Electronic Supplementary Material (ESI) for Dalton Transactions.

A New Bis-phenolate Mesoionic Carbene ligand in early transition metal chemistry

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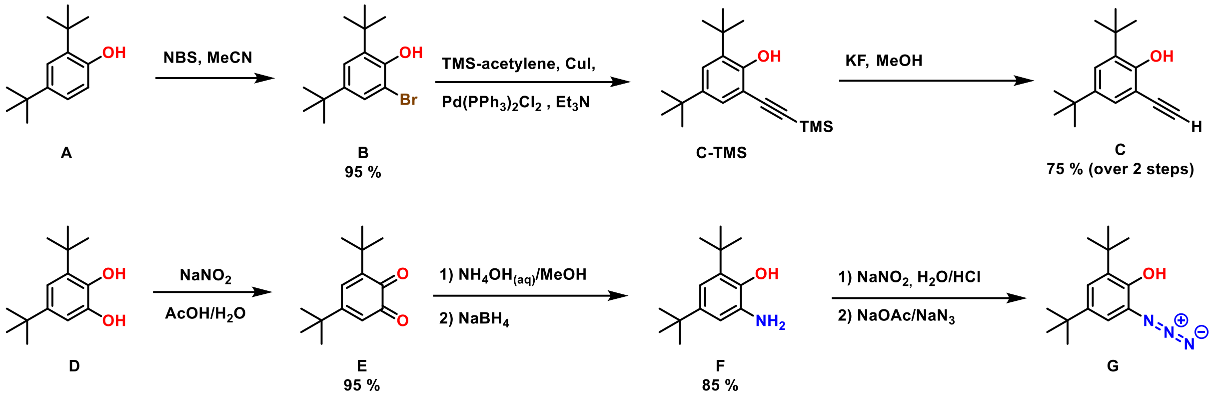
[c]

1. Synthesis of Ligand precursors B – G



Synthesis of ligand precursors

Synthesis of 2-bromo-4,6-di-tert-butylphenol (B):

2,4-di-*tert.*-butylphenol (1 eq, 20,6 g, 100 mmol) were dissolved in MeCN (250 ml) in a 1 L one-neck flask and were cooled to 0°C. In a 250 ml beaker, *N*-bromosuccinimide NBS (1.05 eq, 18.7 g, 105 mmol) was dissolved in MeCN (20 ml) and transferred into a dropping funnel. The NBS solution was added dropwise to the phenol over the course of 2 hours at 0°C and the mixture was stirred over night while warming up to room temperature. The bright yellow reaction mixture was pumped off using a rotary evaporator and the yellow solids were redissolved in diethylether and extracted with water, sat. K_2CO_3 and brine. The organic phase was dried over $MgSO_4$, filtered and the solvent was evaporated to give a yellow microcrystalline solid. Yield 95% (27.1 g, 95 mmol). ^{1}H-NMR ($CDCl_3$, 25°C, 500 MHz) = δ (ppm) 1.32 (s, 9H, C(CH_3)$_3$), 1.44 (s, 9H, C(CH_3)$_3$), 5.67 (s, 1H, O*H*), 7.27 (d, J = 2.4 Hz, 1H, Aryl-H), 7.35 (d, J = 2.4 Hz, 1H, Aryl-H). ^{13}C-NMR ($CDCl_3$, 25°C, 500 MHz) = δ (ppm) 29.6 (C(*C*H$_3$)$_3$), 31.6 (C(*C*H$_3$)$_3$), 34.6 (*C*(CH$_3$)$_3$), 35.7 (*C*(CH$_3$)$_3$), 112.1, 123.8, 126.4, 136.9, 143.9 (all Aryl-*C*), 148. (Aryl-O*H*).

