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SUPPORTING INFORMATION

Siloxane-Containing Derivatives of Benzoic Acid: Chemical Transformation of the Carboxyl Group.

Supp.Inf.2: NMR, ESI HRMS and IR spectra for 3aa-ap

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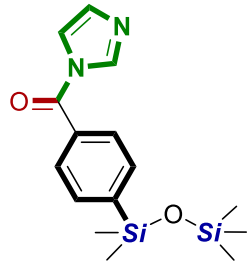
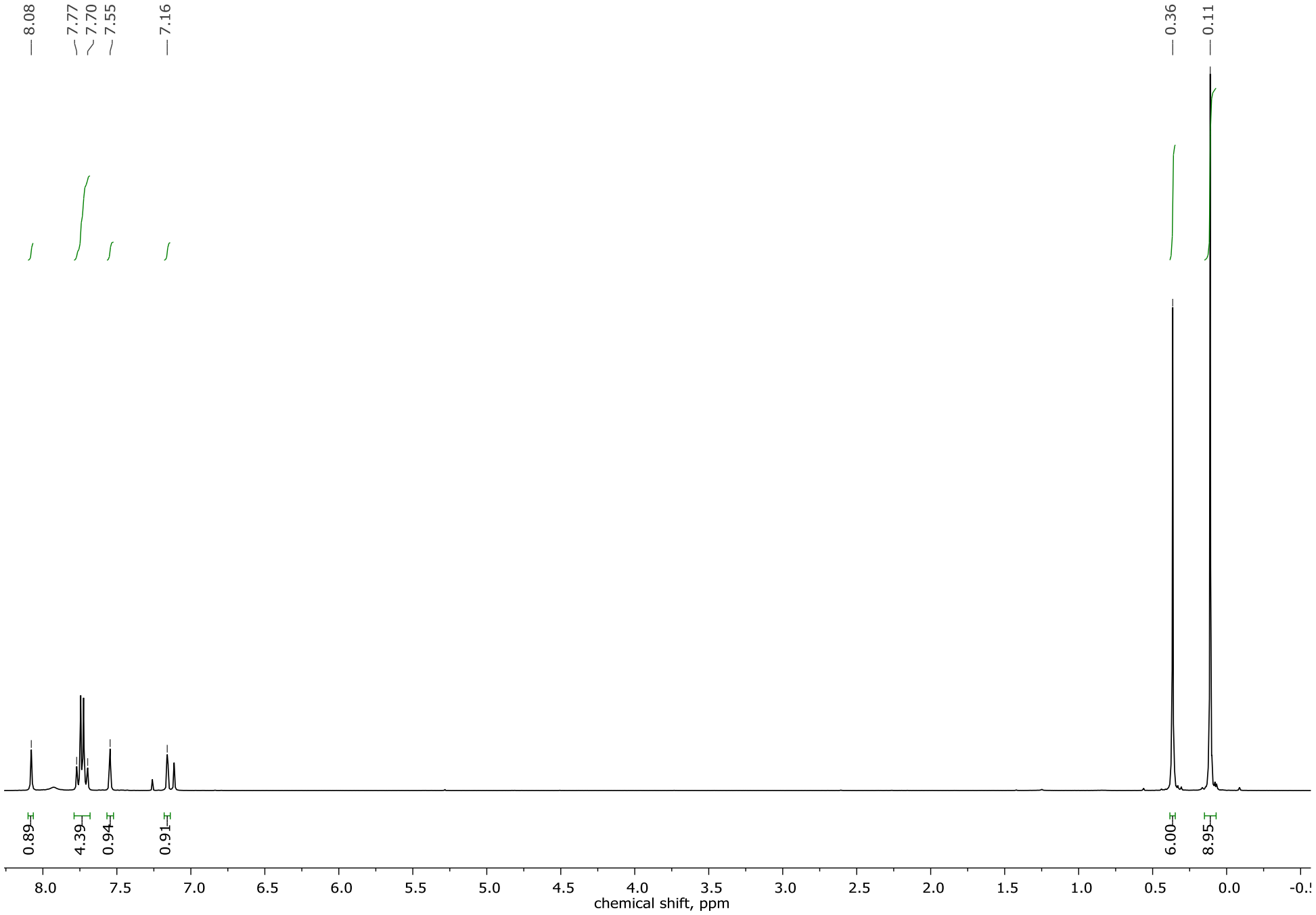


Characterisation data for (1H-imidazol-1-yl)(4-(1,1,3,3,3-pentamethyldisiloxaneyl)phenyl)methanone:

^{1}H NMR (400 MHz, DMSO-d6): δ = 8.08 (s, 1H), δ = 7.77-7.70 (m, 4H), δ = 7.55 (m, 1H), δ = 7.16 (m, 1H), δ = 0.36 (s, 6H), δ = 0.11 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d6): δ = 147.66, 138.32, 134.99, 133.50, 132.36, 130.99, 128.80, 118.16, 2.07, 0.91. ^{29}Si NMR (80 MHz, DMSO-d6): δ = 9.94, -2.77. ^{15}N NMR (40 MHz, DMSO): δ = 266.48, 205.46.

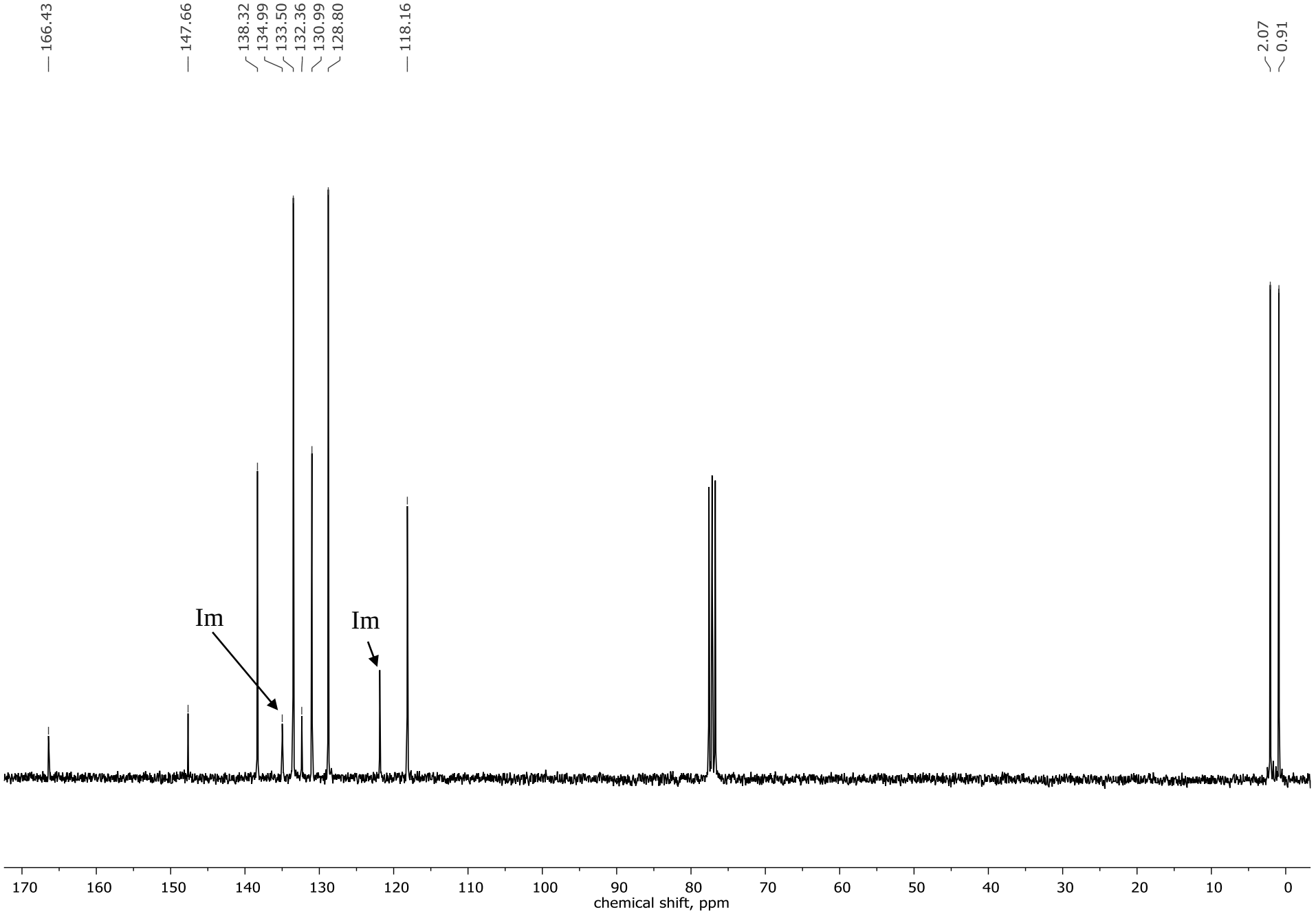
^{1}H NMR

(400 MHz, $CDCl_3$)



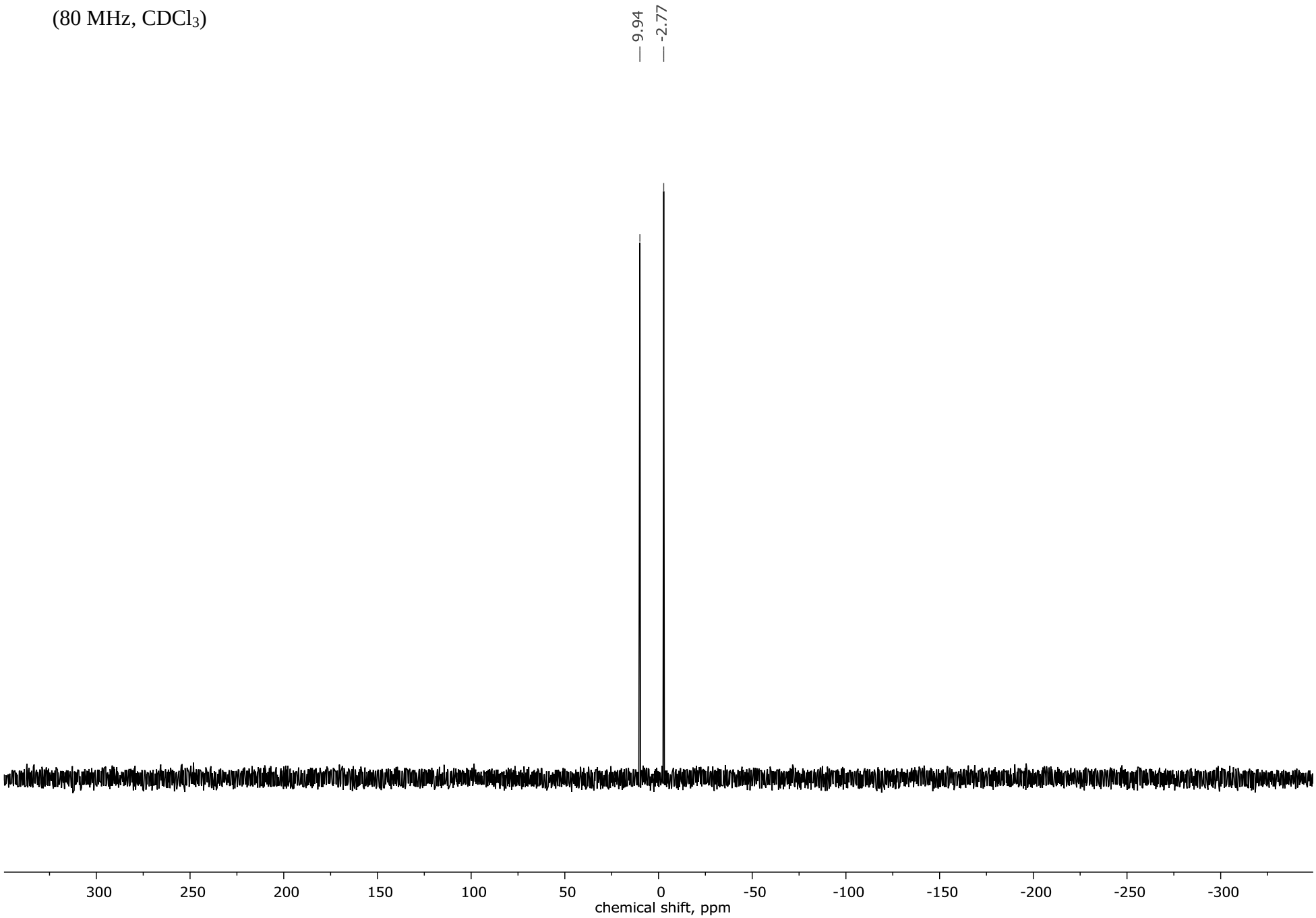
^{13}C NMR

(100 MHz, $CDCl_3$)

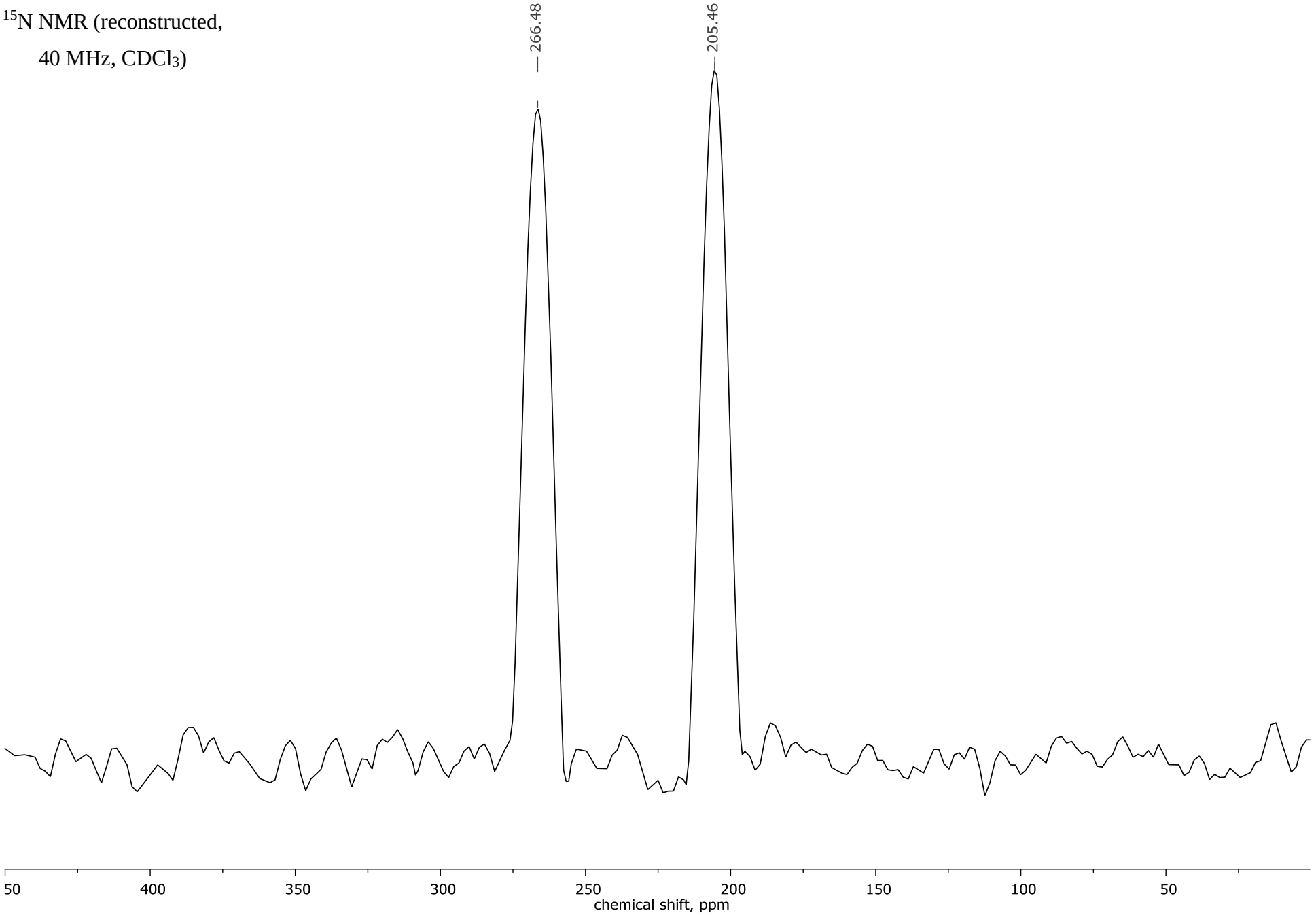


^{29}Si NMR

(80 MHz, $CDCl_3$)

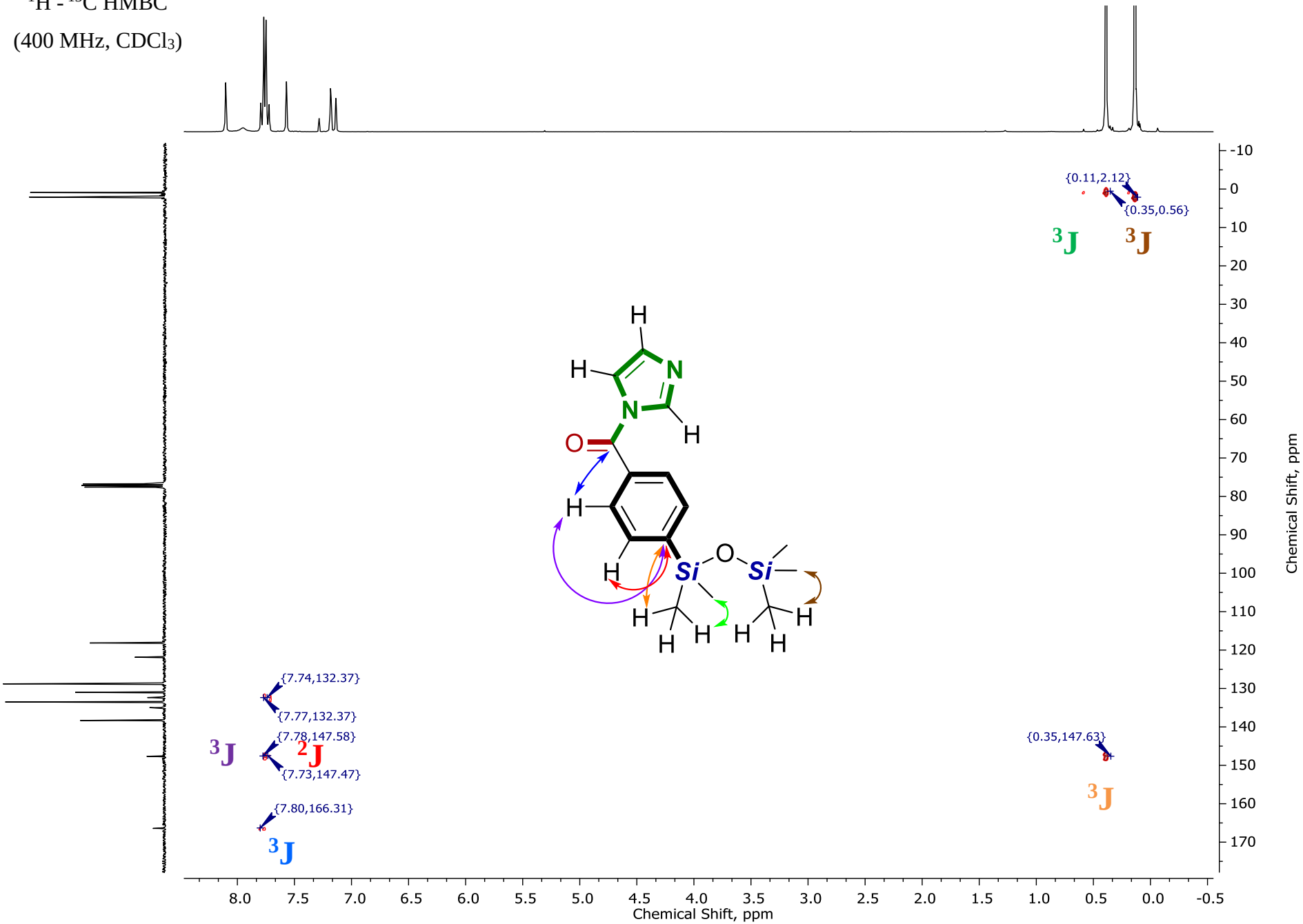


^{15}N NMR (reconstructed,
40 MHz, $CDCl_3$)



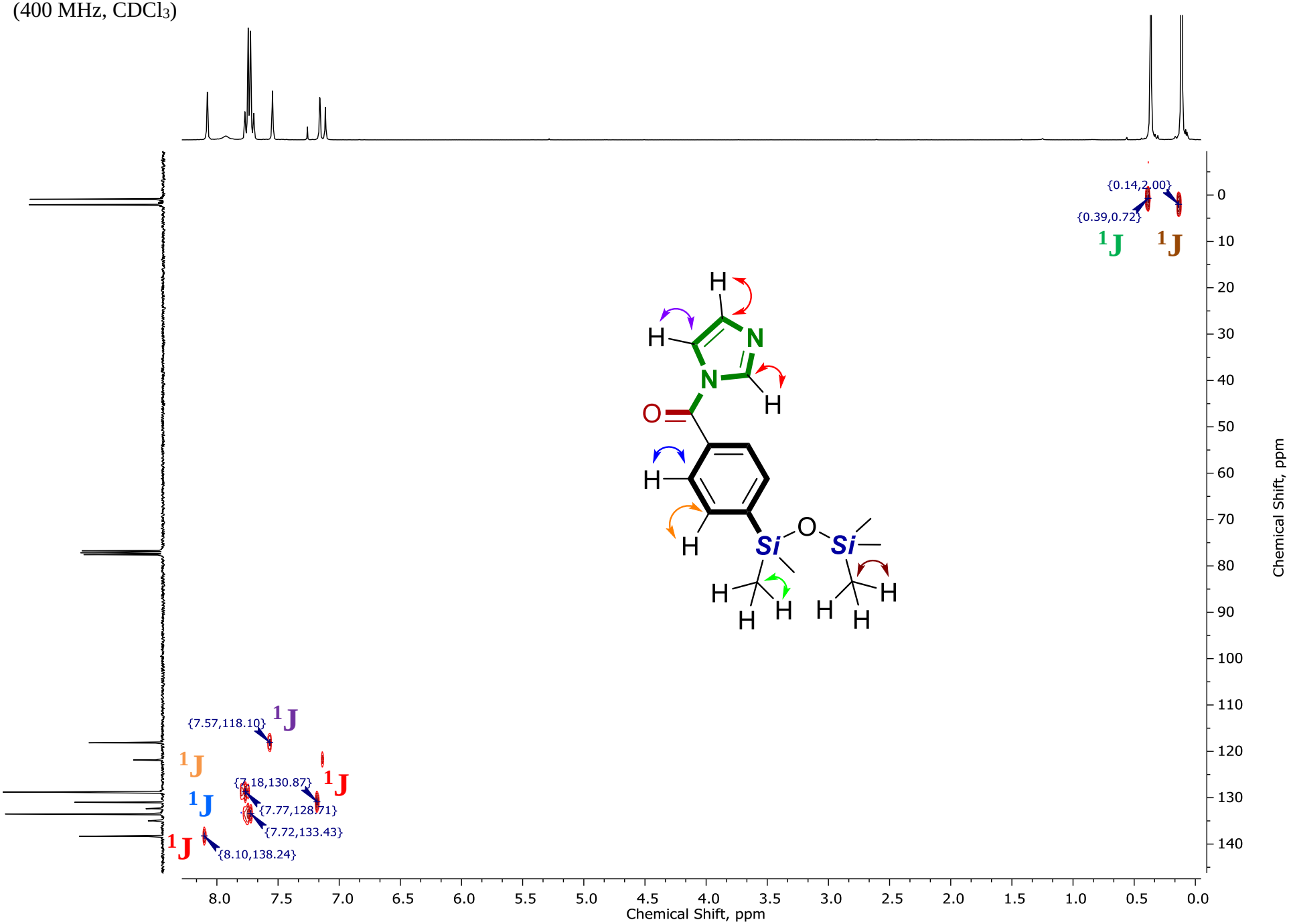
^{1}H - ^{13}C HMBC

(400 MHz, $CDCl_3$)



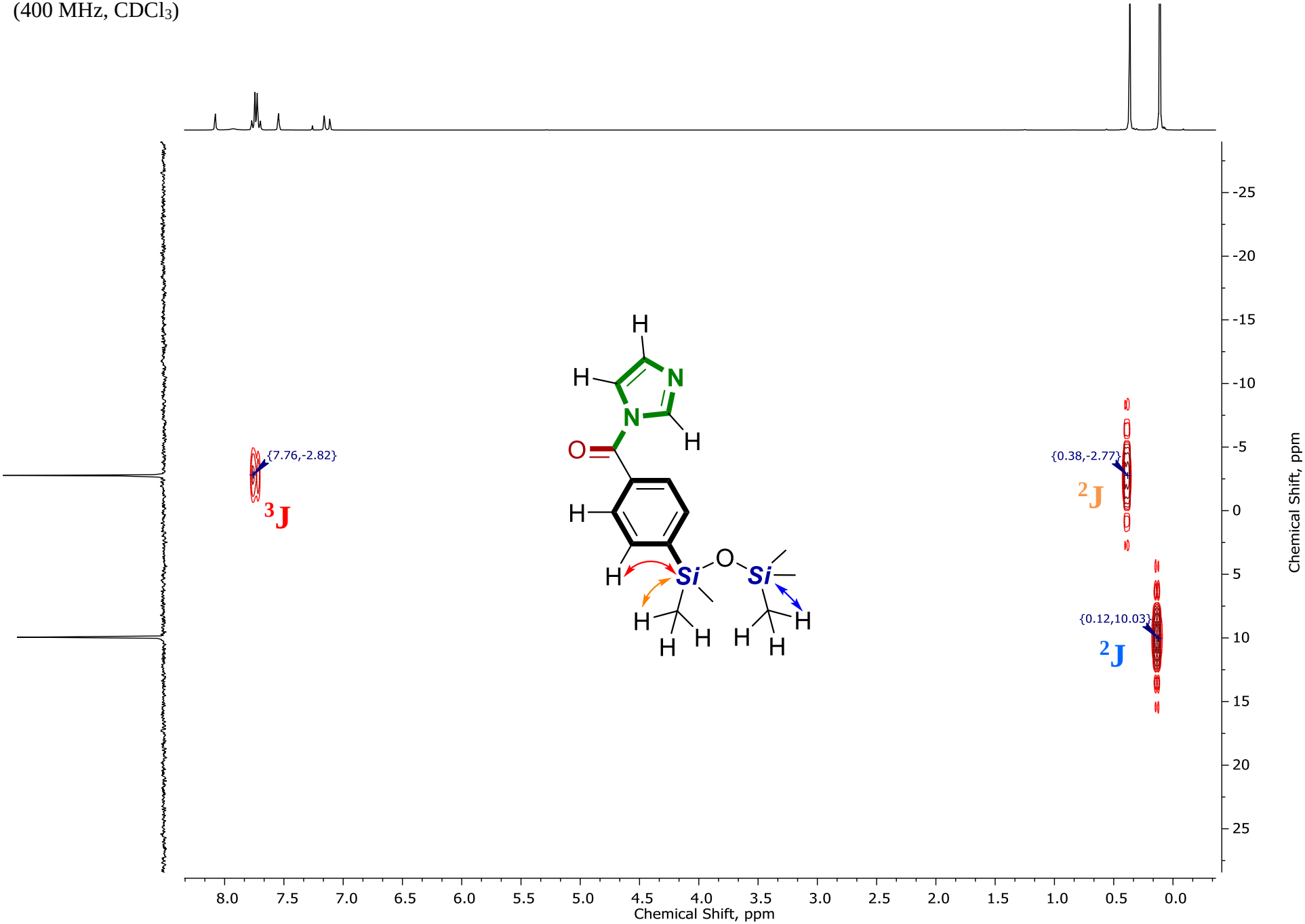
^{1}H - ^{13}C HSQC

(400 MHz, $CDCl_3$)



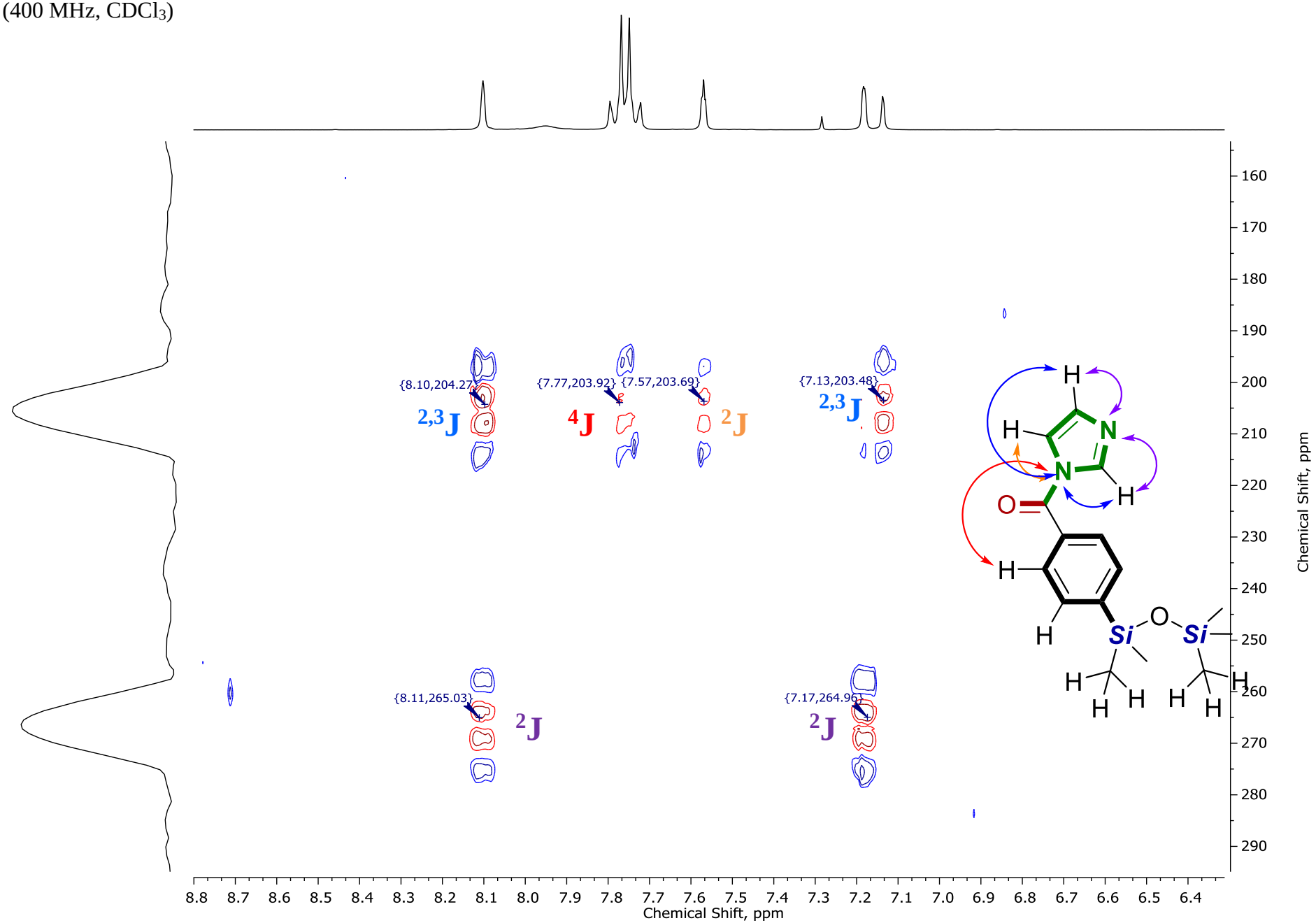
$^{1}H - ^{29}Si$ HMBC

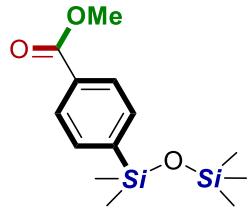
(400 MHz, $CDCl_3$)



$^{1}H - ^{15}N$ HMBC

(400 MHz, $CDCl_3$)



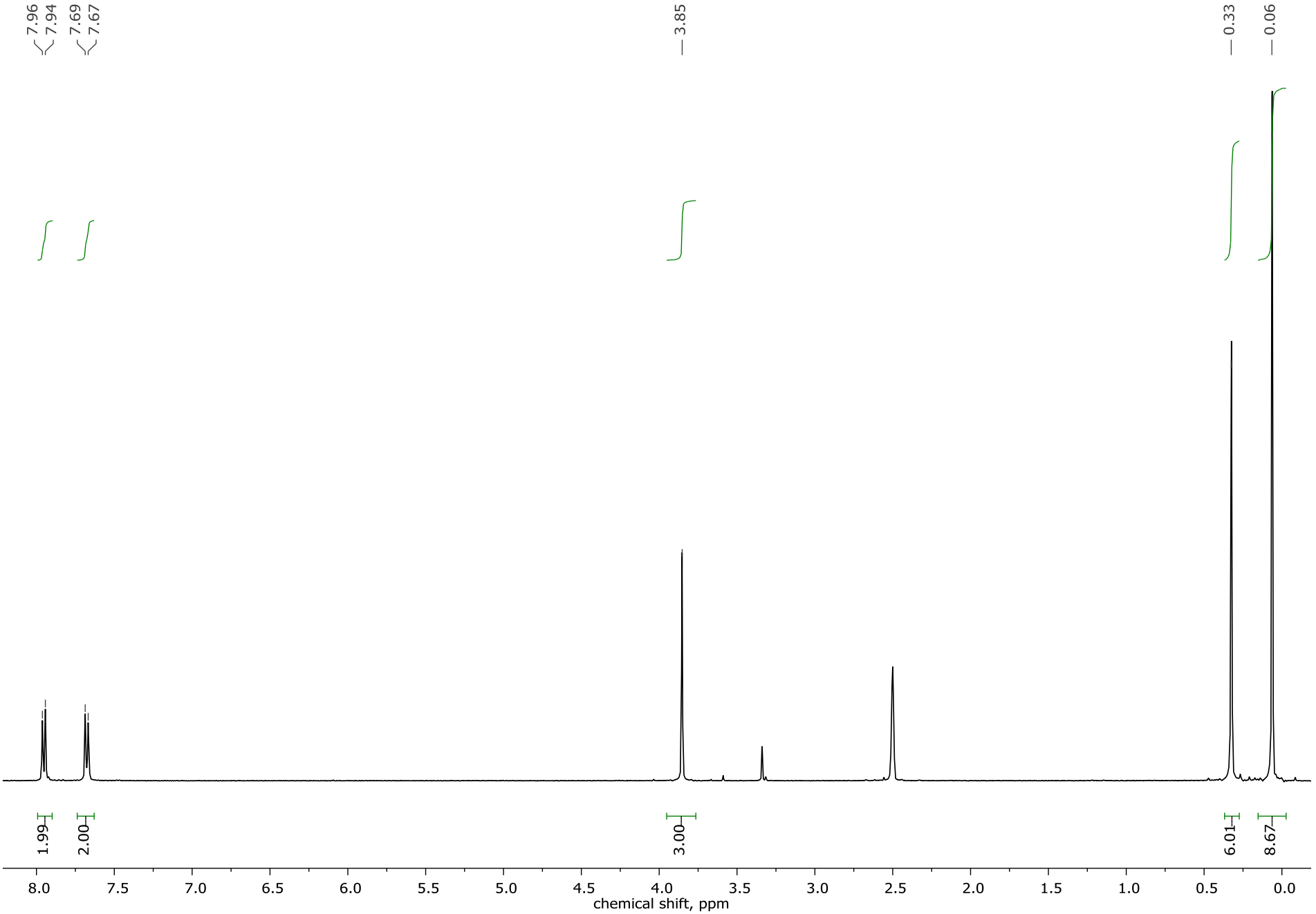


Characterisation data for methyl 4-(1,1,3,3,3-pentamethyldisiloxaneyl)benzoate:

^{1}H NMR (400 MHz, DMSO-d6): δ = 7.95 (d, ^{3}J=8 Hz, 2H), δ = 7.68 (d, ^{3}J=8 Hz, 2H), δ = 3.85 (s, 3H), δ = 0.33 (s, 6H), δ = 0.06 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d6): δ = 166.71, 146.07, 133.52, 130.79, 128.66, 52.57, 2.34, 1.06. ^{29}Si NMR (80 MHz, DMSO-d6): δ = 9.48, -2.06. HRMS (ESI) m/z z $[M + NH_4]^+$: calcd for $[C_{20}H_{26}O_5Si_2 + NH_4]^+$, 420.1657; found, 420.1656; $[M + Na]^+$: calcd for $[C_{20}H_{26}O_5Si_2 + Na]^+$, 425.1211; found, 425.1214; $[M + K]^+$: calcd for $[C_{20}H_{26}O_5Si_2 + K]^+$, 441.0950; found, 441.0948. IR (cm^{-1}): 2957, 1938, 1730, 1601, 1557, 1499, 1436, 1389, 1314-1256, 1187-968, 876-638.

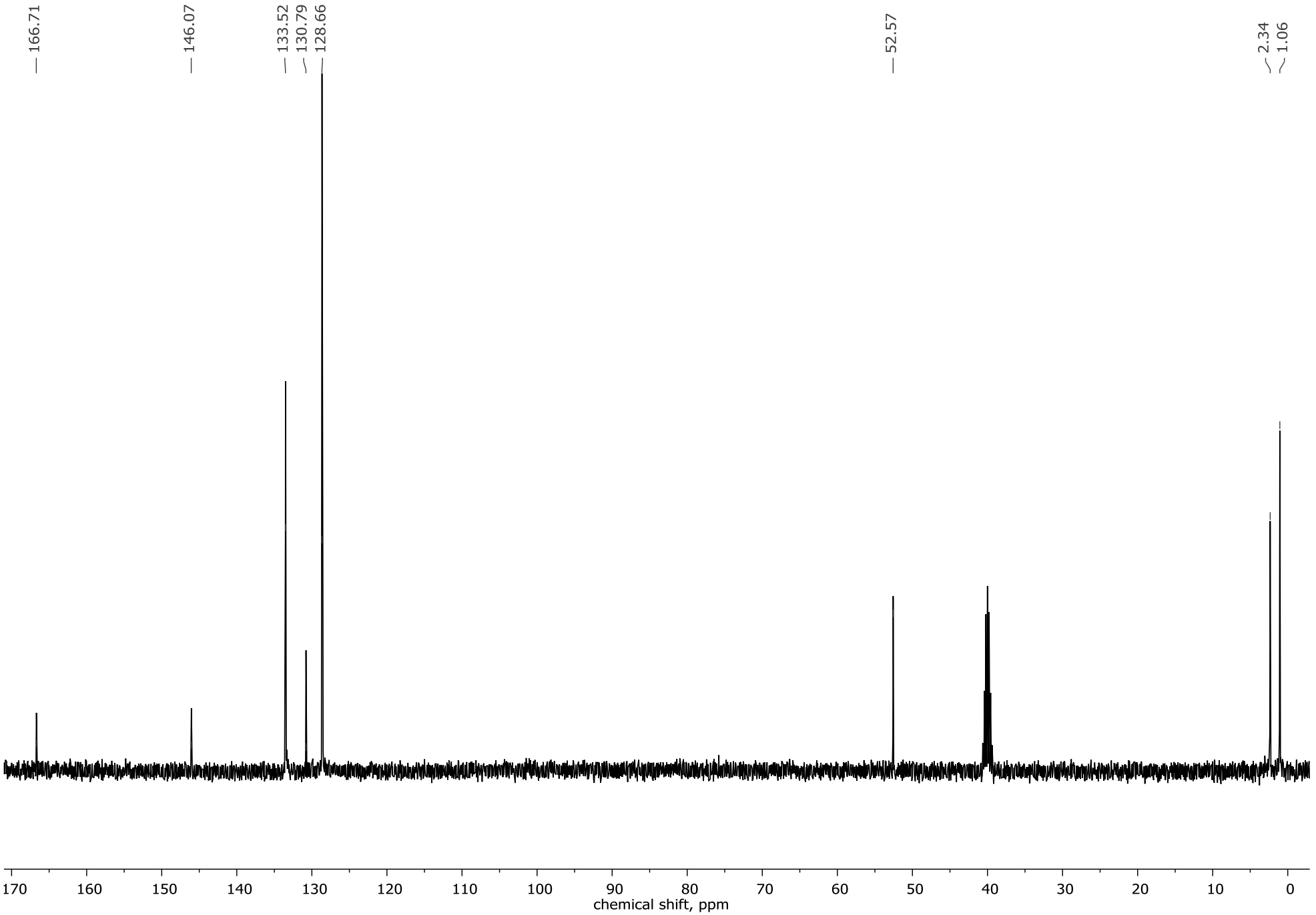
^{1}H NMR

(400 MHz, DMSO-d6)



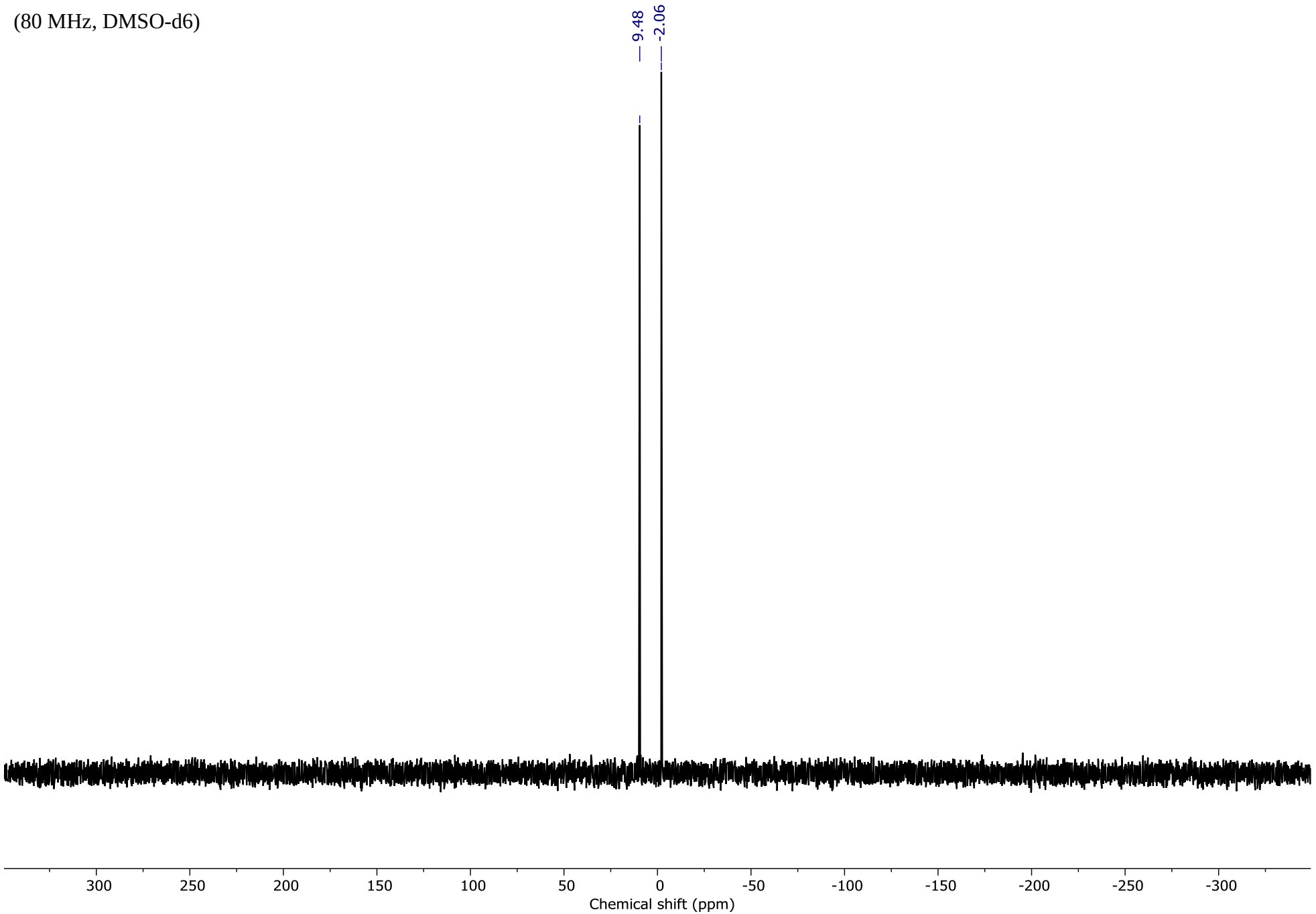
^{13}C NMR

(100 MHz, DMSO-d6)



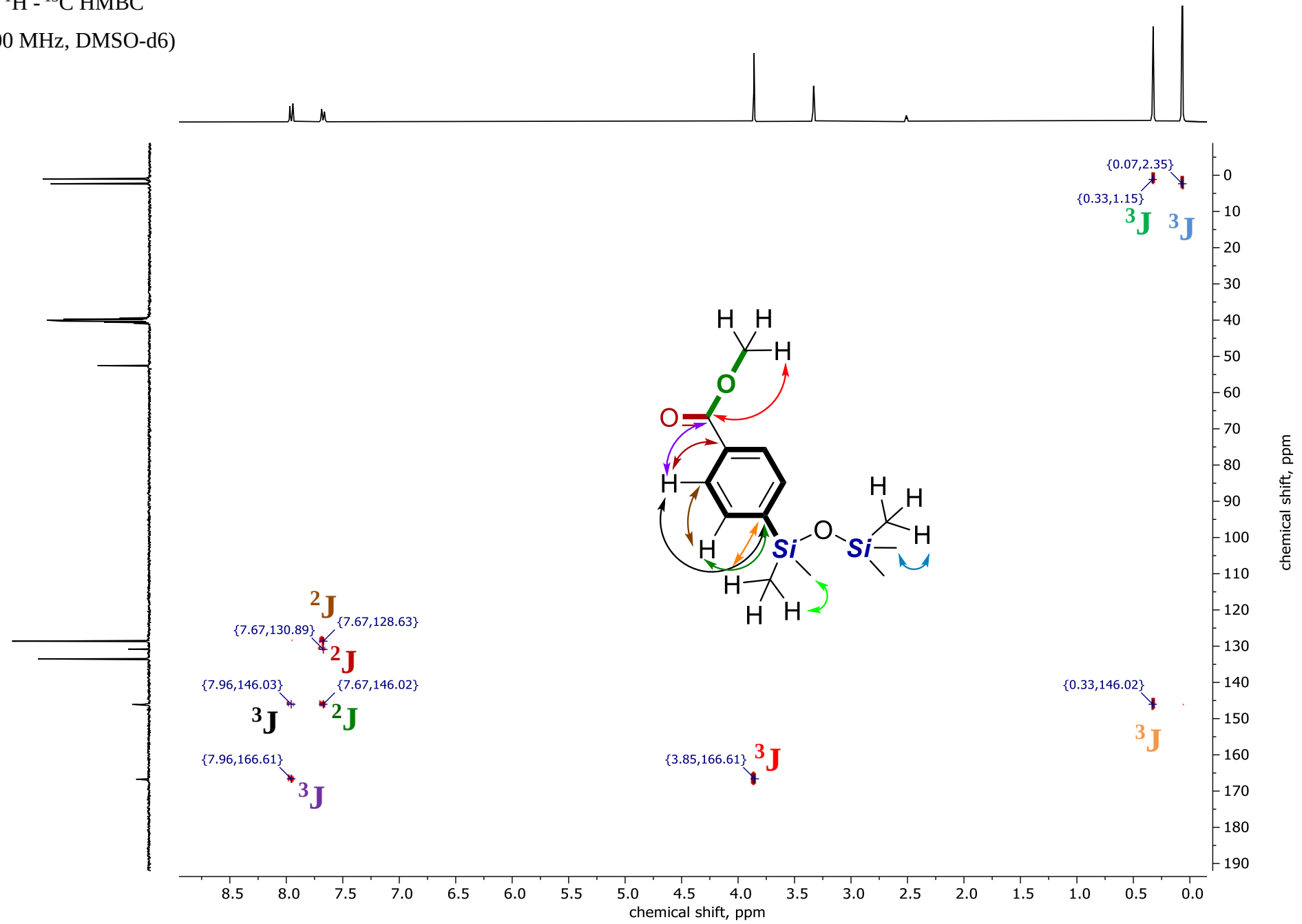
^{29}Si NMR

(80 MHz, DMSO-d6)



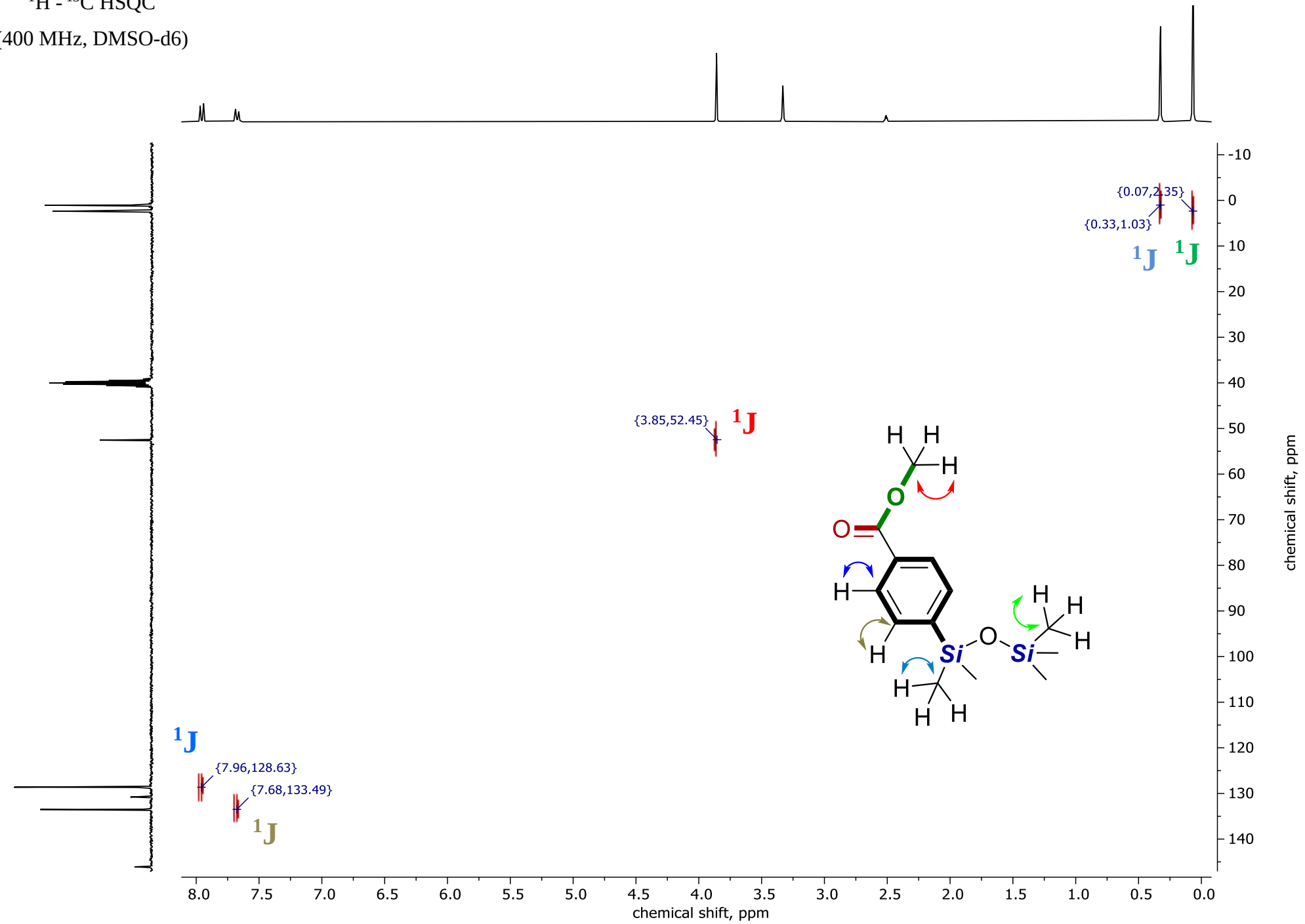
^{1}H - ^{13}C HMBC

(400 MHz, DMSO-d6)



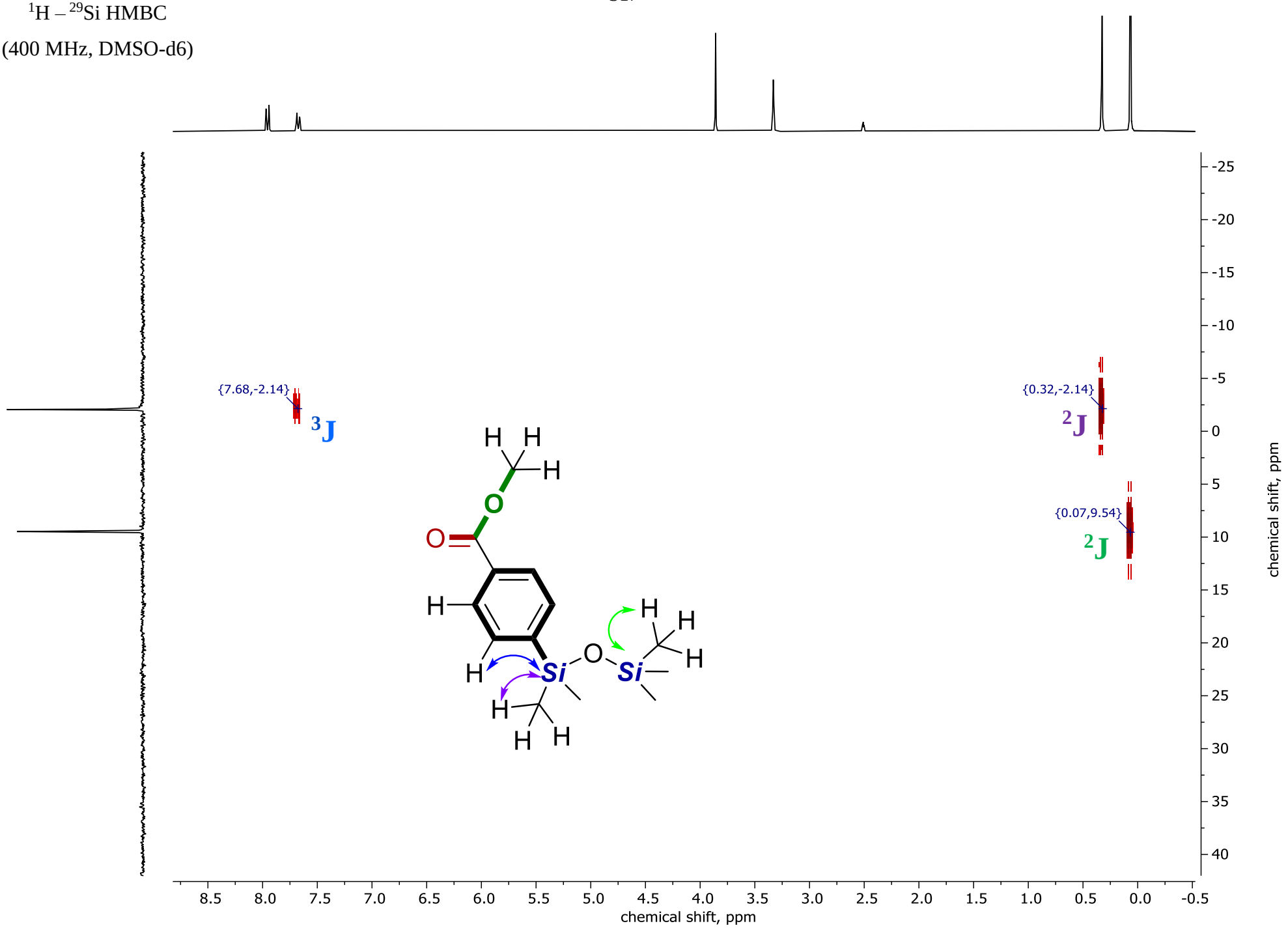
^{1}H - ^{13}C HSQC

(400 MHz, DMSO-d6)

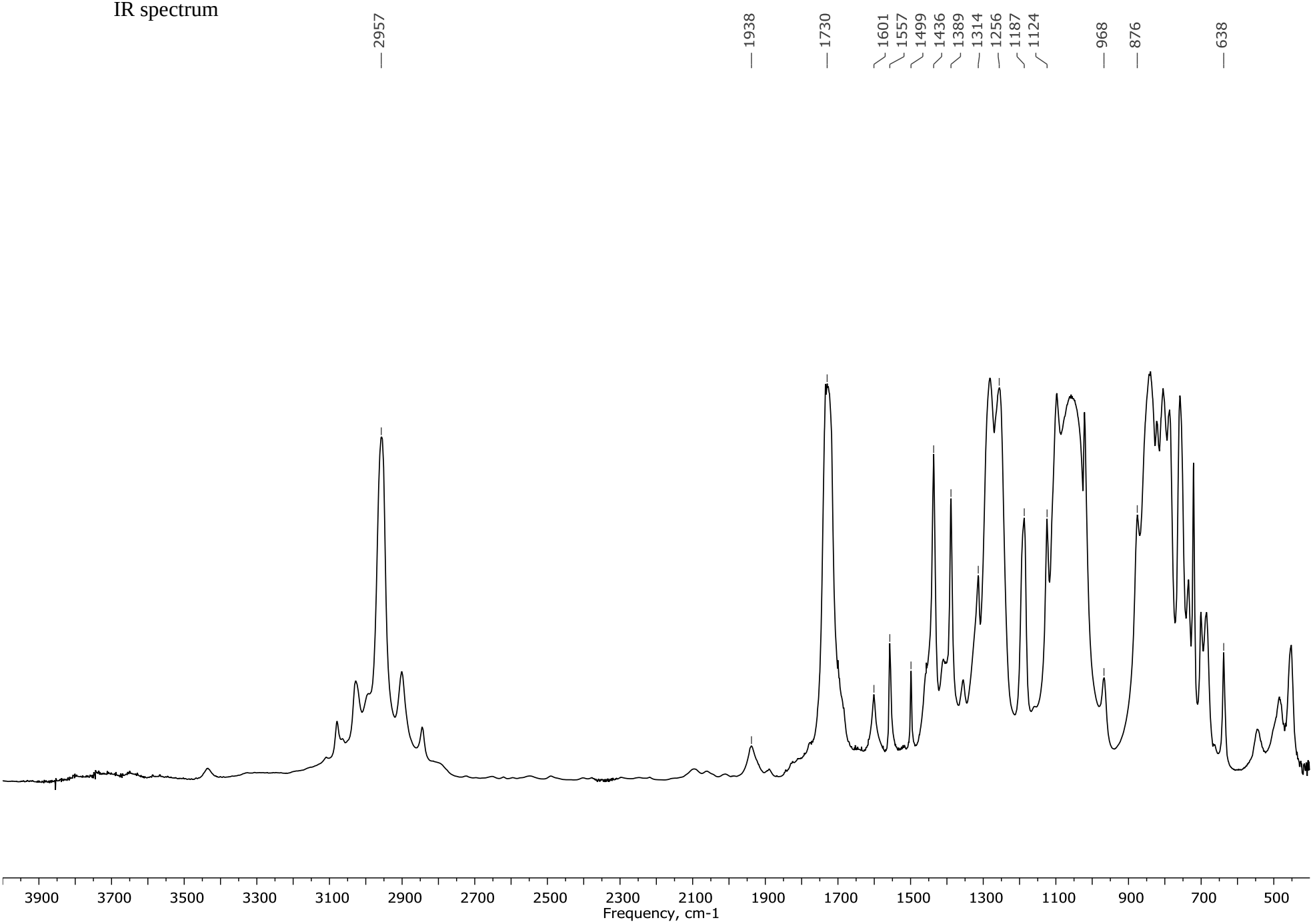


$^{1}H - ^{29}Si$ HMBC

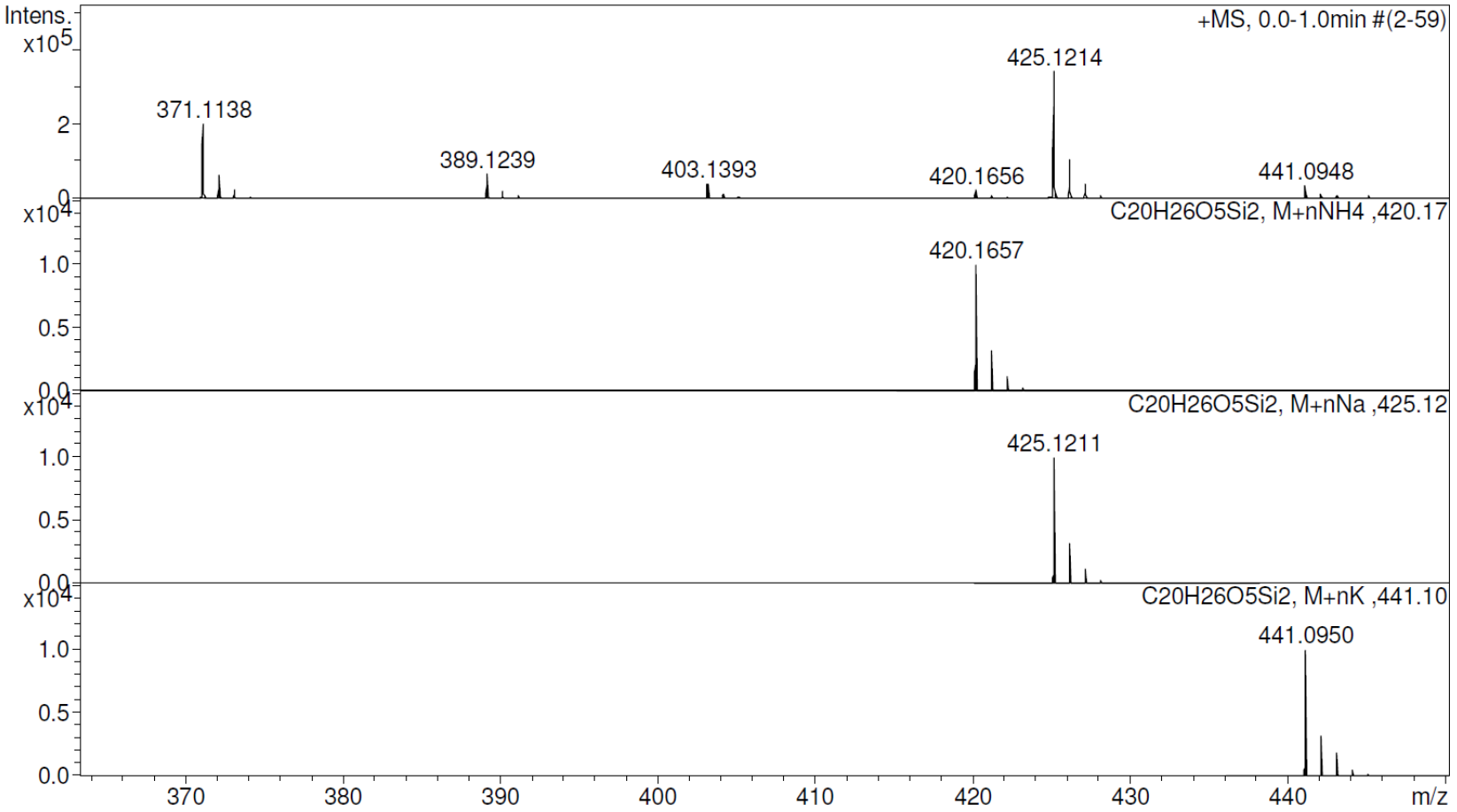
(400 MHz, DMSO-d6)

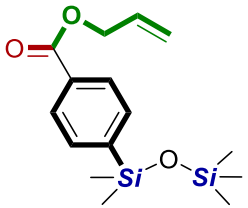


IR spectrum


2957
1938
1730
1601
1557
1499
1436
1389
1314
1256
1187
1124
968
876
638
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

HRMS (ESI)


Intens.
x10^5
+MS, 0.0-1.0min #(2-59)
425.1214
371.1138
389.1239
403.1393
420.1656
441.0948
x10^4
C20H26O5Si2, M+nNH4 ,420.17
420.1657
x10^4
C20H26O5Si2, M+nNa ,425.12
425.1211
x10^4
C20H26O5Si2, M+nK ,441.10
441.0950
m/z

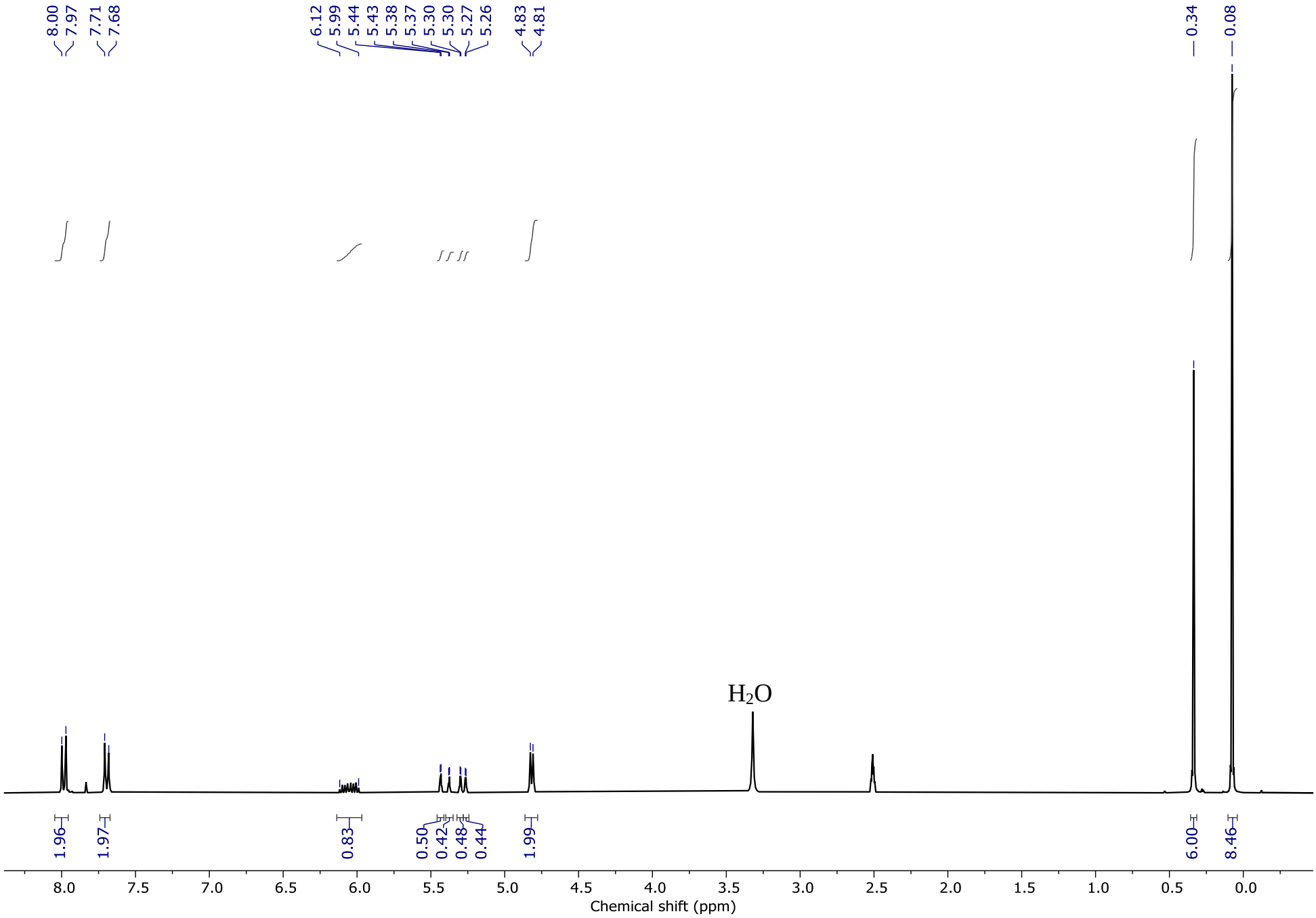


Characterisation data for allyl 4-(1,1,3,3,3-pentamethyldisiloxaneyl)benzoate:

^{1}H NMR (400 MHz, DMSO-*d6*): δ = 7.98 (d, ^{3}J= 11Hz, 2H), δ = 7.69 (d, ^{3}J= 11 Hz, 2H), δ = 6.12-5.99 (m, 1H), δ = 5.44-5.26 (m, 2H), δ = 4.81 (m, 2H), δ = 0.33 (s, 6H), δ = 0.07 (s, 8H). ^{13}C NMR (100 MHz, DMSO-*d6*): δ = 165.39, 145.77, 133.11, 132.58, 130.27, 128.20, 117.82, 65.04, 1.91, 0.60. ^{29}Si NMR (80 MHz, DMSO-*d6*): δ = 9.54, -2.03. HRMS (ESI) m/z z $[M + H]^{+}$: calcd for $[C_{15}H_{24}O_3Si_2 + H]^{+}$, 309.1337; found, 309.1328; $[M + Na]^{+}$: calcd for $[C_{15}H_{24}O_3Si_2 + Na]^{+}$, 331.1156; found, 331.1154. IR (cm^{-1}): 2958, 1724, 1558, 1389, 1275, 1186, 1095-975, 932, 876-638.

