Supporting Information

Iodonium Complexes of the Tertiary Amines Quinuclidine and 1-Ethylpiperidine

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Synthesis

General Considerations

All reagents and solvents were obtained from commercial suppliers and used without further purification. For structural NMR assignments, ^{1}H NMR and ^{1}H-^{15}N NMR correlation spectra were recorded on a Bruker Avance III 500 MHz spectrometer at 25ºC in CD_3CN. Chemical shifts are reported on the δ scale in ppm using the residual solvent signal as internal standard (CD_3CN; δ_H 1.94), or for ^{1}H-^{15}N NMR spectroscopy, to an external d_3-$MeNO_2$ standard. For ^{1}H NMR spectroscopy, each resonance was assigned according to the following conventions: chemical shift (δ) measured in ppm, observed multiplicity, number of hydrogens, observed coupling constant (*J* Hz), and assignment. Multiplicities are denoted as: s (singlet), d (doublet), t (triplet), q (quartet), sept (septet), m (multiplet), and br (broad). For the ^{1}H-^{15}N HMBC spectroscopy, spectral windows of 4 ppm (^{1}H) and 600 ppm (^{15}N) were used, with 1024 points in the direct dimension and 512 increments used in the indirect dimension (resolution ≈ 0.3 ppm/point).

The single crystal X-ray data for [**1**]PF_6 was collected at 170 K using Bruker-Nonius Kappa CCD diffractometer with an APEX-II detector with graphite-monochromatised Mo-Kα (λ = 0.71073 Å) radiation. The program COLLECT[1] was used for the data collection and DENZO/SCALEPACK[2] for the data reduction. The single crystal X-ray data for [**1**]NO_3, [**1**]ClO_4, **I_2·quin** and **I_2·quin_2** were collected at 120 K using an Agilent SuperNova dual wavelength diffractometer with an Atlas detector using mirror-monochromated Cu-Kα (λ = 1.54184 Å) radiation. The single crystal X-ray data for **[$ClCH_2$(quin)][$AgCl_2$]** was collected at 120 K using an Agilent SuperNova diffractometer with an Eos detector using mirror-monochromated Mo-Kα (λ = 0.71073 Å) radiation. The program CrysAlisPro[3] was used for the data collection and reduction on the SuperNova diffractometer, and the intensities were absorption corrected using a gaussian face index absorption correction method. All structures were solved by intrinsic phasing (SHELXT)[4] and refined by full-matrix least squares on F^2 using the OLEX2,[5] utilizing the SHELXL-2015 module.[6] Anisotropic displacement parameters were assigned to non-H atoms and isotropic displacement parameters for all H atoms were constrained to multiples of the equivalent displacement parameters of their parent atoms with U_{iso}(H) = 1.5 U_{eq} (alkyl) of their respective parent atoms. The X-ray single crystal data and CCDC numbers of all new structures are included below. The solid-state structure of [**1**]BF_4 is known,[7] however, the solution-state data has not been previously reported and is therefore included herein.

The following abbreviations are used: 1-Etpip = 1-ethylpiperidine, quin = quinuclidine (1-azabicyclo[2.2.2]octane), py = pyridine, 4-DMAP = N,N-dimethylpyridin-4-amine, DCM = dichloromethane, MeCN = acetonitrile, DIPE = diisopropylether, TBME = ^{t}butylmethylether, DMSO = dimethylsulfoxide.

General Procedure for Synthesis of Quinuclidine Iodonium Complexes

All iodonium complexes of quinuclidine ([**1**]BF_4, [**1**]PF_6, [**1**]NO_3, [**1**]ClO_4) were prepared using the same general method of cation exchange, which is given below using [**1**]PF_6 as an example.

A quinuclidine solution (5.6 mg, 0.05 mmol) in CD_3CN (0.5 mL) was added to $AgPF_6$ (6.3 mg, 0.025 mmol), thoroughly mixed and left for 1 hour to ensure complete formation of the silver(I) complex. I_2 (6.3 mg, 0.025 mmol) was added to immediately give a yellow precipitate and a light orange solution. Samples were prepared immediately prior to the collection of NMR data. The formation of all iodonium complexes ([**1**]BF_4, [**1**]PF_6, [**1**]NO_3, [**1**]ClO_4) was confirmed to be quantitative by ^1H NMR spectroscopy.

For the preparation of crystallographic samples, the same general procedure was followed but using the scaled-up values of: quinuclidine (11.1 mg, 0.1 mmol), $AgPF_6$ (12.6 mg, 0.05 mmol), MeCN (3 mL), and I_2 (12.7 mg, 0.05 mmol).

Characterisation Data

quin: ^{1}H NMR (500 MHz, CD_3CN) δ 2.81 – 2.70 (m, 6H), 1.67 (sept, *J* = 3.1 Hz, 1H), 1.54 – 1.44 (m, 6H); ^{15}N NMR (500 MHz, CD_3CN) δ -366.6.

[**1**]BF_4: ^{1}H NMR (500 MHz, CD_3CN) δ 3.25 – 3.17 (m, 12H), 1.90 (sept, *J* = 3.2 Hz, 2H), 1.74 (m, 12H); ^{15}N NMR (500 MHz, CD_3CN) δ -357.4.

[**1**]PF_6: ^{1}H NMR (500 MHz, CD_3CN) δ 3.26 – 3.16 (m, 12H), 1.90 (sept, *J* = 3.2 Hz, 2H), 1.75 (m, 12H); ^{15}N NMR (500 MHz, CD_3CN) δ -357.3. ^{1}H NMR (500 MHz, d_6-DMSO) δ 3.24 (s.br, 12H), 1.85 (s.br, 2H), 1.69 (s.br, 12H); satisfactory ^{1}H-^{15}N HMBC data could not be collected due to the broadness of the ^{1}H NMR signals. Crystals suitable for single crystal X-ray diffraction were obtained from an MeCN solution vapour diffused with DIPE. Crystal data for [**1**]PF_6: CCDC-2079430, $[C_{14}H_{26}IN_2][PF_6]$, M = 494.23, colourless block, 0.24 x 0.30 x 0.36 mm^3, cubic, space group *Pa*-3, a = 12.3792(3) Å, V = 1897.05(14) Å^3, Z = 4, D_{calc} = 1.730 gcm^{-3}, F000 = 984, μ = 1.83 mm^{-1}, T = 170(1) K, θ_{max} = 27.1°, 705 total reflections, 552 with $I_o > 2\sigma(I_o)$, R_{int} = 0.042, 705 data, 50 parameters, no restraints, GooF = 1.16, 0.25 < dΔρ < -0.81 eÅ^{-3}, $R[F^2 > 2\sigma(F^2)]$ = 0.031, $wR(F^2)$ = 0.068.

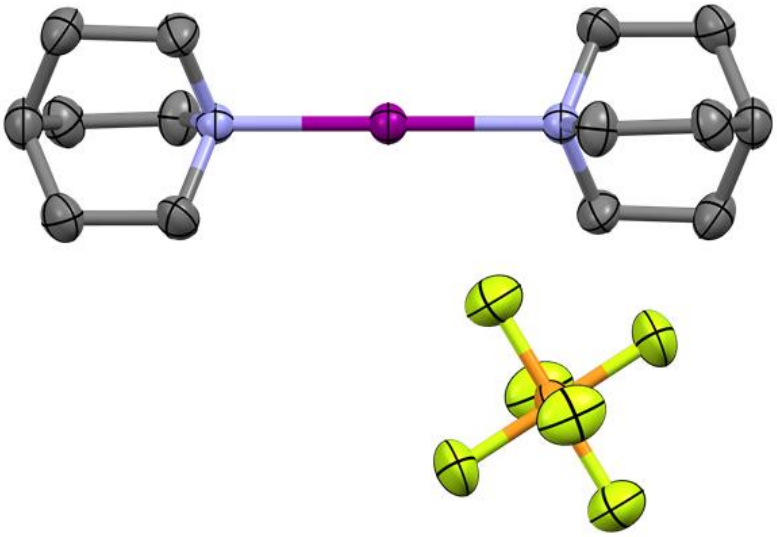


Figure S1: The X-ray crystal structure of [1]PF6 (Hydrogen and disordered atoms omitted for clarity; thermal ellipsoids at 50% probability).

[**1**]NO_3: ^{1}H NMR (500 MHz, CD_3CN) δ 3.25 – 3.16 (m, 12H), 1.90 (sept, *J* = 3.1 Hz, 2H), 1.74 (m, 12H); ^{15}N NMR (500 MHz, CD_3CN) δ -357.4. Crystals suitable for single crystal X-ray diffraction were obtained from an MeCN solution vapour diffused with DIPE. Crystal data for [**1**]NO_3: CCDC-2079431, $[C_{14}H_{26}IN_2][NO_3]$, M = 411.28, colourless plate, 0.06 x 0.14 x 0.21 mm^3, orthorhombic, space group $Pca2_1$, a = 13.8822(3) Å, b = 10.4099(3) Å, c = 11.3834(3) Å, V = 1645.04(7) Å^3, Z = 4, D_{calc} = 1.661 gcm^{-3}, F000 = 832, μ = 15.42 mm^{-1}, T = 120.0(1) K, θ_{max} = 76.2°, 2510 total reflections, 2180 with $I_o > 2\sigma(I_o)$, R_{int} = 0.027, 2510 data, 191 parameters, 1 restraint, GooF = 1.05, 1.03 < dΔρ < -1.37 eÅ^{-3}, $R[F^2 > 2\sigma(F^2)]$ = 0.037, $wR(F^2)$ = 0.099.

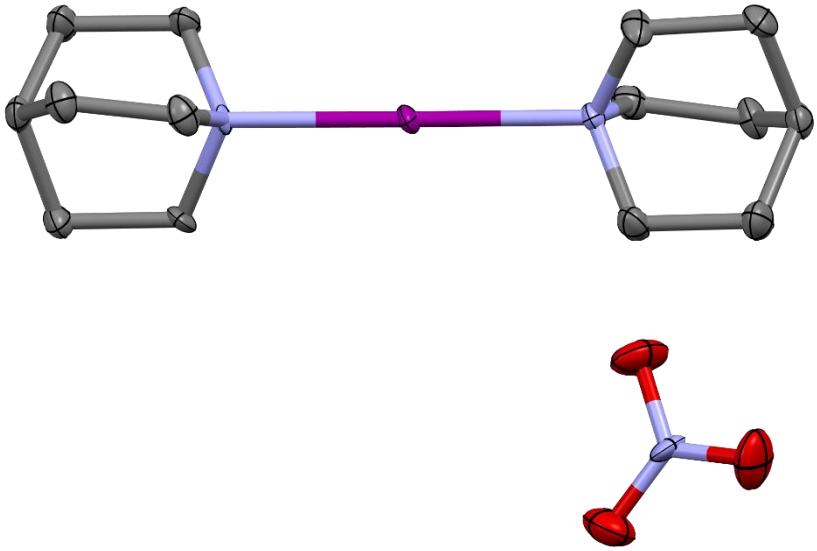


Figure S2: The X-ray crystal structure of [**1**]NO_3 (Hydrogen atoms omitted for clarity; thermal ellipsoids at 50% probability).

[**1**]ClO_4: ^{1}H NMR (500 MHz, CD_3CN) δ 3.26 – 3.16 (m, 12H), 1.90 (sept, *J* = 3.1 Hz, 2H), 1.75 (m, 12H); ^{15}N NMR (500 MHz, CD_3CN) δ -357.4. Crystals suitable for single crystal X-ray diffraction were obtained from an MeCN solution vapour diffused with TBME. Crystal data for [**1**]ClO_4: CCDC-2079432, $[C_{14}H_{26}IN_2][ClO_4]$, M = 448.72, colourless block, 0.10 x 0.11 x 0.13 mm^3, cubic, space group $P2_13$, a = 11.9987(2) Å, V = 1727.44(9) $Å^3$, Z = 4, D_{calc} = 1.725 gcm^{-3}, F000 = 904, μ = 16.16 mm^{-1}, T = 120.0(1) K, θ_{max} = 75.8°, 1130 total reflections, 1078 with $I_o > 2\sigma(I_o)$, R_{int} = 0.019, 1130 data, 68 parameters, no restraints, GooF = 1.04, 0.31 < dΔρ < -0.95 $eÅ^{-3}$, $R[F^2 > 2\sigma(F^2)]$ = 0.023, $wR(F^2)$ = 0.057.

