Supporting Information

Impact of SCILL catalysts for the S-S coupling of thiols to disulfides

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NMR characterization

^{1}H-NMR spectra were recorded on a Bruker UltraShield 500 MHz spectrometer, operating at 11.74 T, corresponding to the resonance frequency of 500.13 MHz for the 1H nucleus, equipped with a direct detection four nuclei probe head (BBO) and field gradients on Z axis. Samples were analyzed in 5 mm NMR tubes (Norell 507). The chemical shifts are reported in ppm, using the TMS as internal standard. Typical parameters for ^{1}H NMR spectra were: 45° pulse, 8.30 s acquisition times, 8.01 kHz spectral window, 16 scans, 20 K data points delay time 1 s. The FID was not processed prior to Fourier transformation. The average acquisition time of the ^{1}H NMR spectra was approximately 2.5 min.

The resonance frequency for the ^{13}C nucleus is 125.77 MHz, 45° pulse, 1.67 s acquisition times, 39.68 kHz spectral window, 1024 scans, 20 K data points delay time 1 s. The average acquisition time of the ^{13}C NMR spectra was approximately 47 min.

1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide [Bmim][NTf$_2$]

^{1}H-NMR (500.13 MHz, DMSO-d$_6$, δ ppm, *J* Hz): 9.09 (s, 1H, H-2), 7.74 (m, 1H, H-4), 7.67 (m, 1H, H-5), 4.16 (t, 2H, 7.2 Hz, H-7), 3.85 (s, 3H, H-6), 1.78 (qv, 2H, 7.2 Hz, H-8), 1.27 (sextet, 2H, 7.5 Hz, H-9), 0.91 (t, 3H, 7.5 Hz, H-10) ^{13}C-NMR (125.77 MHz, DMSO-d$_6$, δ ppm): 136.5 (C-2), 123.6 (C-5), 122.2 (C-4), 119.5 (q, 321.97 Hz, C-11 (CF_3)), 48.5 (C-7), 35.7 (C-6), 31.3 (C-8), 18.7 (C-9), 13.1 (C-10).

1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide [Emim][NTf$_2$]

^{1}H-NMR (500.13 MHz, DMSO-d$_6$, δ ppm, *J* Hz): 9.10 (s, 1H, H-2), 7.76 (m, 1H, H-4), 7.67 (m, 1H, H-5), 4.19 (q, 2H, 7.4 Hz, H-7), 3.85 (s, 3H, H-6), 1.42 (t, 2H, 7.4 Hz, H-8). ^{13}C-NMR (125.77 MHz, DMSO-d$_6$, δ ppm): 136.3 (C-2), 123.6 (C-

5), 121.9 (C-4), 119.5 (q, 321.97 Hz, C-11 (CF_3)), 44.2 (C-7), 35.6 (C-6), 15.0 (C-8).

1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide [Bmpyrr][NTf$_2$]

^{1}H-NMR (500.13 MHz, DMSO-d$_6$, δ ppm, *J* Hz): 3.48-3.40 (m, 4H, H-2, H-5), 3.29 (m, 2H, H-7), 2.97 (s, 3H, H-6), 2.08 (m, 4H, H-3, H-4), 1.68 (m, 2H, H-8), 1.32 (sextet, 2H, 7.4 Hz, H-9), 0.93 (t, 3H, 7.4 Hz, H-10).^{13}C-NMR (125.77 MHz, DMSO-d$_6$, δ ppm): 119.5 (q, 321.97 Hz, C-11 (CF_3)), 63.4 (t, C-2, C-5), 62.9 (t, C-7), 47.5 (t, C-6), 24.9 (C-8), 21.1 (C-4, C-3), 19.3 (C-9), 13.4 (C-10).

