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Supporting Information

Strong *in vitro* Cytotoxic Potential of New Ruthenium-Cymene Complexes

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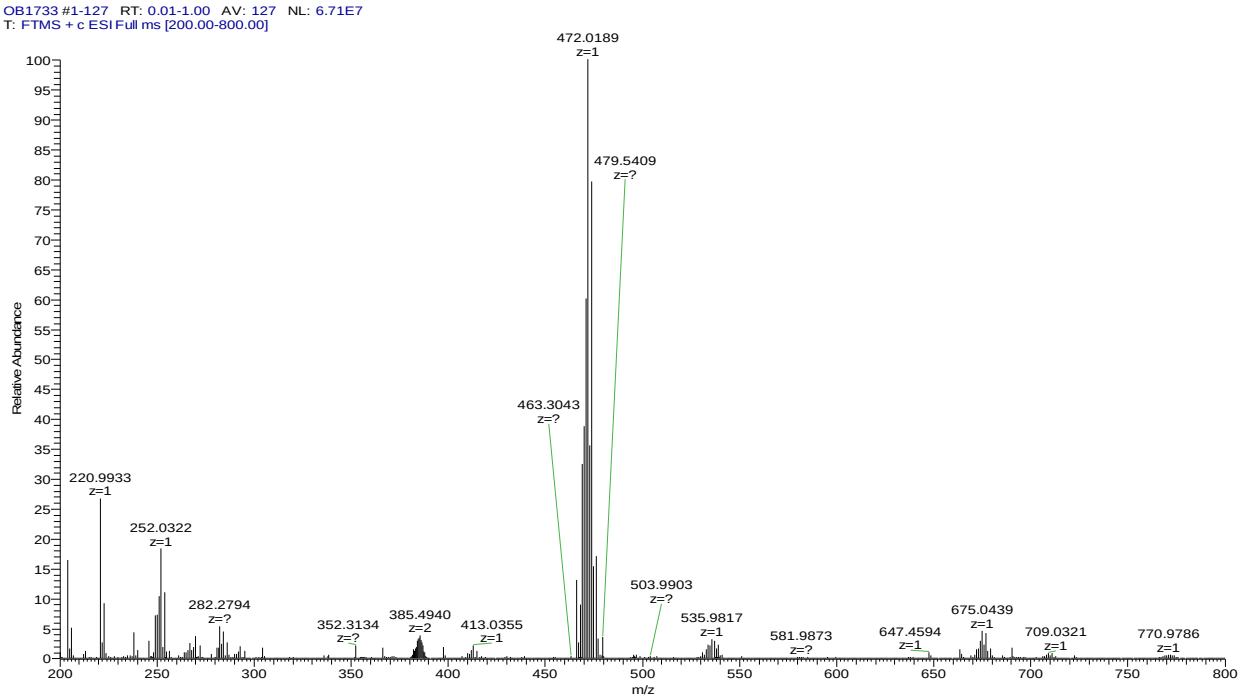
Figure S1: (+)ESI-MS (*m*/*z*) **C1** [(η^6-p-cymene)Ru(L1-H)]$^+$, calculated 472.01776, found 472.0189, in MeOH + 0.1% TFA.



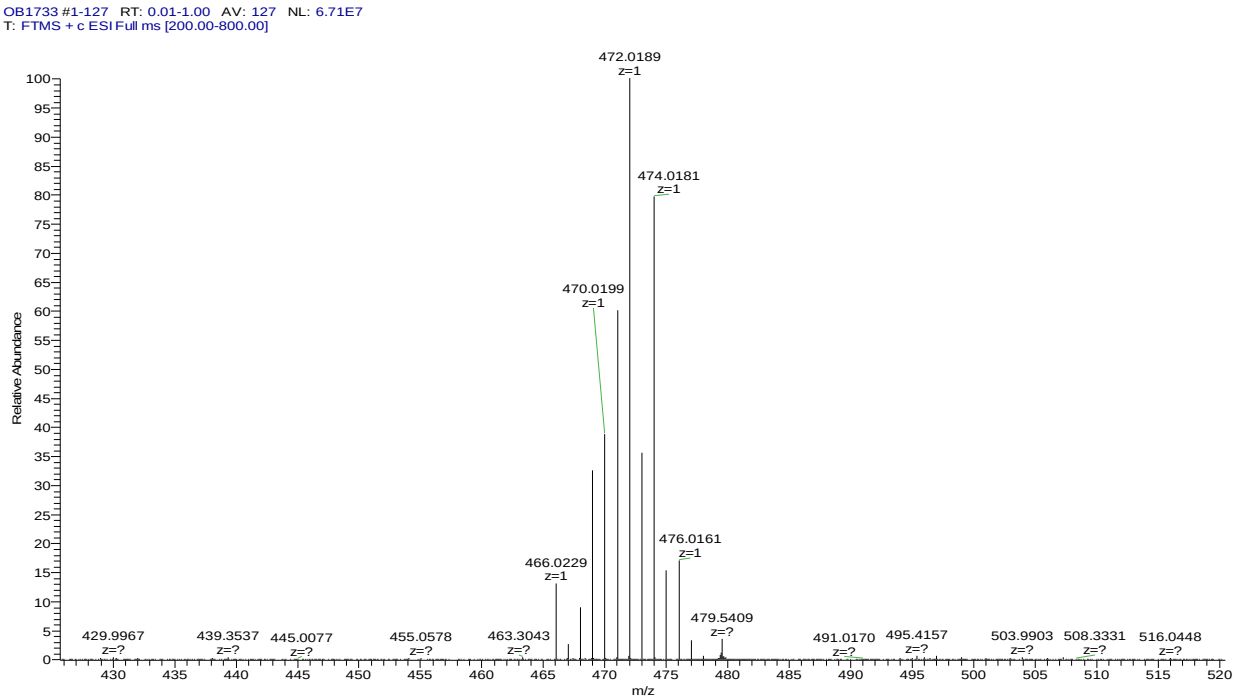
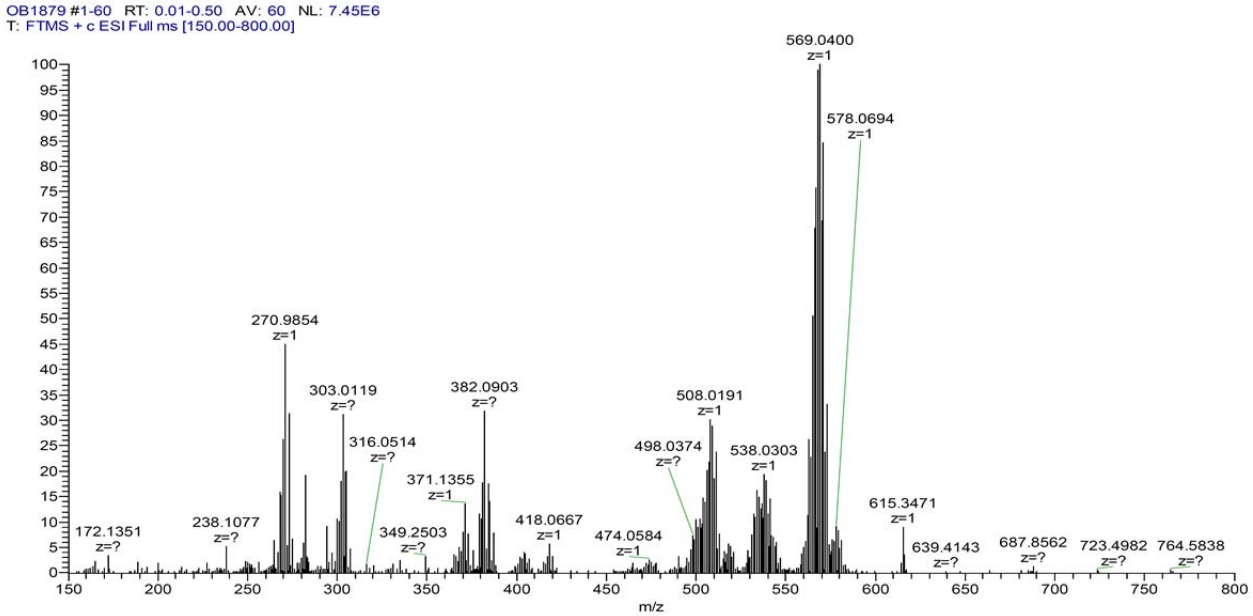


Figure S2: (+)ESI-MS (*m*/*z*) C2: $[(\eta^6\text{-}p\text{-cymene})Ru(L2\text{-}H)]^+$ Calculated 382.084664, found 382.0903, in MeOH + 0.1% TFA.



