Electronic Supplementary Material (ESI) for New Journal of Chemistry.

SUPPORTING INFORMATION

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

Supp.Inf.3: NMR, ESI HRMS and IR spectra for 3ba-bm

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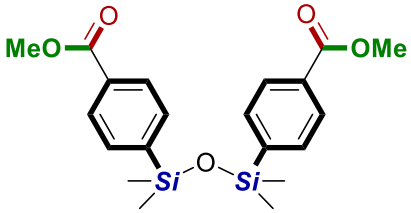
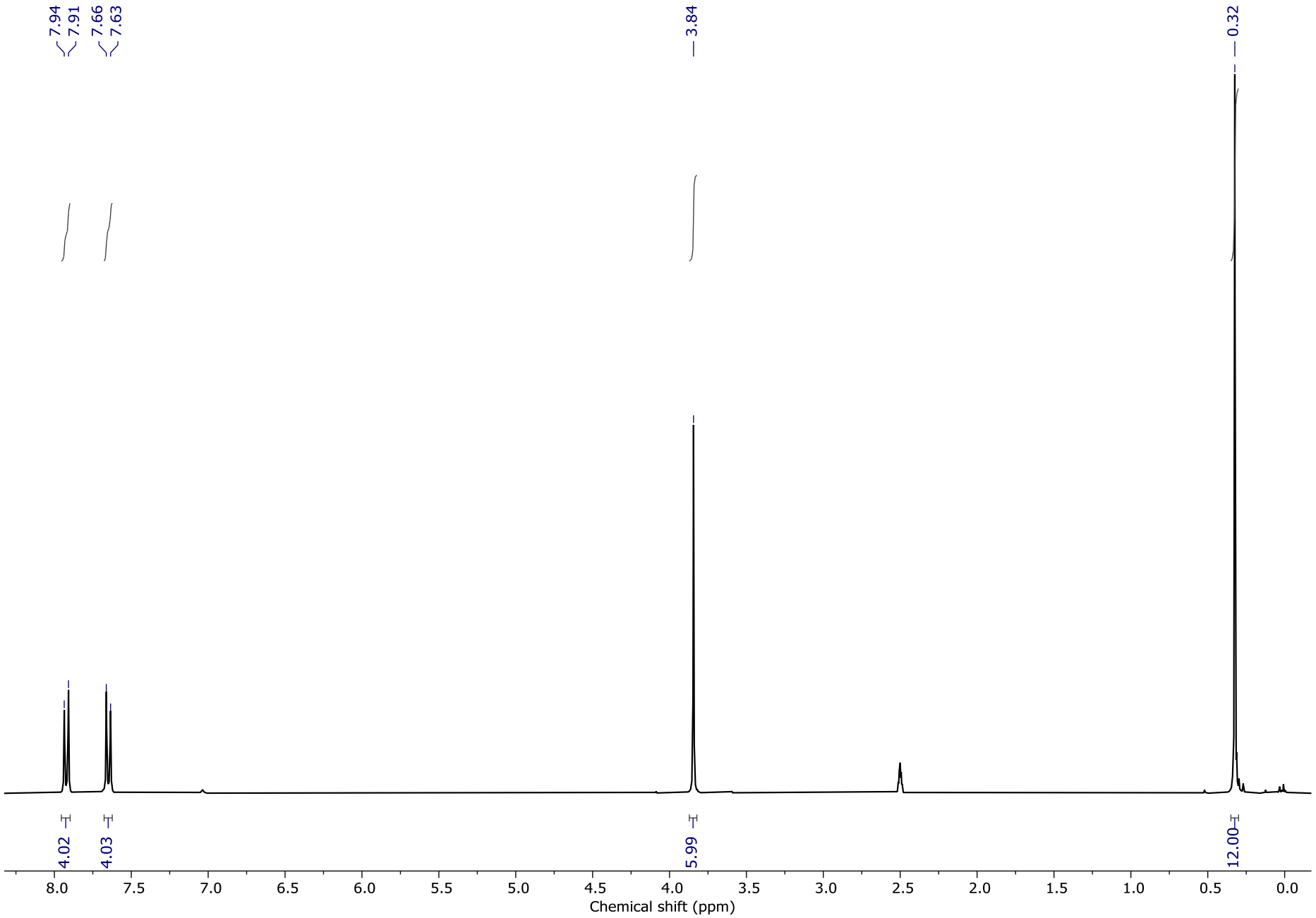


Characterisation data for dimethyl 4,4'-(1,1,3,3-tetramethyldisiloxane-1,3-diyl)dibenzoate:

^{1}H NMR (400 MHz, DMSO-d6): δ = 7.93 (d, ^{3}J=11 Hz, 4H), δ = 7.65 (d, ^{3}J=11 Hz, 4H), δ = 3.84 (s, 6H), δ = 0.32 (s, 12H). ^{13}C NMR (100 MHz, DMSO-d6): δ = 166.17, 145.04, 133.03, 130.38, 128.14, 52.03, 0.42. ^{29}Si NMR (80 MHz, DMSO-d6): δ = -0.30. HRMS (ESI) m/z [M + NH_4] $^{+}$: calcd for [$C_{20}H_{26}O_5Si_2$ + NH_4]$^{+}$, 420.1657; found, 420.1656; [M + Na] $^{+}$: calcd for [$C_20H_{26}O_5Si_2$ + Na]$^{+}$, 425.1211; found, 425.1214; [M + K] $^{+}$: calcd for [$C_20H_{26}O_5Si_2$ + K]$^{+}$, 441.0950; found, 441.0948. IR (cm-1): 3424, 2955, 1723, 1282, 1098.

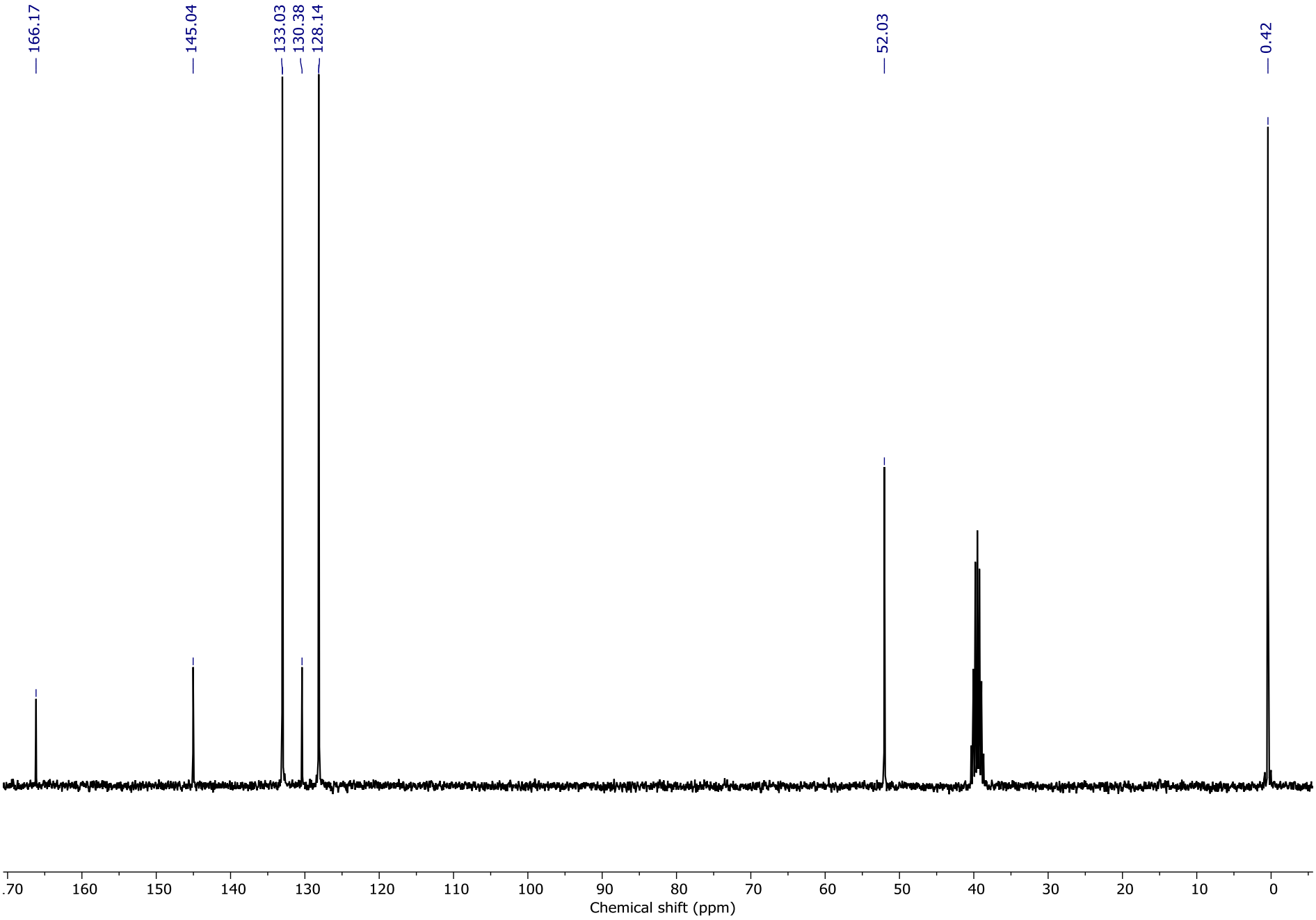
^{1}H NMR

(400 MHz, DMSO-d6)



^{13}C NMR

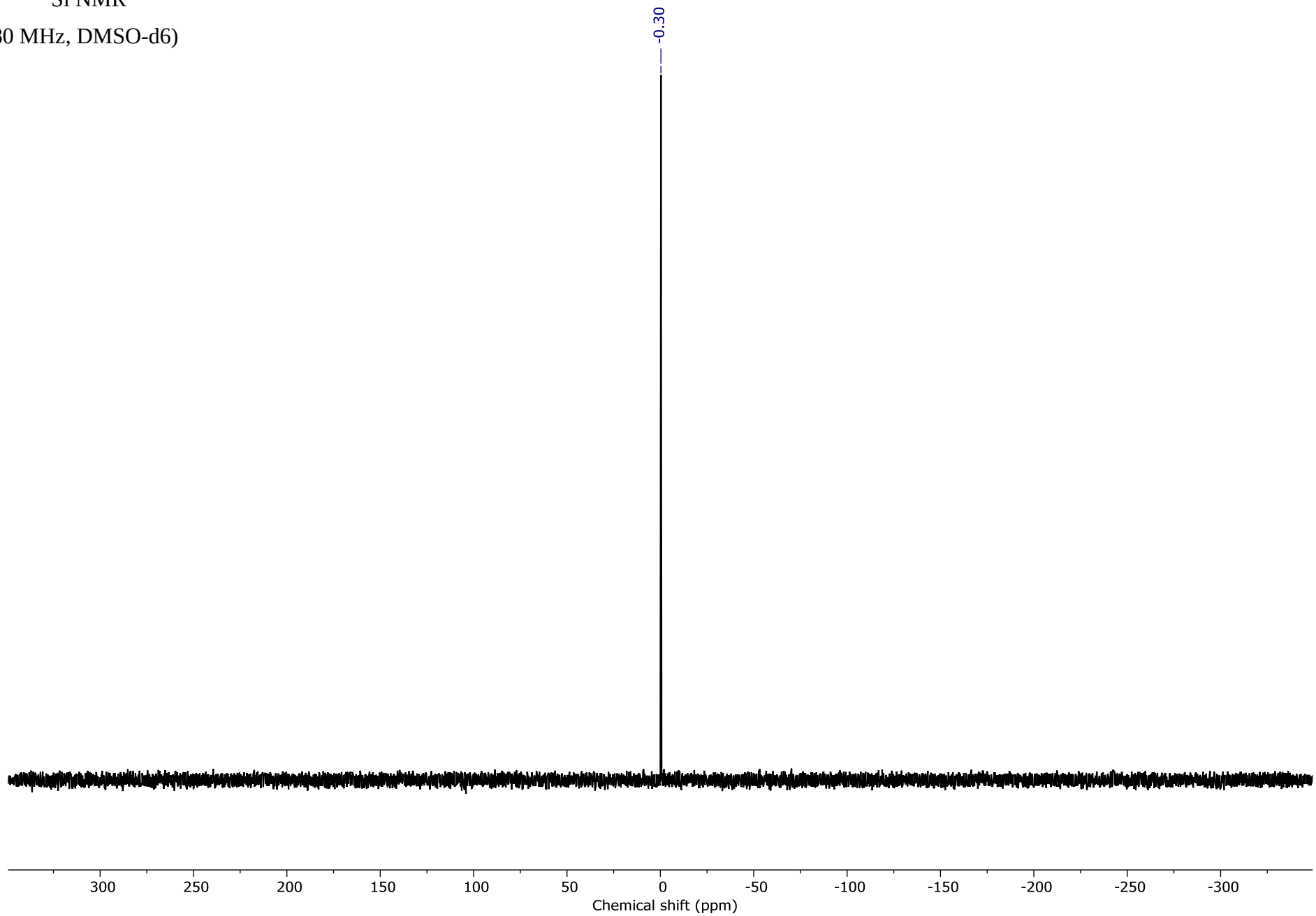
(100 MHz, DMSO-d6)



^{29}Si NMR

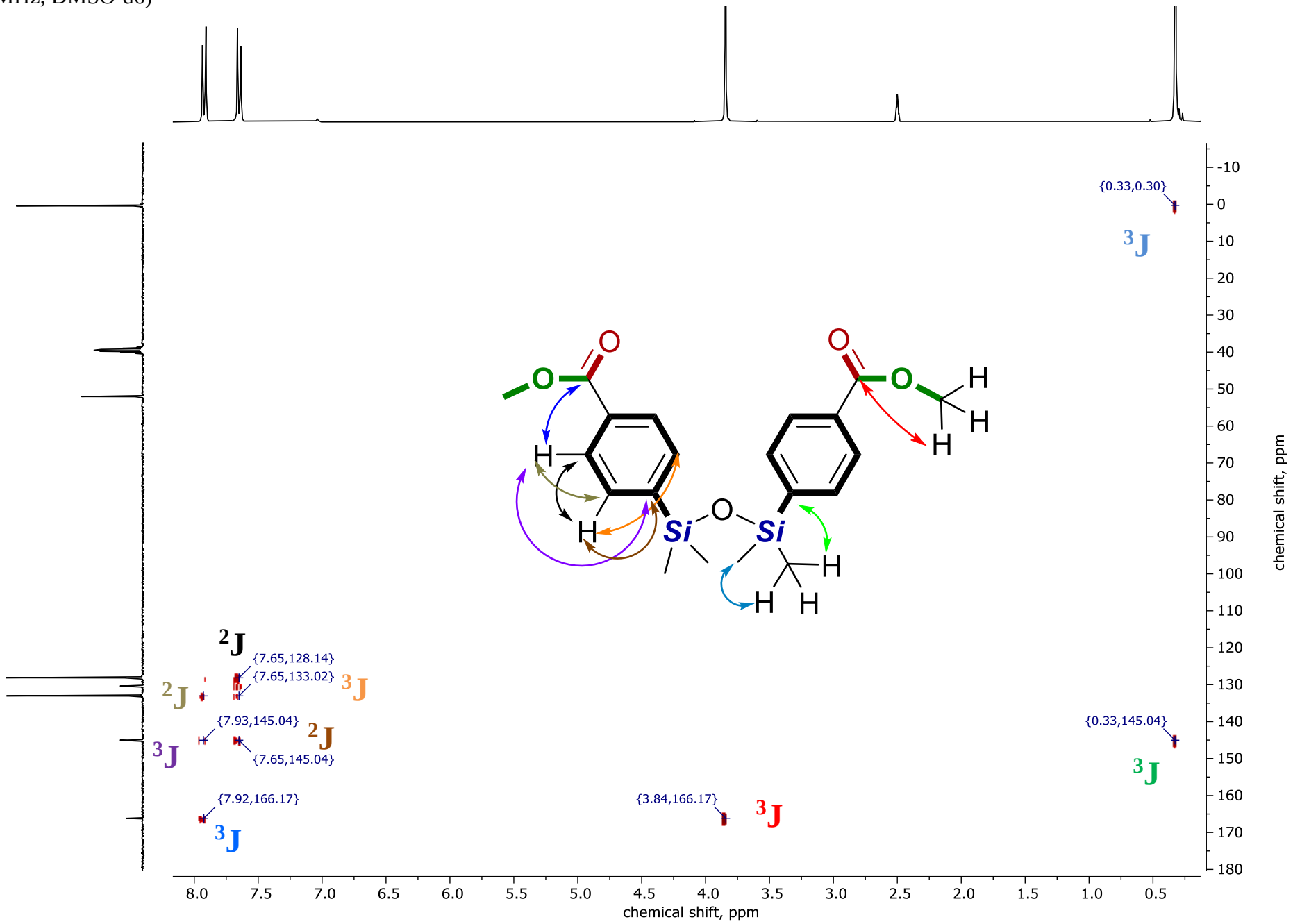
(80 MHz, DMSO-d6)

S5



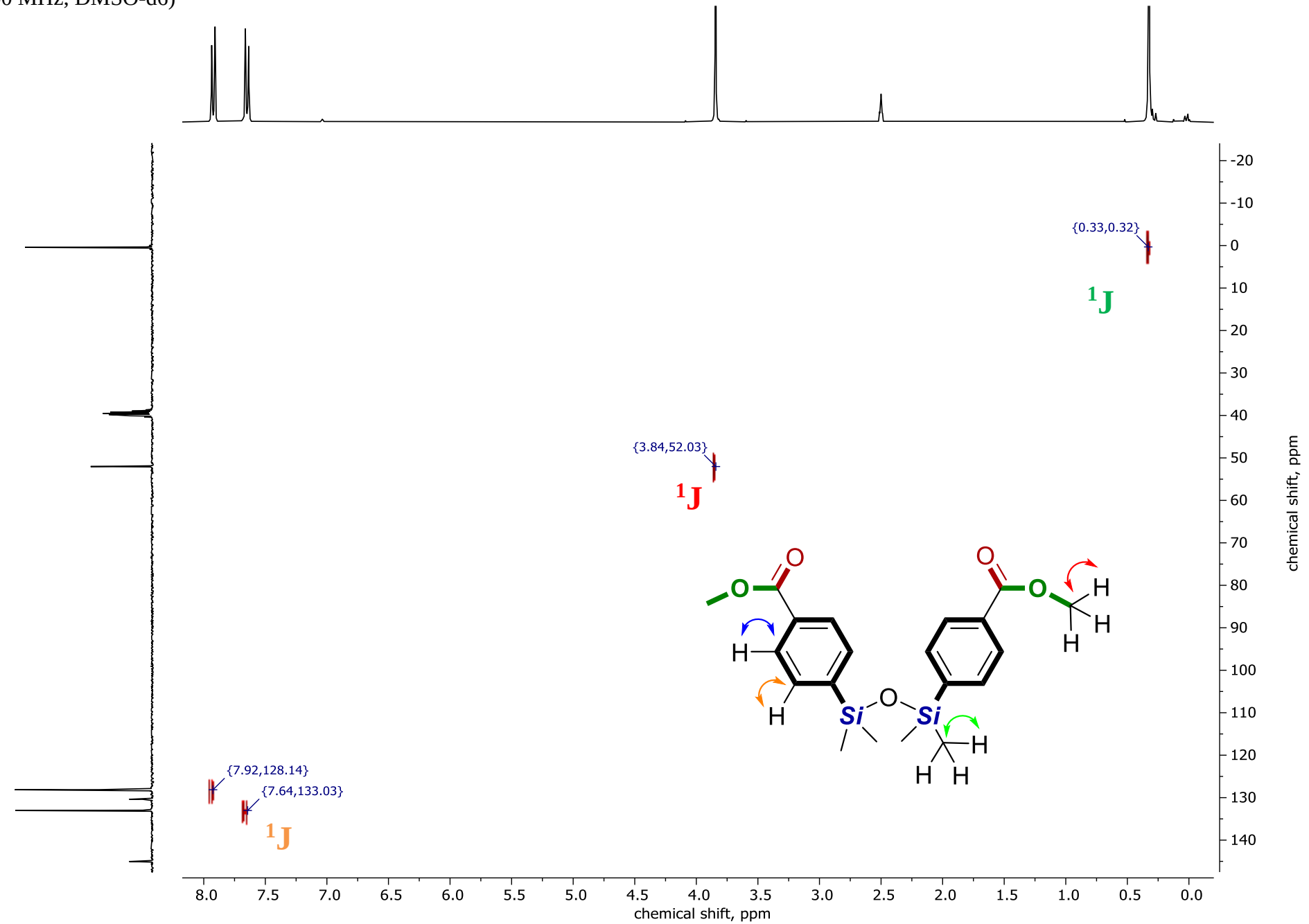
$^{1}H - ^{13}C$ HMBC

(400 MHz, DMSO-d6)



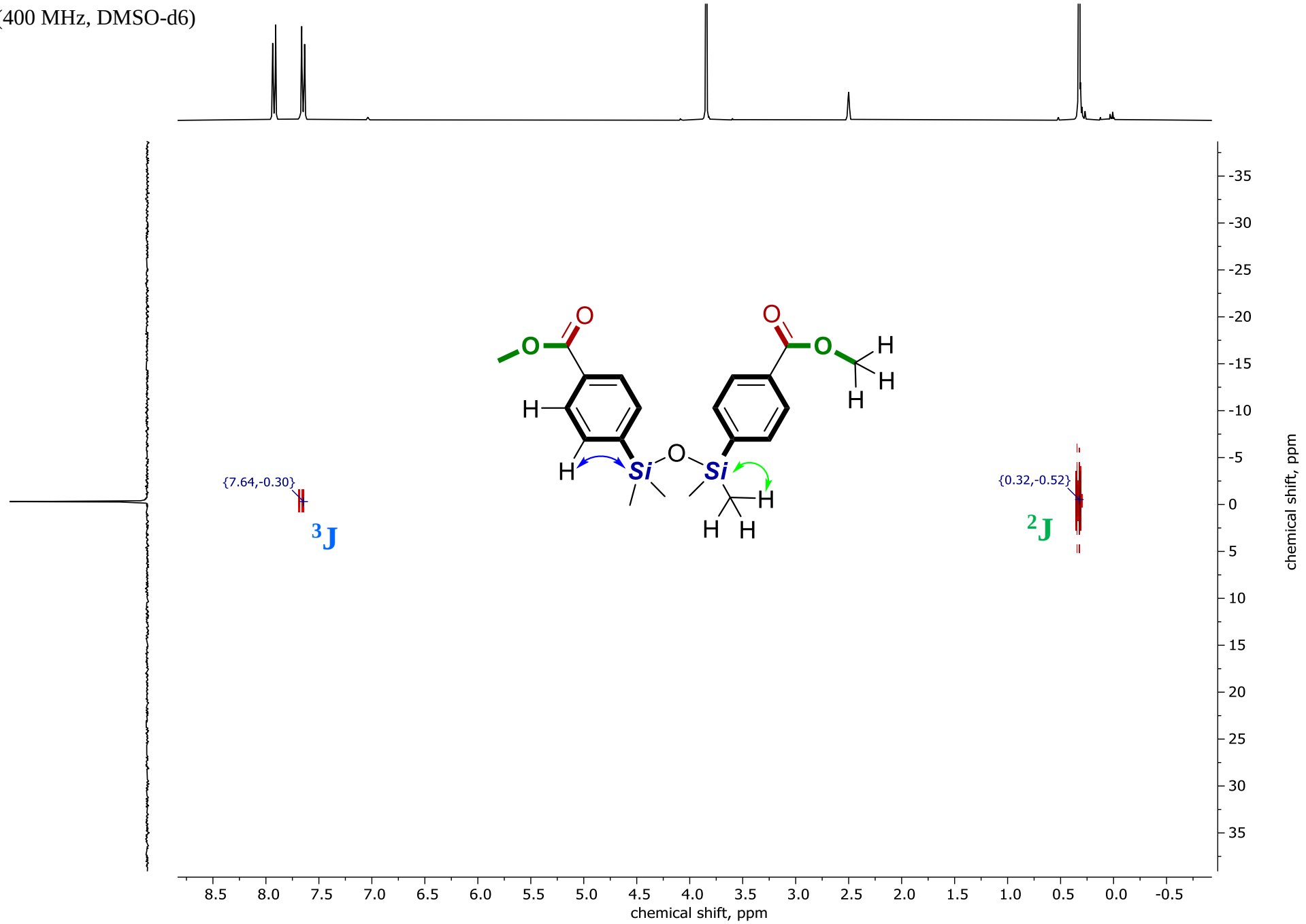
$^{1}H - ^{13}C$ HSQC

(400 MHz, DMSO-d6)

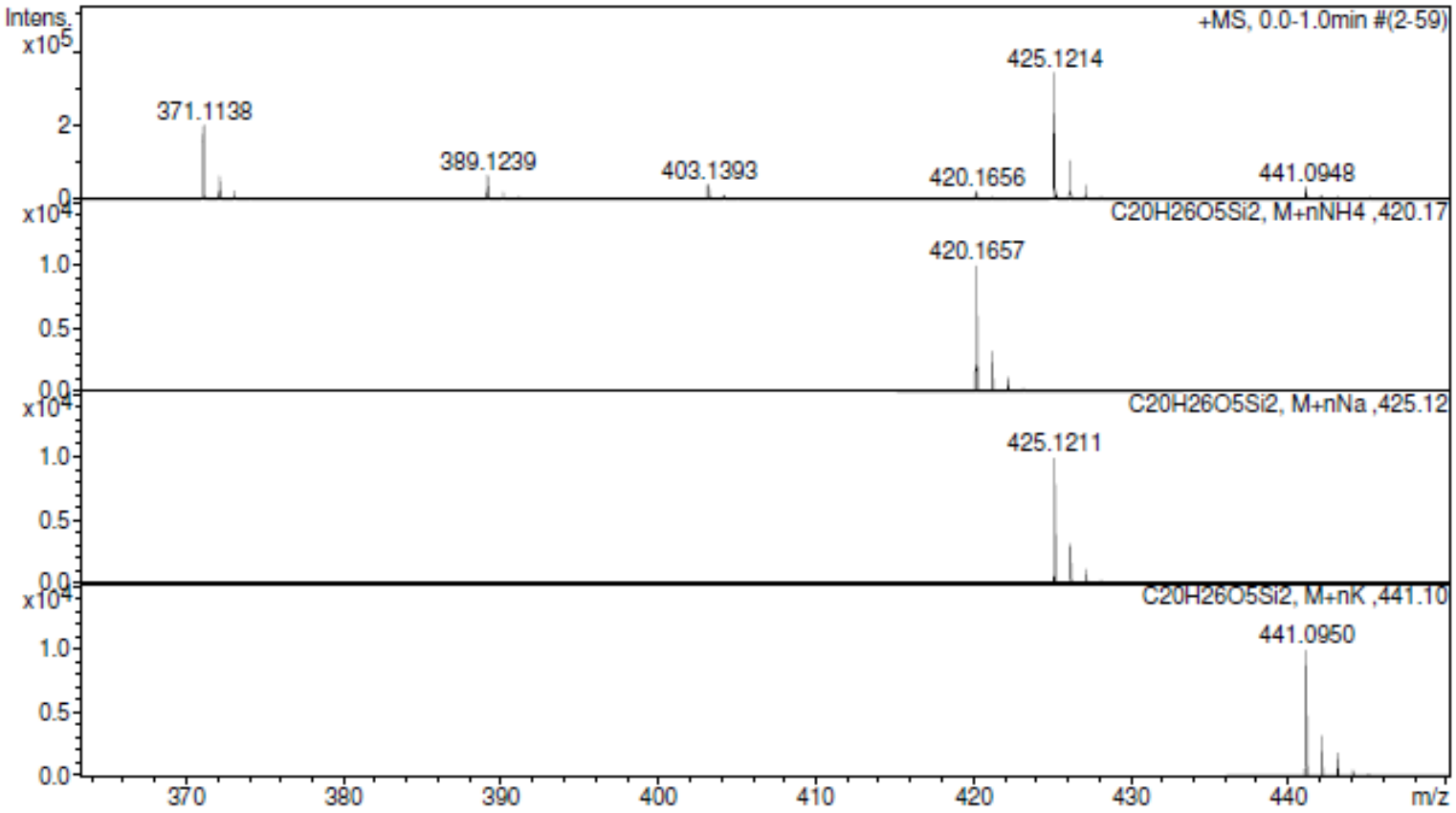


$^{1}H - {}^{29}Si$ HMBC

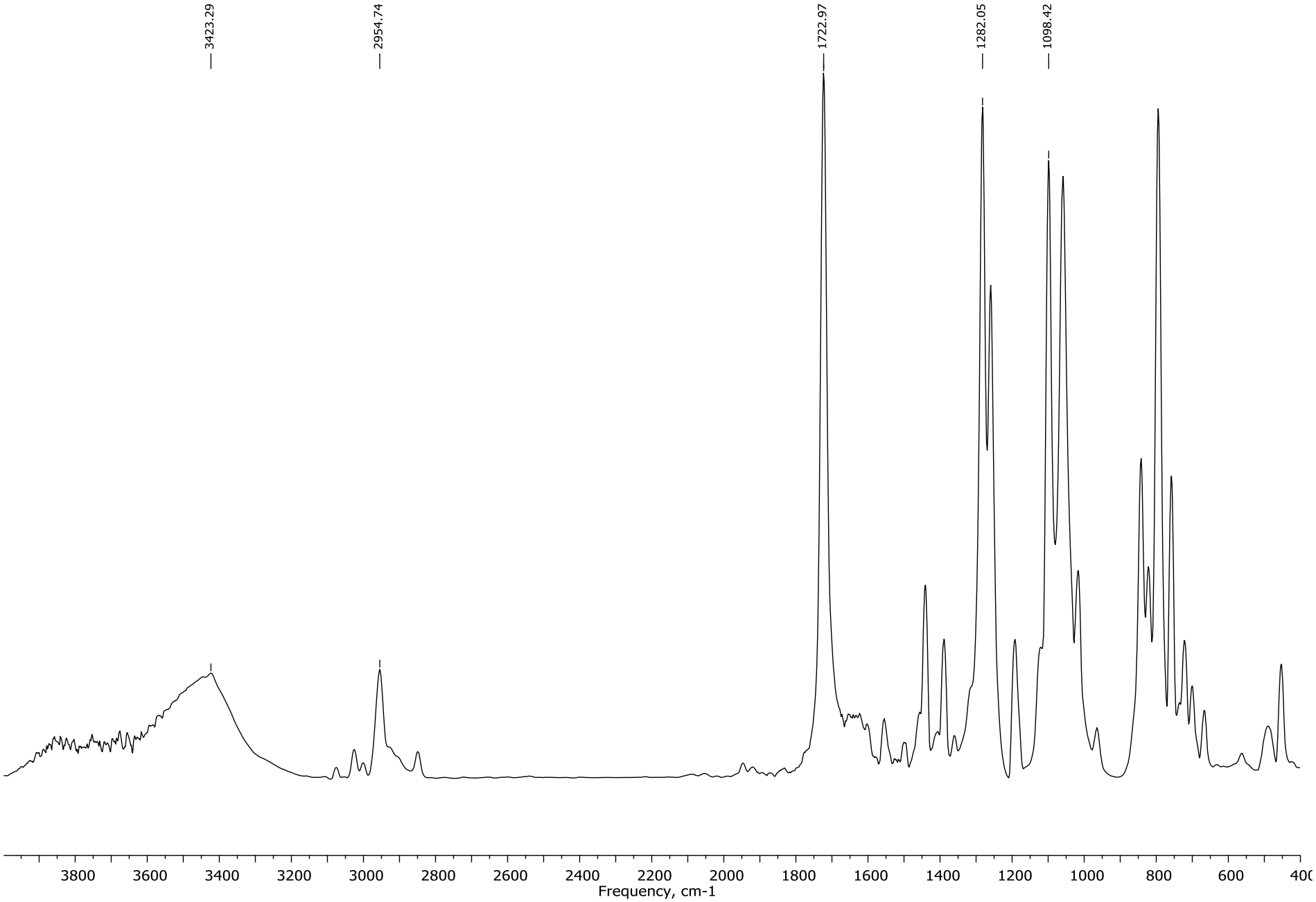
(400 MHz, DMSO-d6)

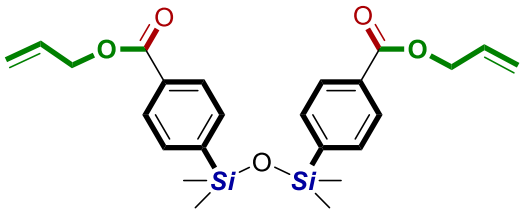


HRMS (ESI)


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

IR Spectrum


3423.29
2954.74
1722.97
1282.05
1098.42
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
Frequency, cm-1

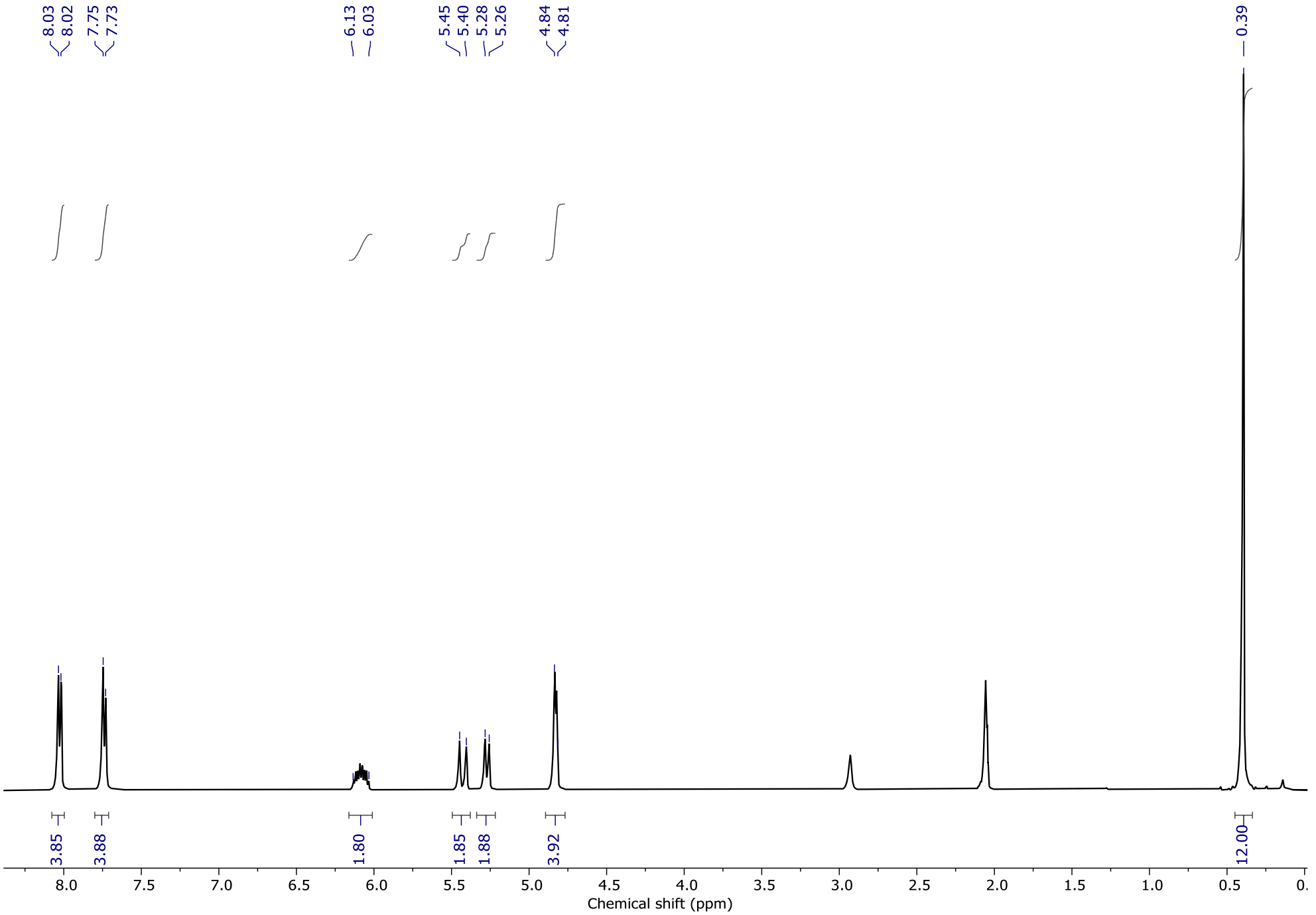


Characterisation data for diallyl 4,4'-(1,1,3,3-tetramethyldisiloxane-1,3-diyl)dibenzoate:

^{1}H NMR (400 MHz, acetone-d6): δ = 8.03 (d, ^{3}J=6 Hz, 4H), δ = 7.74 (d, ^{3}J=6 Hz, 4H), δ = 6.13-6.03 (m, 2H), δ = 5.45-5.26 (m, 4H), δ = 4.83 (m, 4H), δ = 0.39 (s, 12H). ^{13}C NMR (100 MHz, acetone-d6): δ = 166.39, 146.37, 134.02, 133.56, 131.81, 129.25, 118.13, 65.96, 0.77. ^{29}Si NMR (80 MHz, acetone-d6): δ = -0.31. HRMS (ESI) m/z [M + H] $^{+}$: calcd for [$C_{24}H_{30}O_5Si_2$ + H] $^{+}$, 455.1705; found, 455.1710. IR (cm^{-1}): 3429, 3080-2900, 1942, 1717, 1649, 1601, 1557, 1498, 1455-1361, 1313-1260, 1186, 1128-663.

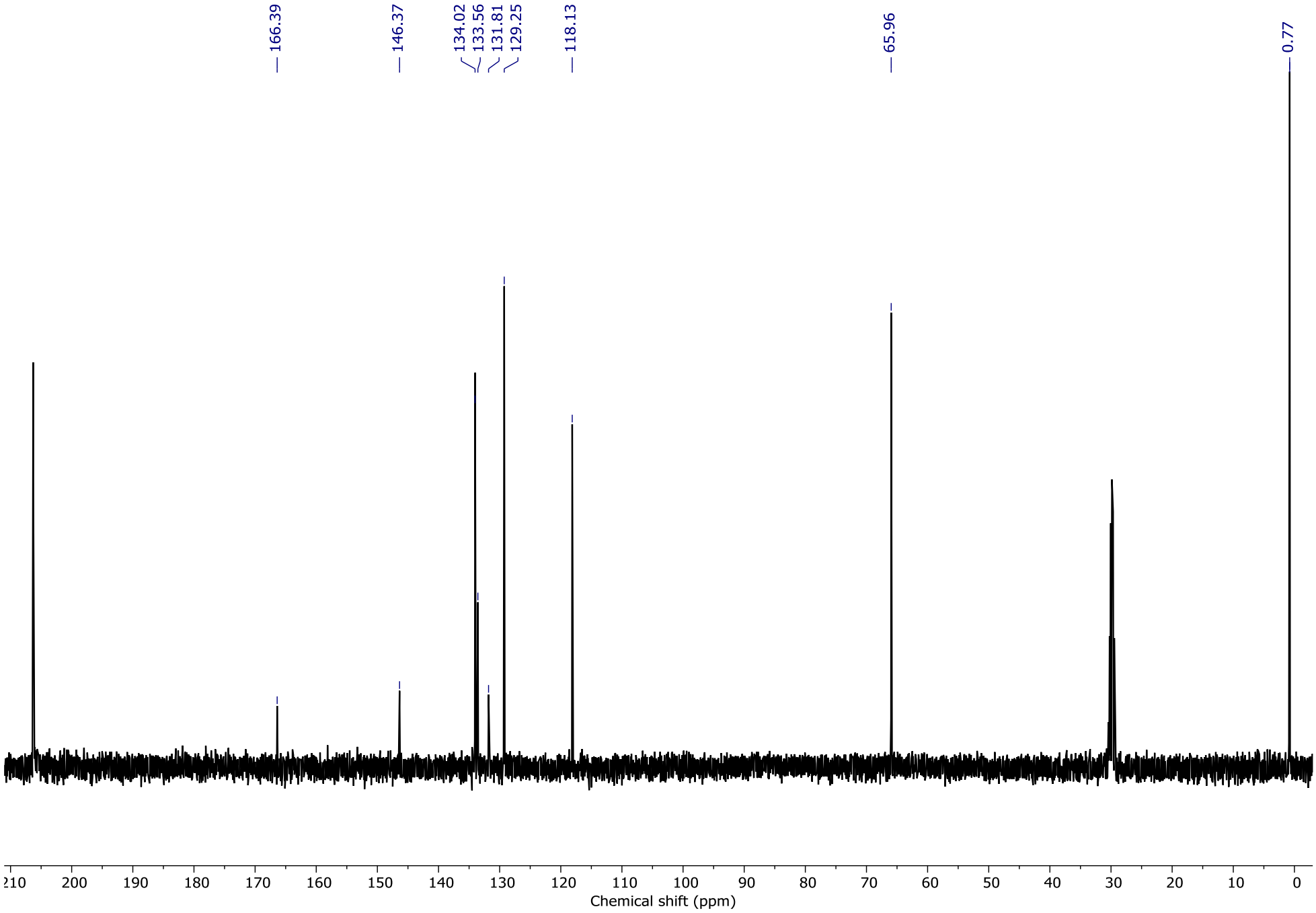
^{1}H NMR

(400 MHz, acetone-d6)



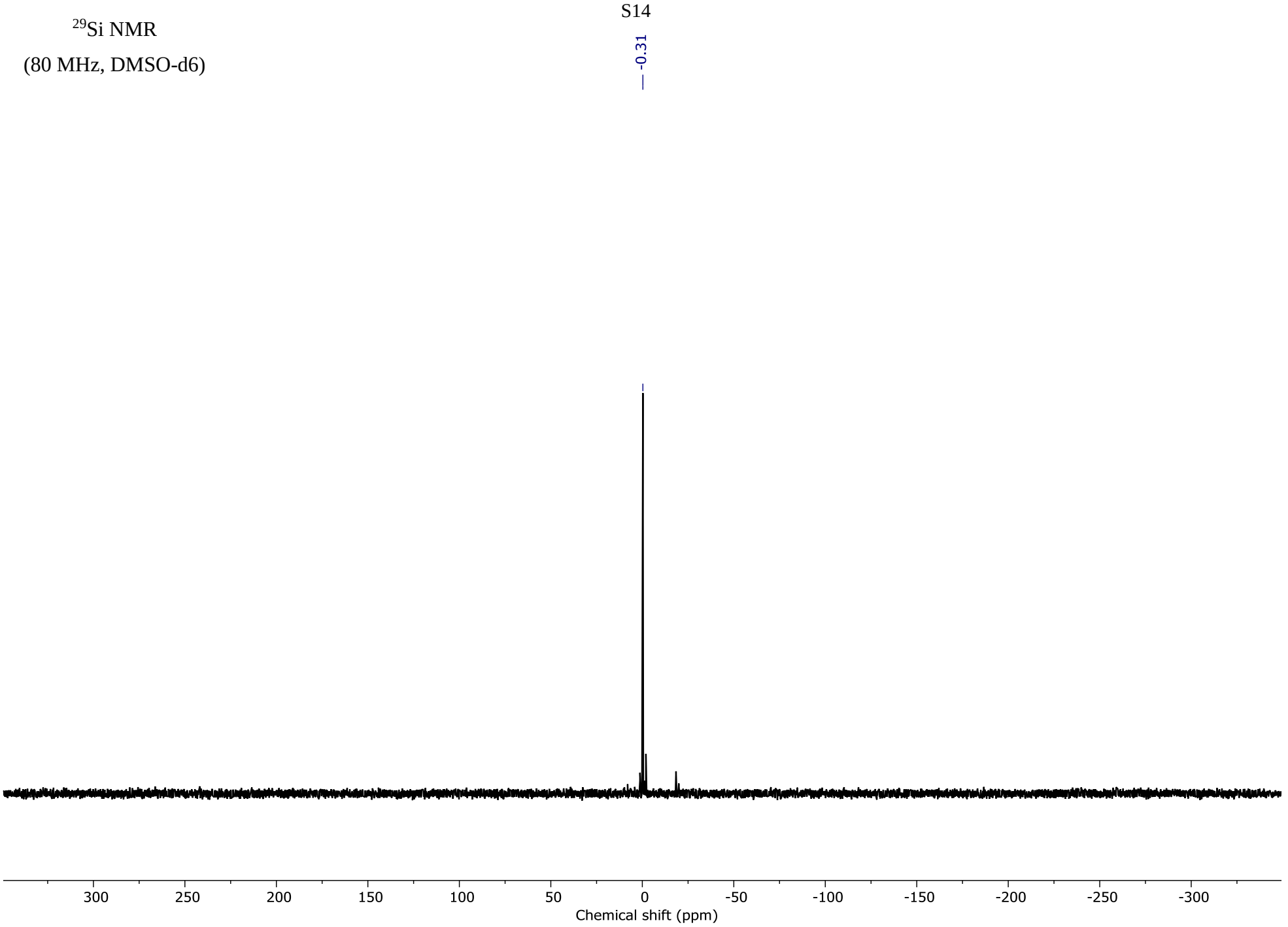
^{13}C NMR

(100 MHz, acetone-d6)



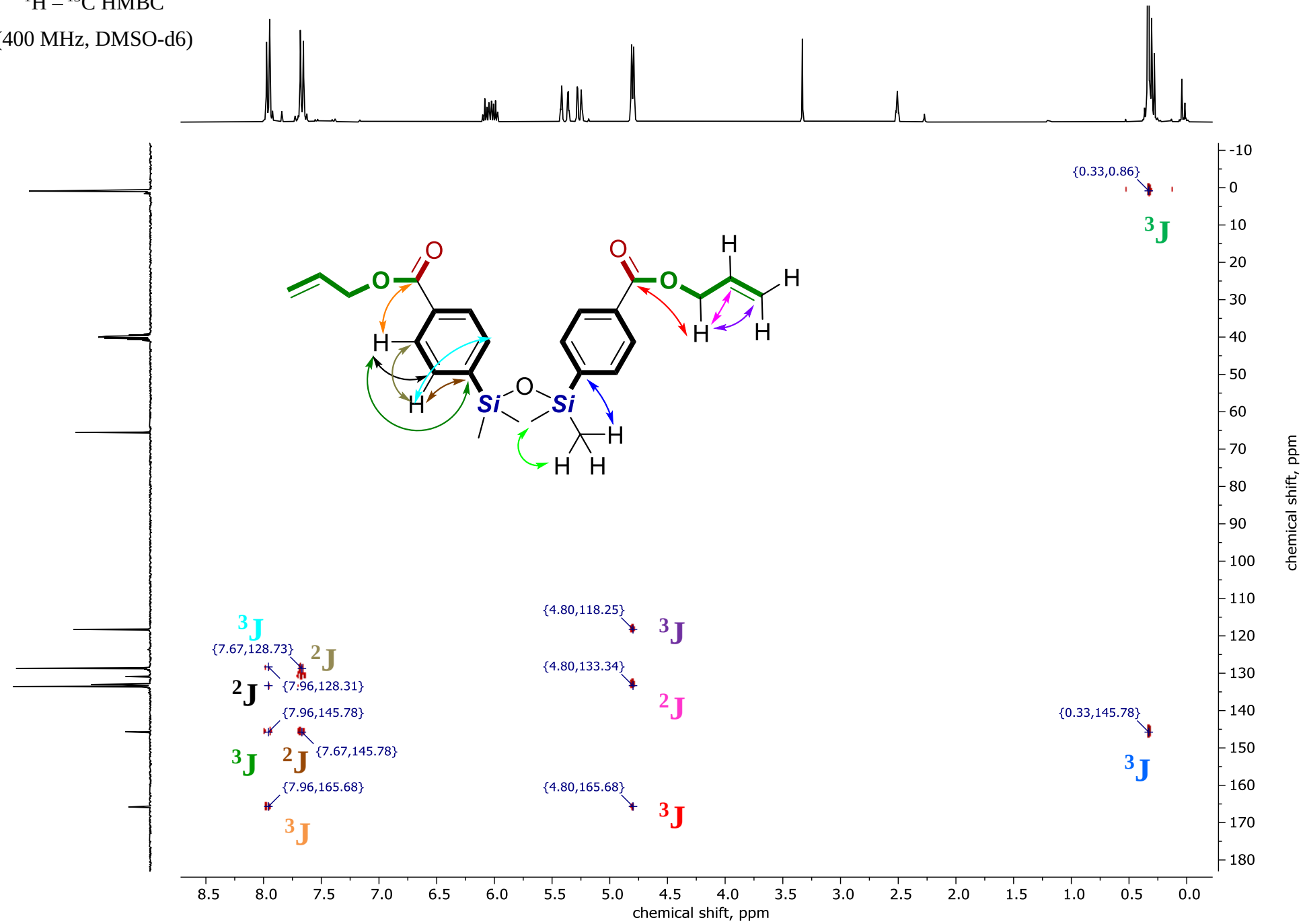
^{29}Si NMR

(80 MHz, DMSO-d6)



