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Supplementary information

Quantum defects as versatile anchors for carbon nanotube functionalization

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Supplementary Data

Quantum defects as versatile anchors for carbon nanotube functionalization

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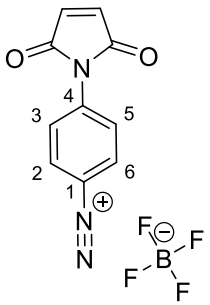
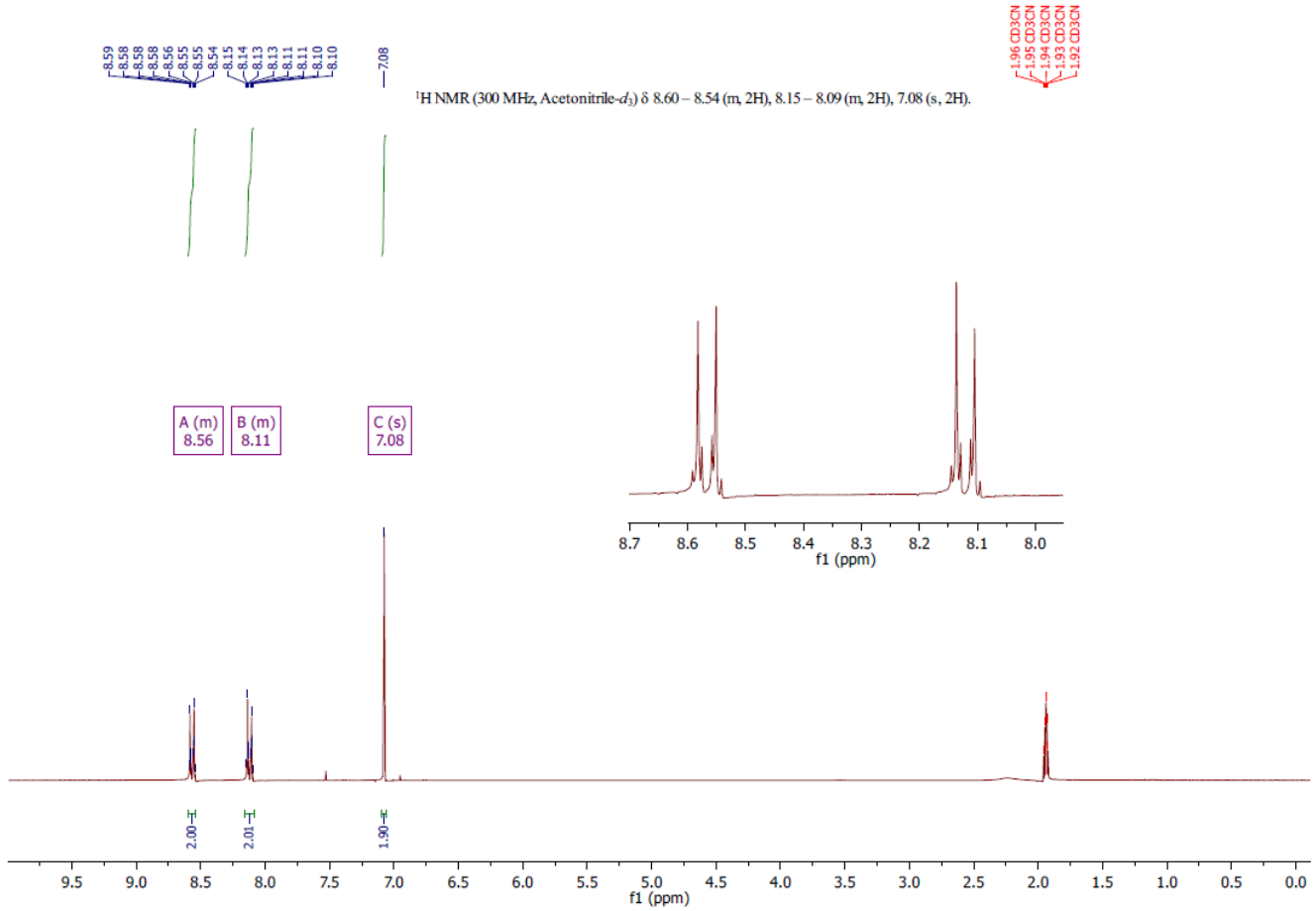
NMR spectra were measured on a Bruker Avance III HD 300 with a 5 mm probe at room temperature, using standard glass NMR tubes. ^{1}H and ^{13}C shifts are reported relative to (residual) solvent peaks. MestReNova 10 was used for analysis. ESI-TOF-MS spectra were acquired on a Bruker micrOTOF using direct injection. Small amounts of methanol were added to the acetonitrile solutions to enhance the ESI-MS signal.

