Catalytic oxygenation of sp^3 "C-H" bonds with Ir(III) complexes of chelating triazoles and mesoionic carbenes

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Supporting Information

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Table S1: Crystallographic details for the molecular structures of complexes **4** - **6**

	4	**5 • $CHCl_3$ • 0.25 H_2O**	**6 • CH_2Cl_2**
Chemical formula	$C_{20}H_{27}N_4Cl_1Ir\ P_1F_6$	$C_{76}H_{116}N_{24}Cl_4Ir_4\ P_4F_{24}\ O\ C_4H_4Cl_{12}$	$C_{20}H_{31}N_6Cl_1Ir\ P_1F_6\ CH_2Cl_2$
M_r	696.08	3349.88	813.05
Crystal system	monoclinic	monoclinic	triclinic
Space group	P2(1)/n	C2/c	P-1
a (Å)	9.121(5)	37.887(5)	7.681(1)
b (Å)	28.247(5)	8.061(5)	12.408(2)
c (Å)	9.246(5)	20.793(5)	16.186(3)
α (°)	90	90	78.662(4)
β (°)	93.306(5)	111.380(5)	85.451(4)
γ (°)	90	90	72.021(4)
V (Å^3)	2378(2)	5913(4)	1438.4(5)
Z	4	2	2
Densitiy (g cm^{-3})	1.944	1.881	1.877
F(000)	1352	3264	796
Radiation Type	MoK_α	MoK_α	MoK_α
μ (mm^{-1})	5.857	4.993	5.038
Crystal size	0.12 x 0.11 x 0.03	0.12 x 0.11 x 0.07	0.24 x 0.22 x 0.17
Meas. Refl.	16300	15612	10986
Indep. Refl.	4183	5248	6333
Obsvd. [$I > 2\sigma(I)$] refl.	3188	3919	5349
R_{int}	0.0576	0.0430	0.0243
R [$F^2 > 2\sigma(F^2)$], wR(F^2)	0.0399, 0.0890	0.0429, 0.1053	0.0446, 0.1389
S	1.096	1.063	1.159
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.686, -2.333	2.695, -2.381	2.522, -2.593
CCDC	1002759	1010867	1002758