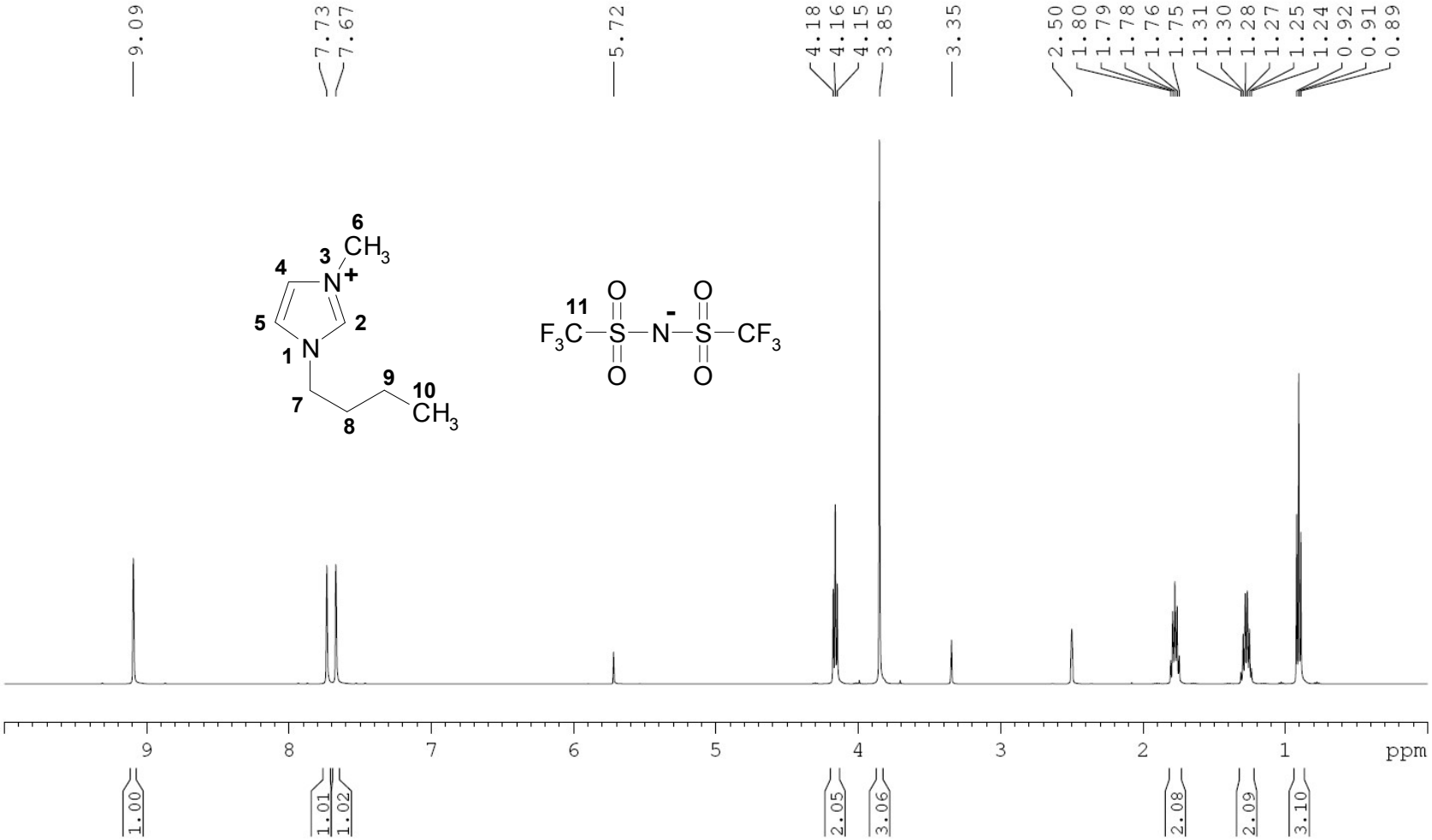

Fig. SI1. ^{1}H-NMR (500.13 MHz, DMSO-d_6) spectrum of [Bmim][NTf_2].

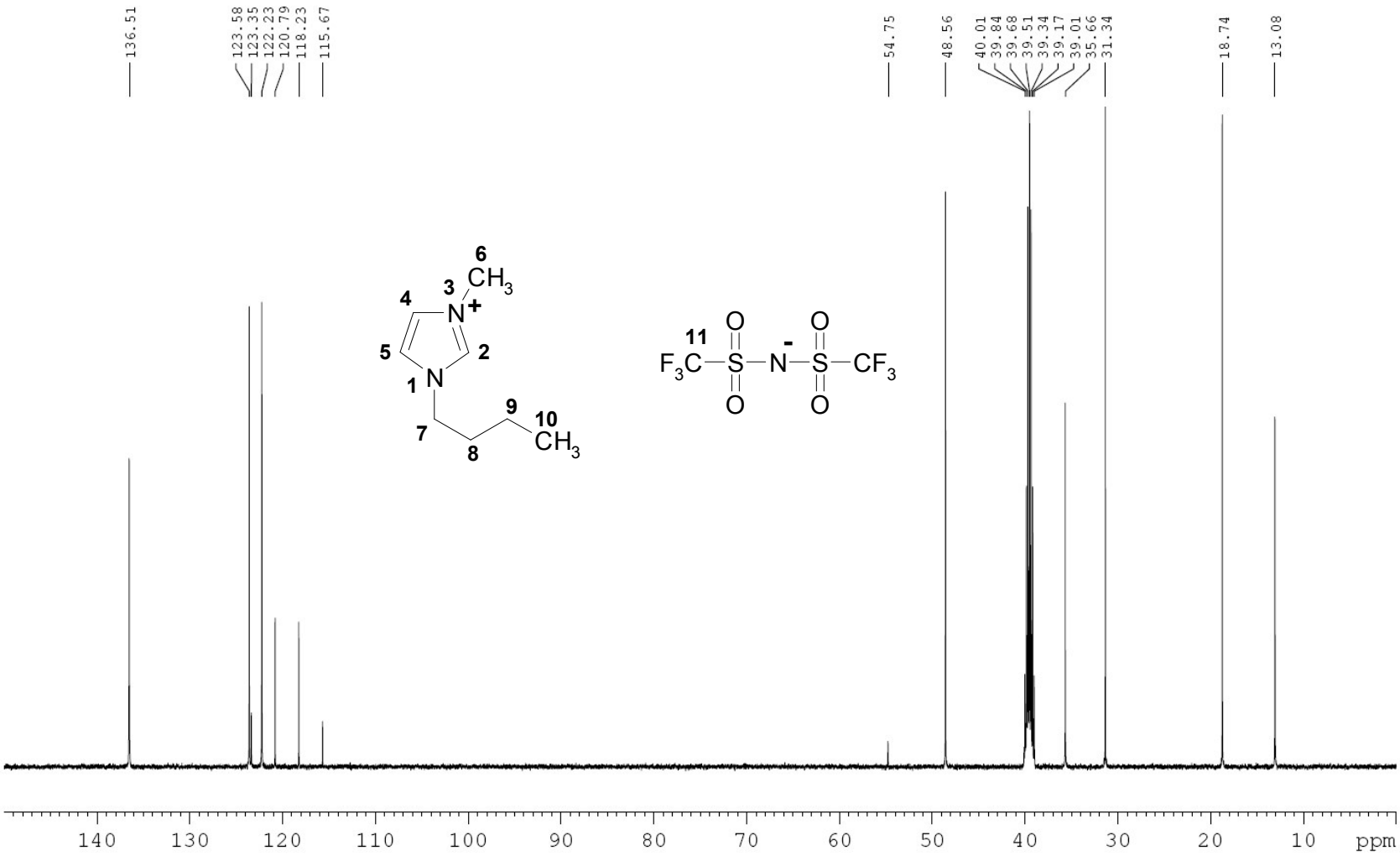

Fig. SI2. ^{13}C-NMR (125.77 MHz, DMSO-d_6) spectrum of [Bmim][NTf_2].

