Supporting Information

Efficient access to polisusbstituted tetrahydrofurans by electrophilic cyclization of vinylsilyl alcohols

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Computational Details

DFT calculations were carried out by using the GAUSSIAN09 package.[S1] B3LYP method (Becke Three Parameter Hybrid Functionals) was applied.[S2] A split-valence double-zeta basis set with polarization functions 6-31G(d,p) was used for all atoms.[S3] Geometry full optimizations were performed in gas-phase without symmetry restrictions, and they were confirmed as minima by vibrational analysis.[S4] Solvent effects were taken into account by using PCM algorithm with dichloromethane (ε = 8.93) as a solvent[S5] and added to Gibbs free energies previously computed in gas phase, by following the equation:

$$G_{toluene} = G_{gas} + (E_{toluene} - E_{gas}) \qquad \text{eq. S1}$$

Transition States were obtained by first scanning the Potential Energy Surface along the bond that will be formed and then applying the synchronous transit-guided quasi-Newton method QST3 at the approximate geometry of the TS.[S6] Once located, they were confirmed by vibrational analysis.
p-Toluene sulfonic acid and p-toluene sulfonate anion were also subjected to the shown procedure and their energy summed to the suitable molecule in order to keep molecular charges offset and compare energies with different number of atoms.

Table S1. Relative Gibbs free energies in solution for all stationary points in pathways **a** and **b**.

Stationary Point	ΔG (kcal/mol)
II	0.00
I	1.46

TSII	2.22
TSI	6.76
IV	-4.92
II	-4.65
4b	-36.82
5b	-33.32

Table S2. Relative Gibbs free energies in solution for all stationary points in pathways **c** and **d**.

Stationary Point	ΔG (kcal/mol)
VI	0.00
V	1.08
TSIV	3.15
TSIII	4.26
VIII	-6.89
VII	-5.46
4e	-34.23
5e	-33.99

Table S3. Relative Gibbs free energies in solution for all stationary points in pathways **e** and **f**.

Stationary Point	ΔG (kcal/mol)
X	0.00
IX	4.66
TSVI	3.04
TSV	12.26
XII	-5.79
XI	-0.76
4h	-34.64
5h	-33.74

(S1) Gaussian 09, Revision **D.01**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A., Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, M. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin,

K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

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(S3) a) A. Sygula, C. Muck-Lichtenfeld, S. Grimme, L. Kobryn, *Phys. Chem. Chem. Phys.,* 2010, **12**, (26), 7091-7097. b) J. R. Otero, D. Josa, Cabaleiro, E. M. Lago, *Phys. Chem. Chem. Phys.,* 2011, **13**, (47), 21139-21145. c) A. Sygula, S. Saebø, T. Janowski, P. Pulay, A. A. Sasith Karunarathna, *Chem. Phys. Lett.,* 2011, **512**, (4–6), 155-160. d) J. Rodríguez-Otero, D. Josa, E. M. Cabaleiro-Lago, M. Rellán-Piñeiro, *Chem. Phys. Lett.,* 2013, **557**, 170-175. e) J. Rodríguez-Otero, D. Josa, E. M. Cabaleiro-Lago, L. A. Santos, T. C. Ramalho, *J. Phys. Chem. A,* 2014, **118**, (40), 9521-9528.

(S4) a) R. Ditchfield, W. J. Hehre, J. A. Pople, *J. Chem. Phys.*, 1971, **54**, 724. b) W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257. c) P. C. Hariharan, J. A. Pople, *Theor. Chem. Acc.*, 1973, **28**, 213-222. d) P. C. Hariharan, J. A. Pople, *Mol. Phys.*, 1974, **27**, 209-214. e) M. S. Gordon , *Chem. Phys. Lett.*, 1980, **76**, 163-168. f) M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, D. J. DeFrees, J. A. Pople, M. S. Gordon, *J. Chem. Phys.*, 1982, **77**, 3654-3665. g) R. C. Binning Jr., L. A. Curtiss, *J. Comp. Chem.*, 1990, **11**, 1206-1216. h) J.-P. Blaudeau, M. P. McGrath, L. A. Curtiss, L. Radom, *J. Chem. Phys*., 1997, **107**, 5016-5021. i) V. A. Rassolov, J. A. Pople, M. A. Ratner, T. L. Windus, *J. Chem. Phys.*, 1998, **109**, 1223-1229. j) V. A. Rassolov, M. A. Ratner, J. A. Pople, P. C. Redfern, L. A. Curtiss, *J. Comp. Chem.*, 2001, **22**, 976-984.

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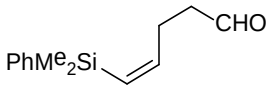
(S6) a) C. Peng, H. B. Schlegel, *Israel J. of Chem.,* 1993*,* **33**, 449. b) C. Peng, P. Y. Ayala, H. B. Schlegel, M. J. Frisch, *J. Comp. Chem*., 1996, **17**, 49.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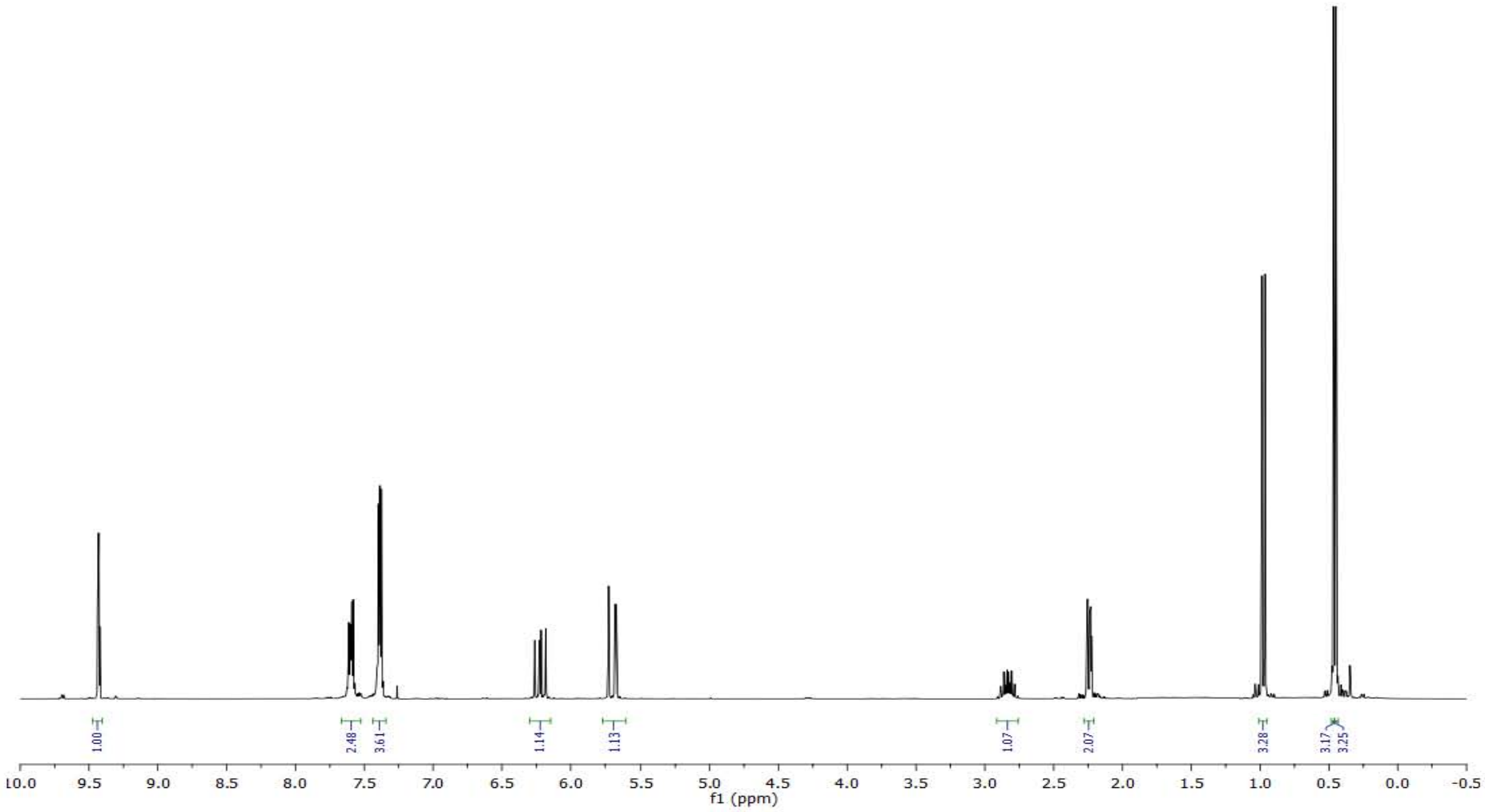
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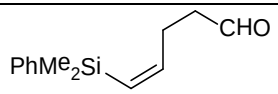
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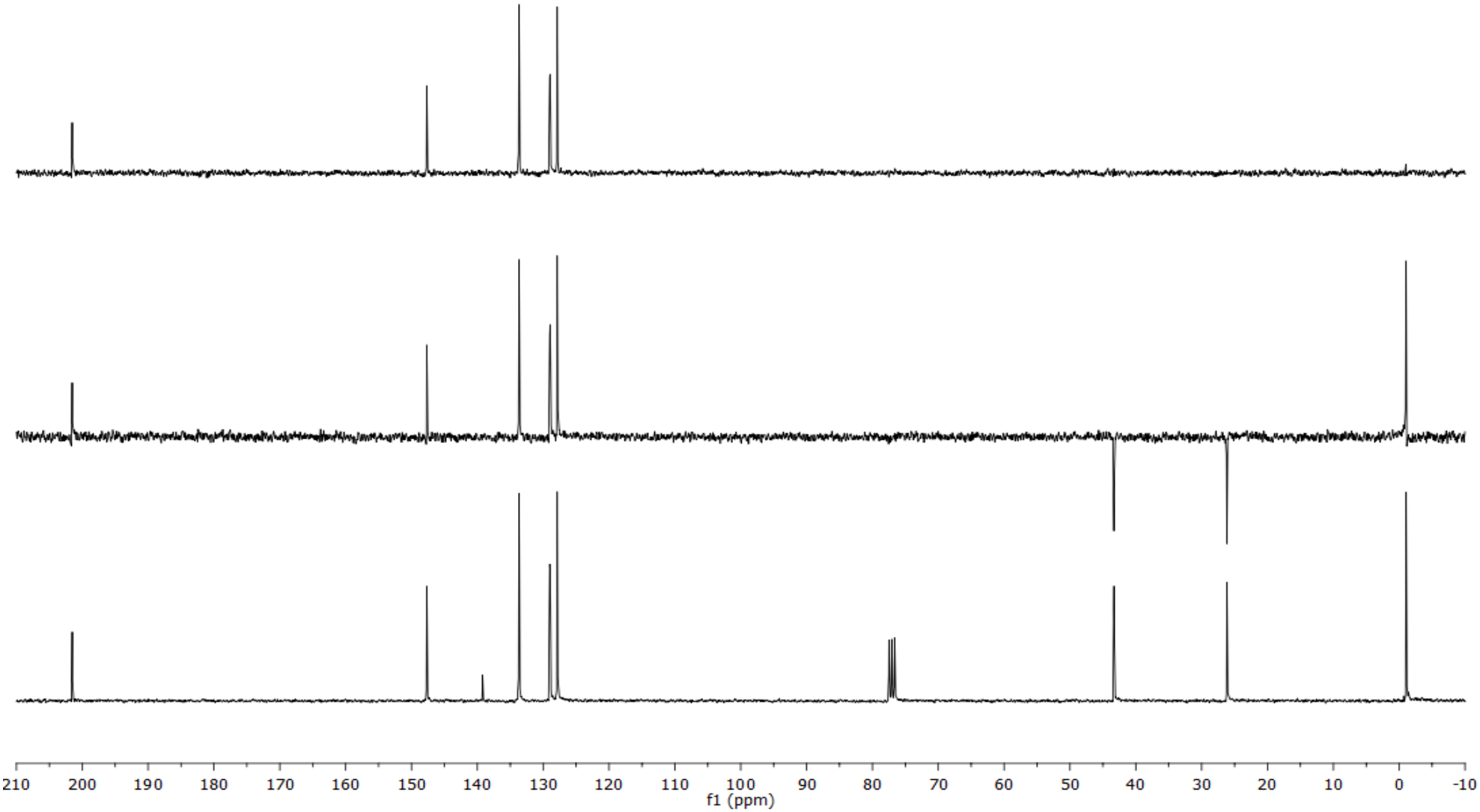
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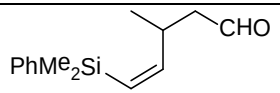
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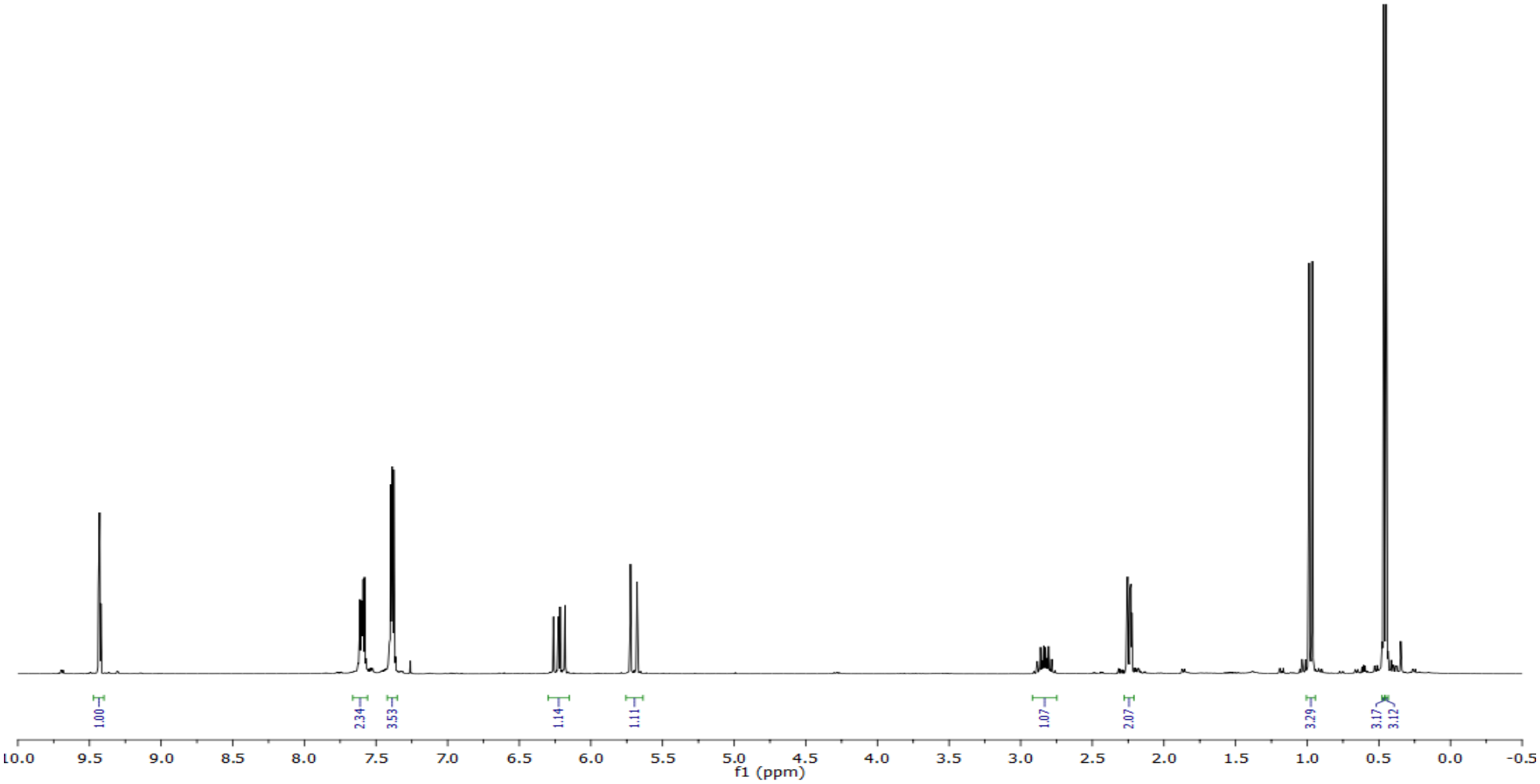
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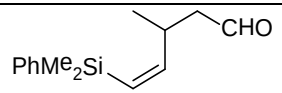
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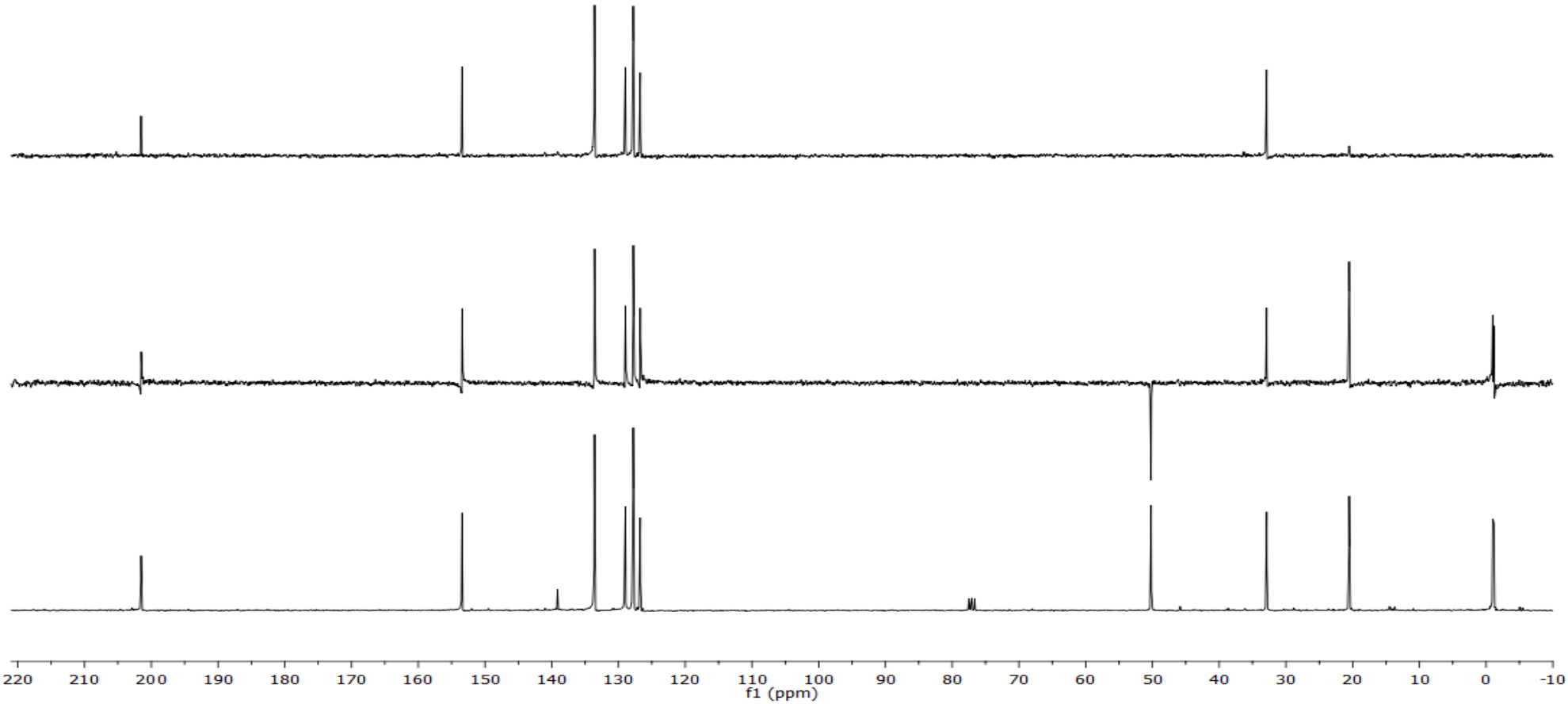
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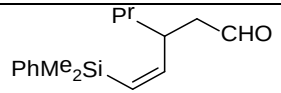
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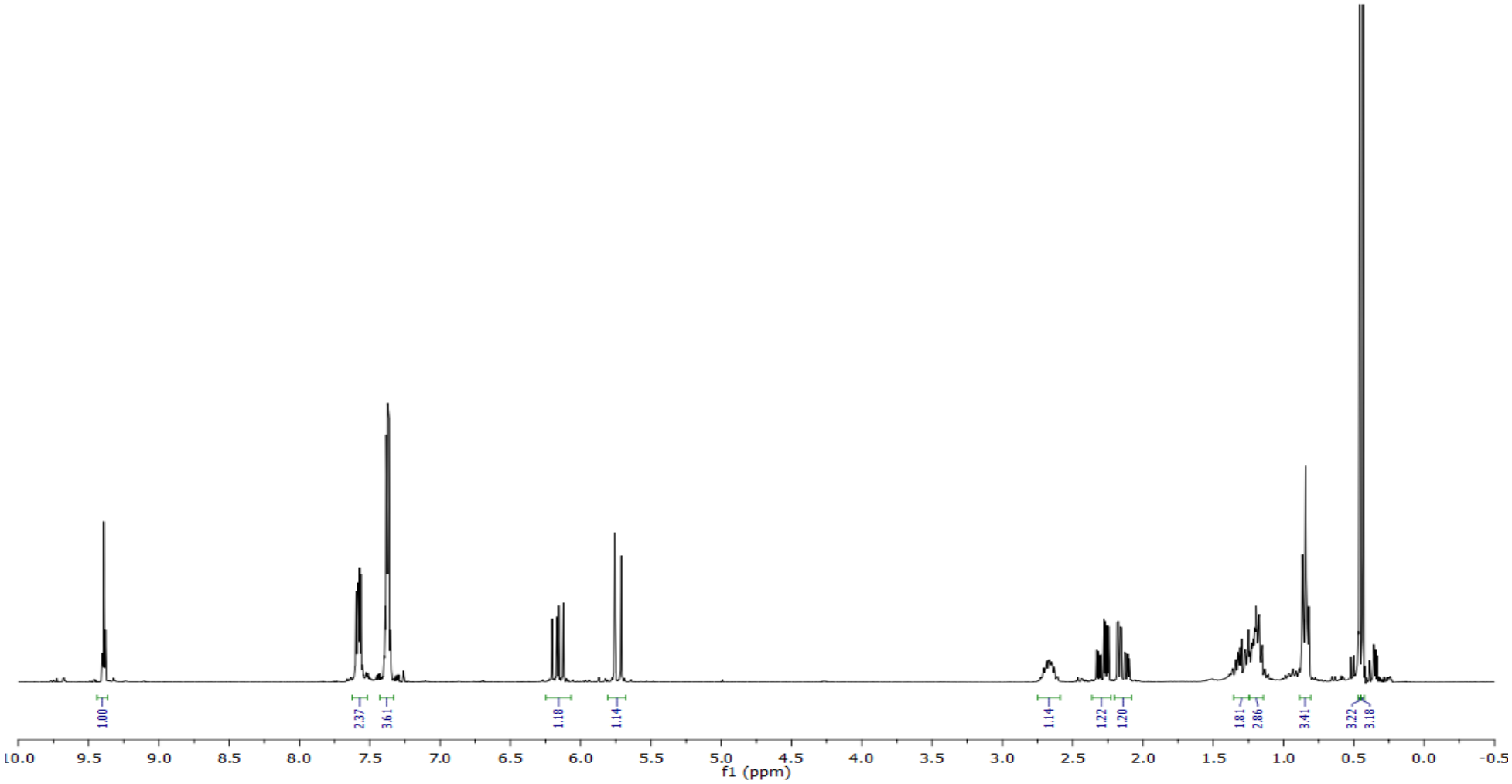
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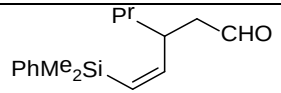
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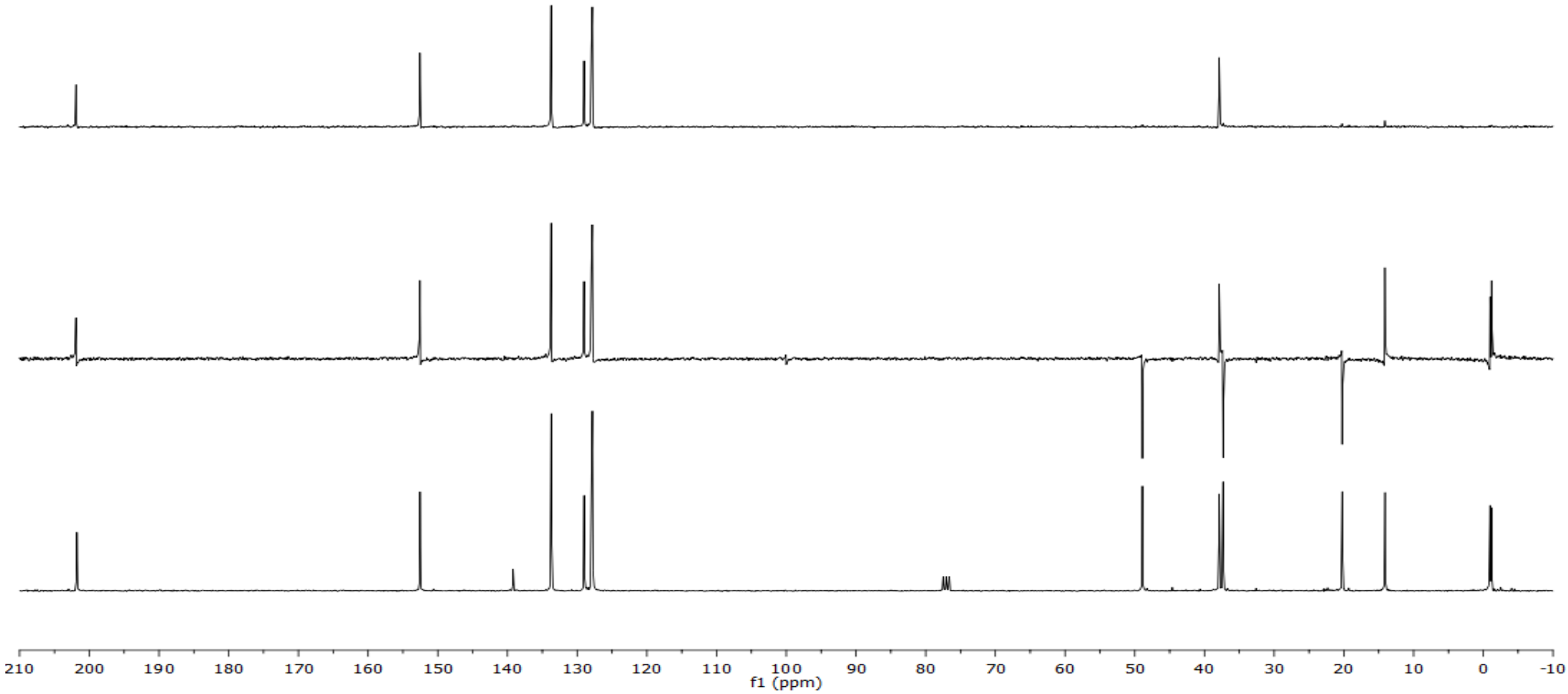
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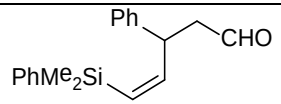
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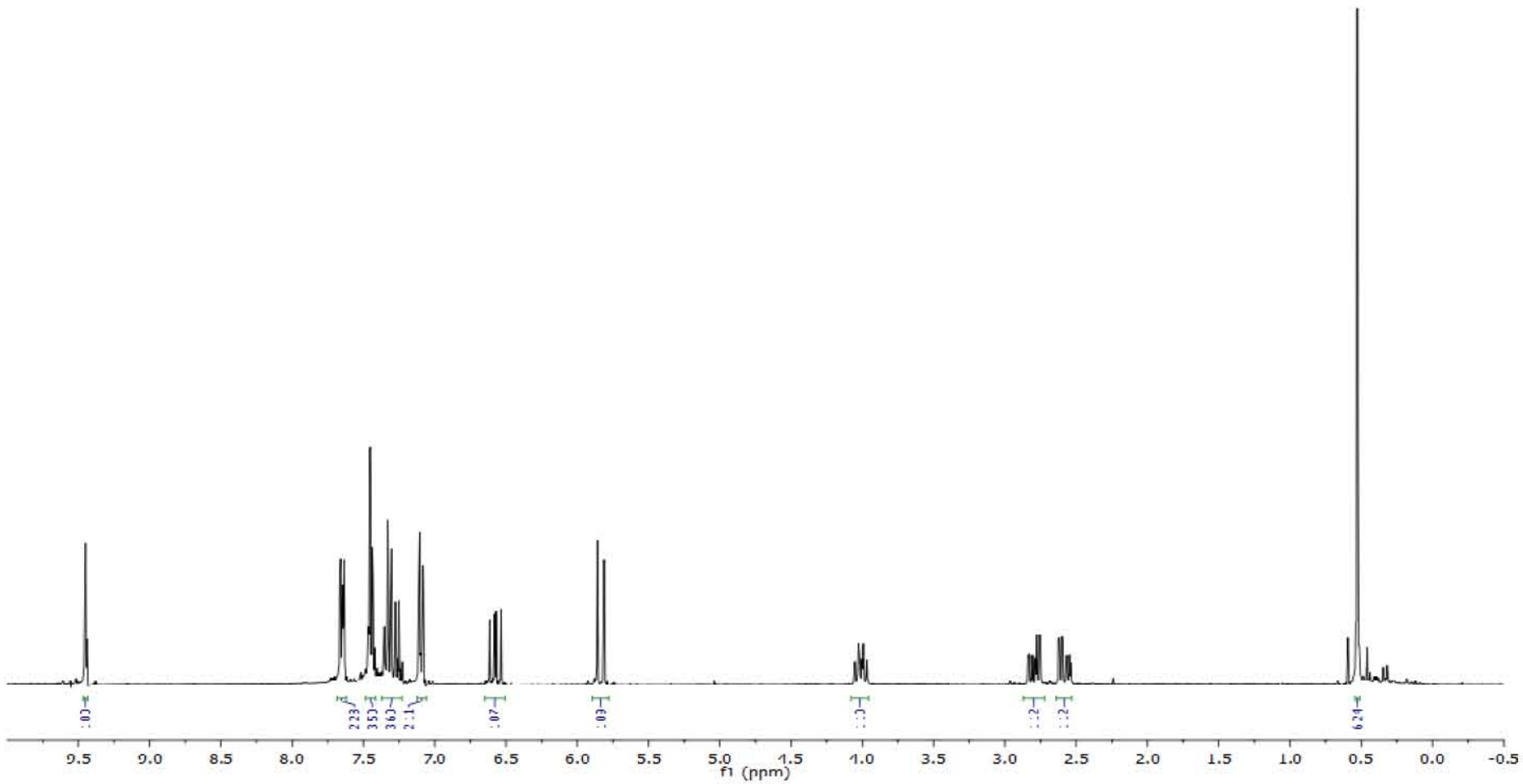
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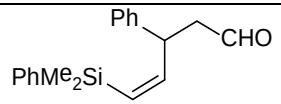
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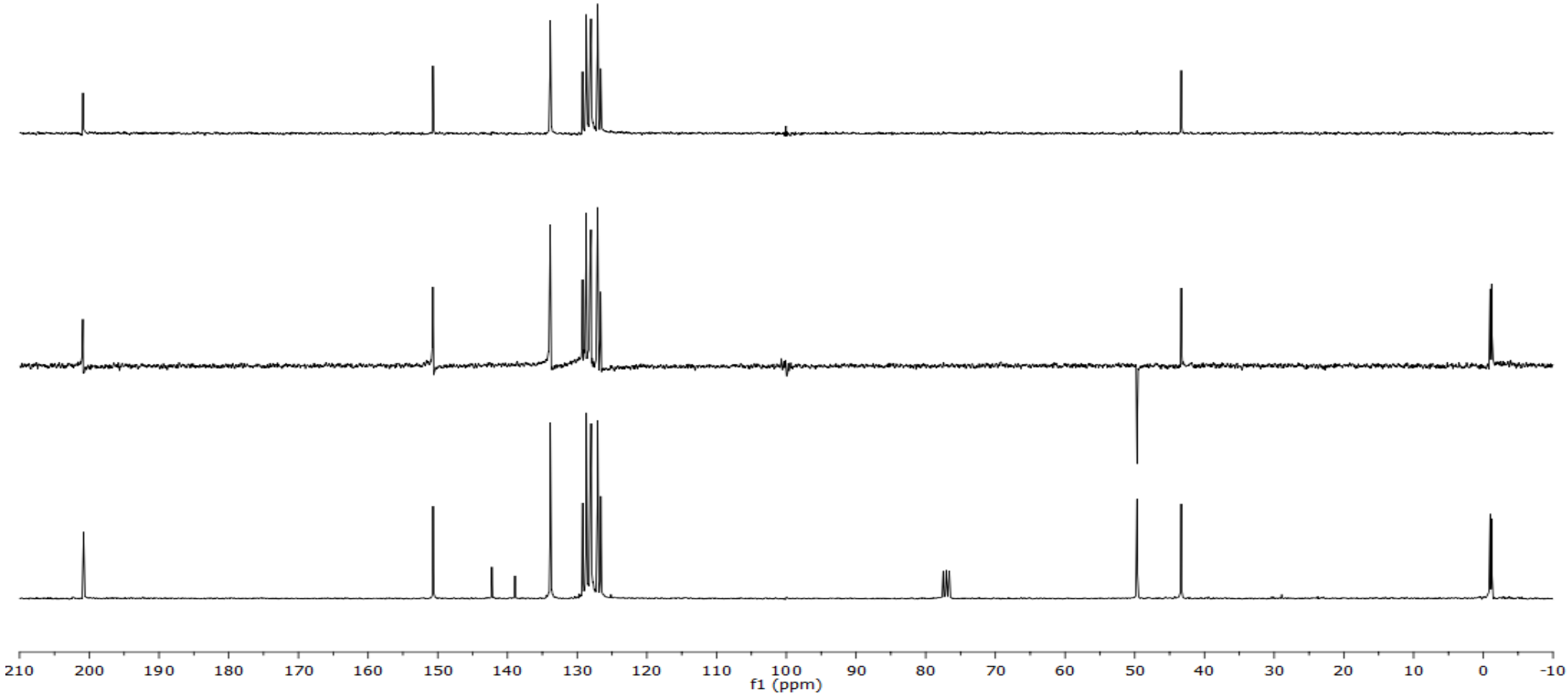
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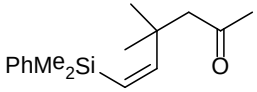
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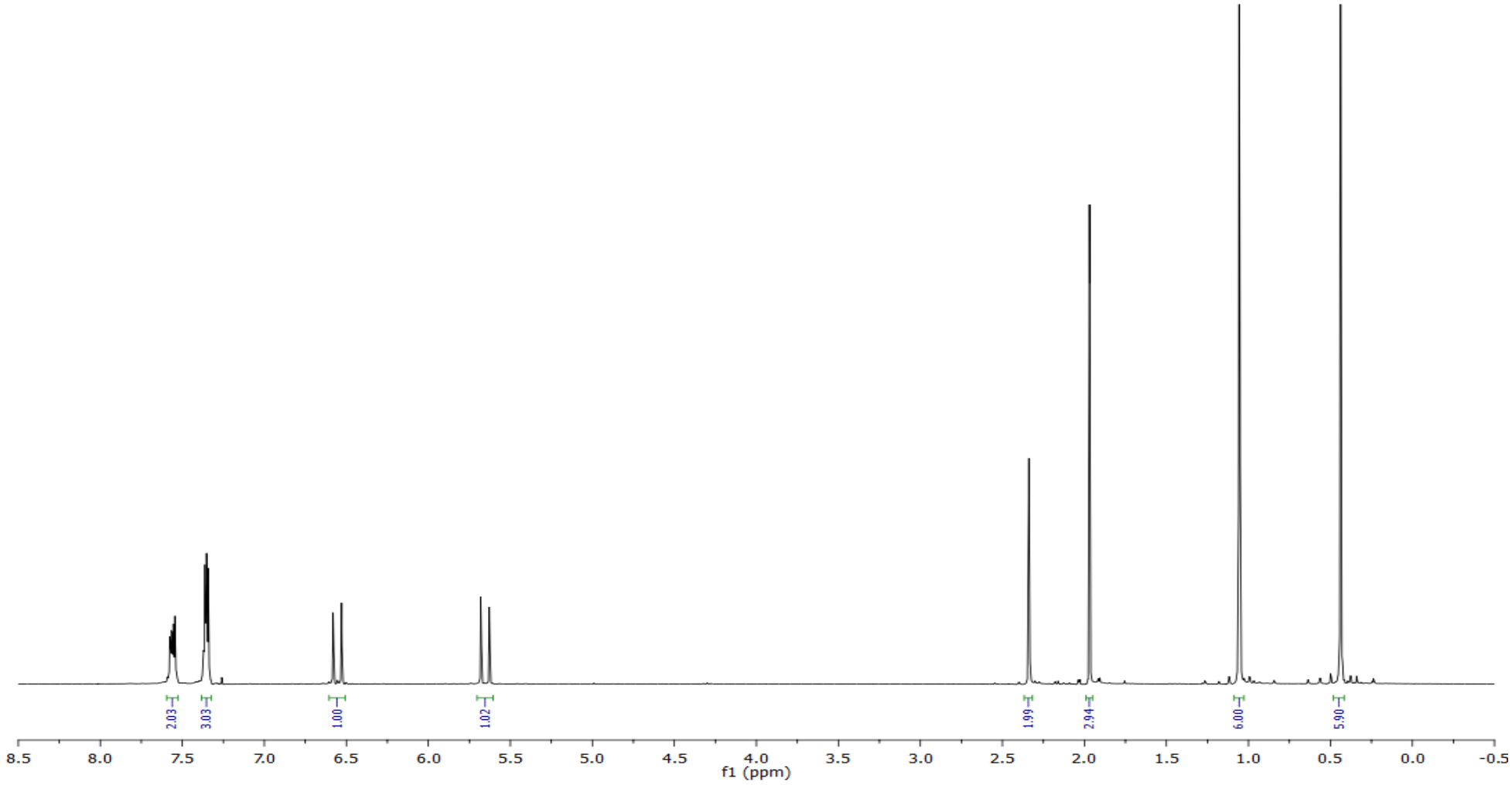
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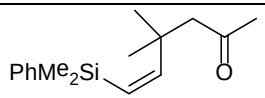
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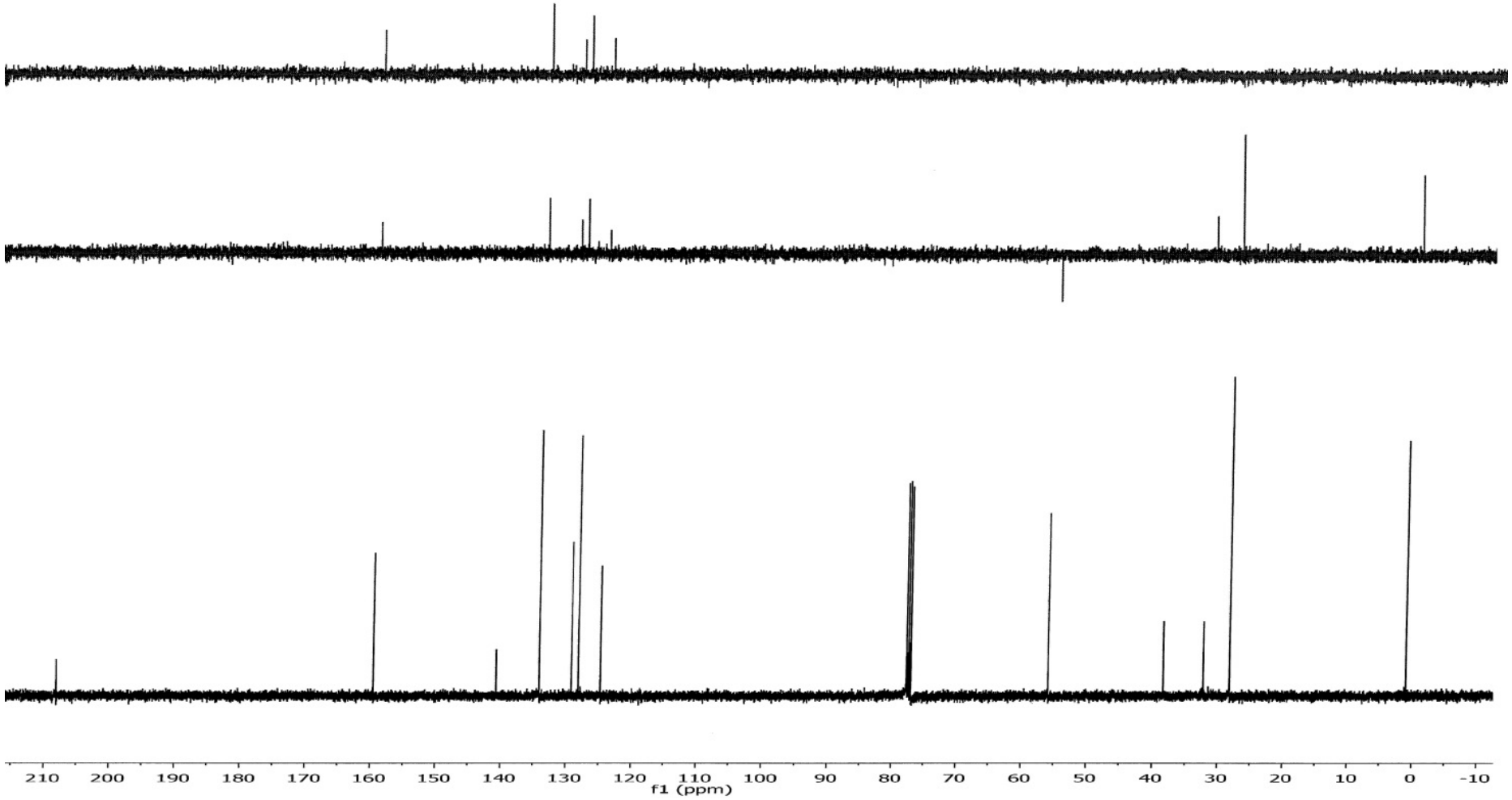
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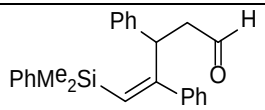
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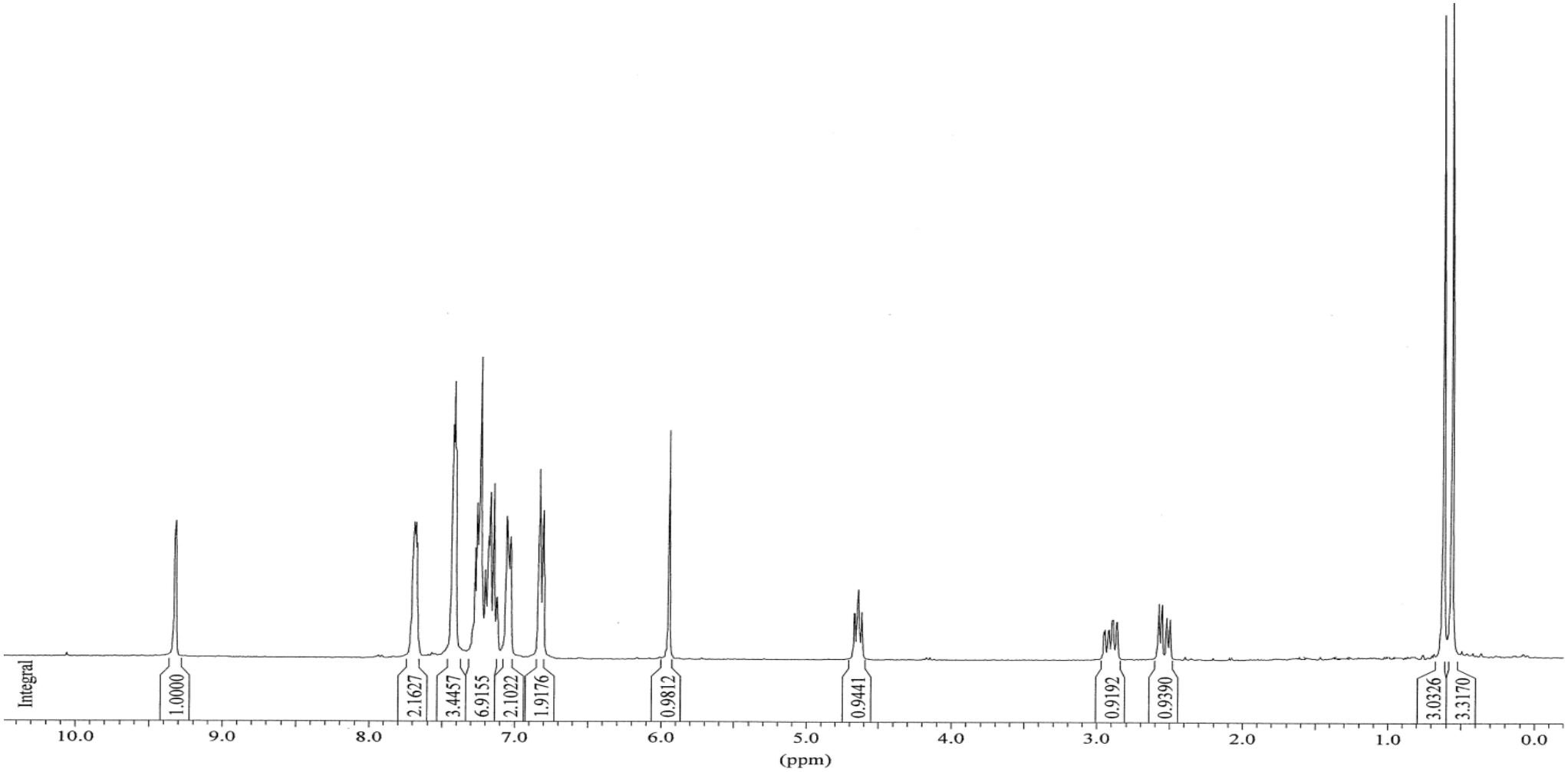
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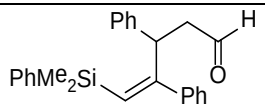