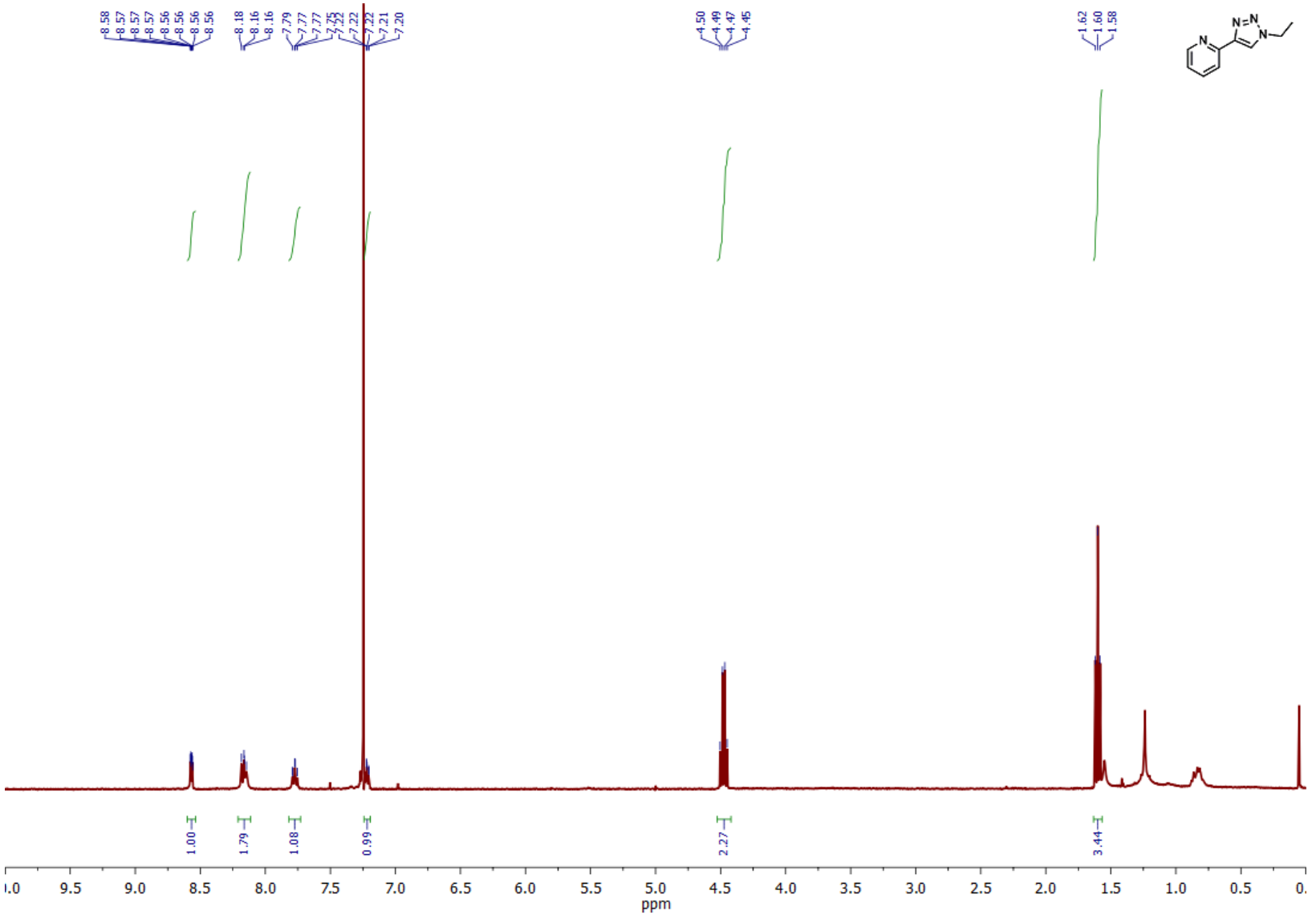

Figure S1: ^{1}H-NMR spectra of L^{2} at 25°C

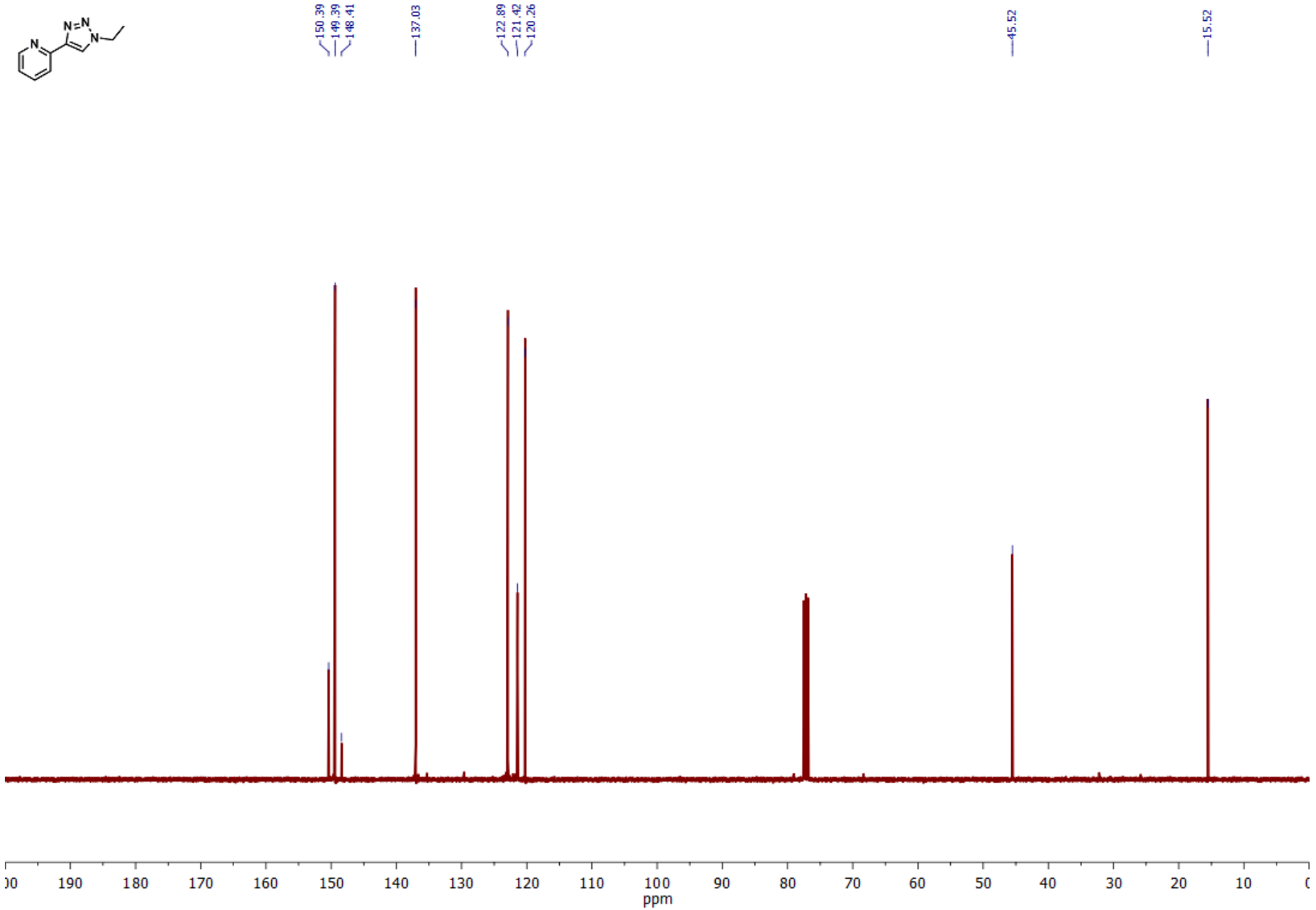

Figure S2: ^{13}C-NMR spectra of L^2 at 25°C

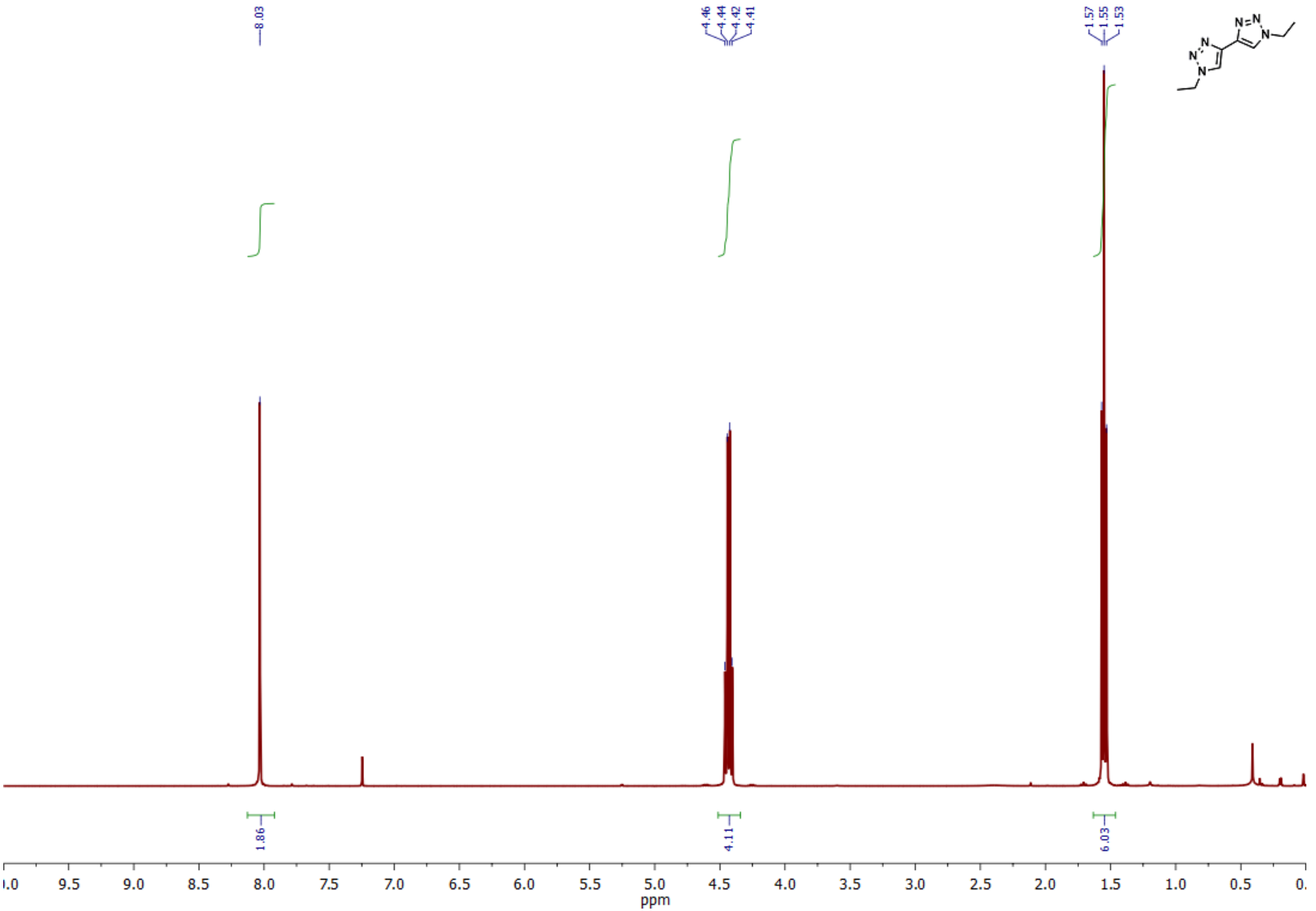

Figure S3: ^{1}H-NMR spectra of L^{3} at 25°C