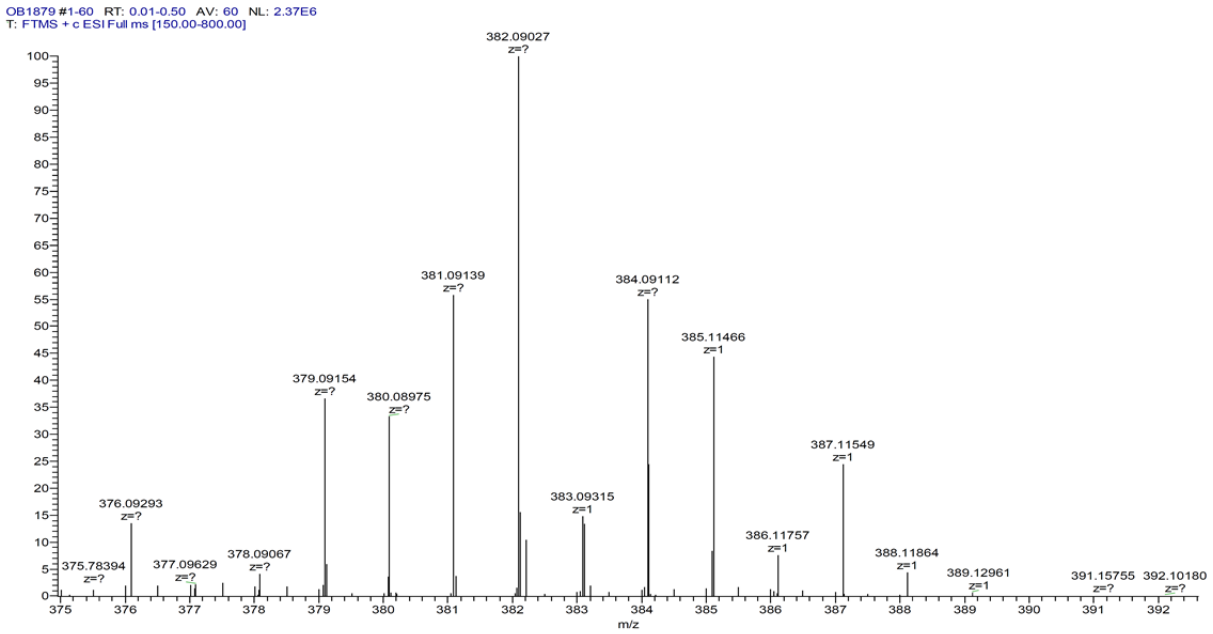


Figure S3: ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of ligand L1

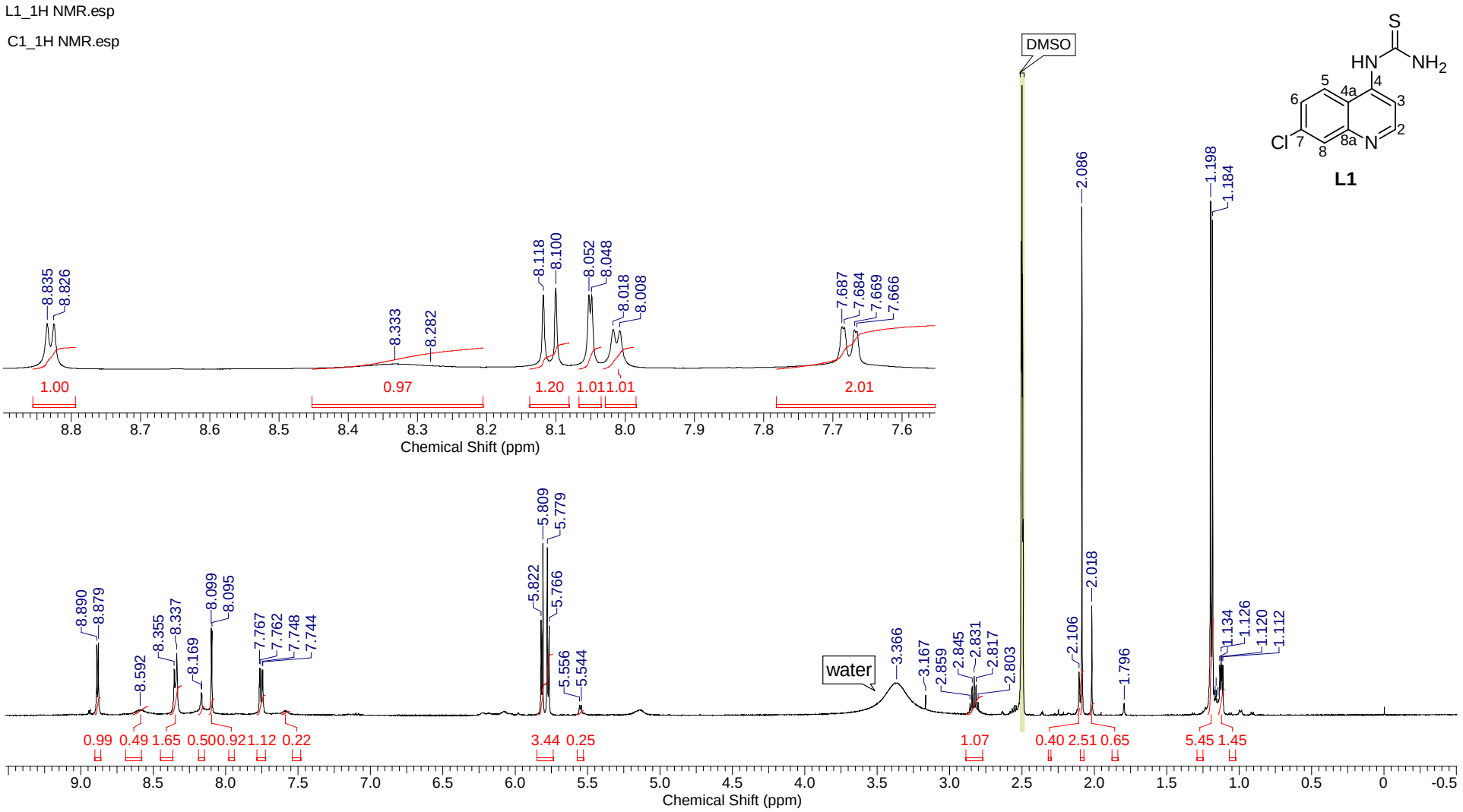


Figure S4: $^{13}C\{^{1}H\}$ NMR (125 MHz, DMSO-d_6)spectrum of ligand L1

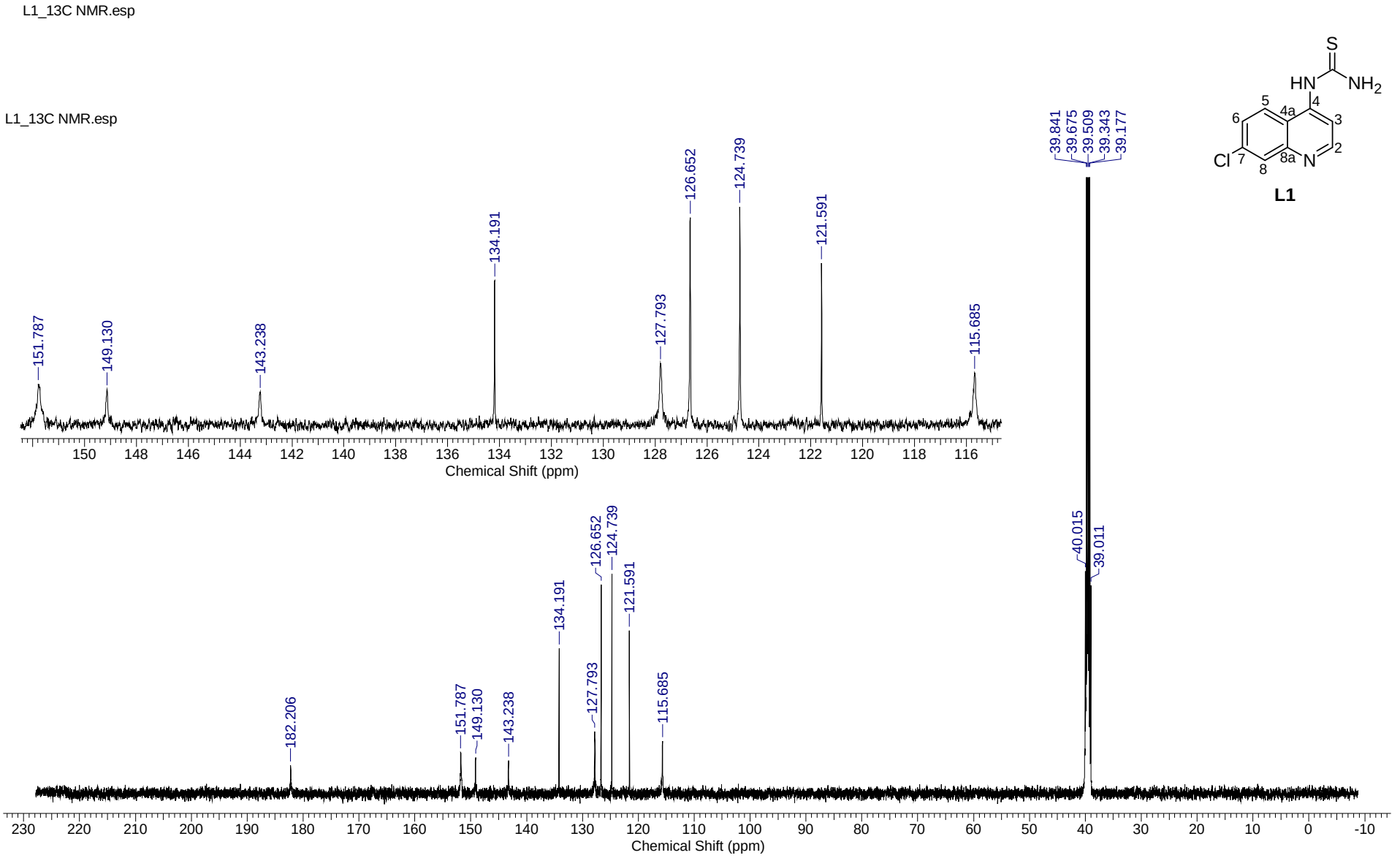


Figure S5: ^{1}H NMR (200 MHz, DMSO-d_6) spectrum of complex C1

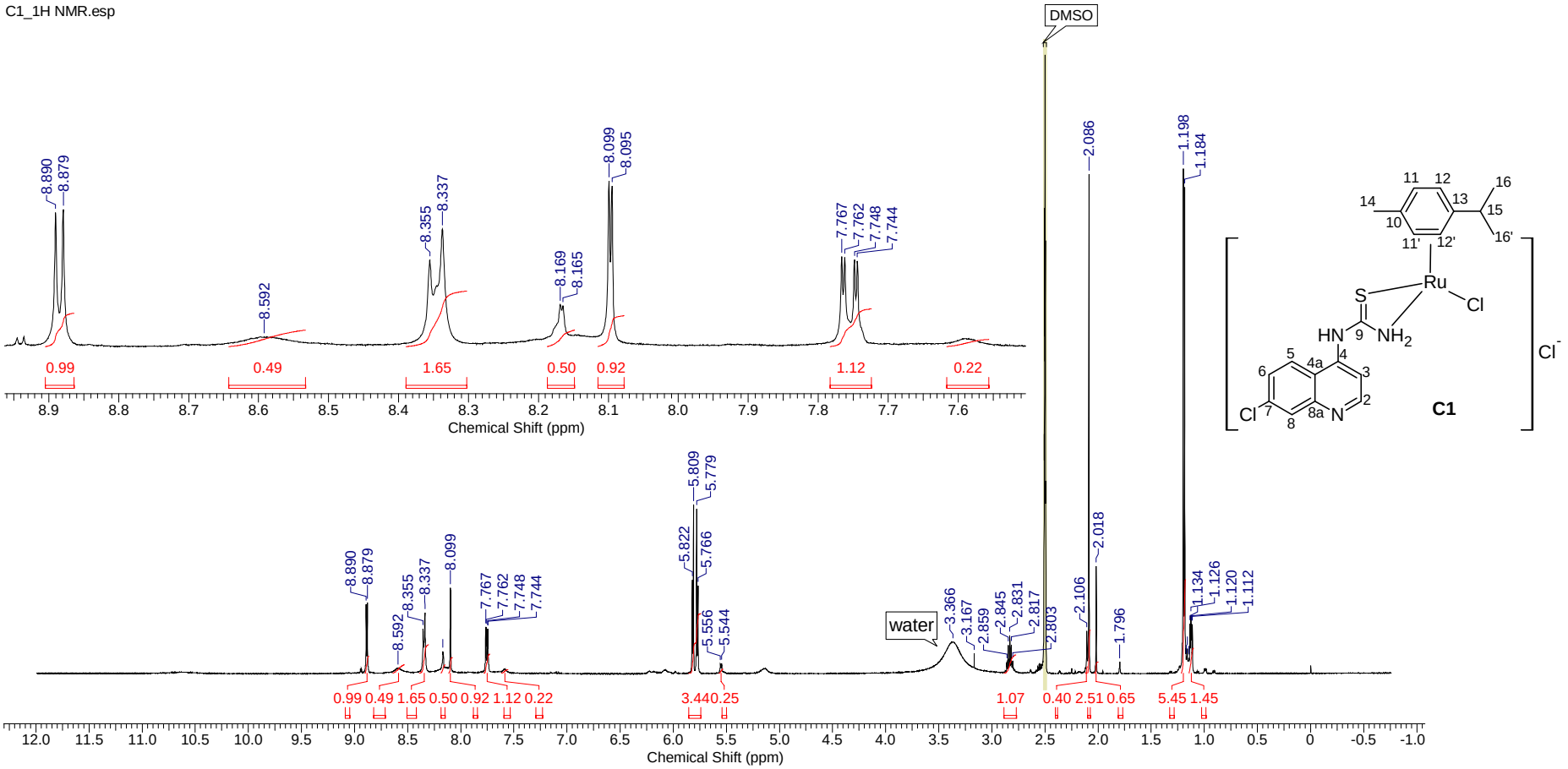


Figure S6: $^{13}C\{^{1}H\}$ NMR (50 MHz, DMSO-d_6) spectrum of ligand C1

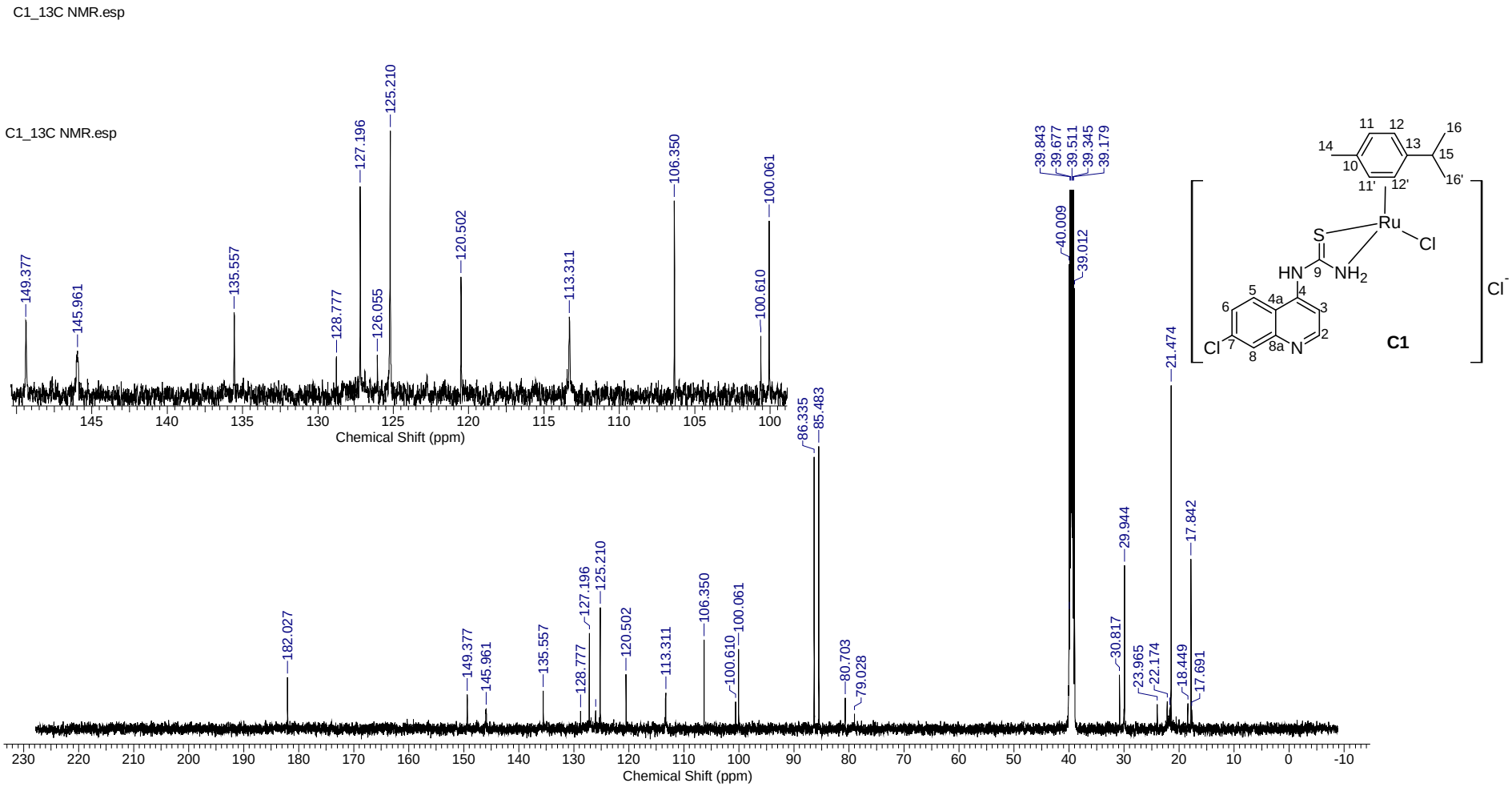


Figure S7: ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of ligand L1

δ_H 9.22 (1H, br s, S=C-NH), 9.07 (1H, d, $^{3}J_{(H2, H3)}$ = 6.7 Hz, H2), 9.05 (1H, br s, S=C-NH), 8.99 (1H, d, $^{3}J_{(H2, H3)}$ = 6.7 Hz, H3), 8.81 (1H, d, $^{3}J_{(H5, H6)}$ = 9.2 Hz, H5), 8.22 (1H, d, $^{4}J_{(H6, H8)}$ = 2.1 Hz, H8), 7.91 (1H, dd, $^{3}J_{(H5, H6)}$ = 9.2 Hz, $^{4}J_{(H6, H8)}$ = 2.1 Hz, H6).