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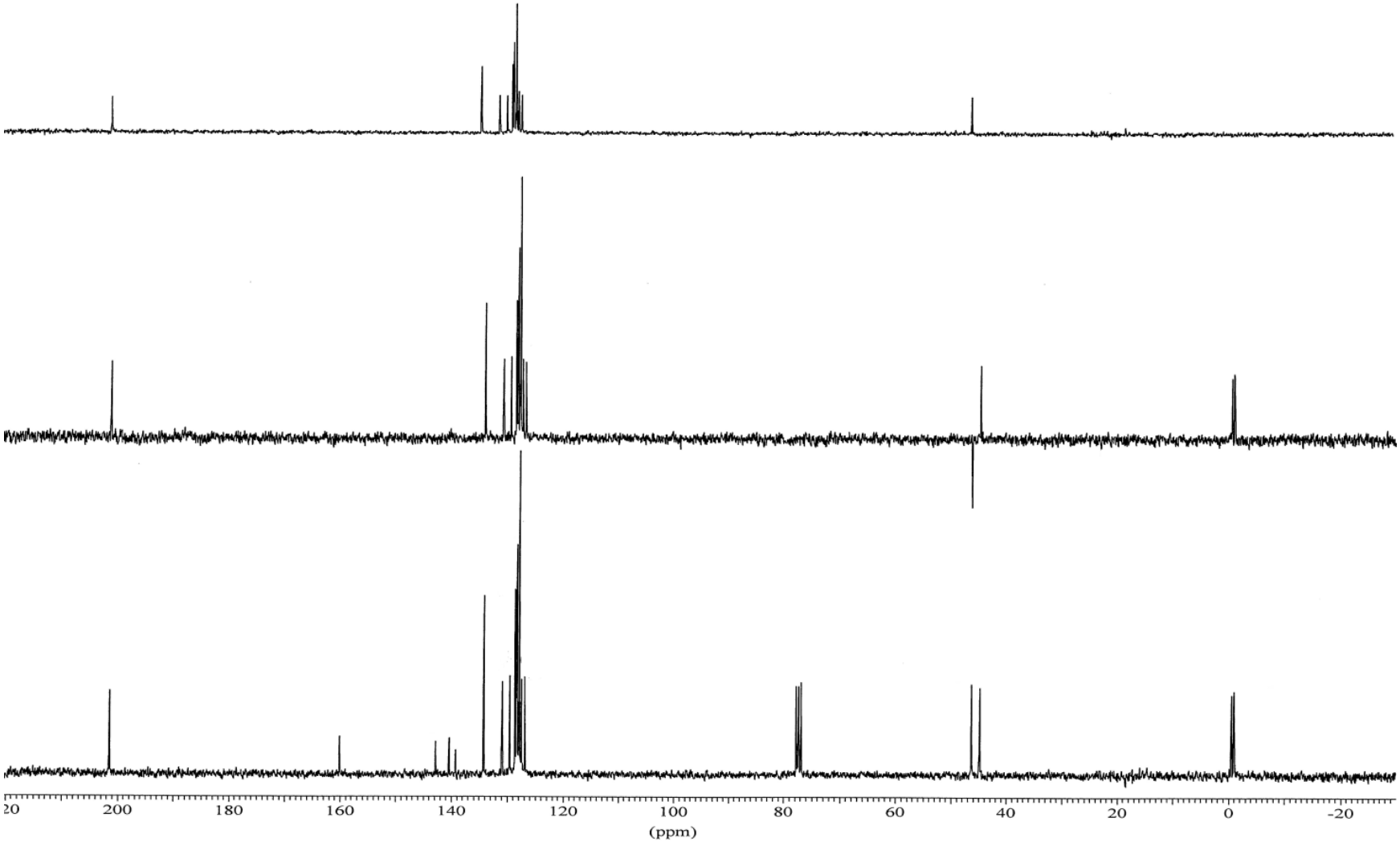

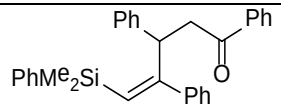
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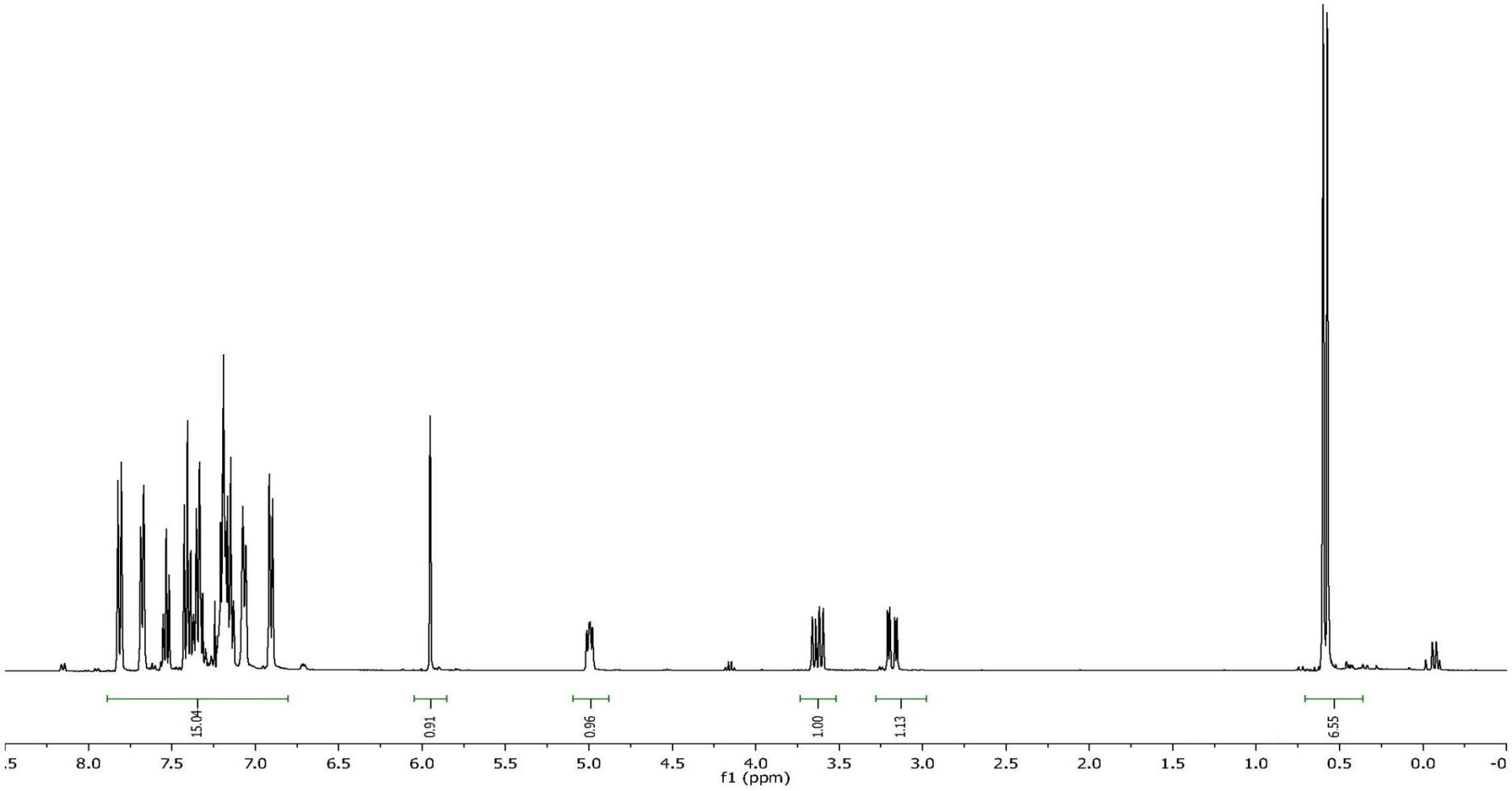
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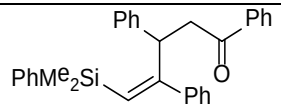
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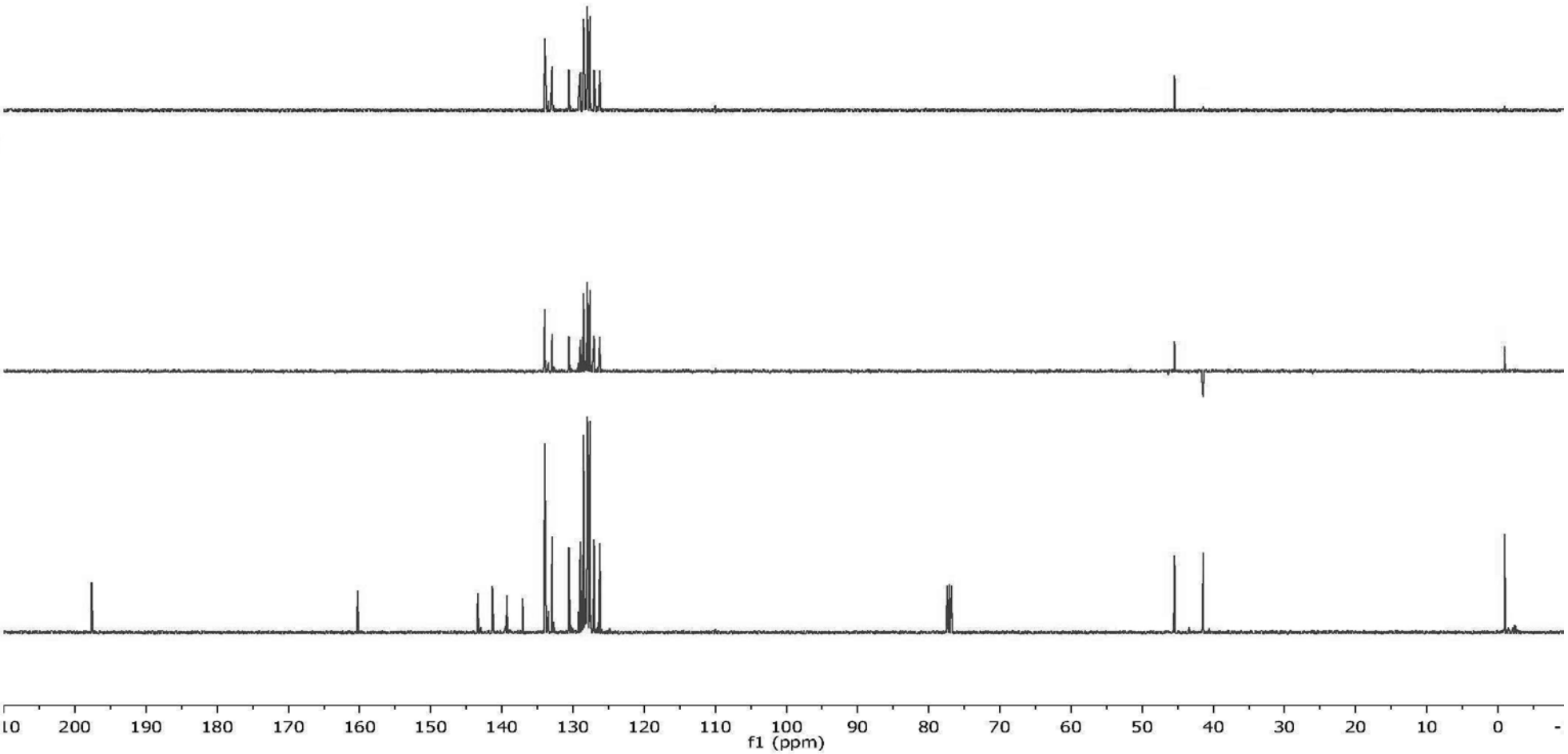
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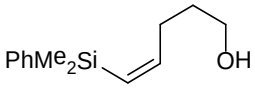
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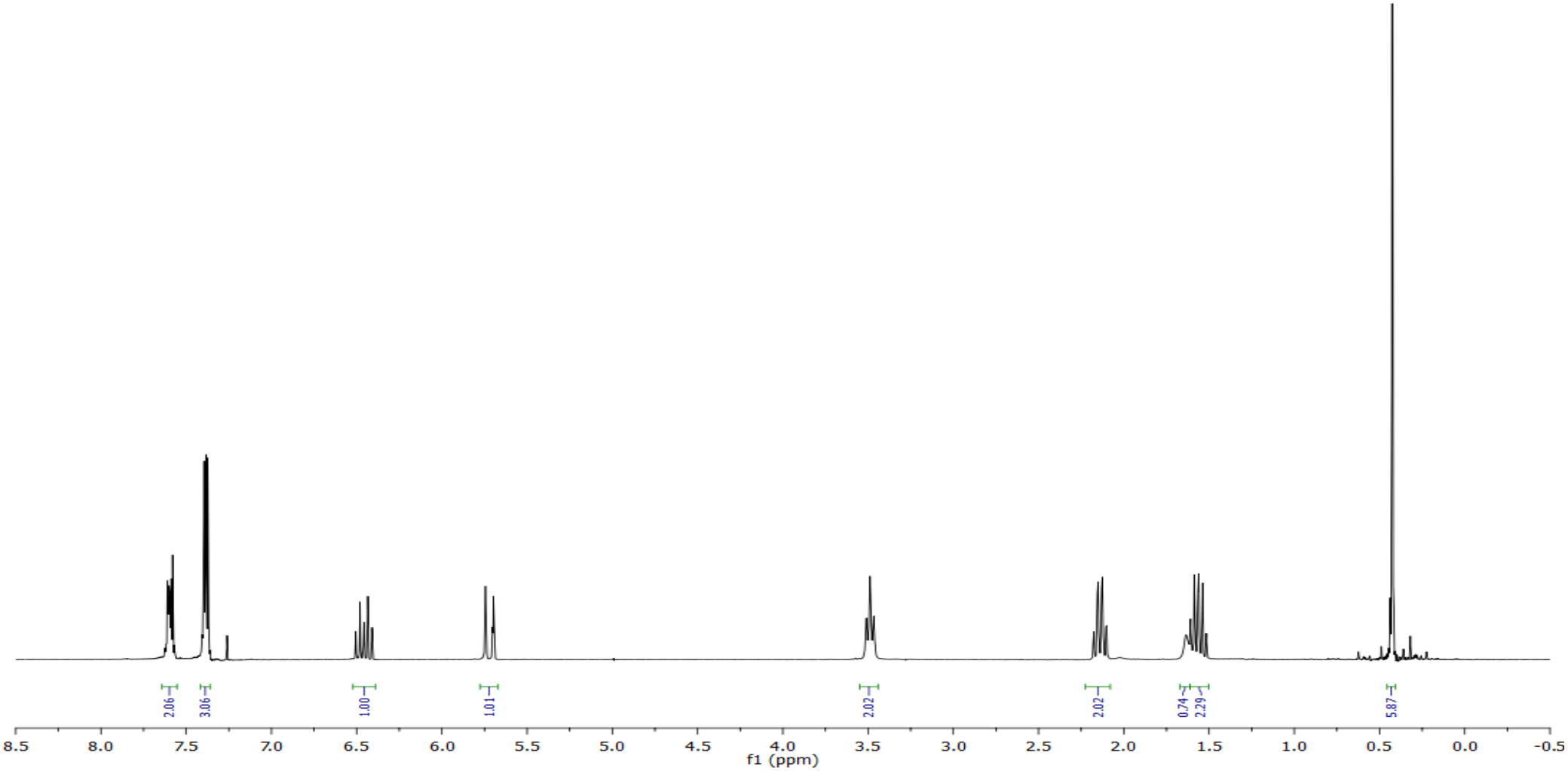
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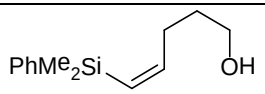
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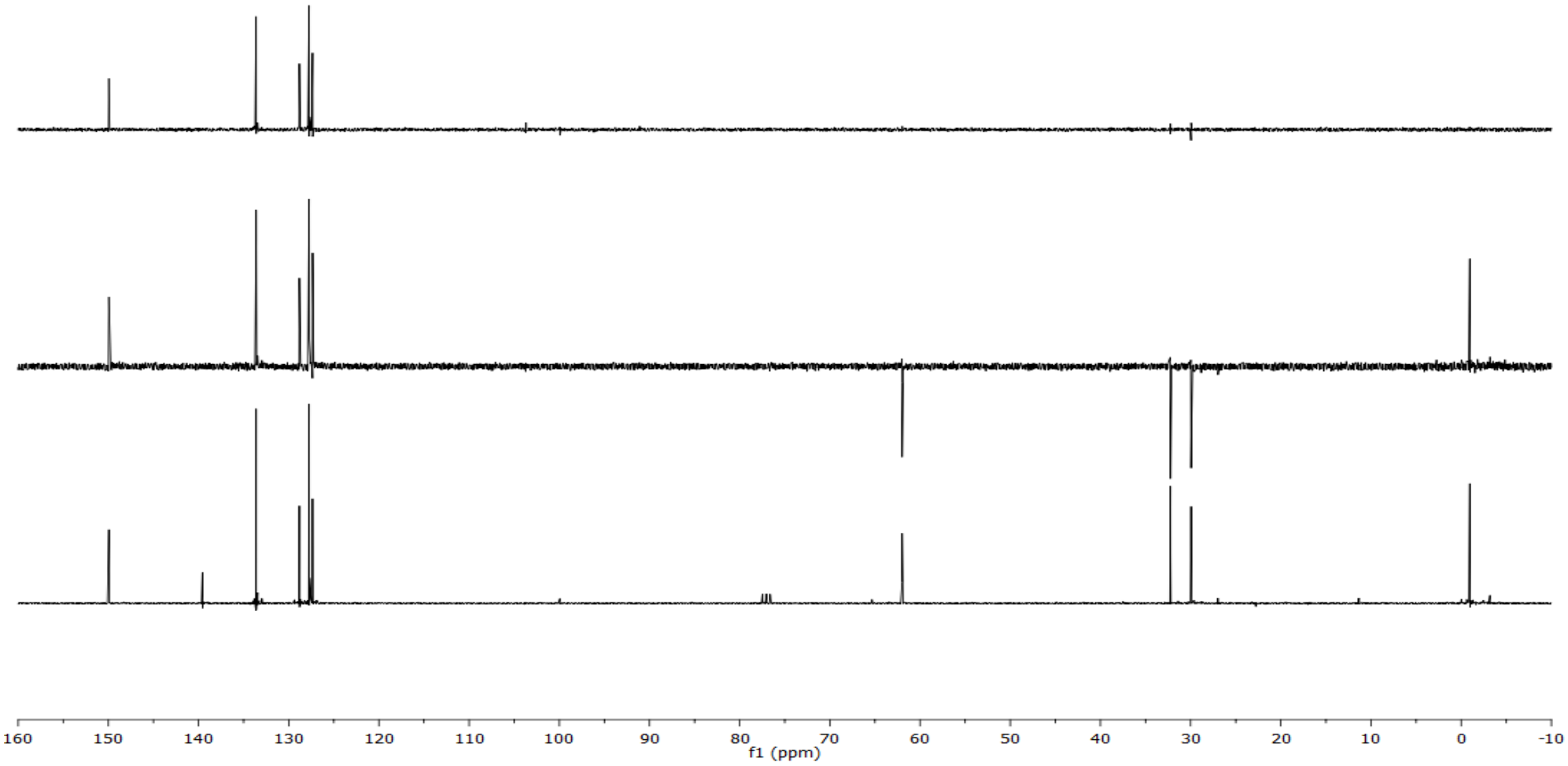
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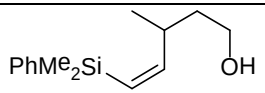
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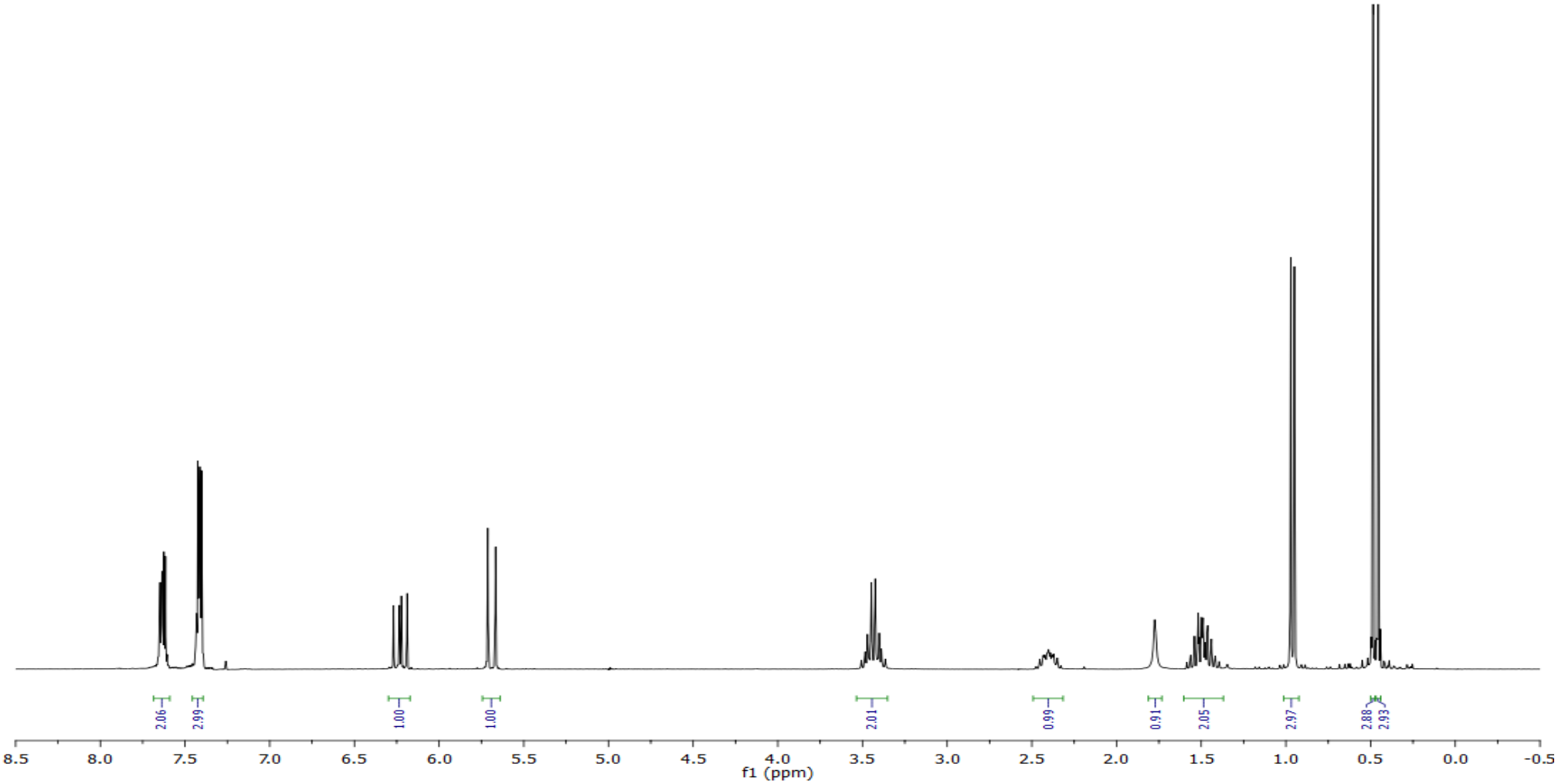
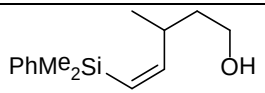
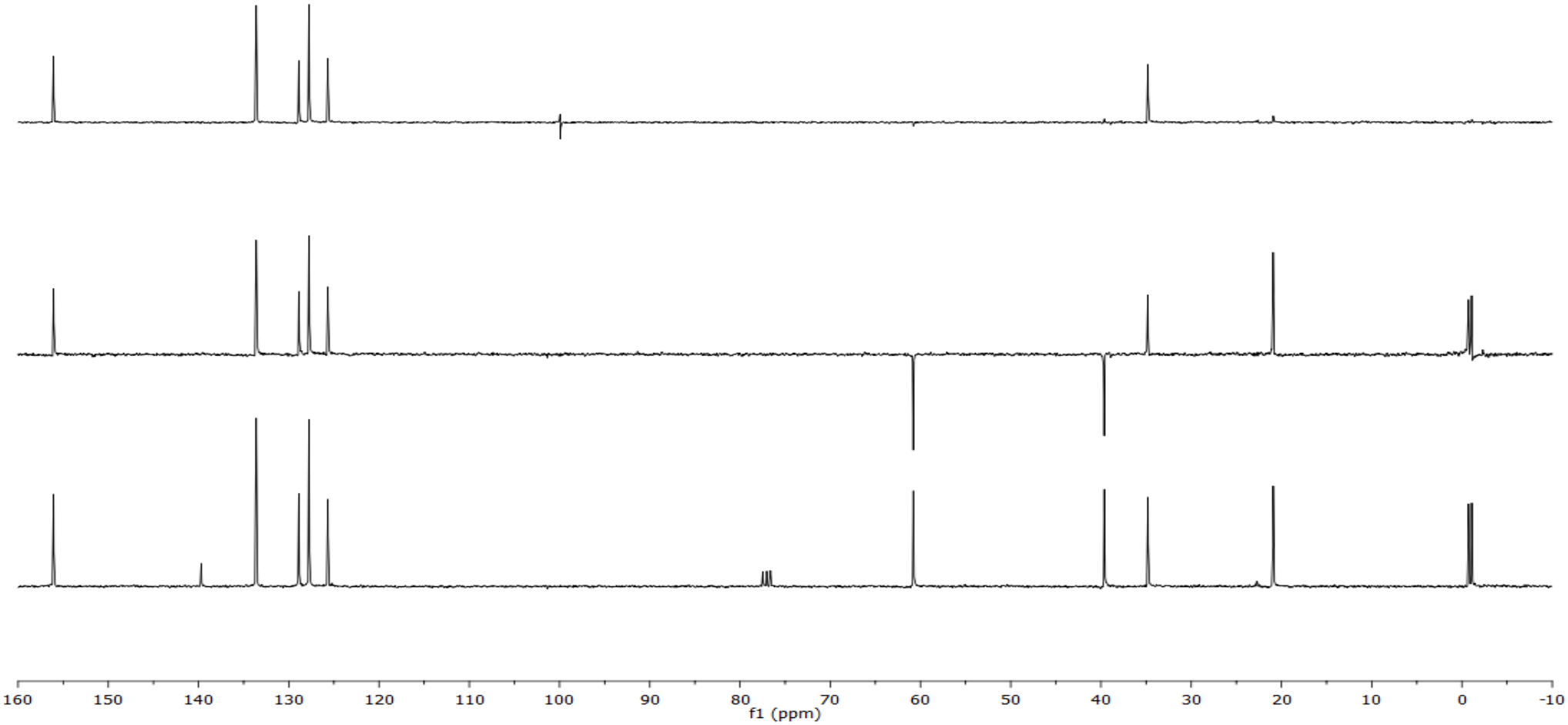
OH