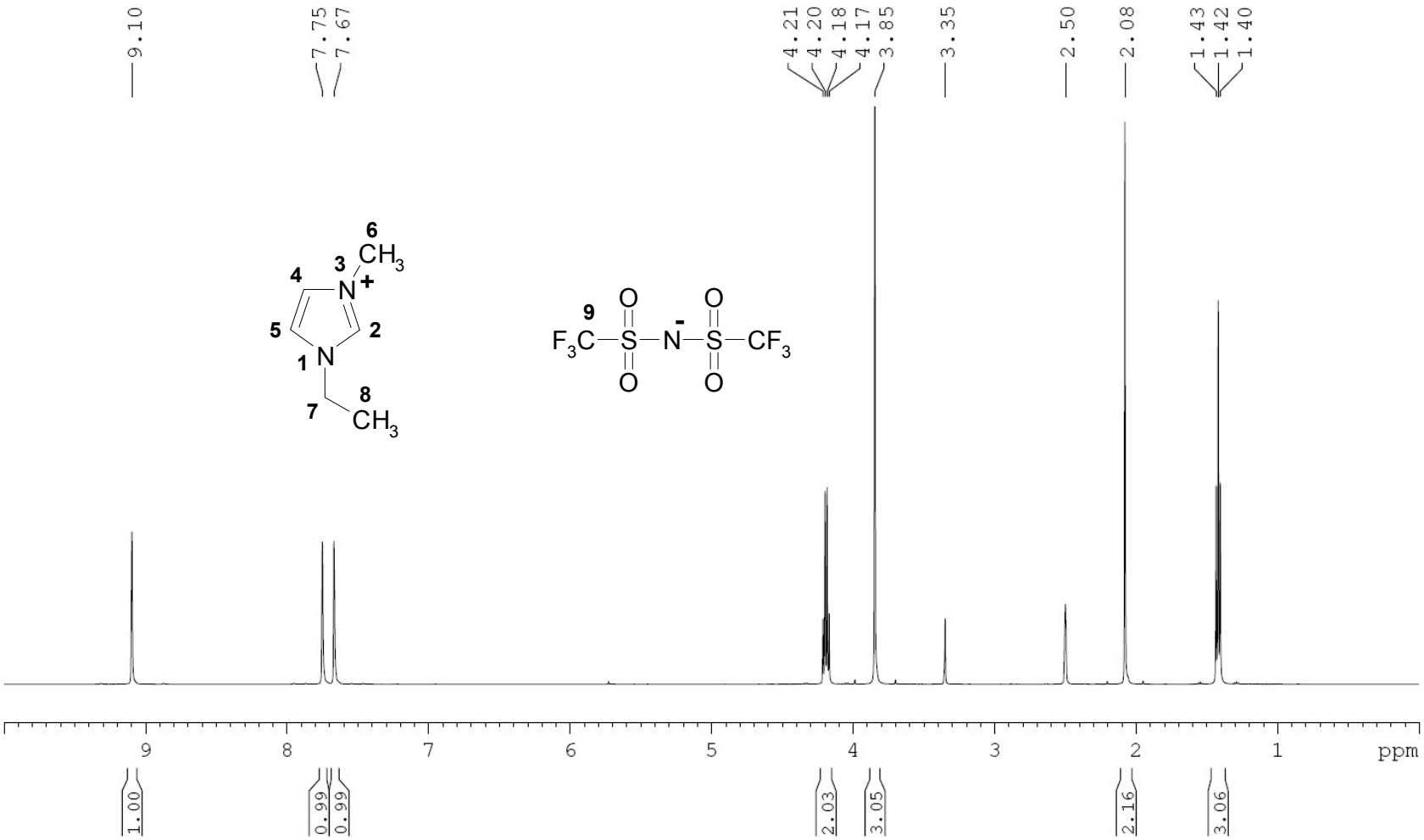

Fig. SI3. ^{1}H-NMR (500.13 MHz, DMSO-d_6) spectrum of [Emim][NTf_2].