4-(*N*-Maleimido)phenyldiazonium tetrafluoroborate



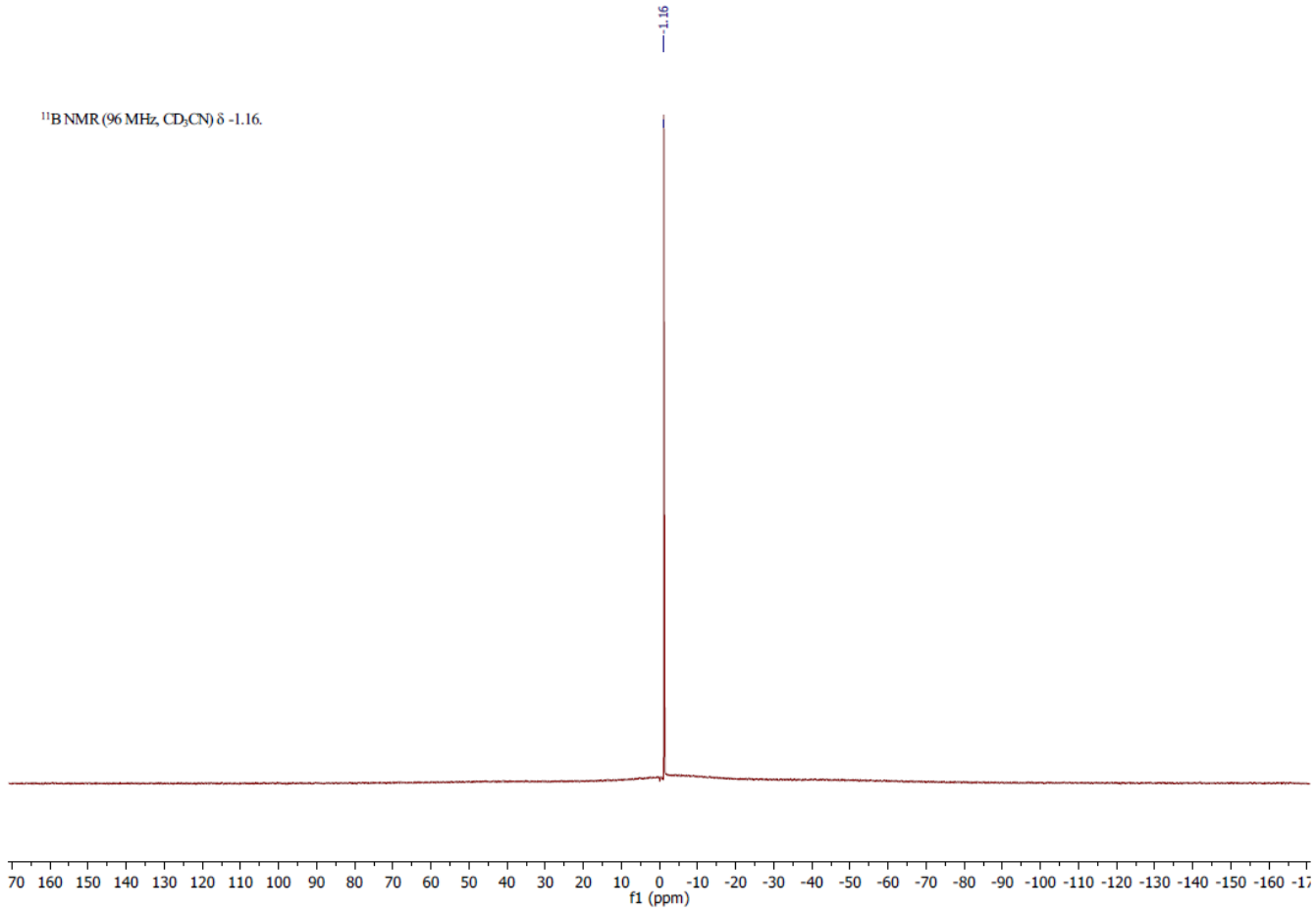
^{1}H-NMR (300 MHz**,** CD_3CN)**:** δ(ppm) = 8.56 (m, 2 H, $H_{2,6}$), 8.09 to 8.15 (m, 2 H, $H_{3,5}$), 7.08 (s, 2 H, $H_{maleimide}$).
^{11}B-NMR (96 MHz**,** CD_3CN)**:** δ(ppm) = −1.16 (s).
^{19}F-NMR (282 MHz**,** CD_3CN)**:** δ(ppm) = −151.48 (s), −151.54 (s) (two signals due to the two NMR-active boron isotopomers).
^{13}C-NMR (75 MHz**,** CD_3CN)**:** δ(ppm) = 169.4, 144.8, 136.5, 134.7, 127.4, 111.2.
HRMS (ESI (pos.) [*m/z*]): calculated ($C_{10}H_6N_3O_2$ [M^+]): 200.0455, found: 200.0448; calculated ($C_{10}H_6NO_2$ [M-N_2]$^+$): 172.0393, found: 172.0389; ($C_{11}H_{10}NO_3$ [M-N_2+MeOH]$^+$): 204.0645, found: 204.0655.
The ^{1}H-NMR data is corresponding to the literature.[1]

