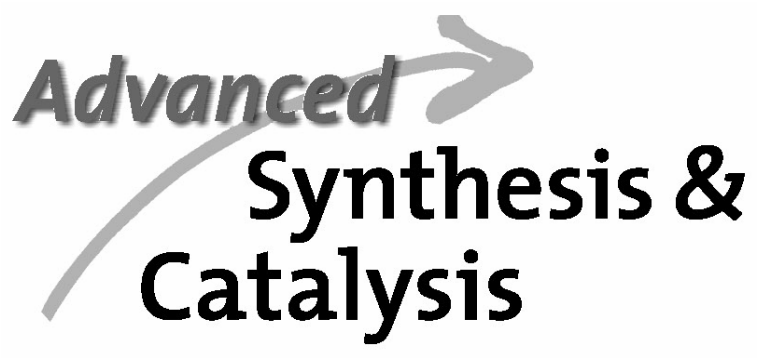

Supporting Information

Supporting Information for

Expeditious and Practical Synthesis of Lycopene

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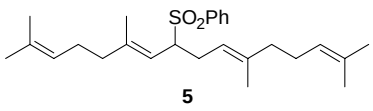
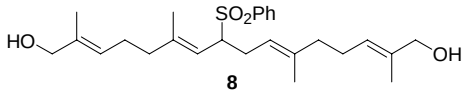
Experimental Procedure

8-Benzenesulfonyl-2,6,11,15-tetramethylhexadeca-2,6,10,14-tetraene (5): To a stirred solution of geranyl sulfone **3** (5.00 g 17.93 mmol) in DMF (50 mL) at –20 °C was added *t*-BuOK (2.33 g, 19.72 mmol). The resulting orange mixture was stirred at that temperature for 30 min, and a solution of geranyl bromide **4** (4.28 g, 19.72 mmol) in DMF (10 mL) was added. The mixture was stirred at –20 °C for 1 h, and quenched with 1 M HCl solution (20 mL). The mixture was extracted with EtOAc (50 mL), washed with 1 M HCl (10 mL × 3), dried over anhyd Na_2SO_4, filtered, and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography to give the coupling product **5** (7.10 g, 17.12 mmol) in 95% yield. Data for **5**: ^{1}H NMR δ 1.19 (d, *J* = 1.3 Hz, 3H), 1.57 (s, 3H), 1.59 (s, 3H), 1.60 (s, 3H), 1.65 (s, 3H), 1.68 (s, 3H), 1.90-2.07 (m, 8H), 2.35 (ddd, *J* = 14.0, 10.9, 7.4 Hz, 1H), 2.89 (ddd, *J* = 14.0, 7.2, 3.3 Hz, 1H), 3.73 (ddd, *J* = 10.9, 10.5, 3.3 Hz, 1H), 4.97 (t, *J* = 7.3 Hz, 1H), 5.02 (d, *J* = 10.5 Hz, 1H), 7.47-7.55 (m, 2H), 7.58-7.66 (m, 1H), 7.82-7.88 (m, 2H) ppm; ^{13}C NMR δ 16.3, 16.4, 17.6, 17.6, 25.6, 25.6, 26.2, 26.3, 26.5, 39.6, 39.6, 64.7, 116.9, 118.5, 123.5, 123.9, 128.6, 129.1, 131.4, 131.9, 133.3, 138.0, 138.5, 145.1 ppm; IR (KBr) 2917, 1447, 1304, 1146, 1085 cm^{-1}; HRMS (FAB$^+$) m/z calcd for $C_{26}H_{39}O_2S$ 415.2671, found 415.2665.



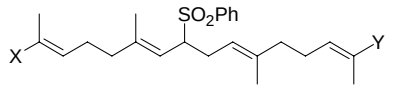
5

8-Benzenesulfonyl-2,6,11,15-tetramethylhexadeca-2,6,10,14-tetraene-1,16-diol (8): To a stirred suspension of SeO_2 (0.54 g, 4.82 mmol, 2 equiv) and salicylic acid (0.34 g, 2.41 mmol, 1 equiv) in CH_2Cl_2 (15 mL) at 0 °C was added a 3.0 M solution of TBHP in toluene (5.0 mL, 14.46 mmol, 6 equiv). The mixture was stirred at that temperature for 1.5 h, and a solution of **5** (1.00 g, 2.41 mmol, 1 equiv) in CH_2Cl_2 (5 mL) was slowly added for 10 min. The reaction mixture was stirred at 0 °C for 3 h, diluted with CH_2Cl_2 (30 mL), washed with 10% NaOH solution (10 mL × 3) and then saturated $Na_2S_2O_3$ solution (10 mL × 3), dried over anhyd Na_2SO_4, filtered, and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography to give the diol **8** (0.51 g, 1.15 mmol) in 48% yield, together with



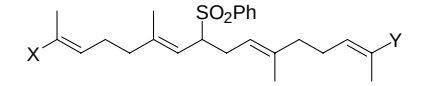
8

the mono-alcohol **9** (0.29 g, 0.68 mmol, 28% yield) and the hydroxyl-aldehyde **10** (0.13 g, 0.29 mmol, 12% yield). Data for **8**: ^{1}H NMR δ 1.24 (d, *J* = 1.3 Hz, 3H), 1.58 (s, 3H), 1.63 (s, 3H), 1.65 (s, 3H), 1.92-2.24 (m, 8H), 2.36 (ddd, *J* = 14.3, 10.0, 7.3 Hz, 1H), 2.77 (ddd, *J* = 14.3, 7.4, 3.7 Hz, 1H), 3.76 (ddd, *J* = 10.3, 10.0, 3.7 Hz, 1H), 3.95 (s, 2H), 3.97 (s, 2H), 5.00 (d, *J* = 10.3 Hz, 1H), 5.00 (t, *J* = 7.3 Hz, 1H), 5.33 (br s, 2H), 7.48-7.67 (m, 3H), 7.80-7.89 (m, 2H) ppm; ^{13}C NMR δ 13.6, 13.6, 16.1, 16.4, 25.4, 25.8, 26.7, 39.1, 39.2, 64.6, 68.5, 68.6, 116.9, 118.8, 124.6, 125.2,128.7, 128.9, 133.4, 134.8, 135.3, 137.9, 138.1, 144.8 ppm; IR (KBr) 3413, 1447, 1301, 1144, 1084, 1013 cm^{-1}; HRMS (CI$^+$) m/z calcd for $C_{26}H_{39}O_4S$ 447.2569, found 447.2568.



9: X = CH_3, Y = CH_2OH or X = CH_2OH, Y = CH_3

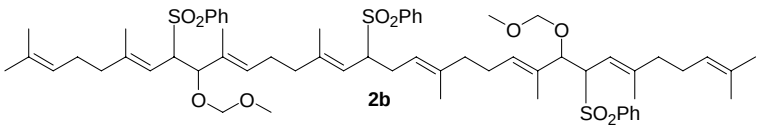
Data for **9**: ^{1}H NMR δ 1.17 (s, 3H), 1.58 (s, 3H), 1.61 (s, 3H), 1.63 (s, 3H), 1.68 (s, 3H), 1.90-2.22 (m, 8H), 2.32-2.46 (m, 1H), 2.80-2.91 (m, 1H), 3.75 (ddd, *J* = 10.3, 10.1, 3.7 Hz, 1H), 3.95 (s, 2H), 4.93-5.10 (m, 3H), 5.34 (br t, *J* = 5.7 Hz, 1H), 7.46-7.67 (m, 3H), 7.78-7.92 (m, 2H) ppm.



10: X = CH_2OH, Y = CHO or X = CHO, Y = CH_2OH

Data for **10**: ^{1}H NMR δ 1.24 (s, 3H), 1.62 (s, 3H), 1.66 (s, 3H), 1.72 (s, 3H), 1.86-2.25 (m, 6H), 2.32-2.50 (m, 3H), 2.73-2.90 (m, 1H), 3.75 (dt, J_d = 3.7, J_t = 10.4 Hz, 1H), 3.99 (s, 2H), 4.99 (d, *J* = 10.4 Hz, 1H), 5.03 (t, *J* = 6.6 Hz, 1H), 5.34 (br s, 1H), 6.41 (t, *J* = 6.6 Hz, 1H), 7.45-7.68 (m, 3H), 7.78-7.93 (m, 2H), 9.34 (s, 1H) ppm.

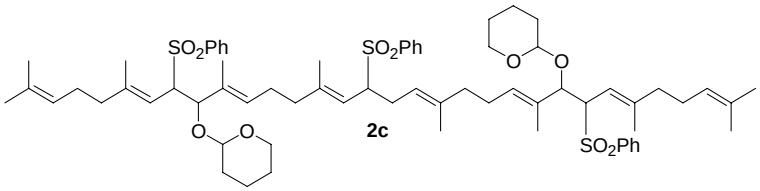
2b, MOM(methoxymethyl)-protection of the diol 2a: To a stirred solution of **2a** (1.73 g, 1.73 mmol, 1 equiv) in dimethoxy methane (6.2 mL, 40 equiv) at room temperature was added P_2O_5 (0.50 g, 3.46 mmol, 2 equiv). The resulting yellow solution was stirred for 9 h, and P_2O_5 (0.25 g, 1.73 mmol, 1 equiv) was added again. Stirring for another 3 h, the reaction mixture was diluted with toluene (40 mL), washed with saturated $NaHCO_3$ solution (10 mL × 3), dried over anhyd Na_2SO_4, filtered, and concentrated under reduced pressure. The crude product was purified by silica gel (deactivated by Et_3N) column chromatography to give **2b** (1.71 g, 1.58 mmol) in 91% yield. Data for **2b**: ^{1}H NMR δ 1.00 (s, 3H), 1.10-1.26 (m, 6H), 1.35-1.38 (m, 3H), 1.49-1.68 (m, 18H), 1.76-2.11 (m, 16H), 2.26-2.45 (m, 1H), 2.78-2.93 (m, 1H), 3.48 (s, 3H), 3.50 (s, 3H), 3.68-3.87 (m, 2H), 4.08-4.21 (m,



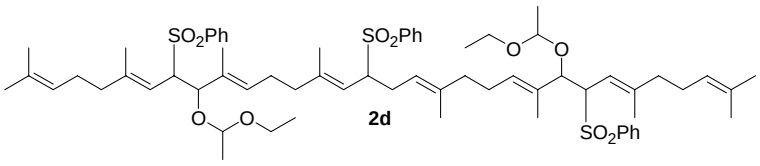
2b

1H), 4.50-4.87 (m, 4H), 4.58 (s, 2H), 4.61 (s, 2H), 4.88-5.08 (m, 4H), 5.30-5.52 (m, 2H), 7.44-7.69 (m, 9H), 7.78-7.90 (m, 6H) ppm; IR (KBr) 2917, 1447, 1303, 1145, 1025 cm^{-1}; HRMS (FAB^+) m/z calcd for $C_{46}H_{63}O_2S$ [$C_{62}H_{87}O_{10}S_3 - 2(C_6H_6SO_2) - 2(C_2H_6O_2)$] 679.4549, found 679.4563.

2c, THP(tetrahydropyranyl)-protection of the diol 2a: To a stirred solution of **2a** (0.74 g, 0.74 mmol, 1 equiv) in CH_2Cl_2 (30 mL) were added 3,4-dihydro-2*H*-pyran (0.35 mL, 3.7 mmol, 5 equiv) and 10-camphorsulfonic acid (0.09 g, 0.37 mmol, 0.5 equiv). The reaction mixture was stirred at room temperature for 14 h, diluted with CH_2Cl_2 (20 mL), washed with saturated $NaHCO_3$ solution (20 mL × 2), dried over anhyd K_2CO_3, filtered, and concentrated under reduced pressure. The crude product was purified by silica gel (deactivated by Et_3N) column chromatography to give **2c** (0.85 g, 0.73 mmol) in 98% yield. Data for **2c**: ^1H NMR δ 1.02-1.22 (m, 9H), 1.32-1.71 (m, 21H), 1.71-1.83 (m, 12H), 1.83-2.08 (m, 16H), 2.26-2.40 (m, 1H), 2.68-2.83 (m, 1H), 3.32-3.61 (m, 2H), 3.61-3.90 (m, 2H), 4.06-4.38 (m, 3H), 4.48-4.55 (m, 2H), 4.72-5.10 (m, 8H), 5.30-5.52 (m, 2H), 7.41-7.66 (m, 9H), 7.77-7.91 (m, 6H) ppm; IR (KBr) 2942, 1447, 1303, 1144, 1077, 1021 cm^{-1}; HRMS (FAB^+) m/z calcd for $C_{46}H_{63}O_2S$ [$C_{68}H_{95}O_{10}S_3 - 2(C_6H_6SO_2) - 2(C_5H_{10}O_2)$] 679.4549, found 679.4550.

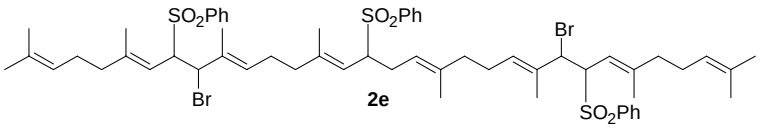


2d, EOE(1-ethoxyethyl)-protection of the diol 2a: To a stirred solution of **2a** (1.00 g, 1.00 mmol, 1 equiv) in CH_2Cl_2 (10 mL) at 0 °C were added ethyl vinyl ether (0.80 mL, 8.00 mmol, 8 equiv) and pyridinium *p*-toluenesulfonate (0.13 g, 0.50 mmol, 0.5 equiv). The mixture was stirred at 0 °C for 1 h, and warmed to and stirred at room temperature for 14 h. The mixture was then diluted with CH_2Cl_2 (20 mL), washed with saturated $NaHCO_3$ (10 mL × 3), dried over anhyd K_2CO_3, filtered, and concentrated under reduced pressure. The crude product was purified by silica gel (deactivated by Et_3N) column chromatography to give **2d** (1.09 g, 0.84 mmol) in 95% yield. Data for **2d**: ^1H NMR δ 1.00-1.42 (m, 24H), 1.43-1.74 (m, 18H), 1.76-2.10 (m, 16H), 2.25-2.46 (m, 1H), 2.78-2.95 (m, 1H), 3.24-3.44 (m, 1H), 3.44-3.62 (m, 1H),



3.62-3.85 (m 4H), 4.05-4.22 (m 1H), 4.45-4.90 (m, 5H), 4.90-5.10 (m, 5H), 5.27-5.52 (m 2H), 7.42-7.68 (m, 9H), 7.77-7.92 (m, 6H) ppm**;** IR (KBr) 2929, 1447, 1305, 1146, 1093, 1026 cm^{-1}; HRMS (FAB^+) m/z calcd for $C_{46}H_{63}O_2S$ [$C_{66}H_{95}O_{10}S_3 - 2(C_6H_6SO_2) - 2(C_4H_{10}O_2)$] 679.4549, found 679.4536.