Synthesis of 2,4-di-tert-butyl-6-ethynylphenol (C):

Compound **B** (1 eq, 6g, 21 mmol) was dissolved in a one-necked schlenk flask in Et_3N (150 ml) and the mixture was carefully degassed using freeze-pump-thaw techniques (three times). To the degassed mixture was added $Pd(PPh_3)_2Cl_2$ (0.05 eq, 736 mg, 1.05 mmol), copper iodide (0.05 eq, 200 mg. 1.05 mmol) and TMS-acetylene (1.2 eq, 2.48 g, 25.2 mmol, 3,5 ml) and the mixture was heated under Argon at 75°C for 18 h in the closed flask. The reaction mixture was cooled to room temperature and filtered through a plug of silica. The silica plug was washed with Et_2O (300 ml). The combined organic phases were extracted using 1M HCl (2 times, 50 ml each), sat. NH_4Cl (2 times, 50 ml each) and brine (2 times, 50 ml each). The ether phase was dried over $MgSO_4$ and was filtered again over a plug of slicia. The silica plug was again washed with Et_2O (100 ml) and the combined washings were evaporated yielding a orange-yellow solid being the TMS-protected alkyne (**C-TMS**).

^{1}H-NMR ($CDCl_3$, 25°C, 500 MHz) = δ (ppm) 0.29 (s, 9H, $Si(CH_3)_3$), 1.28 (s, 9H, $C(CH_3)_3$), 1.40 (s, 9H, $C(CH_3)_3$), 6.09 (s,1H, O*H*), 7.21 (d, *J* = 2.4 Hz, 1H, Aryl-*H*), 7.28 (d, *J* = 2.4 Hz, 1H, Aryl-*H*). ^{1}H-NMR ($CDCl_3$, 25°C, 500 MHz) = δ (ppm) 0.2 ($Si(CH_3)_3$), 29.6 ($C(CH_3)_3$), 31.6 ($C(CH_3)_3$), 34.4 ($C(CH_3)_3$), 35.1 ($C(CH_3)_3$), 100.5 (*C*CH), 101.7 (C*C*H), 109.4, 125.6 (Aryl-*C*H), 125.8 (Aryl-*C*H), 134.9, 142.2, 153.7 (Aryl-*C*-OH).

The crude alkyne was dissolved in MeOH and potassium fluoride (1.3 eq, 1.59 g, 27.3 mmol) was added and the reaction mixture was stirred for 6 h at room temperature. Et_2O (250 ml) was added and the reaction mixture was washed with water (3 times, 50 ml each) and brine (3 times, 50 ml each). The organic phase was dried over $MgSO_4$ and filtered through a plug of silica. The silica plug was washed with Et_2O (100 ml) and the combined organic phases were evaporated yielding alkyne **C** as a yellow solid. Yield: 75% (over both steps, 3.63 g, 15.8 mmol). ^{1}H-NMR ($CDCl_3$, 25°C, 500 MHz) = δ (ppm) 1.28 (s, 9H, $C(CH_3)_3$), 1.41 (s, 9H, $C(CH_3)_3$), 3.45 (s, 1H, CC*H*), 6.01 (s,1H, O*H*), 7.25 (d, *J* = 2.4 Hz, 1H, Aryl-*H*), 7.32 (d, *J* = 2.4 Hz, 1H, Aryl-*H*). ^{1}H-NMR ($CDCl_3$, 25°C, 500 MHz) = δ (ppm) 29.6 ($C(CH_3)_3$), 31.6 ($C(CH_3)_3$), 34.4 ($C(CH_3)_3$), 35.1 ($C(CH_3)_3$), 79.7 (*C*CH), 83.9 (C*C*H), 108.1, 125.9, 126.2, 135.2, 142.3 (all Aryl-*C*), 154.0 (Aryl-*C*-OH).