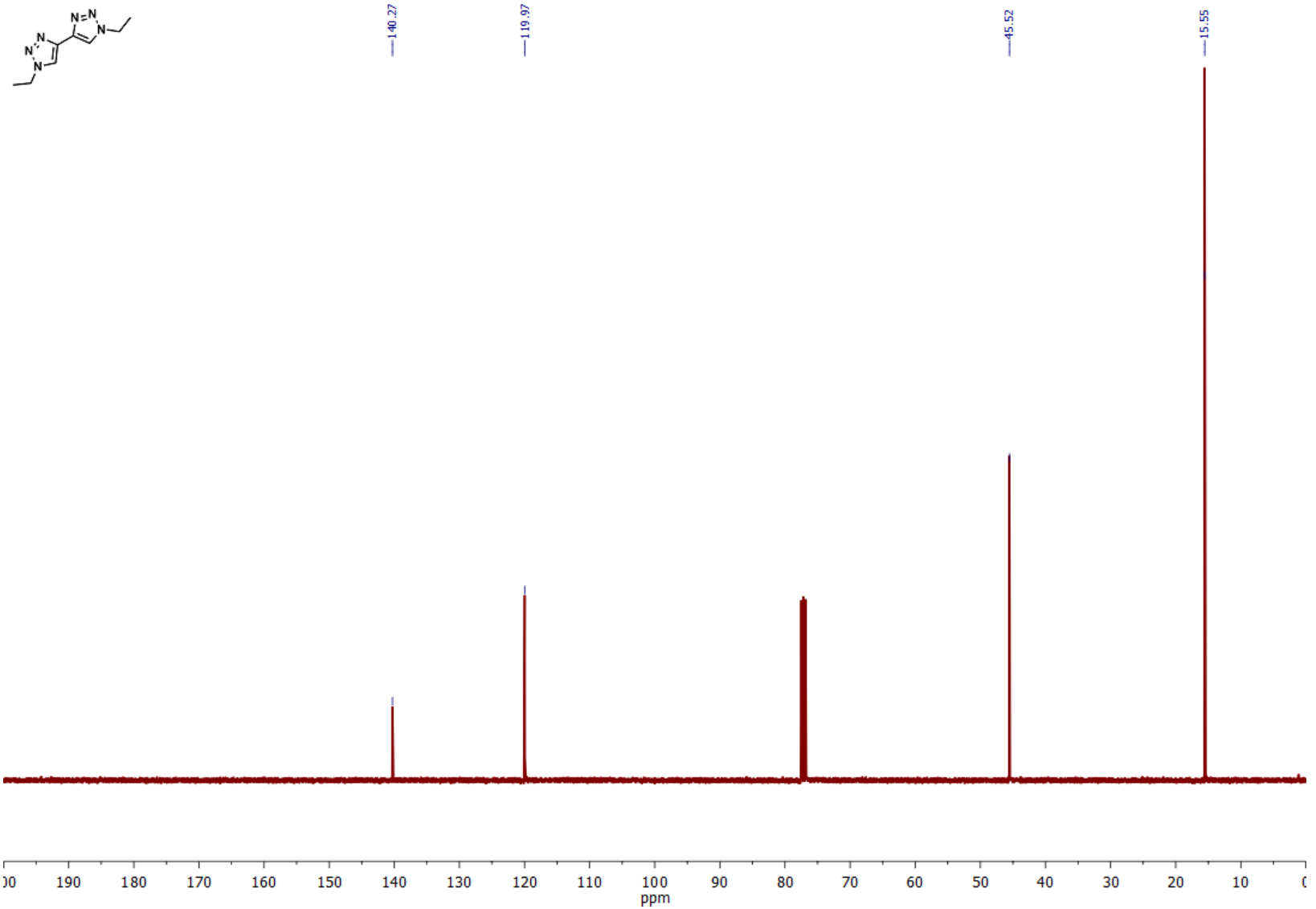

Figure S4: ^{13}C-NMR spectra of L^3 at 25°C

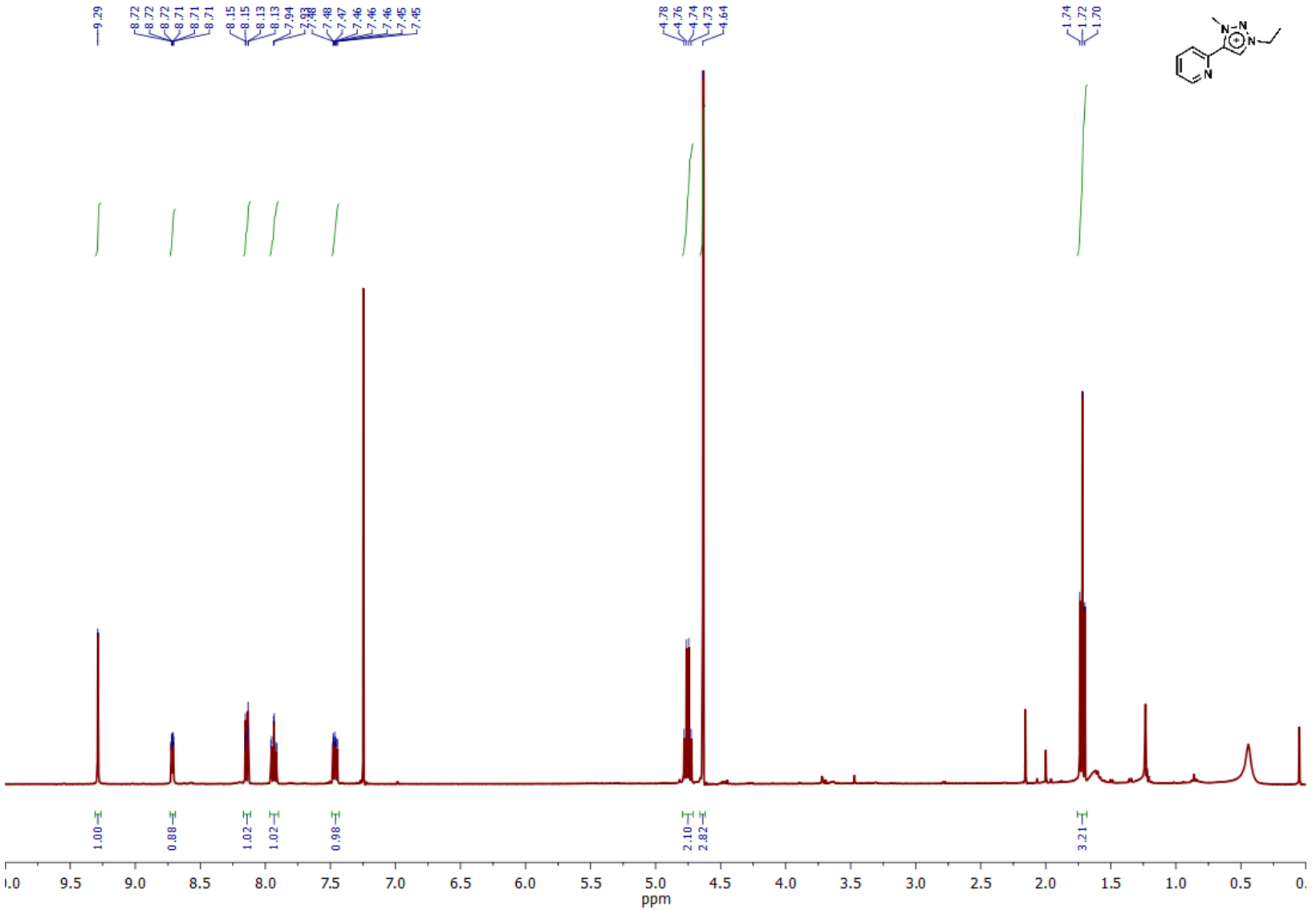

Figure S5: ^{1}H-NMR spectra of $HL^{4}(BF_4)$ at 25°C

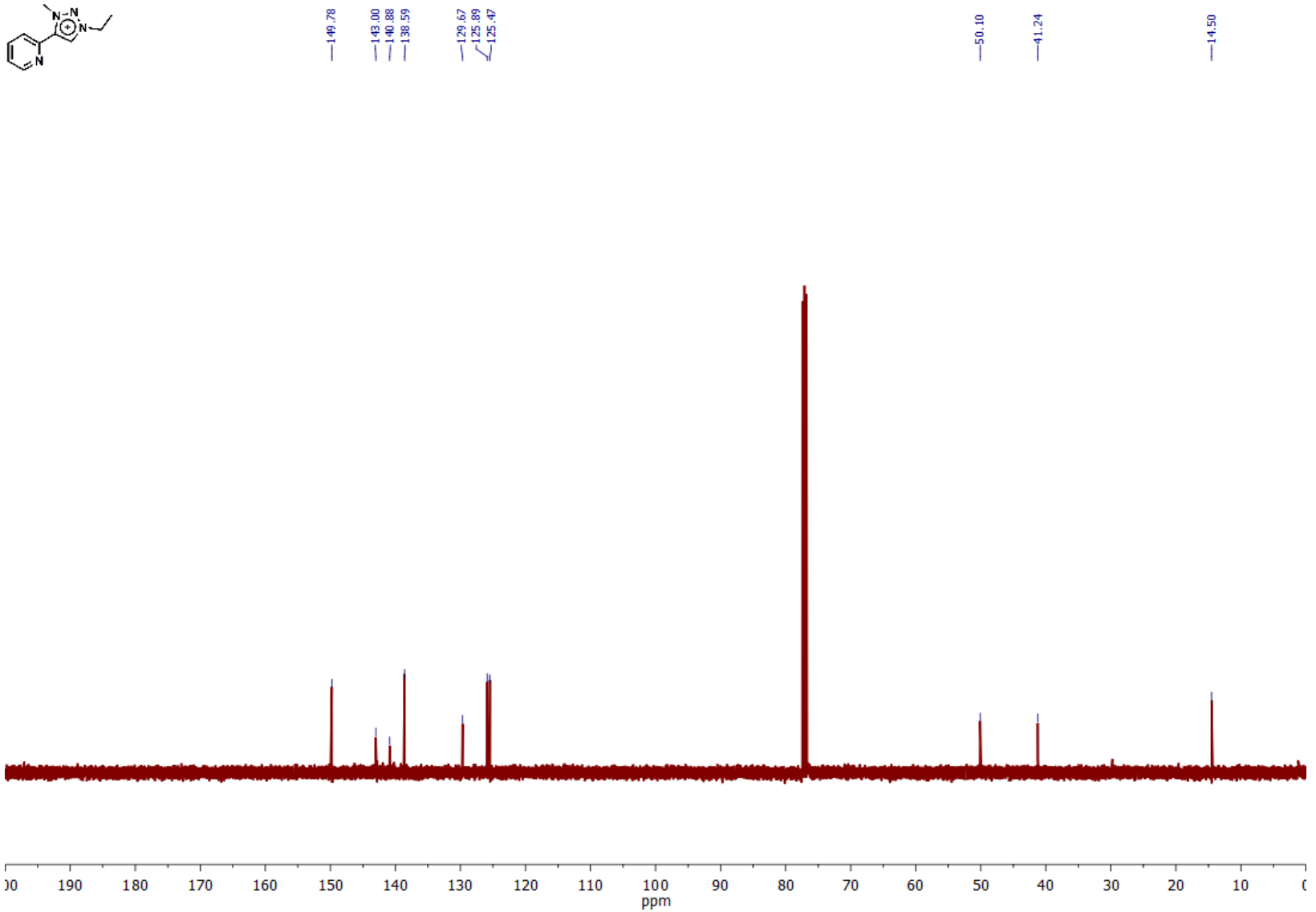

