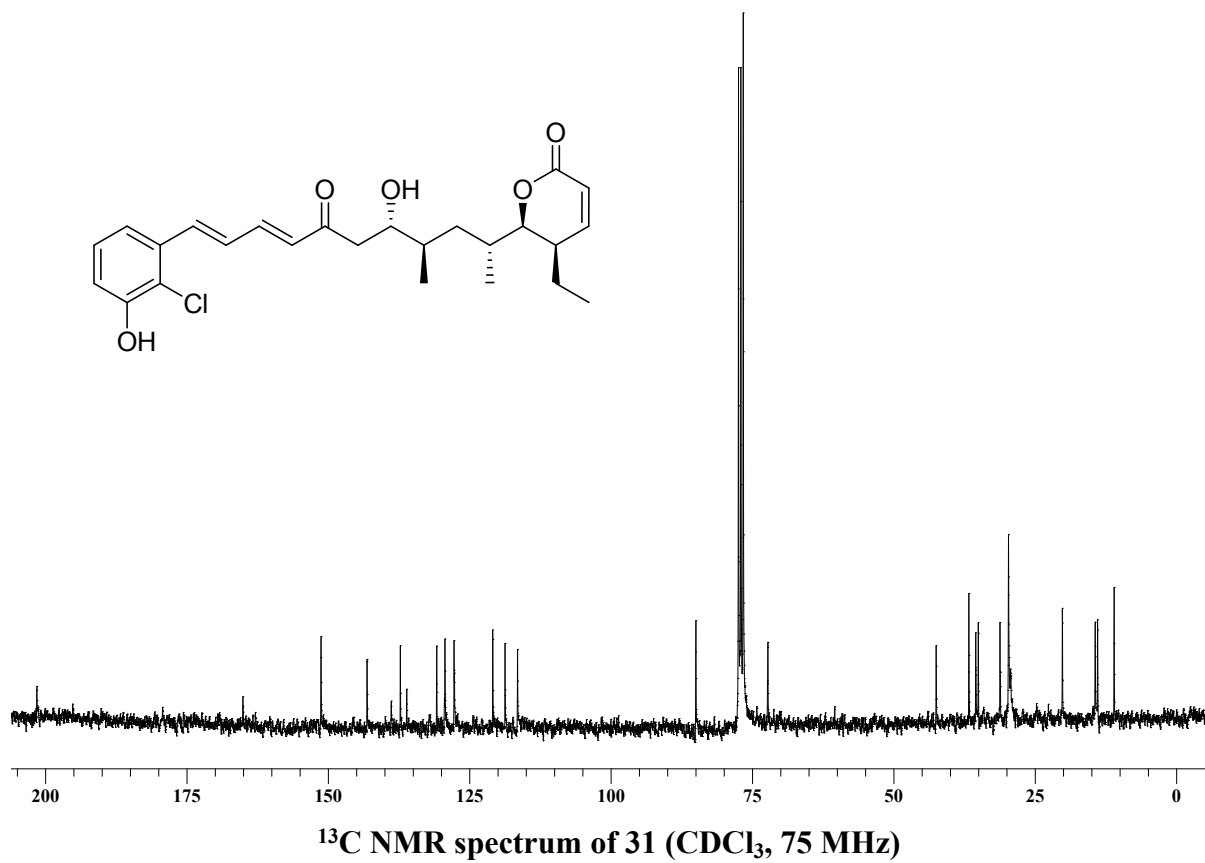
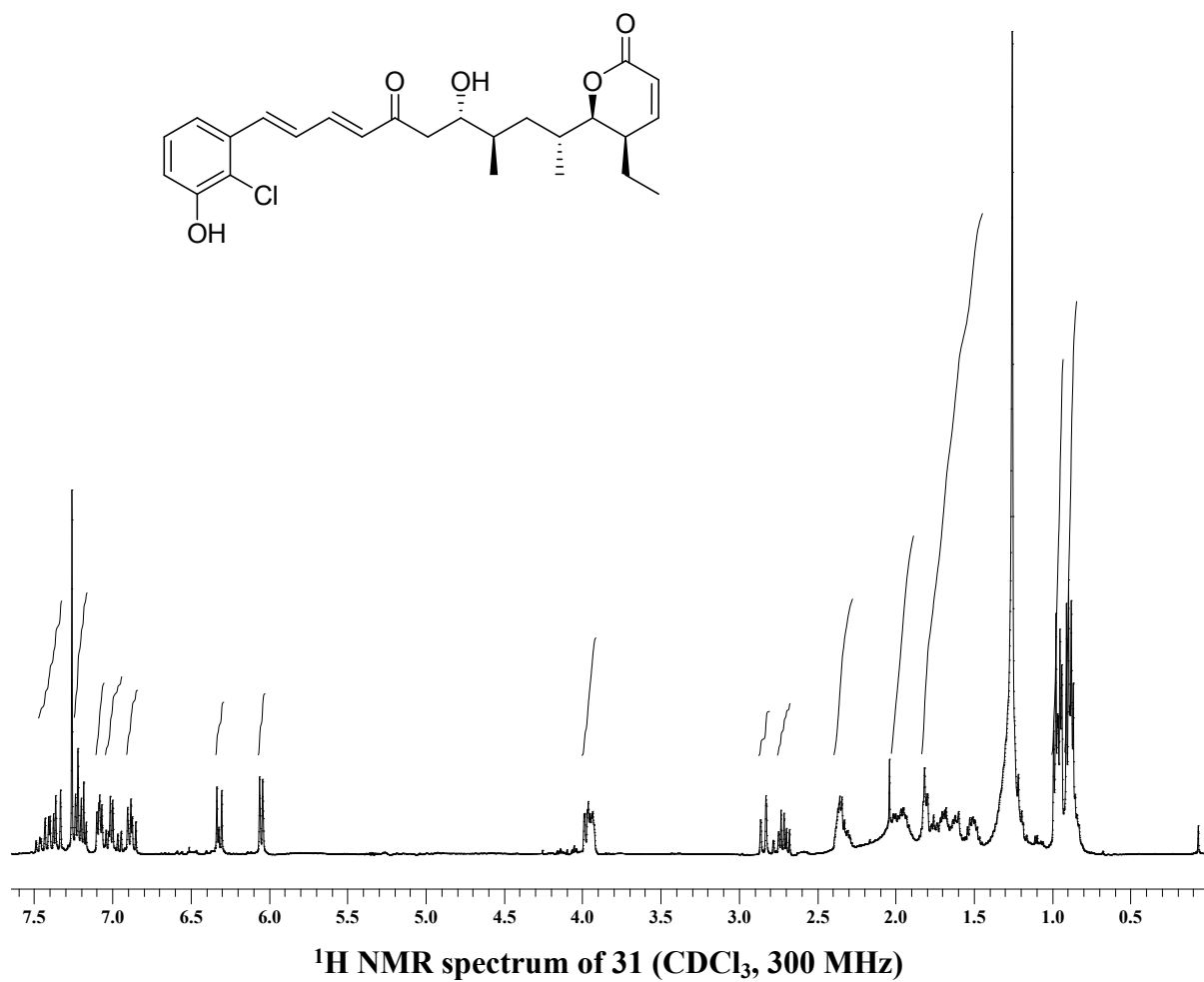


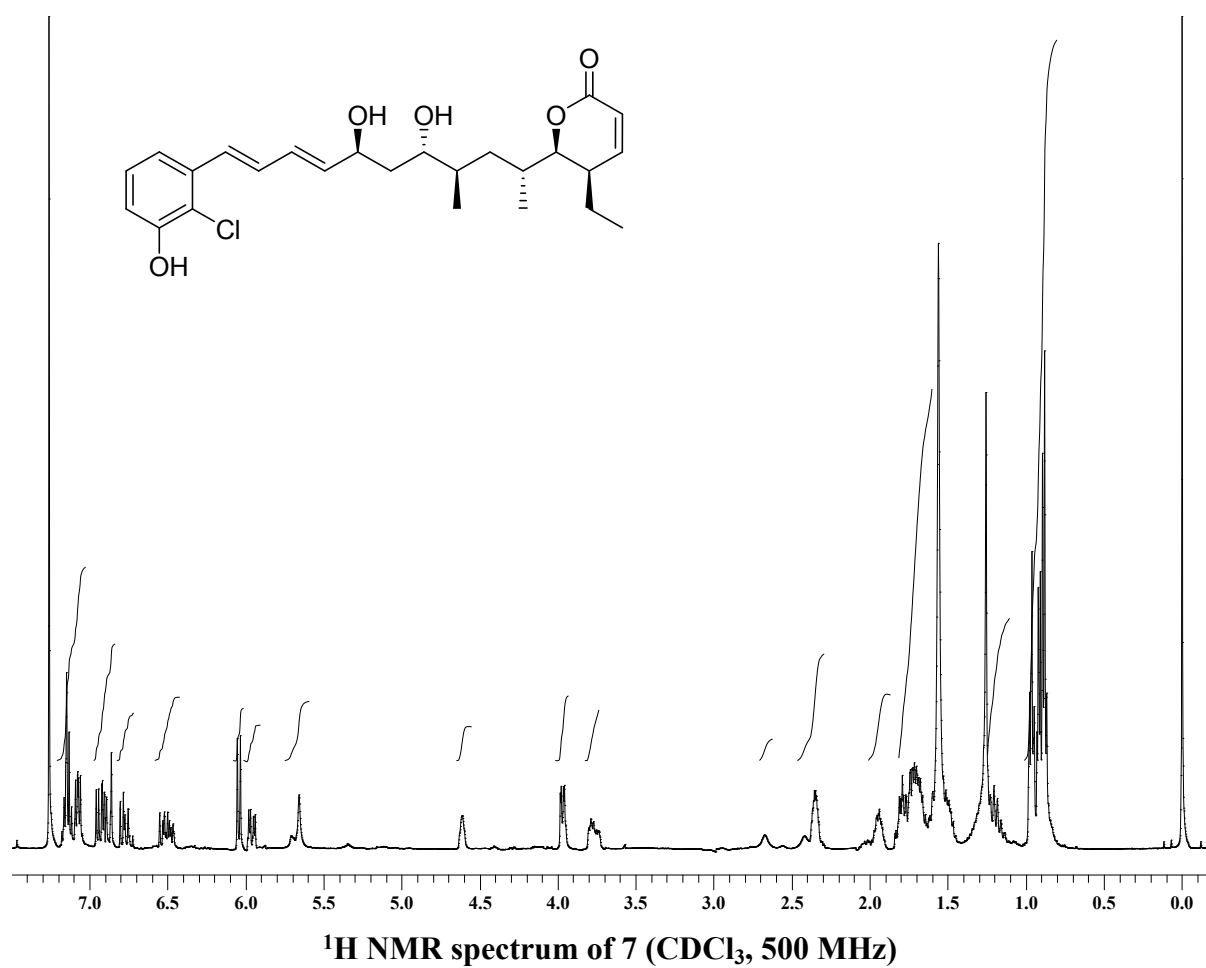


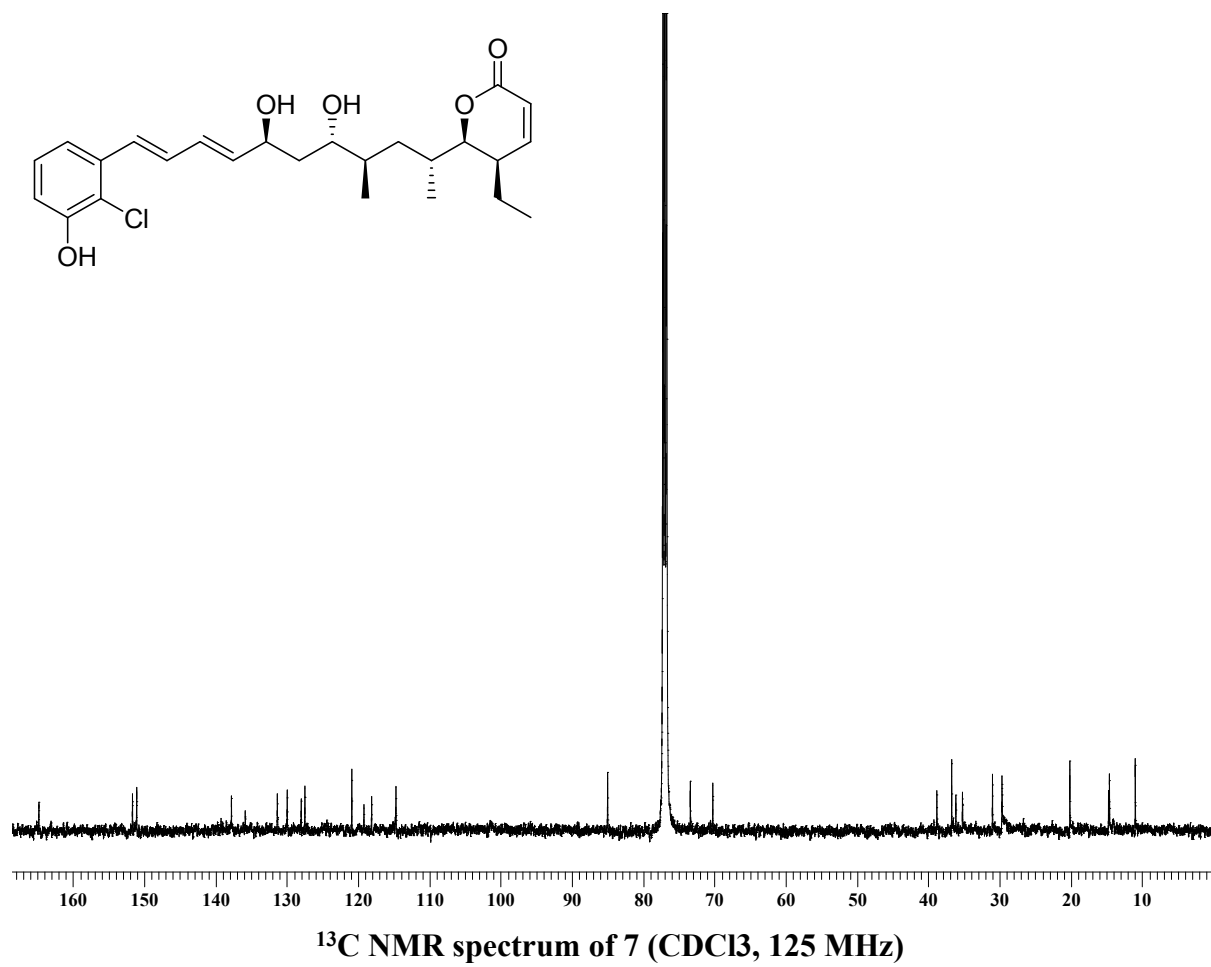










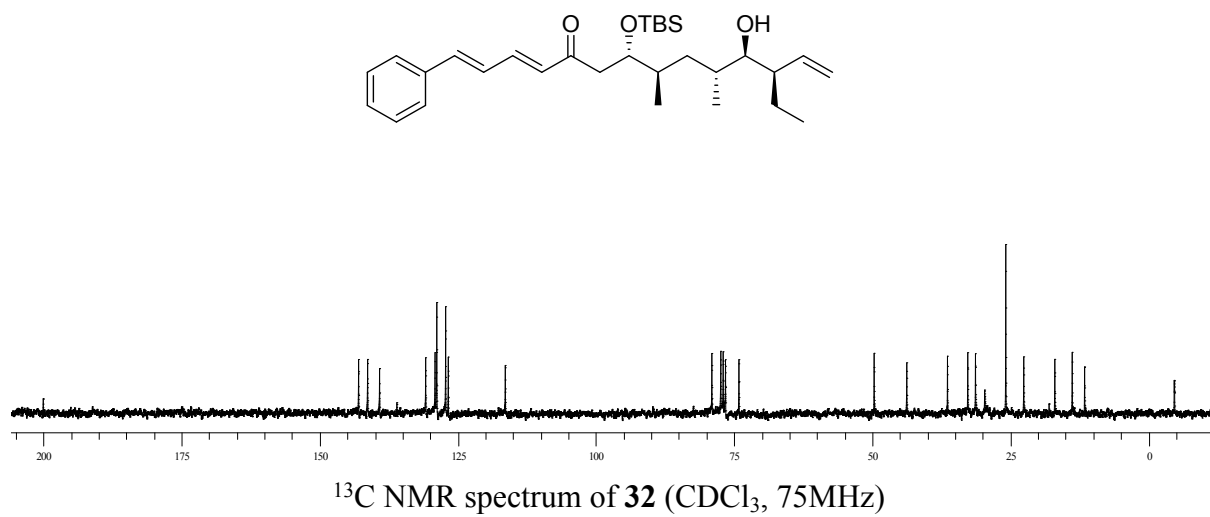
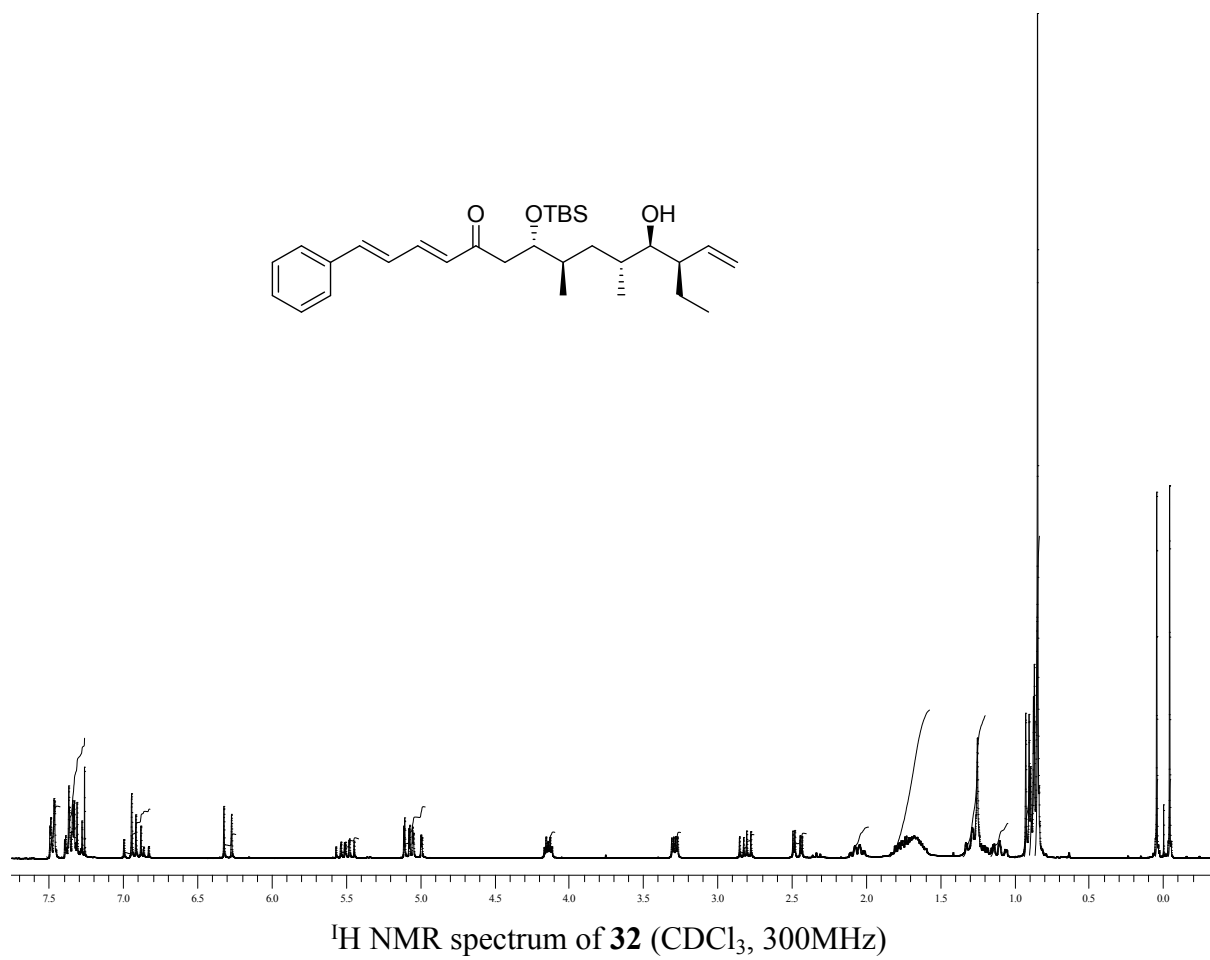


¹H and ¹³C NMR tabular comparison between the natural and synthetic (–)-bitungolide B in CDCl₃:

S.No	Natural (500 MHz, CDCl ₃)	Synthetic (500 MHz, CDCl ₃)
1	7.16 (m, 1H)	7.16 (m, 1H)
2	7.14 (m, 1H)	7.14 (m, 1H)
3	7.08 (dd, <i>J</i> = 9.8, 6.4, 1H)	7.07 (dd, <i>J</i> = 9.8, 6.7, 1H)
4	6.88 (d, <i>J</i> = 15.5, 1H)	6.88 (d, <i>J</i> = 15.3, 1H)
5	6.78 (dd, <i>J</i> = 15.5, 10.4, 1H)	6.78 (dd, <i>J</i> = 14.8, 9.8, 1H)
6	6.77 (dd, <i>J</i> = 8.0, 2.0, 1H)	6.90 (m, 1H)
7	6.53 (ddd, <i>J</i> = 15.3, 10.4, 1.0 1H)	6.52 (ddd, <i>J</i> = 15.8, 9.9, 1.9 1H)
8	6.05 (d, <i>J</i> = 9.8, 1H)	6.05 (d, <i>J</i> = 9.8, 1H)
9	5.96 (dd, <i>J</i> = 15.3, 5.8, 1H)	5.96 (dd, <i>J</i> = 15.3, 5.9, 1H)
10	5.65 (brs, OH)	5.66 (brs, OH)
11	4.62 (m, 1H)	4.61 (m, 1H)