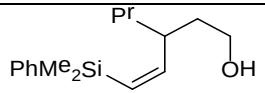
2b


2.06
2.99
1.00
1.00
2.01
0.99
0.91
2.05
2.97
2.88
2.93
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

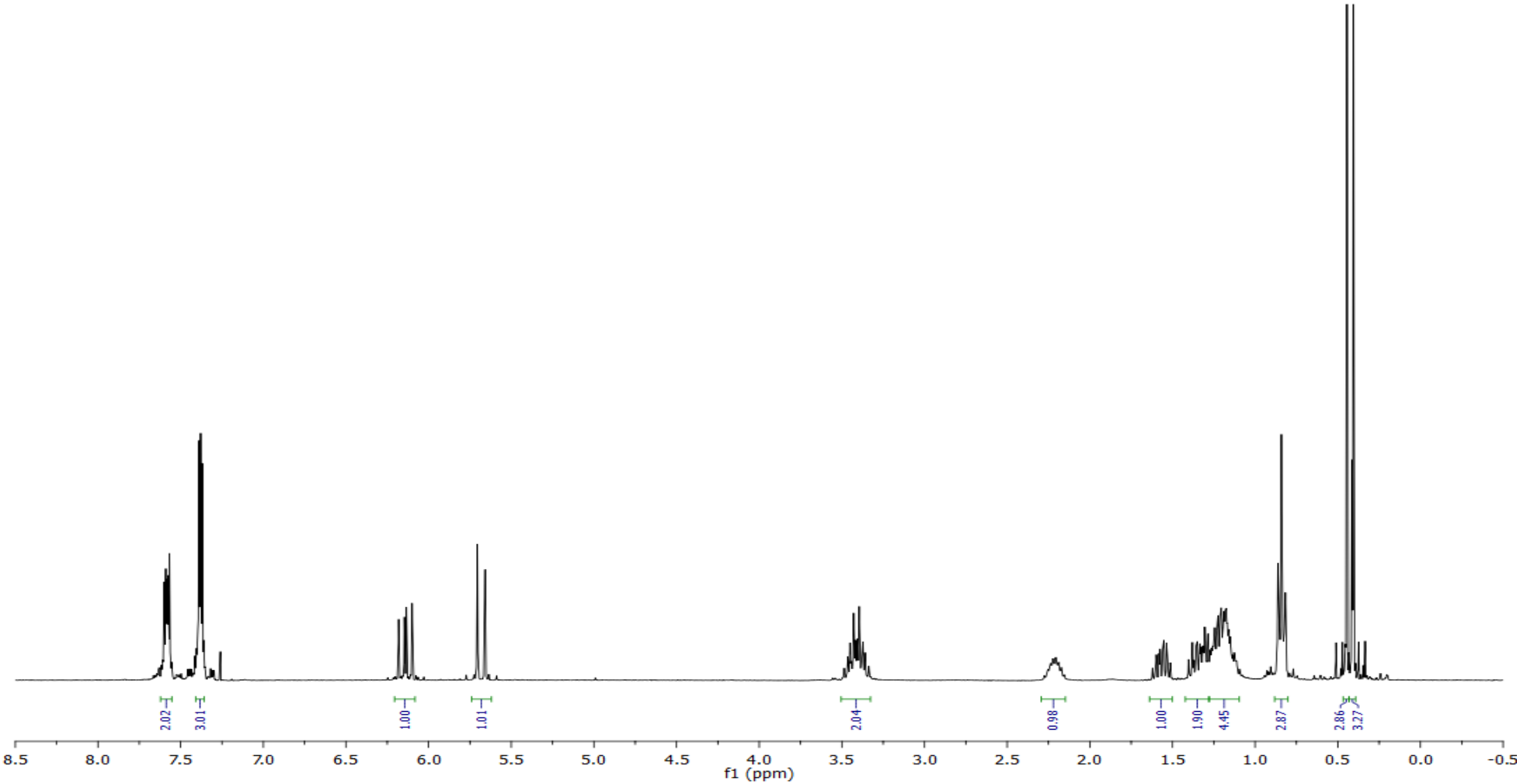

PhMe2Si
OH

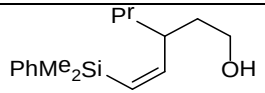
2b


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

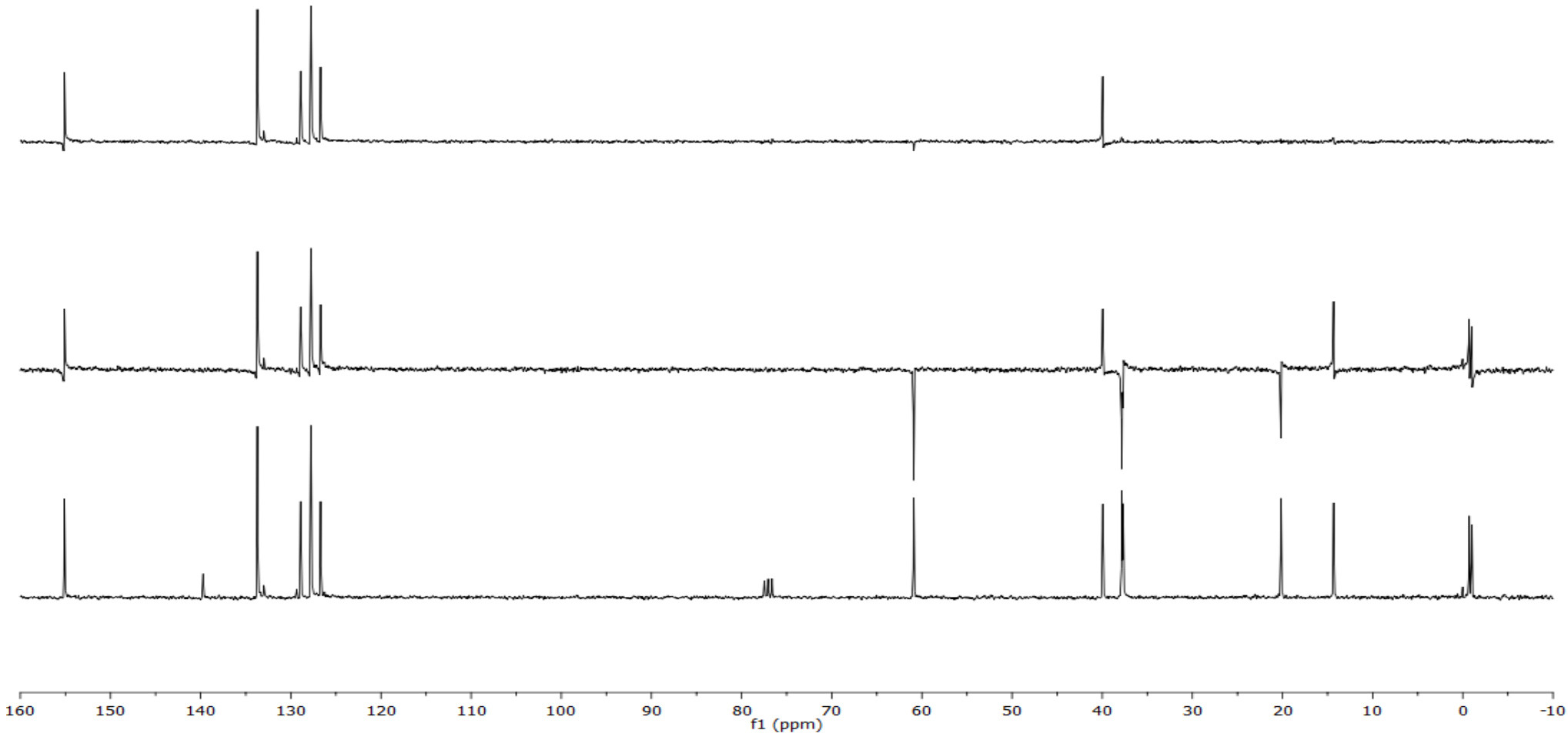

Pr
PhMe2Si
OH

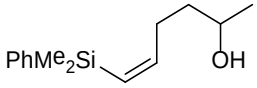
2c


2.02
3.01
1.00
1.01
2.04
0.98
1.00
1.90
4.45
2.87
2.86
3.27
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

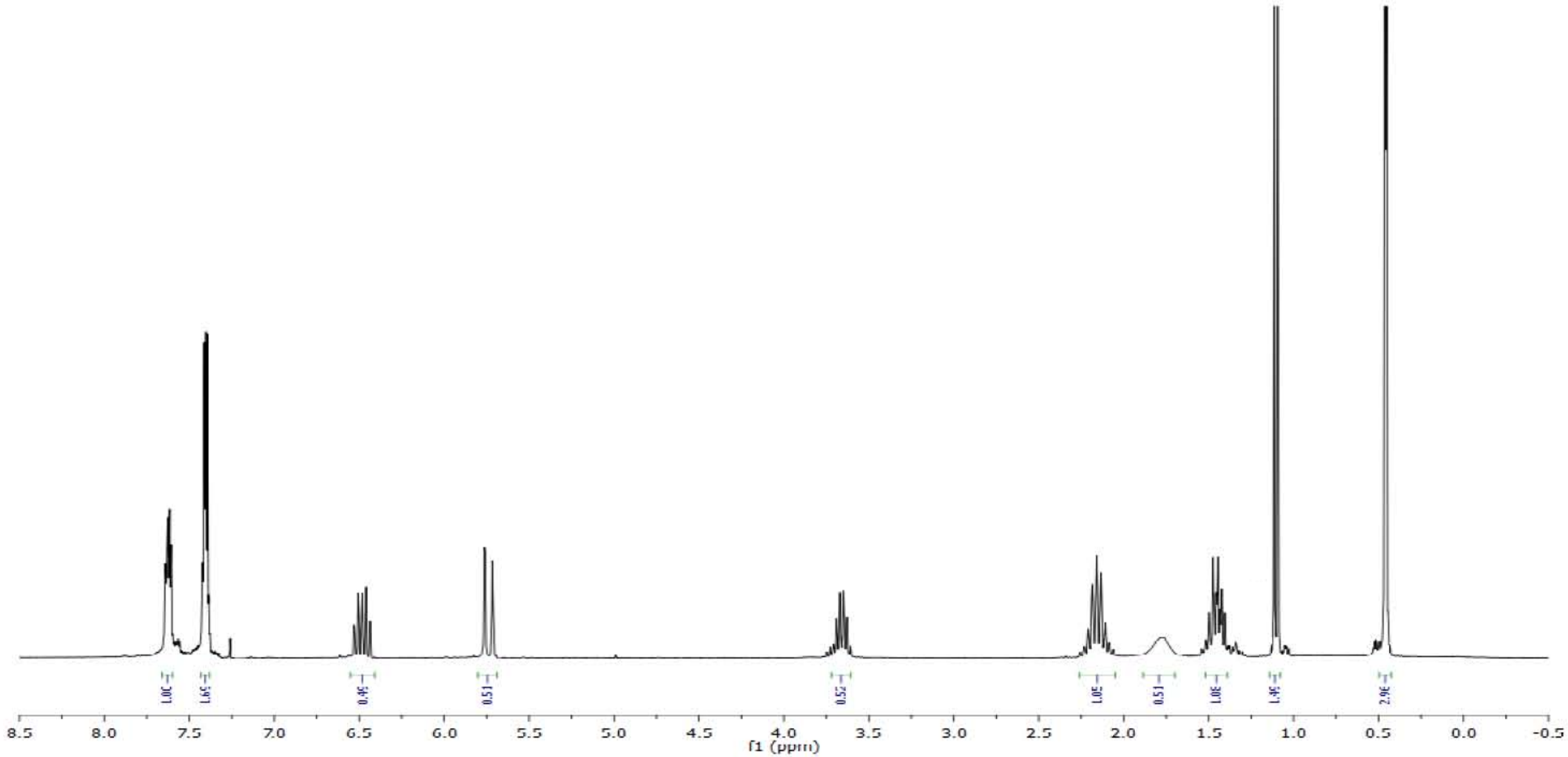

Pr
PhMe2Si
OH

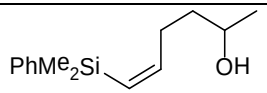
2c


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

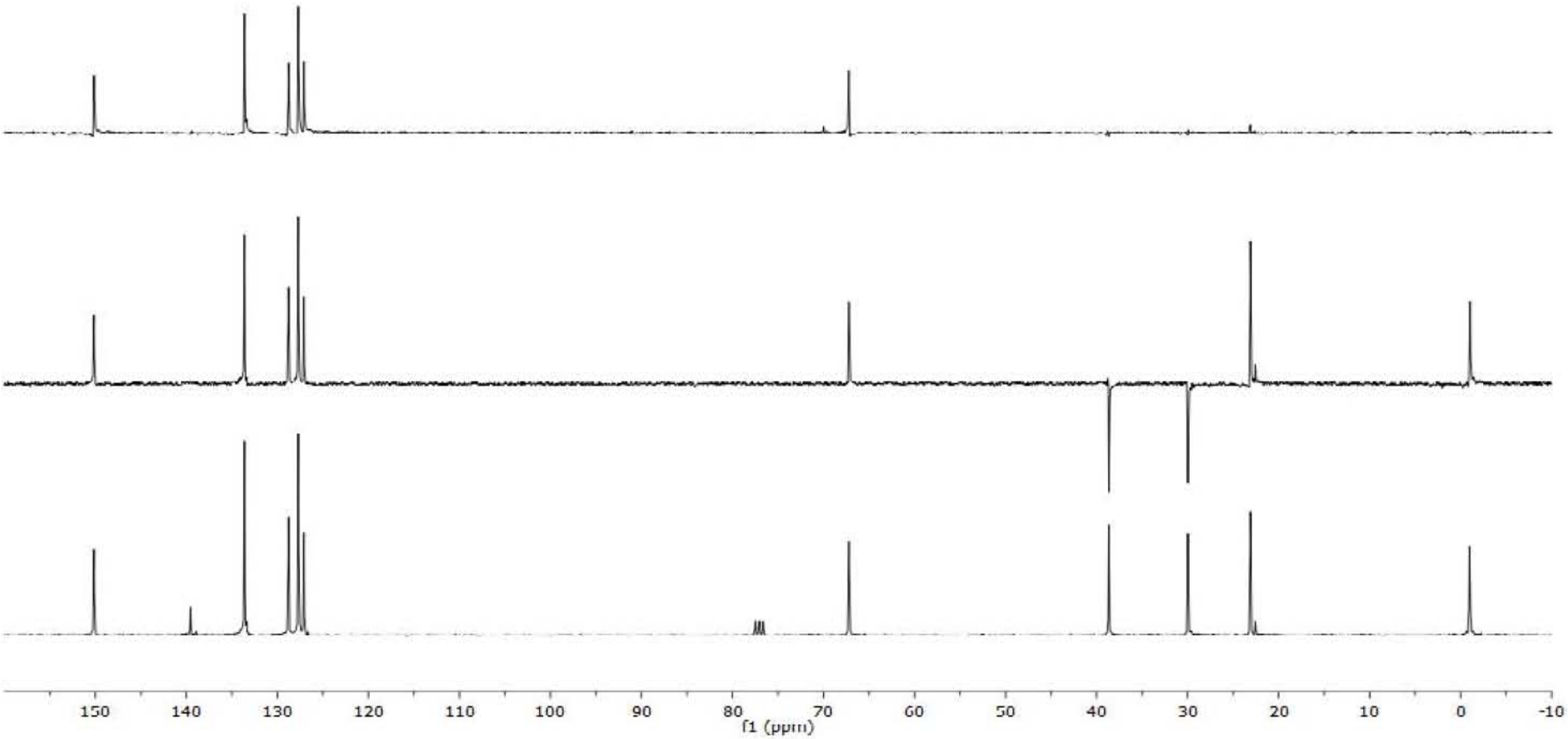

PhMe2Si
OH

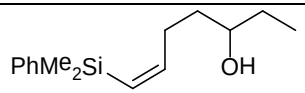
2e


1.00
5.97
0.96
0.51
0.52
1.05
0.51
1.06
1.96
2.96
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

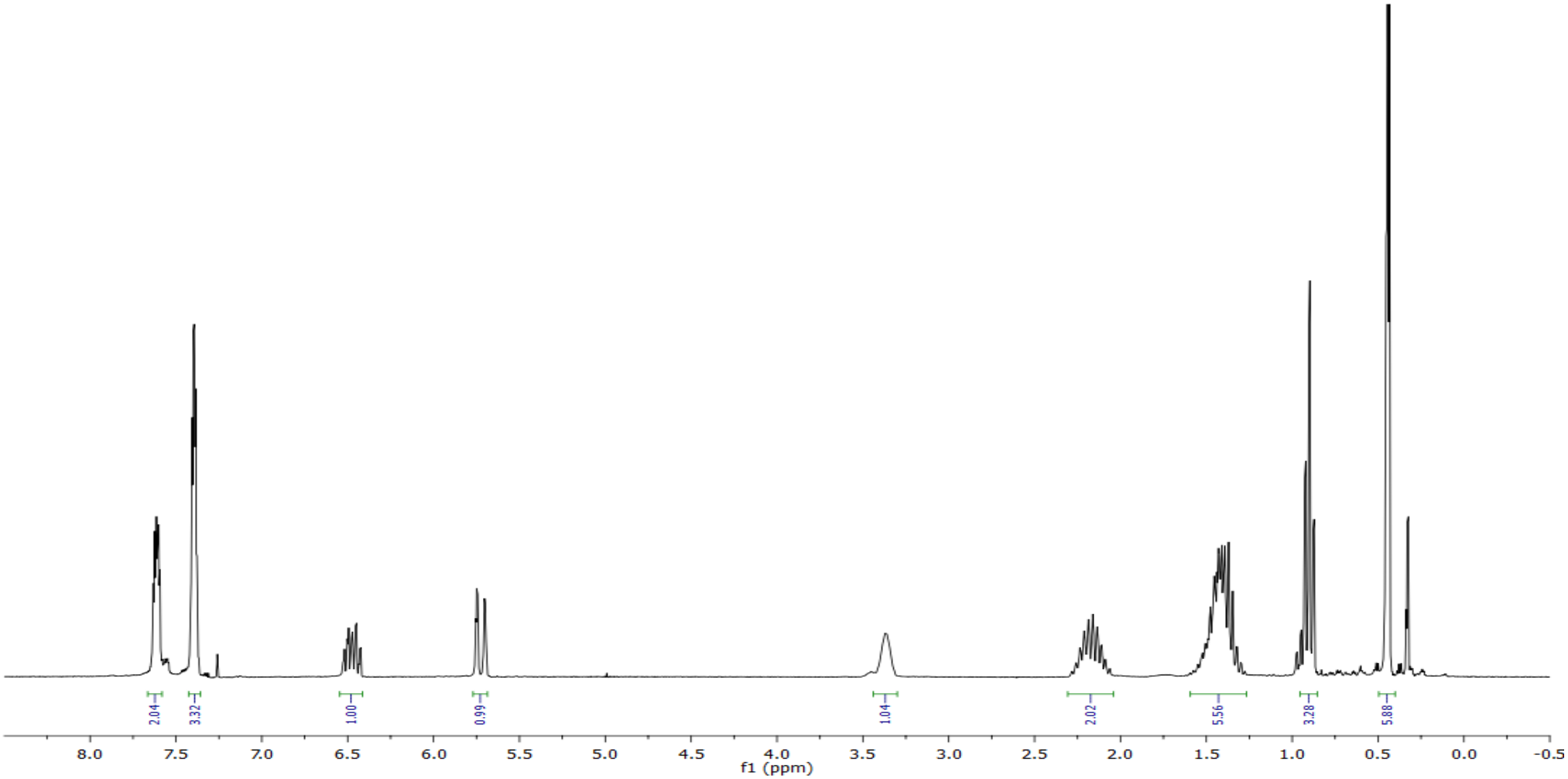

PhMe2Si
OH

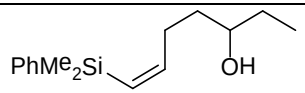
2e


150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

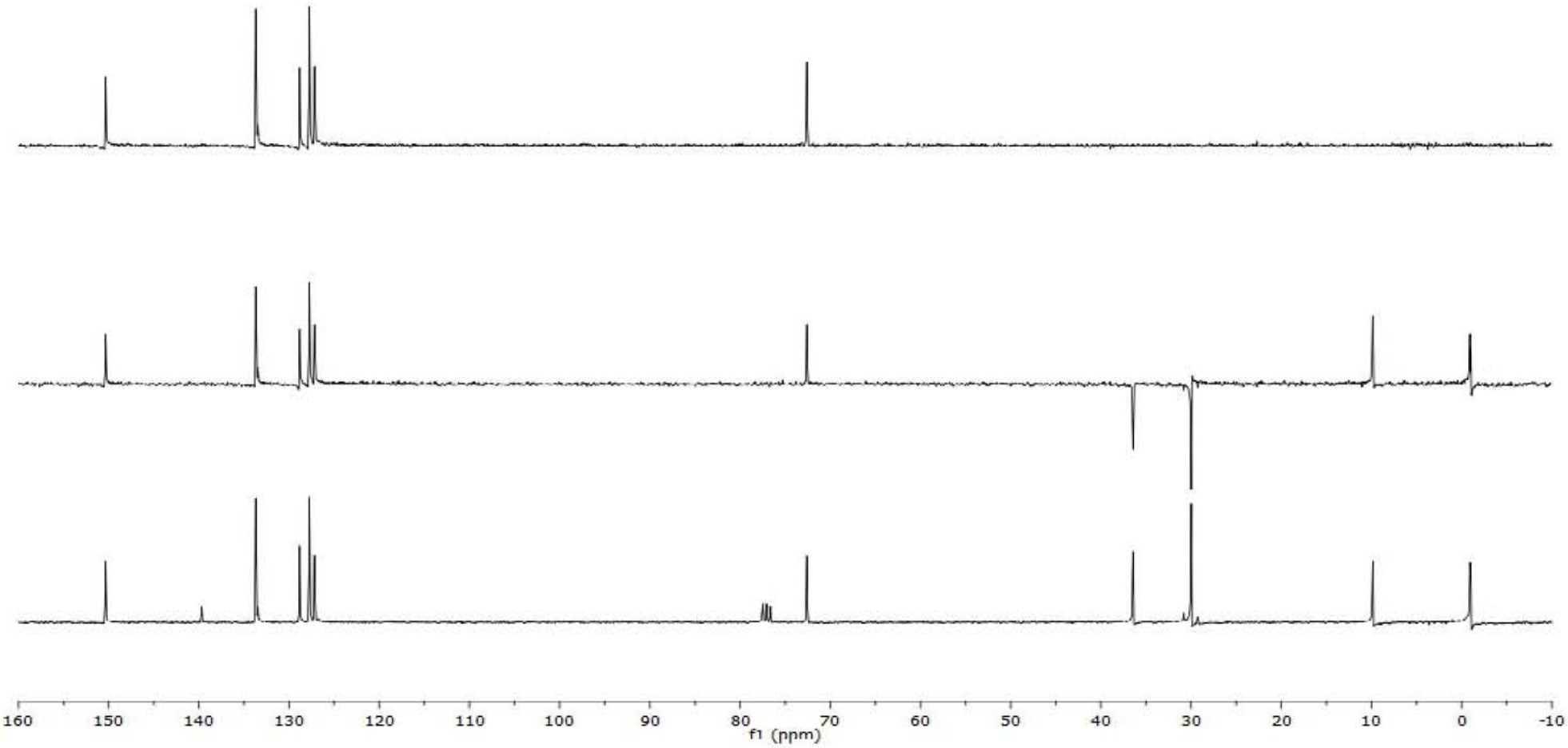

PhMe2Si
OH

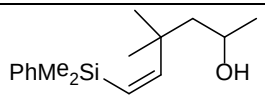
2f


2.04
3.32
1.00
0.99
1.04
2.02
5.56
3.28
5.88
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

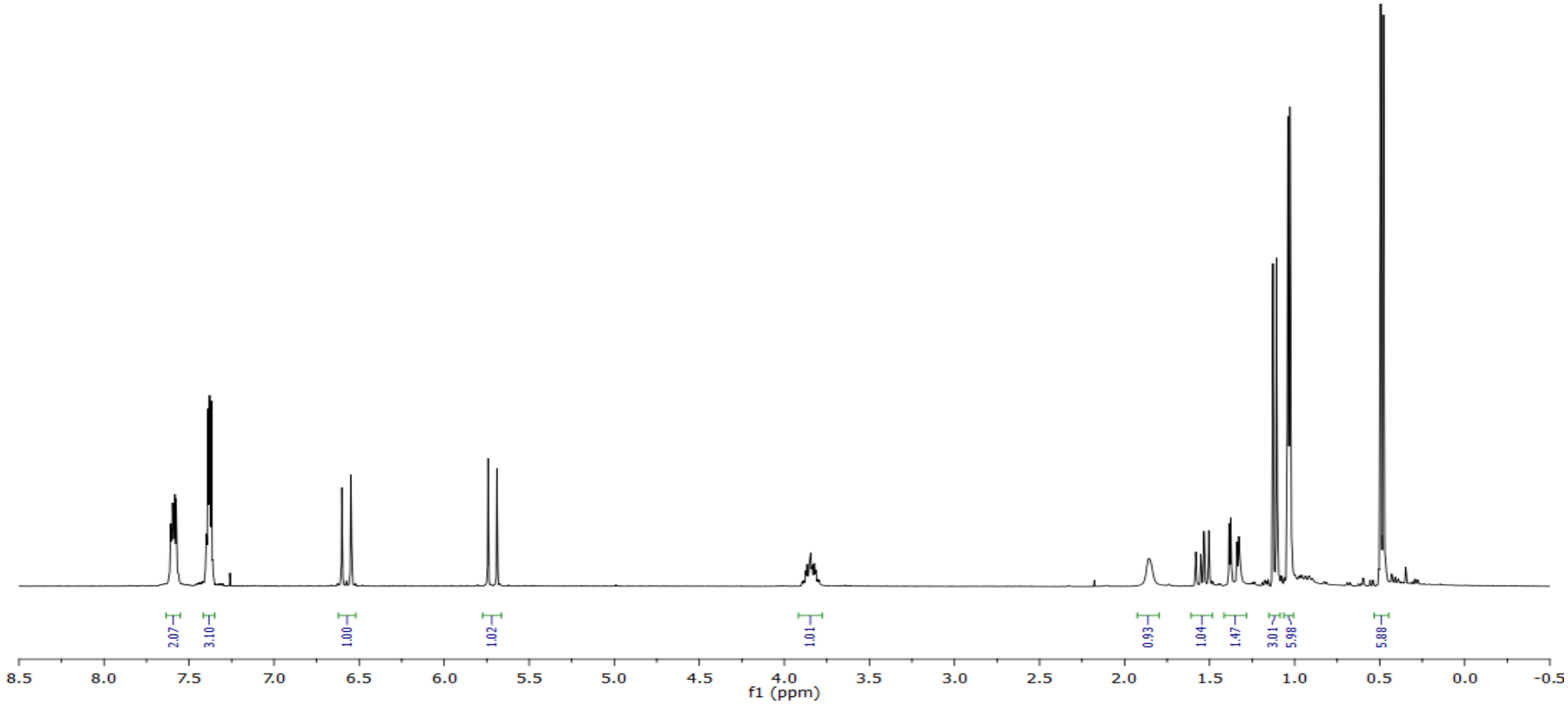

PhMe2Si
OH

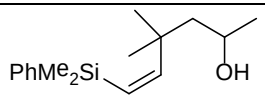
2f


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

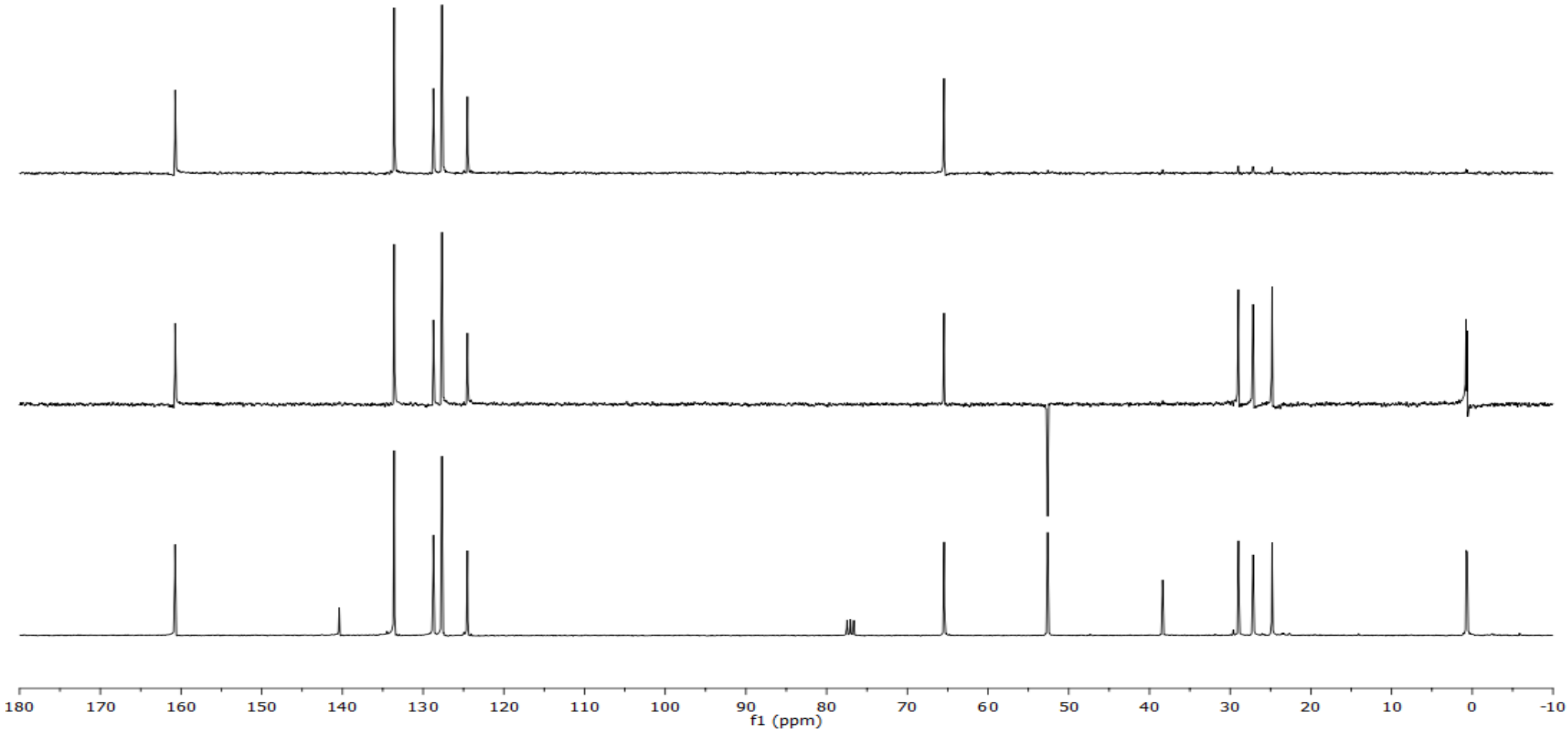

PhMe2Si
OH

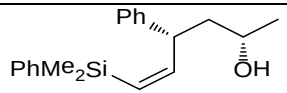
2g


2.07
3.10
1.00
1.02
1.01
0.93
1.04
1.47
3.01
5.98
5.88
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