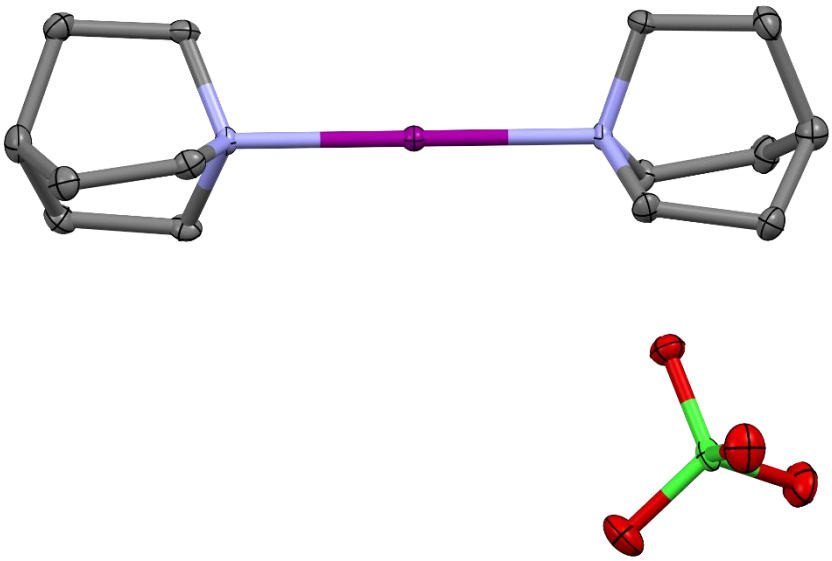


Figure S3: The X-ray crystal structure of [**1**]ClO_4 (Hydrogen atoms omitted for clarity; thermal ellipsoids at 50% probability).

I_2·quin: Crystals suitable for single crystal X-ray diffraction were obtained in a trace amount by evaporation of a 1:4 MeCN:DIPE mixture of complex [**1**]BF_4. Crystal data for **I_2·quin**: CCDC-2079433, $C_7H_{13}I_2N$, M = 364.98, orange plate, 0.02 x 0.05 x 0.06 mm^3, monoclinic, space group $P2_1/c$, a = 10.0222(7) Å, b = 7.9210(5) Å, c = 13.7704(10) Å, β = 110.604(8)°, V = 1023.25(13) $Å^3$, Z = 4, D_{calc} = 2.369 gcm^{-3}, F000 = 672, μ = 47.77 mm^{-1}, T = 120.0(1) K, θ_{max} = 72.1°, 1742 total reflections, 1411 with $I_o > 2\sigma(I_o)$, R_{int} = 0.106, 1742 data, 91 parameters, 18 restraints, GooF = 1.02, 2.52 < dΔρ < -2.72 $eÅ^{-3}$, $R[F^2 > 2\sigma(F^2)]$ = 0.066, $wR(F^2)$ = 0.168.

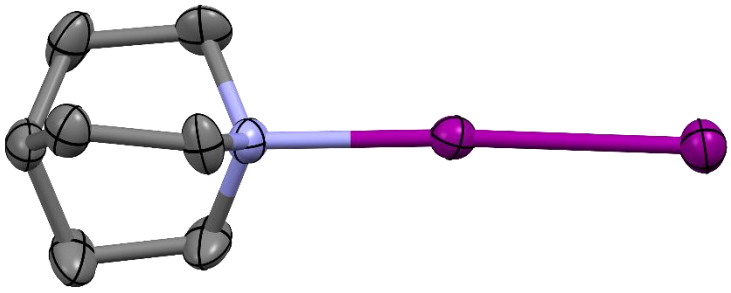


Figure S4: The X-ray crystal structure of **I_2·quin** (Hydrogen atoms omitted for clarity; thermal ellipsoids at 50% probability).

Deliberately synthesised from an equimolar combination of quinuclidine and elemental iodine, and crystals suitable for single crystal X-ray diffraction were obtained by evaporation of a 1:4 MeCN:DIPE mixture. Crystal data for **I_2·quin_2**: CCDC-2079434, $C_7H_{13}I_2N$, M = 364.98, orange plate, 0.01 x 0.05 x 0.08 mm^3, triclinic, space group *P*-1 (No. 2), a = 6.7067(7) Å, b = 8.4046(8) Å, c = 9.5027(7) Å, α = 91.599(7)°, β = 104.779(8)°, γ = 97.372(8)°, V = 512.61(8) $Å^3$, Z = 2, D_{calc} = 2.365 gcm^{-3}, F000 = 336, μ = 47.68 mm^{-1}, T = 120.0(1) K, θ_{max} = 76.5°, 1843 total reflections, 1572 with $I_o > 2\sigma(I_o)$, R_{int} = 0.098, 1843 data, 91 parameters, no restraints, GooF = 1.01, 1.76 < dΔρ < -1.30 $eÅ^{-3}$, $R[F^2 > 2\sigma(F^2)]$ = 0.045, $wR(F^2)$ = 0.120.

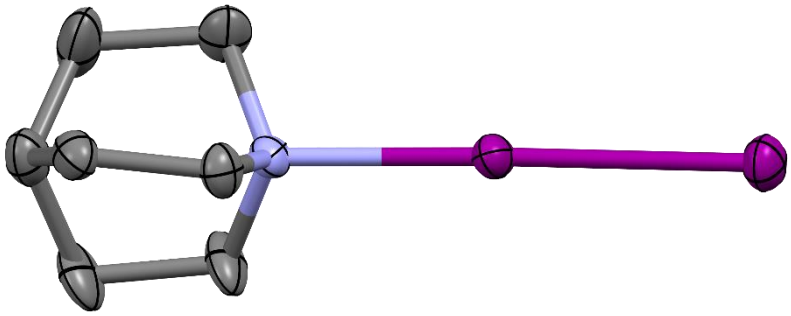


Figure S5: The X-ray crystal structure of **I_2·quin_2** (Hydrogen atoms omitted for clarity; thermal ellipsoids at 50% probability).

The synthesis of $[1]^+$ when performed using DCM as the solvent (instead of MeCN) gave **$[ClCH_2(quin)][AgCl_2]$** as the major product recovered, and crystals suitable for single crystal X-ray diffraction were obtained from a DCM solution vapour diffused with pentane. Crystal data for **$[ClCH_2(quin)][AgCl_2]$**: CCDC-2084411, $[C_8H_{15}ClN][AgCl_2]$, M = 339.43, colourless needle, 0.11 x 0.16 x 0.49 mm^3, tetragonal, space group $I4_1cd$, a = 18.1238(3) Å, c = 13.8565(3) Å, V = 4551.47(18) $Å^3$, Z = 16, D_{calc} = 1.981 gcm^{-3}, F000 = 2688, μ = 2.43 mm^{-1}, T = 120.0(1) K, θ_{max} = 26.3°, 2292 total reflections, 2216 with $I_o > 2\sigma(I_o)$, R_{int} = 0.022, 2292 data, 119 parameters, 1 restraint, GooF = 1.06, 0.24 < dΔρ < -0.46 $eÅ^{-3}$, $R[F^2 > 2\sigma(F^2)]$ = 0.020, $wR(F^2)$ = 0.043.

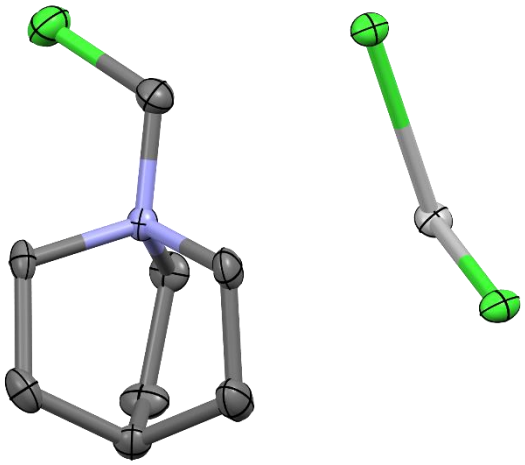


Figure S6: The X-ray crystal structure of **$[ClCH_2(quin)][AgCl_2]$** (Hydrogen atoms omitted for clarity; thermal ellipsoids at 50% probability).

General Procedure for Synthesis of 1-Ethylpiperidine Iodonium Complexes

All iodonium complexes of 1-ethylpiperidine ([**2**]BF_4, [**2**]PF_6, [**2**]NO_3, [**2**]ClO_4) were prepared using the same general method of cation exchange, which is given below using [**2**]NO_3 as an example.

A 1-ethylpiperidine solution (6.9 µL, 0.05 mmol) in CD_3CN (0.5 mL) was added to $AgNO_3$ (4.2 mg, 0.025 mmol), thoroughly mixed and left for 5 minutes to ensure complete formation of the silver(I) complex. I_2 (6.3 mg, 0.025 mmol) was added to immediately give a yellow precipitate and a light orange solution. Samples were prepared immediately prior to the collection of NMR data. Complete decomposition of all iodonium complexes ([**2**]BF_4, [**2**]PF_6, [**2**]NO_3, [**2**]ClO_4) to [H(1-Etpip)][Anion] (Anion = BF_4, PF_6, NO_3, ClO_4) within (a maximum of) 30 minutes was confirmed by ^{1}H NMR spectroscopy.

1-Etpip: ^{1}H NMR (500 MHz, CD_3CN) δ 2.30 (s.br, 4H), 2.27 (q, *J* = 7.2 Hz, 2H), 1.56 – 1.47 (m, 4H), 1.40 (s.br, 2H), 0.99 (t, *J* = 7.2 Hz, 3H); ^{15}N NMR (500 MHz, CD_3CN) δ -329.4.

[**2**]NO_3 (between 0-30 minutes after addition of I_2): ^{1}H NMR (500 MHz, CD_3CN) δ 3.04 (s.br, 4H), 2.99 (q, 7.3 Hz, 2H), 1.85 – 1.74 (m, 4H), 1.59 (s.br, 2H), 1.25 (t, *J* = 7.3 Hz, 3H); ^{15}N NMR (500 MHz, CD_3CN) δ -331.1.

[**2**]NO_3 (1 hour after addition of I_2): ^{1}H NMR (500 MHz, CD_3CN) δ 3.10 (s.br, 4H), 3.04 (q, 7.3 Hz, 2H), 1.89 – 1.76 (m, 4H), 1.61 (s.br, 2H), 1.28 (t, *J* = 7.3 Hz, 3H), N—H signal not observed due to H/D exchange; ^{15}N NMR (500 MHz, CD_3CN) δ -327.5.

[H(1-Etpip)]NO_3: Prepared by addition of HNO_3 to 1-Etpip. ^{1}H NMR (500 MHz, CD_3CN) δ 8.29 (s.br, 1H), 3.45 (d, *J* = 12.3 Hz, 2H), 3.11 – 3.02 (m, 2H), 2.84 – 2.73 (m, 2H), 1.86 (d, *J* = 14.4 Hz, 2H), 1.78 – 1.64 (m, 3H), 1.47 – 1.37 (m, 1H), 1.24 (t, *J* = 7.3 Hz, 3H); ^{15}N NMR (500 MHz, CD_3CN) δ -327.1.

NMR Spectra

Figure S7: The ^{1}H NMR spectrum of complex **quin** in CD_3CN.

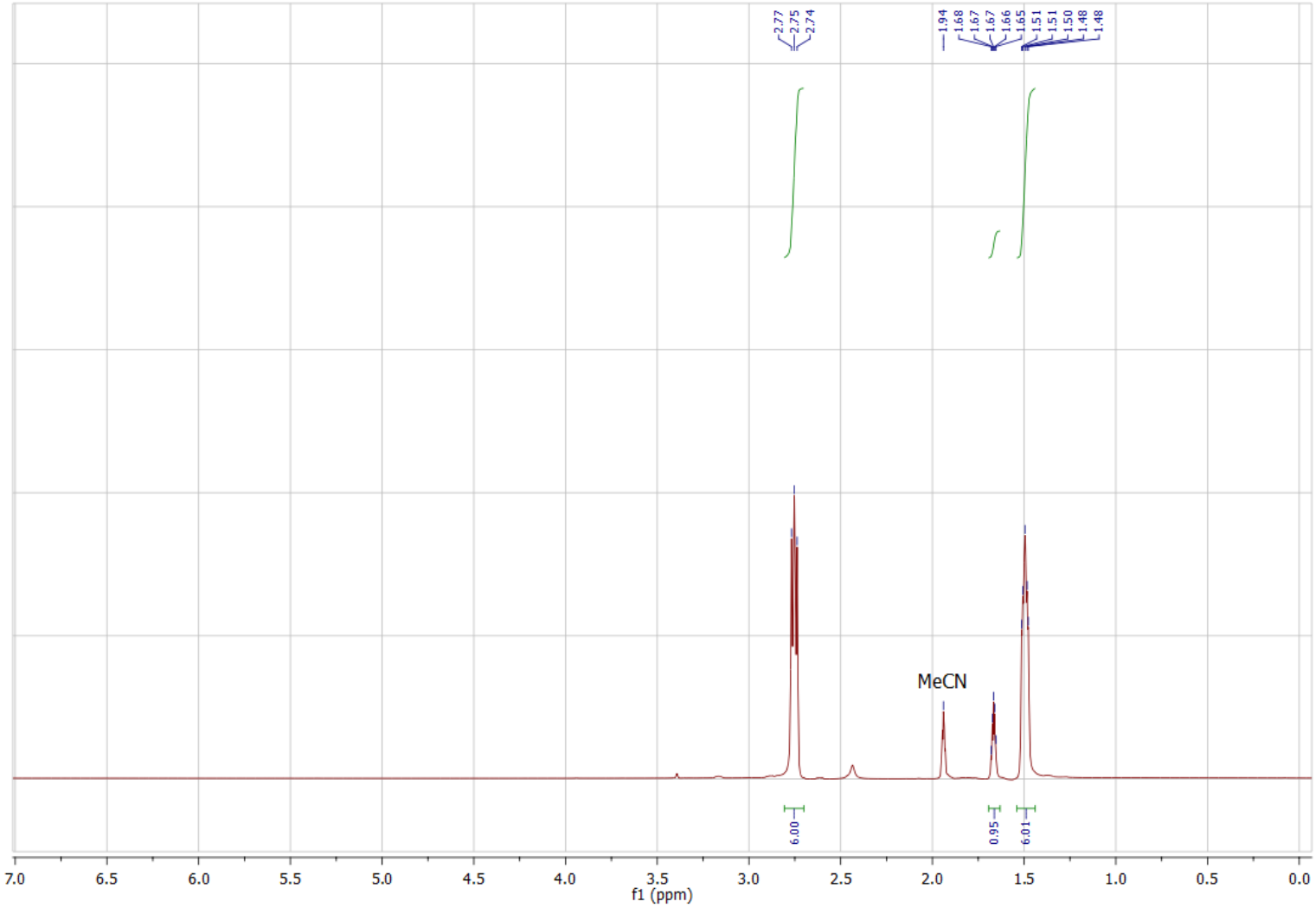


Figure S8: The ^{1}H-^{15}N HMBC spectrum of complex **quin** in CD_3CN.