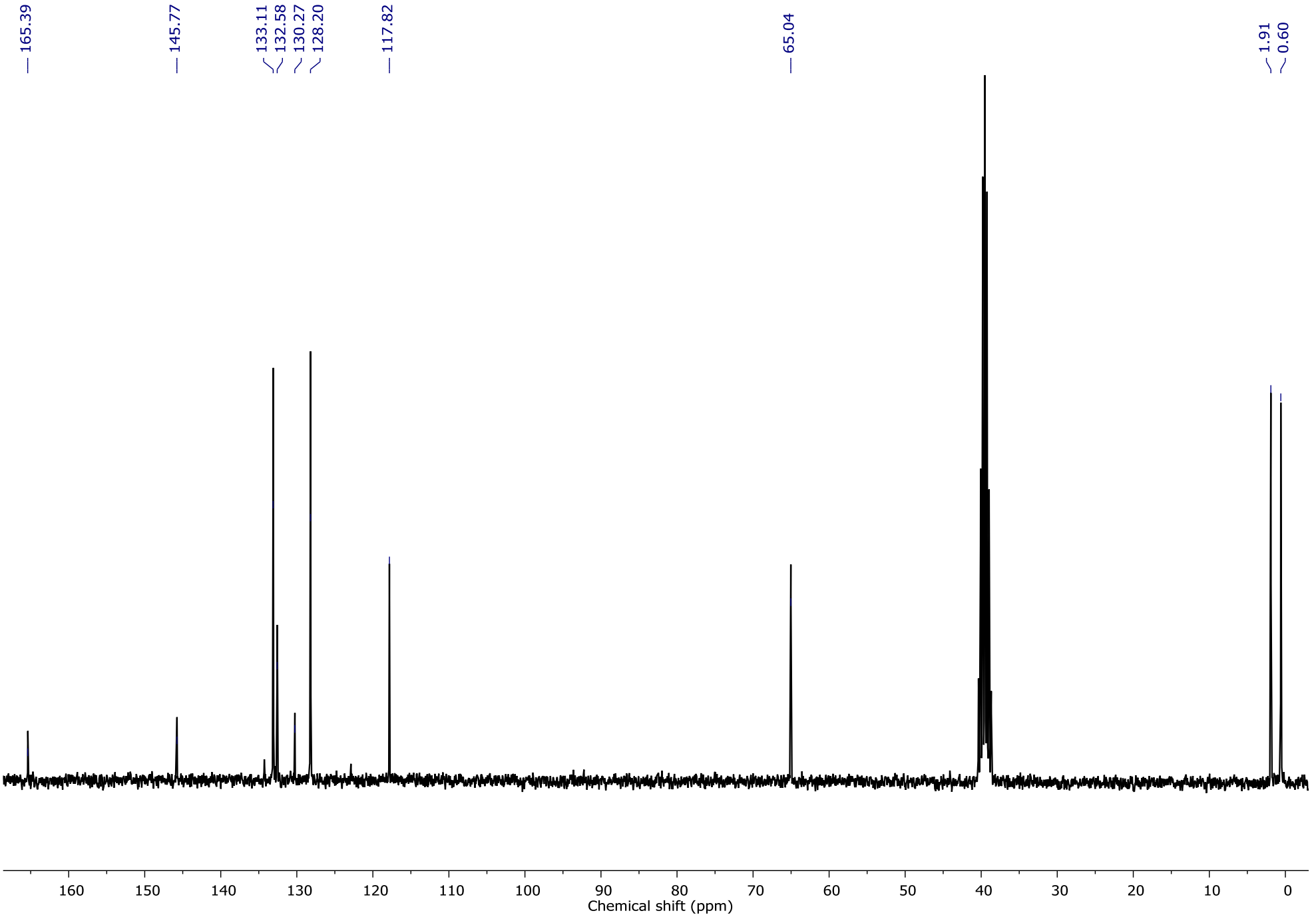
^{1}H NMR

(400 MHz, DMSO-d6)



^{13}C NMR

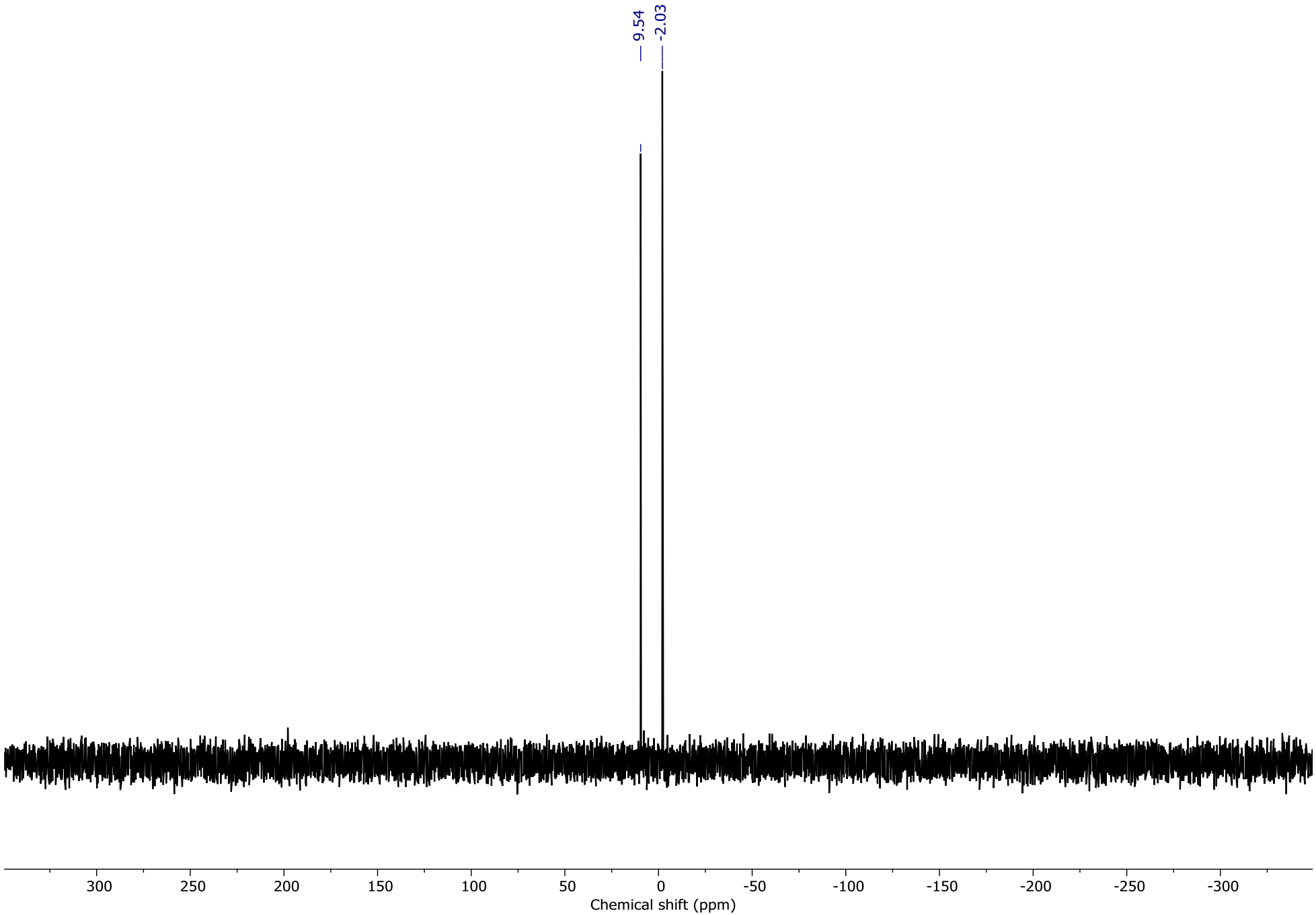
(100 MHz, DMSO-d6)



^{29}Si NMR

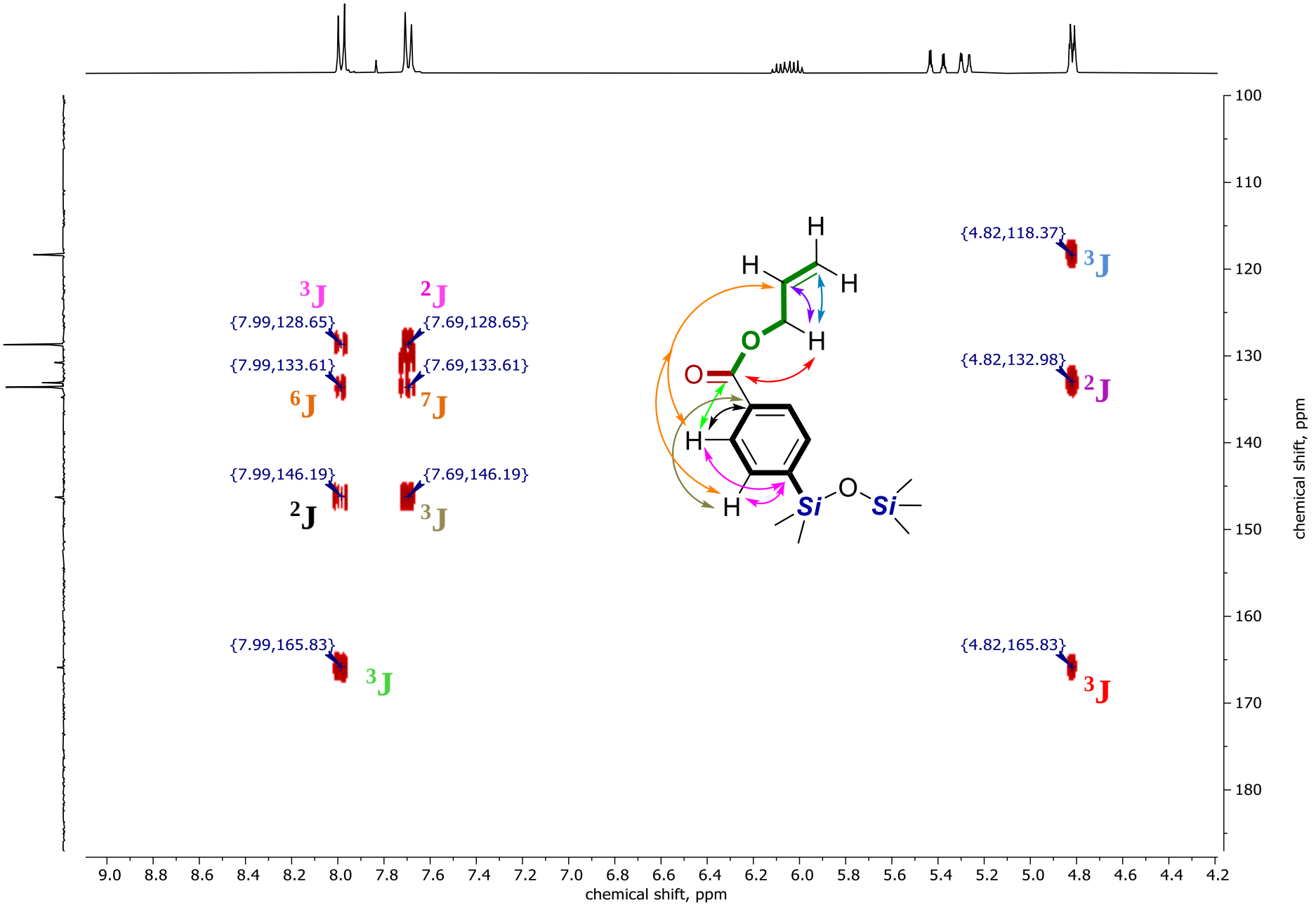
(80 MHz, DMSO-d6)

S23



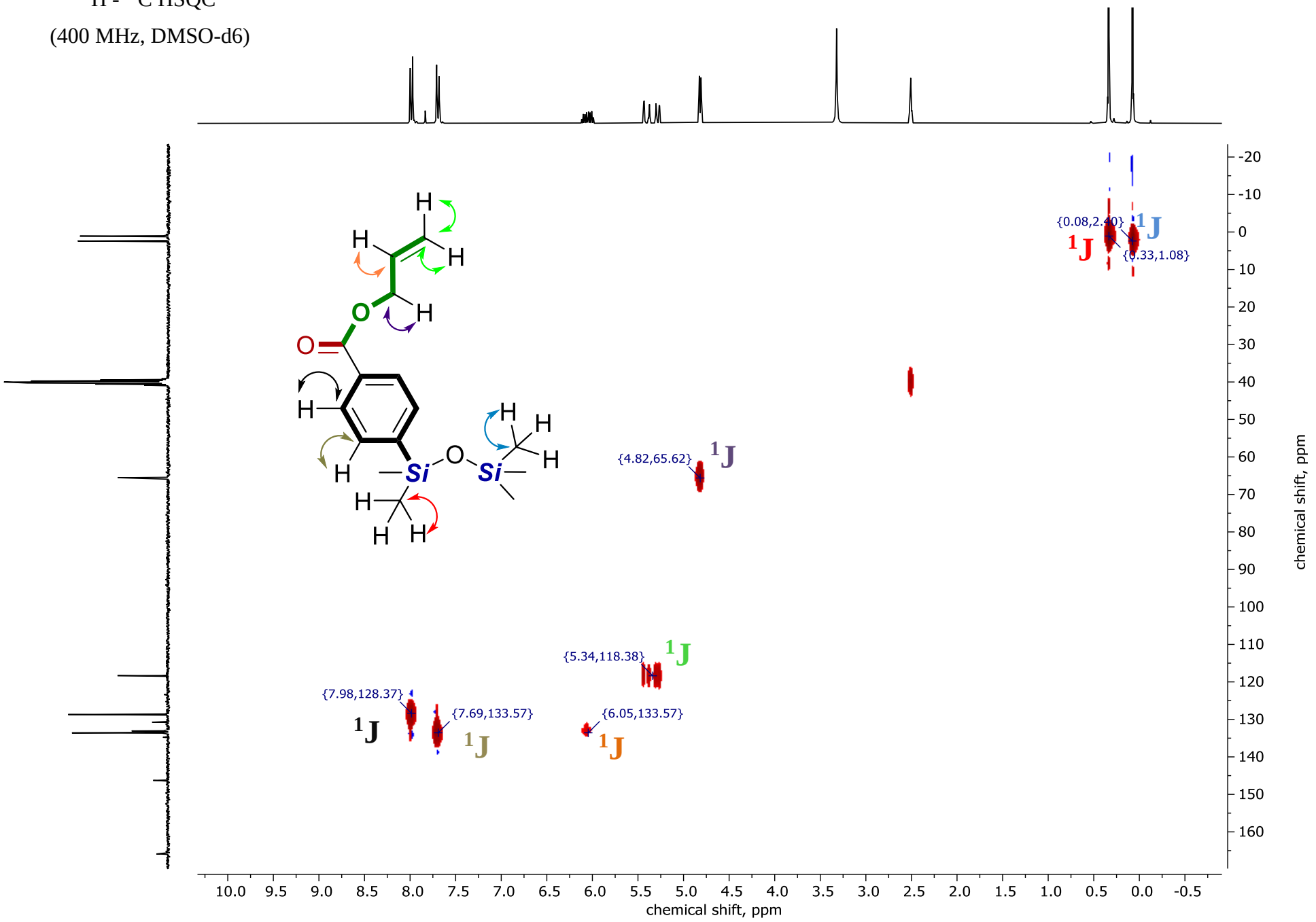
^{1}H - ^{13}C HMBC

(400 MHz, DMSO-d6)



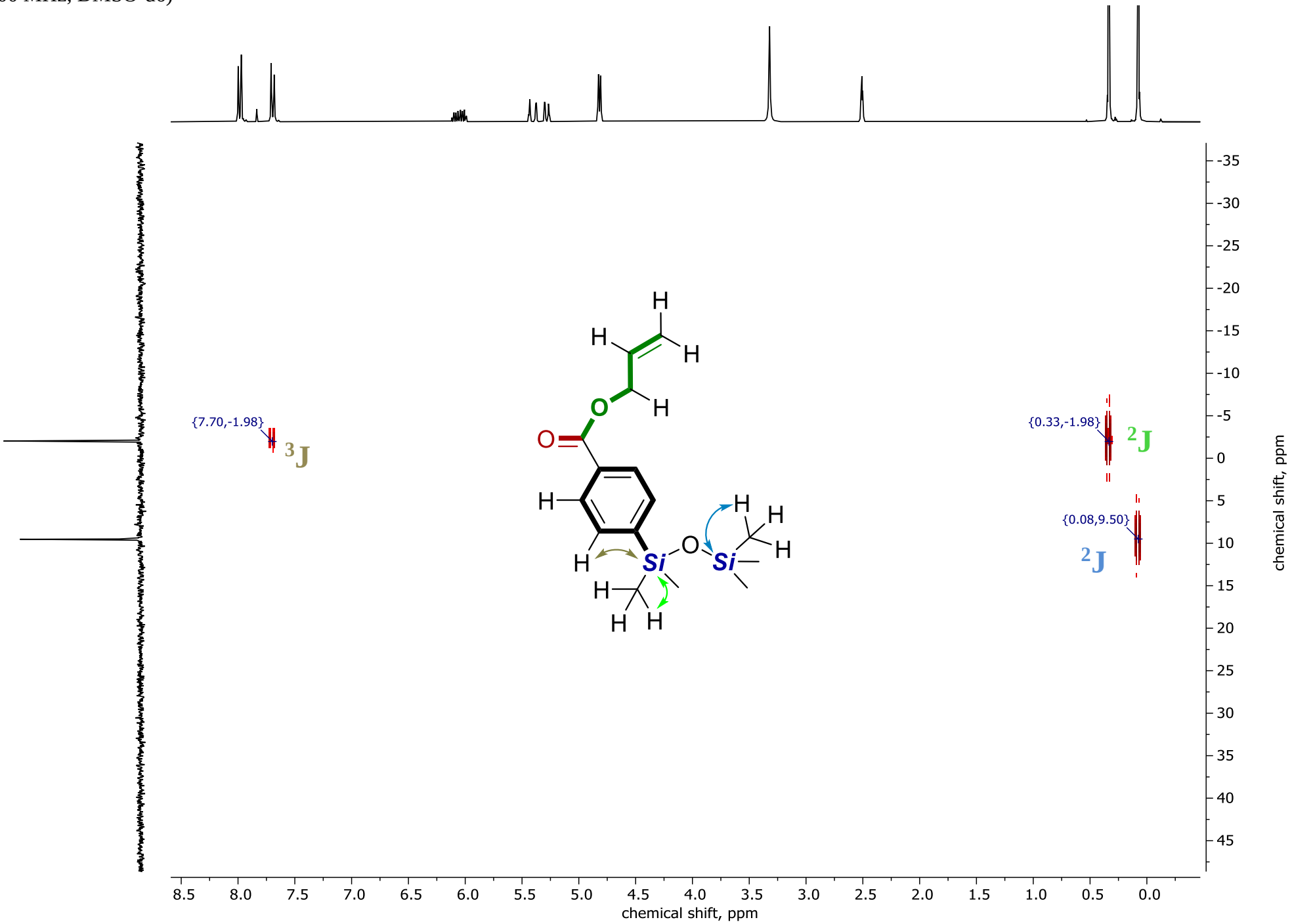
^{1}H - ^{13}C HSQC

(400 MHz, DMSO-d6)

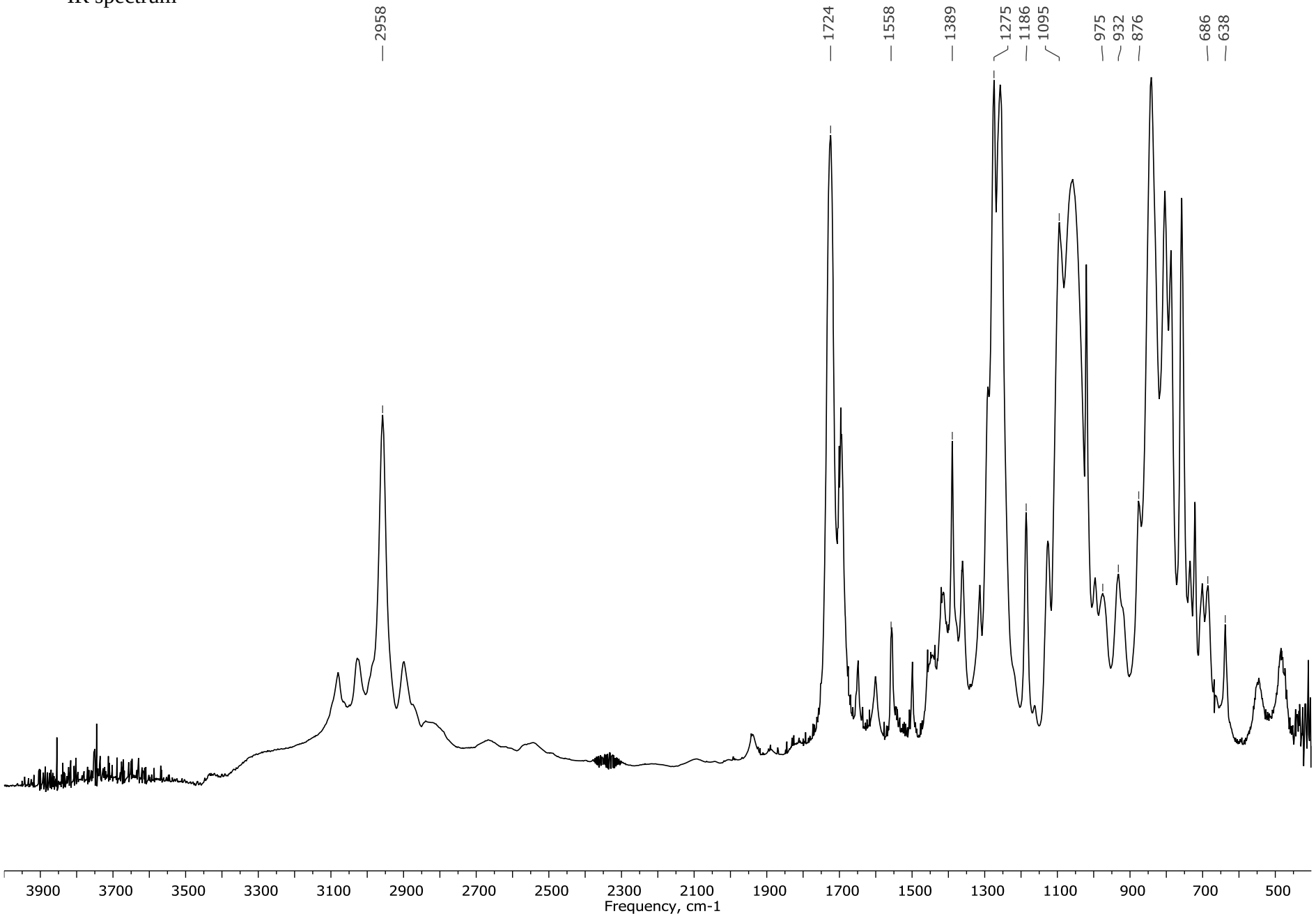


^{1}H - ^{29}Si HMBC

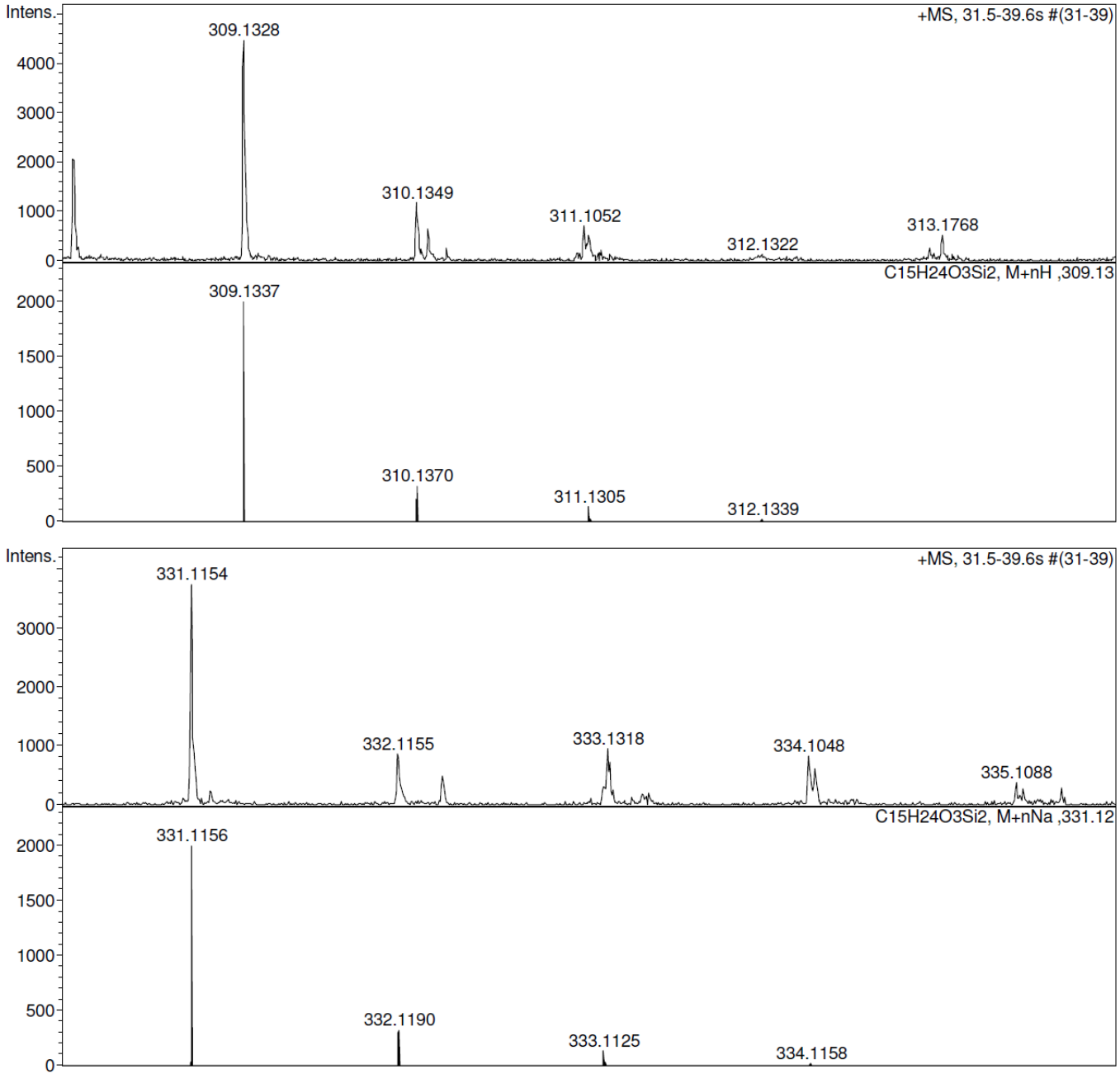
(400 MHz, DMSO-d6)

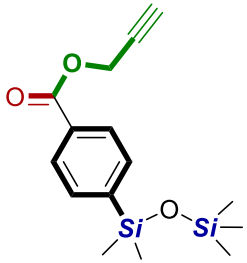


IR spectrum


2958
1724
1558
1389
1275
1186
1095
975
932
876
686
638
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

HRMS (ESI)


Intens.
+MS, 31.5-39.6s #(31-39)
309.1328
310.1349
311.1052
312.1322
313.1768
C15H24O3Si2, M+nH ,309.13
309.1337
310.1370
311.1305
312.1339
Intens.
+MS, 31.5-39.6s #(31-39)
331.1154
332.1155
333.1318
334.1048
335.1088
C15H24O3Si2, M+nNa ,331.12
331.1156
332.1190
333.1125
334.1158

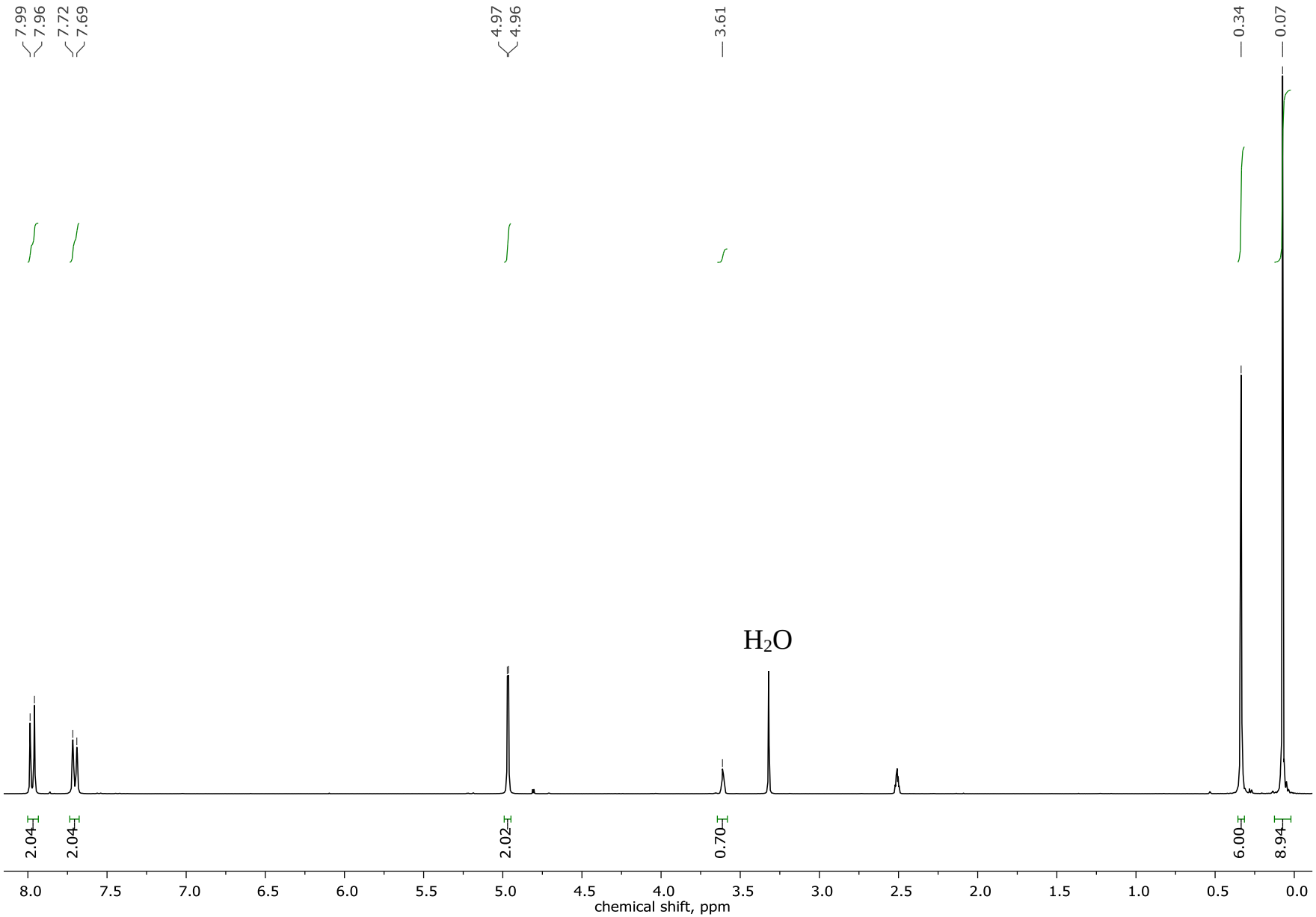


Characterisation data for prop-2-yn-1-yl 4-(1,1,3,3,3-pentamethyldisiloxaneyl)benzoate:

^{1}H NMR (400 MHz, DMSO-*d6*): δ = 7.96 (d, ^{3}J=11 Hz, 2H), δ = 7.71 (d, ^{3}J=11 Hz, 2H), δ = 4.97 (d, ^{4}J=3 Hz, 2H), δ = 3.61 (m, 1H), δ = 0.34 (s, 6H), δ = 0.07 (s, 9H). ^{13}C NMR (100 MHz, DMSO-*d6*): δ = 165.48, 146.59, 133.62, 130.14, 128.74, 78.78, 78.38, 52.94, 2.37, 1.05. ^{29}Si NMR (80 MHz, DMSO-*d6*): δ = -9.57, -2.04. IR (cm^{-1}): 3310, 2958, 1730, 1389, 1274, 1259, 1186, 1123-982, 876-788, 757-638.

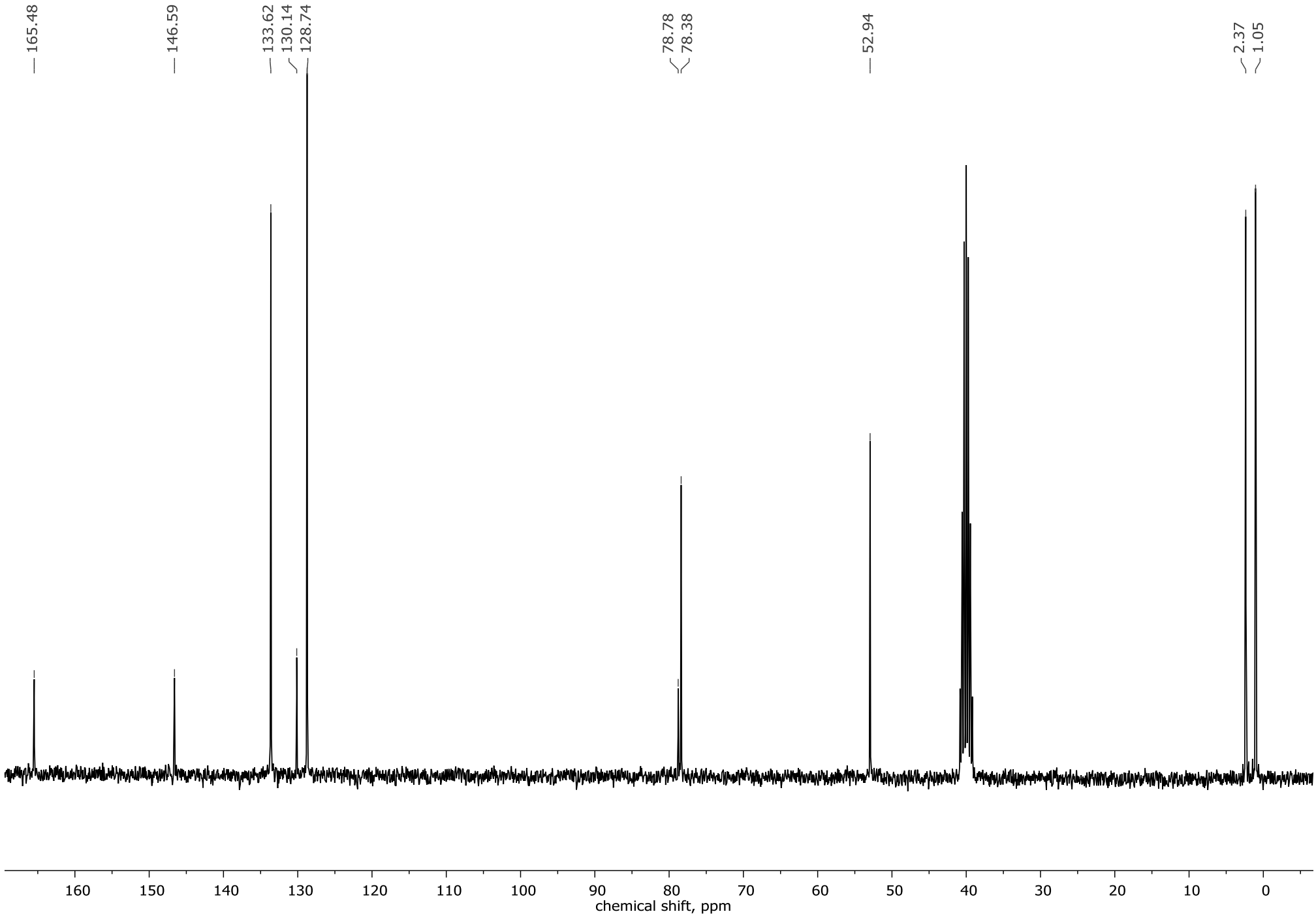
^{1}H NMR

(400 MHz, DMSO-d6)



^{13}C NMR

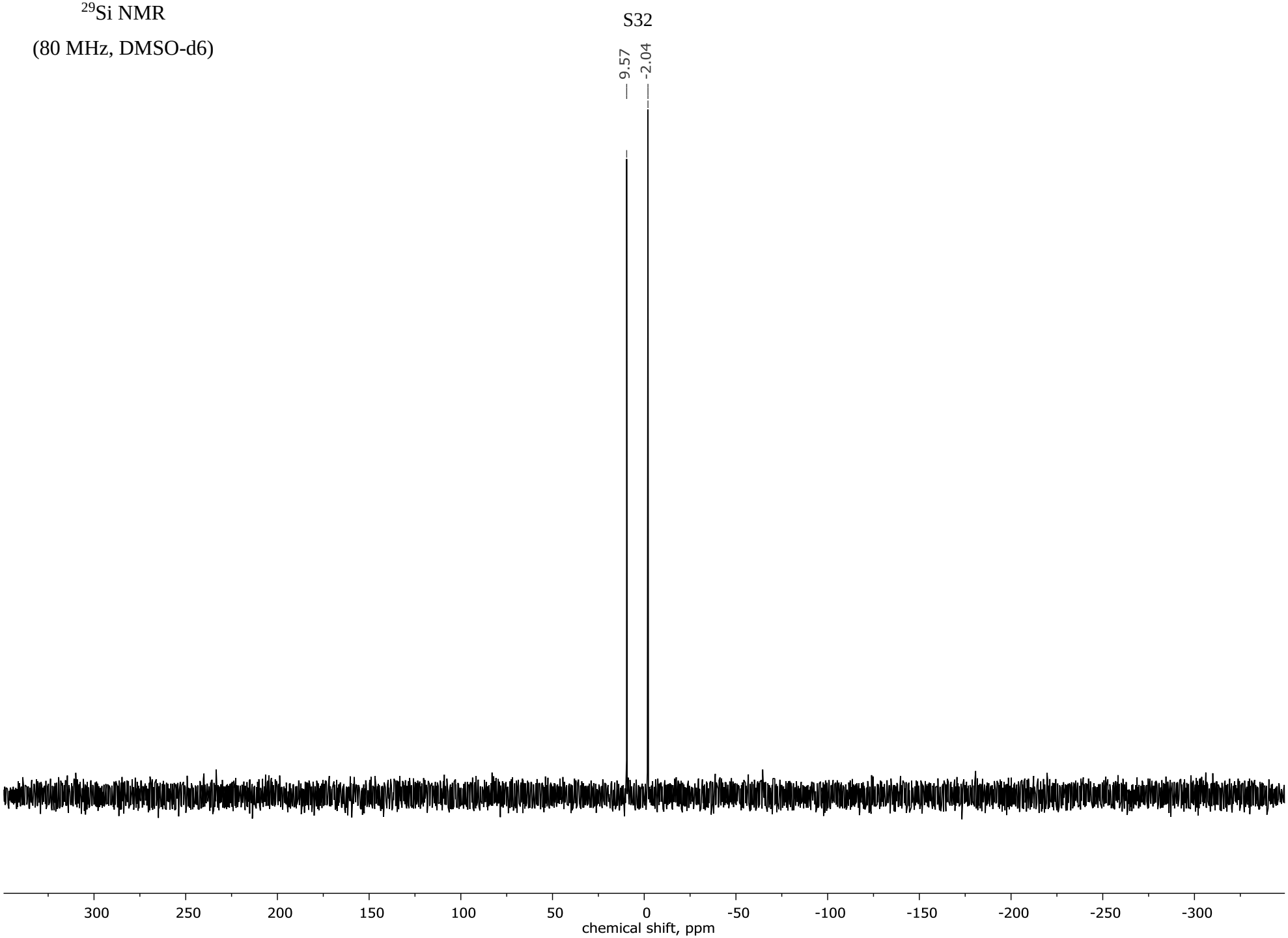
(100 MHz, DMSO-d6)



^{29}Si NMR

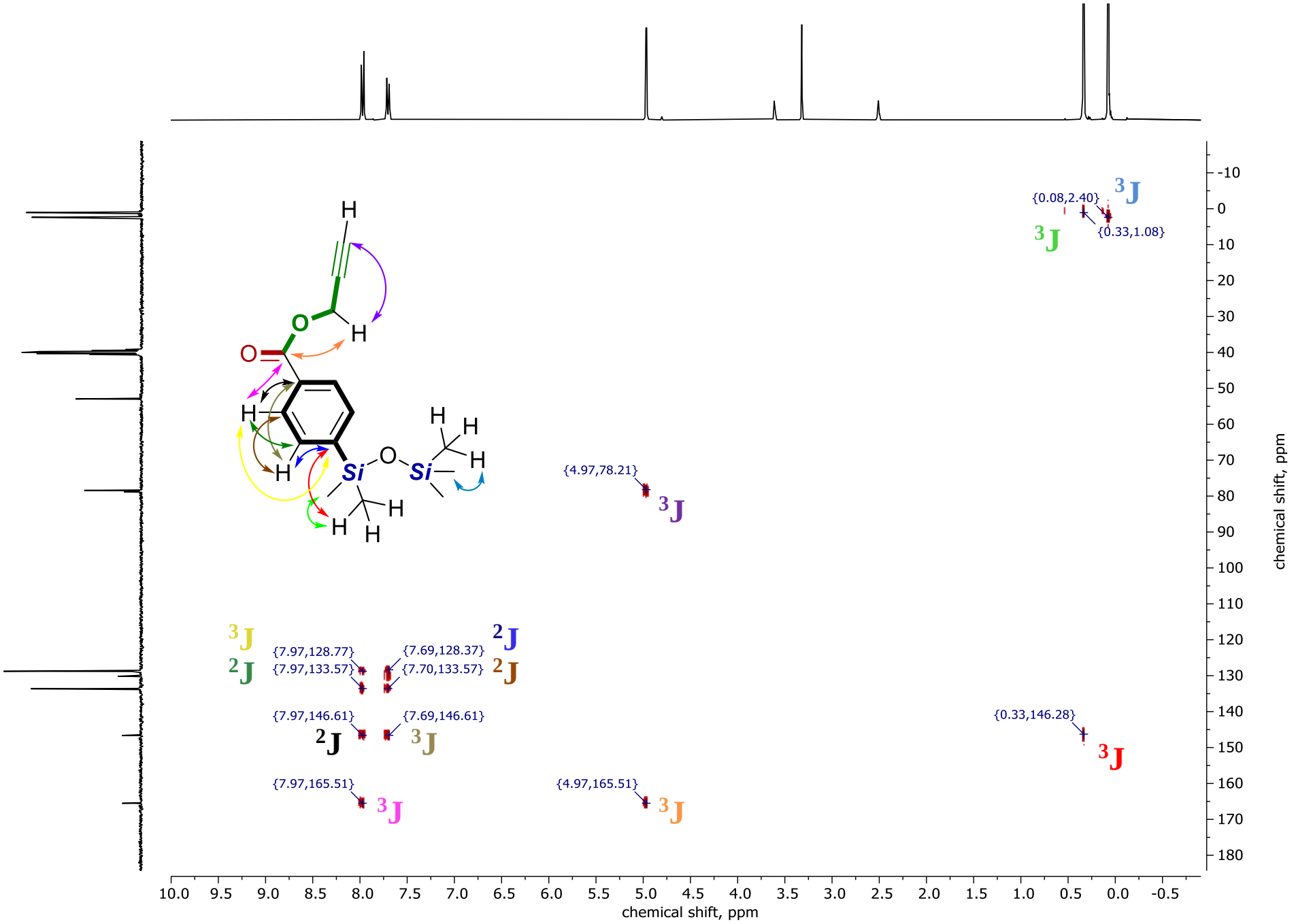
(80 MHz, DMSO-d6)

S32



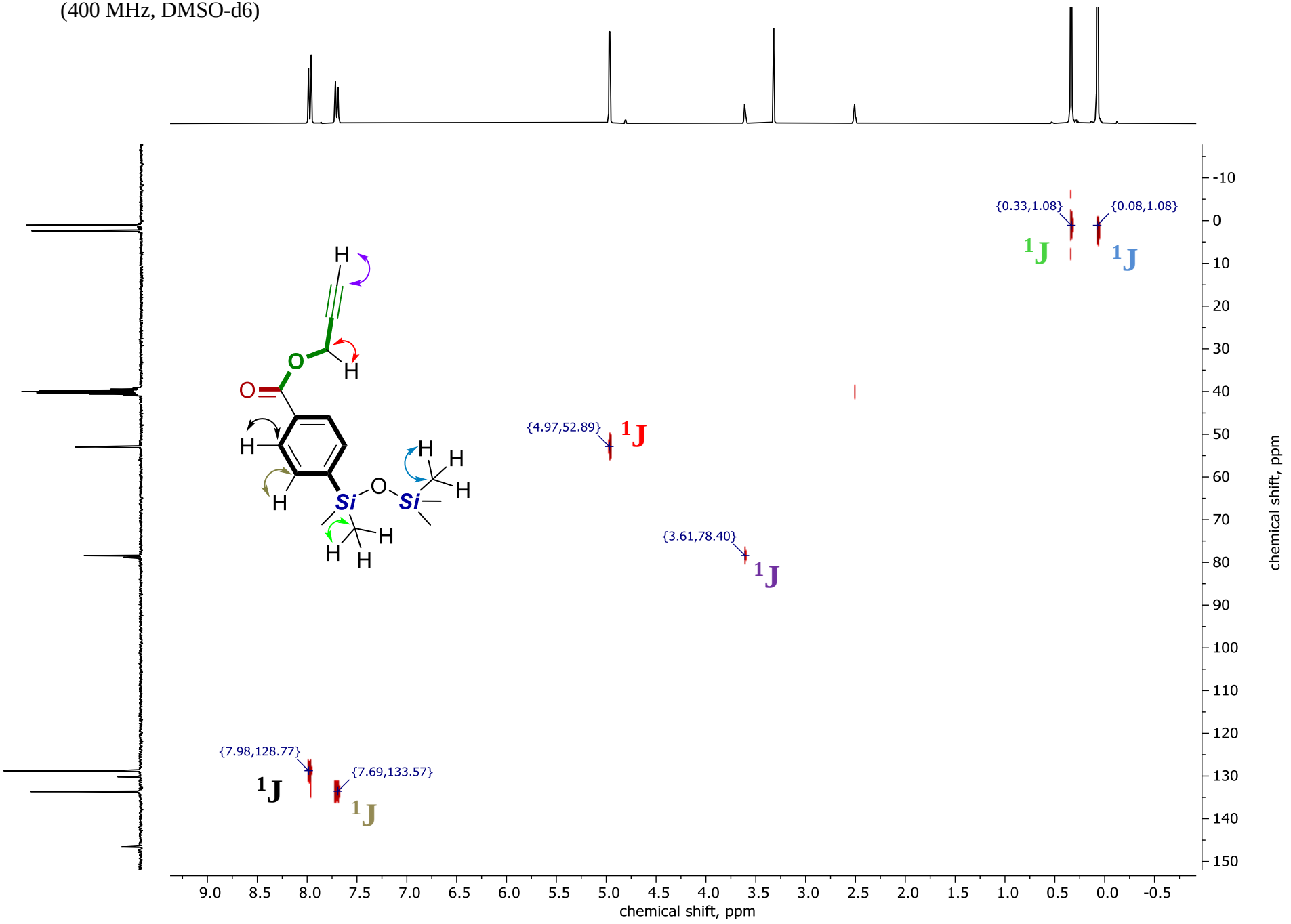
^{1}H - ^{13}C HMBC

(400 MHz, DMSO-d6)



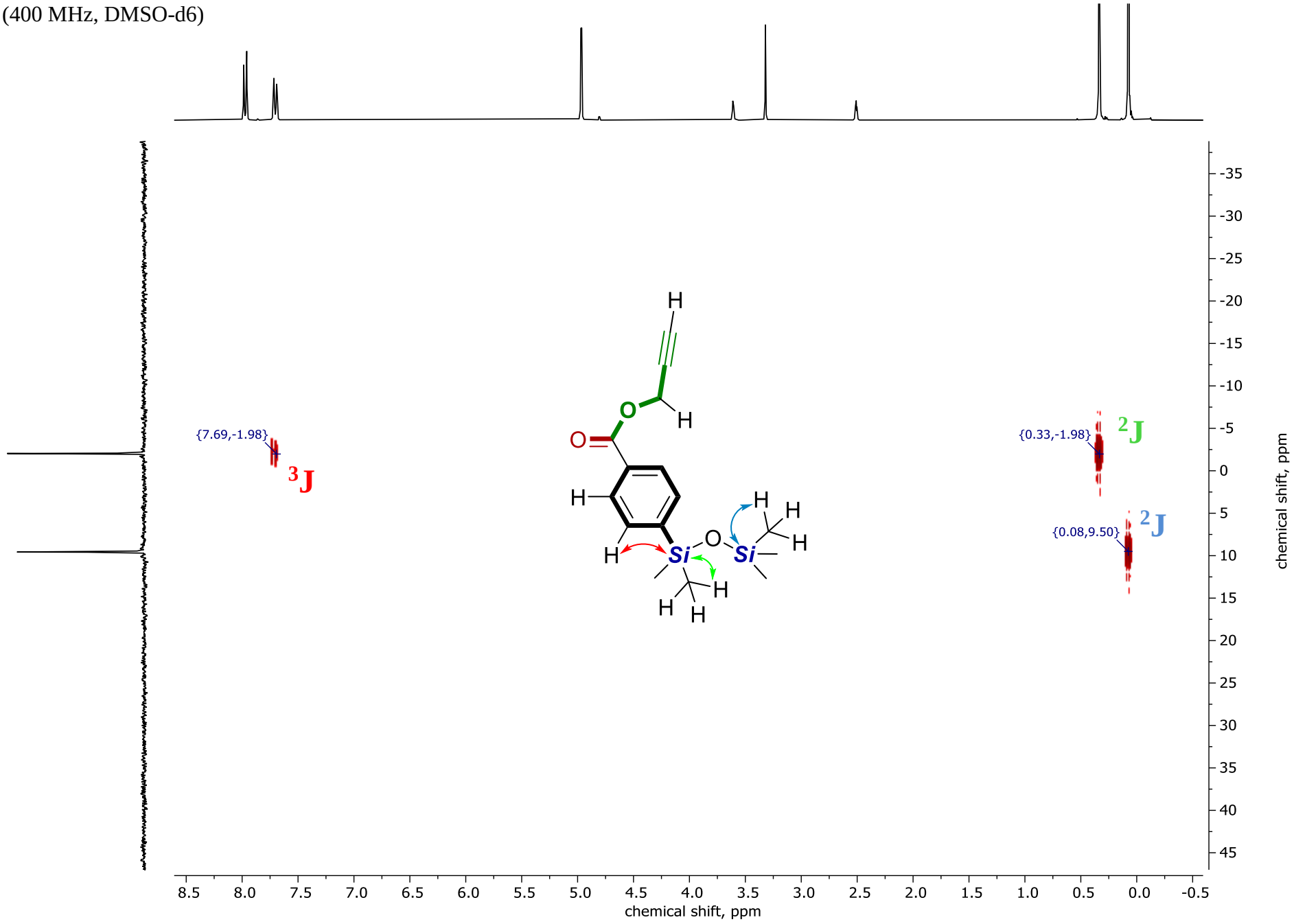
^{1}H - ^{13}C HSQC

(400 MHz, DMSO-d6)

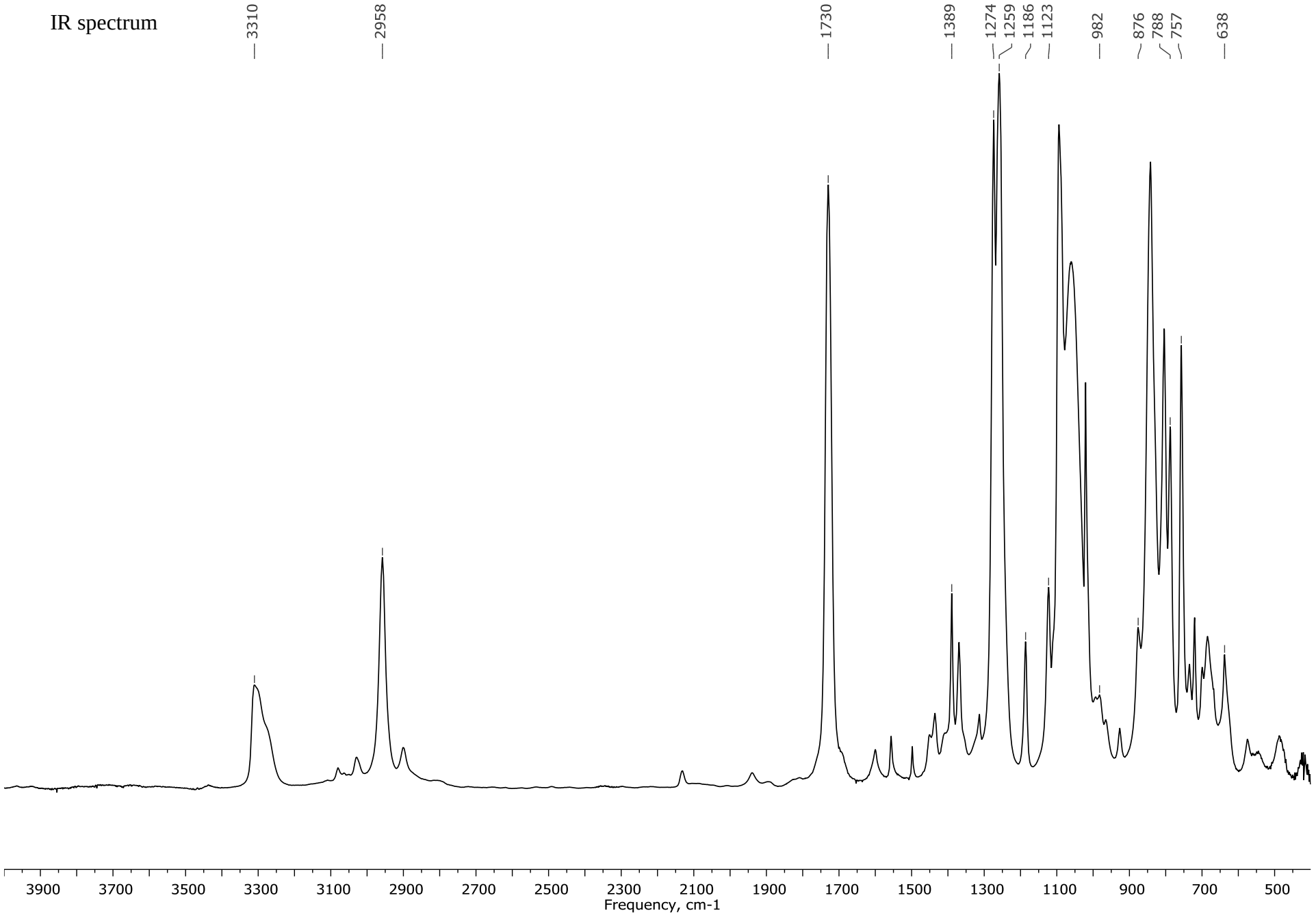


^{1}H - ^{29}Si HMBC

(400 MHz, DMSO-d6)



IR spectrum


3310
2958
1730
1389
1274
1259
1186
1123
982
876
788
757
638
3900
3700
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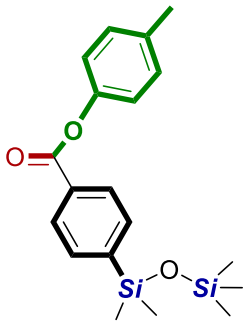
1700
1500
1300
1100
900
700
500
Frequency, cm-1

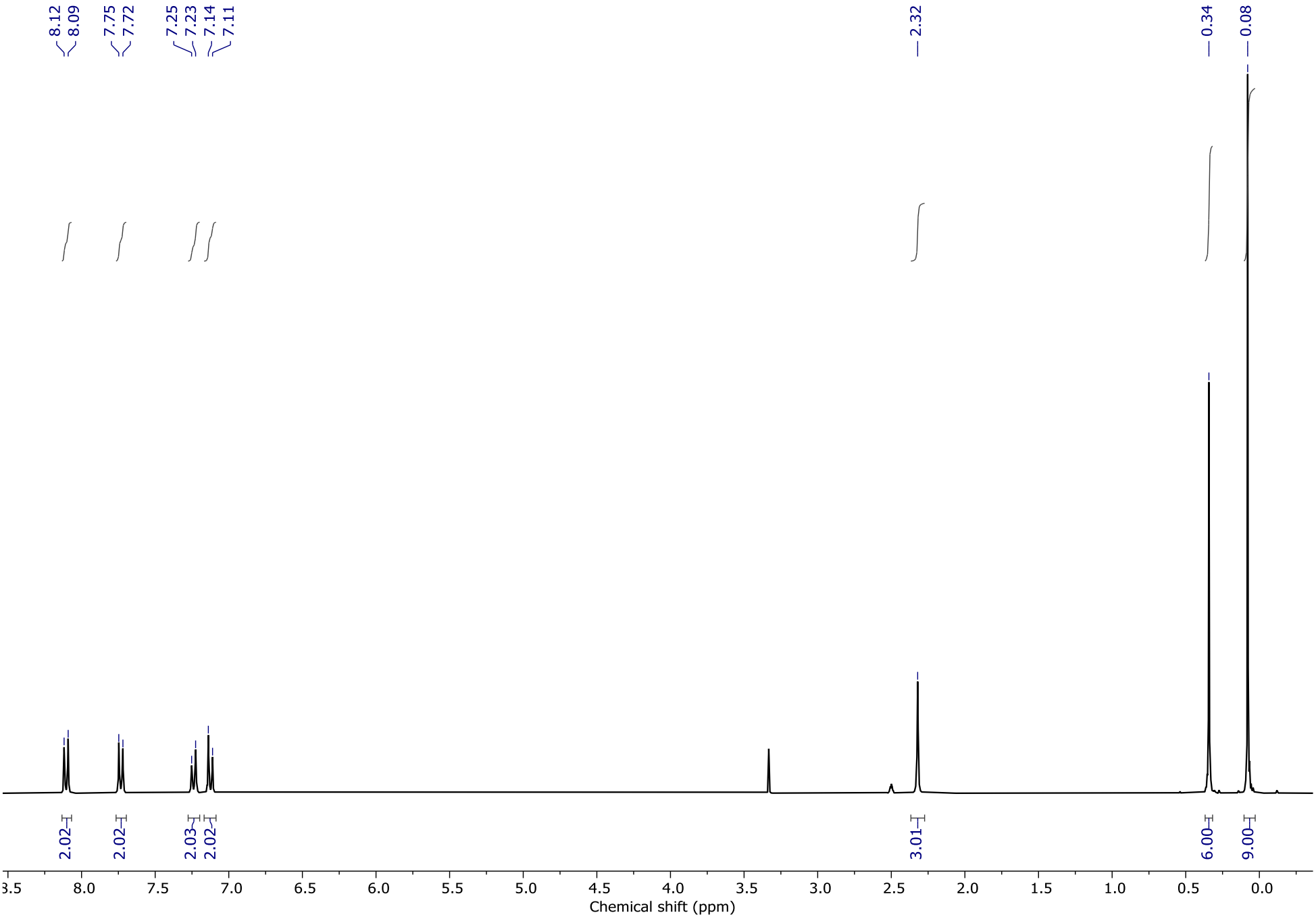


Characterisation data for p-tolyl 4-(1,1,3,3,3-pentamethyldisiloxaneyl)benzoate:

^{1}H NMR (400 MHz, DMSO-d6): δ = 8.11 (d, ^{3}J=11 Hz, 2H), δ = 7.74 (d, ^{3}J=1 Hz, 2H), δ = 7.24 (d, ^{3}J=11 Hz, 2H), δ = 7.13 (d, ^{3}J=11 Hz, 2H), δ = 2.32 (s, 3H), δ = 0.34 (s, 6H), δ = 0.08 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d6): δ = 164.62, 148.37, 146.39, 135.03, 133.12, 129.80, 129.71, 128.68, 121.42, 20.34, 1.82, 0.52. ^{29}Si NMR (80 MHz, DMSO-d6): δ = 9.54, -2.09. HRMS (ESI) m/z [M + H] $^{+}$: calcd for $[C_{19}H_{26}O_3Si_2 + H]^{+}$, 359.1493; found, 259.1508. [M + NH_4] $^{+}$: calcd for $[C_{19}H_{26}O_3Si_2 + NH_4]^{+}$, 376.1759; found, 376.1777. [M + Na] $^{+}$: calcd for $[C_{19}H_{26}O_3Si_2 + Na]^{+}$, 381.1313; found, 381.1320. [M + K] $^{+}$: calcd for $[C_{19}H_{26}O_3Si_2 + K]^{+}$, 397.1052; found, 397.1063. IR (cm^{-1}): 2956, 1738, 1509, 1389, 1258, 1199, 1166, 1117,-1018, 875-753.

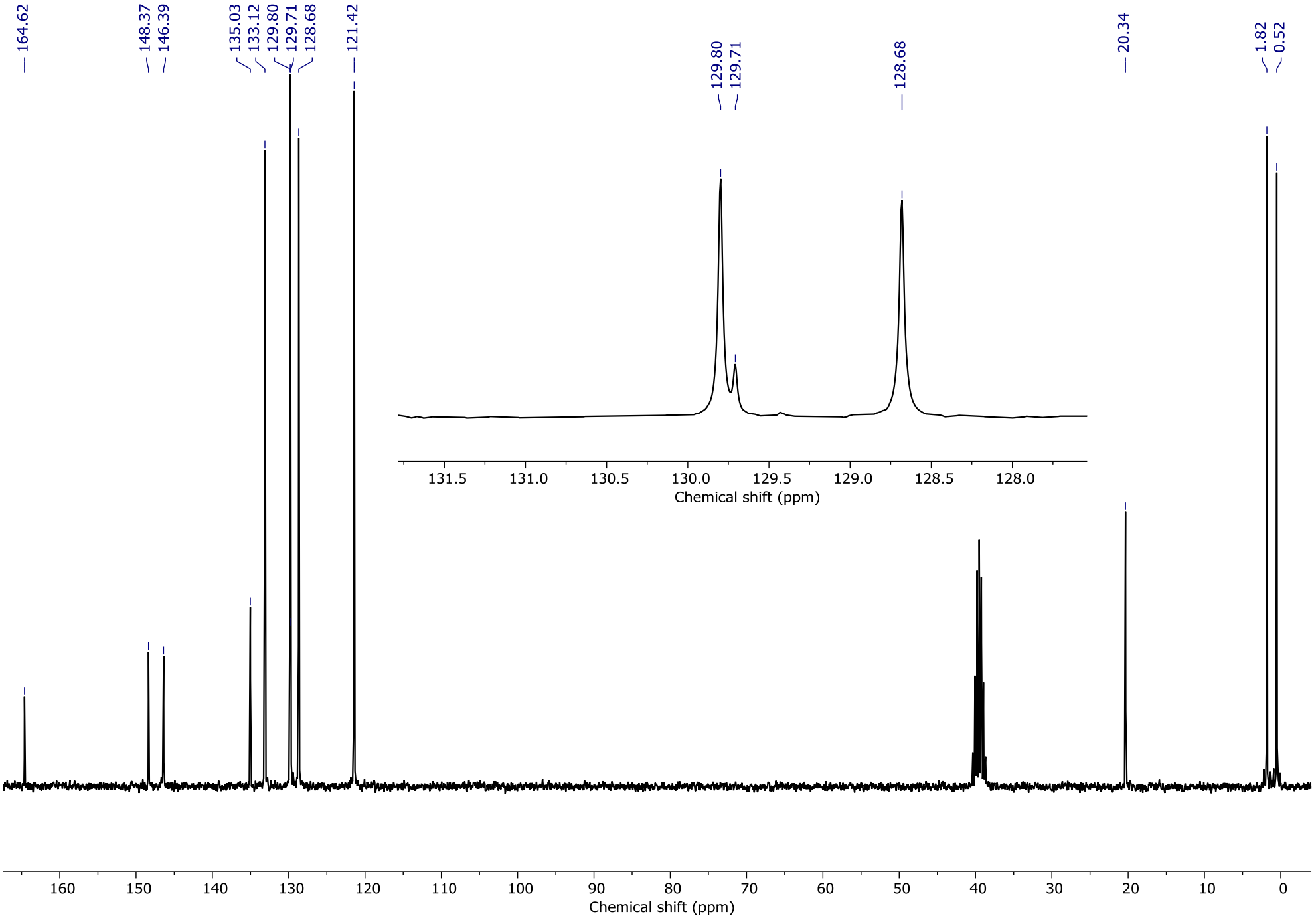
^{1}H NMR

(400 MHz, DMSO-d6)



^{13}C NMR

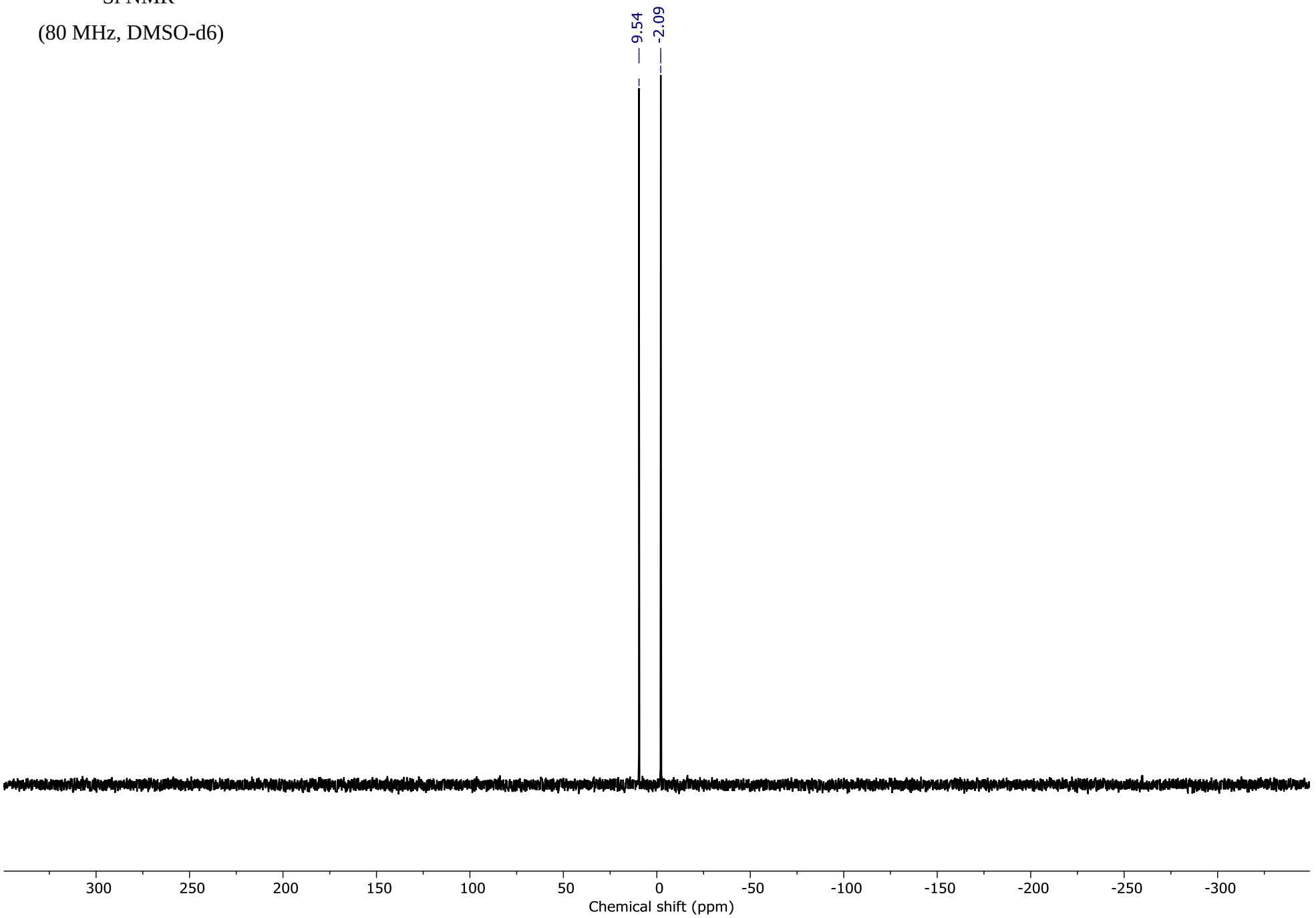
(100 MHz, DMSO-d6)



^{29}Si NMR

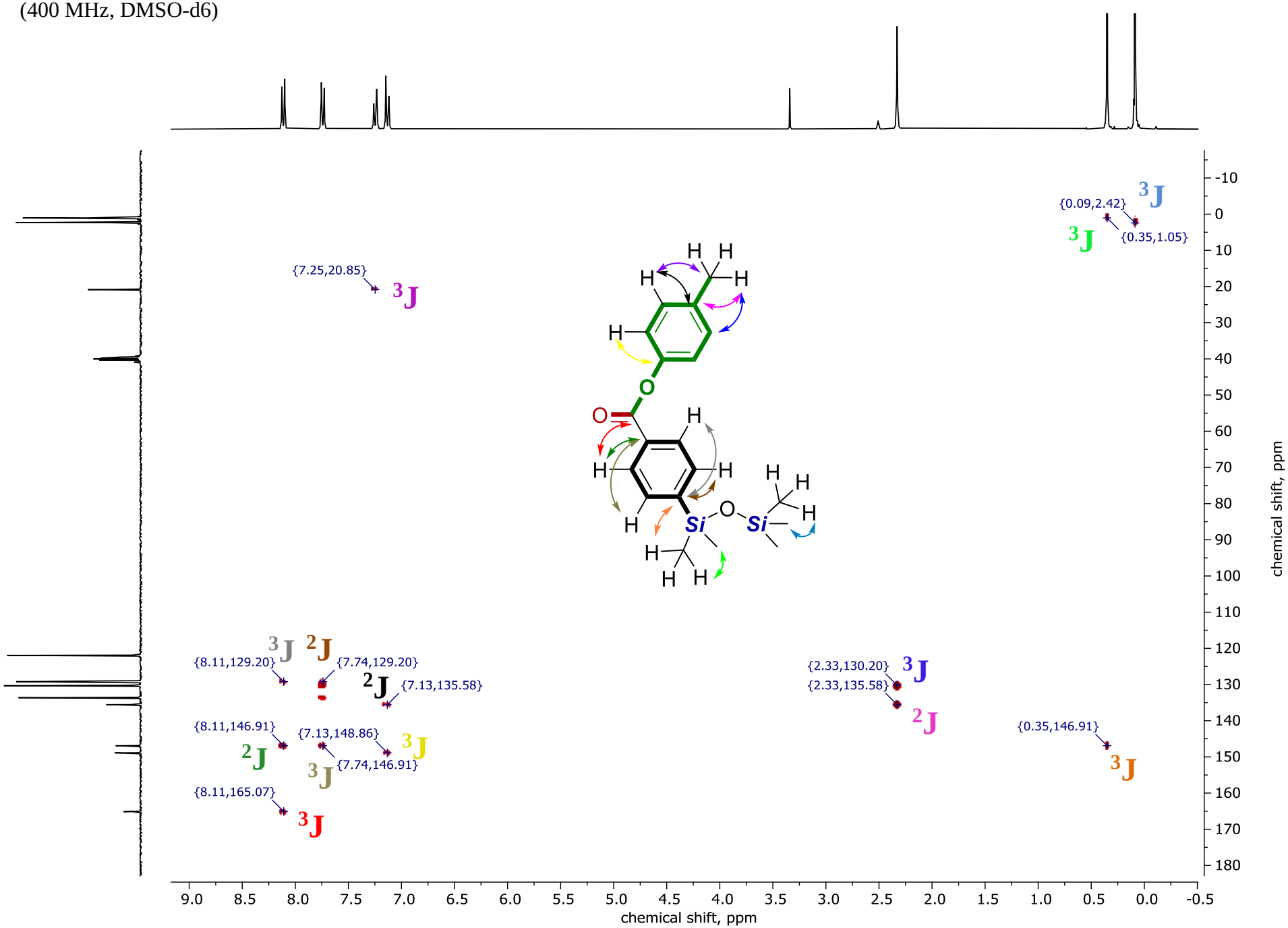
(80 MHz, DMSO-d6)

S40



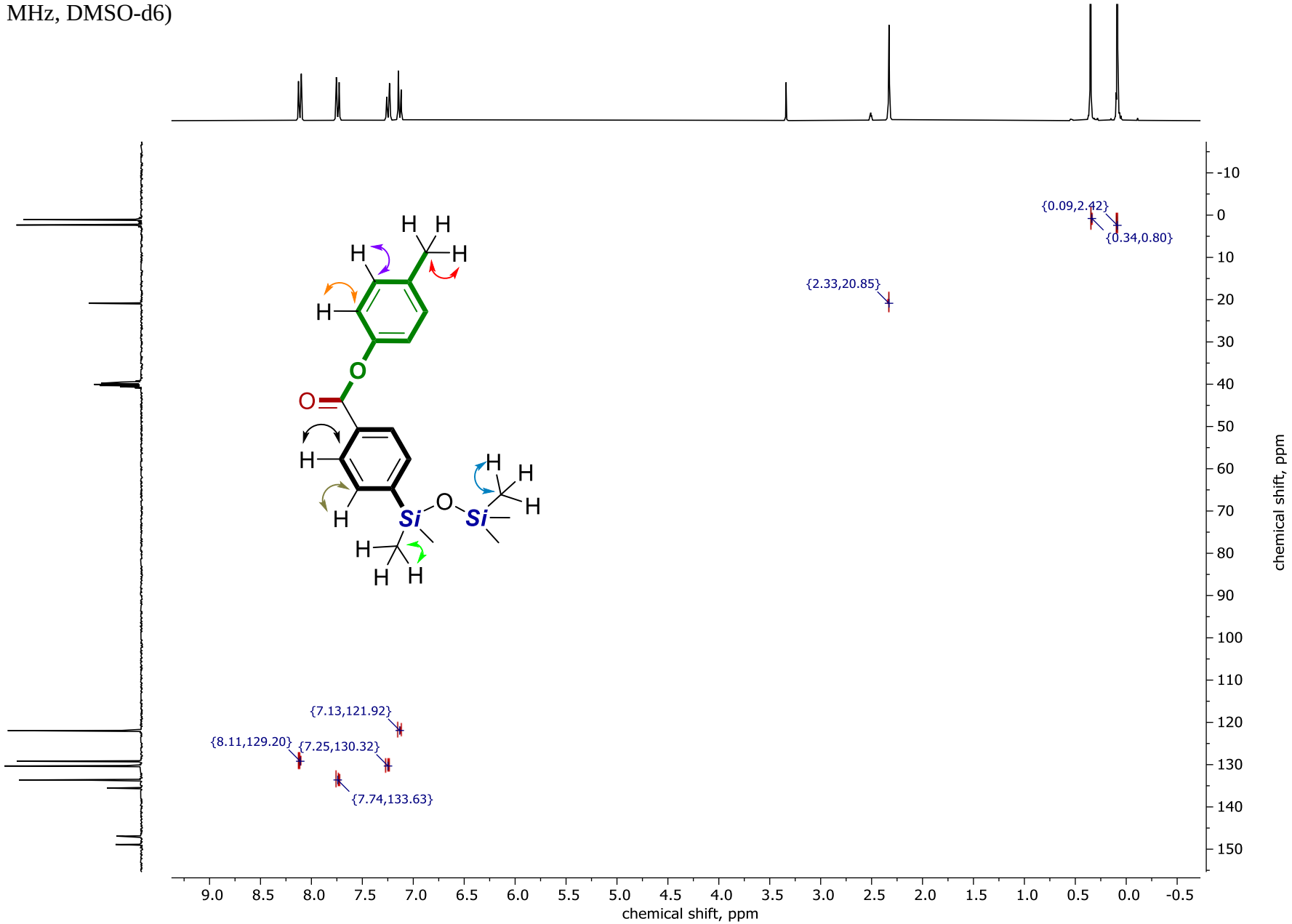
^{1}H - ^{13}C HMBC

(400 MHz, DMSO-d6)



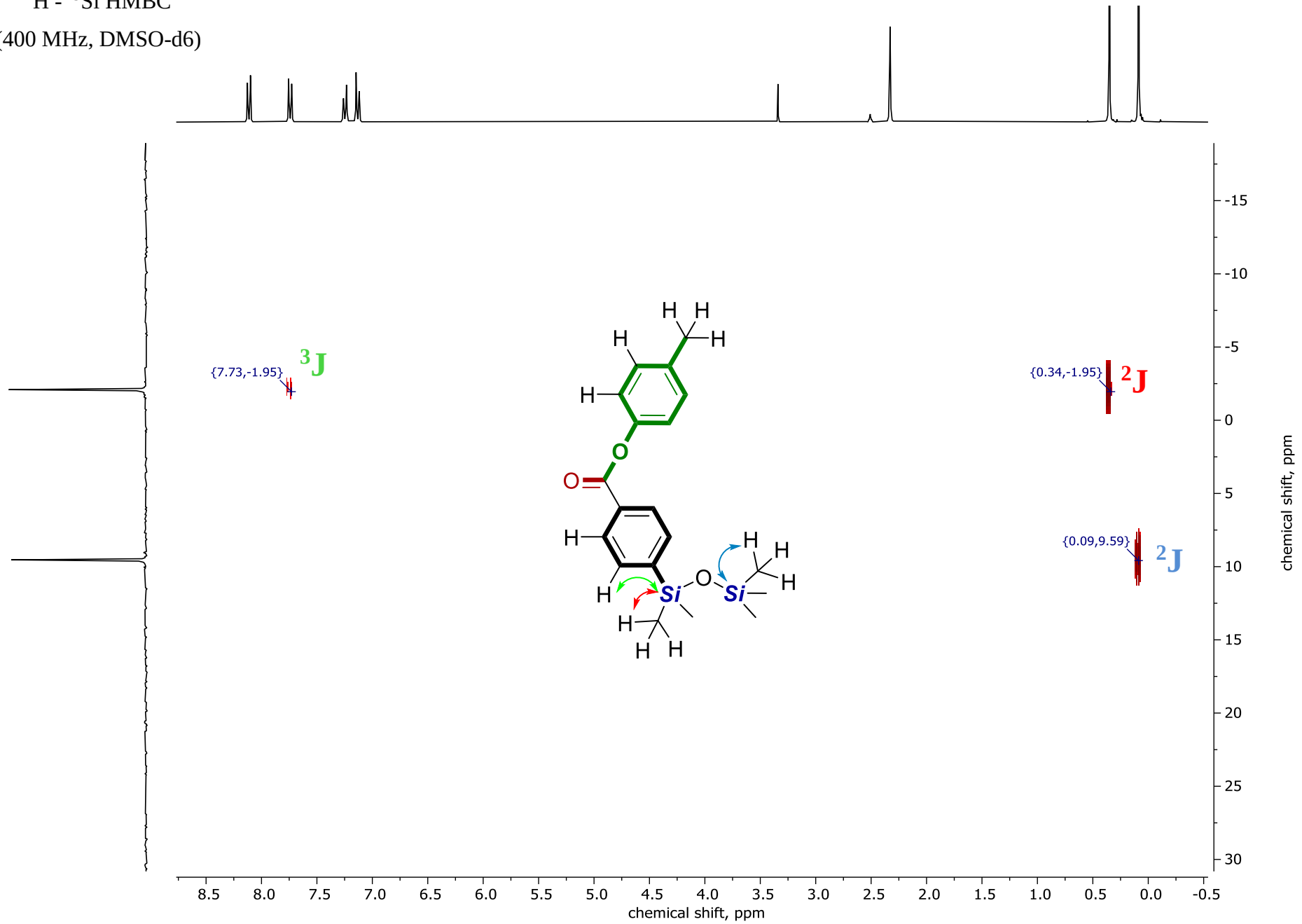
^{1}H - ^{13}C HSQC

(400 MHz, DMSO-d6)