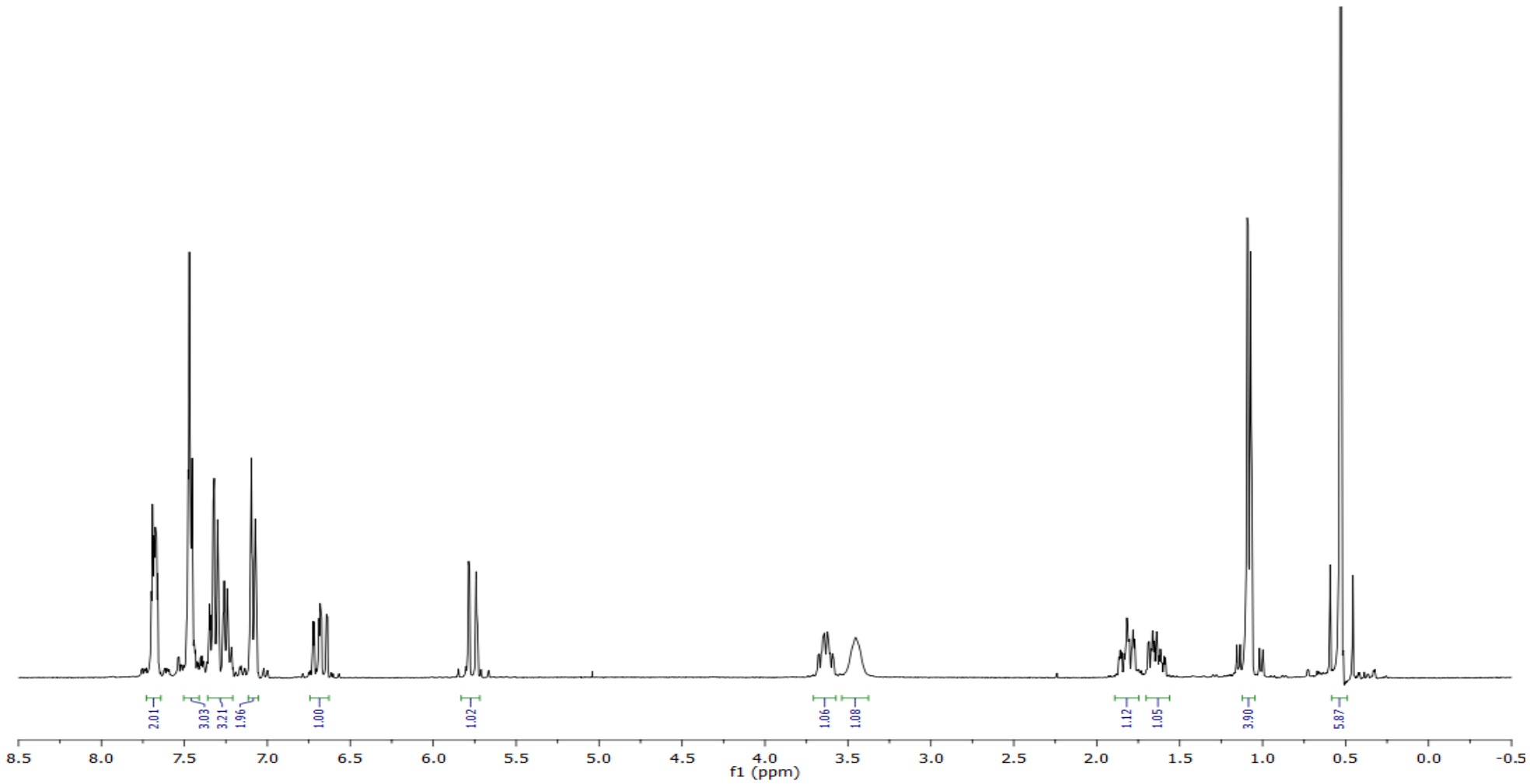

PhMe2Si
OH

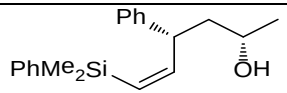
2g


180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

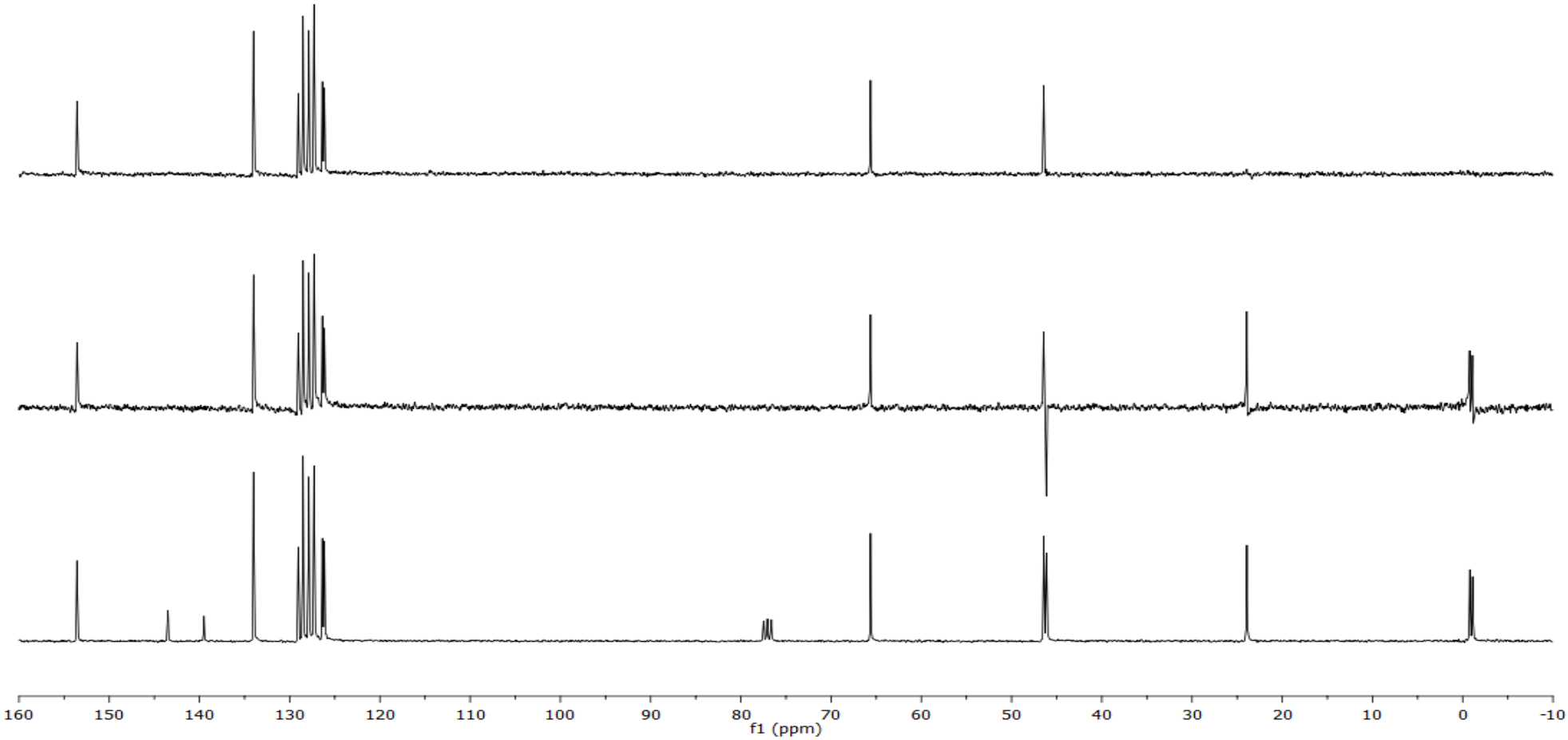

Ph
PhMe2Si
OH

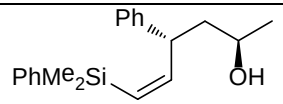
2h


2.01
3.03
3.21
1.96
1.00
1.02
1.06
1.08
1.12
1.05
3.90
5.87
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

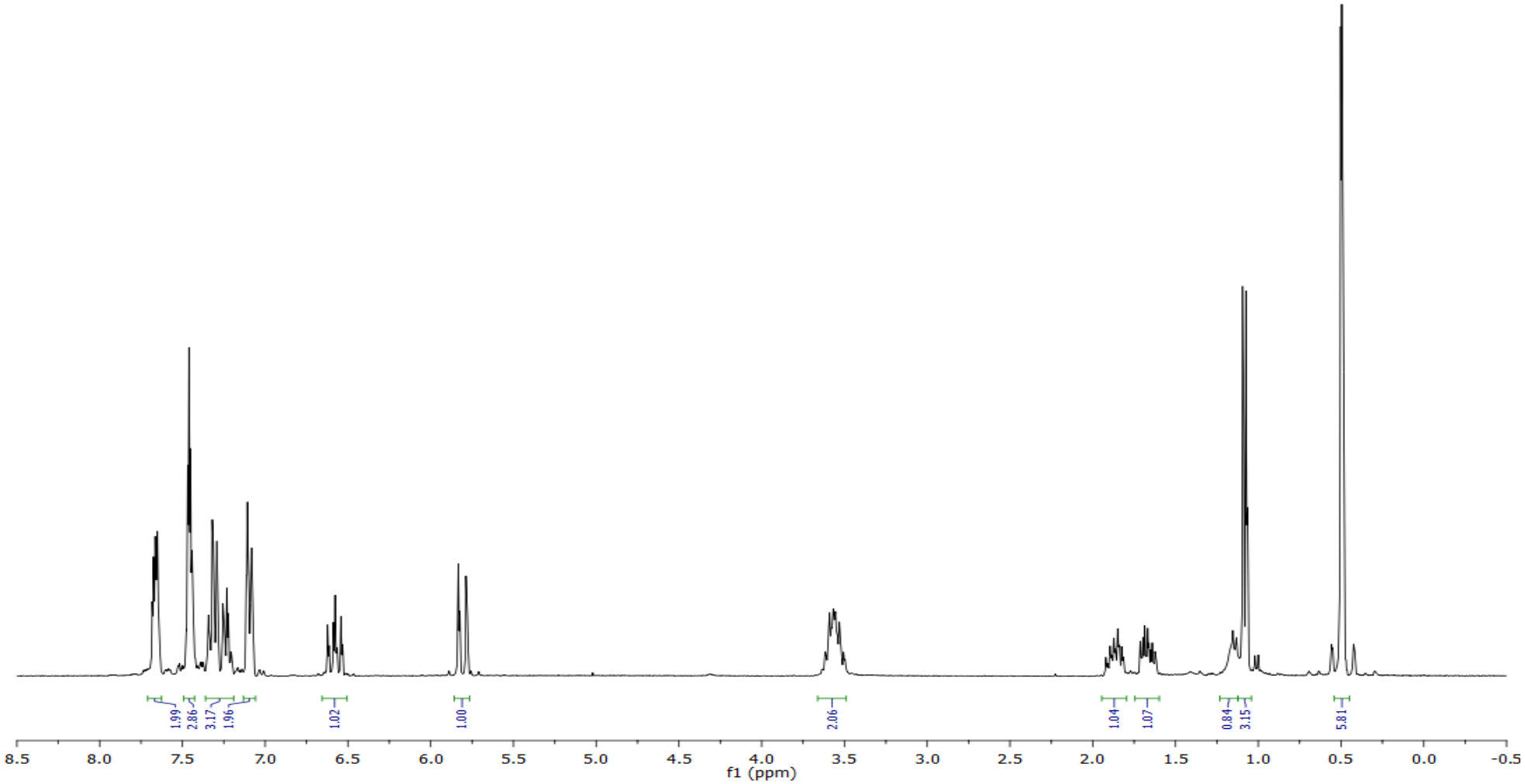

Ph
PhMe2Si
OH

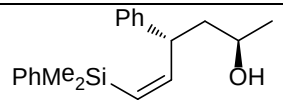
2h


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

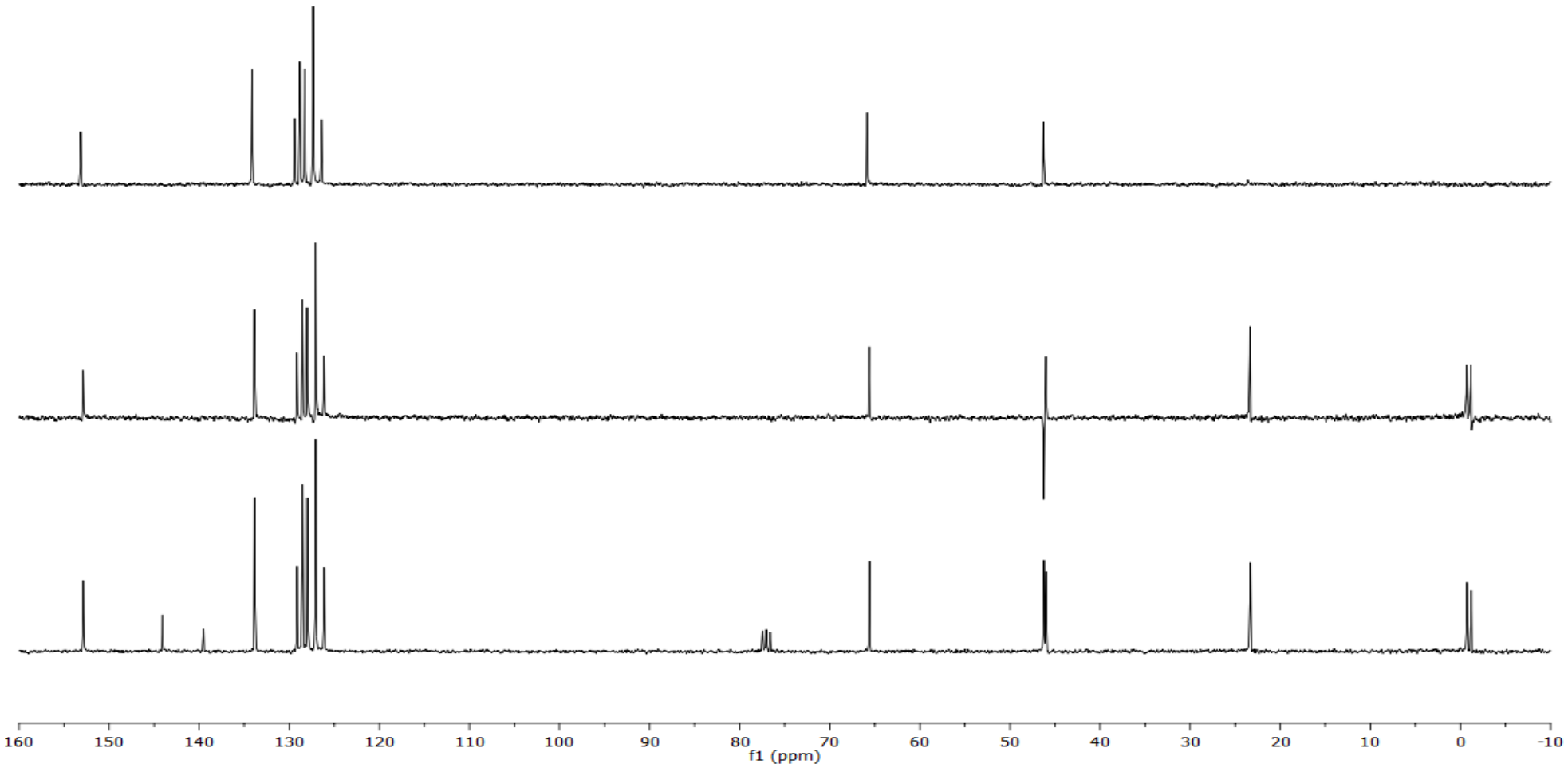

Ph
PhMe2Si
OH

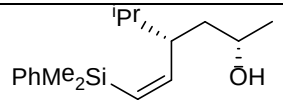
3h


1.99
2.86
3.17
1.96
1.02
1.00
2.06
1.04
1.07
0.84
3.15
5.81
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

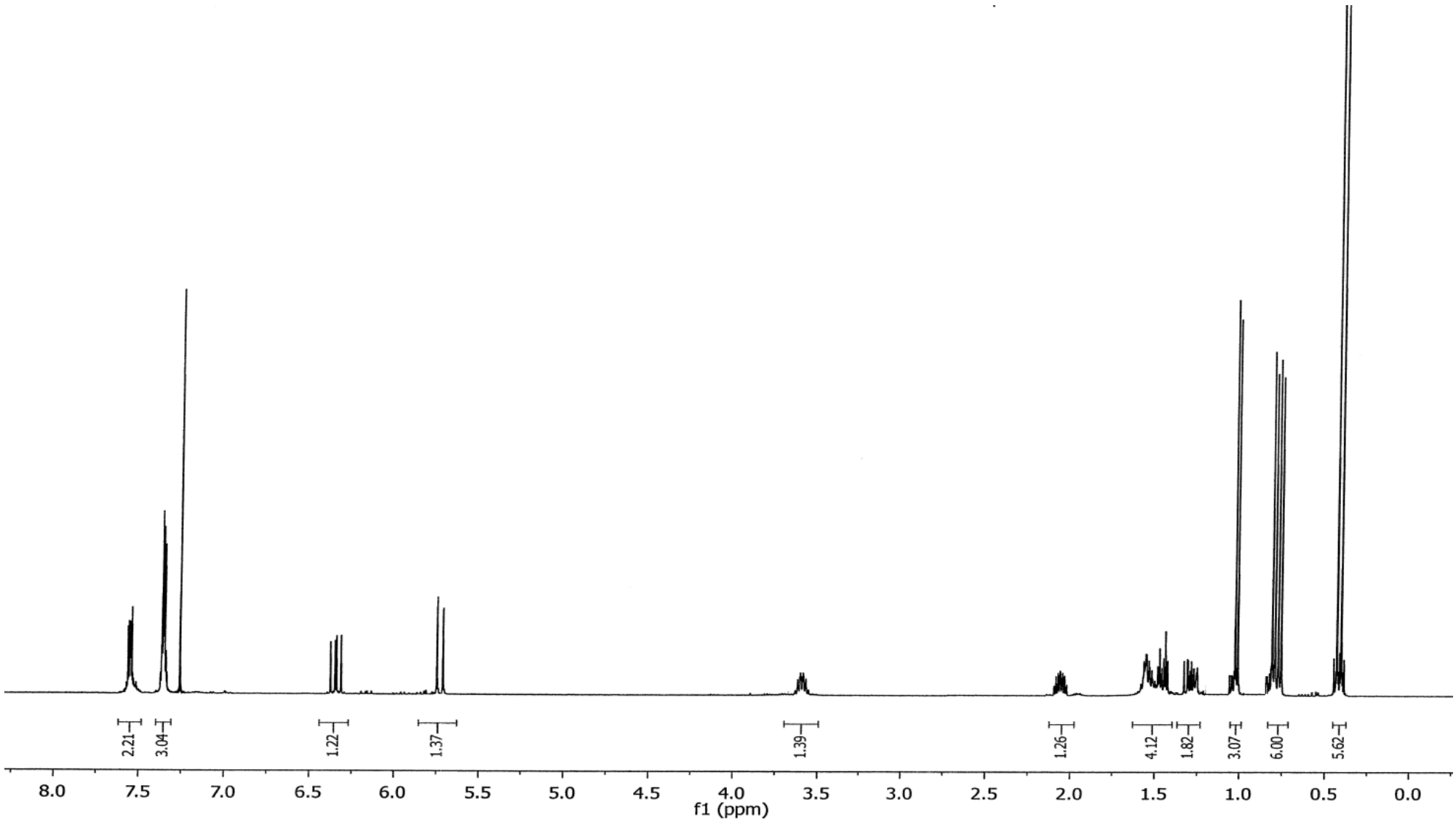

Ph
PhMe2Si
OH

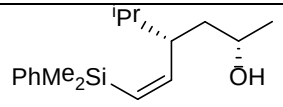
3h


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

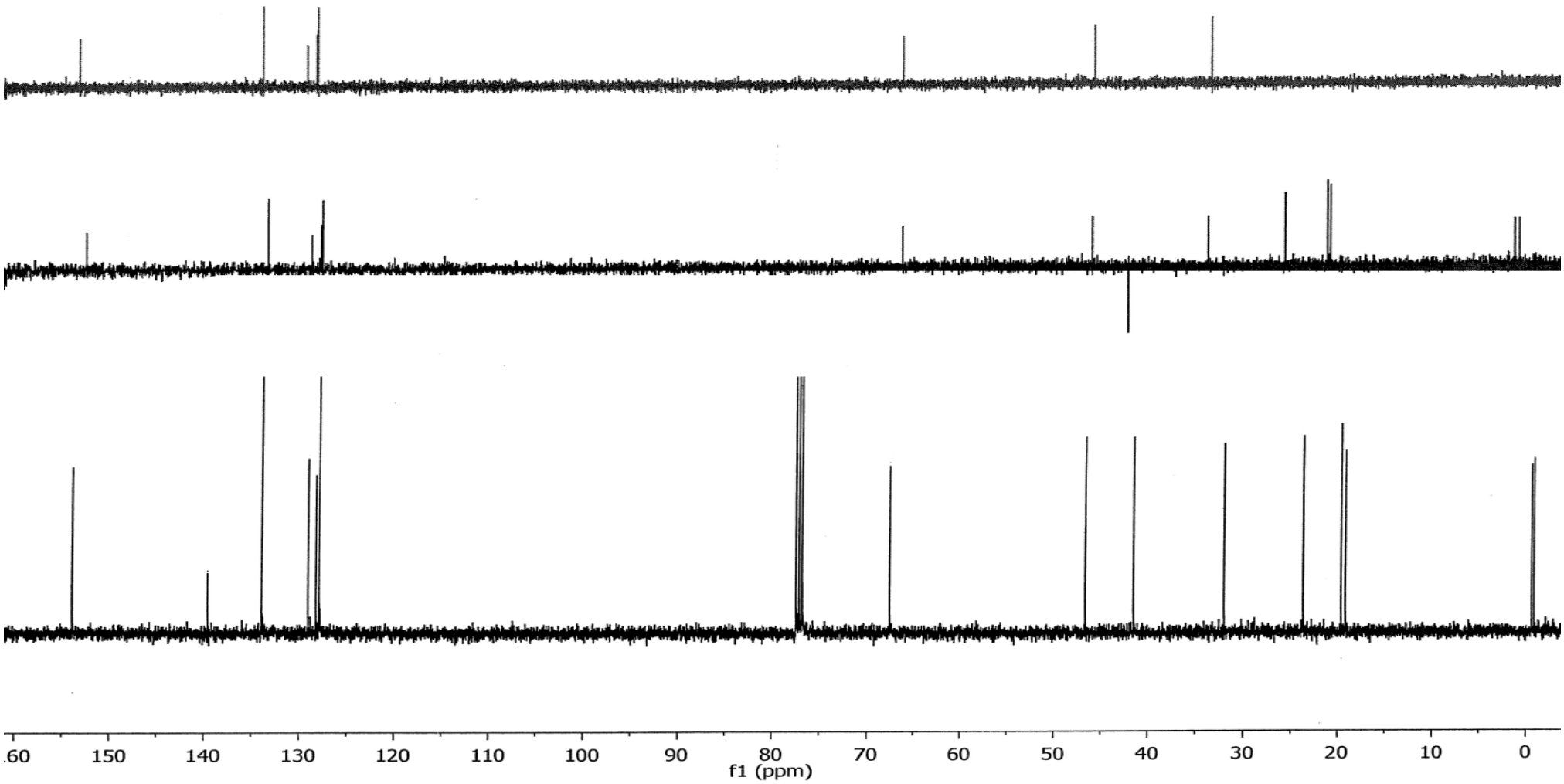

iPr
PhMe2Si
OH

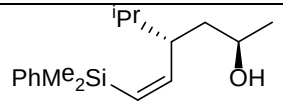
2i


2.21
3.04
1.22
1.37
1.39
1.26
4.12
1.82
3.07
6.00
5.62
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

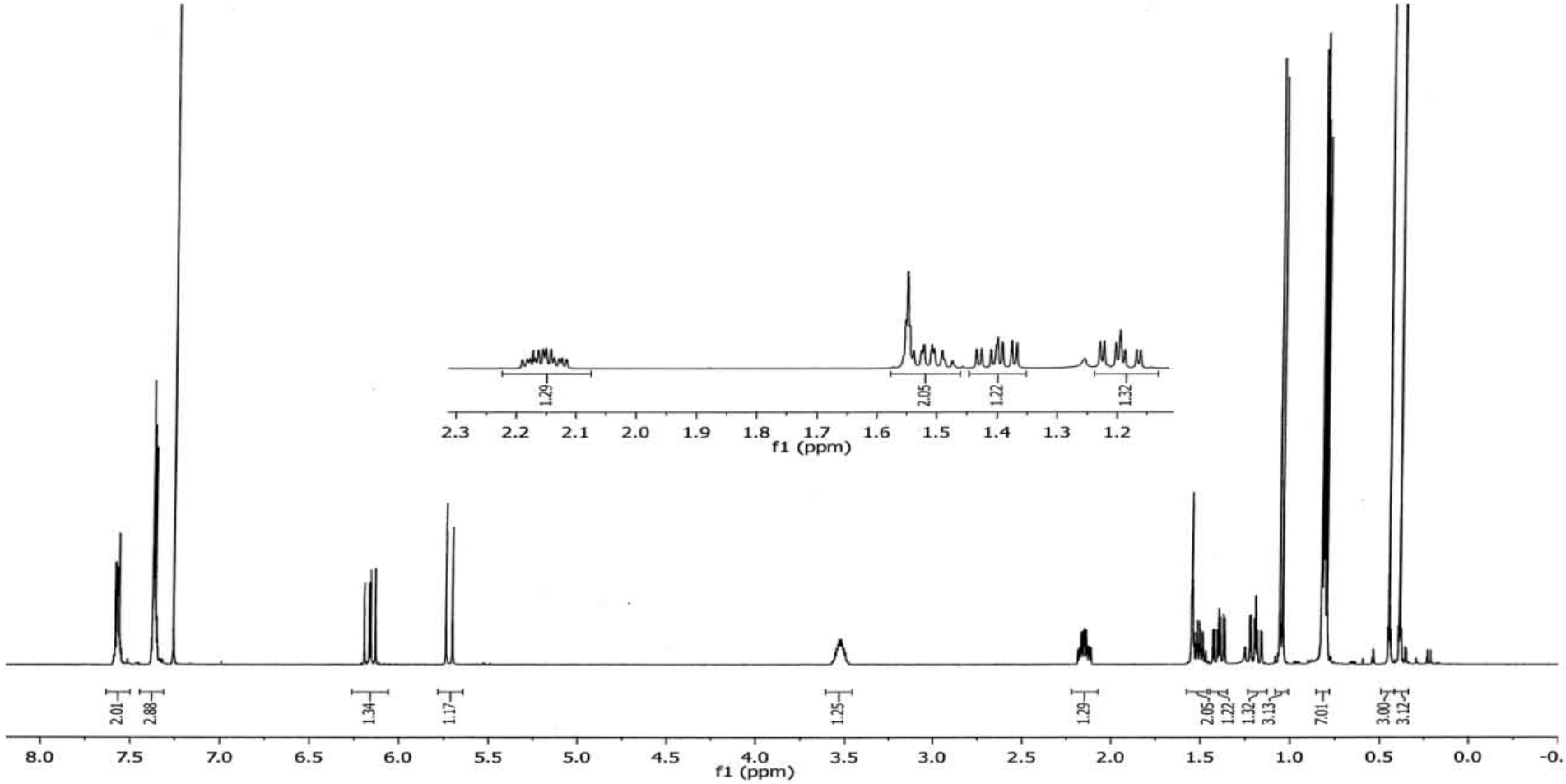

iPr
PhMe2Si
OH

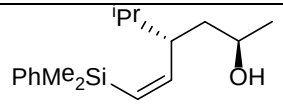
2i


.60
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

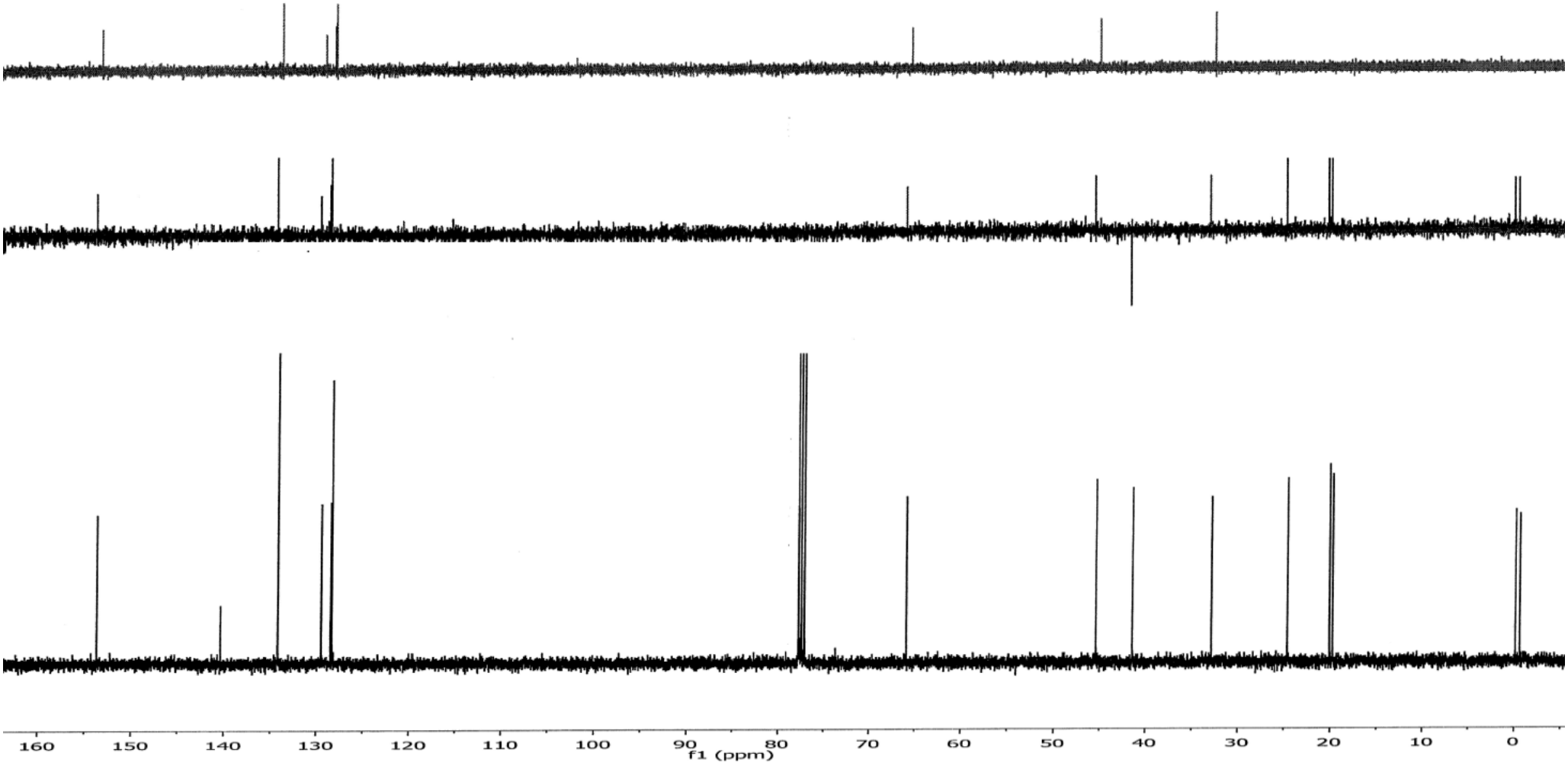

iPr
PhMe2Si
OH

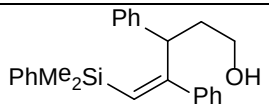
3i


2.01
2.88
1.34
1.17
1.25
1.29
2.05
1.22
1.32
3.13
7.01
3.00
3.12
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)
1.29
2.05
1.22
1.32
2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2
f1 (ppm)

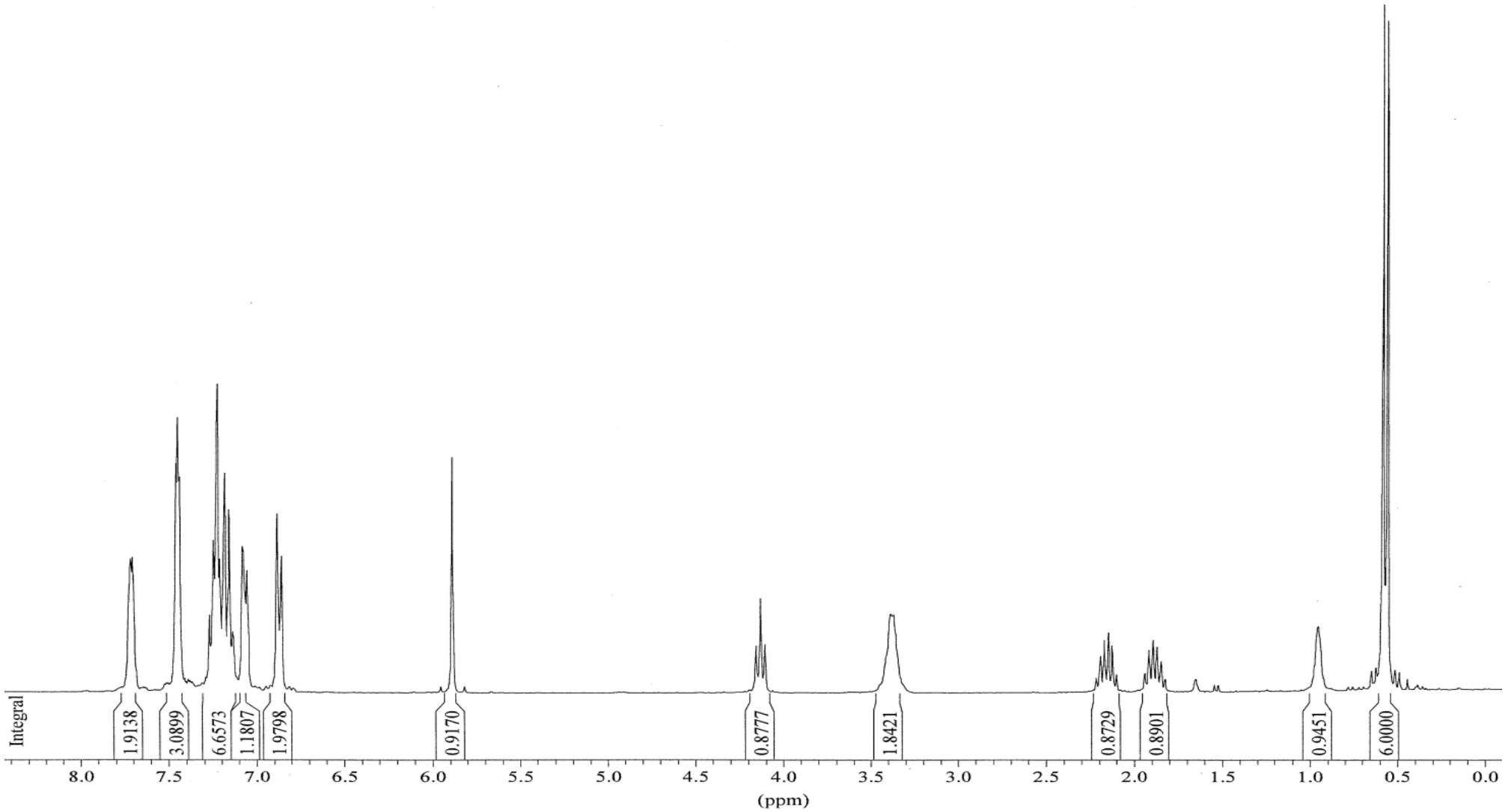

iPr
PhMe2Si
OH

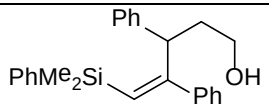
3i


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

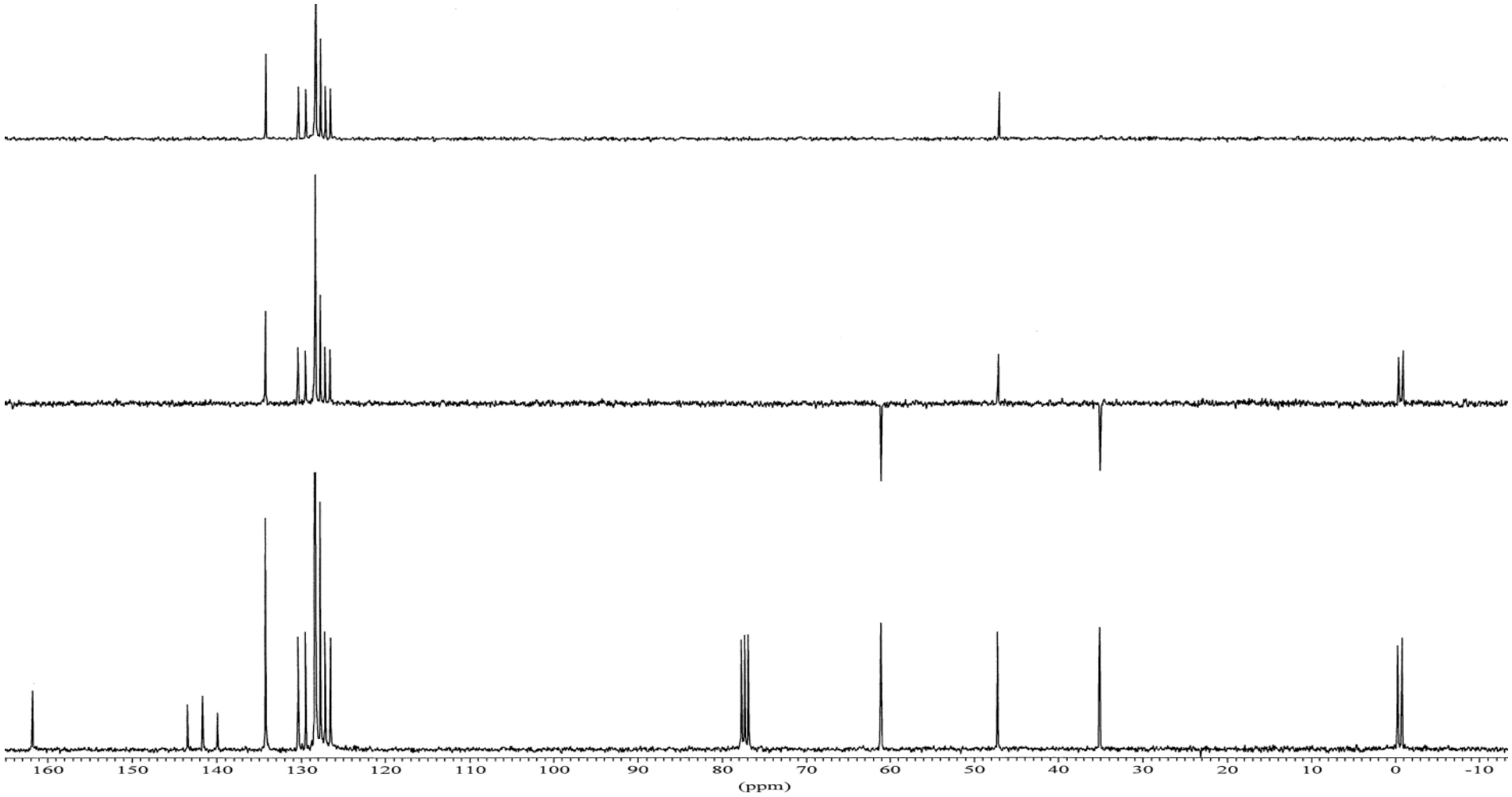

Ph
PhMe2Si
OH
Ph

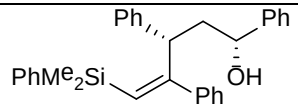
2j


Integral
1.9138
3.0899
6.6573
1.1807
1.9798
0.9170
0.8777
1.8421
0.8729
0.8901
0.9451
6.0000
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