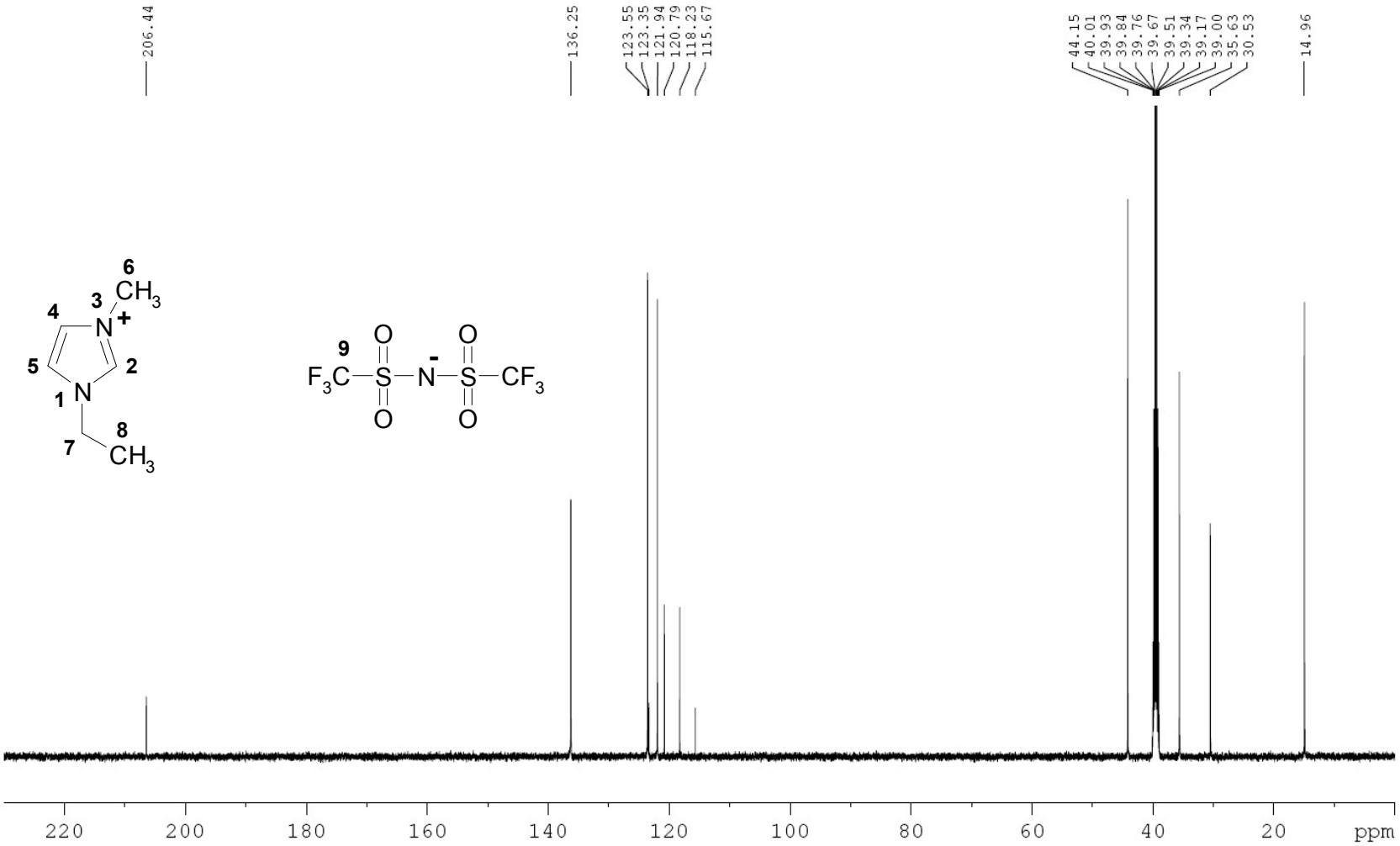

Fig. SI4. ^{13}C-NMR (125.77 MHz, DMSO-d_6) spectrum of [Emim][NTf$_2$].

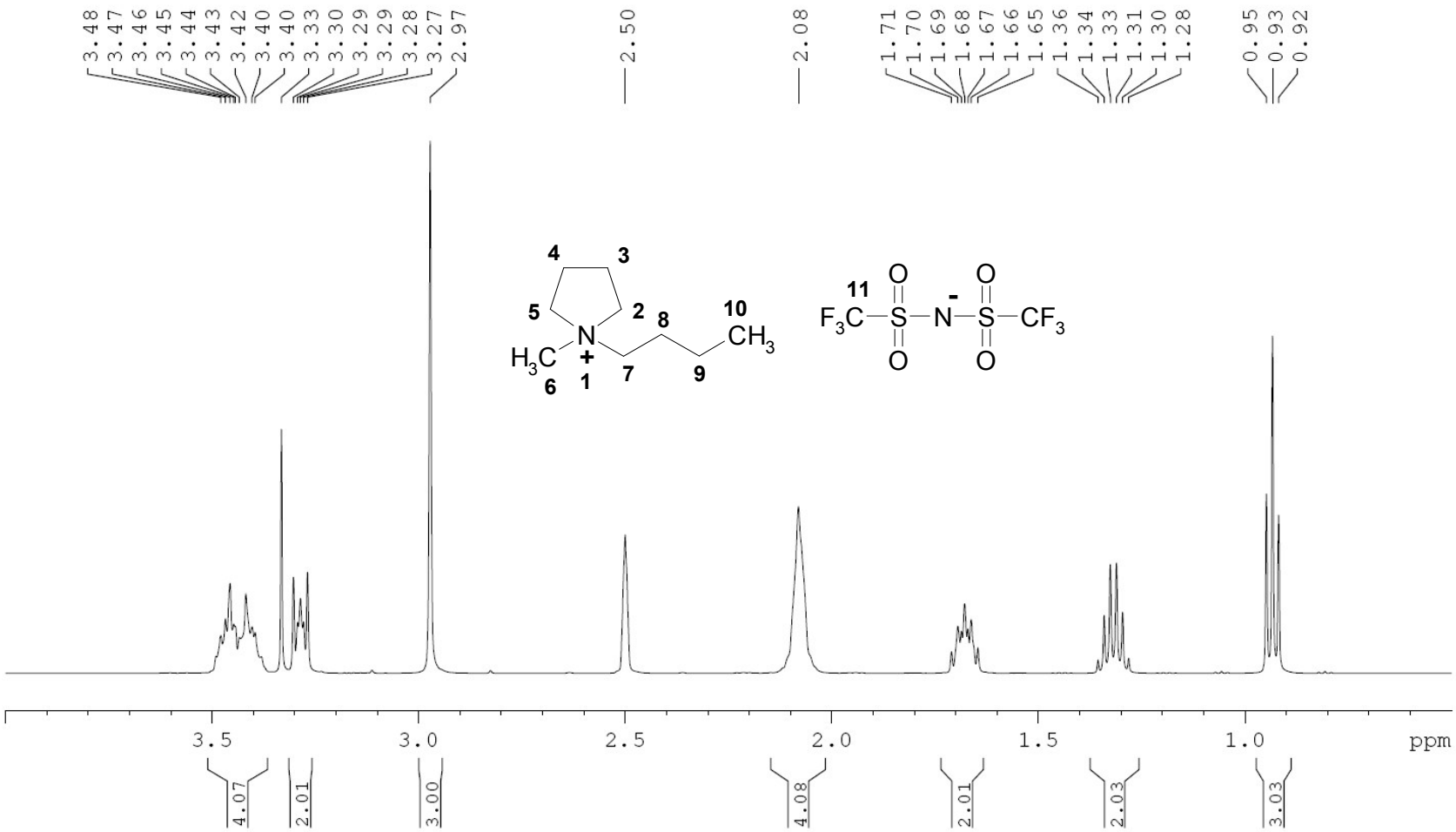

Fig. SI5. ^{1}H-NMR (500.13 MHz, DMSO-d_6) spectrum of [Bmpyrr][NTf_2].