Figure S6: ^{13}C-NMR spectra of $HL^4(BF_4)$ at 25°C

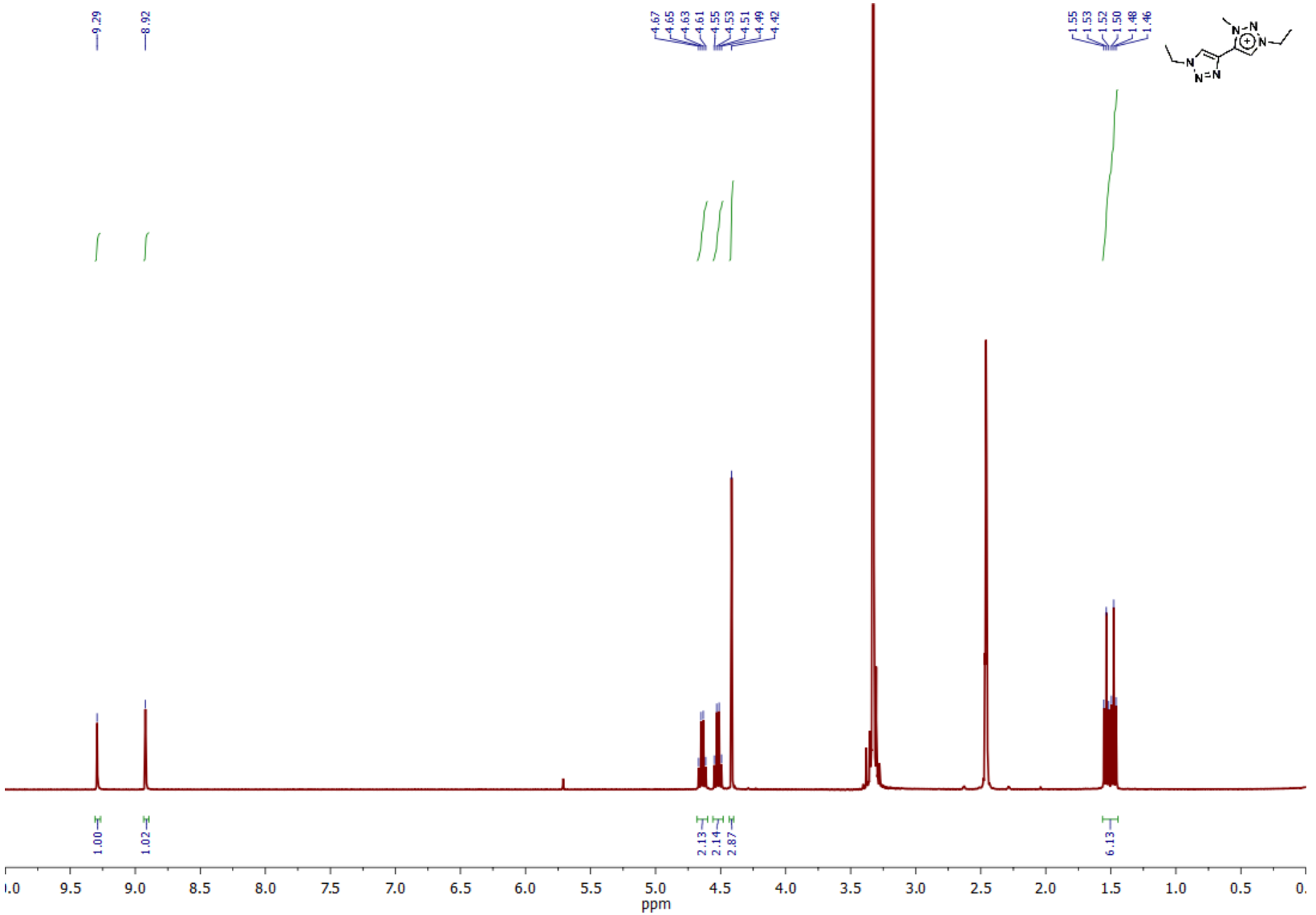

Figure S7: ^{1}H-NMR spectra of $HL^{5}(BF_4)$ at 25°C

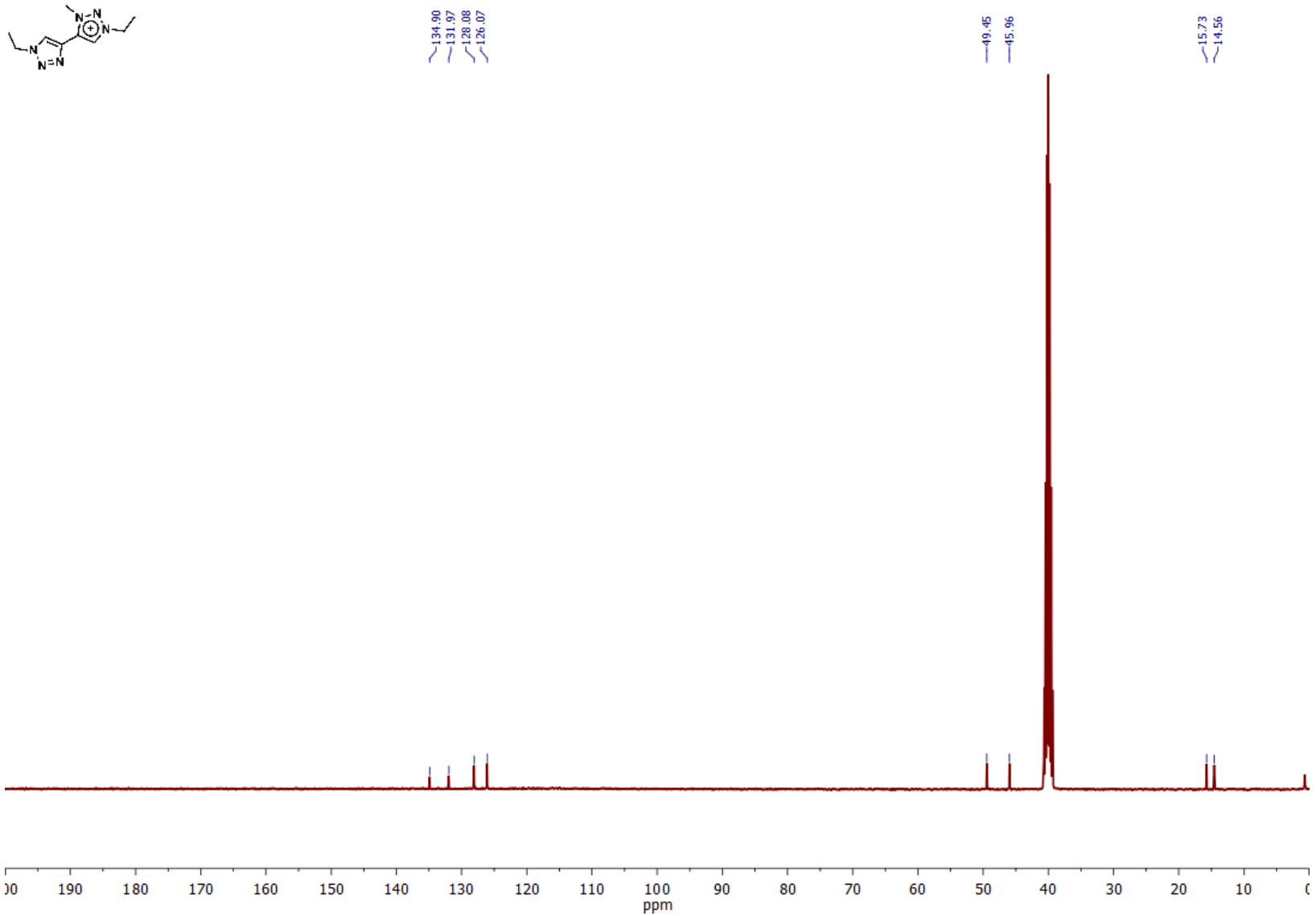

Figure S8: ^{13}C-NMR spectra of $HL^5(BF_4)$ at 25°C

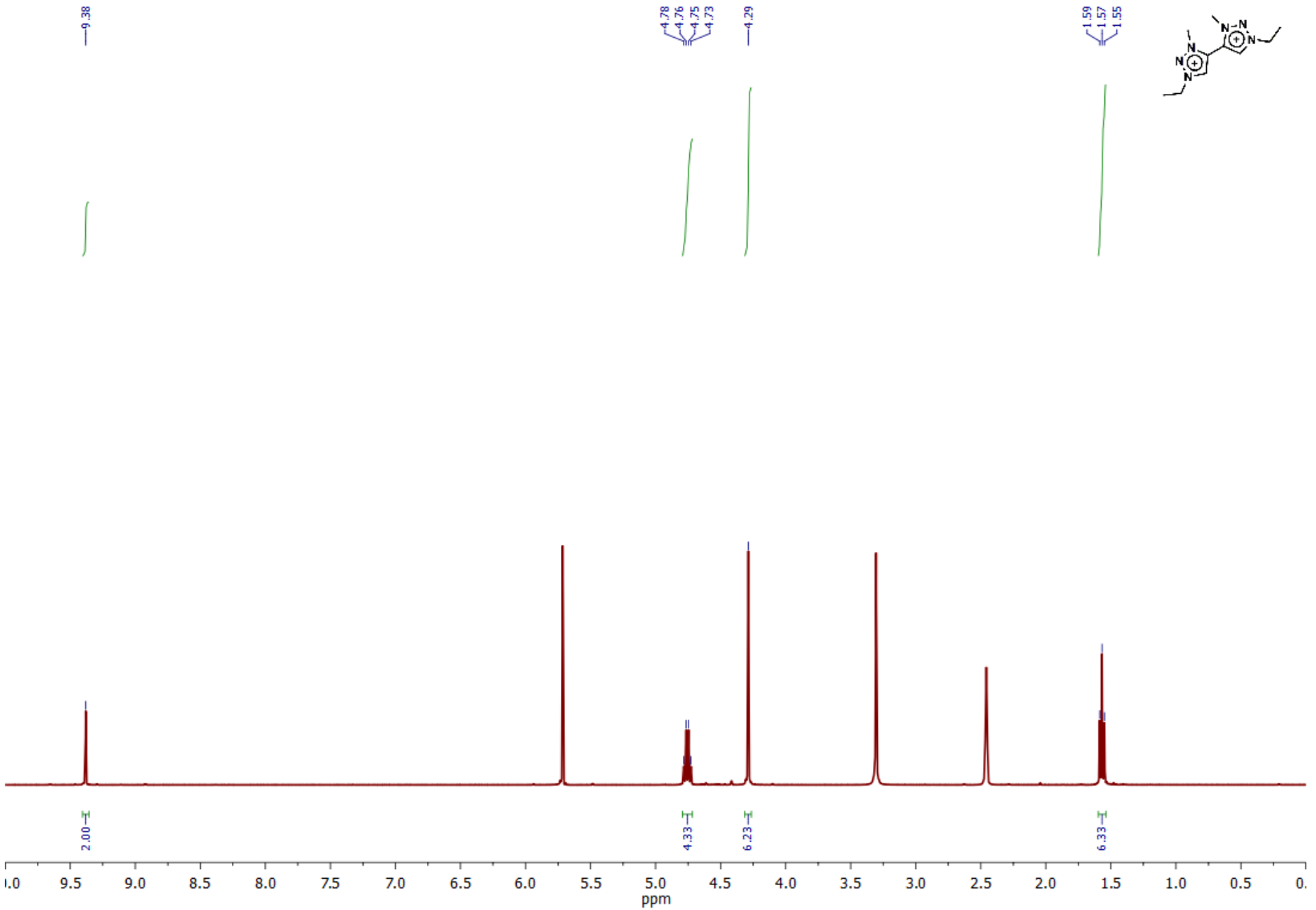