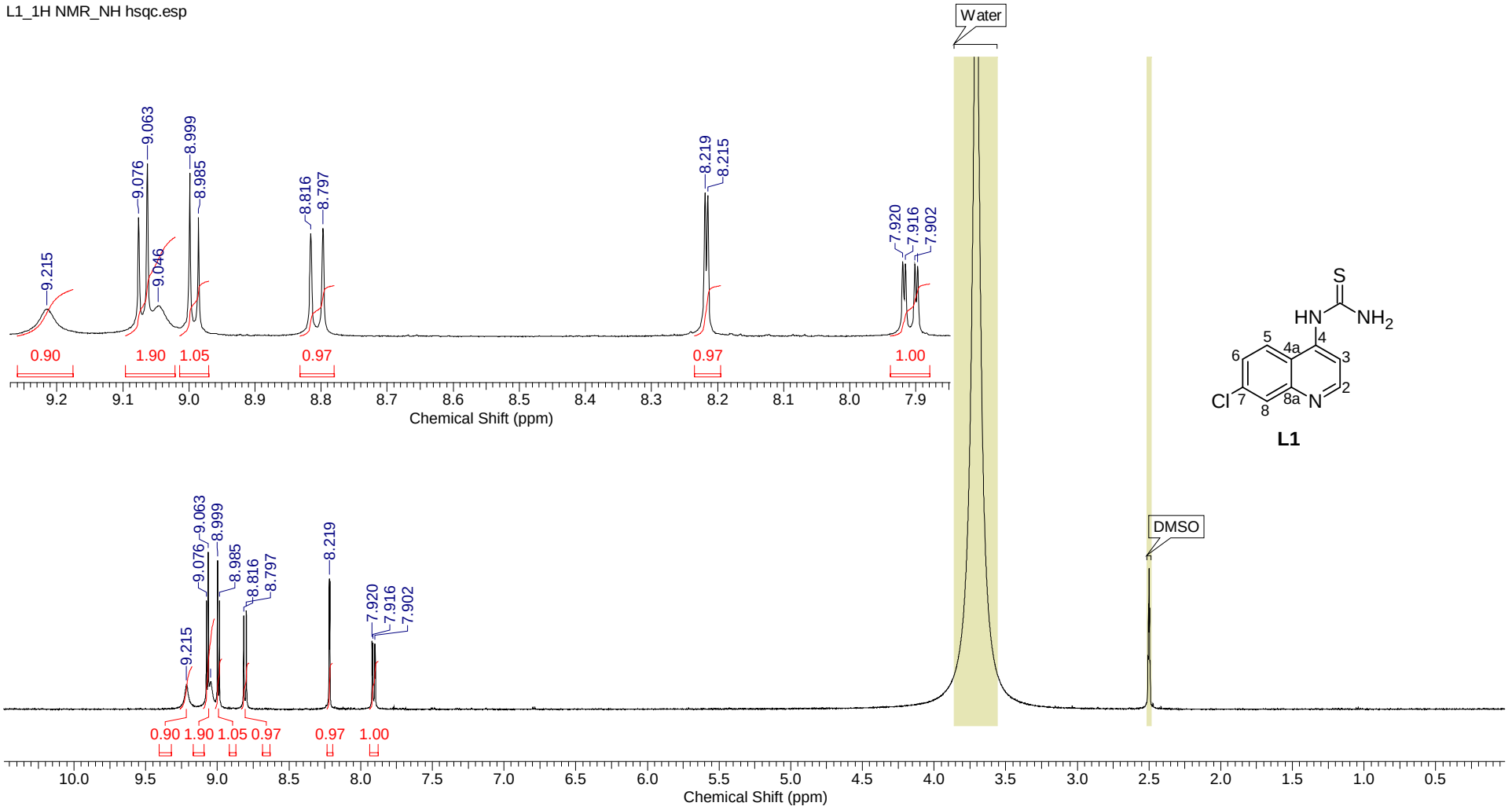


Figure S8: ^{1}H-^{15}N HSQCNMR (500 MHz, DMSO-d_6) spectrum of ligand L1

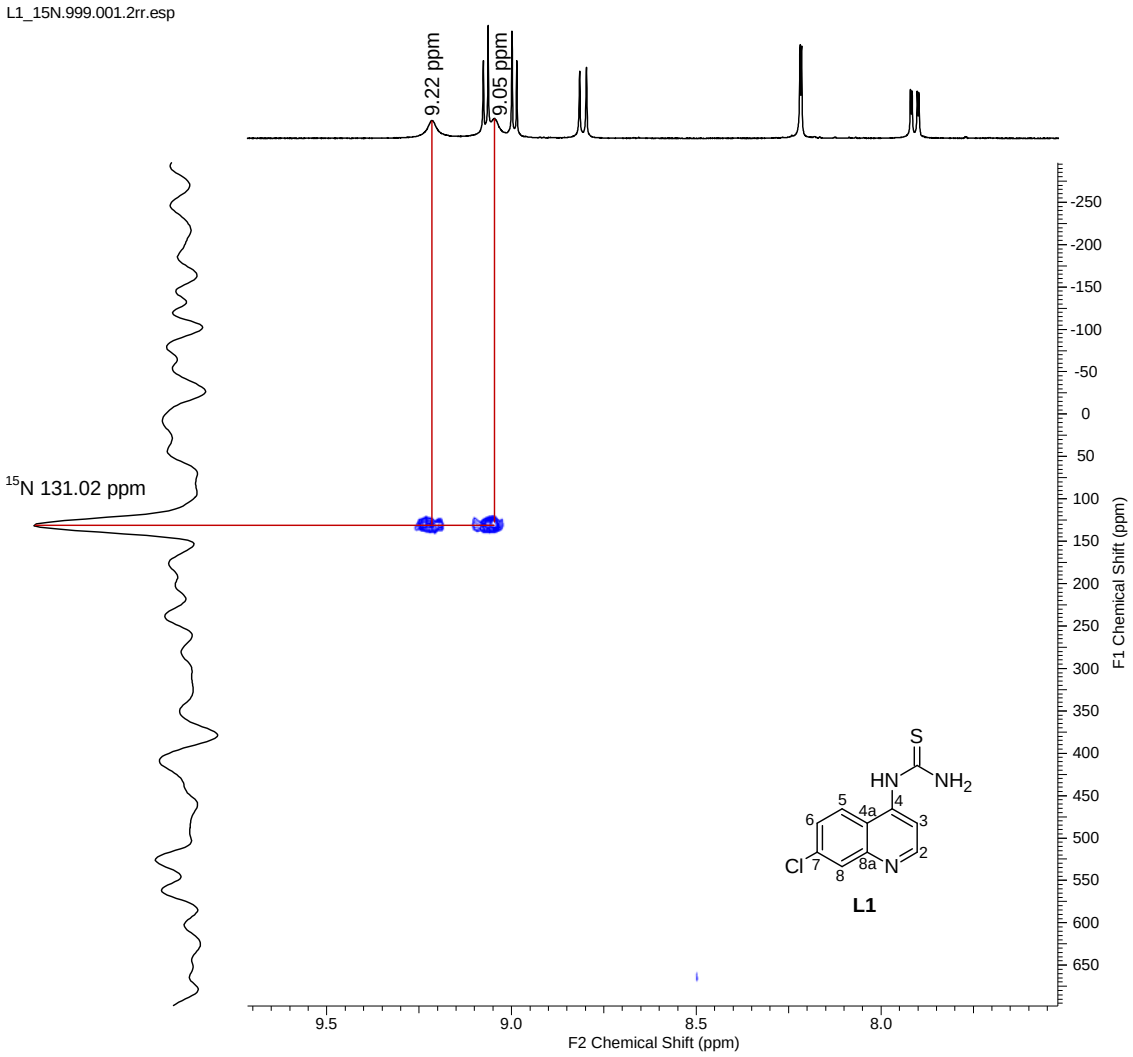


Figure S9: ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of complex C1

δ_H 8.90 (1H, d, $^{3}J_{(H2, H3)}$ = 5.5 Hz, H2), 8.67 (1H, bs S=C-NH), 8.57-8.47 (3H, m, H3, H5 and S=C-NH), 8.12 (1H, d, $^{4}J_{(H6, H8)}$ = 2.1 Hz, H8), 7.76 (1H, dd, $^{3}J_{(H5, H6)}$ = 9.0 Hz, $^{4}J_{(H6, H8)}$ = 2.3 Hz, H6), 5.73 - 5.84 (4H, m, H11, H11", H12 and H12'), 2.88-2.76 (1H, m, H15), 2.08 (3H, s, H14), 1.19 (6H, d, $^{3}J_{(H15, H16)}$ = 7.02 Hz, H16 and H16').

C1_1H NMR_NH hsqc.esp

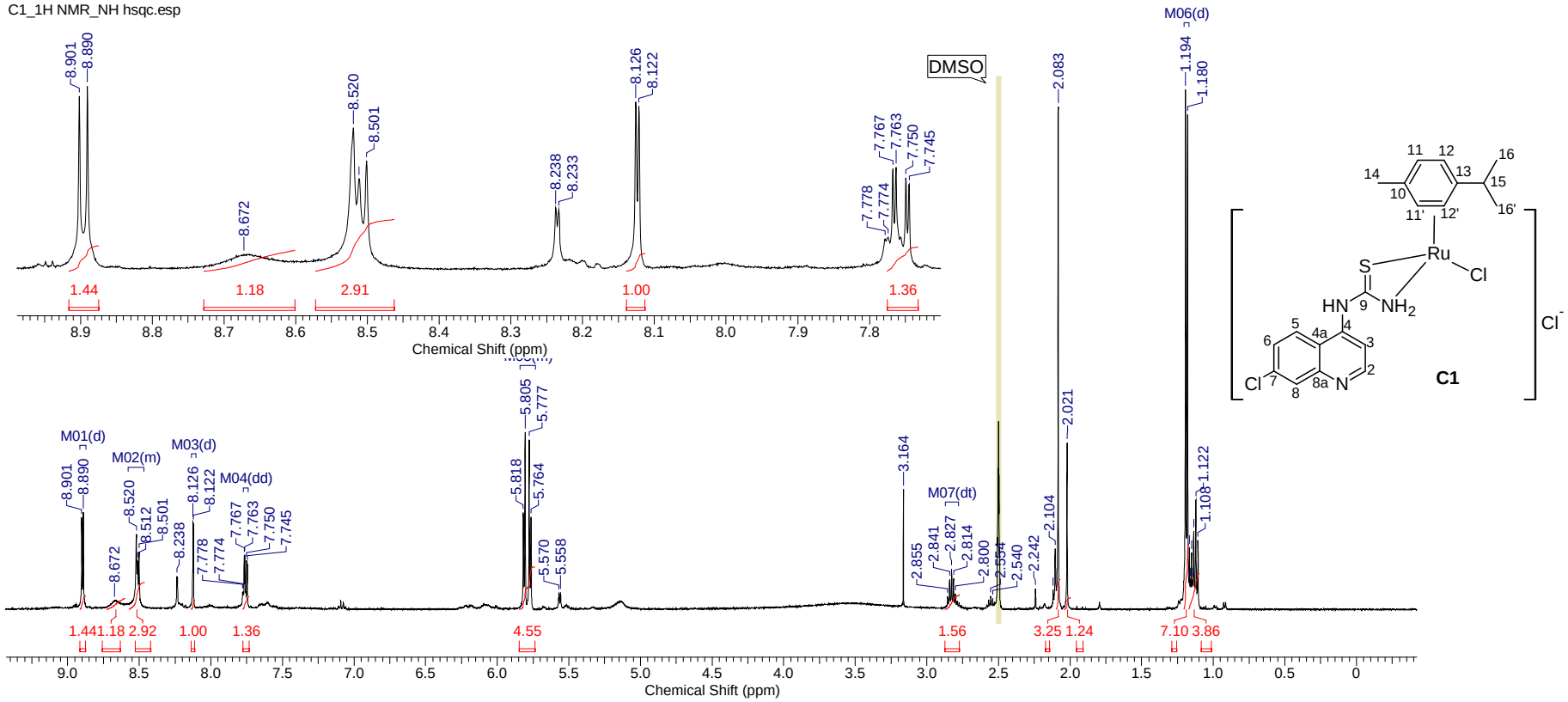


Figure S10: ^{1}H-^{15}N HSQC NMR (500 MHz, DMSO-d_6) spectrum of complex C1 (selected part of spectrum)