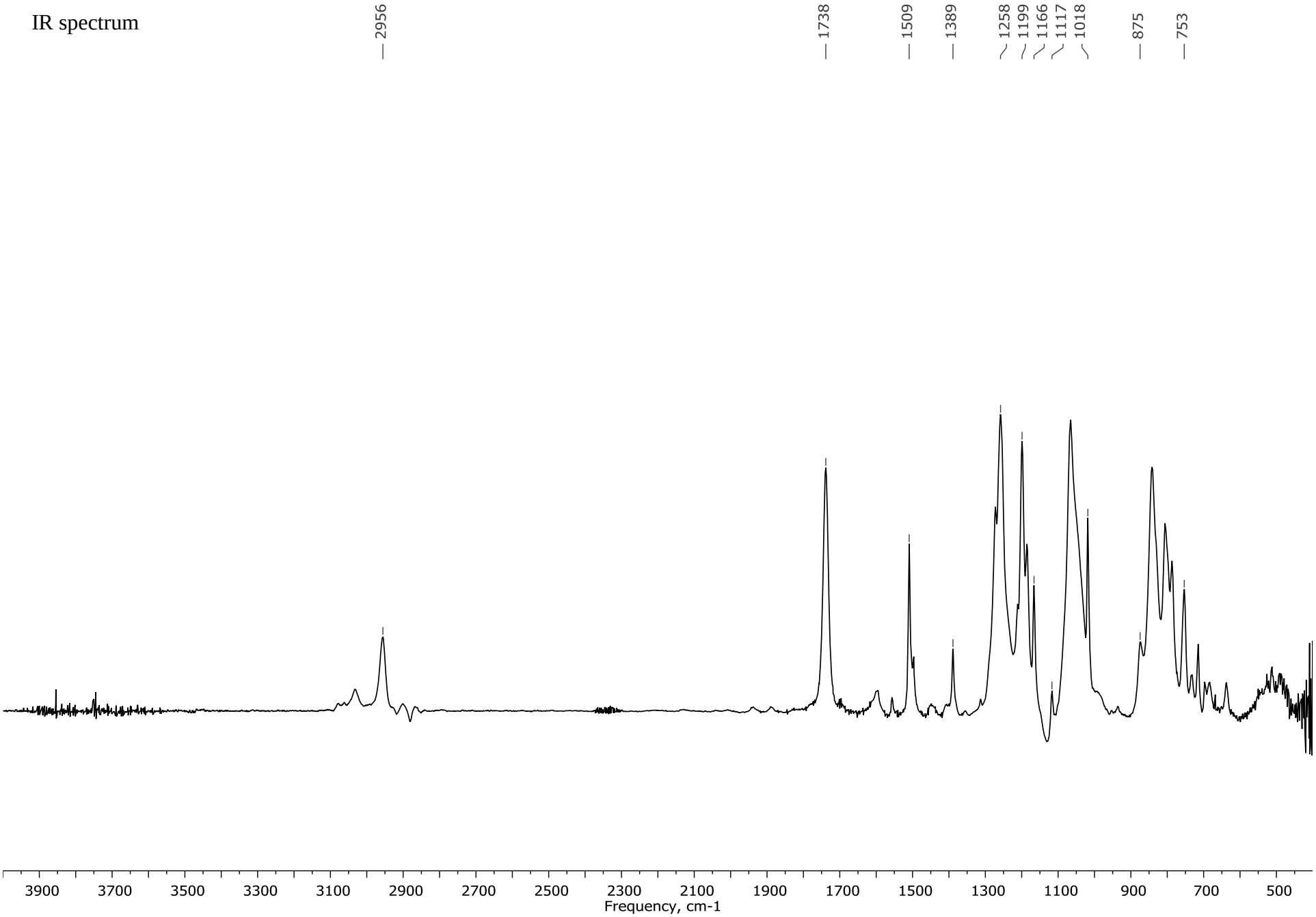


^{1}H - ^{29}Si HMBC

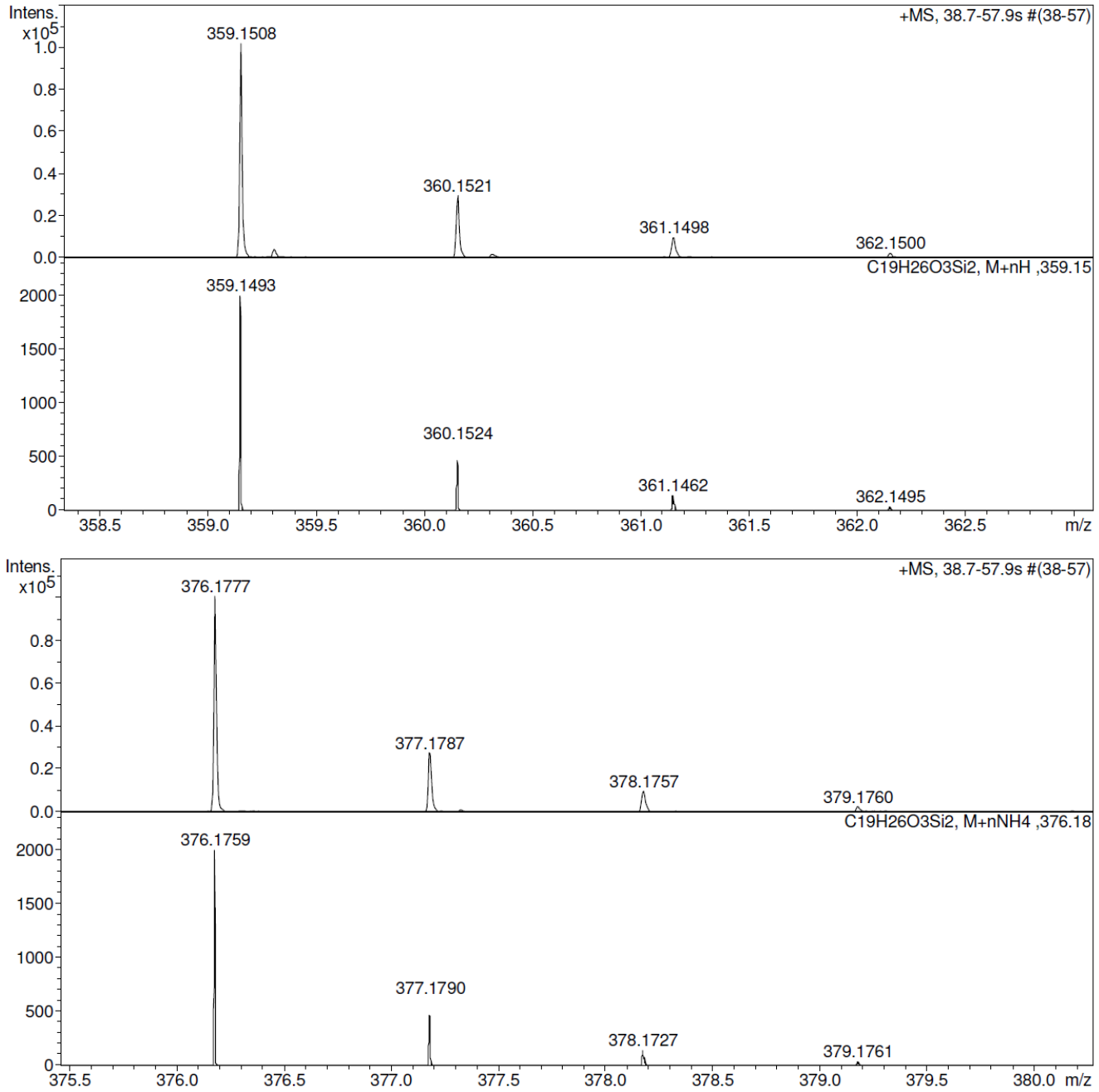
(400 MHz, DMSO-d6)

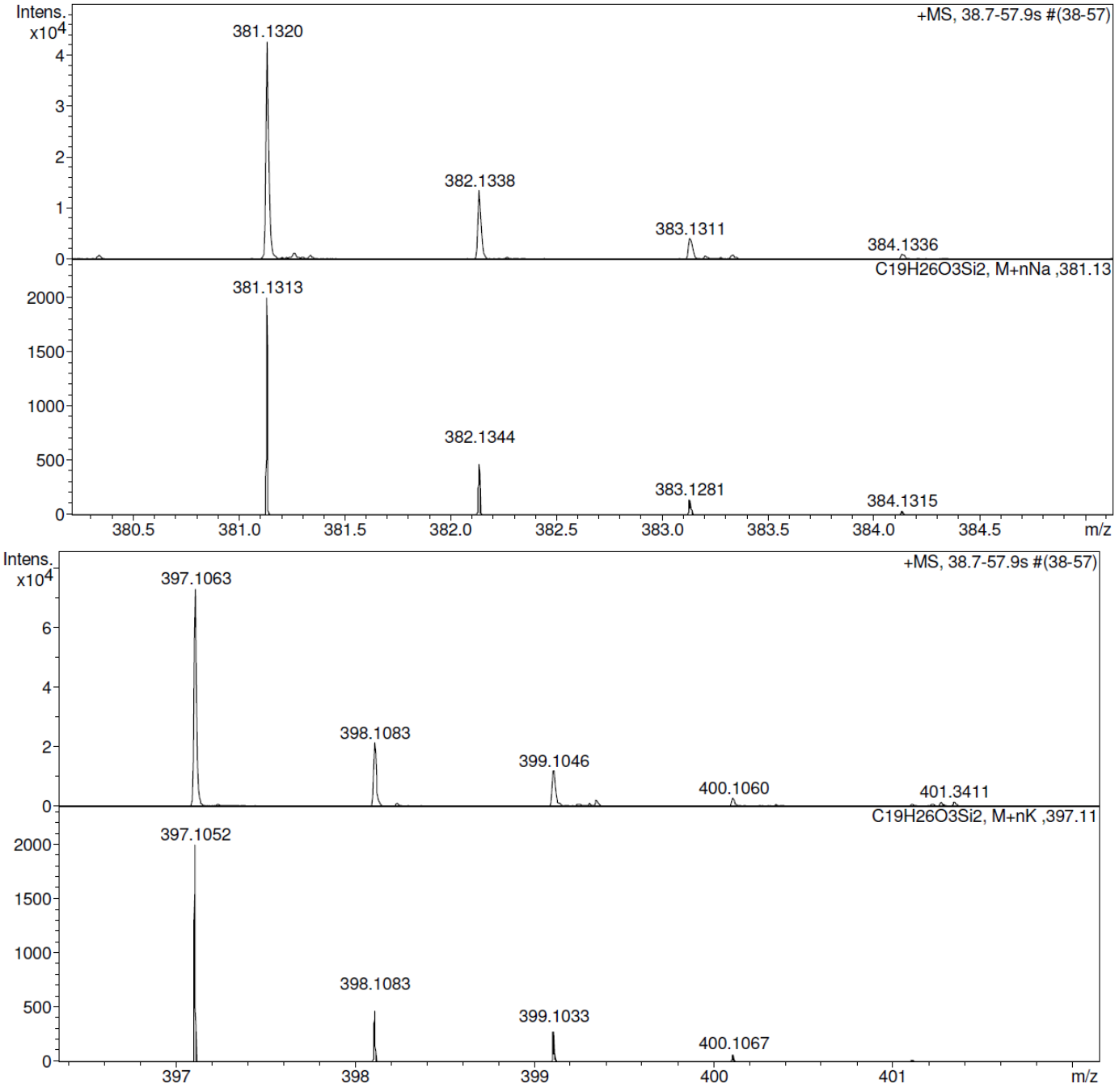


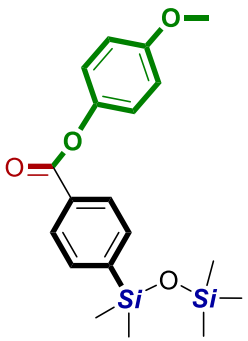
IR spectrum


2956
1738
1509
1389
1258
1199
1166
1117
1018
875
753
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

HRMS (ESI)


Intens.
x10^5
+MS, 38.7-57.9s #(38-57)
359.1508
360.1521
361.1498
362.1500
C19H26O3Si2, M+nH ,359.15
359.1493
360.1524
361.1462
362.1495
m/z
Intens.
x10^5
+MS, 38.7-57.9s #(38-57)
376.1777
377.1787
378.1757
379.1760
C19H26O3Si2, M+nNH4 ,376.18
376.1759
377.1790
378.1727
379.1761
m/z


Intens.
x10^4
+MS, 38.7-57.9s #(38-57)
381.1320
382.1338
383.1311
384.1336
C19H26O3Si2, M+nNa ,381.13
381.1313
382.1344
383.1281
384.1315
m/z
Intens.
x10^4
+MS, 38.7-57.9s #(38-57)
397.1063
398.1083
399.1046
400.1060
401.3411
C19H26O3Si2, M+nK ,397.11
397.1052
398.1083
399.1033
400.1067
m/z

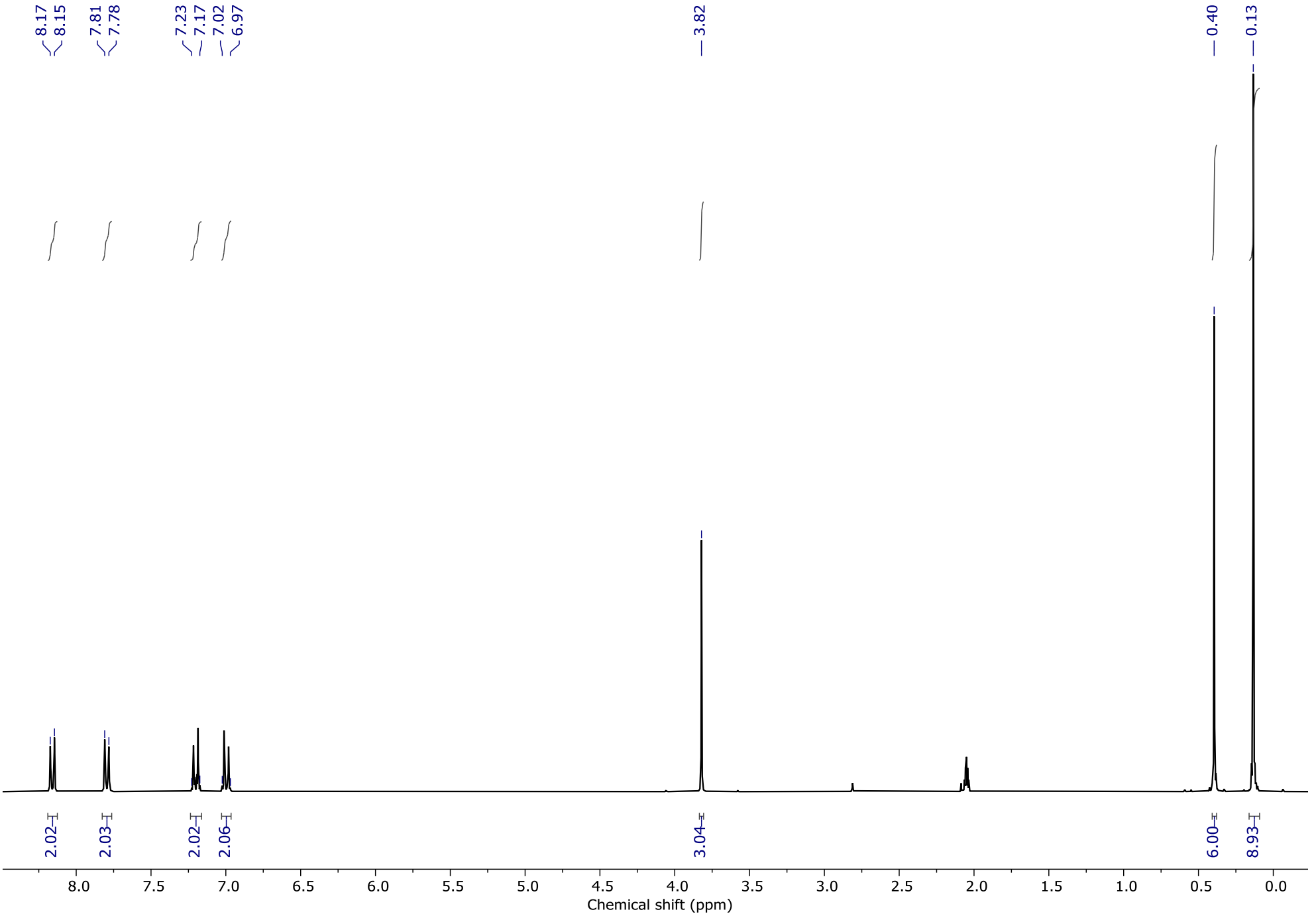


Characterisation data for 4-methoxyphenyl 4-(1,1,3,3,3-pentamethyldisiloxaneyl)benzoate:

^{1}H NMR (400 MHz, acetone-d6): δ = 8.16 (d, ^{3}J=11 Hz, 2H), δ = 7.80 (d, ^{3}J=11 Hz, 2H), δ = 7.23-7.17 (m, 2H), δ = 7.02-6.97 (m, 2H), δ = 3.82 (s, 3H), δ = 0.40 (s, 6H), δ = 0.13 (s, 9H). ^{13}C NMR (100 MHz, acetone-d6): δ = 165.87, 158.40, 147.64, 145.50, 134.11, 131.30, 129.70, 123.44, 115.21, 55.89, 2.04, 0.89. ^{29}Si NMR (80 MHz, acetone-d6): δ = 9.38, -2.38. HRMS (ESI) m/z $[M + NH_4]^+$: calcd for $[C_{19}H_{26}O_4Si_2 + NH_4]^+$, 392.1078; found, 392.1727. IR (cm^{-1}): 2956, 2837, 1734, 1609, 1507, 1389, 1255, 1196, 1066, 871-638.

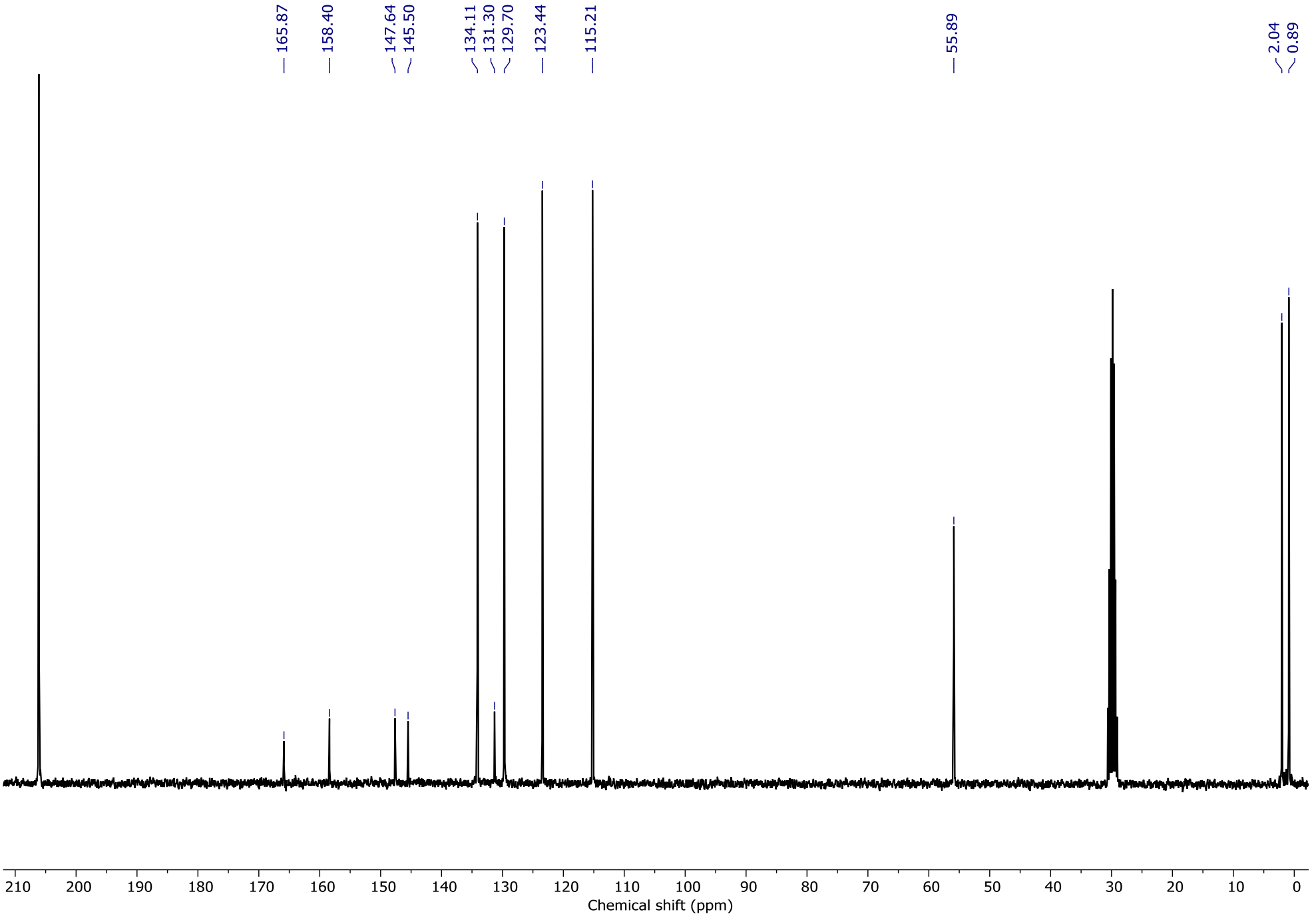
^{1}H NMR

(400 MHz, acetone-d6)



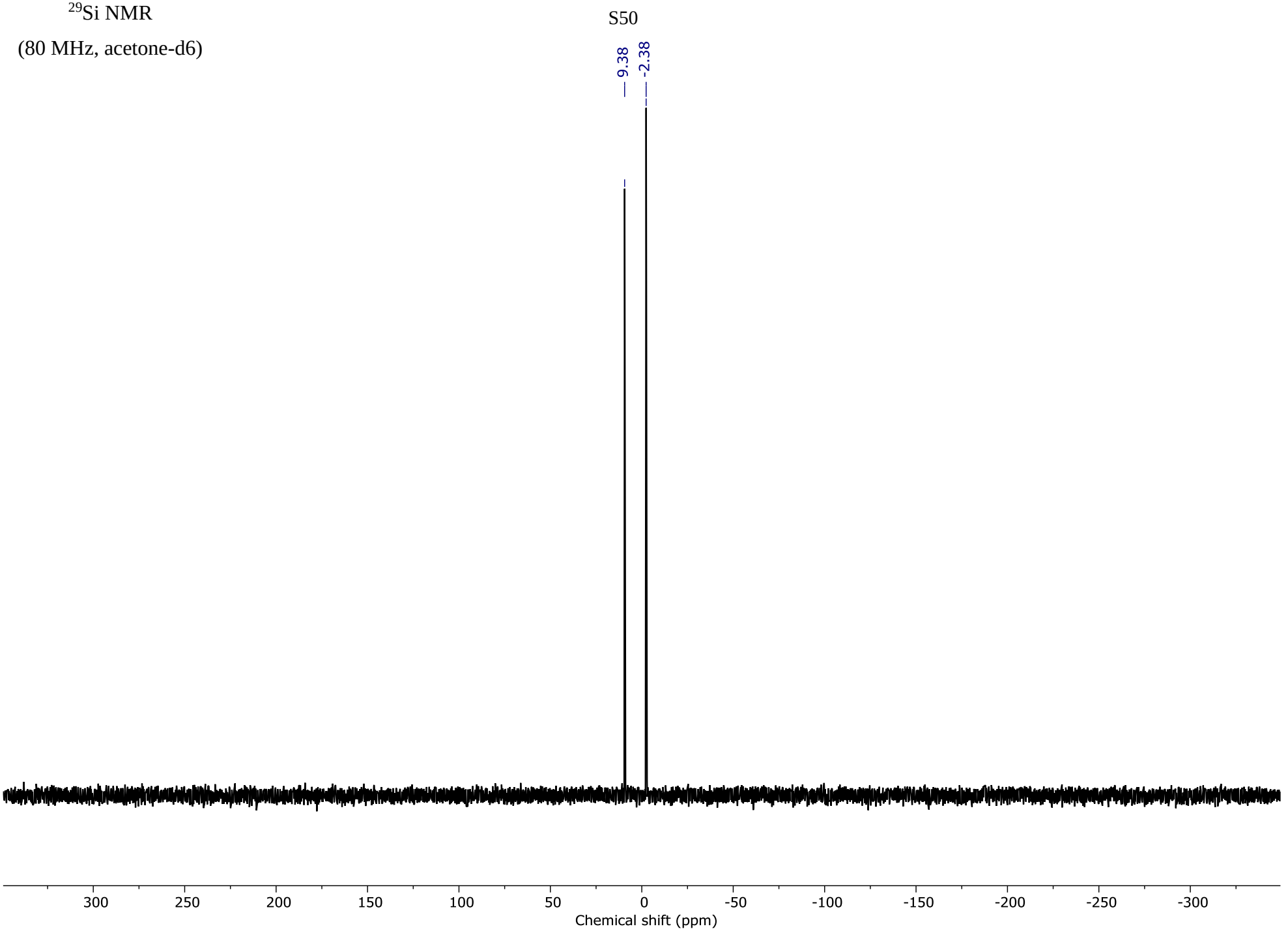
^{13}C NMR

(100 MHz, acetone-d6)



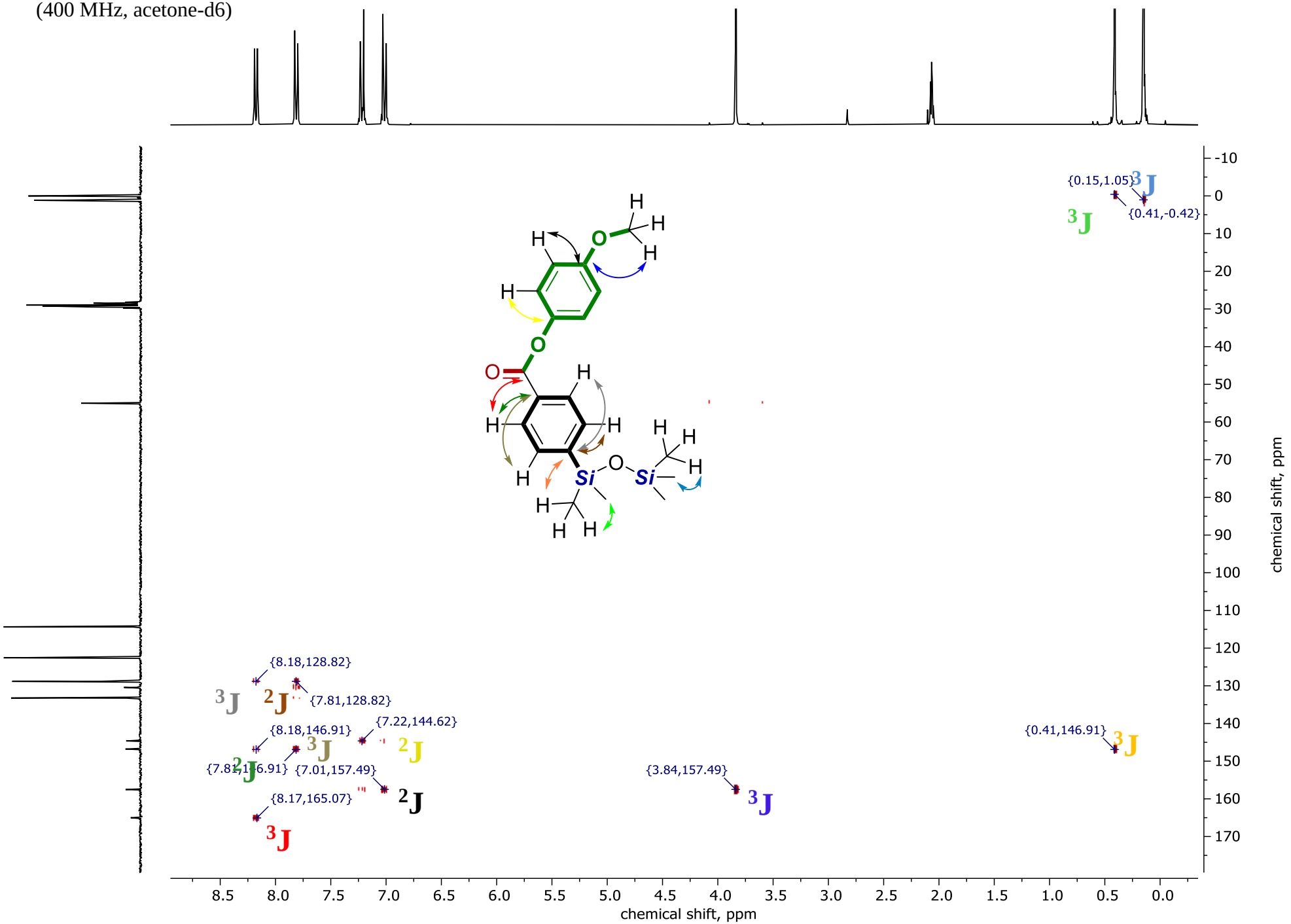
^{29}Si NMR

(80 MHz, acetone-d6)



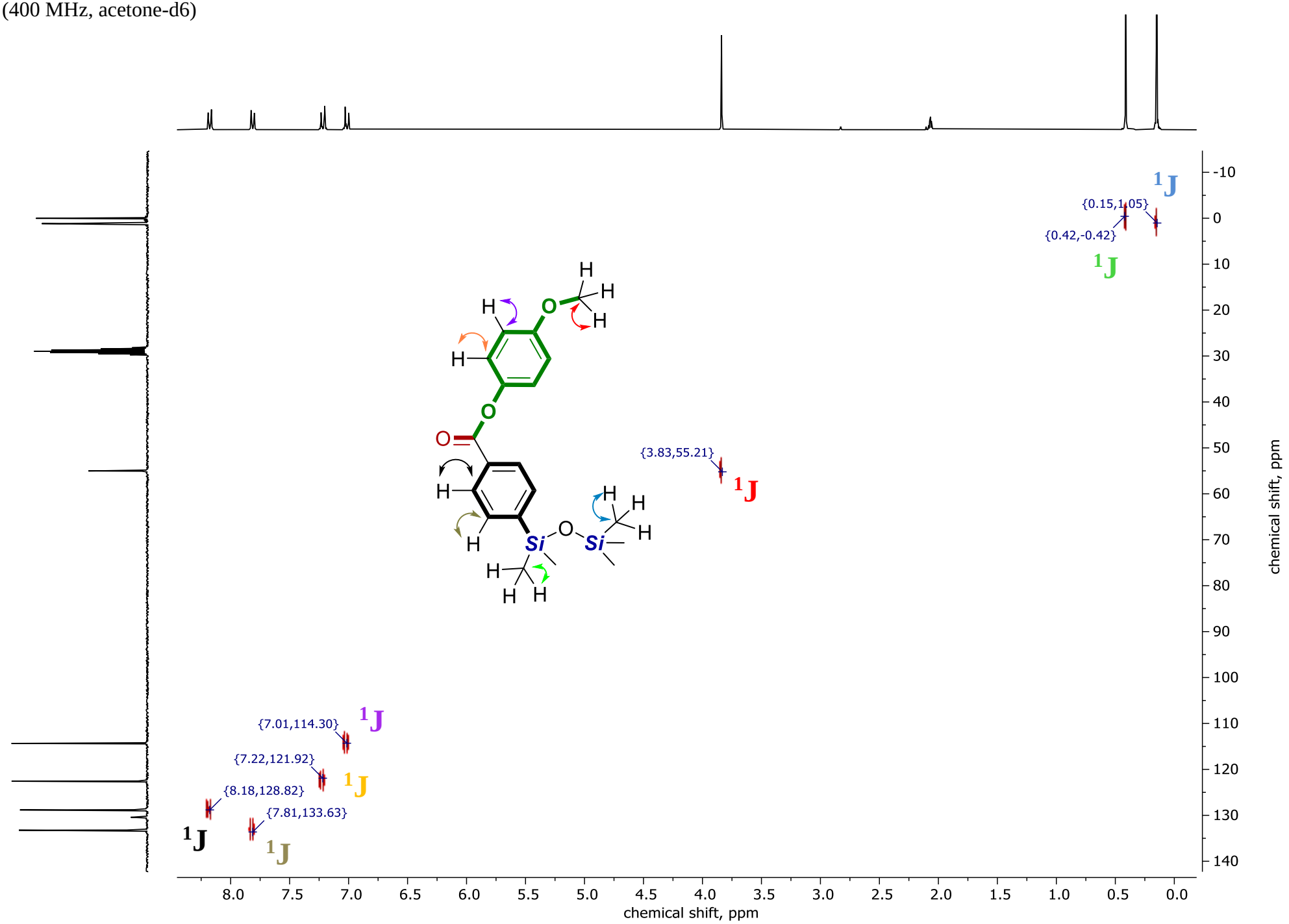
^{1}H - ^{13}C HMBC

(400 MHz, acetone-d6)



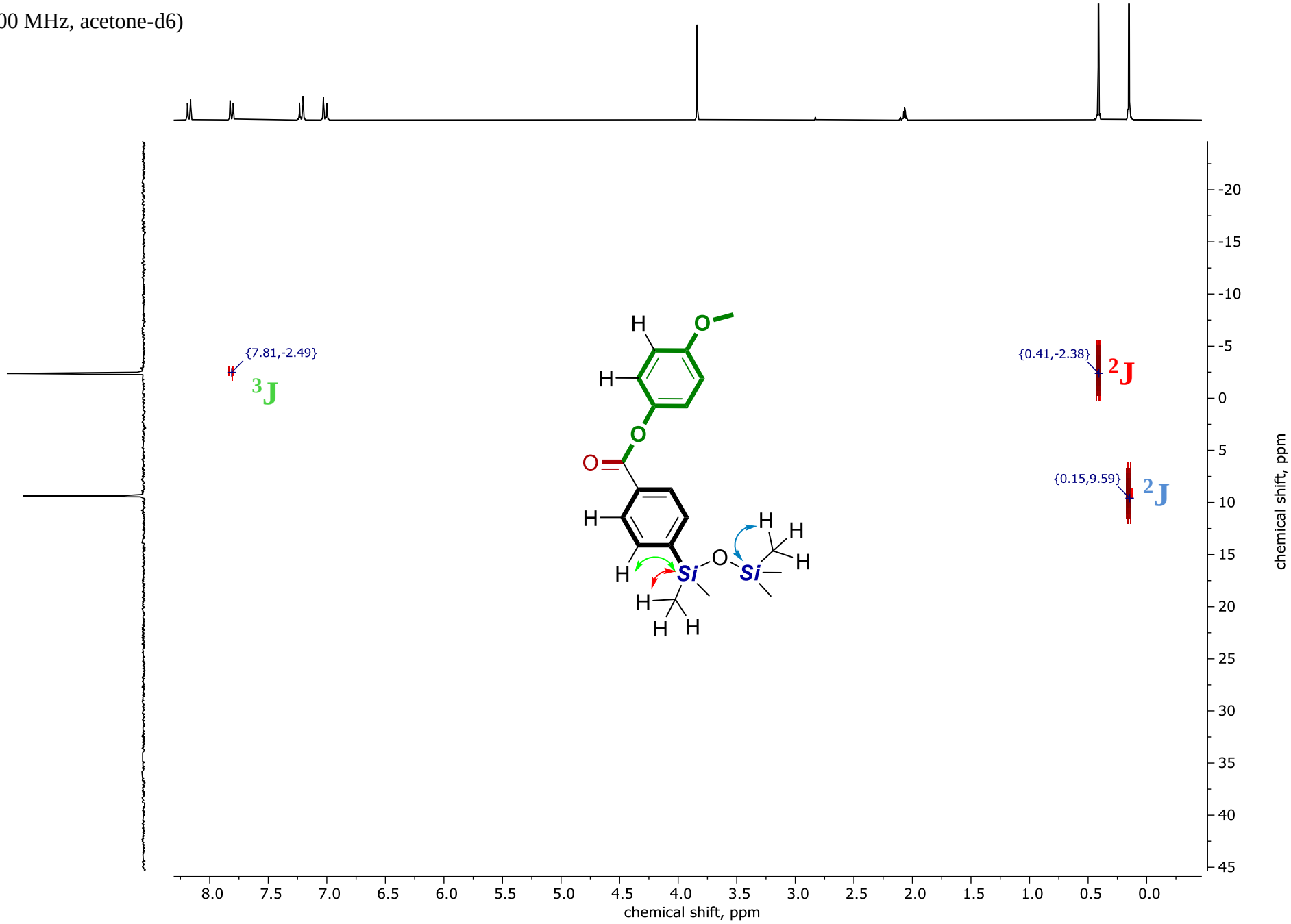
^{1}H - ^{13}C HSQC

(400 MHz, acetone-d6)

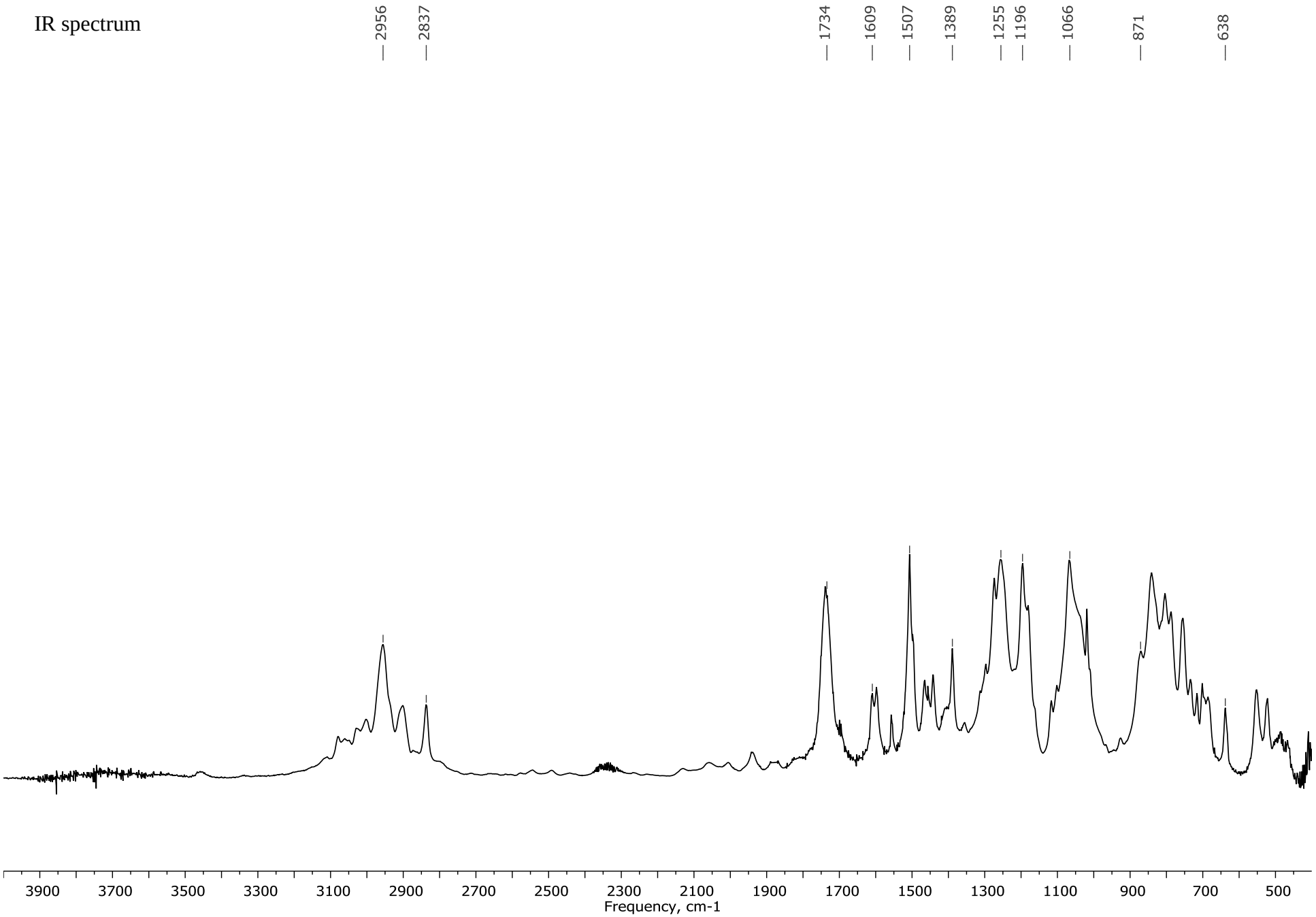


^{1}H - ^{29}Si HMBC

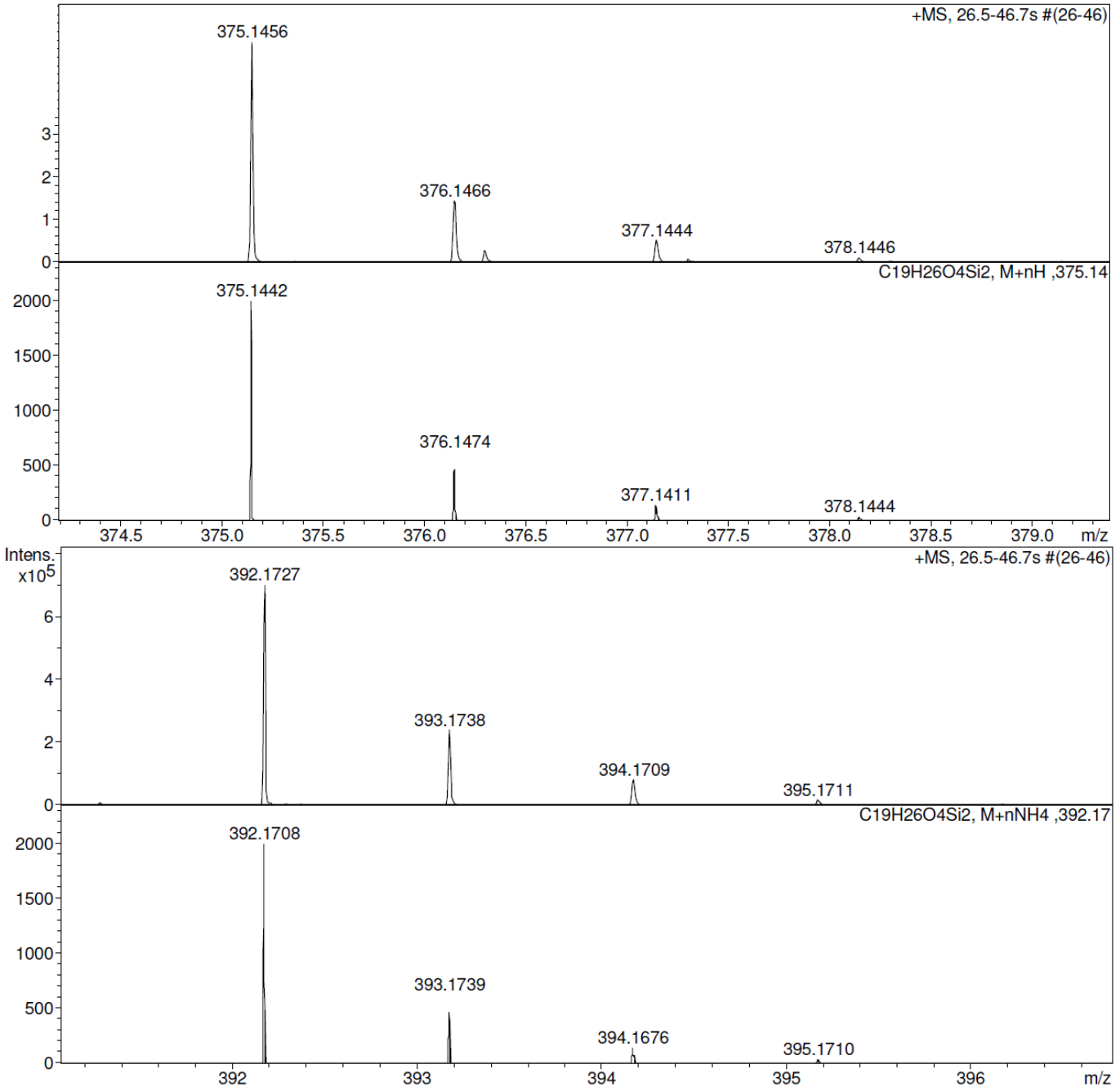
(400 MHz, acetone-d6)

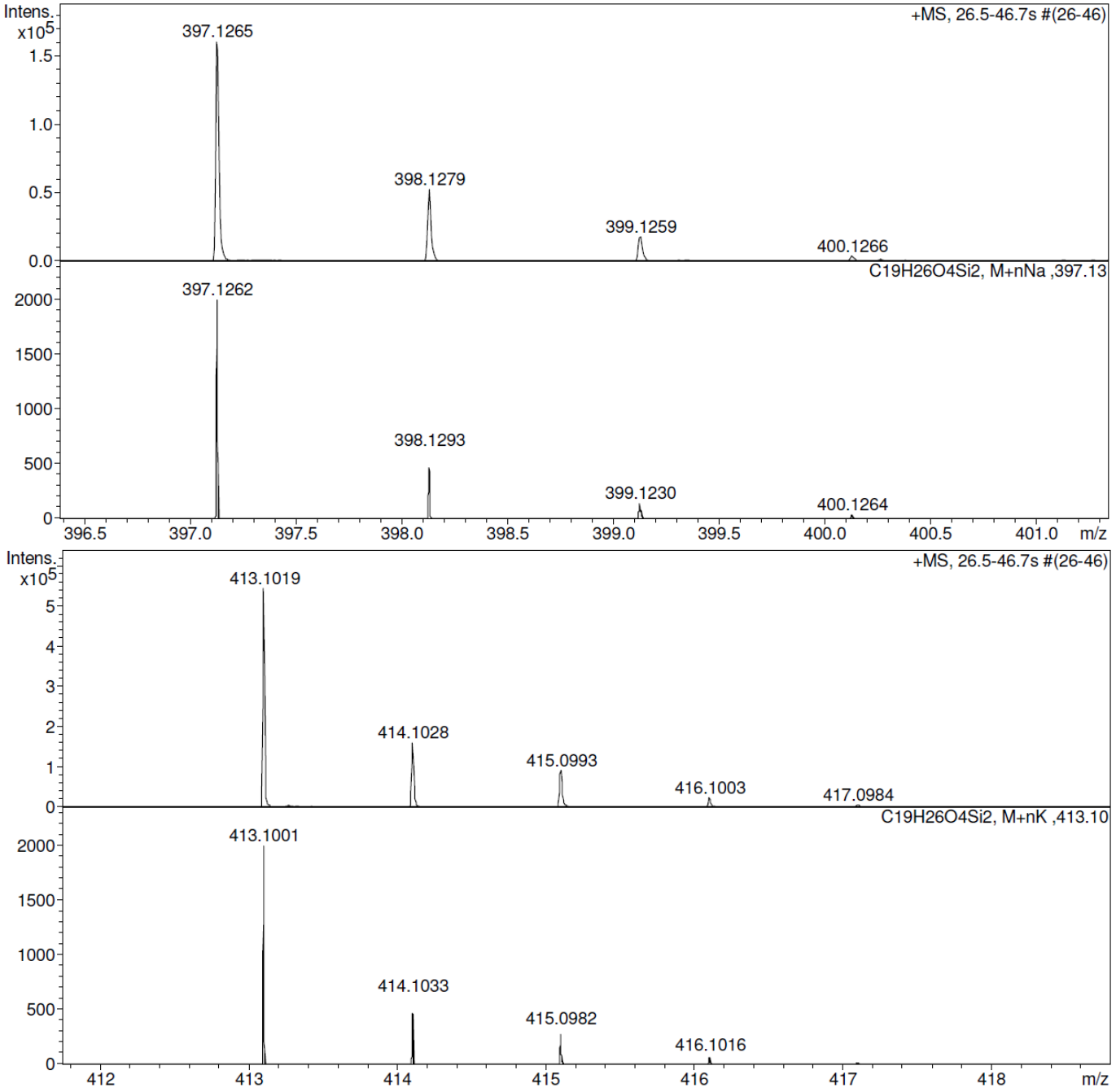


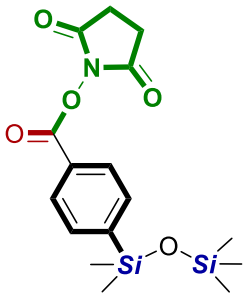
IR spectrum


2956
2837
1734
1609
1507
1389
1255
1196
1066
871
638
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

HRMS (ESI)


+MS, 26.5-46.7s #(26-46)
375.1456
376.1466
377.1444
378.1446
C19H26O4Si2, M+nH ,375.14
375.1442
376.1474
377.1411
378.1444
374.5
375.0
375.5
376.0
376.5
377.0
377.5
378.0
378.5
379.0
m/z
Intens.
x10^5
+MS, 26.5-46.7s #(26-46)
392.1727
393.1738
394.1709
395.1711
C19H26O4Si2, M+nNH4 ,392.17
392.1708
393.1739
394.1676
395.1710
392
393
394
395
396
m/z


Intens.
x10^5
+MS, 26.5-46.7s #(26-46)
397.1265
398.1279
399.1259
400.1266
C19H26O4Si2, M+nNa ,397.13
397.1262
398.1293
399.1230
400.1264
m/z
Intens.
x10^5
+MS, 26.5-46.7s #(26-46)
413.1019
414.1028
415.0993
416.1003
417.0984
C19H26O4Si2, M+nK ,413.10
413.1001
414.1033
415.0982
416.1016
m/z

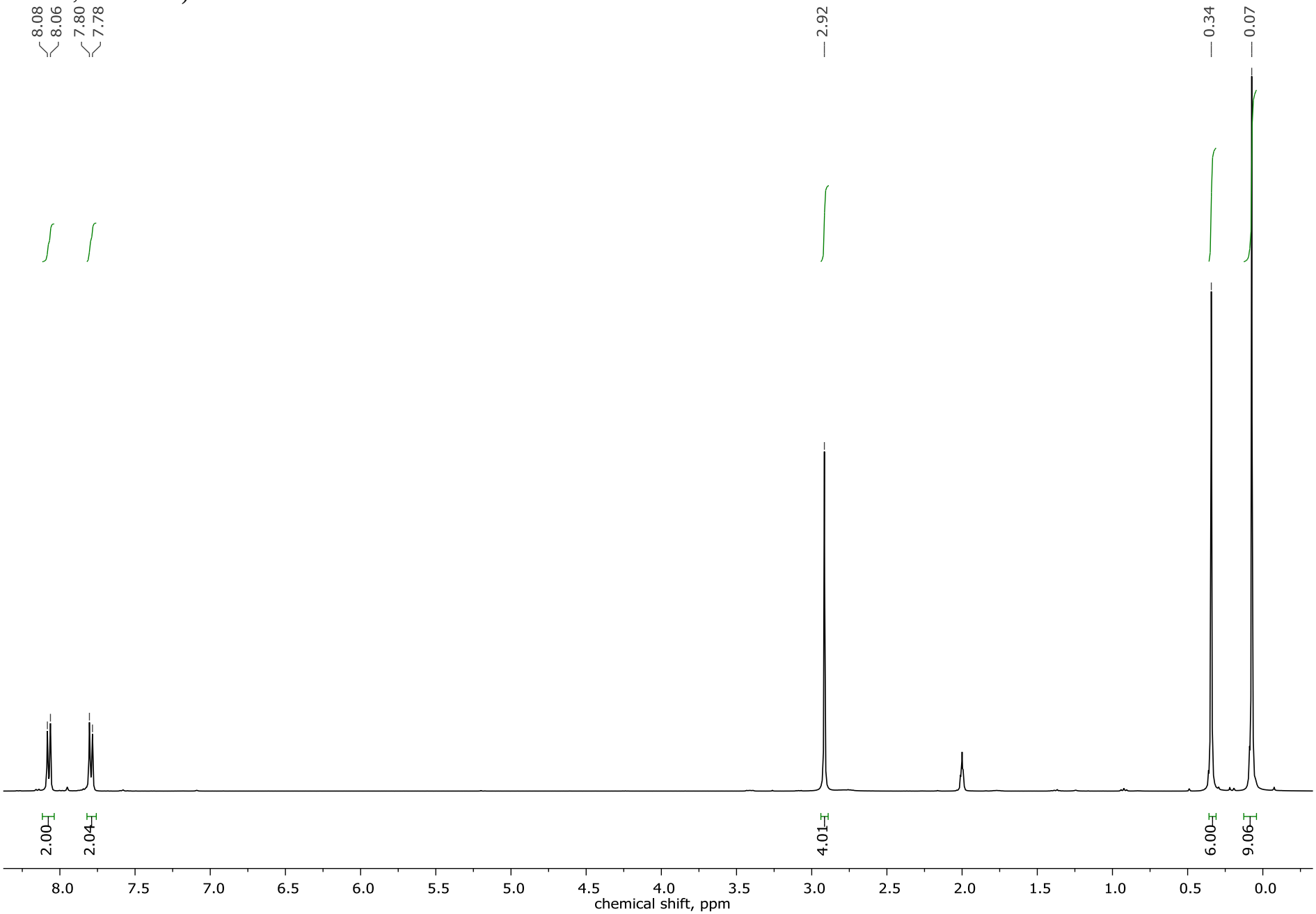


Characterisation data for 2,5-dioxopyrrolidin-1-yl 4-(1,1,3,3,3-pentamethyldisiloxaneyl)benzoate:

^{1}H NMR (400 MHz, acetone-d6): δ = 8.07 (d, ^{3}J=8 Hz, 2H), δ = 7.79 (d, ^{3}J=8 Hz, 2H), δ = 2.92 (s, 4H), δ = 0.34 (s, 6H), δ =.0.07 (s, 9H). ^{13}C NMR (100 MHz, acetone-d6): δ = 170.49, 162.90, 149.68, 134.50, 129.80, 126.81, 26.38, 2.01, 0.80. ^{29}Si NMR (80 MHz, acetone-d6): δ = 9.68, -2.40. ^{15}N NMR (40 MHz, acetone-d6): δ = 198.61. HRMS (ESI) m/z [M + H] $^{+}$: calcd for $[C_{16}H_{23}NO_5Si_2 + H]^{+}$, 366.1188; found, 366.1190; [M + Na] $^{+}$: calcd for $[C_{16}H_{23}NO_5Si_2 + Na]^{+}$, 388.1007; found, 388.1015; [M + K] $^{+}$: calcd for $[C_{16}H_{23}NO_5Si_2 + K]^{+}$, 404.0746; found, 404.0757. IR (cm^{-1}): 2957, 1774, 1757, 1560, 1427, 1391, 1369, 1254-1186, 1111-987, 842-638.

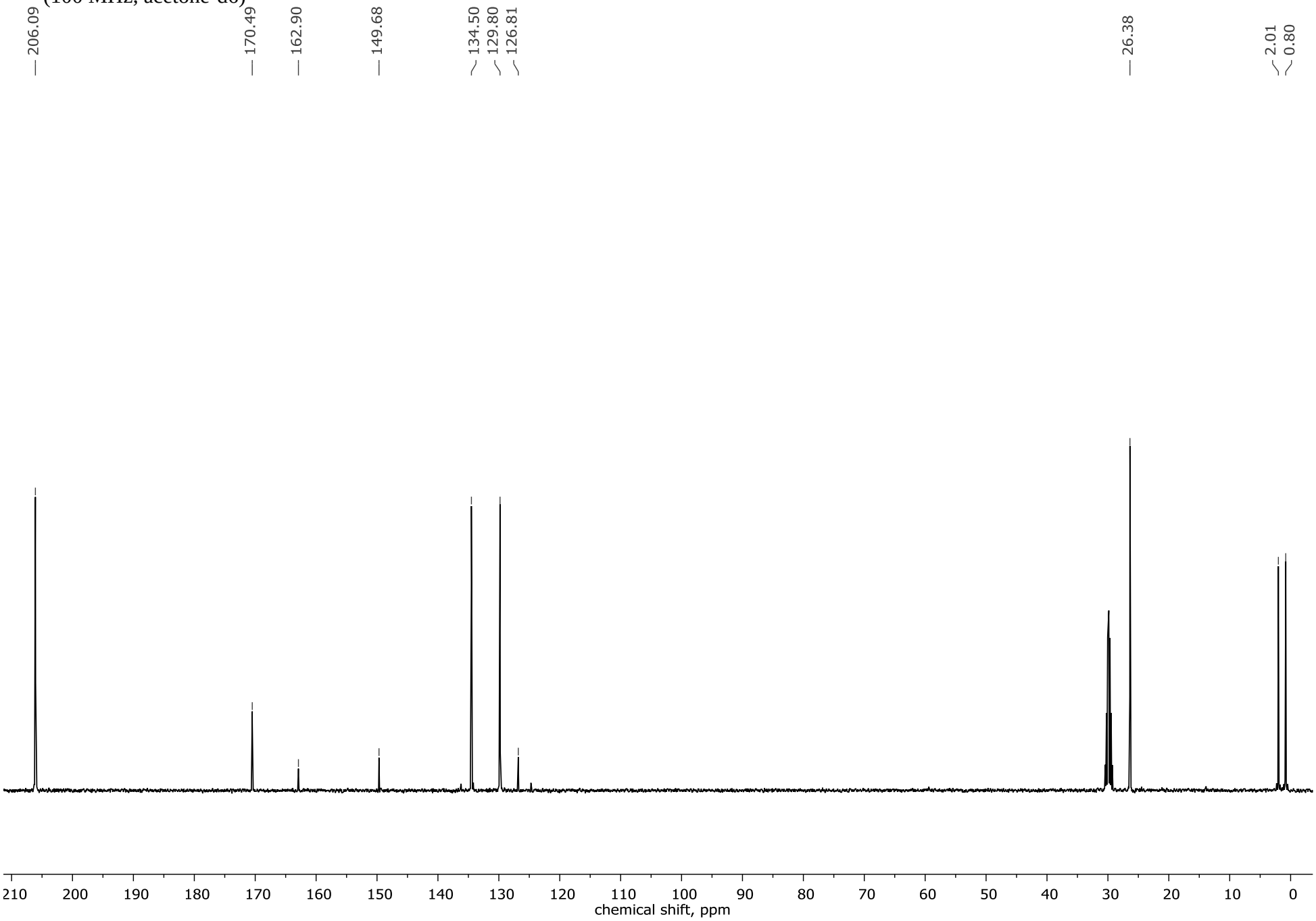
^{1}H NMR

(400 MHz, acetone-d6)



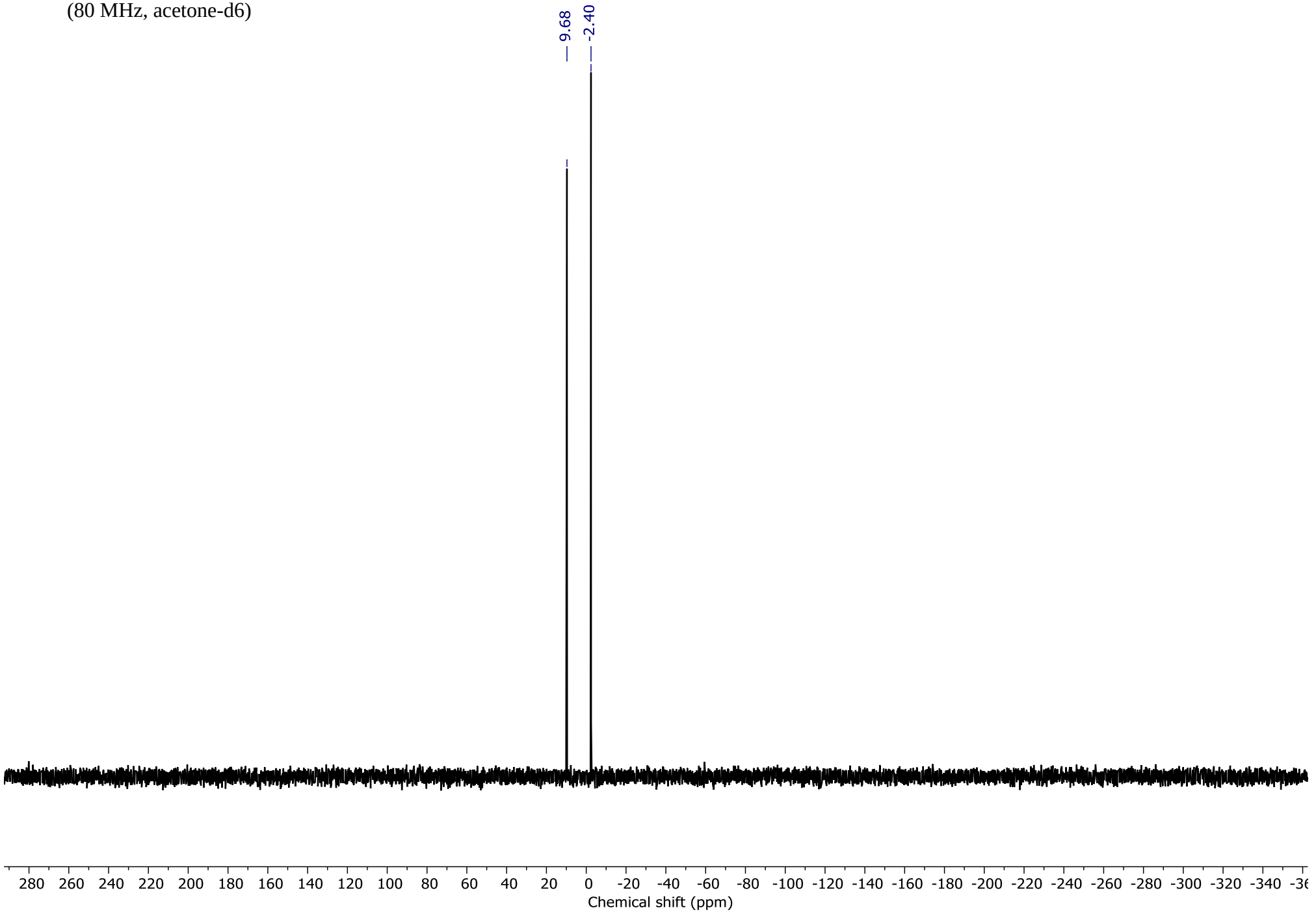
^{13}C NMR

(100 MHz, acetone-d6)



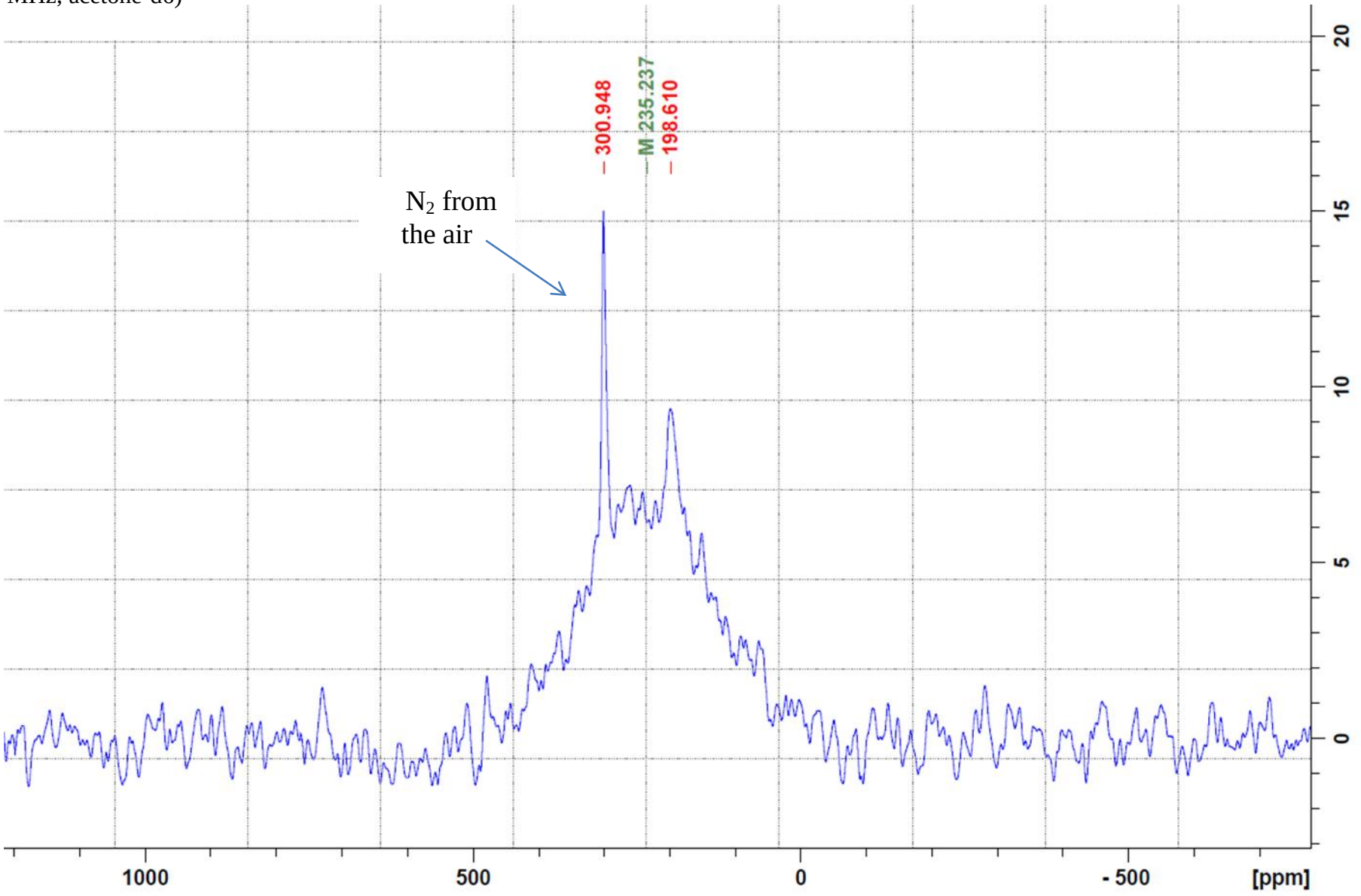
^{29}Si NMR

(80 MHz, acetone-d6)



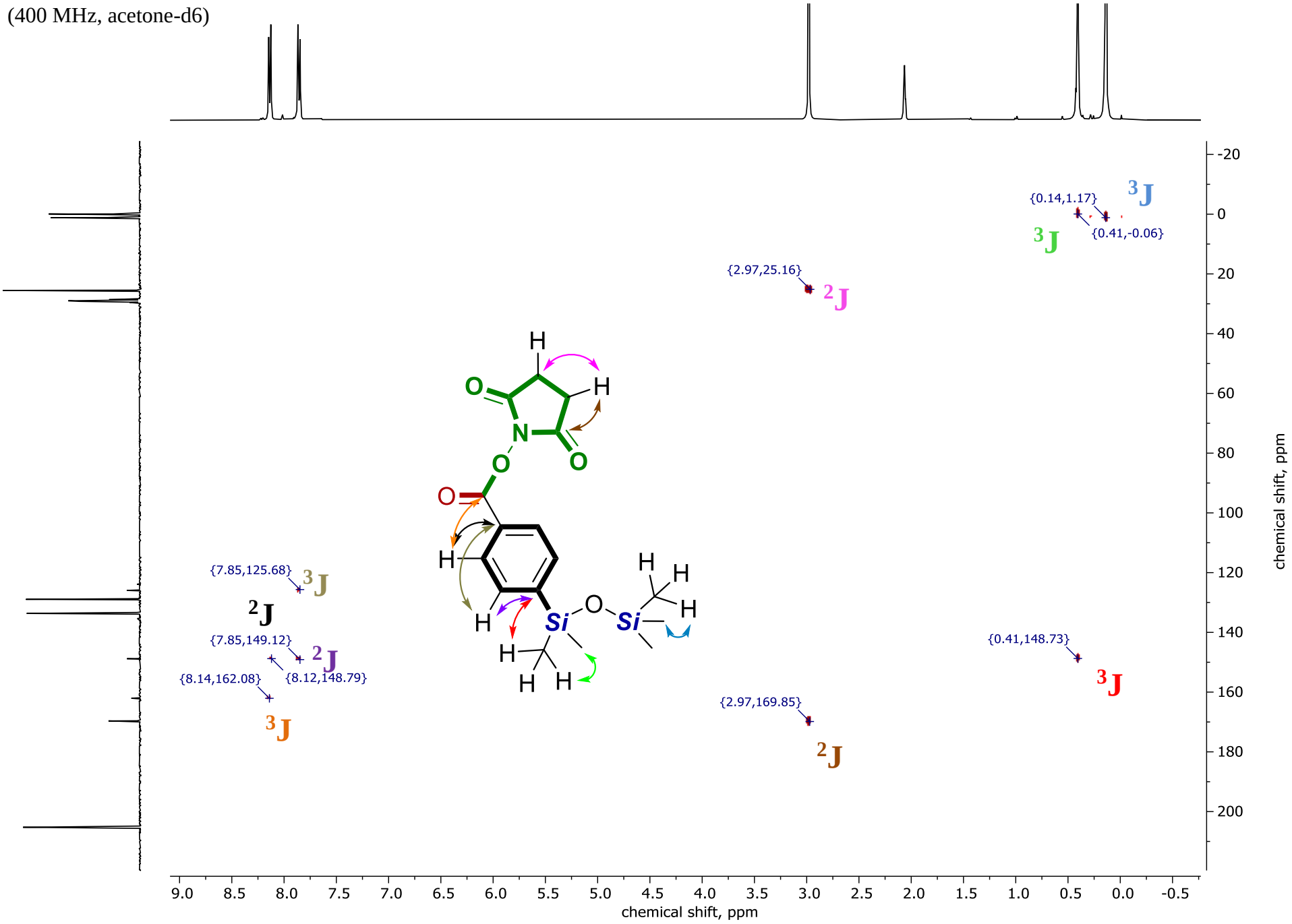
^{15}N NMR

(40 MHz, acetone-d6)



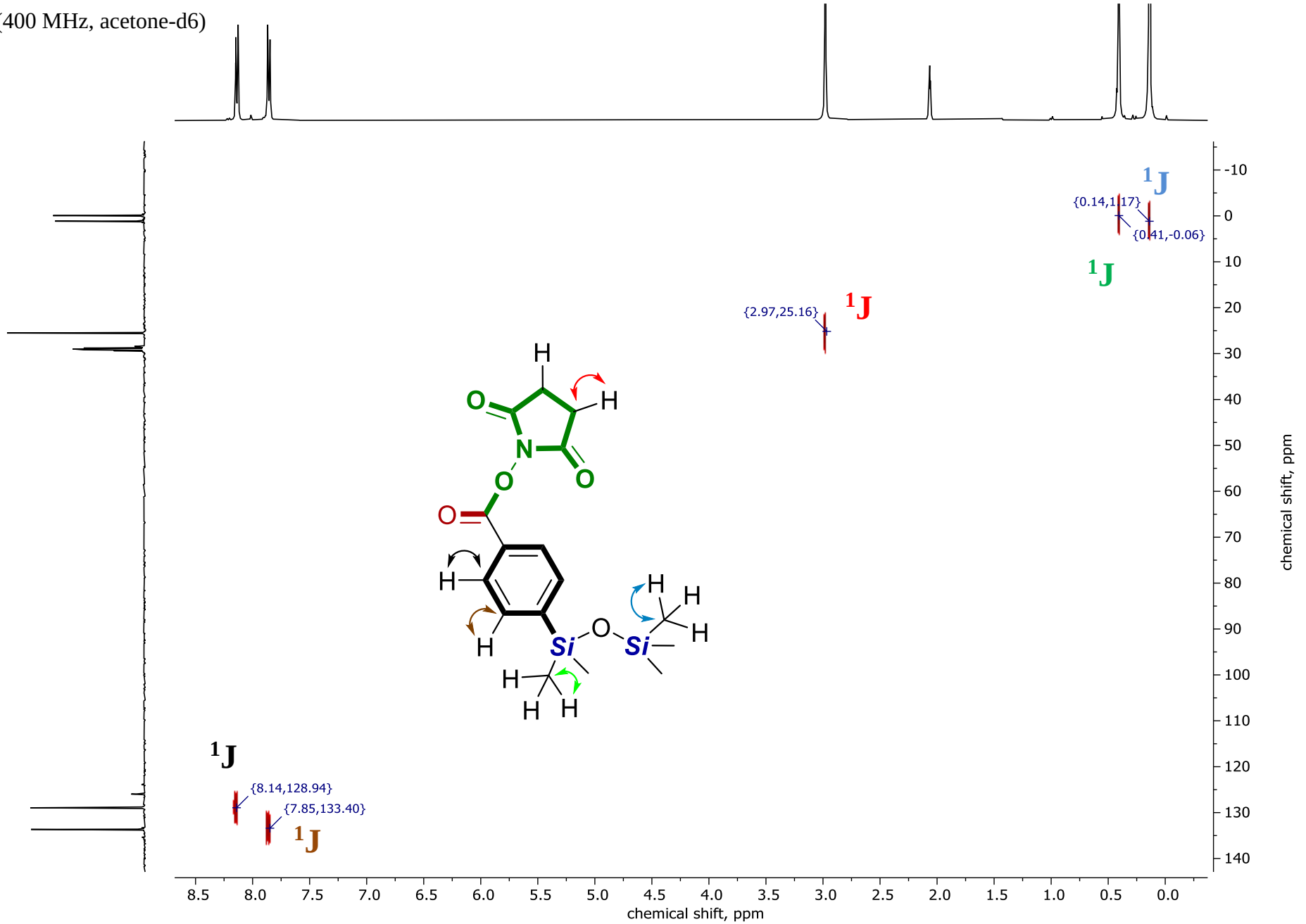
^{1}H - ^{13}C HMBC

(400 MHz, acetone-d6)