3,5-di-tert-butylcyclohexa-3,5-diene-1,2-dione (E)

Synthesis was adapted from the literature.[1] To a stirring solution of 3,5-di-*tert*-butyl-2-hydroxyphenol **D** (11.92 g, 52 mmol, 1 eq.) in glacial acetic acid (150 mL) was added a solution of $NaNO_2$ (7.6 g, 108 mmol, 2.2 eq.) in H_2O (60 mL). The mixture was stirred two more hours, quenched with 2 L of water and filtered. The crude red-brown product **E** was dried under air overnight. (10.9 g, 49.4 mmol, 95 %) ^{1}H-NMR (C_6D_6, 25°C, 500 MHz) = δ (ppm) 0.75 (s, 9H, $C(CH_3)_3$), 1.14 (s, 9H, $C(CH_3)_3$), 5.96 (d, J = 2.4 Hz, 1H, Aryl-H), 6.58 (d, J = 2.4 Hz, 1H, Aryl-H). ^{13}C-NMR (C_6D_6, 25°C, 500 MHz) = δ (ppm) 29.6 ($C(CH_3)_3$), 31.6 ($C(CH_3)_3$), 34.4 ($C(CH_3)_3$), 35.1 ($C(CH_3)_3$), 123.1, 133.1, 150.4, 161.4 (all Aryl-*C*), 180.7, 181.4 (Aryl-*C*=O).

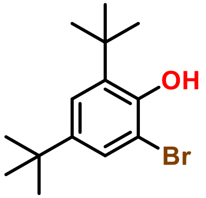
2-amino-4,6-di-tert-butylphenol (F)

Synthesis was adapted from the literature.[2] Quinone **E** (7.91 g, 35.9 mmol, 1 eq.) was solved in a mixture of MeOH and concentrated ammiona solution (200/80 mL) and stirred for 10min. $NaBH_4$ (3.25 g, 85.4 mmol, 2.2 eq.) was added portionwise over a period of 40 min and the mixture was stirred for another hour at room temperature. The reaction was quenched by pouring it slowly in 1 L of ice-water. Extraction with Et_2O (300 ml), subsequent drying of the ether phase over $MgSO_4$ and evaporation of the solvent afforded 4,6-di-*tert.*-butyl-2-amino-phenol **F** as a pale green powder. (7.09 g, 32.1 mmol, 89 %) ^1H-NMR (C_6D_6, 25°C, 500 MHz) = δ (ppm) 1.32 (s, 9H, $C(CH_3)_3$), 1.57 (s, 9H, $C(CH_3)_3$), 2.21 (s, broad, NH_2), 5.97 (s, broad, 1H, O*H*), 6.52 (s, 1H, Aryl-*H*), 7.14 (s, 1H, Aryl-*H*). ^{13}C-NMR (C_6D_6, 25°C, 500 MHz) = δ (ppm) 30.4 ($C(CH_3)_3$), 32.3 ($C(CH_3)_3$), 34.8 ($C(CH_3)_3$), 35.4 ($C(CH_3)_3$), 117.1, 117.8, 132.9, 136.3, 142.5, 145.9 (all Aryl-*C*).

2-azido-4,6-di-tert-butylphenol (G)

Synthesis was adapted from the literature.[3] A solution of $NaNO_2$ (823 mg, 11.9 mmol, 1.2 eq.) in H_2O (10 mL) was added dropwise to a heavily stirred suspension of **F** (2.2 g, 9.94 mmol, 1 eq.) in H_2O/HCl_{konz} (40/40 mL) at 0 °C . The red suspension was stirred for 30 min and then added to a solution of NaN_3 (1.29 g, 19.9 mmol, 2 eq.) und NaOAc (2.45 g, 29.8 mmol, 3 eq.) in H_2O (100 mL) at 0 °C dropwise. (Note: remaining red solids can be washed into the reaction mexutre using acetone). The mixture was stirred at rt overnight and the suspension was extracted 2 times with 100 ml of diethyl ether. The ether was dried over $MgSO_4$, filtered and evaporated to give a crude red, waxy solid of azide **G** (approx. 75 %). Contrary to the literature, we found this compound to be highly unstable and we recommend to use it directly on the same day for the next step. IR $\tilde{\nu}$ (cm^{-1}) = 3529 (OH), 2111 (N_3).