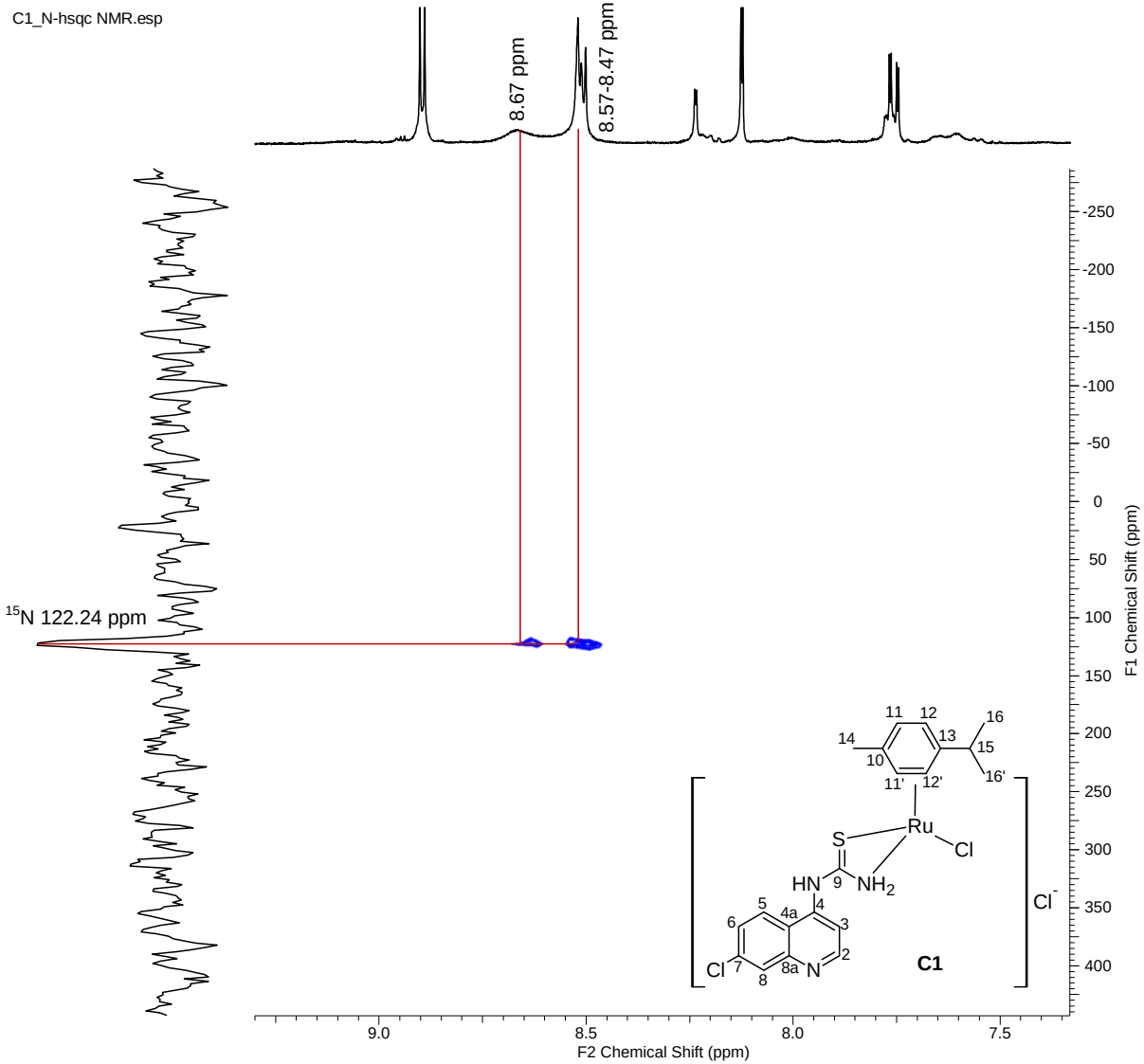


Figure S11: ^{1}H NMR (200 MHz,DMSO-d_6) spectrum of ligand L2xHCl

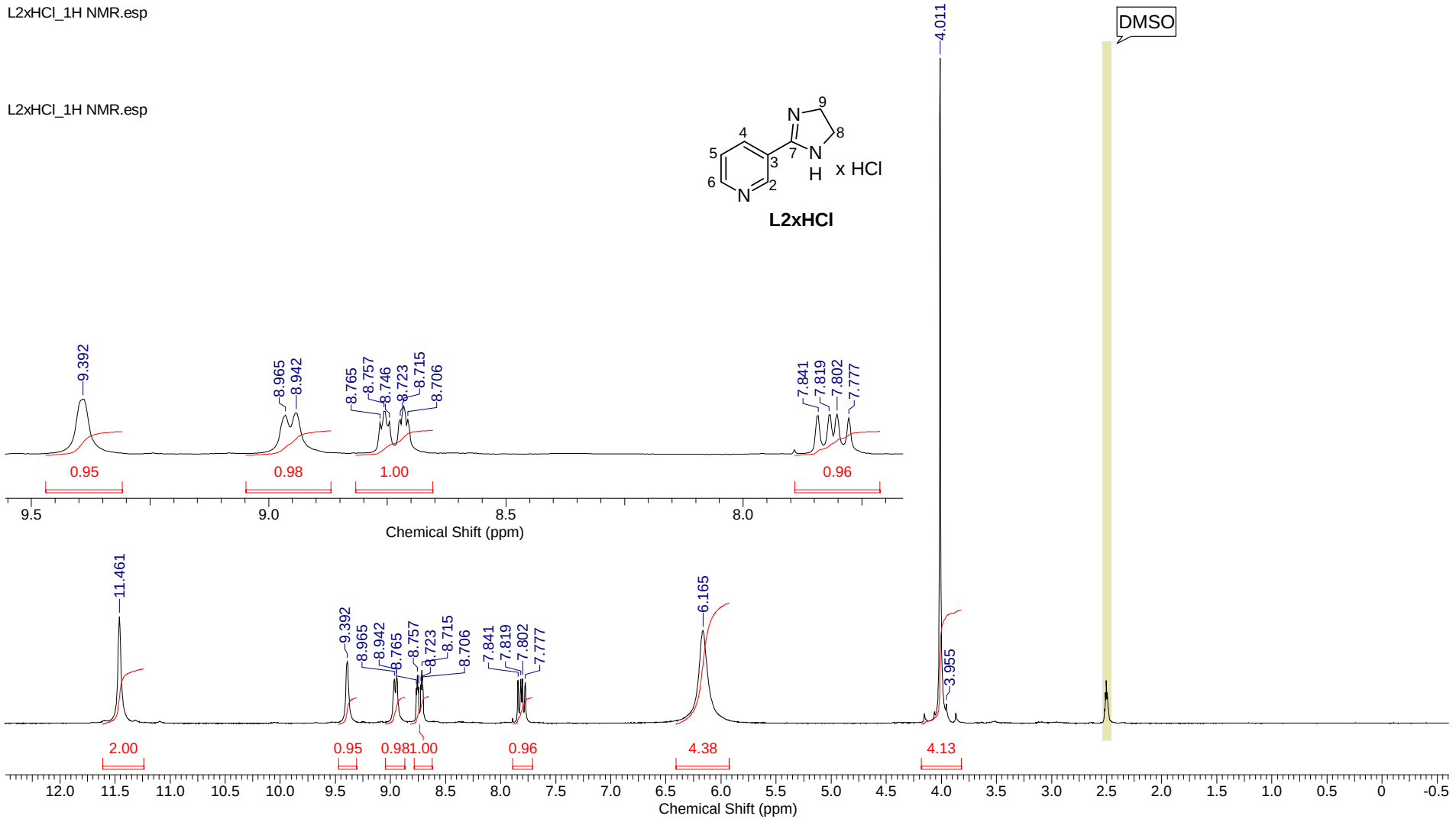


Figure S12: $^{13}C\{^{1}H\}$ NMR (50 MHz, DMSO-d_6) spectrum of ligand L2xHCl

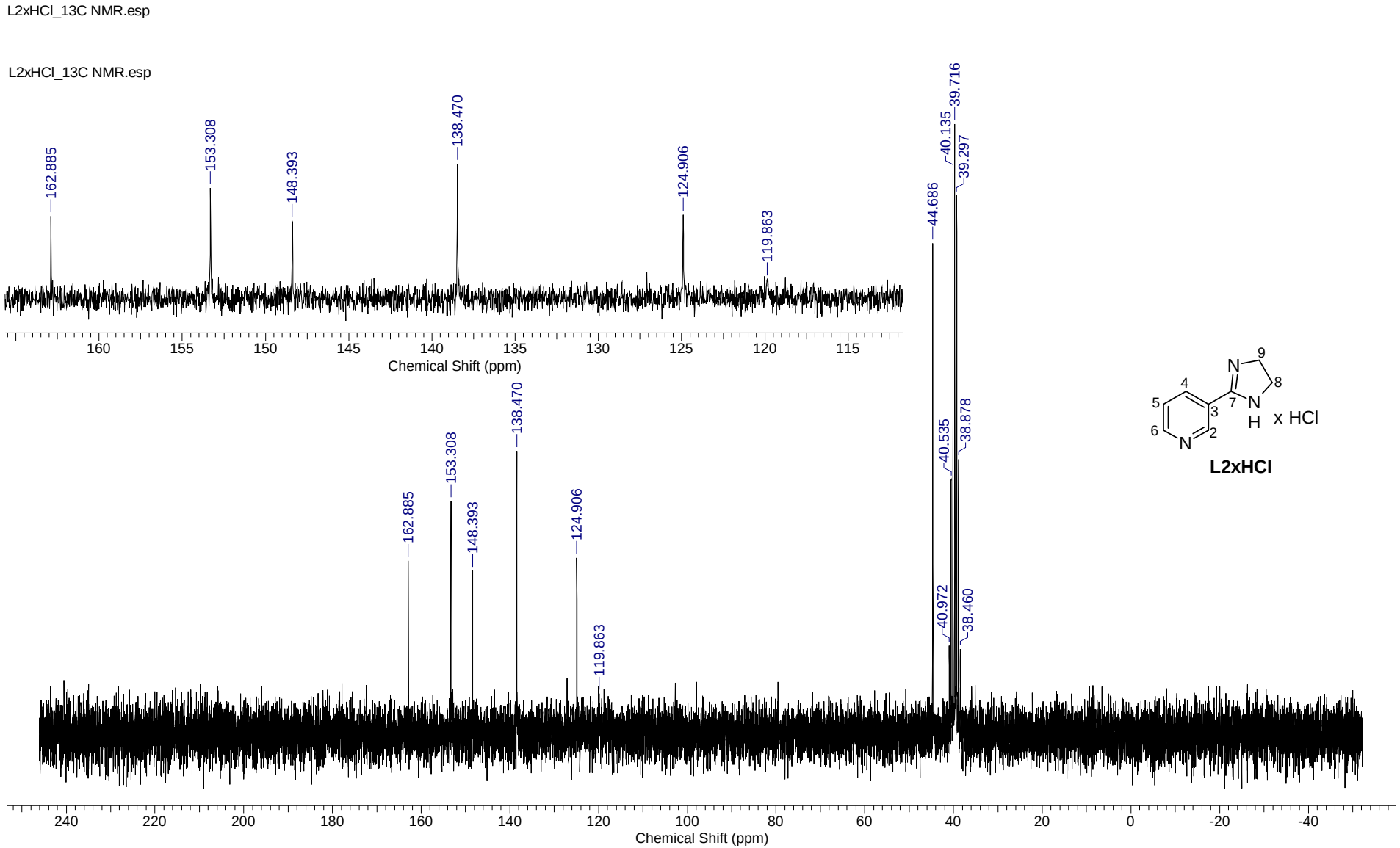


Figure S13: ^{1}H NMR (200 MHz, DMSO-d_6) spectrum of complex C2

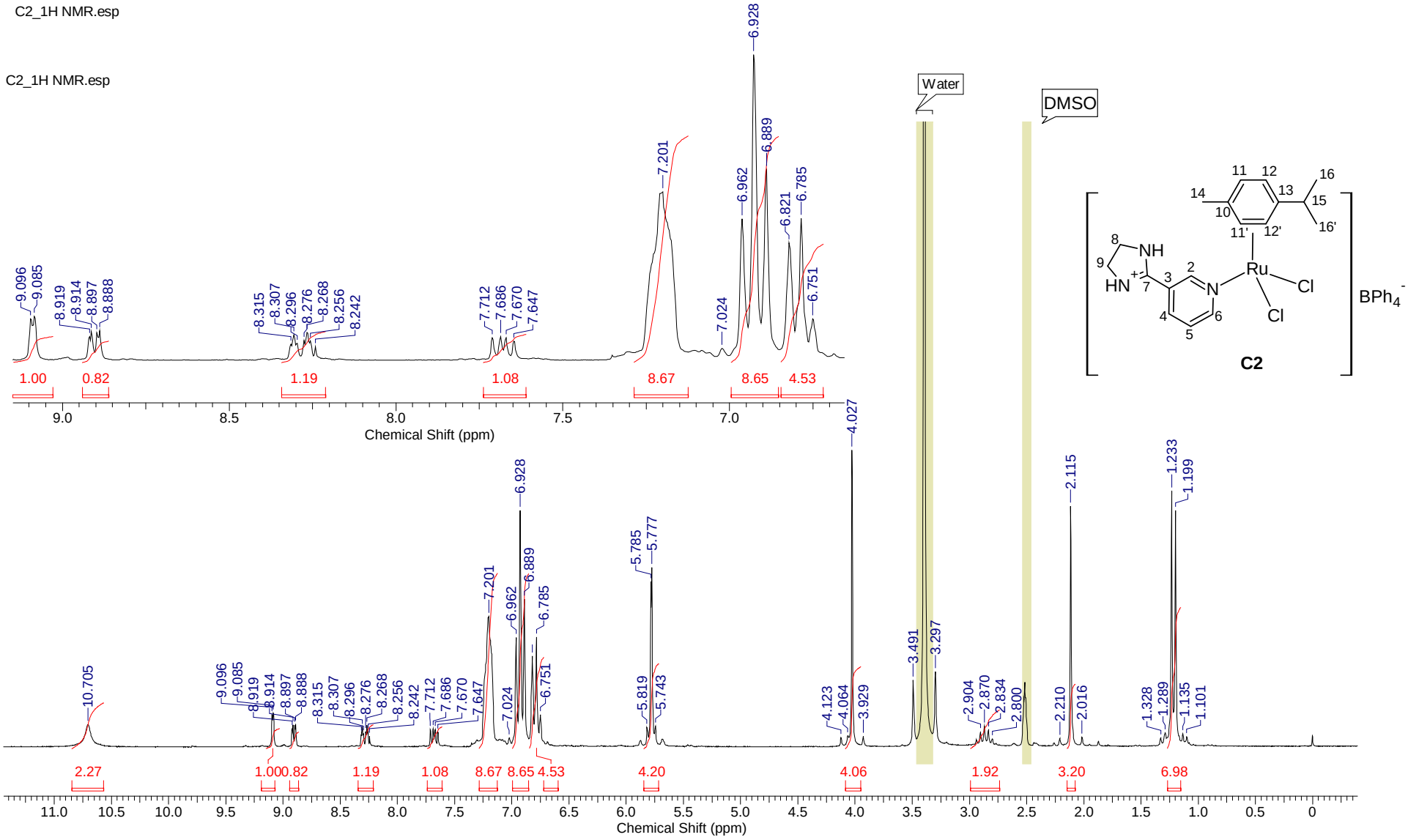


Figure S14: $^{13}C\{^{1}H\}$ NMR (50 MHz, DMSO-d_6) spectrum of ligand C2