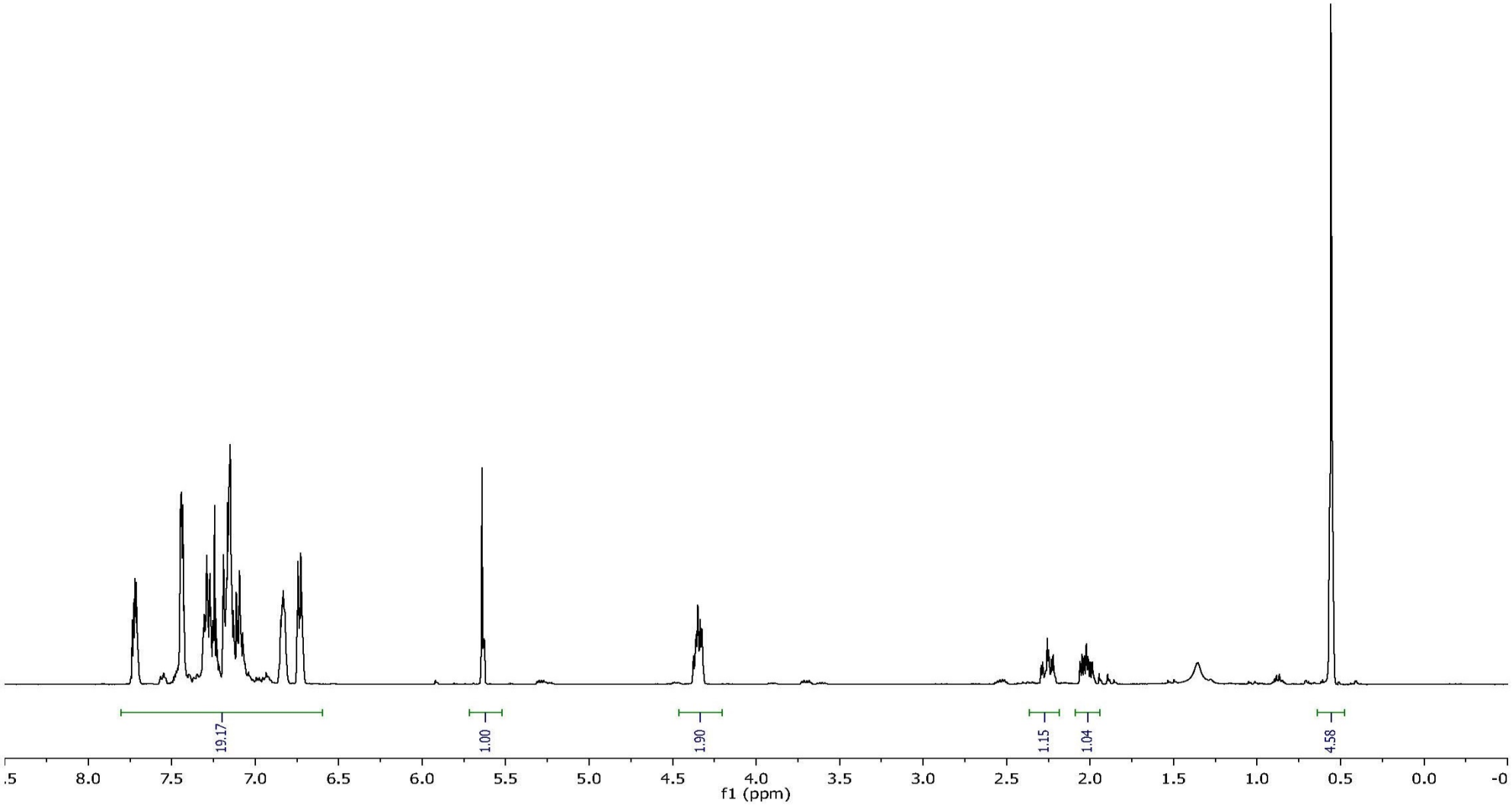

Ph
PhMe2Si
OH
Ph

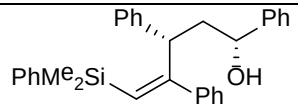
2j


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
(ppm)

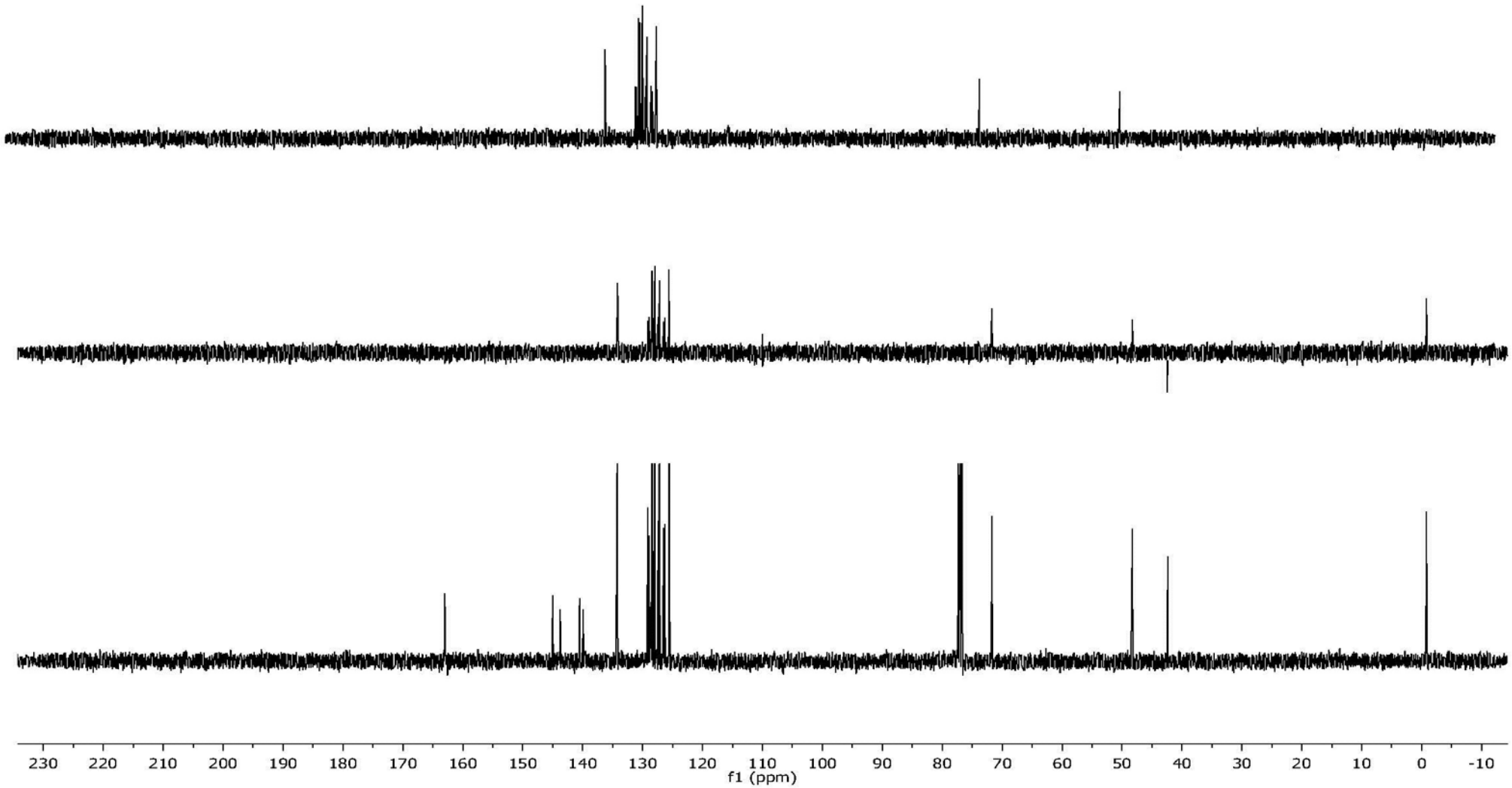

Ph
Ph
PhMe2Si
Ph
OH

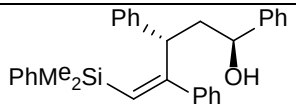
2k


19.17
1.00
1.90
1.15
1.04
4.58
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

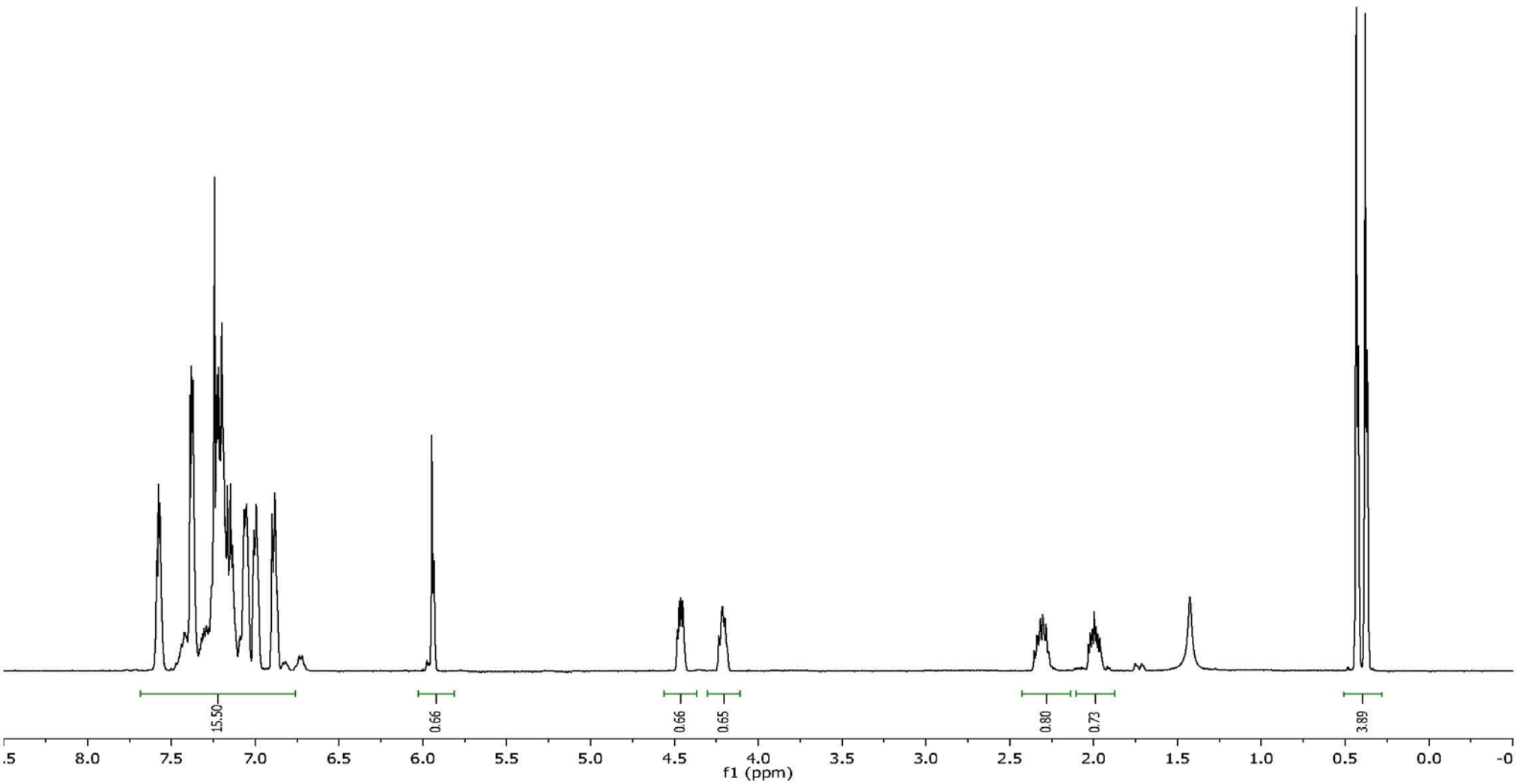

Ph
Ph
PhMe2Si
Ph
OH

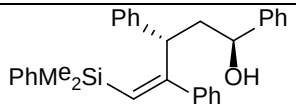
2k


230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

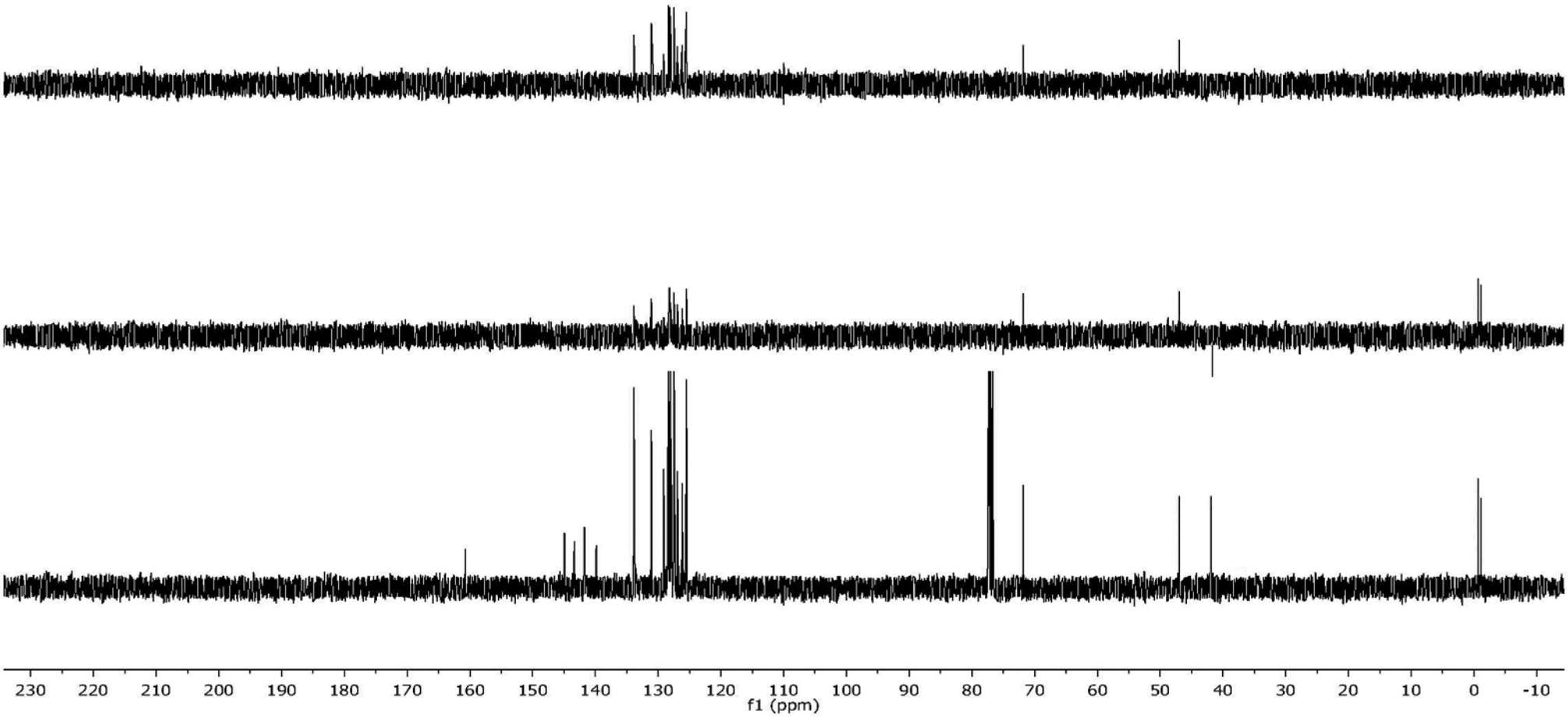

Ph
Ph
PhMe2Si
OH
Ph

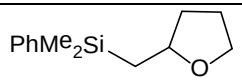
3k


15.50
0.66
0.66
0.65
0.80
0.73
3.89
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

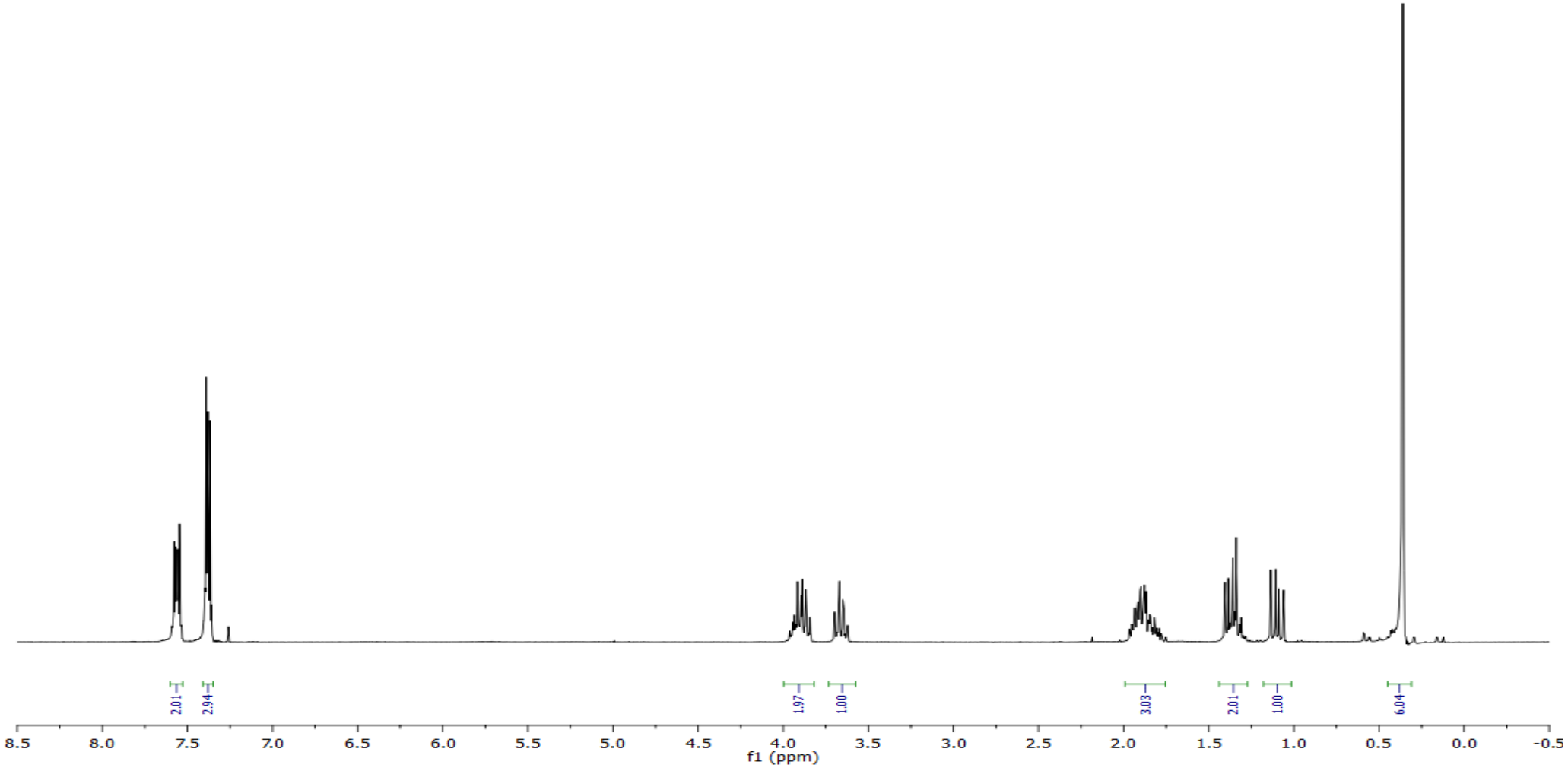

Ph
Ph
PhMe2Si
Ph
OH

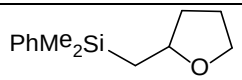
3k


230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

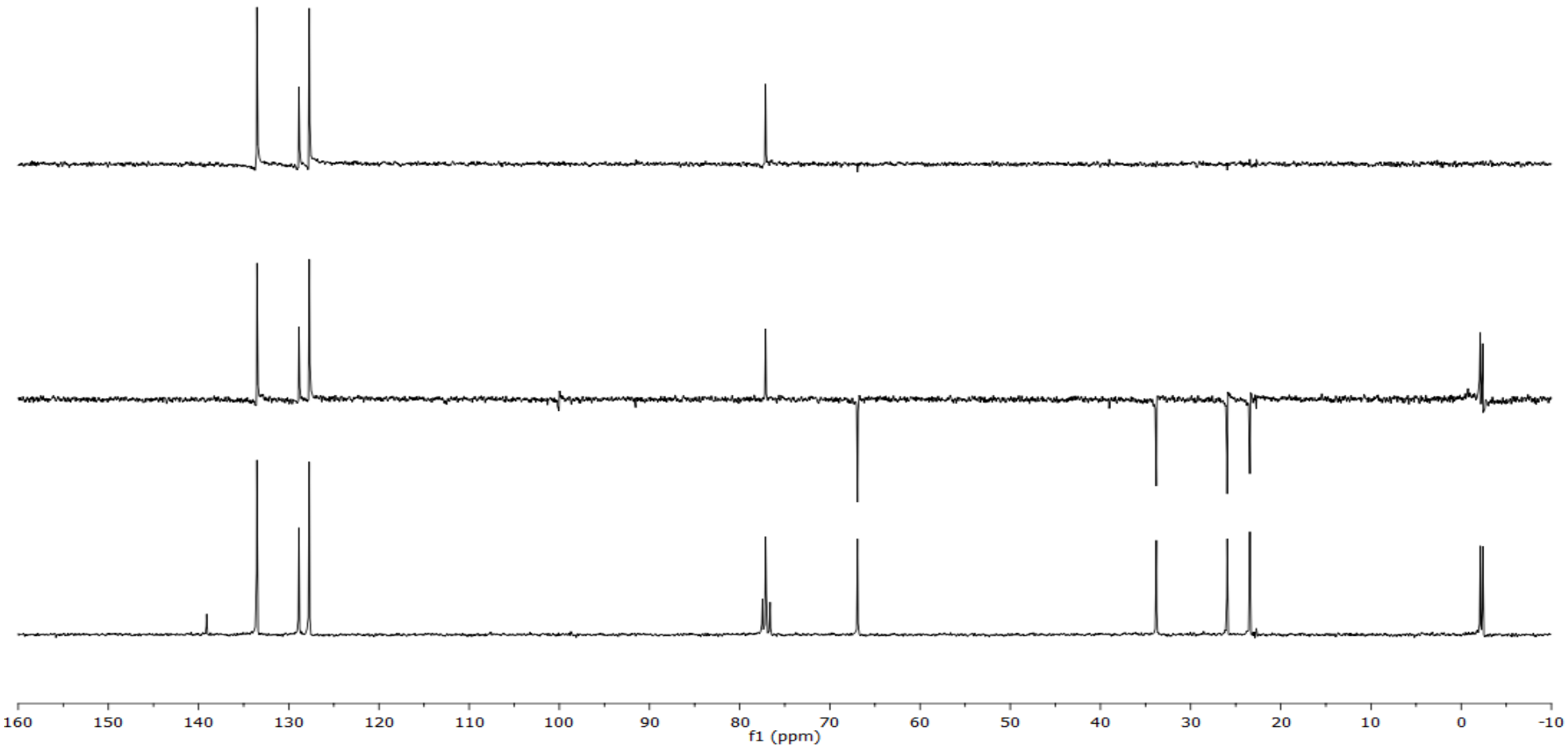

PhMe2Si
O

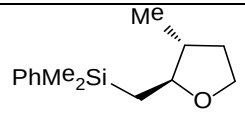
4a


2.01
2.94
1.97
1.00
3.03
2.01
1.00
6.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

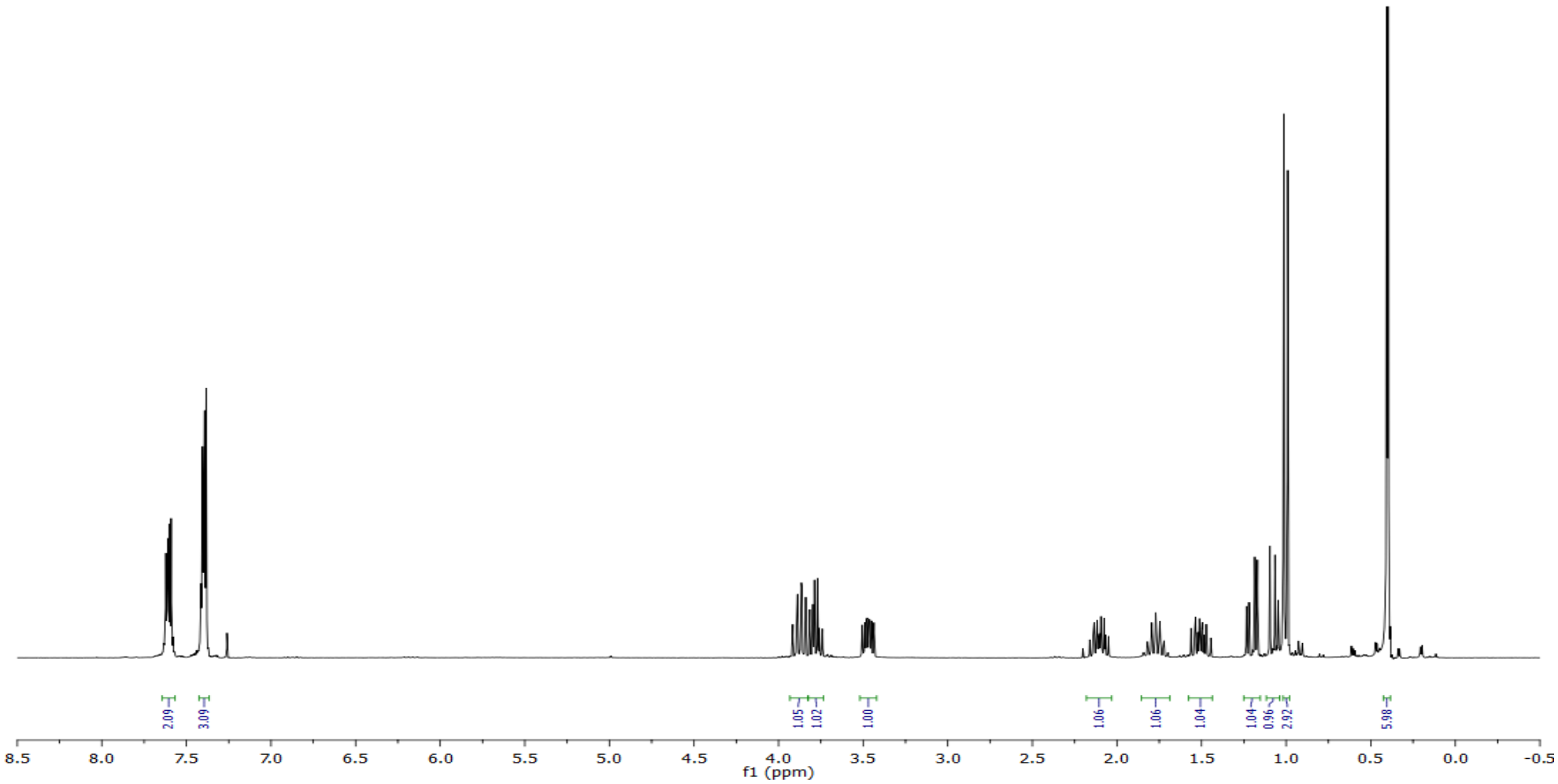

PhMe2Si
O

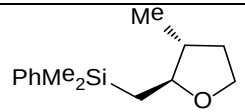
4a


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

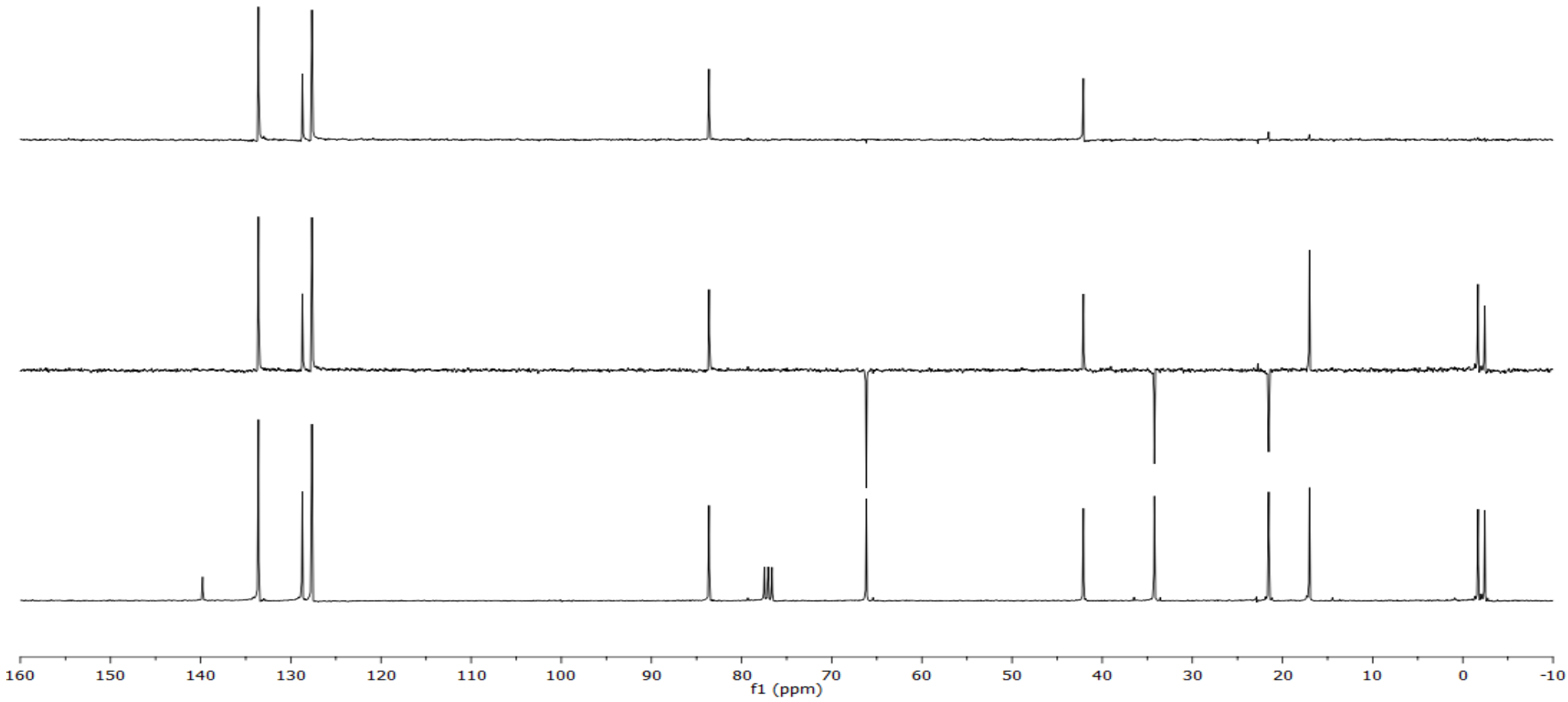

Me
PhMe2Si
O

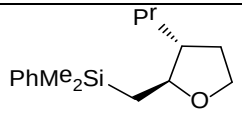
4b


2.09
3.09
1.05
1.02
1.00
1.06
1.06
1.04
1.04
0.96
2.92
5.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