^{1}H-NMR



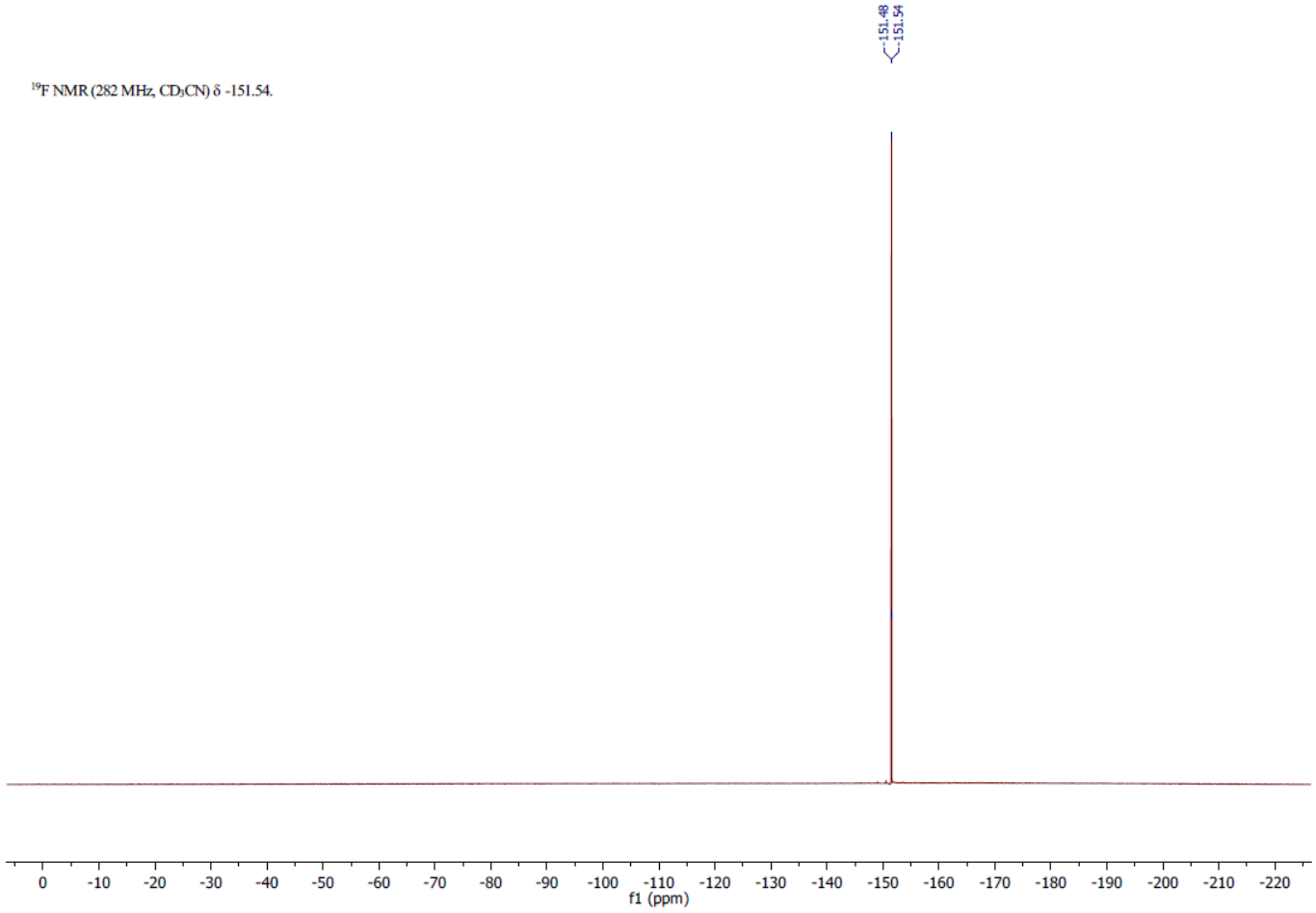
^{1}H NMR (300 MHz, Acetonitrile-d_3) δ 8.60 – 8.54 (m, 2H), 8.15 – 8.09 (m, 2H), 7.08 (s, 2H).