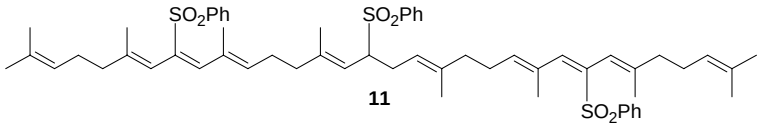
9,24-Dibromo-8,16,25-tris(benzenesulfonyl)-2,6,10,14,19,23,27,31-octamethyldotriaconta-



2e

2,6,10,14,18,22,26,30-octaene (2e): To a stirred solution of **2a** (3.68 g, 3.69 mmol, 1 equiv) in CH_2Cl_2 (50 mL) at 0 °C were added pyridine (1.5 mL, 18.45 mmol, 5 equiv) and PBr_3 (0.43 mL, 4.42 mmol, 1.2 equiv). The mixture was stirred at 0 °C for 1h, diluted with CH_2Cl_2 (30 mL), washed with 1 M HCl solution (10 mL × 3), dried over anhyd $MgSO_4$, filtered, and concentrated under reduced pressure to give the bromination product **2e** (3.99 g, 3.54 mmol) in 96% crude yield. Data for **2e**: ^{1}H NMR δ 1.06-1.36 (m, 9H), 1.42-1.73 (m, 21H), 1.80-2.22 (m, 16H), 2.22-2.50 (m, 1H), 2.74-2.93 (m, 1H), 3.63-4.02 (m, 2H), 4.08-4.40 (m, 1H), 4.53-4.86 (m, 2H), 4.86-5.16 (m, 4H), 5.16-5.72 (m, 4H), 7.43-7.68 (m, 9H), 7.75-7.97 (m, 6H) ppm; IR (KBr) 2920, 1663, 1447, 1375, 1304, 1145, 1083, 955 cm^{-1}; HRMS (FAB^+) m/z calcd for $C_{52}H_{72}BrO_4S_2$ [$C_{58}H_{77}Br_2O_6S_3 - (C_6H_5SO_2) - Br$] 903.4055, found 903.4055.

8,16,25-tris(benzenesulfonyl)-2,6,10,14,19,23,27,31-octamethyldotriaconta-

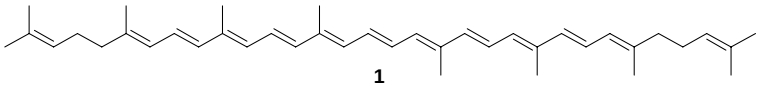


11

2,6,8,10,14,18,22,24,26,30-decaene (11): To a stirred solution of **2e** (0.40 g, 0.35 mmol, 1 equiv) in CH_2Cl_2 (20 mL) at 0 °C was added KOMe (0.13g , 1.77 mmol, 5 equiv). The mixture was stirred at that temperature for 1 h, diluted with CH_2Cl_2 (20 mL), washed with 1 M HCl solution (10 mL × 2), dried over anhyd Na_2SO_4, filtered, and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography to give **11** (0.29 g, 0.30 mmol) in 85% yield. Data for **11**: ^{1}H NMR δ 1.00 (s, 3H), 1.03 (s, 3H), 1.27 (s, 3H), 1.59 (s, 3H), 1.60 (s, 3H), 1.62 (s, 3H), 1.64 (s, 3H), 1.67 (s, 3H), 1.68 (s, 3H), 1.69 (s, 3H), 1.96-2.10 (m, 12H), 2.12-2.26 (m, 4H), 2.38 (ddd, J = 14.4, 10.8, 7.2 Hz, 1H), 2.88 (ddd, J = 14.4, 7.2, 3.6 Hz, 1H), 3.77 (dt, J_d = 3.6, J_t = 10.4 Hz, 1H), 4.95-5.10 (br s, 4H), 5.76 (s, 1H),

5.77 (s, 1H), 5.85 (t, J = 7.2 Hz, 1H), 5.88 (t, J = 7.2 Hz, 1H), 7.27 (s, 1H), 7.30 (s, 1H), 7.42-7.68 (m, 9H), 7.75-7.90 (m, 6H) ppm; ^{13}C NMR δ 14.3, 16.3, 16.4, 16.8, 17.3, 17.4, 17.9, 25.9, 26.2, 26.4, 26.8, 27.1, 27.1, 29.9, 38.8, 38.8, 39.3, 39.9, 56.3, 64.8, 110.5, 115.4, 177.8, 119.7, 123.7, 123.8, 128.6, 128.7, 128.7, 129.1, 129.1, 129.2, 132.2, 132.6, 132.9, 133.0, 133.7, 135.1, 135.6, 137.9, 138.2, 138.8, 139.8, 139.8, 141.8, 142.0, 142.4, 143.2, 144.6, 146.6, 148.1, 148.2 ppm; IR (KBr) 1447, 1303, 1146, 1086 cm^{-1}; HRMS (FAB^{+}) m/z calcd for $C_{58}H_{75}O_6S_3$ 963.4726, found 963.4712.

Double elimination reactions to Lycopene (1). From 2b: To a stirred solution of **2b** (1.67 g, 1.54 mmol) in cyclohexane (15 mL) and benzene (25 mL) was added KOMe (3.78 g, 53.9 mmol). The mixture was heated to 70~80 °C for 15 h, cooled to room temperature, and 1 M HCl (60 mL) was carefully added. The reaction mixture was extracted with a 2:1 (*v*:*v*) solution (60 mL) of hexane and benzene, dried over anhyd Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting red solid was diluted with hexane (50 mL) and washed with CH_3CN (10 mL × 3). The hexane layer was concentrated under reduced pressure to give Lycopene **1** (0.61 g, 1.14 mmol) in 74% crude yield, which presumably contained a certain amount of 9-(*Z*) isomers. The crude product was purified by recrystallization from MeOH and THF to provide all (*E*)-Lycopene **1** (0.46 g, 0.86 mmol) in 56% yield as a dark red crystal.

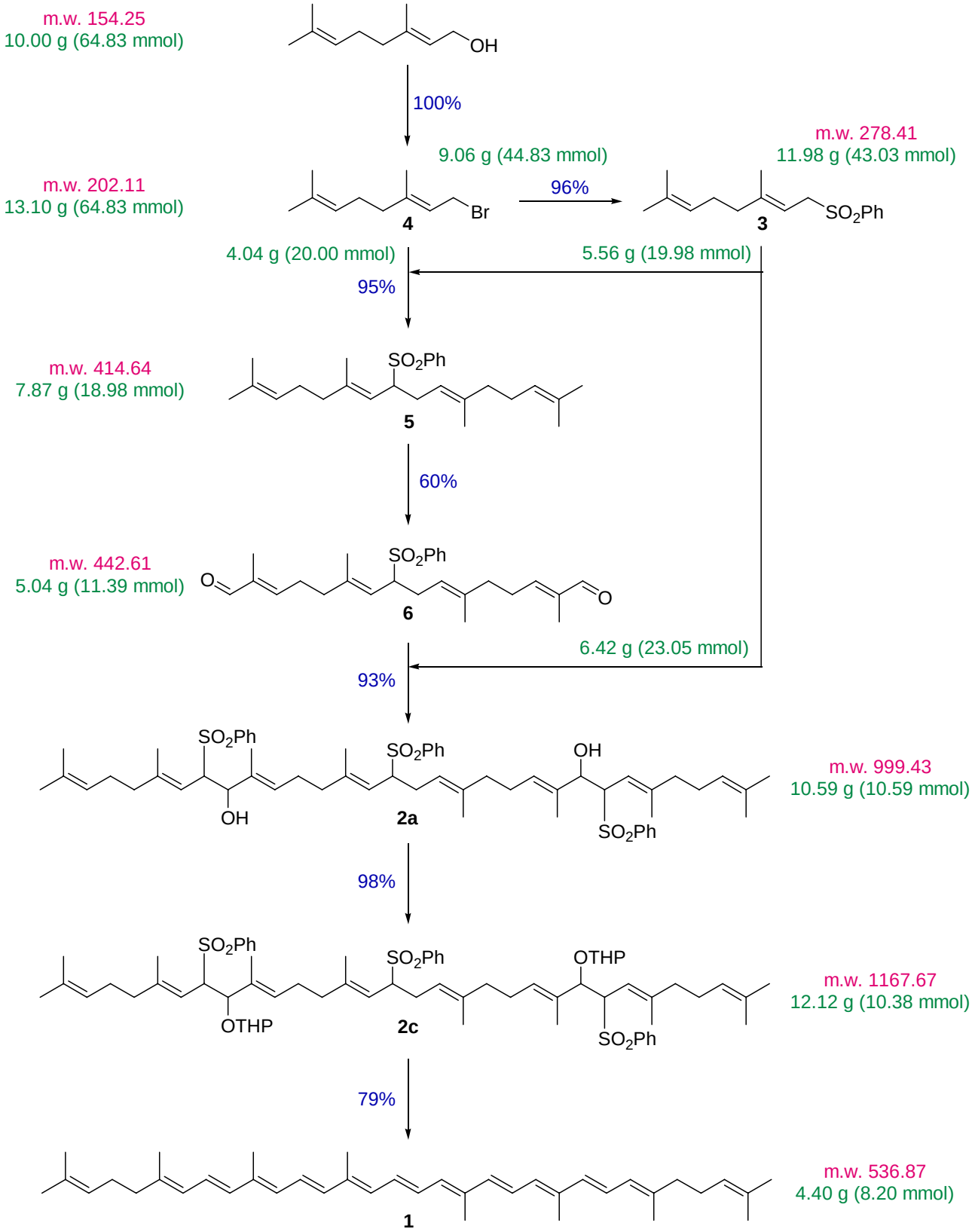


1

From 2d: The elimination reaction of **2d** (0.70 g, 0.61 mmol) by KOMe (1.28 g, 18.30 mmol) in cyclohexane (20 mL) and benzene (25 mL) at 70~80 °C for 18 h produced Lycopene **1** (0.24 g, 0.45 mmol) in 73% crude yield, which was purified by recrystallization to give all (*E*)-Lycopene **1** (0.17 g, 0.32 mmol) in 52% yield.

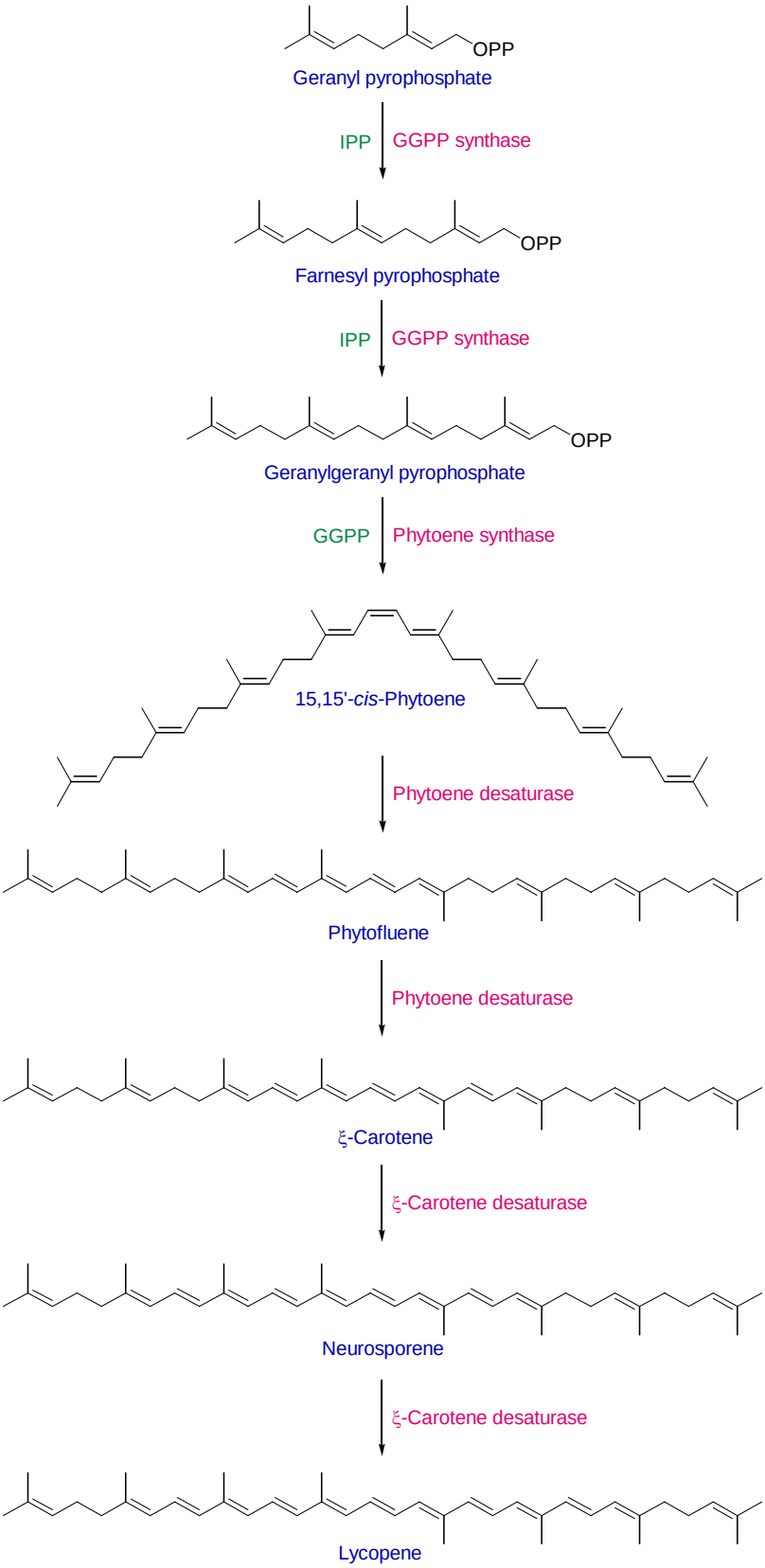
From 2e: The elimination reaction of **2e** (0.31 g, 0.27 mmol) by KOMe (0.58 g, 8.27 mmol) in cyclohexane (10 mL) and benzene (5 mL) at 70~80 °C for 11 h produced Lycopene **1** (0.11 g, 0.21 mmol) in 76% crude yield, which was purified by recrystallization to give all (*E*)-Lycopene **1** (0.083 g, 0.15 mmol) in 57% yield.