2. NMR spectra



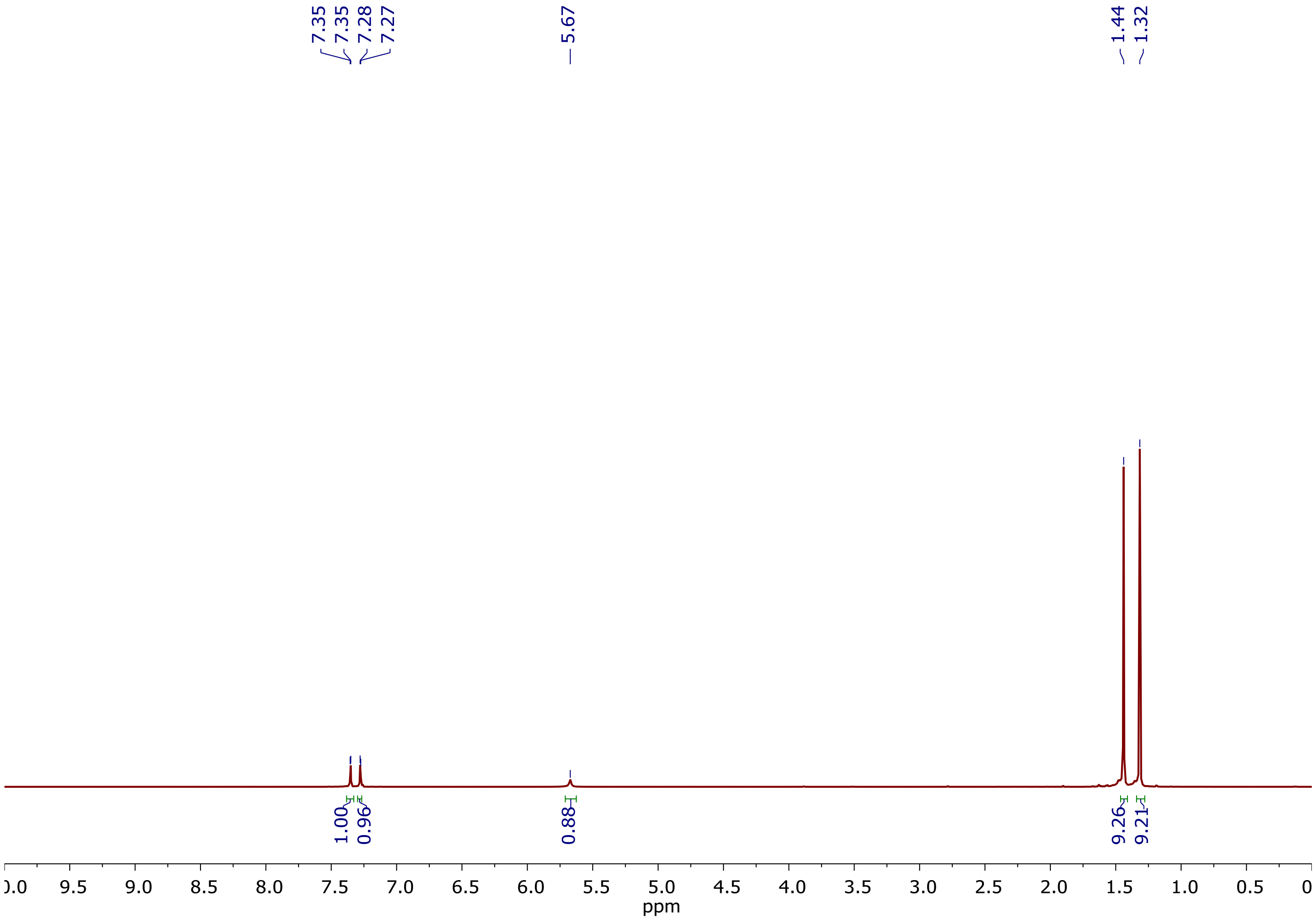


Figure S 1: ^{1}H-NMR of **B** in $CDCl_3$