^{11}B-NMR



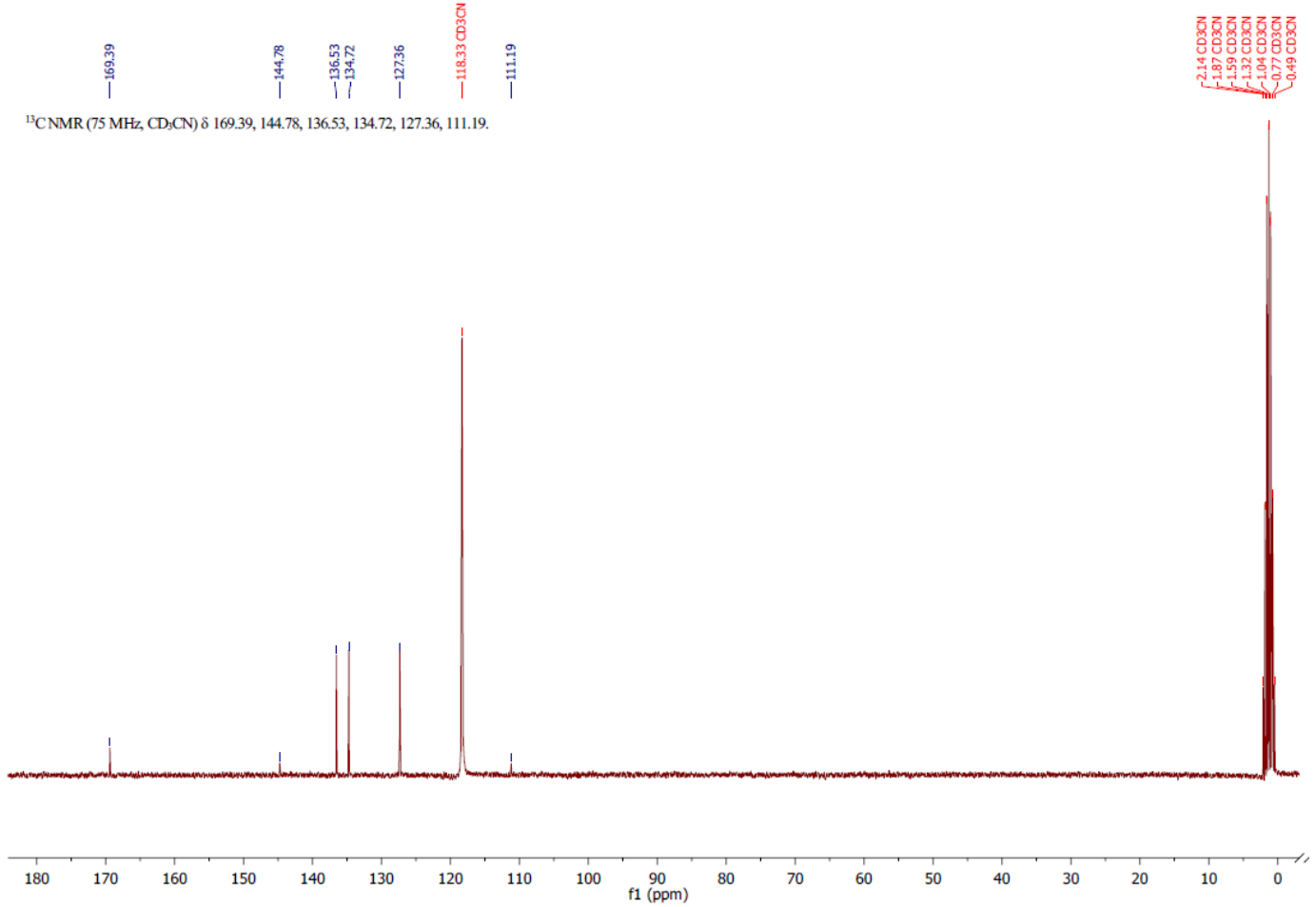
^{11}B NMR (96 MHz, CD_3CN) δ -1.16.