Figure S9: ^{1}H-NMR spectra of $H_2L^6(BF_4)$ at 25°C

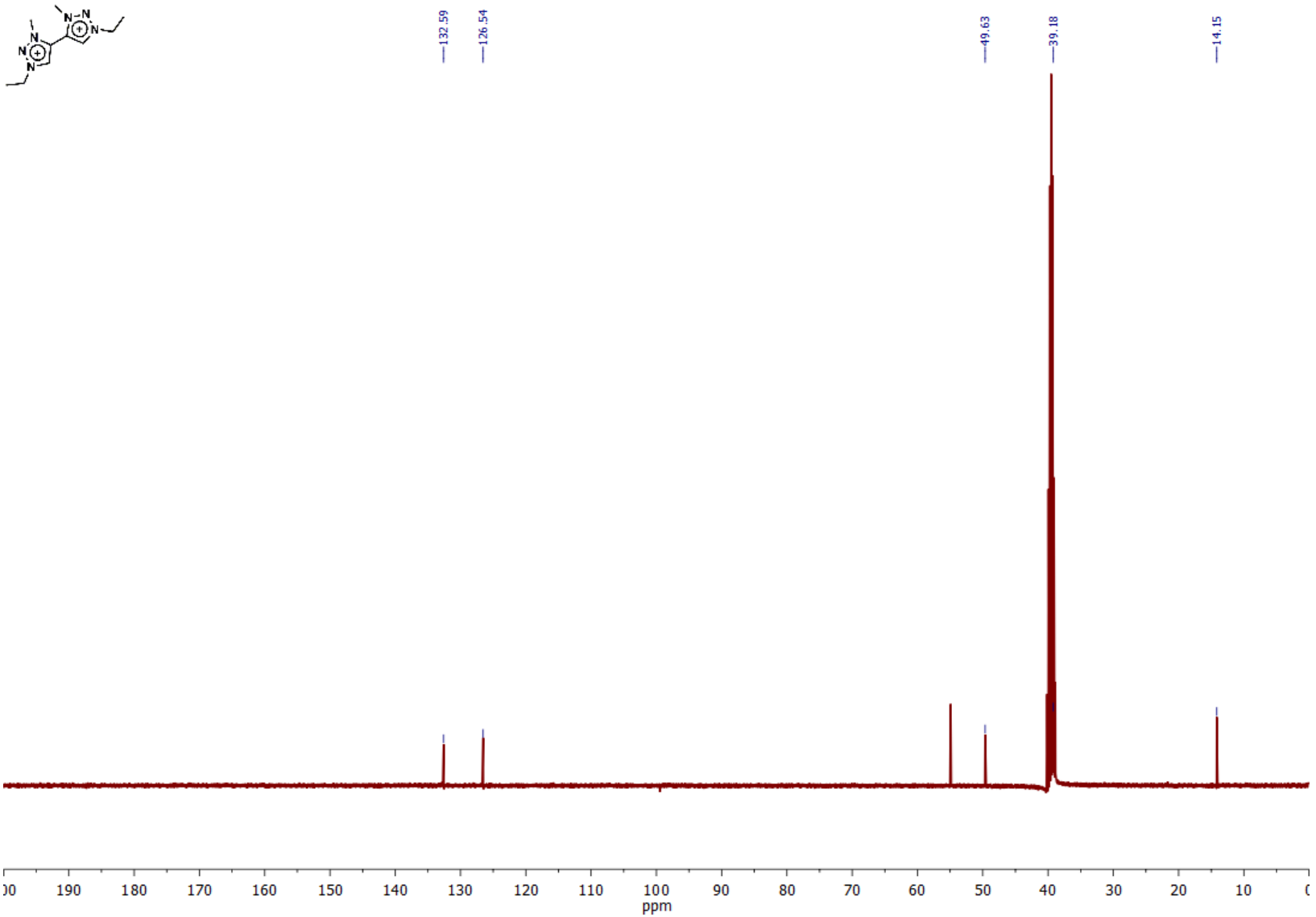

Figure S10: ^{13}C-NMR spectra of $H_2L^6(BF_4)$ at 25°C

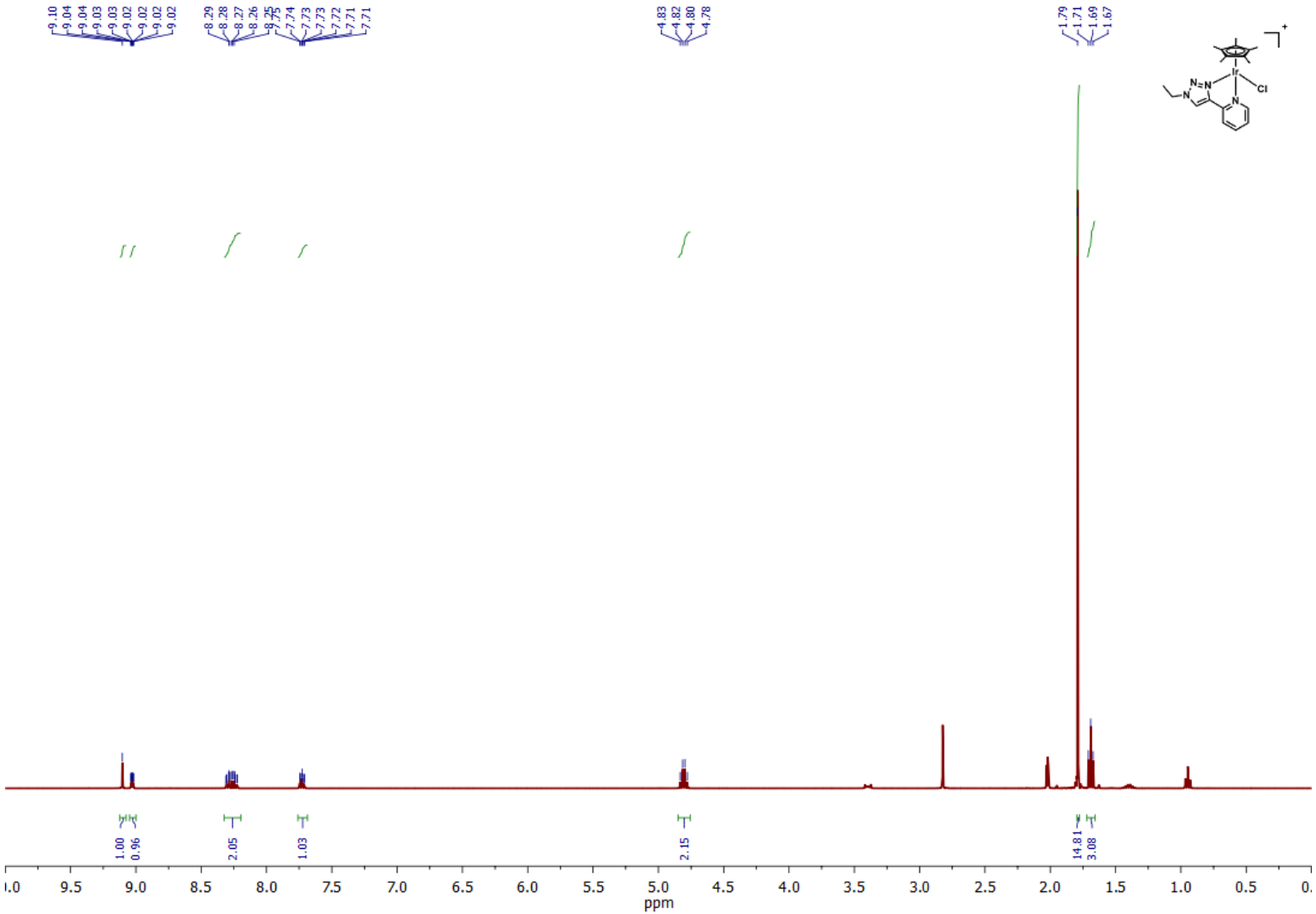

Figure S11: ^{1}H-NMR spectra of 2 at 25°C