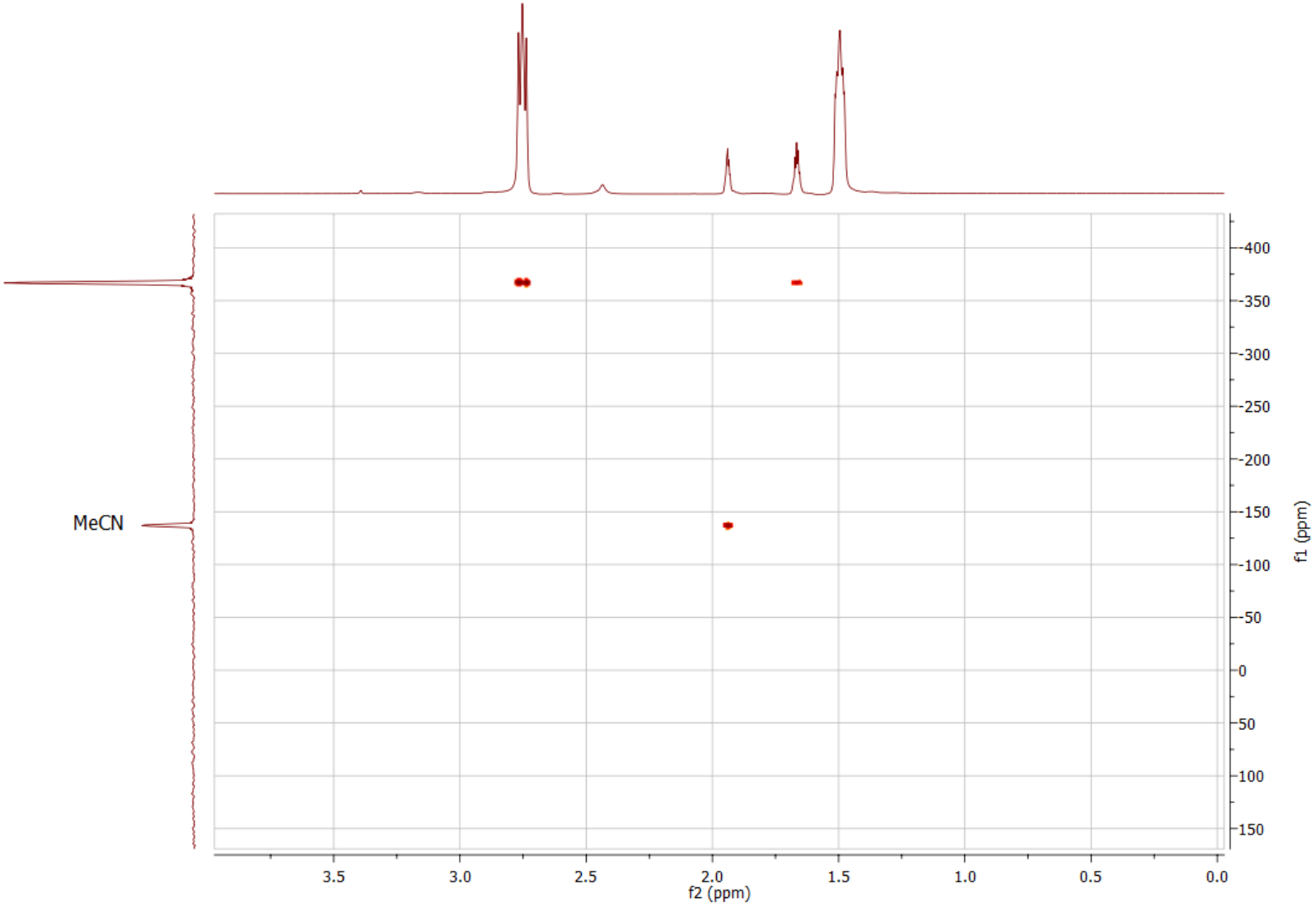


Figure S9: The ^{1}H NMR spectrum of complex [**1**]BF_4 in CD_3CN.

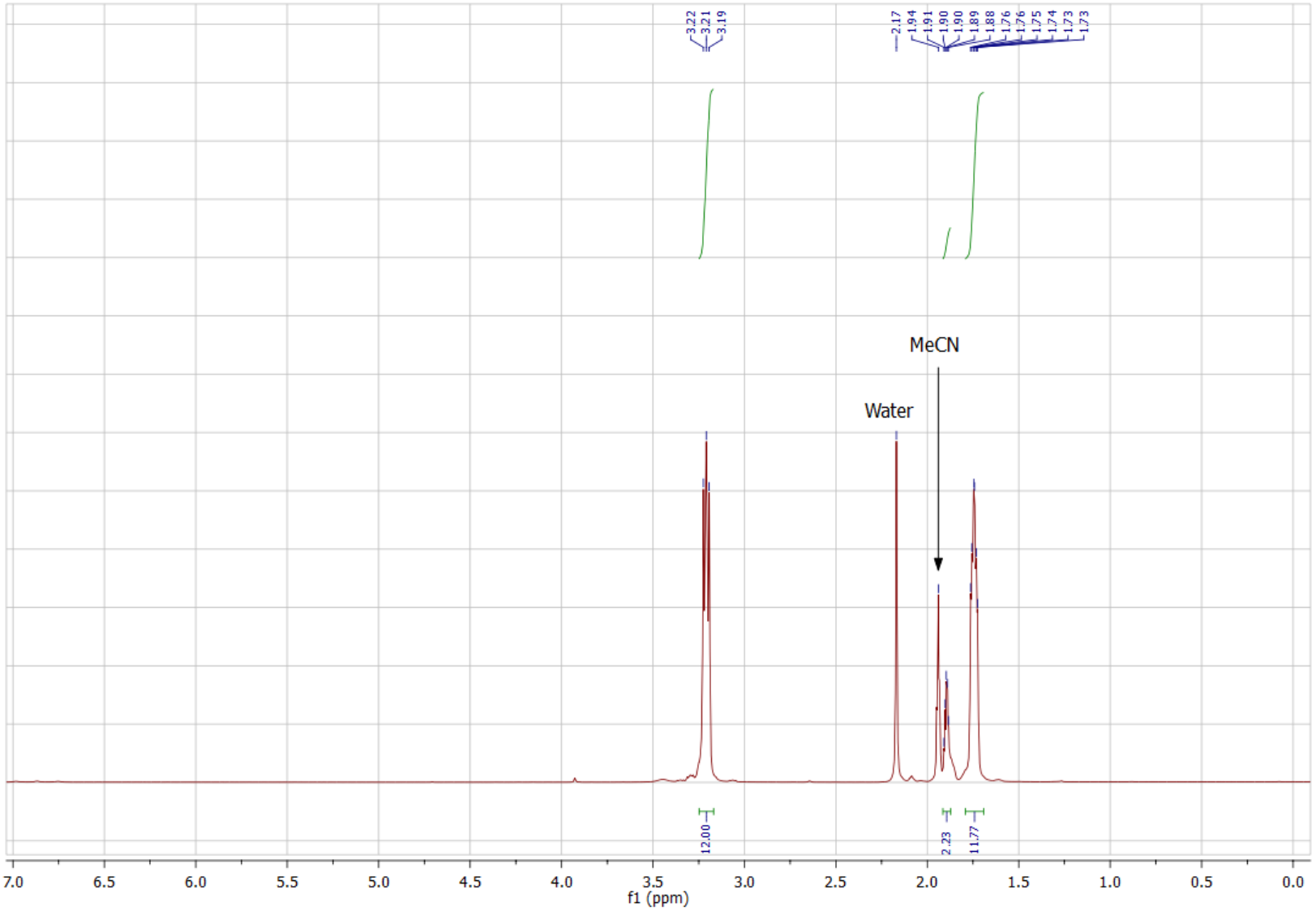


Figure S10: The ^{1}H-^{15}N HMBC spectrum of complex [**1**]BF_4 in CD_3CN.

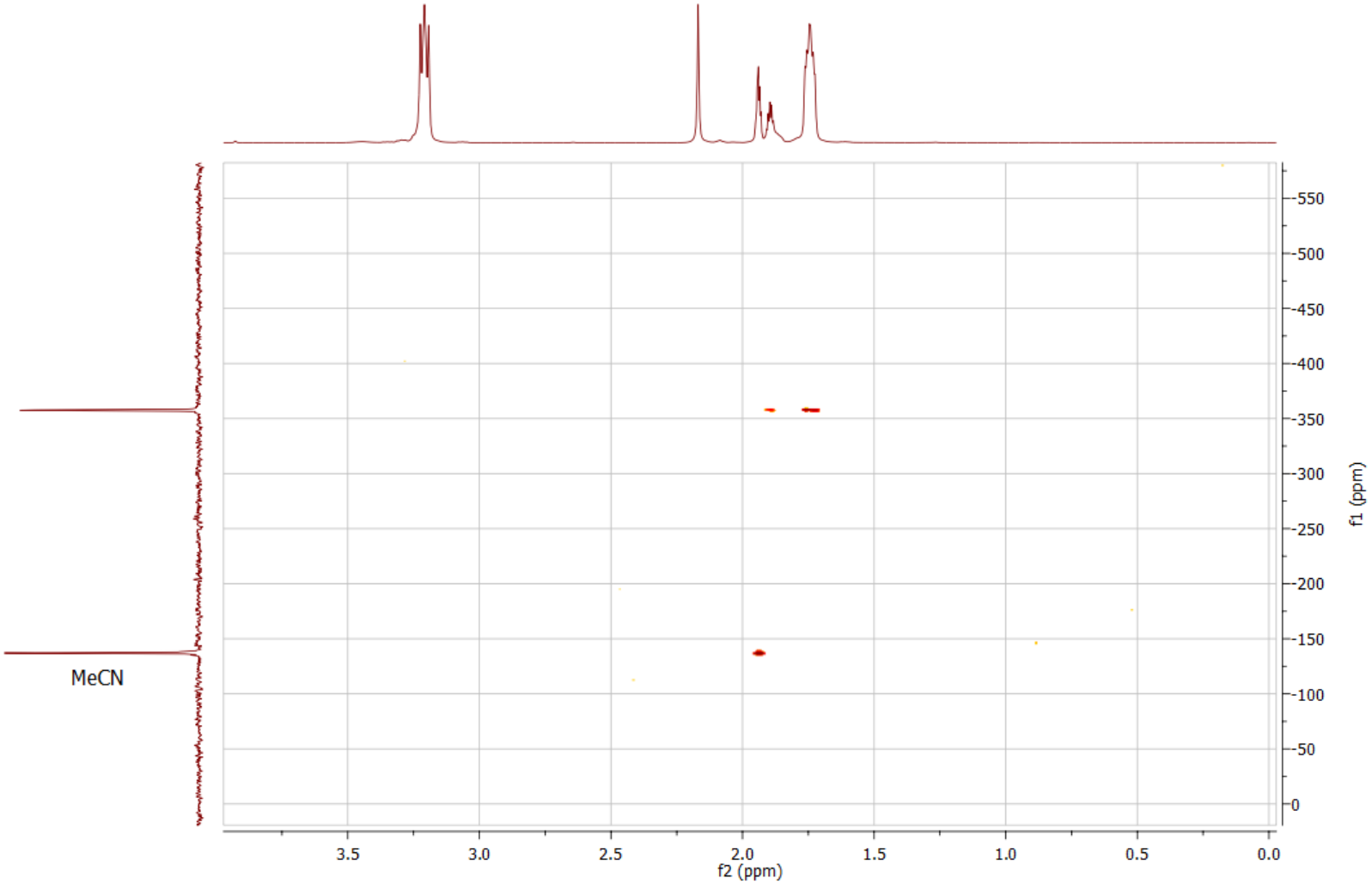


Figure S11: The ^{1}H NMR spectrum of complex [**1**]PF_6 in CD_3CN.