^{19}F-NMR

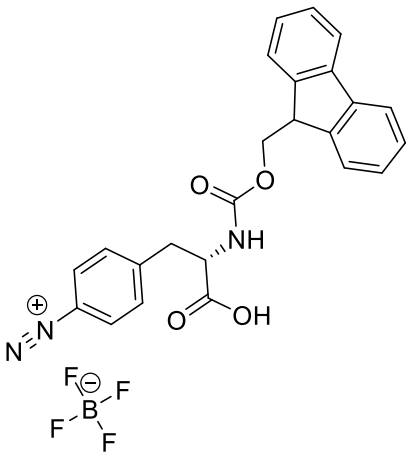


^{19}F NMR (282 MHz, CD_3CN) δ -151.54.

^{13}C-NMR



Fmoc-L-4-diazonium-phenylalanine tetrafluoroborate



^{1}H-NMR (300 MHz, CD_3CN): δ(ppm) = 8.35 (d, J = 8.5 Hz, 2H), 7.84 (d, J = 7.5 Hz, 2H), 7.76 (d, J = 8.4 Hz, 2H), 7.61 (dd, J = 7.5, 4.6 Hz, 2H), 7.43 (t, J = 7.5 Hz, 2H), 7.35 (t, J = 7.5 Hz, 2H), 6.13 (d, J= 8.7 Hz, 1H), 4.53 (s, 1H), 4.30 (d, J = 6.2 Hz, 2H), 4.18 (t, J = 6.8 Hz, 1H), 3.50 –3.41 (m, 1H), 3.27 –3.16 (m, 1H).