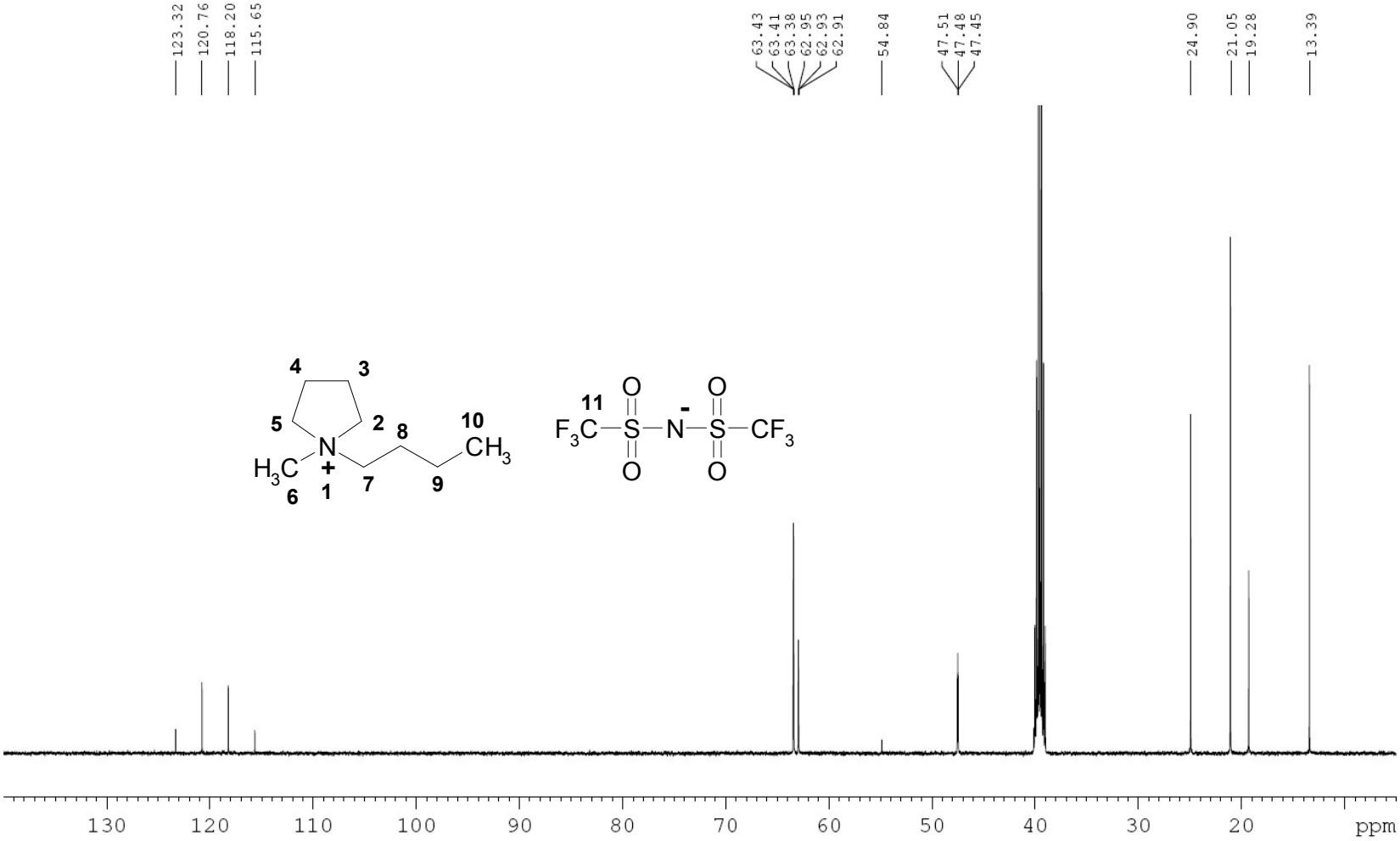

Fig. SI6. ^{13}C-NMR (125.77 MHz, DMSO-d_6) spectrum of [Bmpyrr][NTf_2].

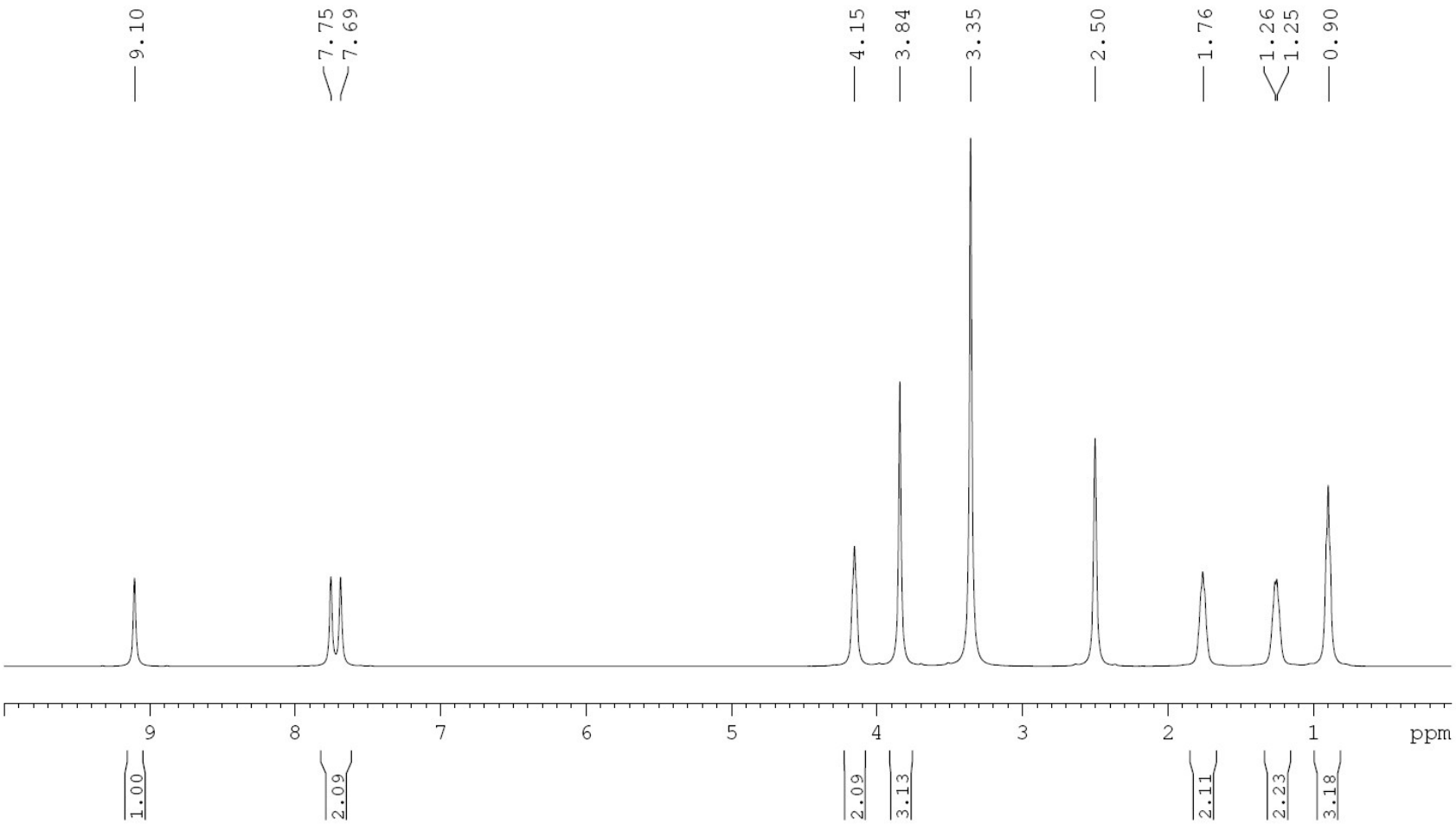

Fig. SI7. ^{1}H-NMR (500.13 MHz, DMSO-d_6) spectrum of 5% Pt/OMS-2/[Bmim][NTf_2].