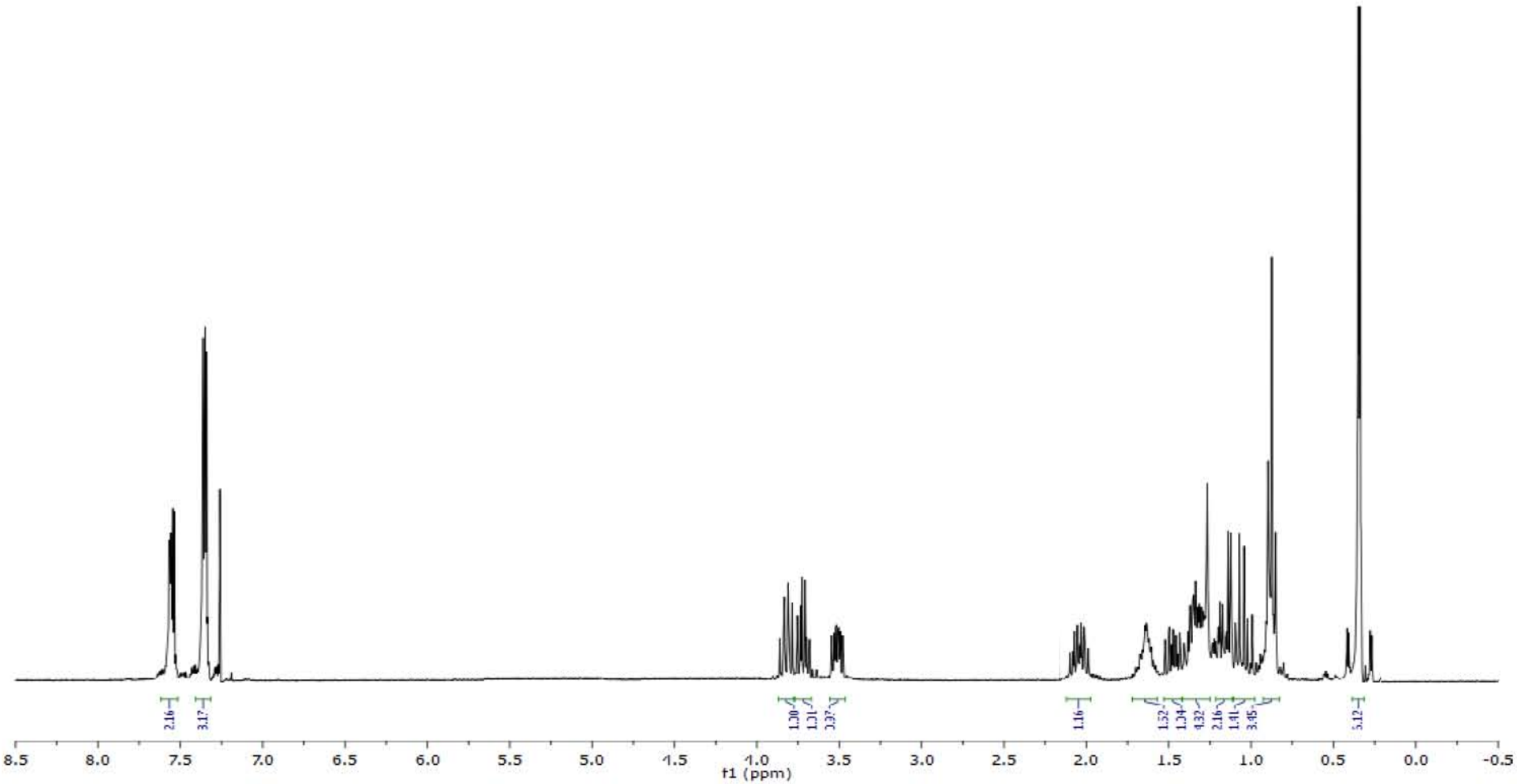

Me
PhMe2Si
O

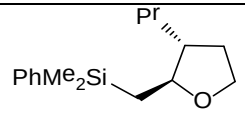
4b


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

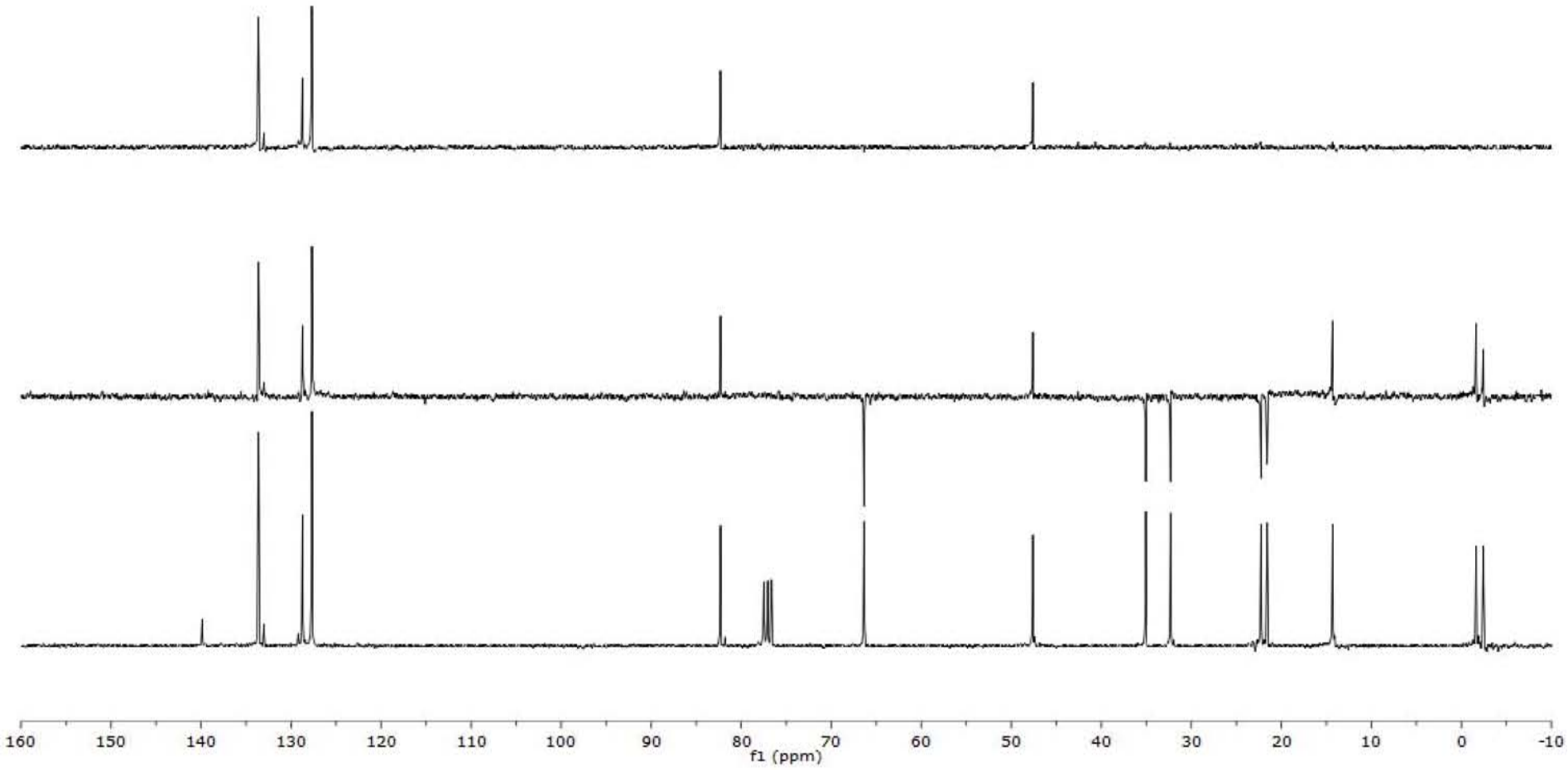

Pr
PhMe2Si
O

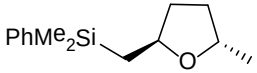
4c


2.16
3.17
1.00
1.31
3.37
1.16
1.52
1.34
4.32
2.16
1.41
3.45
3.12
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

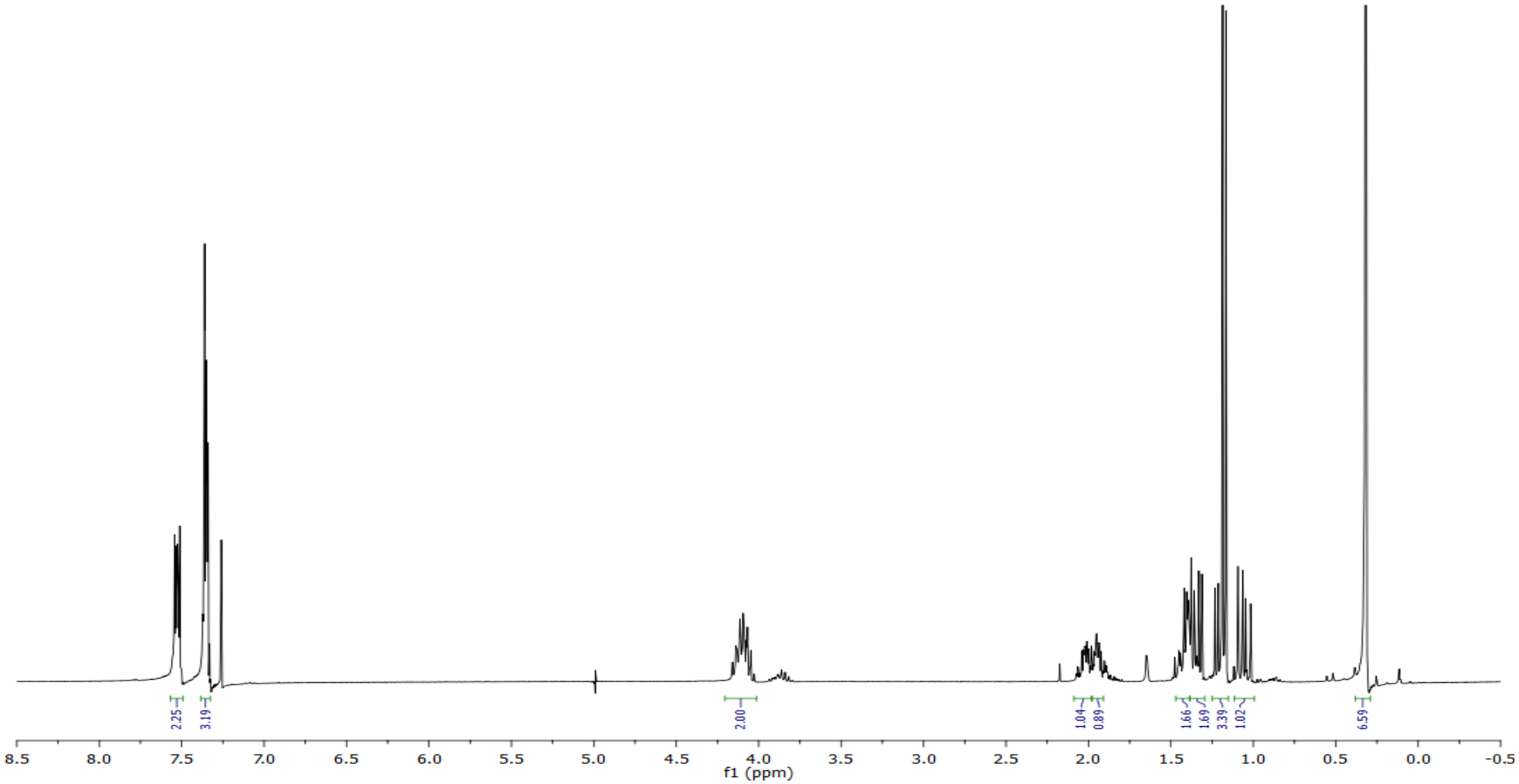

Pr
PhMe2Si
O

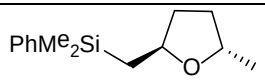
4c


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

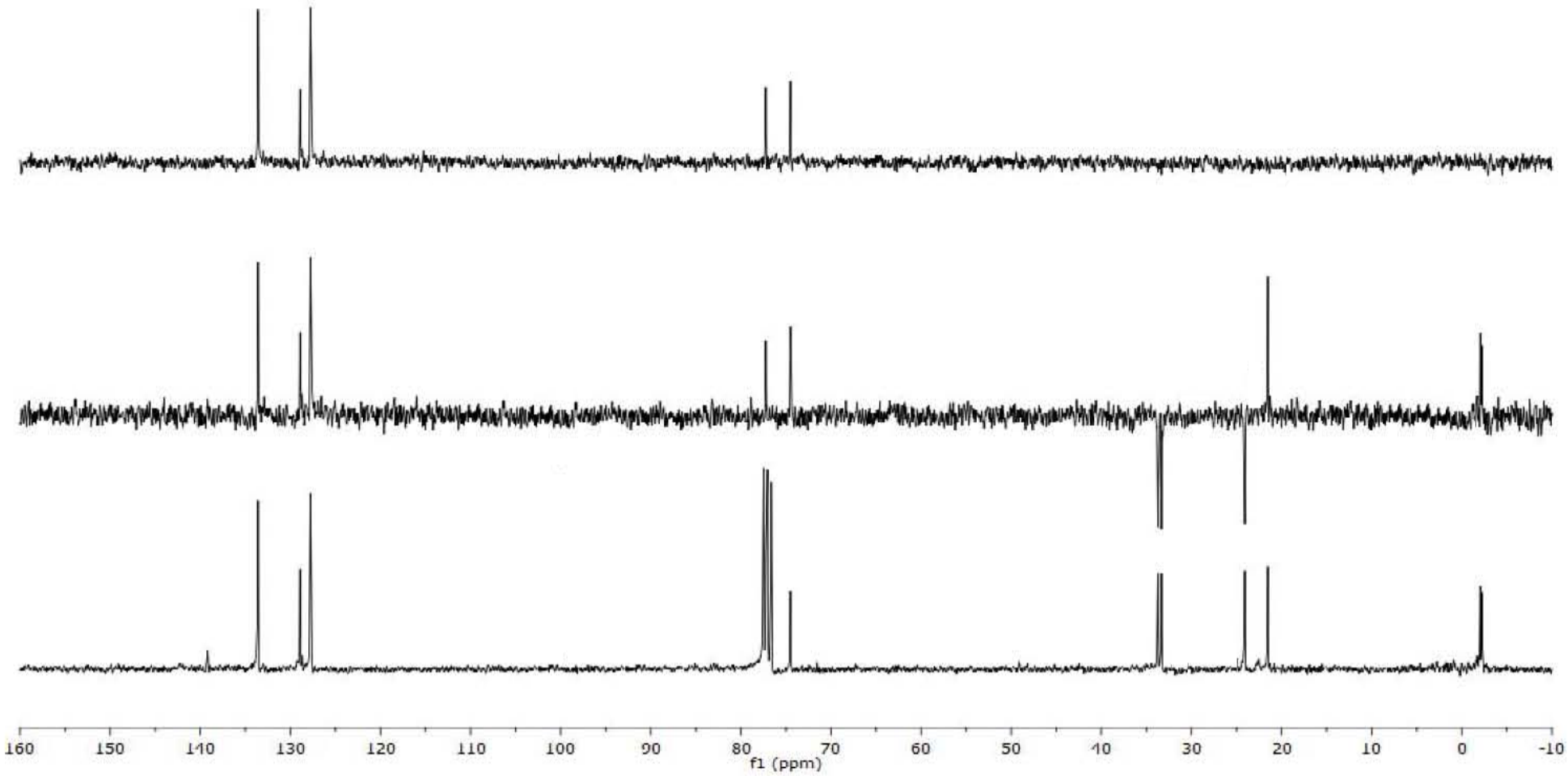

PhMe2Si
O

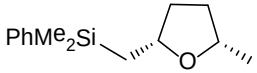
4e


2.25
3.19
2.00
1.04
0.89
1.66
1.69
3.39
1.02
6.59
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

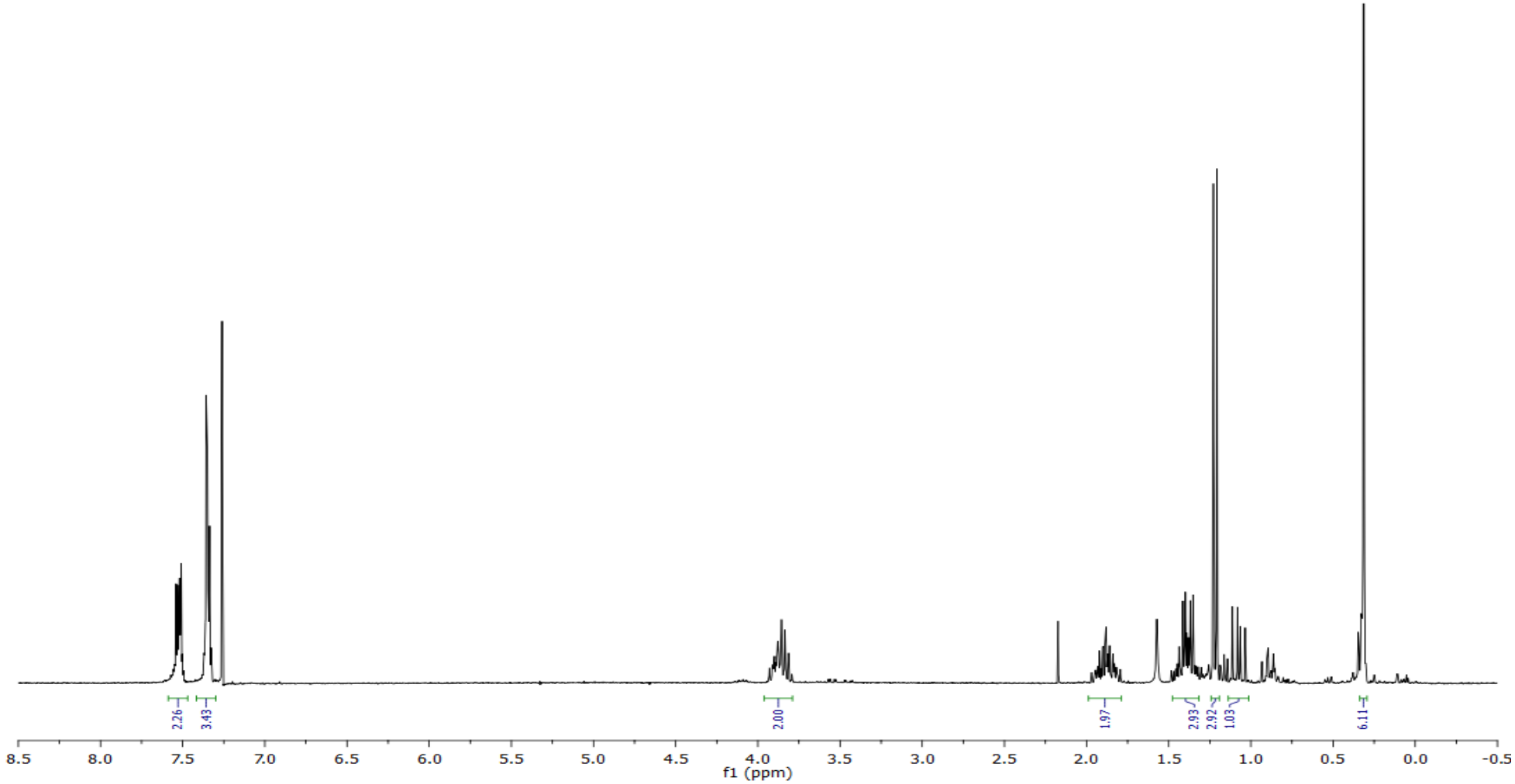

PhMe2Si
O

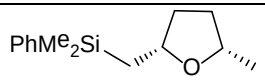
4e


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

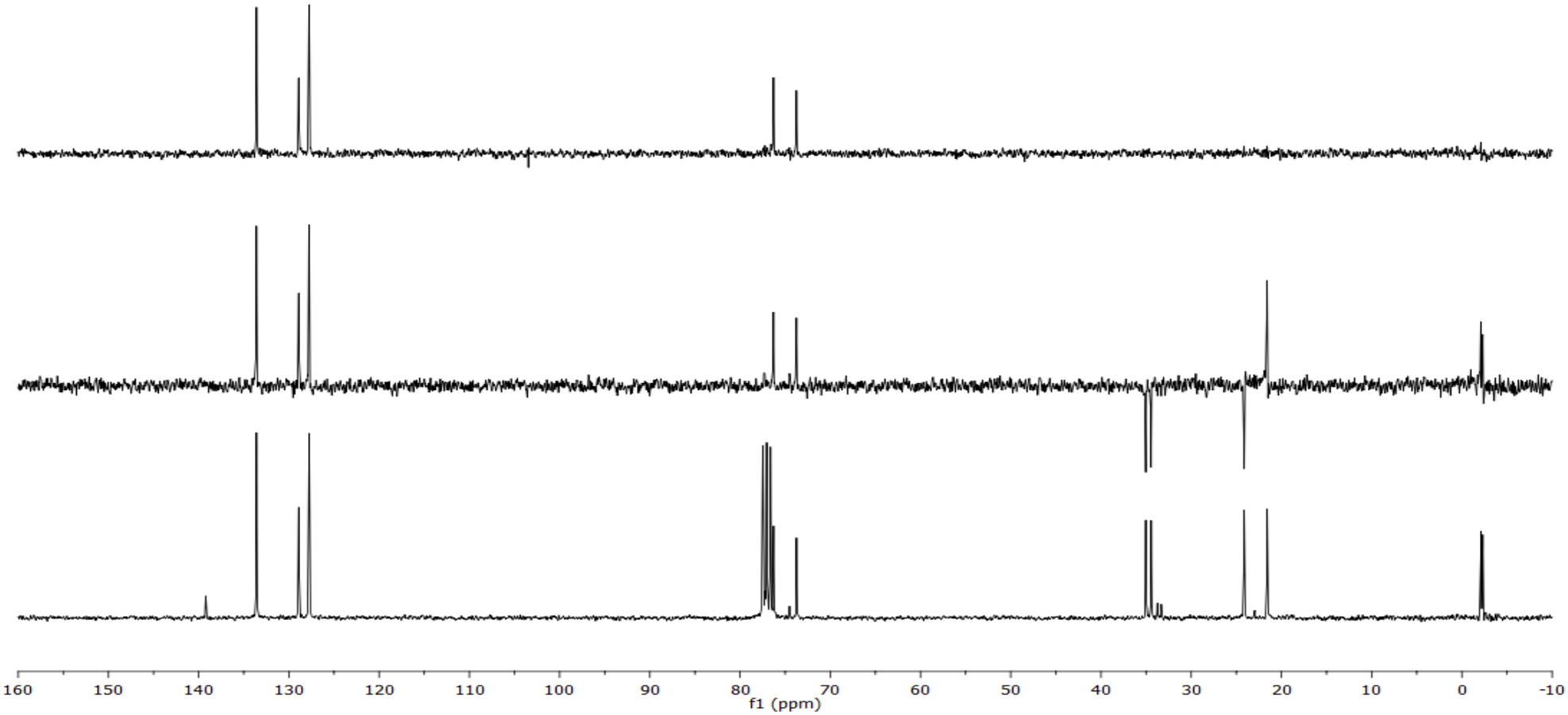

PhMe2Si
O

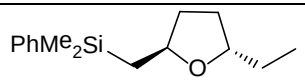
5e


2.26
3.43
2.00
1.97
2.93
2.92
1.03
6.11
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

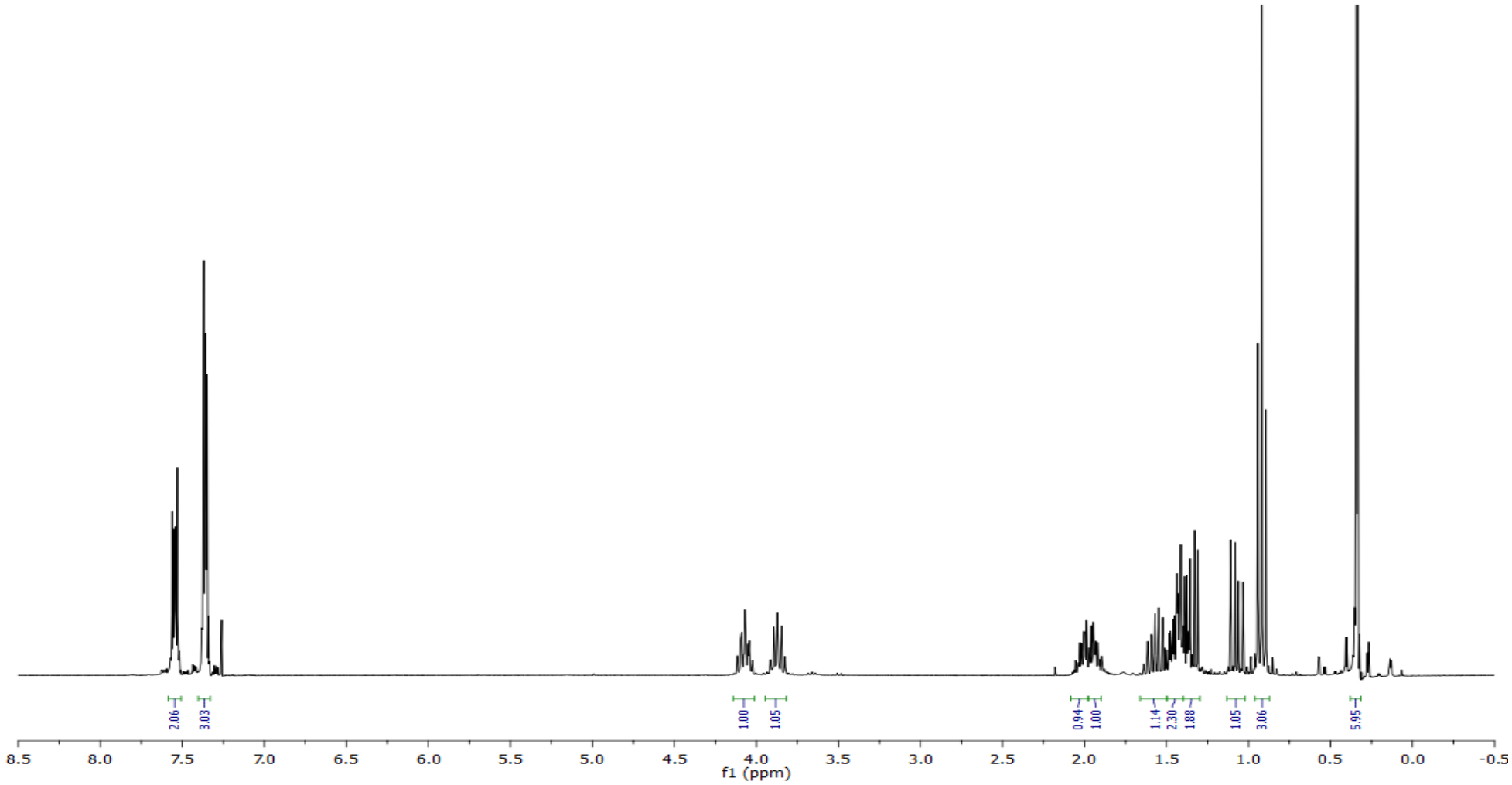

PhMe2Si
O

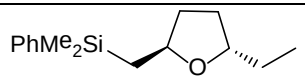
5e


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

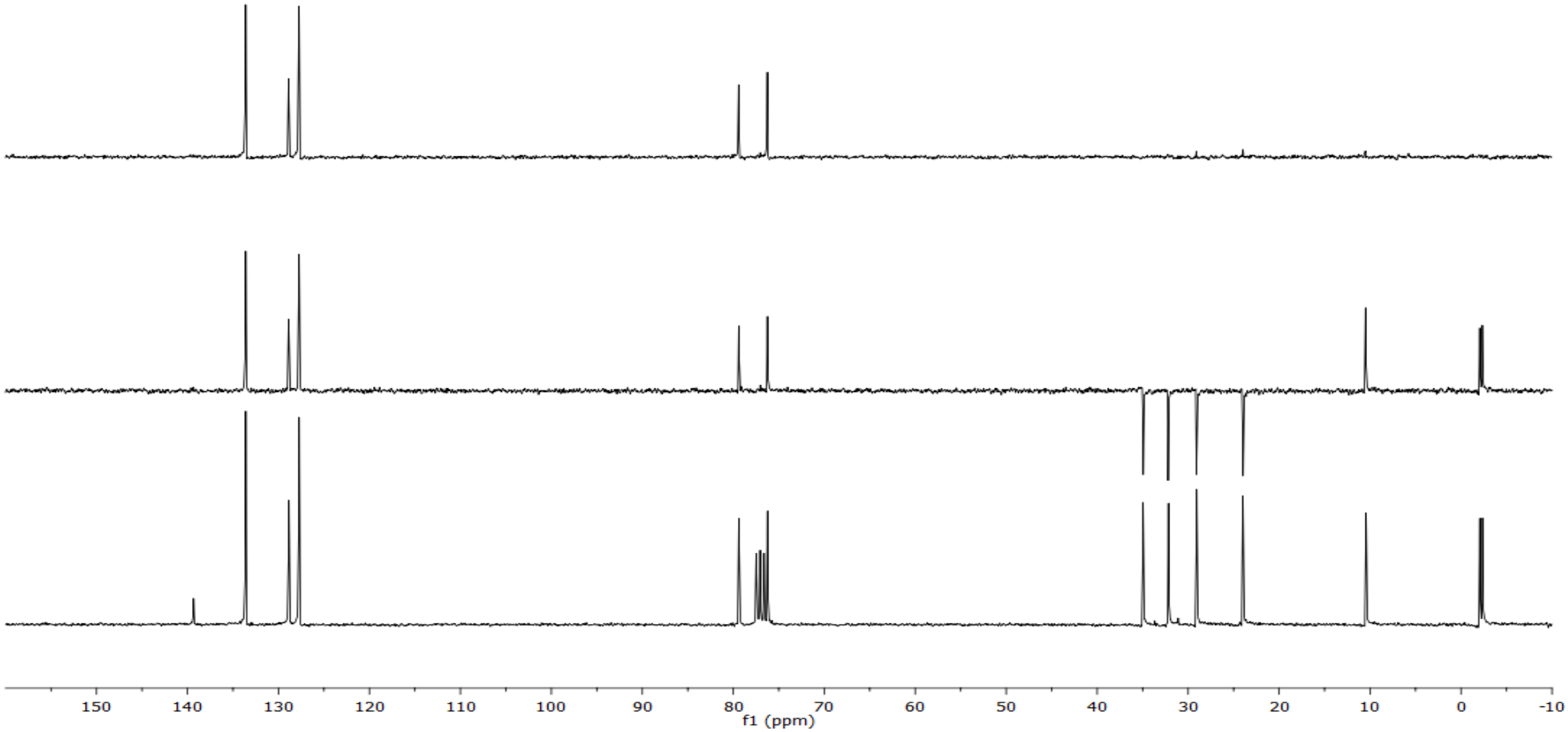

PhMe2Si
O

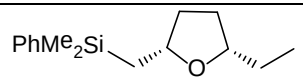
4f


2.06
3.03
1.00
1.05
0.94
1.00
1.14
2.30
1.88
1.05
3.06
5.95
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

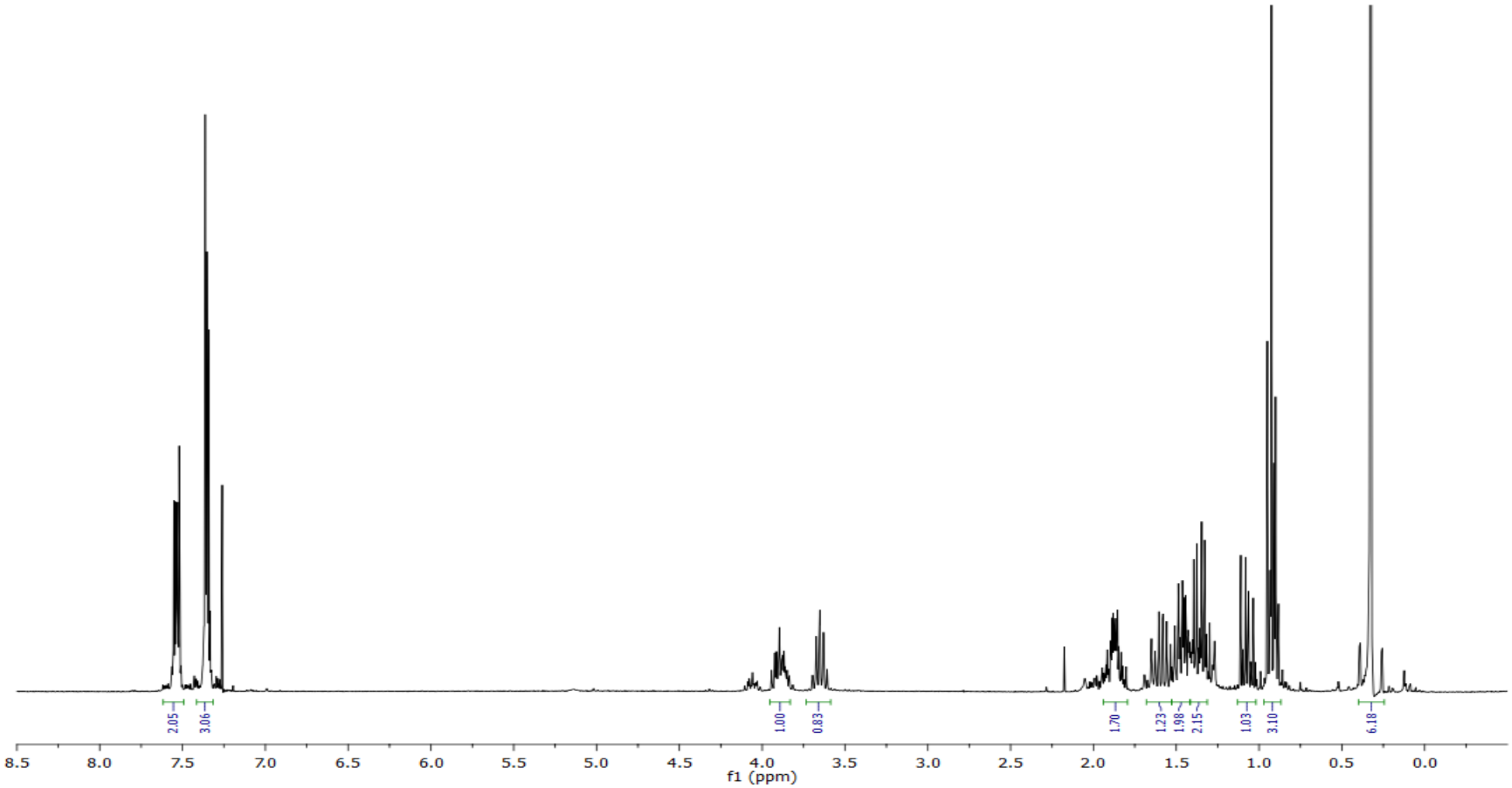

PhMe2Si
O

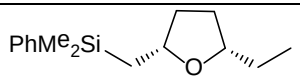
4f


150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

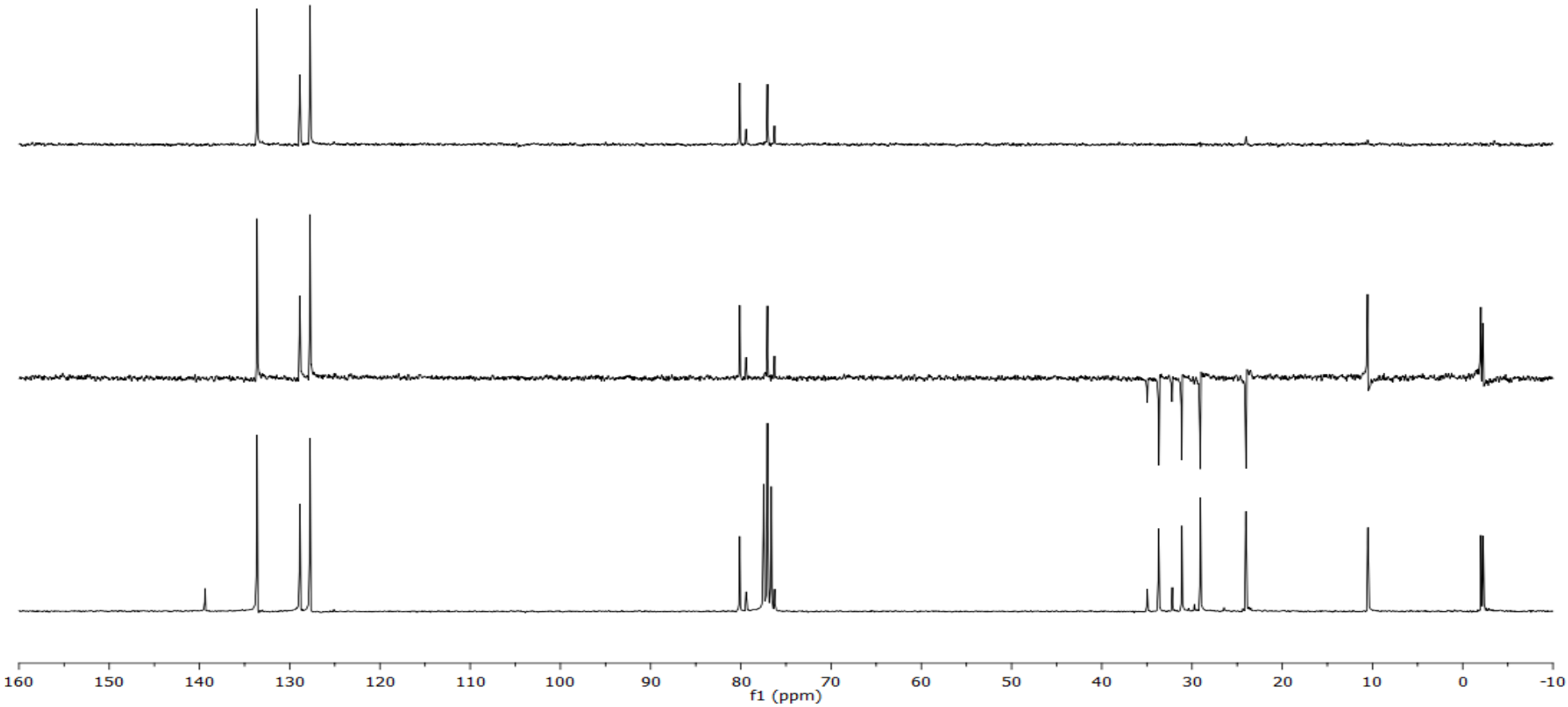

PhMe2Si
O

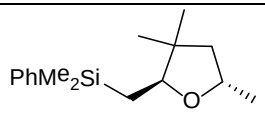
5f


2.05
3.06
1.00
0.83
1.70
1.23
1.98
2.15
1.03
3.10
6.18
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