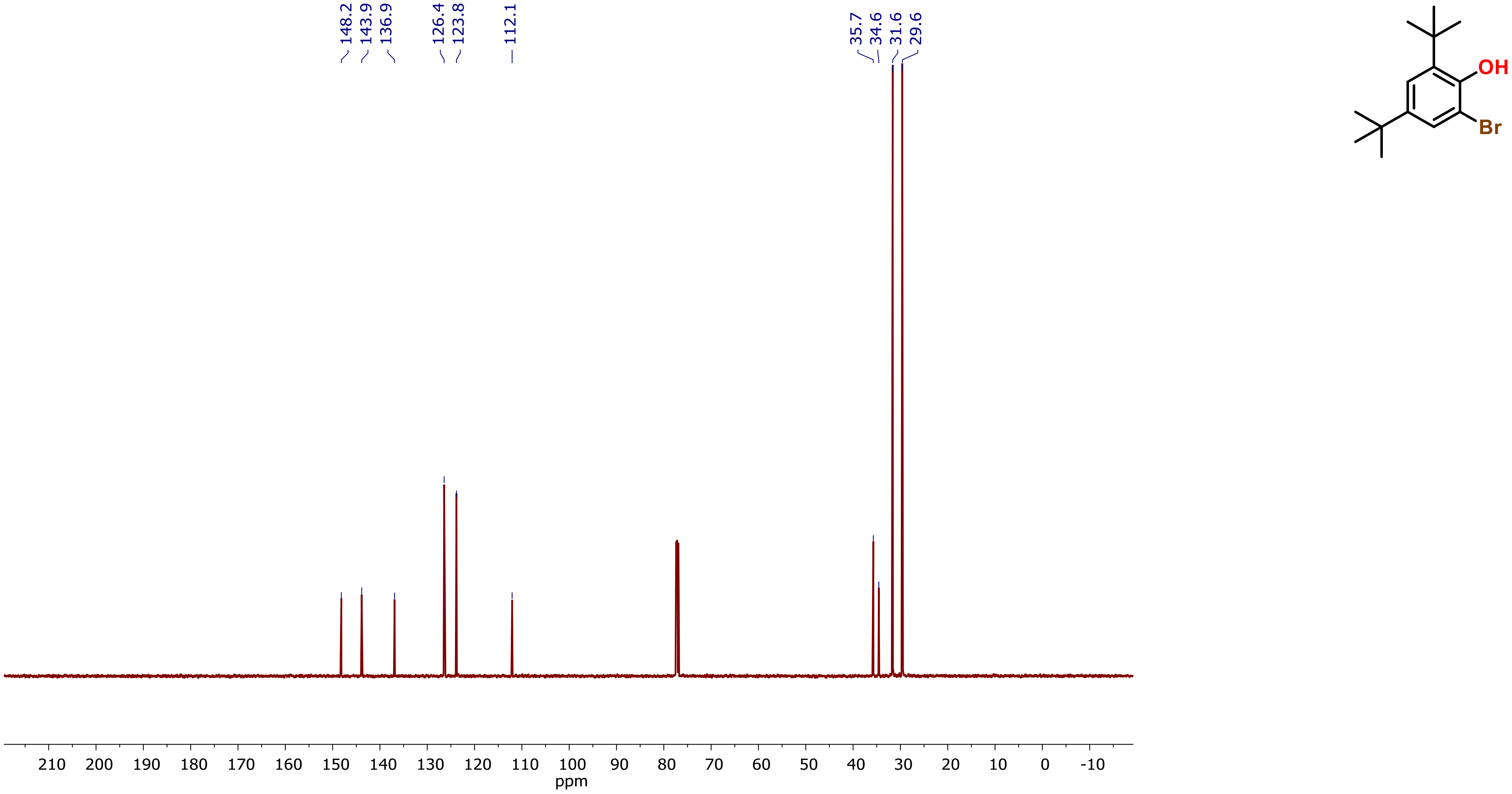


Figure S 2: ^{13}C-NMR of **B** in $CDCl_3$