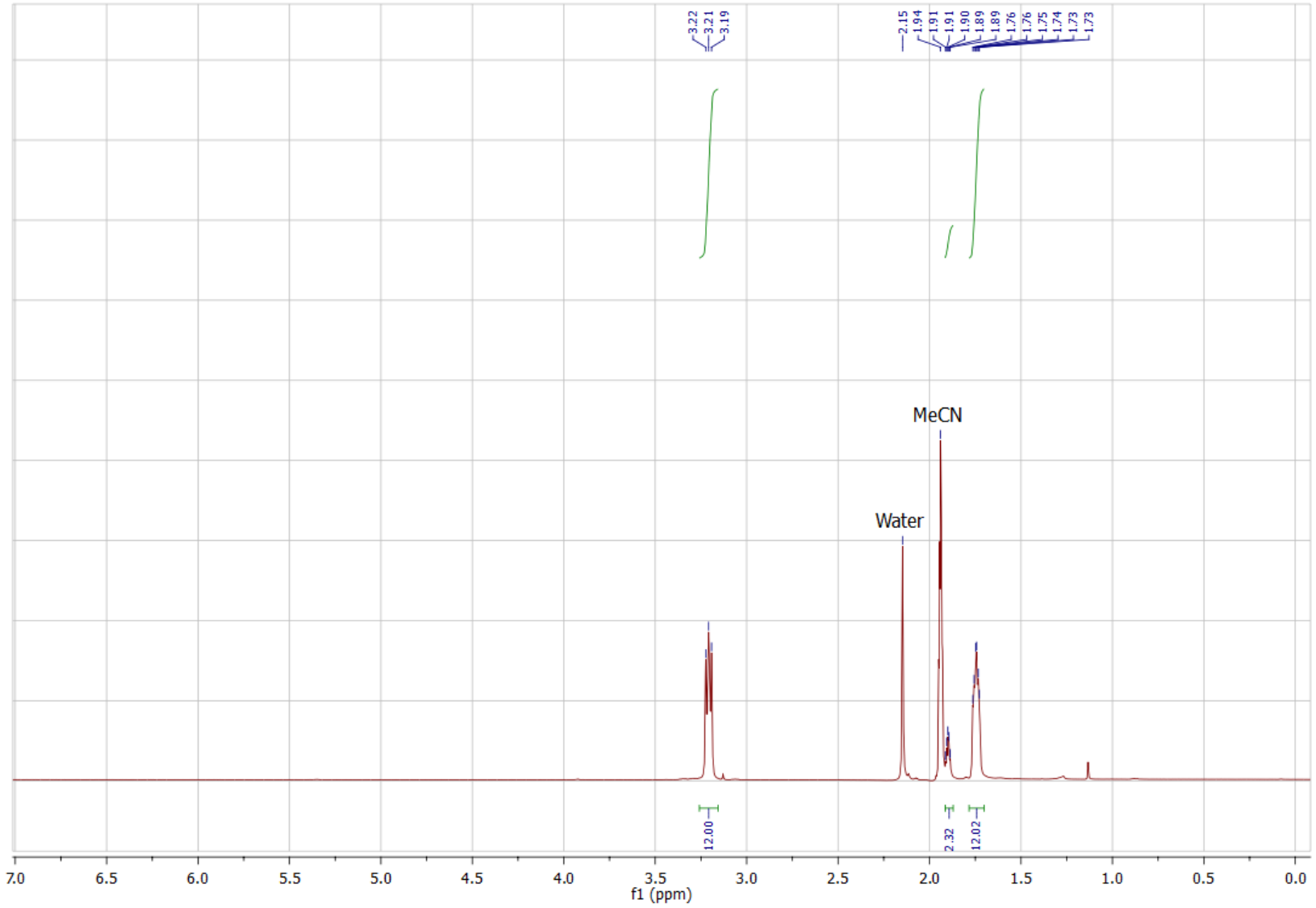


Figure S12: The ^{1}H-^{15}N HMBC spectrum of complex [**1**]PF_6 in CD_3CN.

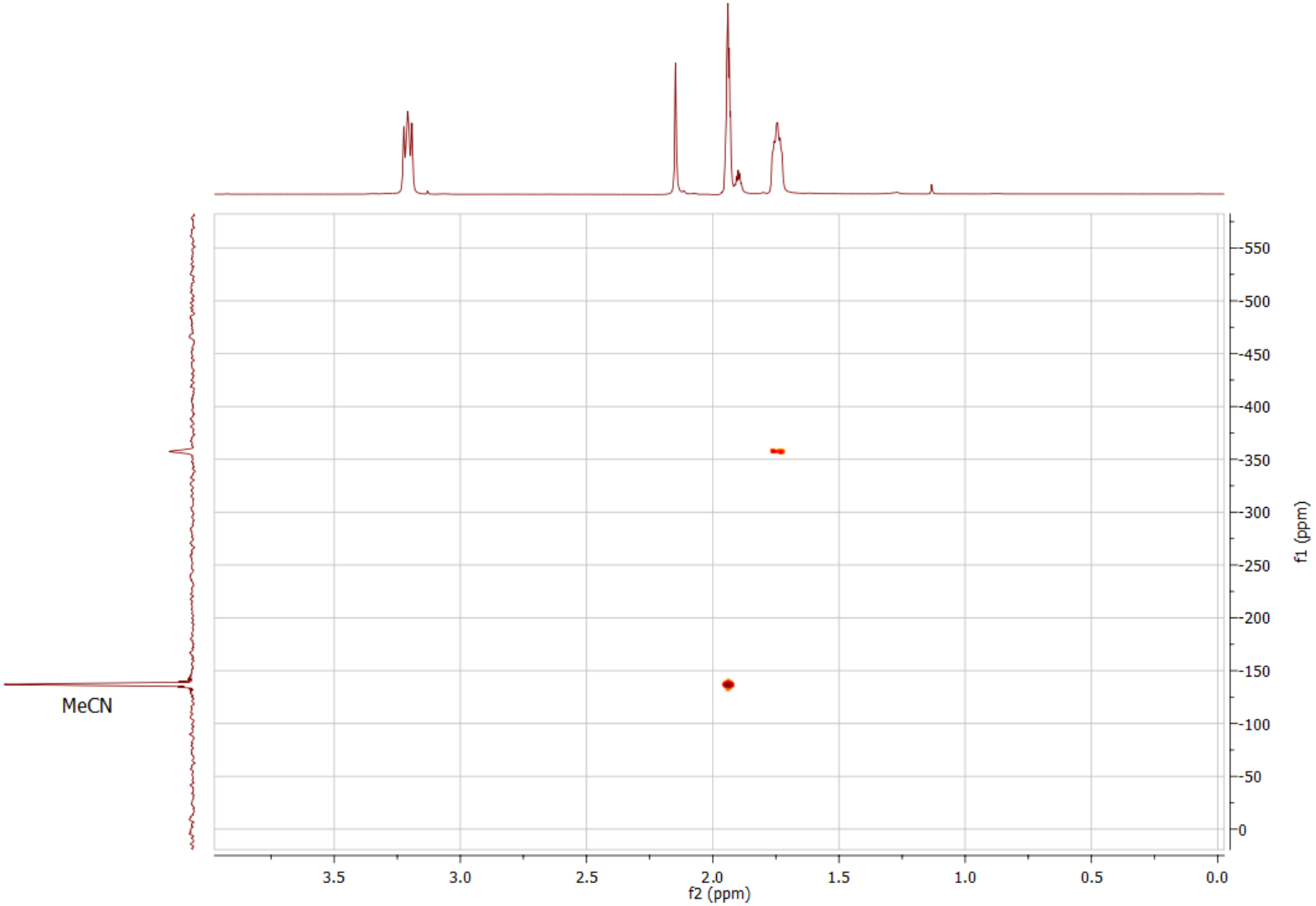


Figure S13: The ^{1}H NMR spectrum of complex [**1**]PF_6 in d_6-DMSO.

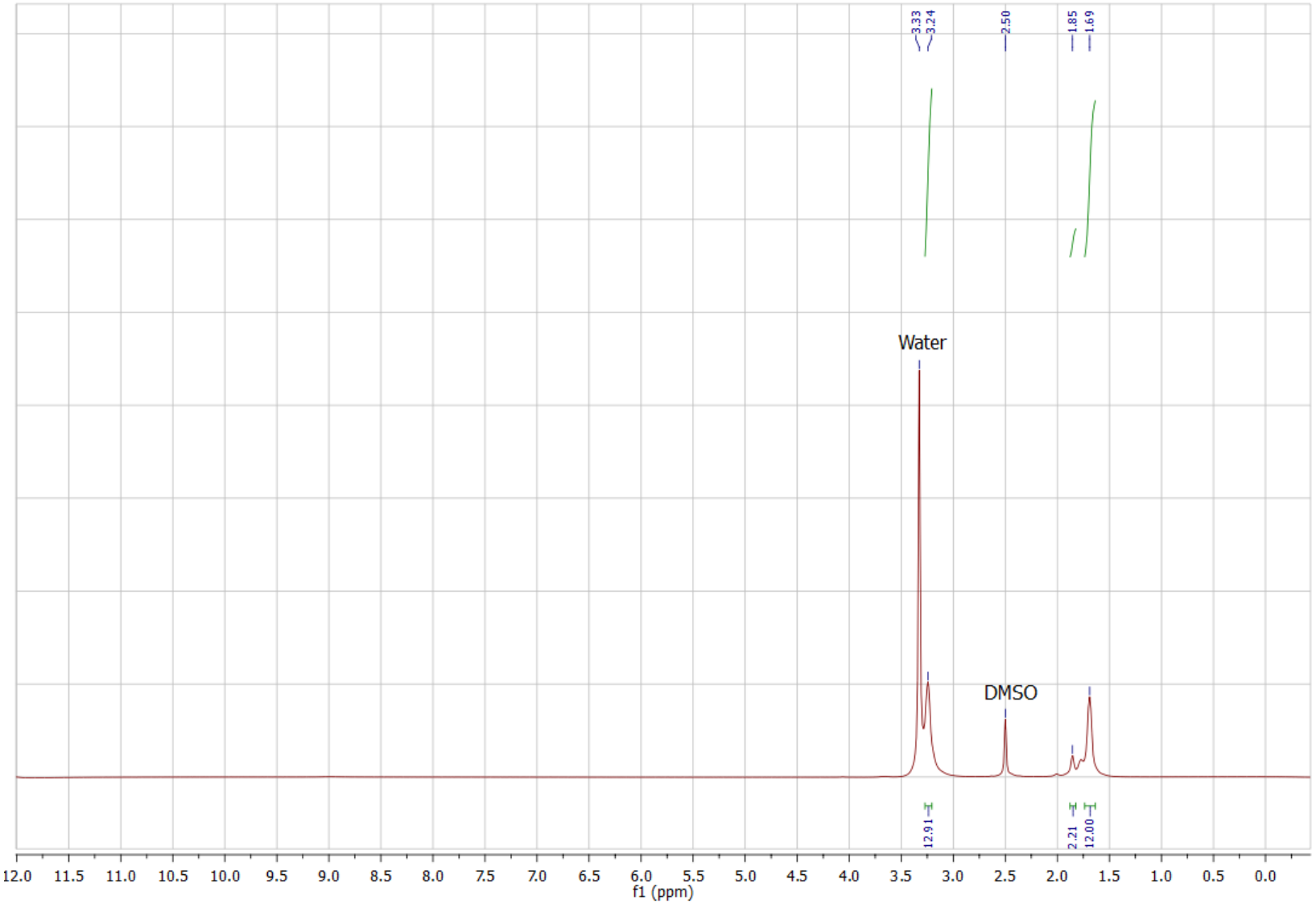


Figure S14: The ^{1}H NMR spectrum of complex [**1**]NO_3 in CD_3CN.