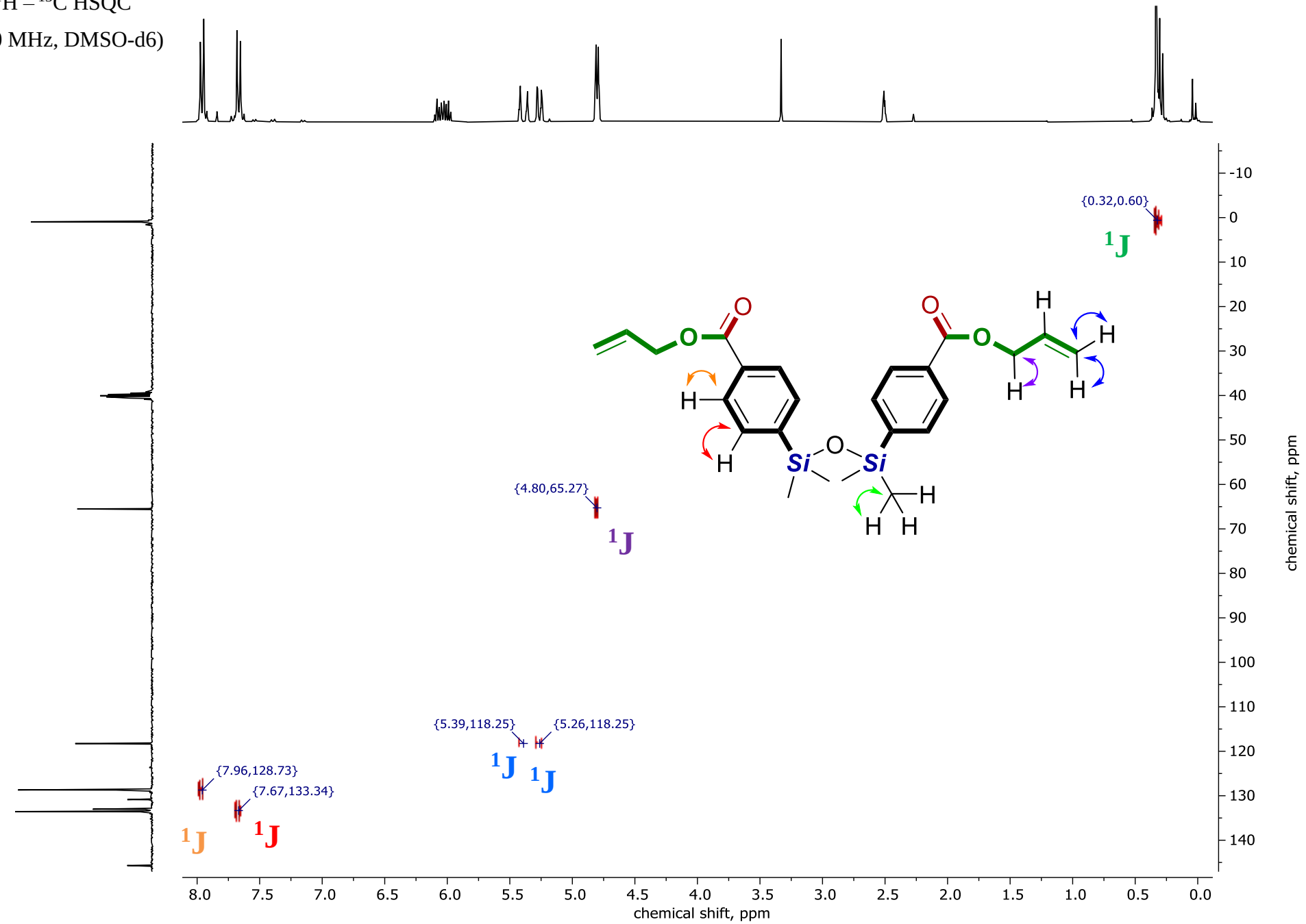
$^{1}H - ^{13}C$ HMBC

(400 MHz, DMSO-d6)



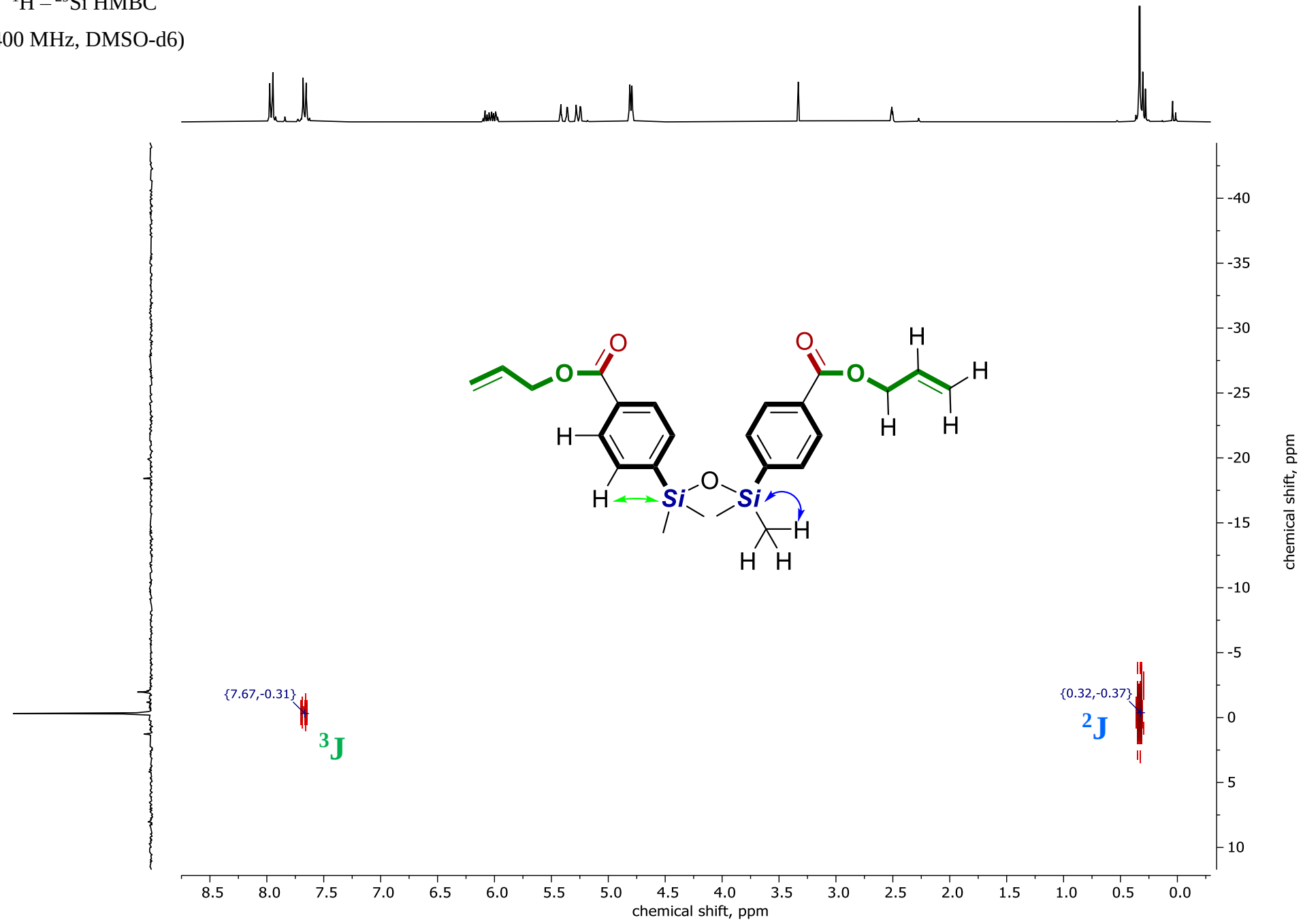
$^{1}H - ^{13}C$ HSQC

(400 MHz, DMSO-d6)

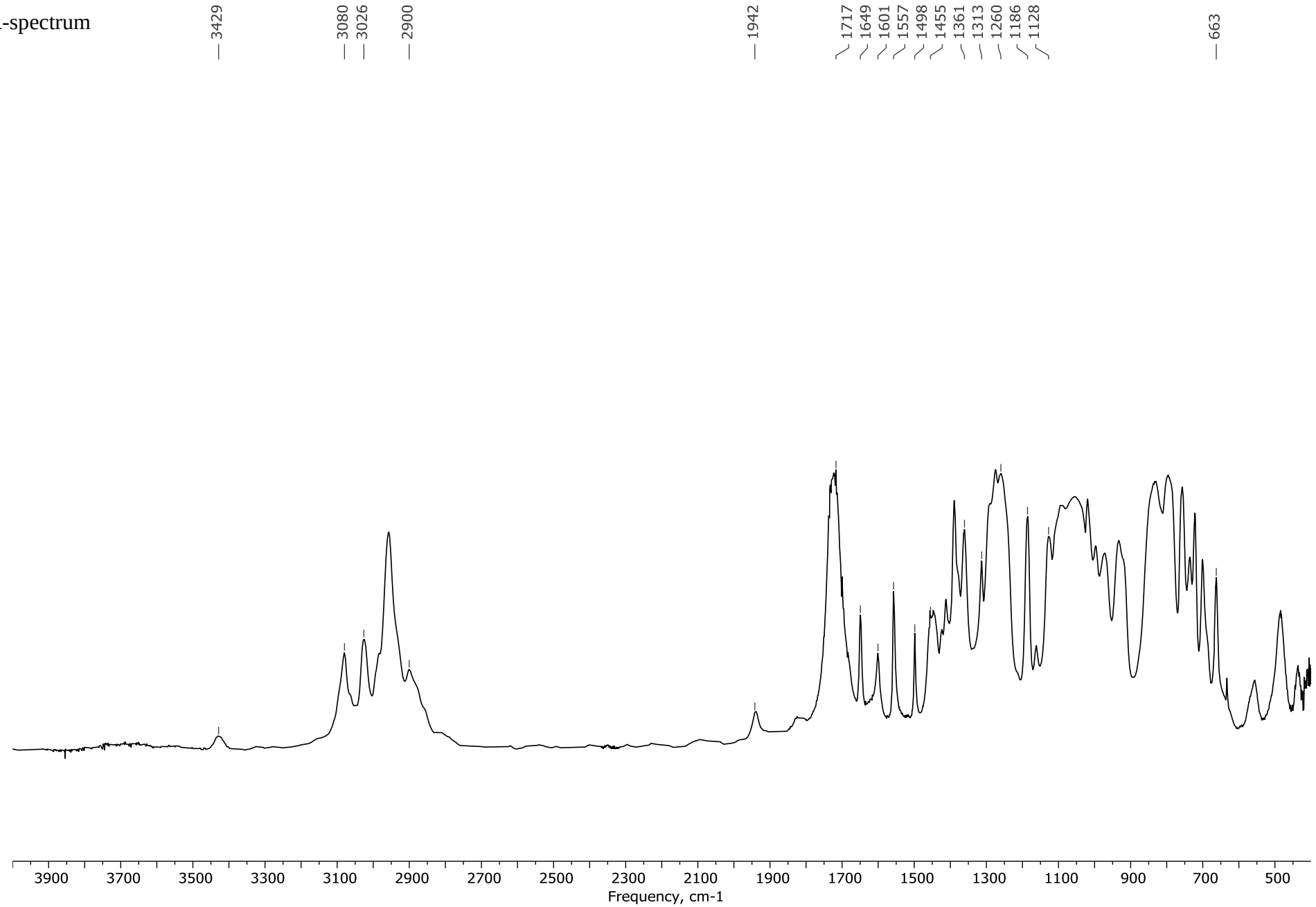


$^{1}H - {}^{29}Si$ HMBC

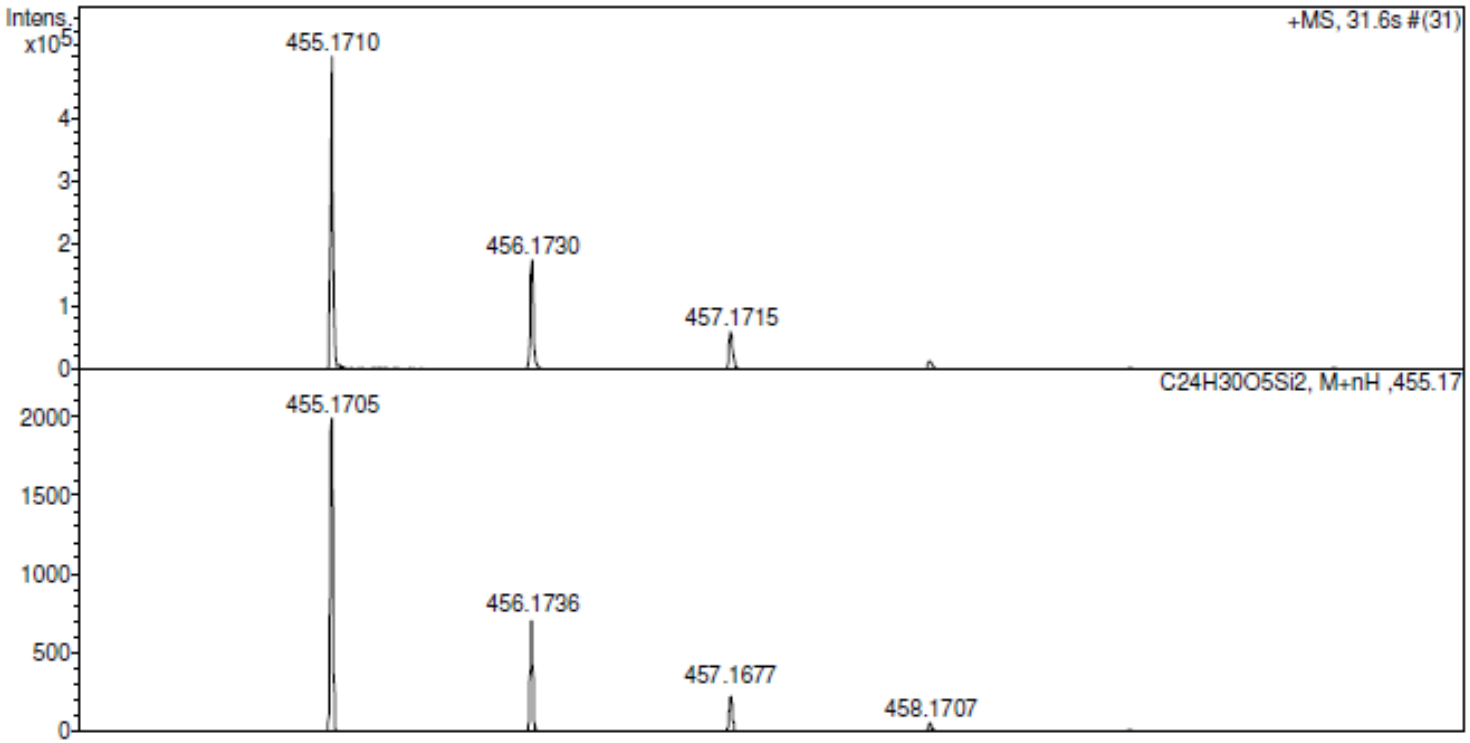
(400 MHz, DMSO-d6)

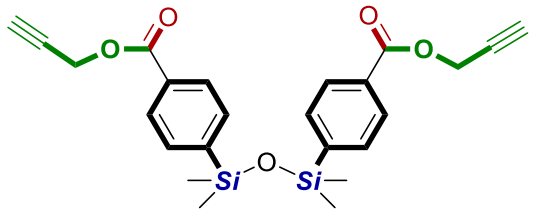


IR-spectrum


3429
3080
3026
2900
1942
1717
1649
1601
1557
1498
1455
1361
1313
1260
1186
1128
663
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, 31.6s #(31)
455.1710
456.1730
457.1715
C24H30O5Si2, M+nH ,455.17
455.1705
456.1736
457.1677
458.1707

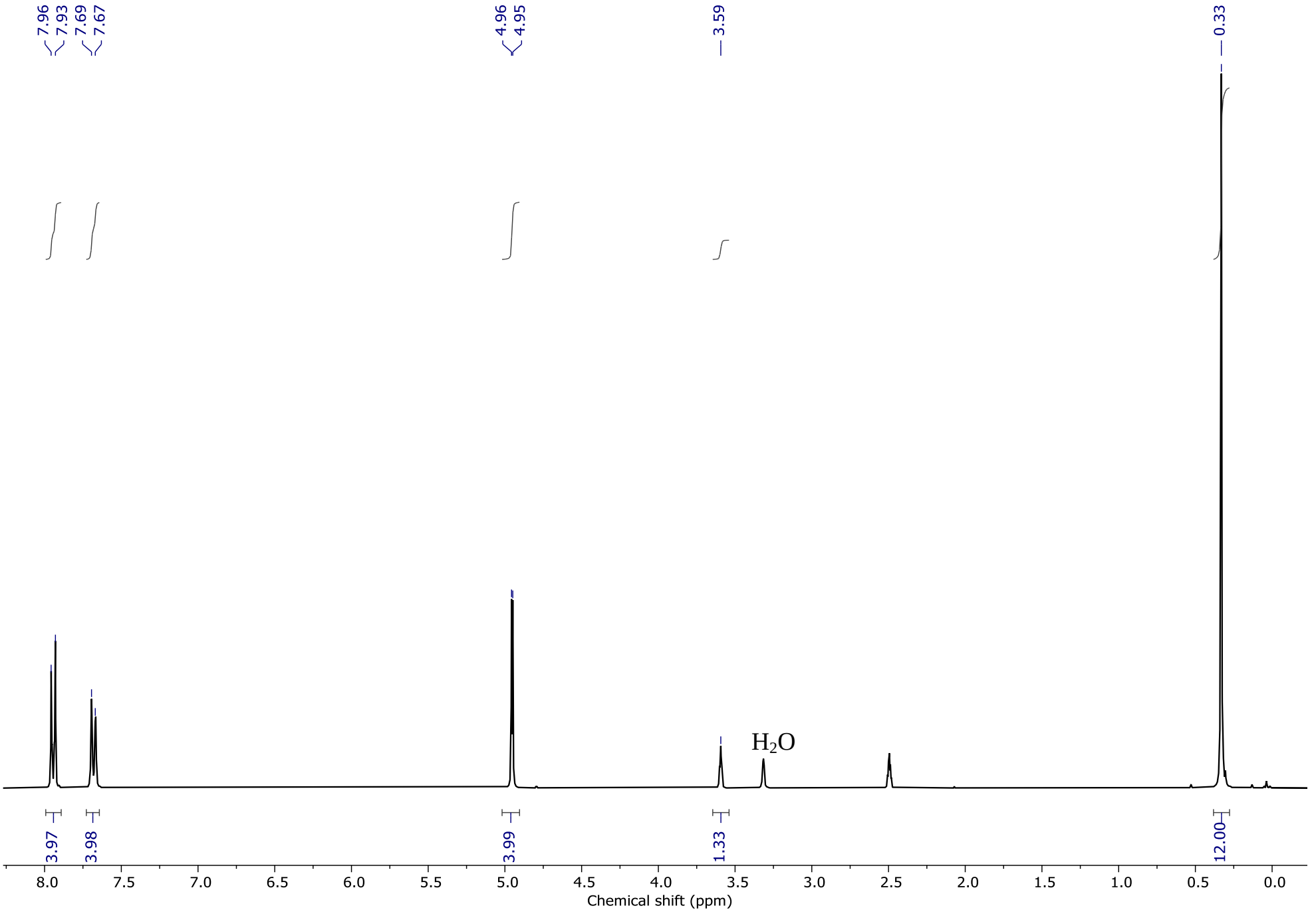


Characterisation data for di(prop-2-yn-1-yl) 4,4'-(1,1,3,3-tetramethyldisiloxane-1,3-diyl)dibenzoate:

^{1}H NMR (400 MHz, DMSO-d6): δ = 7.95 (d, ^{3}J=11 Hz, 4H), δ = 7.69 (d, ^{3}J=11 Hz, 4H), δ = 4.96 (d, ^{3}J=3, 4H), δ = 3.59 (m, 1H), δ = 0.33 (s, 12H). ^{13}C NMR (100 MHz, DMSO-d6): δ = 165.46, 146.07, 133.66, 130.25, 128.78, 78.77, 78.39, 52.96, 0.95. ^{29}Si NMR (80 MHz, DMSO): δ = -0.21. HRMS (ESI) m/z $[M + H]^+$: calcd for $[C_{24}H_{26}O_5Si_2 + H]^+$, 451.1392; found, 451.1391; $[M + K]^+$: calcd for $[C_{24}H_{26}O_5Si_2 + K]^+$, 489.0950; found, 489.0953; $[M + Na]^+$: calcd for $[C_{24}H_{26}O_5Si_2 + Na]^+$, 473.1211; found, 473.1206. IR (cm^{-1}): 3291, 2964, 1715, 1281, 1100, 825-651.

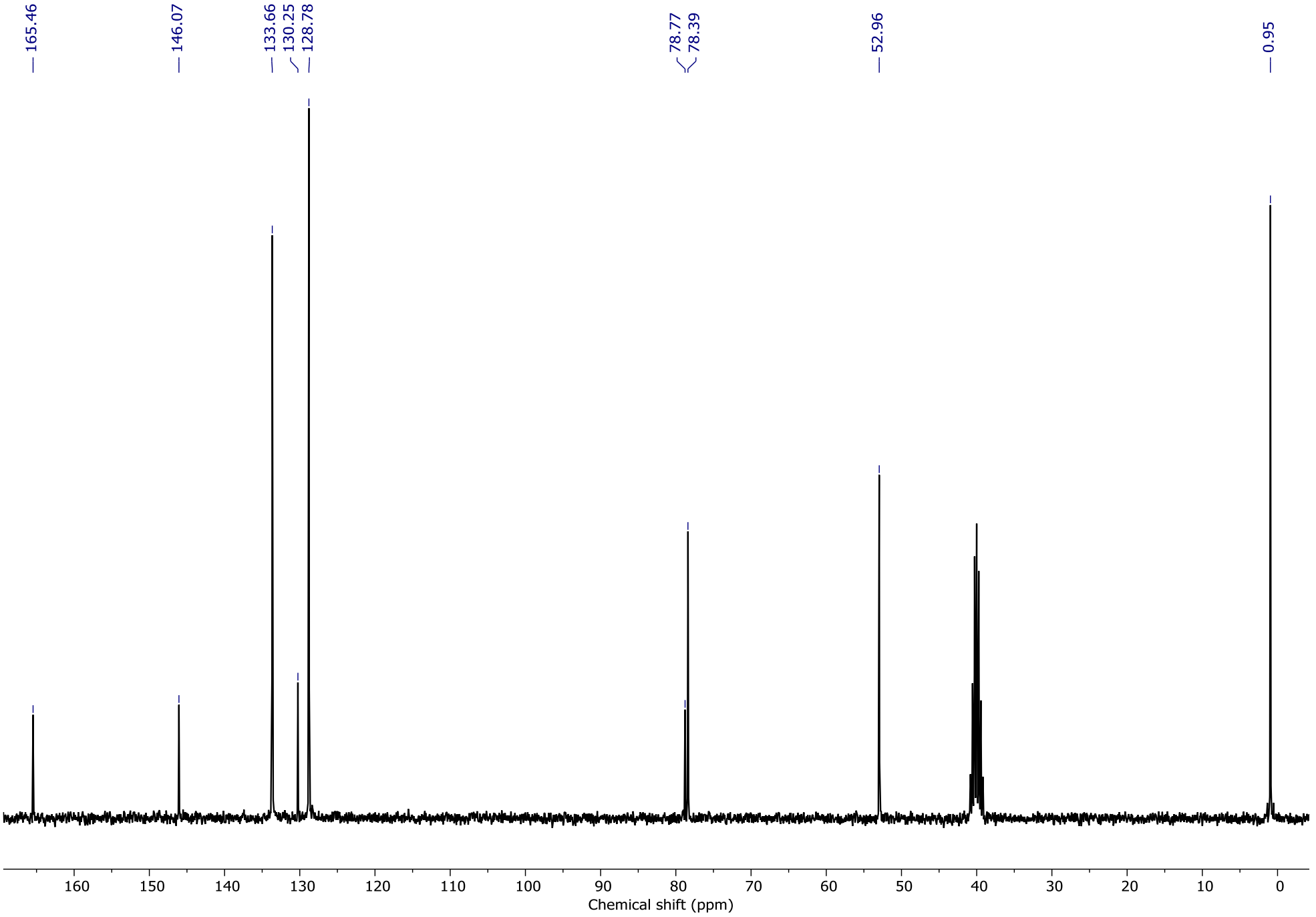
^{1}H NMR

(400 MHz, DMSO-d6)



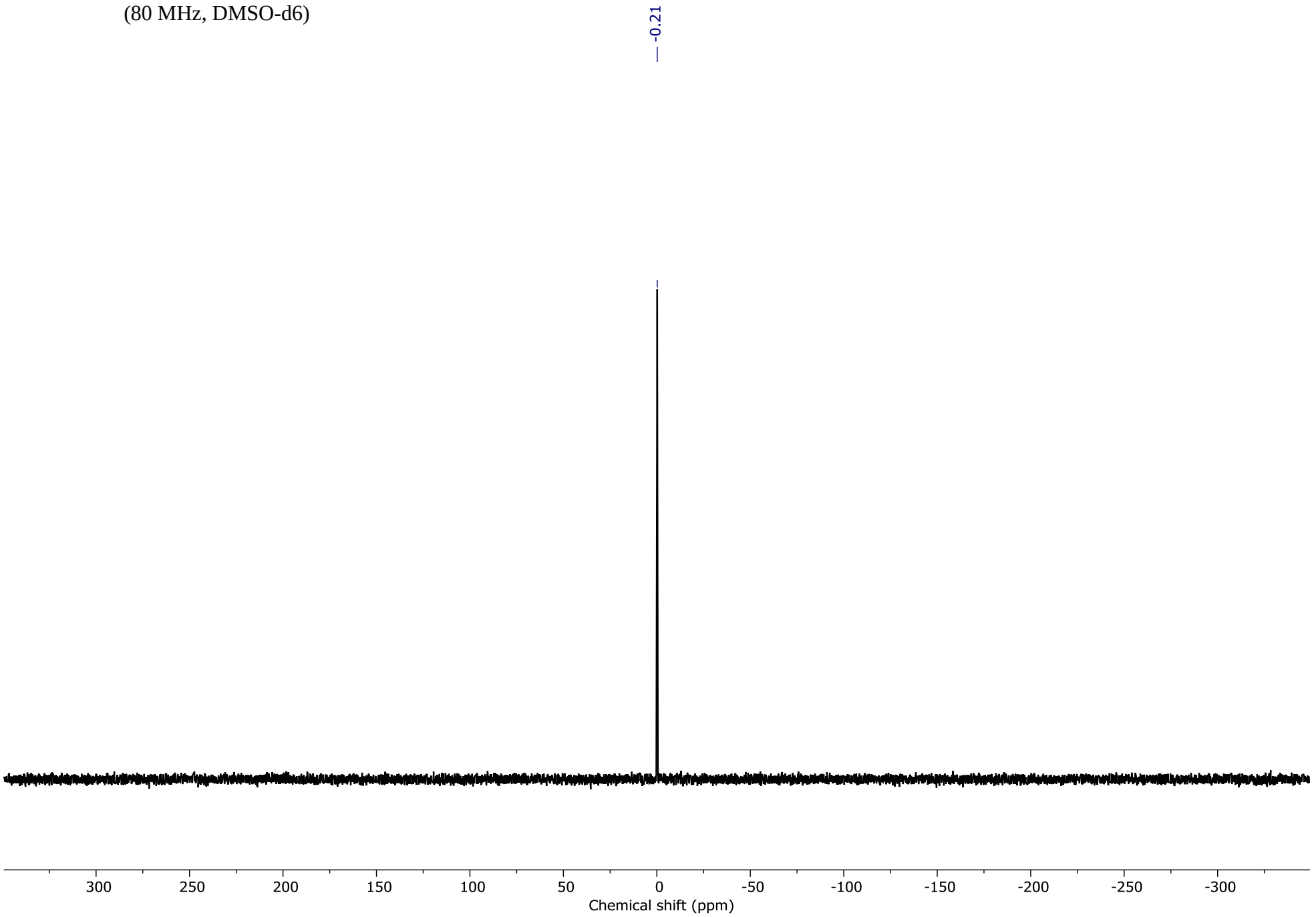
^{13}C NMR

(100 MHz, DMSO-d6)



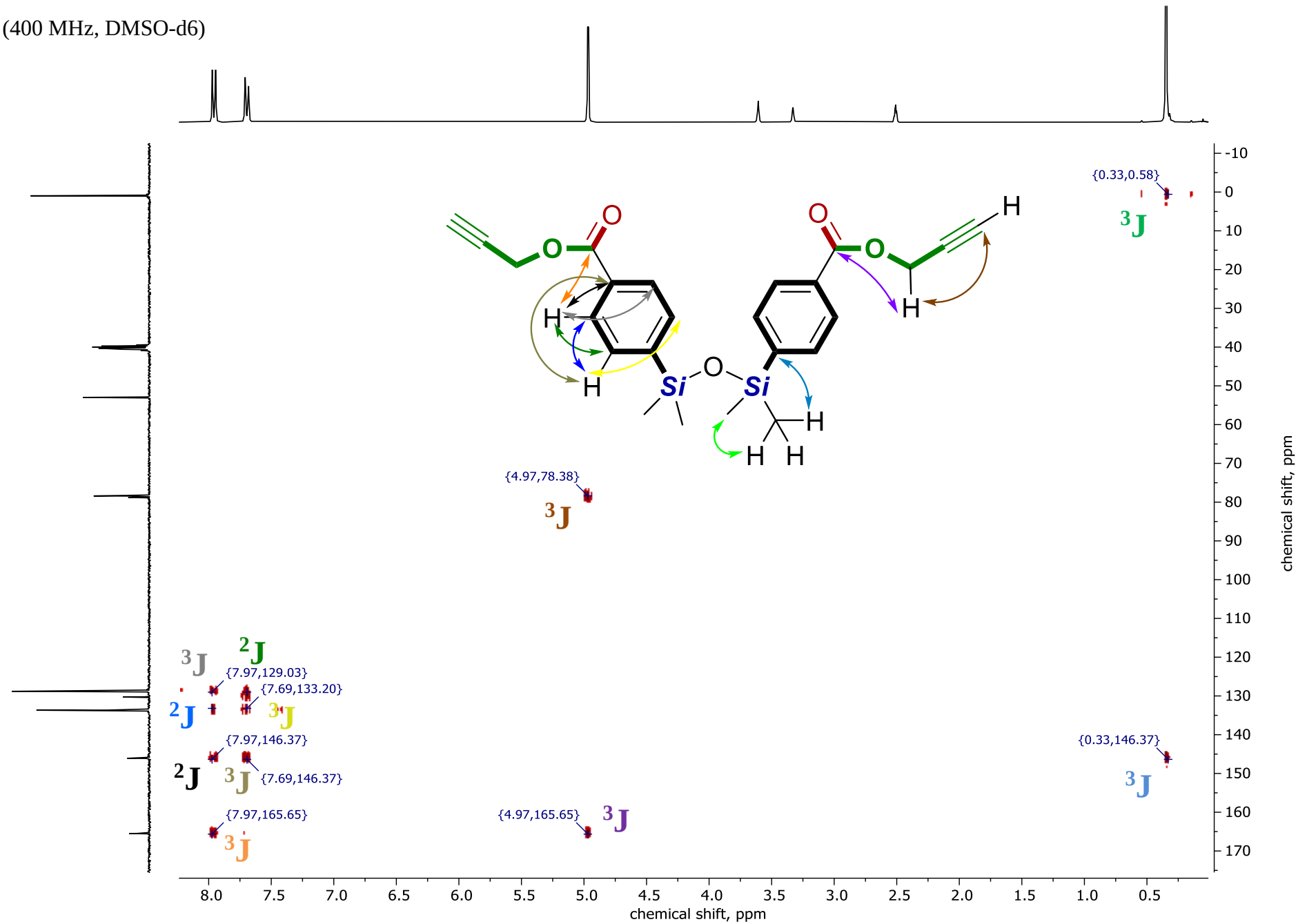
^{29}Si NMR

(80 MHz, DMSO-d6)



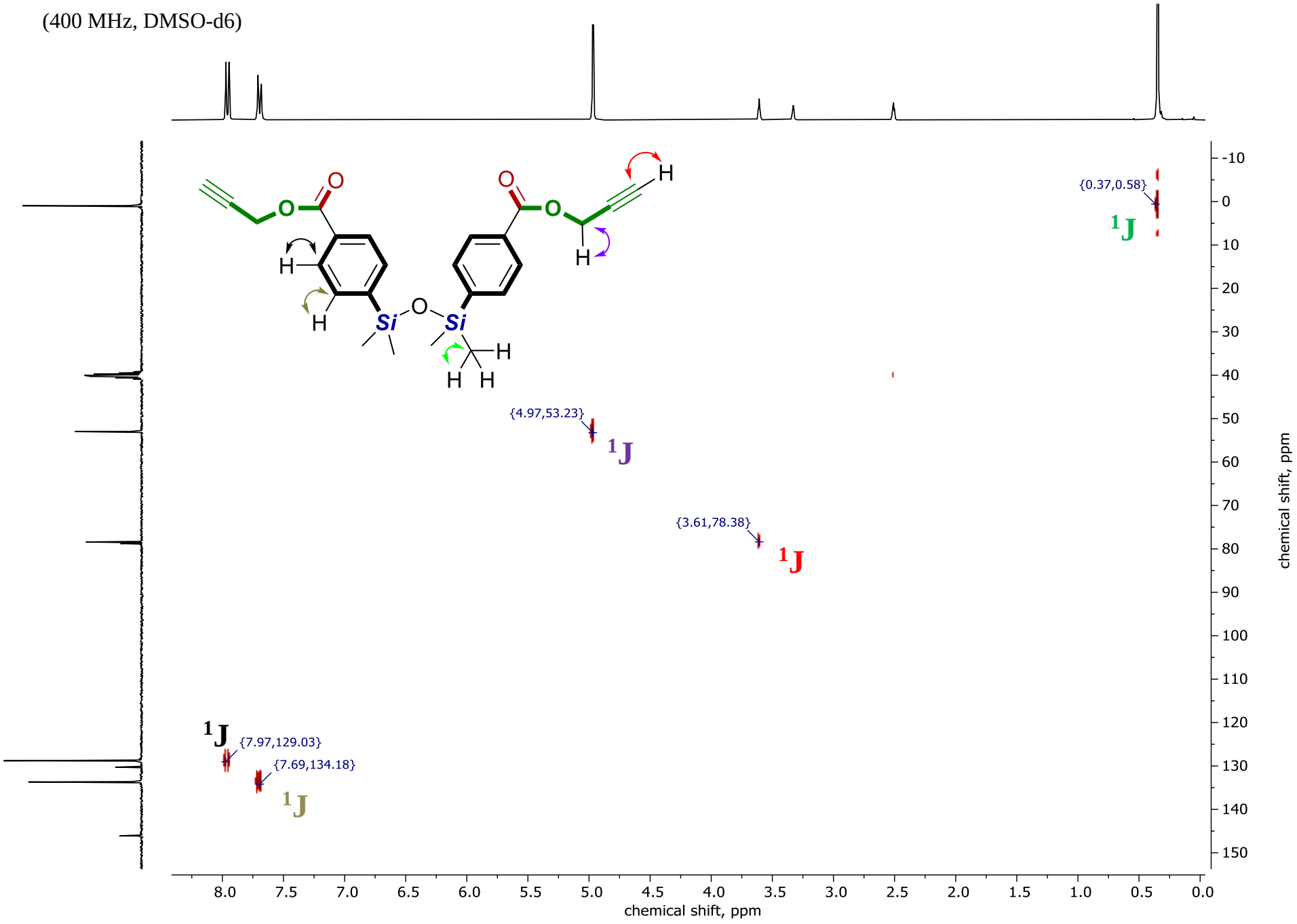
$^{1}H - ^{13}C$ HMBC

(400 MHz, DMSO-d6)



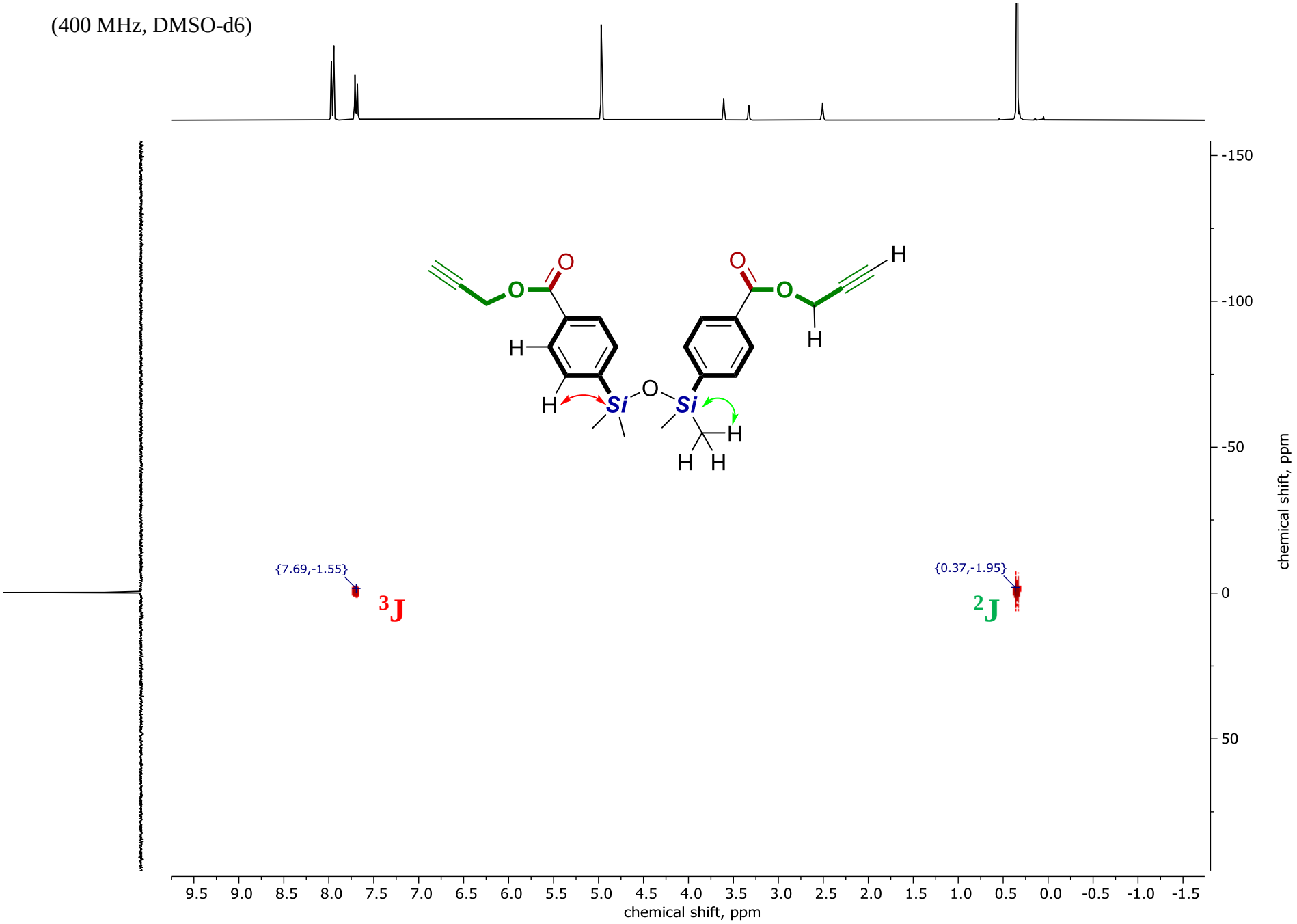
$^{1}H - ^{13}C$ HSQC

(400 MHz, DMSO-d6)

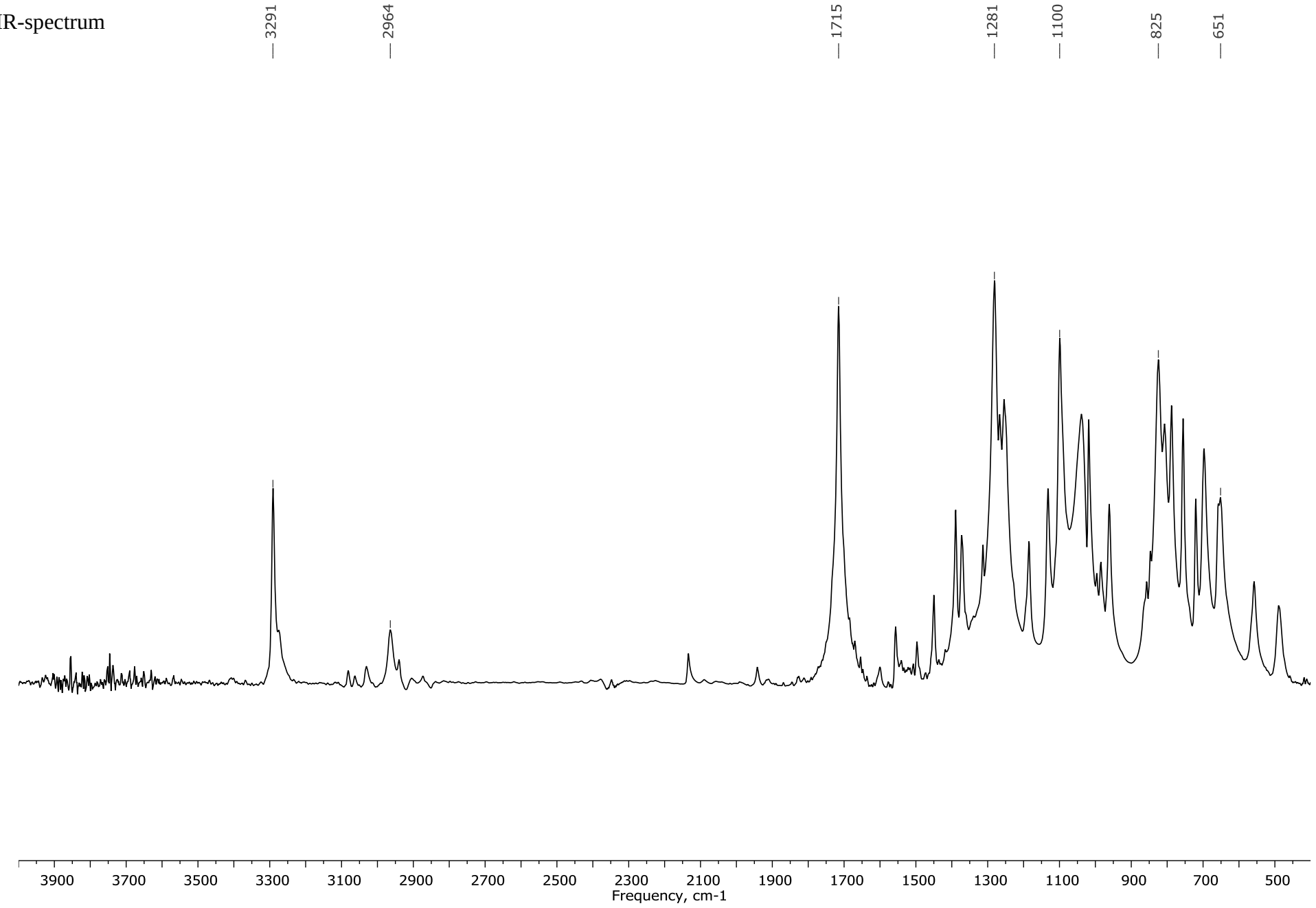


$^{1}H - {}^{29}Si$ HMBC

(400 MHz, DMSO-d6)



IR-spectrum


3291
2964
1715
1281
1100
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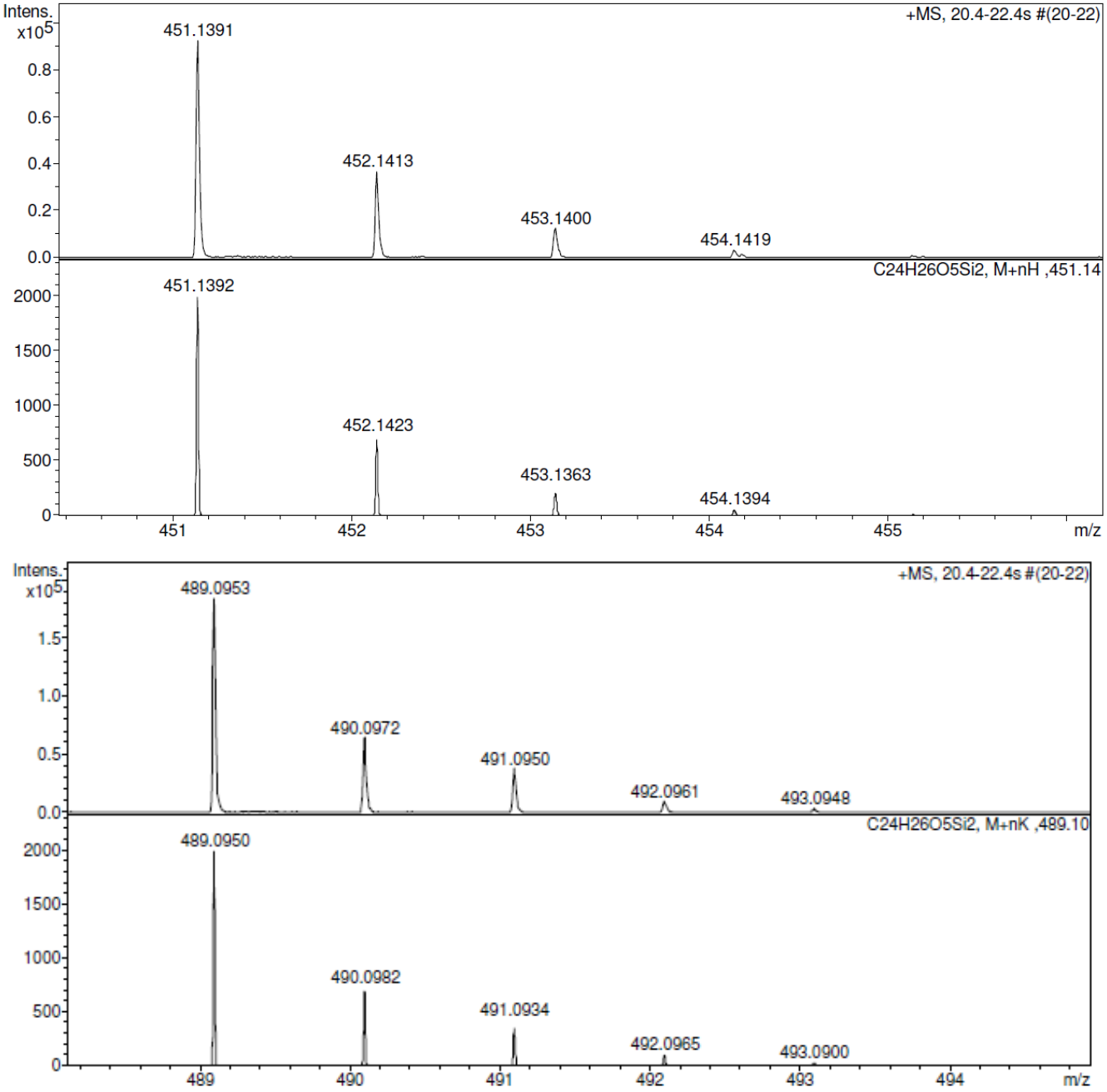
651
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

HRMS (ESI)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x10^5
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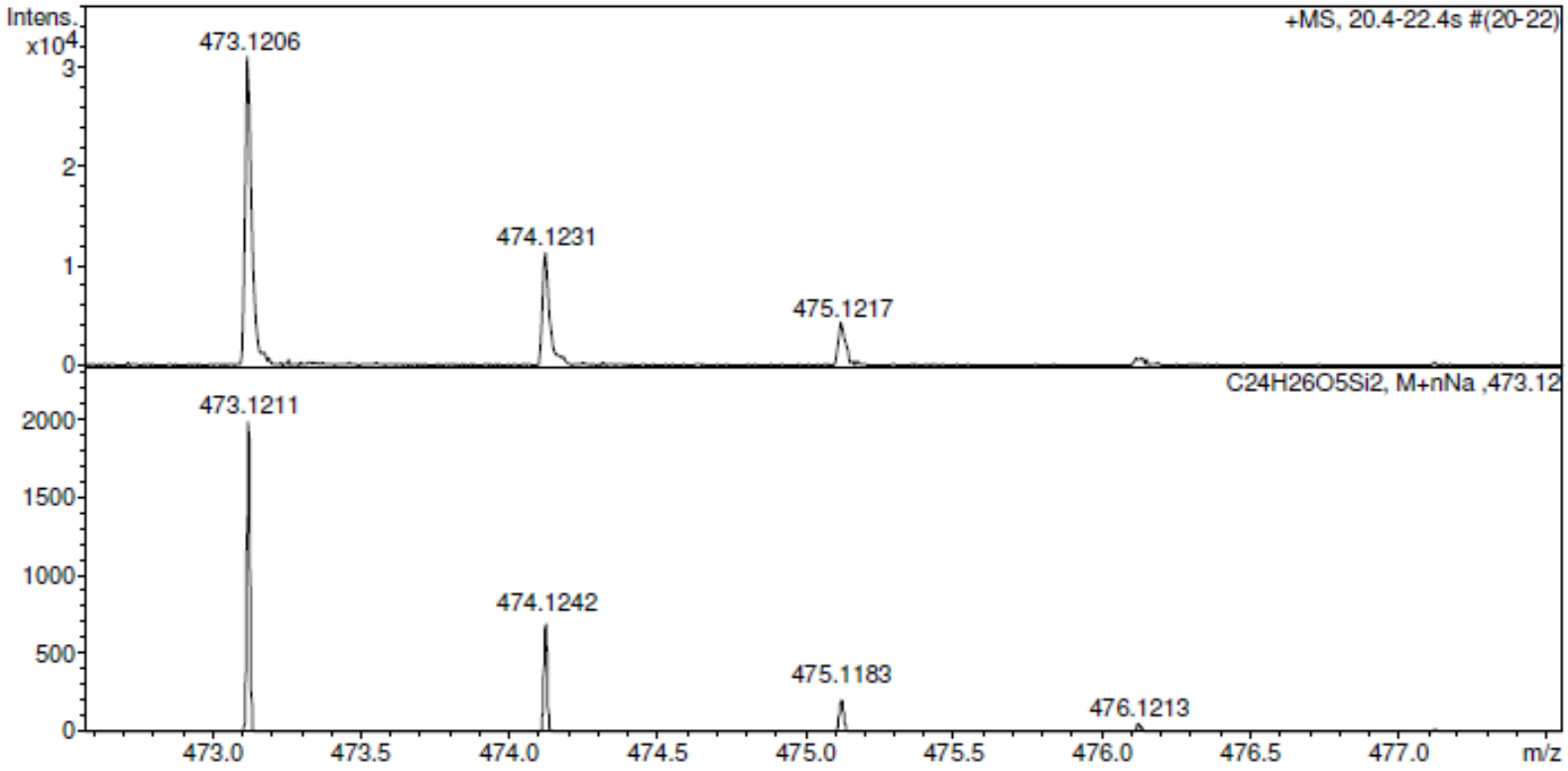
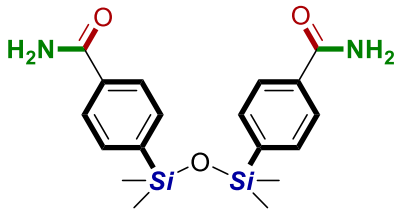
451.1391
452.1413
453.1400
454.1419
C24H26O5Si2, M+nH ,451.14
451.1392
452.1423
453.1363
454.1394
m/z
Intens.
x10^5
+MS, 20.4-22.4s #(20-22)
489.0953
490.0972
491.0950
492.0961
493.0948
C24H26O5Si2, M+nK ,489.10
489.0950
490.0982
491.0934
492.0965
493.0900
m/z


Intens.
x10^4
3
2
1
0
473.1206
474.1231
475.1217
+MS, 20.4-22.4s #(20-22)
C24H26O5Si2, M+nNa ,473.12
2000
1500
1000
500
0
473.1211
474.1242
475.1183
476.1213
473.0
473.5
474.0
474.5
475.0
475.5
476.0
476.5
477.0
m/z

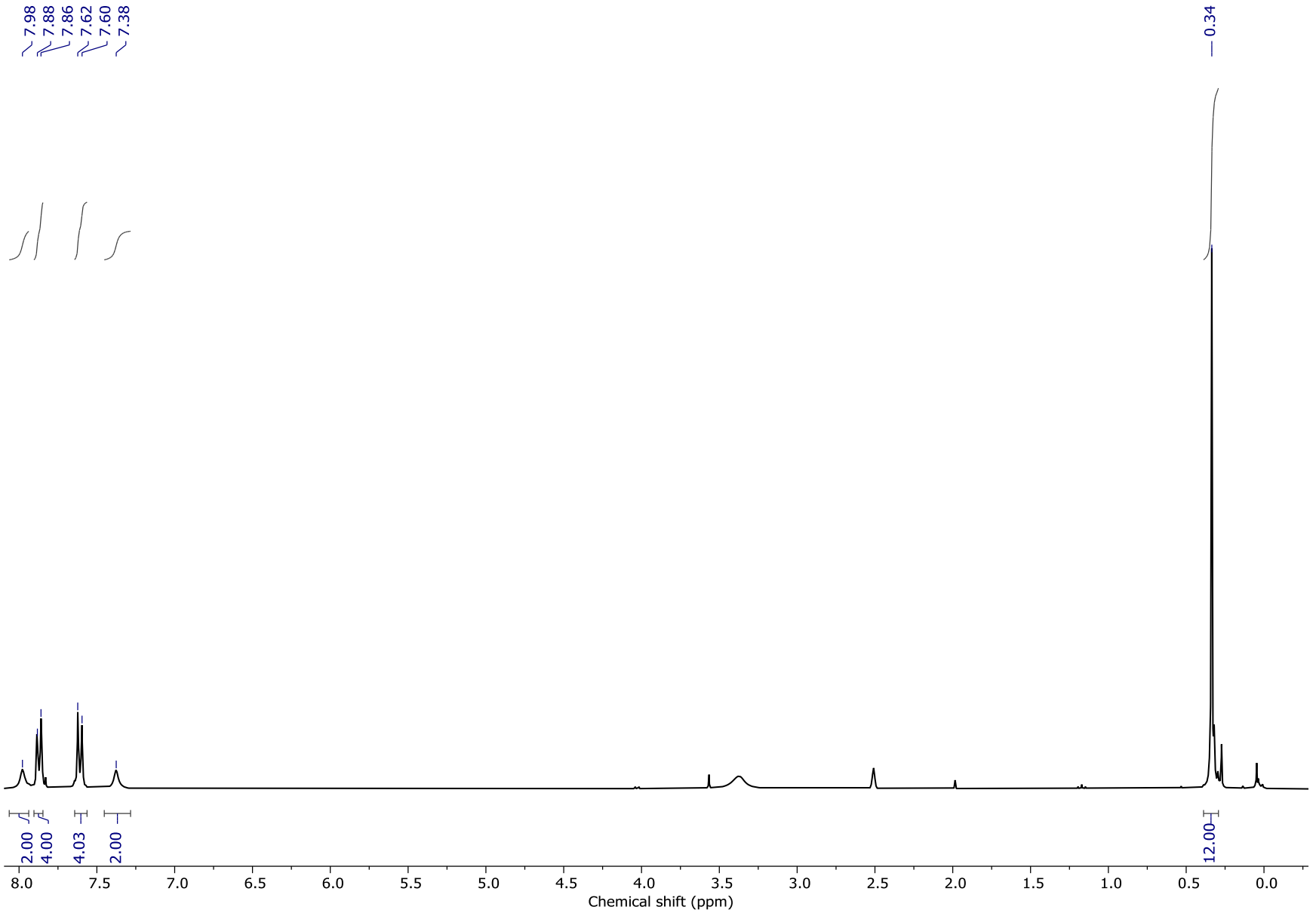


Characterisation data for 4,4'-(1,1,3,3-tetramethyldisiloxane-1,3-diyl)dibenzamide:

^{1}H NMR (400 MHz, DMSO-d6): δ = 7.98 (br s, 2H), δ = 7.87 (d, ^{3}J=11 Hz, 4H), δ = 7.61 (d, ^{3}J=11 Hz, 4H), δ = 7.38 (br s, 2H), δ = 0.34 (s, 12H). ^{13}C NMR (100 MHz, DMSO-d6): δ = 167.95, 142.63, 135.18, 132.66, 126.67, 0.67. ^{29}Si NMR (80 MHz, DMSO-d6): δ = -0.56. ^{15}N NMR (40 MHz, DMSO-d6): δ = 103.21.