12	3.97 (dd, <i>J</i> = 10.4, 3.0, 1H)	3.97 (dd, <i>J</i> = 10.8, 2.9, 1H)
13	3.80 (m, 1H)	3.79 (m, 1H)
14	2.73 (brs, OH)	2.68 (brs, OH)
15	2.47 (brs, OH)	2.43 (brs, OH)
16	2.36 (m, 1H)	2.36 (m, 1H)
17	1.95 (m, 1H)	1.95 (m, 1H)
18	1.83 (m, 1H), 1.80 (m, 1H), 1.74 (m, 1H), 1.72 (m, 1H), 1.69 (m, 1H),	1.84 – 1.67 (m, 5H)
19	1.50 (m, 1H)	1.50 (m, 1H)
20	1.20 (ddd, <i>J</i> = 13.0, 10.0, 2.0 1H)	1.20 (ddd, <i>J</i> = 12.8, 10.8, 1.9 1H)
21	0.96 (t, 7.6, 3H)	0.96 (t, 7.9, 3H)

22	0.91 (d, 6.4, 3H)	0.91 (d, 6.9, 3H)
23	0.89 (d, 6.7, 3H)	0.89 (d, 6.9, 3H)

S.No	Natural (125 MHz, CDCl₃)	Synthetic (125 MHz, CDCl₃)
1	164.9	164.8
2	151.6	151.6
3	151.2	151.1
4	137.8	137.8
5	135.8	135.8
6	131.3	131.3
7	129.9	129.9
8	128.0	128.0
9	127.5	127.5
10	120.9	120.9
11	119.0	119.1
12	118.1	118.1
13	114.7	114.7
14	85.0	85.0
15	73.4	73.4
16	70.3	70.3
17	38.7	38.8
18	36.7	36.7
19	36.1	36.1
20	35.2	35.2
21	31.0	31.0
22	20.1	20.1
23	14.7	14.7
24	14.6	14.6
25	11.0	11.0



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