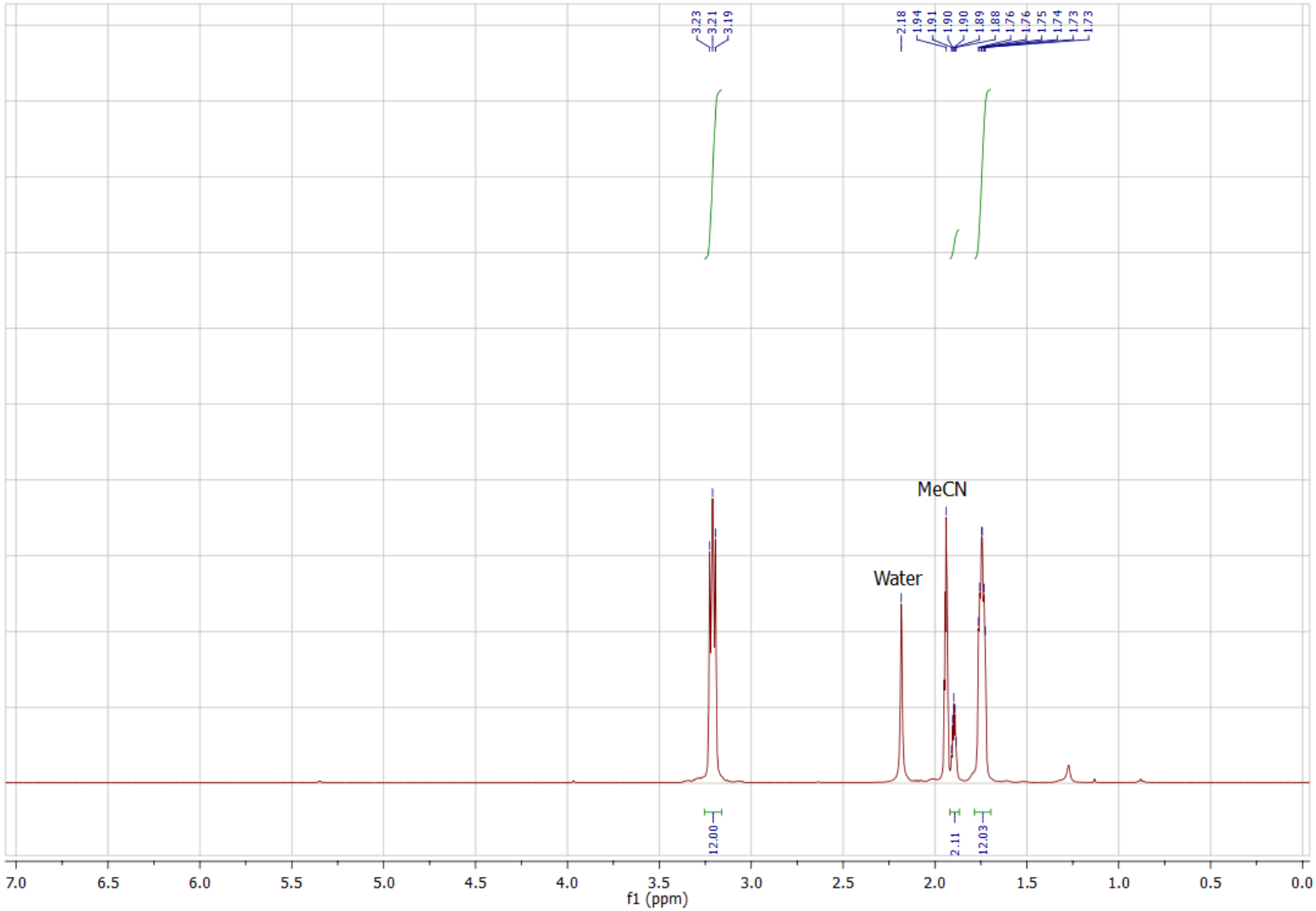


Figure S15: The ^{1}H-^{15}N HMBC spectrum of complex [**1**]NO_3 in CD_3CN.

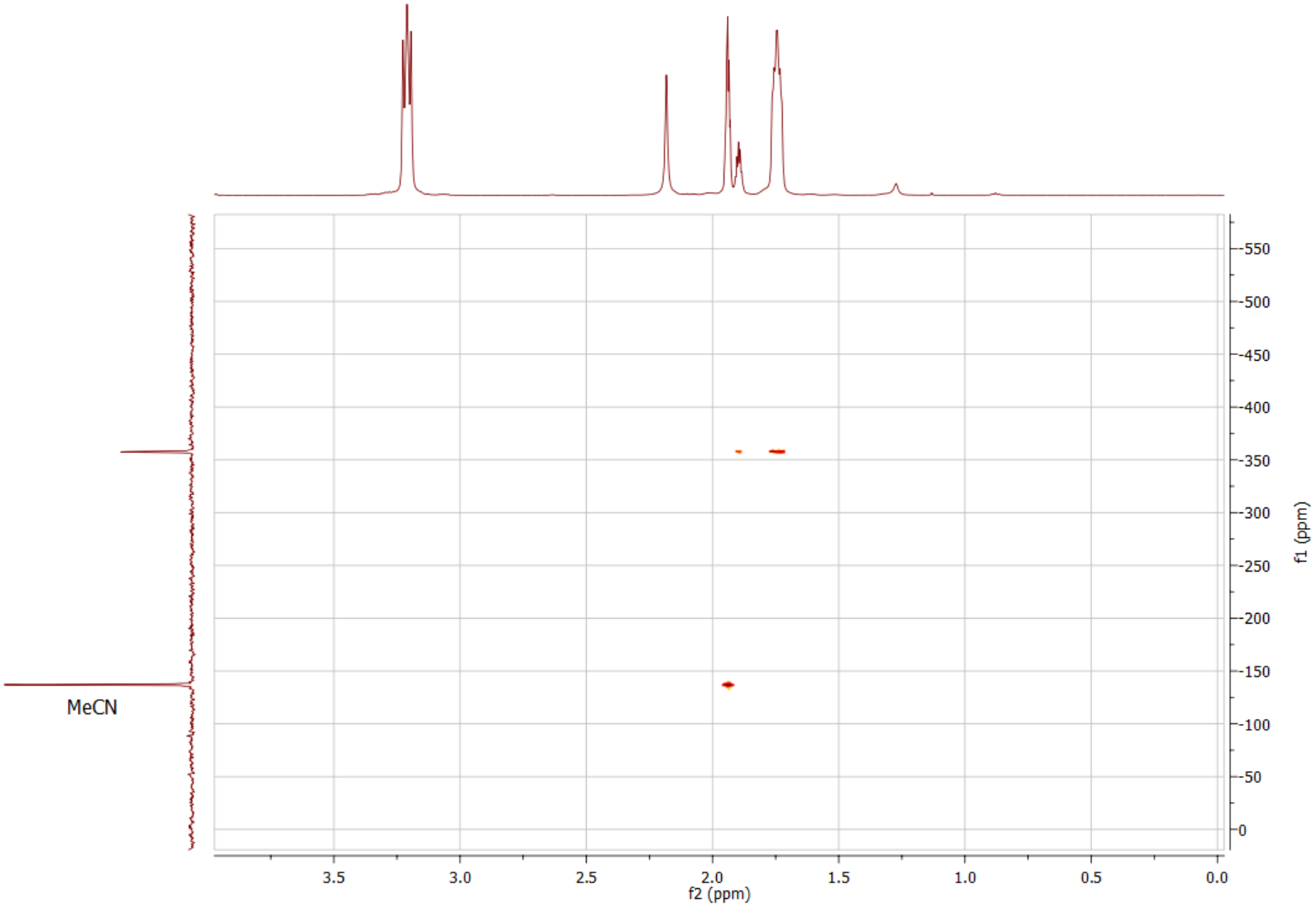


Figure S16: The ^{1}H NMR spectrum of complex [**1**]ClO_4 in CD_3CN.

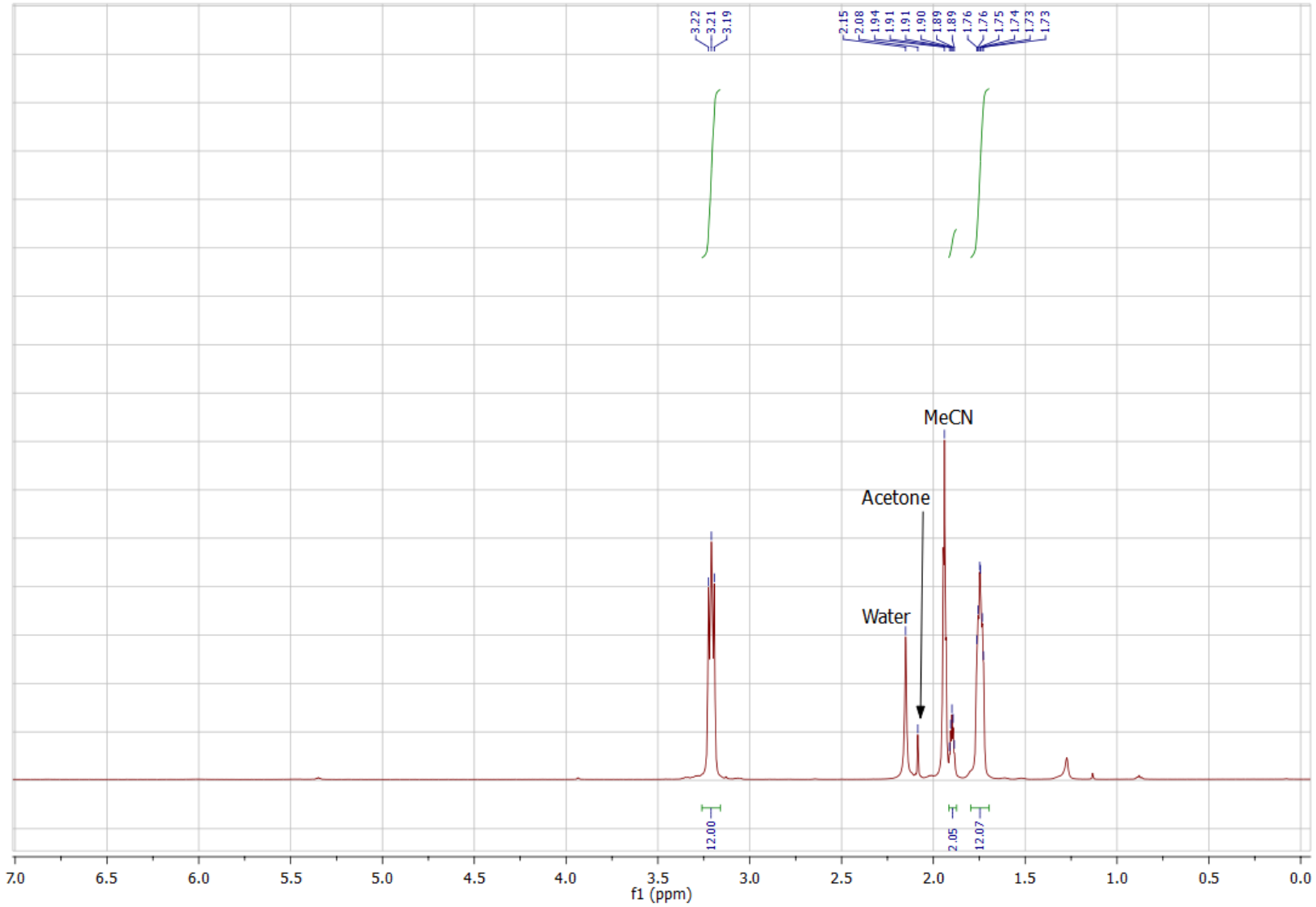


Figure S17: The ^{1}H-^{15}N HMBC spectrum of complex [**1**]ClO_4 in CD_3CN.

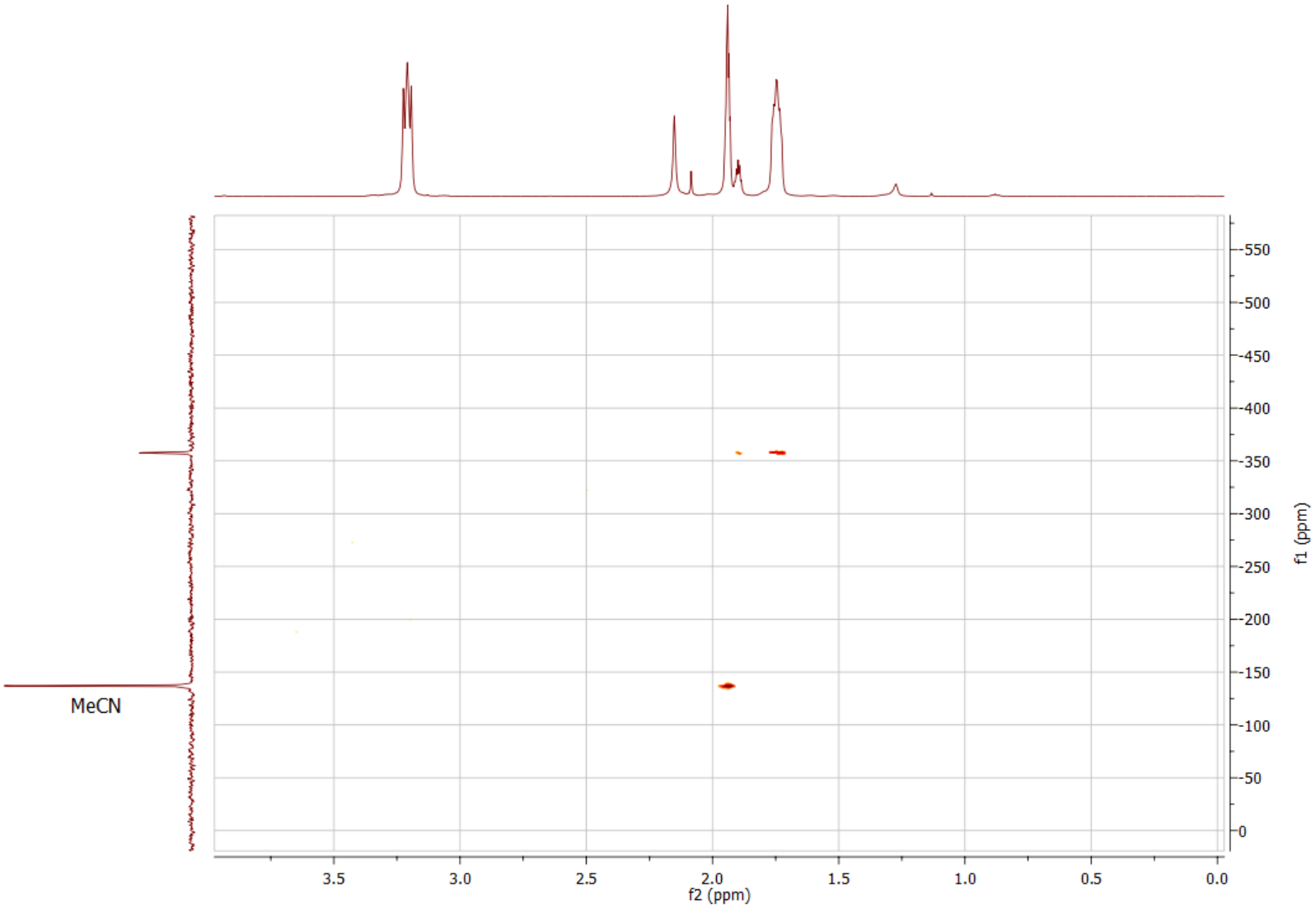


Figure S18: The ^{1}H NMR spectrum of 1-Etpip in CD_3CN.