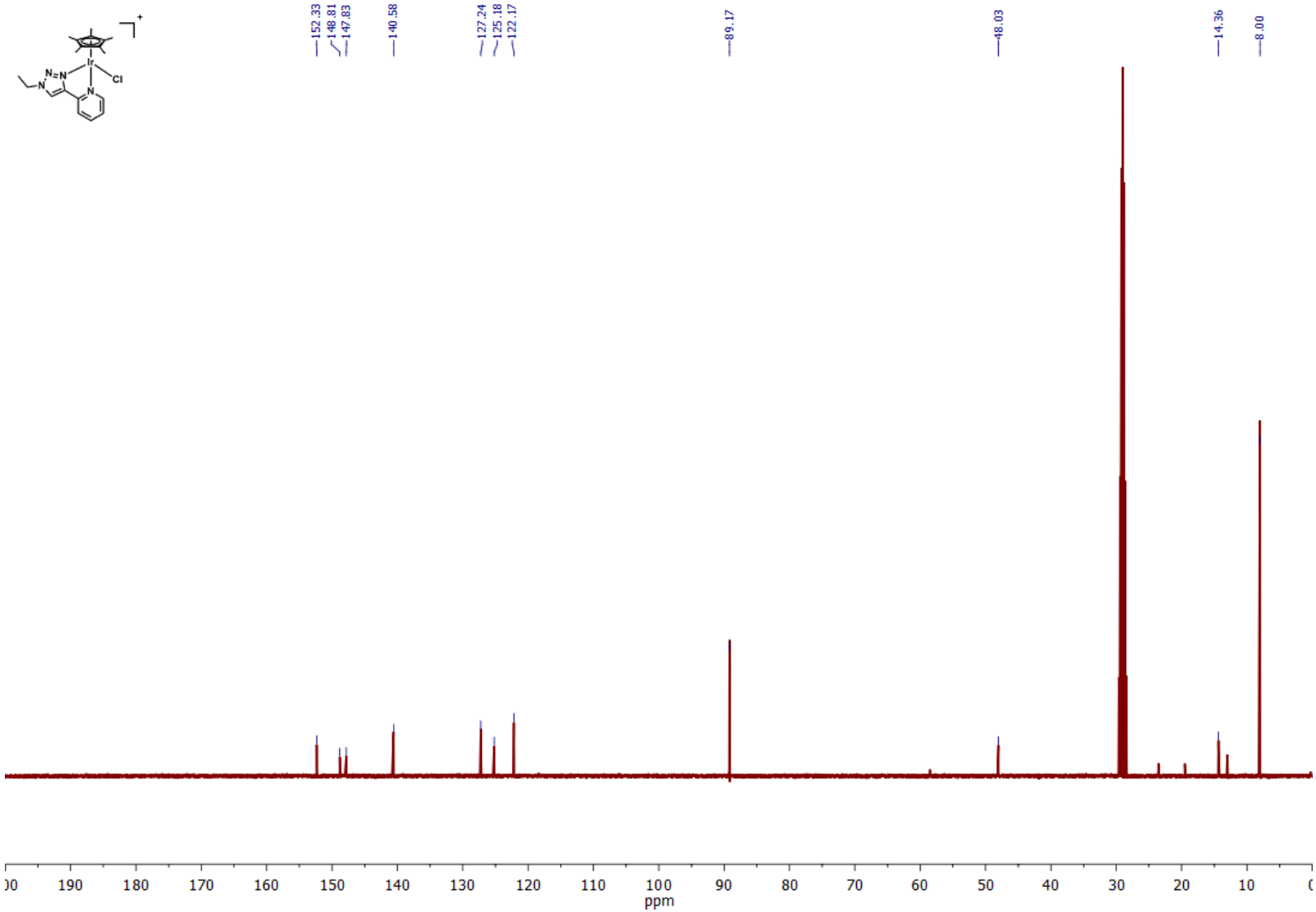

Figure S12: ^{13}C-NMR spectra of 2 at 25°C

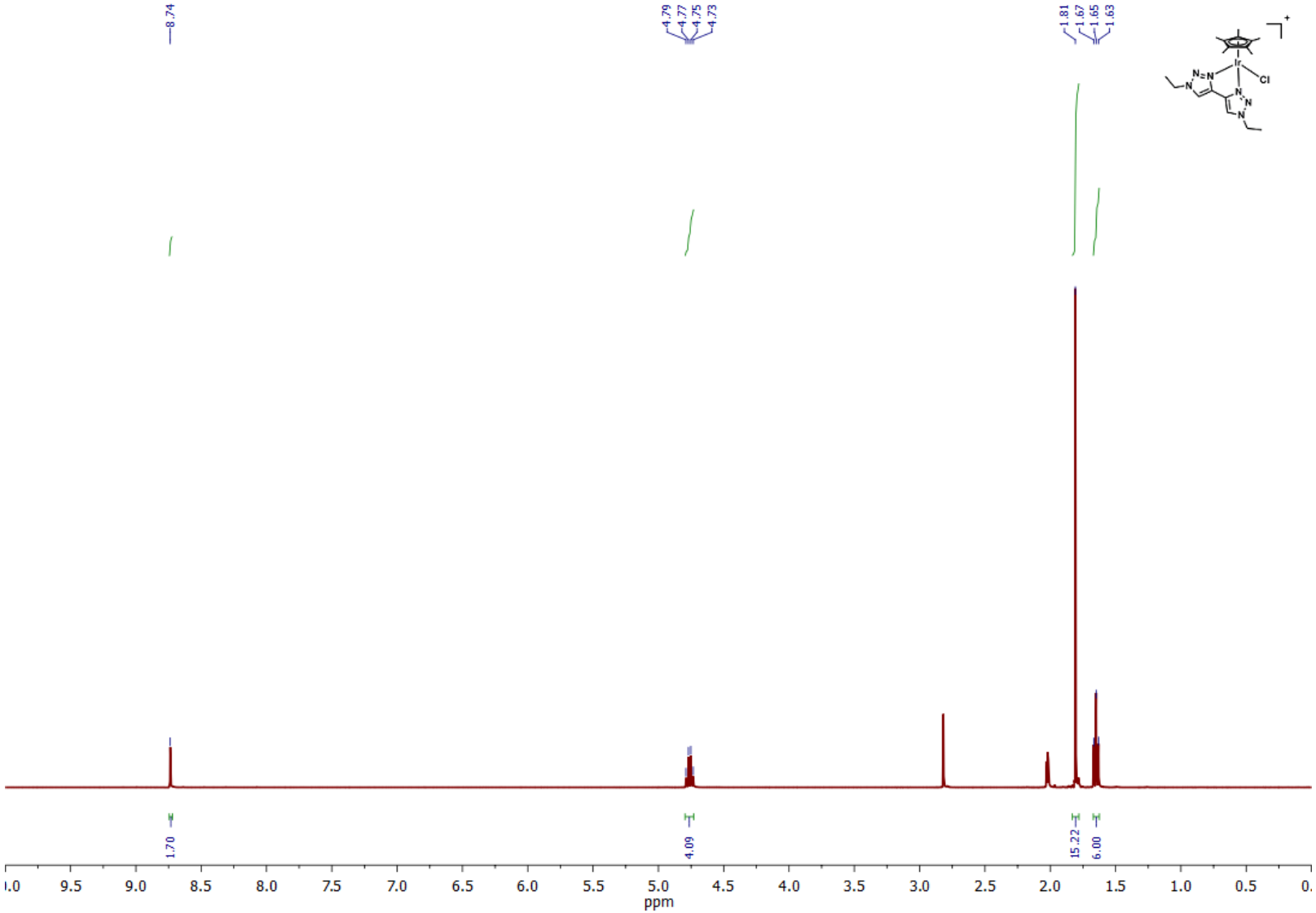

Figure S13: [1]H-NMR spectra of 3 at 25°C

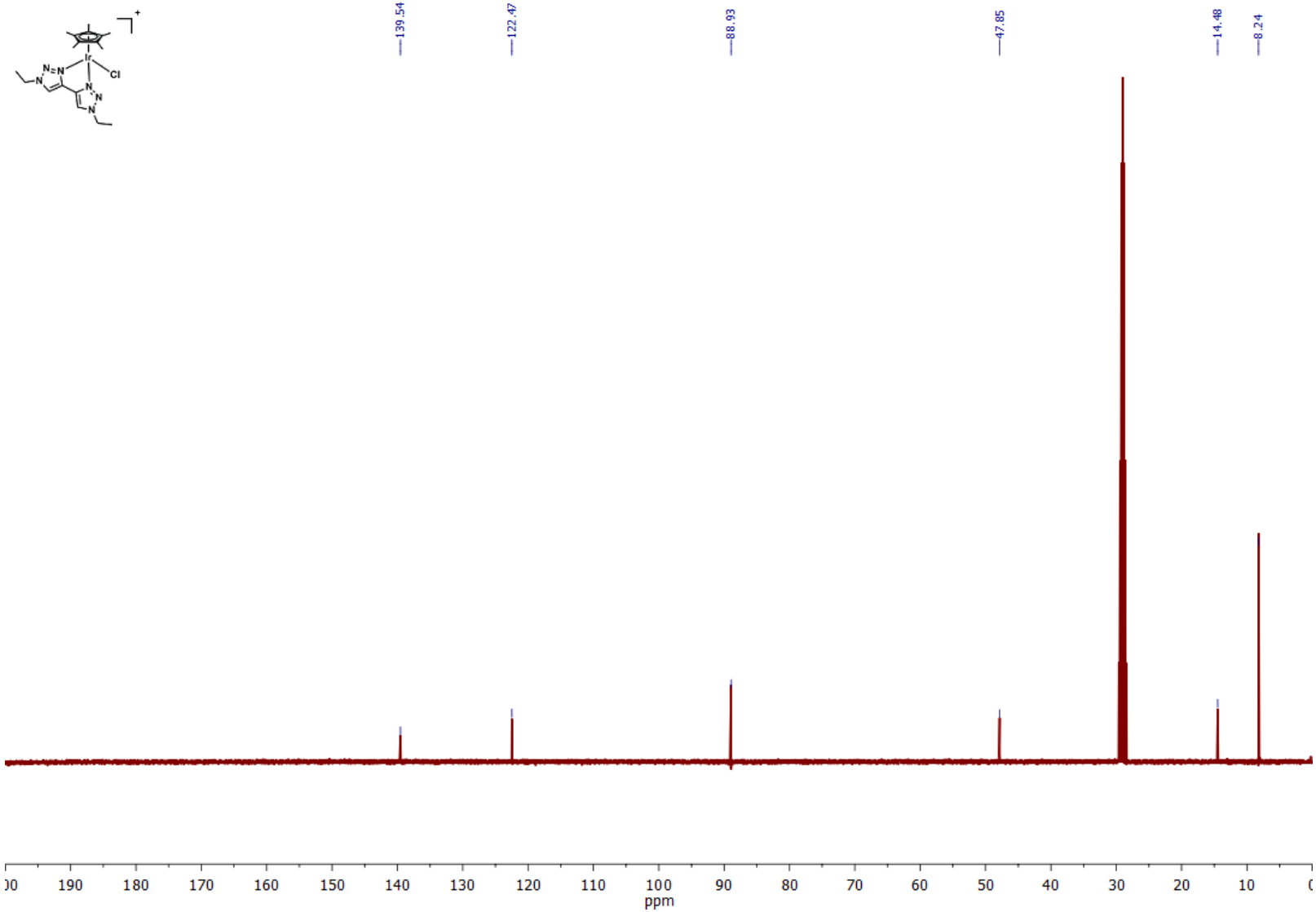

Figure S14: ^{13}C-NMR spectra of 3 at 25°C