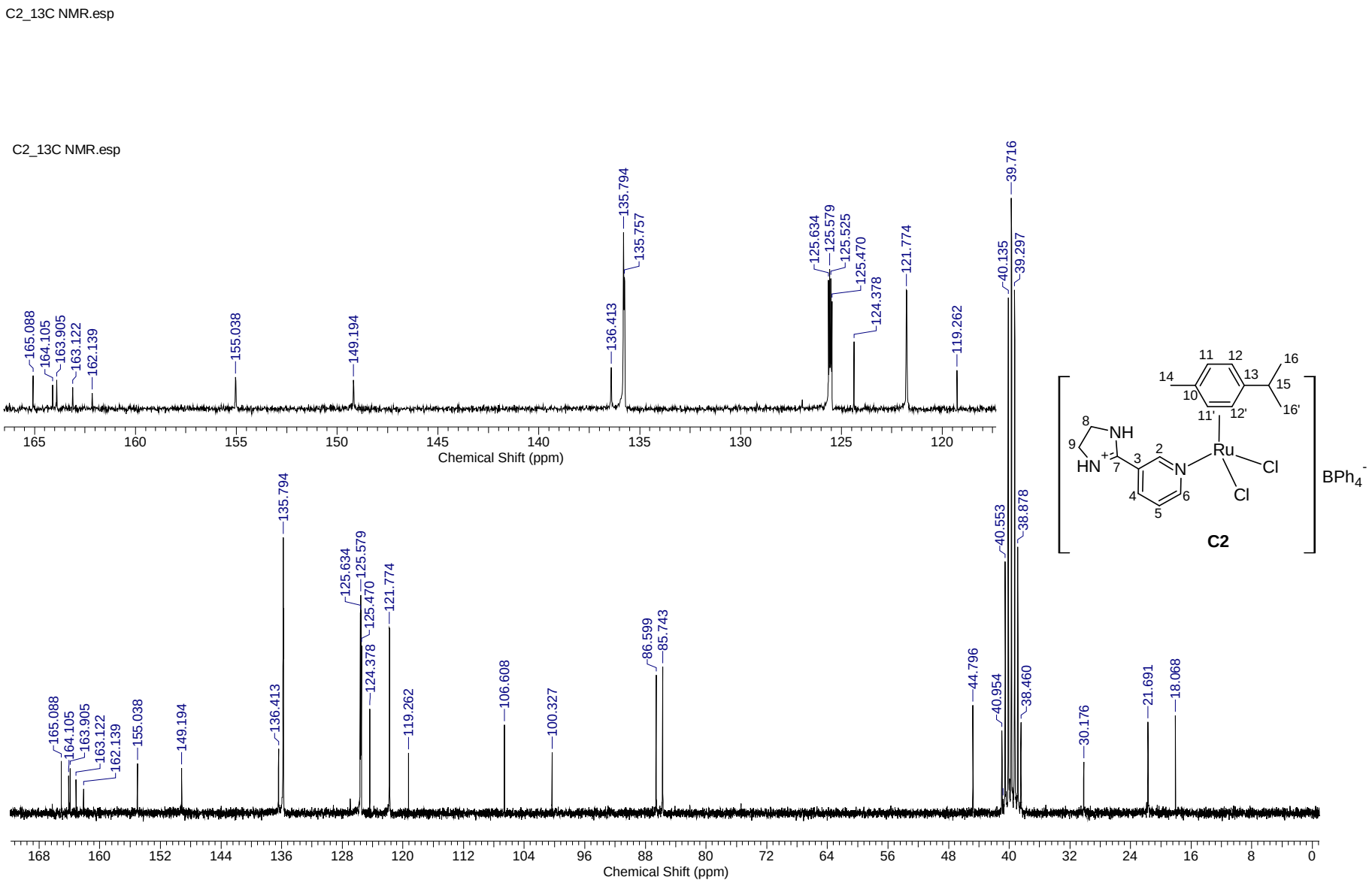


Figure S15: ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of ligand L2 (as base)

δ_H 9.29 (1H, d, $^{3}J_{(H2, H4)}$ = 1.7 Hz, H2), 8.77 (1H, d, $^{3}J_{(H5, H6)}$ = 4.5 Hz, $^{4}J_{(H4, H6)}$ = 1.5 Hz, H6), 8.57 (1H, dt, $^{3}J_{(H4, H5)}$ = 8.2 Hz, $^{3}J_{(H2, H4)}$ = 1.8 Hz, H4), 7.58 (1H, ddd, $^{3}J_{(H4, H5)}$ = 8.1 Hz, $^{3}J_{(H5, H6)}$ = 4.9 Hz, J = 0.7 Hz, H5), 3.85 (4H, s, H8 and H9).