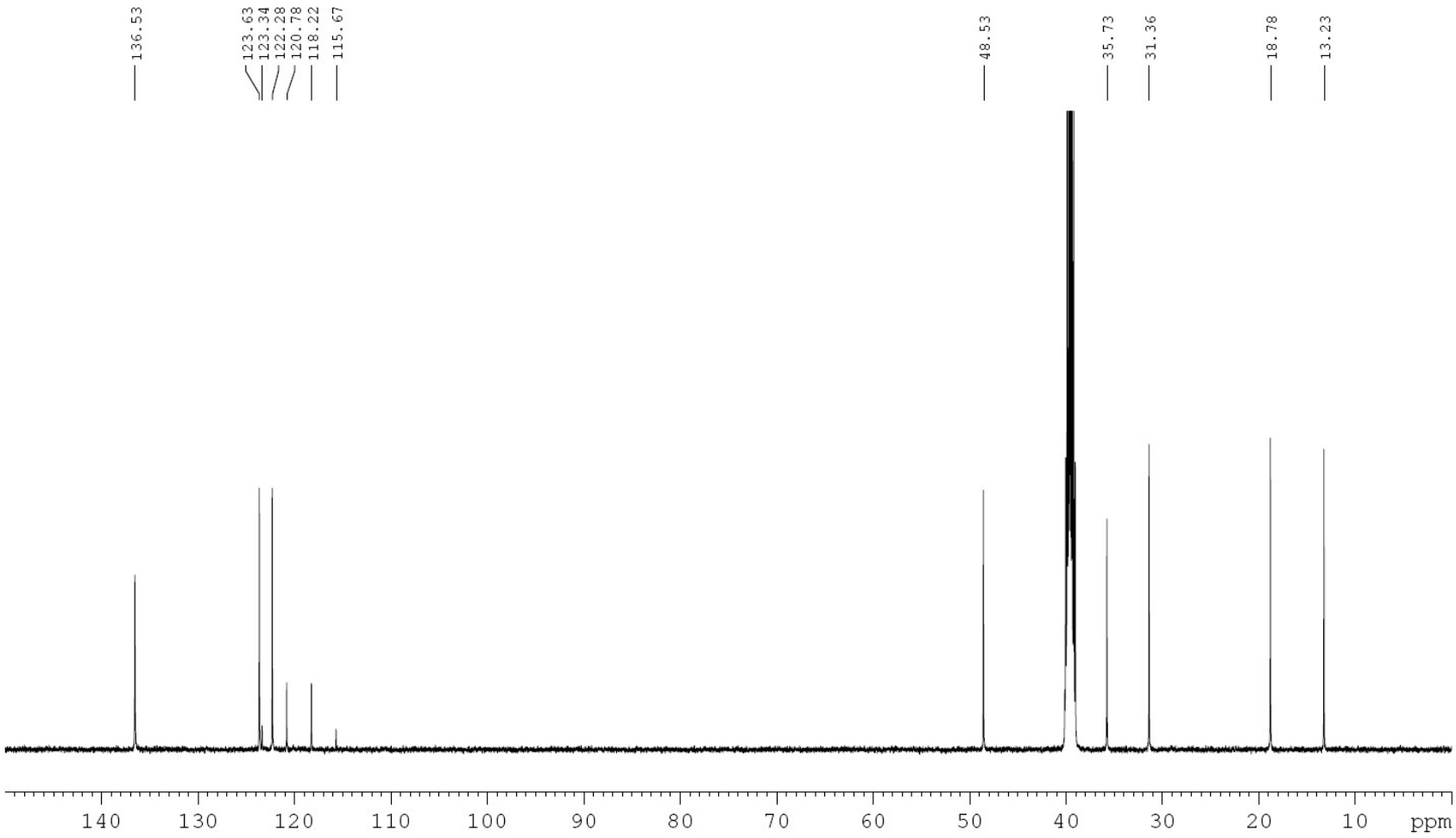

Fig. SI8. ^{13}C-NMR (125.77 MHz, DMSO-d_6) spectrum of 5% Pt/OMS-2/[Bmim][NTf_2].