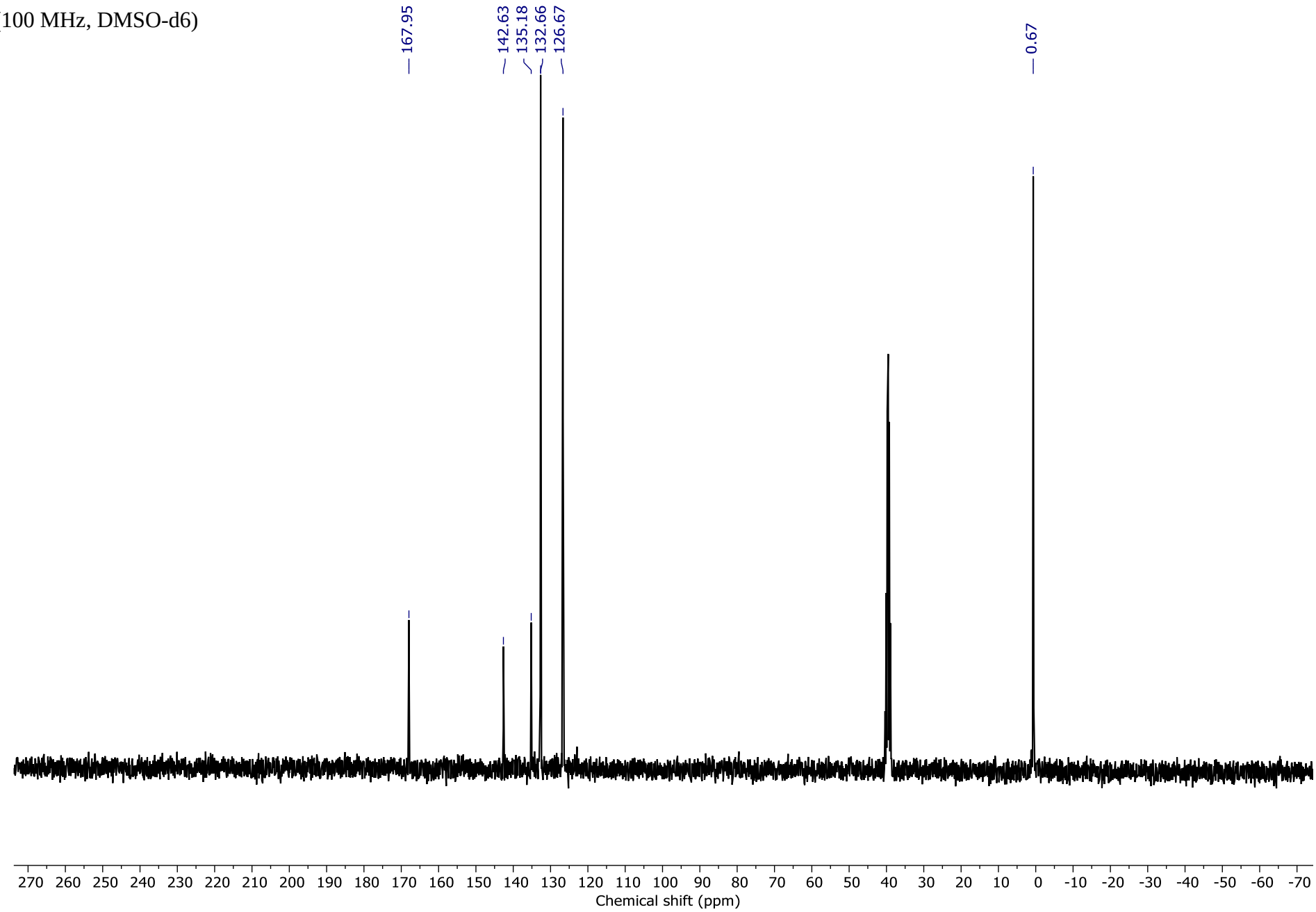
^{1}H NMR

(400 MHz, DMSO-d6)



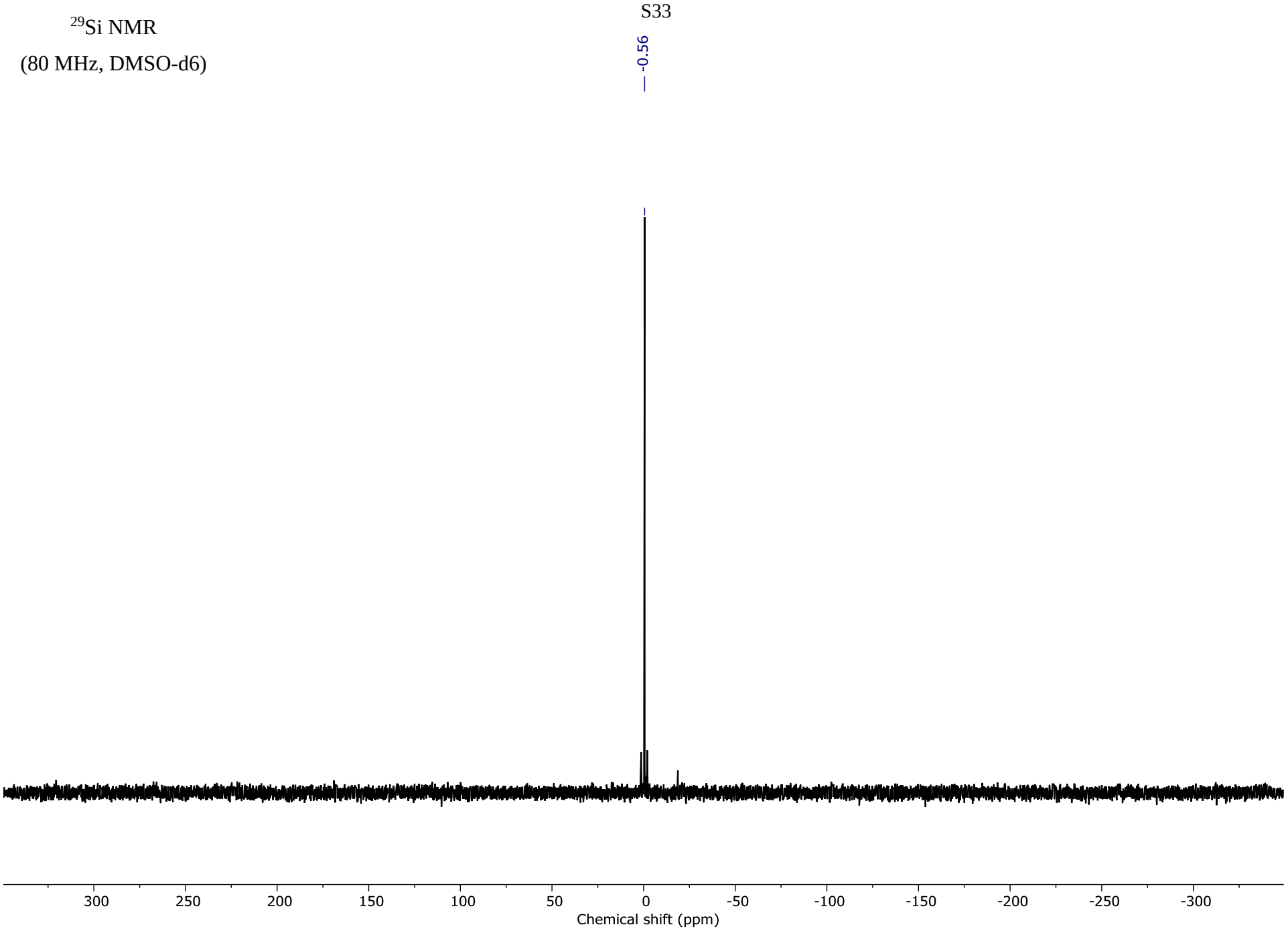
^{13}C NMR

(100 MHz, DMSO-d6)



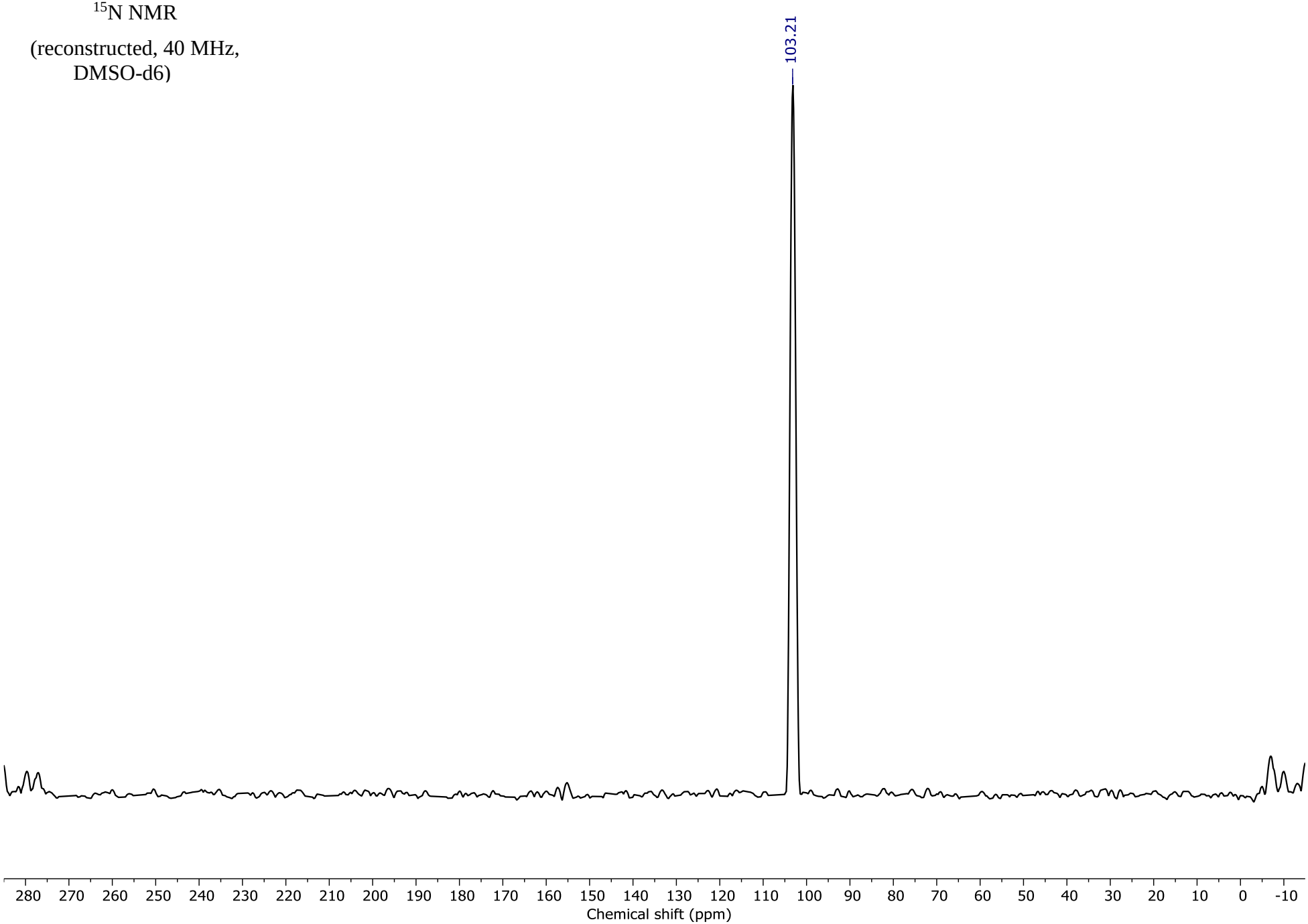
^{29}Si NMR

(80 MHz, DMSO-d6)



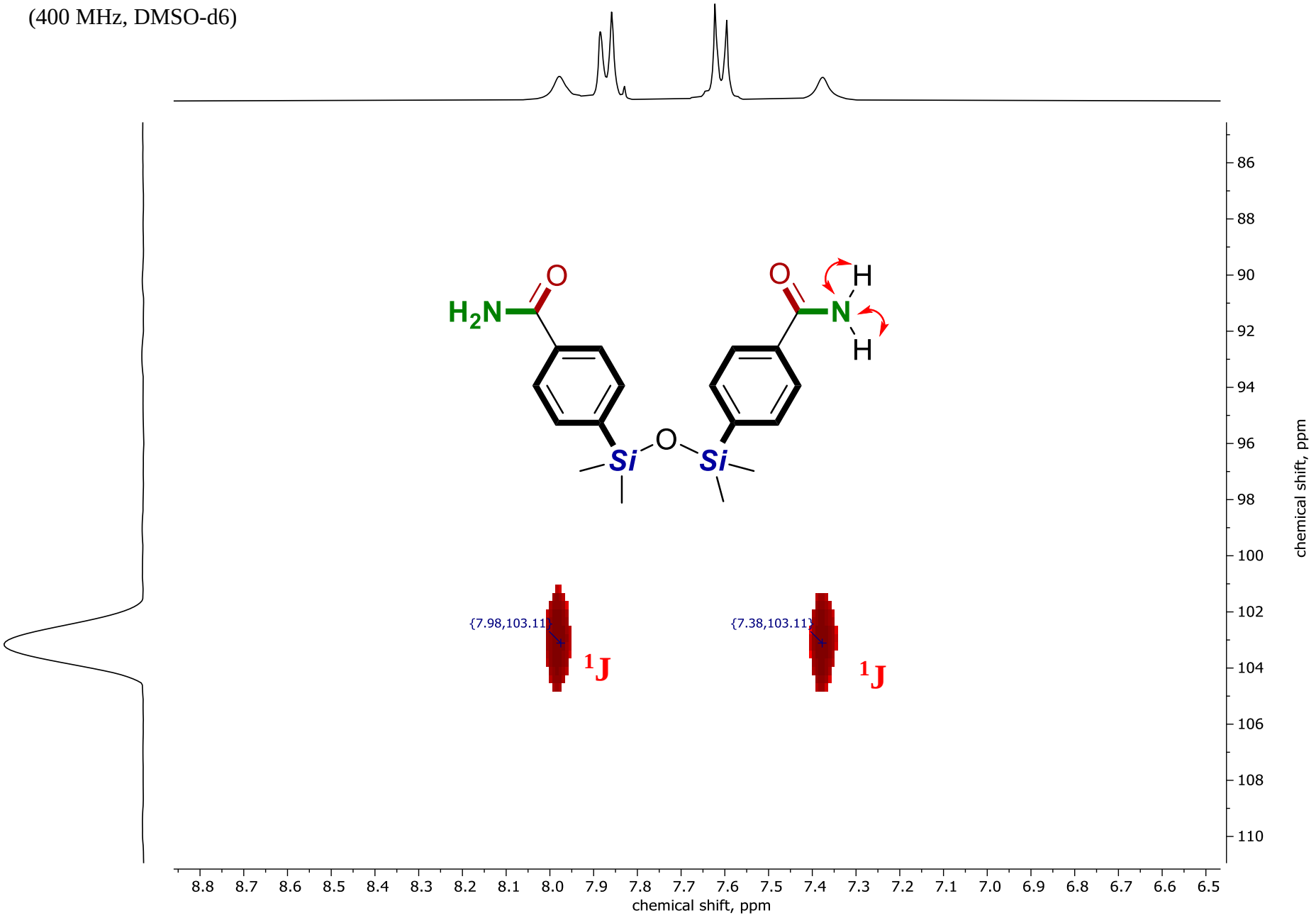
^{15}N NMR

(reconstructed, 40 MHz, DMSO-d6)



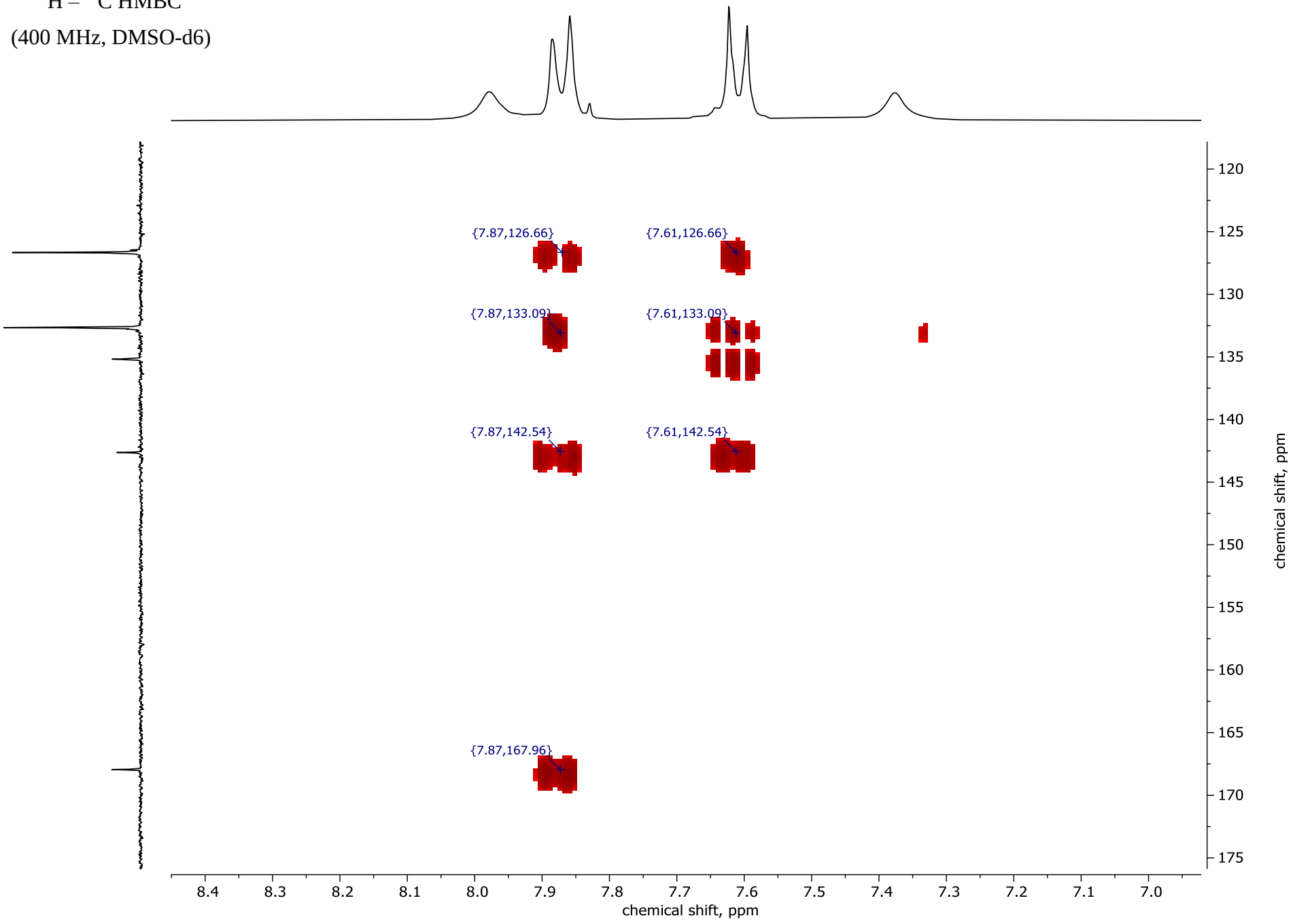
$^{1}H - {}^{15}N$ HMBC

(400 MHz, DMSO-d6)



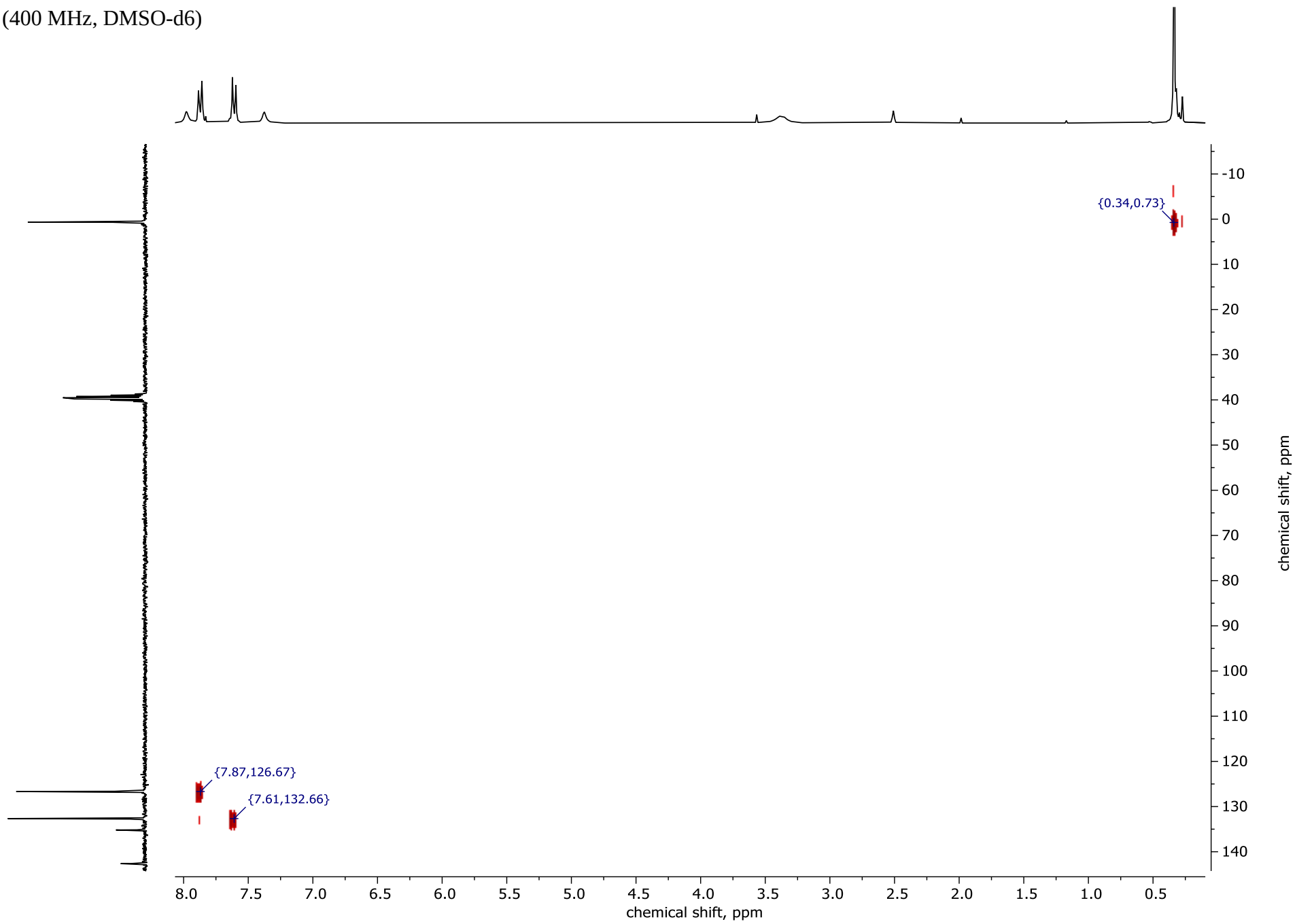
$^{1}H - ^{13}C$ HMBC

(400 MHz, DMSO-d6)



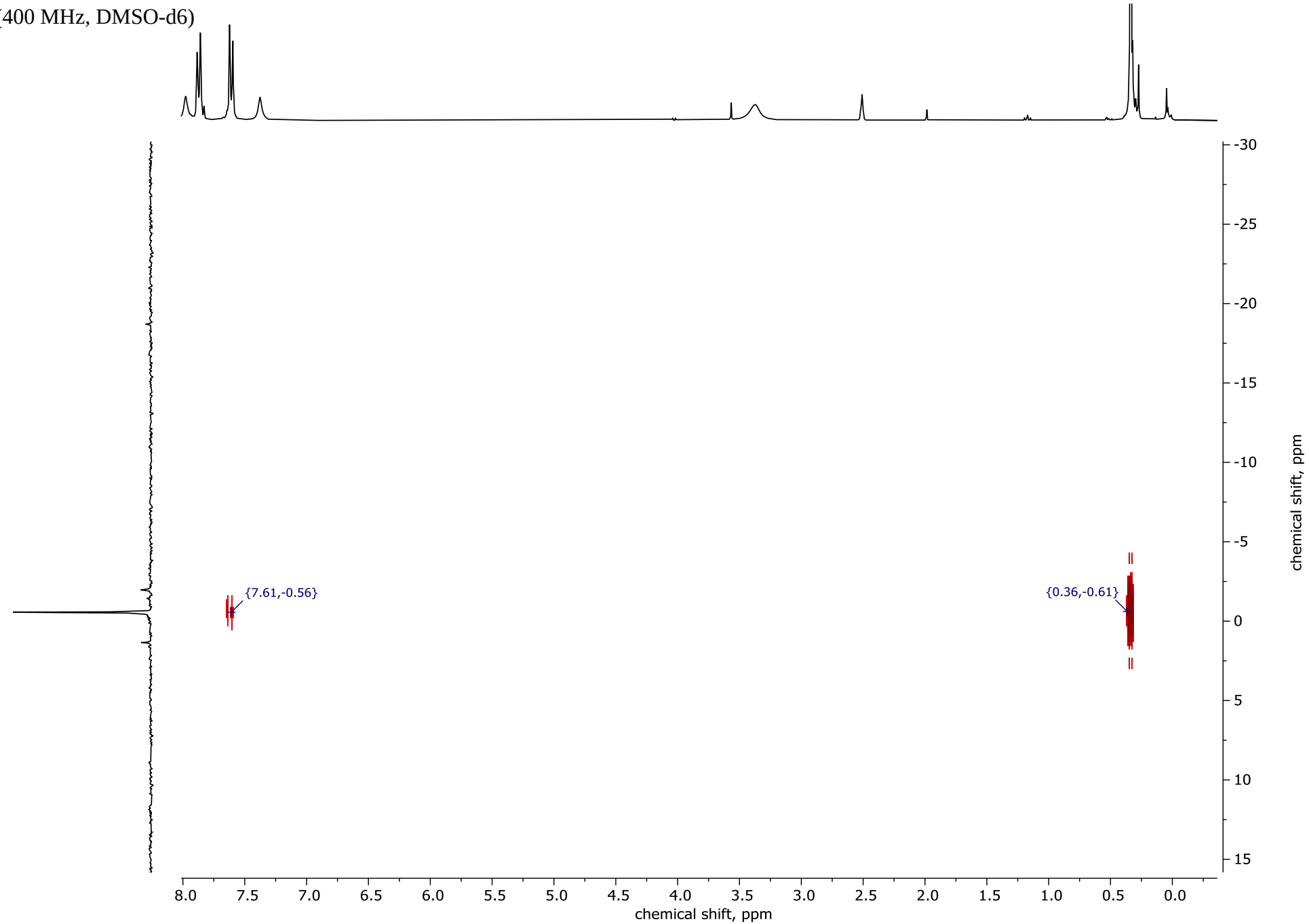
$^{1}H - ^{13}C$ HSQC

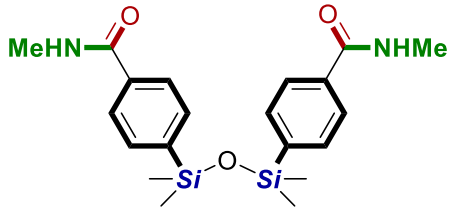
(400 MHz, DMSO-d6)



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

(400 MHz, DMSO-d6)



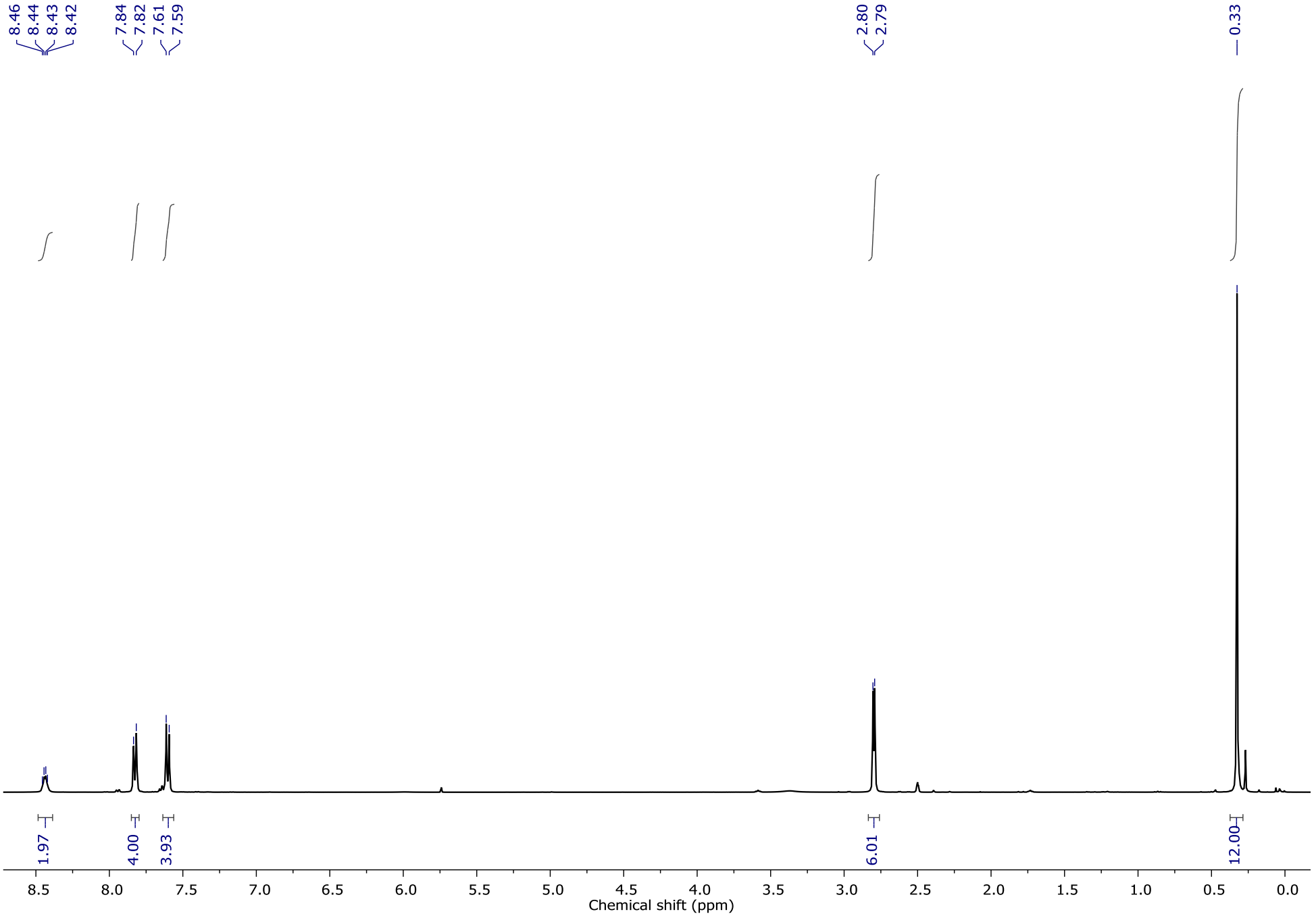


Characterisation data for 4,4'-(1,1,3,3-tetramethyldisiloxane-1,3-diyl)bis(N-methylbenzamide):

^{1}H NMR (400 MHz, DMSO-d6): δ = 8.44 (m, 2H), δ = 7.83 (d, ^{3}J= 8 Hz, 4H), δ = 7.60 (d, ^{3}J= 8Hz, 4H), δ = 2.80 (d, ^{3}J= 4.6 Hz, 6H), δ = 0.33 (s, 12H). ^{13}C NMR (100 MHz, DMSO-d6): δ = 167.09, 142.82, 135.90, 133.18, 126.74, 26.68, 1.10. ^{29}Si NMR (80 MHz, DMSO-d6): δ = -0.57. ^{15}N NMR (40 MHz, DMSO-d6): δ = 99.46. HRMS (ESI) m/z [M + H] $^{+}$: calcd for $[C_{20}H_{28}N_2O_3Si_2 + H]^{+}$, 401.1711; found, 401.1706; [M + Na] $^{+}$: calcd for $[C_{20}H_{28}N_2O_3Si_2 + Na]^{+}$, 423.1531; found, 423.1526; [M + K] $^{+}$: calcd for $[C_{20}H_{28}N_2O_3Si_2 + K]^{+}$,439.1270; found, 439.1263. IR (cm^{-1}): 3325, 2958, 1635, 1545, 1411, 1319, 1254, 1111, 1067, 830, 791.

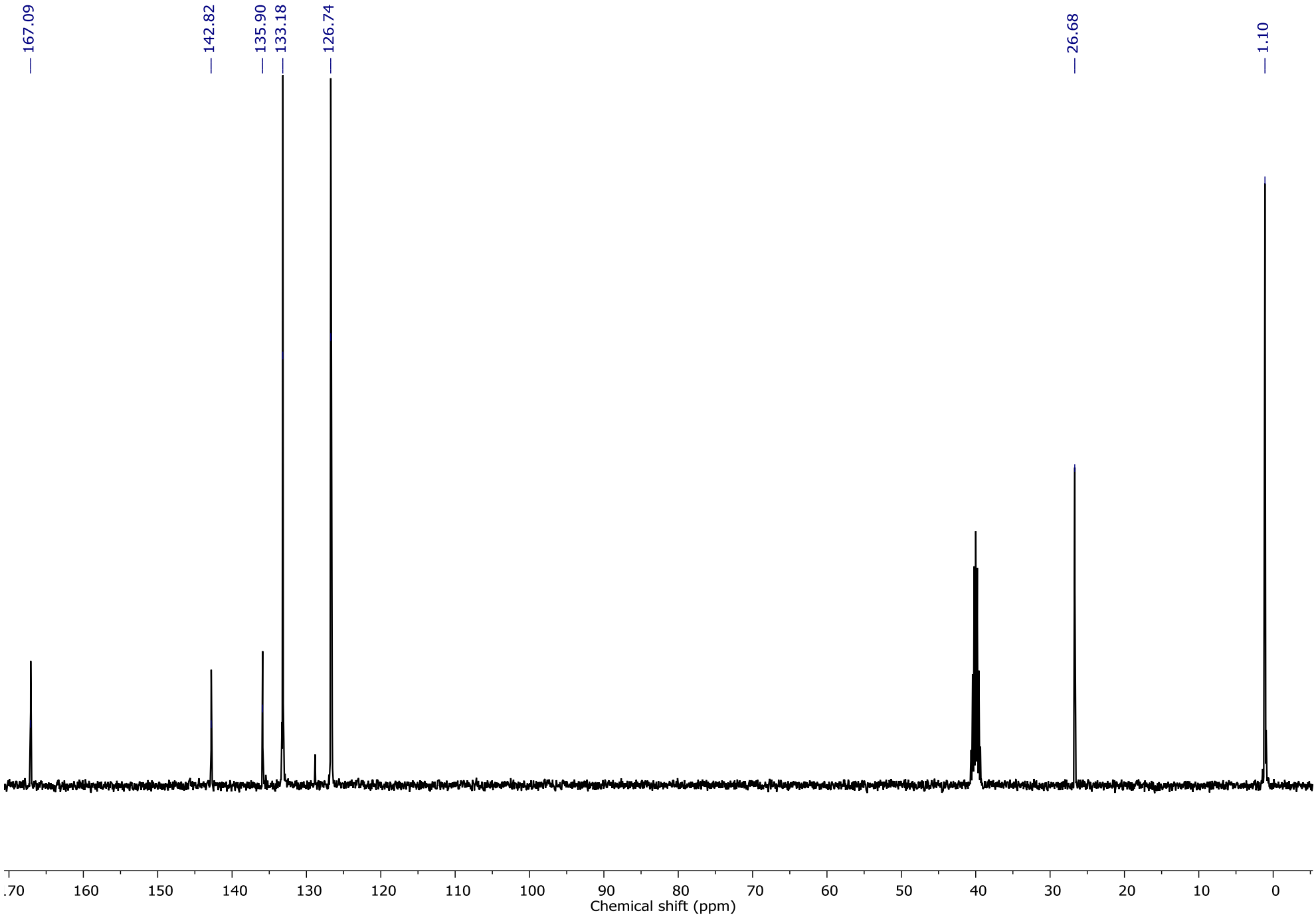
^{1}H NMR

(400 MHz, DMSO-d6)



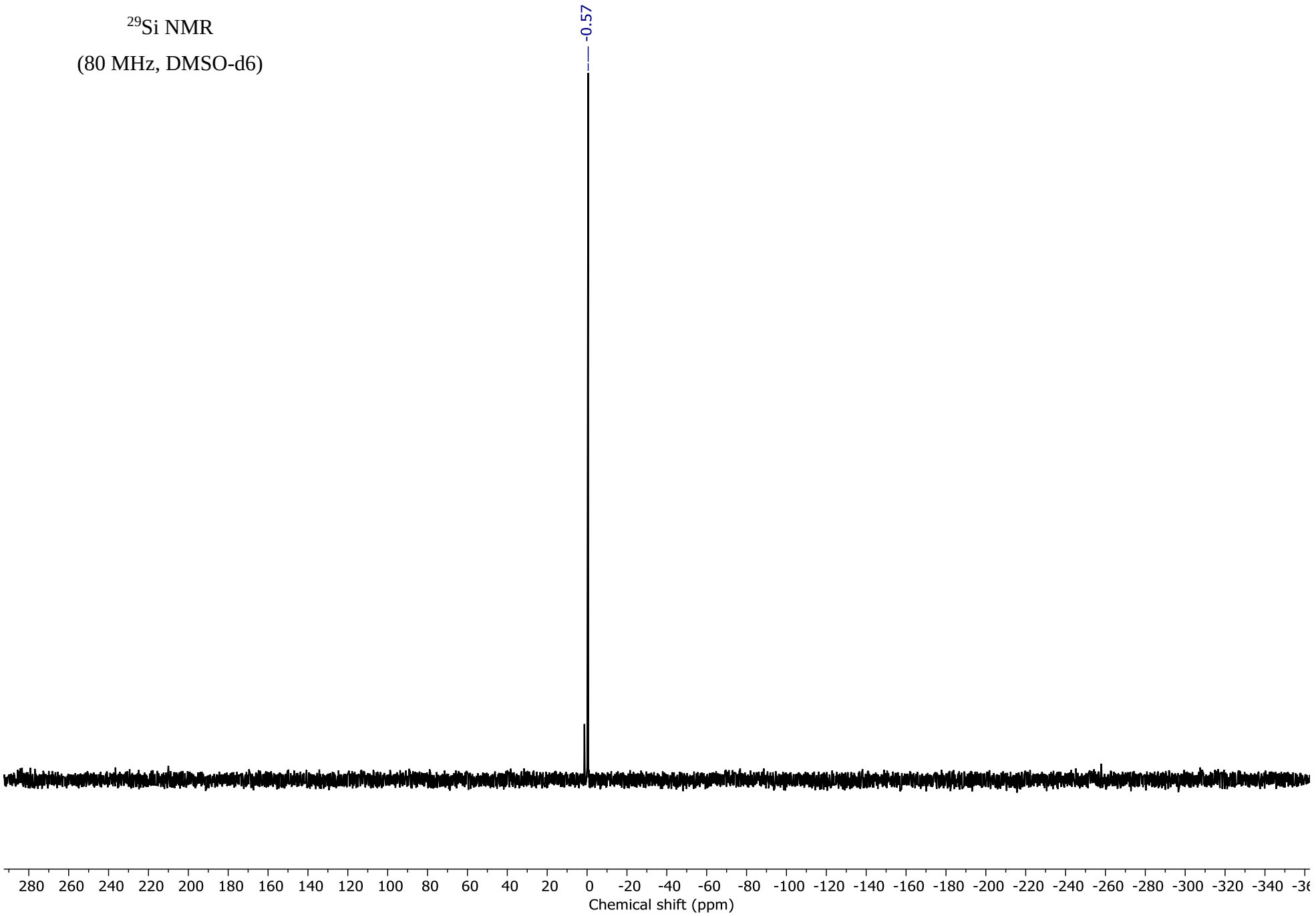
^{13}C NMR

(100 MHz, DMSO-d6)



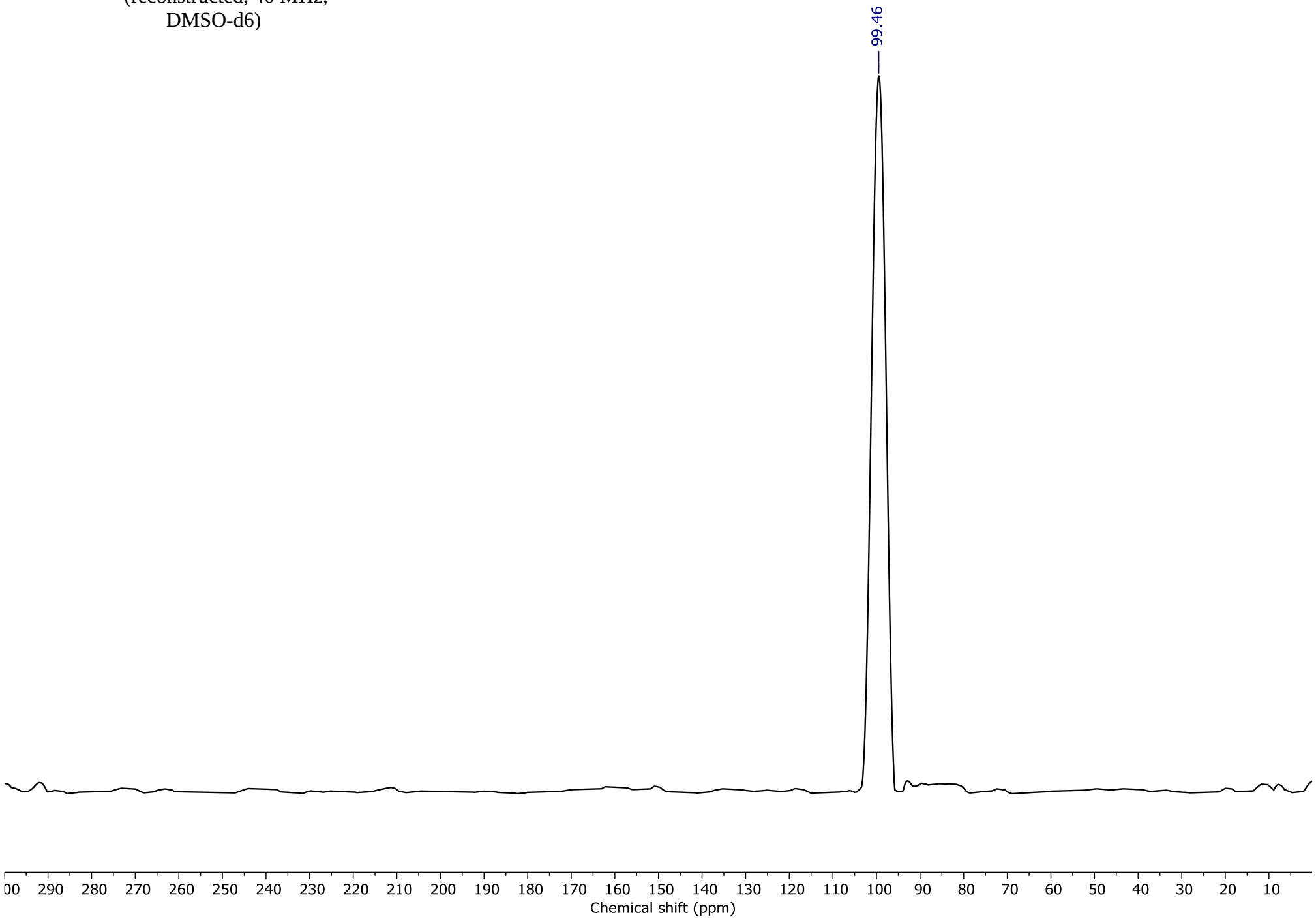
^{29}Si NMR

(80 MHz, DMSO-d6)