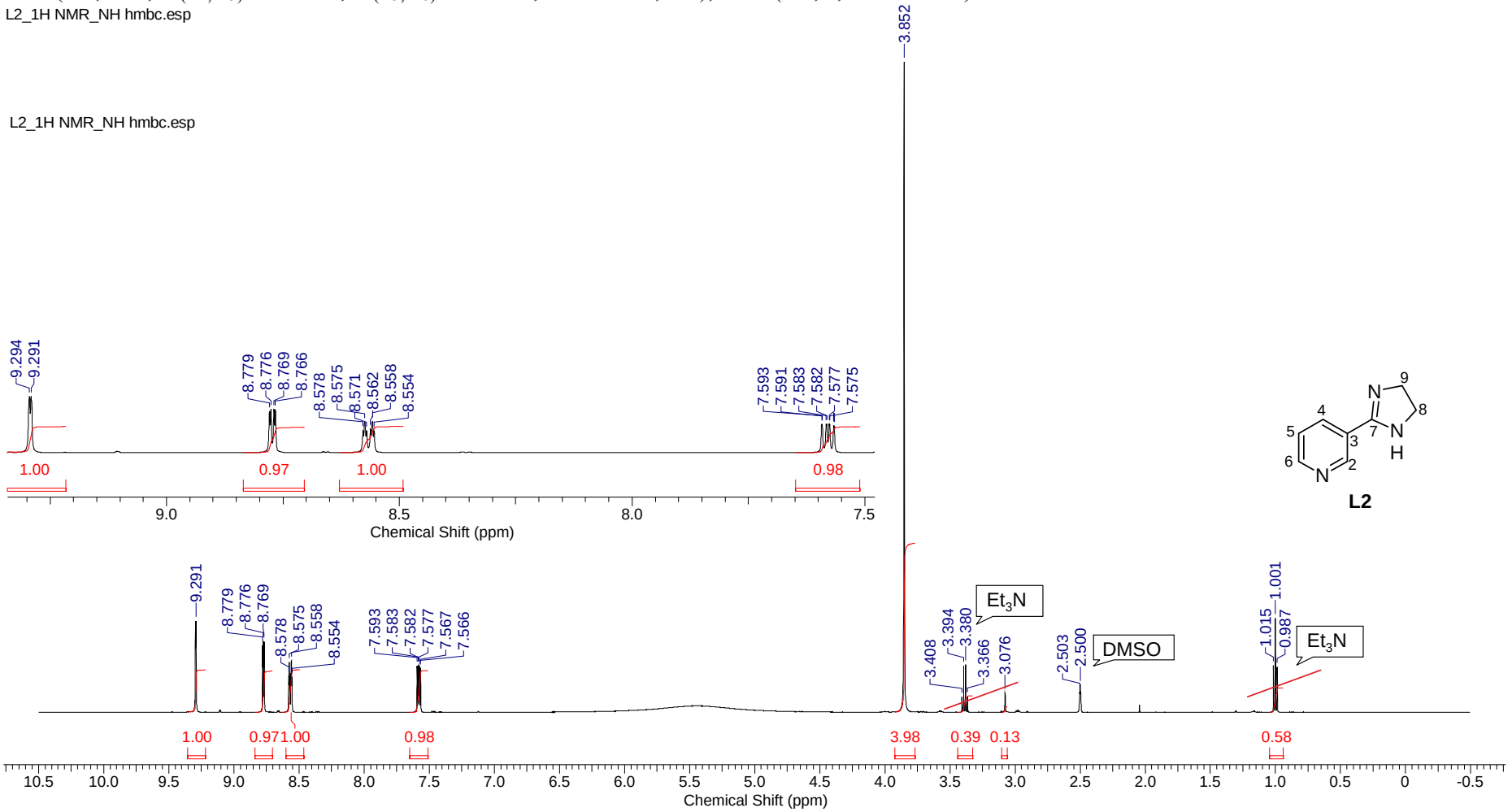


Figure S16: ^{1}H-^{15}N HMBC NMR (500 MHz, DMSO-d_6) spectrum of ligand L2

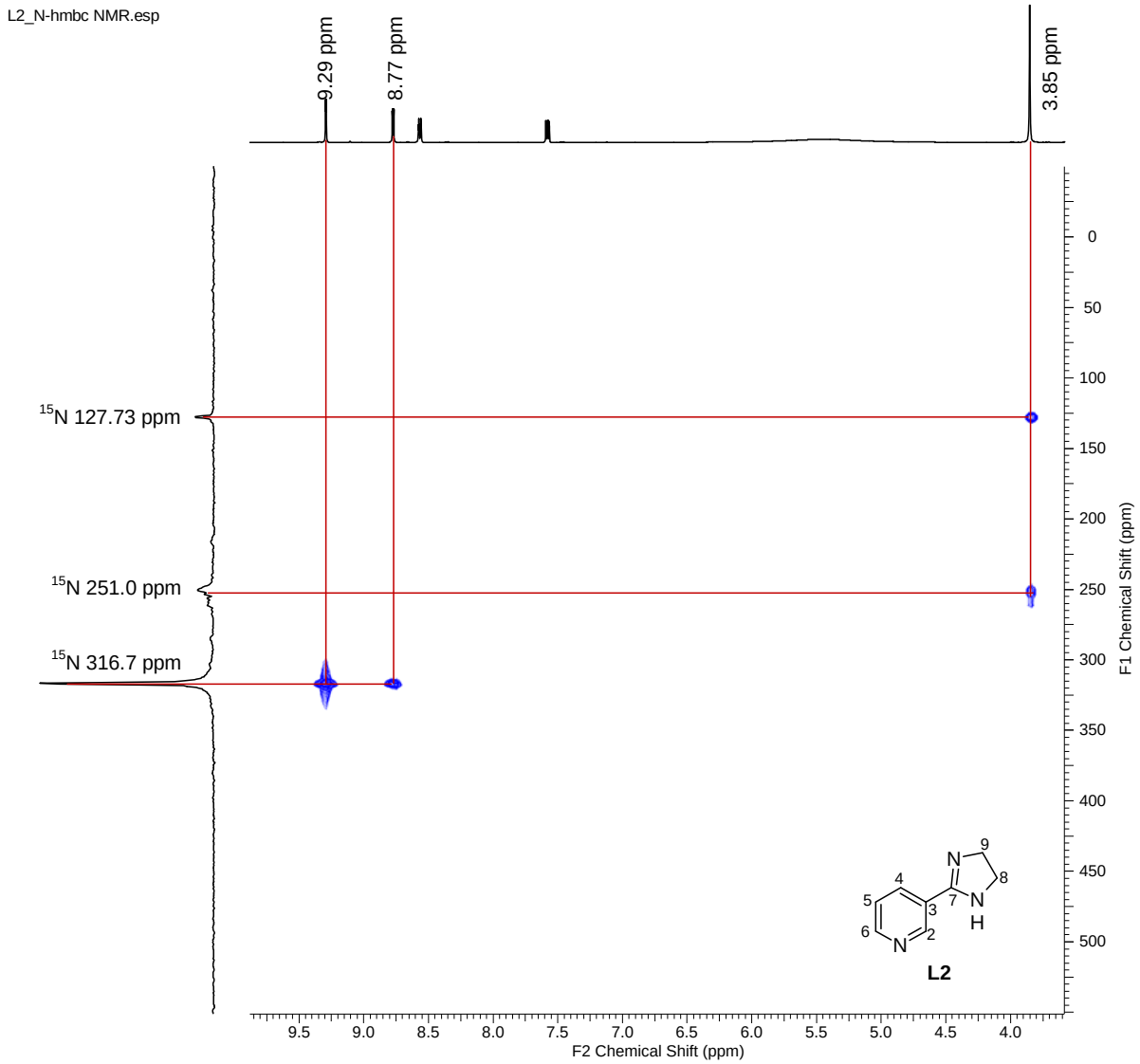


Figure S17: ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of complex C2:
δ_H 9.08 (1H, d, $^{3}J_{(H2, H4)}$ = 1.9 Hz, H2), 8.90 (1H, dd, $^{3}J_{(H5, H6)}$ = 4.8 Hz, $^{3}J_{(H4, H6)}$ = 1.5 Hz, H6), 8.29 (1H, dt, $^{3}J_{(H4, H5)}$ = 8.0 Hz, $^{3}J_{(H2, H4)}$ = 2.0 Hz, H4), 7.70 (1H, ddd, $^{3}J_{(H4, H5)}$ = 8.8 Hz, $^{3}J_{(H5, H6)}$ = 4.8 Hz, J = 0.7 Hz, H5), 7.21-7.15 (8H, m, H2-BPh_4), 6.92 (8H, t, $^{3}J_{(H2', H3', H4')}$ = 7.4 Hz, H3-BPh_4), 6.82-6.76 (4H, m, H4-BPh_4), 5.84-5.75 (4H, m, H11, H11", H12 and H12'), 4.0 (4H, s, H8 and H9), 2.88-2.78 (1H, m, H15), 2.09 (3H, s, H14), 1.19 (6H, d, $^{3}J_{(H15, H16)}$ = 7.0 Hz, H16 and H16').

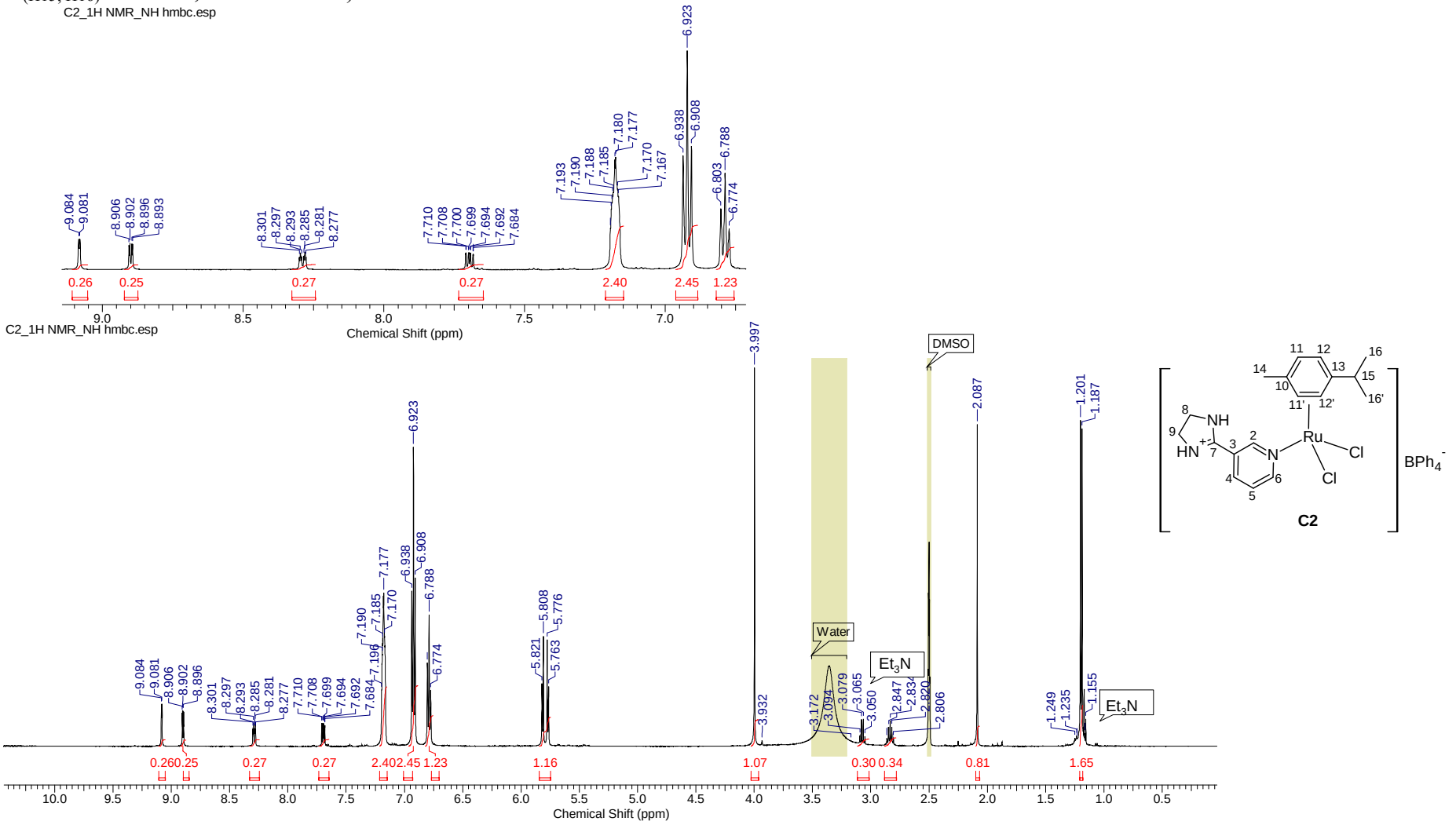


Figure S18: ^{1}H-^{15}N HMBC NMR (500 MHz, DMSO-d_6) spectrum of complex C2 (selected part of spectrum)

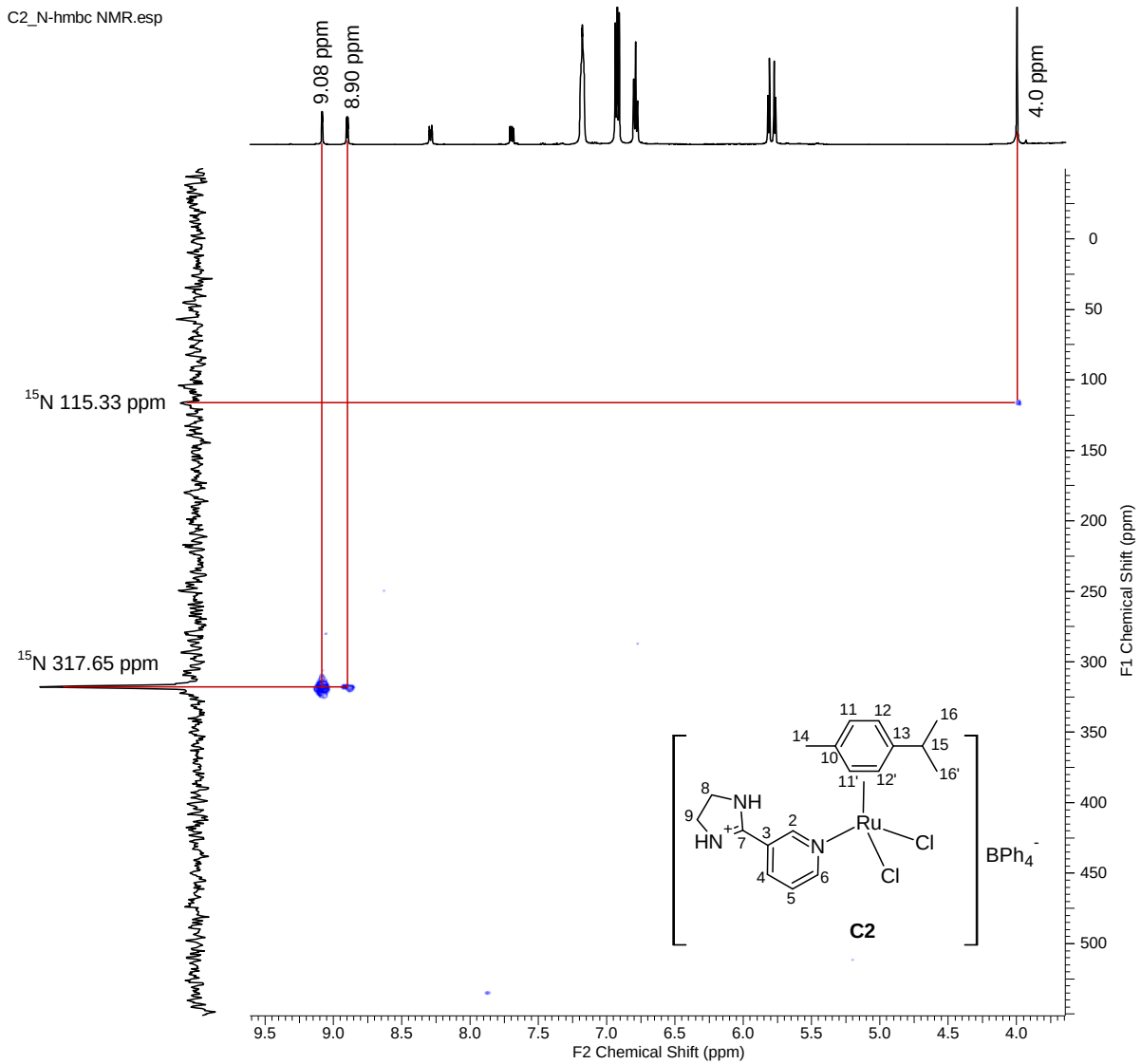
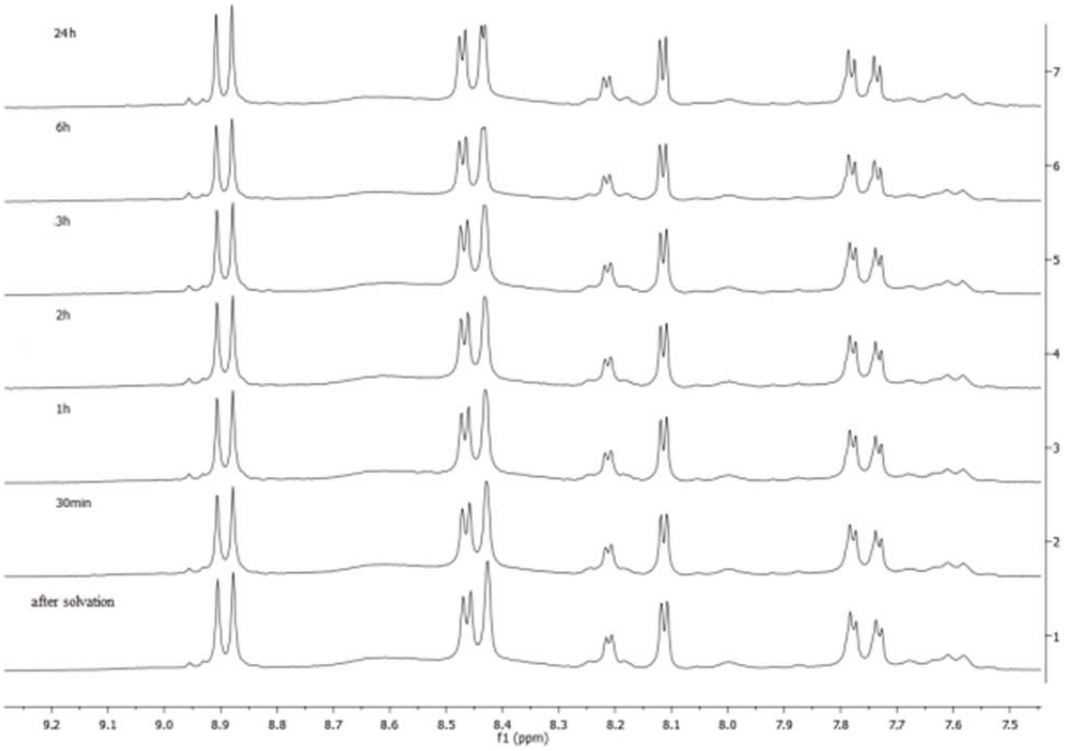