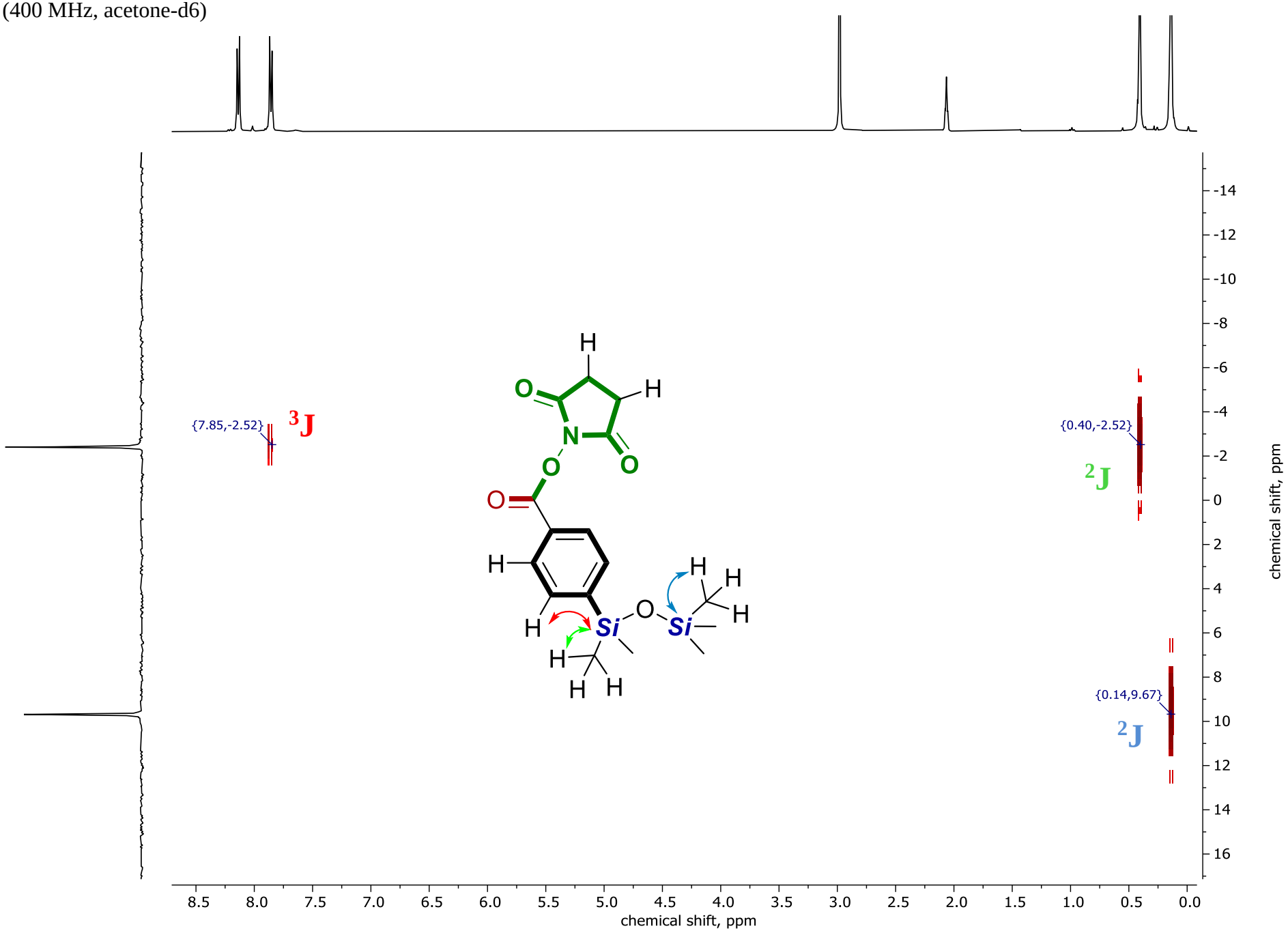
^{1}H - ^{13}C HSQC

(400 MHz, acetone-d6)

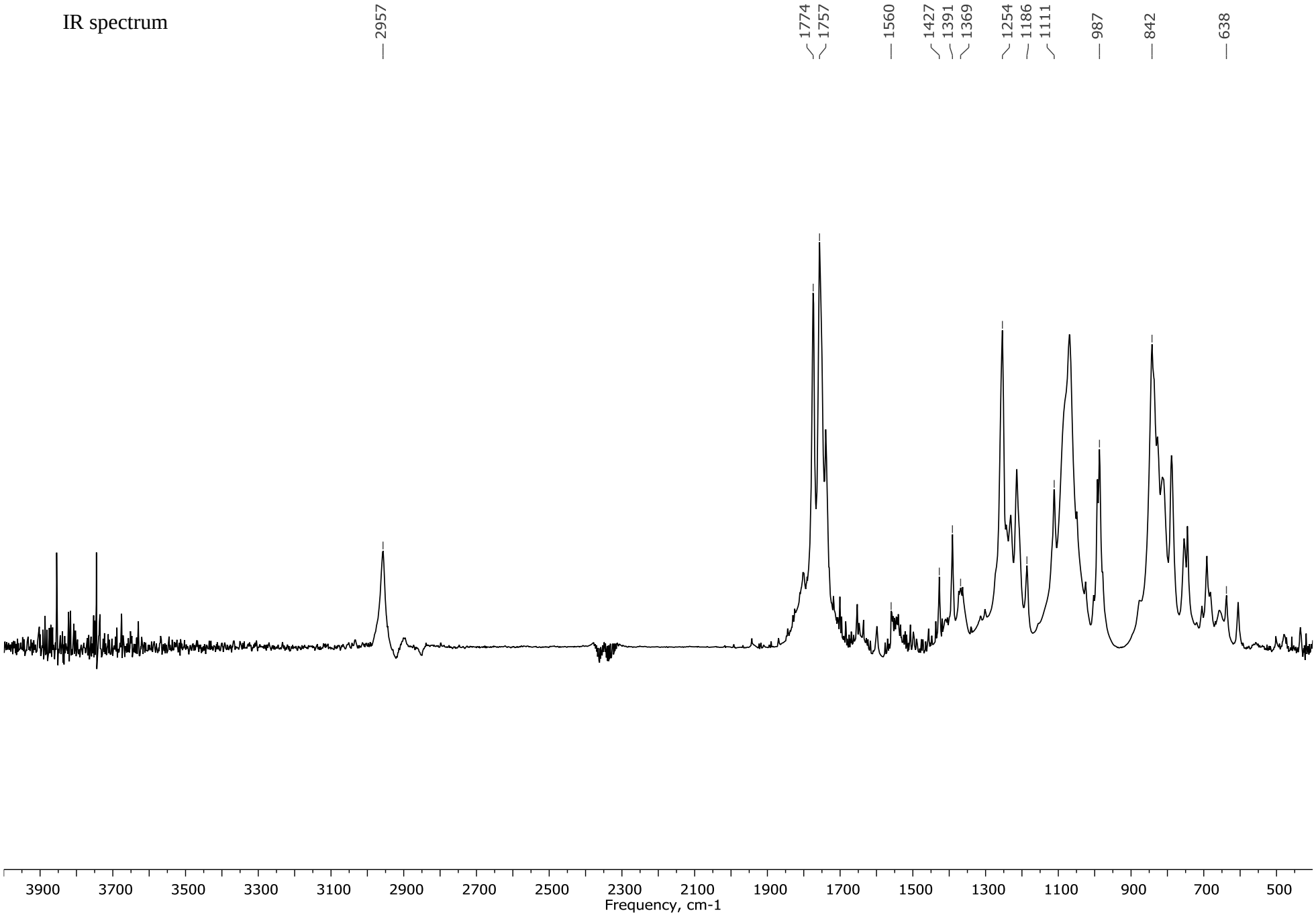


^{1}H - ^{29}Si HMBC

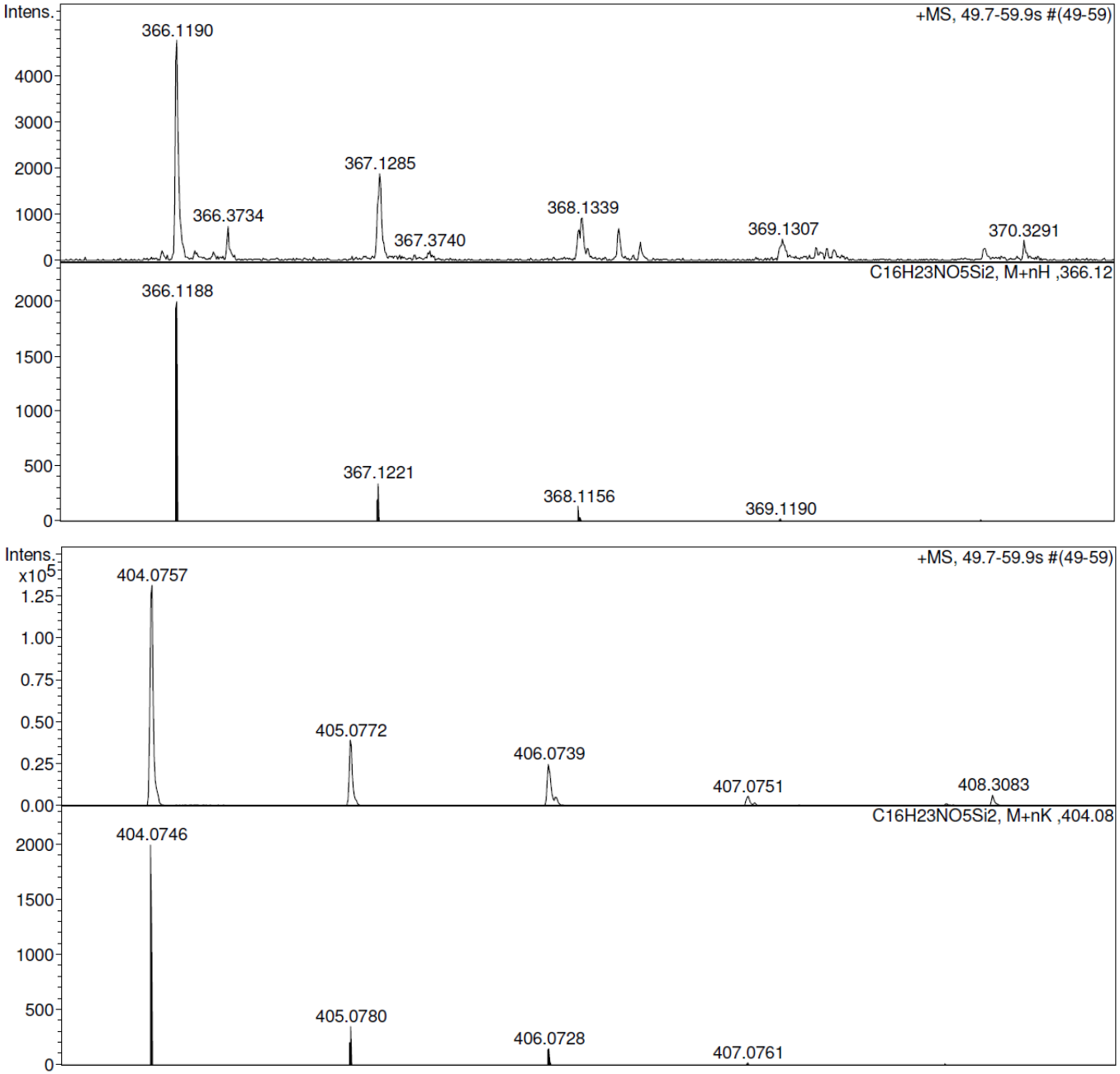
(400 MHz, acetone-d6)

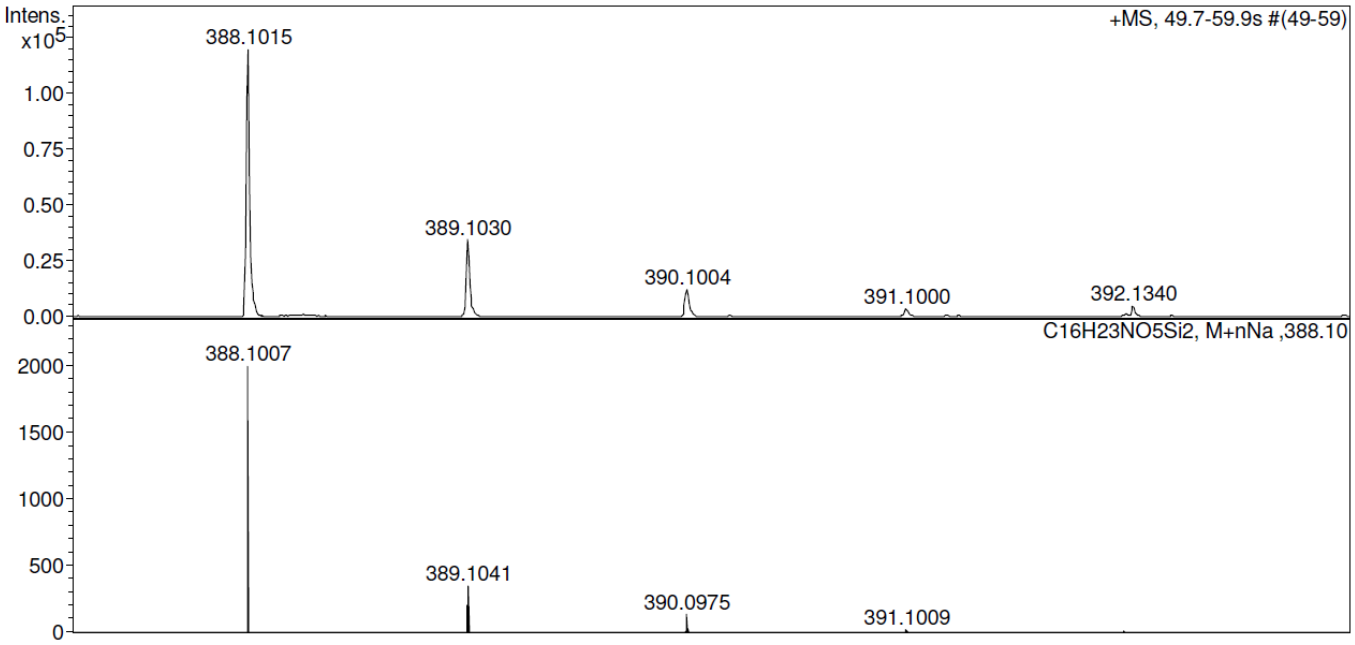


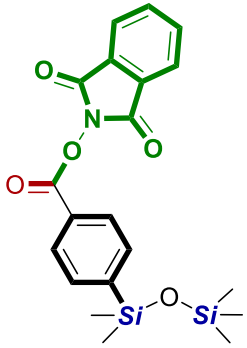
IR spectrum


2957
1774
1757
1560
1427
1391
1369
1254
1186
1111
987
842
638
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

HRMS (ESI)


Intens.
+MS, 49.7-59.9s #(49-59)
366.1190
366.3734
367.1285
367.3740
368.1339
369.1307
370.3291
C16H23NO5Si2, M+nH ,366.12
366.1188
367.1221
368.1156
369.1190
Intens.
x10^5
+MS, 49.7-59.9s #(49-59)
404.0757
405.0772
406.0739
407.0751
408.3083
C16H23NO5Si2, M+nK ,404.08
404.0746
405.0780
406.0728
407.0761



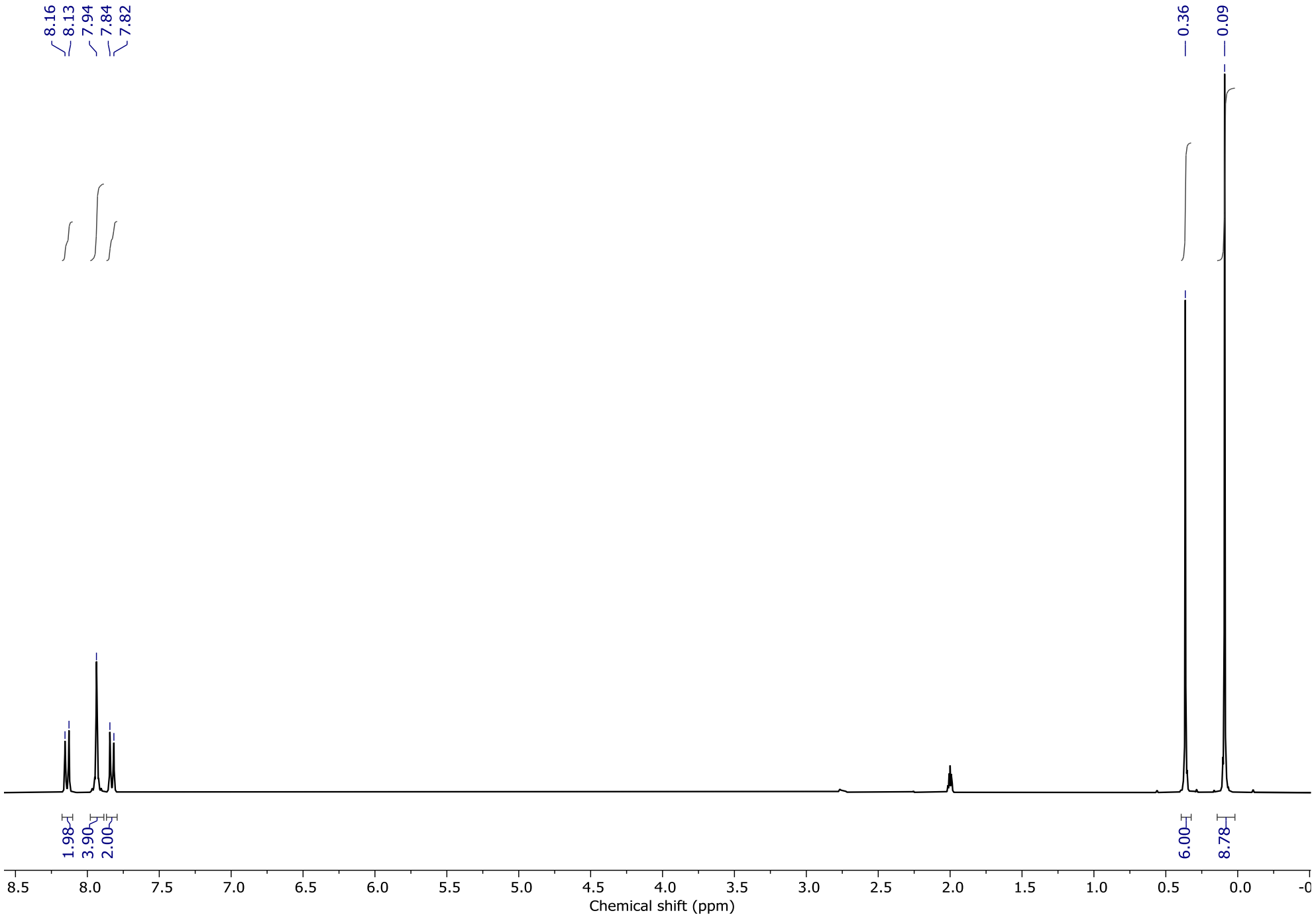


Characterisation data for 1,3-dioxoisoindolin-2-yl 4-(1,1,3,3,3-pentamethyldisiloxaneyl)benzoate:

^{1}H NMR (400 MHz, acetone-d6): δ = 8.15 (d, ^{3}J=11 Hz, 2H), δ = 7.94 (m, 4H), δ = 7.83 (d, ^{3}J=11 Hz, 2H), δ = 0.36 (s, 6H), δ = 0.09 (s, 9H). ^{13}C NMR (100 MHz, acetone-d6): δ = 163.84, 162.76, 149.98, 136.16, 134.58, 129.96, 129.79, 126.54, 124.71, 2.04, 0.83. ^{29}Si NMR (80 MHz, acetone-d6): δ = 9.71, -2.39. ^{15}N NMR (40 MHz, acetone-d6): δ = 207.49. HRMS (ESI) m/z [M + H] $^{+}$: calcd for [$C_{20}H_{23}NO_6Si_2$ + H]$^{+}$, 431.1215; found, 431.1474. IR (cm^{-1}): 2959, 1768, 1741, 1601, 1467, 1362, 1252, 1187, 1089, 1034-1006, 877-607.

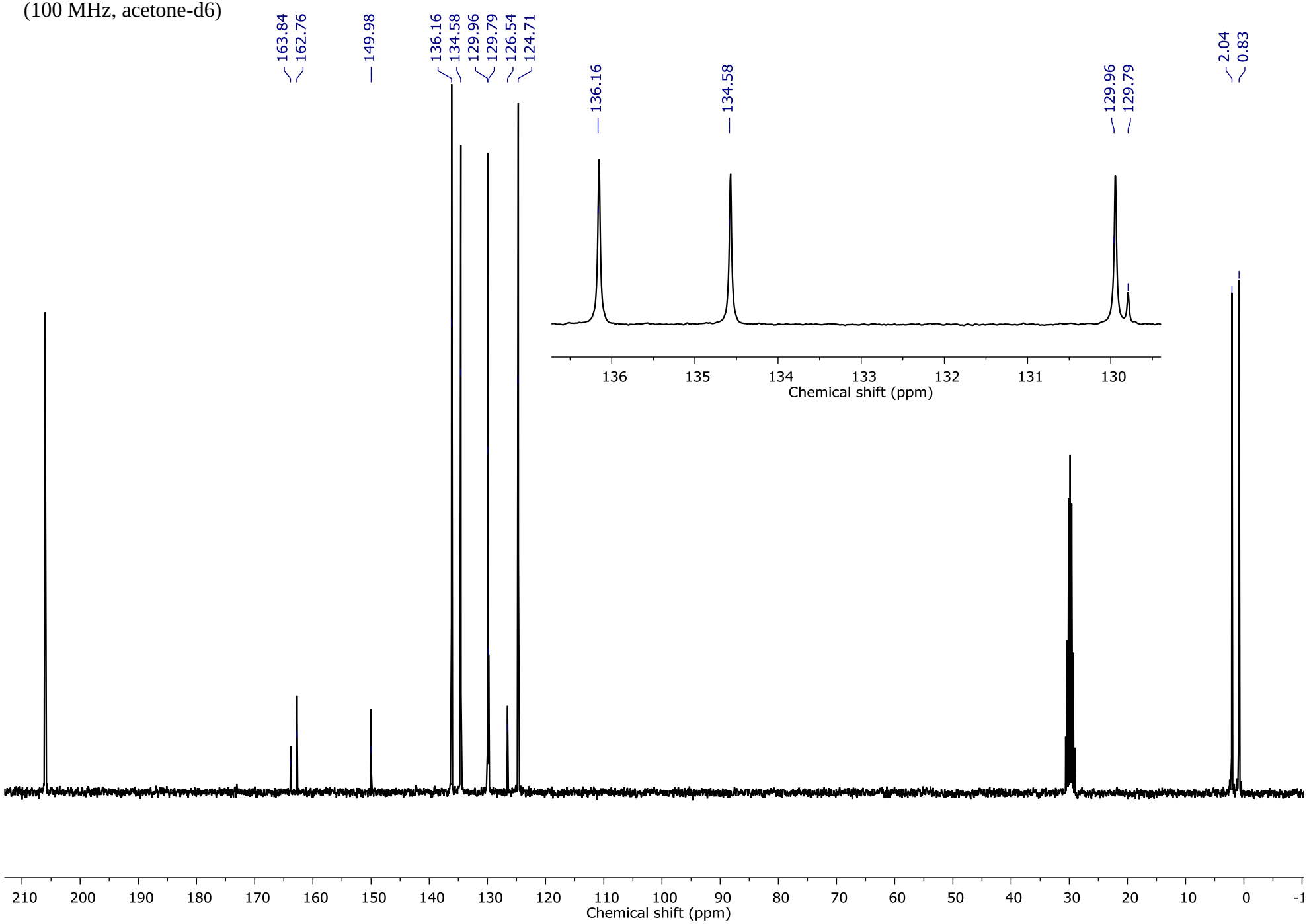
^{1}H NMR

(400 MHz, acetone-d6)



^{13}C NMR

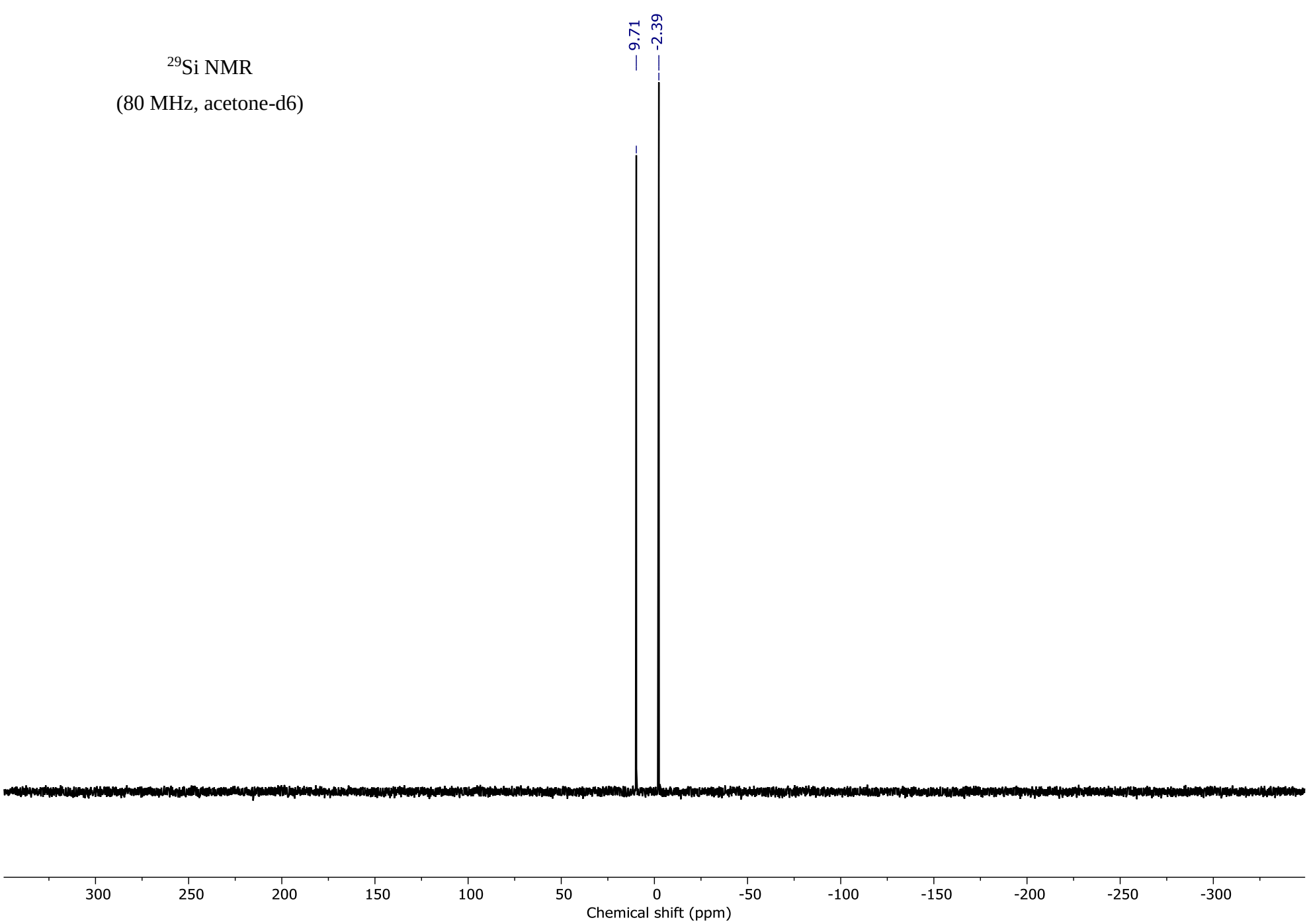
(100 MHz, acetone-d6)



S70

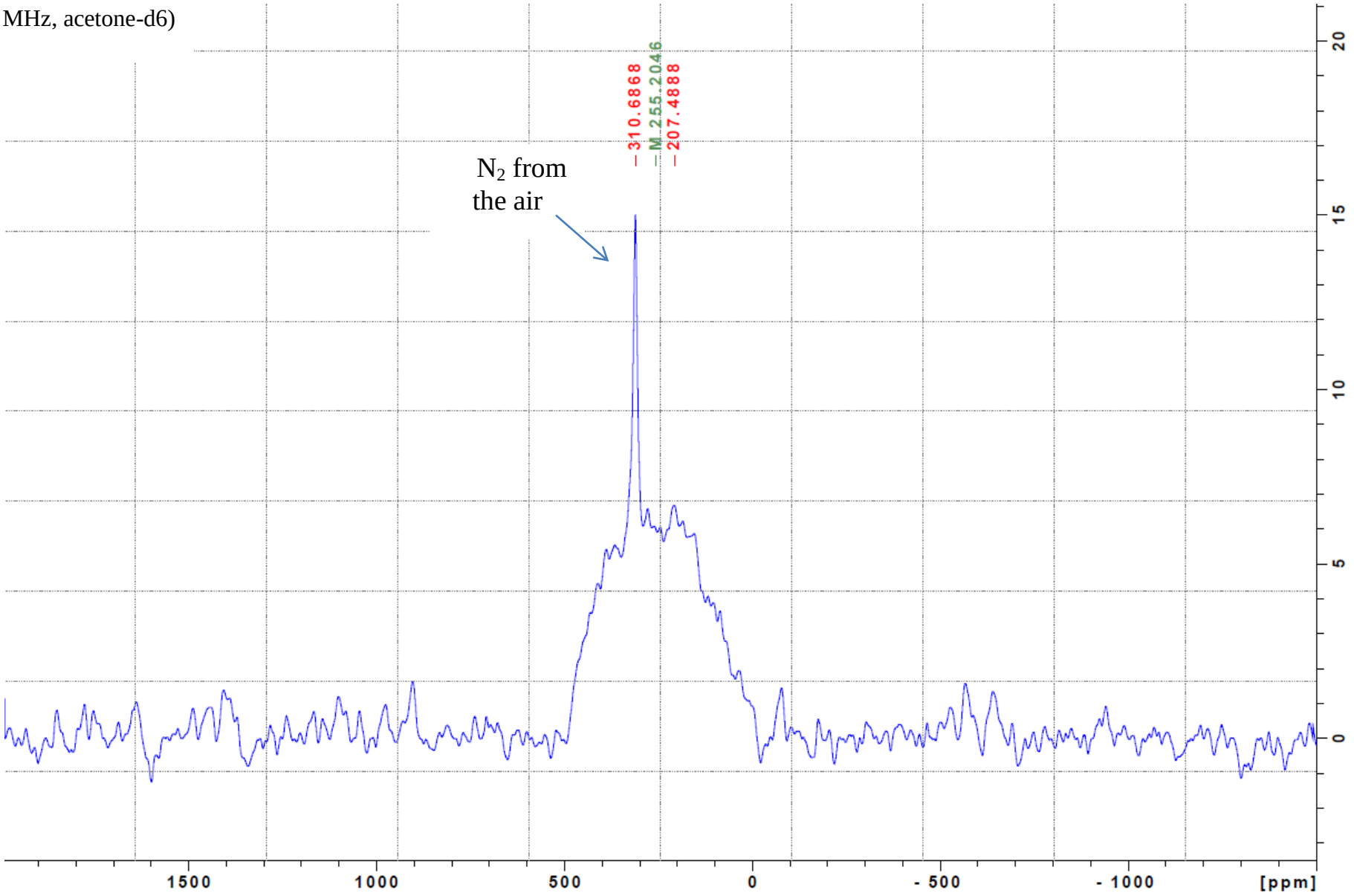
^{29}Si NMR

(80 MHz, acetone-d6)



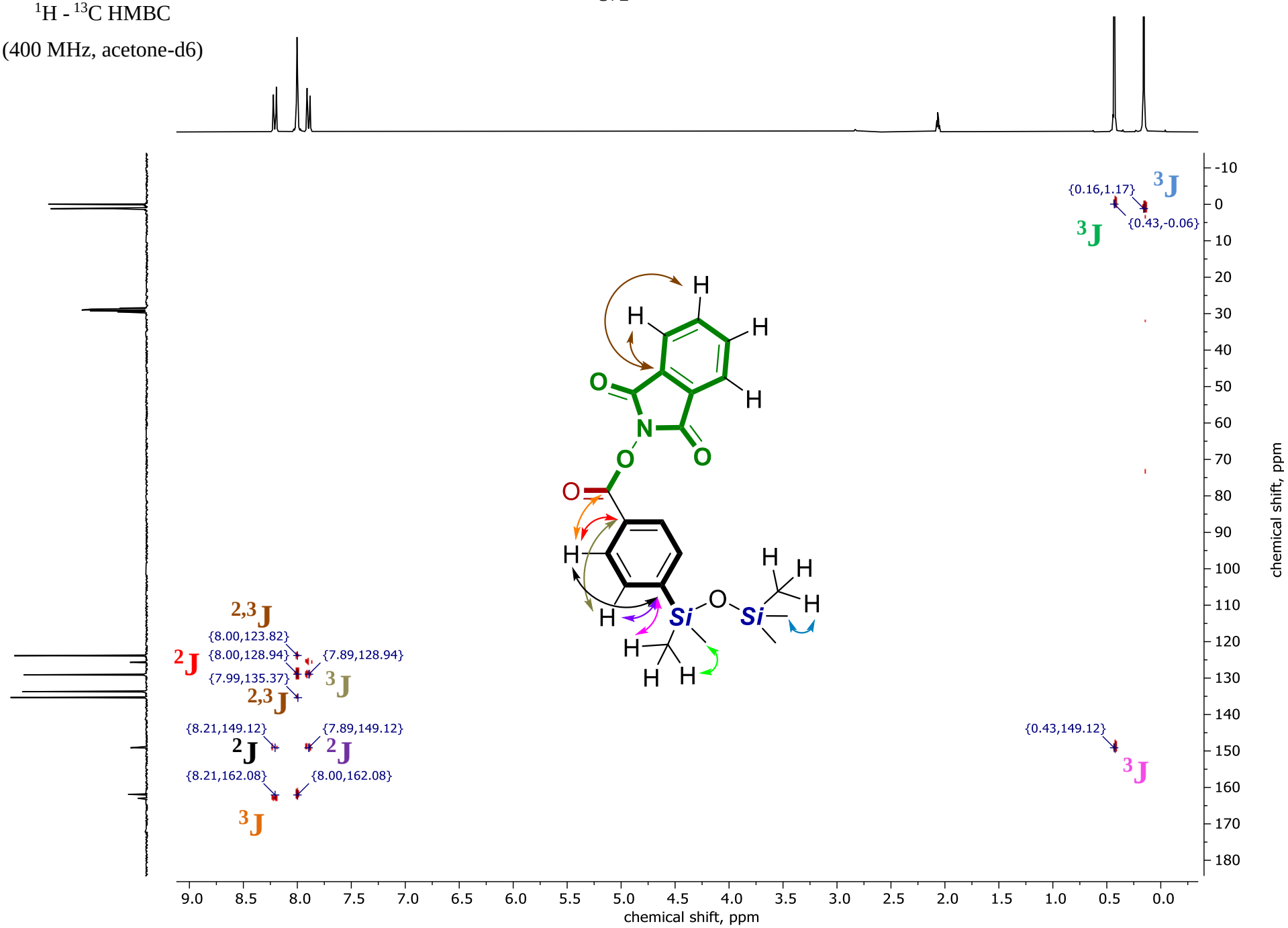
^{15}N NMR

(40 MHz, acetone-d6)



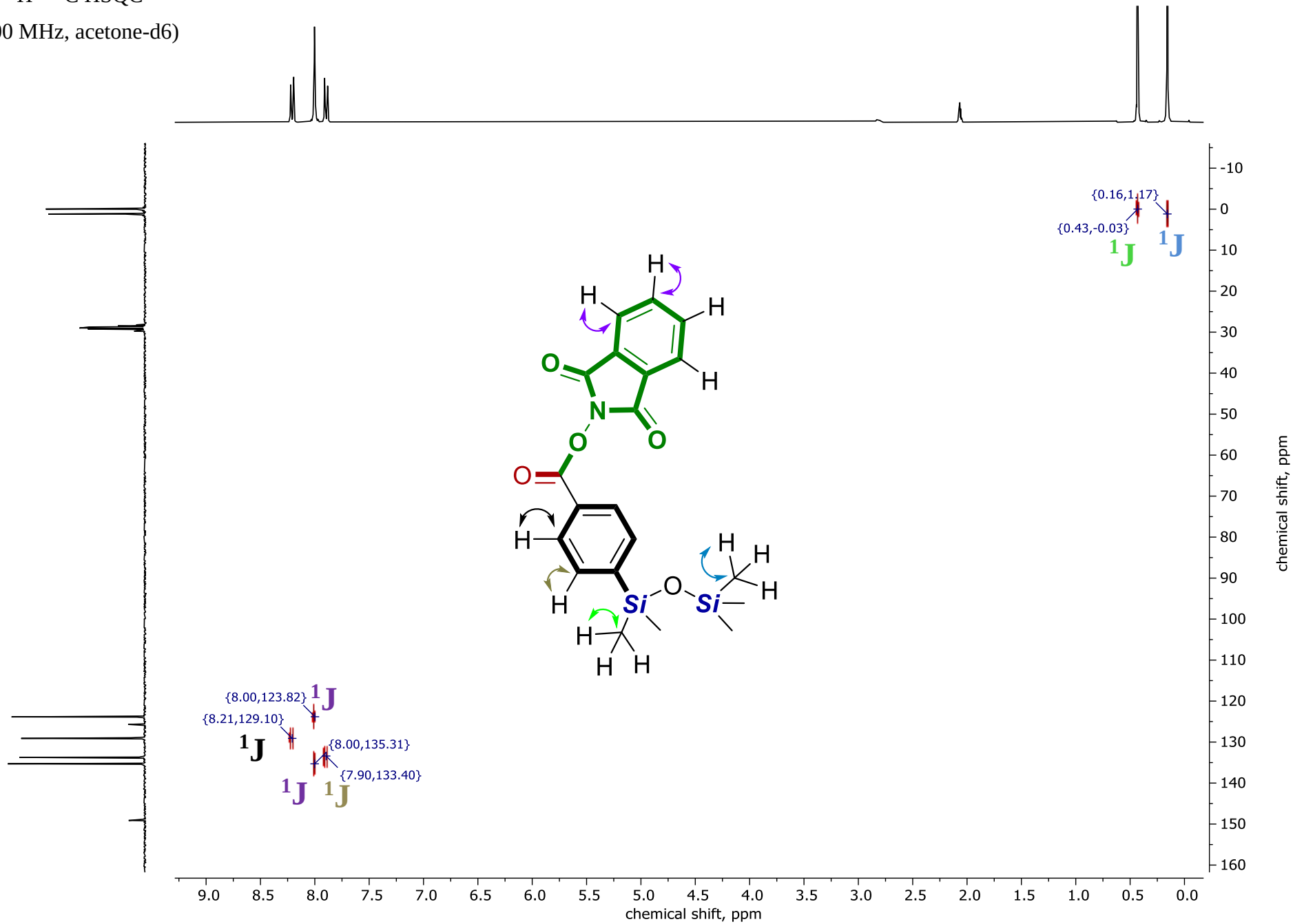
^{1}H - ^{13}C HMBC

(400 MHz, acetone-d6)



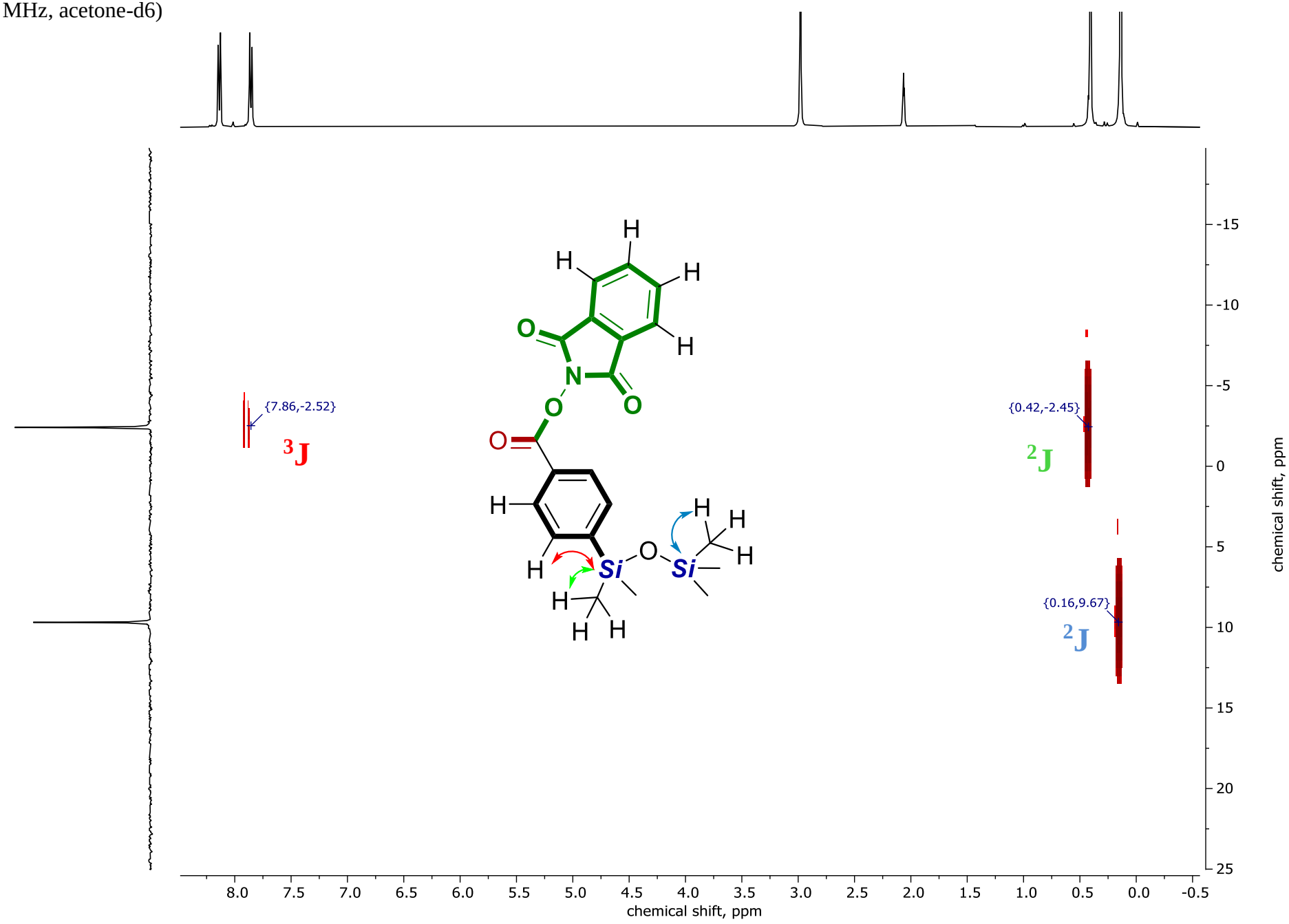
^{1}H - ^{13}C HSQC

(400 MHz, acetone-d6)

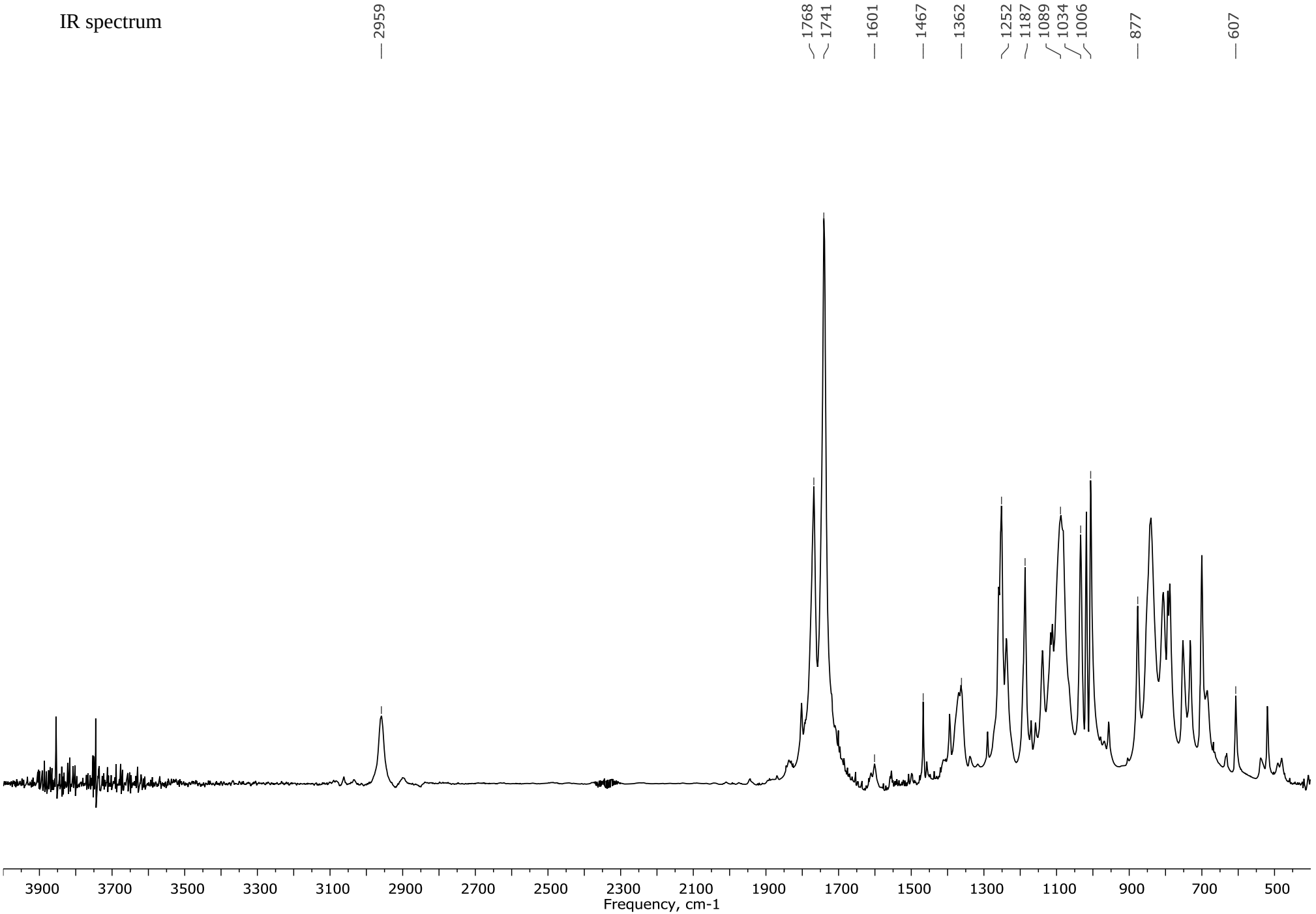


^{1}H - ^{29}Si HMBC

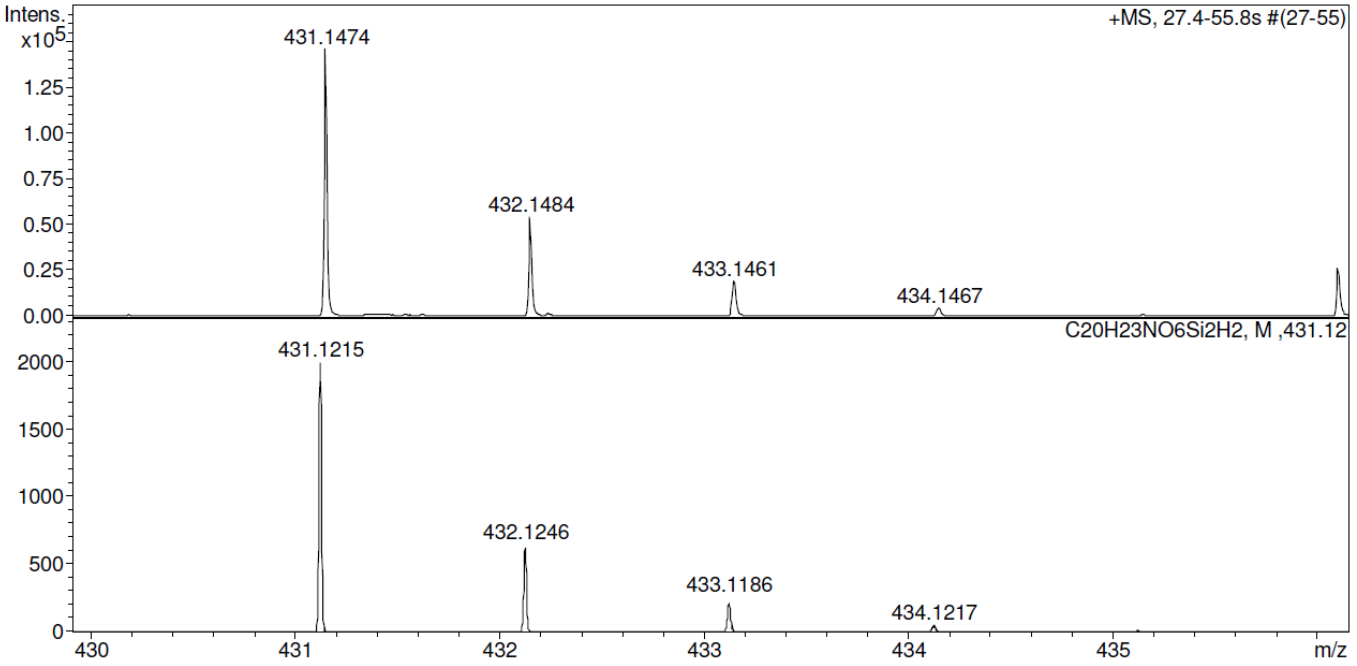
(400 MHz, acetone-d6)

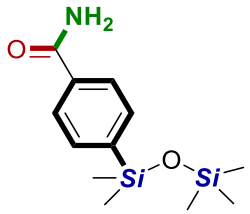


IR spectrum


2959
1768
1741
1601
1467
1362
1252
1187
1089
1034
1006
877
607
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

HRMS (ESI)



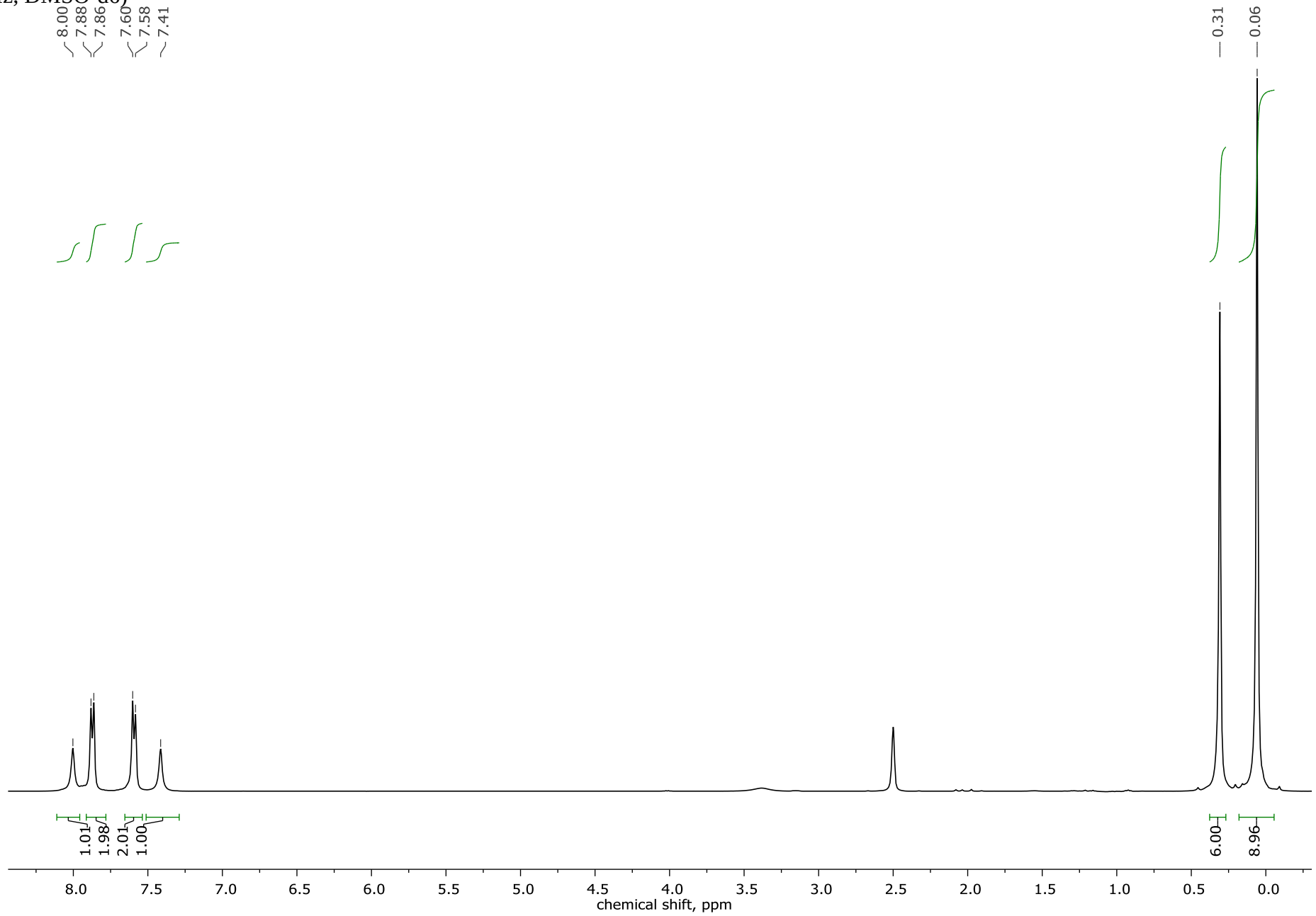


Characterisation data for 4-(1,1,3,3,3-pentamethyldisiloxanyl)benzamide:

^{1}H NMR (400 MHz, DMSO-d6): δ = 8.00 (br s, 1H), δ = 7.87 (d, ^{3}J=8, 2H), δ = 7.59 (d, ^{3}J=8, 2H), δ = 7.41 (br s, 1H), δ = 0.31 (s, 6H), δ = 0.06 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d6): δ = 167.94, 142.97, 135.10, 132.64, 126.67, 1.99, 0.74. ^{29}Si NMR (80 MHz, DMSO-d6): δ = 9.14, -2.08. ^{15}N NMR (40 MHz, DMSO-d6): δ = 103.05. IR (cm^{-1}): 2958, 1653, 1610, 1547, 1405, 1251, 1067, 840-685.

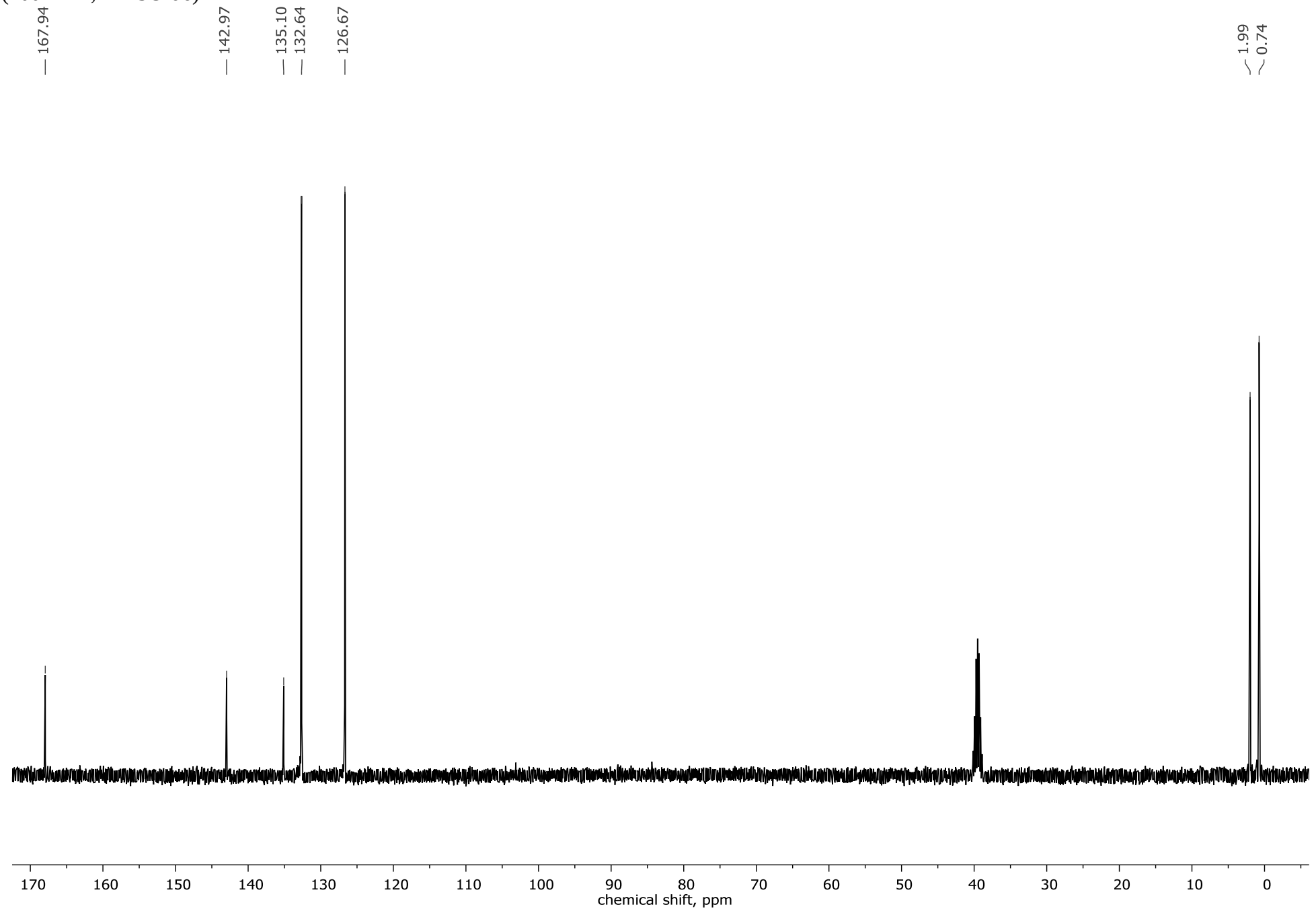
^{1}H NMR

(400 MHz, DMSO-d6)



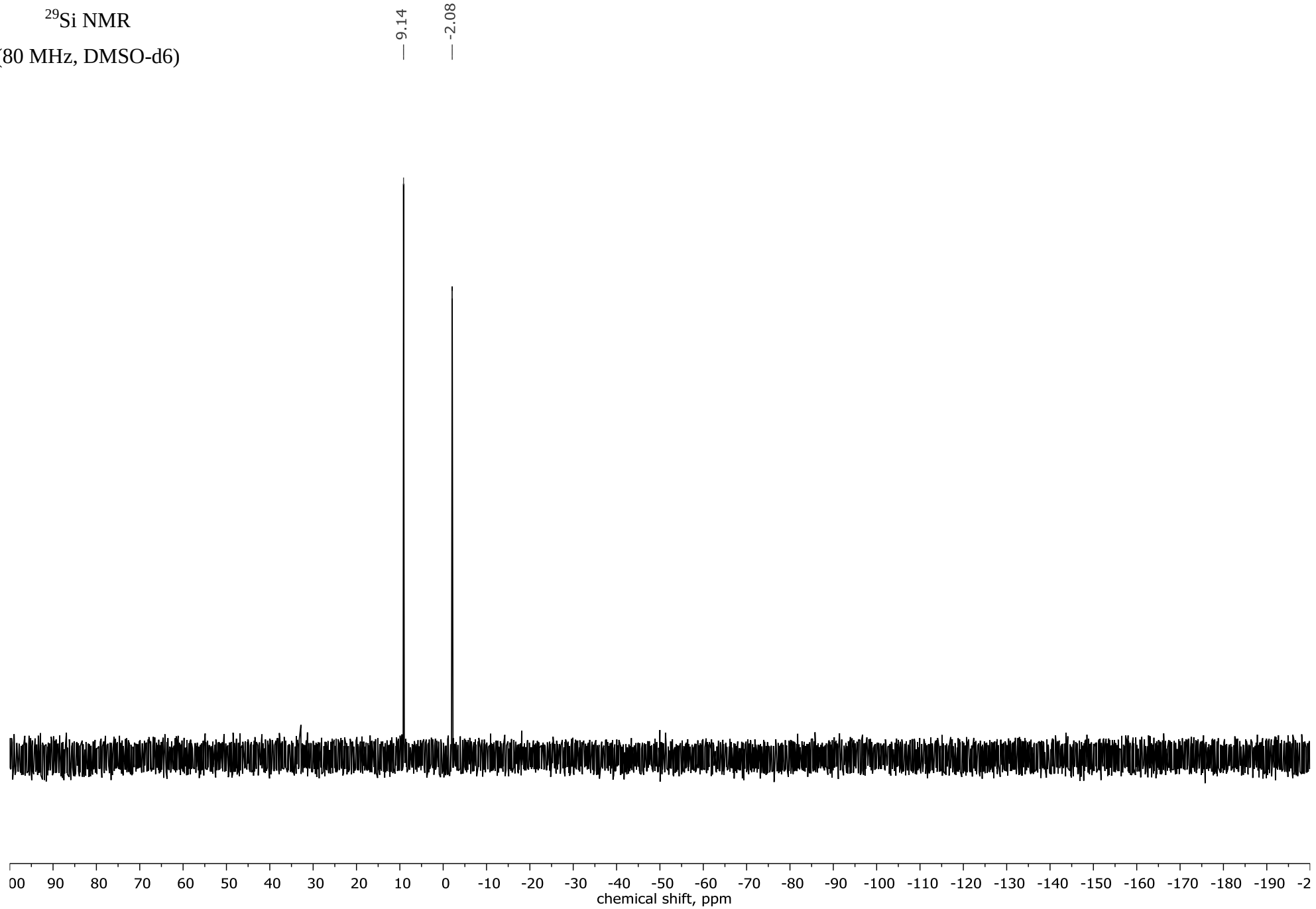
^{13}C NMR

(100 MHz, DMSO-d6)



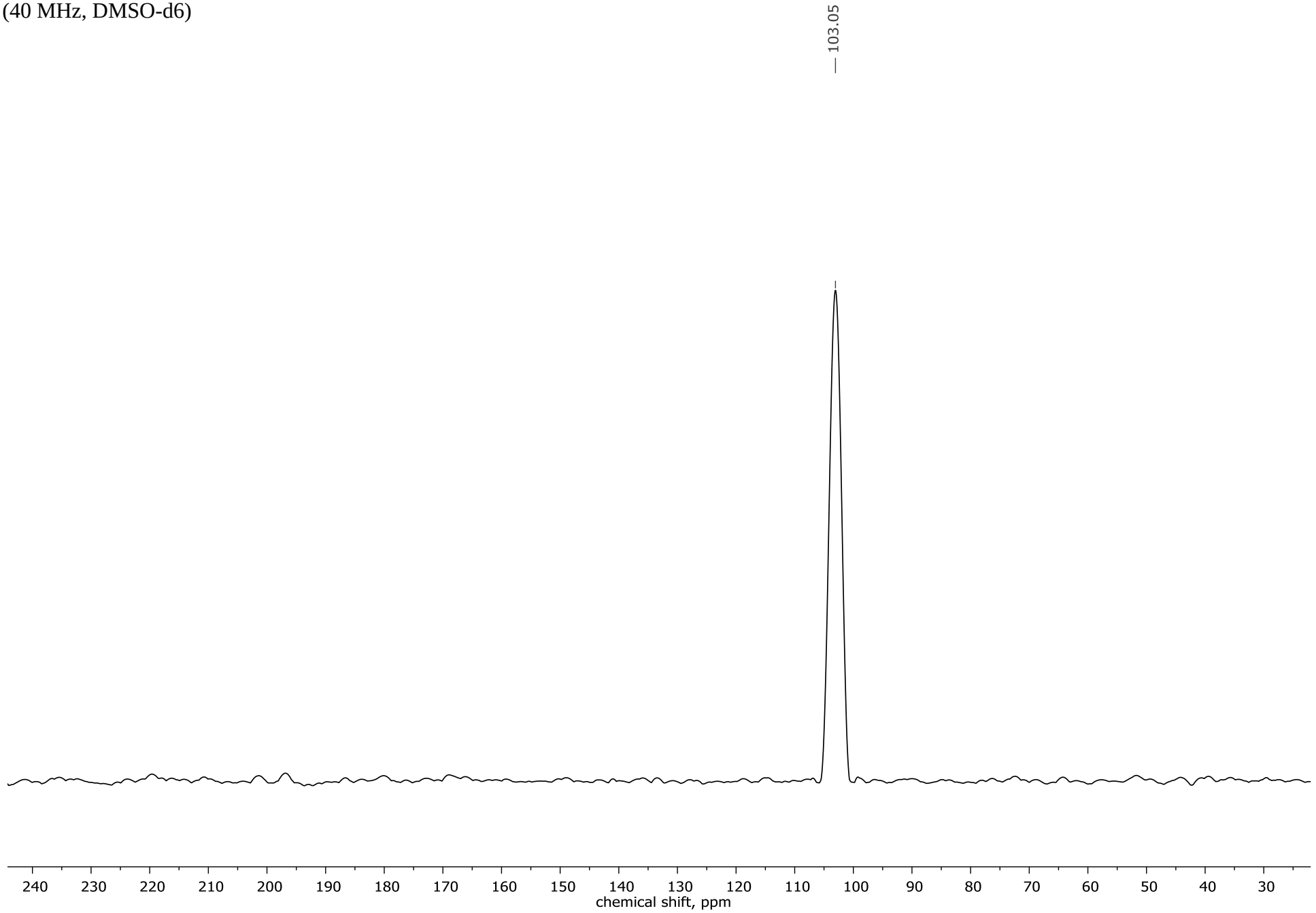
^{29}Si NMR

(80 MHz, DMSO-d6)



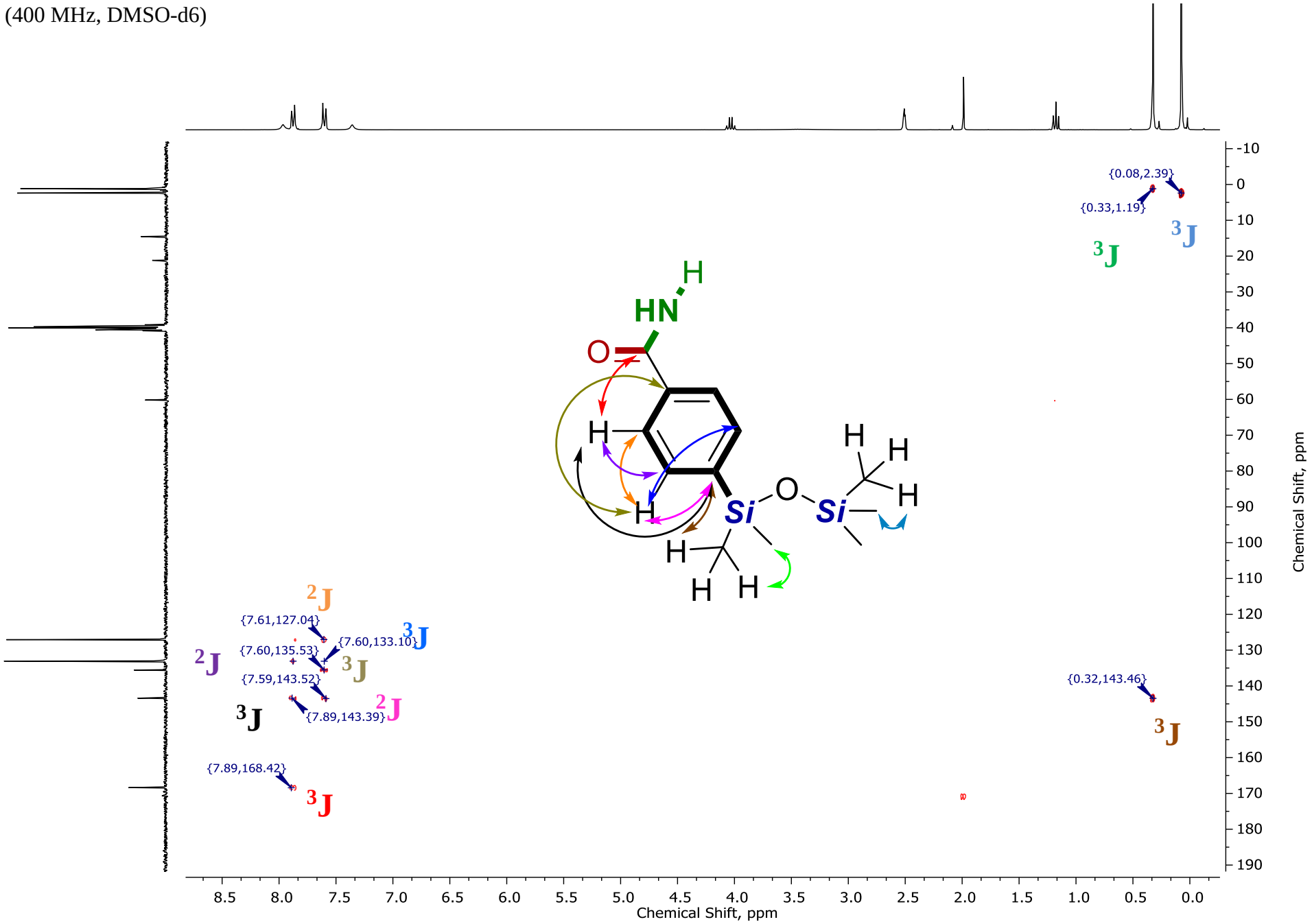
15N NMR

(40 MHz, DMSO-d6)



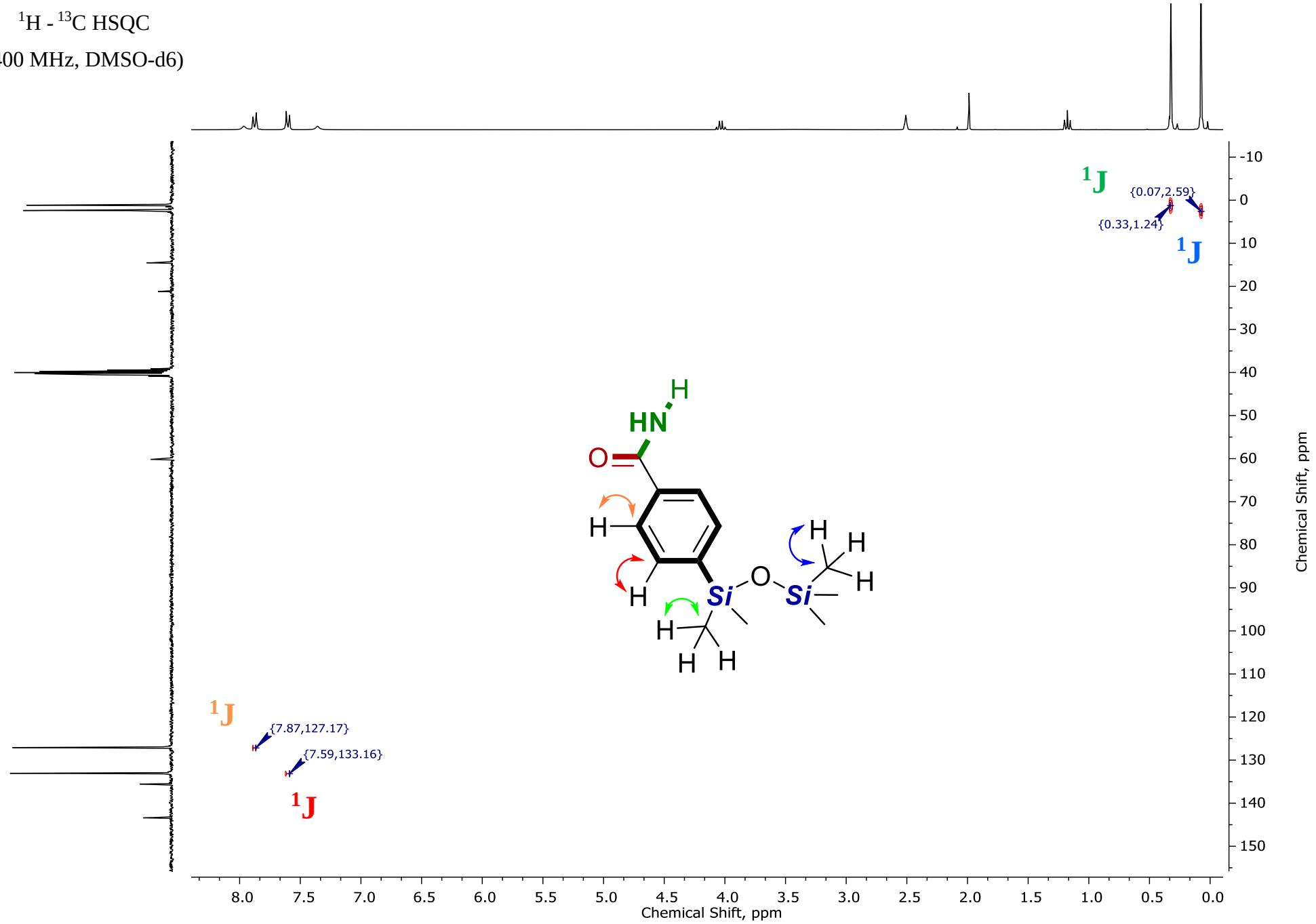
^{1}H - ^{13}C HMBC

(400 MHz, DMSO-d6)