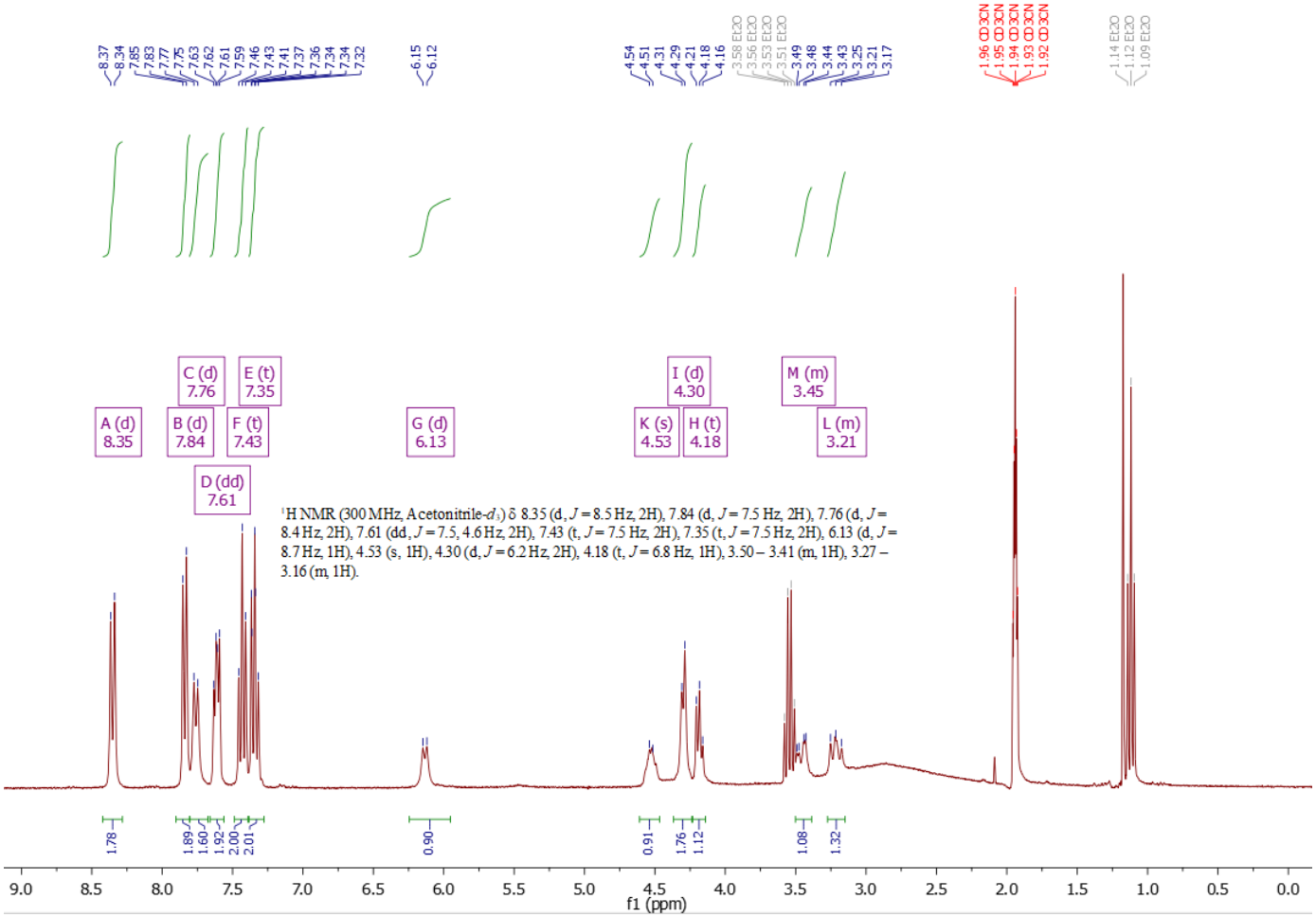
^{11}B-NMR (96 MHz, CD_3CN): δ(ppm) = −1.15(s).

^{19}F-NMR (282 MHz, CD_3CN): δ(ppm) = −151.47 (s), −151.53 (s) (two signals due to the two NMR-active boron isotopomers).