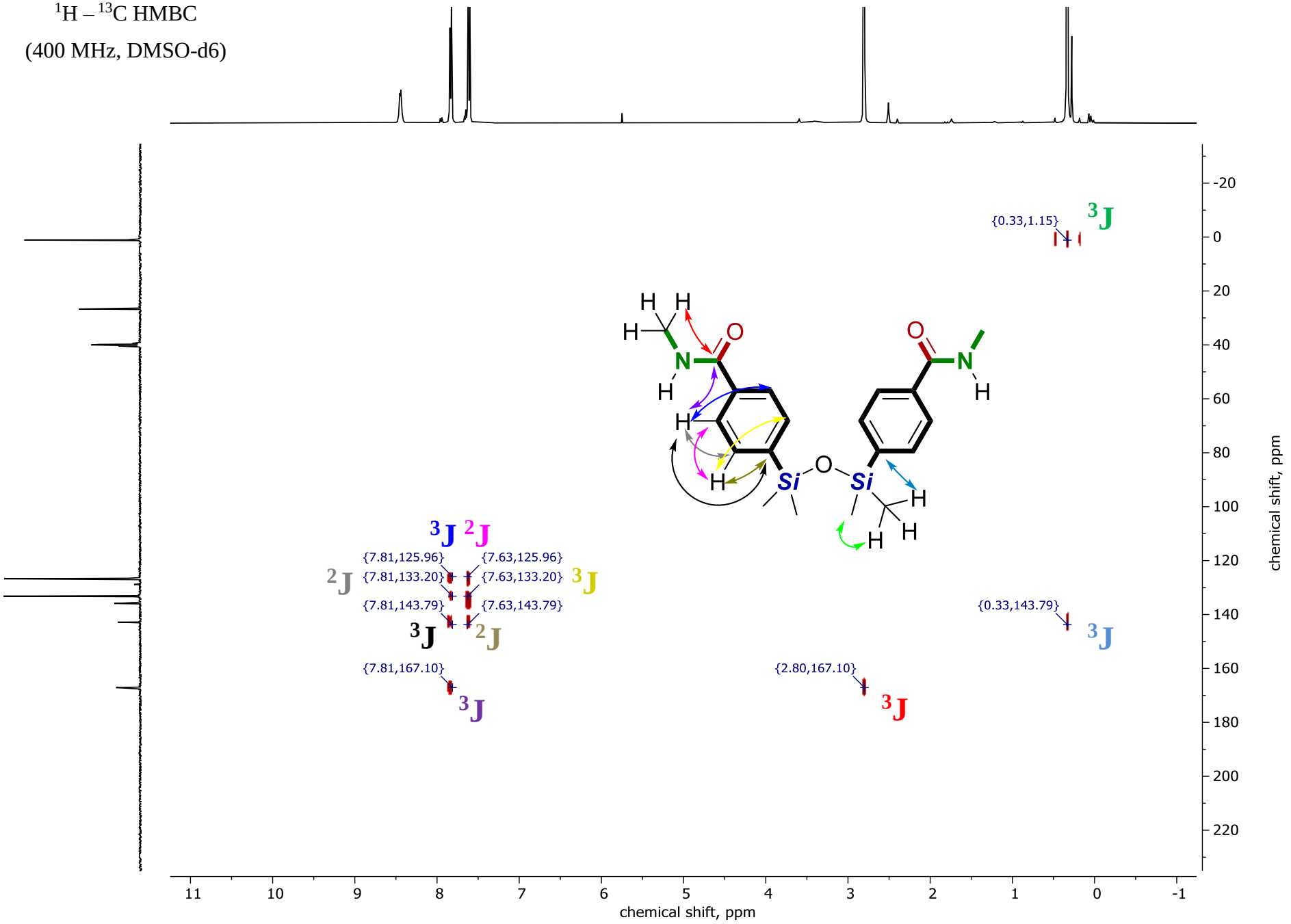
^{15}N NMR

(reconstructed, 40 MHz, DMSO-d6)



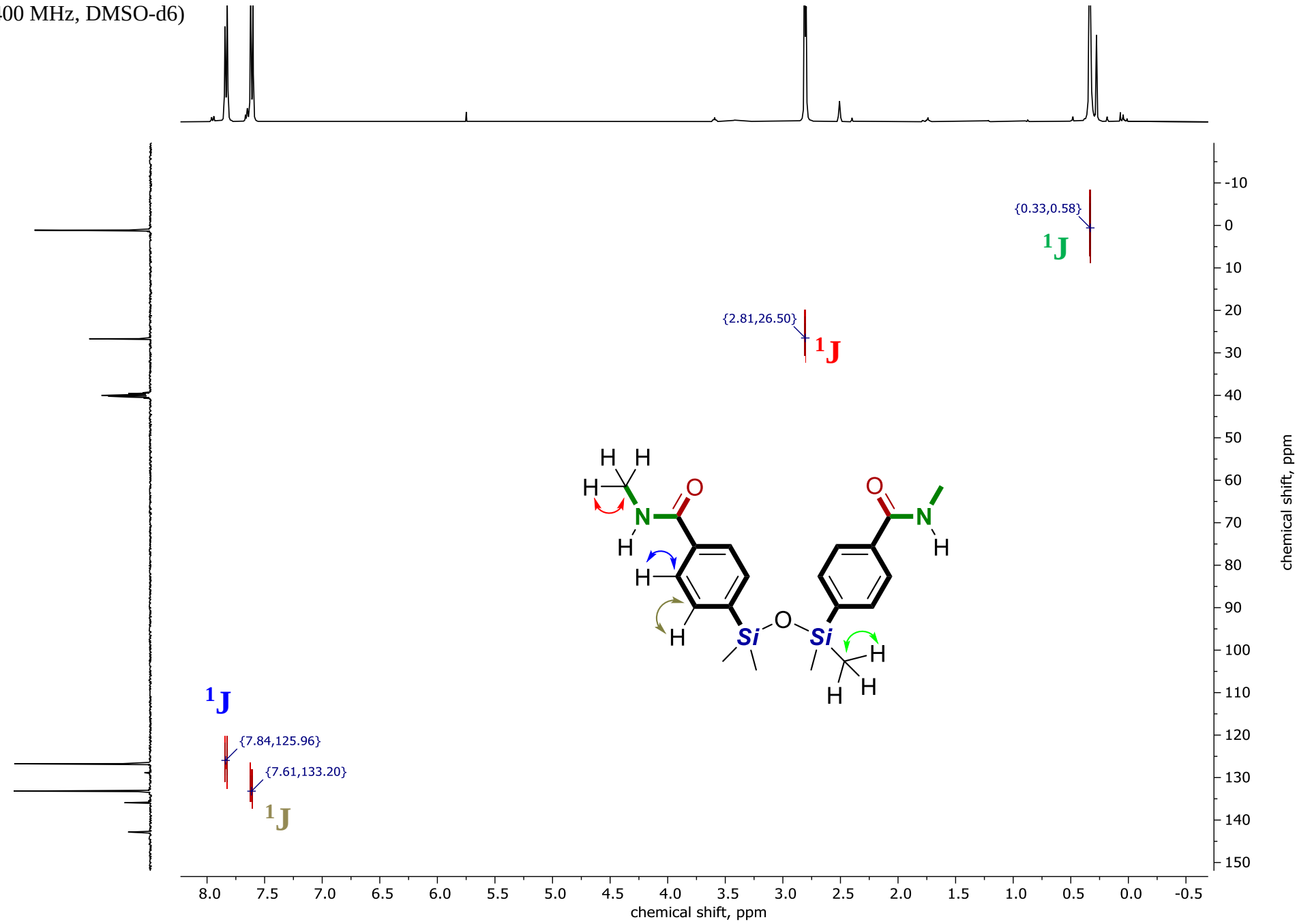
$^{1}H - {}^{13}C$ HMBC

(400 MHz, DMSO-d6)



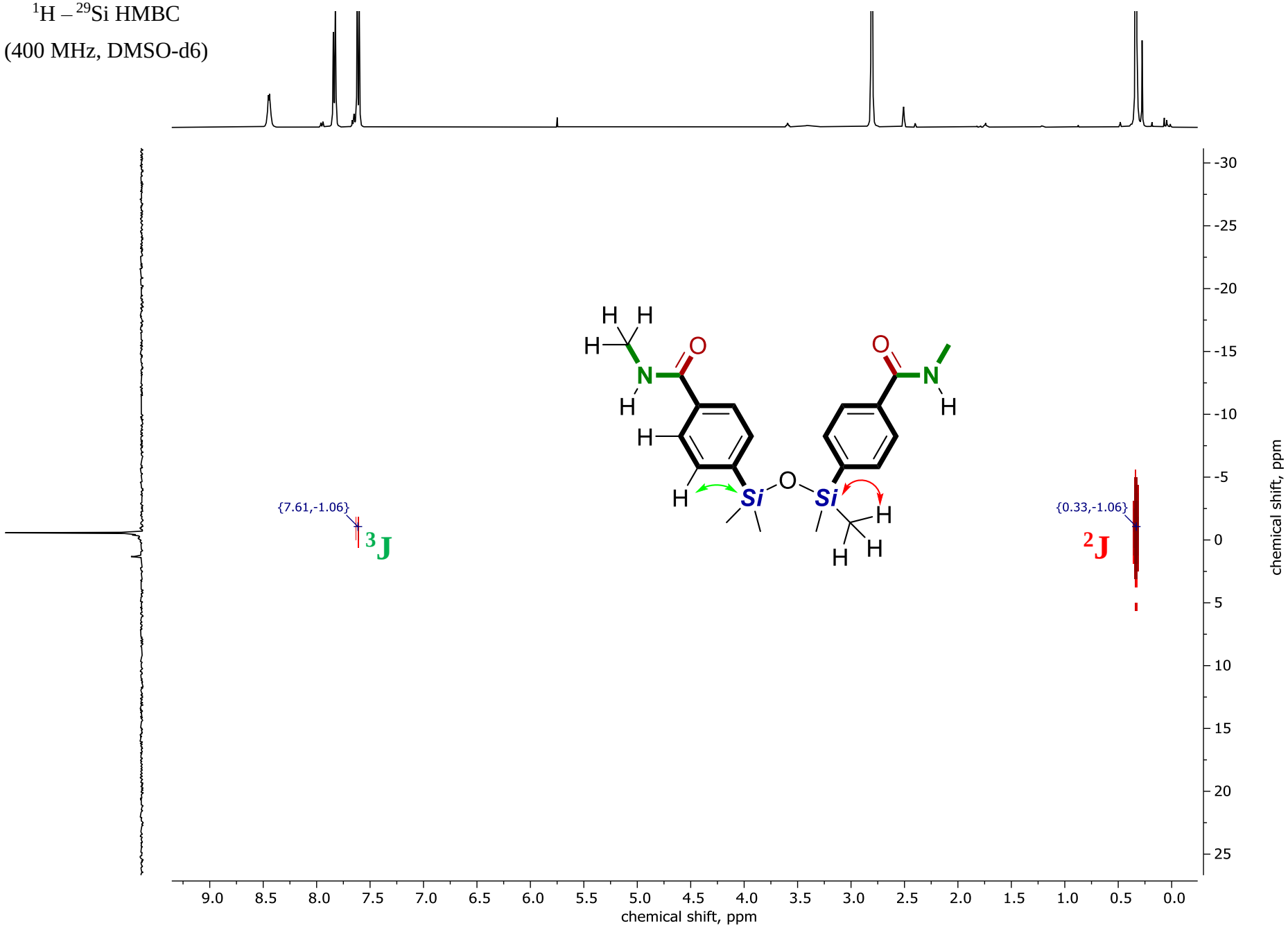
$^{1}H - ^{13}C$ HSQC

(400 MHz, DMSO-d6)



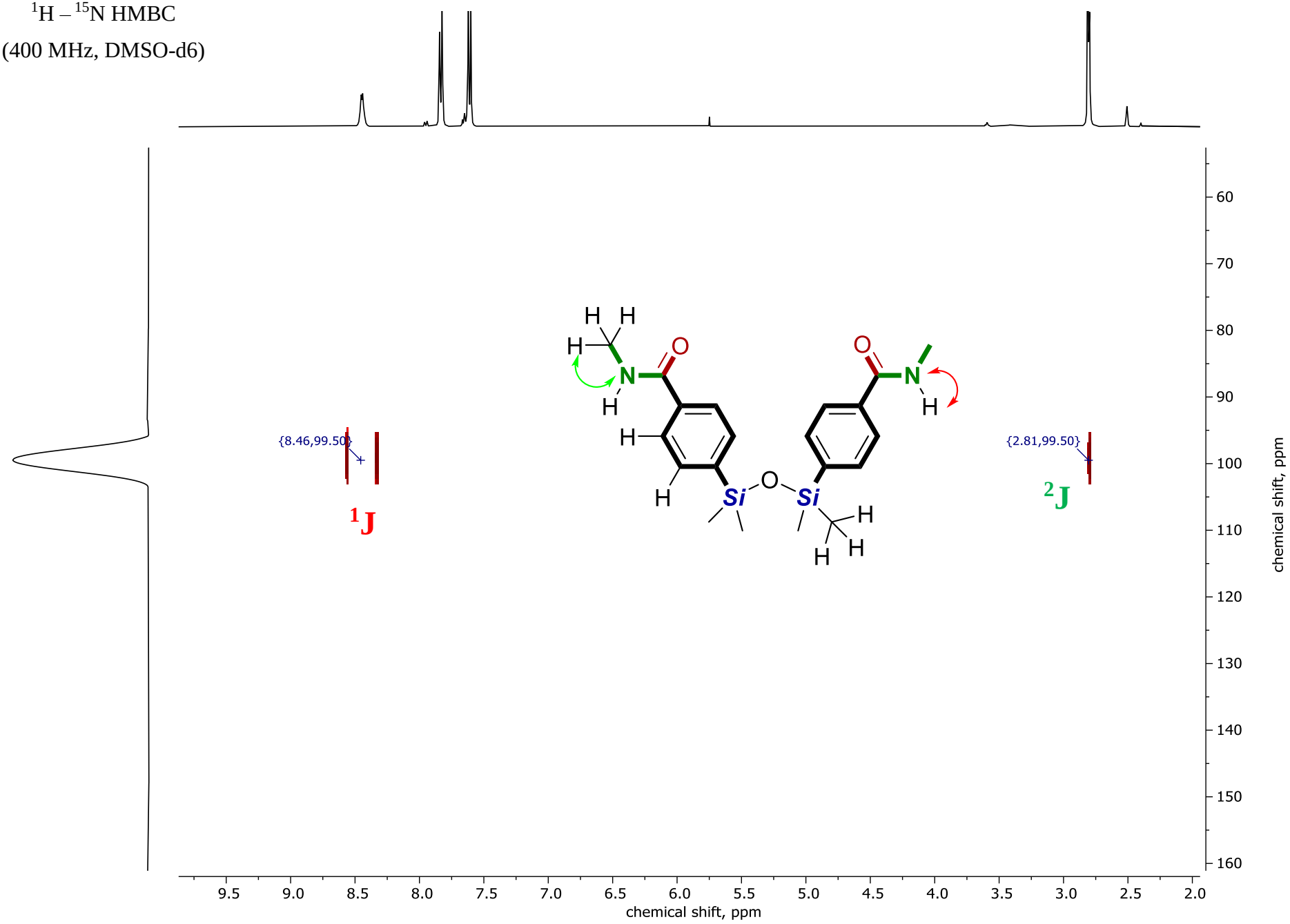
$^{1}H - ^{29}Si$ HMBC

(400 MHz, DMSO-d6)



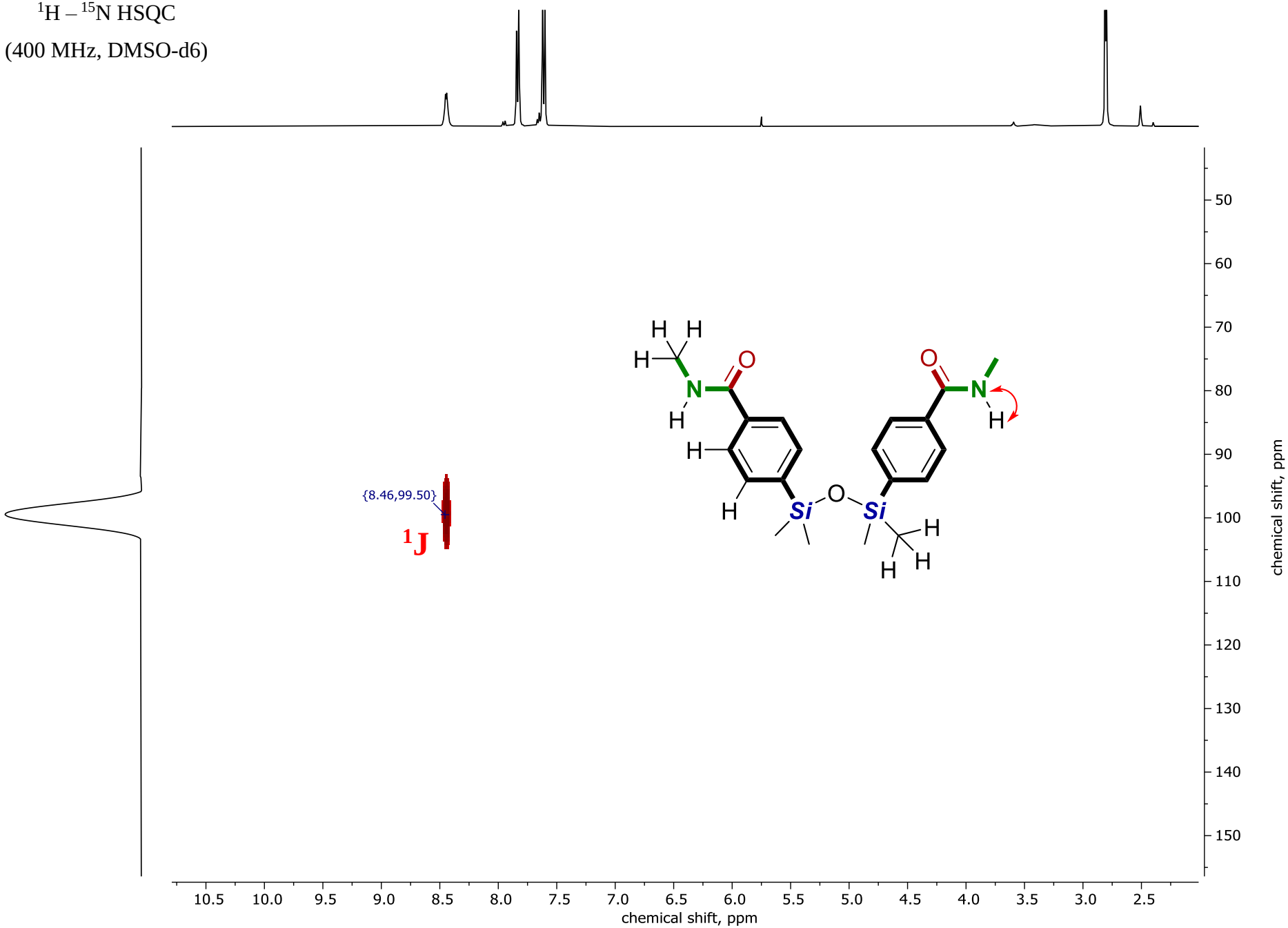
$^{1}H - {}^{15}N$ HMBC

(400 MHz, DMSO-d6)

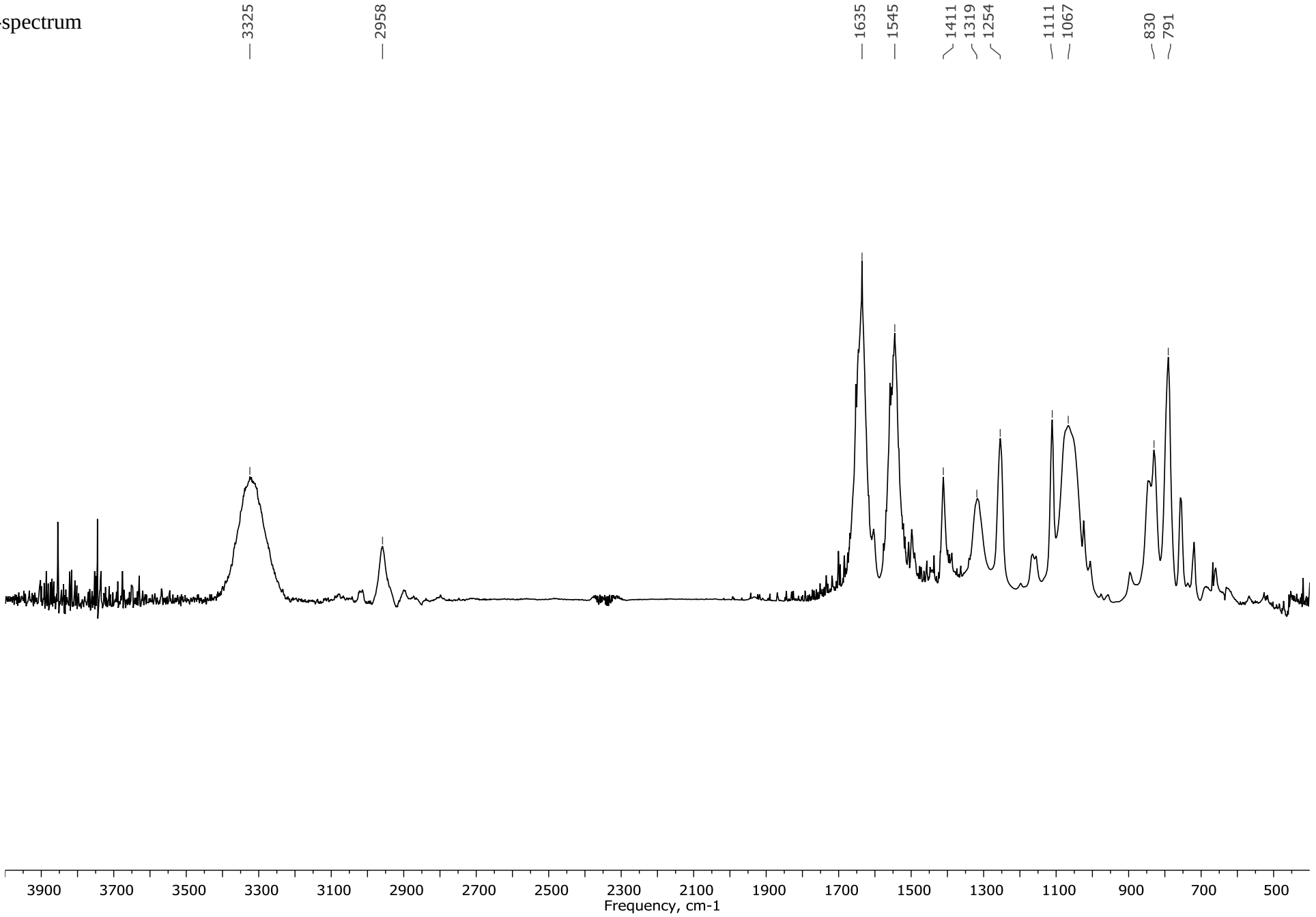


$^{1}H - ^{15}N$ HSQC

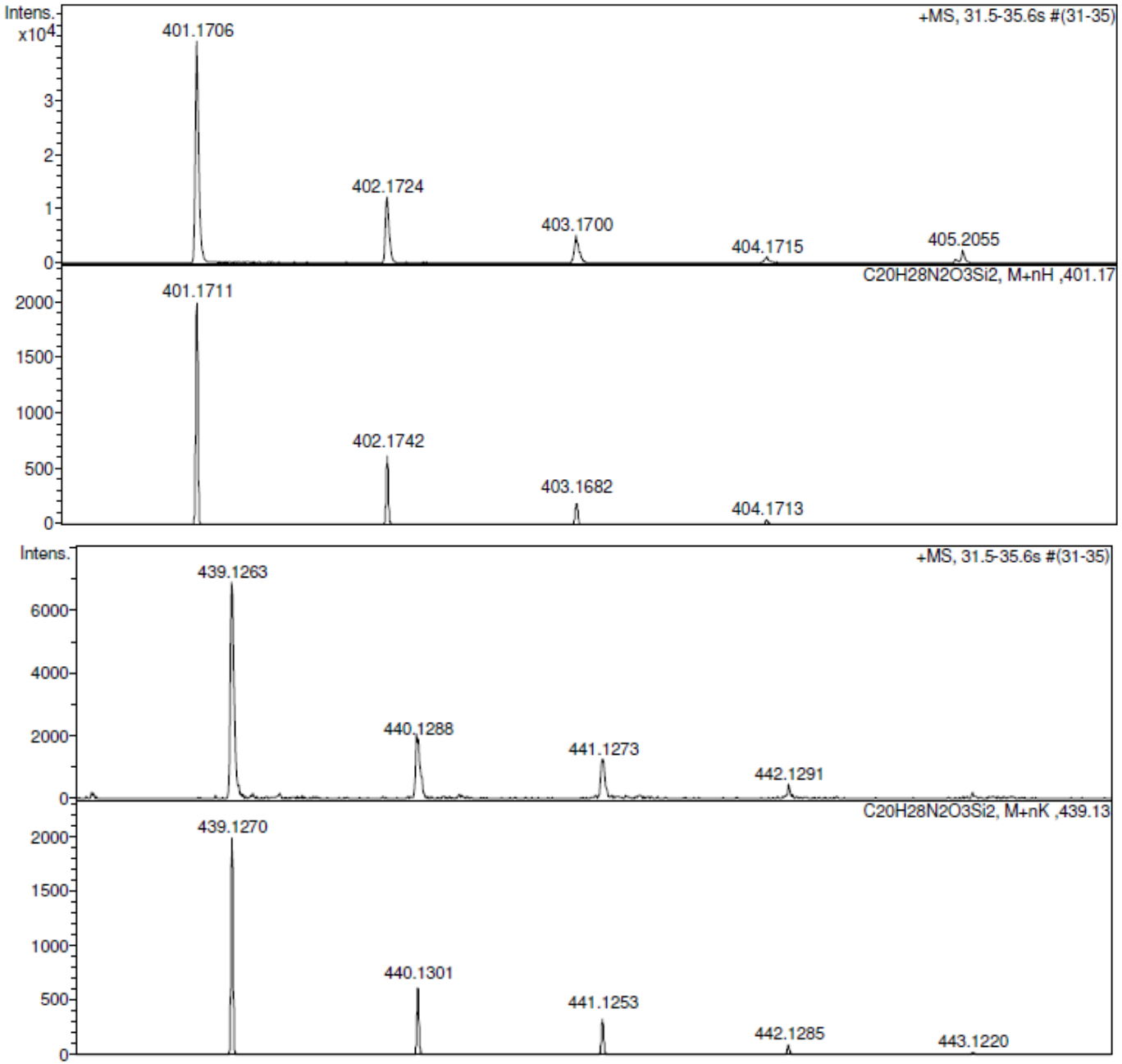
(400 MHz, DMSO-d6)

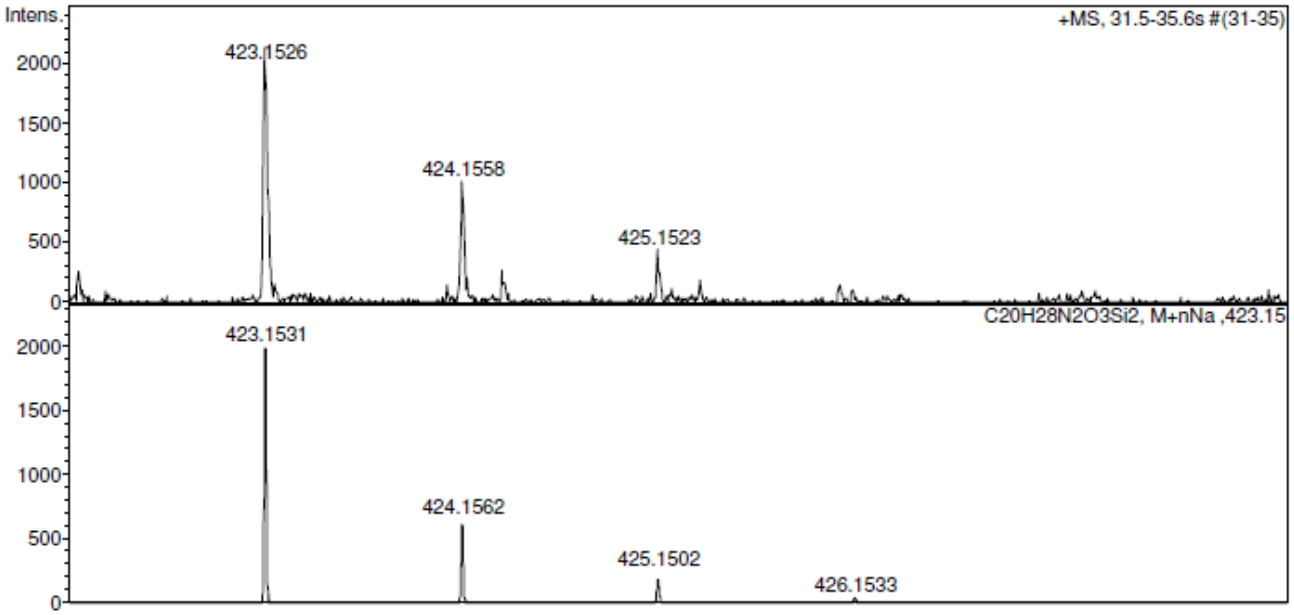


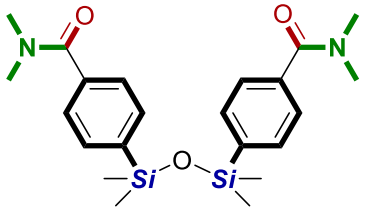
IR-spectrum


3325
2958
1635
1545
1411
1319
1254
1111
1067
830
791
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, 31.5-35.6s #(31-35)
401.1706
402.1724
403.1700
404.1715
405.2055
C20H28N2O3Si2, M+nH ,401.17
401.1711
402.1742
403.1682
404.1713
Intens.
+MS, 31.5-35.6s #(31-35)
439.1263
440.1288
441.1273
442.1291
C20H28N2O3Si2, M+nK ,439.13
439.1270
440.1301
441.1253
442.1285
443.1220


Intens.
+MS, 31.5-35.6s #(31-35)
423.1526
424.1558
425.1523
2000
1500
1000
500
0
C20H28N2O3Si2, M+nNa ,423.15
423.1531
424.1562
425.1502
426.1533

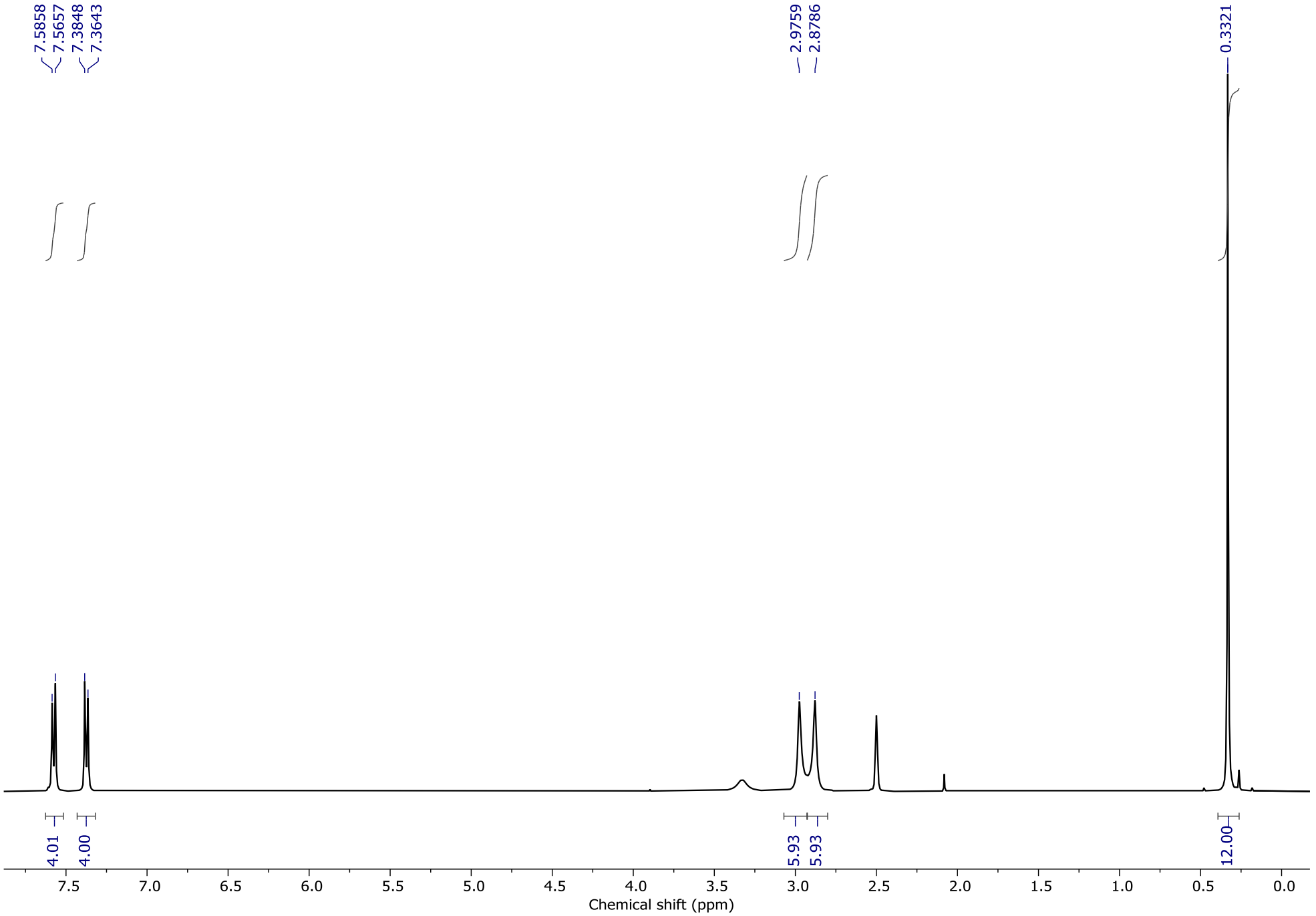


Characterisation data for 4,4'-(1,1,3,3-tetramethyldisiloxane-1,3-diyl)bis(N,N-dimethylbenzamide):

^{1}H NMR (400 MHz, DMSO-d6): δ =7.58 (d, ^{3}J=8 Hz, 4H); δ = 7.37 (d, ^{3}J=8 Hz, 4H); δ = 2.98 (s, 6H); δ = 2.88 (s, 6H) ; δ = 0.33 (s, 12H). ^{13}C NMR (100 MHz, DMSO-d6): δ = 170.43, 140.82, 137.97, 133.13, 126.60, 35.11, 1.44. ^{29}Si NMR (80 MHz, DMSO-d6): δ = -0.61. ^{15}N NMR (40 MHz, DMSO-d6): δ = HRMS (ESI) m/z [M + H] $^{+}$: calcd for $[C_{22}H_{32}N_2O_3Si_2 + H]^{+}$, 429.2024; found, 429.2024; [M + Na] $^{+}$: calcd for $[C_{22}H_{32}N_2O_3Si_2 + Na]^{+}$, 451.1844; found, 451.1840; [M + K] $^{+}$: calcd for $[C_{22}H_{32}N_2O_3Si_2 + K]^{+}$, 467.158; found, 467.1588. IR (cm^{-1}): 2955, 1628, 1507-1398, 1254, 1074, 833, 790.

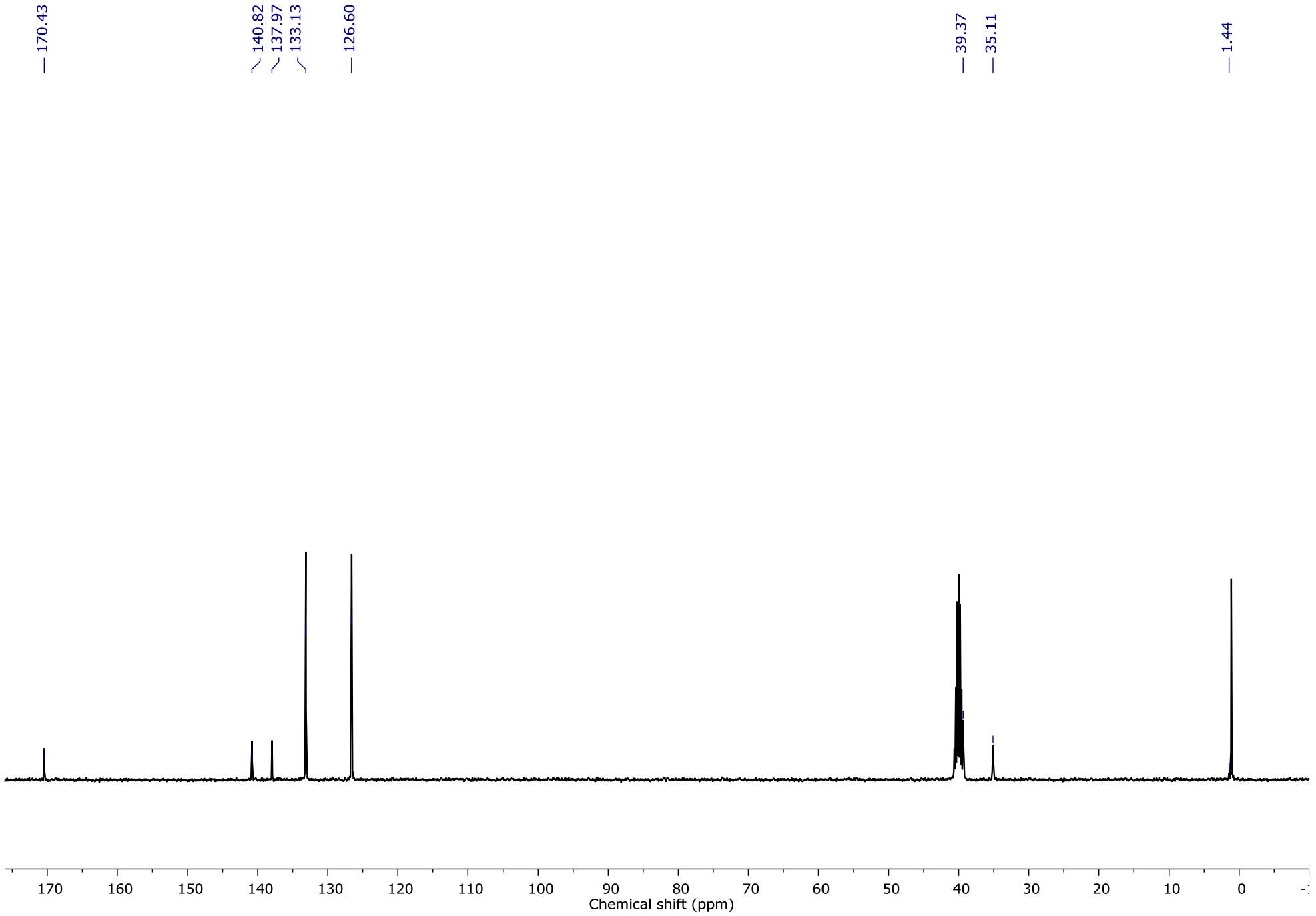
^{1}H NMR

(400 MHz, DMSO-d6)



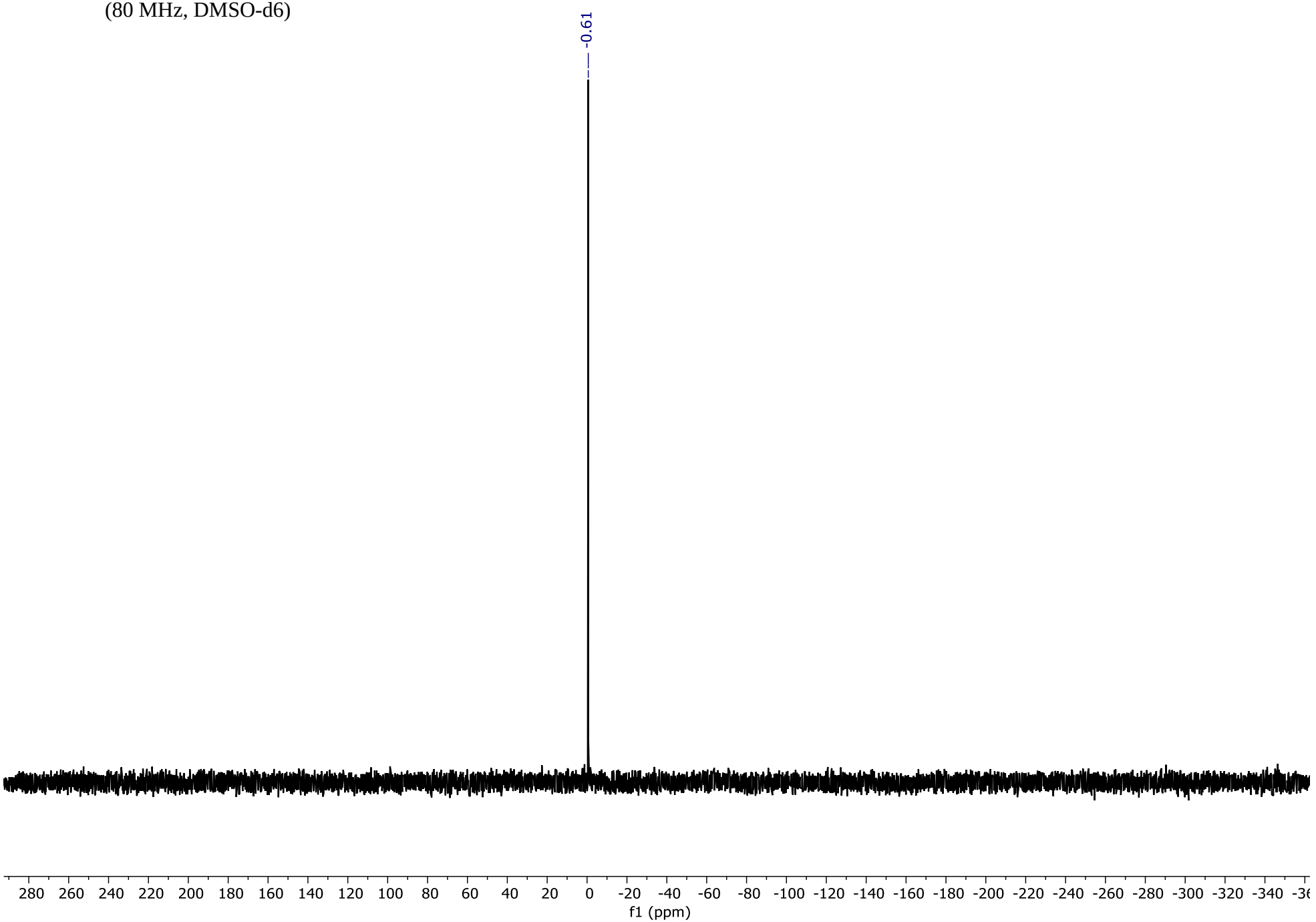
^{13}C NMR

(100 MHz, DMSO-d6)



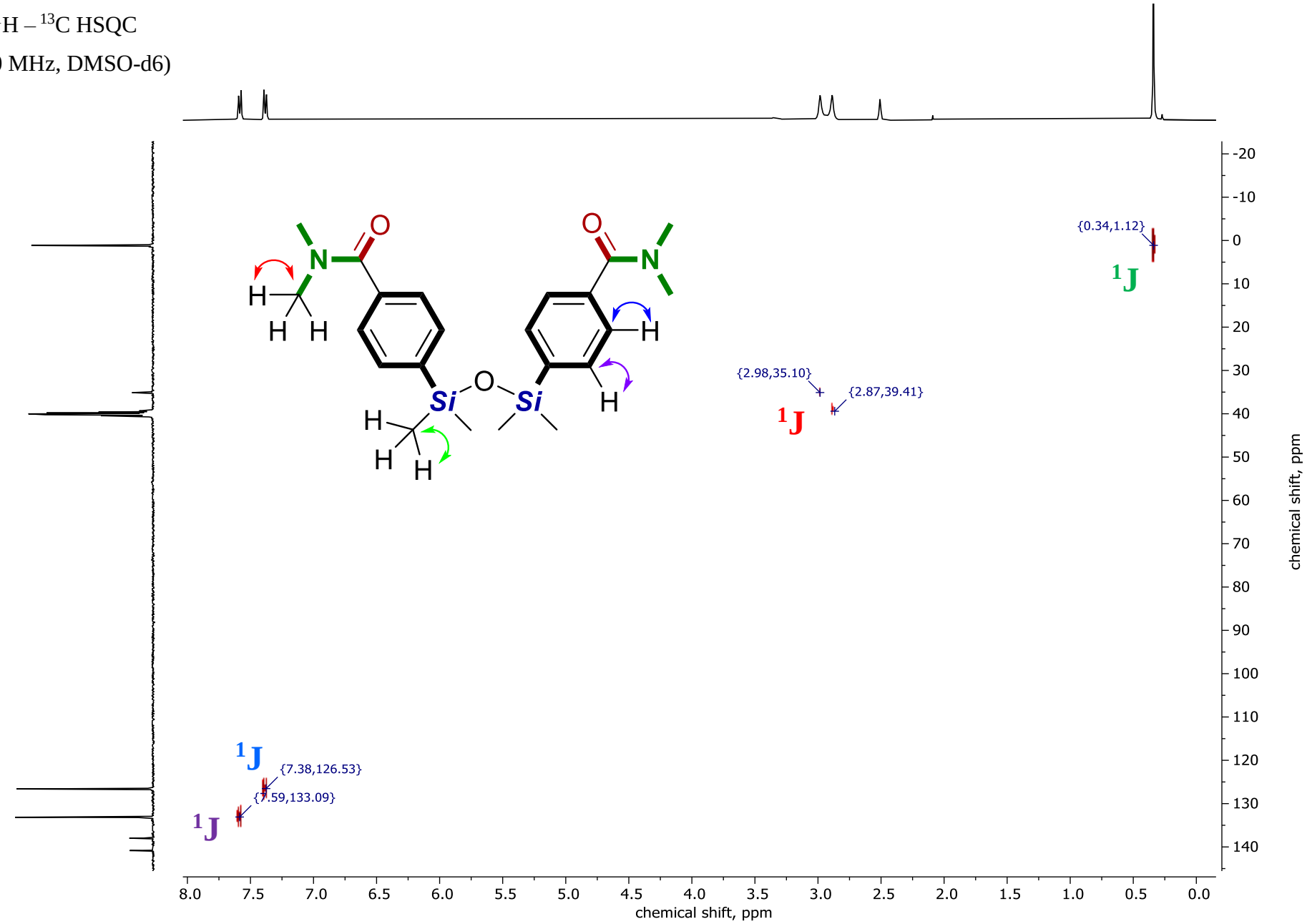
^{29}Si NMR

(80 MHz, DMSO-d6)



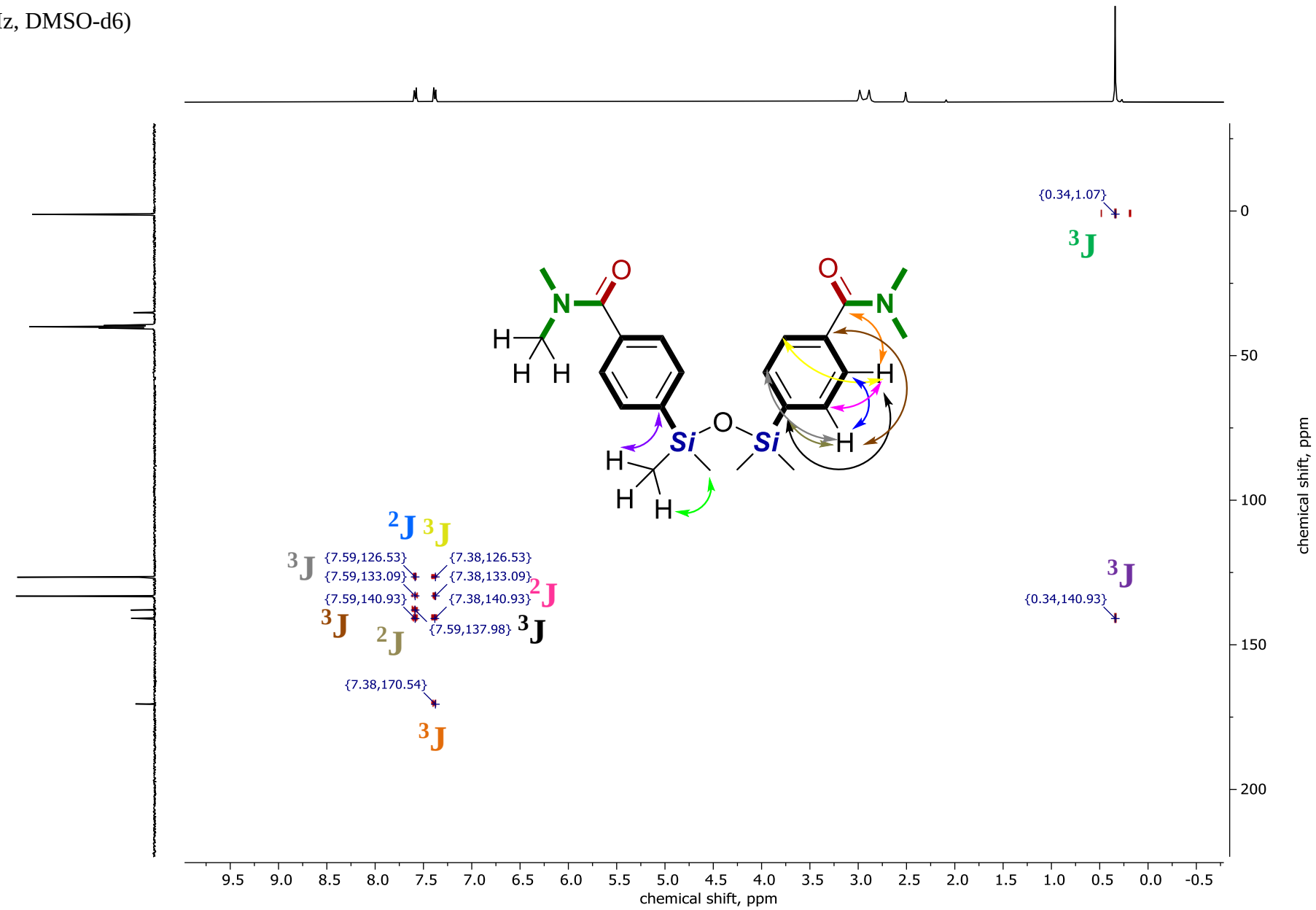
$^{1}H - ^{13}C$ HSQC

(400 MHz, DMSO-d6)