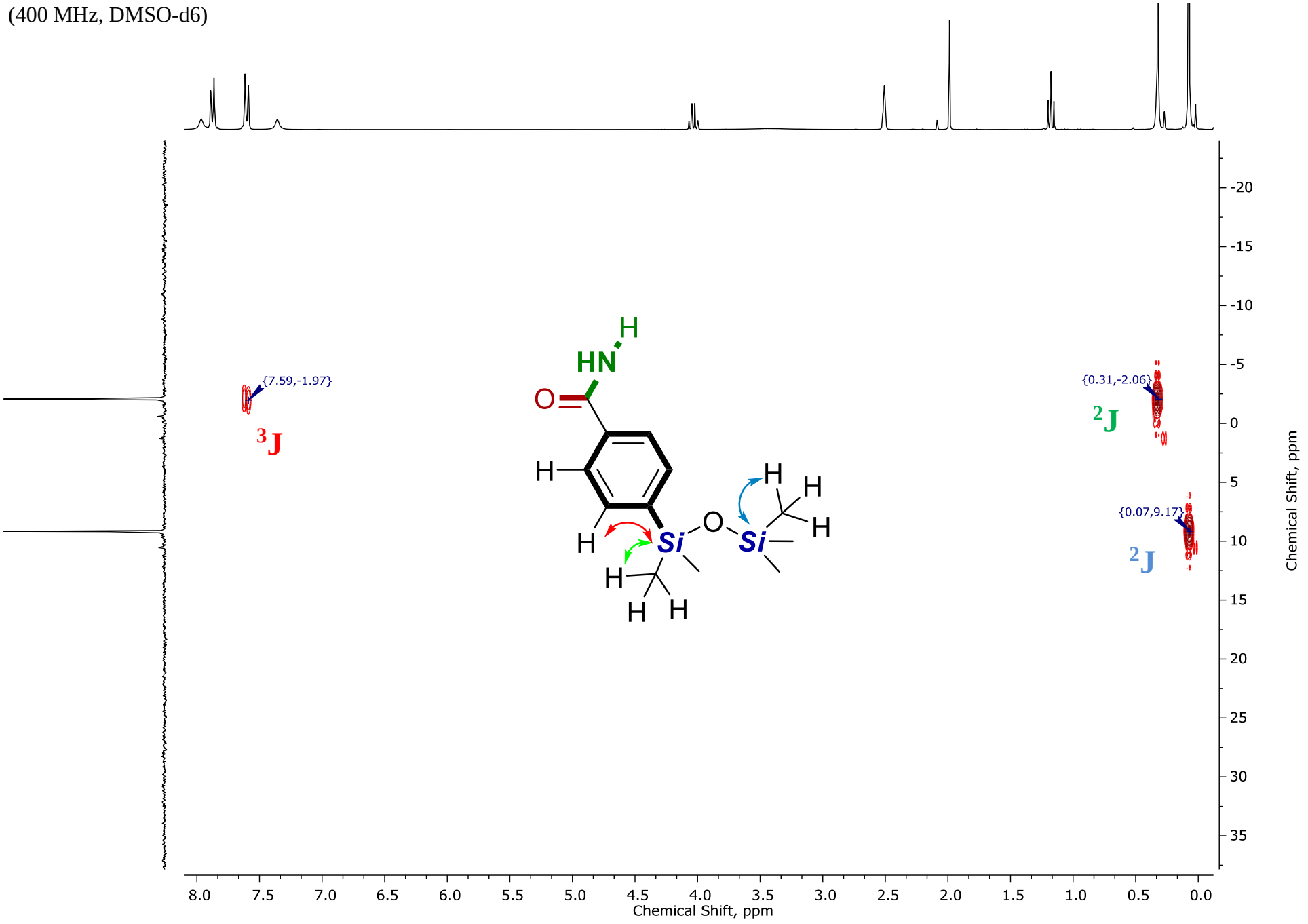
^{1}H - ^{13}C HSQC

(400 MHz, DMSO-d6)



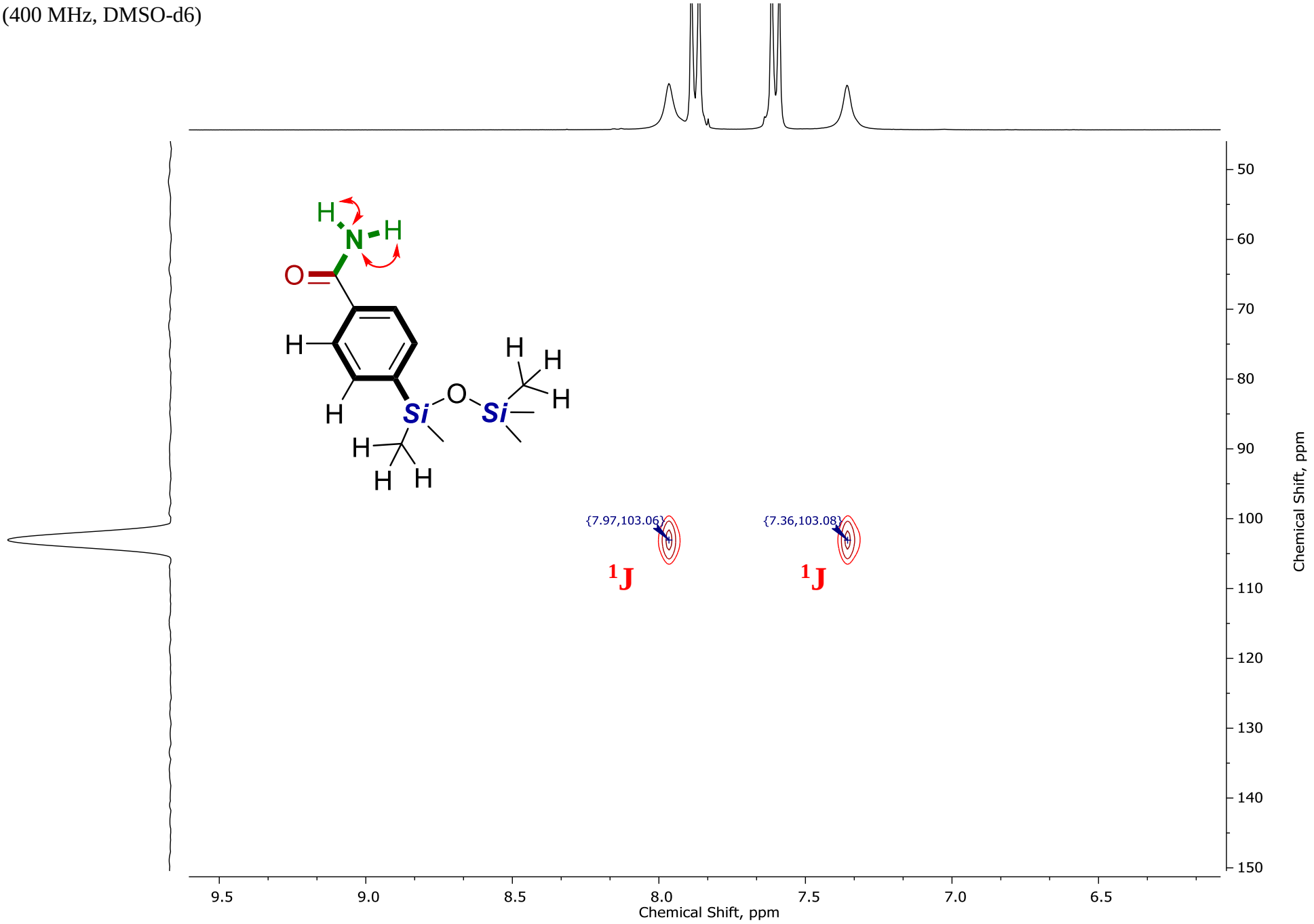
$^{1}H - ^{29}Si$ HMBC

(400 MHz, DMSO-d6)

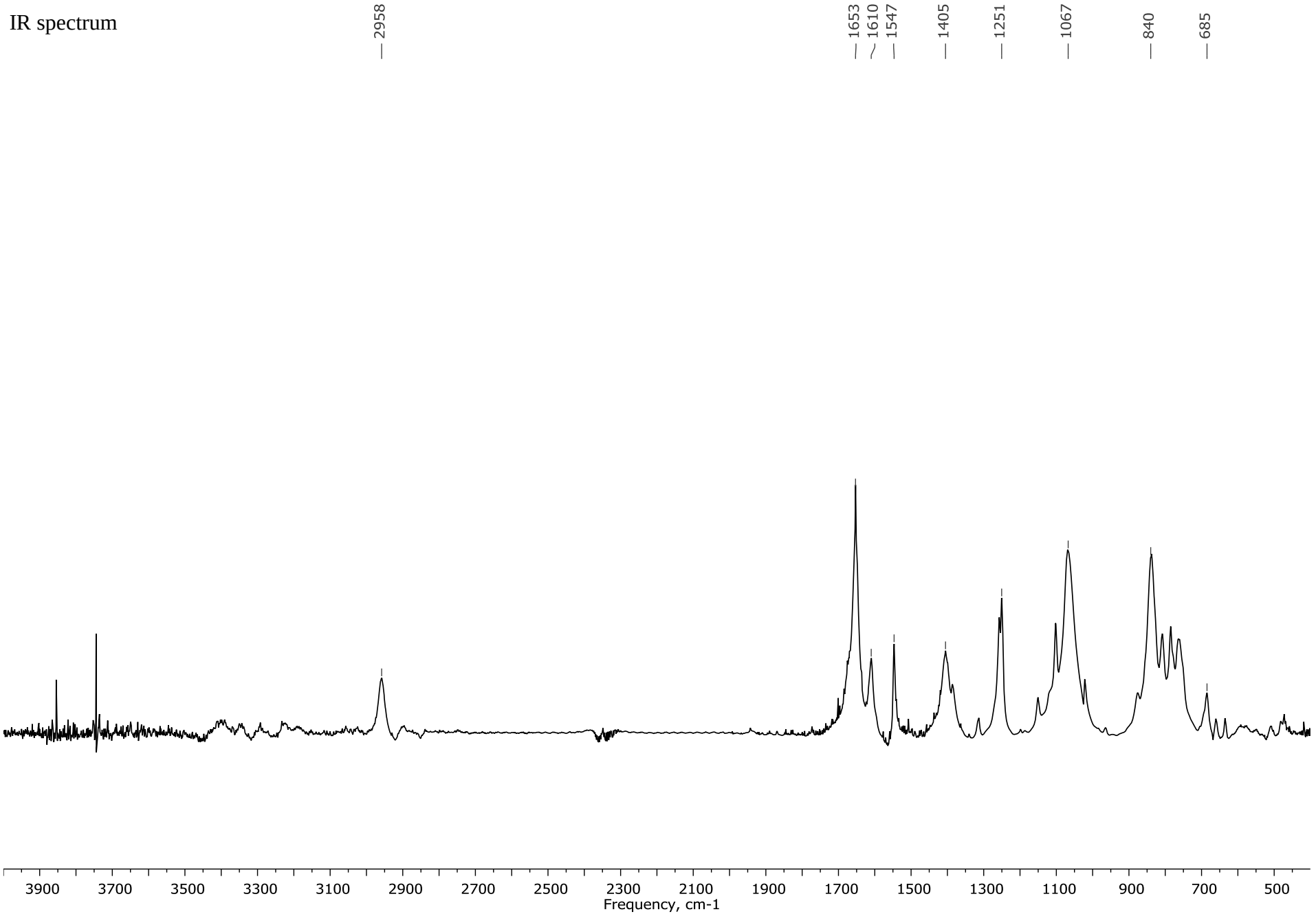


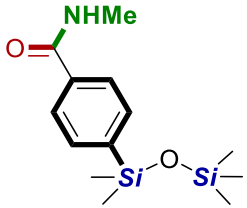
$^{1}H - ^{15}N$ HSQC

(400 MHz, DMSO-d6)



IR spectrum


2958
1653
1610
1547
1405
1251
1067
840
685
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

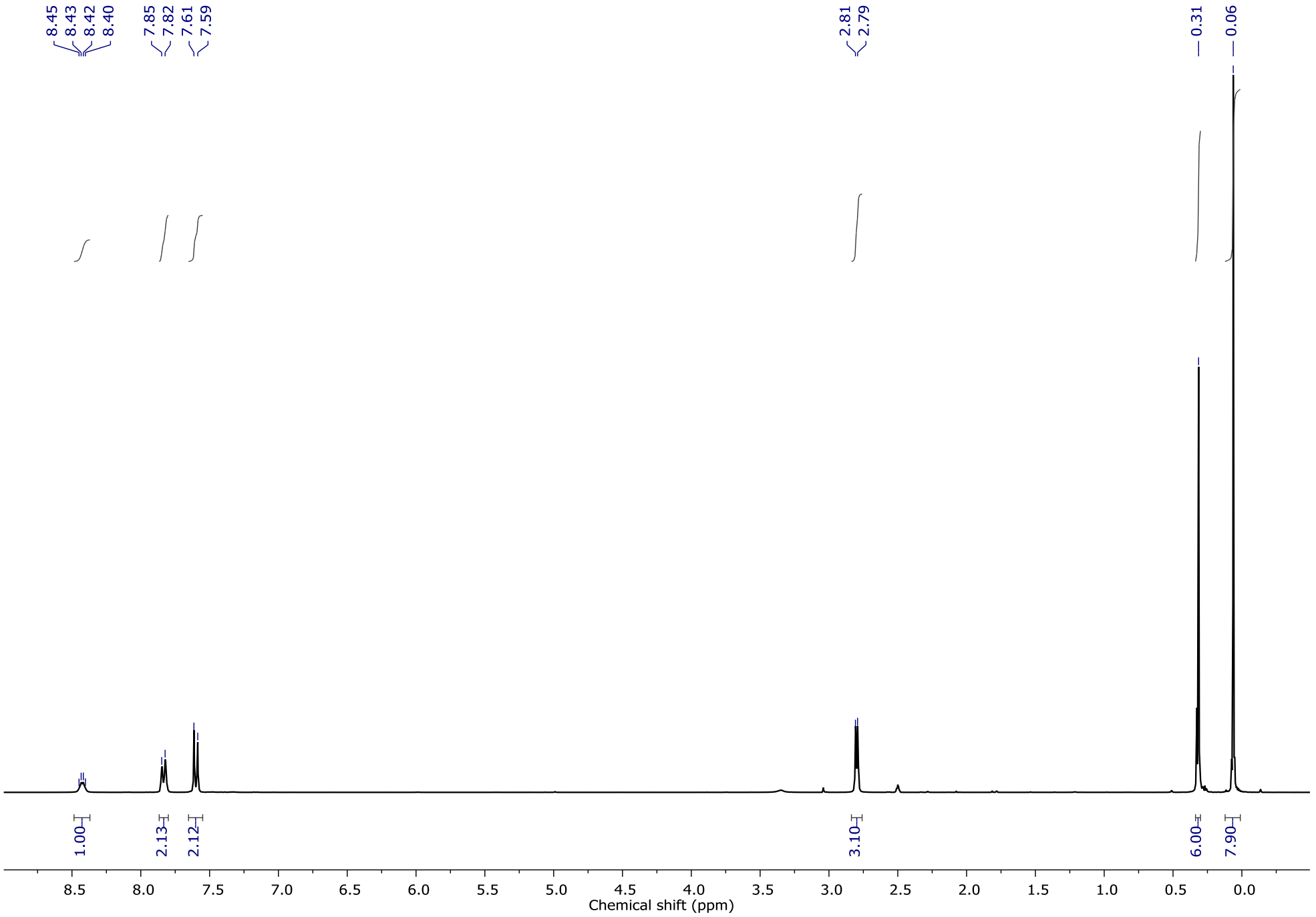


Characterisation data for N-methyl-4-(1,1,3,3,3-pentamethyldisiloxanyl)benzamide:

^{1}H NMR (400 MHz, DMSO-d6): δ = 8.43 (m, 1H), δ = 7.84 (d, ^{3}J=11 Hz, 2H), δ = 7.60 (d, ^{3}J=11 Hz, 2H), δ = 2.80 (d, ^{3}J=6 Hz, 3H), δ = 0.31 (s, 6H), δ = 0.06 (s, 7H). ^{13}C NMR (100 MHz, DMSO-d6): δ = 166.58, 142.64, 135.32, 132.60, 126.20, 26.16, 1.87, 0.63. ^{29}Si NMR (80 MHz, DMSO-d6): δ = 9.62, -2.09. ^{15}N NMR (40 MHz, DMSO-d6): δ = 99.40. HRMS (ESI) m/z [M + H] $^{+}$: calcd for $[C_{13}H_{23}NO_2Si_2 + H]^{+}$, 282.1340; found, 282.1351. IR (cm^{-1}): 3323, 2958, 1636, 1543, 1411, 1318, 1255, 1160-1036, 877-639.

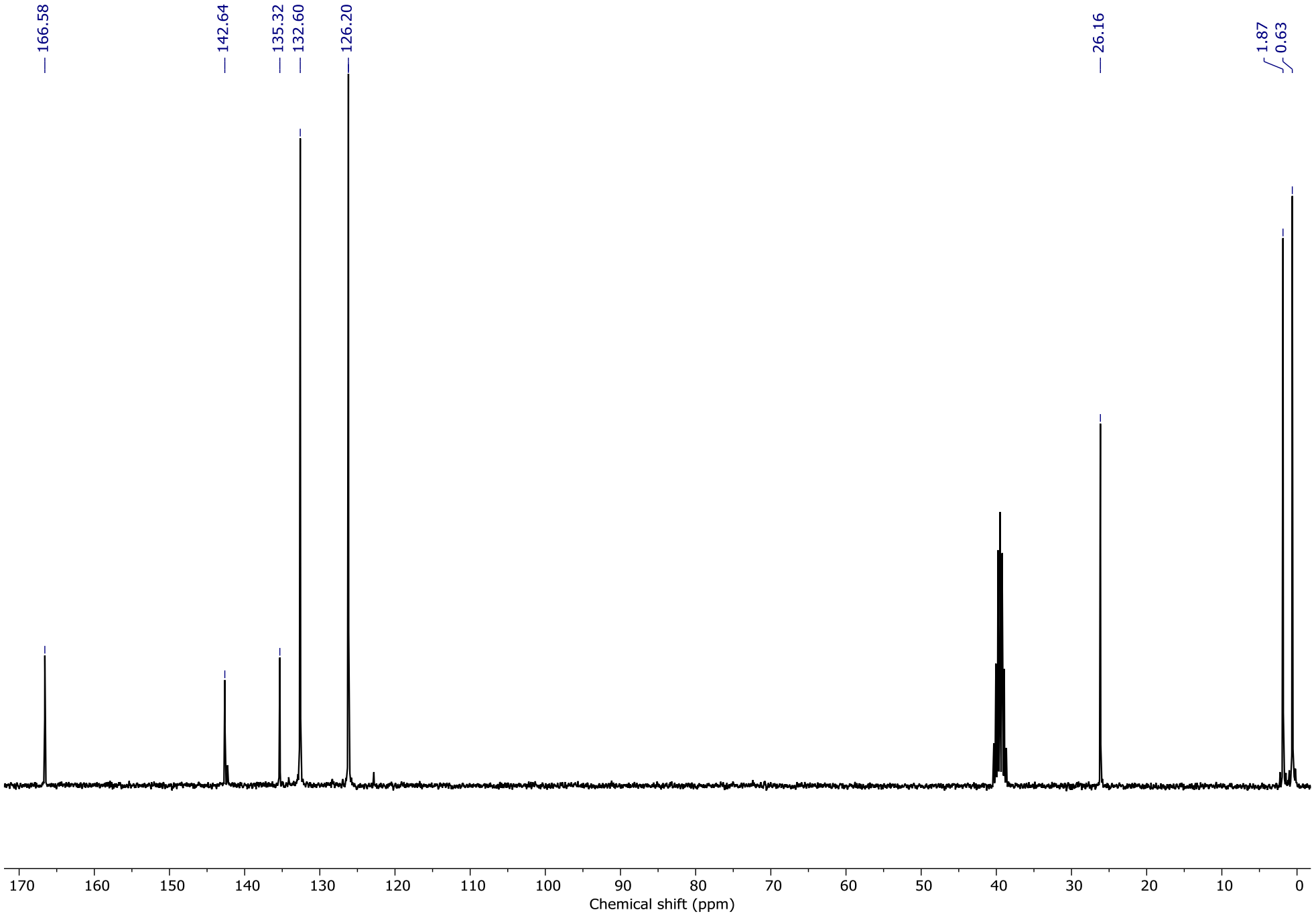
^{1}H NMR

(400 MHz, DMSO-d6)



^{13}C NMR

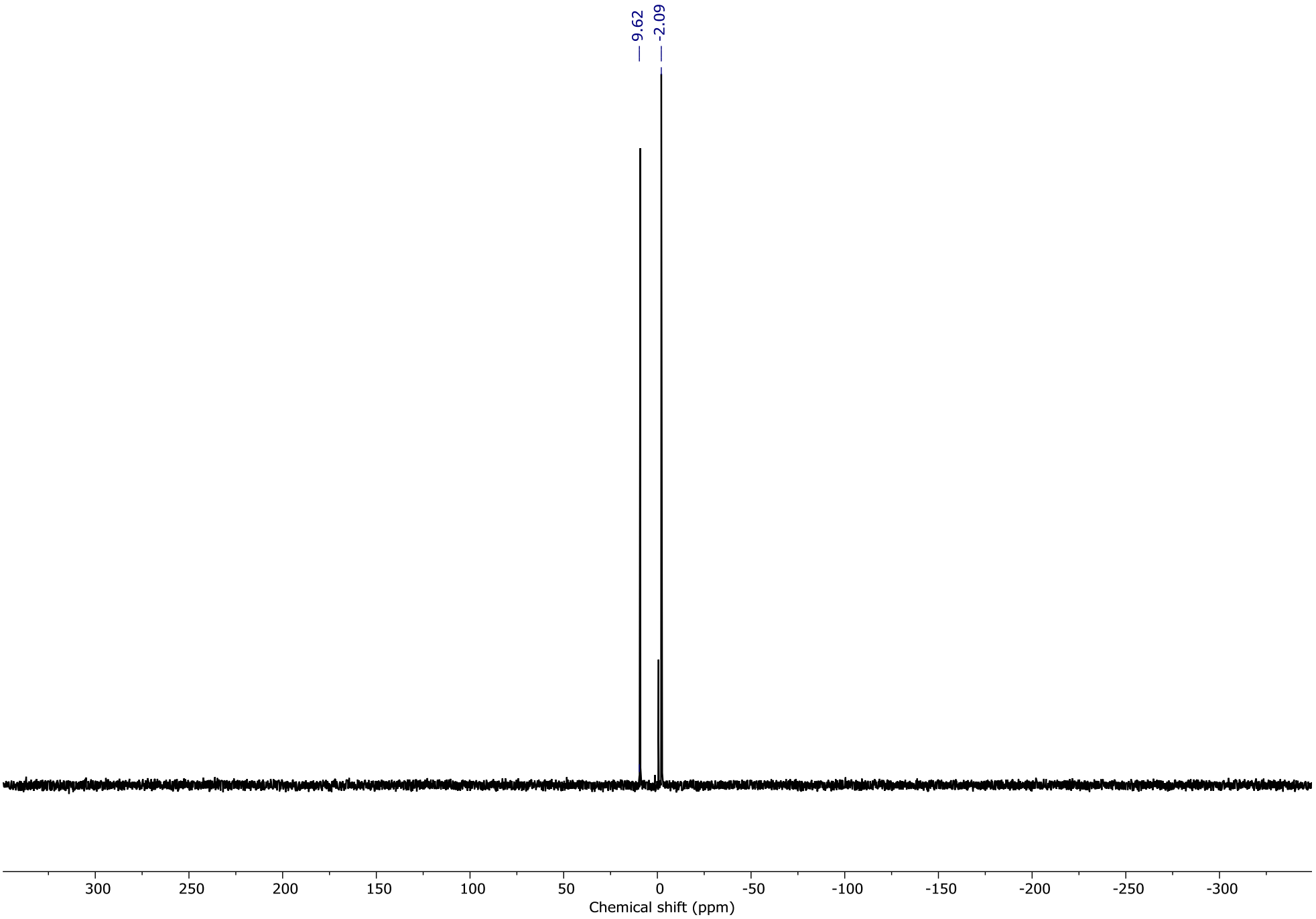
(100 MHz, DMSO-d6)



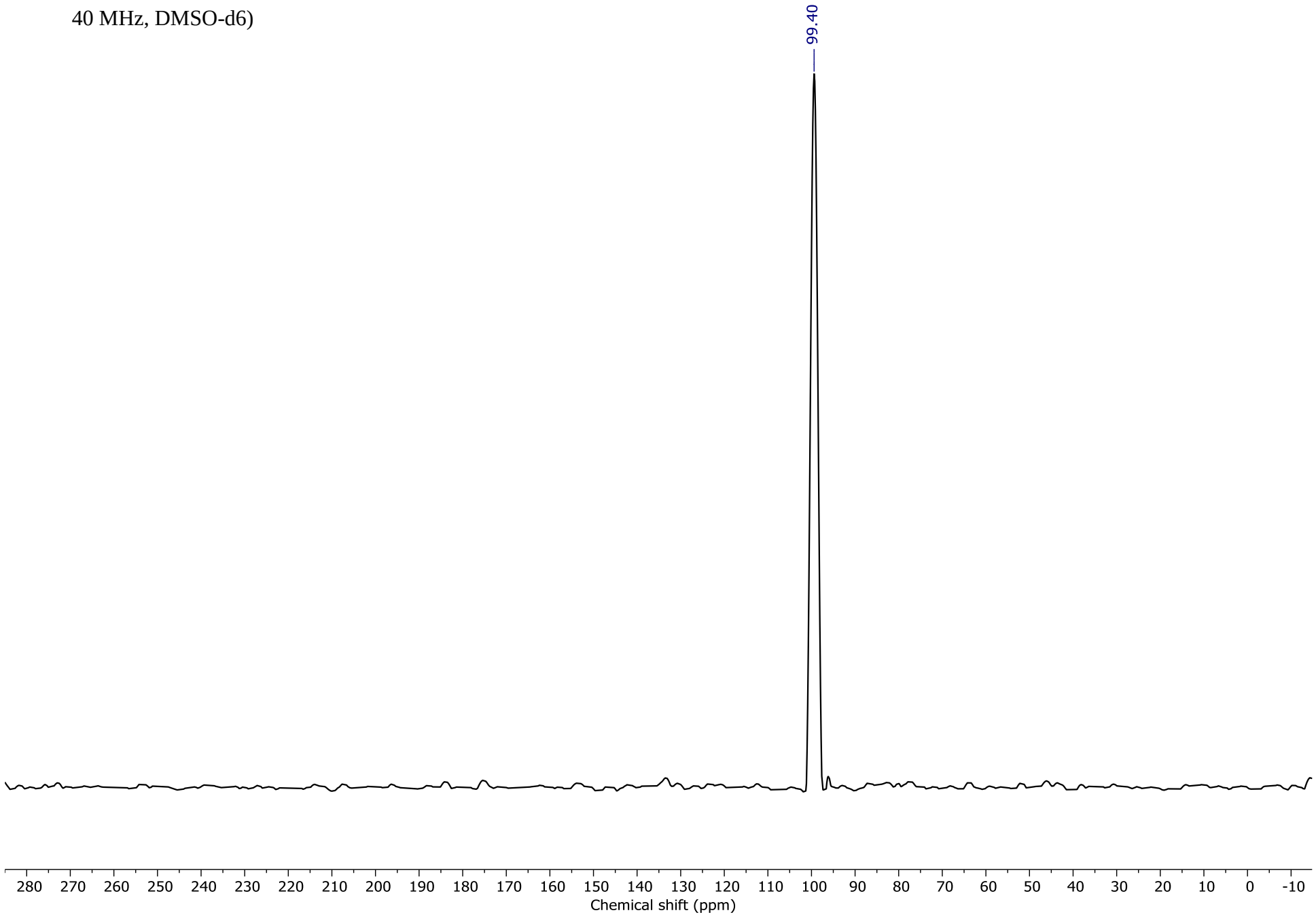
^{29}Si NMR

(80 MHz, DMSO-d6)

S89

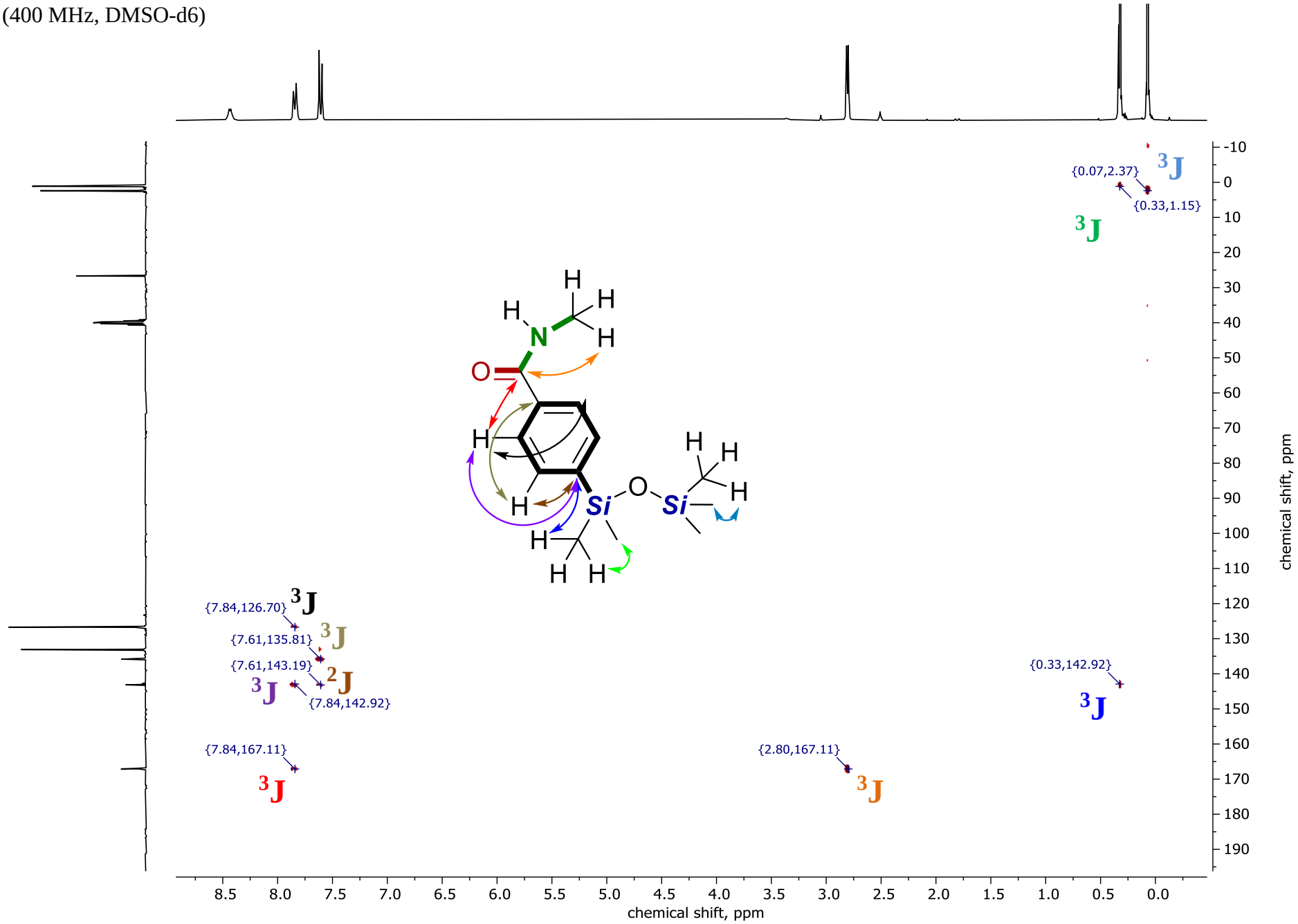


^{15}N NMR (reconstructed, 40 MHz, DMSO-d6)



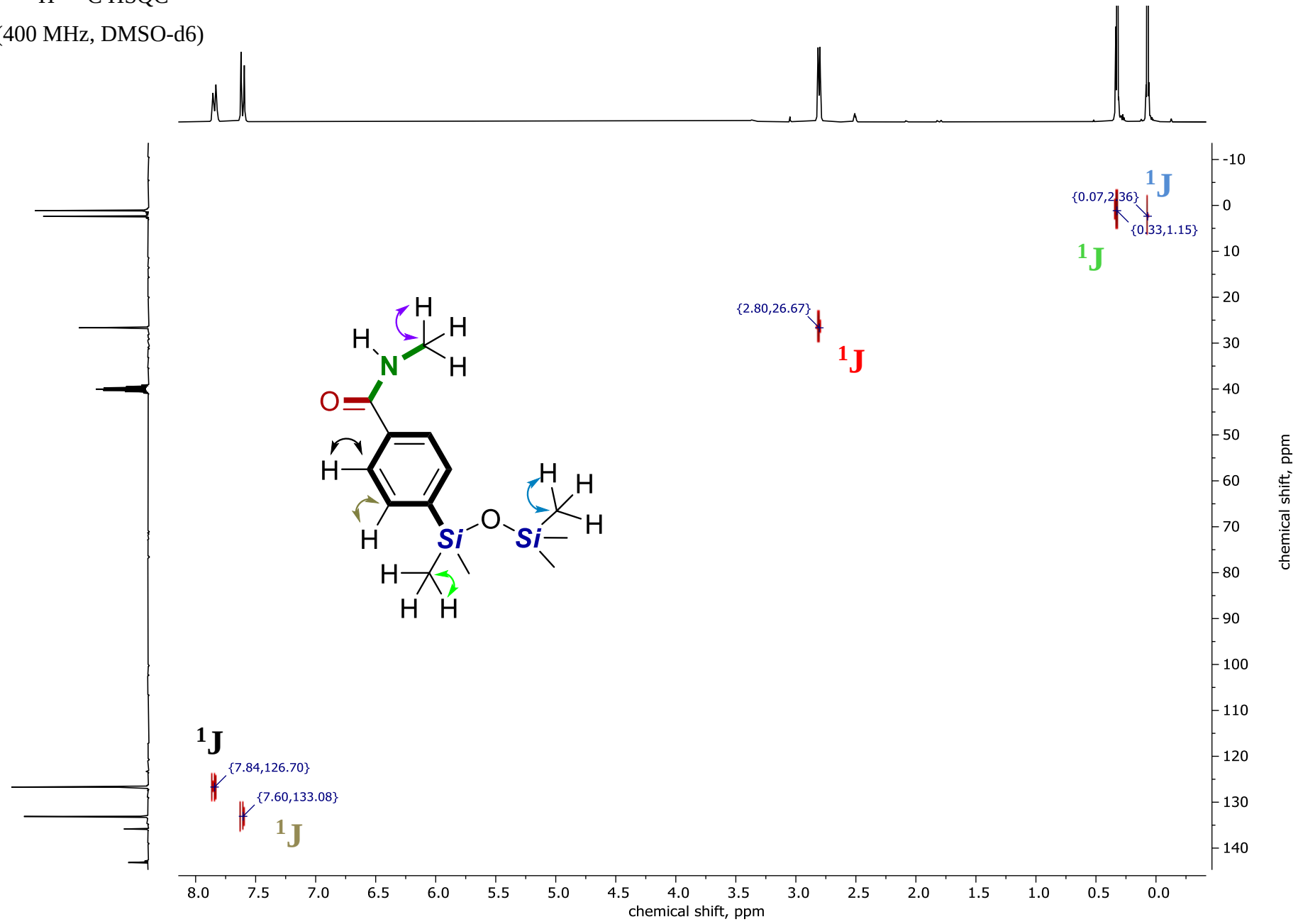
^{1}H - ^{13}C HMBC

(400 MHz, DMSO-d6)



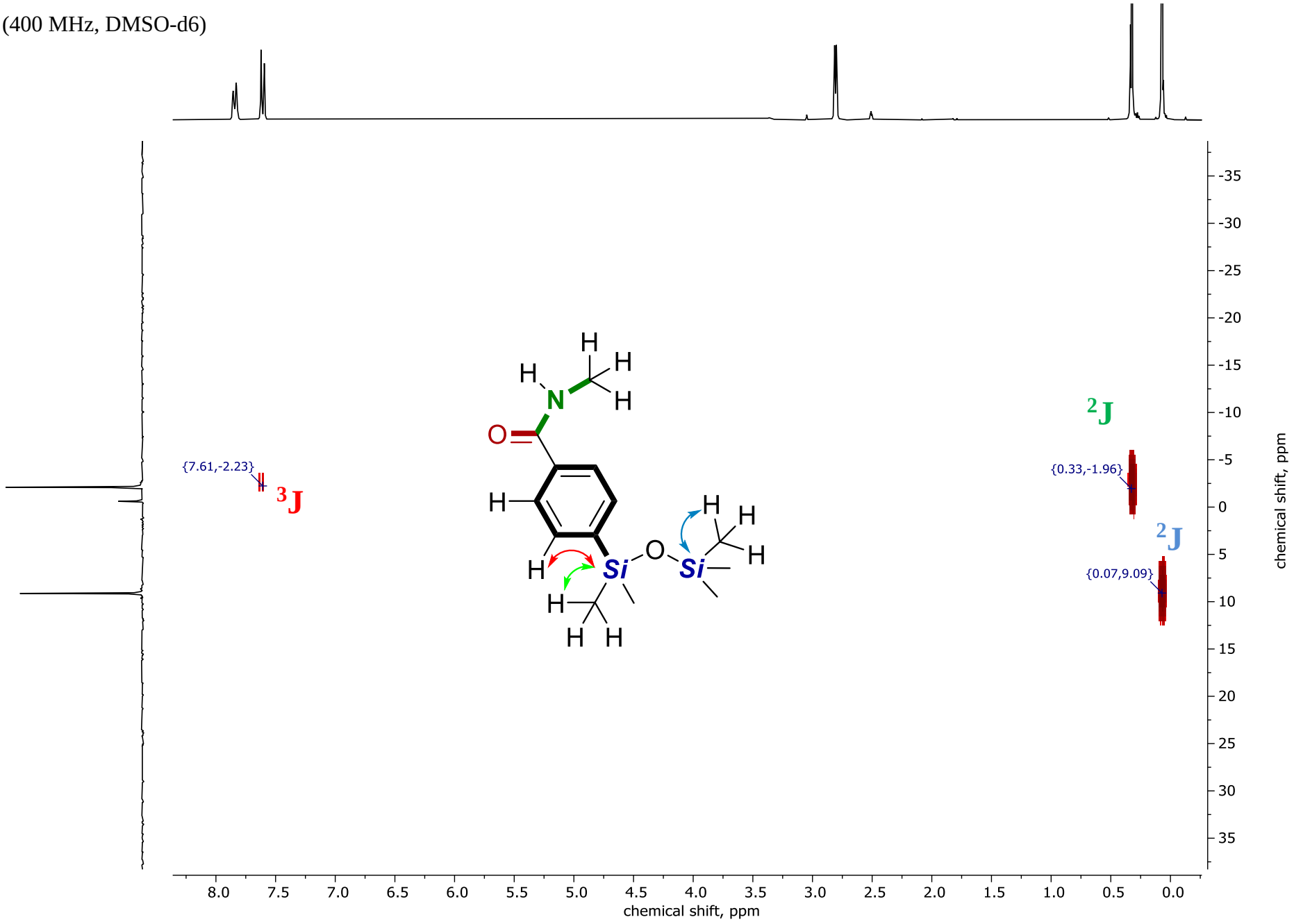
^{1}H - ^{13}C HSQC

(400 MHz, DMSO-d6)



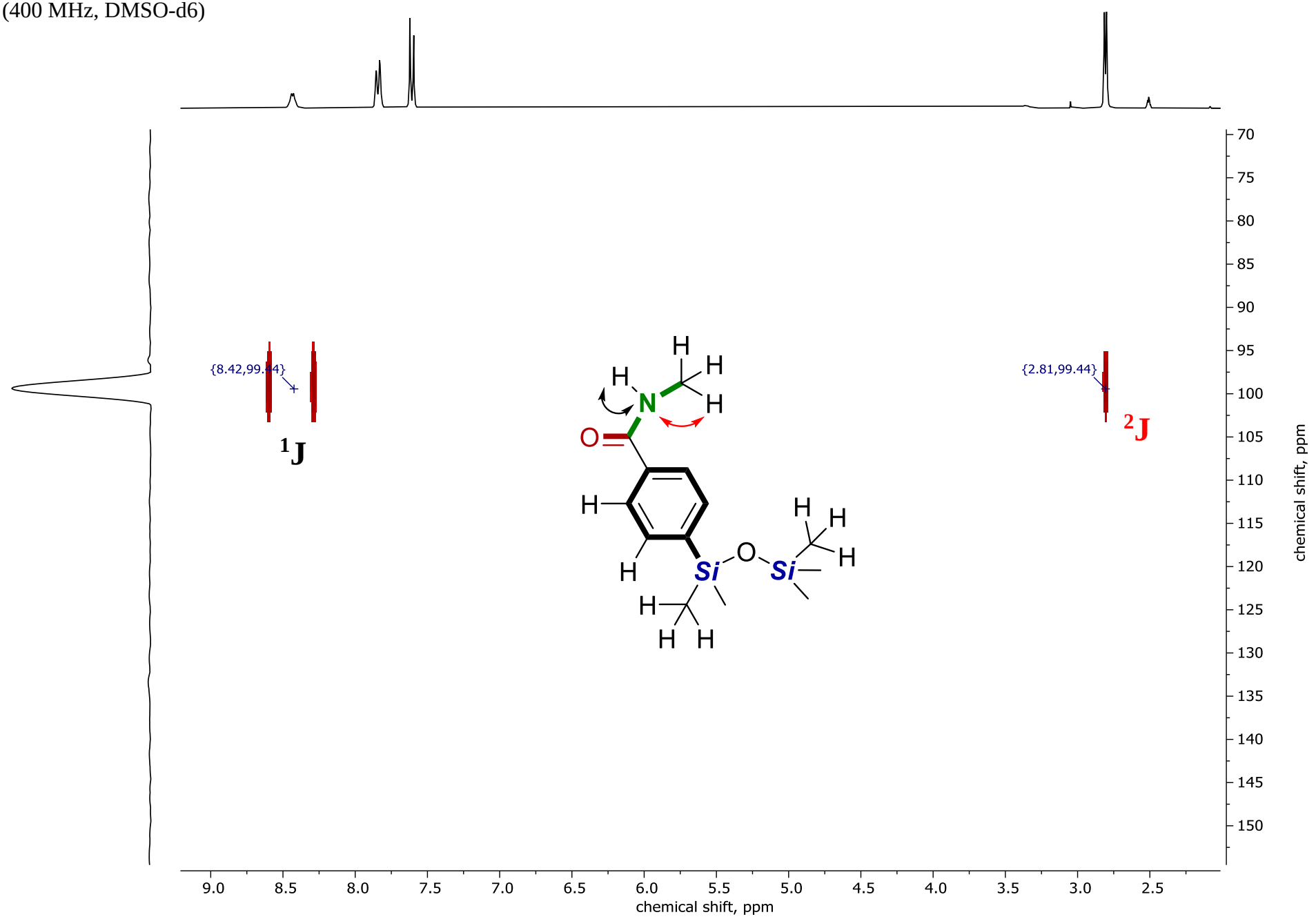
^{1}H - ^{29}Si HMBC

(400 MHz, DMSO-d6)



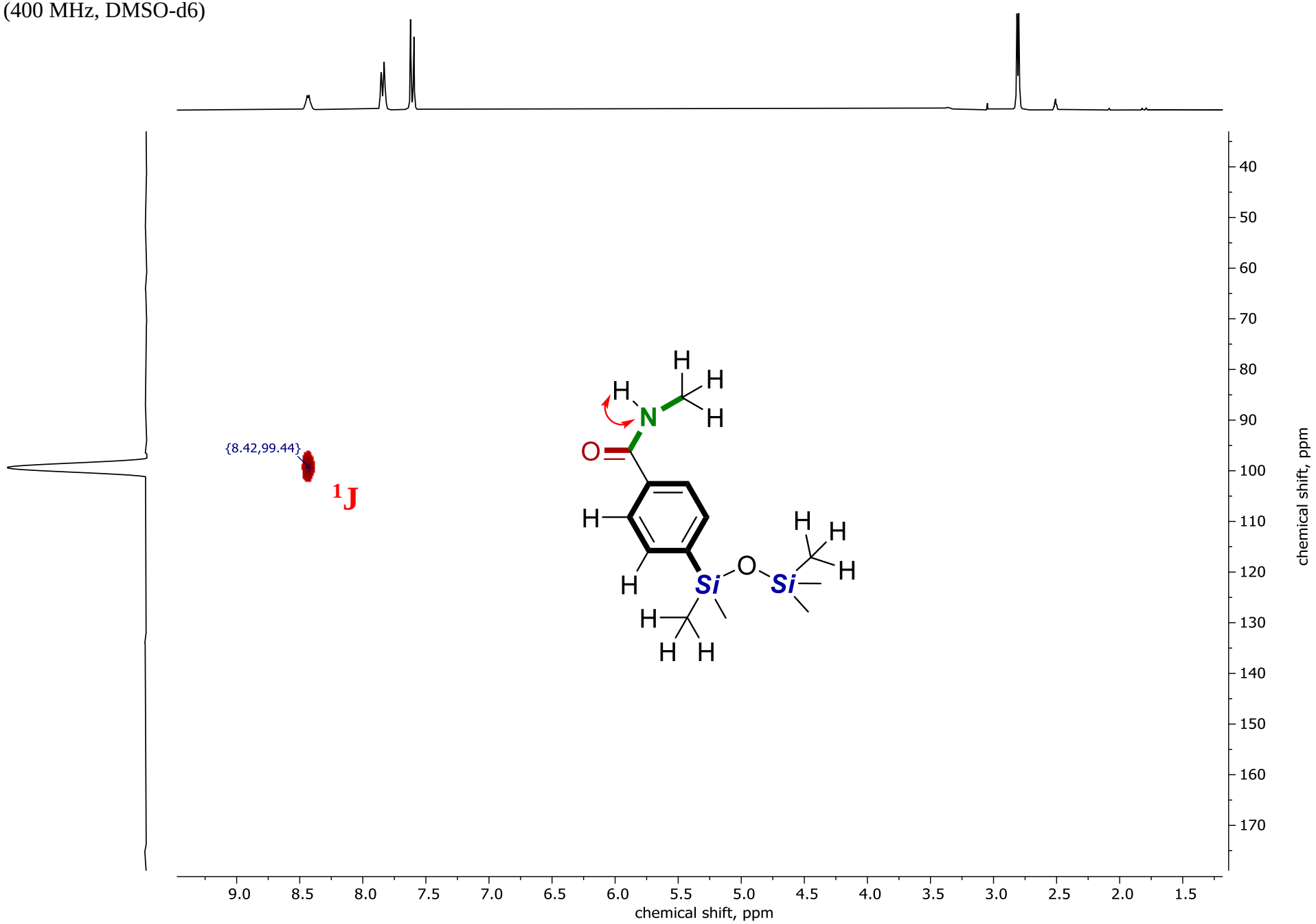
$^{1}H - ^{15}N$ HMBC

(400 MHz, DMSO-d6)

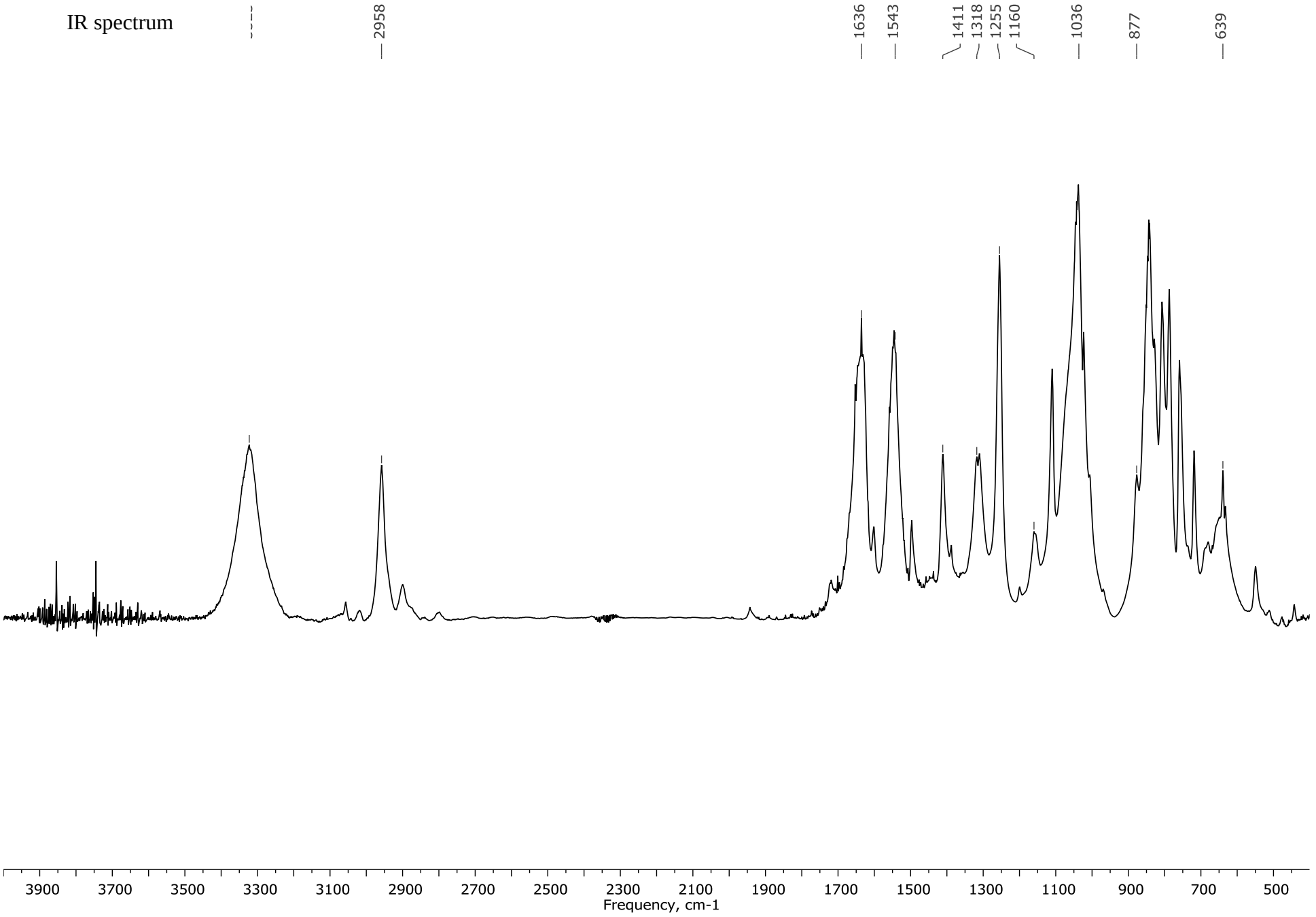


$^{1}H - ^{15}N$ HSQC

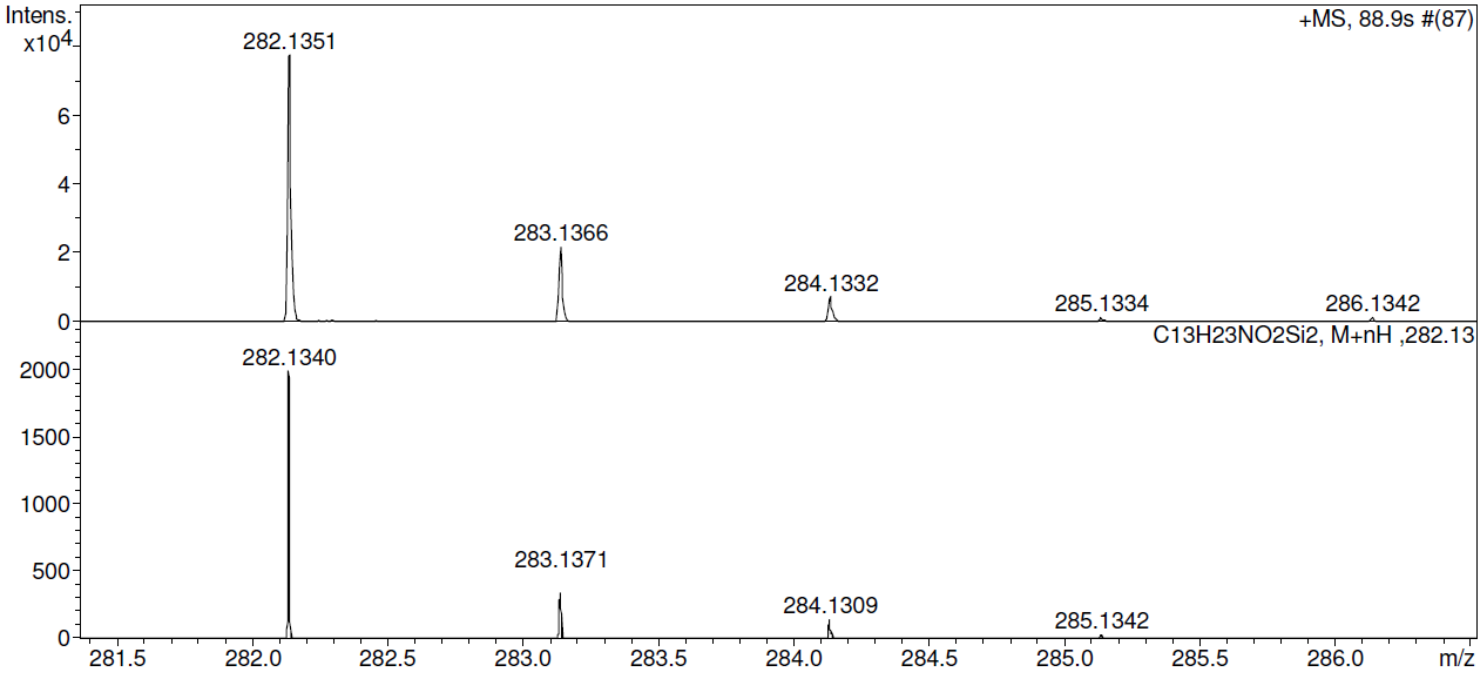
(400 MHz, DMSO-d6)

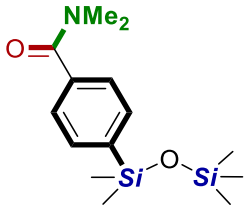


IR spectrum


2958
1636
1543
1411
1318
1255
1160
1036
877
639
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

HRMS (ESI)


Intens.
x10^4
+MS, 88.9s #(87)
282.1351
283.1366
284.1332
285.1334
286.1342
C13H23NO2Si2, M+nH ,282.13
282.1340
283.1371
284.1309
285.1342
m/z

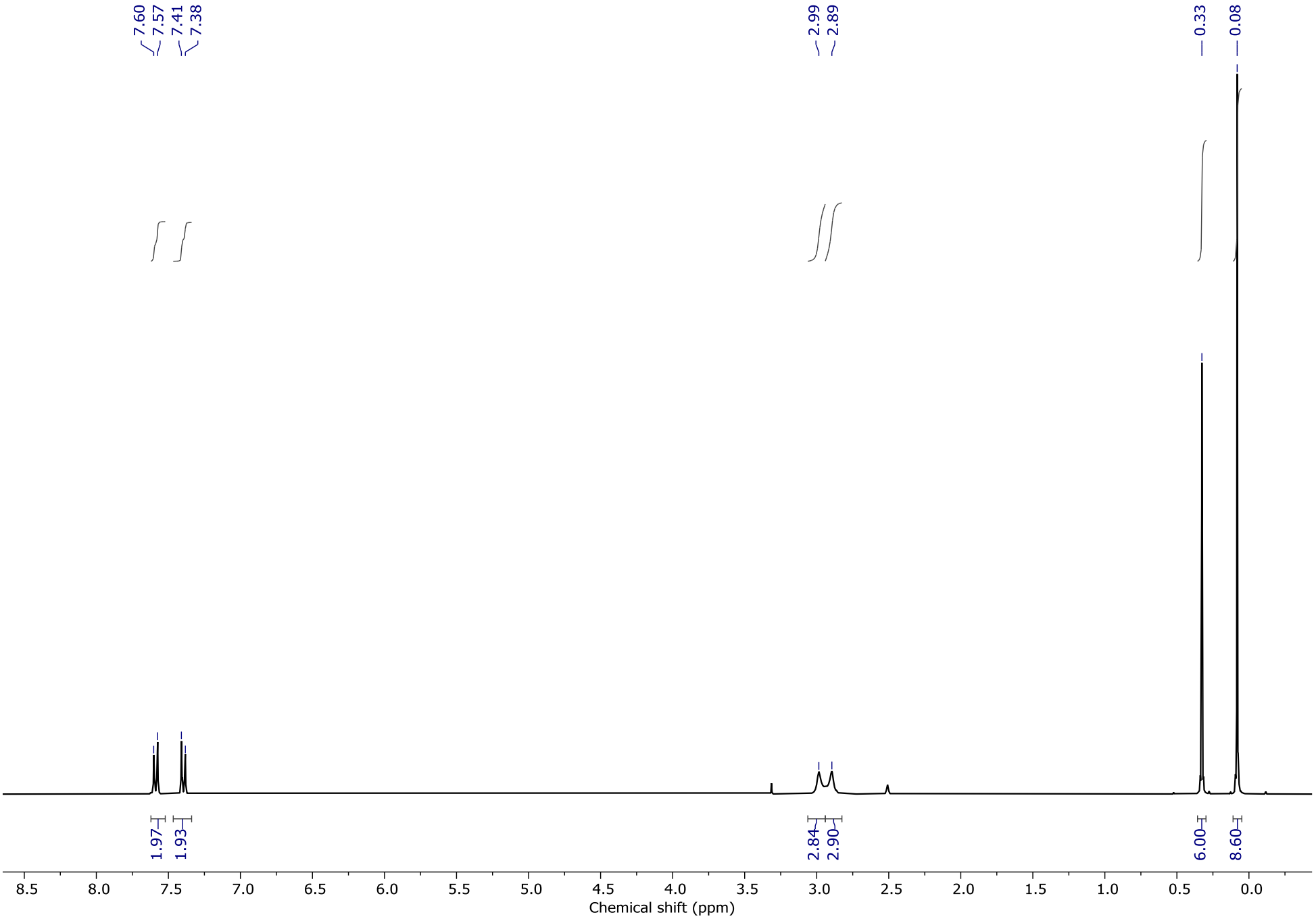


Characterisation data for N,N-dimethyl-4-(1,1,3,3,3-pentamethyldisiloxanyl)benzamide:

^{1}H NMR (400 MHz, DMSO-d6): δ = 7.59 (d, ^{3}J=11 Hz, 2H), δ = 7.40 (d, ^{3}J=11 Hz, 2H), δ = 2.99 (s, 3H), δ = 2.89 (s, 3H), δ = 0.33 (s, 6H), δ = 0.08 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d6): δ = 169.96, 140.68, 137.38, 132.58, 126.07, 34.60, 1.91, 0.68. ^{29}Si NMR (80 MHz, DMSO-d6): δ = 9.15, -2.10. It appeared to be feasible to obtain neither ^{15}N NMR nor ^{1}H – ^{15}N HMBC due to the symmetry of the molecule and ^{15}N relaxation characteristics. HRMS (ESI) m/z [M + H] $^{+}$: calcd for $[C_{14}H_{25}NO_2Si_2 + H]^{+}$, 296.1497; found, 296.1501; [M + Na] $^{+}$: calcd for $[C_{14}H_{25}NO_2Si_2 + Na]^{+}$, 318.1316; found, 318.1314; [M + K] $^{+}$: calcd for $[C_{14}H_{25}NO_2Si_2 + K]^{+}$, 334.1055; found, 334.1055. IR (cm^{-1}): 3620-3189, 2956, 1932, 1720, 1636, 1545-1394, 1257, 1118-1020, 876-676.

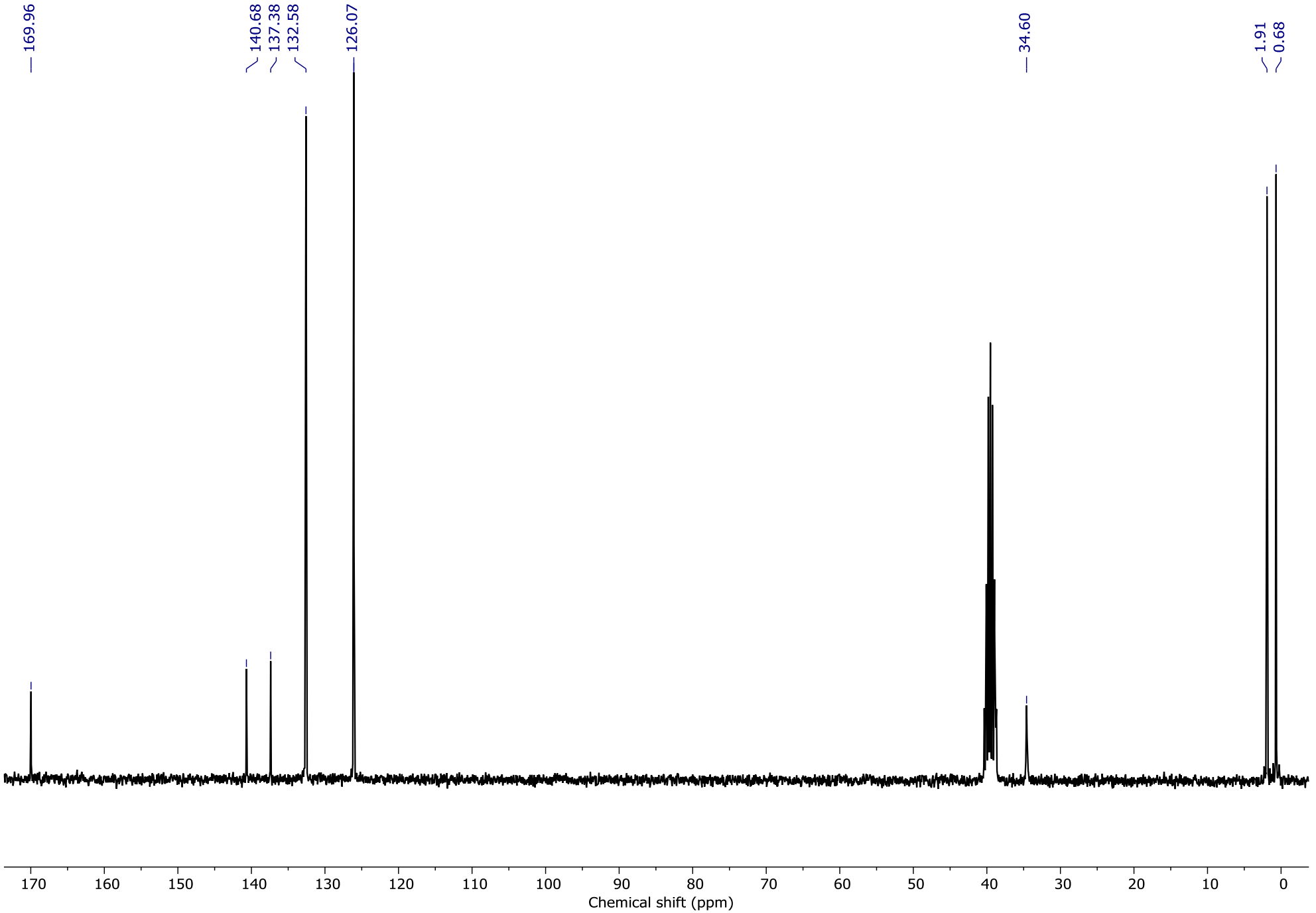
^{1}H NMR

(400 MHz, DMSO-d6)



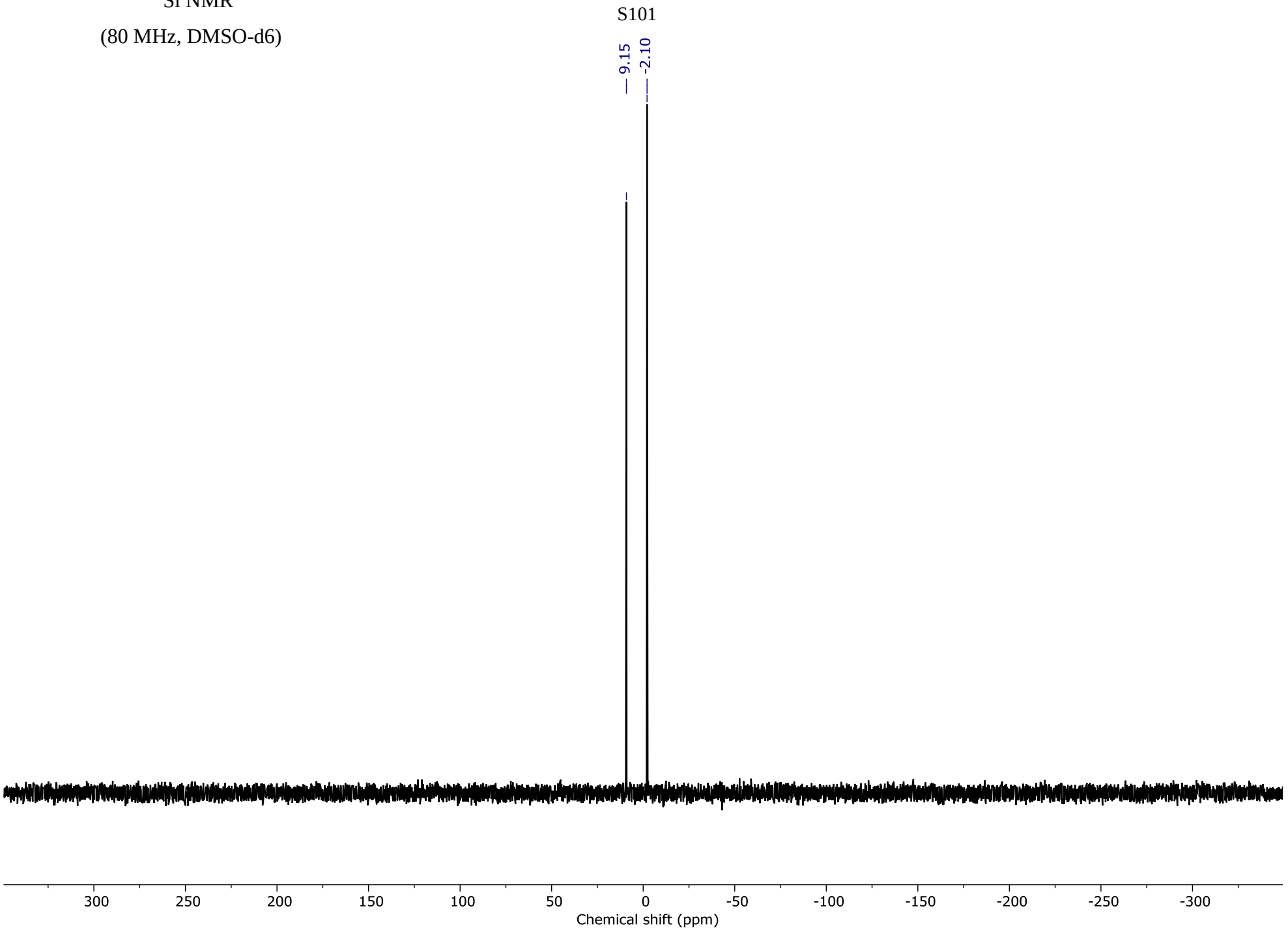
^{13}C NMR

(100 MHz, DMSO-d6)



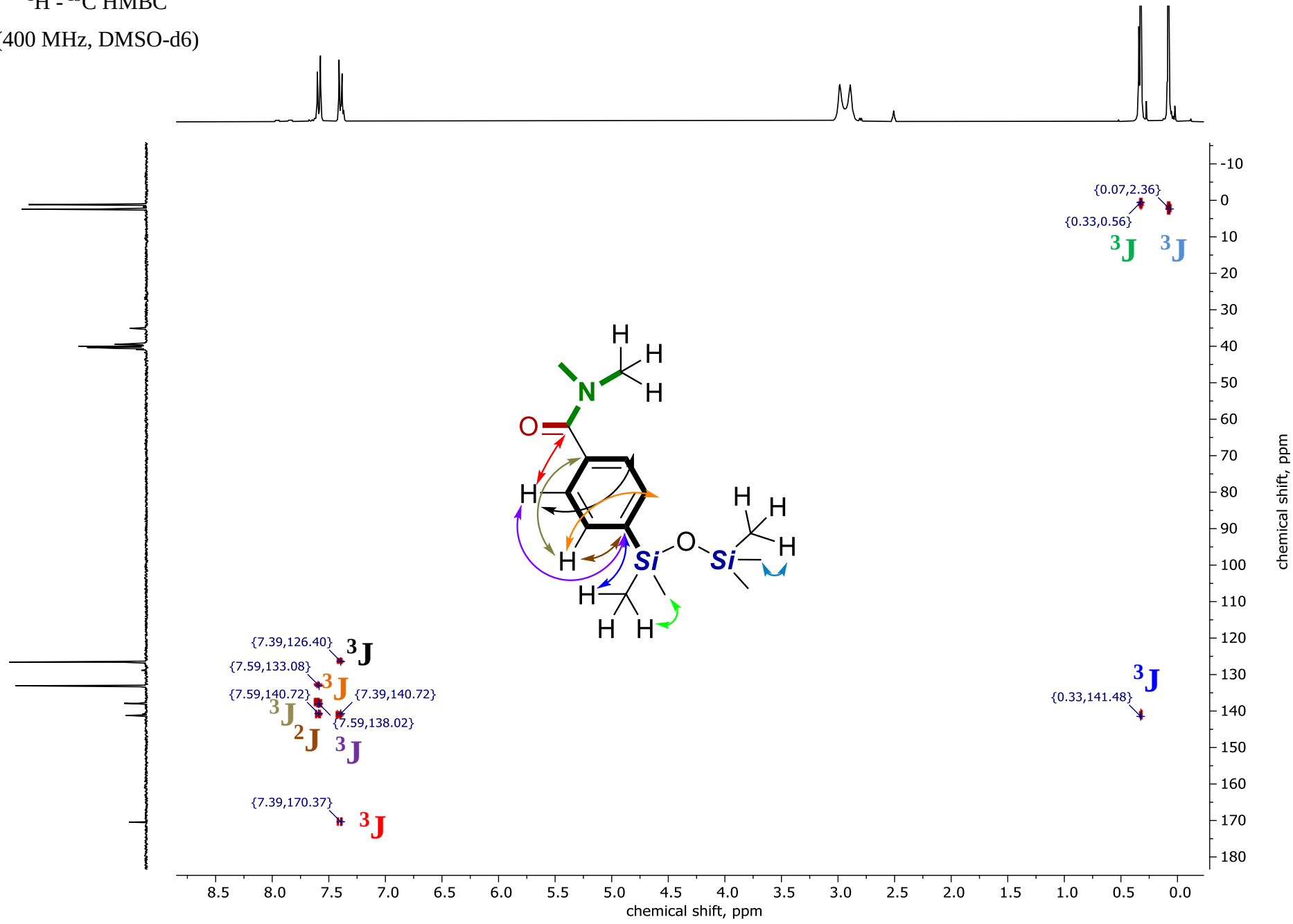
^{29}Si NMR

(80 MHz, DMSO-d6)



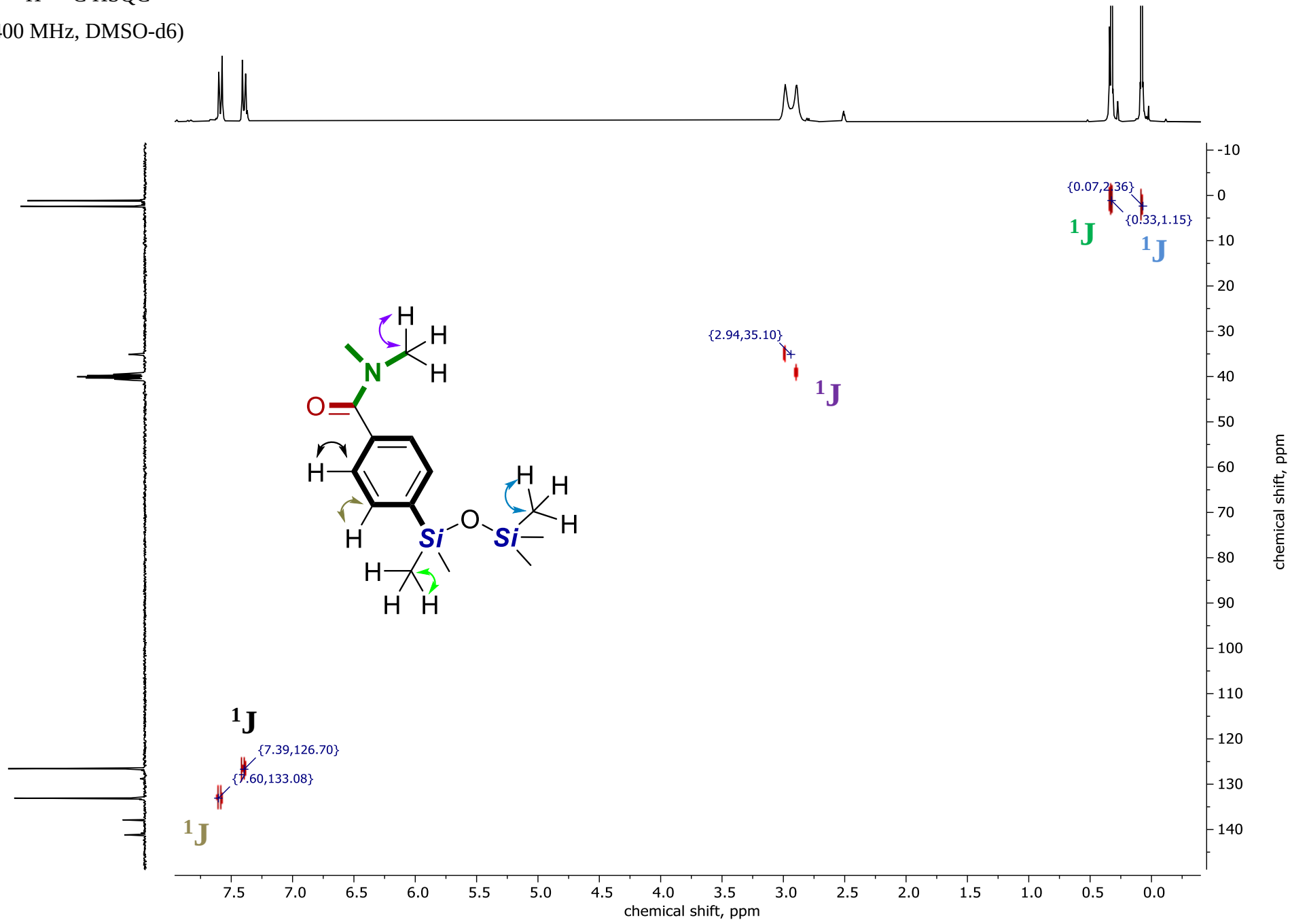
^{1}H - ^{13}C HMBC

(400 MHz, DMSO-d6)