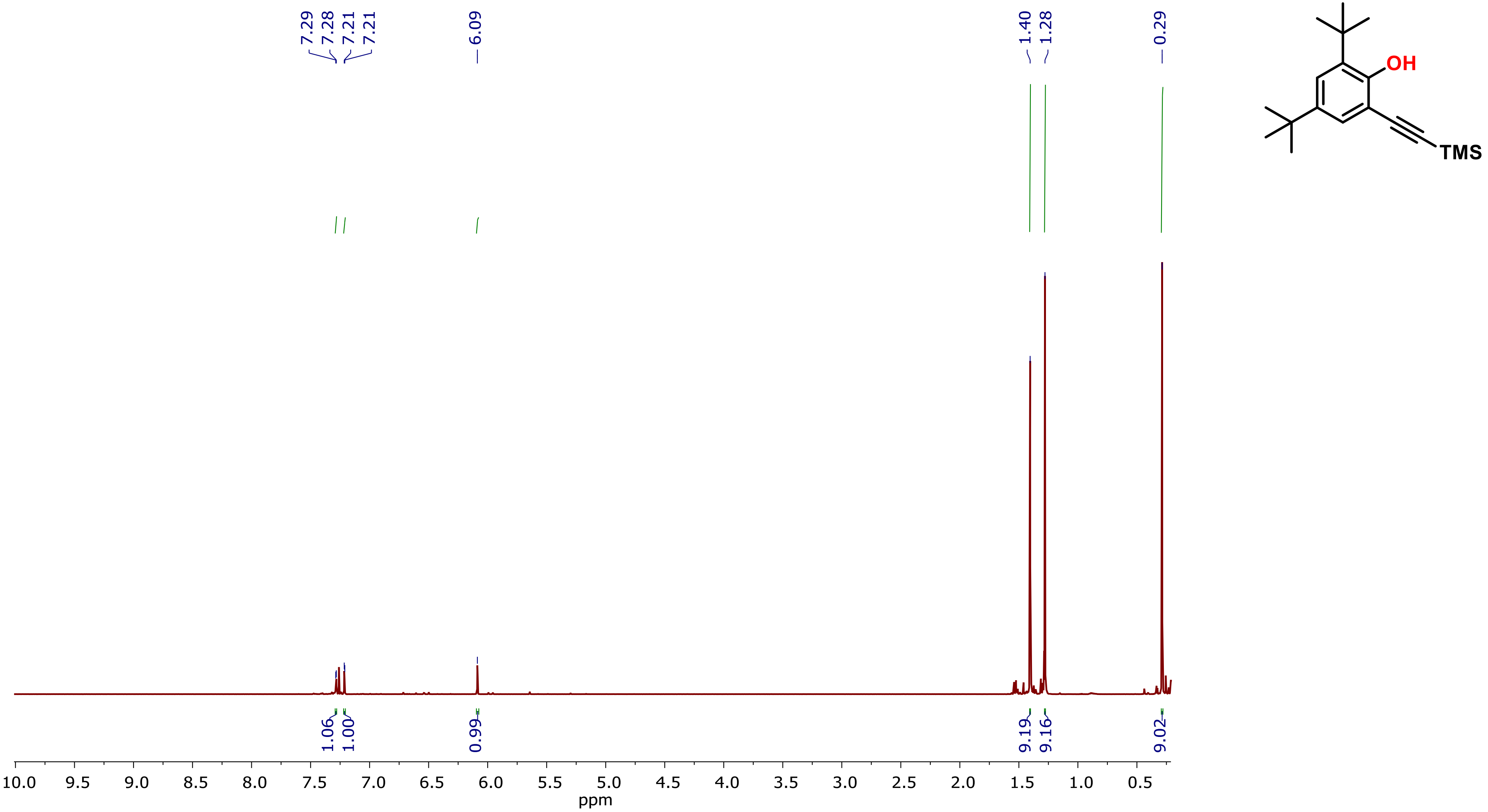


Figure S 3: ^{1}H-NMR of crude **C-TMS** in $CDCl_3$