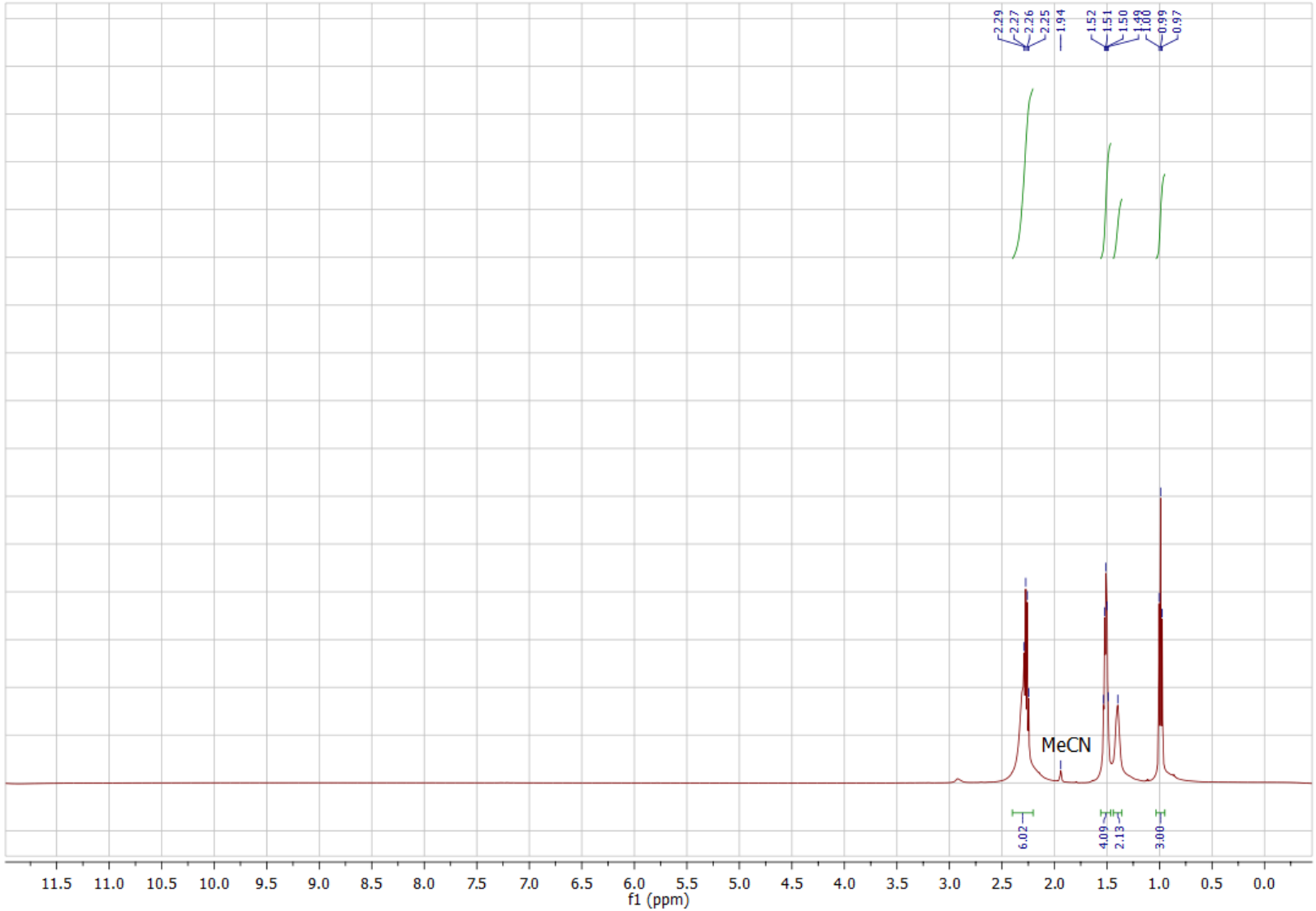


Figure S19: The ^{1}H-^{15}N HMBC spectrum of 1-Etpip in CD_3CN.

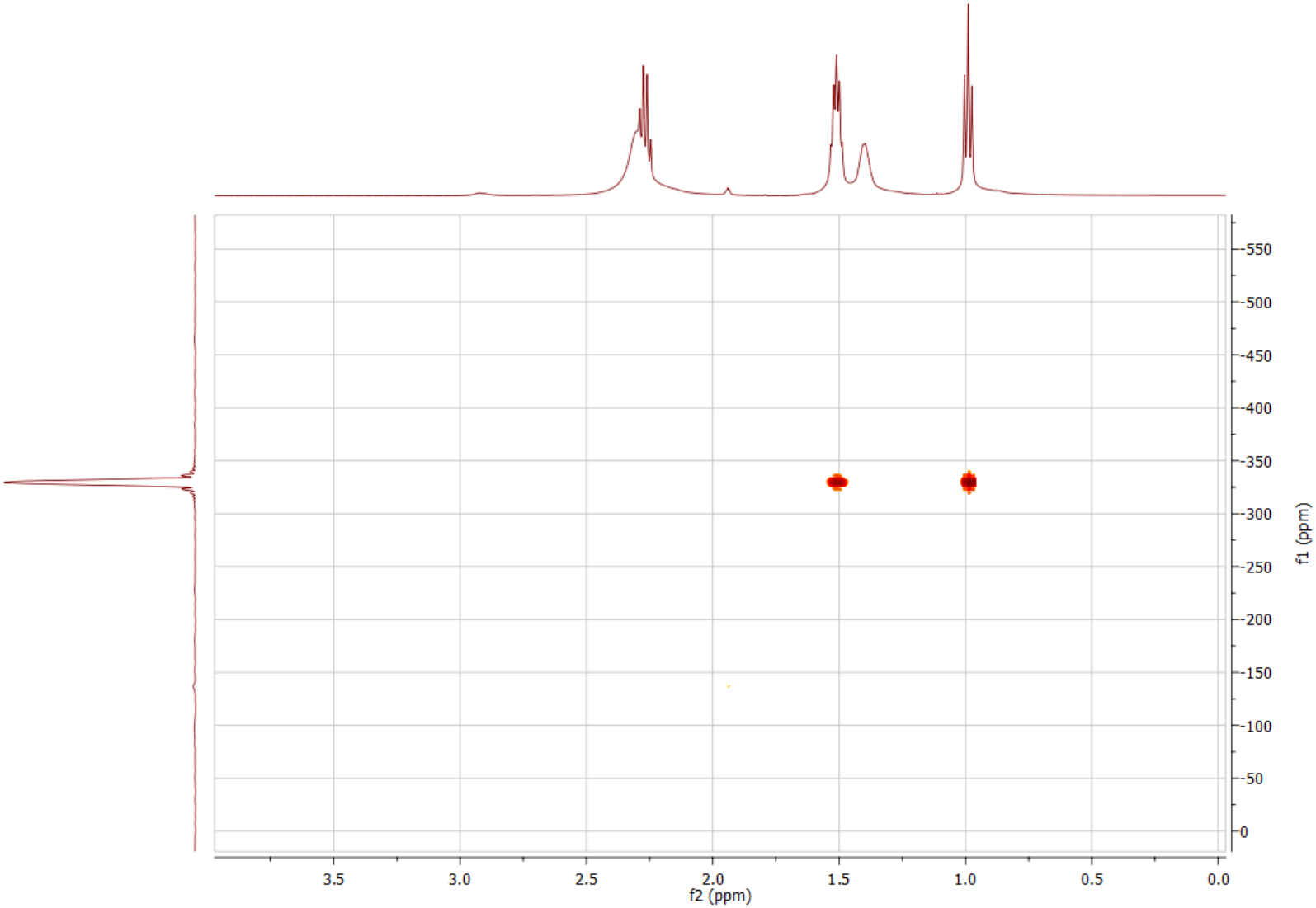


Figure S20: The ^{1}H NMR spectrum of complex [**2**]NO_3 (between 0-30 minutes after addition of I_2) in CD_3CN.

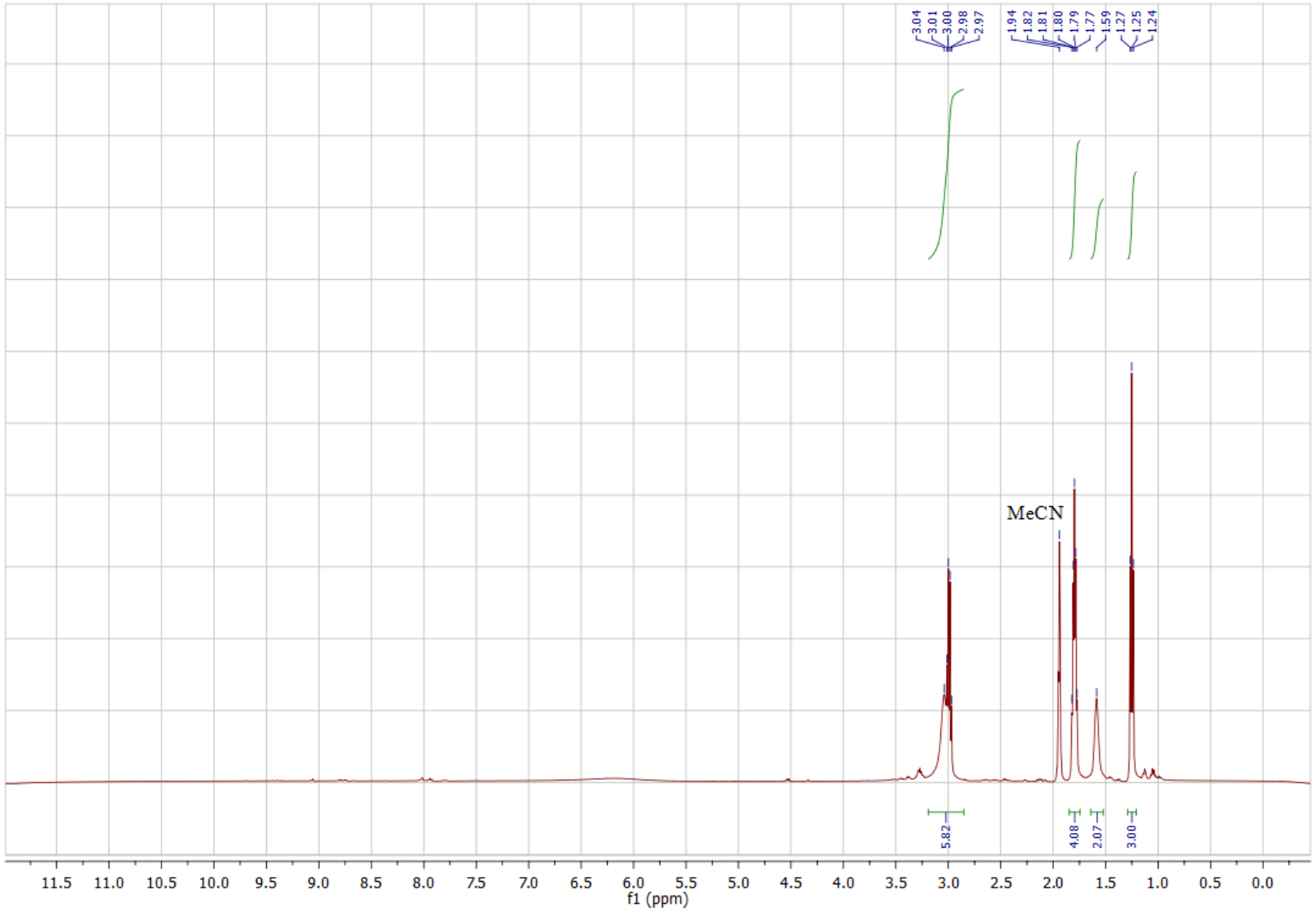


Figure S21: The ^{1}H-^{15}N HMBC spectrum of complex [**2**]NO_3 (between 0-30 minutes after addition of I_2) in CD_3CN.