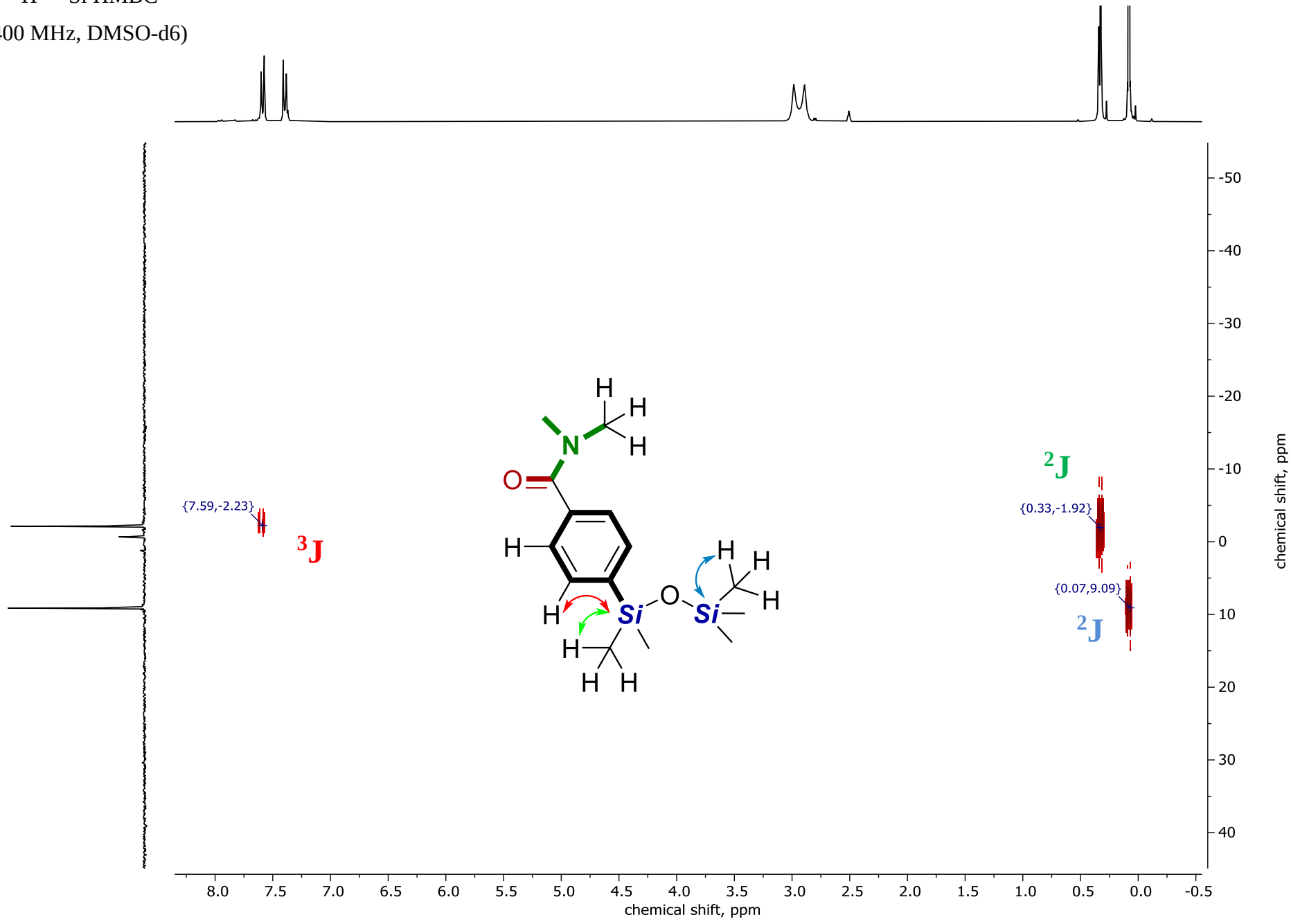
^{1}H - ^{13}C HSQC

(400 MHz, DMSO-d6)

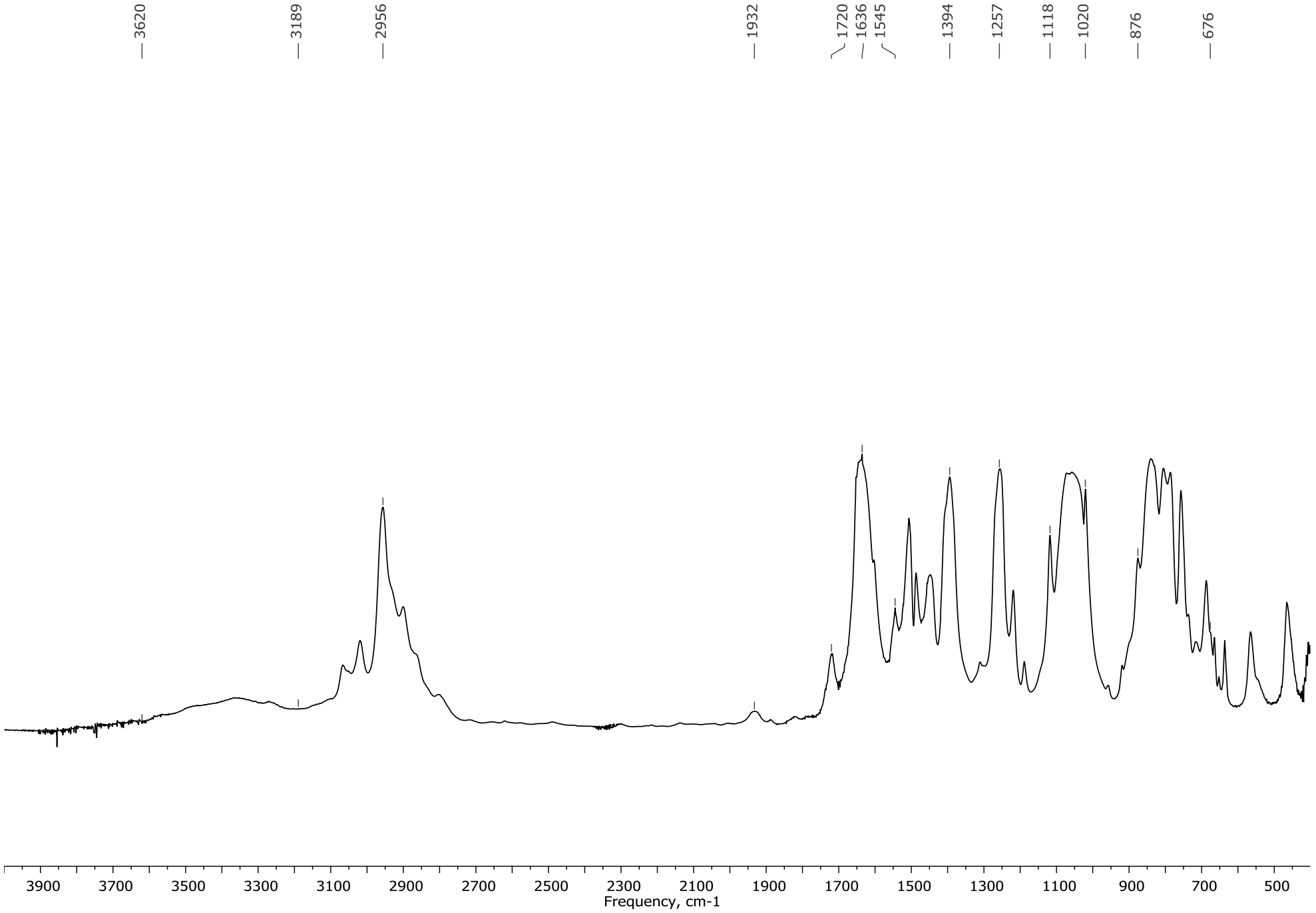


^{1}H - ^{29}Si HMBC

(400 MHz, DMSO-d6)



IR spectrum


3620
3189
2956
1932
1720
1636
1545
1394
1257
1118
1020
876
676
3900
3700
3500
3300
3100
2900
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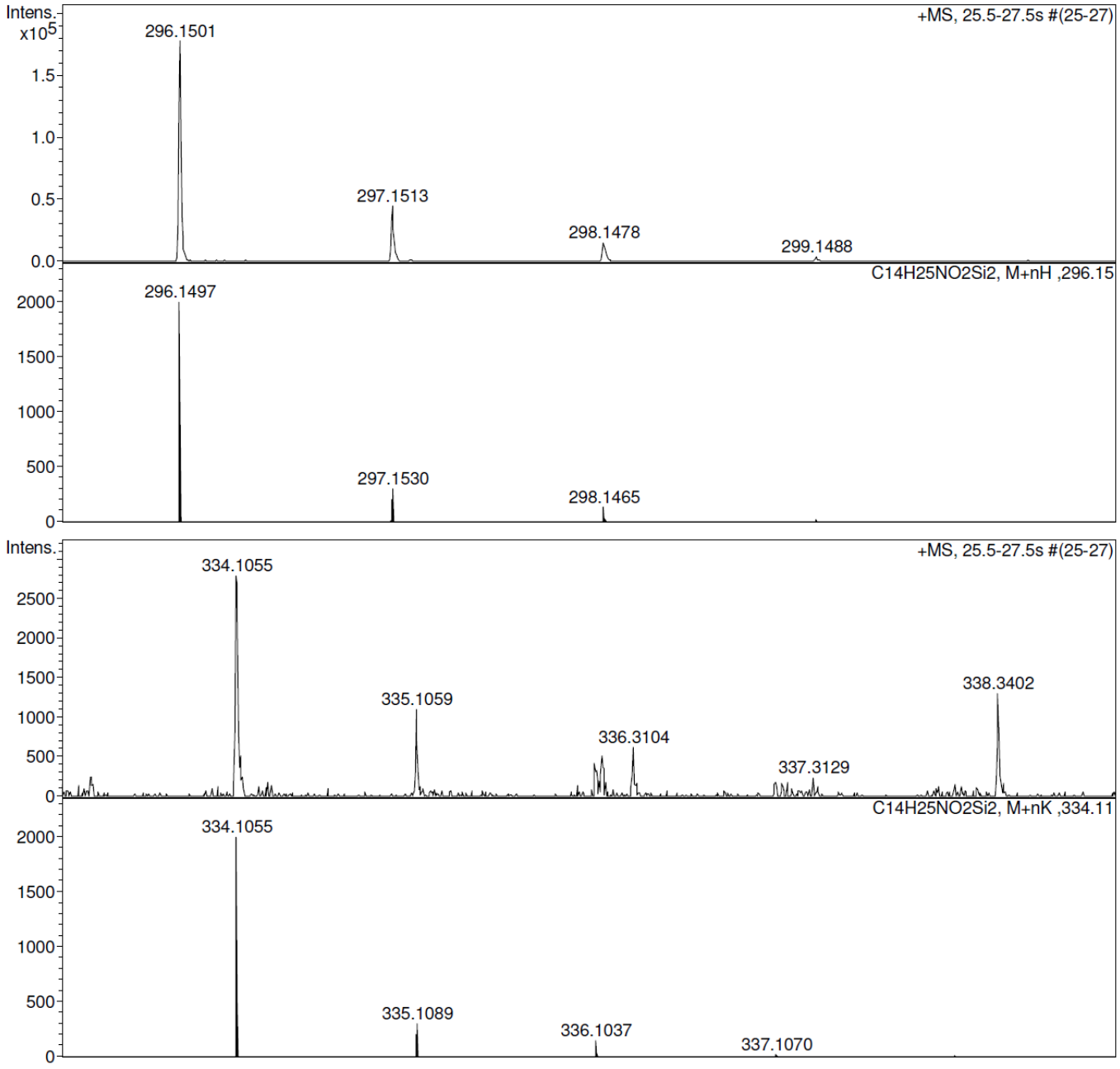
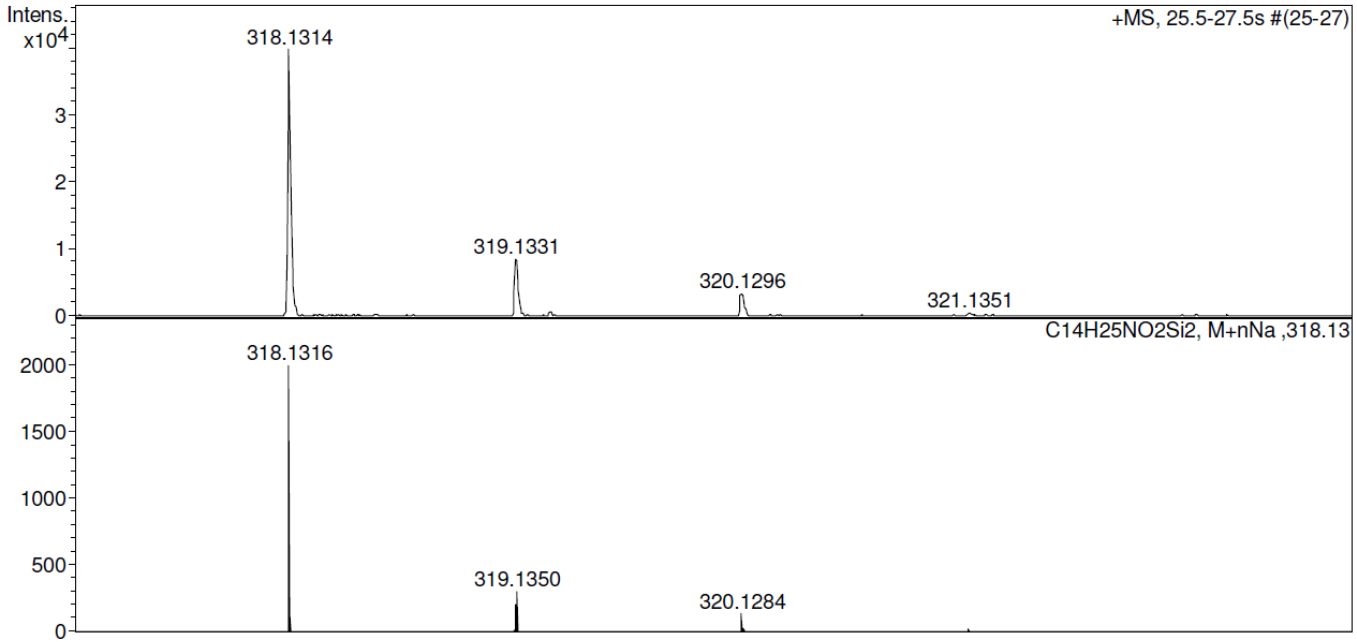
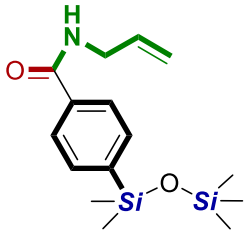
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

HRMS (ESI)


Intens.
x10^5
1.5
1.0
0.5
0.0
296.1501
297.1513
298.1478
299.1488
+MS, 25.5-27.5s #(25-27)
C14H25NO2Si2, M+nH ,296.15
2000
1500
1000
500
0
296.1497
297.1530
298.1465
Intens.
2500
2000
1500
1000
500
0
334.1055
335.1059
336.3104
337.3129
338.3402
+MS, 25.5-27.5s #(25-27)
C14H25NO2Si2, M+nK ,334.11
2000
1500
1000
500
0
334.1055
335.1089
336.1037
337.1070


Intens.
x10^4
+MS, 25.5-27.5s #(25-27)
318.1314
319.1331
320.1296
321.1351
C14H25NO2Si2, M+nNa ,318.13
318.1316
319.1350
320.1284

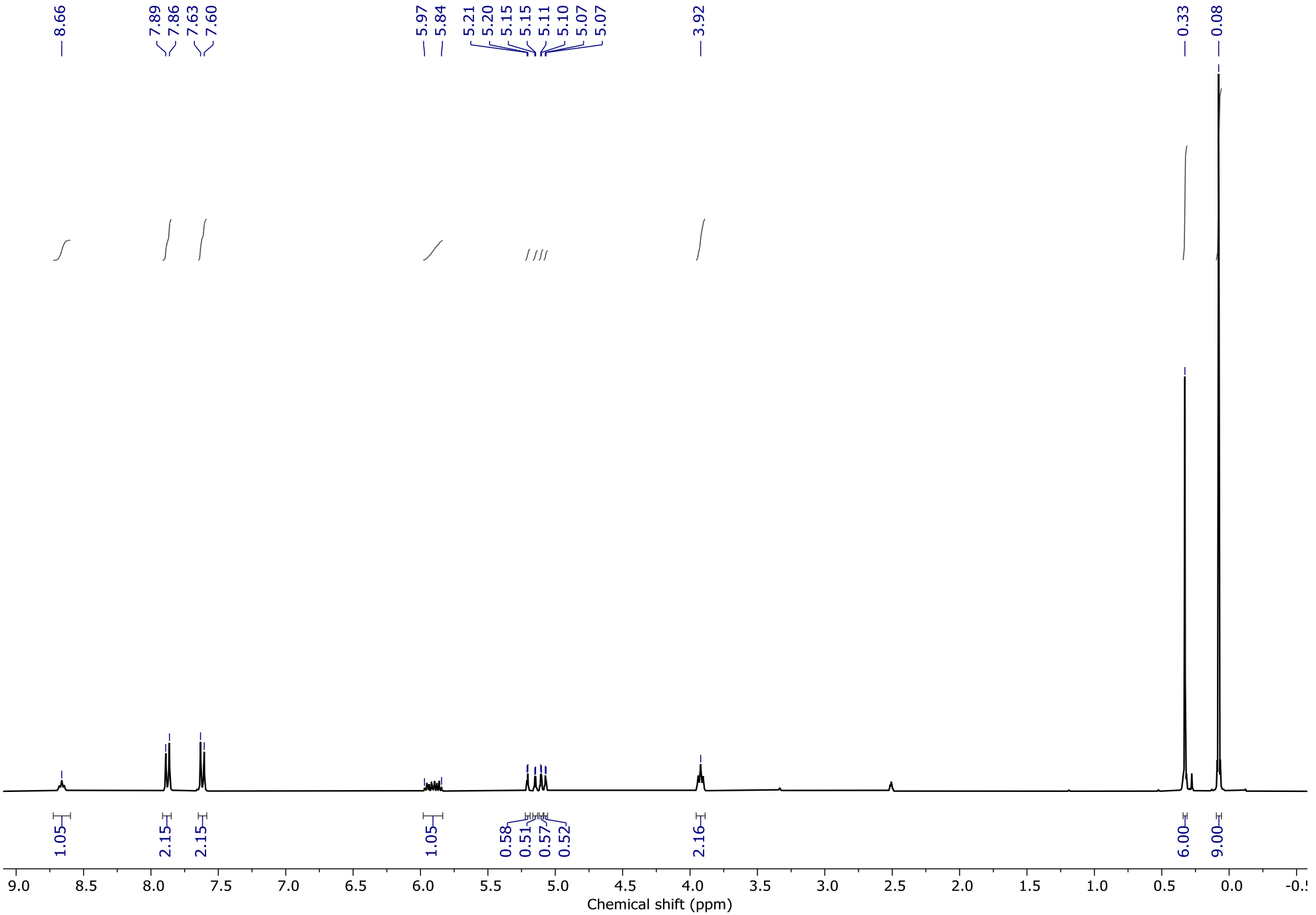


Characterisation data for N-allyl-4-(1,1,3,3,3-pentamethyldisiloxanyl)benzamide:

^{1}H NMR (400 MHz, DMSO): δ = 8.66 (t, ^{3}J=8, 1H), δ = 7.88 (d, ^{3}J=11, 2H), δ = 7.62 (d, ^{3}J=11, 2H), δ = 5.97-5.84 (m, 1H), δ = 5.21-5.07 (m, 2H), δ = 3.92 (m, 2H), δ = 0.33 (s, 6H), δ = 0.08 (s, 9H). ^{13}C NMR (100 MHz, DMSO): δ = 165.99, 142.83, 135.38, 135.21, 132.62, 126.36, 115.00, 41.46, 1.90, 0.66. ^{29}Si NMR (80 MHz, DMSO): δ = 9.17, -2.08. ^{15}N NMR (40 MHz, DMSO): δ = 109.66. HRMS (ESI) m/z [M + H] $^{+}$: calcd for $[C_{15}H_{25}NO_2Si_2 + H]^{+}$, 282.1340; found, 282.1351. IR (cm^{-1}): 3574-3138, 2959, 1934, 1721, 1642, 1543, 1429, 1284, 1057, 920, 816-638.

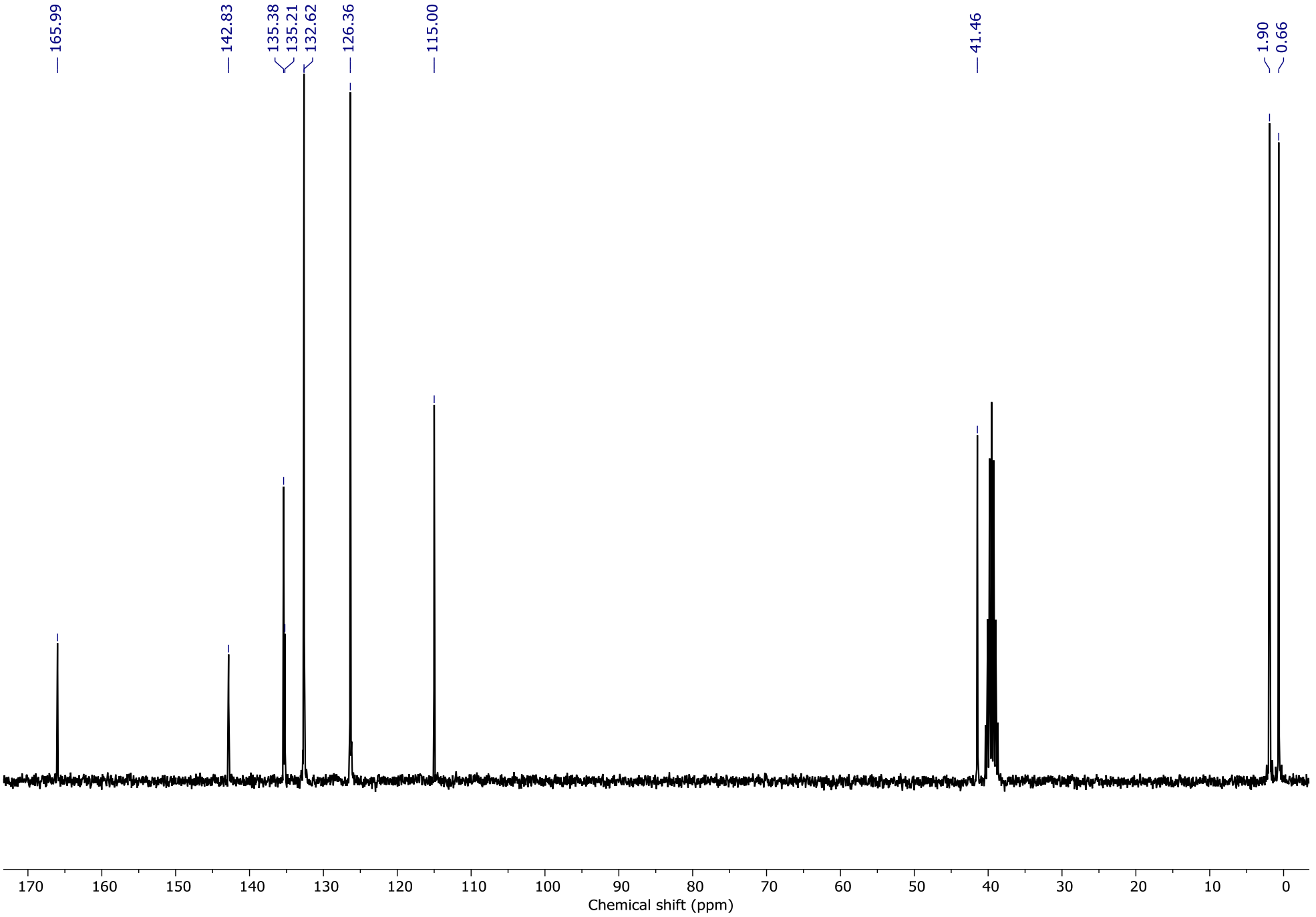
^{1}H NMR

(400 MHz, DMSO-d6)



^{13}C NMR

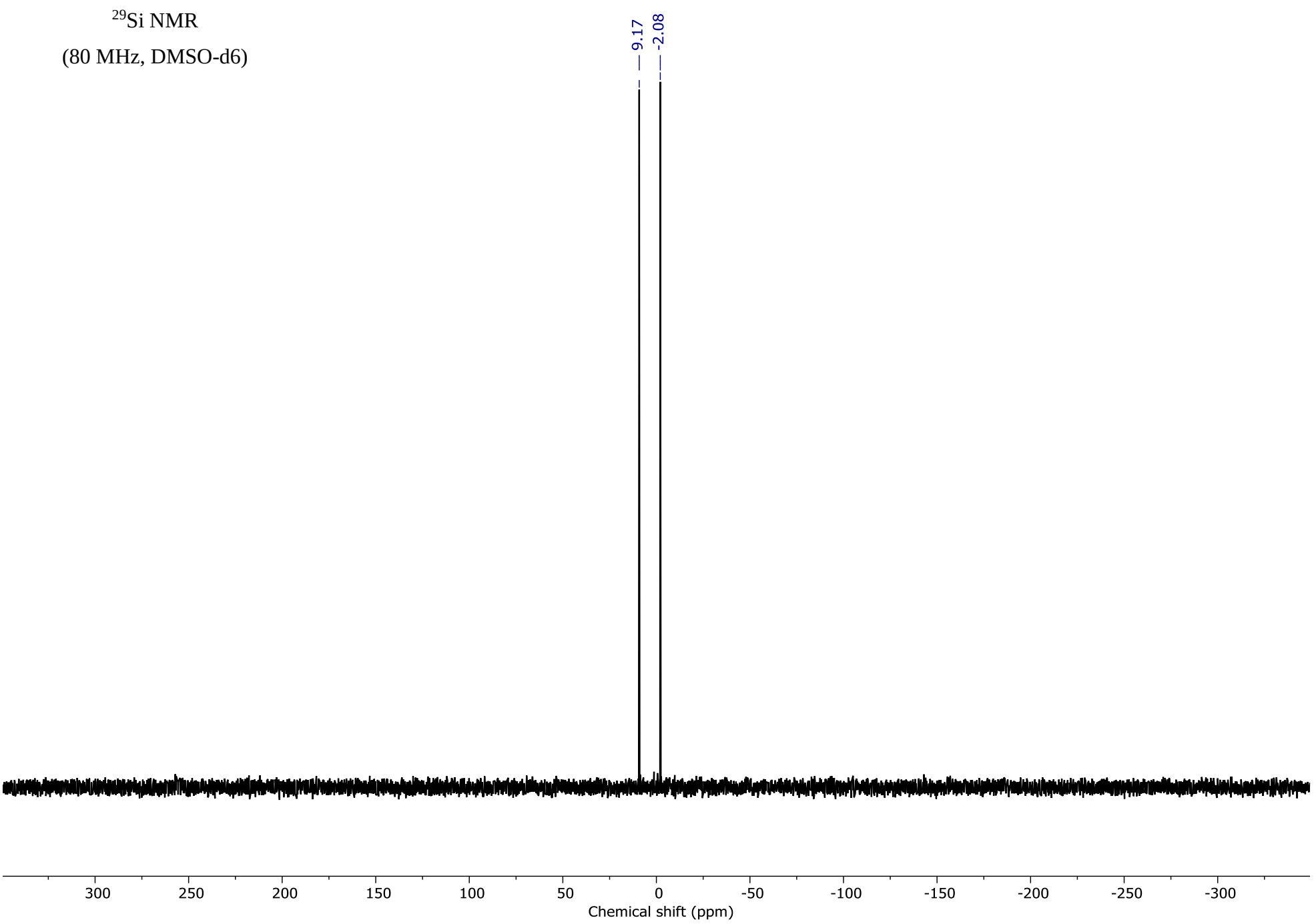
(100 MHz, DMSO-d6)



S111

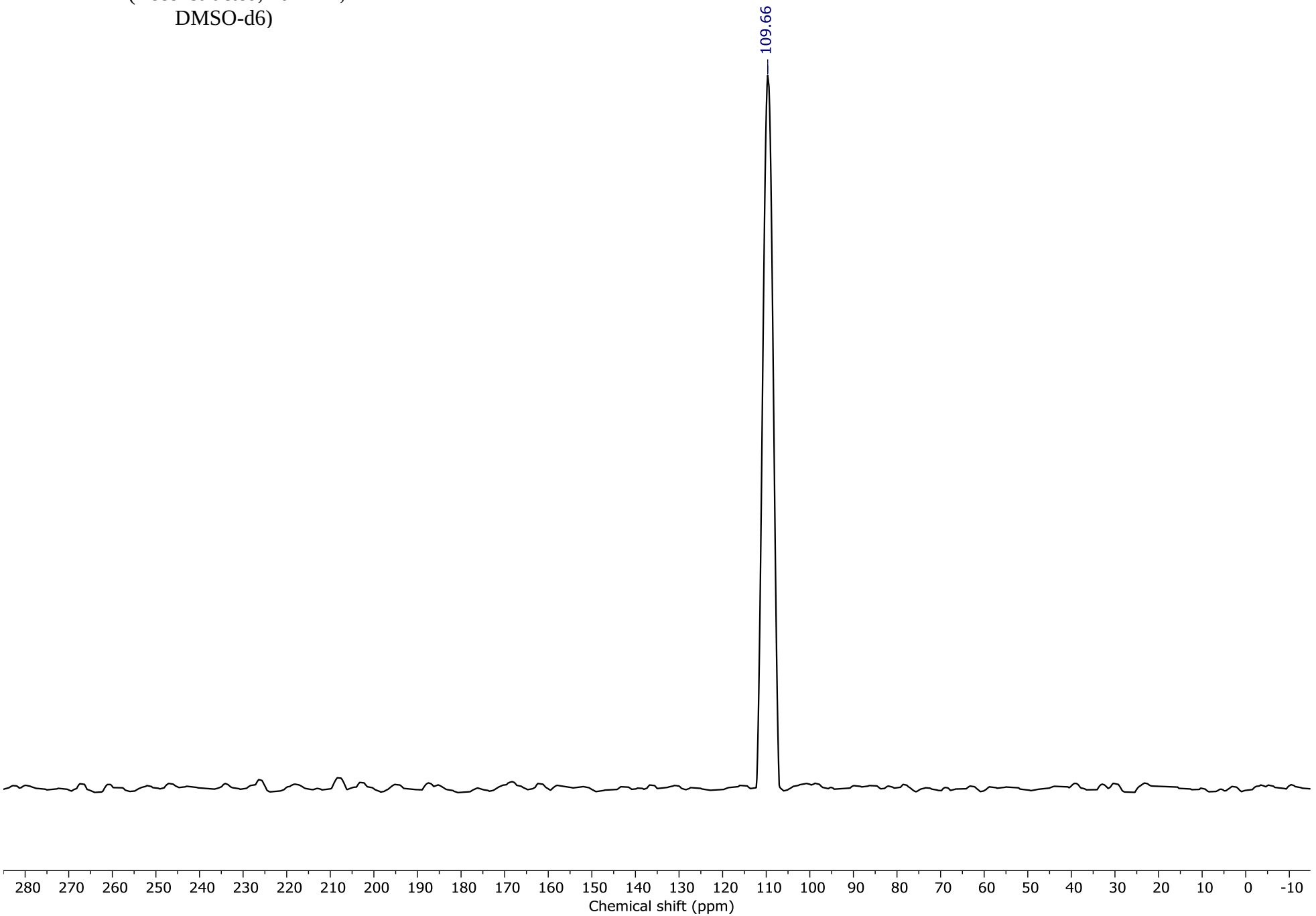
^{29}Si NMR

(80 MHz, DMSO-d6)



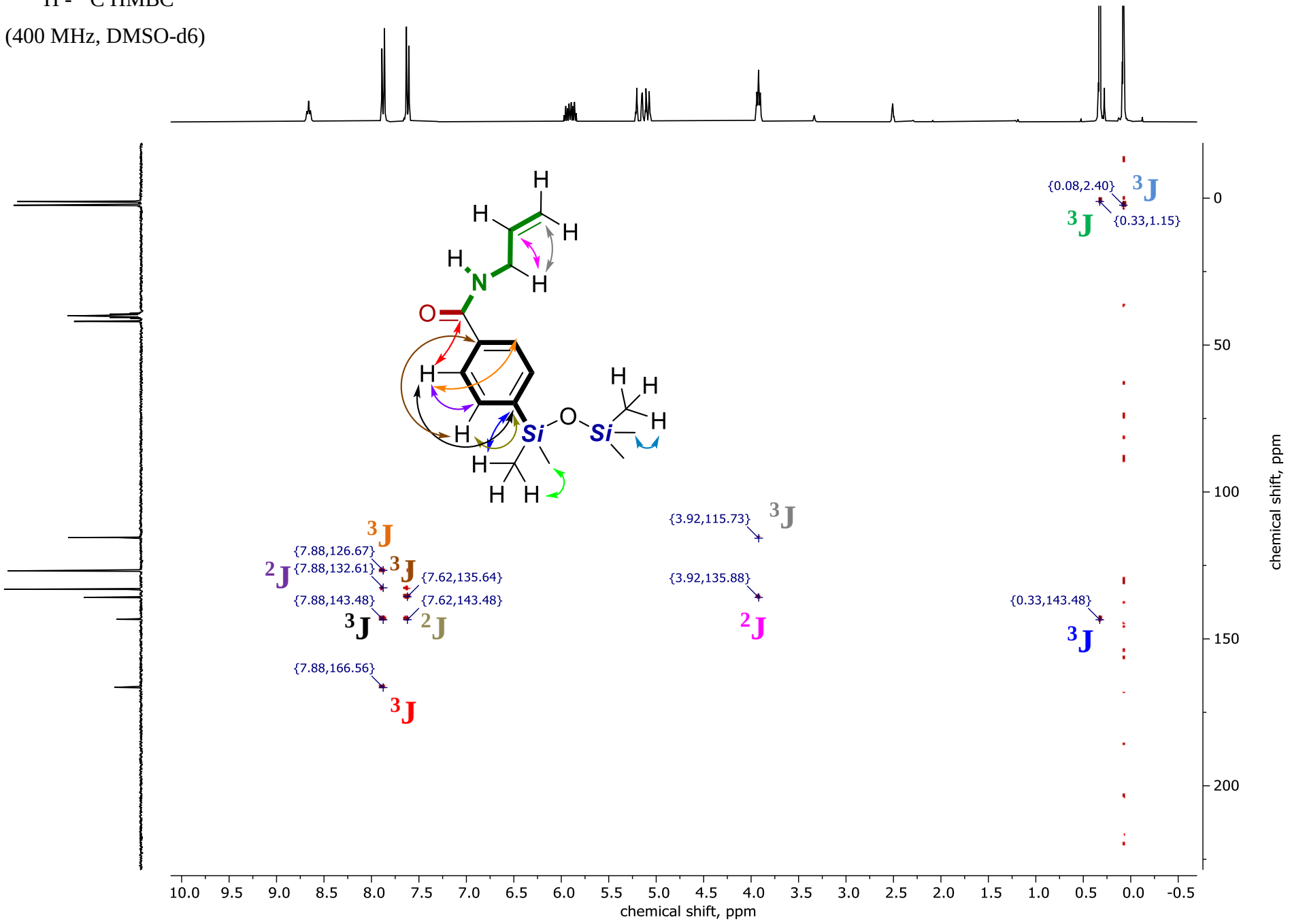
^{15}N NMR

(Reconstructed, 40 MHz, DMSO-d6)



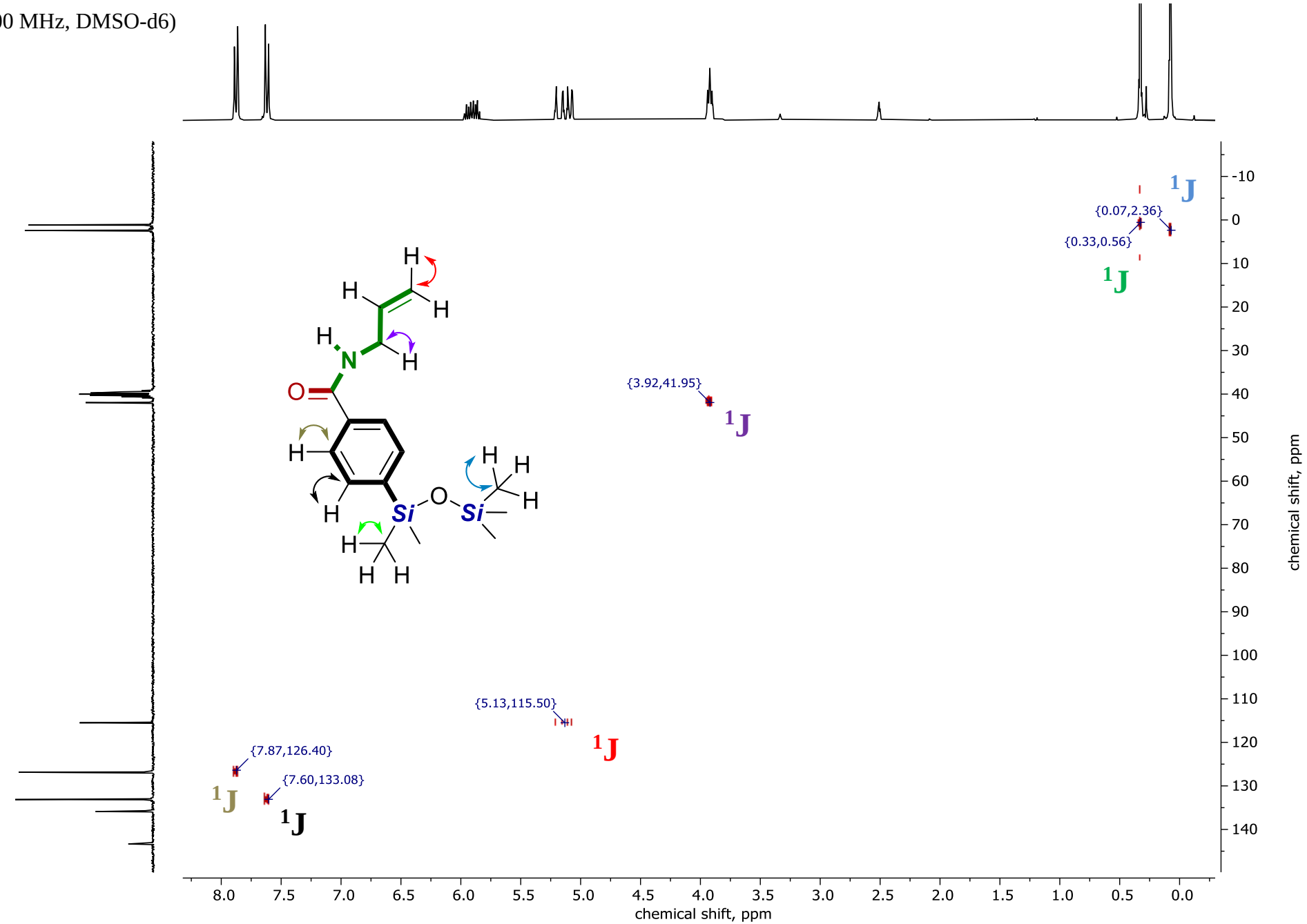
^{1}H - ^{13}C HMBC

(400 MHz, DMSO-d6)



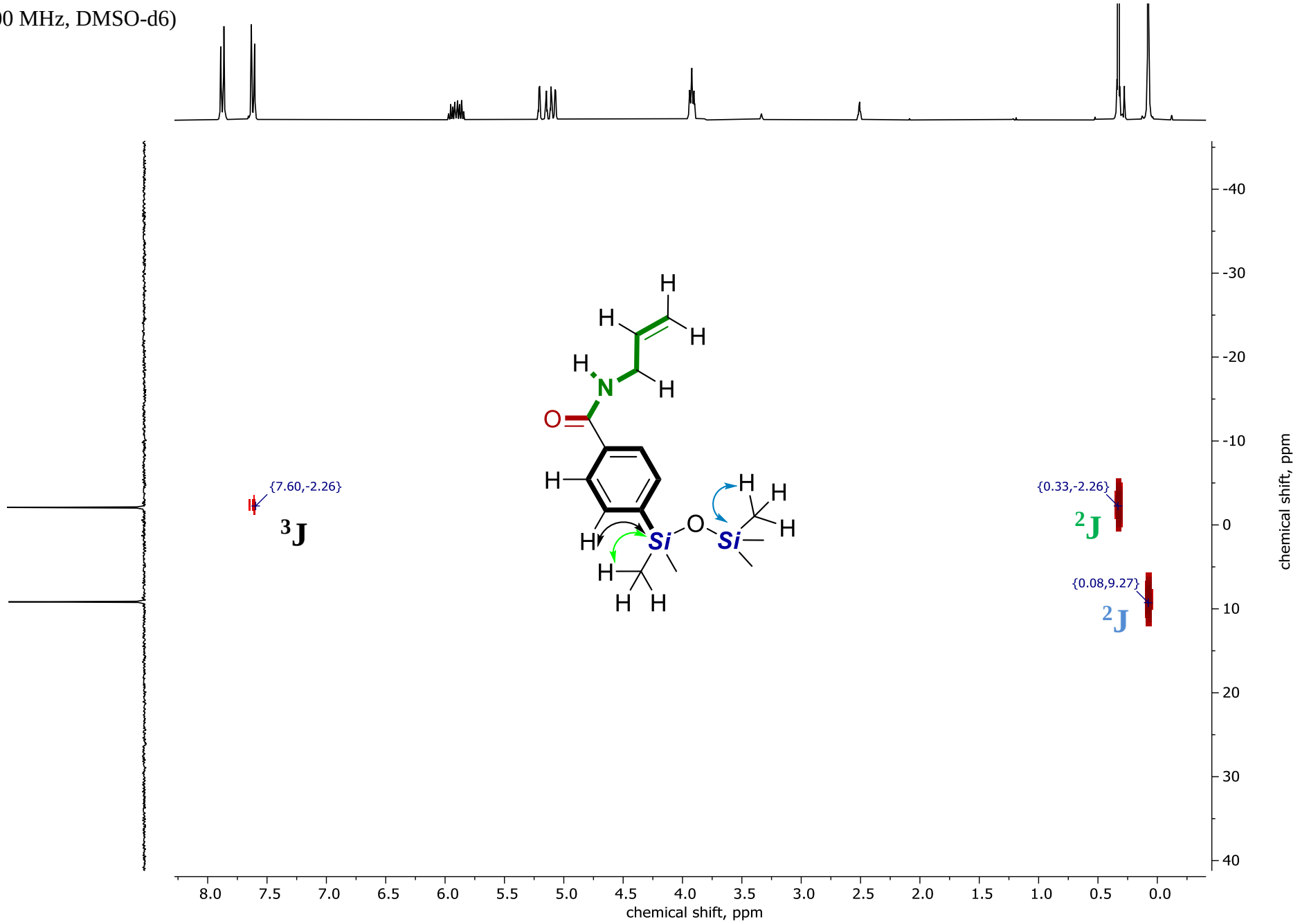
^{1}H - ^{13}C HSQC

(400 MHz, DMSO-d6)



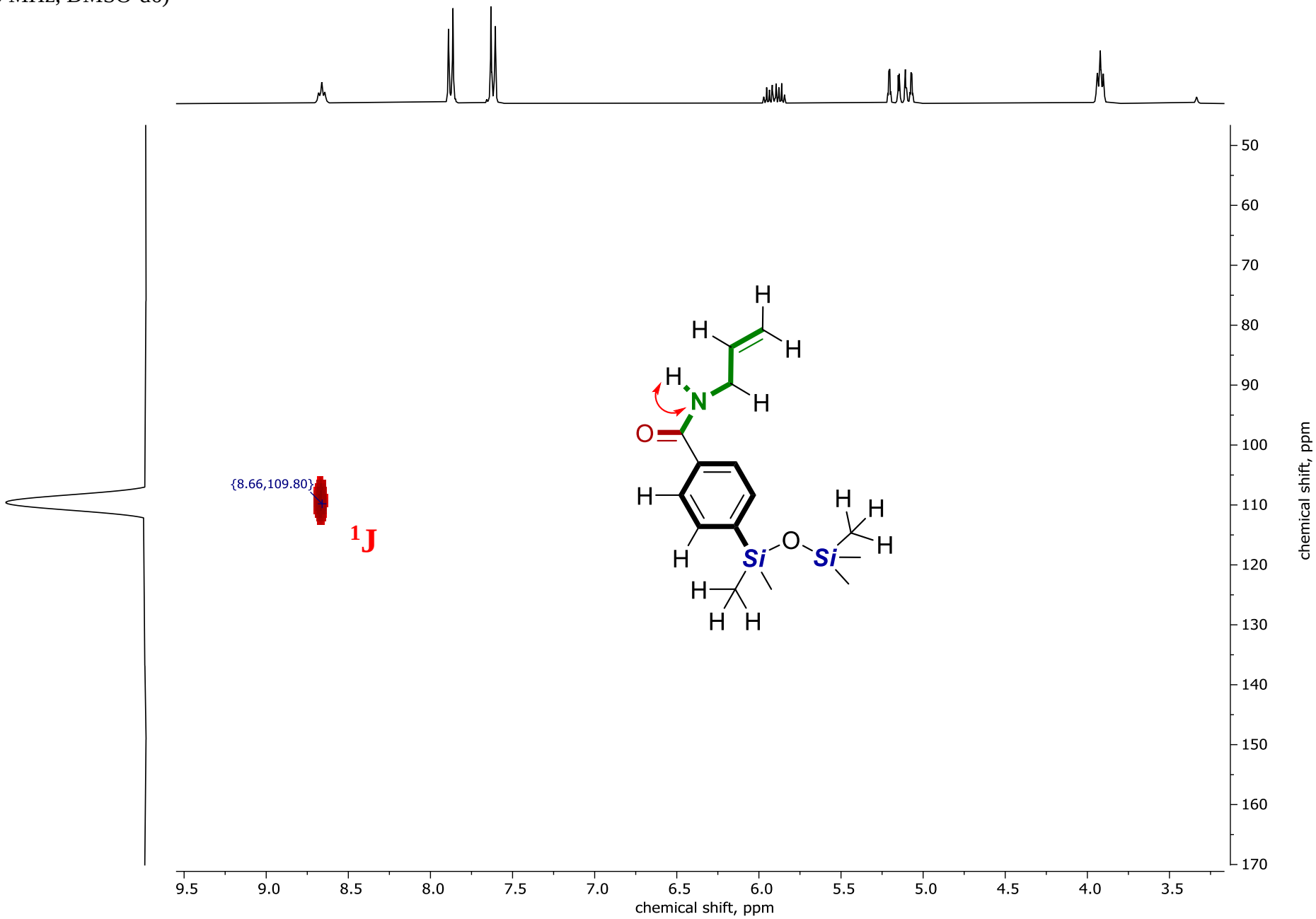
^{1}H - ^{29}Si HMBC

(400 MHz, DMSO-d6)

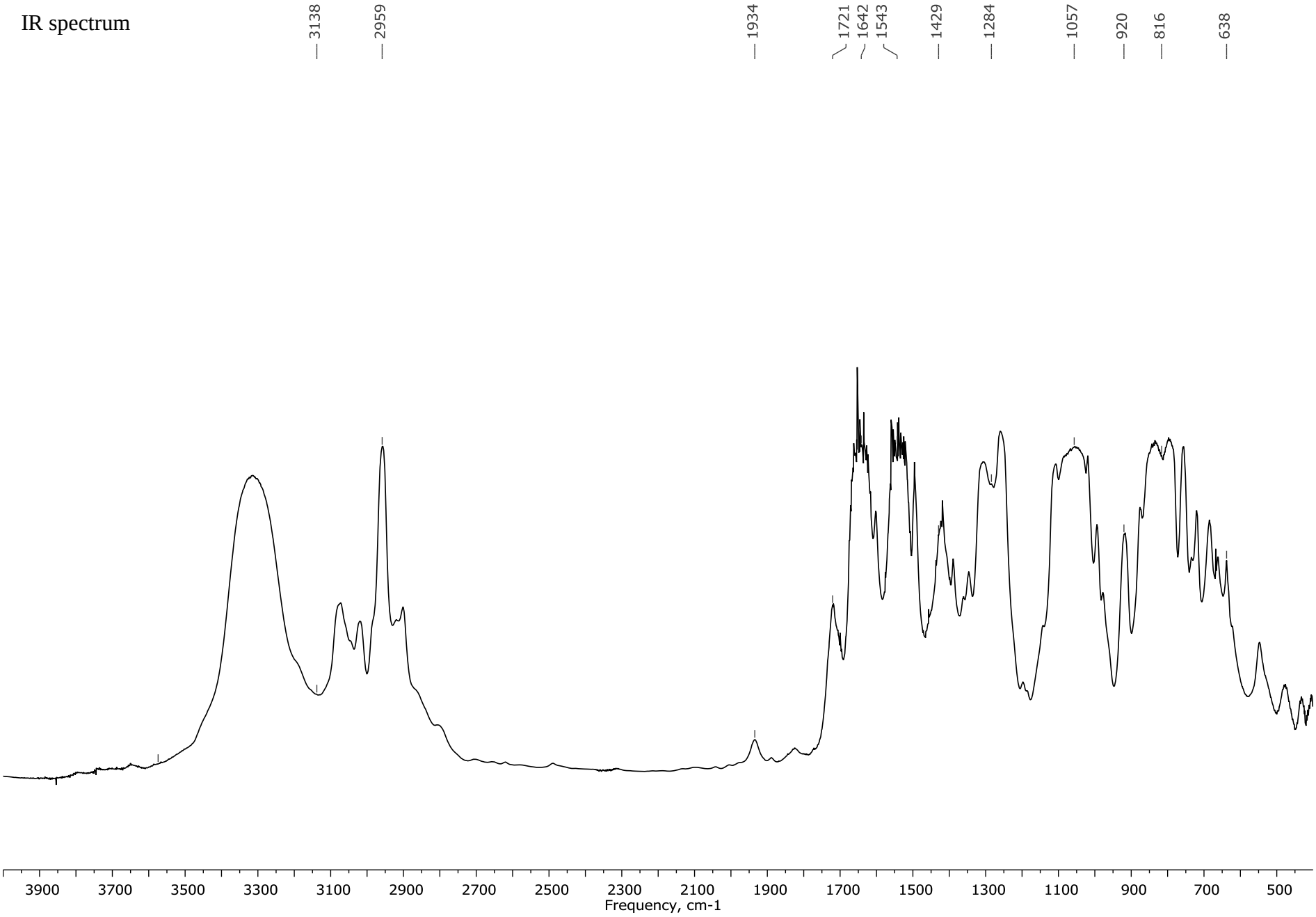


$^{1}H - ^{15}N$ HSQC

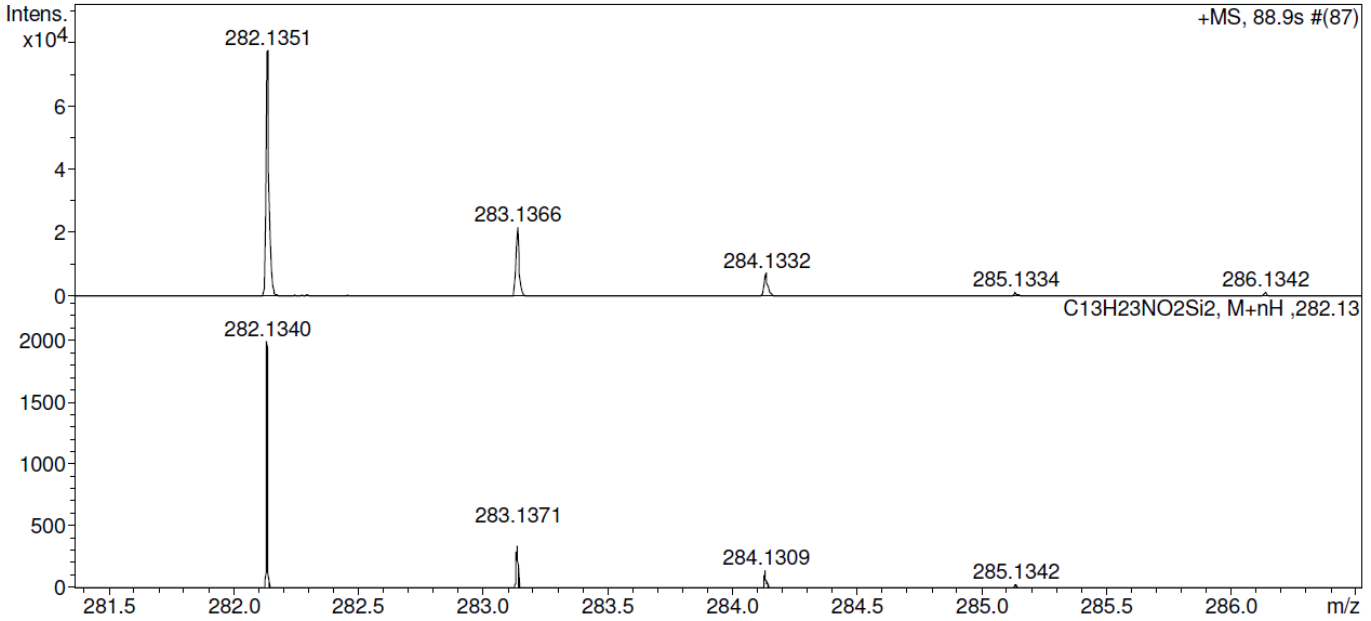
(400 MHz, DMSO-d6)

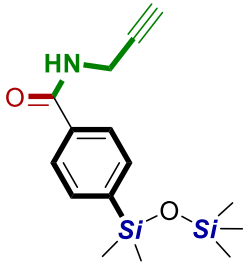


IR spectrum


3138
2959
1934
1721
1642
1543
1429
1284
1057
920
816
638
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

HRMS (ESI)


Intens.
x10^4
+MS, 88.9s #(87)
282.1351
283.1366
284.1332
285.1334
286.1342
C13H23NO2Si2, M+nH ,282.13
282.1340
283.1371
284.1309
285.1342
m/z

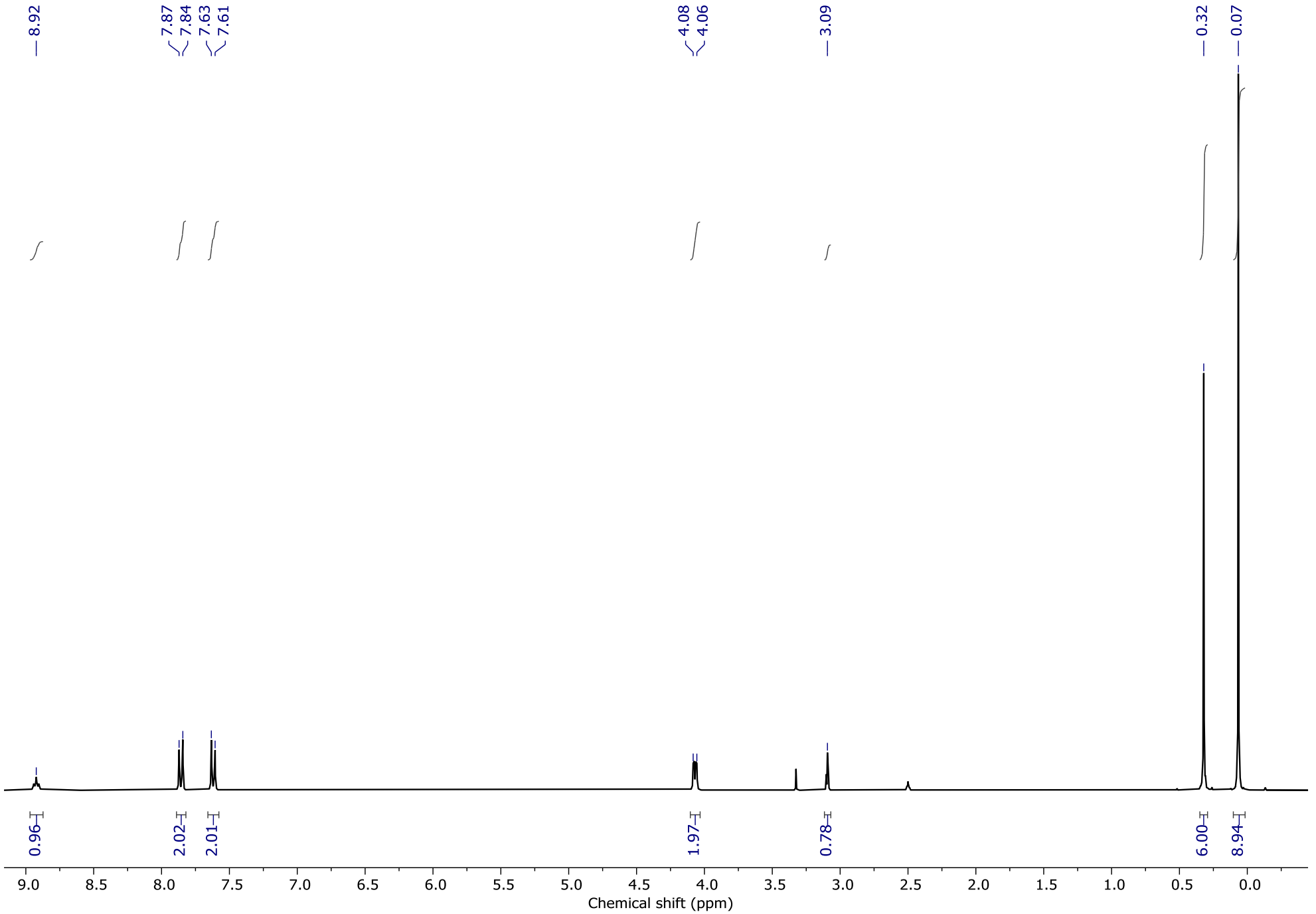


Characterisation data for 4-(1,1,3,3,3-pentamethyldisiloxanyl)-N-(prop-2-yn-1-yl)benzamide:

^{1}H NMR (400 MHz, DMSO): δ = 8.92 (t, ^{3}J=7, 1H), δ = 7.86 (d, ^{3}J=11, 2H), δ = 7.62 (d, ^{3}J=11, 2H), δ = 4.08-4.06 (m, 2H), δ = 3.09 (t, ^{4}J=3, 1H), δ = 0.32 (s, 6H), δ = 0.07 (s, 9H). ^{13}C NMR (100 MHz, DMSO): δ = 165.90, 143.22, 134.59, 132.69, 126.40, 81.23, 72.72, 28.45, 1.90, 0.64. ^{29}Si NMR (80 MHz, DMSO): δ = 9.23, -2.06. ^{15}N NMR (40 MHz, DMSO): δ = 107.75. HRMS (ESI) m/z [M + H] $^{+}$: calcd for $[C_{15}H_{23}NO_2Si_2 + H]^{+}$, 306.1340; found, 306.1340. IR (cm^{-1}): 3327, 3236, 2959, 2120, 1638, 1542, 1423, 1313, 1250, 1112, 1063, 843-639.

^{1}H NMR

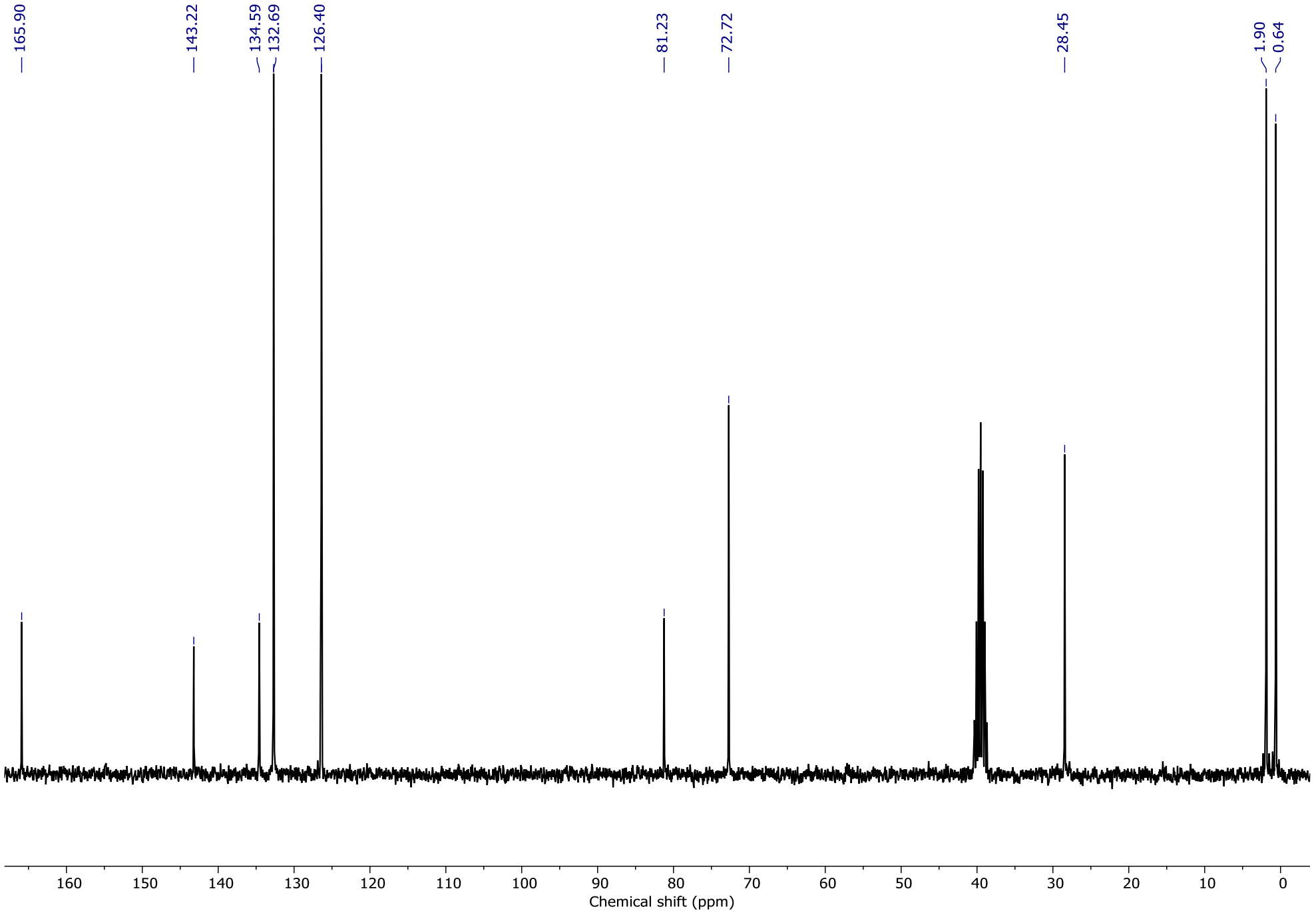
(400 MHz, DMSO-d6)



^{13}C NMR

(100 MHz, DMSO-d6)

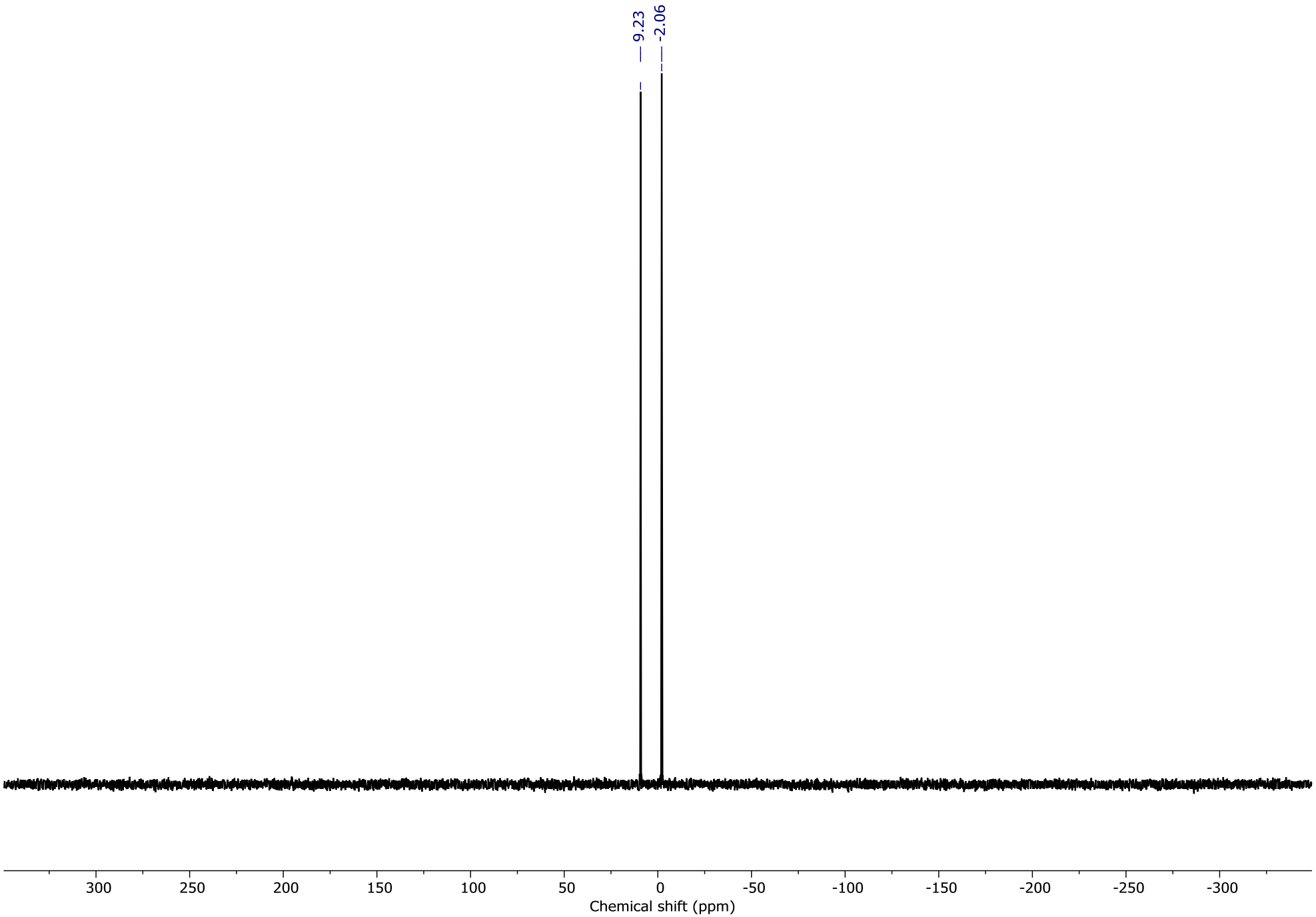
S121



^{29}Si NMR

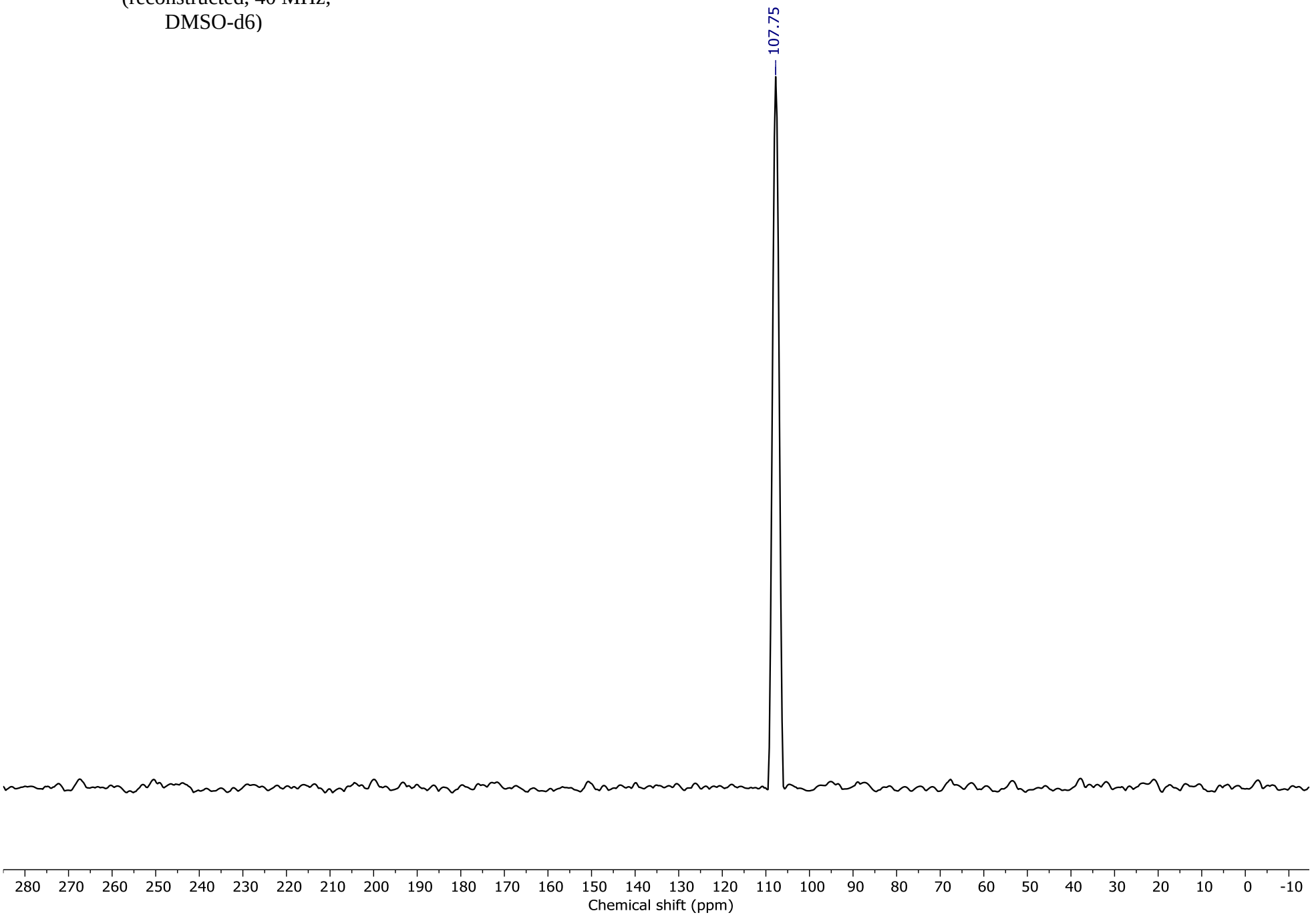
(80 MHz, DMSO-d6)

S122



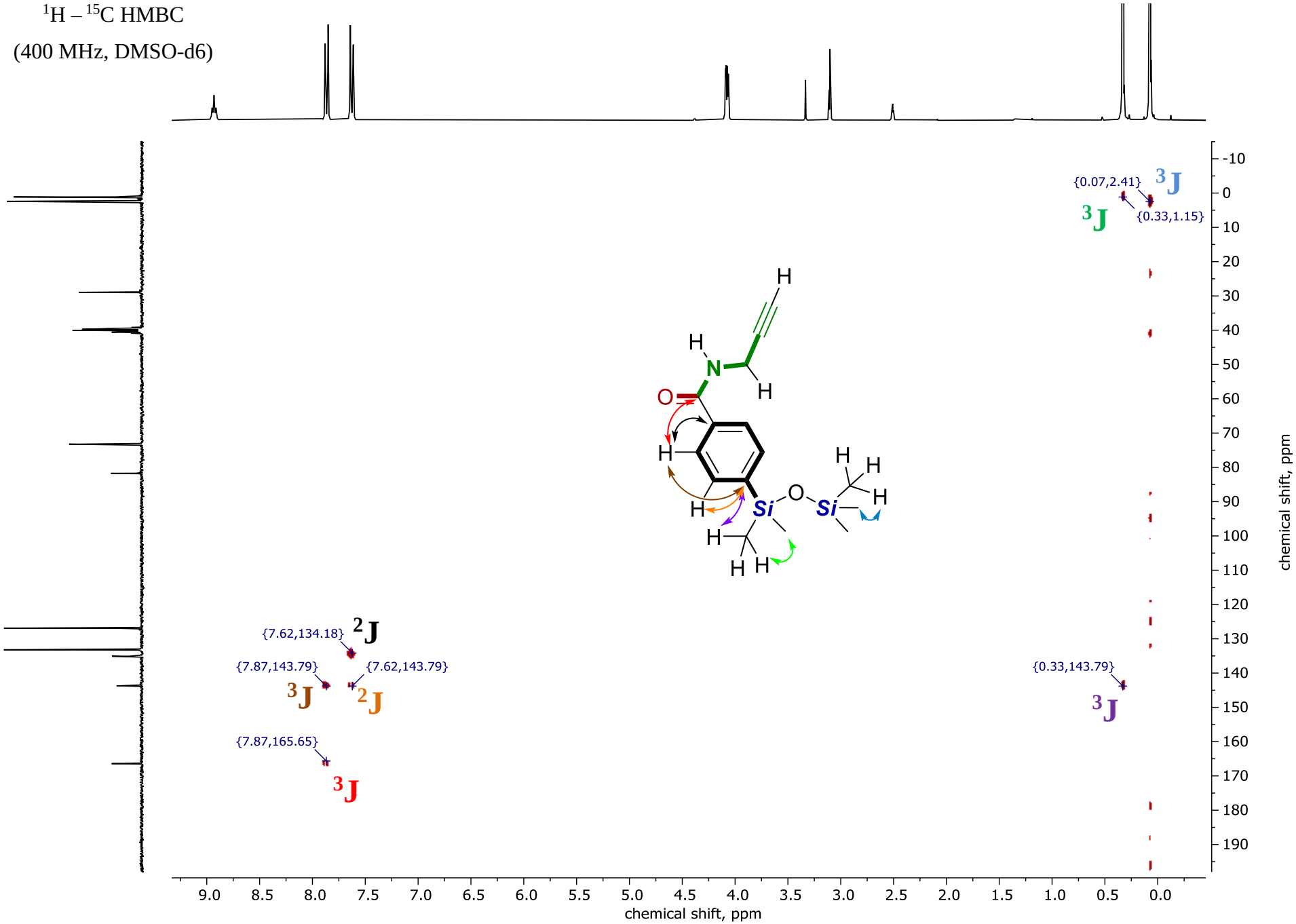
^{15}N NMR

(reconstructed, 40 MHz, DMSO-d6)