Figure S19. Stability of complex C1 in 24h period; ^{1}H NMR spectra were recorded in DMSO-d_6: a) ligand region; b) *p*-cymene region.

a)



b)

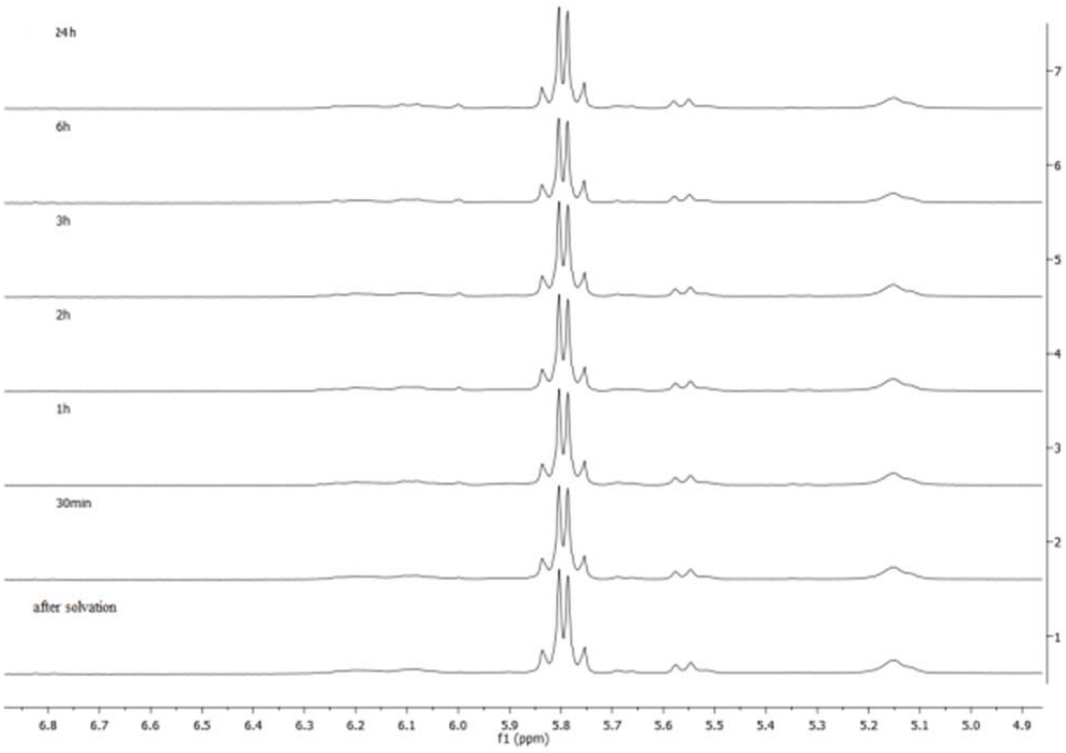
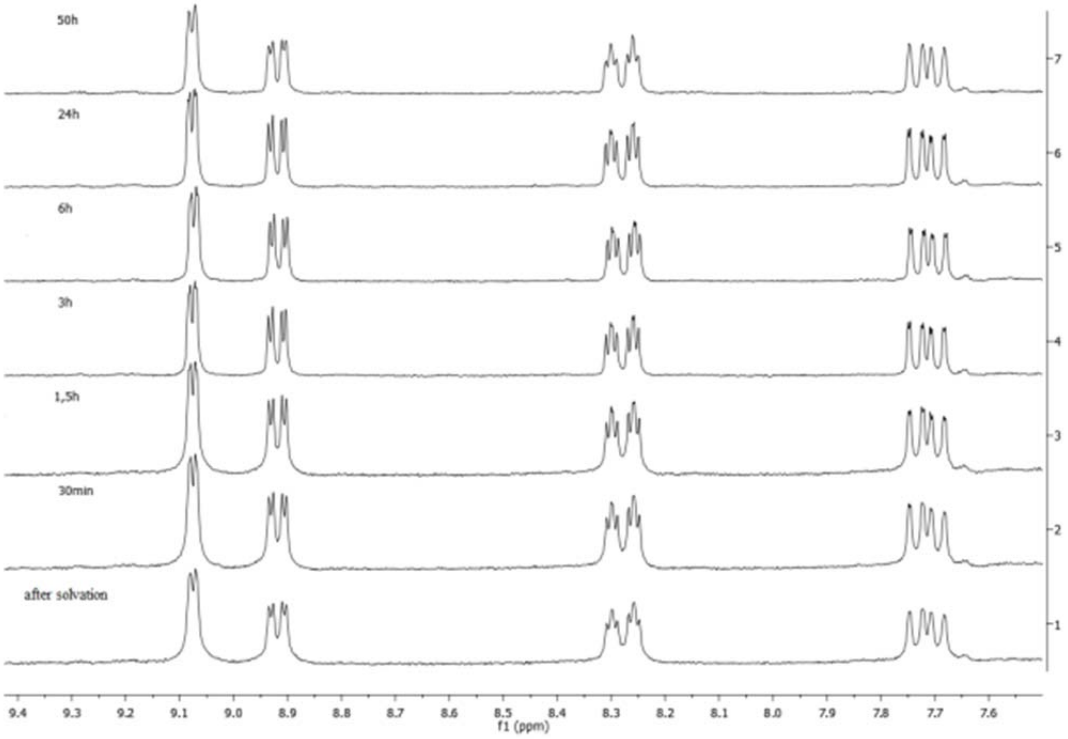


Figure S20. Stability of complex C2 in 24 h period; ^{1}H NMR spectra were recorded in DMSO-d_6: a) ligand region; b) *p*-cymene region.

a)



b)

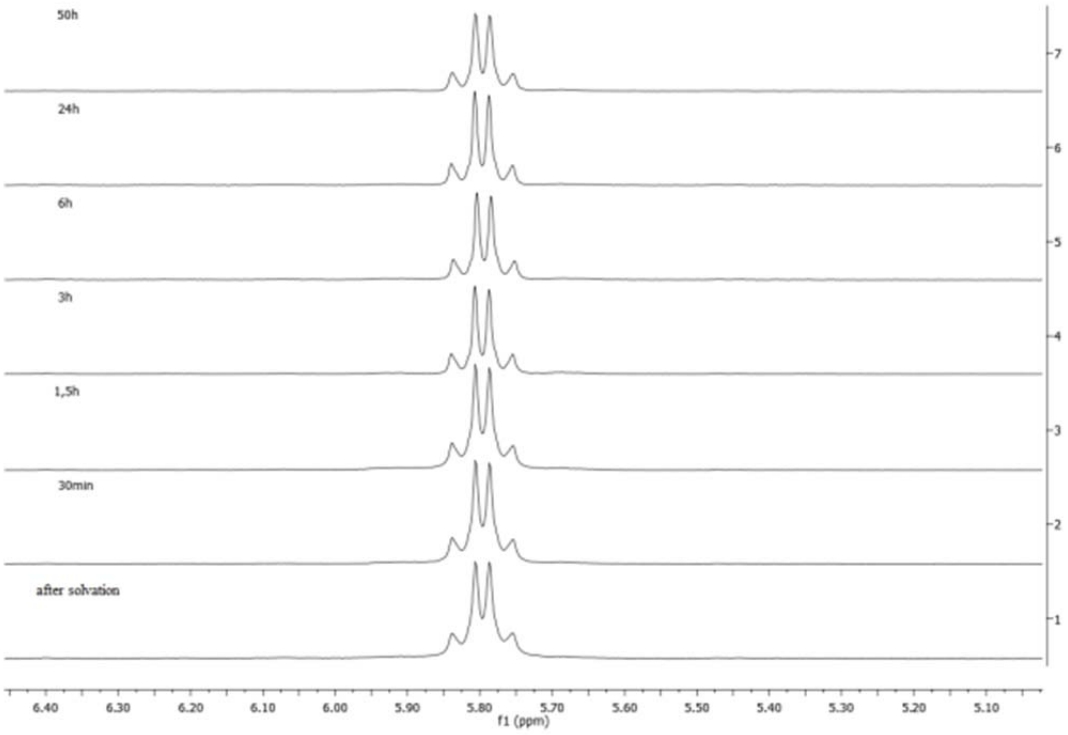


Figure S21. Comparison of ^{1}H NMR spectrum of complex C1 after 24 h period and ^{1}H NMR spectrum of free ligand L1. Spectra were recorded in DMSO-d_6.

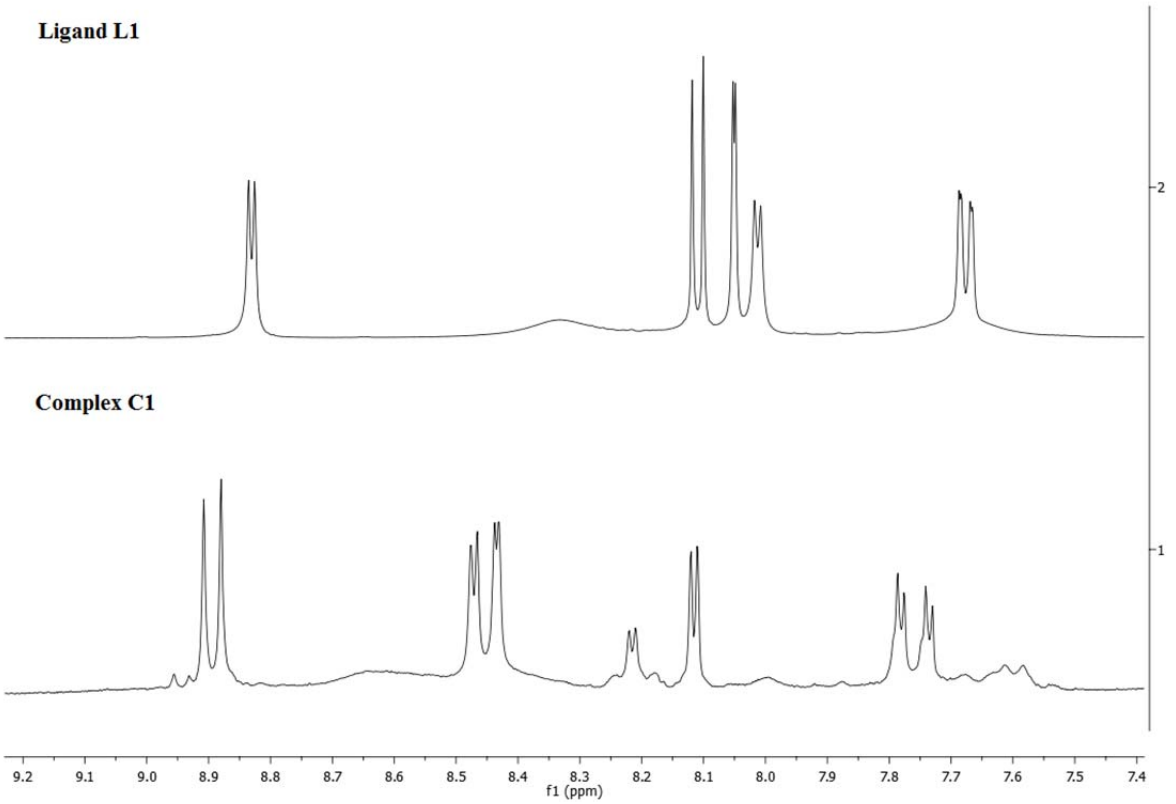


Figure S22. Comparison of ^{1}H NMR spectrum of complex C2 after 24 h period and ^{1}H NMR spectrum of free ligand L2. Spectra were recorded in DMSO-d_6.