Synthetic scheme and yield for Lycopene (1)

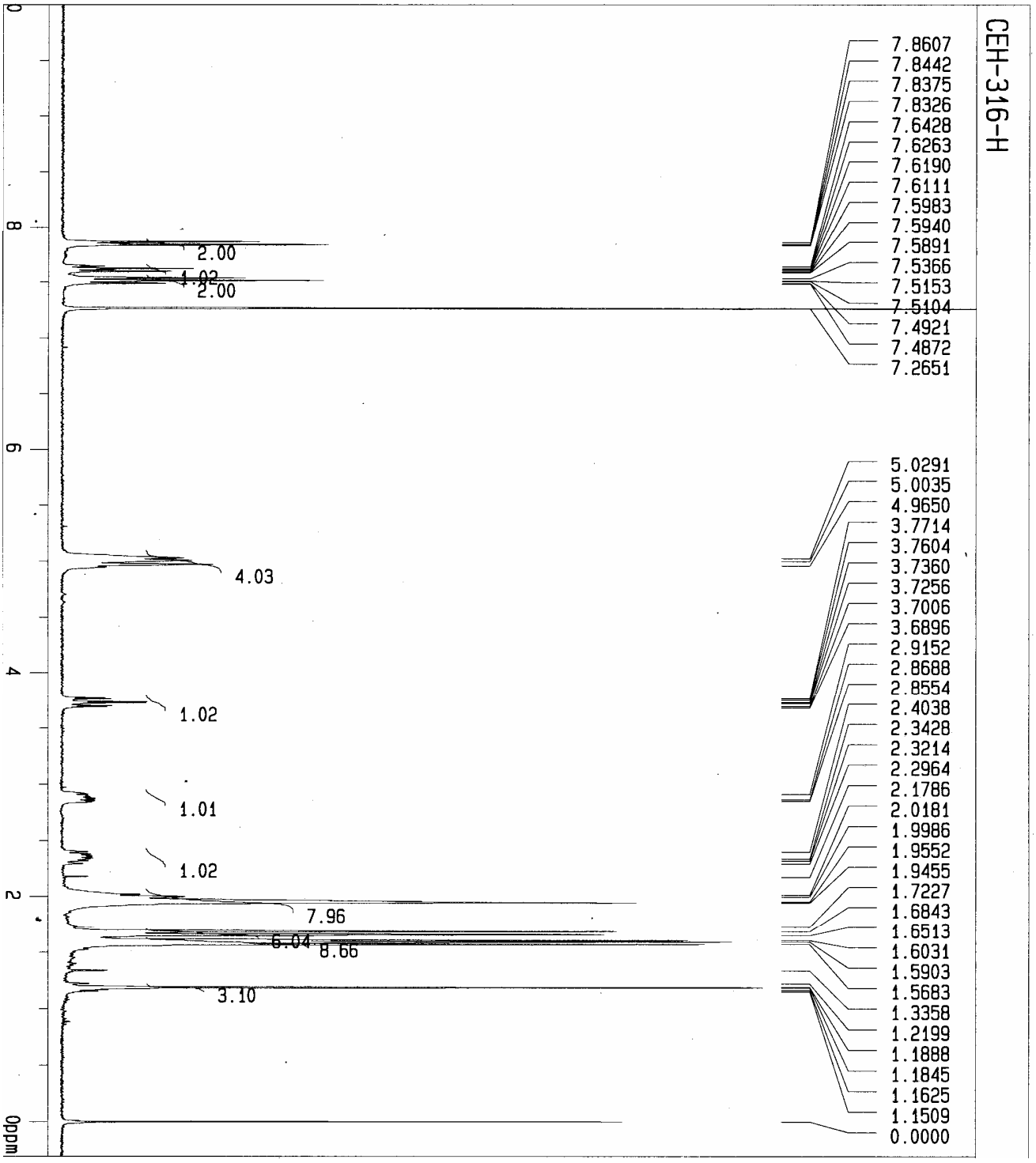


10.00 g (64.83 mmol, 4 equiv) Geraniol can give 4.40 g (8.20 mmol) Lycopene through 7 steps in 51% overall yield.

Biosynthetic pathway for Lycopene



Armstrong, G. *Comprehensive Natural Products Chemistry*; Barton, D., Nakanish, K., Eds; Elsevier: Oxford, 1999; Vol. 2, pp 321-352.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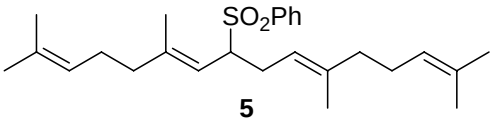
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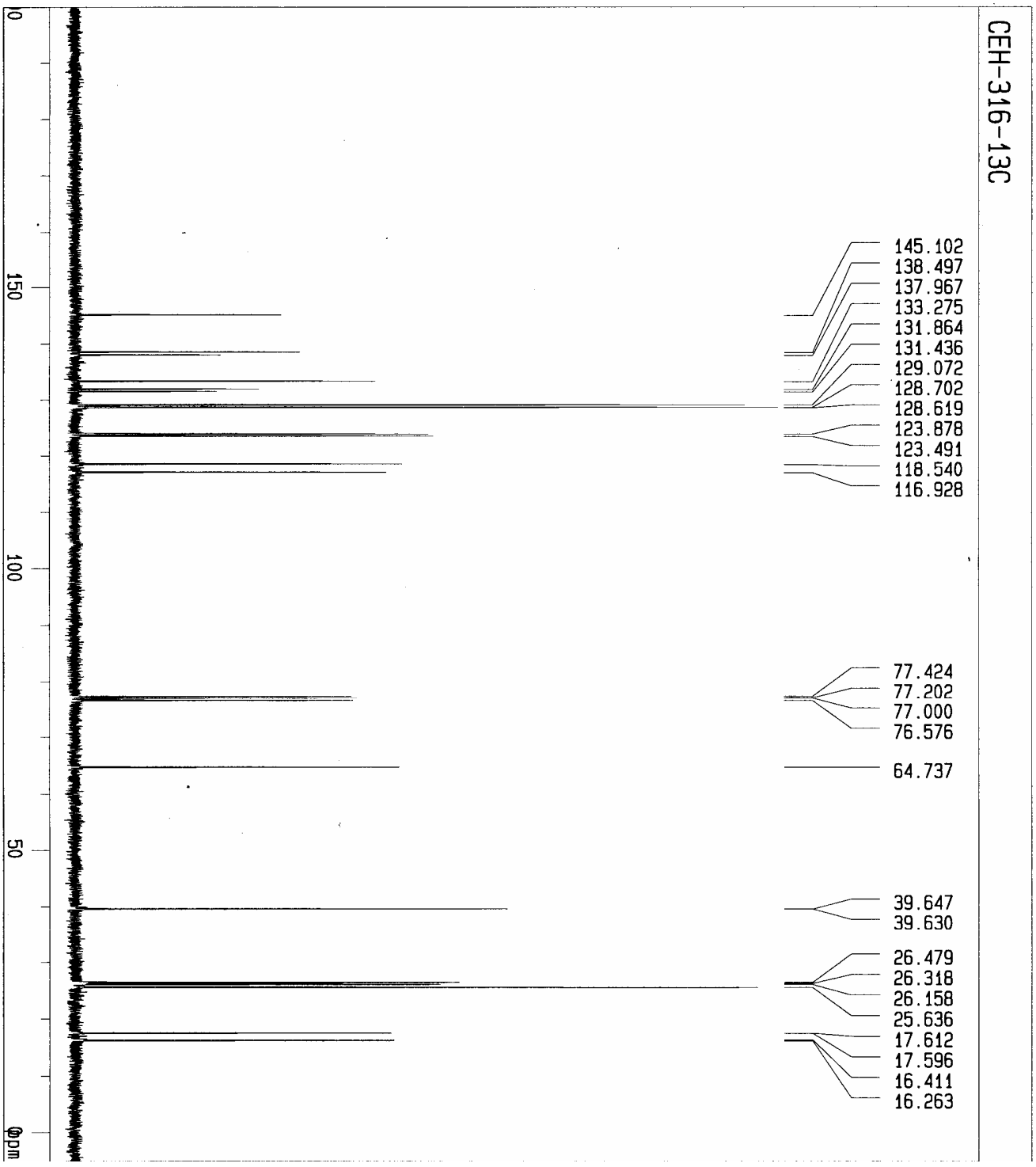
5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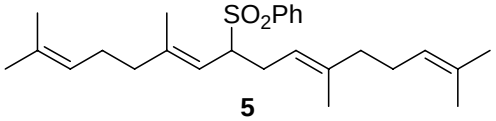
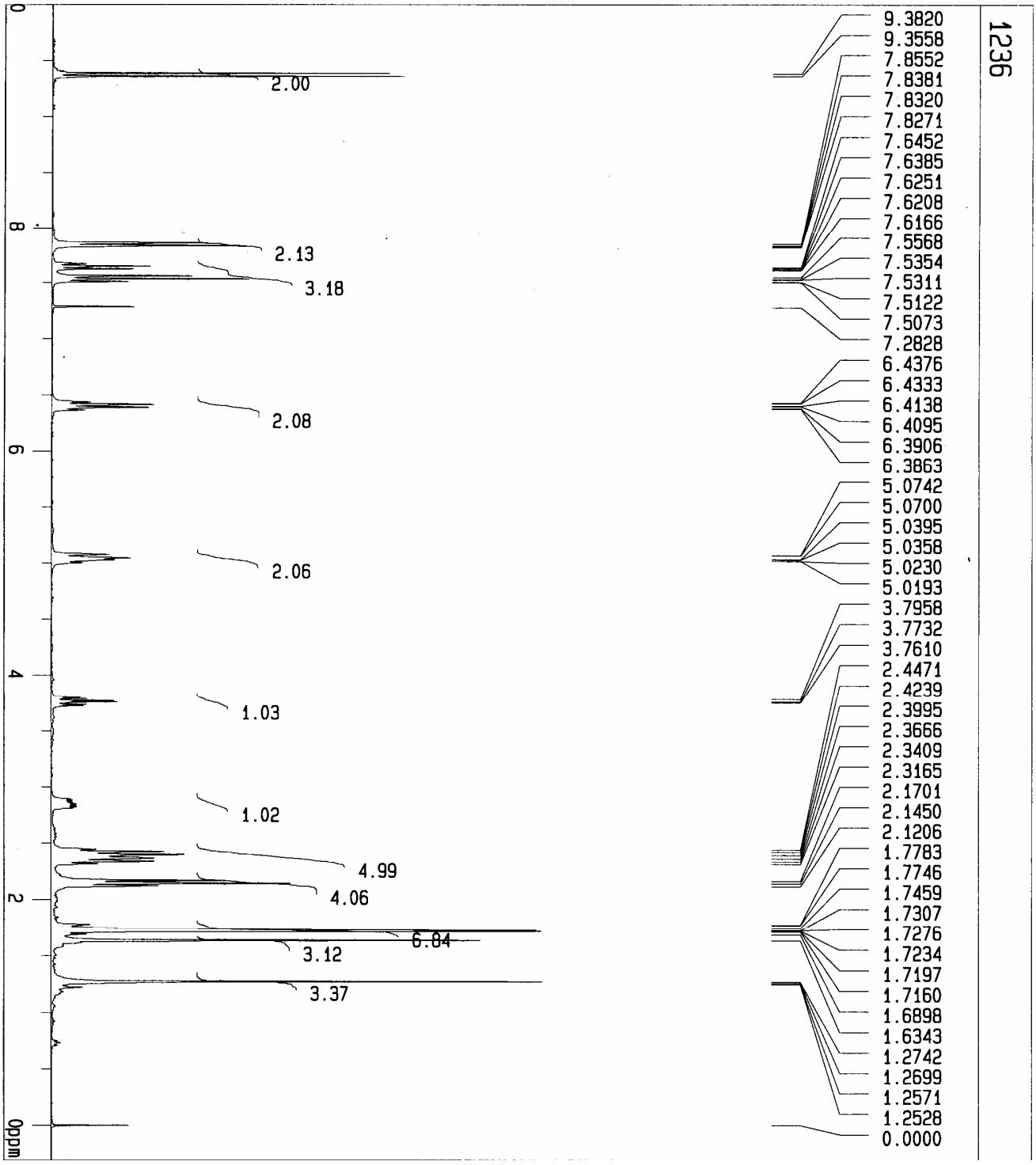
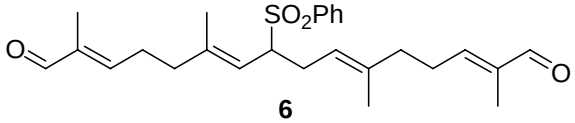
123.491
118.540
116.928
77.424
77.202
77.000
76.576
64.737
39.647
39.630
26.479
26.318
26.158
25.636
17.612
17.596
16.411
16.263
150
100
50
0
ppm

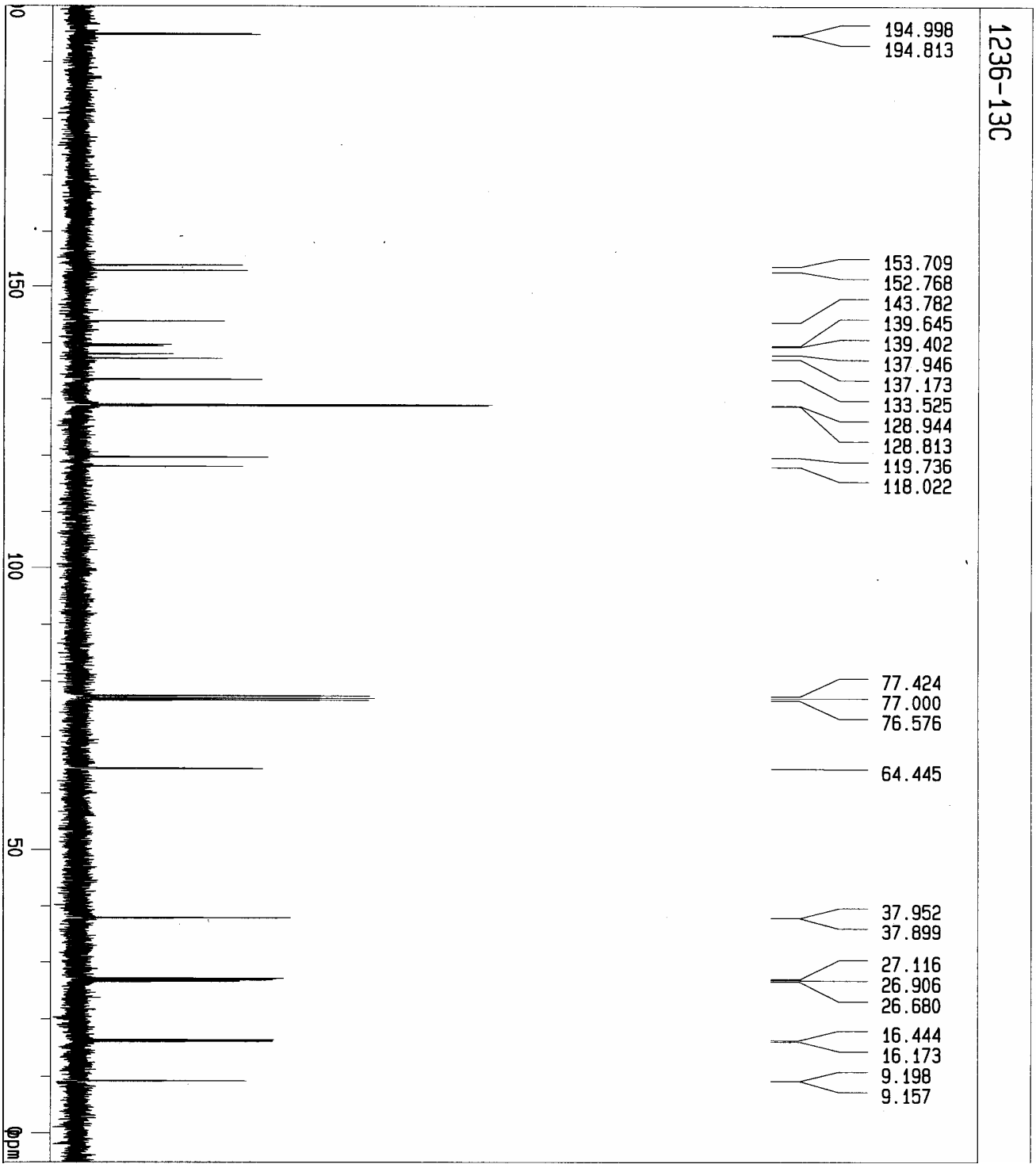

SO2Ph

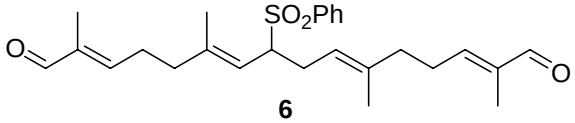
5


1236
9.3820
9.3558
7.8552
7.8381
7.8320
7.8271
7.6452
7.6385
7.6251
7.6208
7.6166
7.5568
7.5354
7.5311
7.5122
7.5073
7.2828
6.4376
6.4333
6.4138
6.4095
6.3906
6.3863
5.0742
5.0700
5.0395
5.0358
5.0230
5.0193
3.7958
3.7732
3.7610
2.4471
2.4239
2.3995
2.3666
2.3409
2.3165
2.1701
2.1450
2.1206
1.7783
1.7746
1.7459
1.7307
1.7276
1.7234
1.7197
1.7160
1.6898
1.6343
1.2742
1.2699
1.2571
1.2528
0.0000
2.00
2.13
3.18
2.08
2.06
1.03
1.02
4.99
4.06
6.84
3.12
3.37
0
8
6
4
2
0ppm