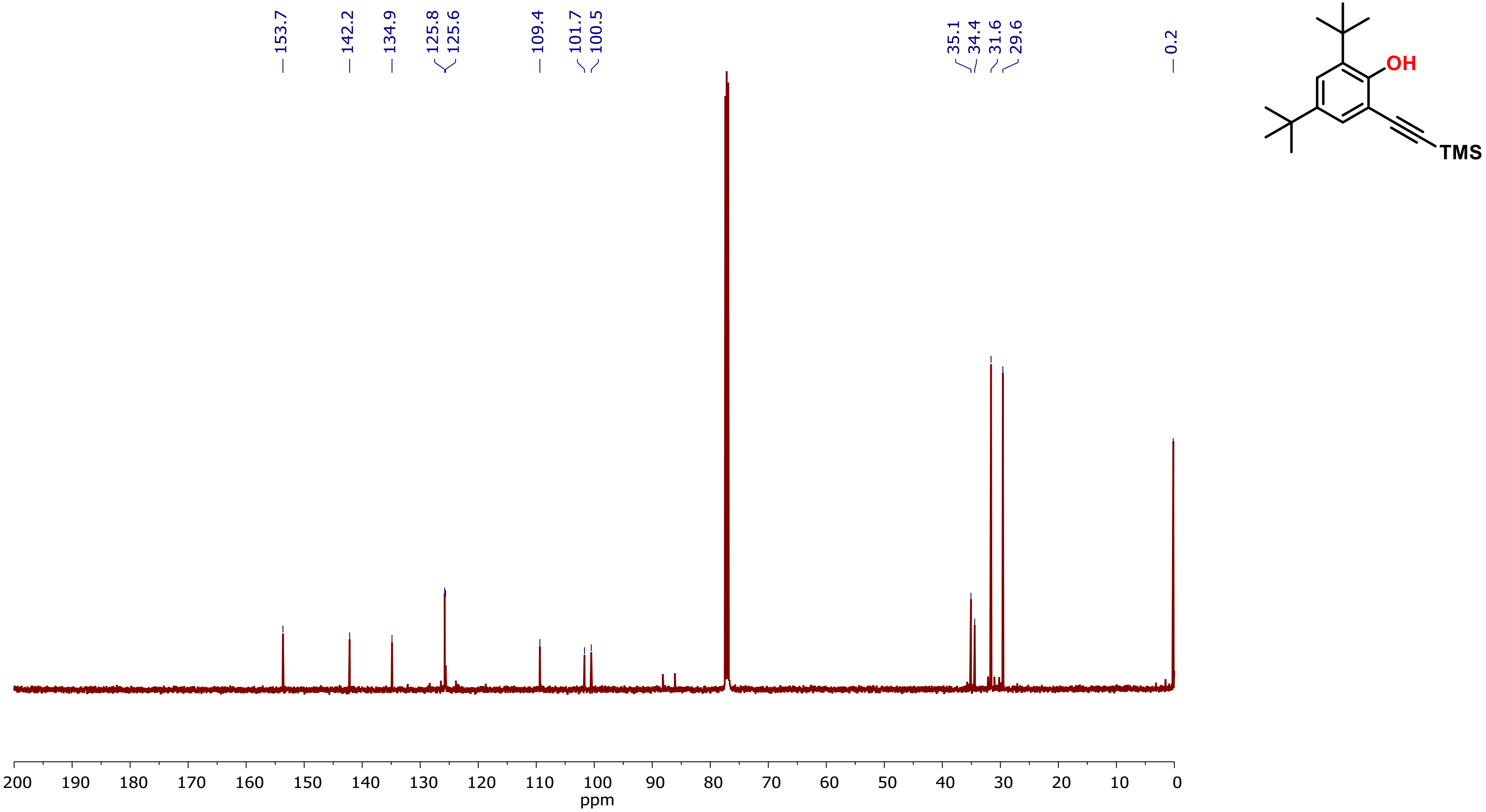


Figure S 4: ^{13}C-NMR of crude **C-TMS** in $CDCl_3$