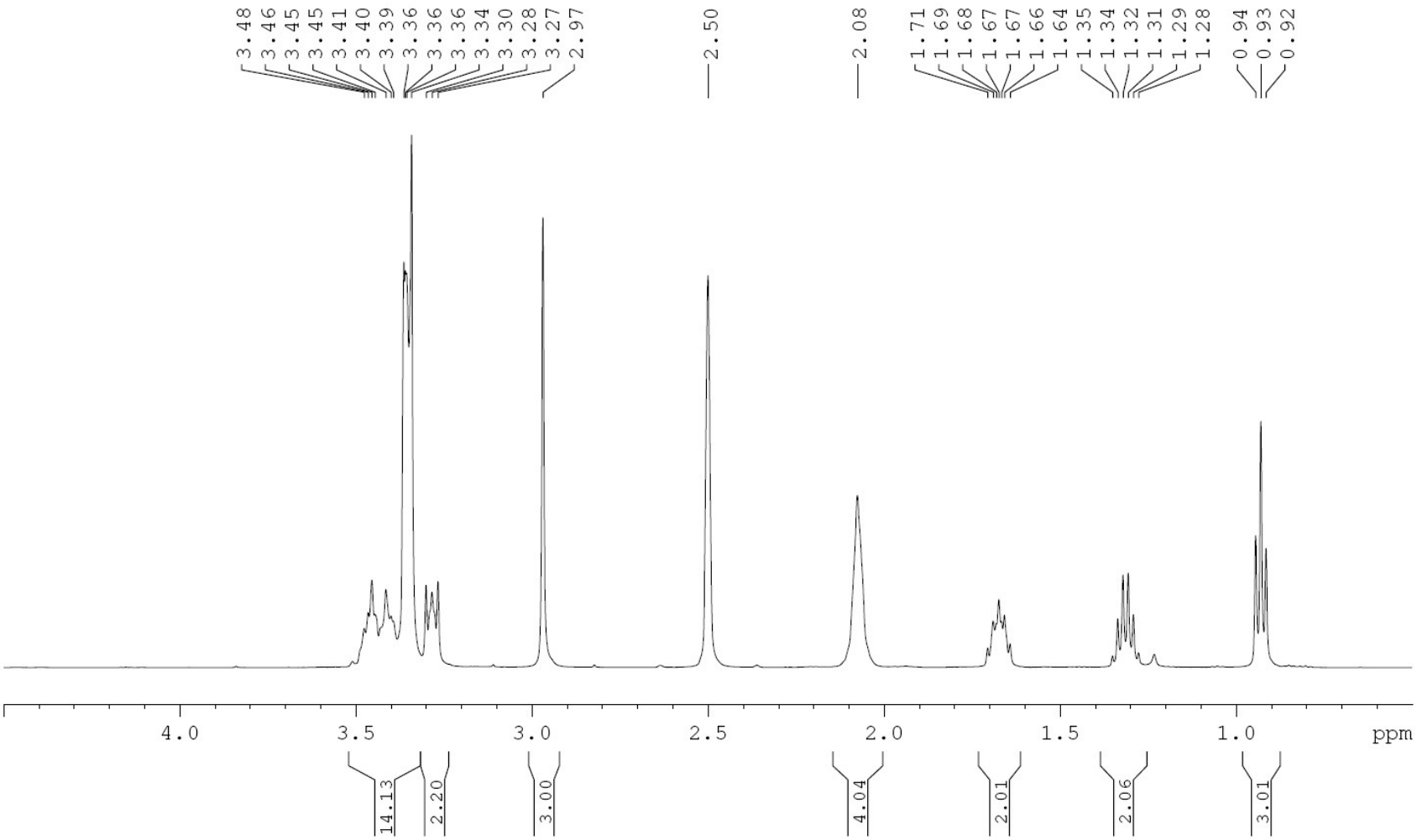

Fig. SI9. ^{1}H-NMR (500.13 MHz, DMSO-d_6) spectrum of 5% Pt/OMS-2/[Bmpyrr][NTf_2].

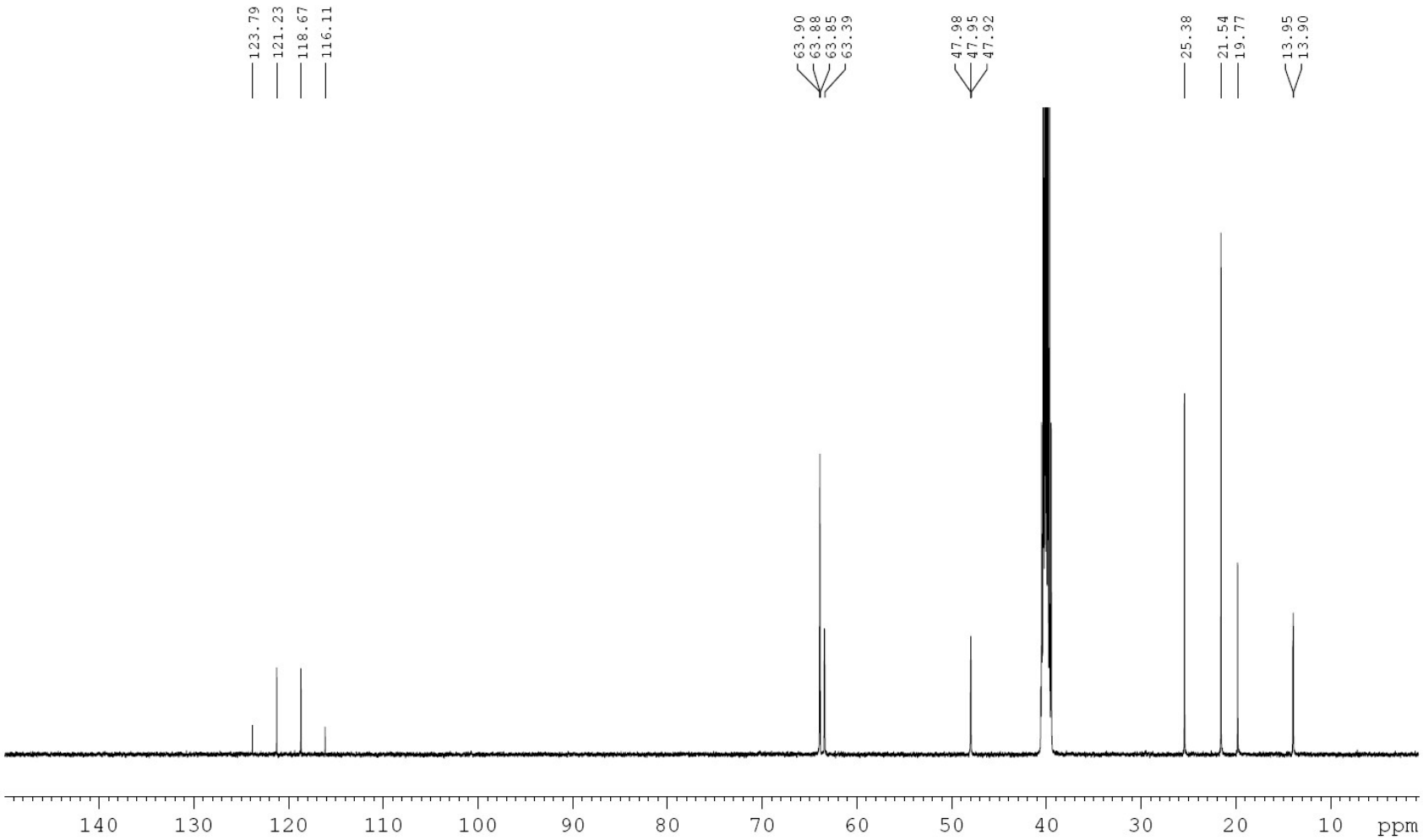

Fig. SI10. ^{13}C-NMR (125.77 MHz, DMSO-d_6) spectrum of 5% Pt/OMS-2/[Bmpyrr][NTf_2]