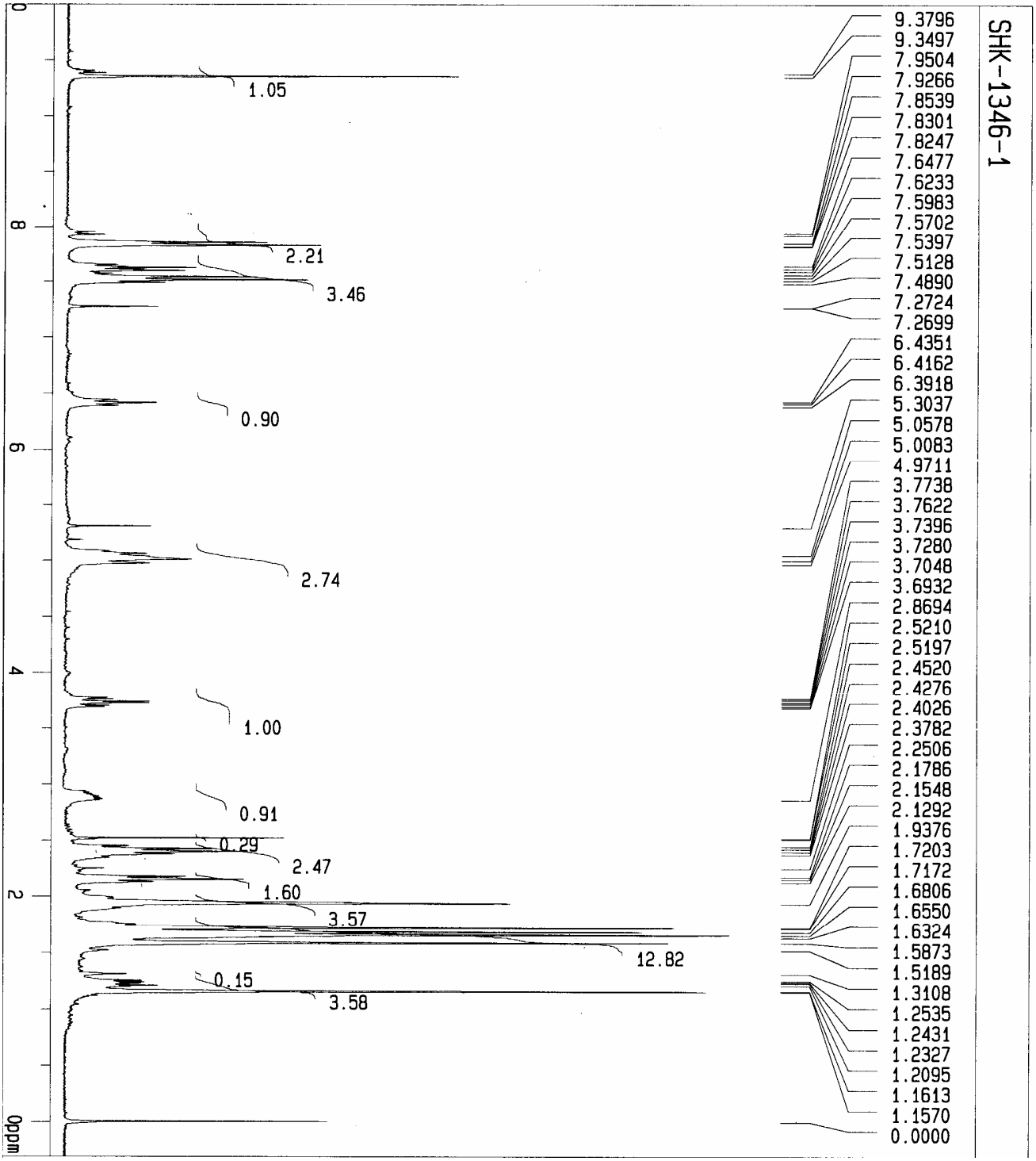

SO2Ph
O
O

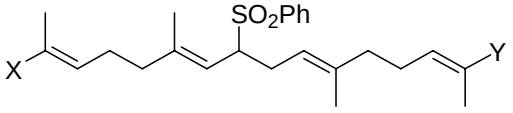
6


1236-13C
194.998
194.813
153.709
152.768
143.782
139.645
139.402
137.946
137.173
133.525
128.944
128.813
119.736
118.022
77.424
77.000
76.576
64.445
37.952
37.899
27.116
26.906
26.680
16.444
16.173
9.198
9.157
ppm

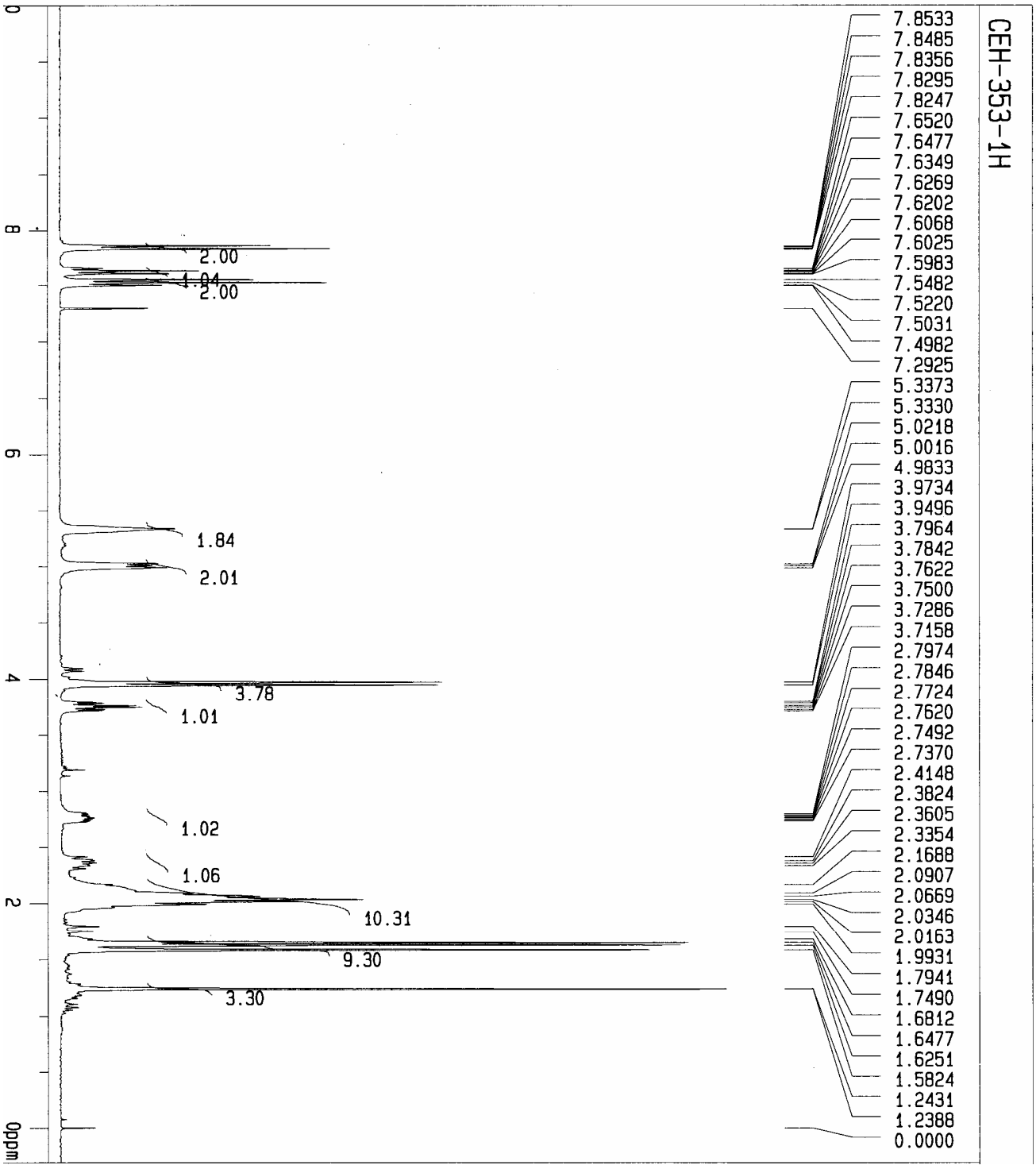

SO2Ph
O
O

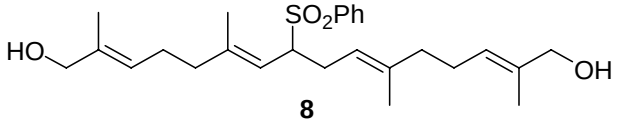
6



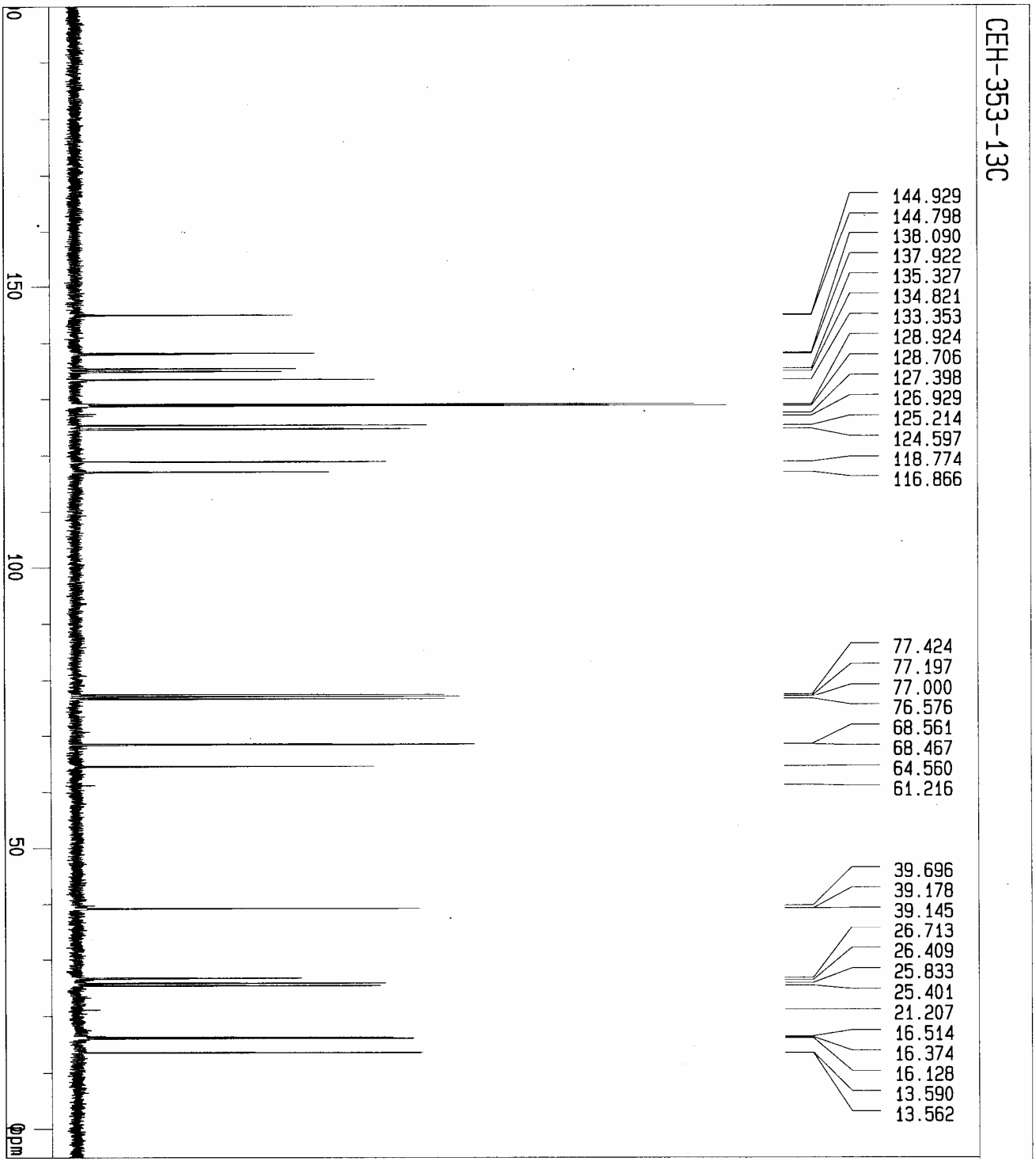


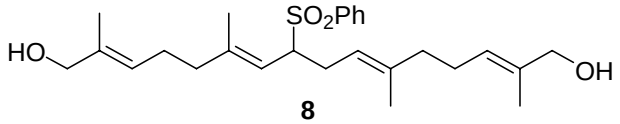
7: X = CH_3, Y = CHO or X = CHO, Y = CH_3