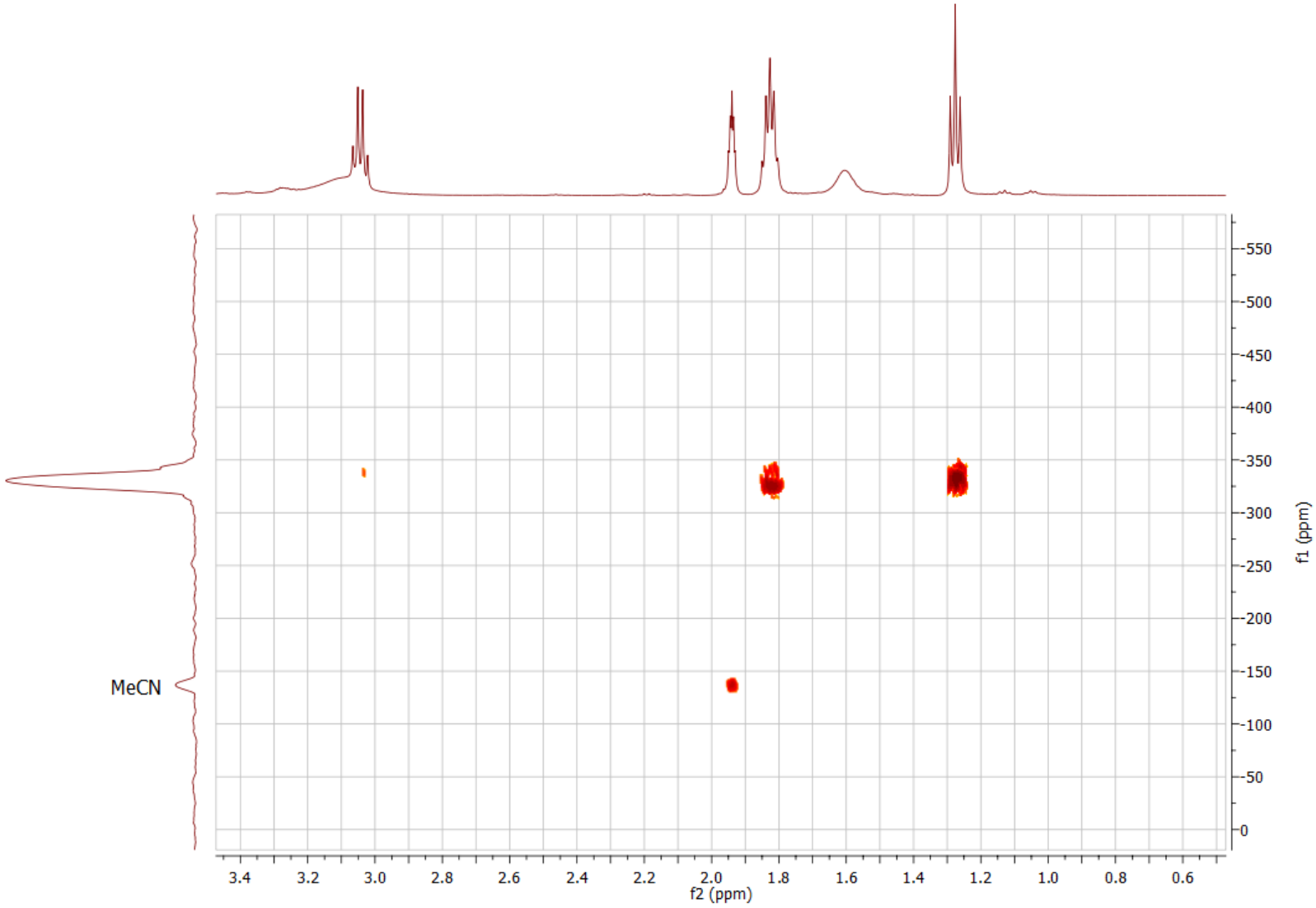


Figure S22: The ^{1}H NMR spectrum of complex [**2**]NO_3 (1 hour after addition of I_2) in CD_3CN.

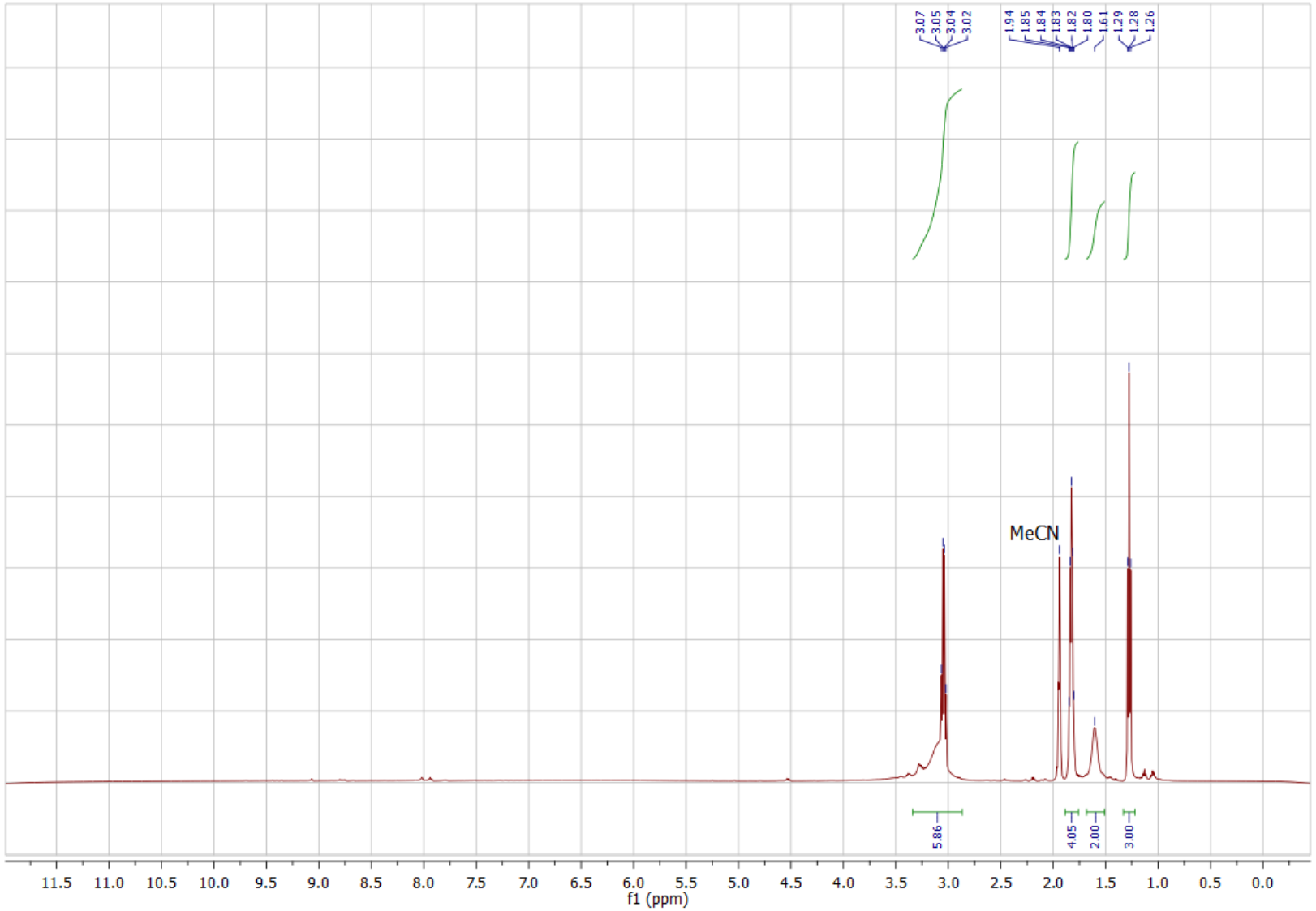


Figure S23: The ^{1}H-^{15}N HMBC spectrum of complex [**2**]NO_3 (1 hour after addition of I_2) in CD_3CN.

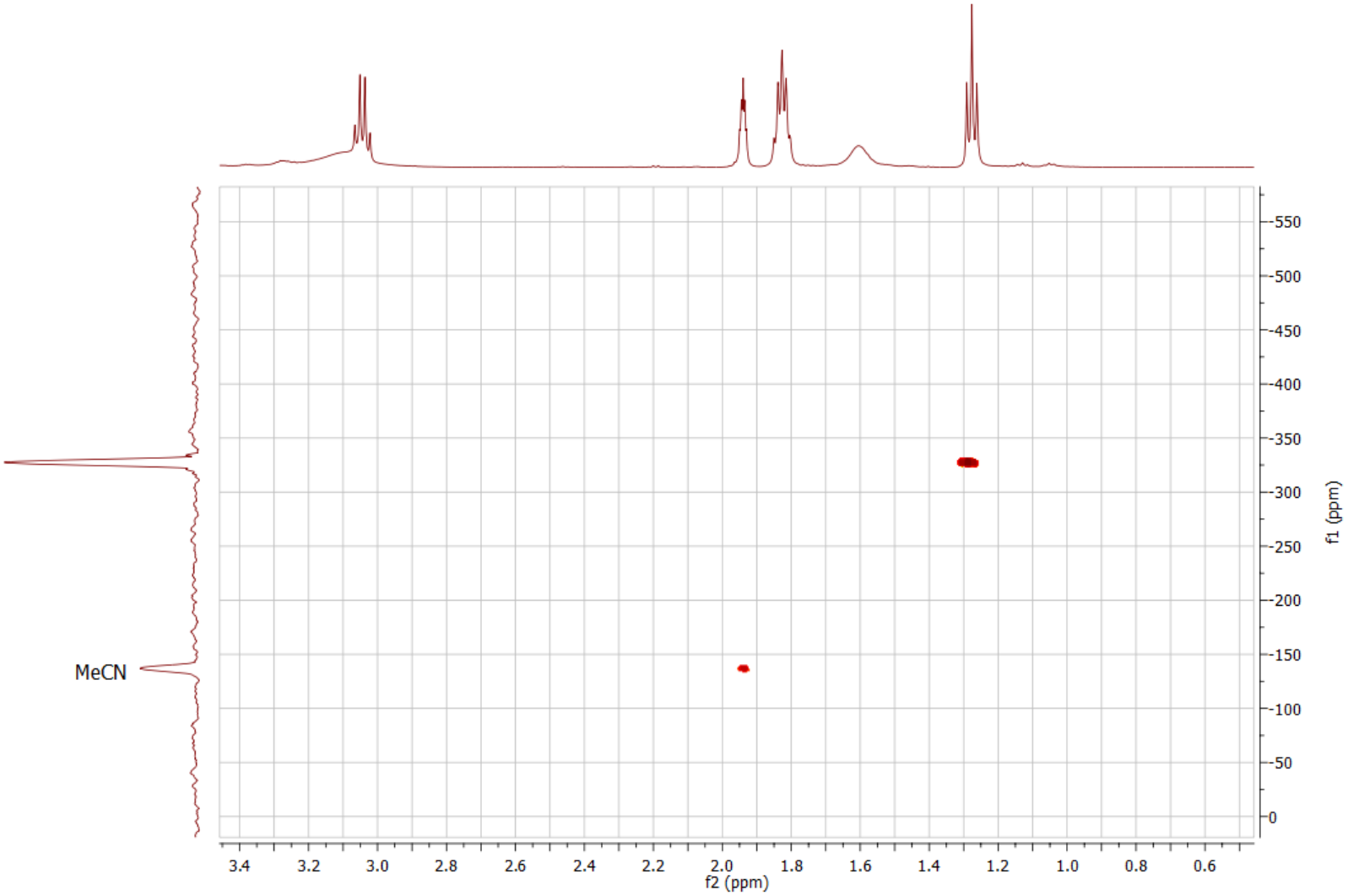


Figure S24: The ^{1}H NMR spectrum of $[H(1\text{-Etpip})]NO_3$ in CD_3CN.