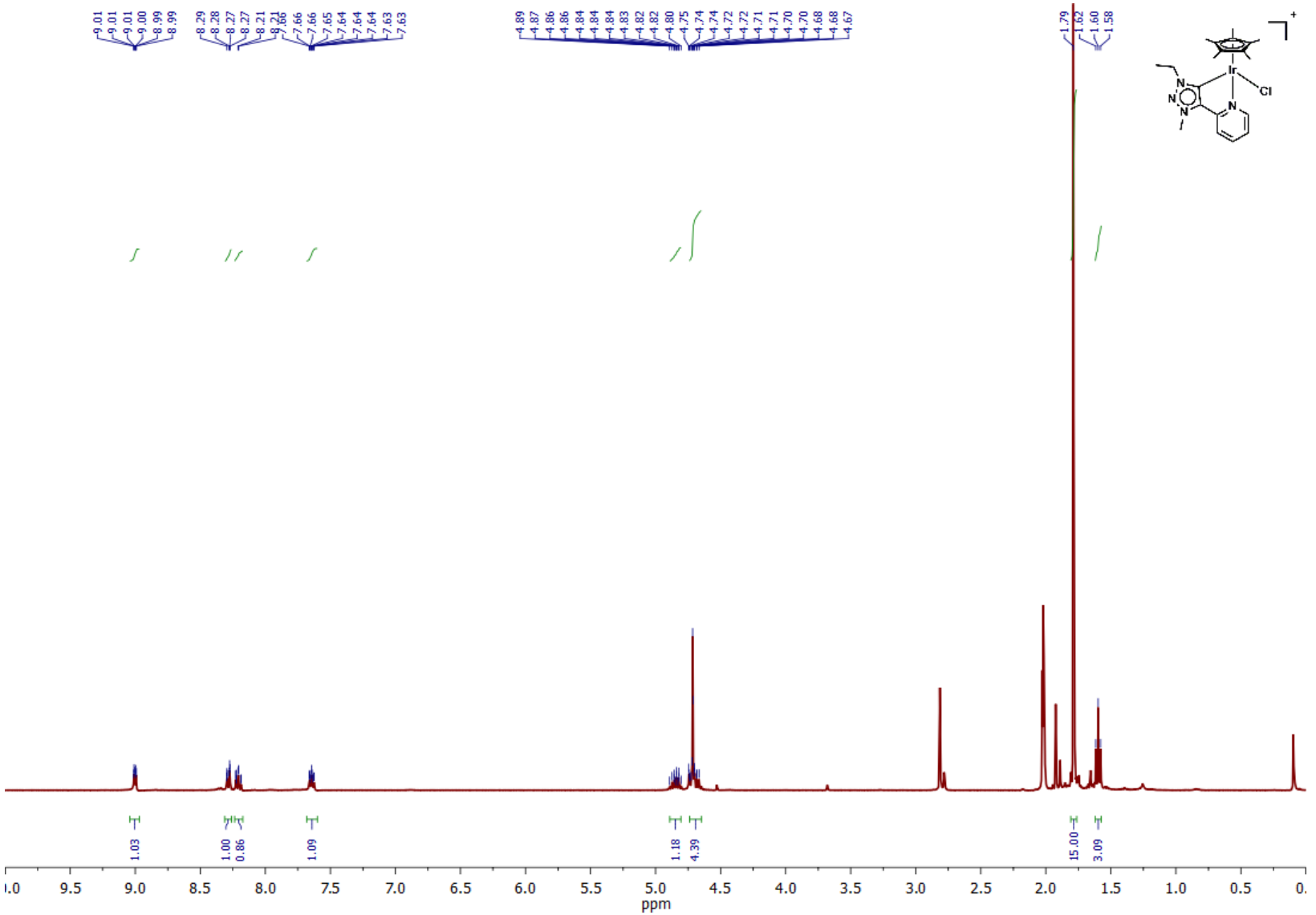

Figure S15: ^{1}H-NMR spectra of 4 at 25°C

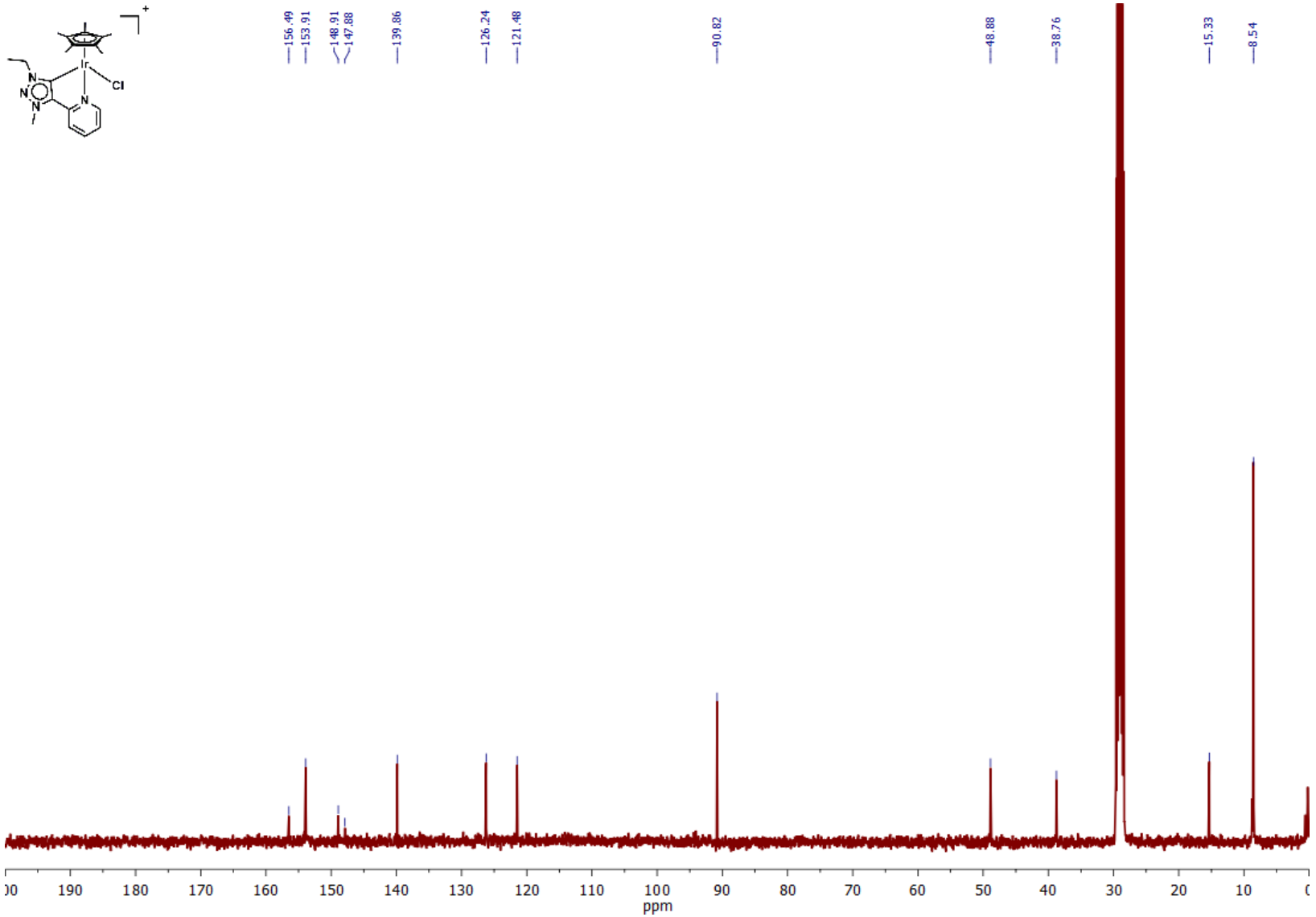

Figure S16: ^{13}C-NMR spectra of 4 at 25°C

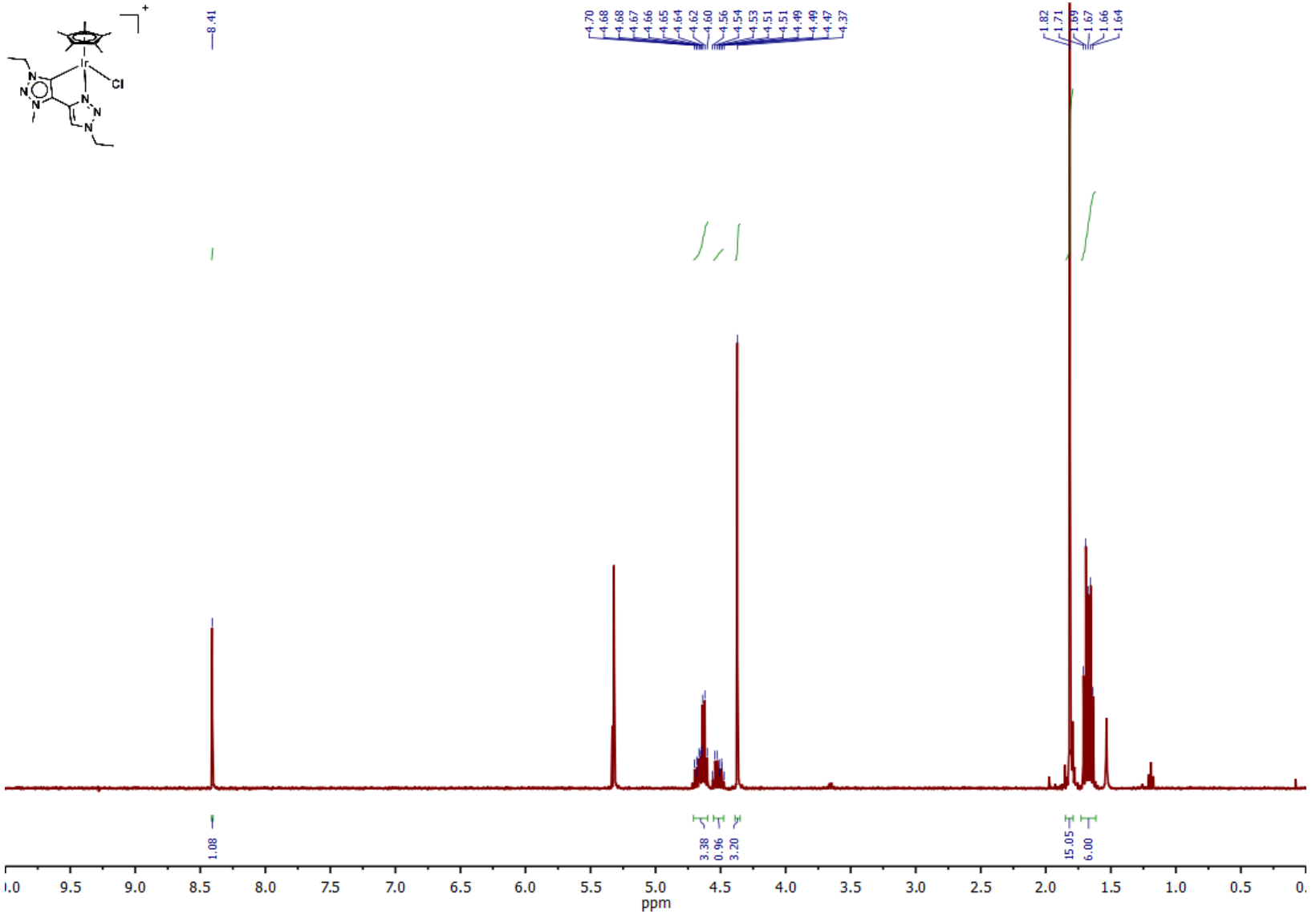

Figure S17: ^{1}H-NMR spectra of 5 at 25°C