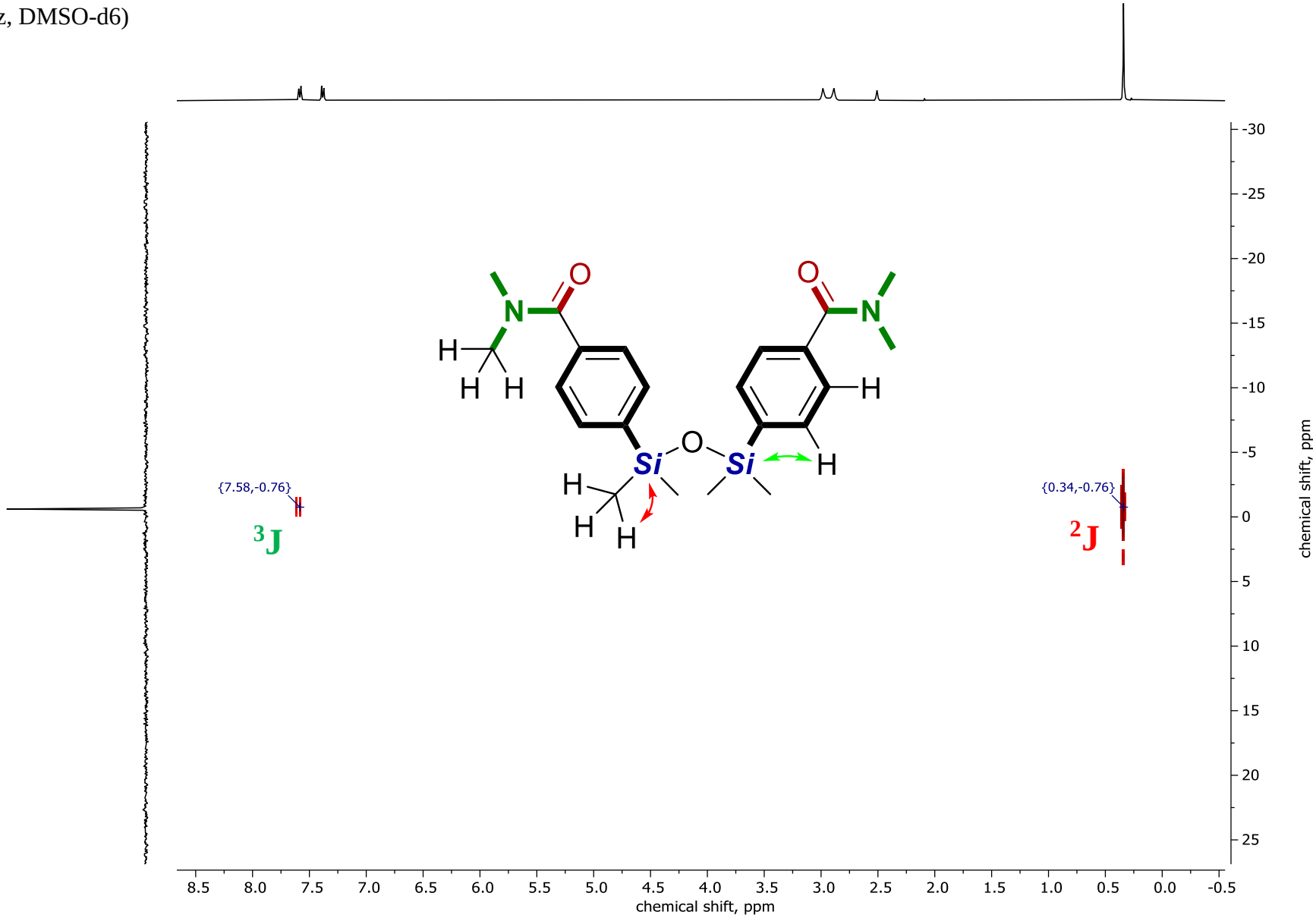
$^{1}H - {}^{13}C$ HMBC

(400 MHz, DMSO-d6)

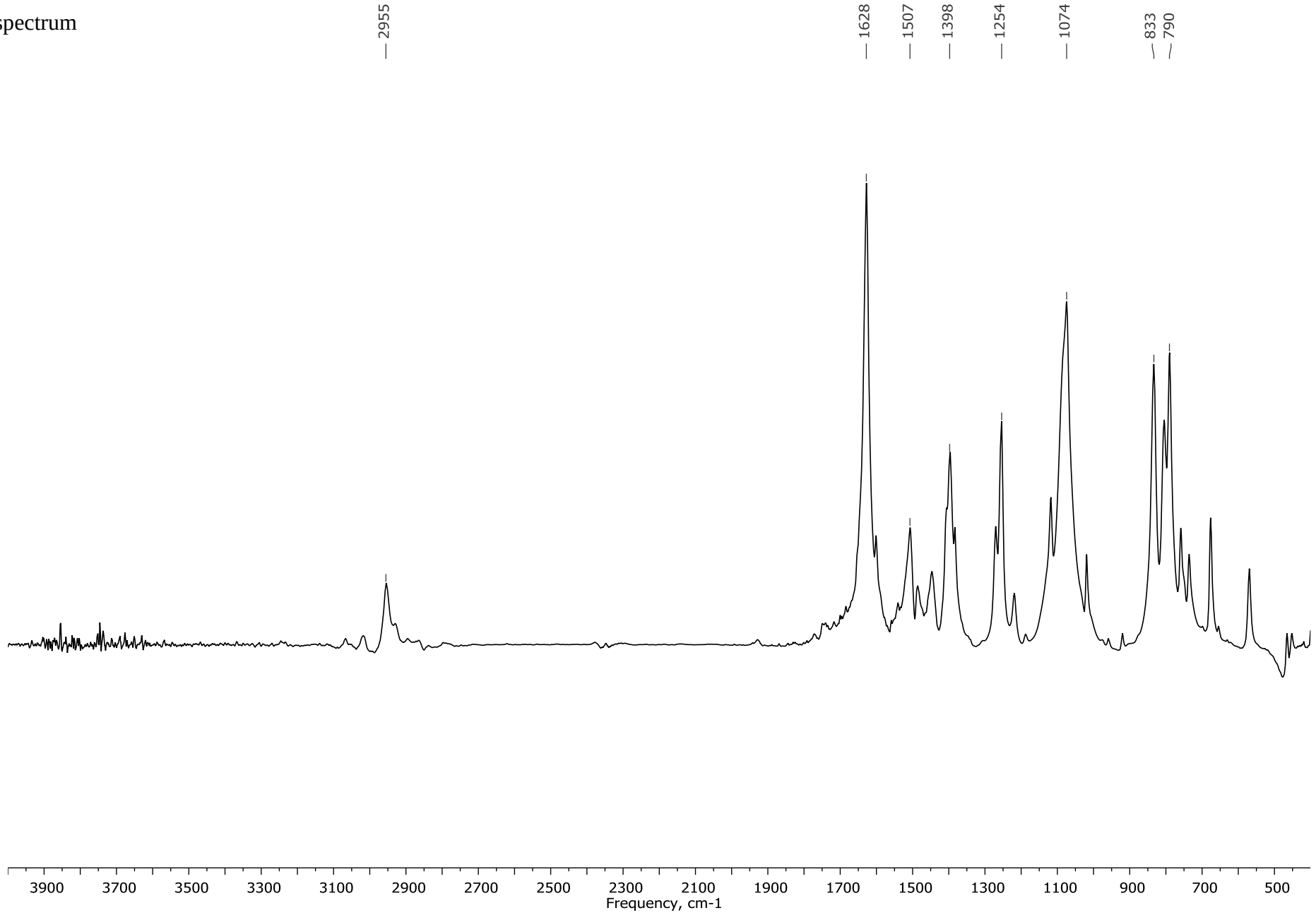


$^{1}H - {}^{29}Si$ HMBC

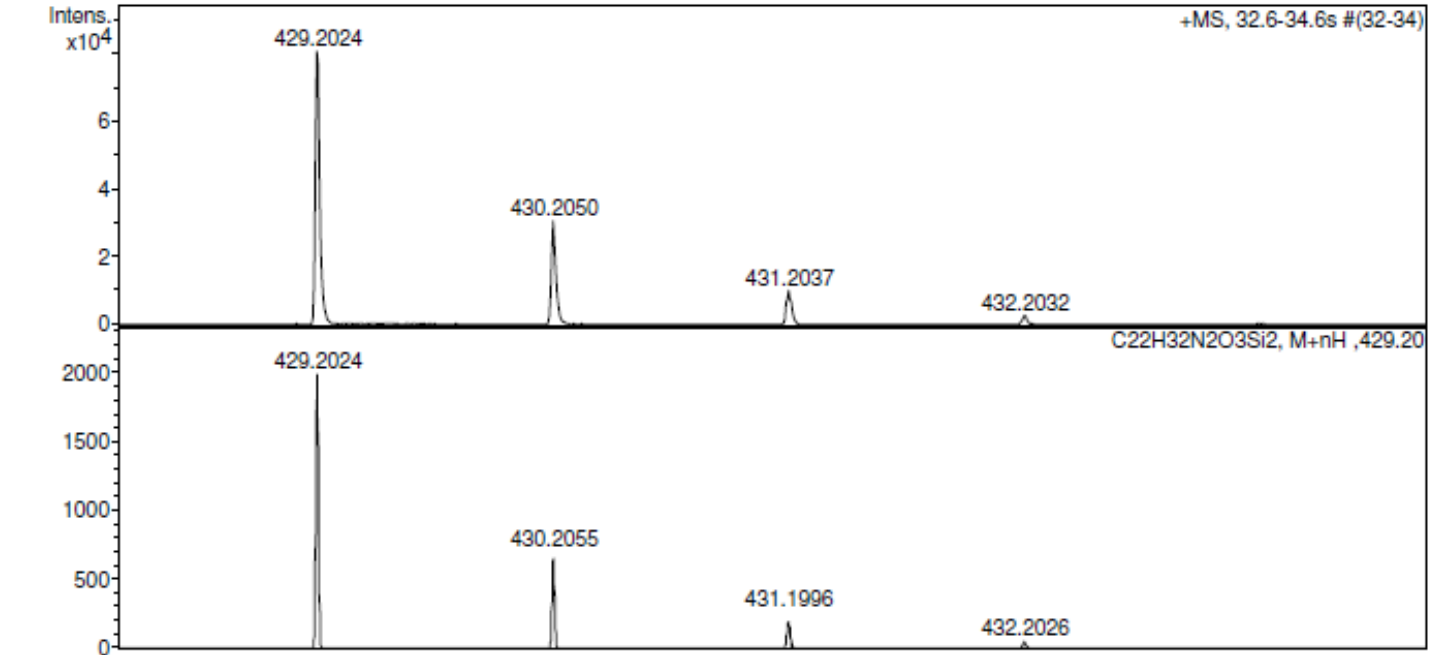
(400 MHz, DMSO-d6)

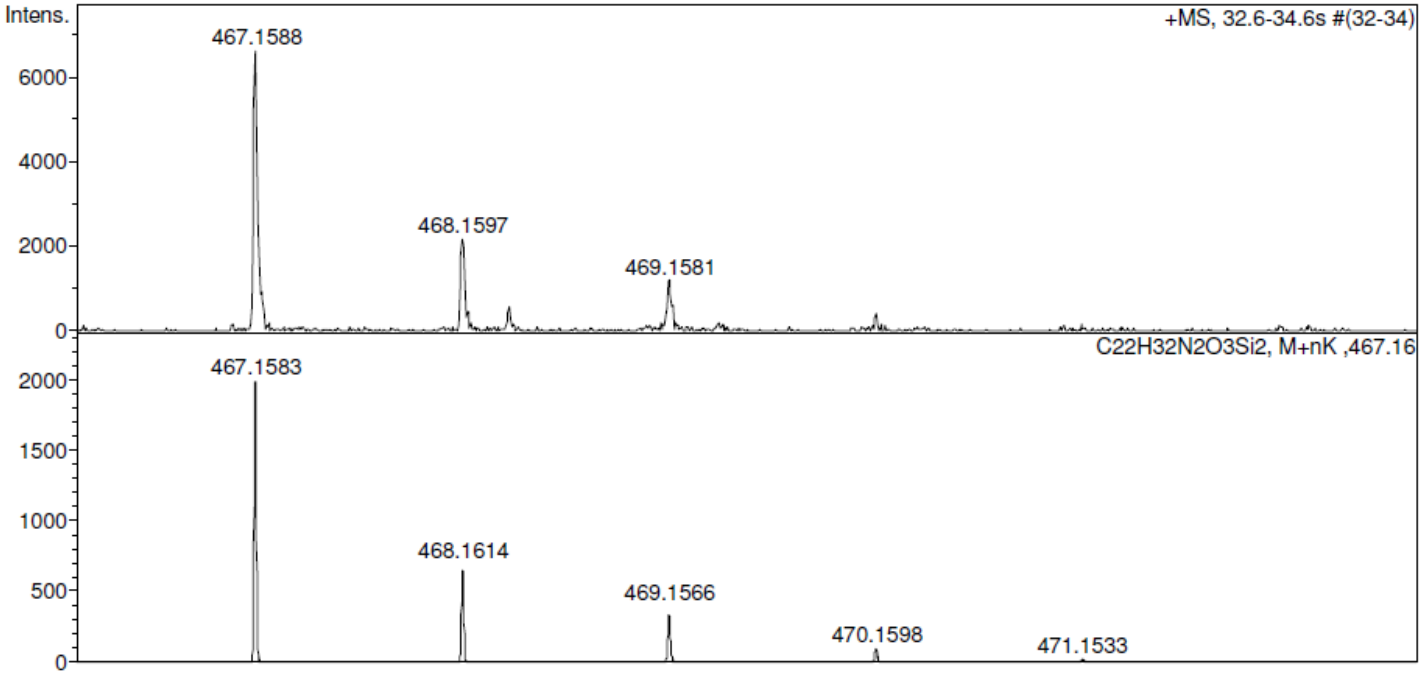


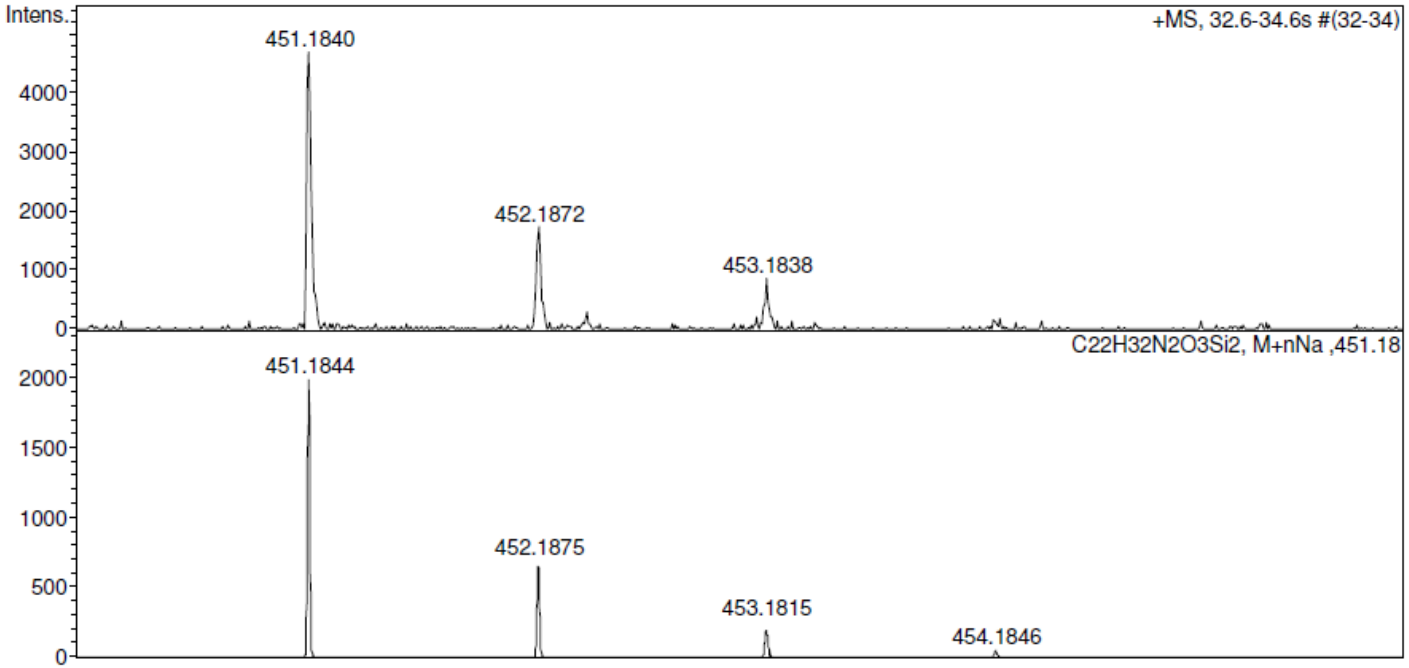
IR-spectrum

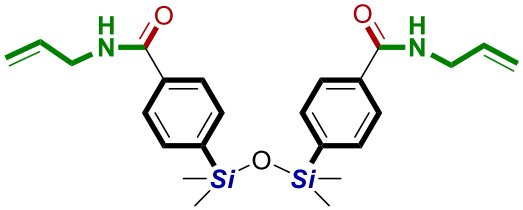

2955
1628
1507
1398
1254
1074
833
790
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

HRMS (ESI)


Intens.
x10^4
+MS, 32.6-34.6s #(32-34)
429.2024
430.2050
431.2037
432.2032
C22H32N2O3Si2, M+nH ,429.20
429.2024
430.2055
431.1996
432.2026


Intens.
+MS, 32.6-34.6s #(32-34)
467.1588
468.1597
469.1581
C22H32N2O3Si2, M+nK ,467.16
467.1583
468.1614
469.1566
470.1598
471.1533


Intens.
+MS, 32.6-34.6s #(32-34)
451.1840
452.1872
453.1838
4000
3000
2000
1000
0
C22H32N2O3Si2, M+nNa ,451.18
451.1844
452.1875
453.1815
454.1846
2000
1500
1000
500
0

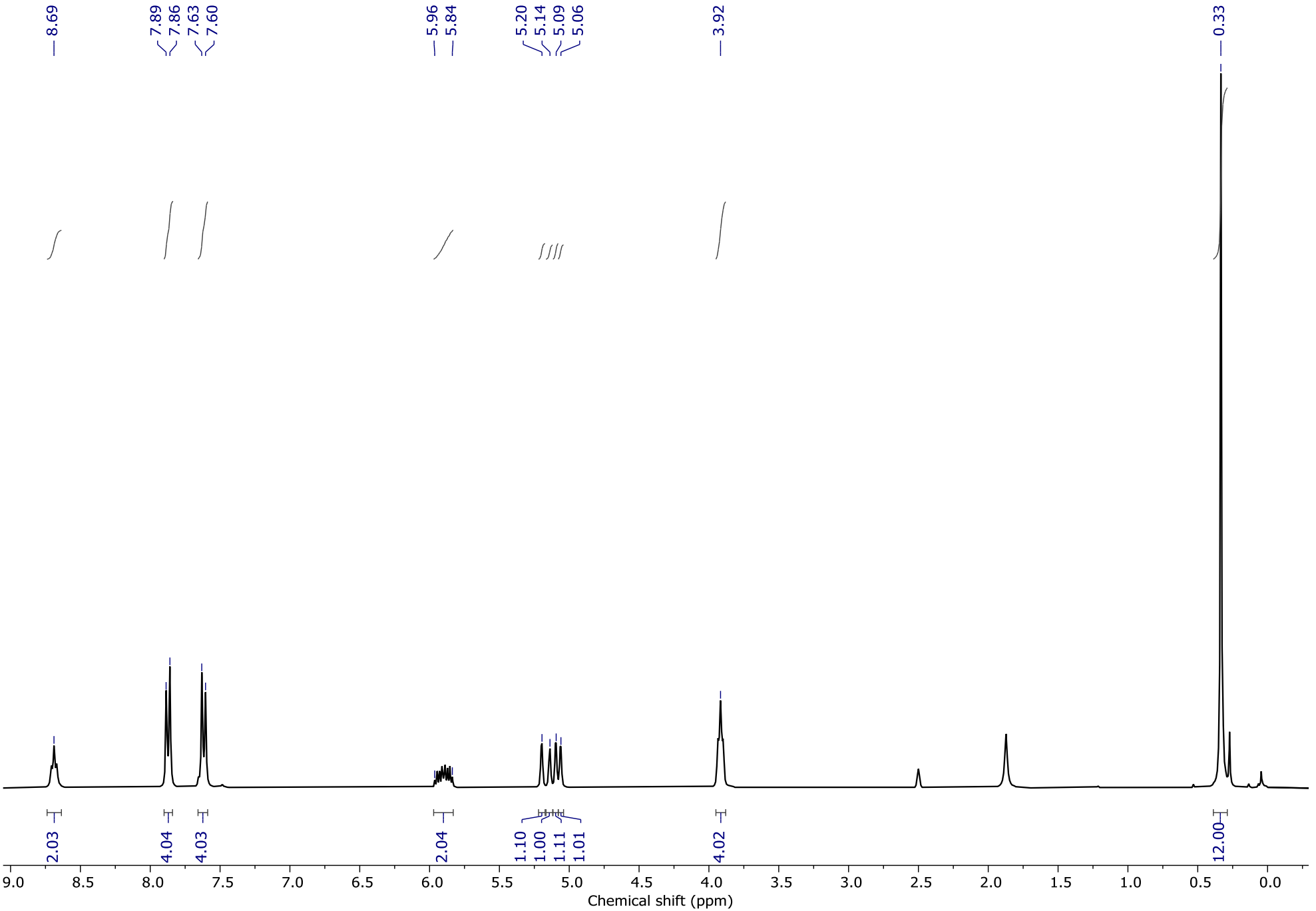


Characterisation data for 4,4'-(1,1,3,3-tetramethyldisiloxane-1,3-diyl)bis(N-allylbenzamide):

^{1}H NMR (400 MHz, DMSO-d6): δ = 8.69 (t, ^{3}J=8 Hz, 2H), δ = 7.87 (d, ^{3}J=11 Hz, 4H), δ = 7.62 (d, ^{3}J=11 Hz, 4H), δ = 5.96-5.84 (m, 2H), δ = 5.20-5.06 (m, 4H), δ = 3.92 (t, ^{3}J=7 Hz, 4H), δ = 0.33 (s, 12H). ^{13}C NMR (100 MHz, DMSO-d6): δ = 173.62, 166.52, 143.00, 135.88, 133.18, 126.92, 115.54, 41.99, 1.13. ^{29}Si NMR (80 MHz, DMSO-d6): δ = -0.56. ^{15}N NMR (40 MHz, DMSO-d6): δ = 109.80. HRMS (ESI) m/z [M + H] $^{+}$: calcd for $[C_{24}H_{32}N_2O_3Si_2 + H]^{+}$, 453.2024; found, 453.2026. IR (cm^{-1}): 3279, 2953, 1636, 1539, 1305, 1254, 1107, 1070, 838-668.

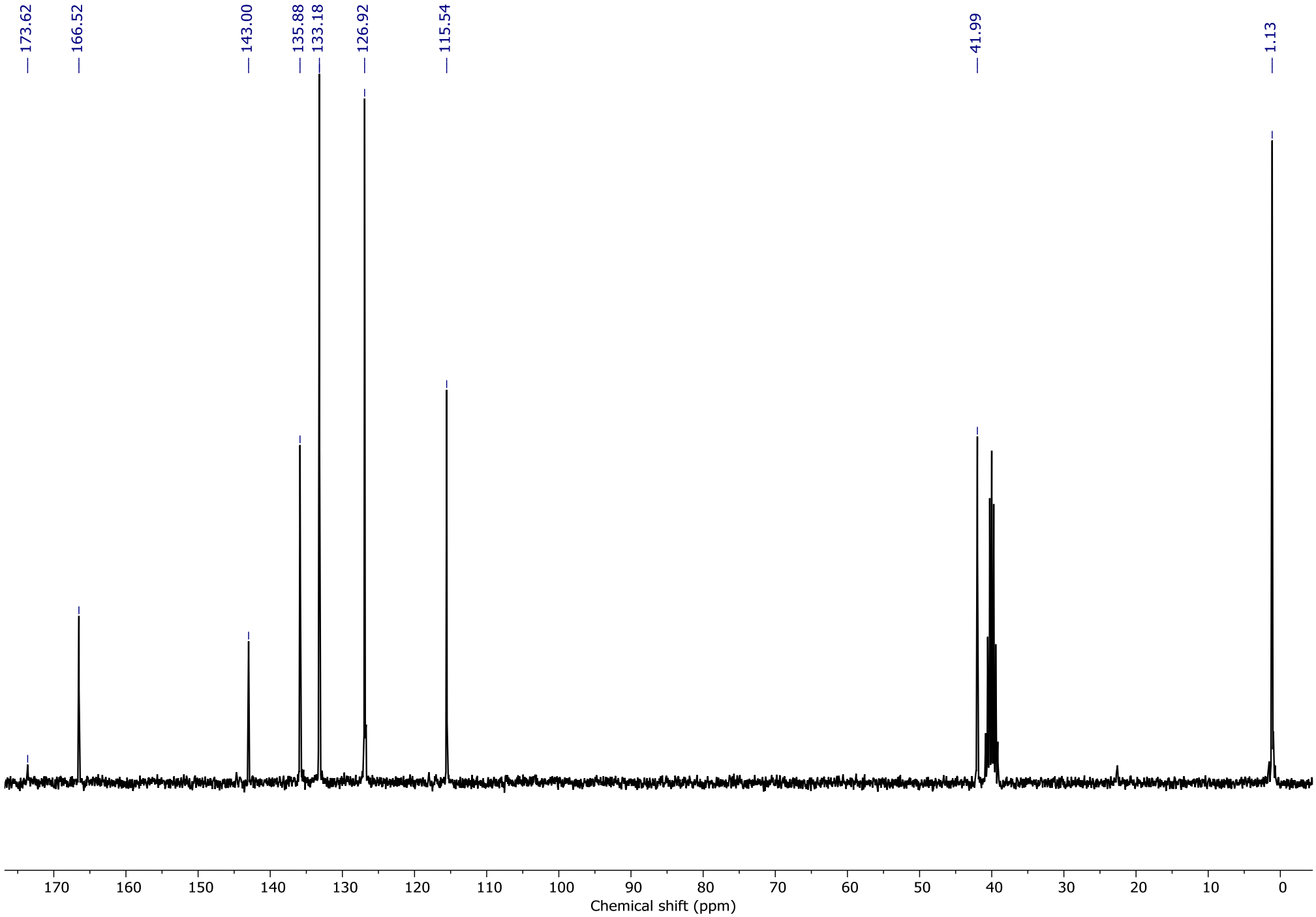
^{1}H NMR

(400 MHz, DMSO-d6)



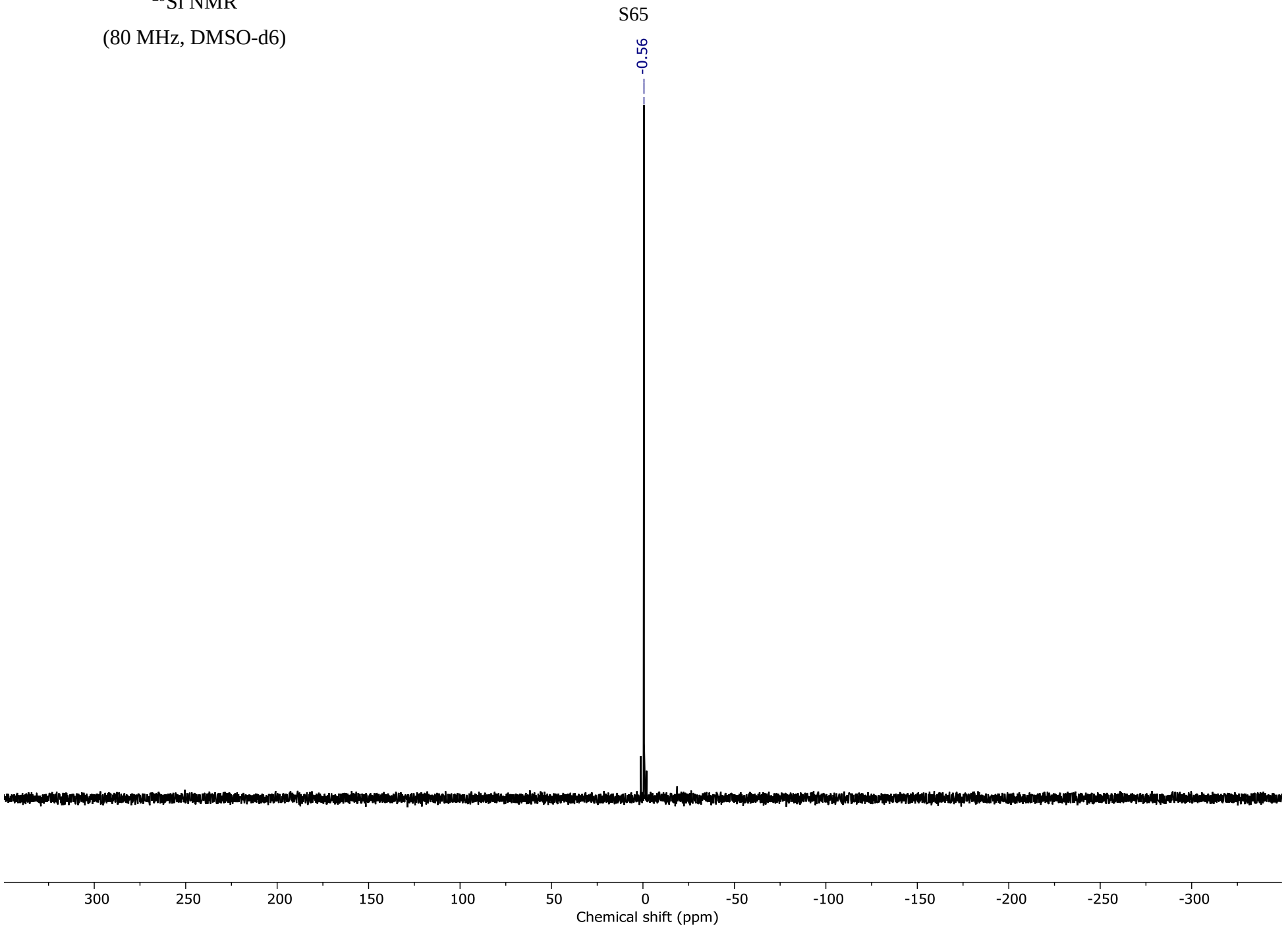
^{13}C NMR

(100 MHz, DMSO-d6)



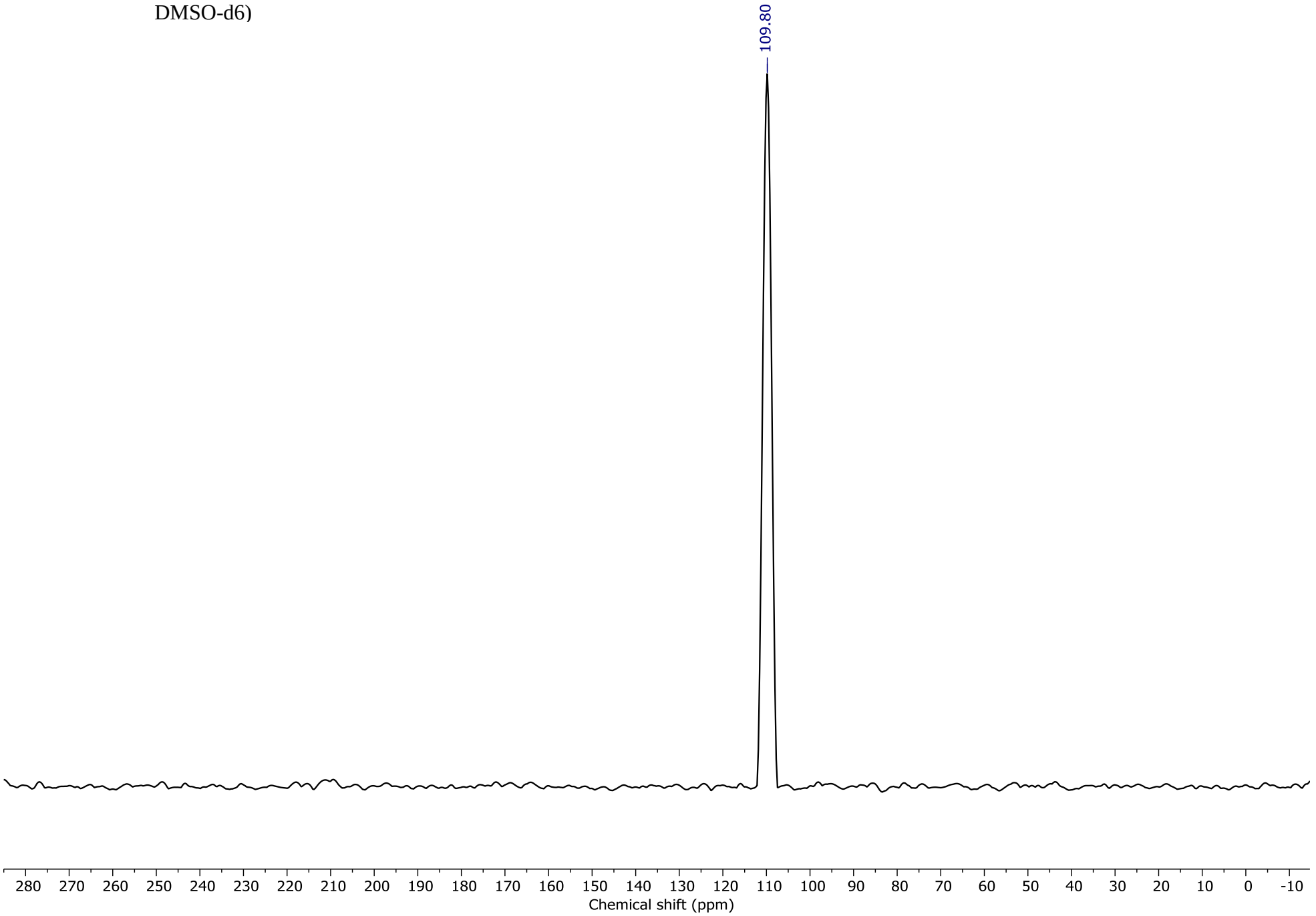
^{29}Si NMR

(80 MHz, DMSO-d6)



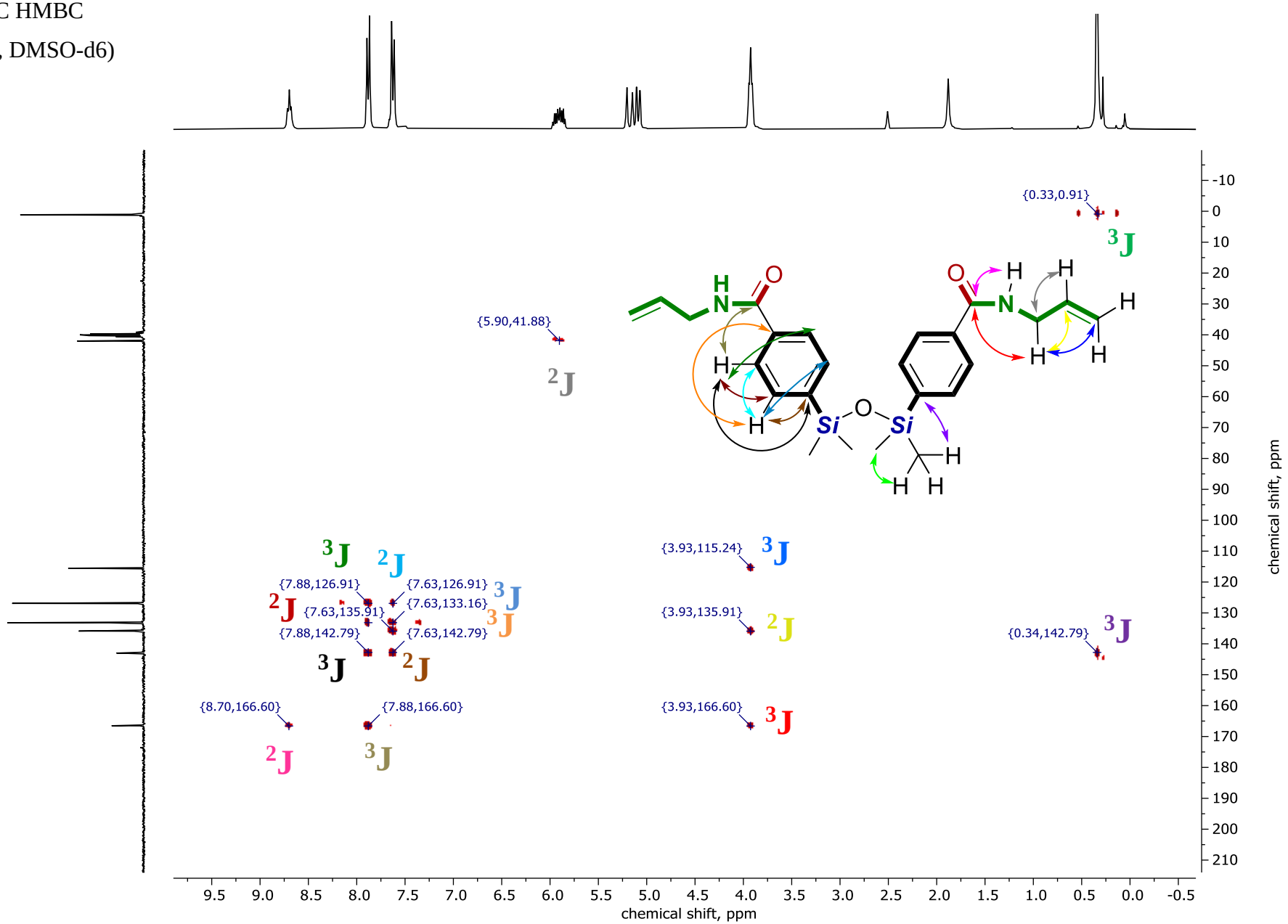
^{15}N NMR

(reconstructed, 40 MHz, DMSO-d6)



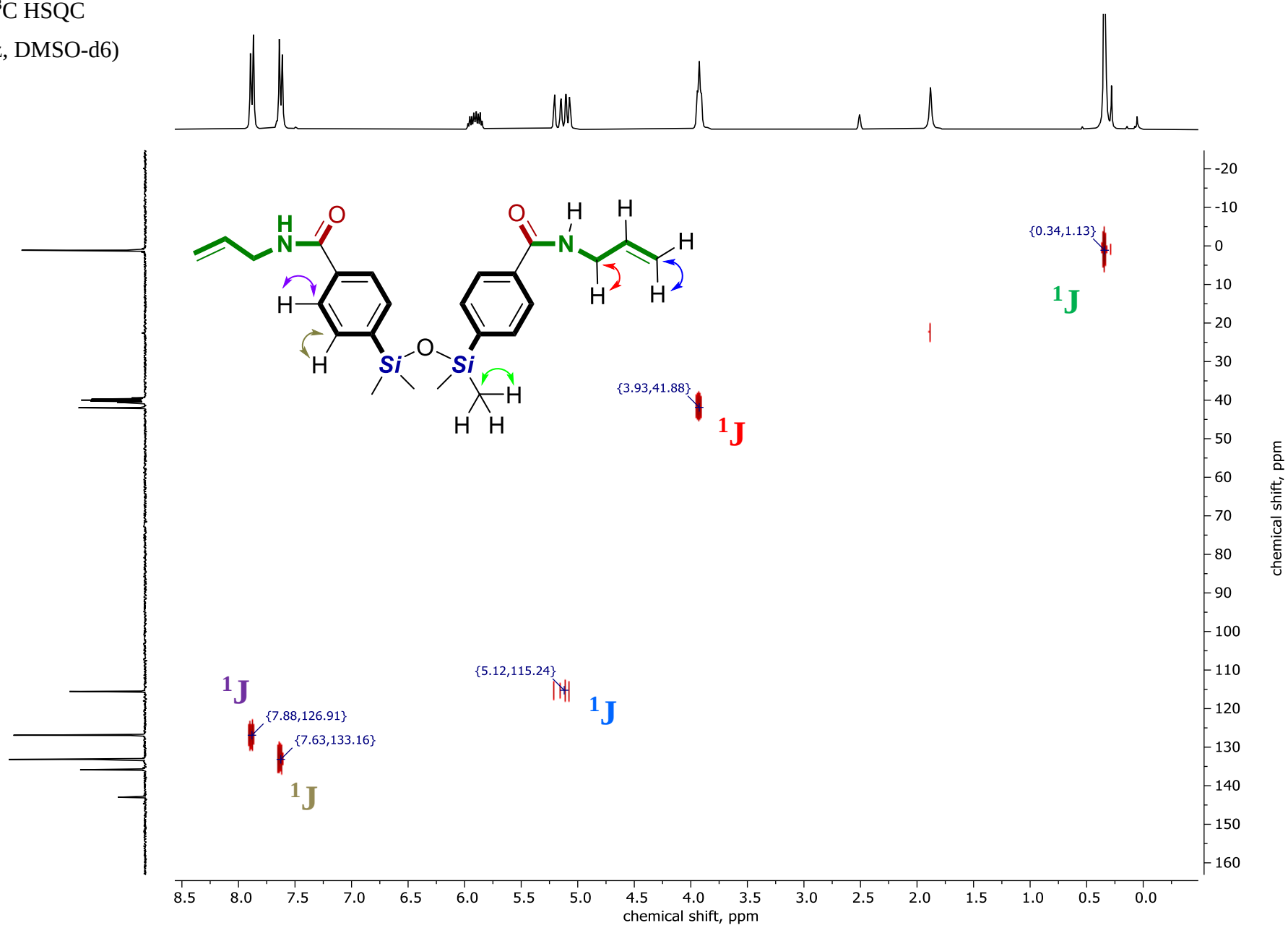
$^{1}H - {}^{13}C$ HMBC

(400 MHz, DMSO-d6)



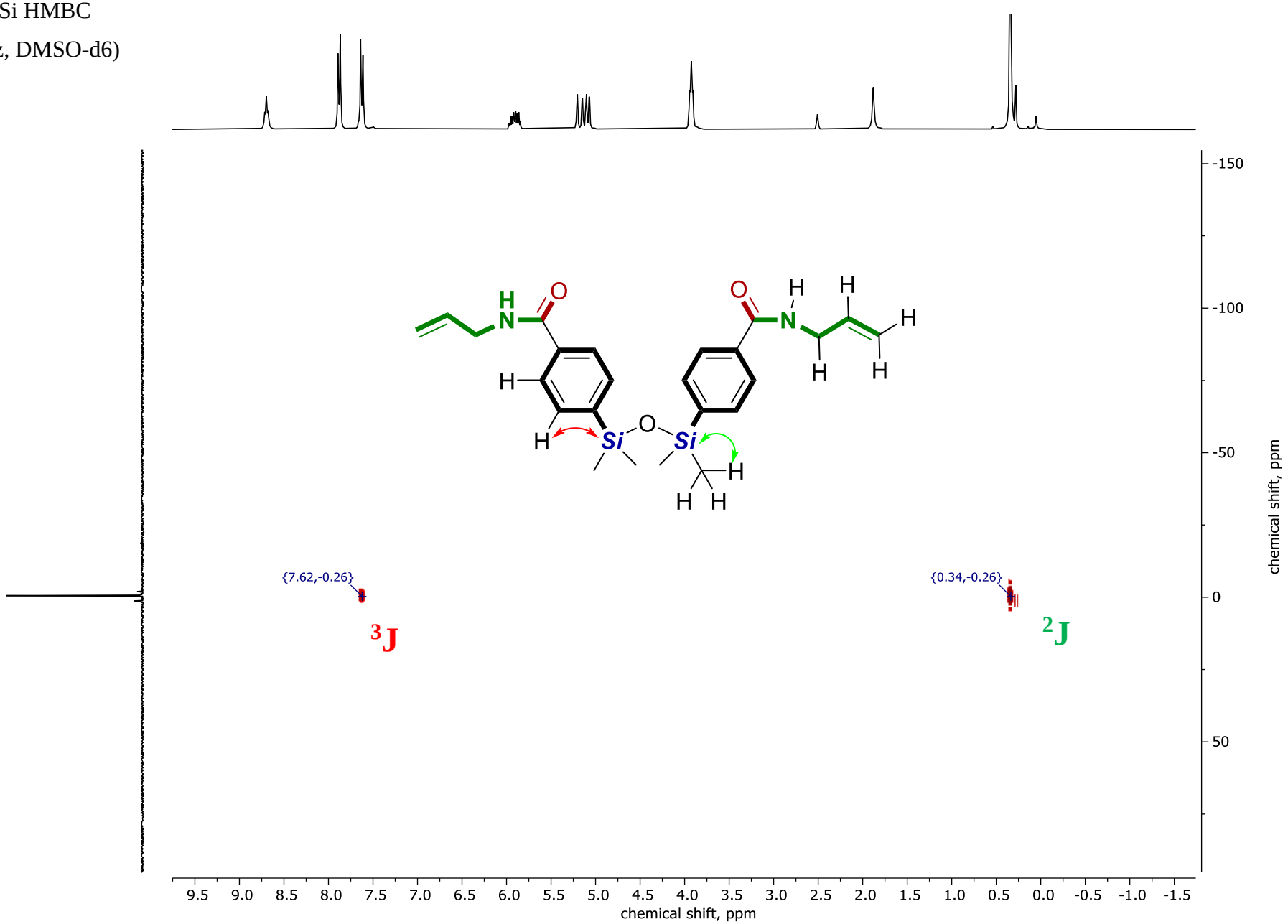
$^{1}H - ^{13}C$ HSQC

(400 MHz, DMSO-d6)



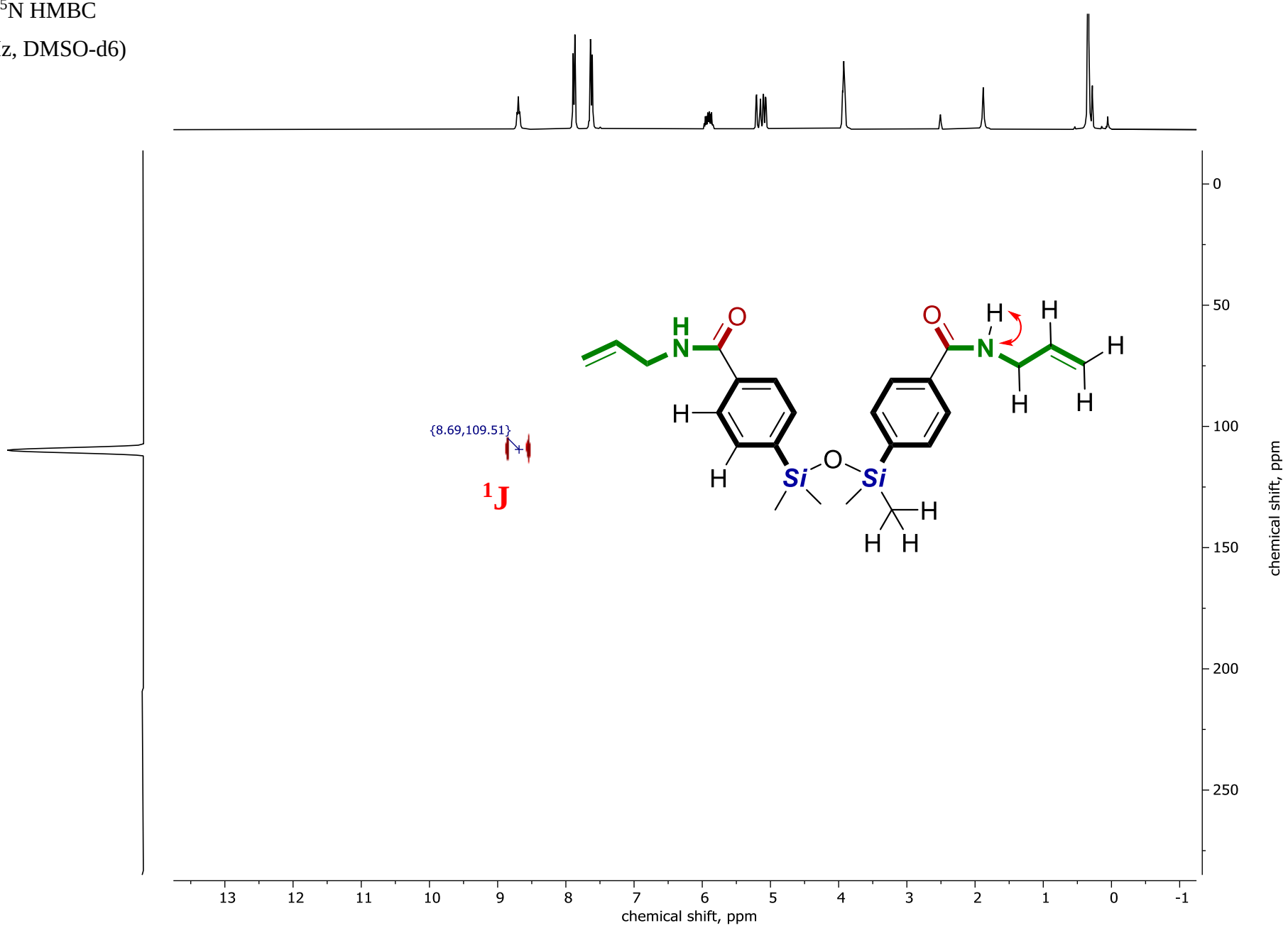
$^{1}H - {}^{29}Si$ HMBC

(400 MHz, DMSO-d6)