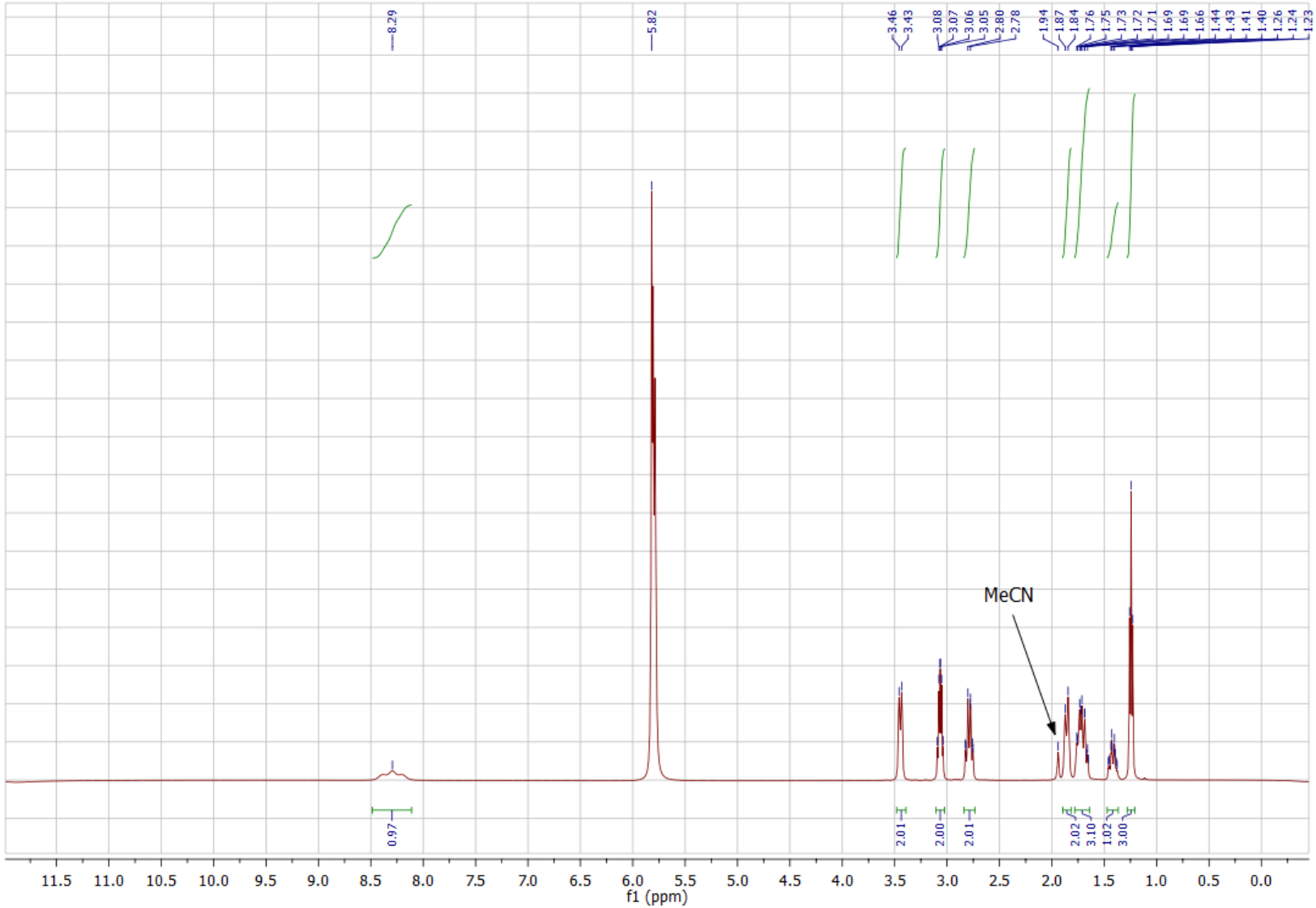
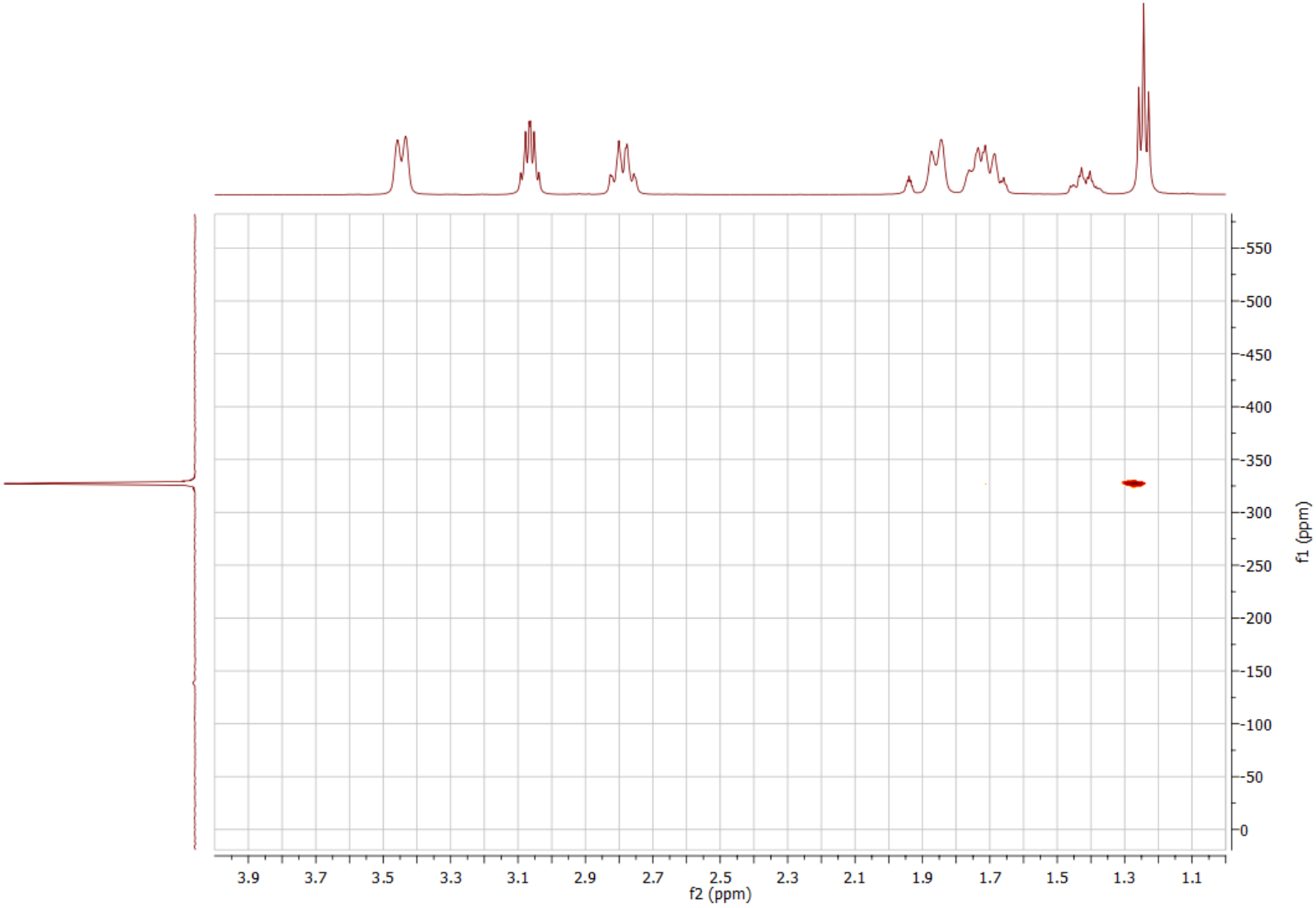


Figure S25: The ^{1}H-^{15}N HMBC spectrum of [H(1-Etpip)]NO_3 in CD_3CN.



Computational Details

Theoretical methods

For the optimizations we have used the M06-2X/def2-TZVP level of theory and the Gaussian-16 program.[8–10] The minimum nature of the compounds has been verified by using frequency calculations (zero imaginary frequencies). The NBO calculations including the Wiberg bond index (WBI) have been computed using the same level of theory (M06-2X/def2-TZVP level of theory) by using the NBO 3.1 version as implemented in Gaussian-16 program.[10,11]

Cartesian Coordinates

[1]$^{+}$

53	0.000000	0.000000	0.000000
7	0.000000	0.000000	2.288211
6	-0.215106	1.385595	2.789174
1	-1.230899	1.666982	2.509950
1	0.473034	2.042410	2.258173
6	0.000000	1.434584	4.315792
1	0.947530	1.920749	4.551987
1	-0.791670	2.021040	4.781089
6	0.000000	0.000000	4.850331
1	0.000000	0.000000	5.938756
6	1.307513	-0.506510	2.789174
1	2.059099	0.232499	2.509950
1	1.532262	-1.430865	2.258173
6	1.242386	-0.717292	4.315792
1	1.189653	-1.780960	4.551987
1	2.146107	-0.324913	4.781089
6	-1.092407	-0.879085	2.789174
1	-0.828200	-1.899481	2.509950
1	-2.005296	-0.611546	2.258173
6	-1.242386	-0.717292	4.315792
1	-2.137183	-0.139790	4.551987
1	-1.354437	-1.696127	4.781089
7	-0.000000	-0.000000	-2.288211
6	0.215106	-1.385595	-2.789174
1	1.230899	-1.666982	-2.509950
1	-0.473034	-2.042410	-2.258173
6	-0.000000	-1.434584	-4.315792
1	-0.947530	-1.920749	-4.551987
1	0.791670	-2.021040	-4.781089
6	-0.000000	-0.000000	-4.850331
1	-0.000000	-0.000000	-5.938756
6	-1.307513	0.506510	-2.789174
1	-2.059099	-0.232499	-2.509950
1	-1.532262	1.430865	-2.258173
6	-1.242386	0.717292	-4.315792
1	-1.189653	1.780960	-4.551987
1	-2.146107	0.324913	-4.781089
6	1.092407	0.879085	-2.789174
1	0.828200	1.899481	-2.509950
1	2.005296	0.611546	-2.258173
6	1.242386	0.717292	-4.315792
1	2.137183	0.139790	-4.551987
1	1.354437	1.696127	-4.781089

[2]$^{+}$

53	0.000000	0.000000	0.000000
7	-2.299148	-0.213489	0.097065
6	-2.720465	-0.787001	-1.214632
1	-2.288145	-1.785560	-1.288923
1	-2.263526	-0.165493	-1.988062
6	-4.233479	-0.810866	-1.407643
6	-4.837887	0.573462	-1.189623
6	-2.879366	1.147588	0.256464
1	-2.458086	1.757833	-0.546097
1	-2.526557	1.559822	1.199801
6	-4.398490	1.145631	0.155846
6	-2.641860	-1.146045	1.209574
1	-2.036767	-2.039732	1.048904
1	-3.686757	-1.442299	1.111187
6	-2.404248	-0.583455	2.597833
1	-3.119491	0.198540	2.849791
1	-2.530921	-1.386688	3.322487
7	2.299148	0.213489	-0.097065
6	2.720465	0.787001	1.214632
1	2.288145	1.785560	1.288923
1	2.263526	0.165493	1.988062
6	4.233479	0.810866	1.407643
6	4.837887	-0.573462	1.189623
6	2.879366	-1.147588	-0.256464
1	2.458086	-1.757833	0.546097
1	2.526557	-1.559822	-1.199801
6	4.398490	-1.145631	-0.155846
6	2.641860	1.146045	-1.209574
1	2.036767	2.039732	-1.048904
1	3.686757	1.442299	-1.111187
6	2.404248	0.583455	-2.597833
1	3.119491	-0.198540	-2.849791
1	2.530921	1.386688	-3.322487
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1	1.395719	0.186246	-2.711149
1	-4.503821	1.244275	-1.987165
1	-5.924608	0.525702	-1.250028
1	-4.832194	0.568849	0.977568
1	-4.749720	2.171236	0.274912
1	-4.697265	-1.535617	-0.736052
1	-4.431511	-1.163546	-2.420669
1	4.431511	1.163546	2.420669
1	4.697265	1.535617	0.736052
1	4.749720	-2.171236	-0.274912
1	4.832194	-0.568849	-0.977568
1	5.924608	-0.525702	1.250028
1	4.503821	-1.244275	1.987165

$[I(4\text{-}DMAP)_2]^+$

53	0.000000	0.000000	0.000000
7	-2.244942	0.000000	0.000000
7	-6.390778	0.000000	0.000000
7	2.244942	-0.000000	0.000000
7	6.390778	-0.000000	0.000000
6	-2.931929	1.151258	0.000000
1	-2.343248	2.060056	0.000000
6	-4.299435	1.201715	0.000000
1	-4.780379	2.166956	0.000000
6	-5.049030	0.000000	0.000000
6	-7.120625	1.258353	0.000000
1	-6.886349	1.848167	0.888353
1	-8.185184	1.049534	0.000000
1	-6.886349	1.848167	-0.888353
6	2.931929	-1.151258	0.000000
1	2.343248	-2.060056	0.000000
6	4.299435	-1.201715	0.000000
1	4.780379	-2.166956	0.000000
6	5.049030	-0.000000	0.000000
6	7.120625	-1.258353	0.000000
1	6.886349	-1.848167	0.888353
1	8.185184	-1.049534	0.000000
1	6.886349	-1.848167	-0.888353
6	-2.931929	-1.151258	-0.000000
1	-2.343248	-2.060056	-0.000000
6	-4.299435	-1.201715	-0.000000
1	-4.780379	-2.166956	-0.000000
6	-7.120625	-1.258353	-0.000000
1	-6.886349	-1.848167	0.888353
1	-8.185184	-1.049534	-0.000000
1	-6.886349	-1.848167	-0.888353
6	2.931929	1.151258	0.000000
1	2.343248	2.060056	0.000000
6	4.299435	1.201715	0.000000
1	4.780379	2.166956	0.000000
6	7.120625	1.258353	0.000000
1	6.886349	1.848167	0.888353
1	8.185184	1.049534	0.000000
1	6.886349	1.848167	-0.888353

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