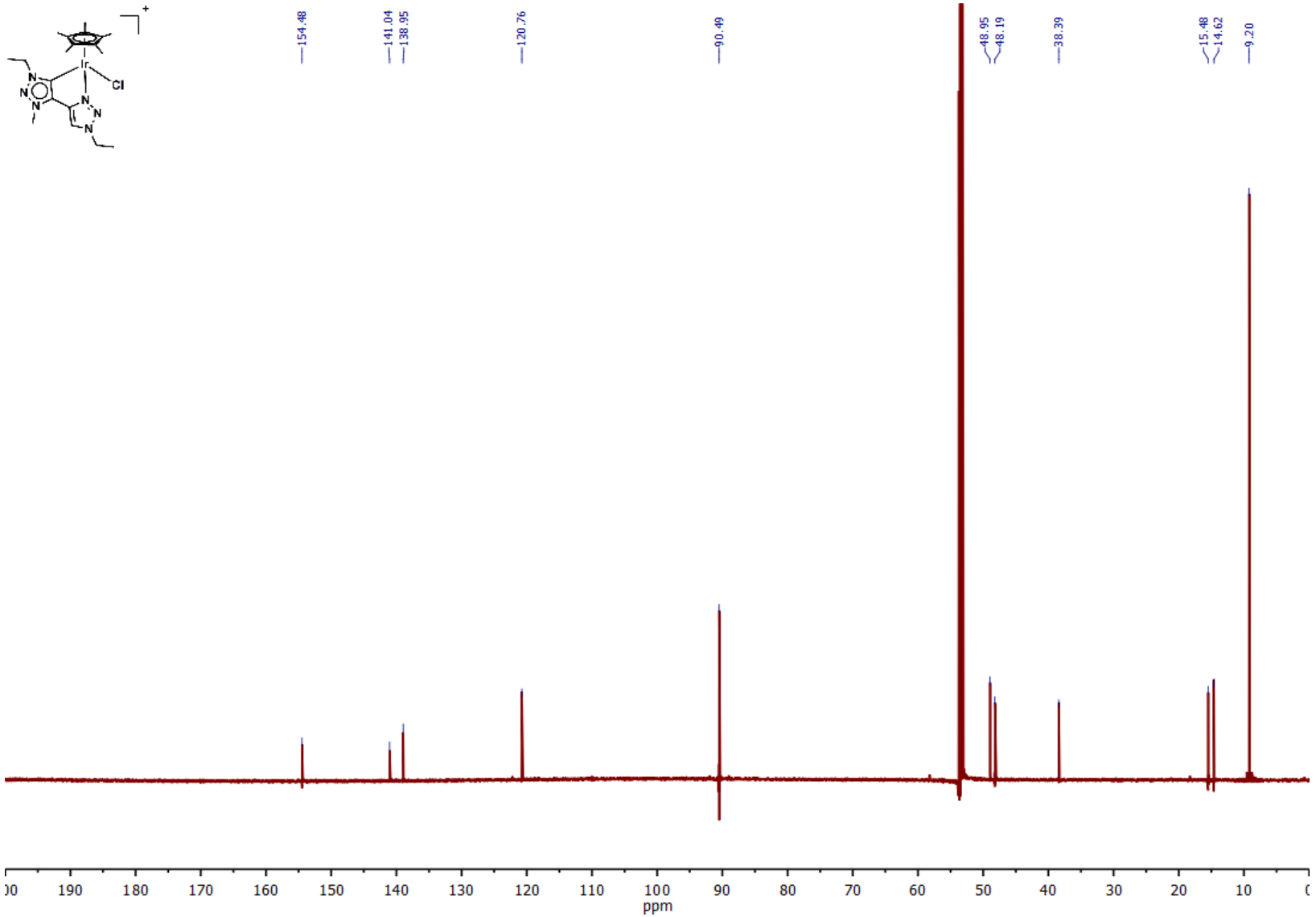

Figure S18: ^{13}C-NMR spectra of 5 at 25°C

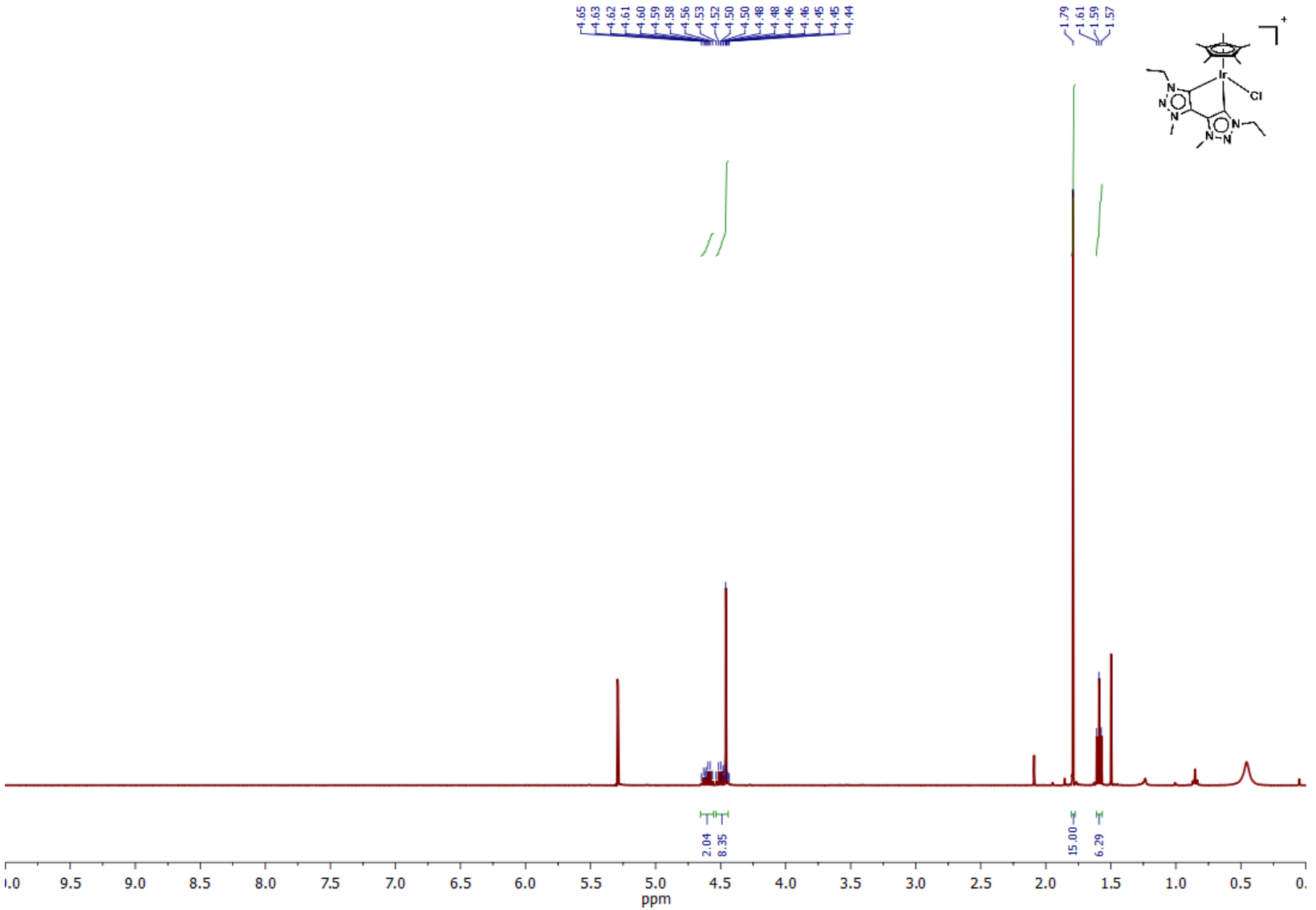

Figure S19: ^{1}H-NMR spectra of 6 at 25°C

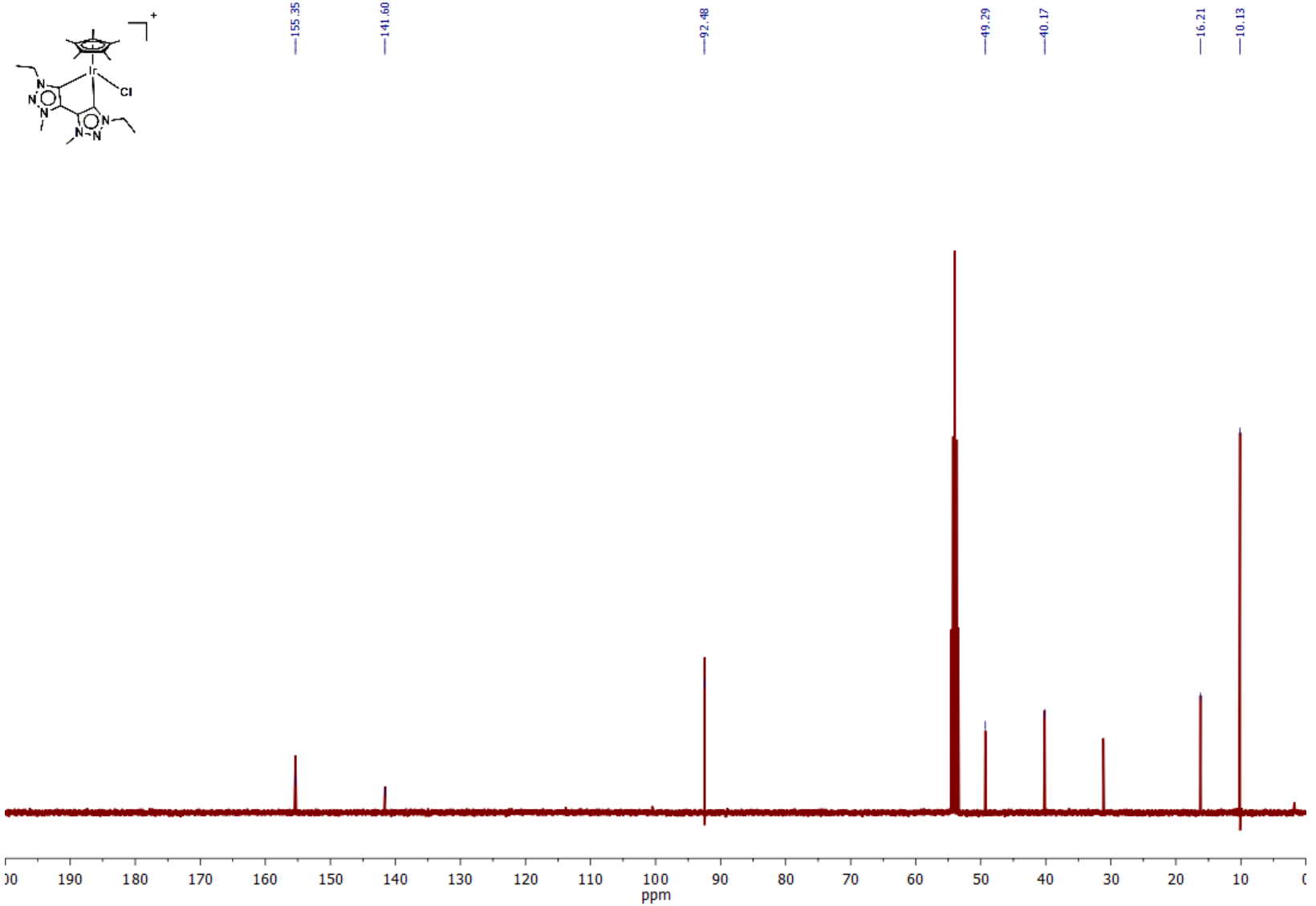

Figure S20: ^{13}C-NMR spectra of 6 at 25°C