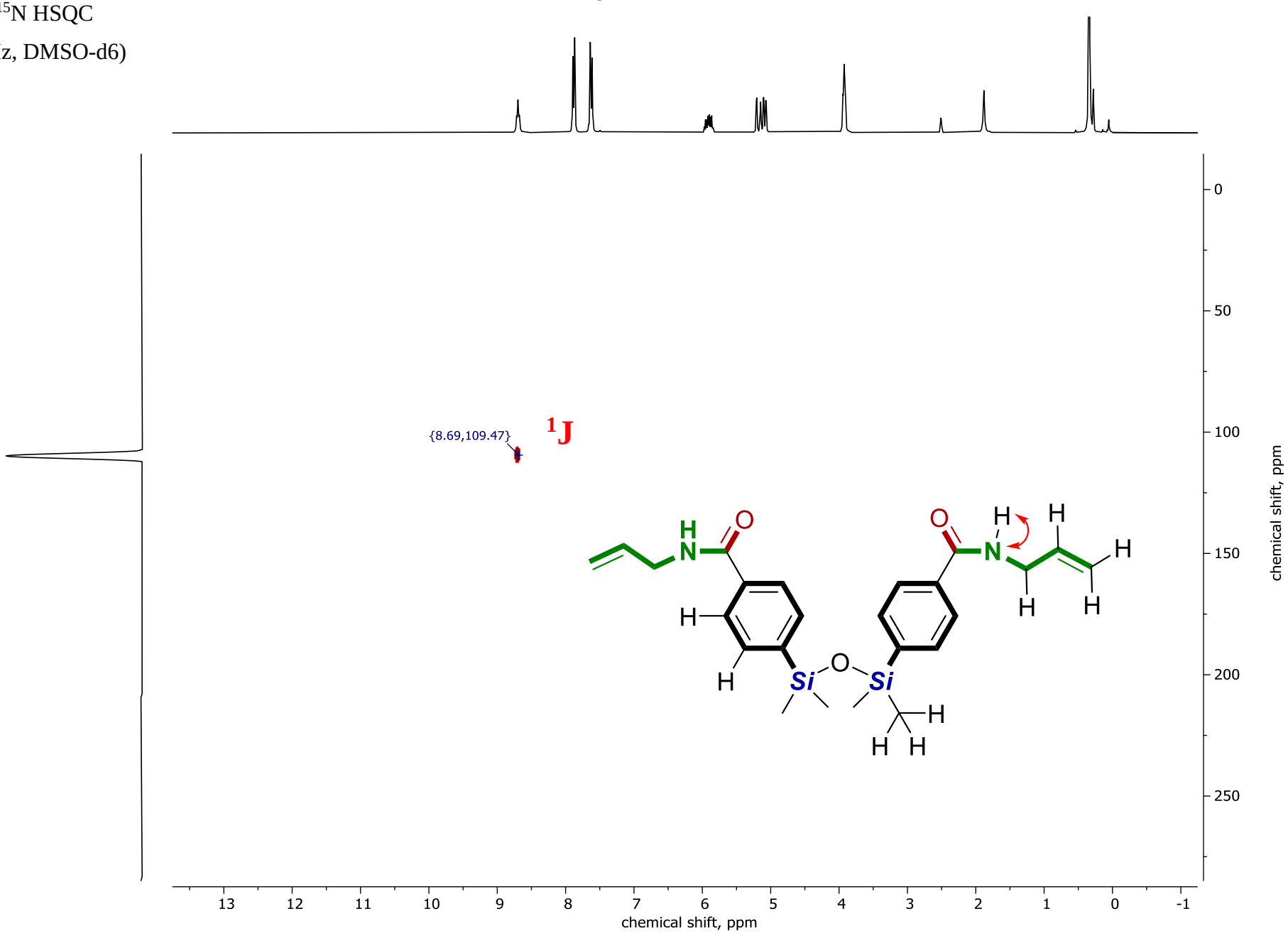
$^{1}H - ^{15}N$ HMBC

(400 MHz, DMSO-d6)

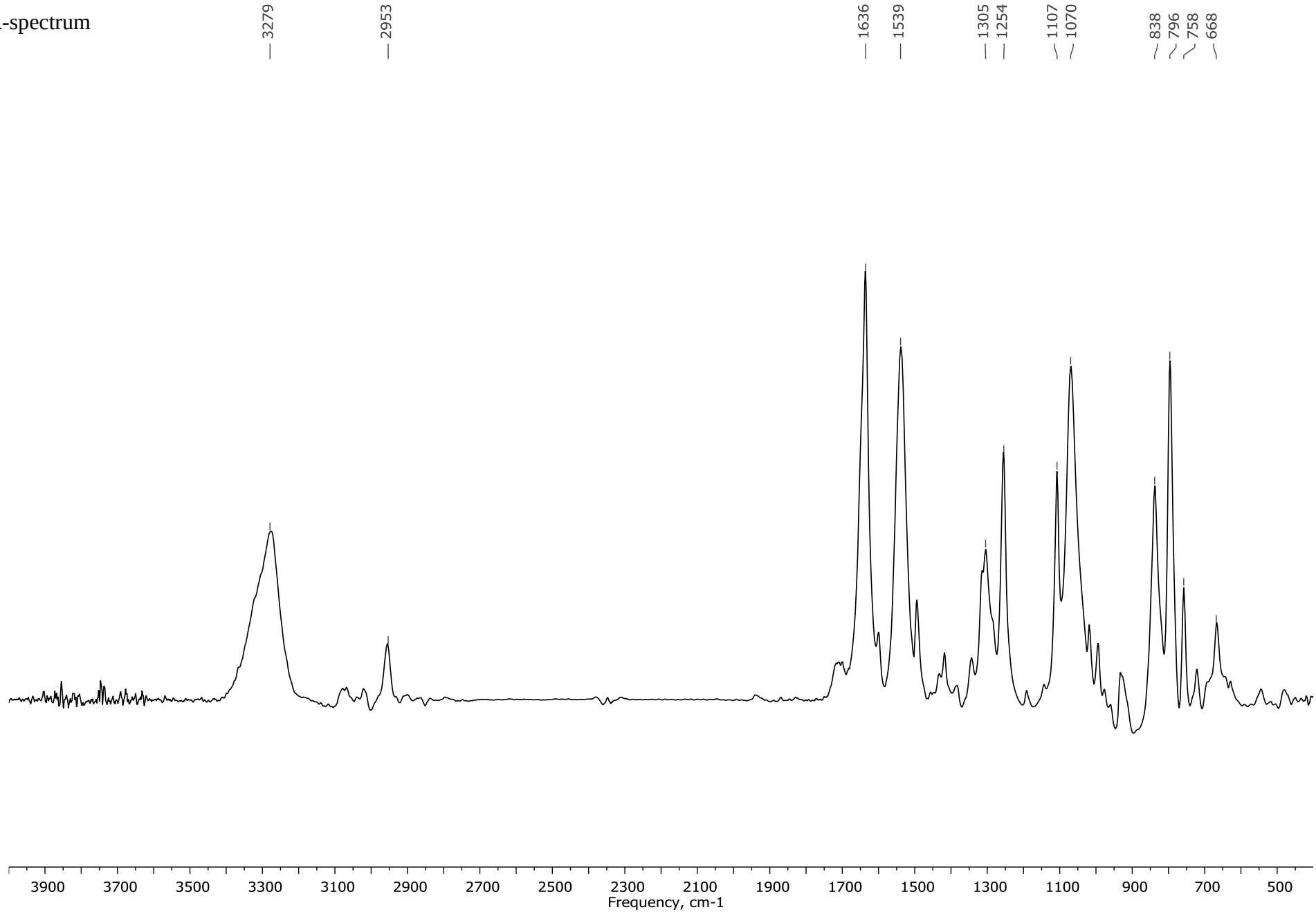


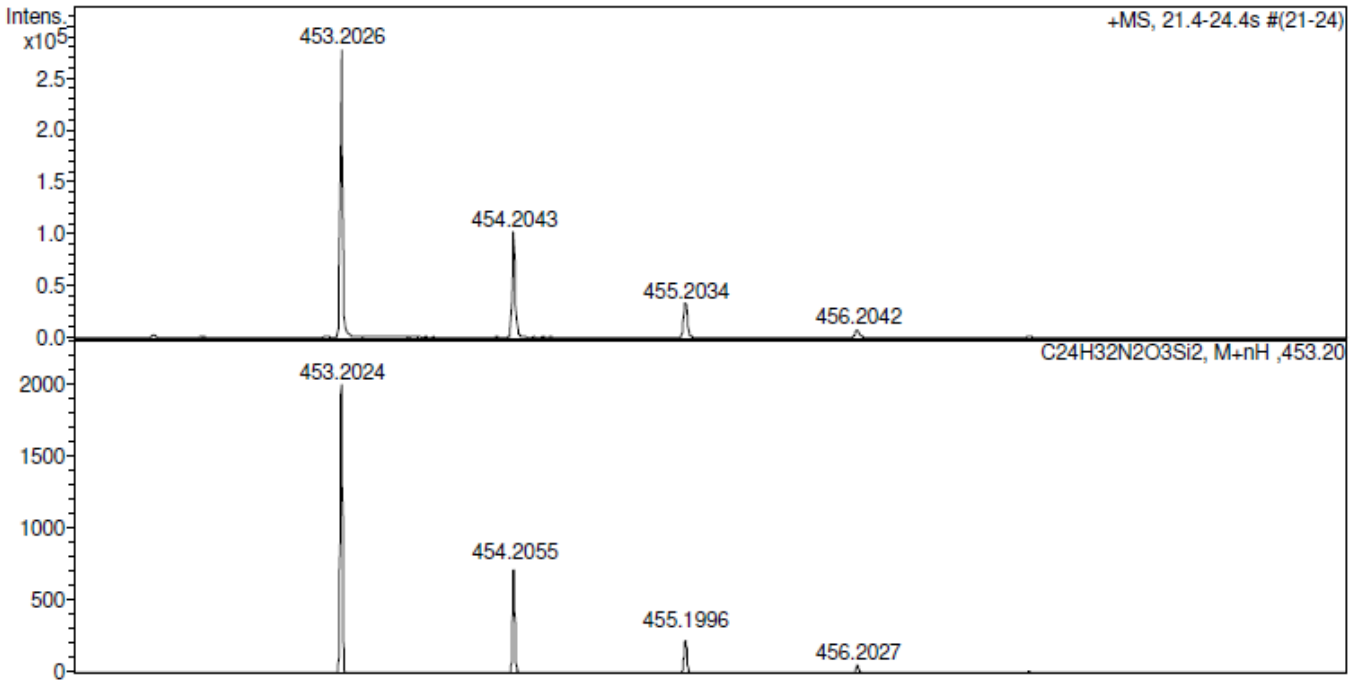
$^{1}H - ^{15}N$ HSQC

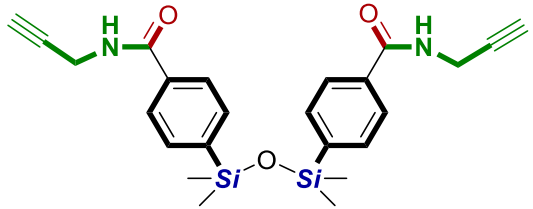
(400 MHz, DMSO-d6)



IR-spectrum


3279
2953
1636
1539
1305
1254
1107
1070
838
796
758
668
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1


Intens.
x10^5
2.5
2.0
1.5
1.0
0.5
0.0
453.2026
454.2043
455.2034
456.2042
+MS, 21.4-24.4s #(21-24)
2000
1500
1000
500
0
453.2024
454.2055
455.1996
456.2027
C24H32N2O3Si2, M+nH ,453.20

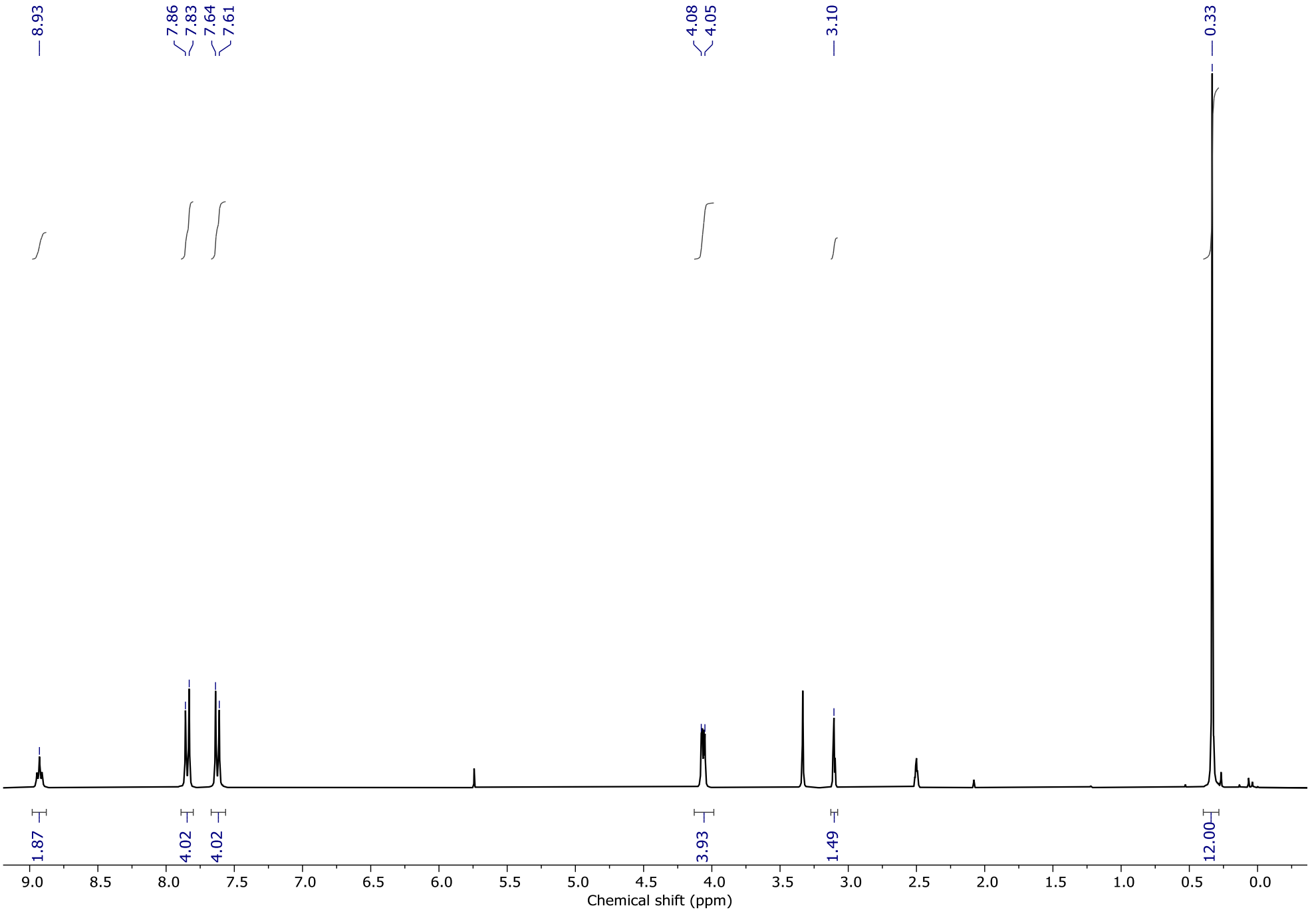


Characterisation data for 4,4'-(1,1,3,3-tetramethyldisiloxane-1,3-diyl)bis(N-(prop-2-yn-1-yl)benzamide):

^{1}H NMR (400 MHz, DMSO-d6): δ = 8.93 (t, ^{3}J=8 Hz, 2H), δ = 7.85 (d, ^{3}J=11 Hz, 4H), δ = 7.63 (d, ^{3}J=11 Hz, 4H), δ = 4.08-4.05 (m, 4H), δ = 3.10 (t, ^{4}J=3 Hz, 2H), δ = 0.33 (s, 12H). ^{13}C NMR (100 MHz, DMSO-d6): δ = 165.91, 142.89, 134.68, 132.78, 126.45, 81.26, 72.79, 28.47, 0.63. ^{29}Si NMR (80 MHz, DMSO-d6): δ = -0.49. ^{15}N NMR (40 MHz, DMSO-d6): δ = 107.75. HRMS (ESI) m/z [M + H] $^{+}$: calcd for $[C_{24}H_{28}N_2O_3Si_2 + H]^{+}$, 449.1711; found, 449.1729. IR (cm^{-1}): 3339, 3234, 1640, 1543, 1313, 1258, 1112, 1065, 838, 794.

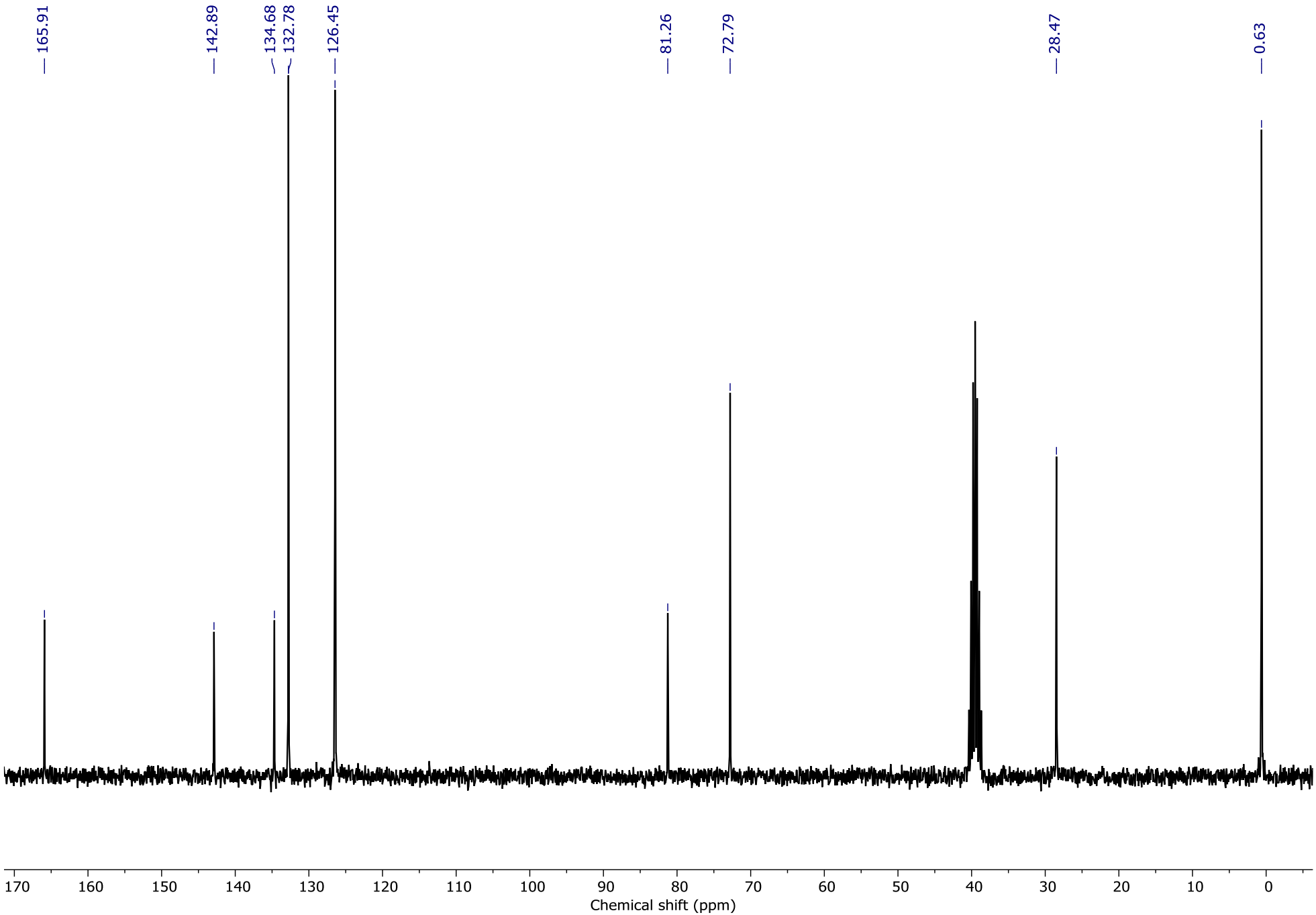
^{1}H NMR

(400 MHz, DMSO-d6)



^{13}C NMR

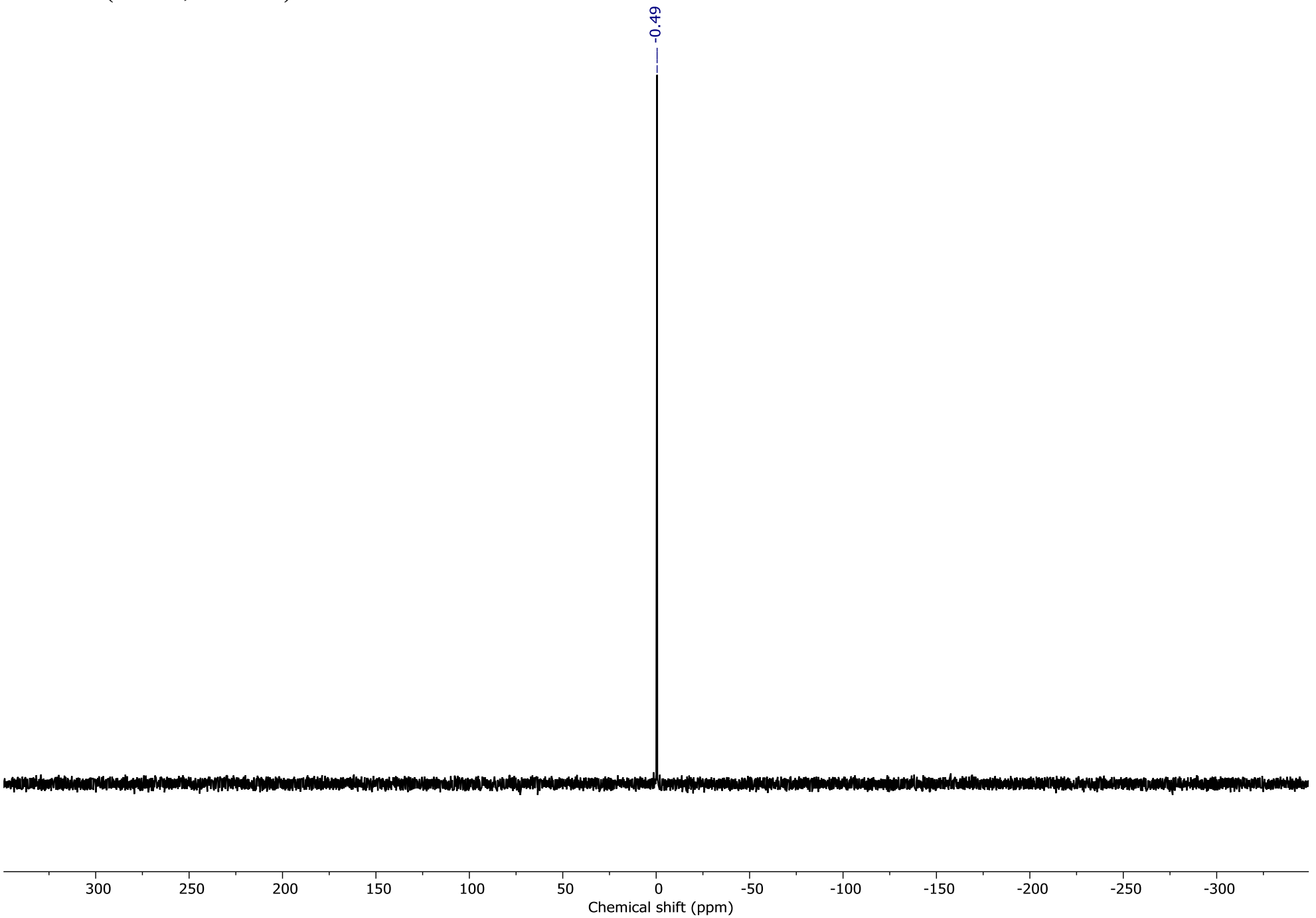
(100 MHz, DMSO-d6)



^{29}Si NMR

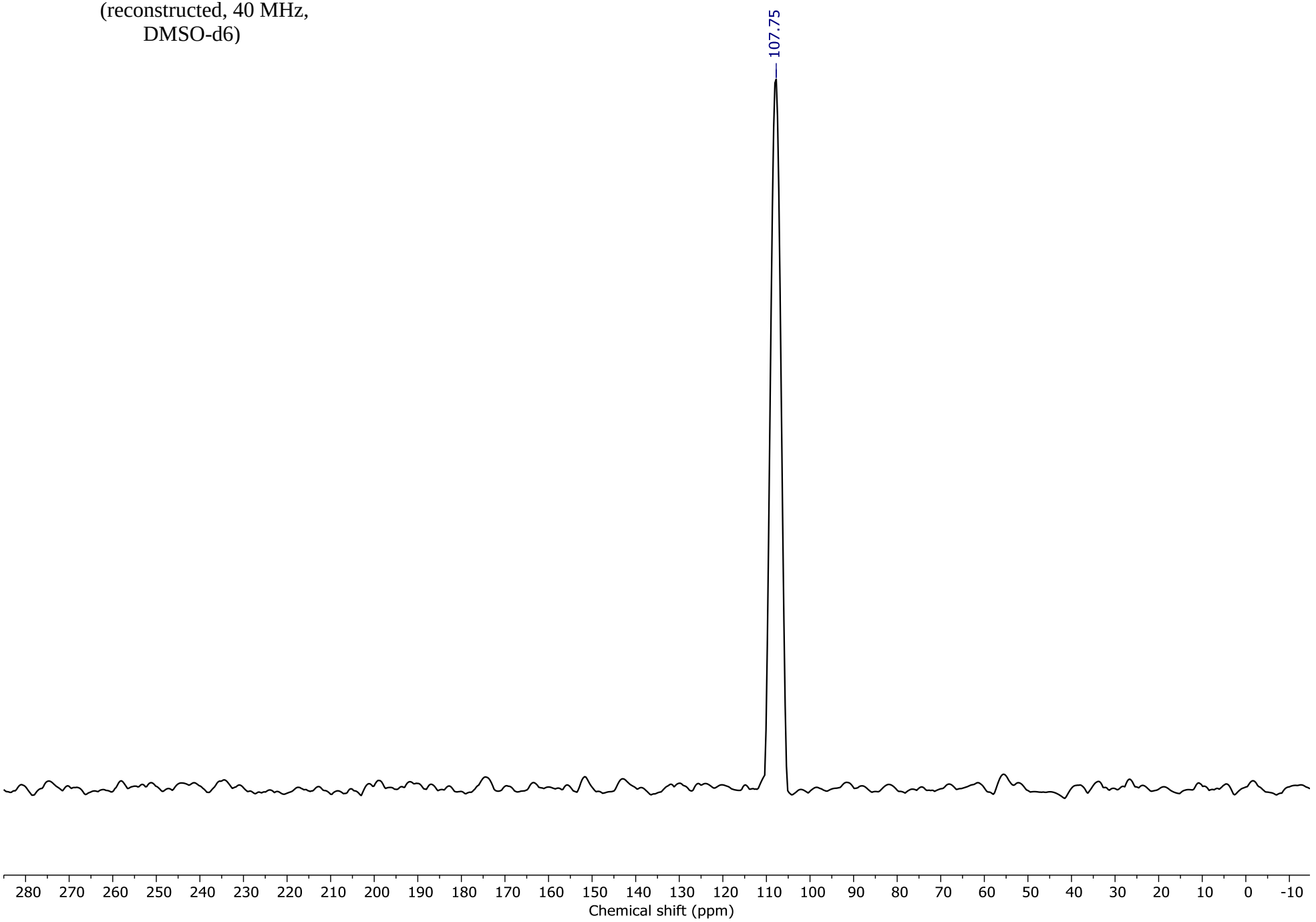
(80 MHz, DMSO-d6)

S77



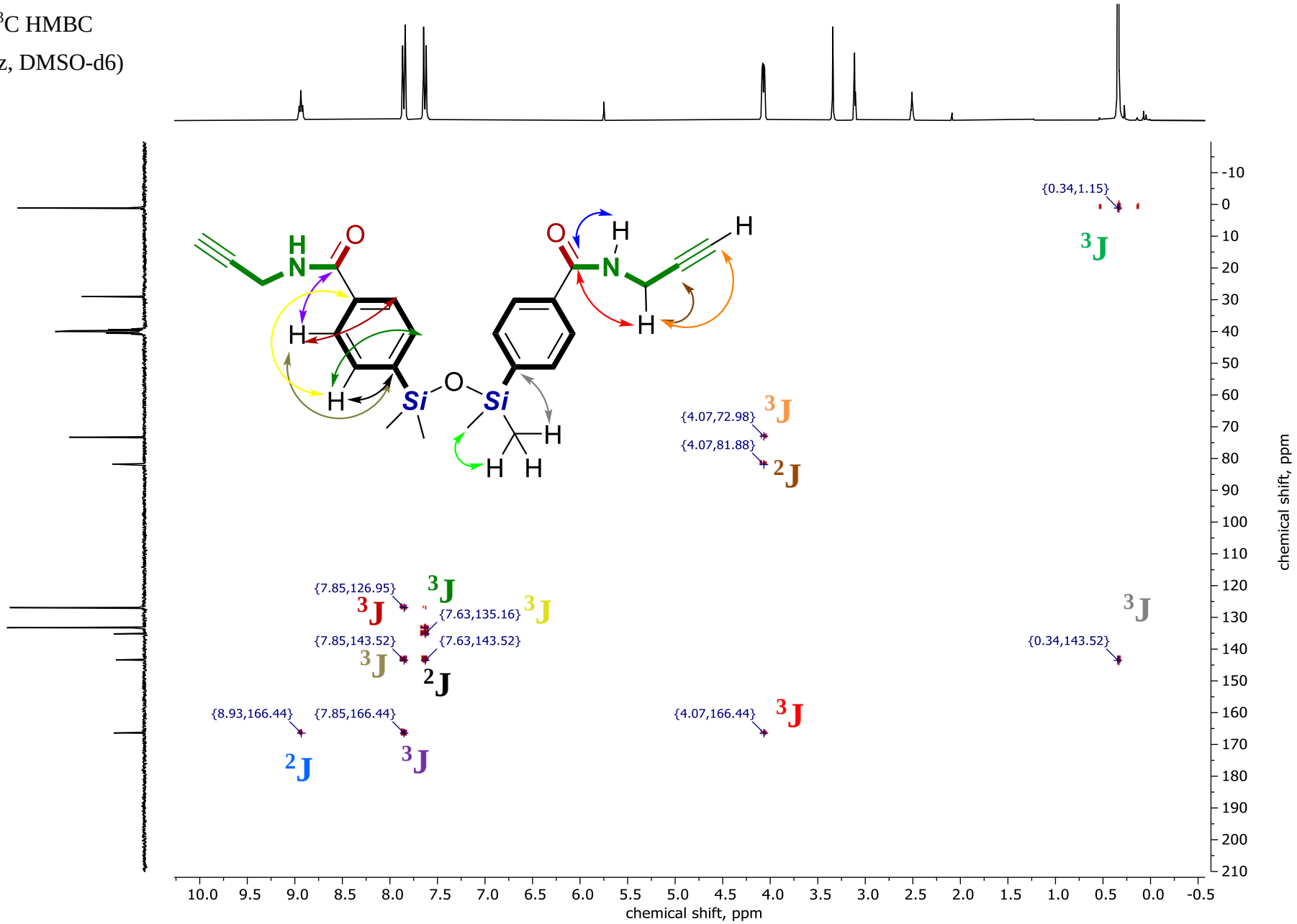
^{15}N NMR

(reconstructed, 40 MHz, DMSO-d6)



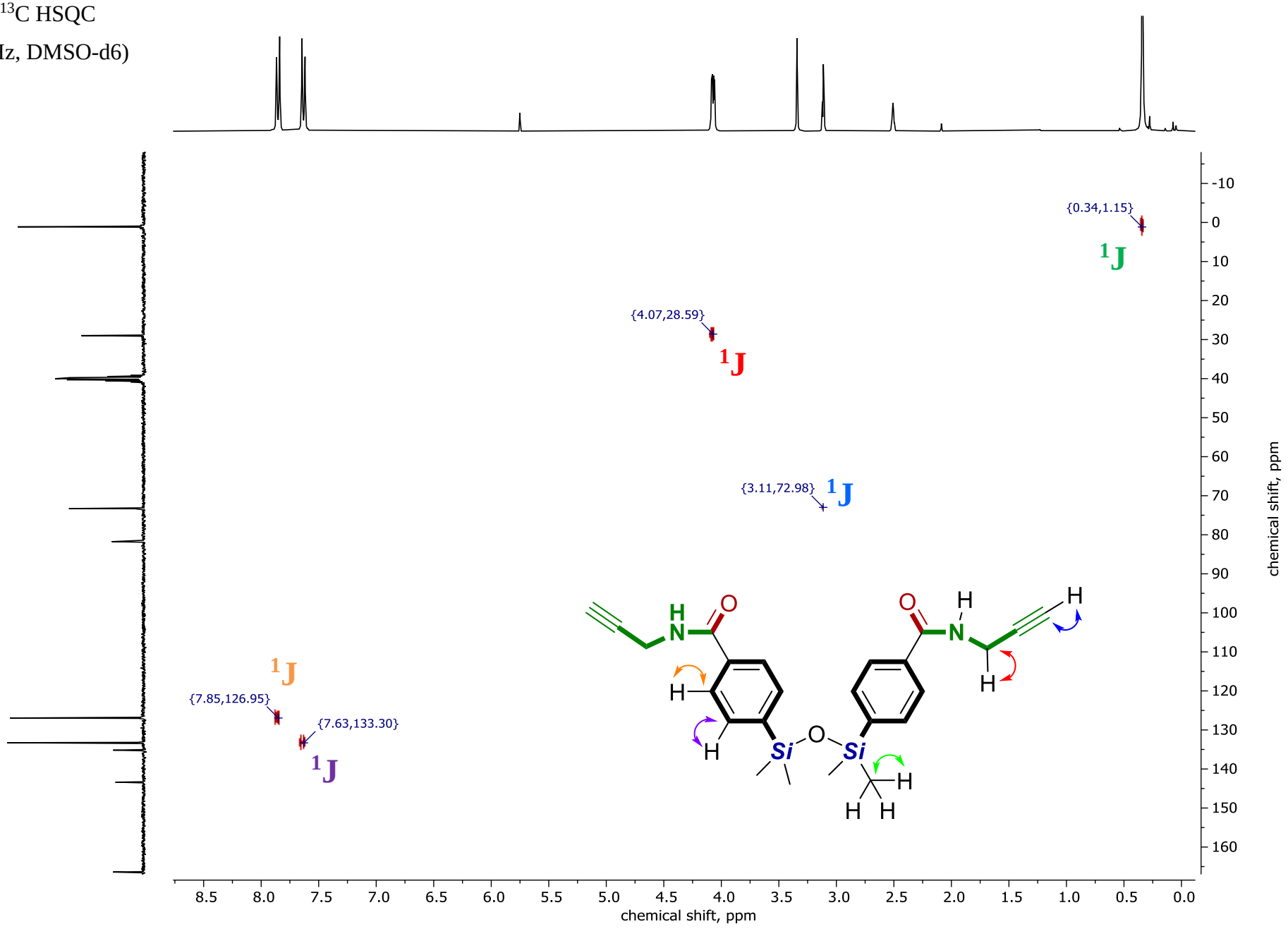
$^{1}H - ^{13}C$ HMBC

(400 MHz, DMSO-d6)



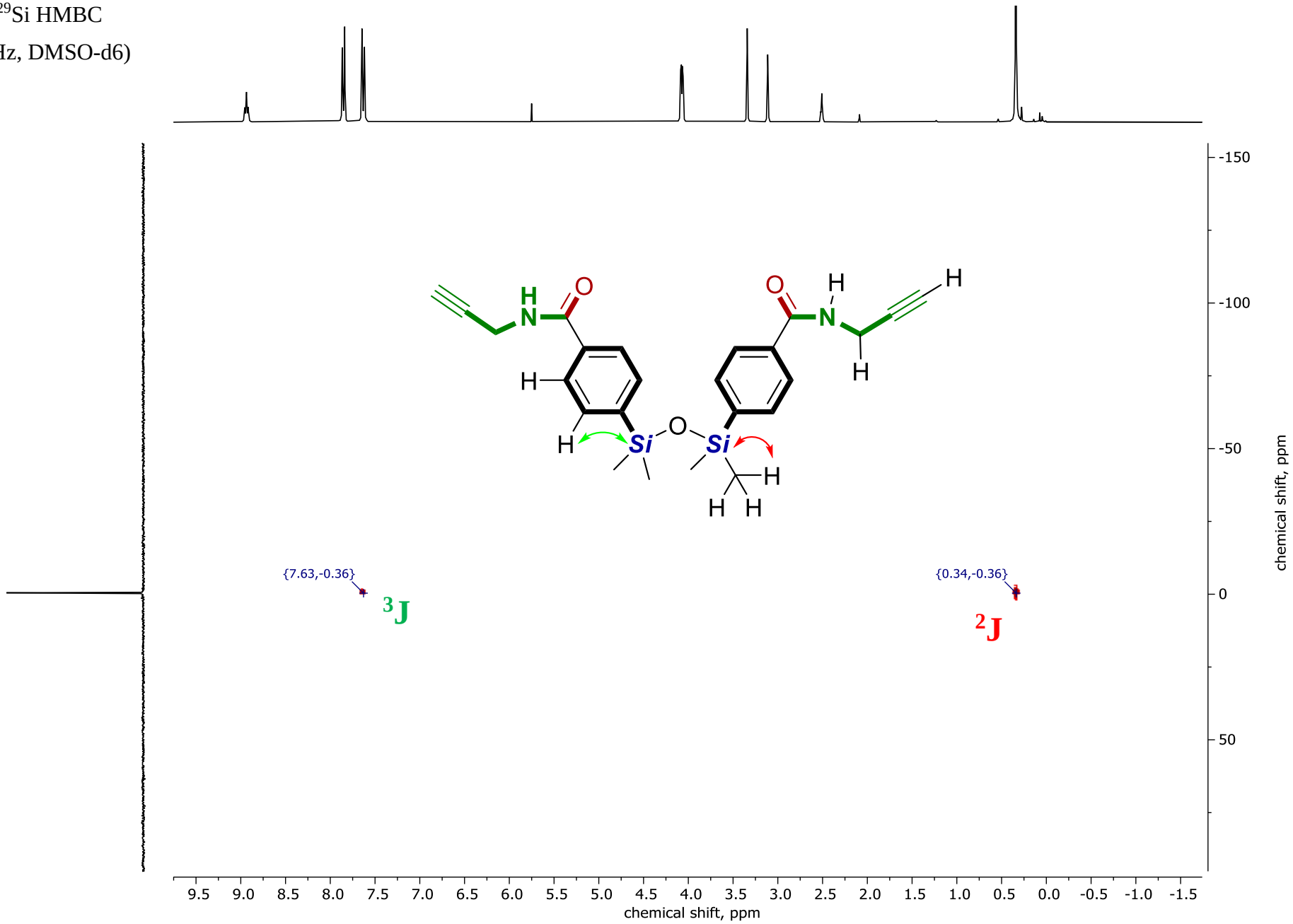
$^{1}H - ^{13}C$ HSQC

(400 MHz, DMSO-d6)



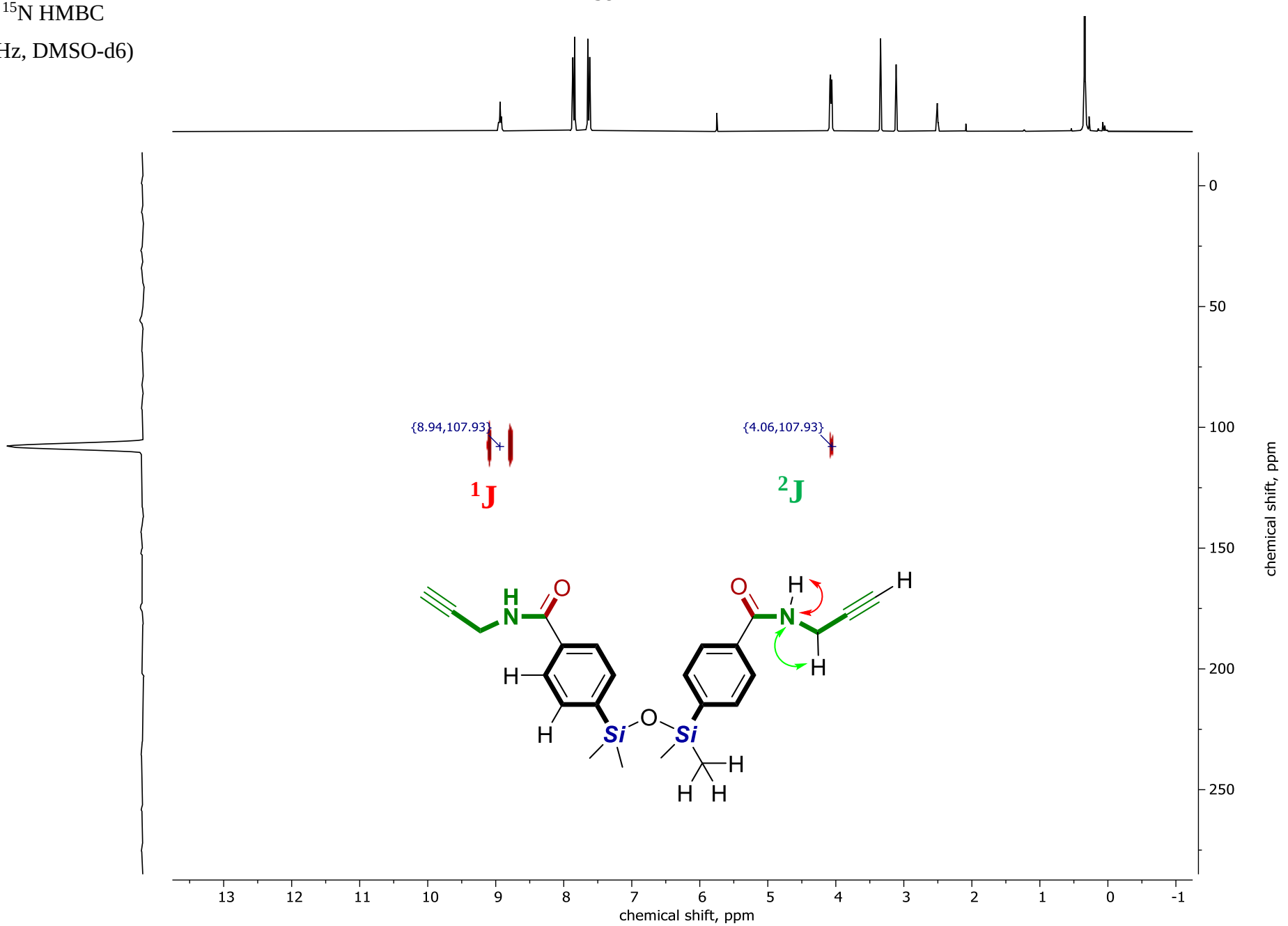
$^{1}H - ^{29}Si$ HMBC

(400 MHz, DMSO-d6)



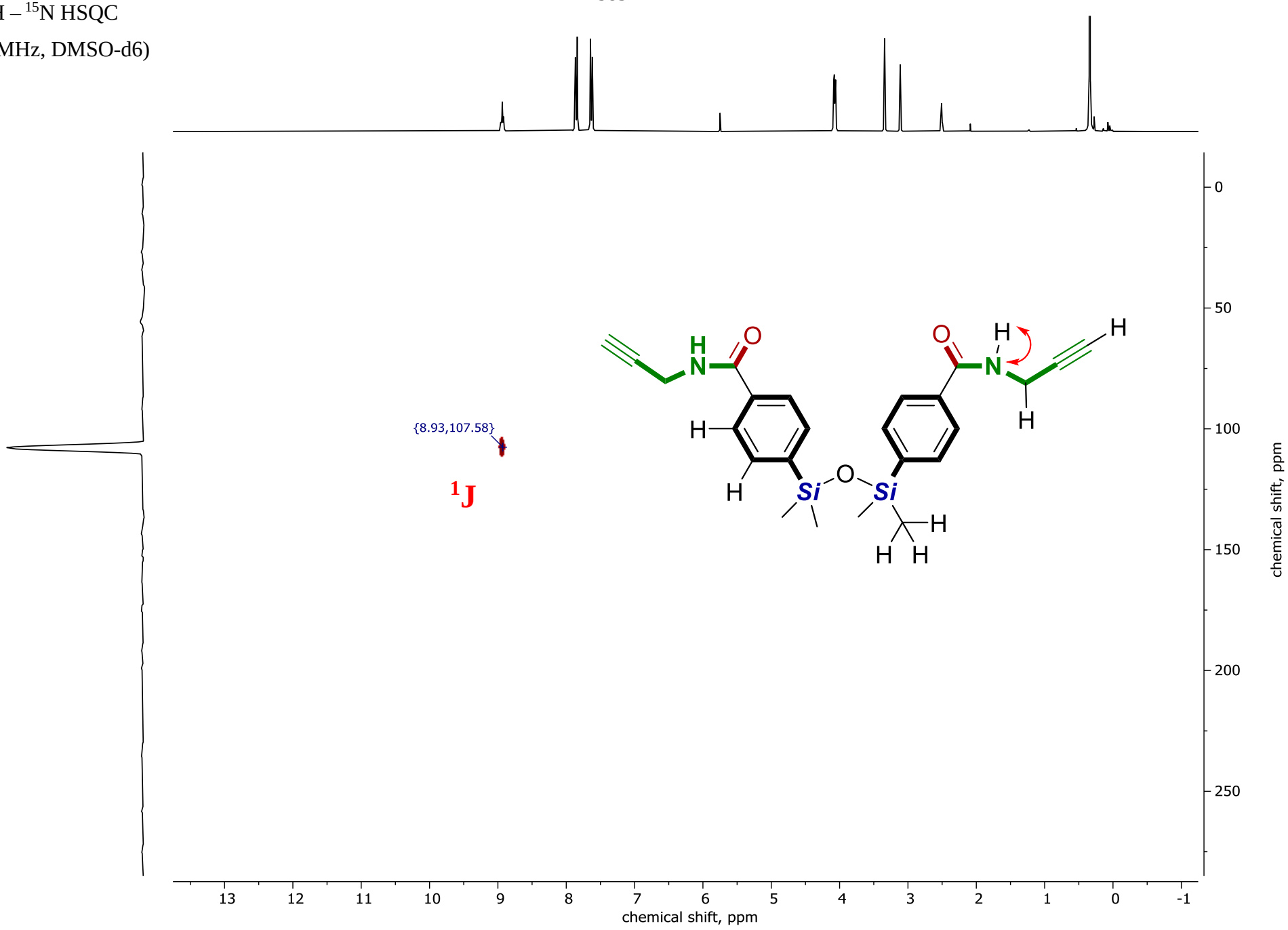
$^{1}H - ^{15}N$ HMBC

(400 MHz, DMSO-d6)

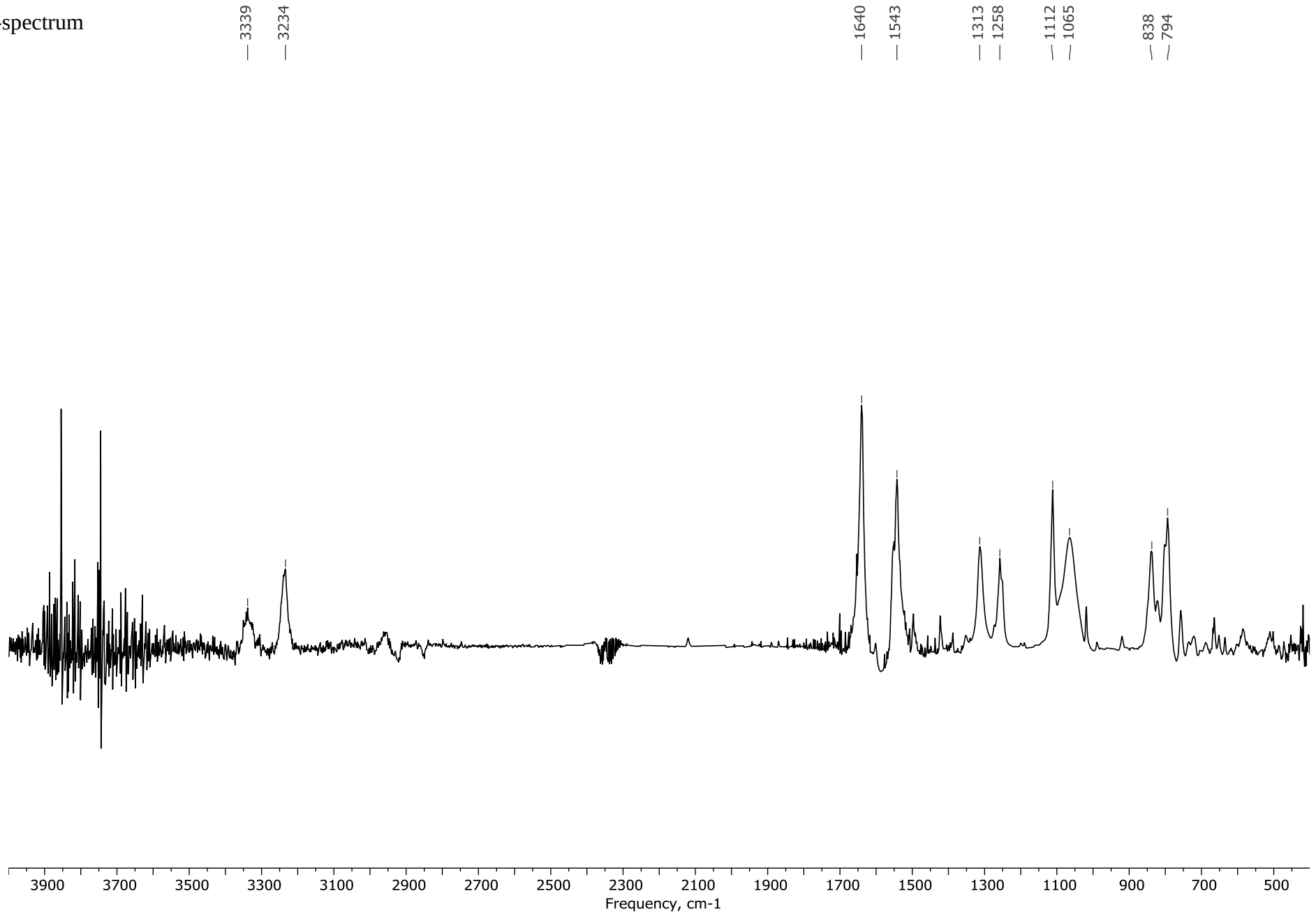


$^{1}H - {}^{15}N$ HSQC

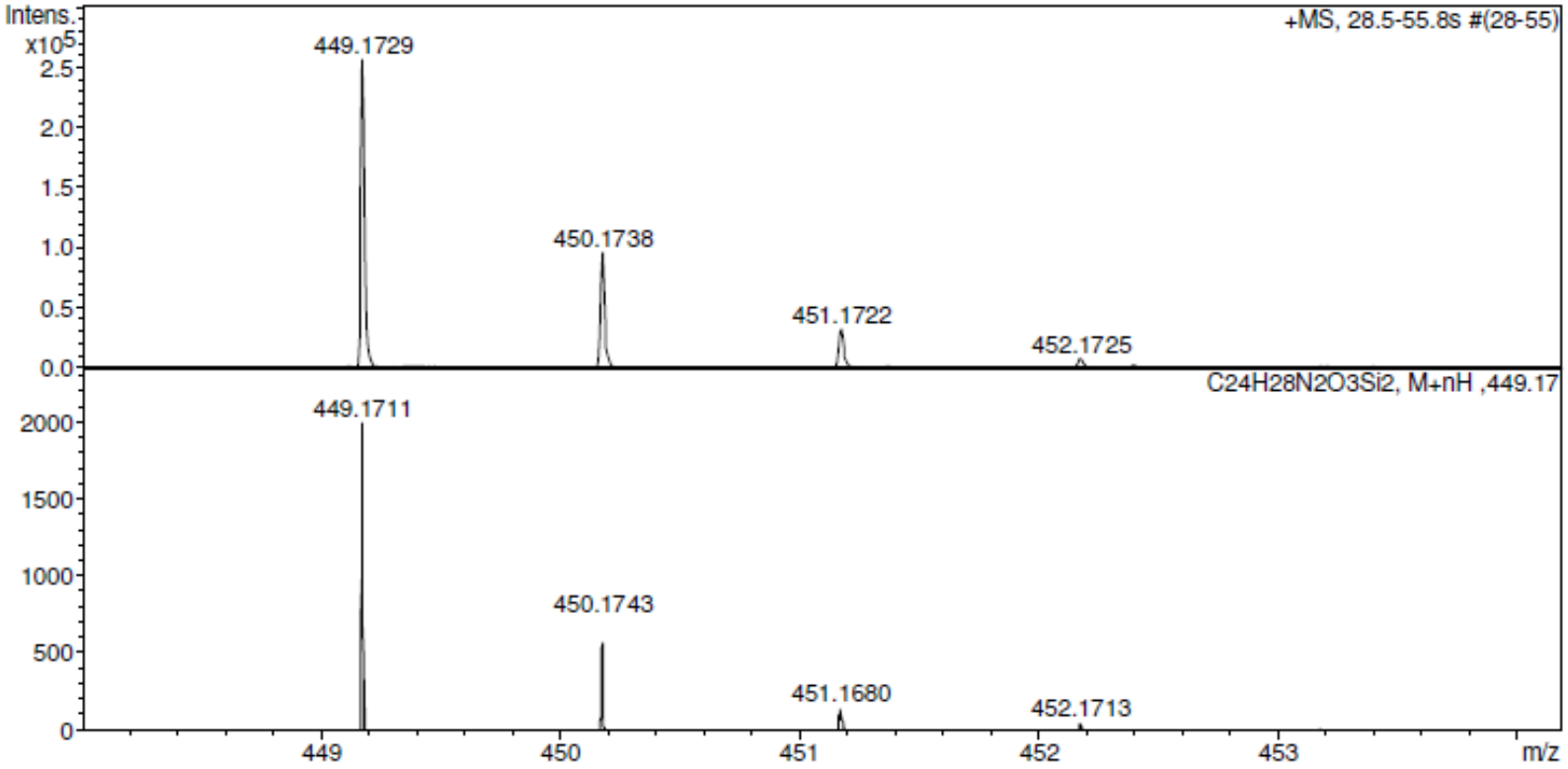
(400 MHz, DMSO-d6)