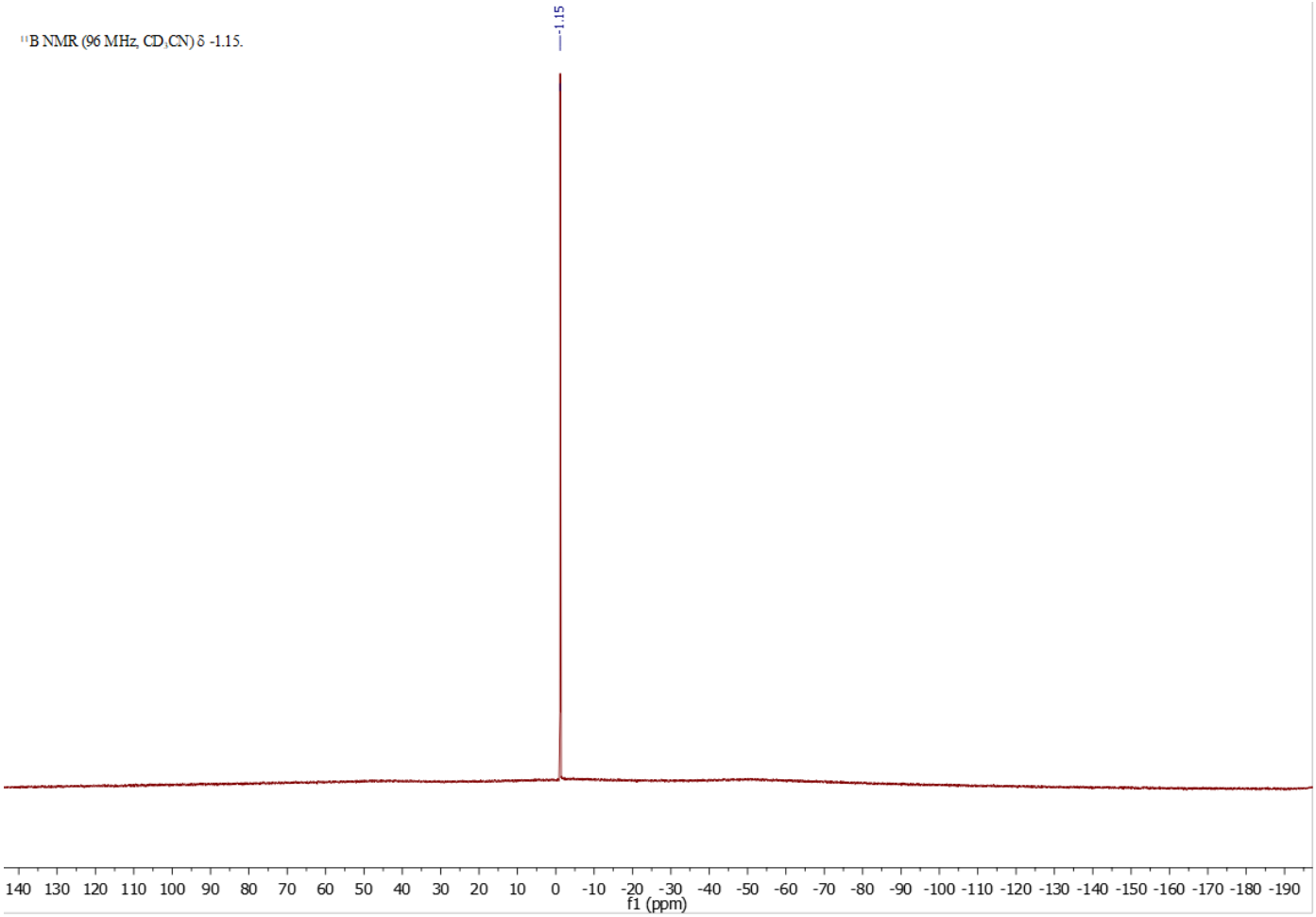
A ^{13}C-NMR was not obtained due to the low solubility of this compound in acetonitrile.

HRMS (ESI (pos.) [*m/z*]): calculated ($C_{24}H_{21}NO_4[M\text{-}N_2]^+$): 386.1392, found: 386.1387.