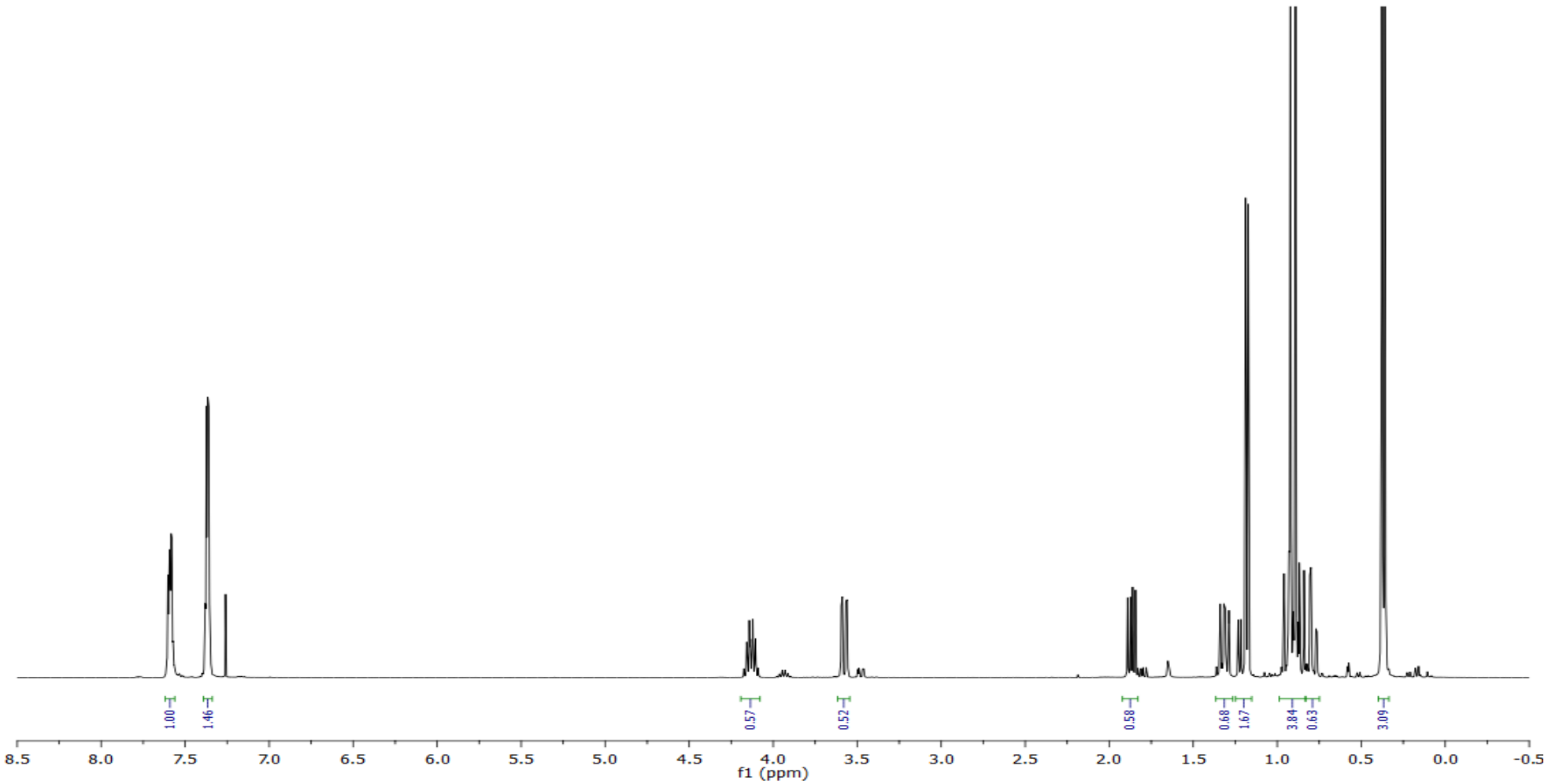

PhMe2Si
O

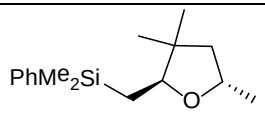
5f


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

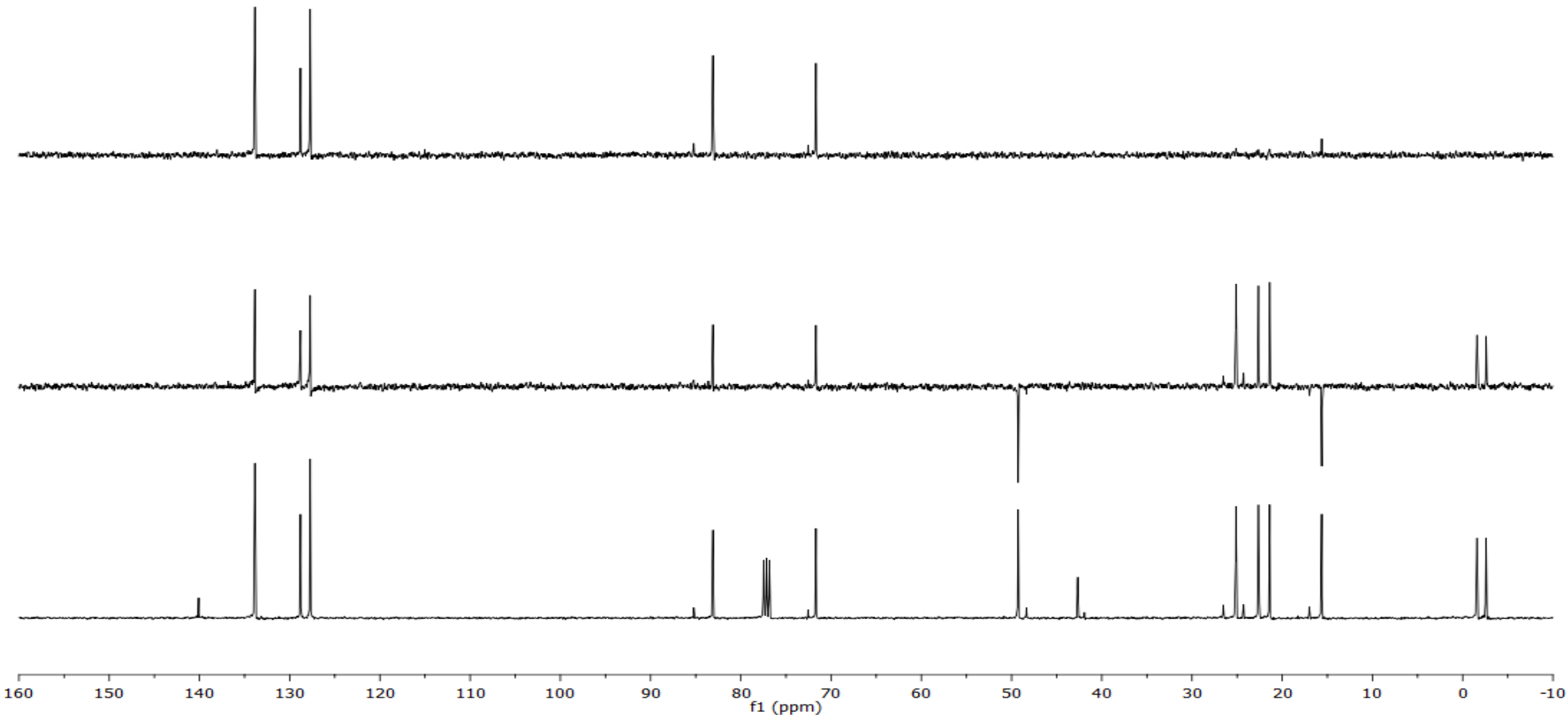

PhMe2Si
O

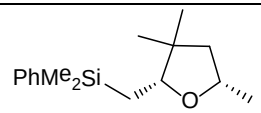
4g


1.00
1.46
0.57
0.52
0.58
0.68
1.67
3.84
0.63
3.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

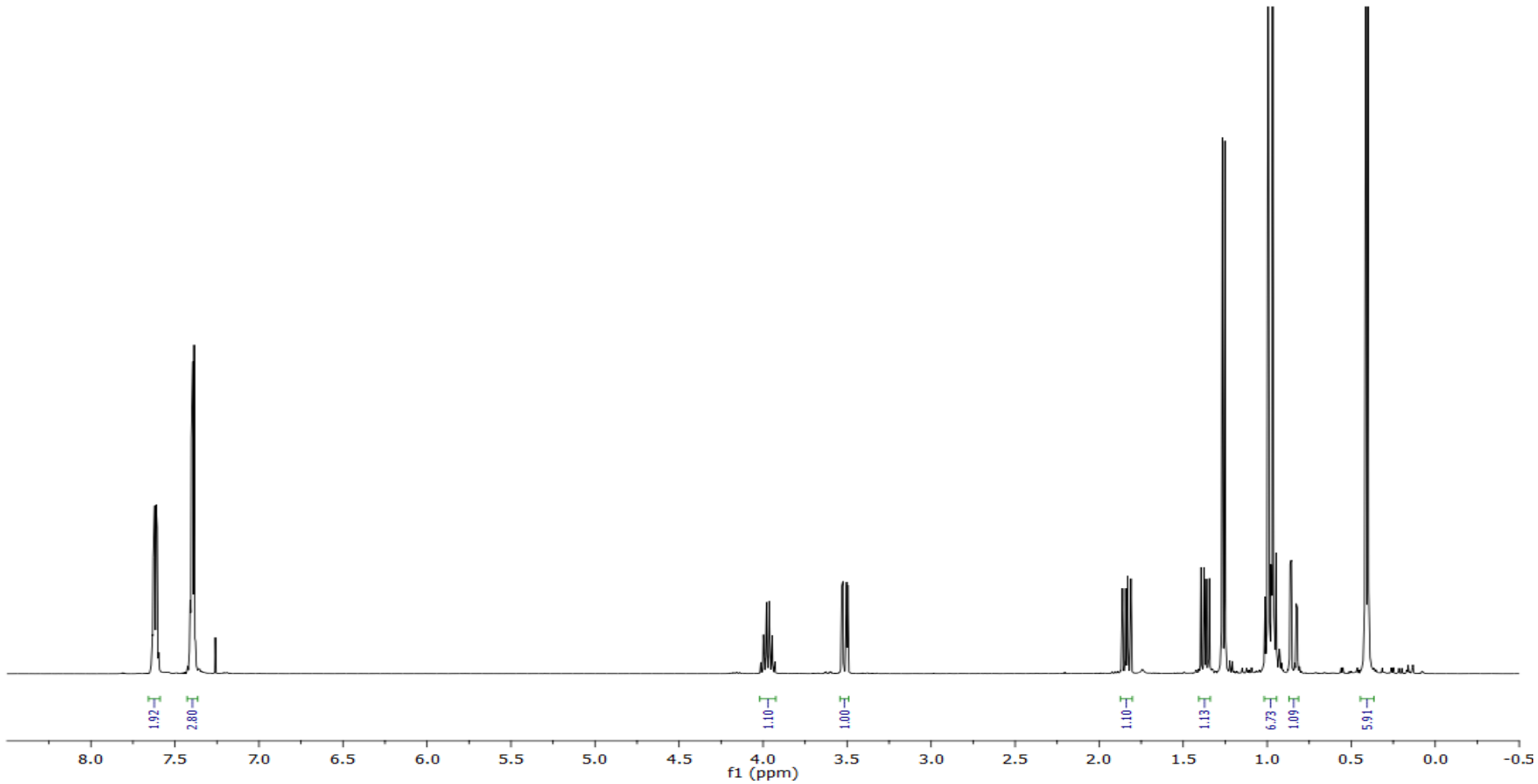

PhMe2Si
O

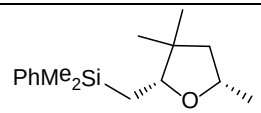
4g


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

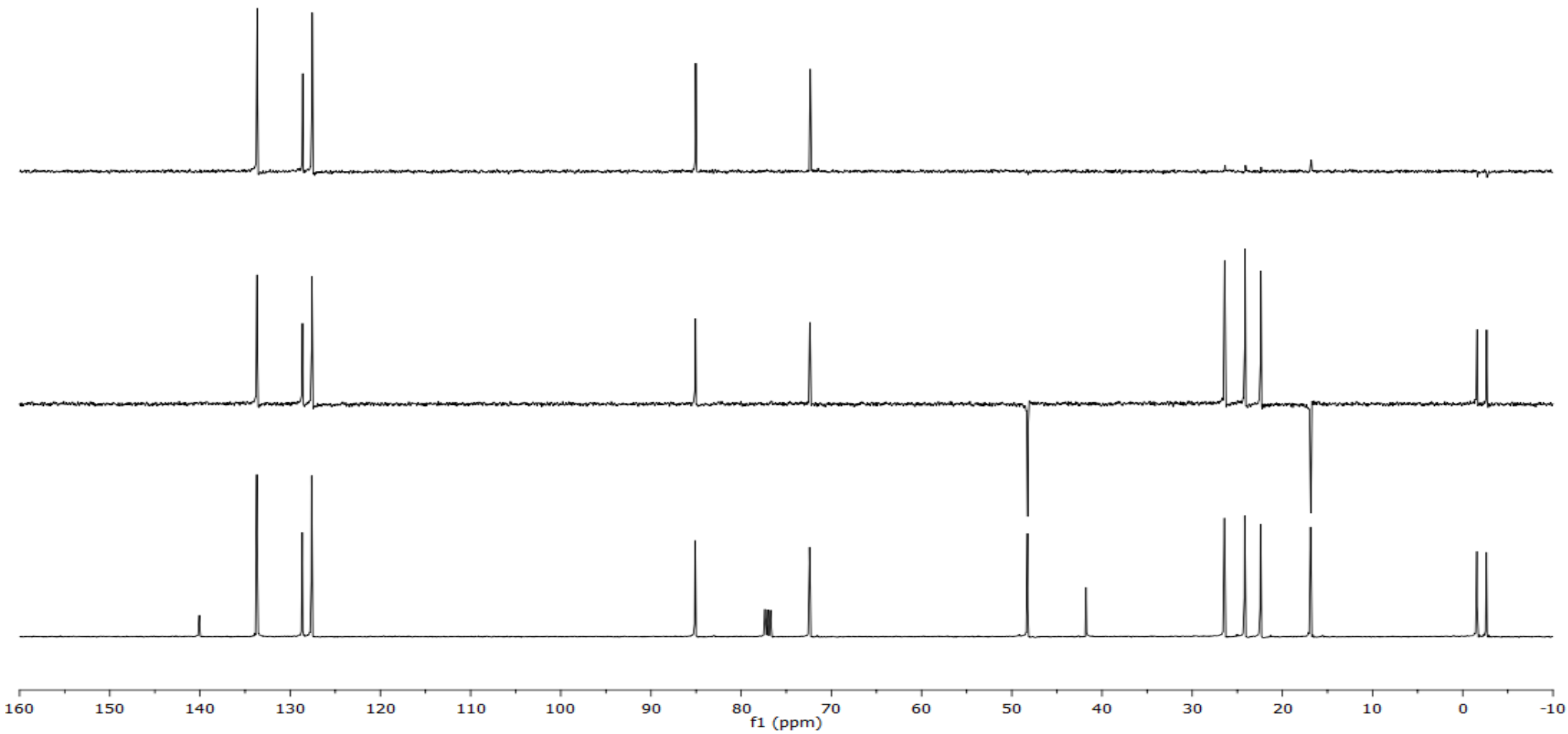

PhMe2Si
O

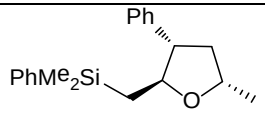
5g


1.92
2.80
1.10
1.00
1.10
1.13
6.73
1.09
5.91
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

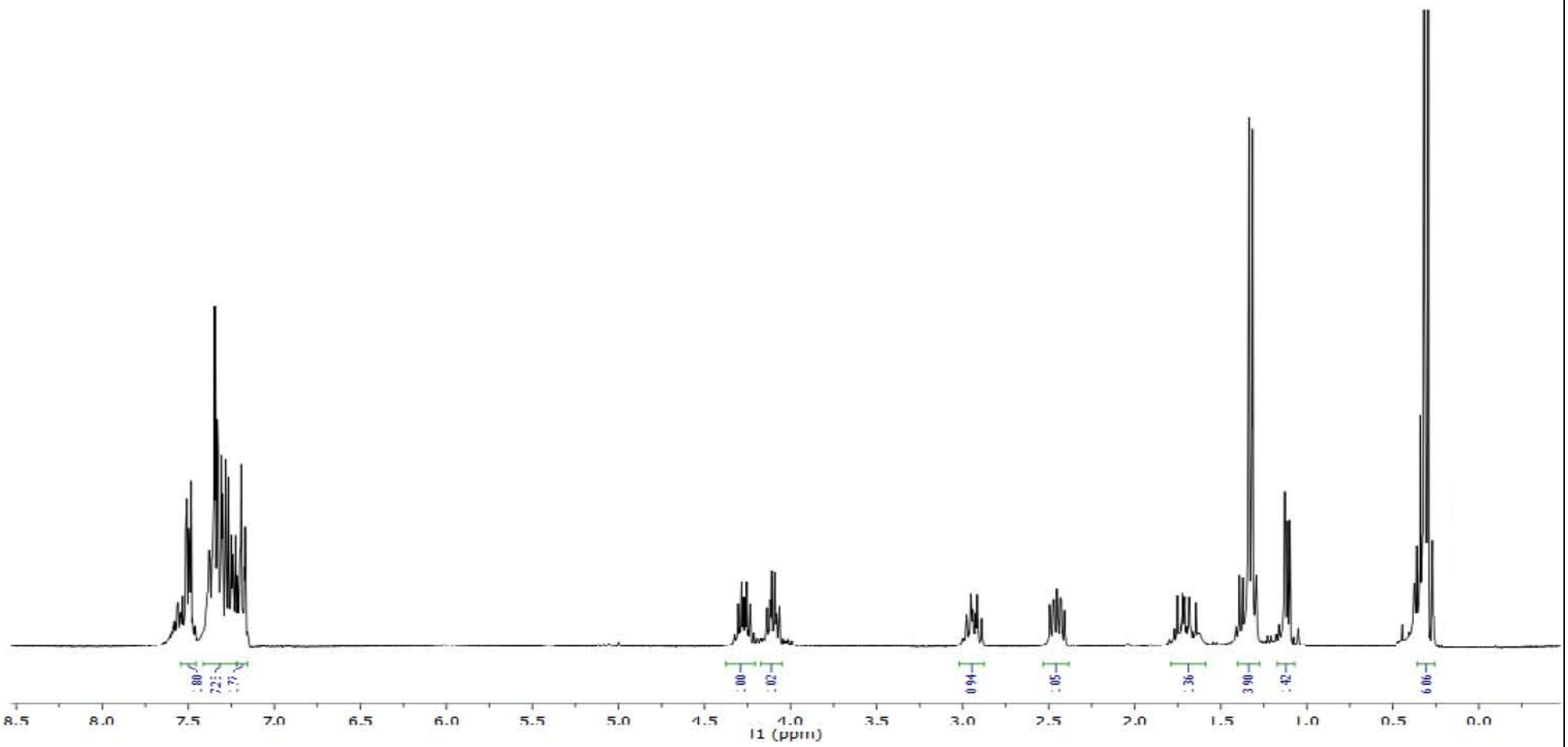

PhMe2Si
O

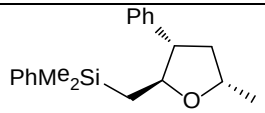
5g


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

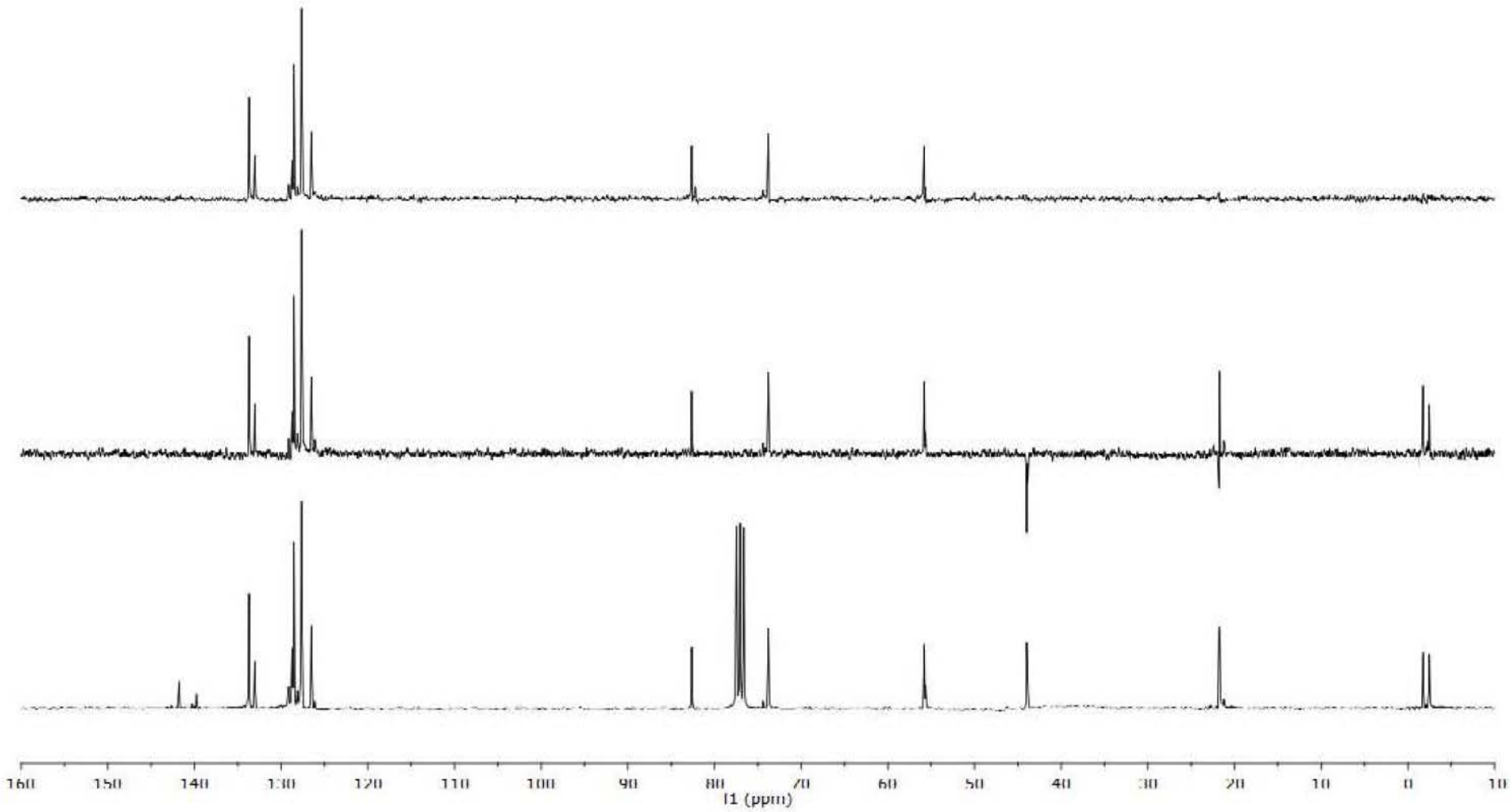

Ph
PhMe2Si
O

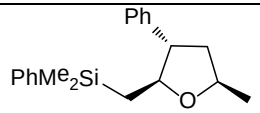
4h


8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

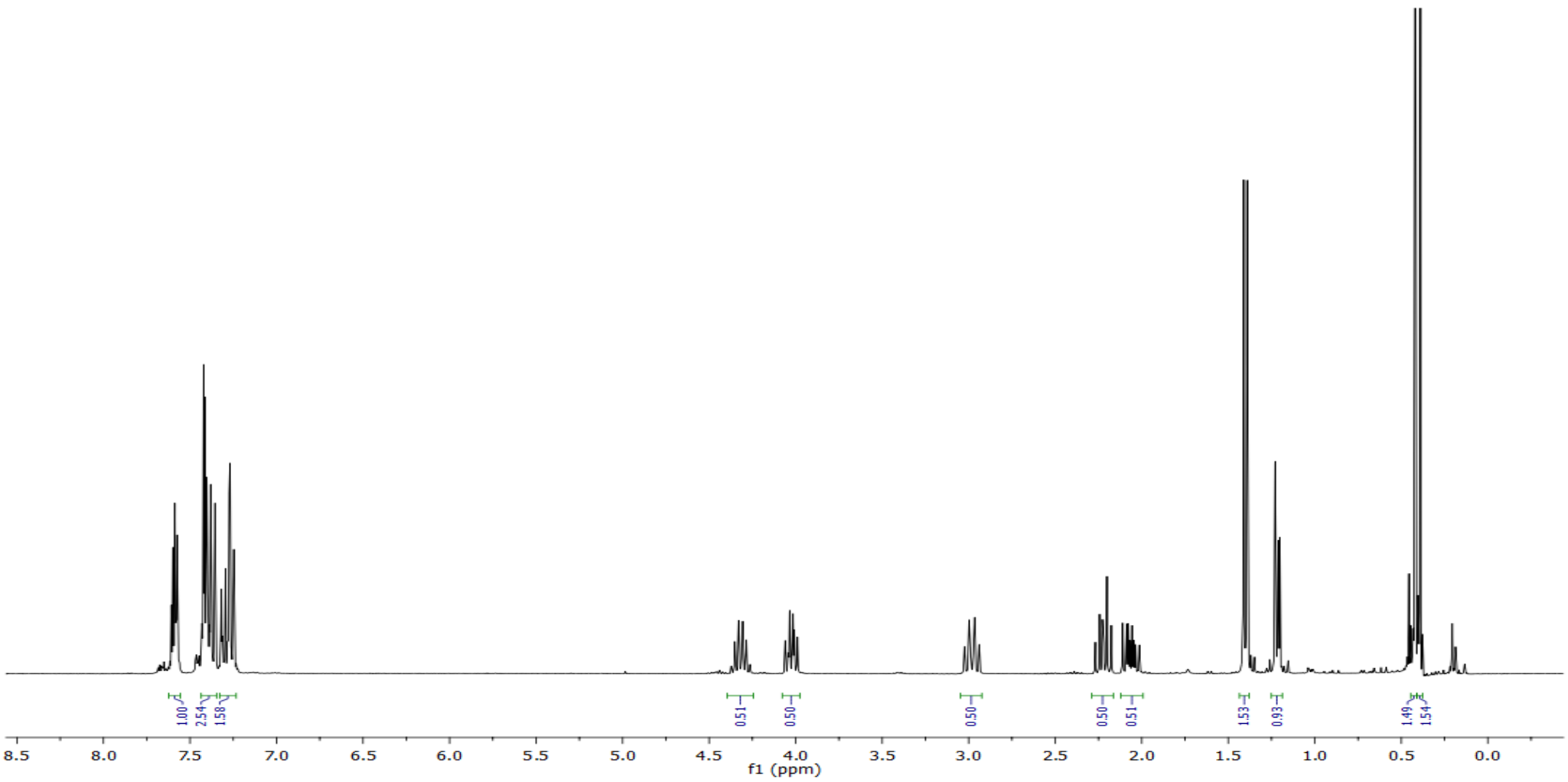

Ph
PhMe2Si
O

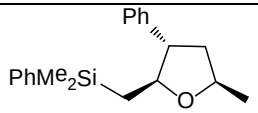
4h


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

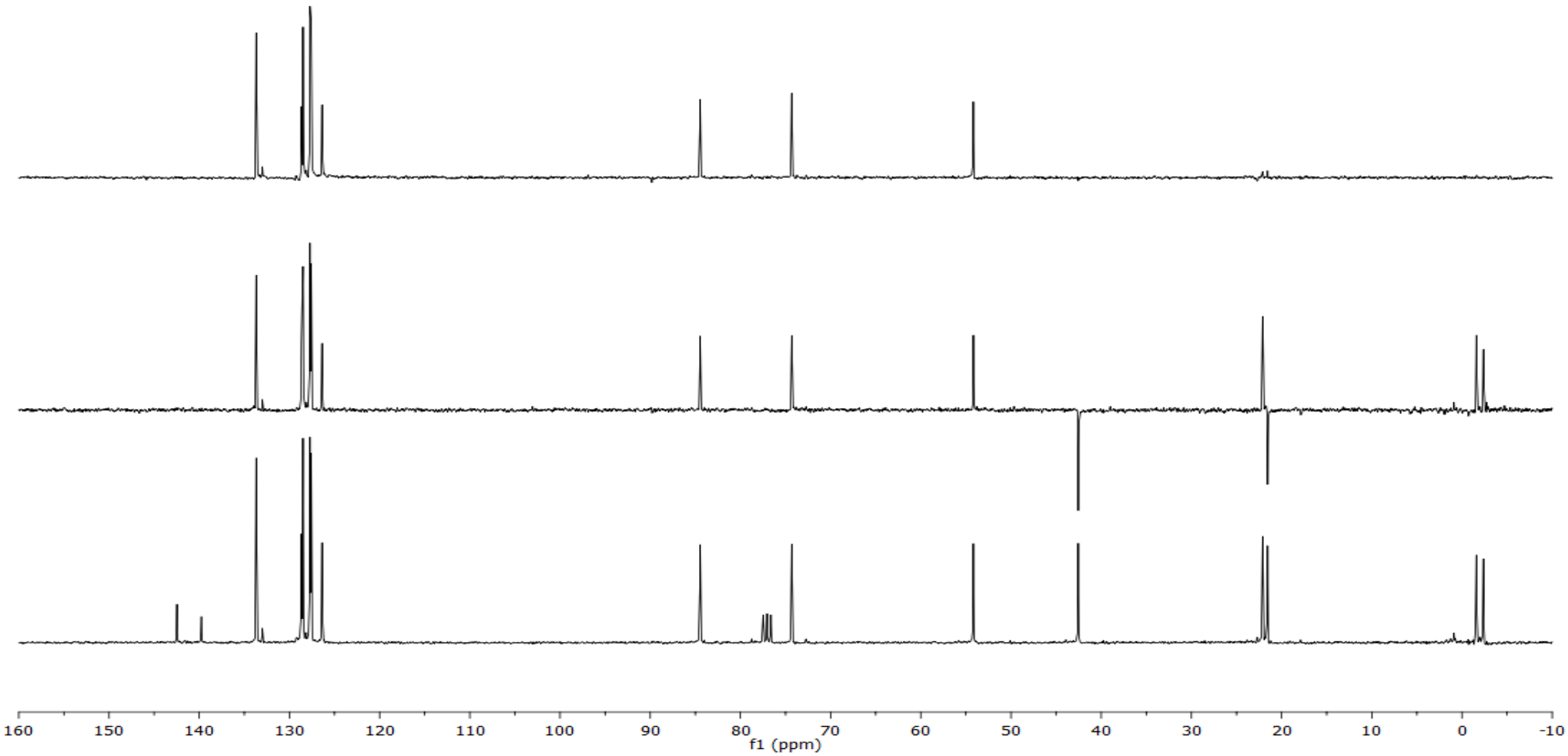

Ph
PhMe2Si
O

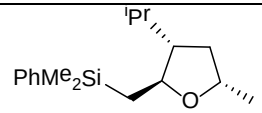
6h


1.00
2.54
1.58
0.51
0.50
0.50
0.50
0.51
1.53
0.93
1.49
1.54
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