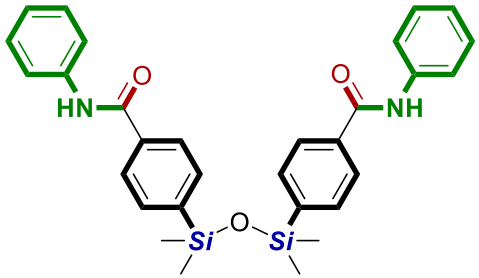


IR-spectrum


3339
3234
1640
1543
1313
1258
1112
1065
838
794
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1

ESI HRMS


Intens.
x10^5
2.5
2.0
1.5
1.0
0.5
0.0
449.1729
450.1738
451.1722
452.1725
+MS, 28.5-55.8s #(28-55)
C24H28N2O3Si2, M+nH ,449.17
2000
1500
1000
500
0
449.1711
450.1743
451.1680
452.1713
449
450
451
452
453
m/z

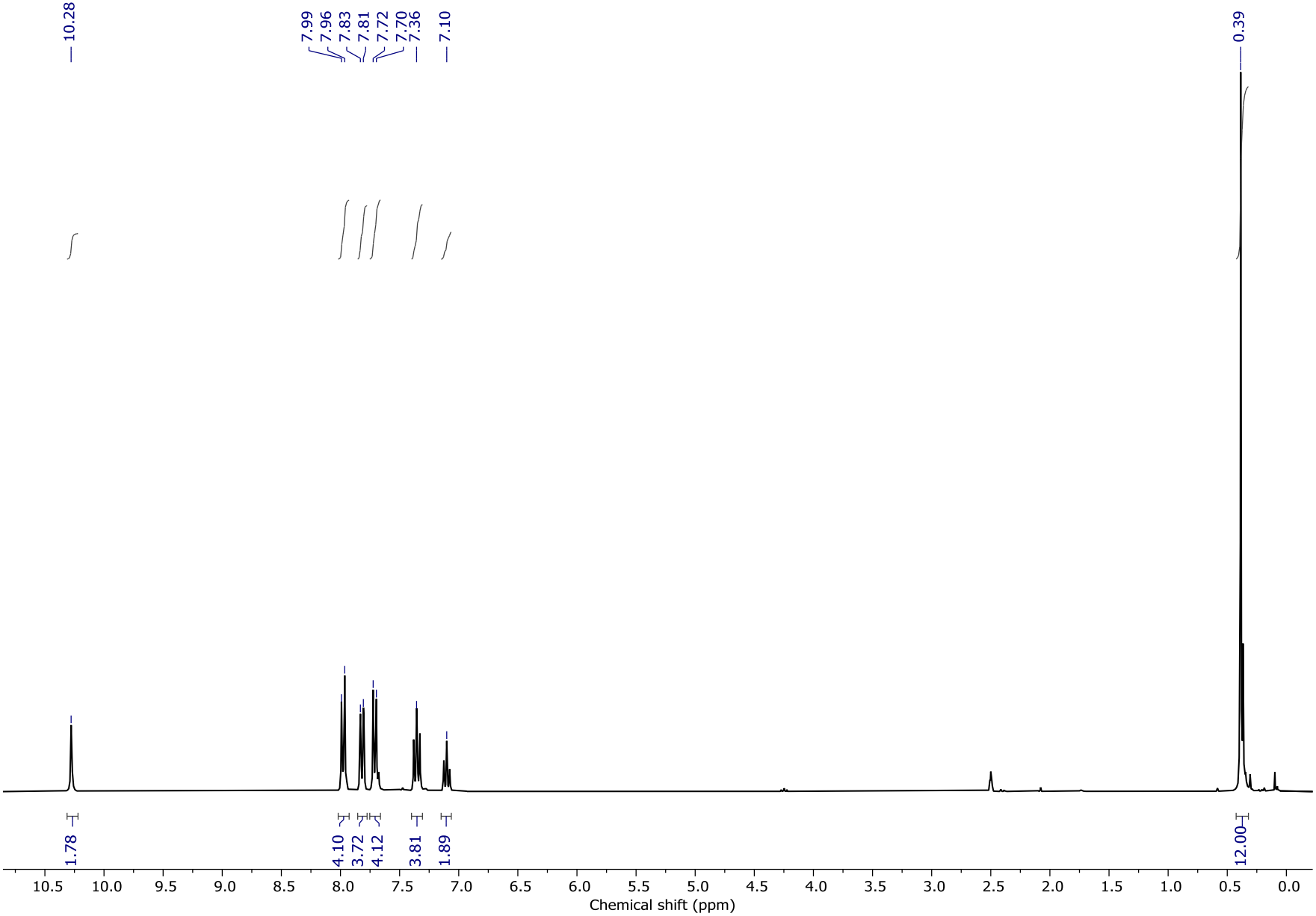


Characterisation data for 4,4'-(1,1,3,3-tetramethyldisiloxane-1,3-diyl)bis(N-phenylbenzamide):

^{1}H NMR (400 MHz, DMSO-d6): δ = 10.28 (s, 2H), δ = 7.98 (d, ^{3}J=11 Hz, 4H), δ = 7.82 (d, ^{3}J=10 Hz, 4H), δ = 7.71 (d, ^{3}J=11 Hz, 4H), δ = 7.36 (t, ^{3}J=10 Hz, 4H), δ = 7.10 (t, ^{3}J=10 Hz, 2H), δ = 0.39 (s, 12H). ^{13}C NMR (100 MHz, DMSO-d6): δ = 166.57, 143.02, 139.16, 135.94, 132.77, 128.56, 126.88, 123.64, 120.34, 0.69. ^{29}Si NMR (80 MHz, DMSO-d6): δ = -0.45. ^{15}N NMR (40 MHz, DMSO): δ = 129.14. HRMS (ESI) m/z [M + H] $^{+}$: calcd for $[C_{30}H_{32}N_2O_3Si_2 + H]^{+}$, 525.2024; found, 525.2082; [M + K] $^{+}$: calcd for $[C_{30}H_{32}N_2O_3Si_2 + K]^{+}$, 563.1583; found, 563.1574; [M + Na] $^{+}$: calcd for $[C_{30}H_{32}N_2O_3Si_2 + Na]^{+}$, 547.1844; found, 547.1843; [M + NH_4] $^{+}$: calcd for $[C_{30}H_{32}N_2O_3Si_2 + NH_4]^{+}$, 542.2290; found, 542.2286. IR (cm^{-1}): 3268-2958, 1648, 1599, 1542, 1443, 1329, 1258, 1050, 832-758.

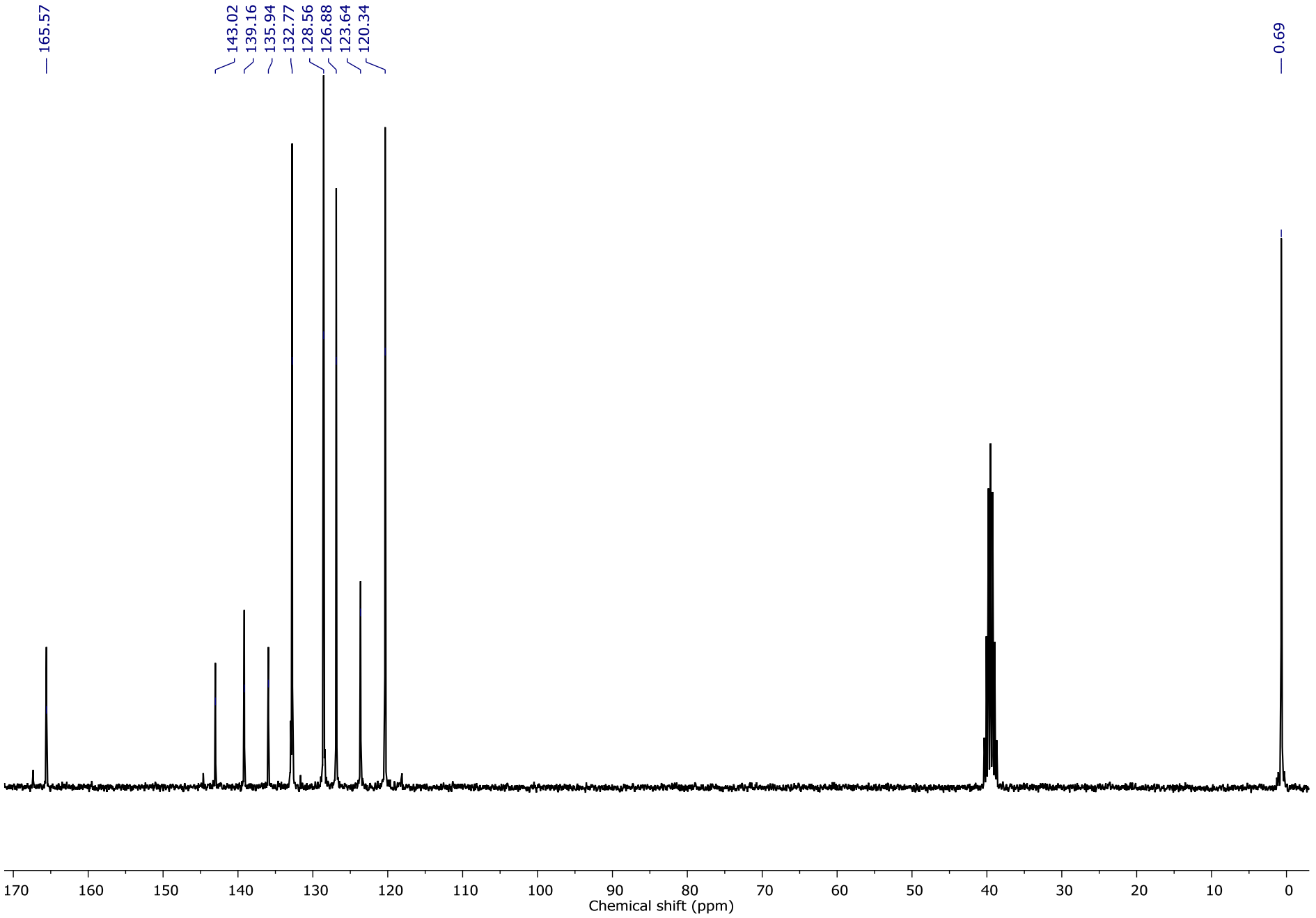
^{1}H NMR

(400 MHz, DMSO-d6)



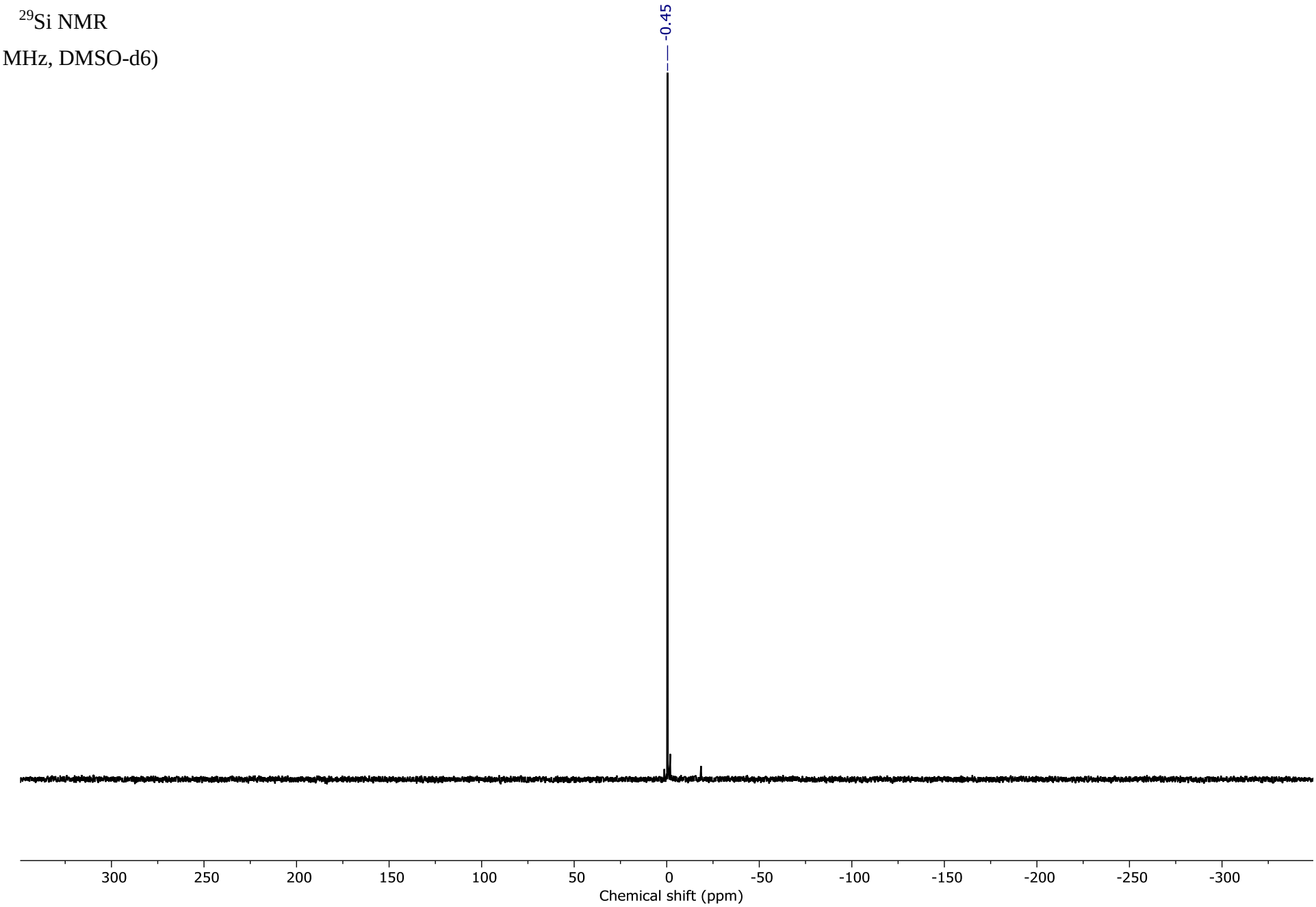
^{13}C NMR

(100 MHz, DMSO-d6)



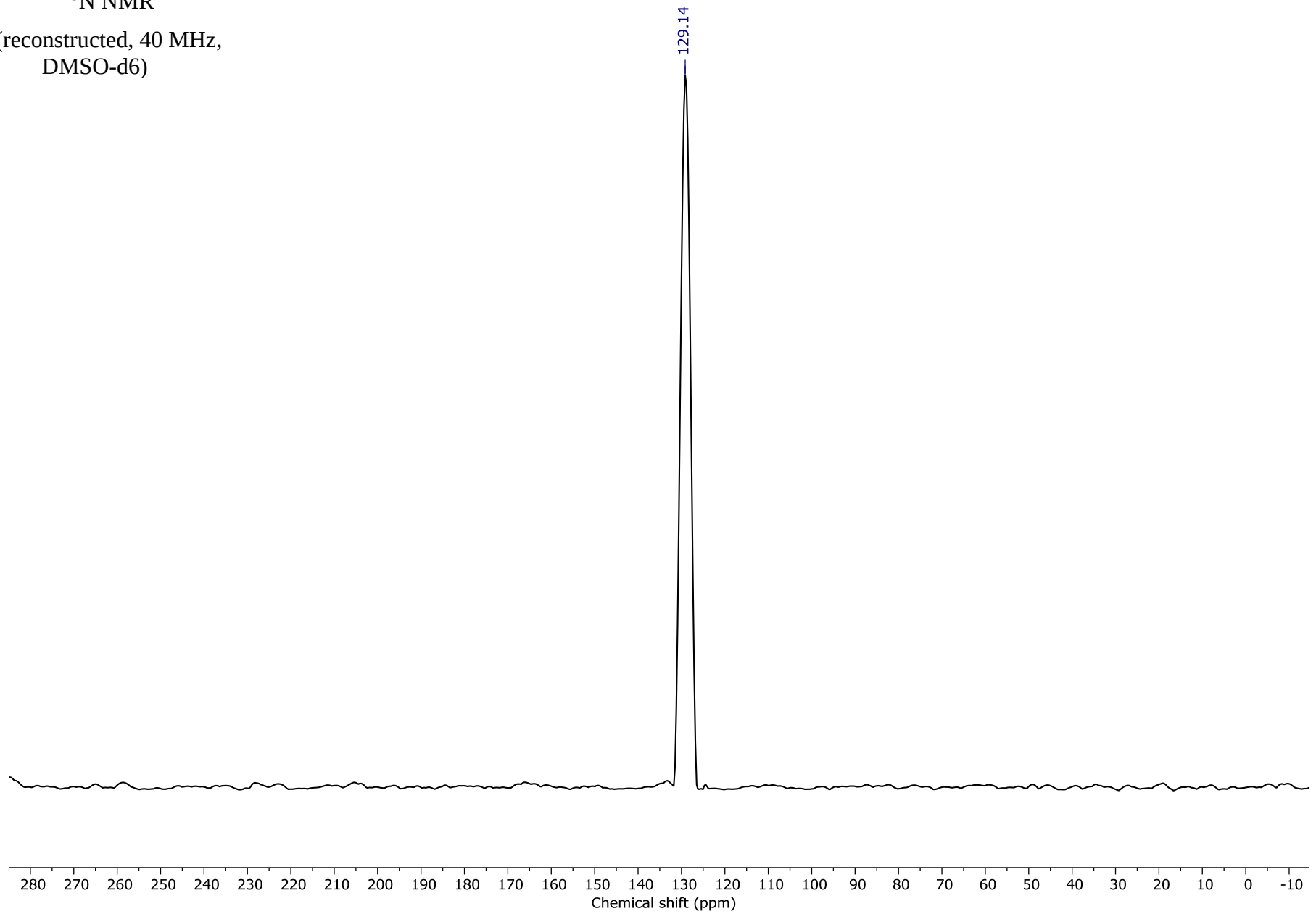
^{29}Si NMR

(80 MHz, DMSO-d6)



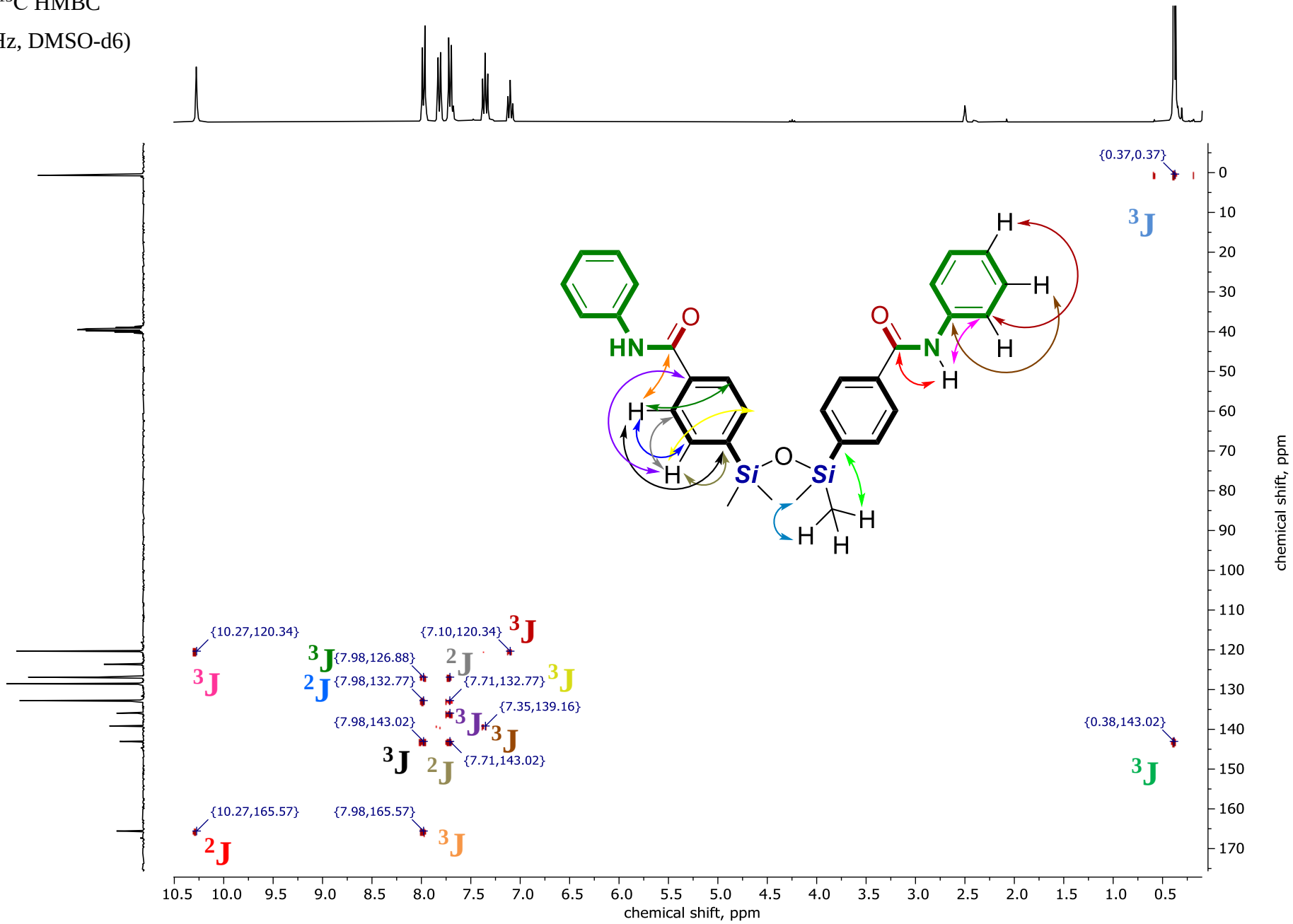
^{15}N NMR

(reconstructed, 40 MHz, DMSO-d6)



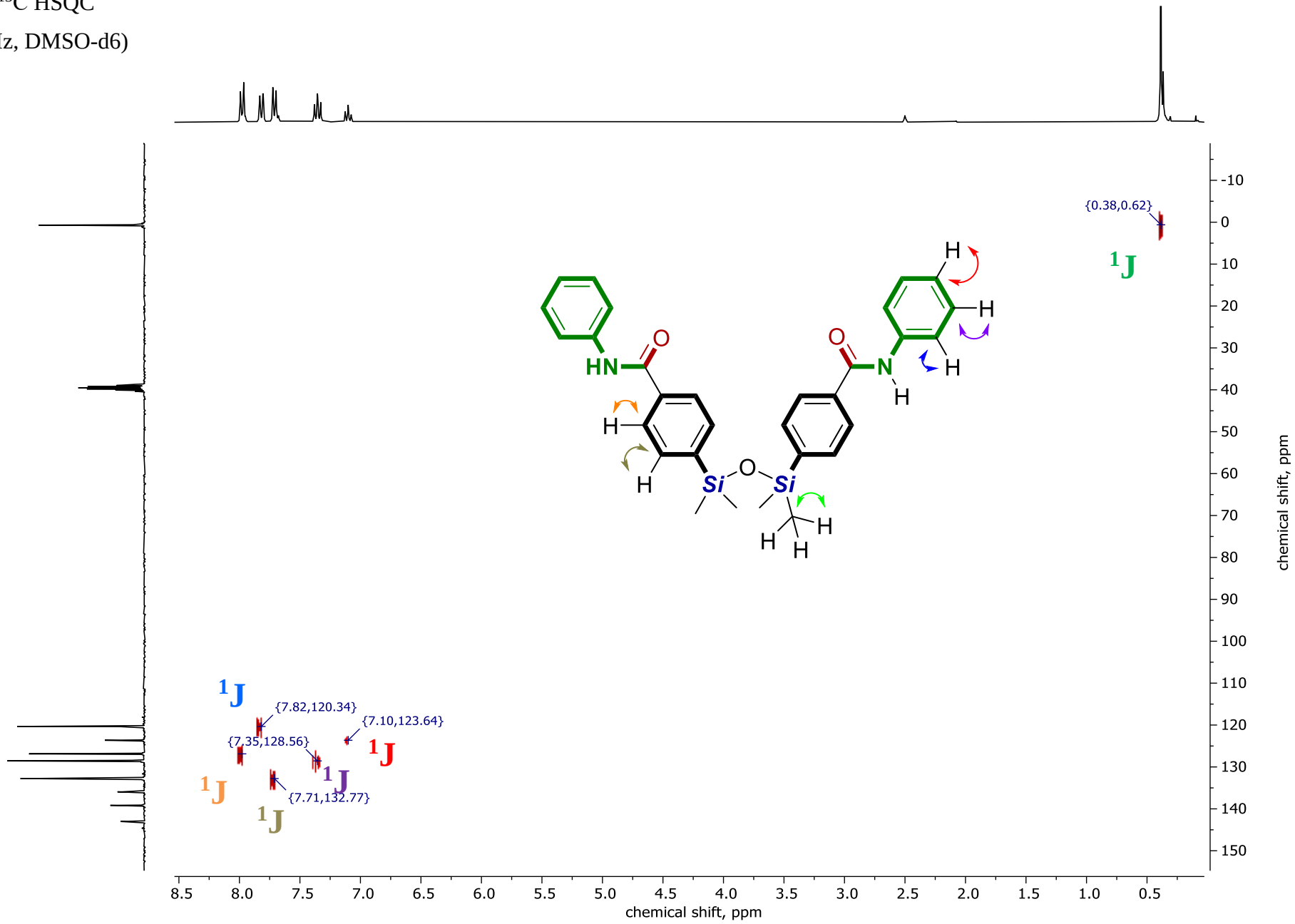
$^{1}H - {}^{13}C$ HMBC

(400 MHz, DMSO-d6)



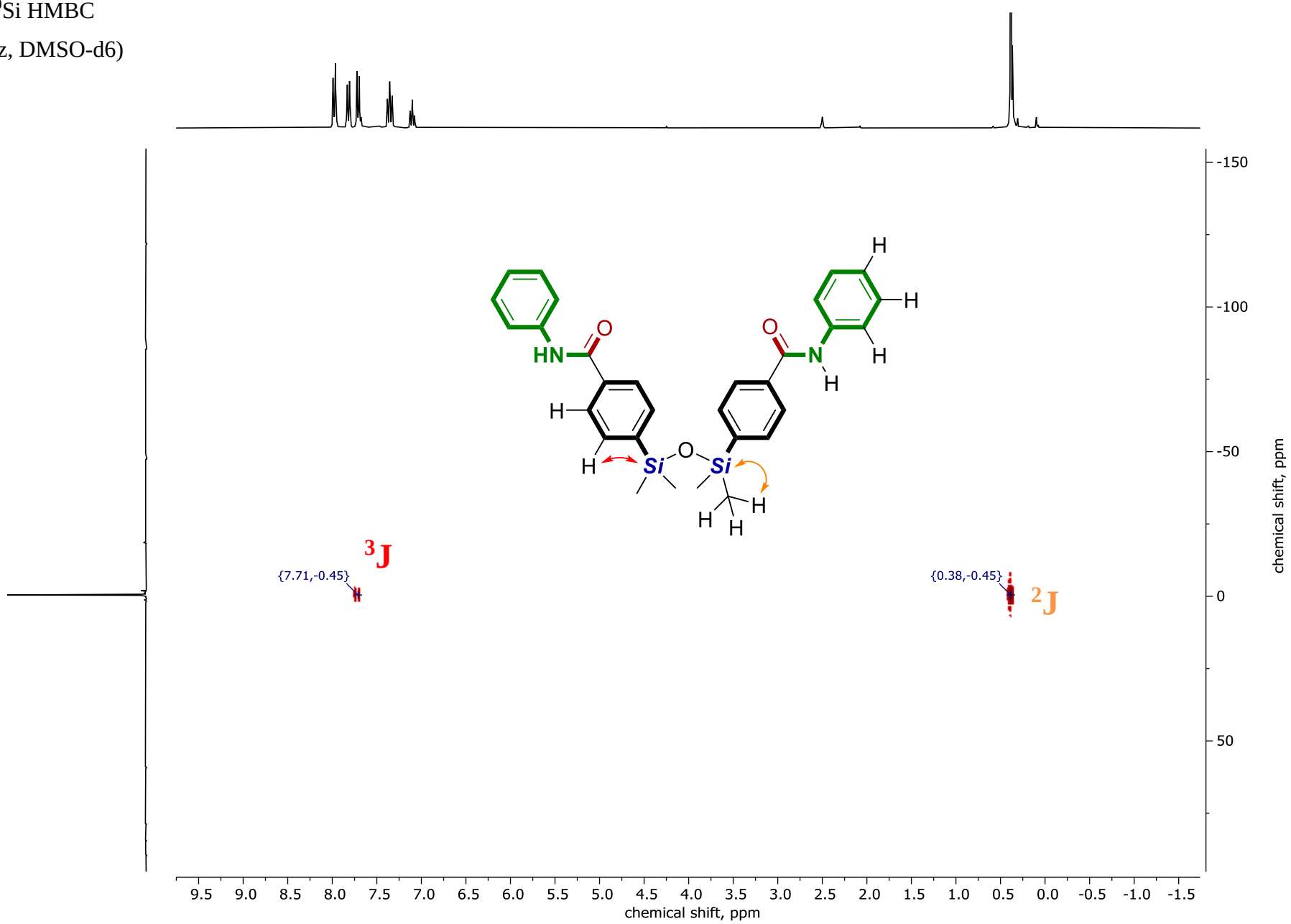
$^{1}H - ^{13}C$ HSQC

(400 MHz, DMSO-d6)



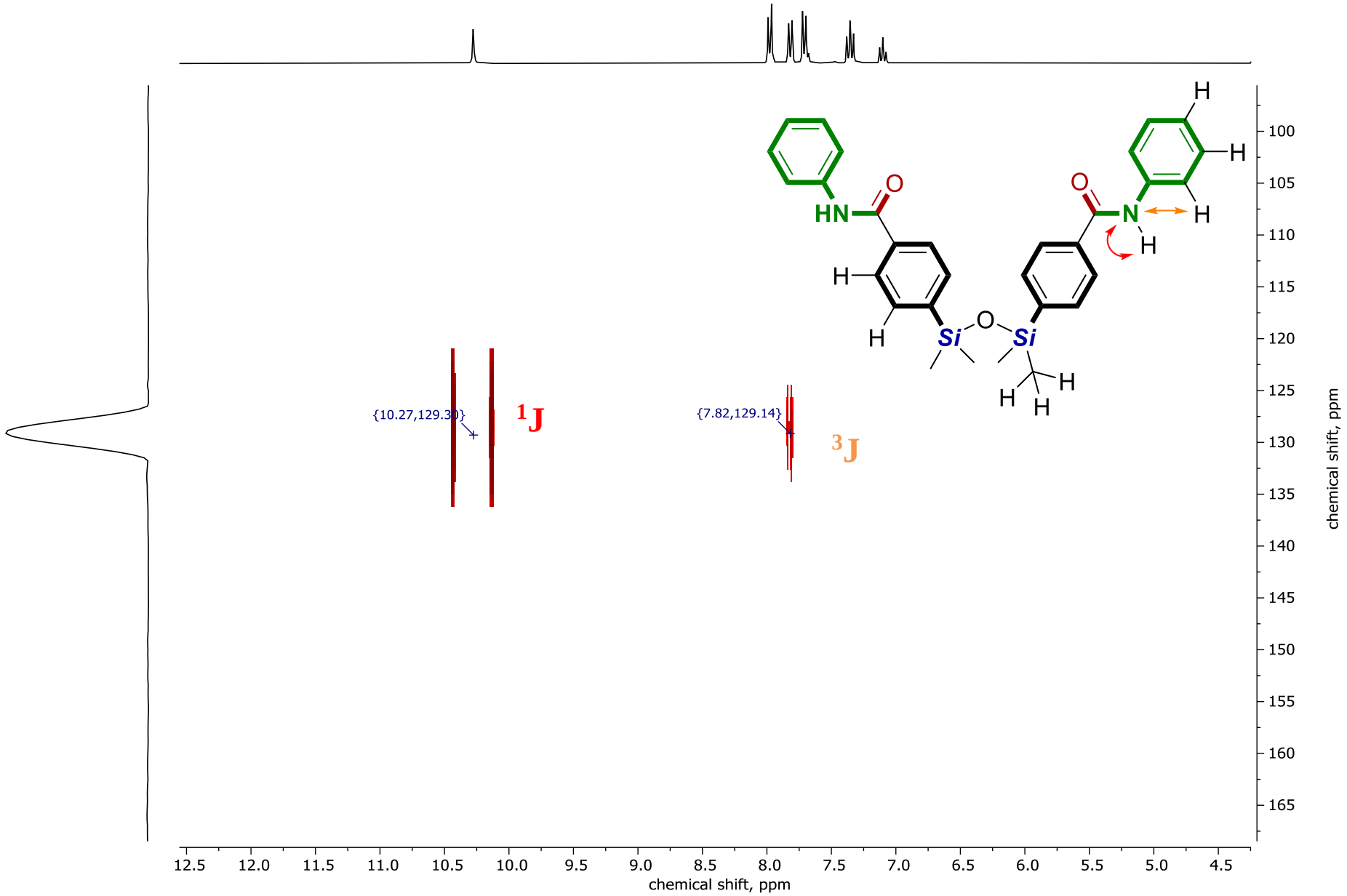
$^{1}H - {}^{29}Si$ HMBC

(400 MHz, DMSO-d6)



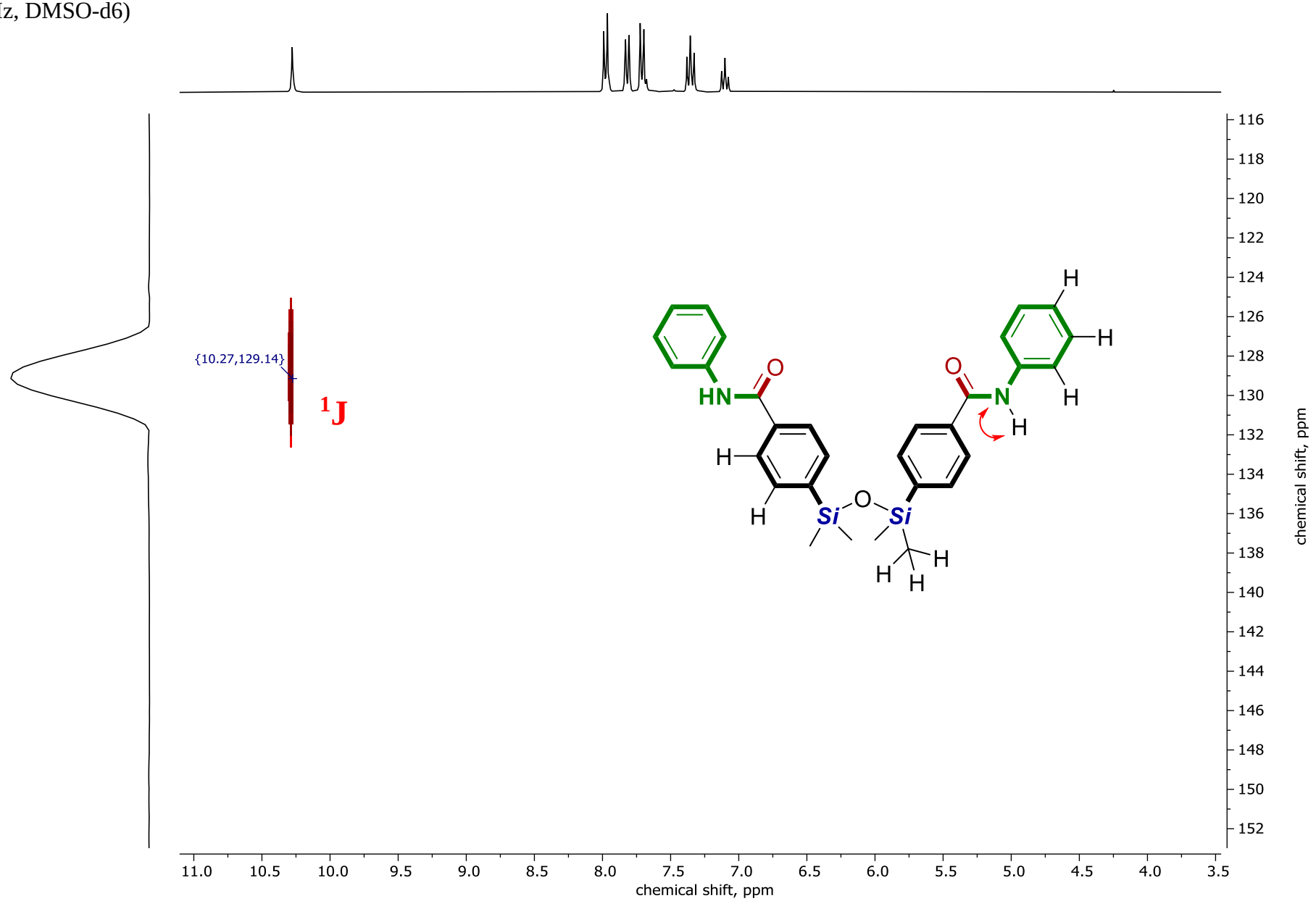
$^{1}H - ^{15}N$ HMBC

(400 MHz, DMSO-d6)

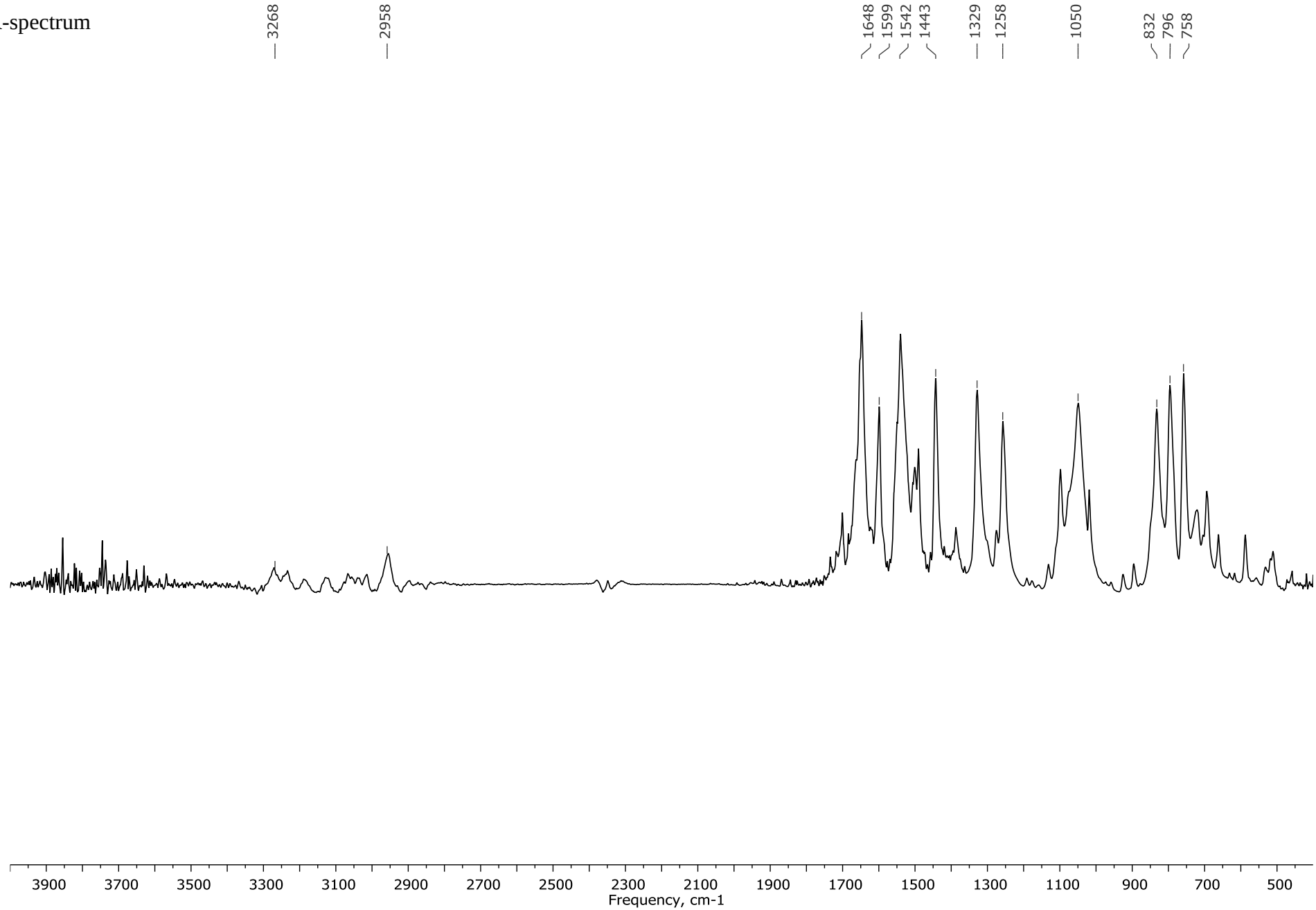


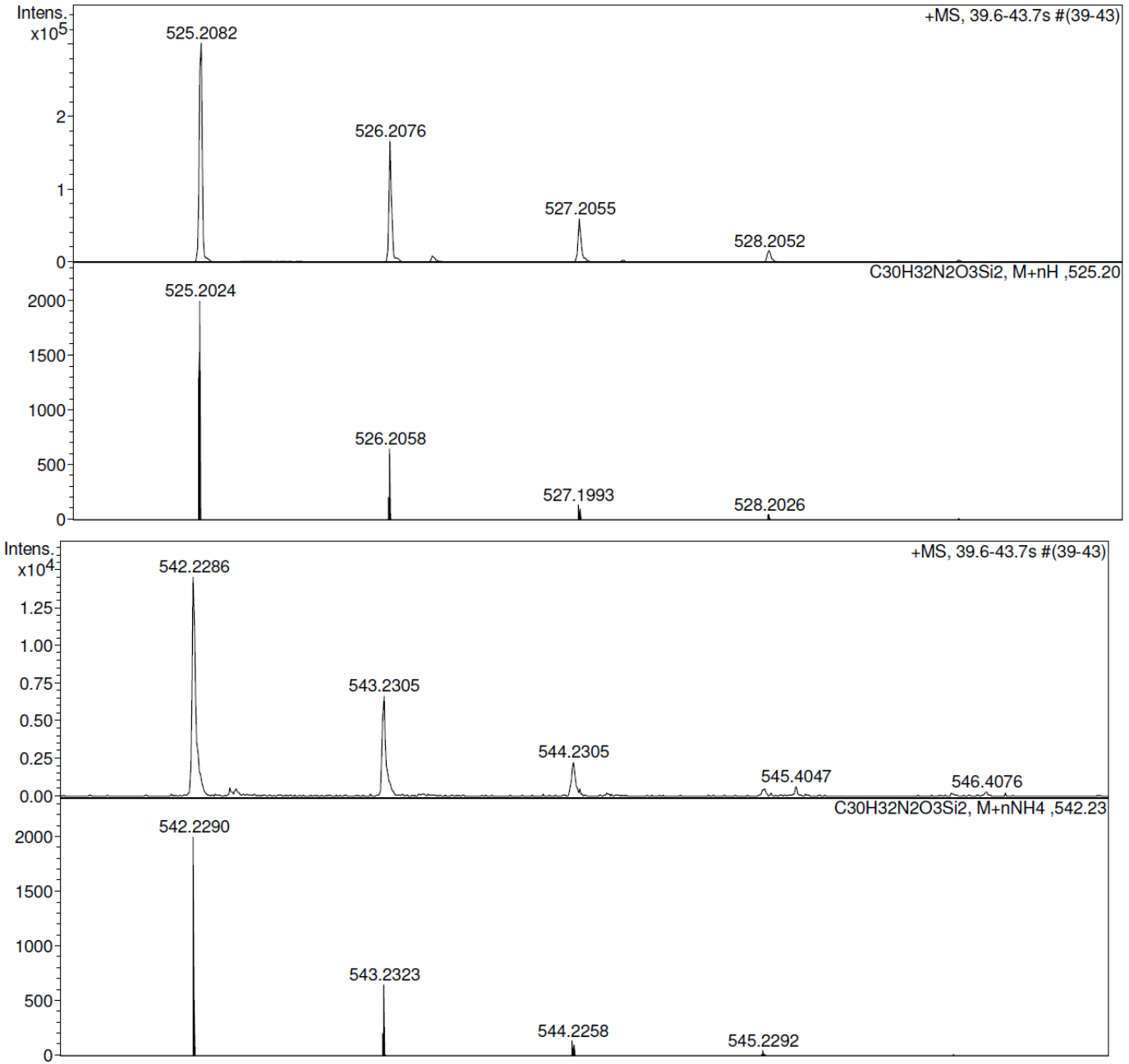
$^{1}H - ^{15}N$ HSQC

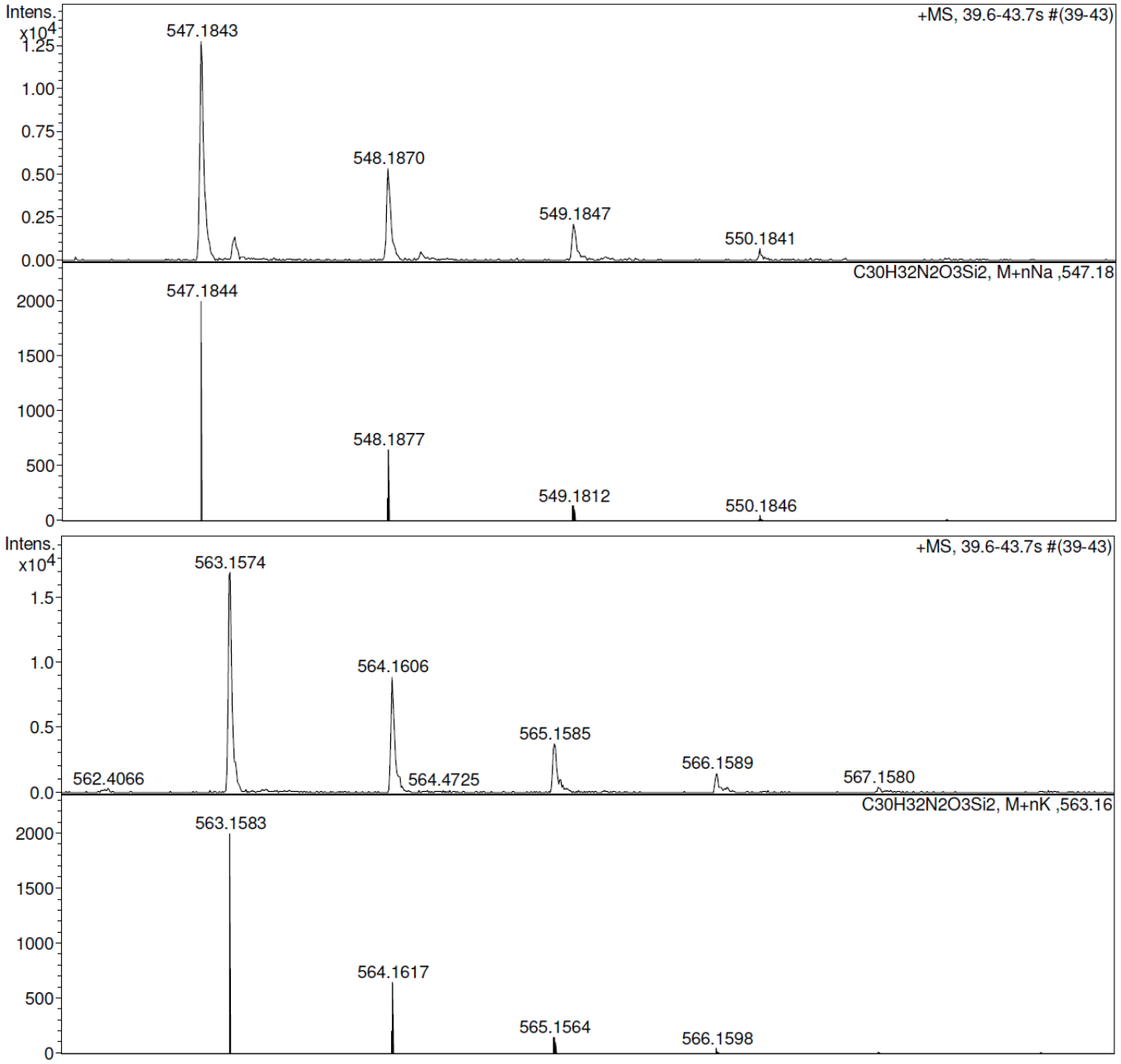
(400 MHz, DMSO-d6)