CEH-353-1H
7.8533
7.8485
7.8356
7.8295
7.8247
7.6520
7.6477
7.6349
7.6269
7.6202
7.6068
7.6025
7.5983
7.5482
7.5220
7.5031
7.4982
7.2925
5.3373
5.3330
5.0218
5.0016
4.9833
3.9734
3.9496
3.7964
3.7842
3.7622
3.7500
3.7286
3.7158
2.7974
2.7846
2.7724
2.7620
2.7492
2.7370
2.4148
2.3824
2.3605
2.3354
2.1688
2.0907
2.0669
2.0346
2.0163
1.9931
1.7941
1.7490
1.6812
1.6477
1.6251
1.5824
1.2431
1.2388
0.0000
2.00
1.04
2.00
1.84
2.01
3.78
1.01
1.02
1.06
10.31
9.30
3.30
ppm

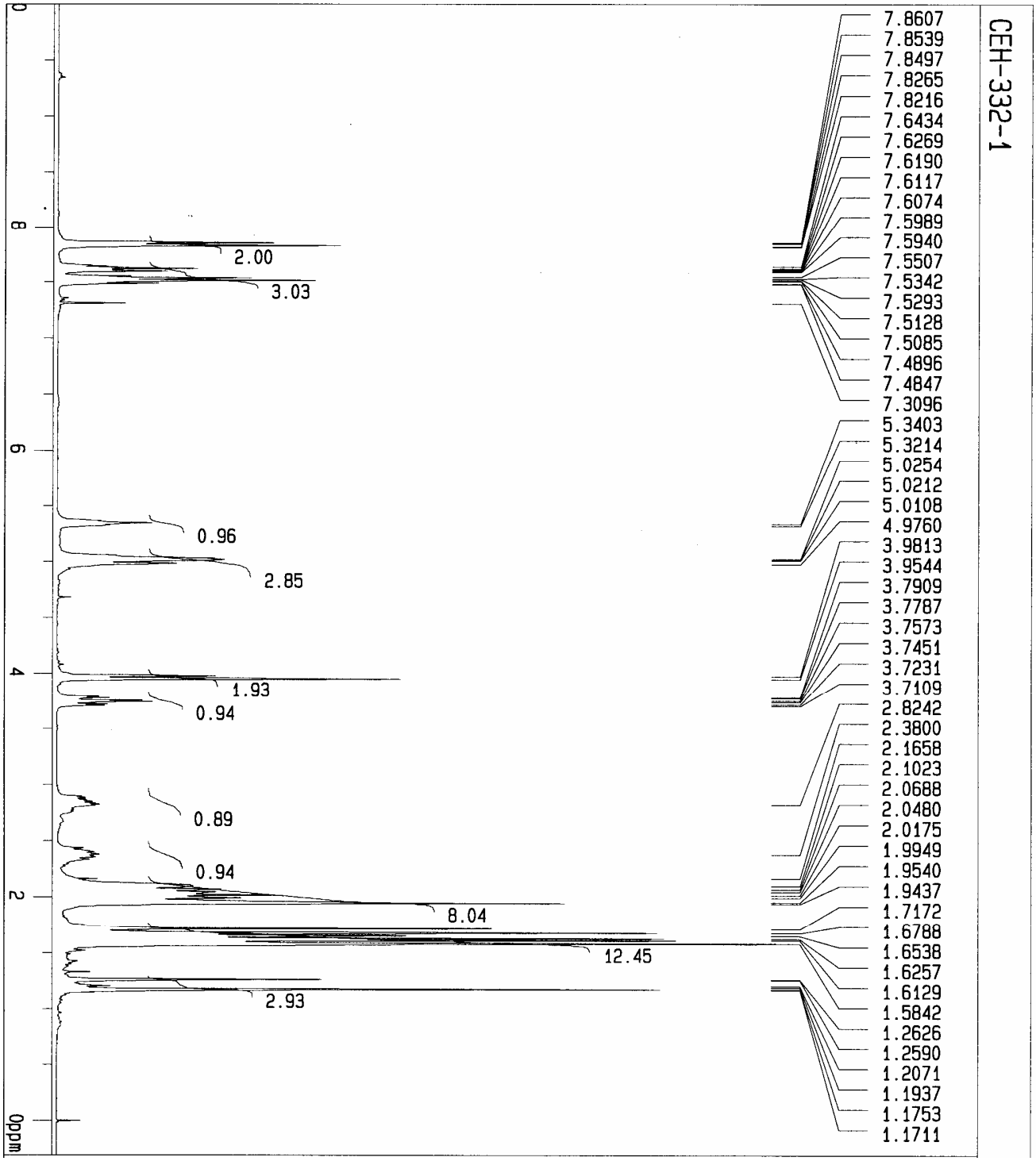

SO2Ph
HO
OH

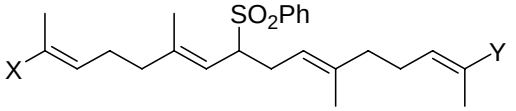
8


CEH-353-13C
144.929
144.798
138.090
137.922
135.327
134.821
133.353
128.924
128.706
127.398
126.929
125.214
124.597
118.774
116.866
77.424
77.197
77.000
76.576
68.561
68.467
64.560
61.216
39.696
39.178
39.145
26.713
26.409
25.833
25.401
21.207
16.514
16.374
16.128
13.590
13.562
150
100
50
0
ppm

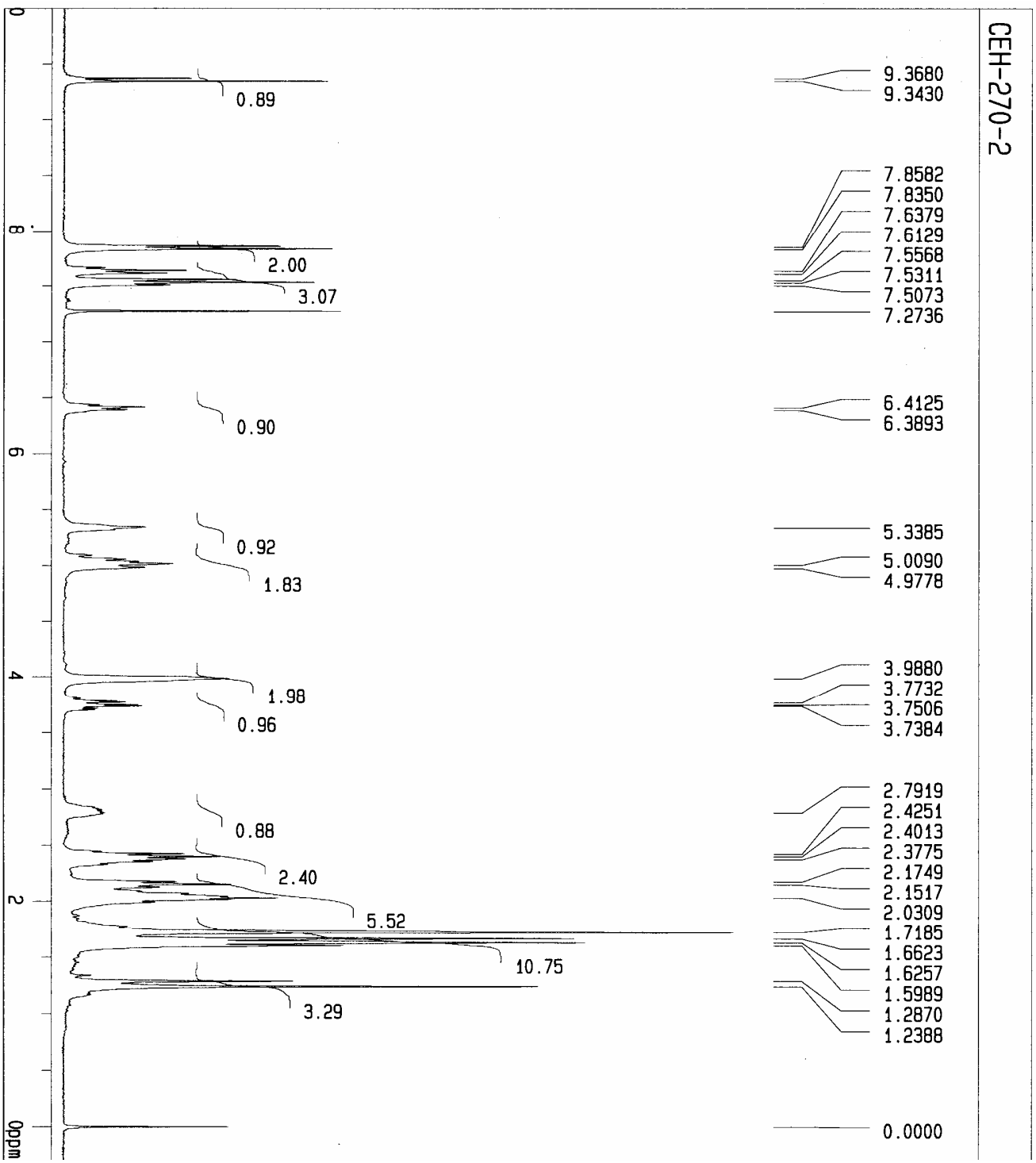

SO2Ph
HO
OH

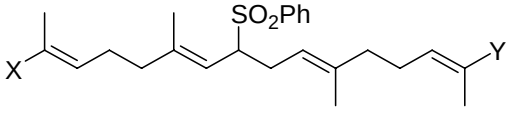
8



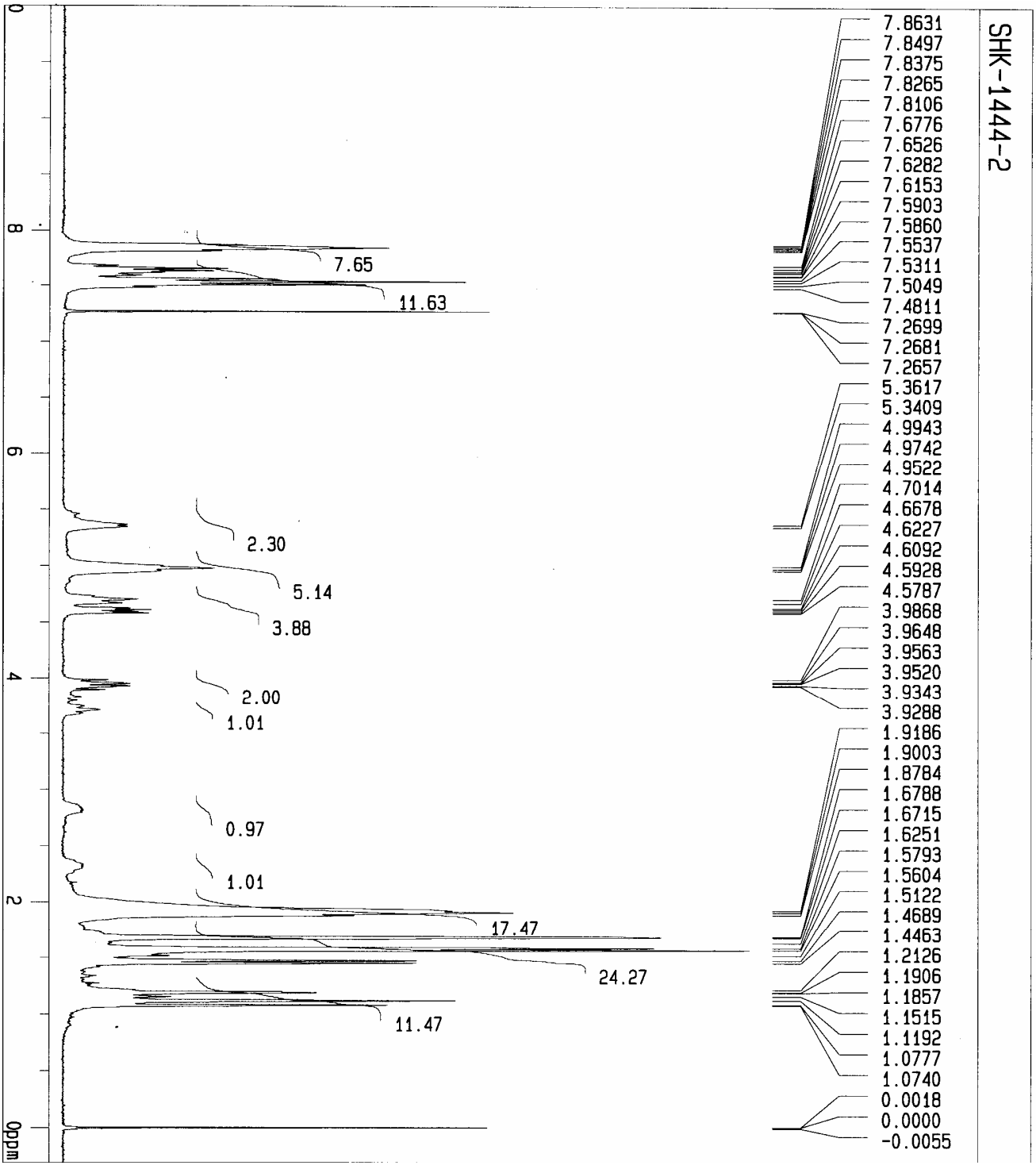


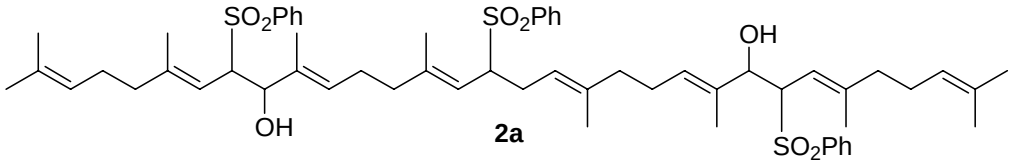
9: X = CH_3, Y = CH_2OH or X = CH_2OH, Y = CH_3