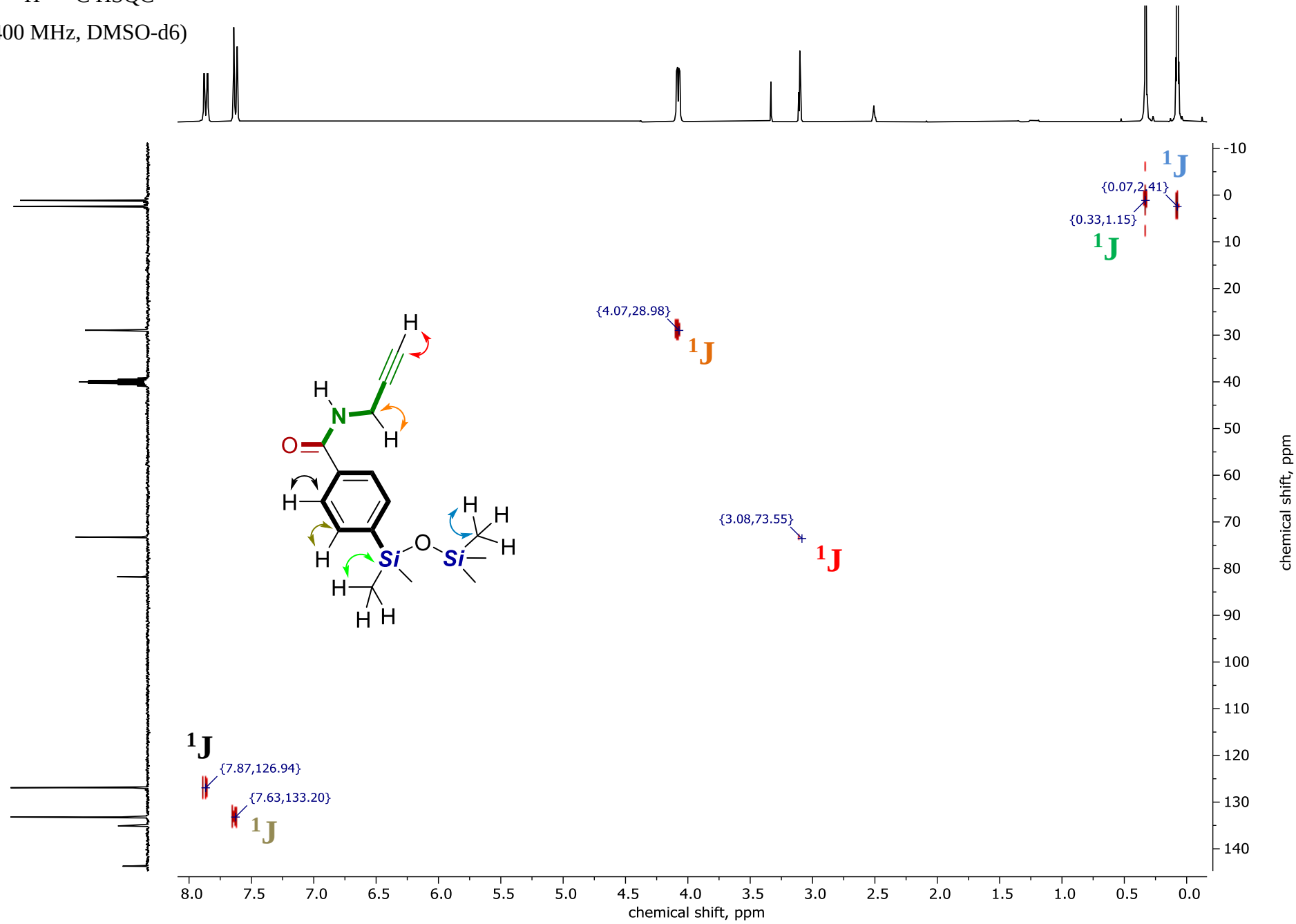
$^{1}H - {}^{15}C$ HMBC

(400 MHz, DMSO-d6)



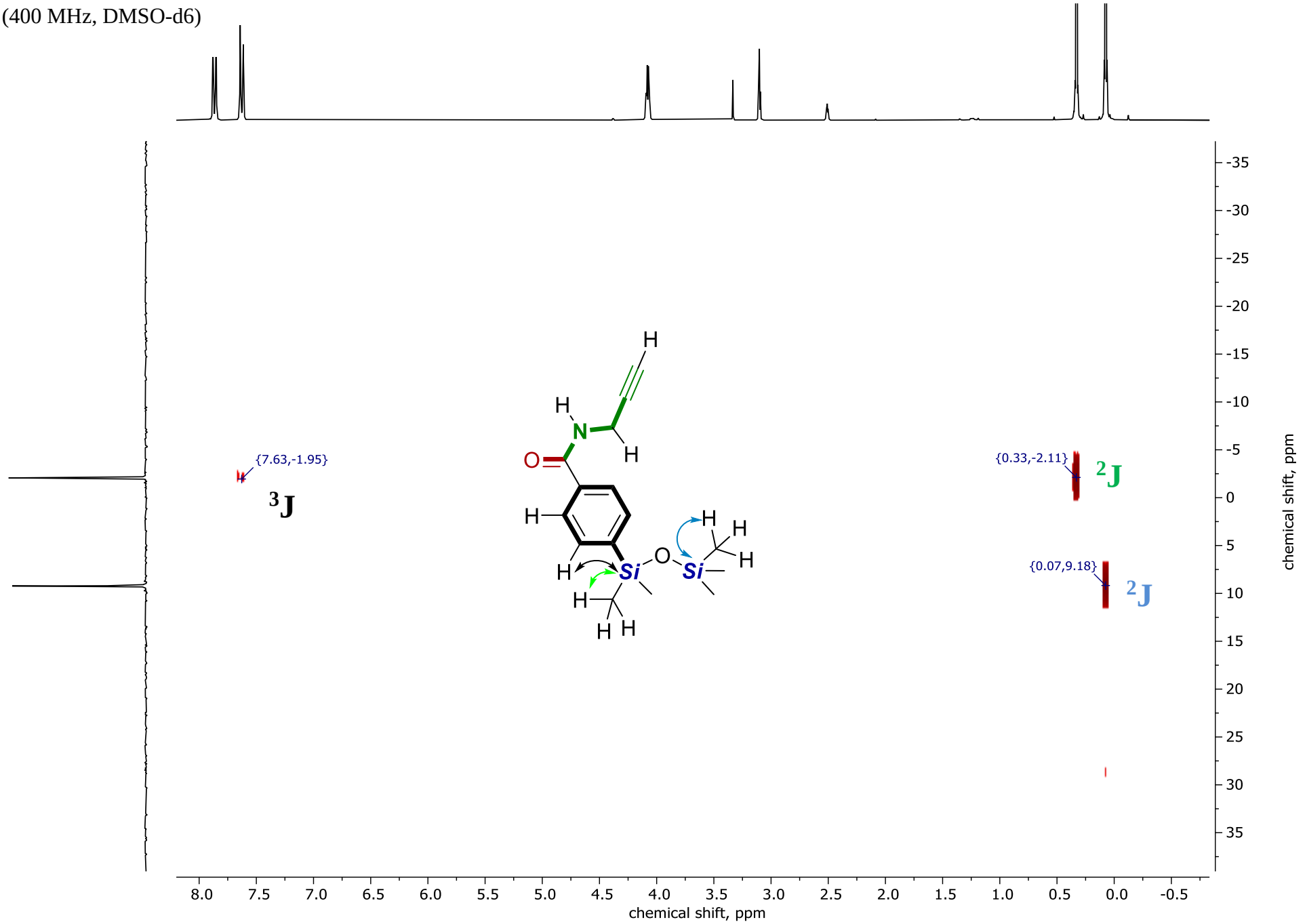
$^{1}H - ^{15}C$ HSQC

(400 MHz, DMSO-d6)



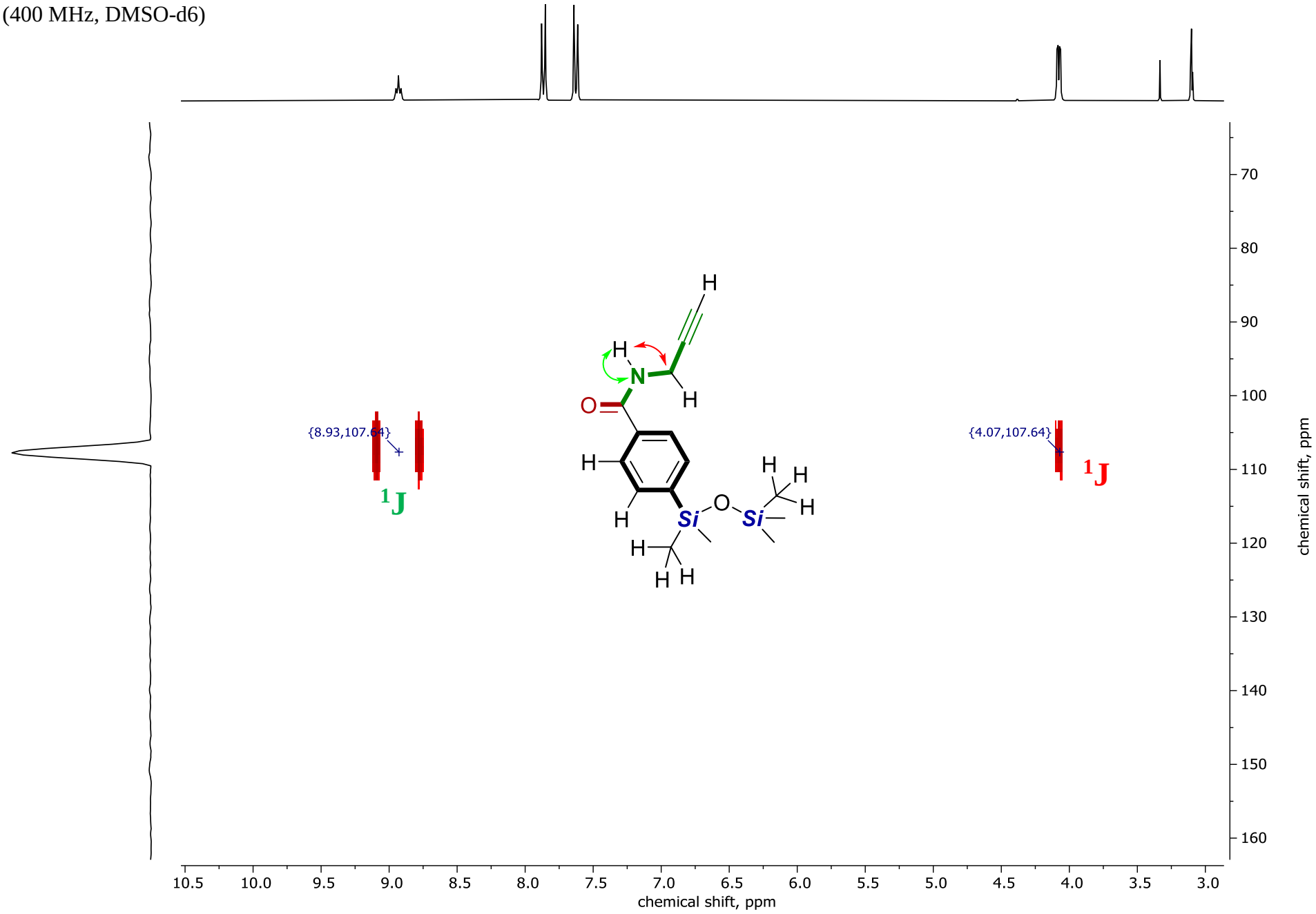
$^{1}H - ^{29}Si$ HMBC

(400 MHz, DMSO-d6)



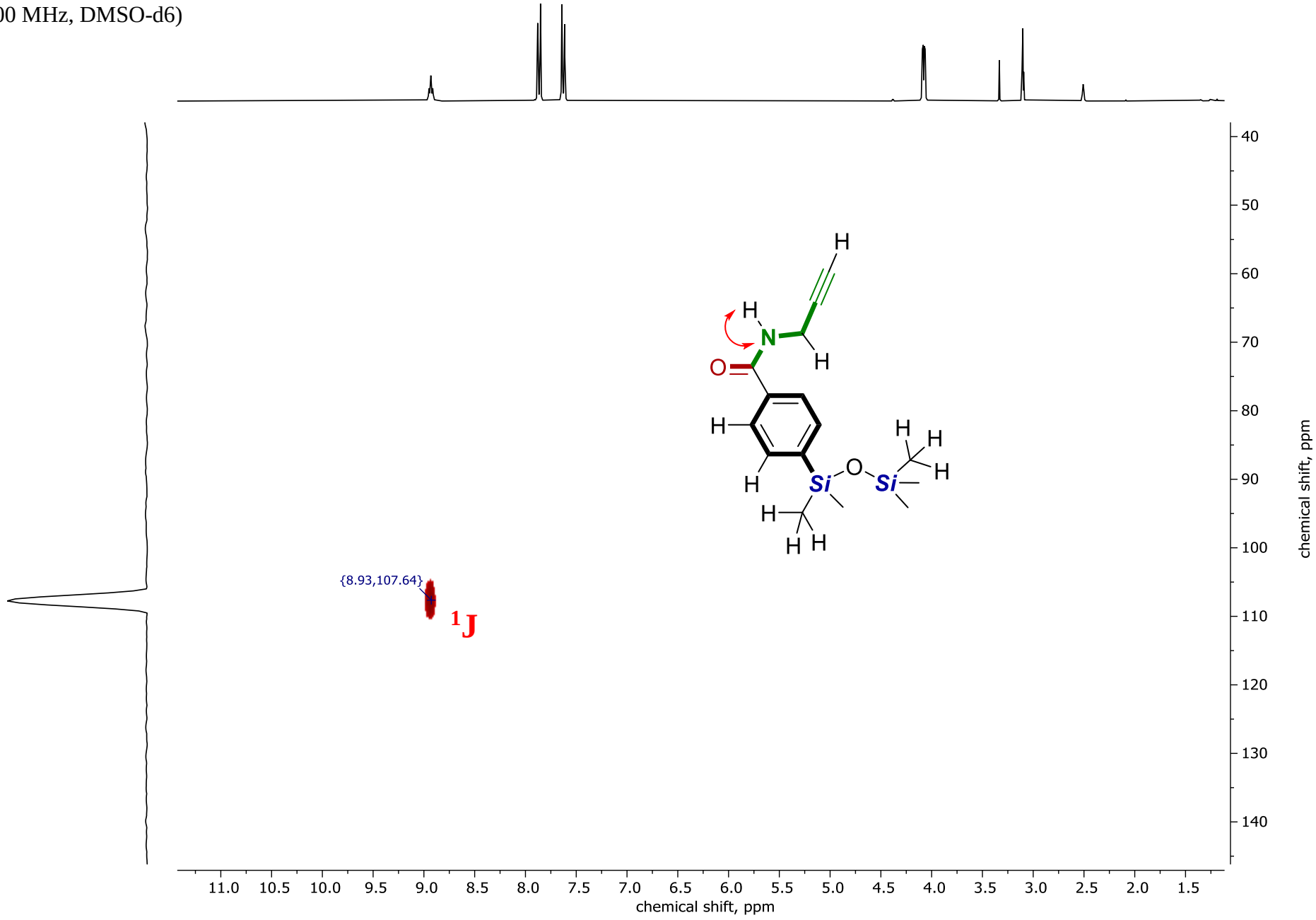
$^{1}H - {}^{15}N$ HMBC

(400 MHz, DMSO-d6)

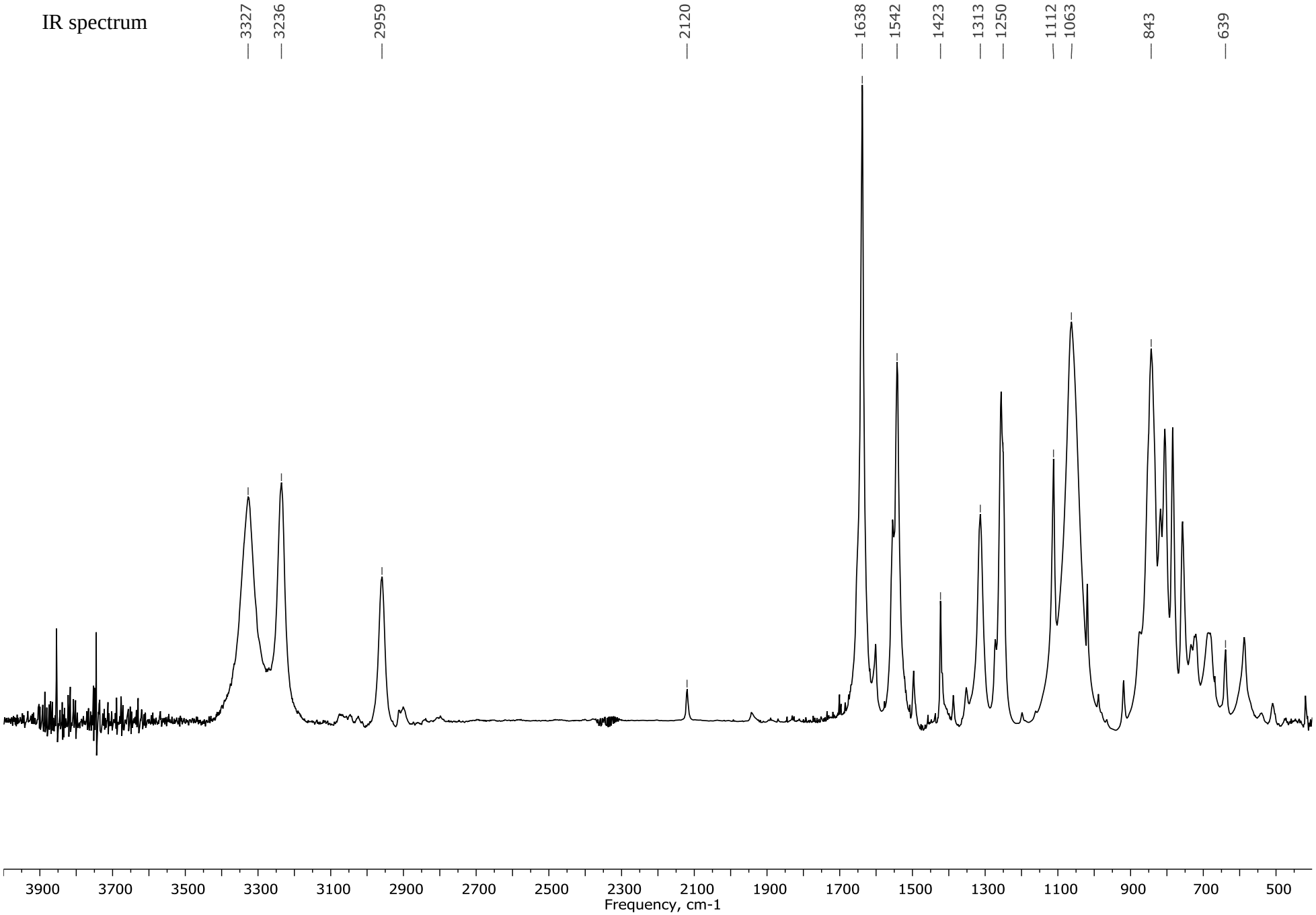


$^{1}H - ^{15}N$ HSQC

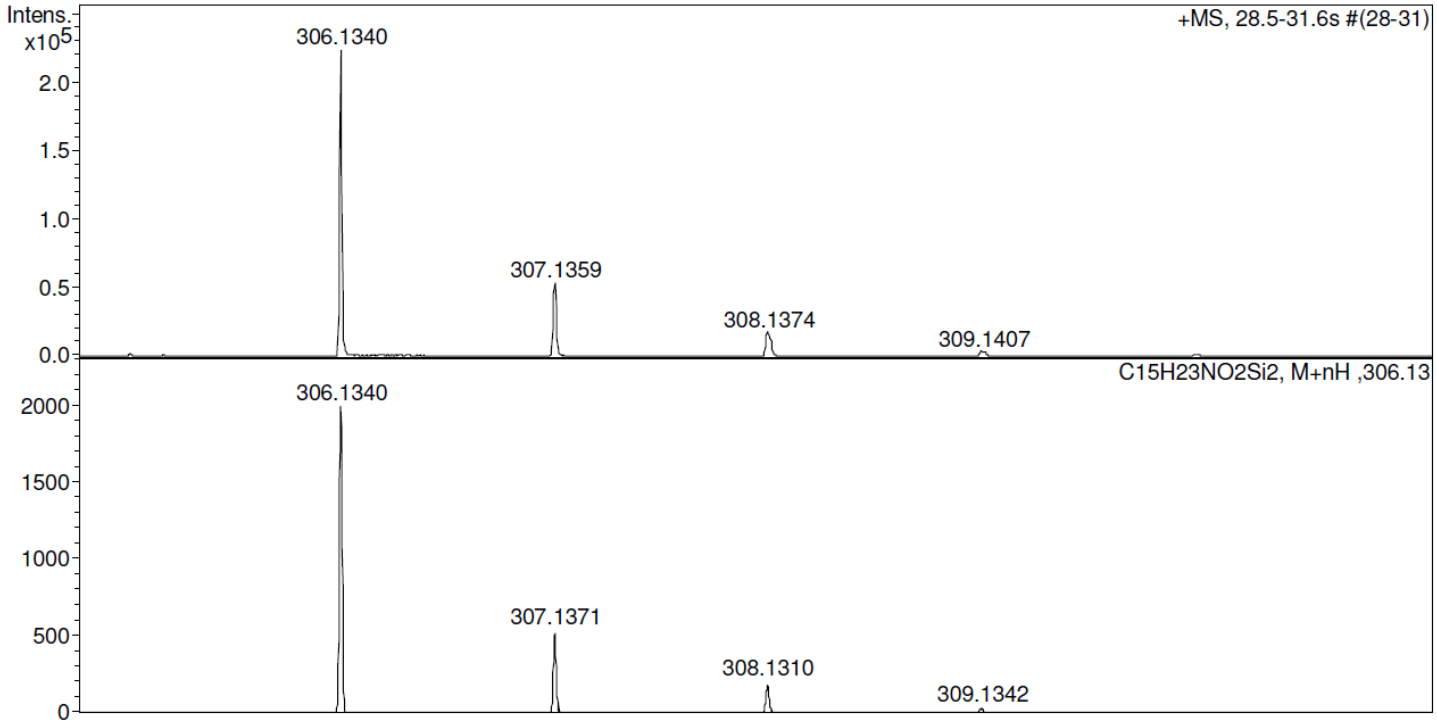
(400 MHz, DMSO-d6)

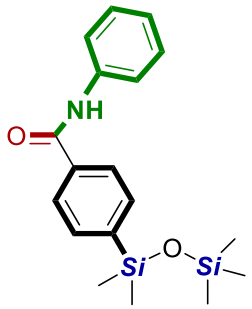


IR spectrum


3327
3236
2959
2120
1638
1542
1423
1313
1250
1112
1063
843
639
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

HRMS (ESI)


Intens.
x10^5
2.0
1.5
1.0
0.5
0.0
306.1340
307.1359
308.1374
309.1407
+MS, 28.5-31.6s #(28-31)
C15H23NO2Si2, M+nH ,306.13
2000
1500
1000
500
0
306.1340
307.1371
308.1310
309.1342

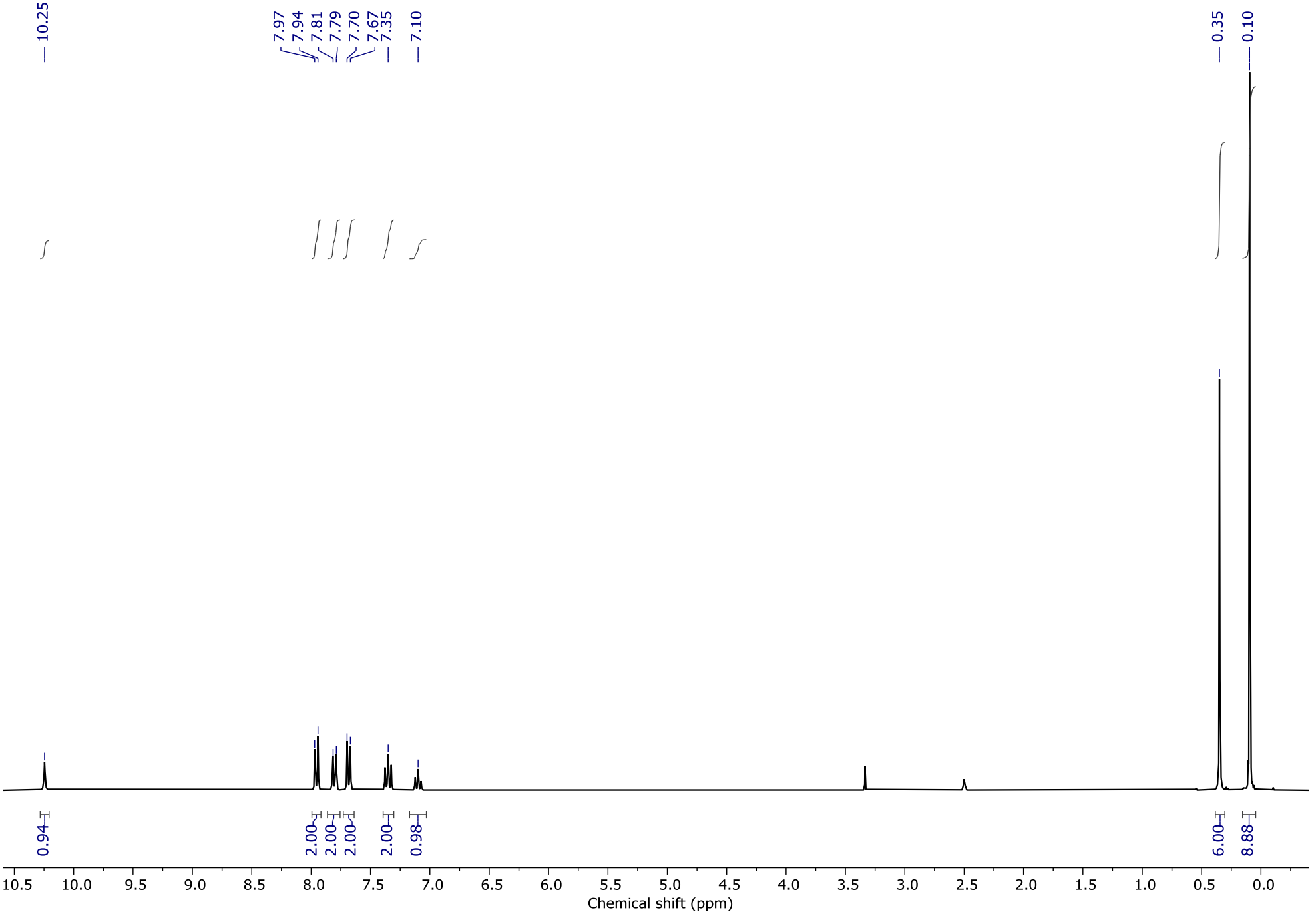


Characterisation data for 4-(1,1,3,3,3-pentamethyldisiloxanyl)-N-phenylbenzamide:

^{1}H NMR (400 MHz, DMSO): δ = 10.25 (s, 1H), δ = 7.96 (d, ^{3}J=11, 2H), δ = 7.80 (d, ^{3}J=11, 2H), δ = 7.69 (d, ^{3}J=11, 2H), δ = 7.35 (t, ^{3}J=10, 2H), δ = 7.10 (t, ^{3}J=10, 1H), δ = 0.35 (s, 6H), δ = 0.10 (s, 9H). ^{13}C NMR (100 MHz, DMSO): δ = 165.56, 143.37, 139.16, 135.83, 132.70, 128.53, 126.78, 123.58, 120.27, 1.93, 0.68. ^{29}Si NMR (80 MHz, DMSO): δ = 9.29, -2.07. ^{15}N NMR (40 MHz, DMSO): δ = 128.85. HRMS (ESI) m/z [M + H] $^{+}$: calcd for $[C_{18}H_{25}NO_2Si_2 + H]^{+}$, 344.1497; found, 344.1505. IR (cm^{-1}): 3305, 2956, 1640, 1602, 1540, 1496, 1444, 1330, 1253, 1082, 840-637.

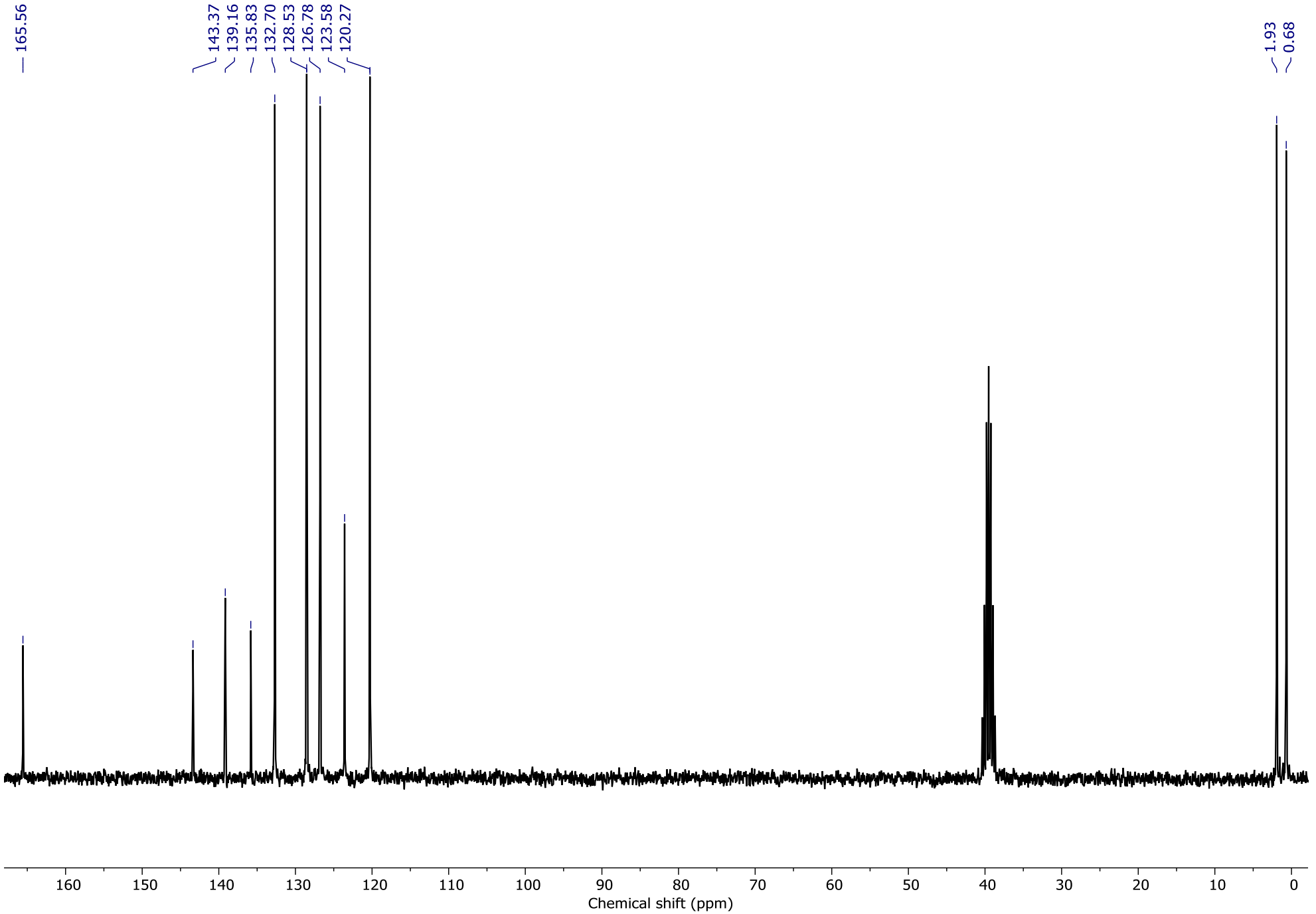
^{1}H NMR

(400 MHz, DMSO-d6)



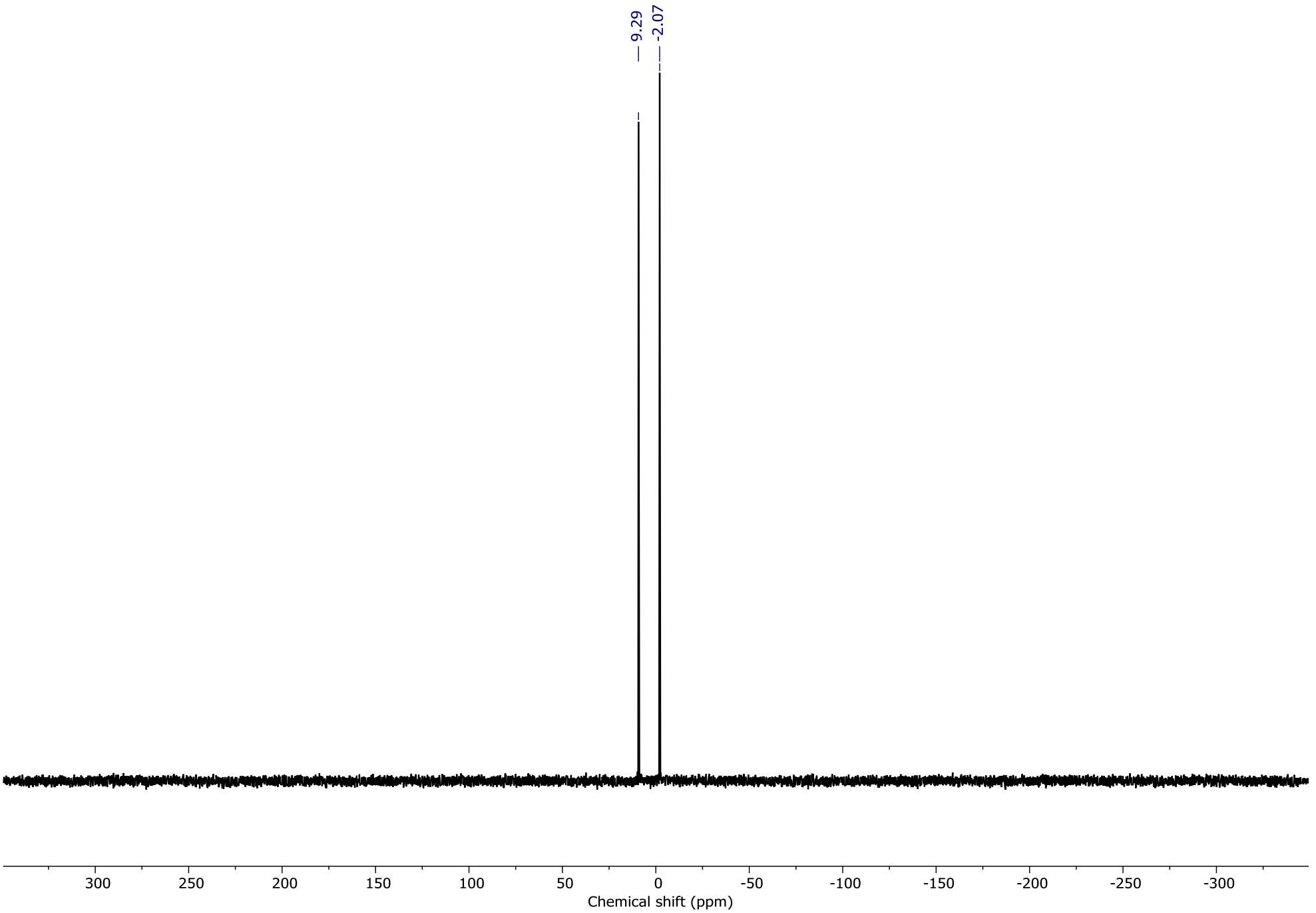
^{13}C NMR

(100 MHz, DMSO-d6)



^{29}Si NMR

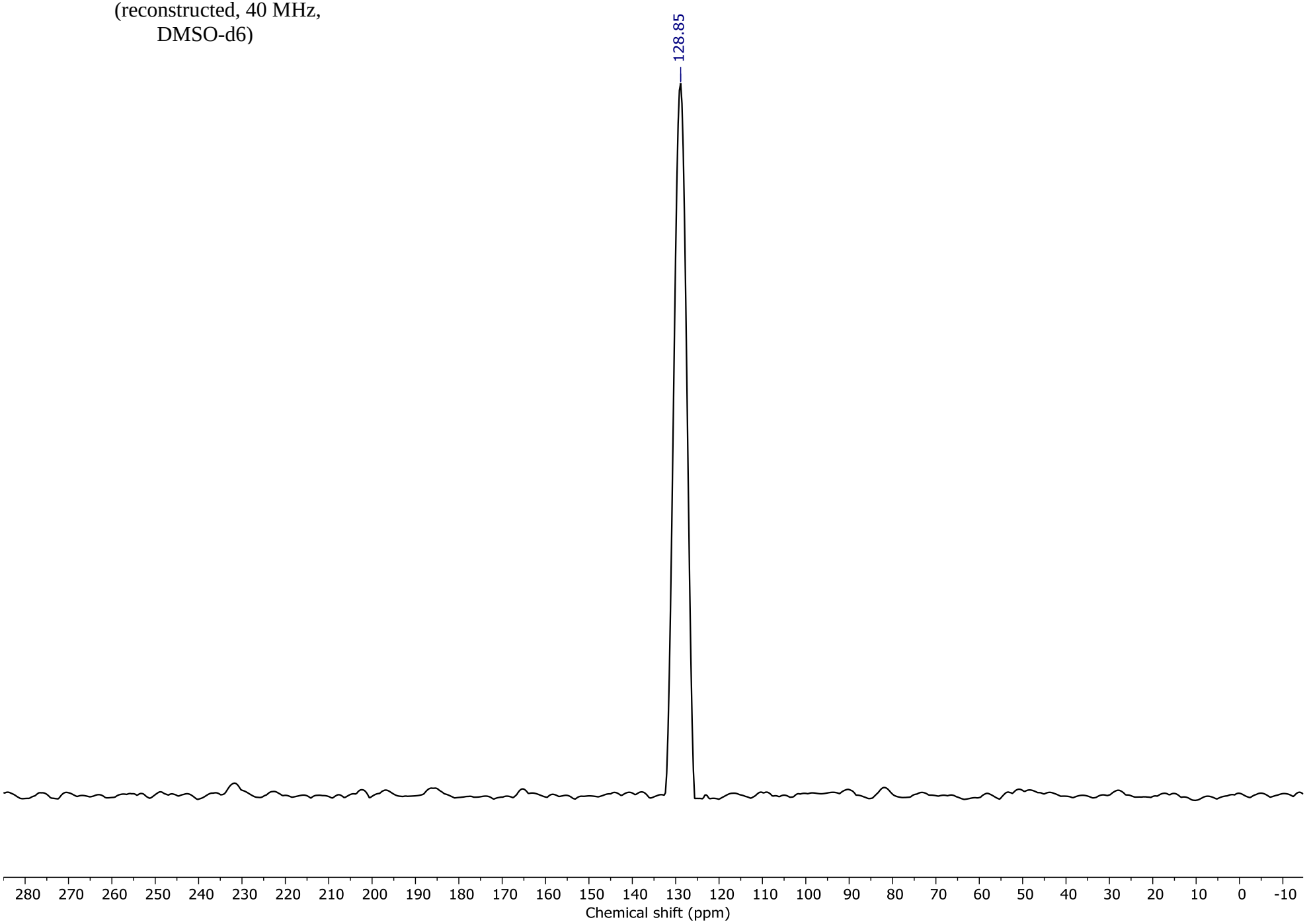
(80 MHz, DMSO-d6)



^{15}N NMR

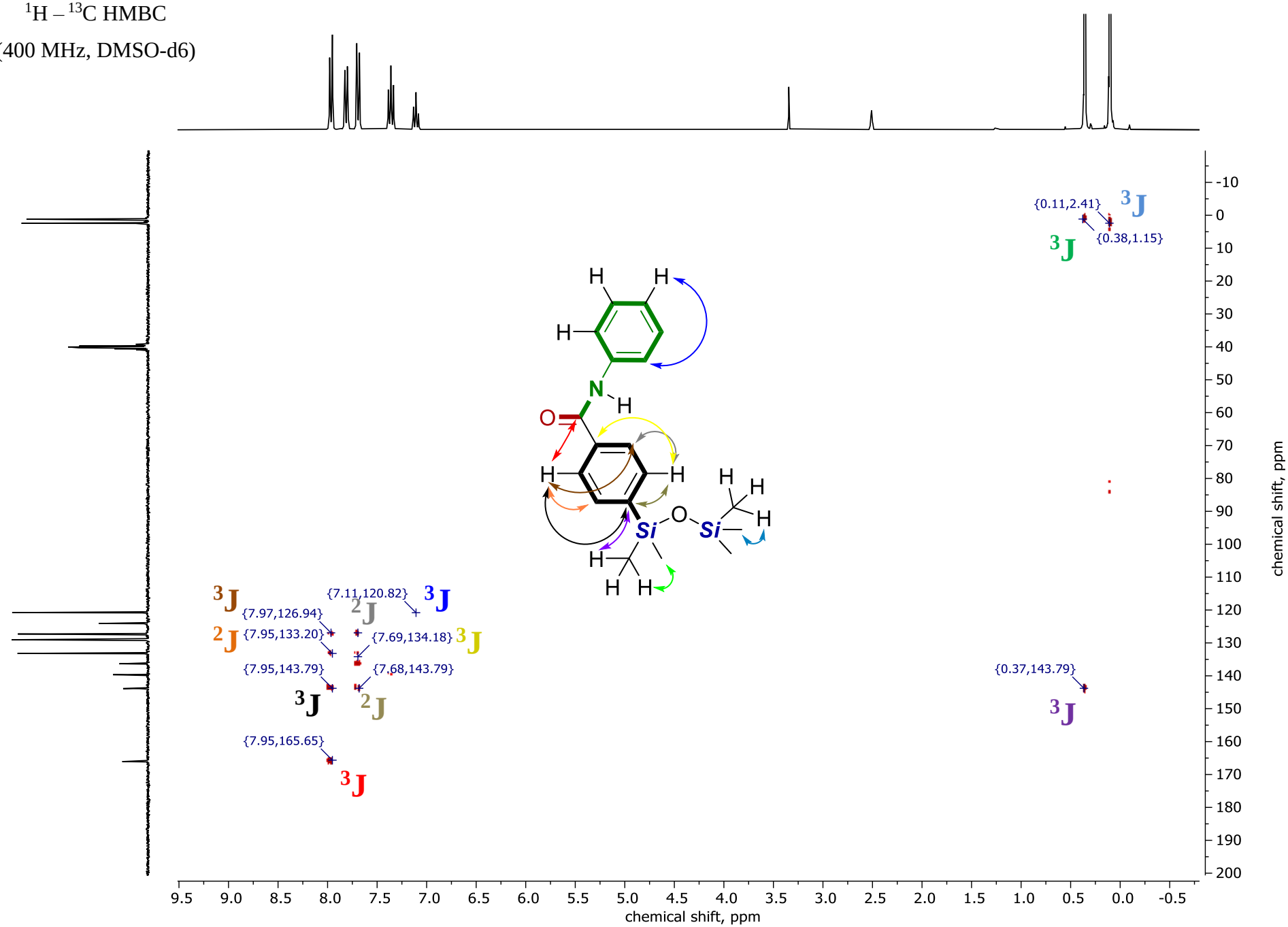
(reconstructed, 40 MHz, DMSO-d6)

S135



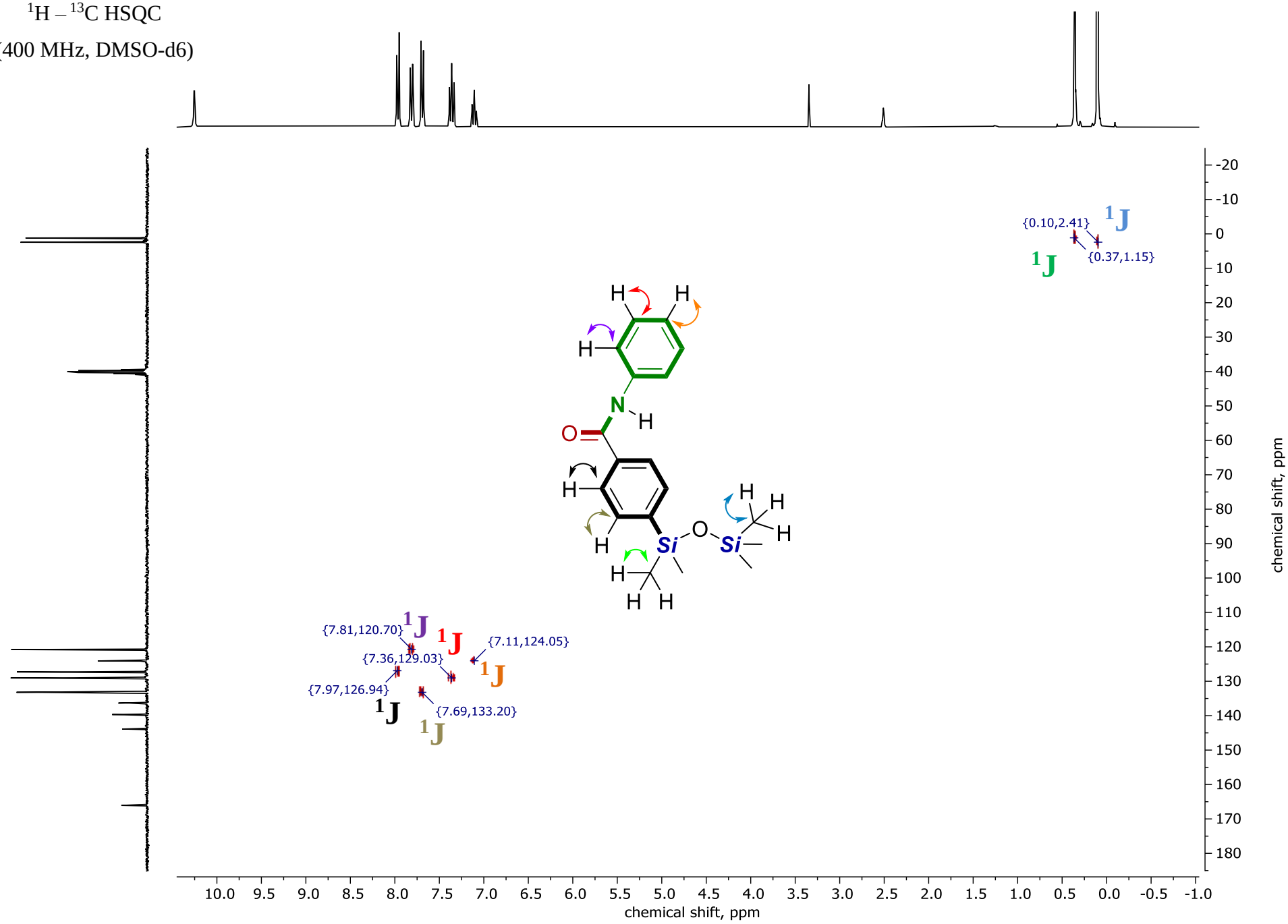
$^{1}H - ^{13}C$ HMBC

(400 MHz, DMSO-d6)



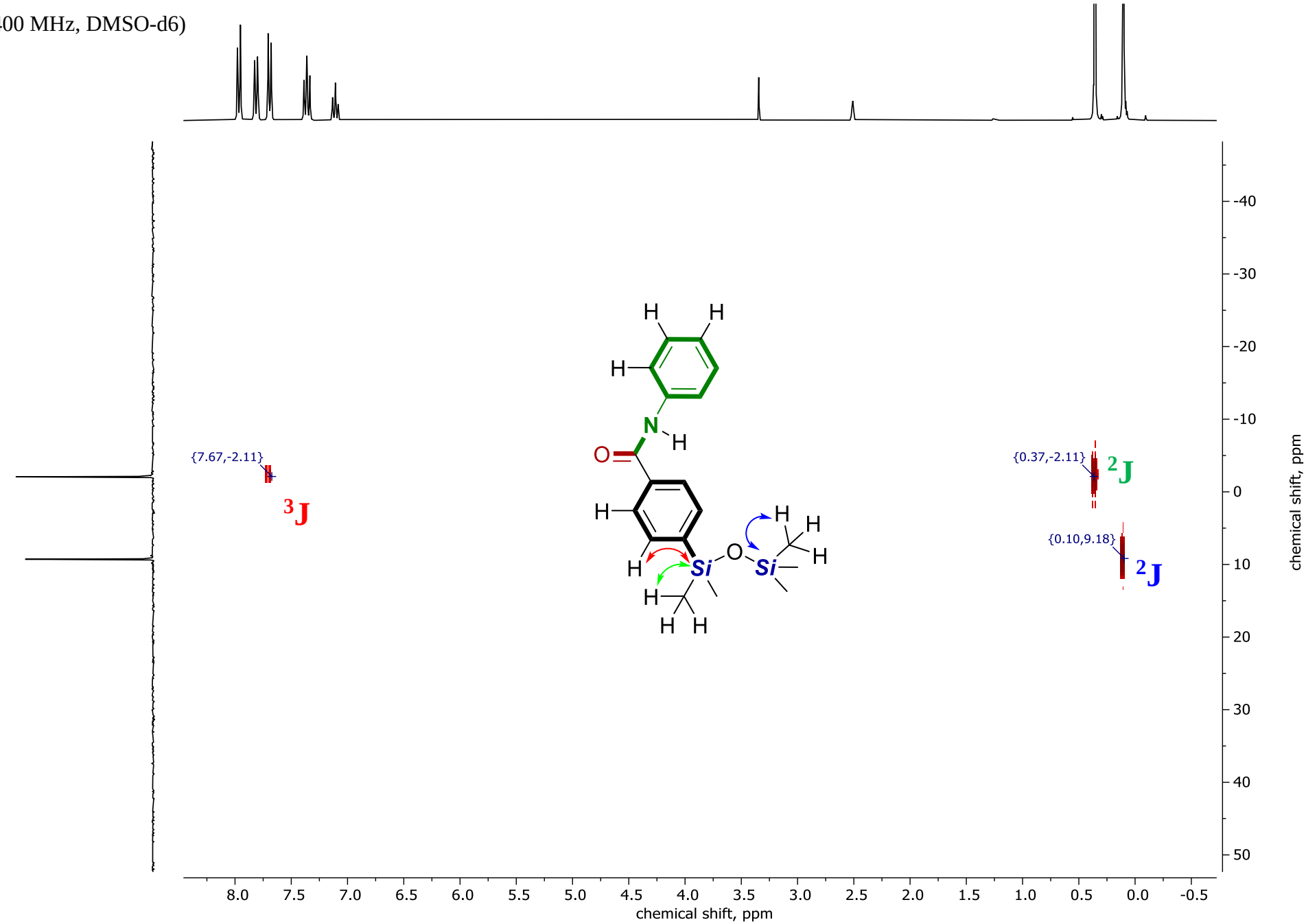
$^{1}H - ^{13}C$ HSQC

(400 MHz, DMSO-d6)



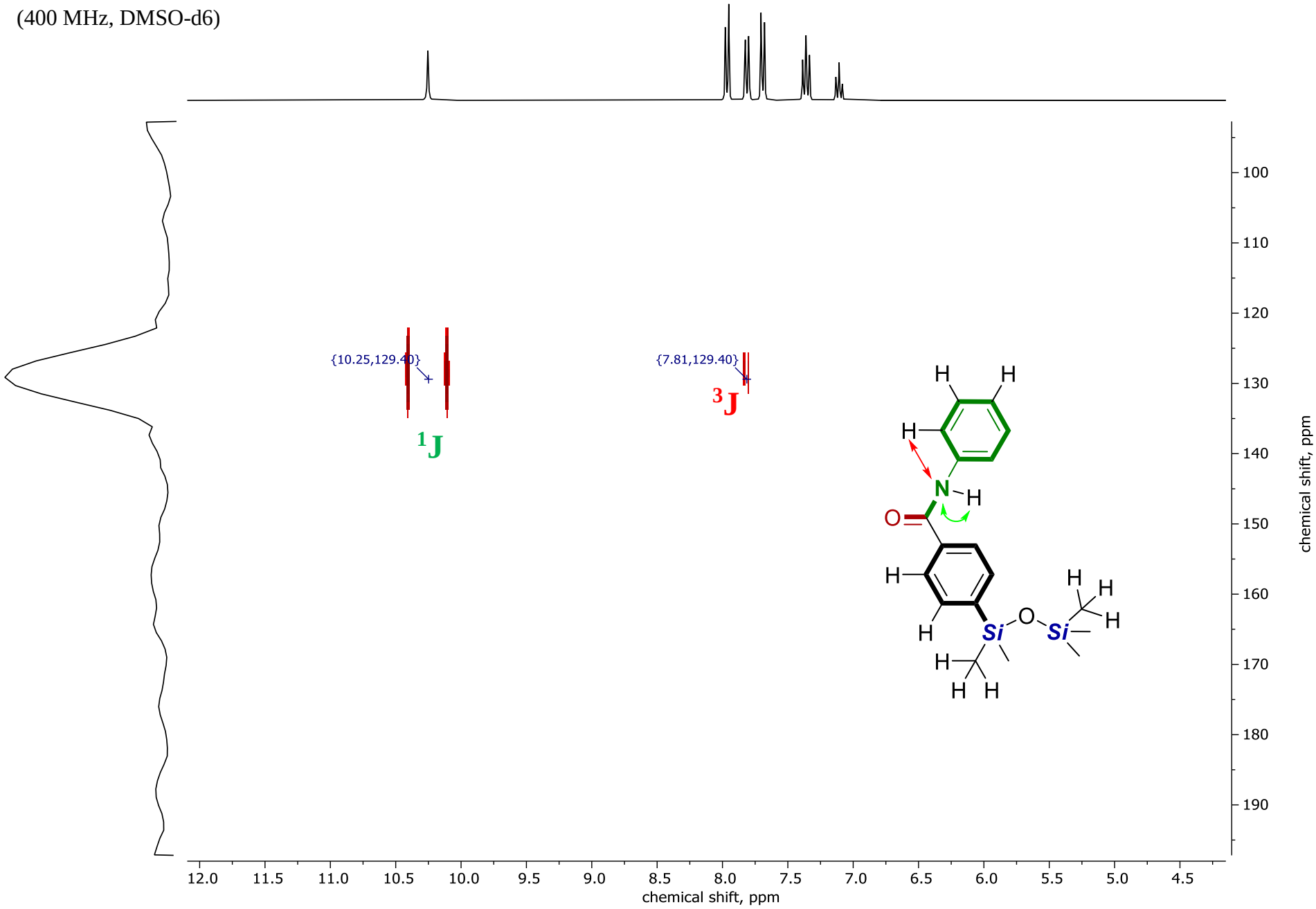
$^{1}H - ^{29}Si$ HMBC

(400 MHz, DMSO-d6)



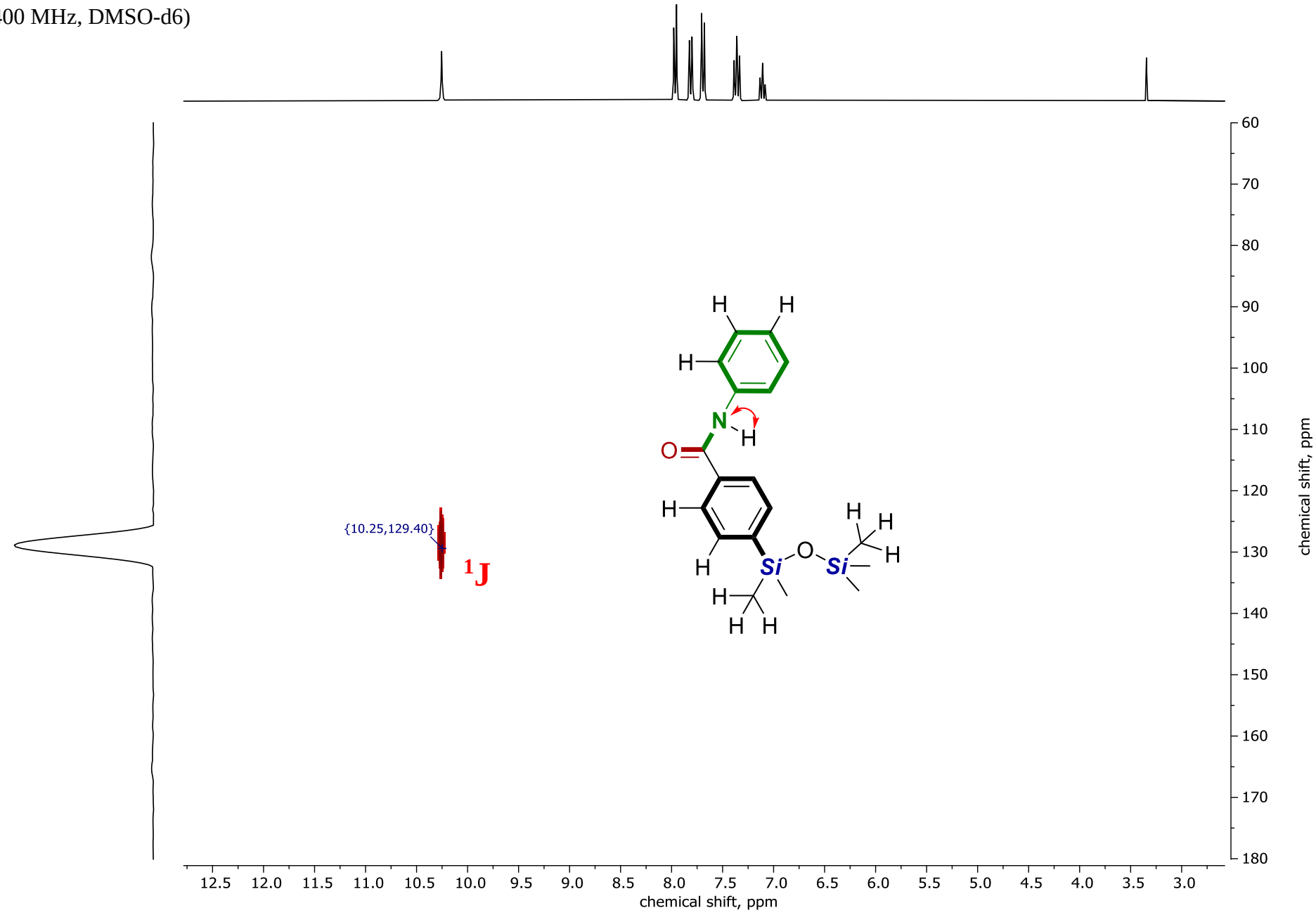
$^{1}H - {}^{15}N$ HMBC

(400 MHz, DMSO-d6)

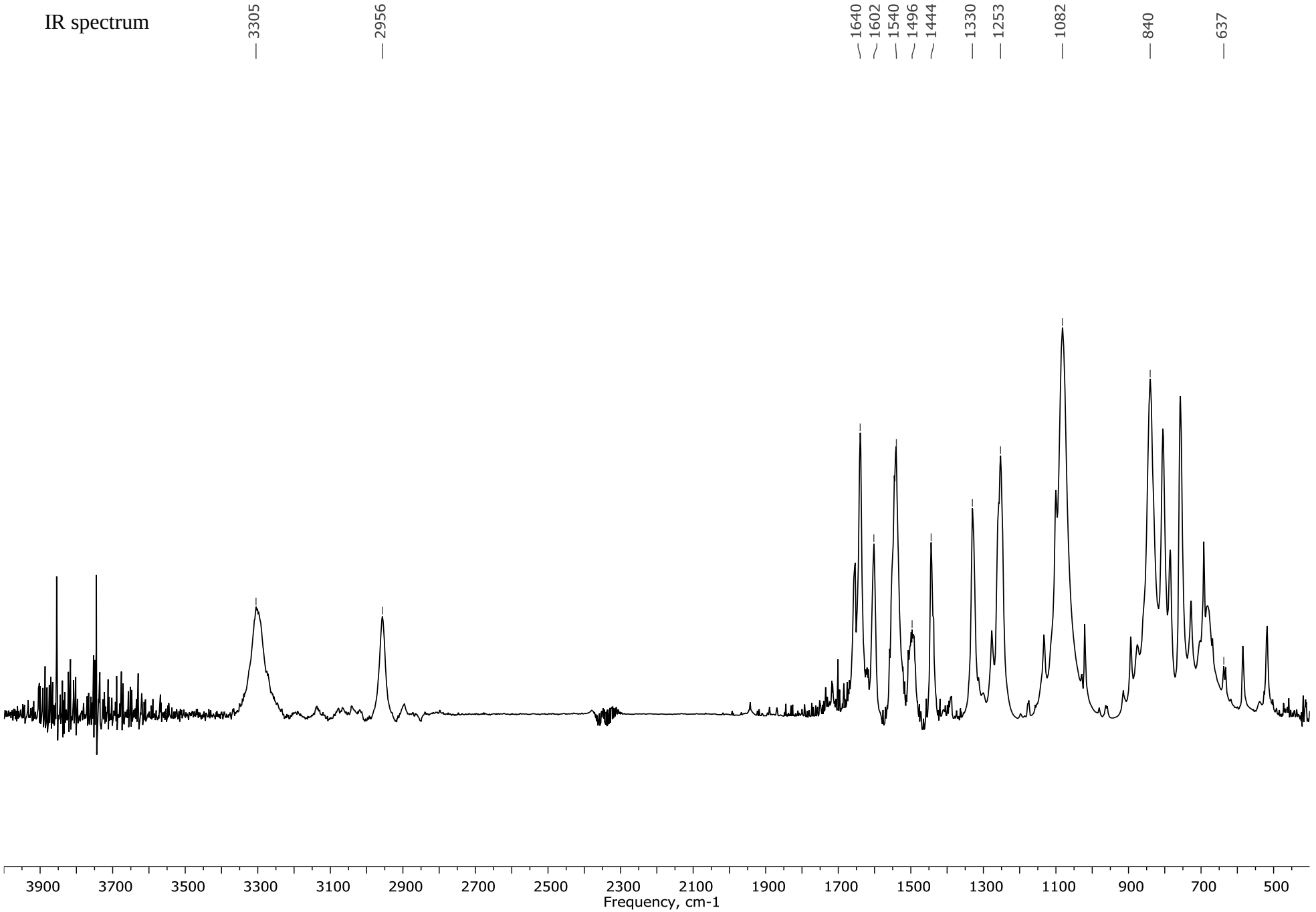


$^{1}H - {}^{15}N$ HSQC

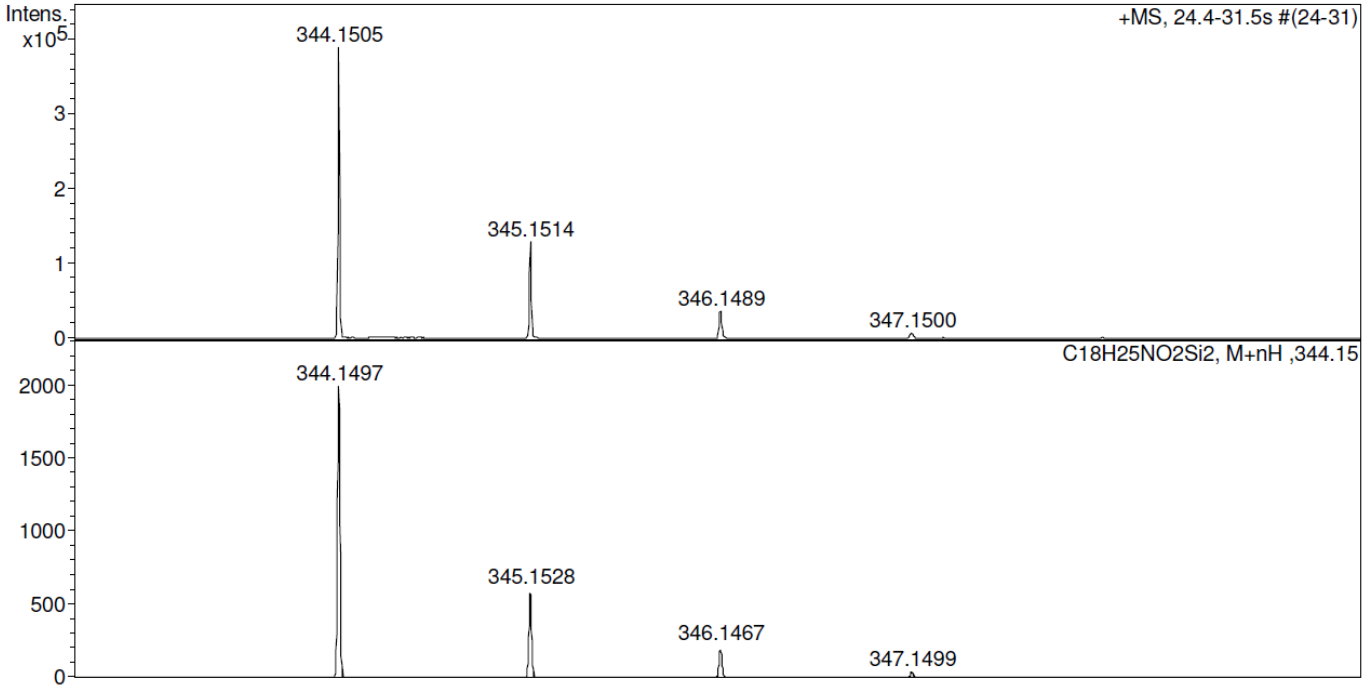
(400 MHz, DMSO-d6)

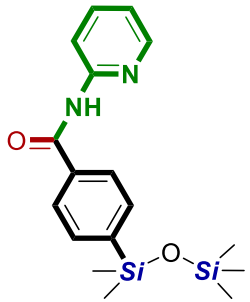


IR spectrum


3305
2956
1640
1602
1540
1496
1444
1330
1253
1082
840
637
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

HRMS (ESI)


Intens.
x10^5
3
2
1
0
344.1505
345.1514
346.1489
347.1500
+MS, 24.4-31.5s #(24-31)
2000
1500
1000
500
0
344.1497
345.1528
346.1467
347.1499
C18H25NO2Si2, M+nH ,344.15

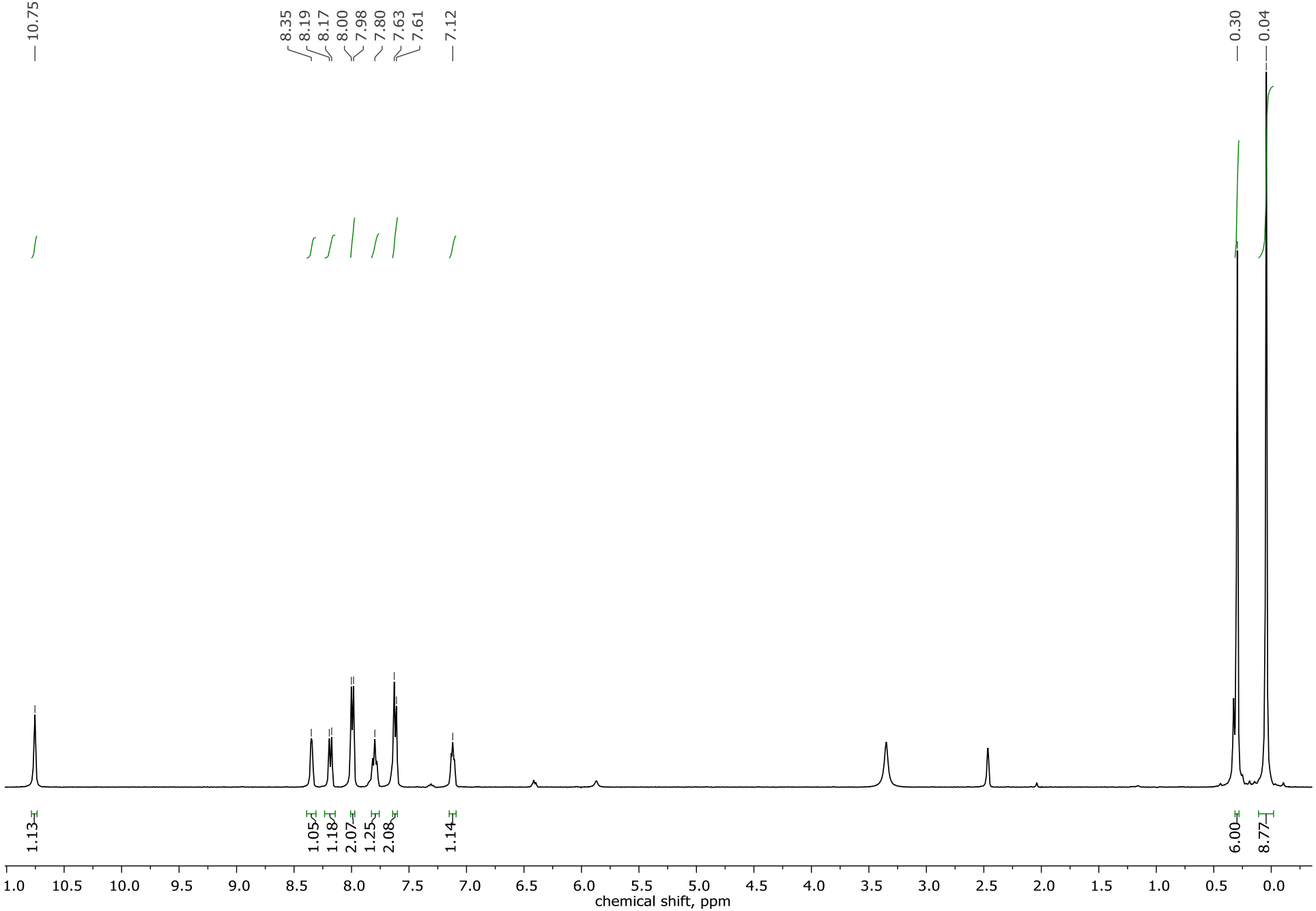


Characterisation data for 4-(1,1,3,3,3-pentamethyldisiloxanyl)-N-(pyridin-2-yl)benzamide:

^{1}H NMR (400 MHz, DMSO): δ = 10.75 (s, 1H), δ = 8.35 (m, 1H), δ = 8.18 (d, ^{3}J=8 Hz, 1H), δ = 7.99 (d, ^{3}J=8 Hz, 2H), δ = 7.80 (t, ^{3}J=8 Hz, 1H), δ = 7.62 (d, ^{3}J=8 Hz, 2H), δ = 7.12 (m, 1H), δ = 0.30 (s, 6H), δ = 0.04 (s, 9H). ^{13}C NMR (100 MHz, DMSO): δ = 166.02, 152.20, 147.93, 143.88, 138.10, 134.90, 132.74, 127.16, 119.82, 114.71, 2.00, 0.74. ^{29}Si NMR (80 MHz, DMSO): δ = 9.31, -2.06. HRMS (ESI) m/z [M + H] $^{+}$: calcd for $[C_{17}H_{24}NO_2Si_2 + H]^{+}$, 345.1449; found, 345.1452. IR (cm^{-1}): 2958, 1675, 1584, 1539, 1442, 1313, 1253, 1313, 1253, 1077, 840-682.