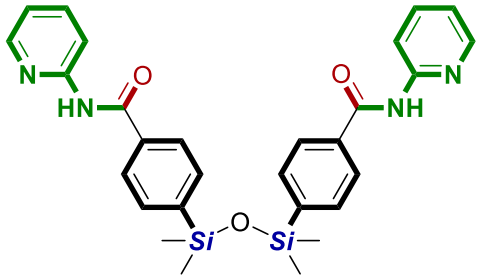


IR-spectrum


3268
2958
1648
1599
1542
1443
1329
1258
1050
832
796
758
3900
3700
3500
3300
3100
2900
2700
2500
2300
2100
1900
1700
1500
1300
1100
900
700
500
Frequency, cm-1


Intens.
x10^5
+MS, 39.6-43.7s #(39-43)
525.2082
526.2076
527.2055
528.2052
C30H32N2O3Si2, M+nH ,525.20
525.2024
526.2058
527.1993
528.2026
Intens.
x10^4
+MS, 39.6-43.7s #(39-43)
542.2286
543.2305
544.2305
545.4047
546.4076
C30H32N2O3Si2, M+nNH4 ,542.23
542.2290
543.2323
544.2258
545.2292


Intens.
x10^4
+MS, 39.6-43.7s #(39-43)
547.1843
548.1870
549.1847
550.1841
C30H32N2O3Si2, M+nNa ,547.18
547.1844
548.1877
549.1812
550.1846
Intens.
x10^4
+MS, 39.6-43.7s #(39-43)
563.1574
564.1606
565.1585
566.1589
562.4066
564.4725
567.1580
C30H32N2O3Si2, M+nK ,563.16
563.1583
564.1617
565.1564
566.1598

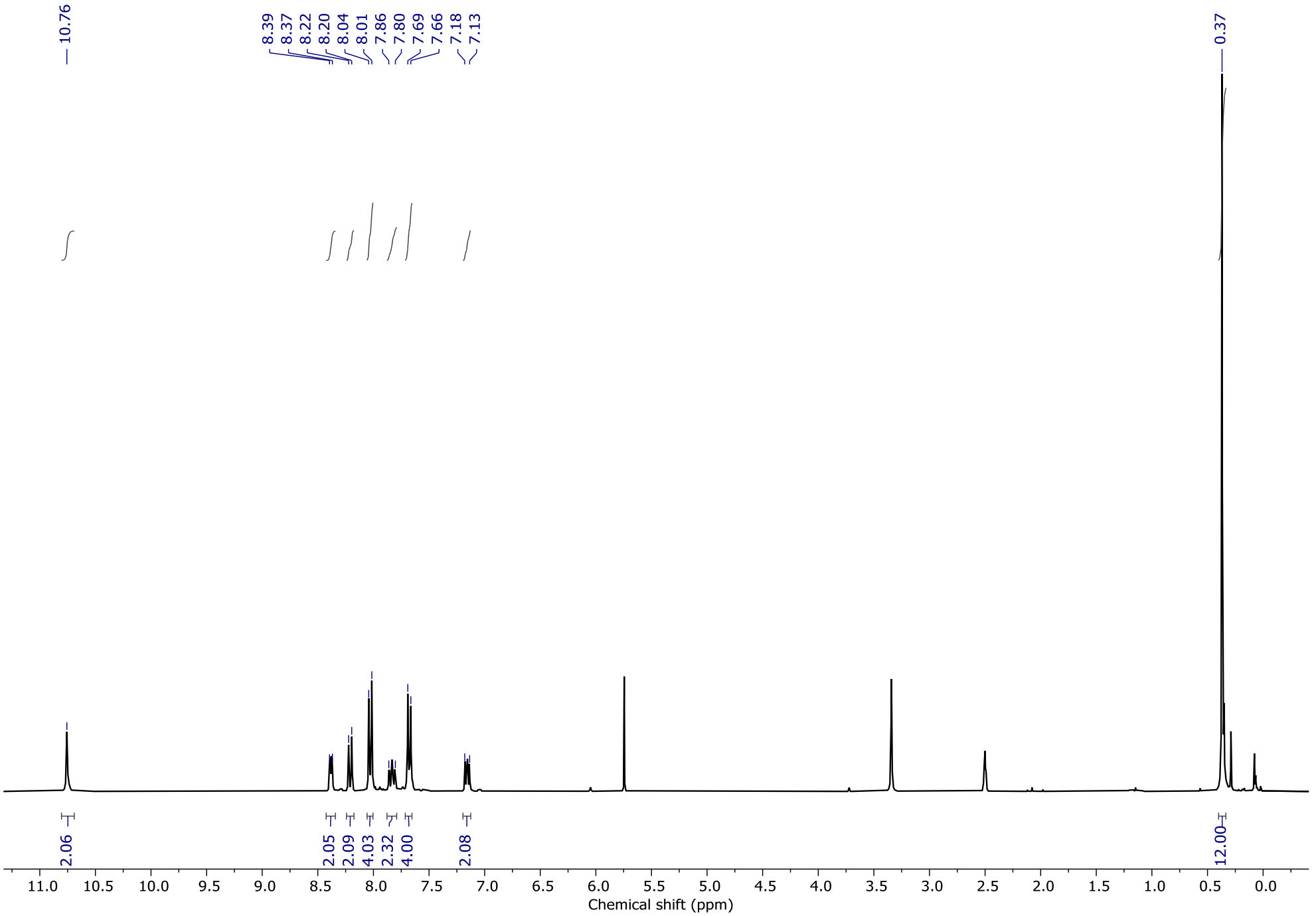


Characterisation data for 4,4'-(1,1,3,3-tetramethyldisiloxane-1,3-diyl)bis(N-(pyridin-2-yl)benzamide):

^{1}H NMR (400 MHz, DMSO-d6): δ = 10.76 (s, 2H), δ = 8.39-8.37 (m, 2H), δ = 8.21 (m, 2H), δ = 8.03(d, ^{3}J= 11Hz, 4H), δ = 7.86-7.80 (m, 2H), δ = 7.68 (d, ^{3}J= 11 Hz, 4H), δ = 7.18-7.13 (m, 2H), δ = 0.37 (s, 12H). ^{13}C NMR (100 MHz, DMSO-d6): δ = 165.97, 152.14, 147.90, 143.46, 138.06, 134.99, 132.76, 127.15, 119.79, 114.70, 0.67. ^{29}Si NMR (80 MHz, DMSO-d6): δ = -0.39. ^{15}N NMR (40 MHz, DMSO-d6): δ = 288.93, 138.27. HRMS (ESI) m/z [M + H] $^{+}$: calcd for $[C_{28}H_{30}N_4O_3Si_2 + H]^{+}$, 527.1929; found, 527.1964; [M + K] $^{+}$: calcd for $[C_{28}H_{30}N_4O_3Si_2 + K]^{+}$, 565.1488; found, 565.1482; [M + Na] $^{+}$: calcd for $[C_{28}H_{30}N_4O_3Si_2 + Na]^{+}$, 549.1749; found, 549.1746. IR (cm^{-1}): 2957, 1676, 1582, 1539, 1437, 1306, 1254, 1074, 831, 794.

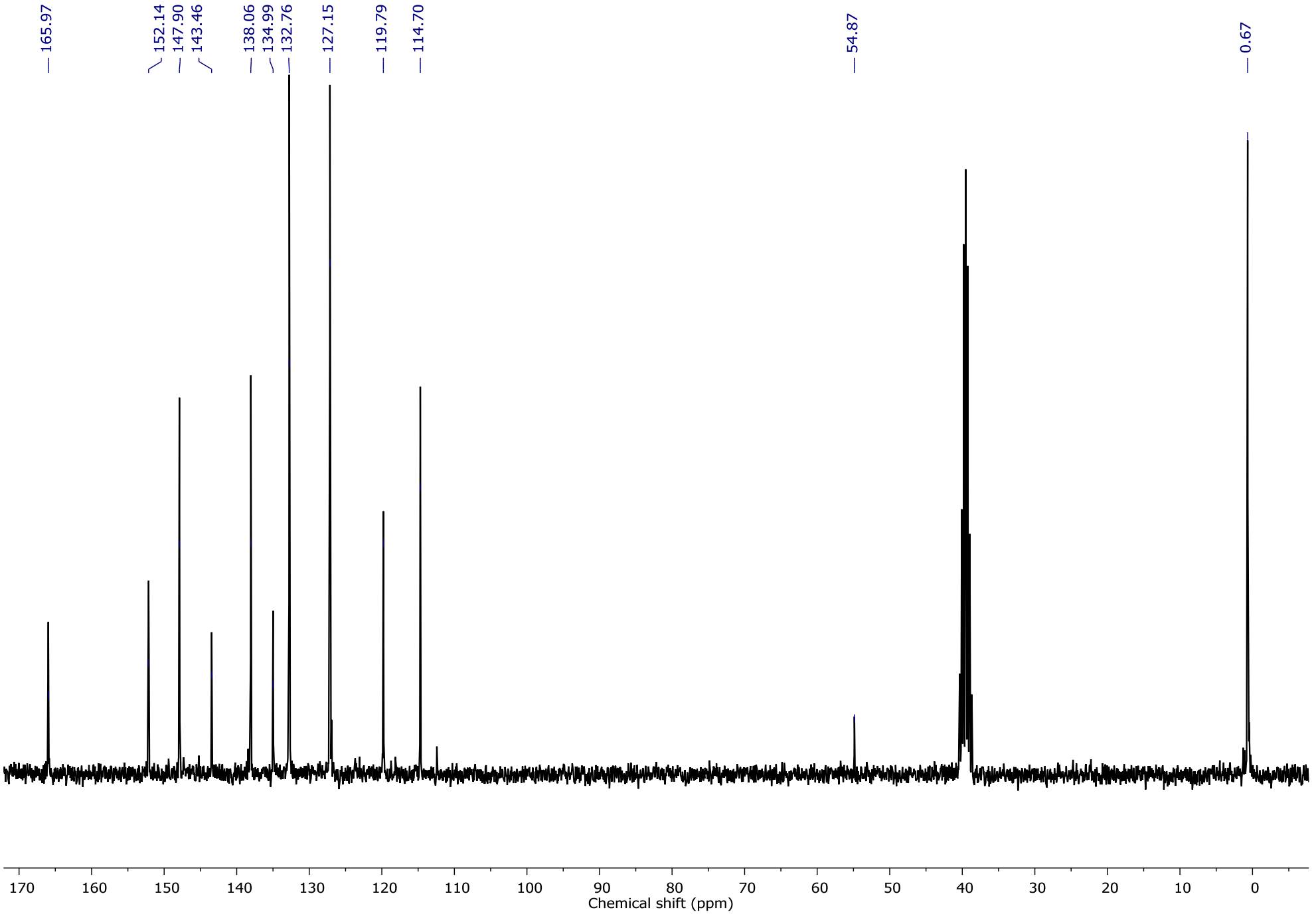
^{1}H NMR

(400 MHz, DMSO-d6)



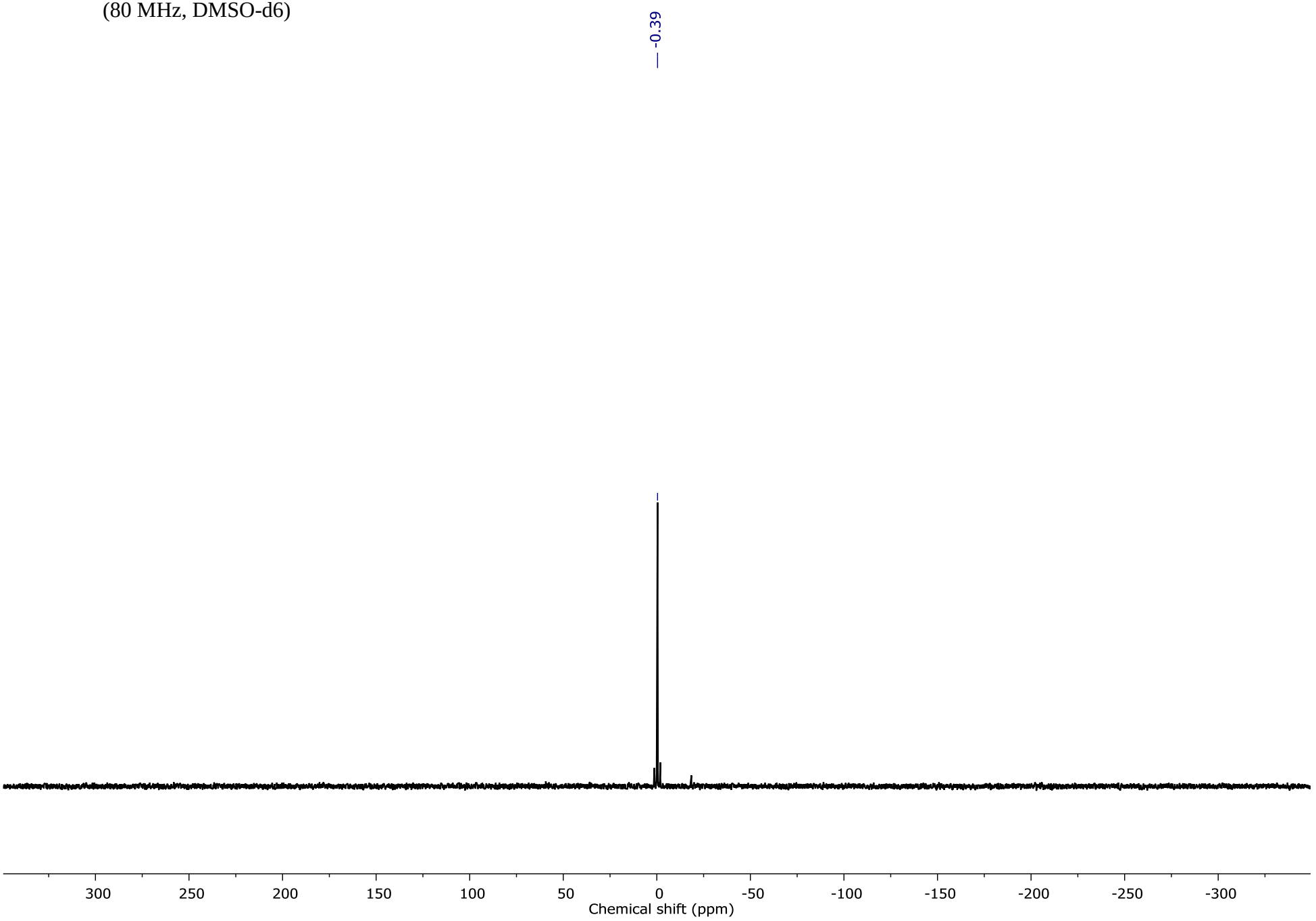
^{13}C NMR

(100 MHz, DMSO-d6)



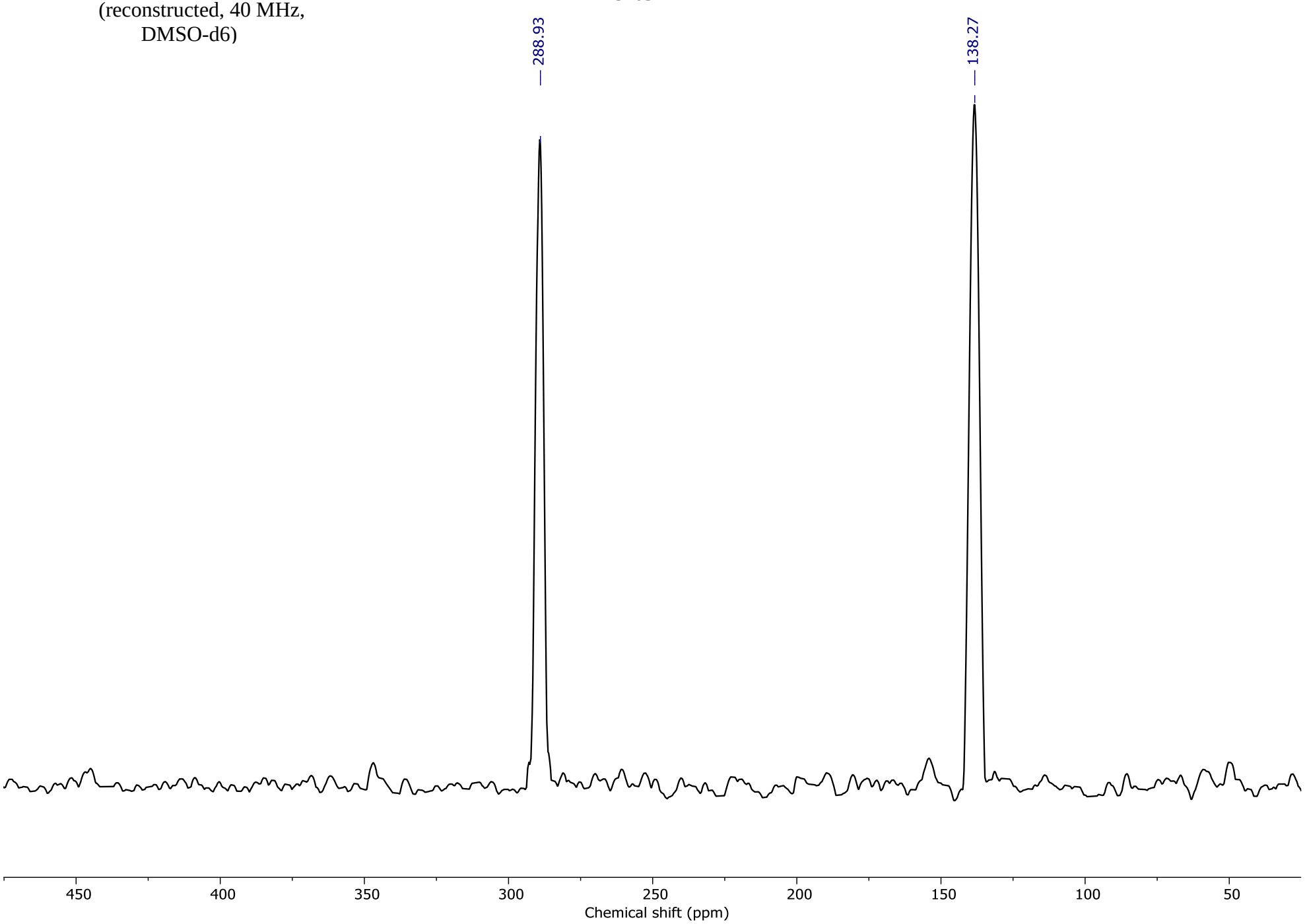
^{29}Si NMR

(80 MHz, DMSO-d6)



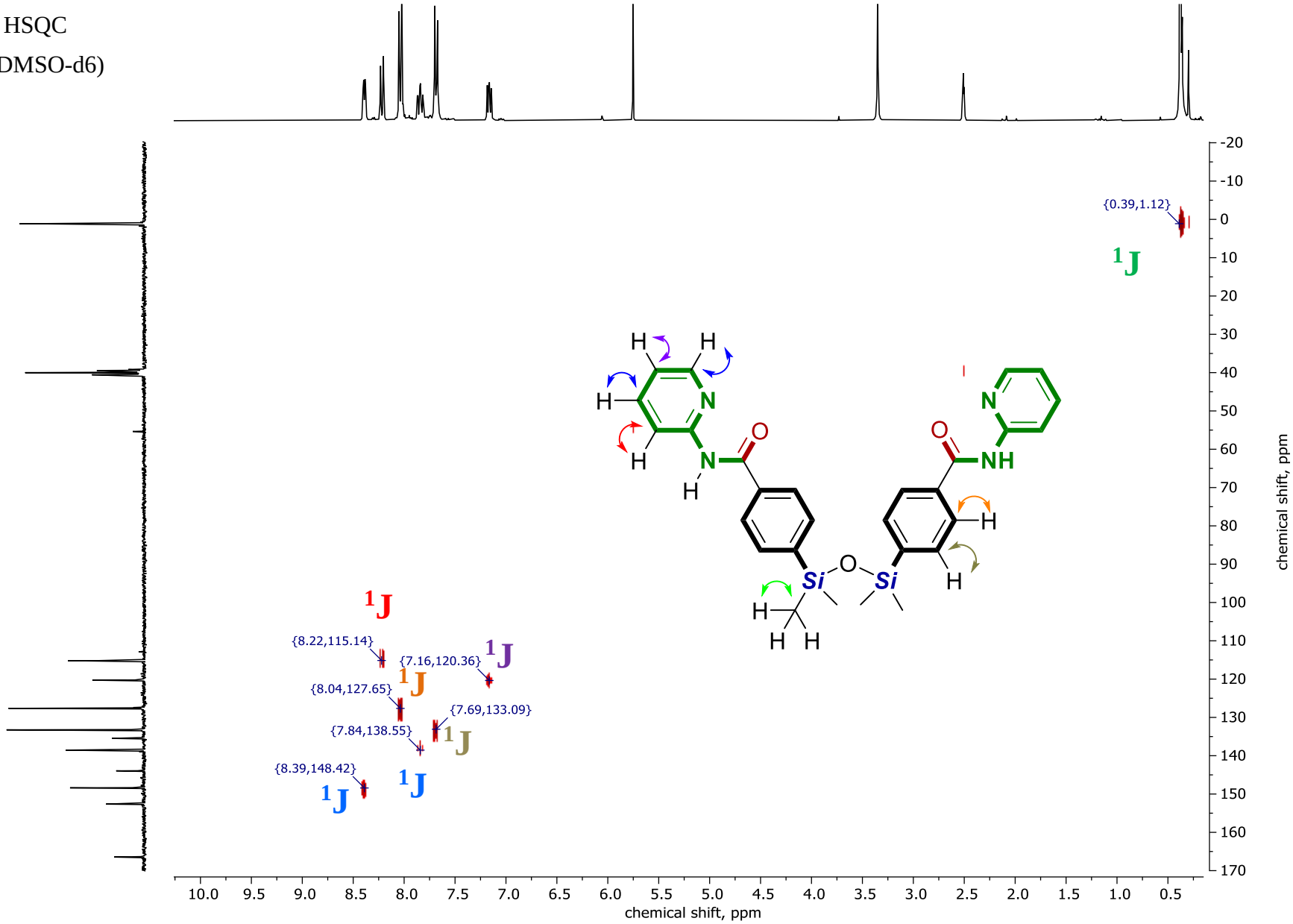
^{15}N NMR

(reconstructed, 40 MHz, DMSO-d6)



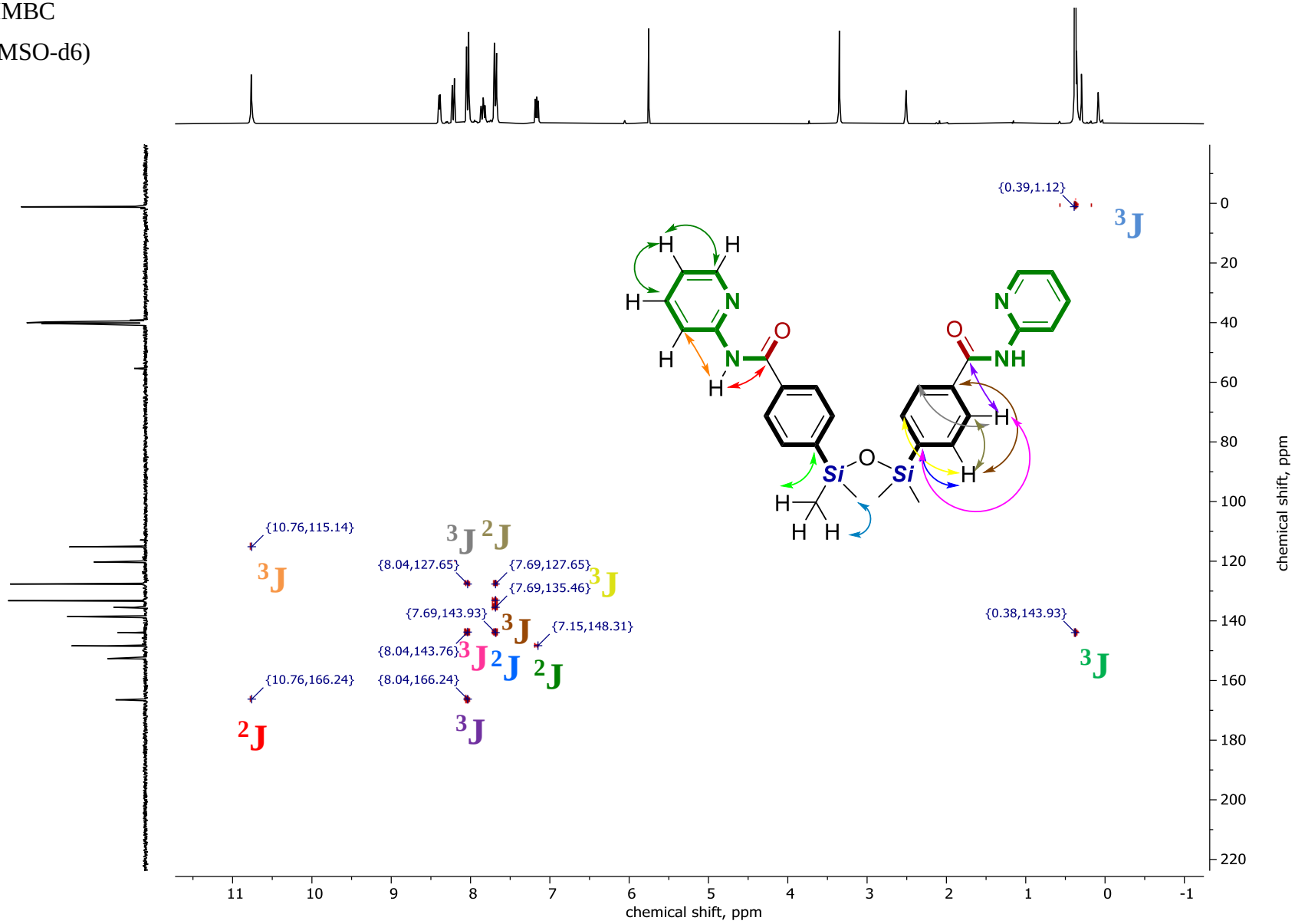
^{1}H - ^{13}C HSQC

(400 MHz, DMSO-d6)



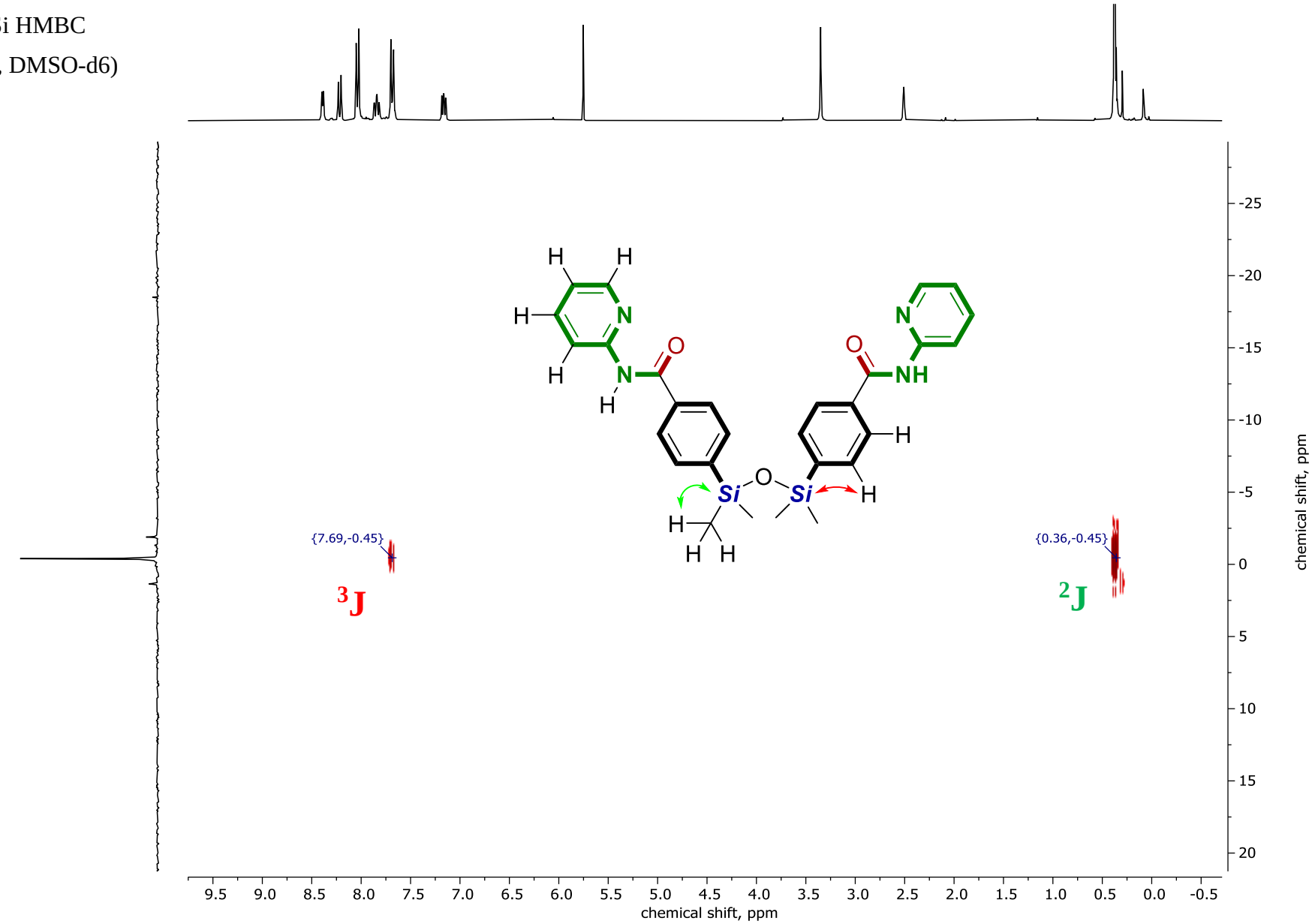
^{1}H - ^{13}C HMBC

(400 MHz, DMSO-d6)



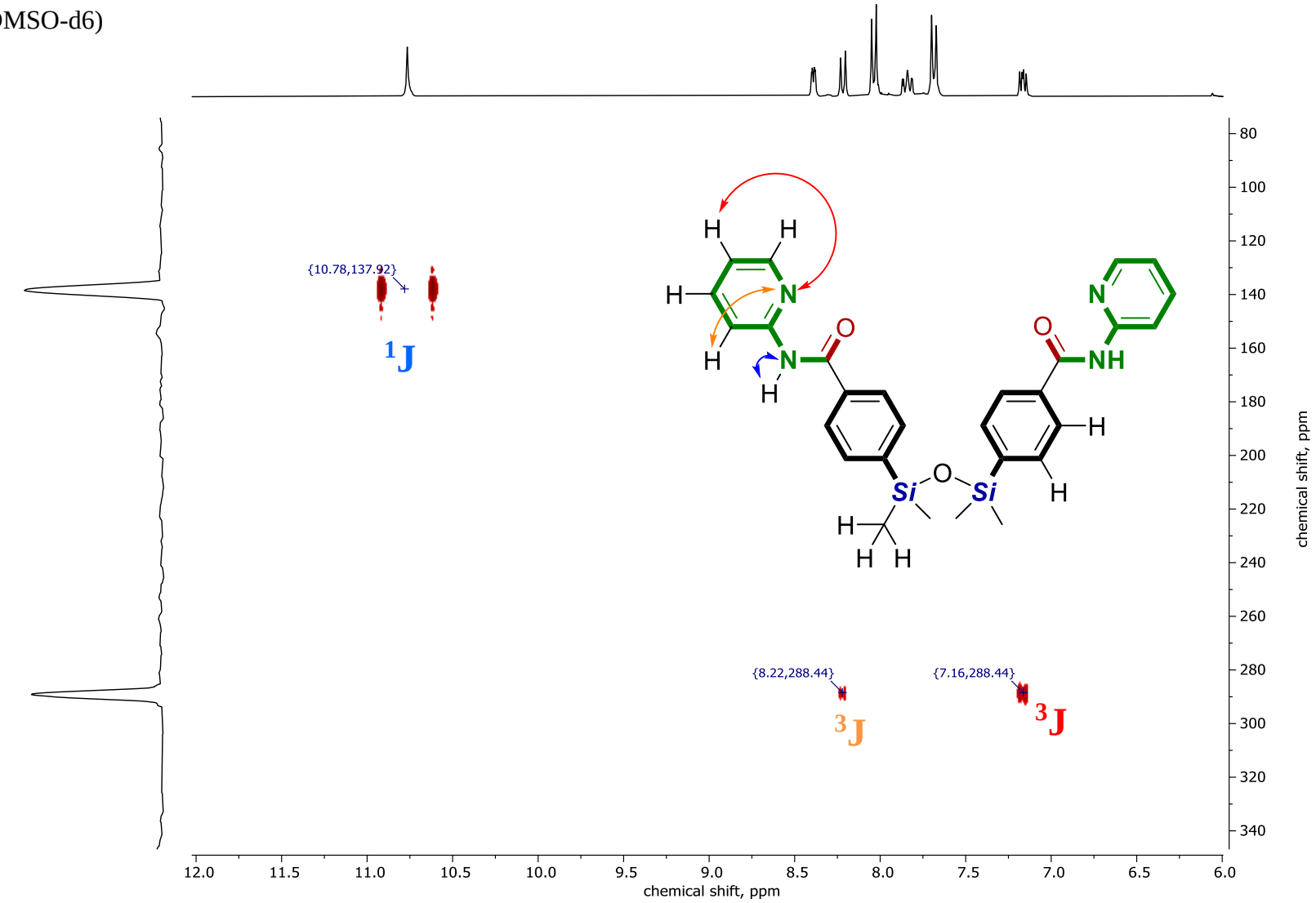
^{1}H - ^{29}Si HMBC

(400 MHz, DMSO-d6)



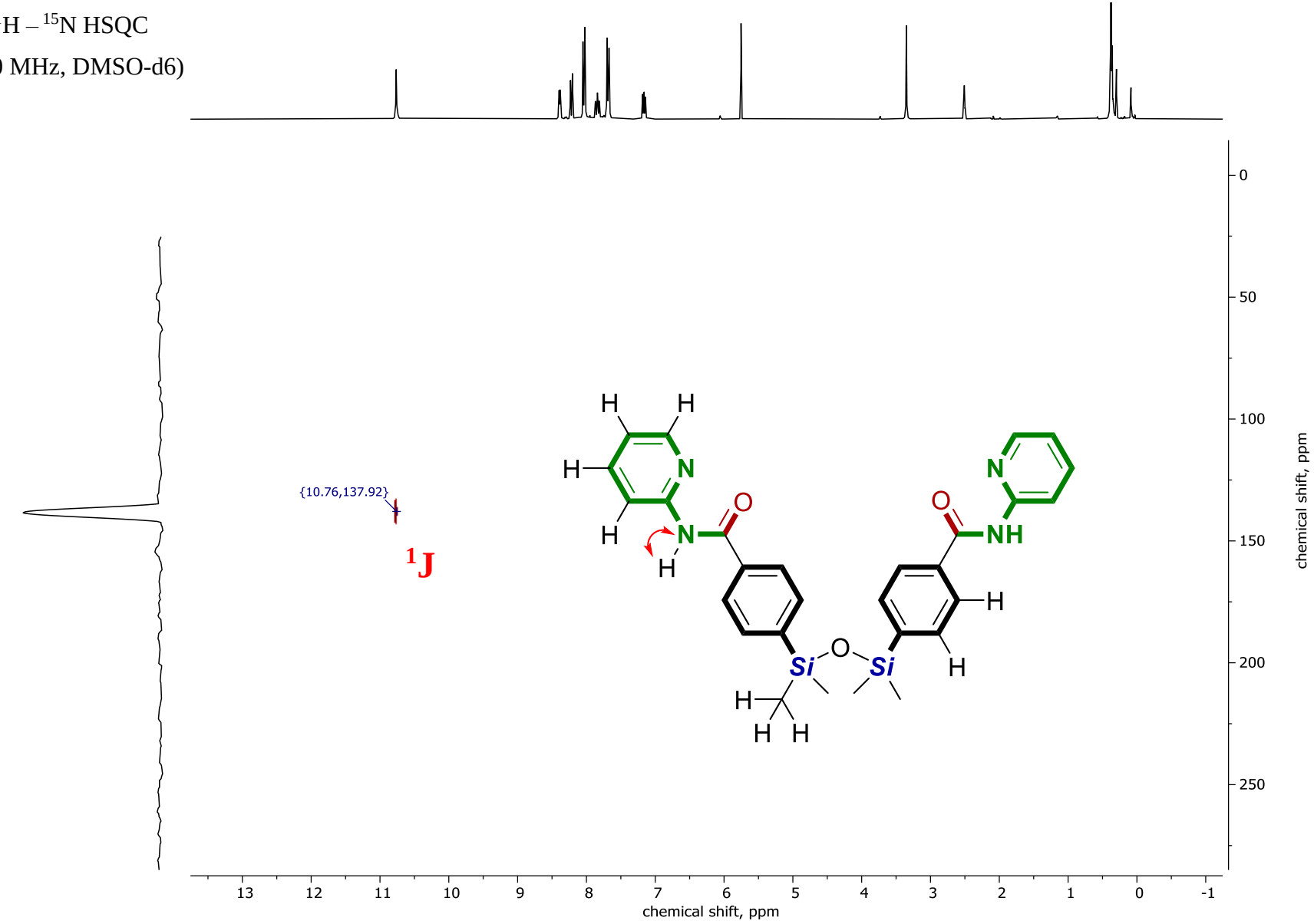
$^{1}H - {}^{15}N$ HMBC

(400 MHz, DMSO-d6)

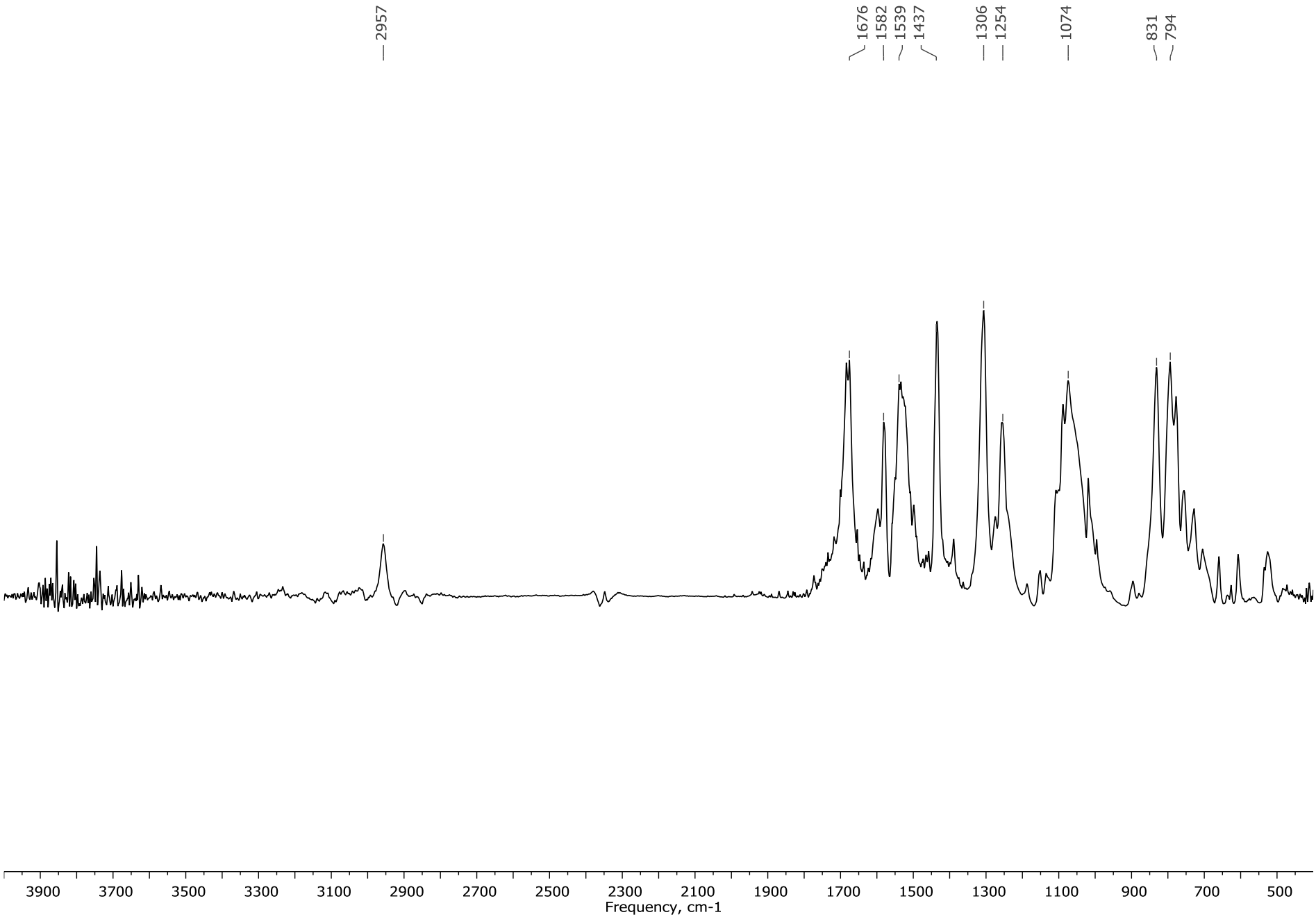


$^{1}H - ^{15}N$ HSQC

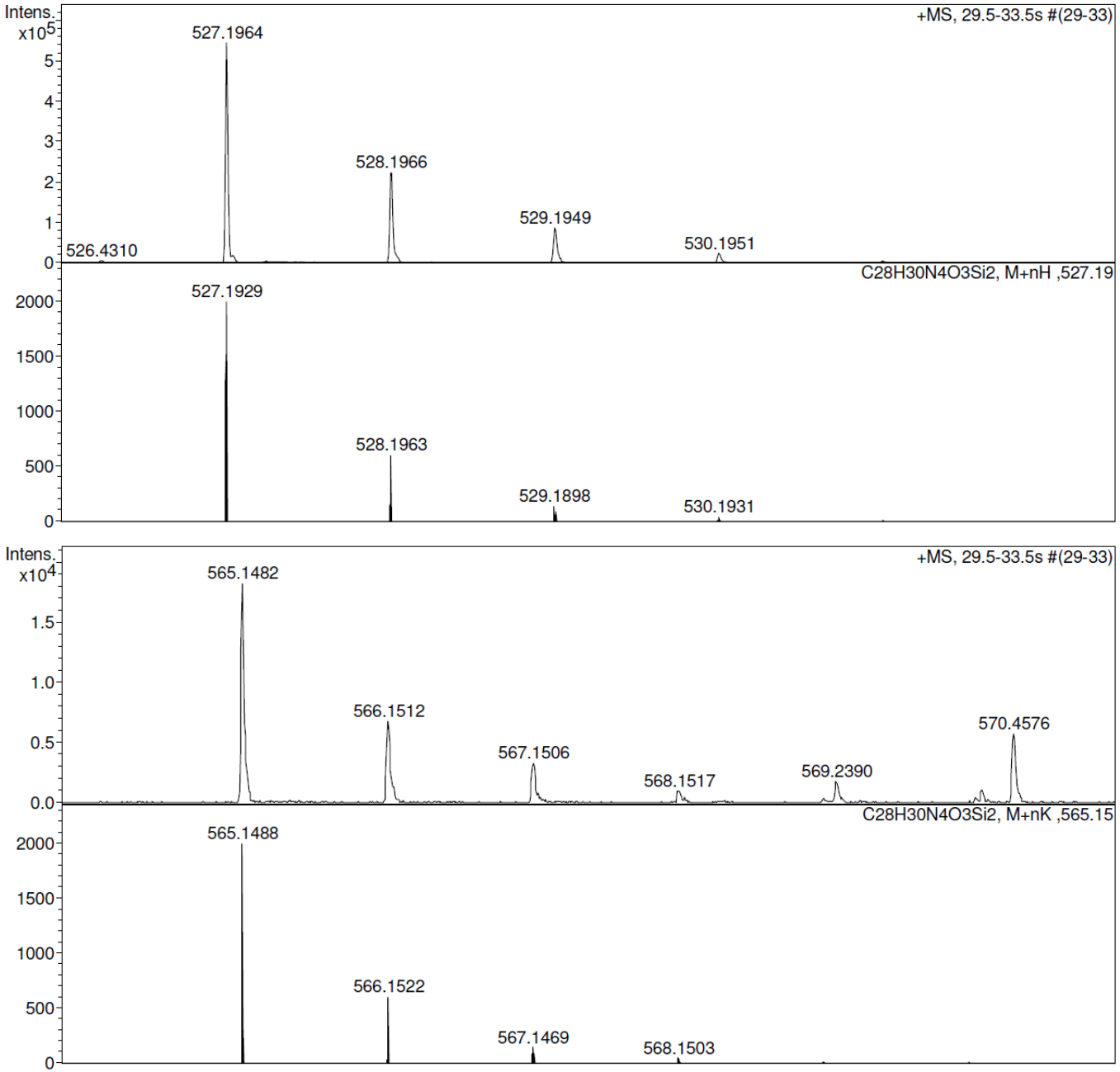
(400 MHz, DMSO-d6)

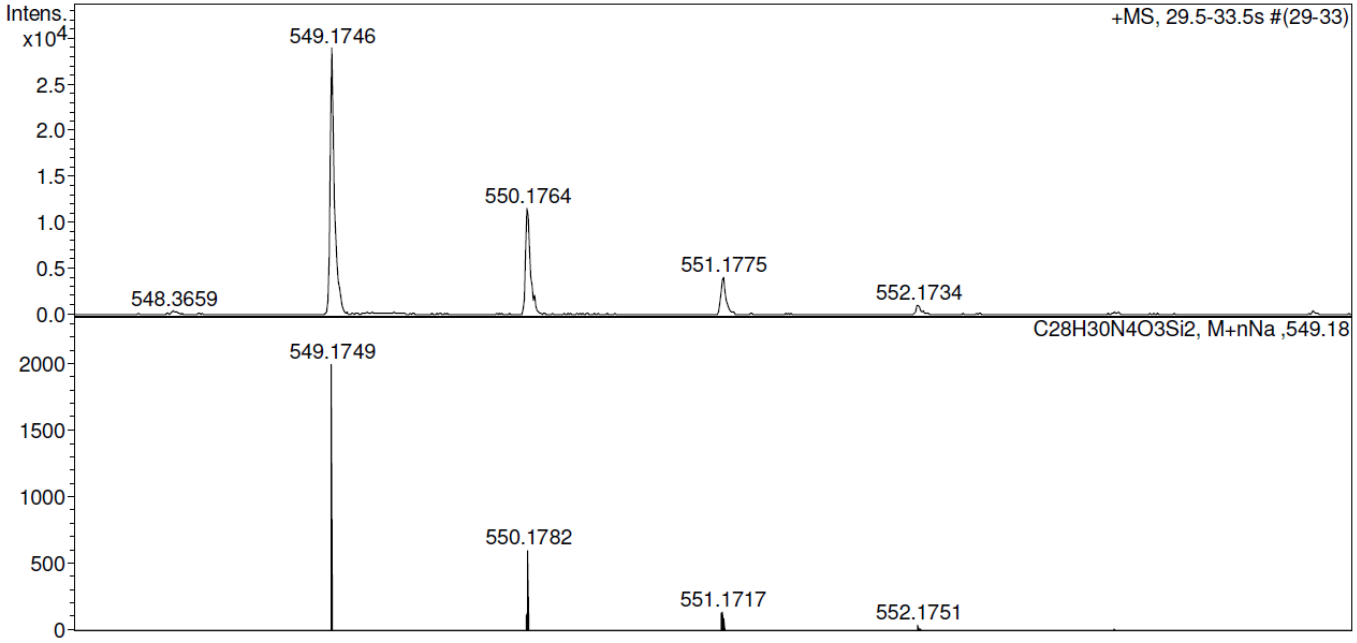


IR-spectrum


2957
1676
1582
1539
1437
1306
1254
1074
831
794
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, 29.5-33.5s #(29-33)
527.1964
528.1966
529.1949
530.1951
526.4310
C28H30N4O3Si2, M+nH ,527.19
527.1929
528.1963
529.1898
530.1931
Intens.
x10^4
+MS, 29.5-33.5s #(29-33)
565.1482
566.1512
567.1506
568.1517
569.2390
570.4576
C28H30N4O3Si2, M+nK ,565.15
565.1488
566.1522
567.1469
568.1503


Intens.
x10^4
2.5
2.0
1.5
1.0
0.5
0.0
549.1746
550.1764
551.1775
548.3659
552.1734
+MS, 29.5-33.5s #(29-33)
C28H30N4O3Si2, M+nNa ,549.18
2000
1500
1000
500
0
549.1749
550.1782
551.1717
552.1751