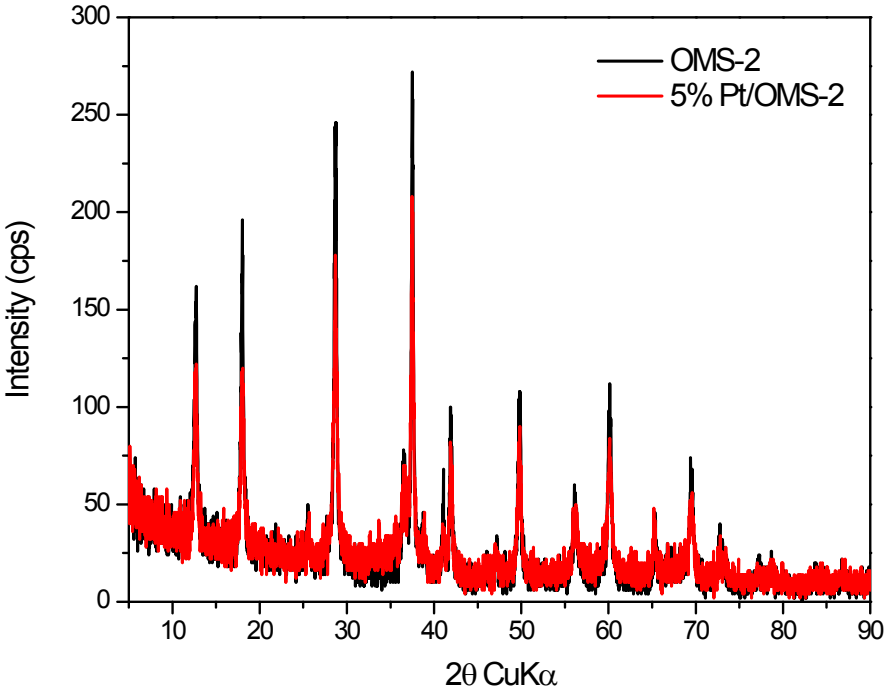

Fig. SI11. XRD patterns of OMS-2 and 5% Pt/OMS-2 samples.

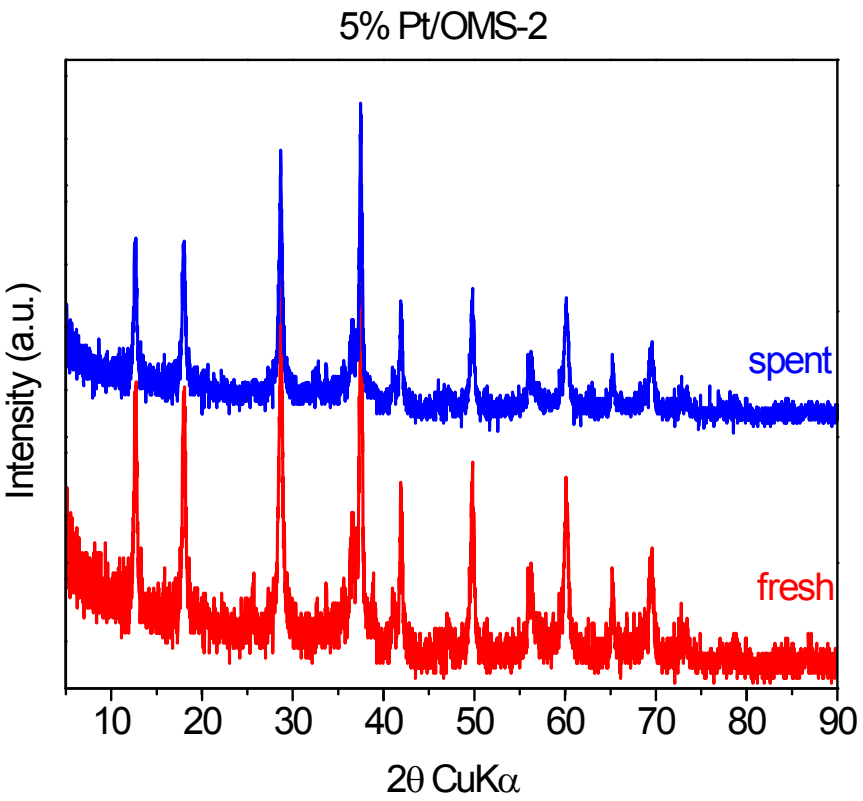

Fig. SI12. XRD patterns of fresh and spent of 5% Pt/OMS-2 samples.

Table SI1. Pt $4f_{7/2}$ and C1s XPS binding energies (eV) comparing a fresh and [Bmim][NTf_2] modified 5% Pt/OMS-2 catalyst as well as the supported and unsupported ionic liquid.

X-ray photoelectron peak	**5% Pt/OMS-2/[Bmim][NTf_2]**	**5% Pt/OMS-2[a]**
Pt $4f_{7/2}$	74.9	74.8
	5% Pt/OMS-2/[Bmim][NTf_2]	**[Bmim][NTf_2][b]**
C1s C aliphatic chain	284.8	284.7
C1s N bonded C aliphatic chain	285.6	285.9
C1s C-C*-N imidazolium ring	286.9	286.5
C 1s N-C*-N imidazolium ring		287.1
C 1s $–SO_2$-CF_3	293.0	292.6

[a]I.J. McManus, H. Daly, H.G. Manyar, S.F.R. Taylor, J.M. Thompson and C. Hardacre, *Faraday Discuss.*, 2016, **188**, 451; [b]O. Hofft, S. Bahr, M. Himmerlich, S. Krischok, J.A. Schaefer and V. Kempter, *Langmuir*, 2006, **22**, 7120.