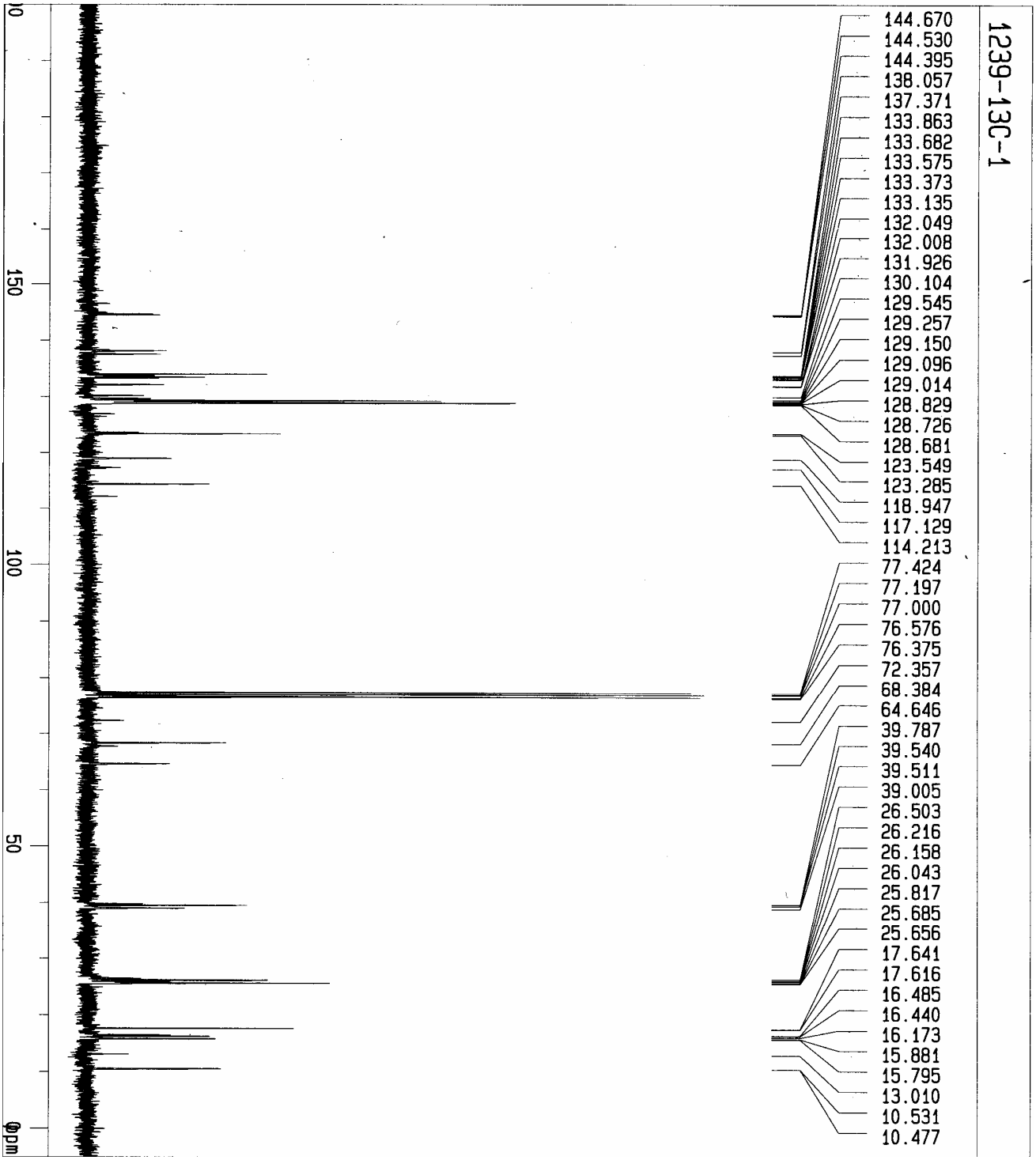


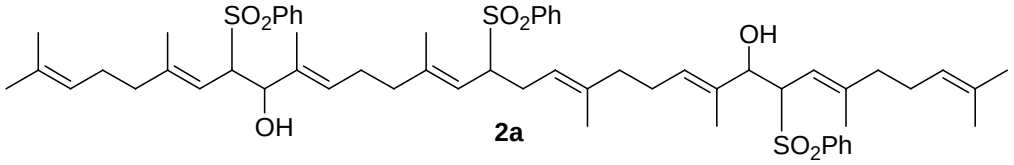
10: X = CH_2OH, Y = CHO or X = CHO, Y = CH_2OH


SHK-1444-2
7.8631
7.8497
7.8375
7.8265
7.8106
7.6776
7.6526
7.6282
7.6153
7.5903
7.5860
7.5537
7.5311
7.5049
7.4811
7.2699
7.2681
7.2657
5.3617
5.3409
4.9943
4.9742
4.9522
4.7014
4.6678
4.6227
4.6092
4.5928
4.5787
3.9868
3.9648
3.9563
3.9520
3.9343
3.9288
1.9186
1.9003
1.8784
1.6788
1.6715
1.6251
1.5793
1.5604
1.5122
1.4689
1.4463
1.2126
1.1906
1.1857
1.1515
1.1192
1.0777
1.0740
0.0018
0.0000
-0.0055
7.65
11.63
2.30
5.14
3.88
2.00
1.01
0.97
1.01
17.47
24.27
11.47
0
8
6
4
2
0ppm

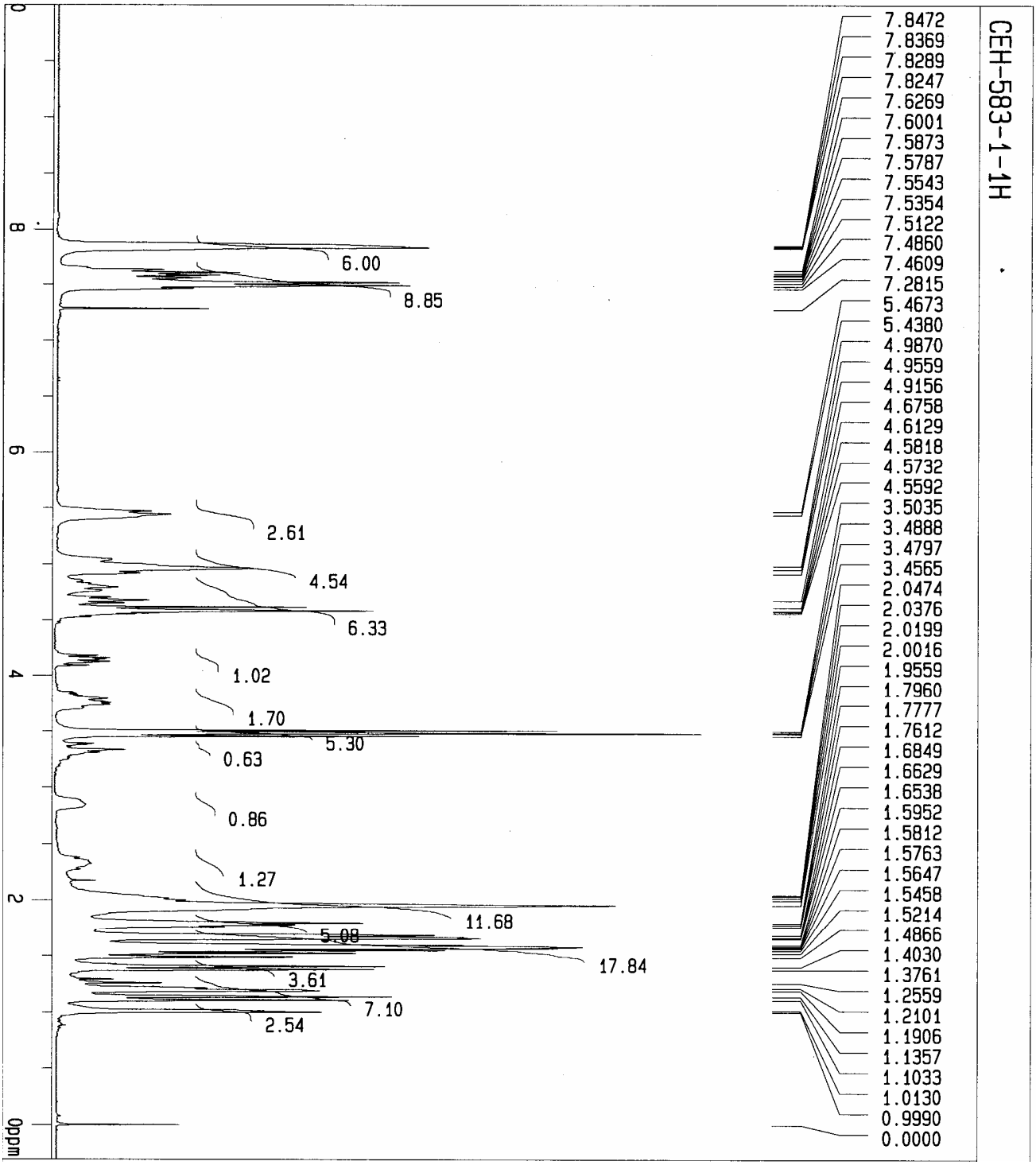

SO2Ph
SO2Ph
OH
OH
SO2Ph

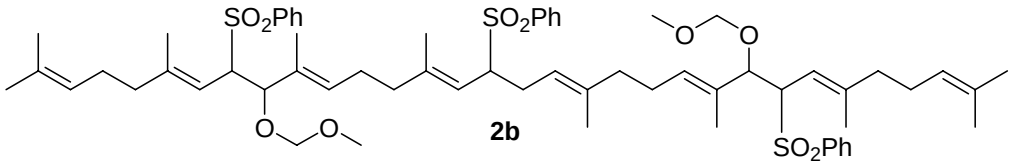
2a


1239-13C-1
144.670
144.530
144.395
138.057
137.371
133.863
133.682
133.575
133.373
133.135
132.049
132.008
131.926
130.104
129.545
129.257
129.150
129.096
129.014
128.829
128.726
128.681
123.549
123.285
118.947
117.129
114.213
77.424
77.197
77.000
76.576
76.375
72.357
68.384
64.646
39.787
39.540
39.511
39.005
26.503
26.216
26.158
26.043
25.817
25.685
25.656
17.641
17.616
16.485
16.440
16.173
15.881
15.795
13.010
10.531
10.477
150
100
50
0
ppm

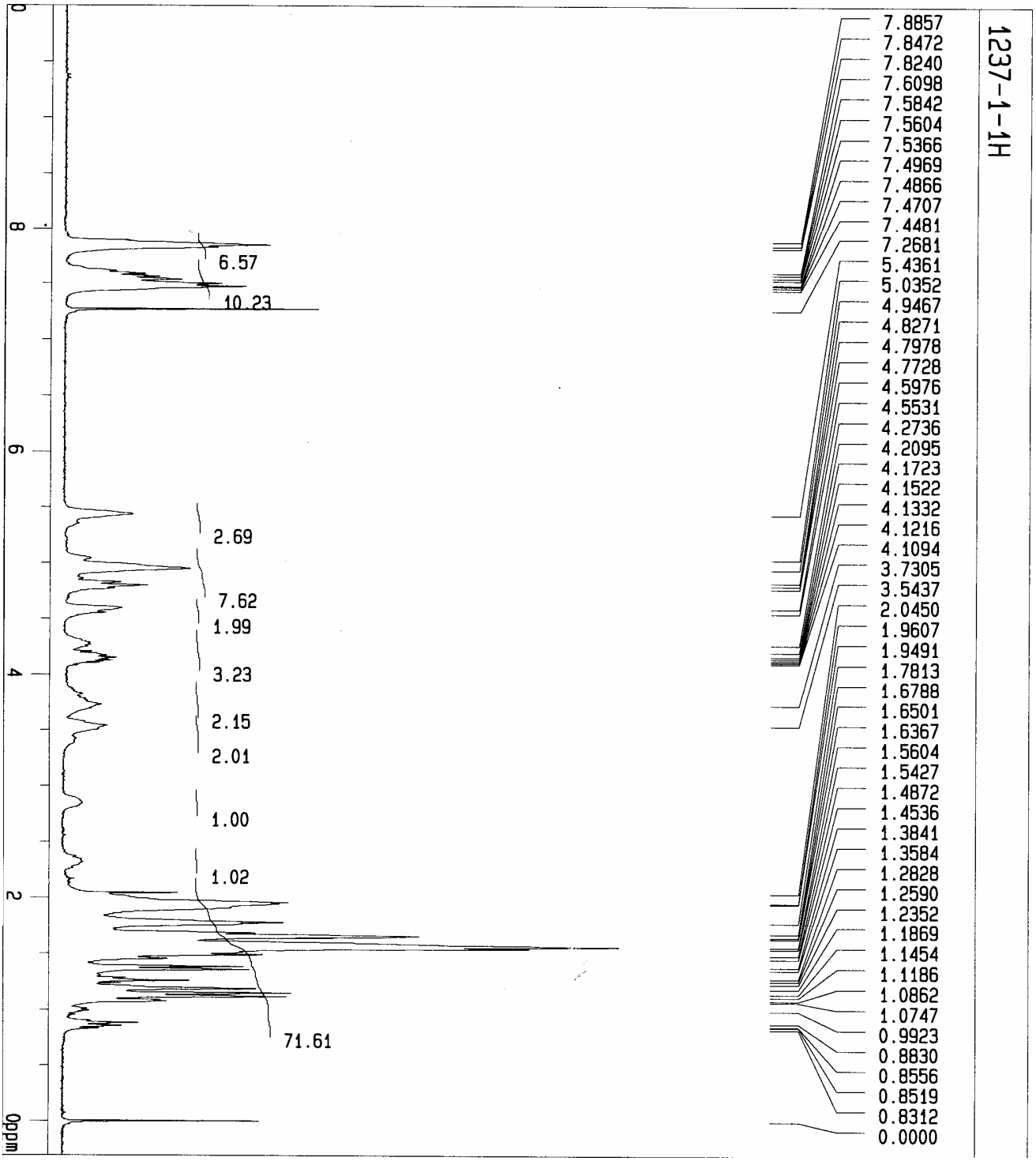

SO2Ph
SO2Ph
OH
OH
SO2Ph

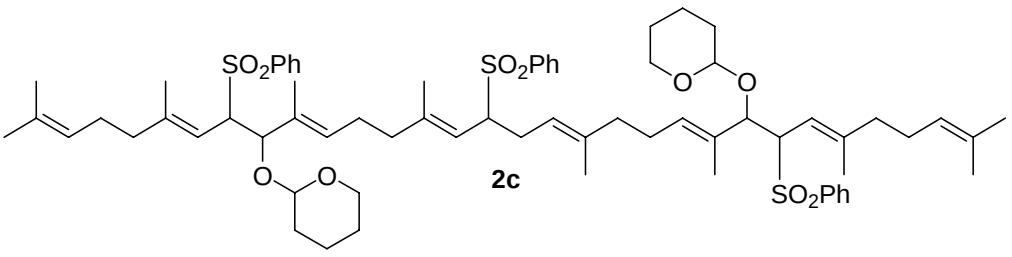
2a


CEH-583-1-1H
7.8472
7.8369
7.8289
7.8247
7.6269
7.6001
7.5873
7.5787
7.5543
7.5354
7.5122
7.4860
7.4609
7.2815
5.4673
5.4380
4.9870
4.9559
4.9156
4.6758
4.6129
4.5818
4.5732
4.5592
3.5035
3.4888
3.4797
3.4565
2.0474
2.0376
2.0199
2.0016
1.9559
1.7960
1.7777
1.7612
1.6849
1.6629
1.6538
1.5952
1.5812
1.5763
1.5647
1.5458
1.5214
1.4866
1.4030
1.3761
1.2559
1.2101
1.1906
1.1357
1.1033
1.0130
0.9990
0.0000
6.00
8.85
2.61
4.54
6.33
1.02
1.70
5.30
0.63
0.86
1.27
11.68
5.08
17.84
3.61
7.10
2.54
0ppm