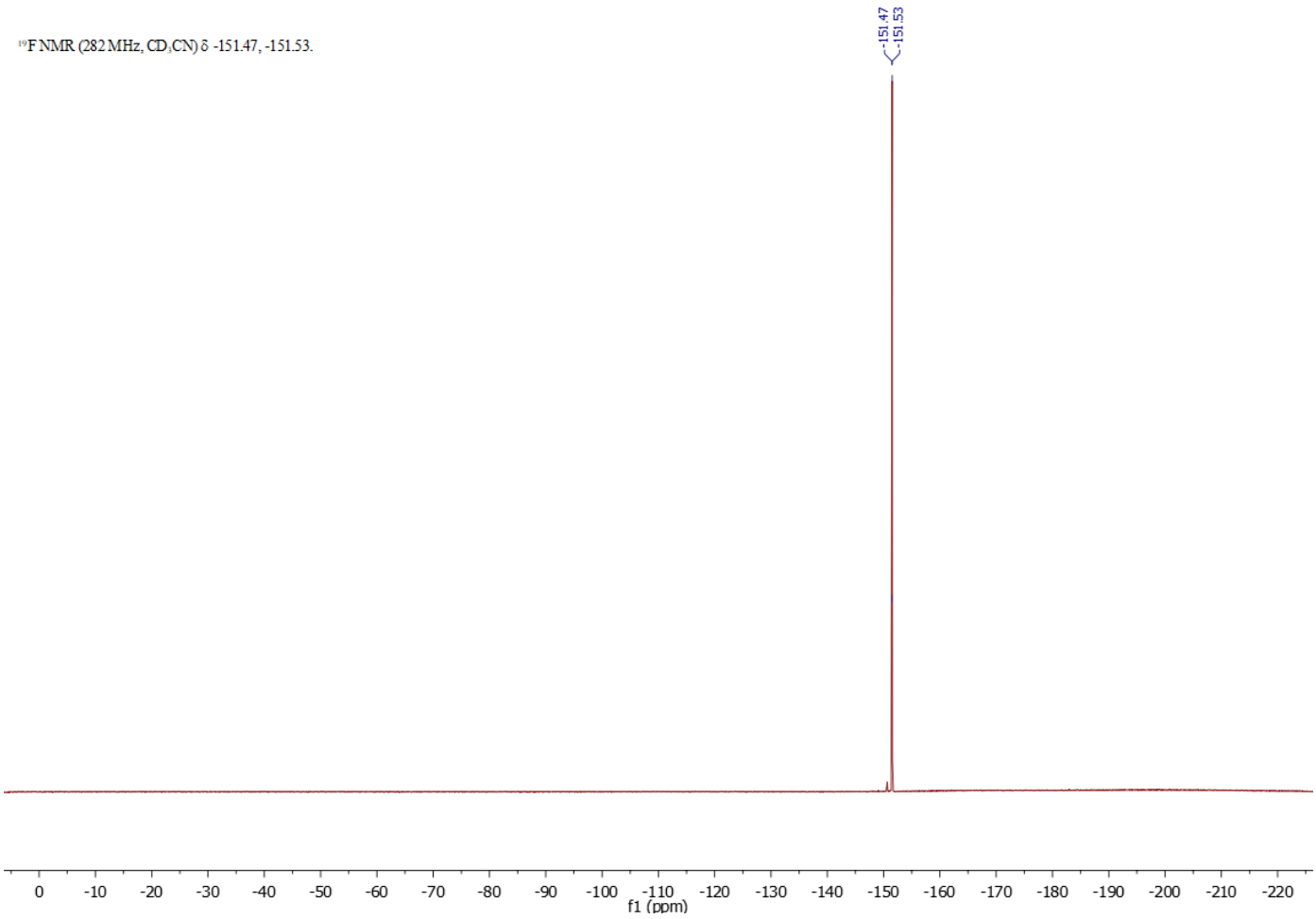
^{1}H-NMR



^{11}B-NMR


^{11}B NMR (96 MHz, CD$_3$CN) δ -1.15.
-1.15
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)

^{19}F-NMR



[1] J. C. Harper, R. Polsky, D. R. Wheeler, S. M. Brozik, *Langmuir* **2008**, *24*, 2206–2211.