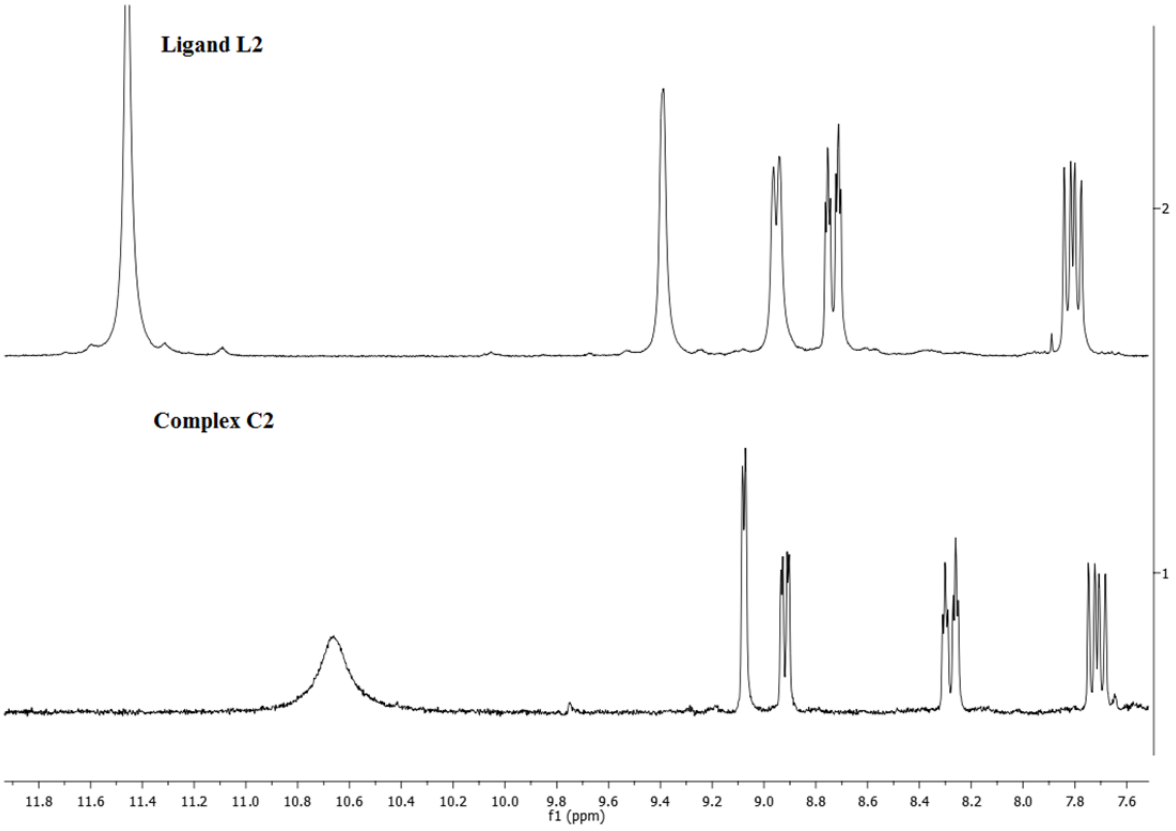


Figure S23. Comparison of ^{1}H NMR spectrum of complex C1 after 24 h period and ^{1}H NMR spectrum of complex [Ru(cymene)Cl$_2$DMSO]. Spectra were recorded in DMSO-d_6.

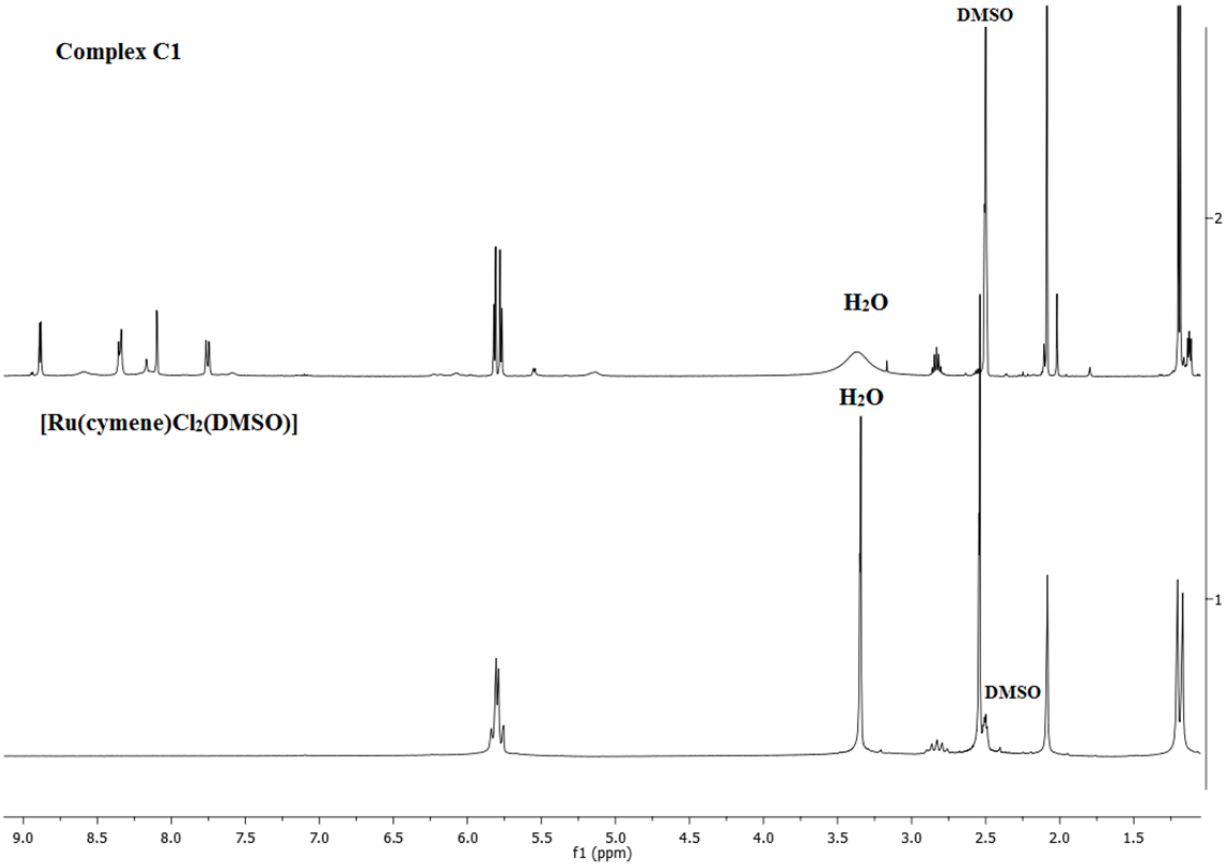


Figure S24. Comparison of ^{1}H NMR spectrum of complex C2 after 24 h period and ^{1}H NMR spectrum of complex [Ru(cymene)Cl$_2$DMSO]. Spectra were recorded in dmso-d_6.

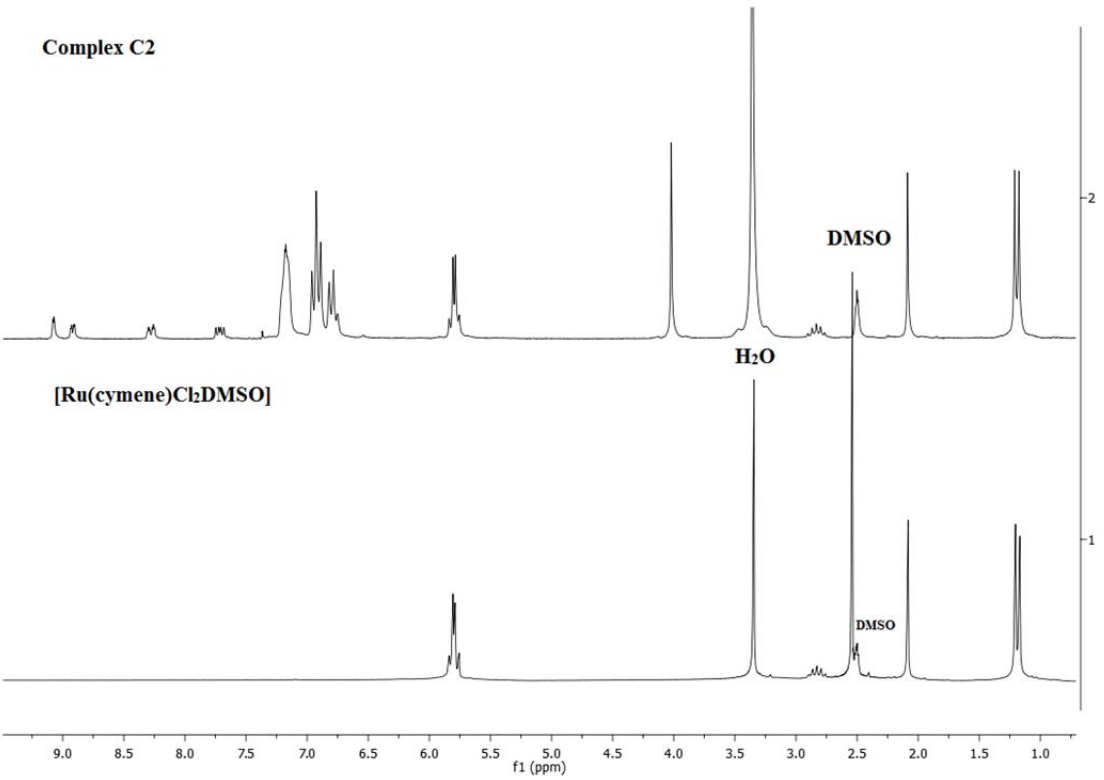


Figure S25: Cell survival after 72h treatment of A549 cell line with ligands L1, L2, complexes C1, C2 and CDDP.

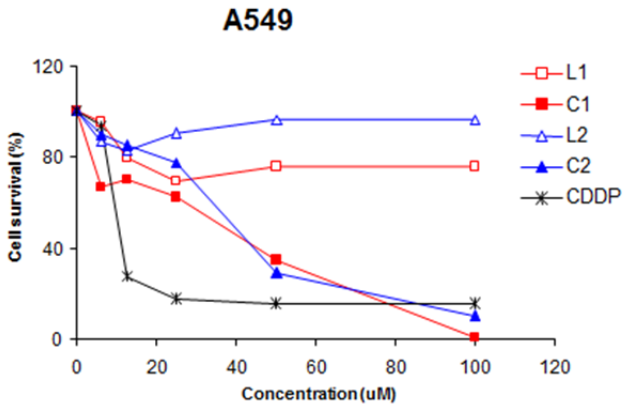


Figure S26:Cell survival after 72h treatment of HeLa cell line with ligands L1, L2, complexes C1, C2 and CDDP

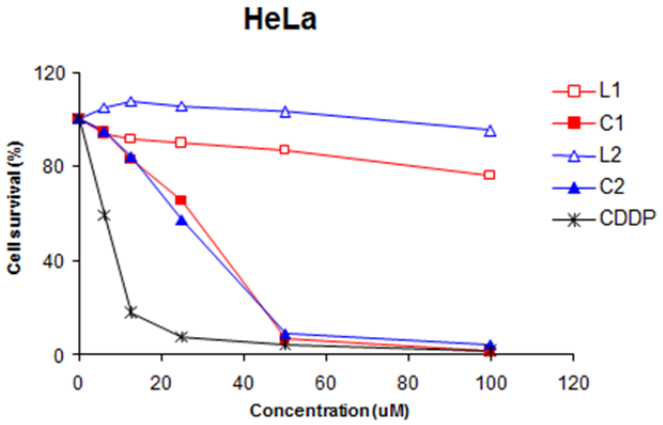


Figure S27: Cell survival after 72h treatment of MDA-MB-231 cell line with ligands L1, L2, complexes C1, C2 and CDDP