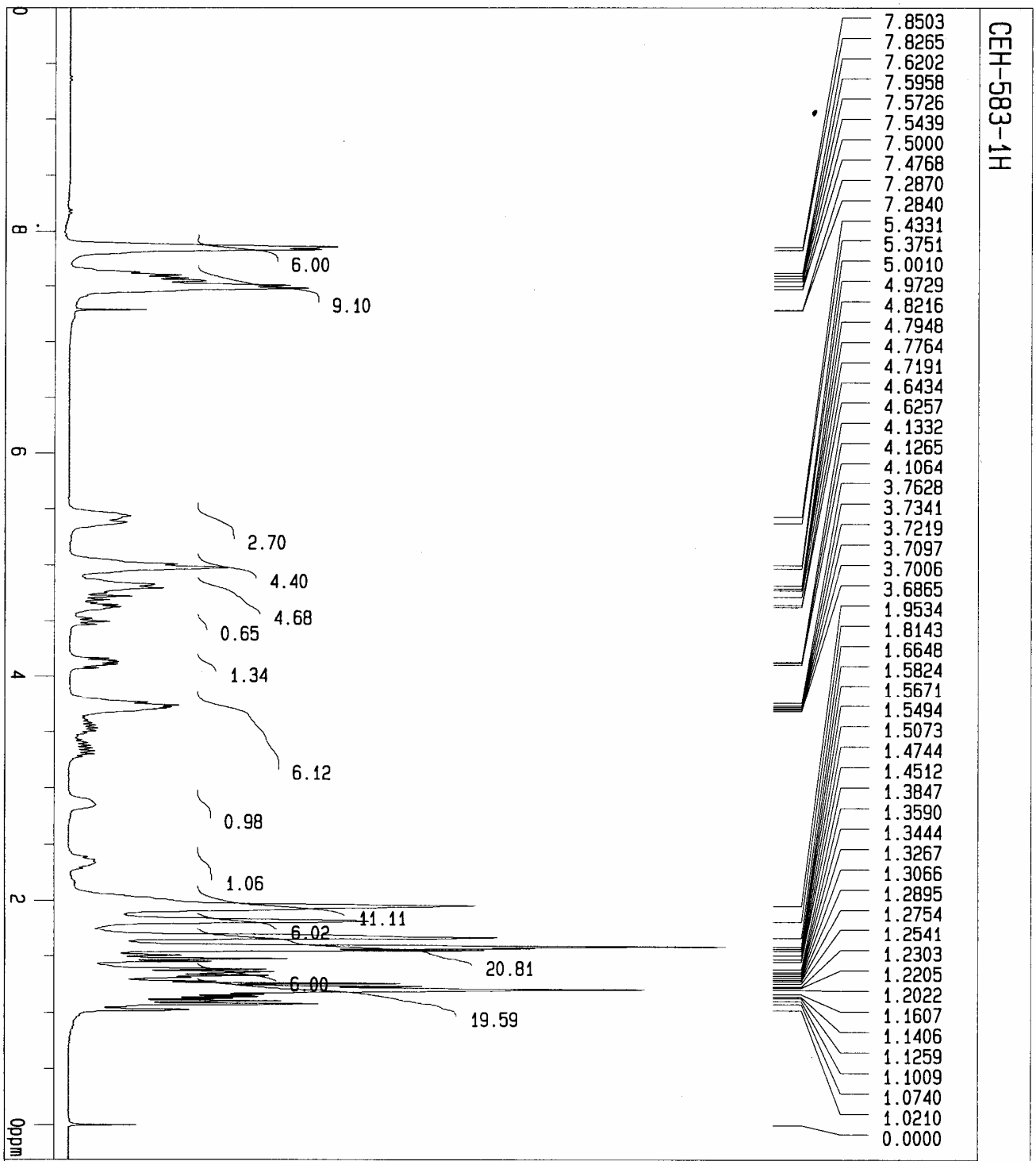

SO2Ph
SO2Ph
O
O
O
O
SO2Ph

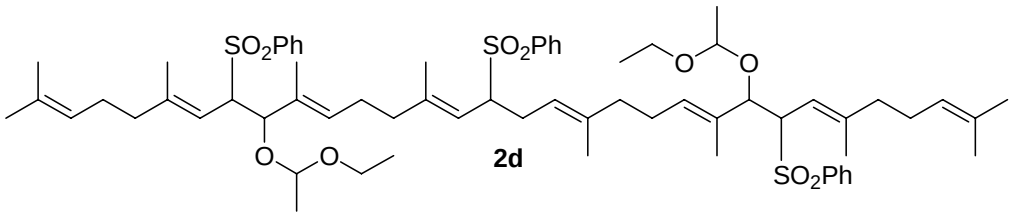
2b


1237-1-1H
7.8857
7.8472
7.8240
7.6098
7.5842
7.5604
7.5366
7.4969
7.4866
7.4707
7.4481
7.2681
5.4361
5.0352
4.9467
4.8271
4.7978
4.7728
4.5976
4.5531
4.2736
4.2095
4.1723
4.1522
4.1332
4.1216
4.1094
3.7305
3.5437
2.0450
1.9607
1.9491
1.7813
1.6788
1.6501
1.6367
1.5604
1.5427
1.4872
1.4536
1.3841
1.3584
1.2828
1.2590
1.2352
1.1869
1.1454
1.1186
1.0862
1.0747
0.9923
0.8830
0.8556
0.8519
0.8312
0.0000
6.57
10.23
2.69
7.62
1.99
3.23
2.15
2.01
1.00
1.02
71.61
0ppm
8
6
4
2

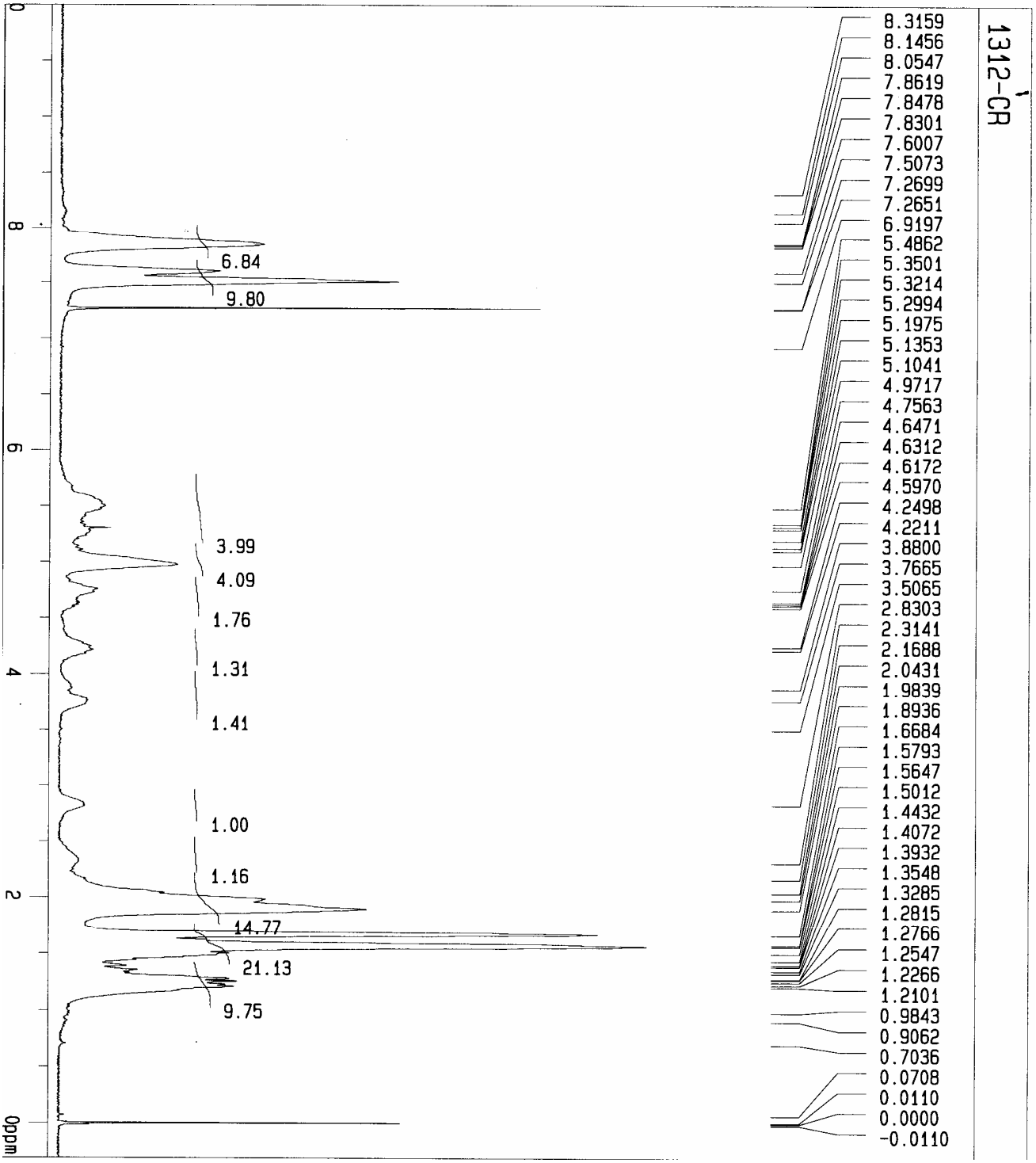

SO2Ph
SO2Ph
O
O
O
O
SO2Ph

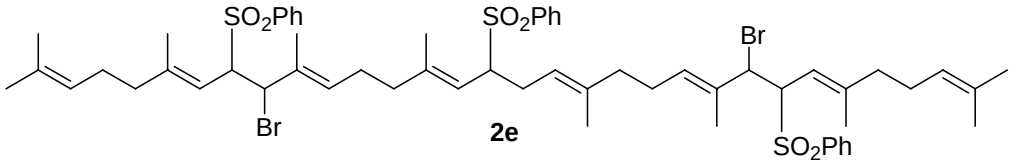
2c


CEH-583-1H
7.8503
7.8265
7.6202
7.5958
7.5726
7.5439
7.5000
7.4768
7.2870
7.2840
5.4331
5.3751
5.0010
4.9729
4.8216
4.7948
4.7764
4.7191
4.6434
4.6257
4.1332
4.1265
4.1064
3.7628
3.7341
3.7219
3.7097
3.7006
3.6865
1.9534
1.8143
1.6648
1.5824
1.5671
1.5494
1.5073
1.4744
1.4512
1.3847
1.3590
1.3444
1.3267
1.3066
1.2895
1.2754
1.2541
1.2303
1.2205
1.2022
1.1607
1.1406
1.1259
1.1009
1.0740
1.0210
0.0000
6.00
9.10
2.70
4.40
4.68
0.65
1.34
6.12
0.98
1.06
11.11
6.02
20.81
6.00
19.59
8
6
4
2
0ppm

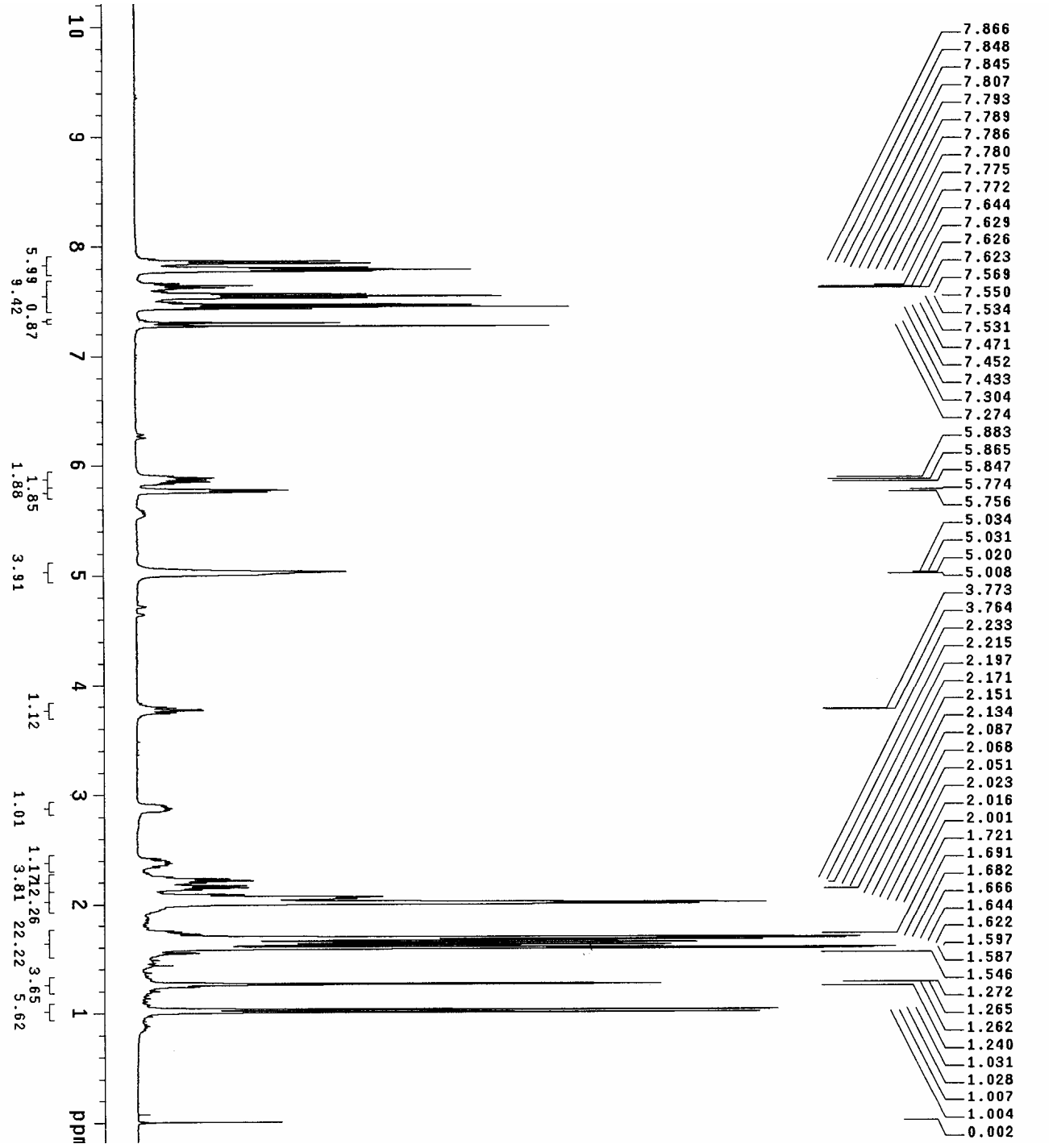

SO2Ph
SO2Ph
O
O
O
O
SO2Ph

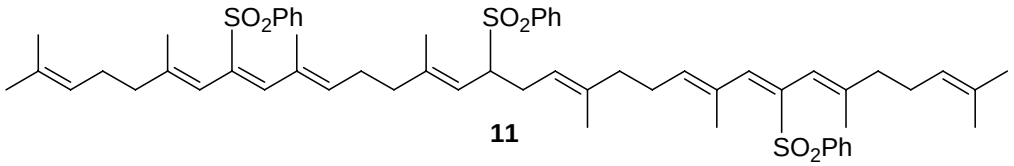
2d


1312-CR
8.3159
8.1456
8.0547
7.8619
7.8478
7.8301
7.6007
7.5073
7.2699
7.2651
6.9197
5.4862
5.3501
5.3214
5.2994
5.1975
5.1353
5.1041
4.9717
4.7563
4.6471
4.6312
4.6172
4.5970
4.2498
4.2211
3.8800
3.7665
3.5065
2.8303
2.3141
2.1688
2.0431
1.9839
1.8936
1.6684
1.5793
1.5647
1.5012
1.4432
1.4072
1.3932
1.3548
1.3285
1.2815
1.2766
1.2547
1.2266
1.2101
0.9843
0.9062
0.7036
0.0708
0.0110
0.0000
-0.0110
6.84
9.80
3.99
4.09
1.76
1.31
1.41
1.00
1.16
14.77
21.13
9.75
ppm