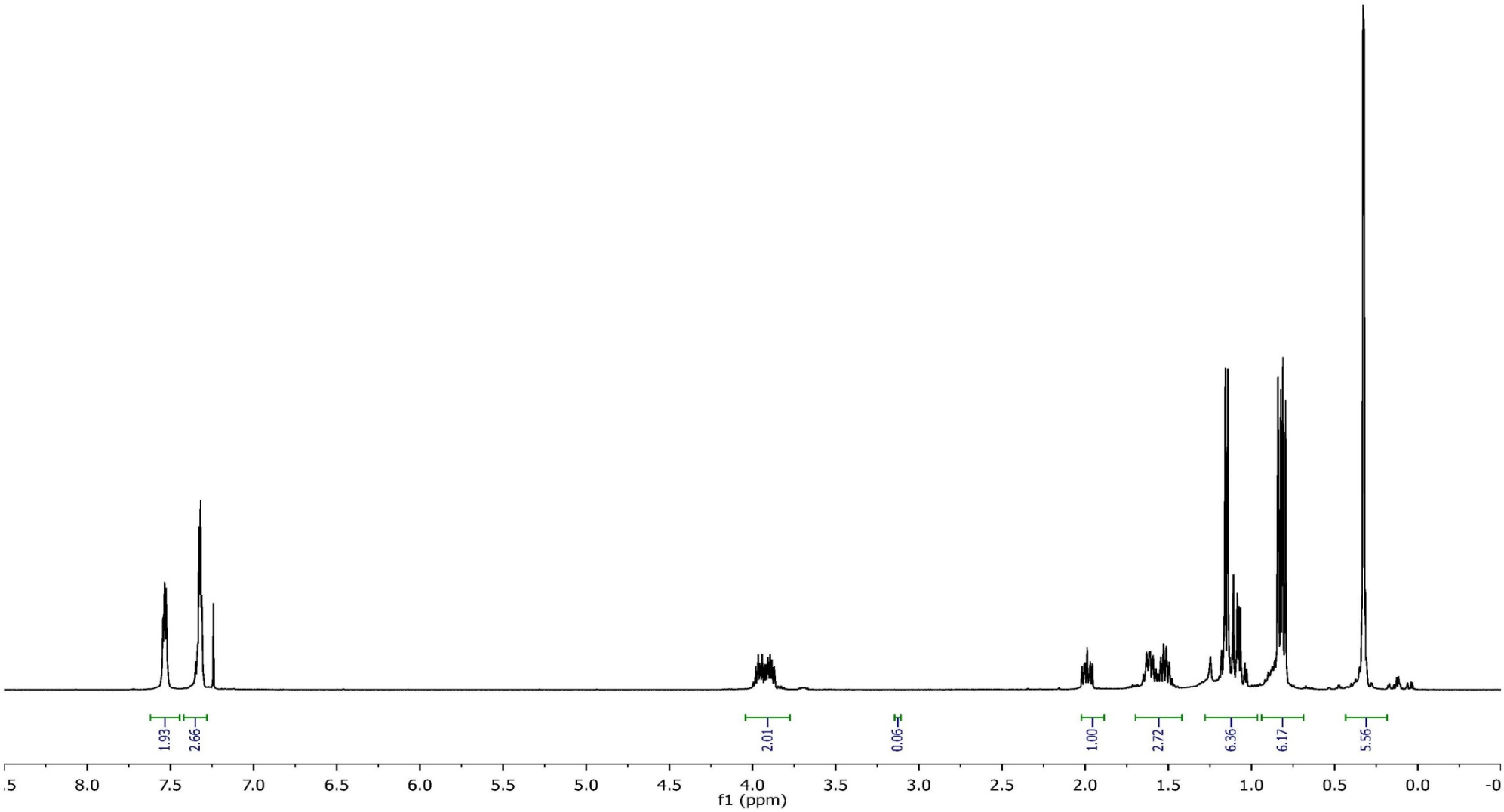

Ph
PhMe2Si
O

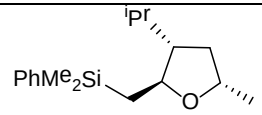
6h


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

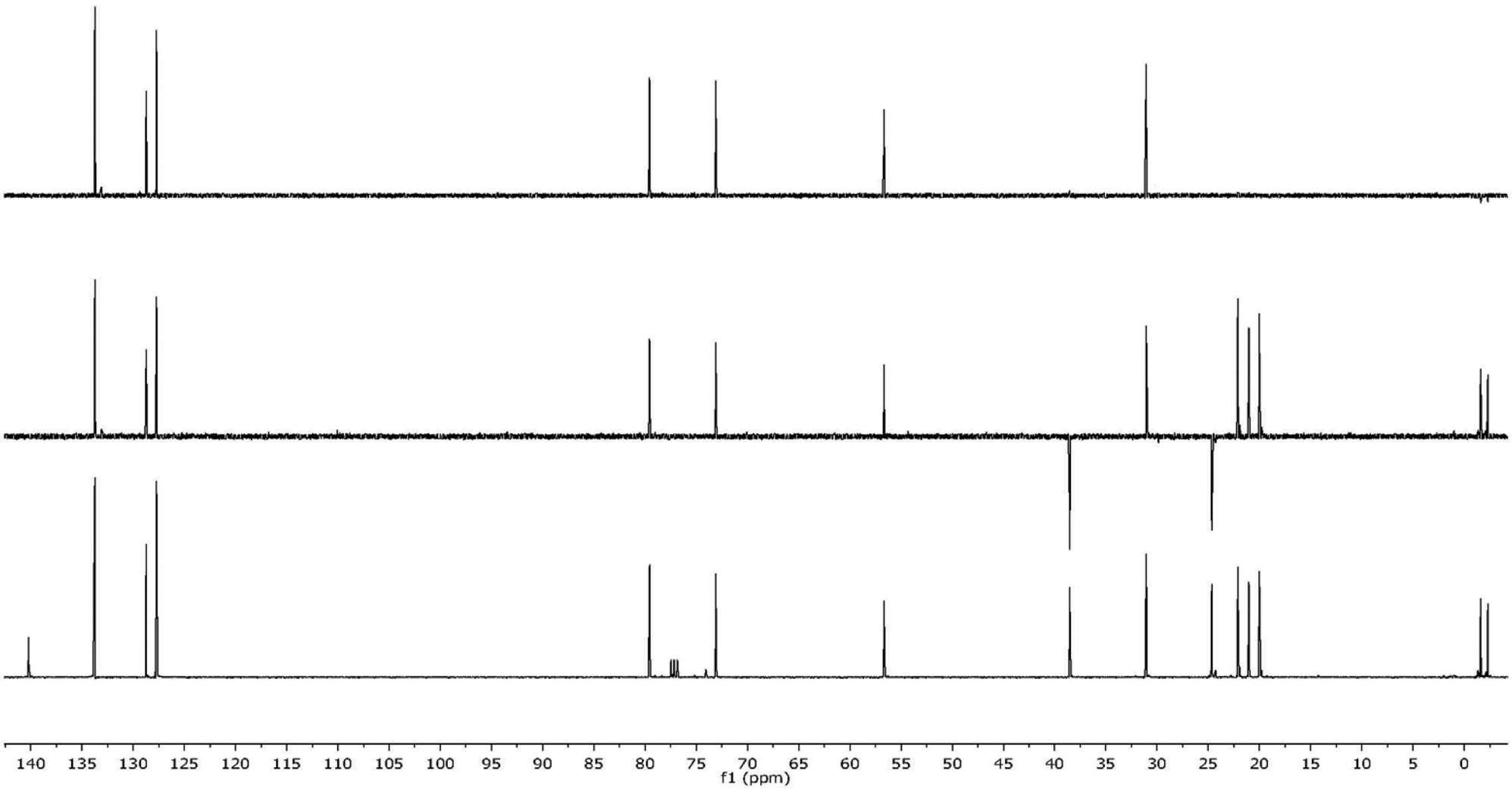

iPr
PhMe2Si
O

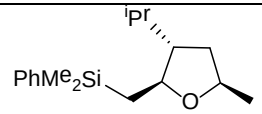
4i


1.93
2.66
2.01
0.06
1.00
2.72
6.36
6.17
5.56
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

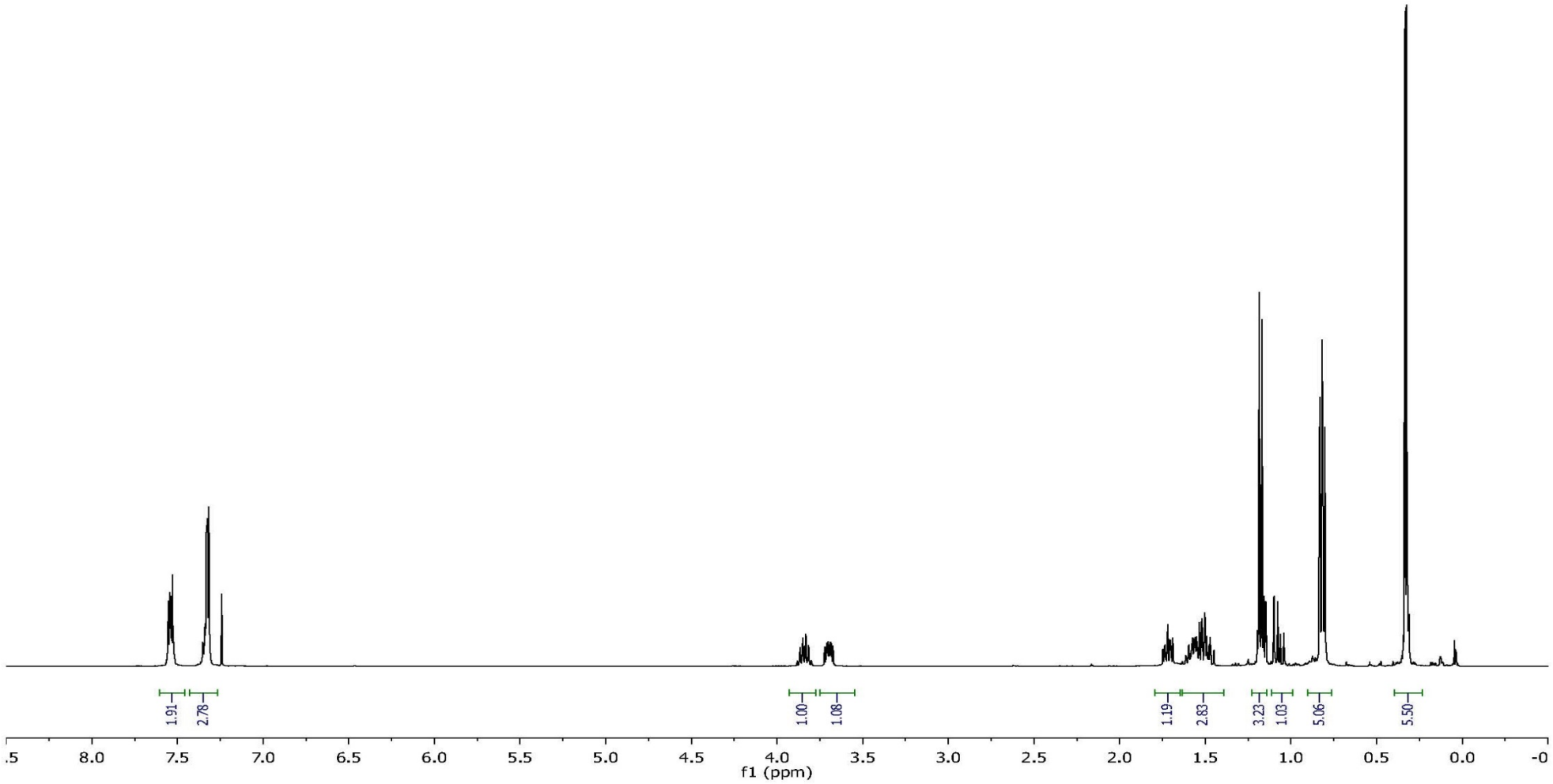

iPr
PhMe2Si
O

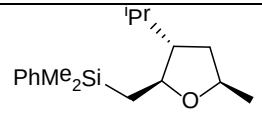
4i


140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

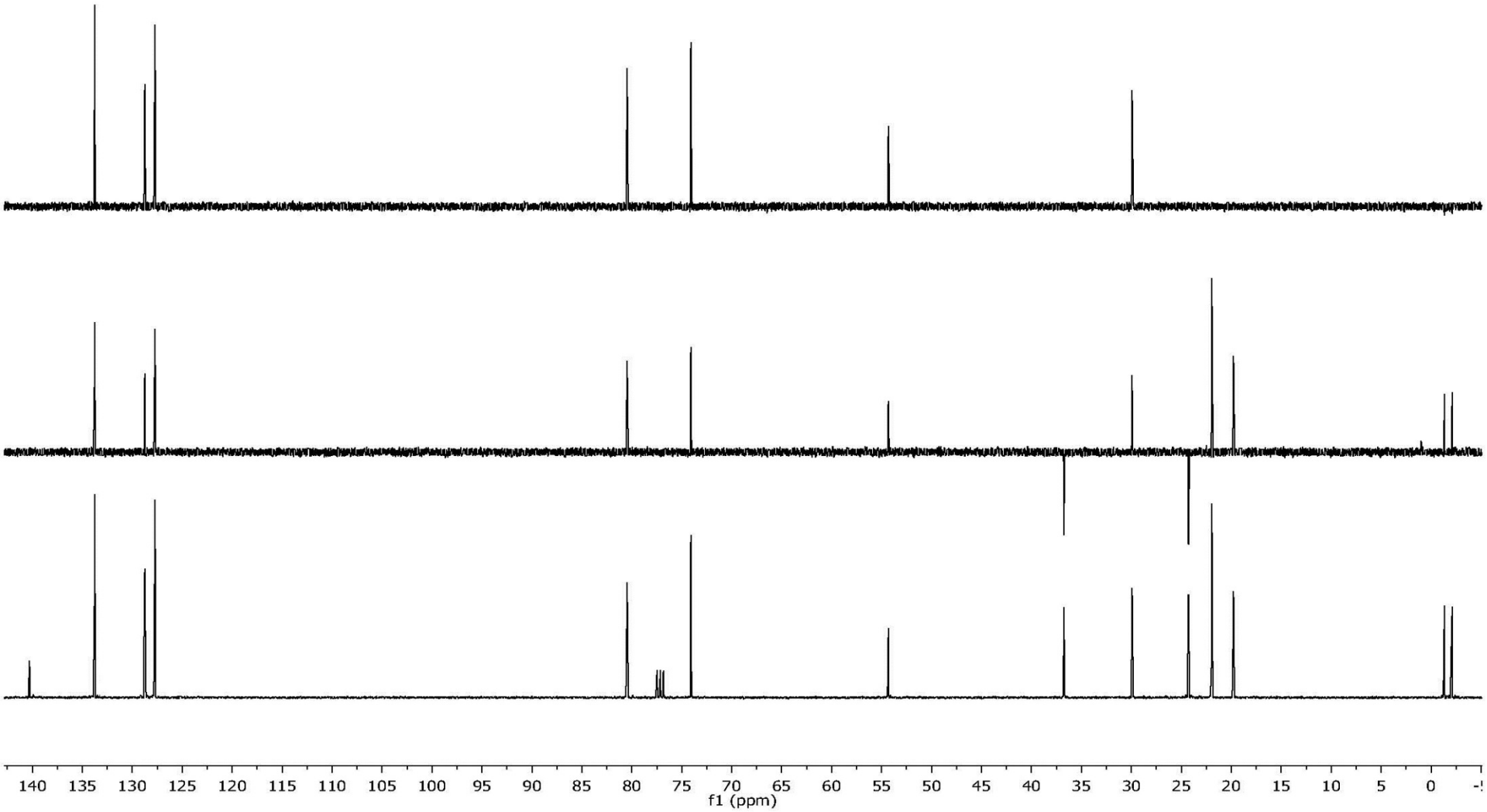

iPr
PhMe2Si
O

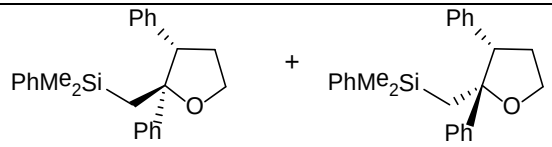
6i


1.91
2.78
1.00
1.08
1.19
2.83
3.23
1.03
5.06
5.50
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

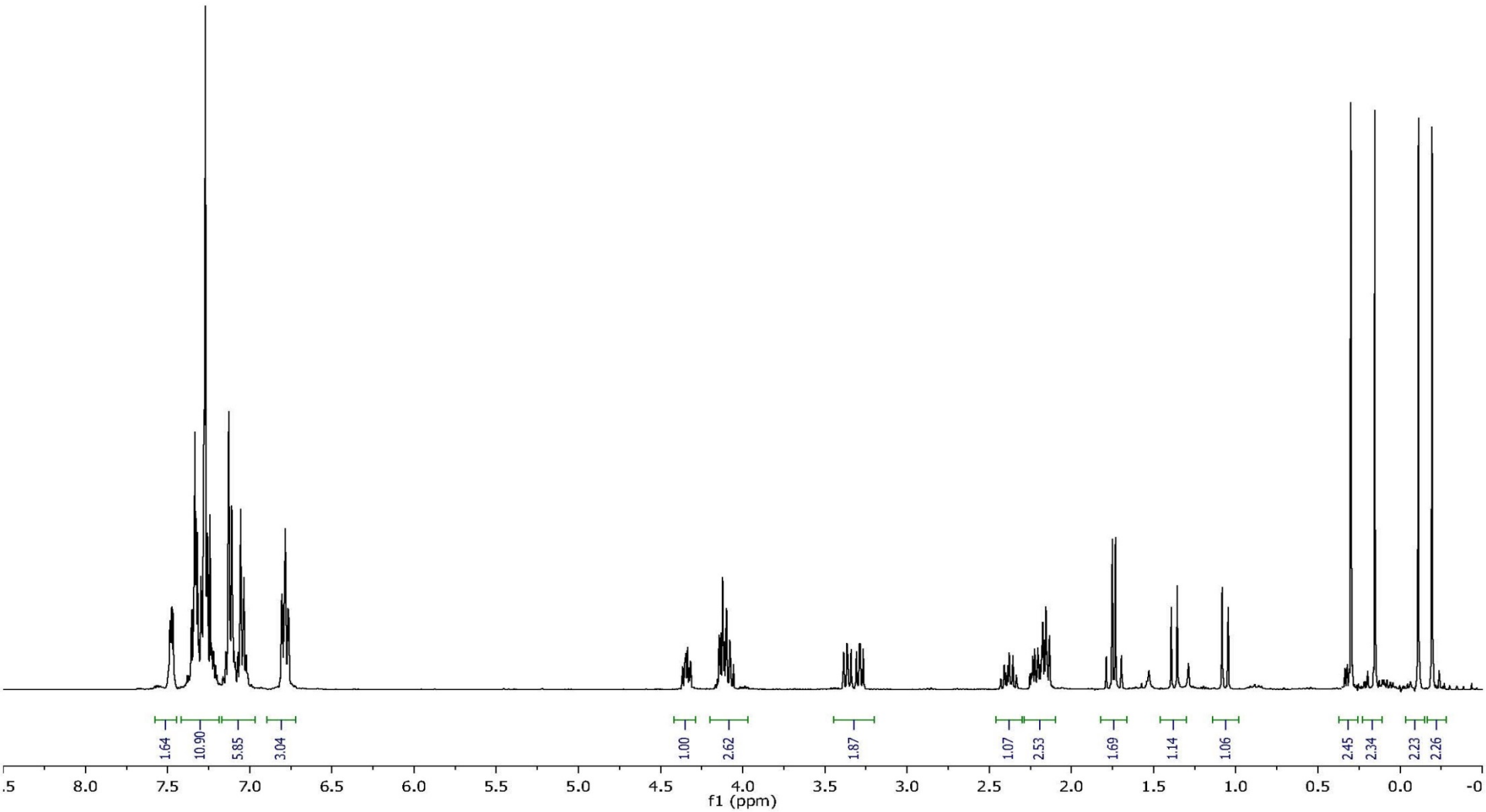

iPr
PhMe2Si
O

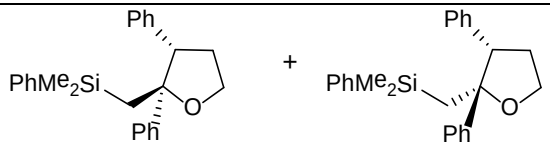
6i


140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

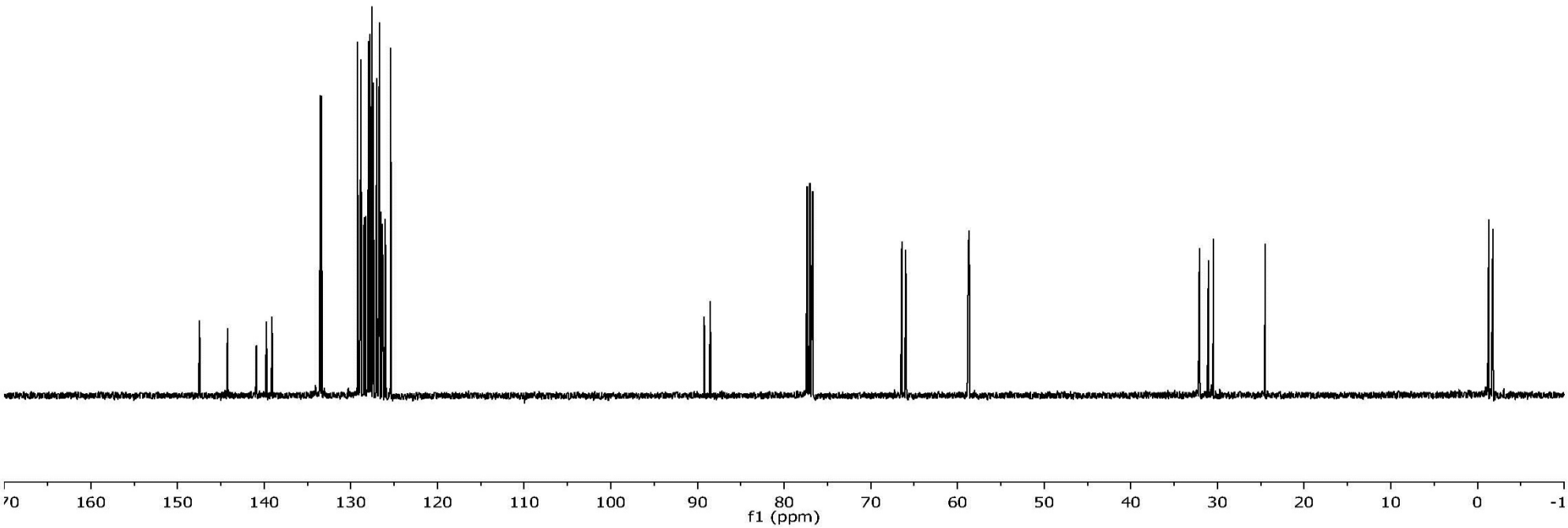

Ph
PhMe2Si
O
Ph
+
Ph
PhMe2Si
O
Ph

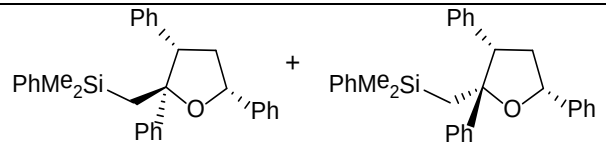
4j + 5j


1.64
10.90
5.85
3.04
1.00
2.62
1.87
1.07
2.53
1.69
1.14
1.06
2.45
2.34
2.23
2.26
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

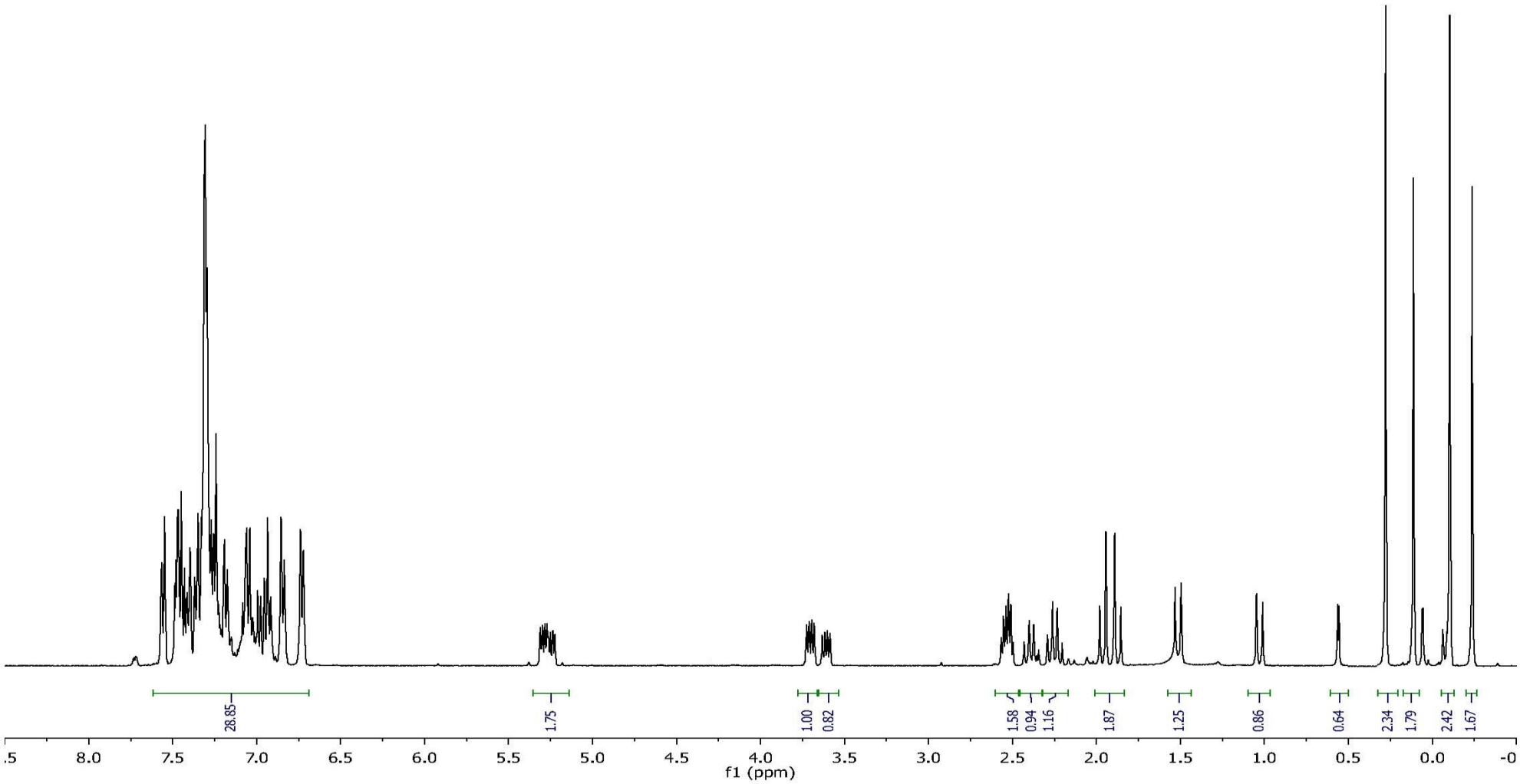

Ph
PhMe2Si
O
Ph
+
Ph
PhMe2Si
O
Ph

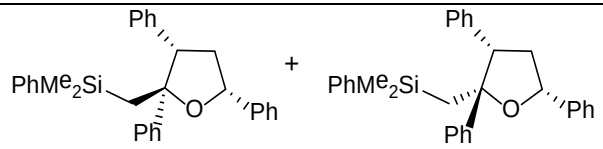
4j + 5j


160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

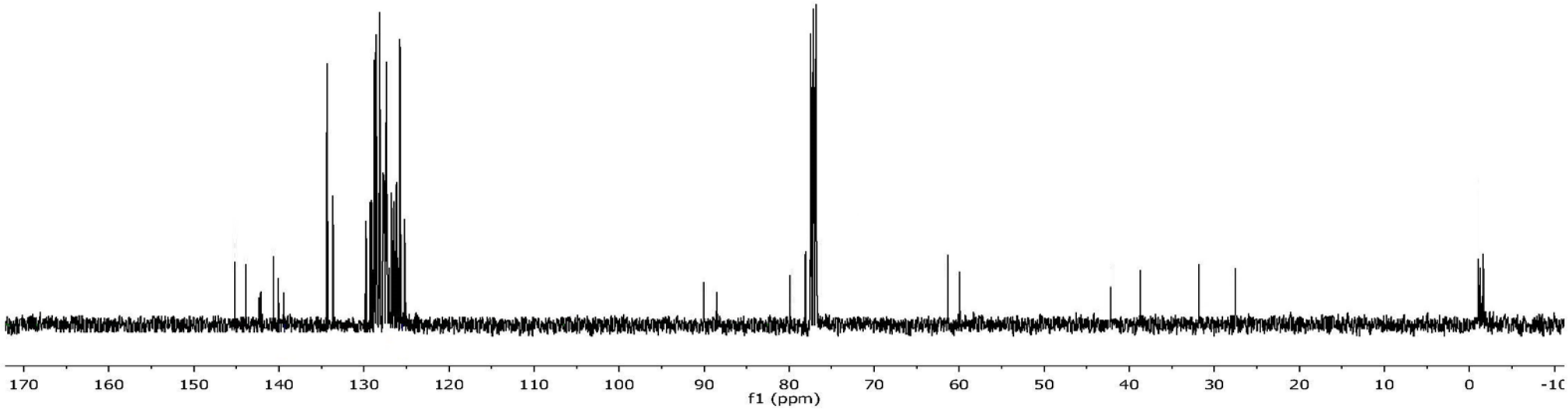

Ph
PhMe2Si
O
Ph
Ph
+
Ph
PhMe2Si
O
Ph
Ph

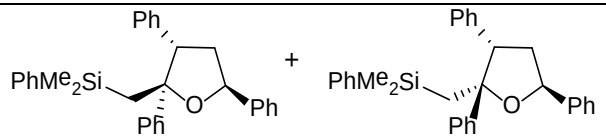
4k + 5k


28.85
1.75
1.00
0.82
1.58
0.94
1.16
1.87
1.25
0.86
0.64
2.34
1.79
2.42
1.67
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

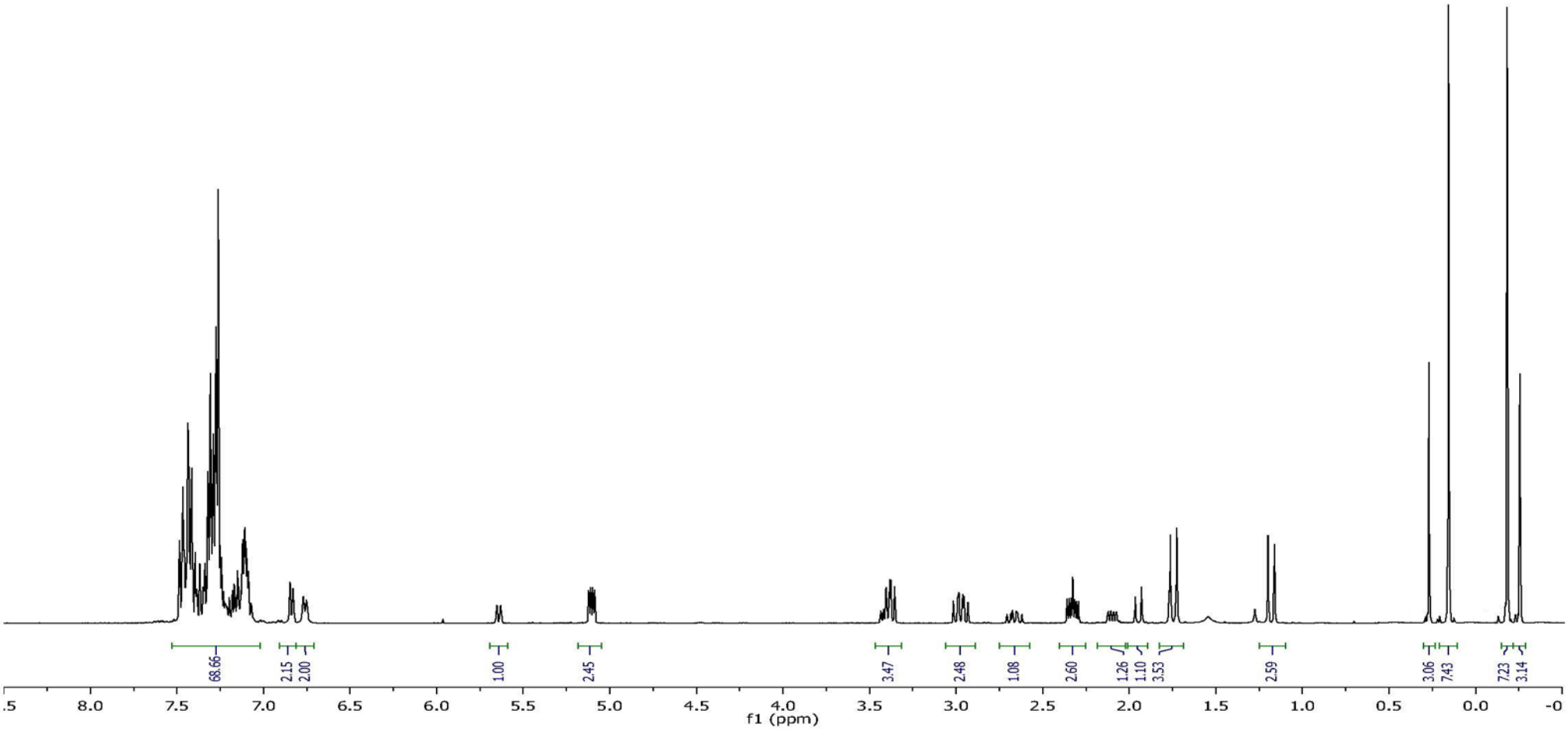

Ph
PhMe2Si
O
Ph
Ph
+
Ph
PhMe2Si
O
Ph
Ph

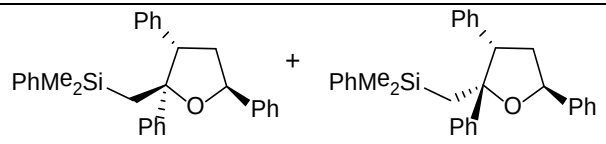
4k + 5k


170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

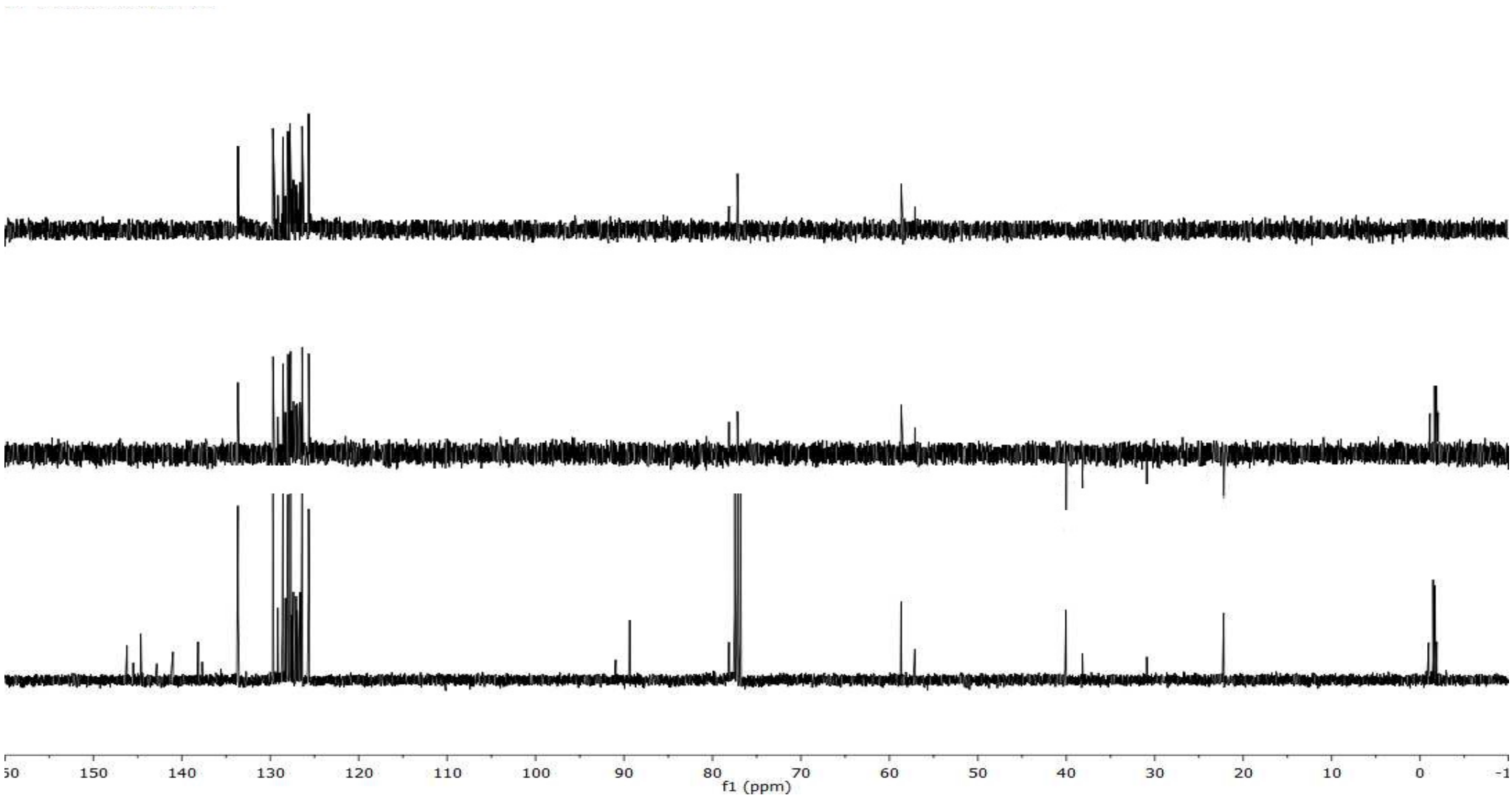

Ph
PhMe2Si
Ph
O
Ph
+
Ph
PhMe2Si
Ph
O
Ph

6k + 7k


68.66
2.15
2.00
1.00
2.45
3.47
2.48
1.08
2.60
1.26
1.10
3.53
2.59
3.06
7.43
7.23
3.14
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Ph
PhMe2Si
O
Ph
Ph
+
Ph
PhMe2Si
O
Ph
Ph

6k + 7k


150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)