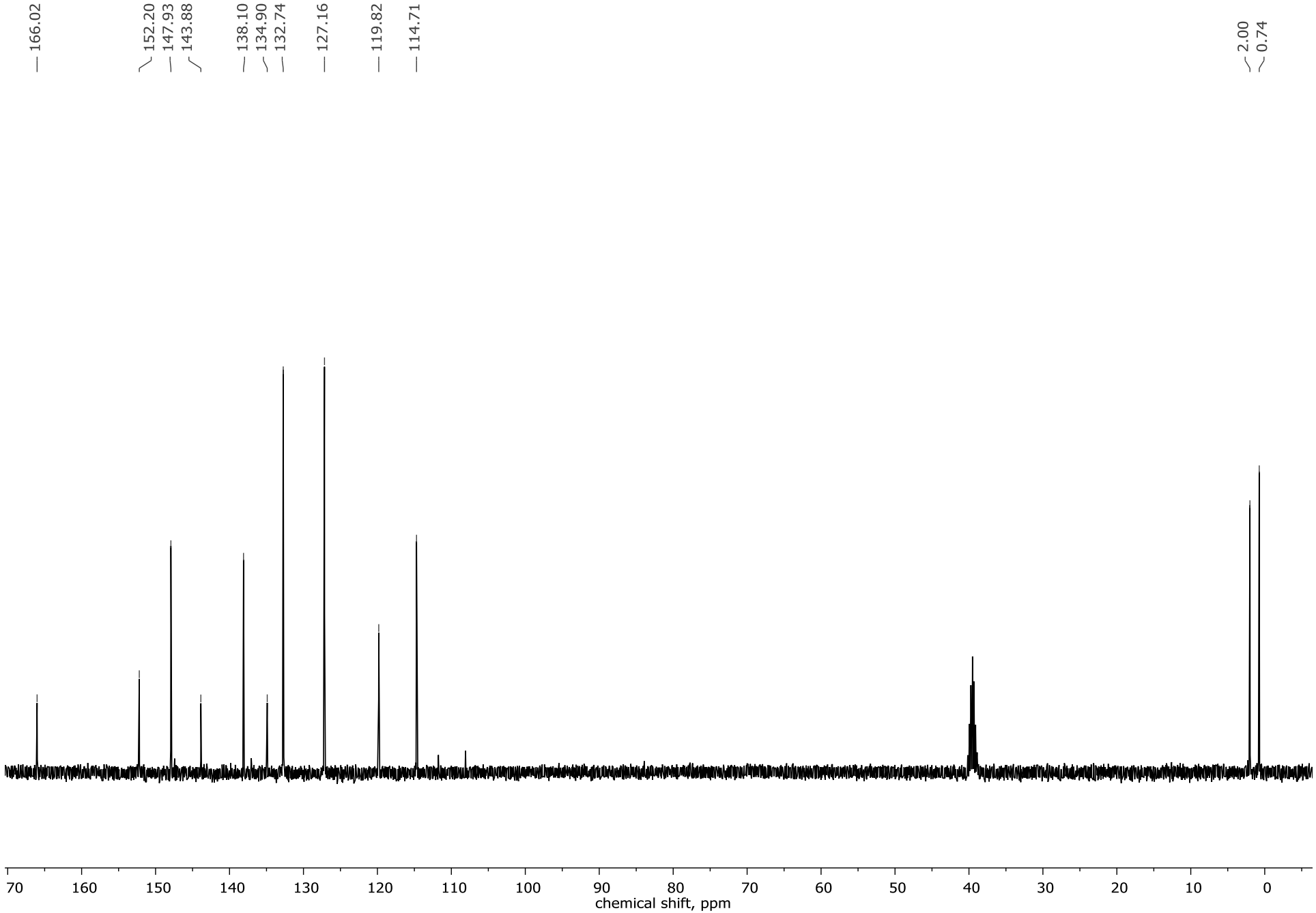
^{1}H NMR

(400 MHz, DMSO-d6)



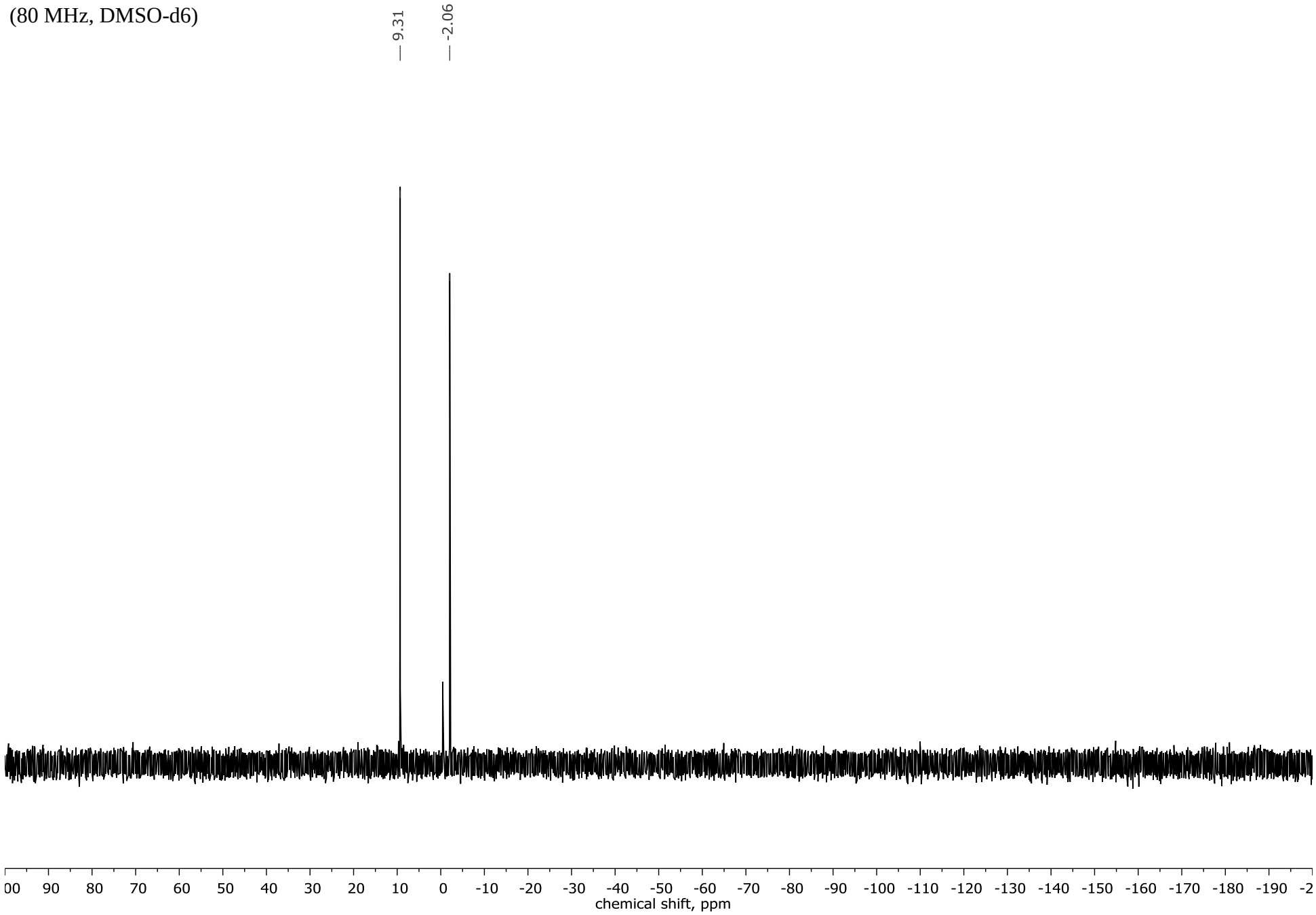
^{13}C NMR

(100 MHz, DMSO-d6)

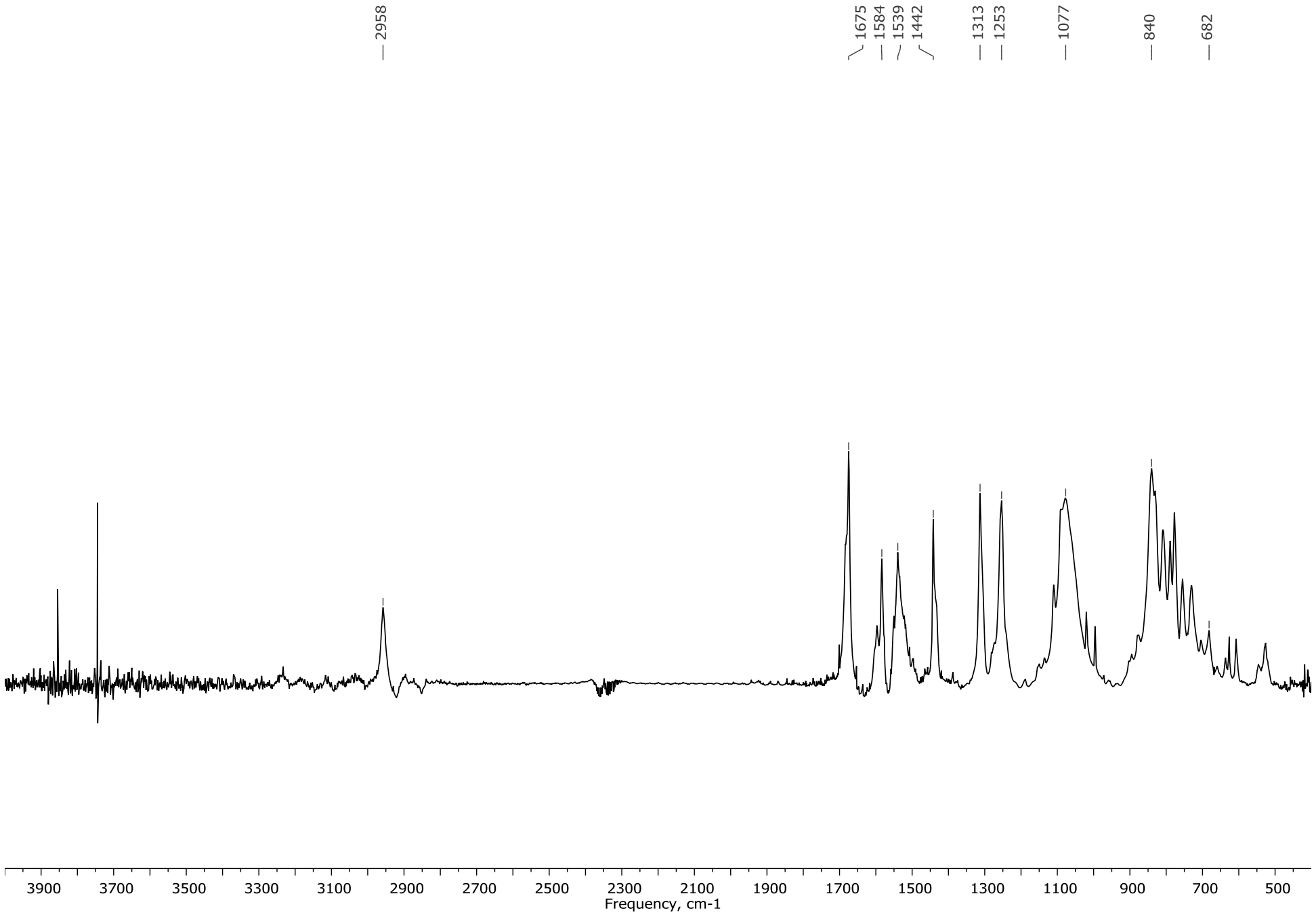


^{29}Si NMR

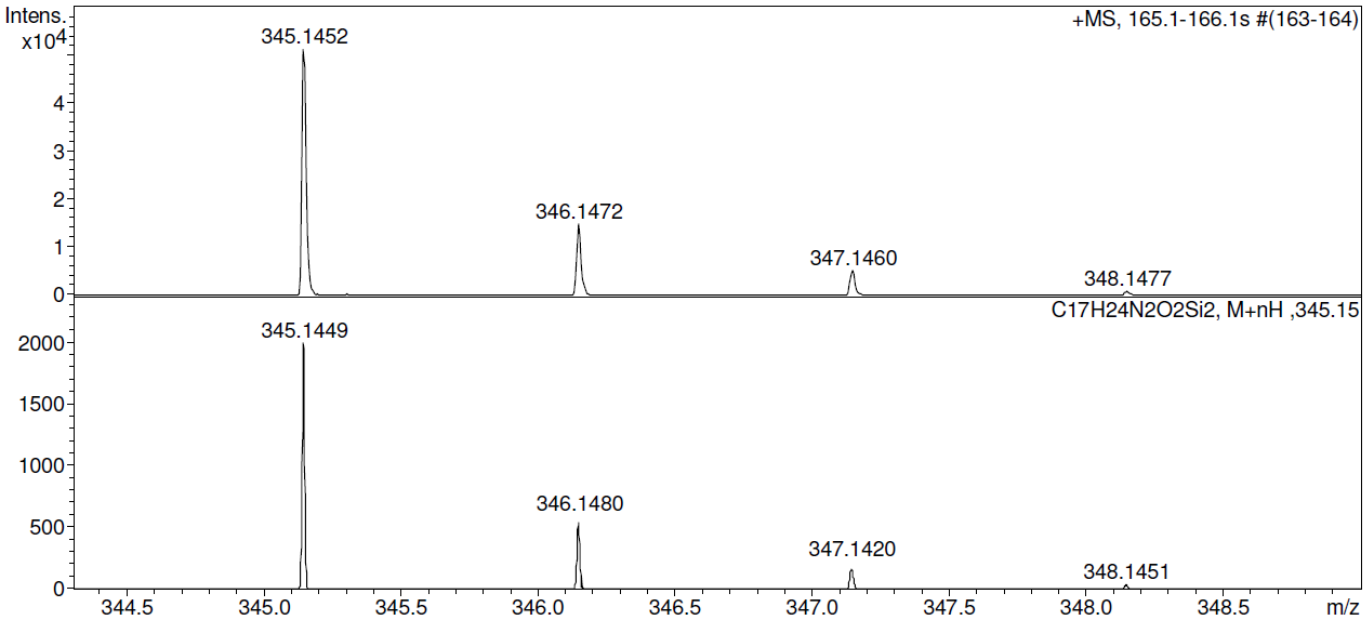
(80 MHz, DMSO-d6)

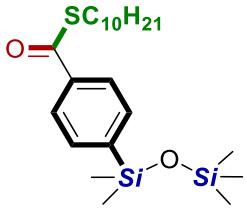


IR spectrum


2958
1675
1584
1539
1442
1313
1253
1077
840
682
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

HRMS (ESI)


Intens.
x10^4
+MS, 165.1-166.1s #(163-164)
345.1452
346.1472
347.1460
348.1477
C17H24N2O2Si2, M+nH ,345.15
345.1449
346.1480
347.1420
348.1451
m/z

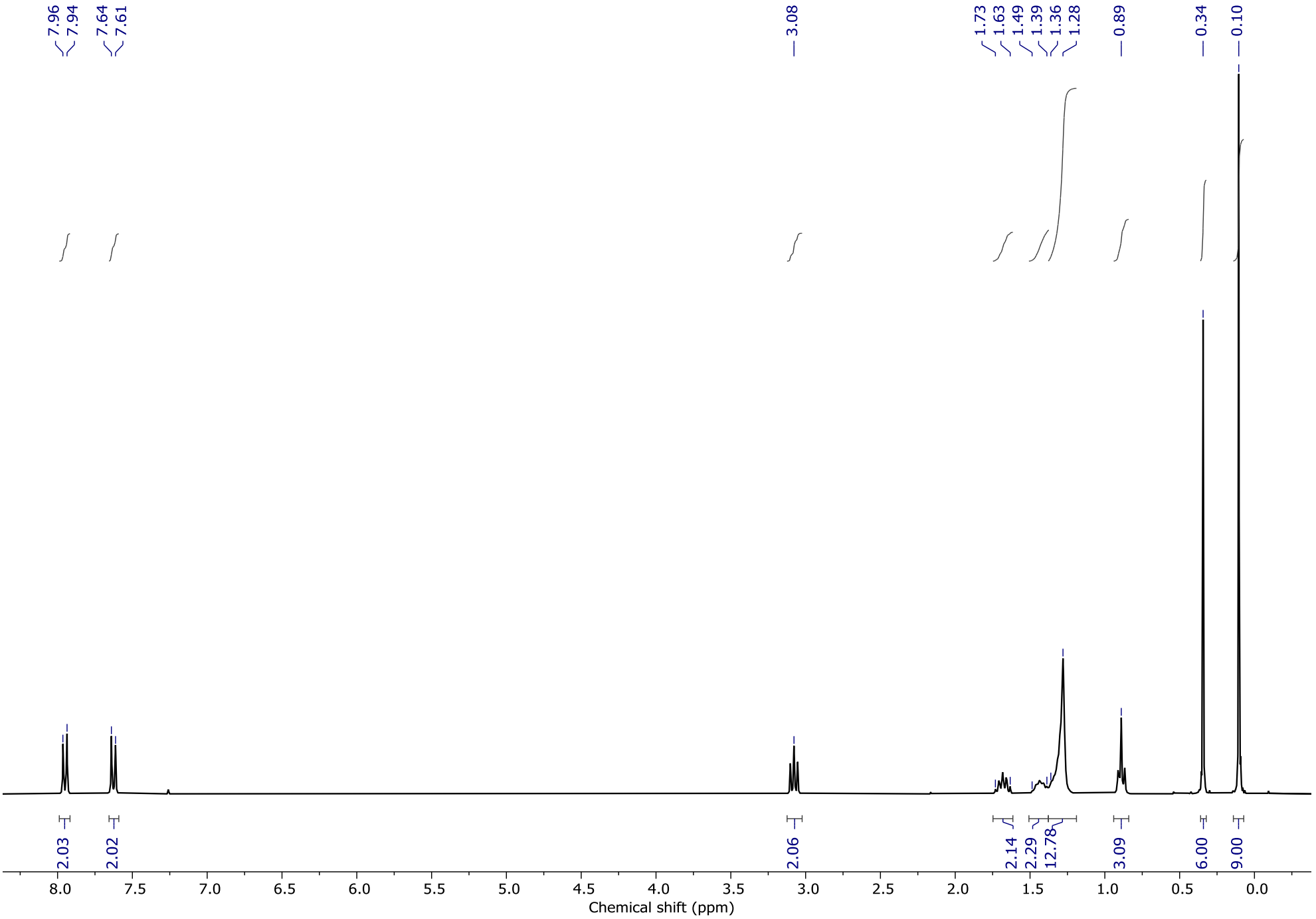


Characterisation data for S-decyl 4-(1,1,3,3,3-pentamethyldisiloxanyl)benzothioate:

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.95 (d, ^{3}J=11 Hz, 2H), δ = 7.63 (d, ^{3}J=11 Hz, 2H), δ = 3.08 (t, ^{3}J=10 Hz, 2H), δ = 1.73-1.63 (m, 2H), δ = 1.49-1.39 (m, 2H), δ = 1.36-1.28 (m, 13H), δ = 0.89 (m, 3H), δ = 0.34 (s, 6H), δ = 0.10 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 192.22, 146.64, 137.69, 133.09, 126.11, 31.88, 29.57, 29.53, 29.49, 29.29, 29.15, 28.99, 28.93, 22.66, 14.08, 1.90, 0.74. ^{29}Si NMR (80 MHz, $CDCl_3$): δ = 9.45, -2.72. HRMS (ESI) m/z $[M + H]^+$: calcd for $[C_{22}H_{40}O_2SSi_2 + H]^+$, 425.2360; found, 425.2368; $[M + NH_4]^+$: calcd for $[C_{22}H_{40}O_2SSi_2 + NH_4]^+$, 442.2626; found, 442.2624; $[M + Na]^+$: calcd for $[C_{22}H_{40}O_2SSi_2 + Na]^+$, 447.2180; found, 447.2161; $[M + K]^+$: calcd for $[C_{22}H_{40}O_2SSi_2 + K]^+$, 463.1919; found, 463.1914. IR (cm^{-1}): 2956-2855, 1669, 1457, 1387, 1254, 1212, 1181, 1058, 916, 842-650.

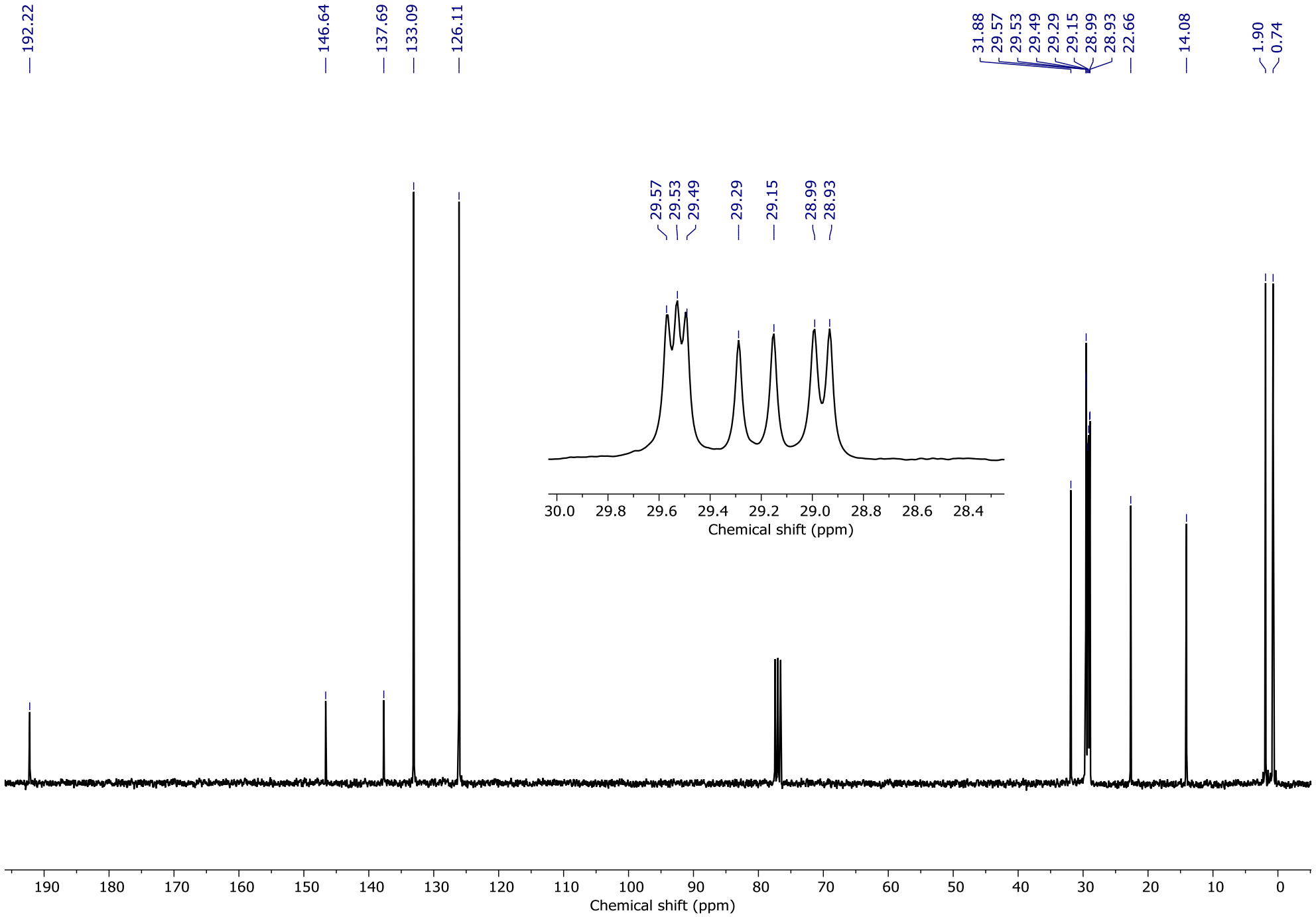
^{1}H NMR

(400 MHz, $CDCl_3$)



^{13}C NMR

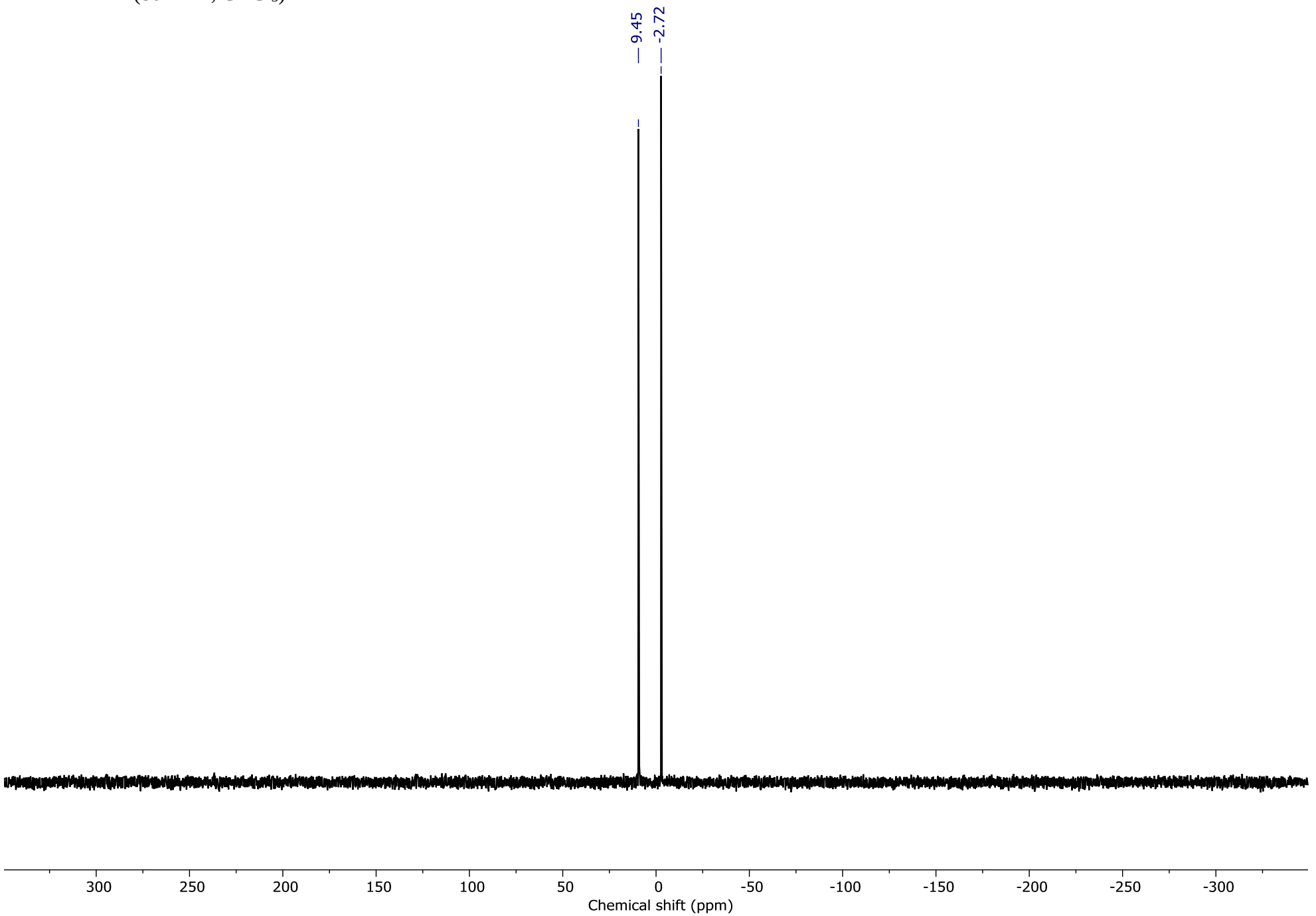
(100 MHz, $CDCl_3$)



^{29}Si NMR

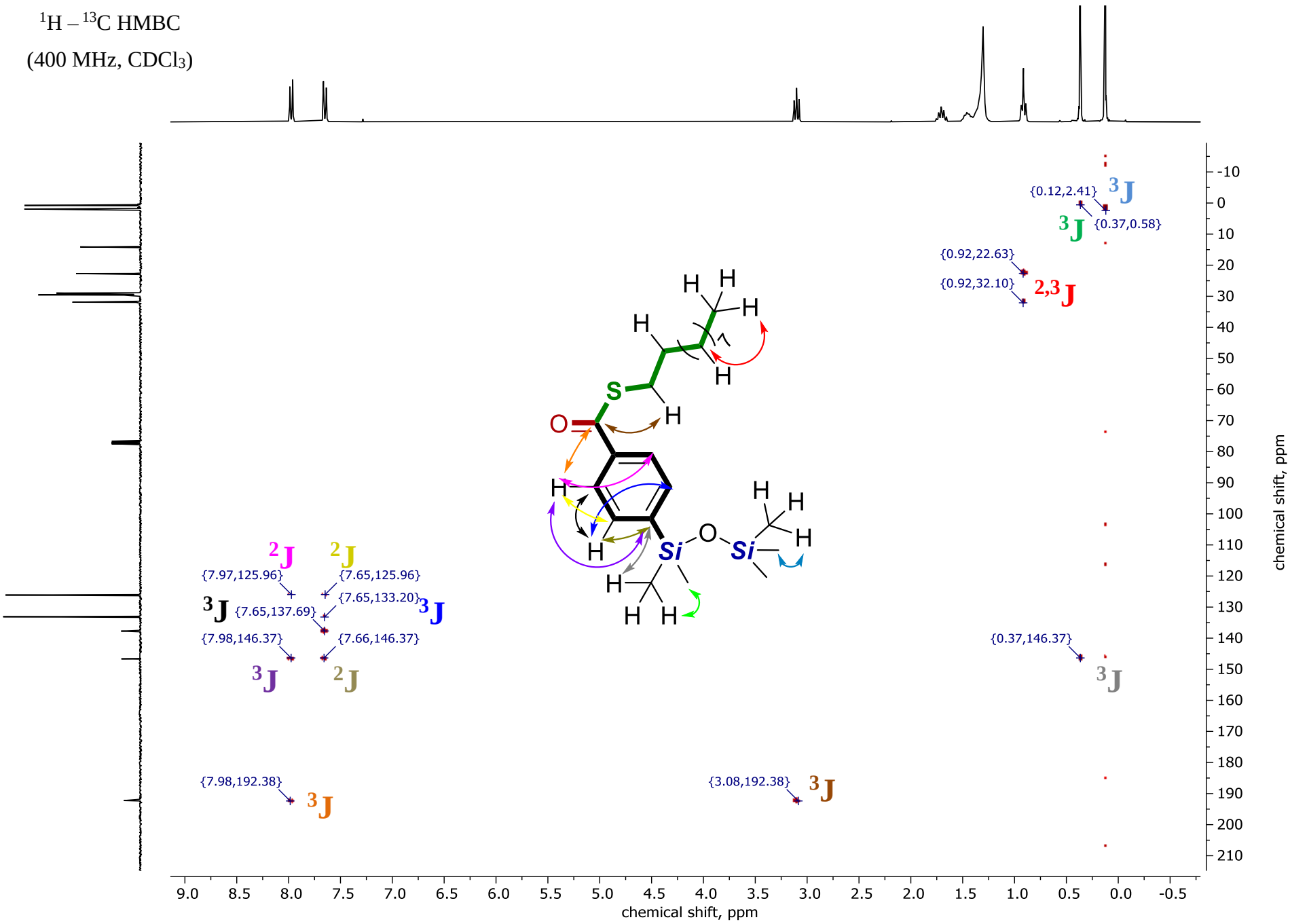
(80 MHz, $CDCl_3$)

S152



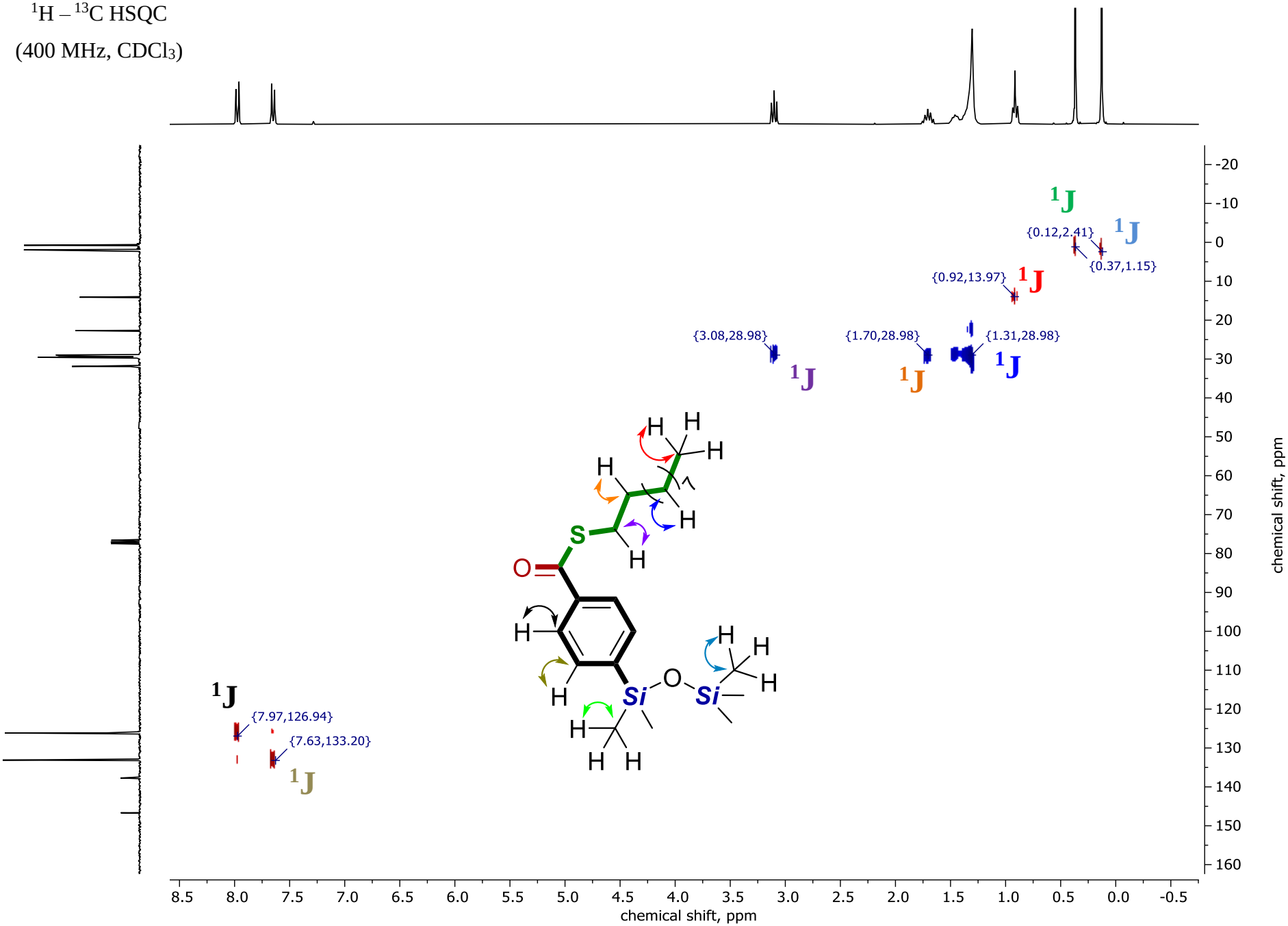
$^{1}H - {}^{13}C$ HMBC

(400 MHz, $CDCl_3$)



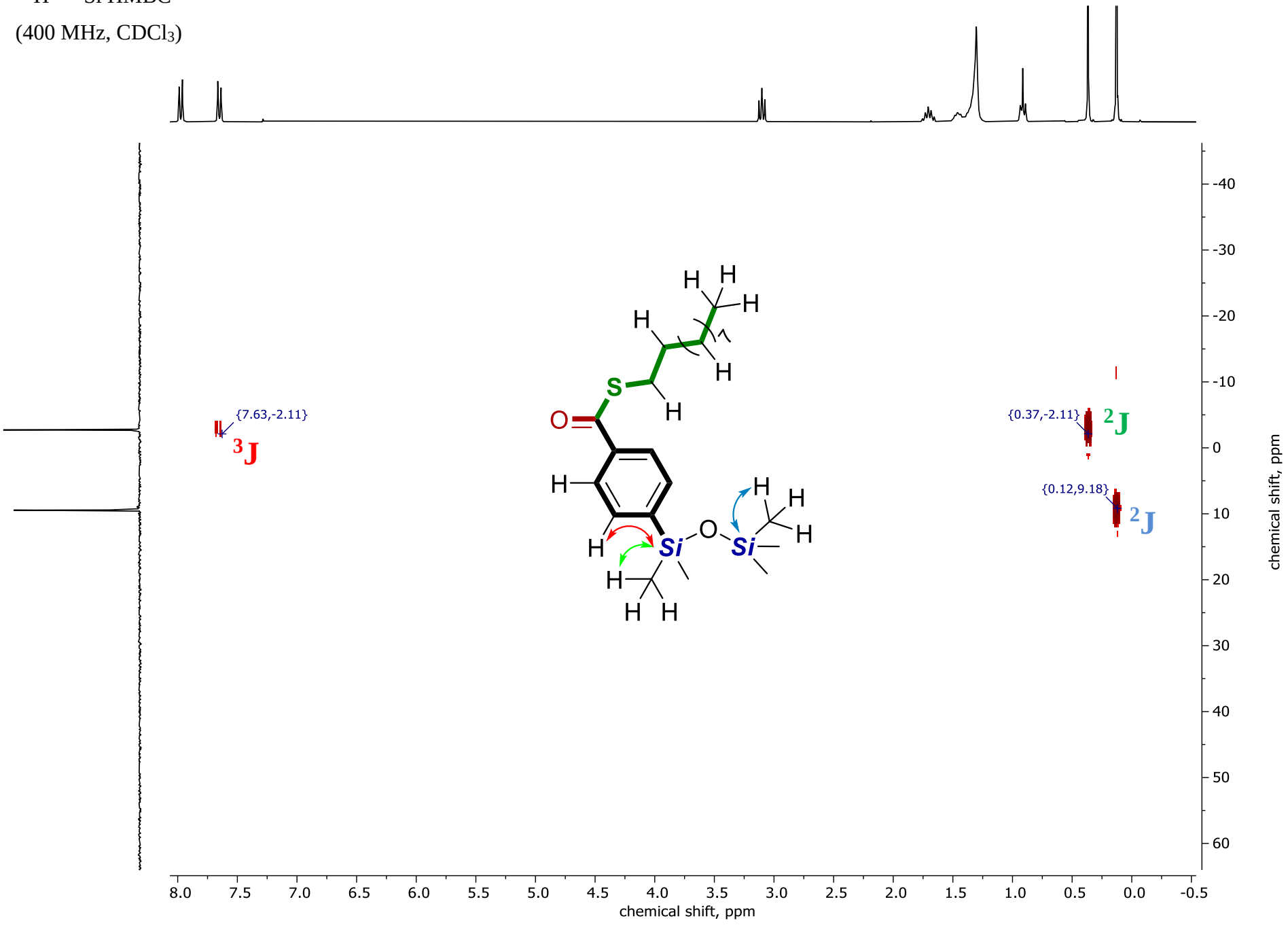
$^{1}H - ^{13}C$ HSQC

(400 MHz, $CDCl_3$)

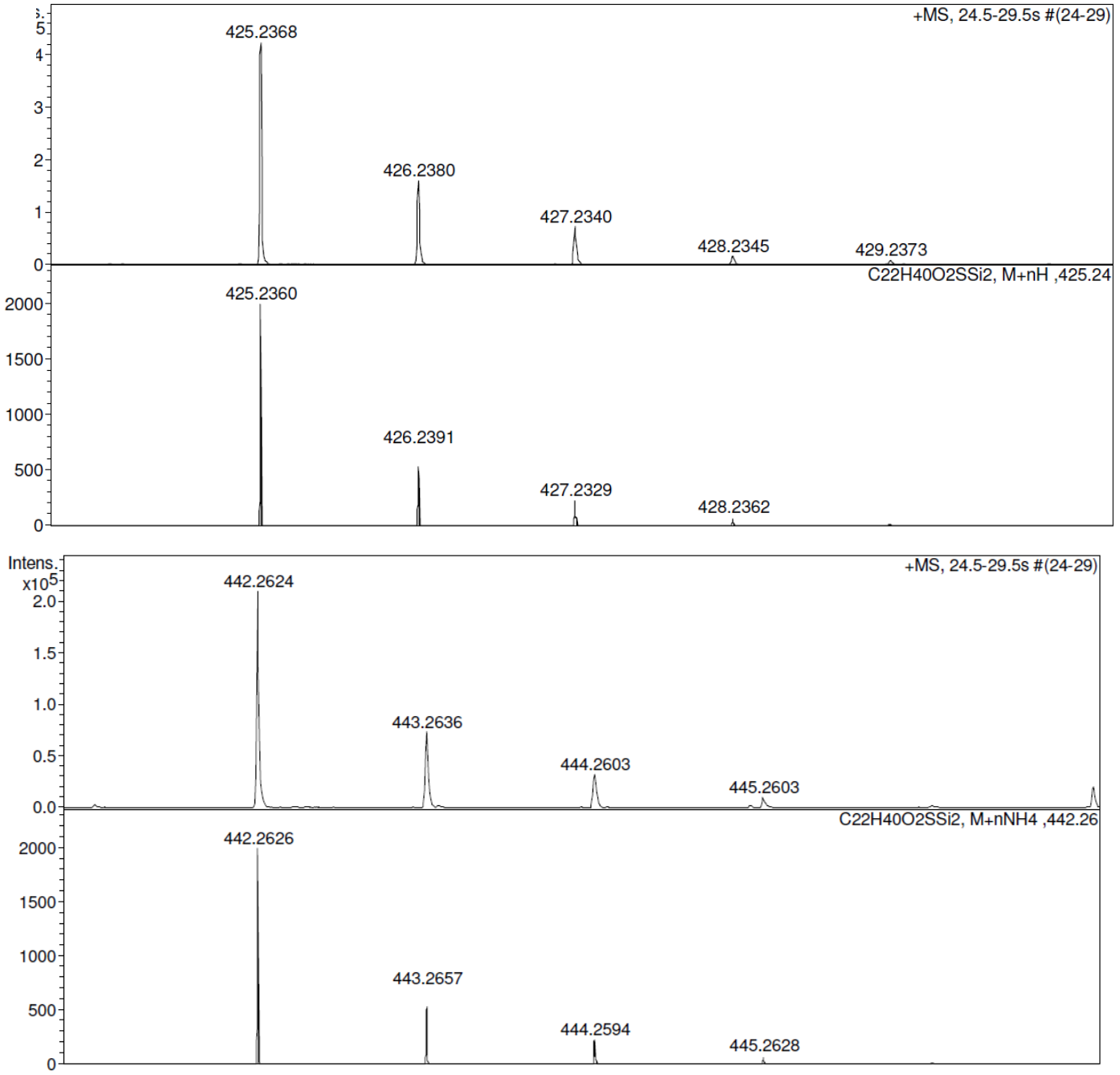


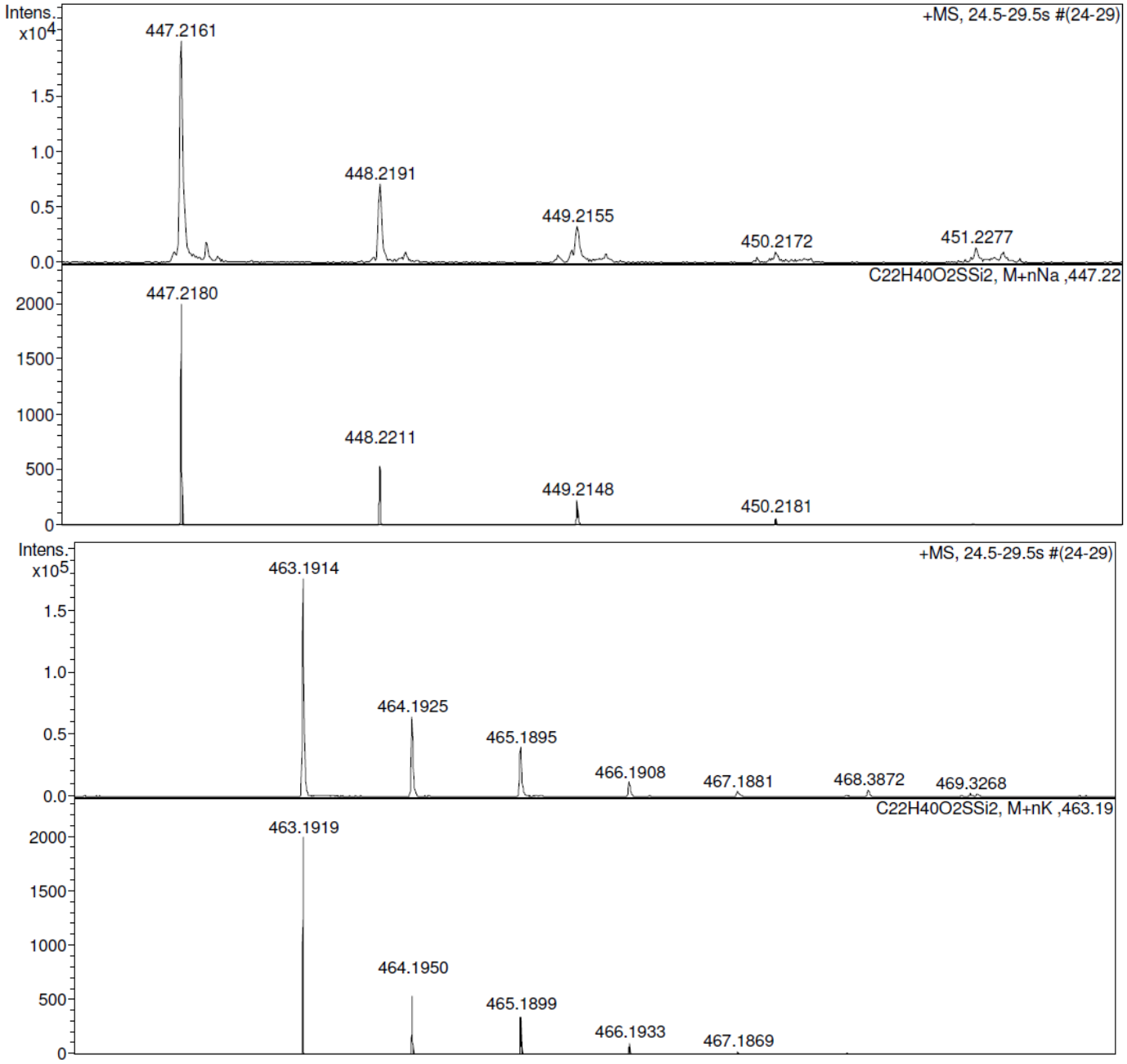
$^{1}H - ^{29}Si$ HMBC

(400 MHz, $CDCl_3$)

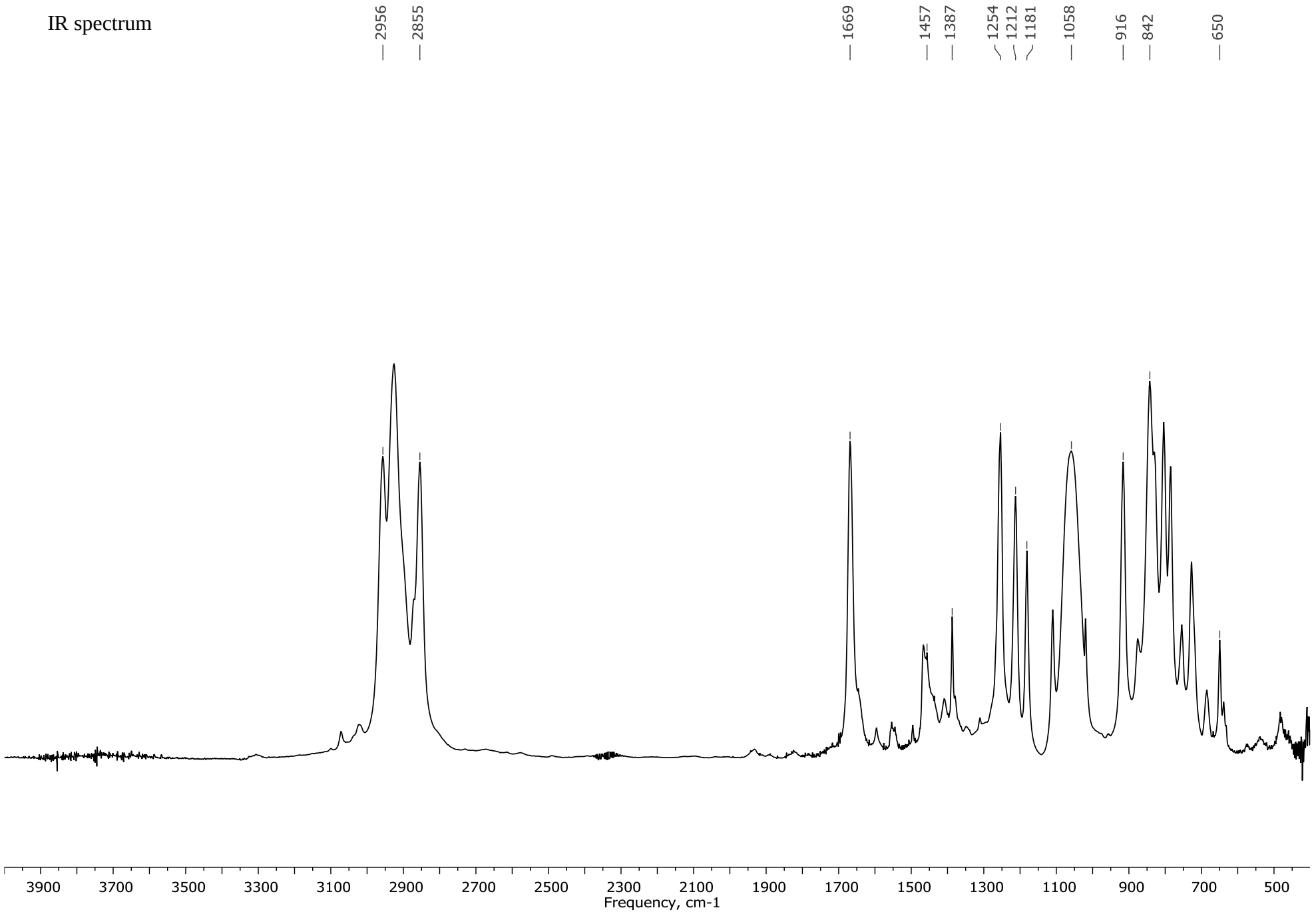


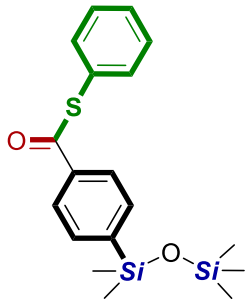
HRMS (ESI)


+MS, 24.5-29.5s #(24-29)
425.2368
426.2380
427.2340
428.2345
429.2373
C22H40O2SSi2, M+nH ,425.24
425.2360
426.2391
427.2329
428.2362
Intens.
x10^5
+MS, 24.5-29.5s #(24-29)
442.2624
443.2636
444.2603
445.2603
C22H40O2SSi2, M+nNH4 ,442.26
442.2626
443.2657
444.2594
445.2628


Intens.
x10^4
+MS, 24.5-29.5s #(24-29)
447.2161
448.2191
449.2155
450.2172
451.2277
C22H40O2SSi2, M+nNa ,447.22
447.2180
448.2211
449.2148
450.2181
Intens.
x10^5
+MS, 24.5-29.5s #(24-29)
463.1914
464.1925
465.1895
466.1908
467.1881
468.3872
469.3268
C22H40O2SSi2, M+nK ,463.19
463.1919
464.1950
465.1899
466.1933
467.1869

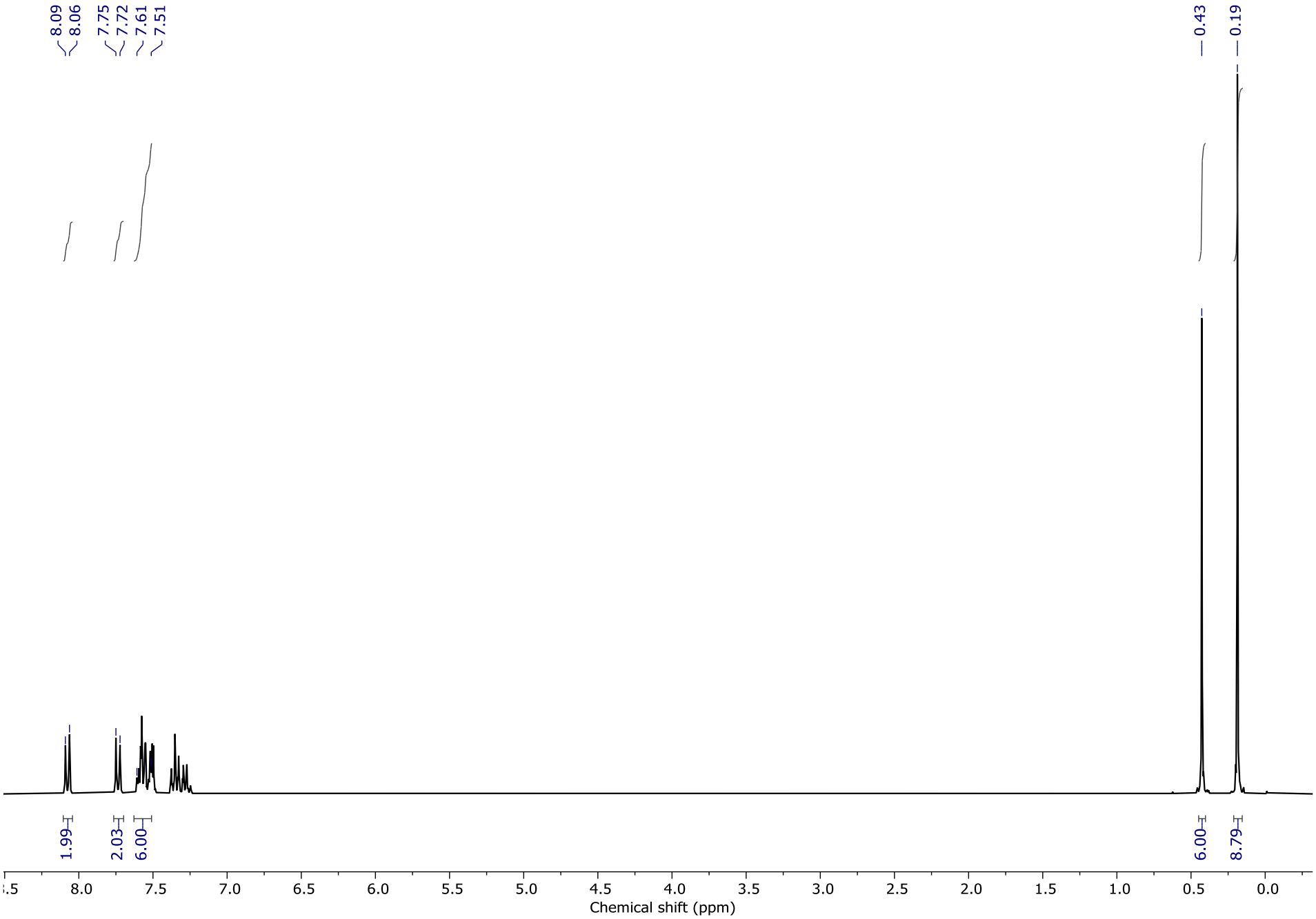
IR spectrum

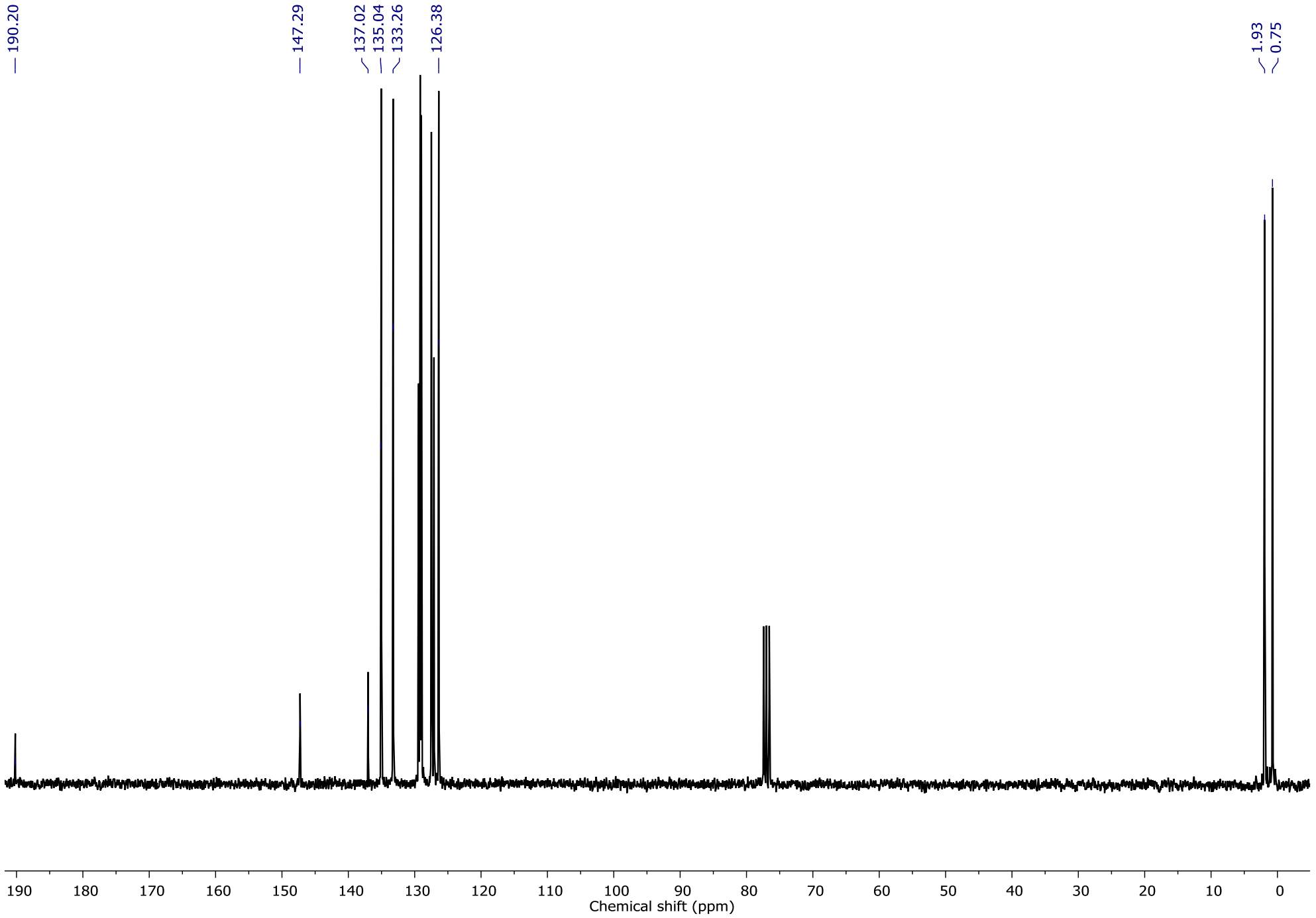

2956
2855
1669
1457
1387
1254
1212
1181
1058
916
842
650
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

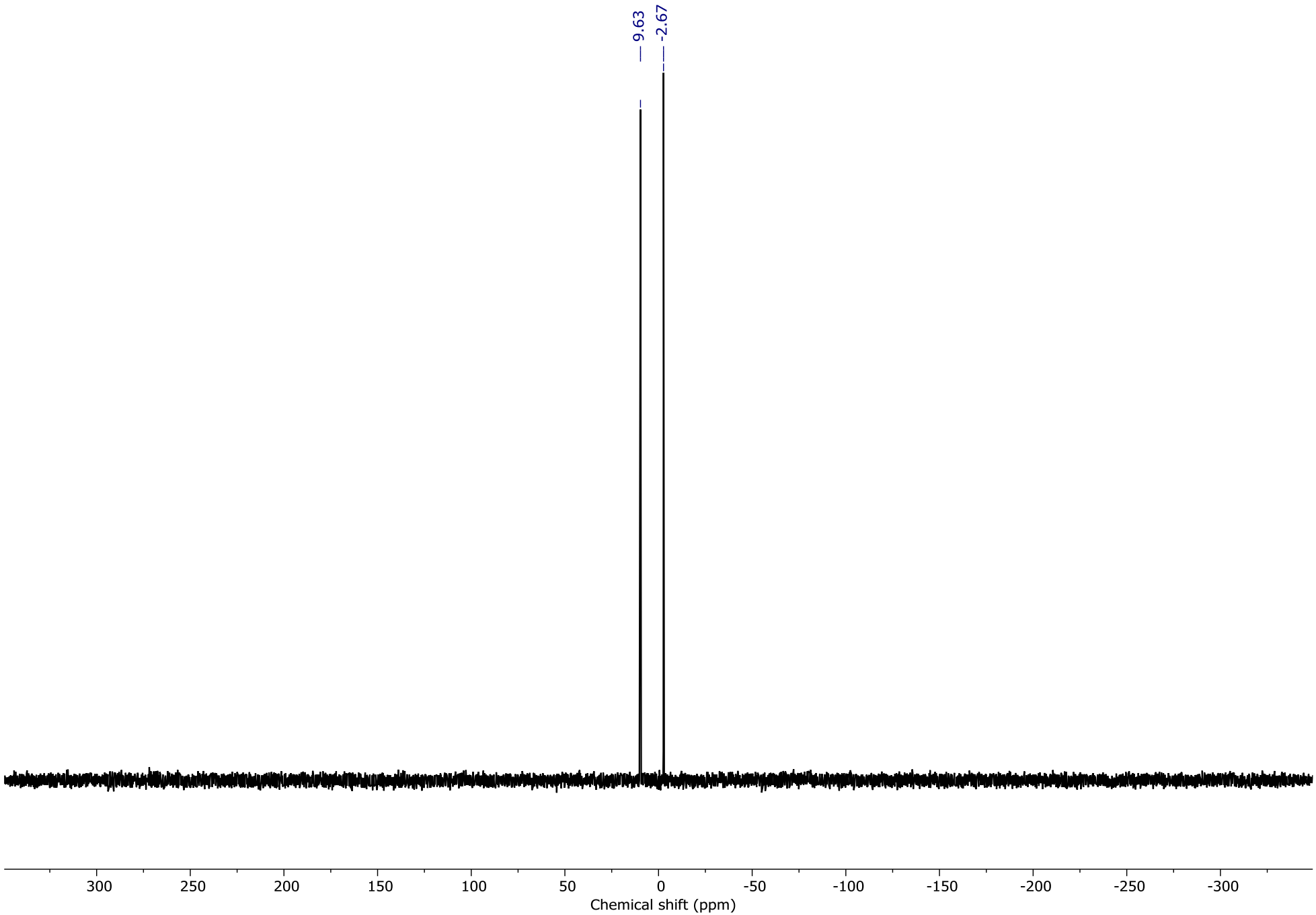


Characterisation data for S-phenyl 4-(1,1,3,3,3-pentamethyldisiloxanyl)benzothioate:

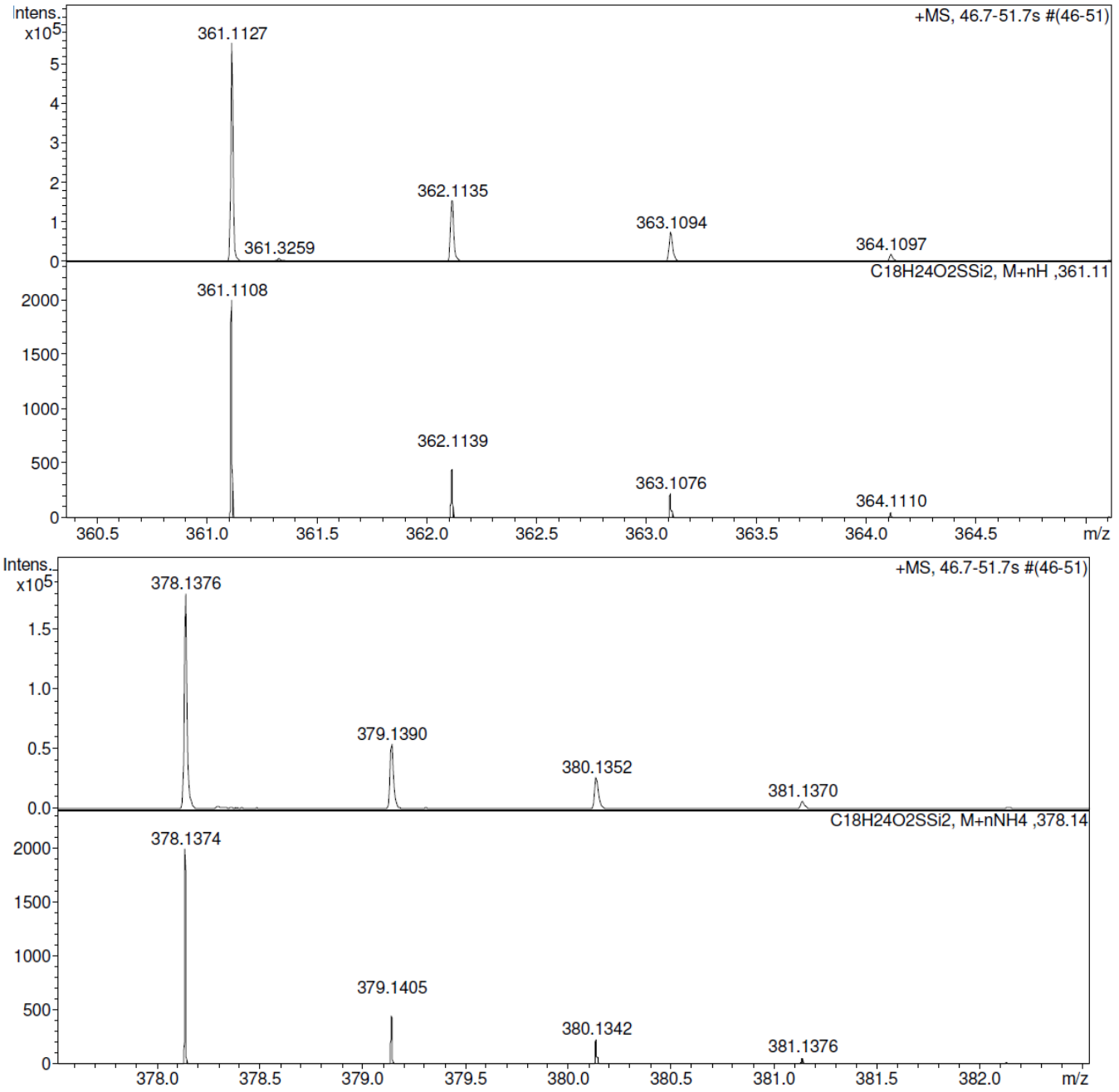
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.08 (d, ^{3}J=11 Hz, 2H), δ = 7.74 (d, ^{3}J=11 Hz, 2H), δ = 7.61-7.51 (m, 6H), δ = 0.43 (s, 6H), δ = 0.19 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 190.20, 147.29, 137.02, 135.04, 133.26, 126.38, 1.93, 0.75. ^{29}Si NMR (80 MHz, $CDCl_3$): δ = 9.63, -2.67. HRMS (ESI) m/z $[M + H]^+$: calcd for $[C_{18}H_{24}O_2SSi_2 + H]^+$, 361.1108; found, 361.1127; $[M + NH_4]^+$: calcd for $[C_{18}H_{24}O_2SSi_2 + NH_4]^+$, 378.1374; found, 378.1376 ; $[M + Na]^+$: calcd for $[C_{18}H_{24}O_2SSi_2 + Na]^+$, 383.0928; found, 383.0924; $[M + K]^+$: calcd for $[C_{18}H_{24}O_2SSi_2 + K]^+$, 399.0667; found, 399.0666. IR (cm^{-1}): 3063, 2899, 1685, 1579, 1479, 1441, 1387, 1254, 1209, 1182, 1052, 903, 842-646.

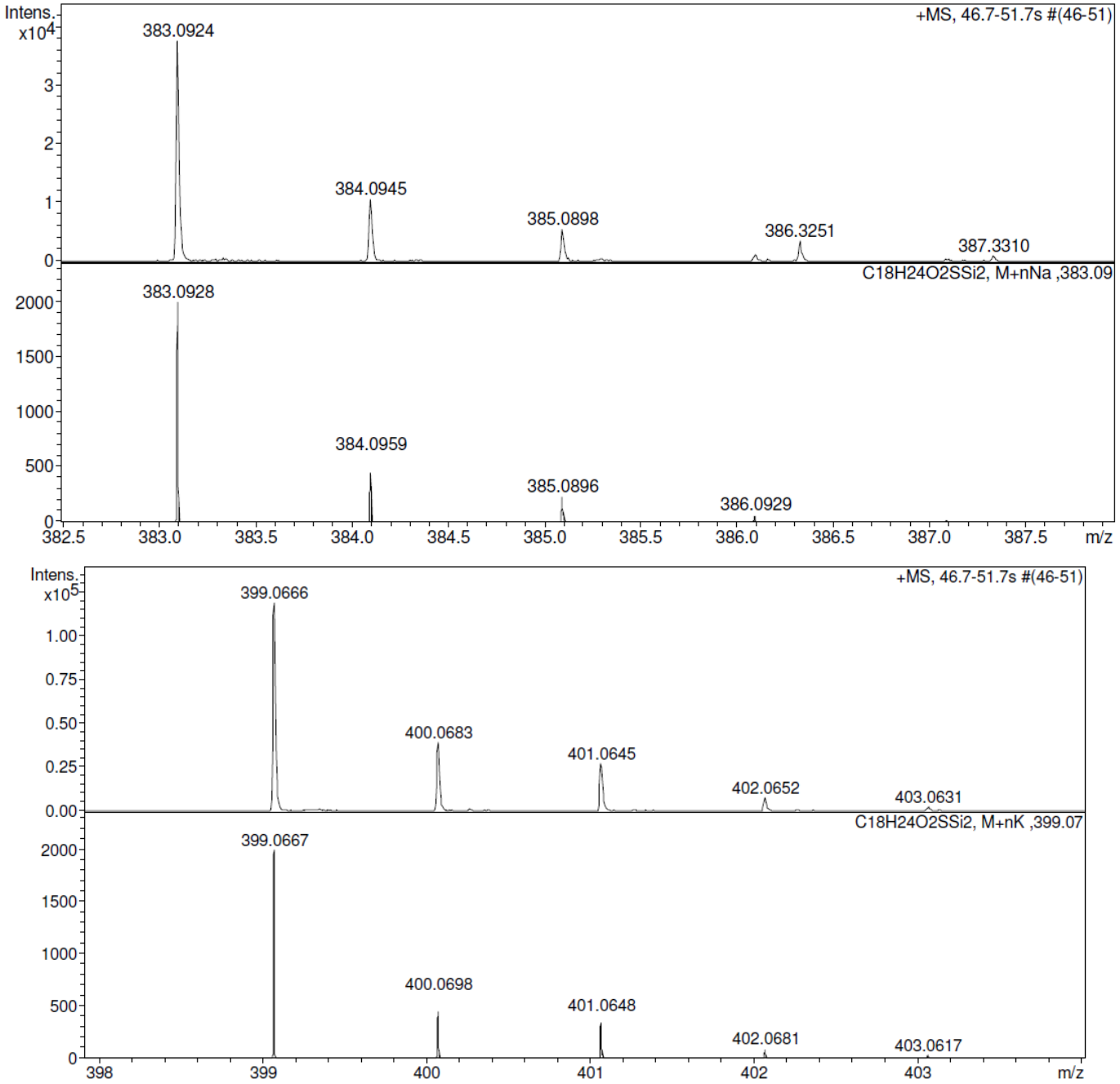

8.09
8.06
7.75
7.72
7.61
7.51
0.43
0.19
1.99
2.03
6.00
6.00
8.79
Chemical shift (ppm)


190.20
147.29
137.02
135.04
133.26
126.38
1.93
0.75
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical shift (ppm)

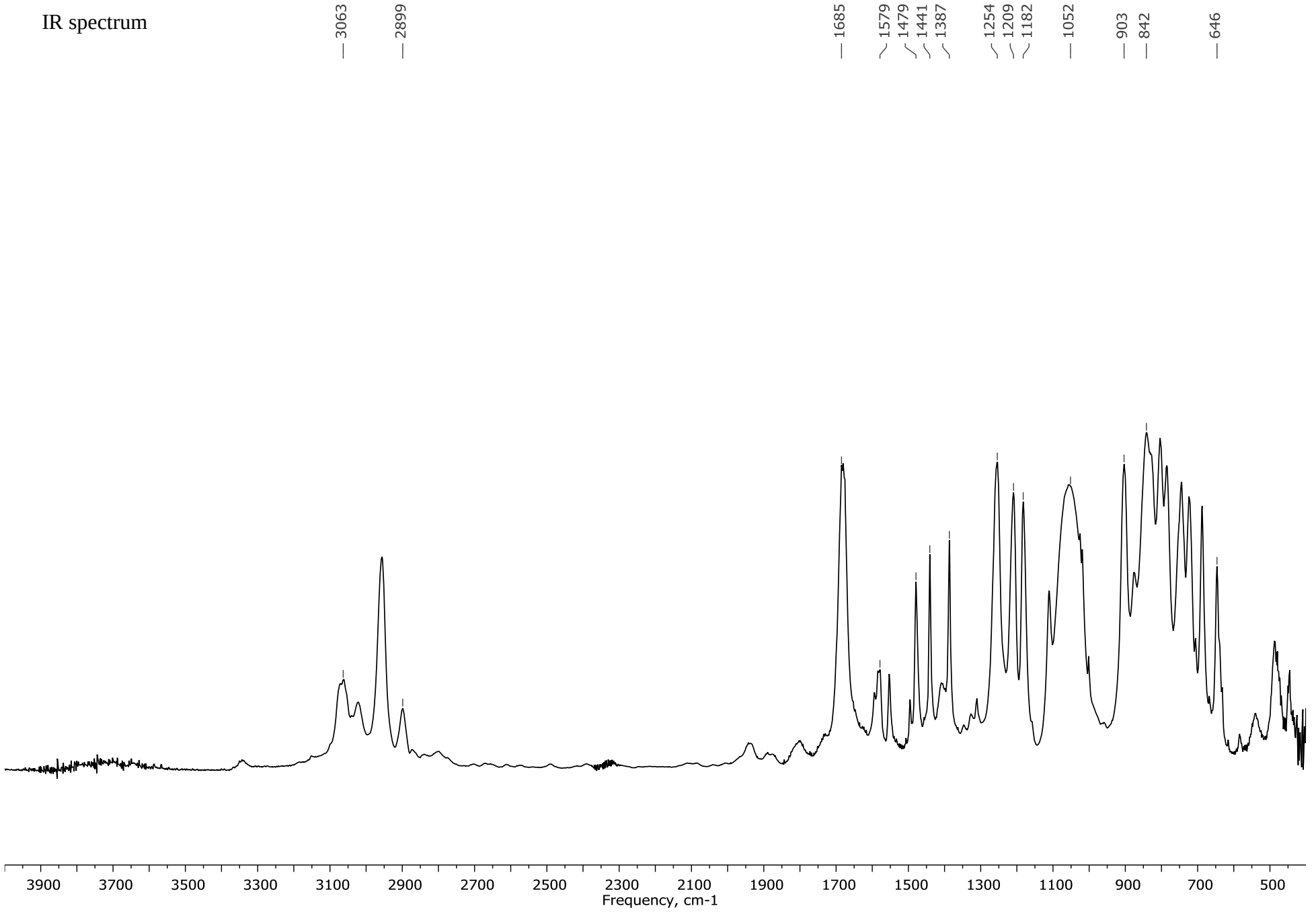

9.63
-2.67
300
250
200
150
100
50
0
-50
-100
-150
-200
-250
-300
Chemical shift (ppm)

HRMS (ESI)


Intens.
x10^5
+MS, 46.7-51.7s #(46-51)
361.1127
362.1135
363.1094
361.3259
364.1097
C18H24O2SSi2, M+nH ,361.11
361.1108
362.1139
363.1076
364.1110
m/z
Intens.
x10^5
+MS, 46.7-51.7s #(46-51)
378.1376
379.1390
380.1352
381.1370
C18H24O2SSi2, M+nNH4 ,378.14
378.1374
379.1405
380.1342
381.1376
m/z


Intens.
x10^4
+MS, 46.7-51.7s #(46-51)
383.0924
384.0945
385.0898
386.3251
387.3310
C18H24O2SSi2, M+nNa ,383.09
383.0928
384.0959
385.0896
386.0929
m/z
Intens.
x10^5
+MS, 46.7-51.7s #(46-51)
399.0666
400.0683
401.0645
402.0652
403.0631
C18H24O2SSi2, M+nK ,399.07
399.0667
400.0698
401.0648
402.0681
403.0617
m/z

IR spectrum


3063
2899
1685
1579
1479
1441
1387
1254
1209
1182
1052
903
842
646
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1