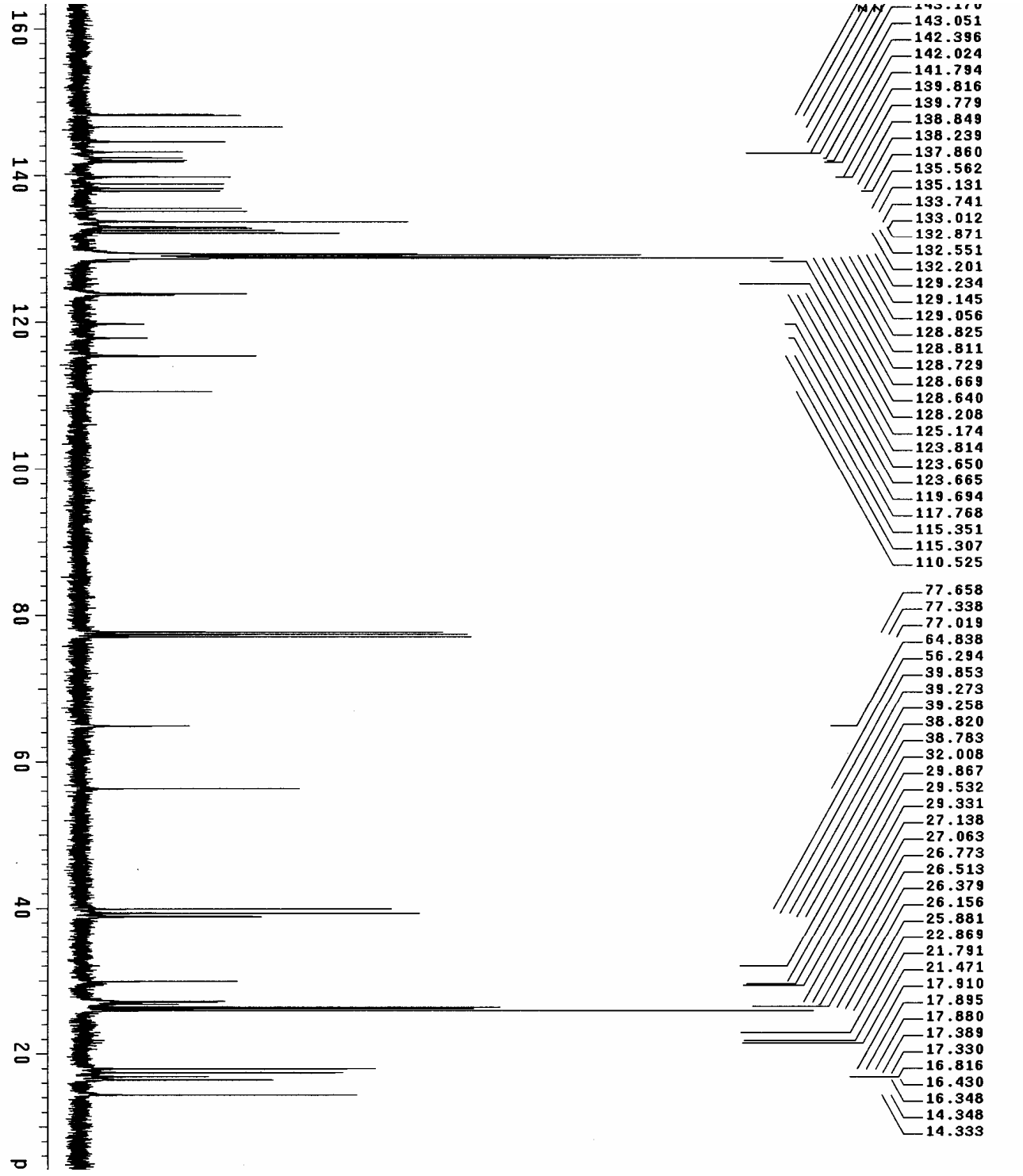

SO2Ph
SO2Ph
Br
Br
SO2Ph

2e


7.866
7.848
7.845
7.807
7.793
7.789
7.786
7.780
7.775
7.772
7.644
7.629
7.626
7.623
7.569
7.550
7.534
7.531
7.471
7.452
7.433
7.304
7.274
5.883
5.865
5.847
5.774
5.756
5.034
5.031
5.020
5.008
3.773
3.764
2.233
2.215
2.197
2.171
2.151
2.134
2.087
2.068
2.051
2.023
2.016
2.001
1.721
1.691
1.682
1.666
1.644
1.622
1.597
1.587
1.546
1.272
1.265
1.262
1.240
1.031
1.028
1.007
1.004
0.002
5.99
0.87
9.42
1.85
1.88
3.91
1.12
1.01
1.17
12.26
3.81
22.22
3.65
5.62
ppm


SO2Ph
SO2Ph
SO2Ph

11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120
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80
60
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138.239
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77.019
64.838
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27.138
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26.156
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22.869
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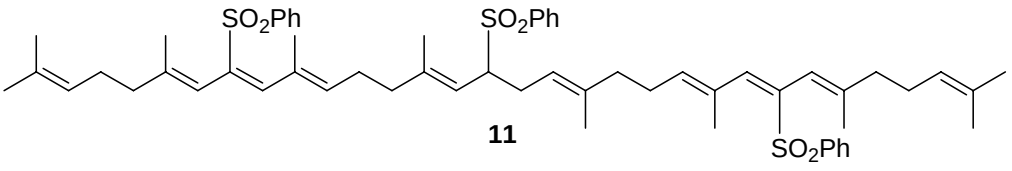
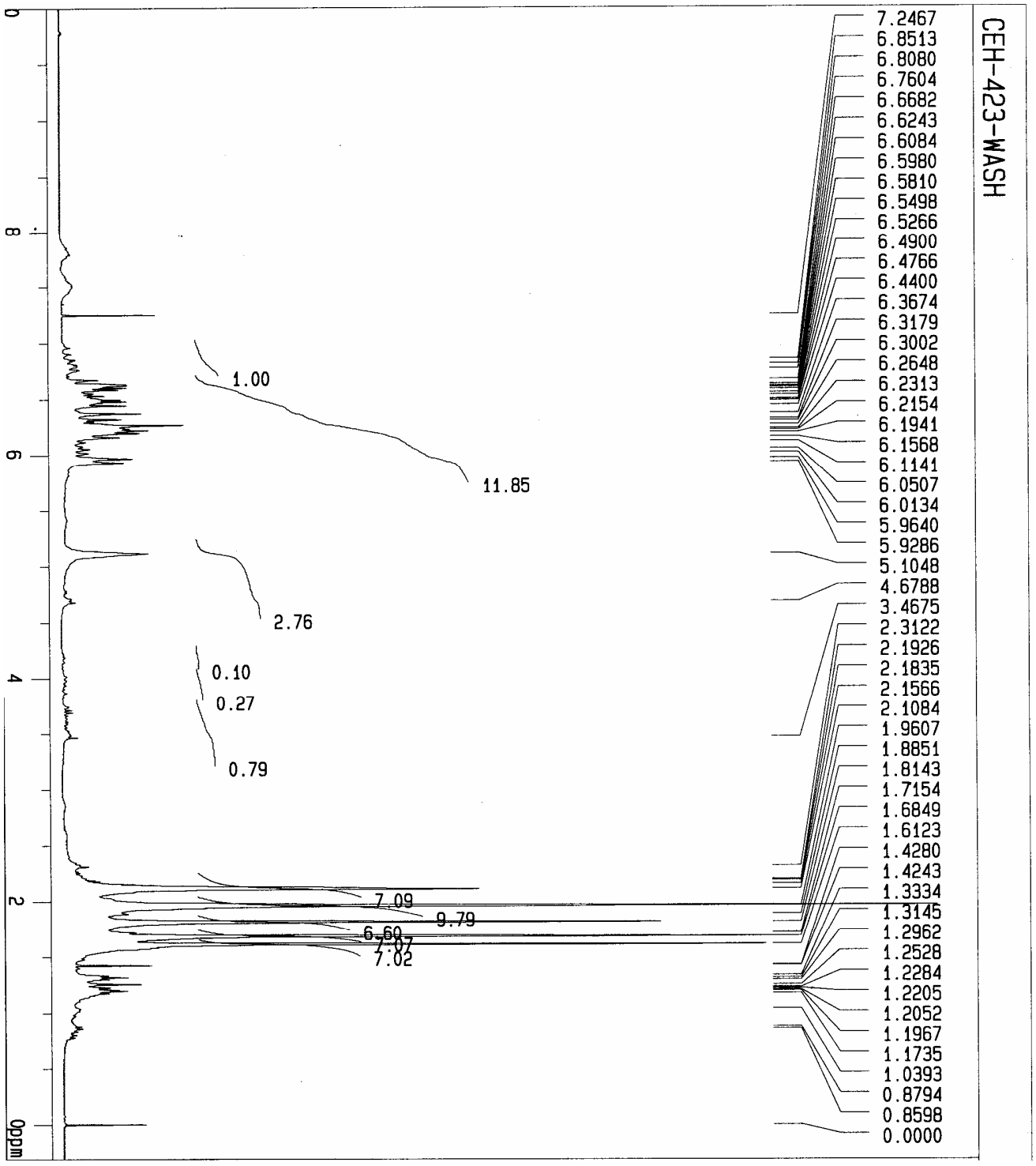
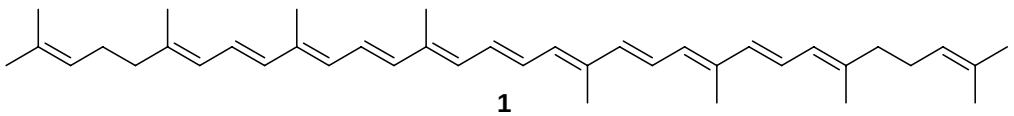

SO2Ph
SO2Ph
SO2Ph

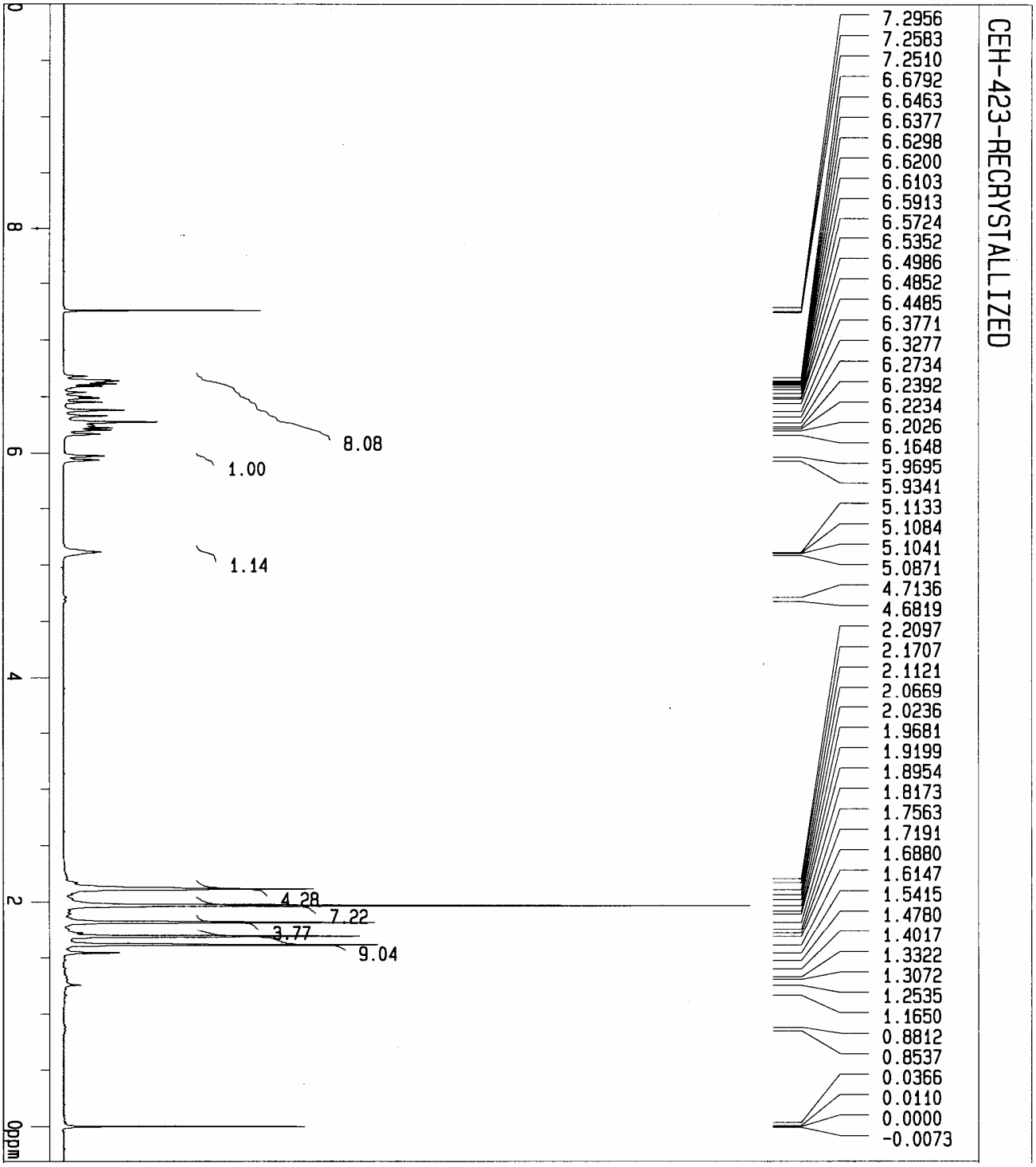
11

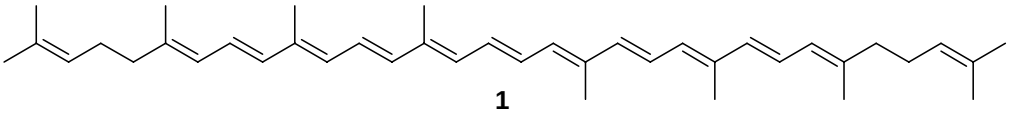




1

Crude product





1

Recystallized product