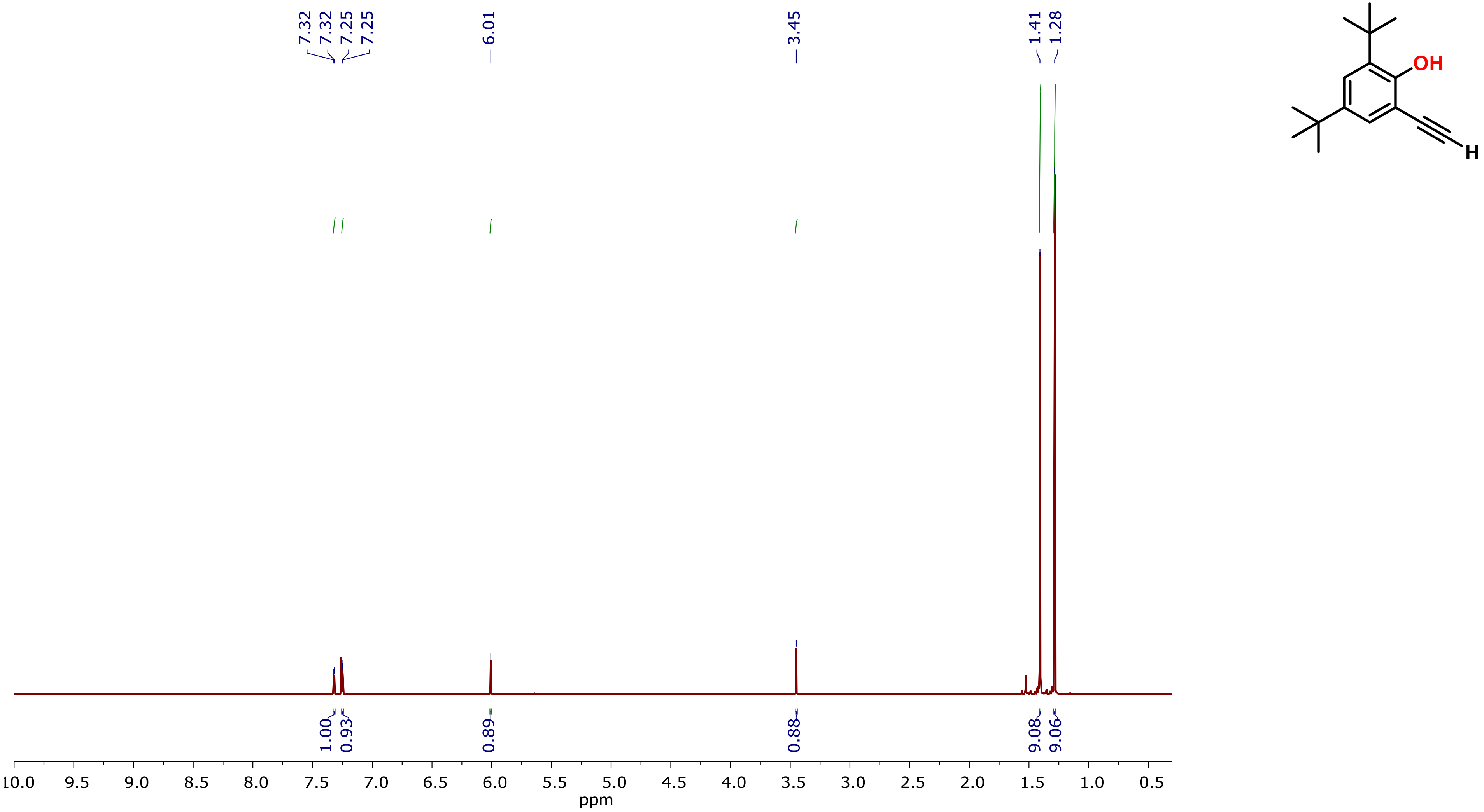


Figure S 5: ^{1}H-NMR of **C** in $CDCl_3$

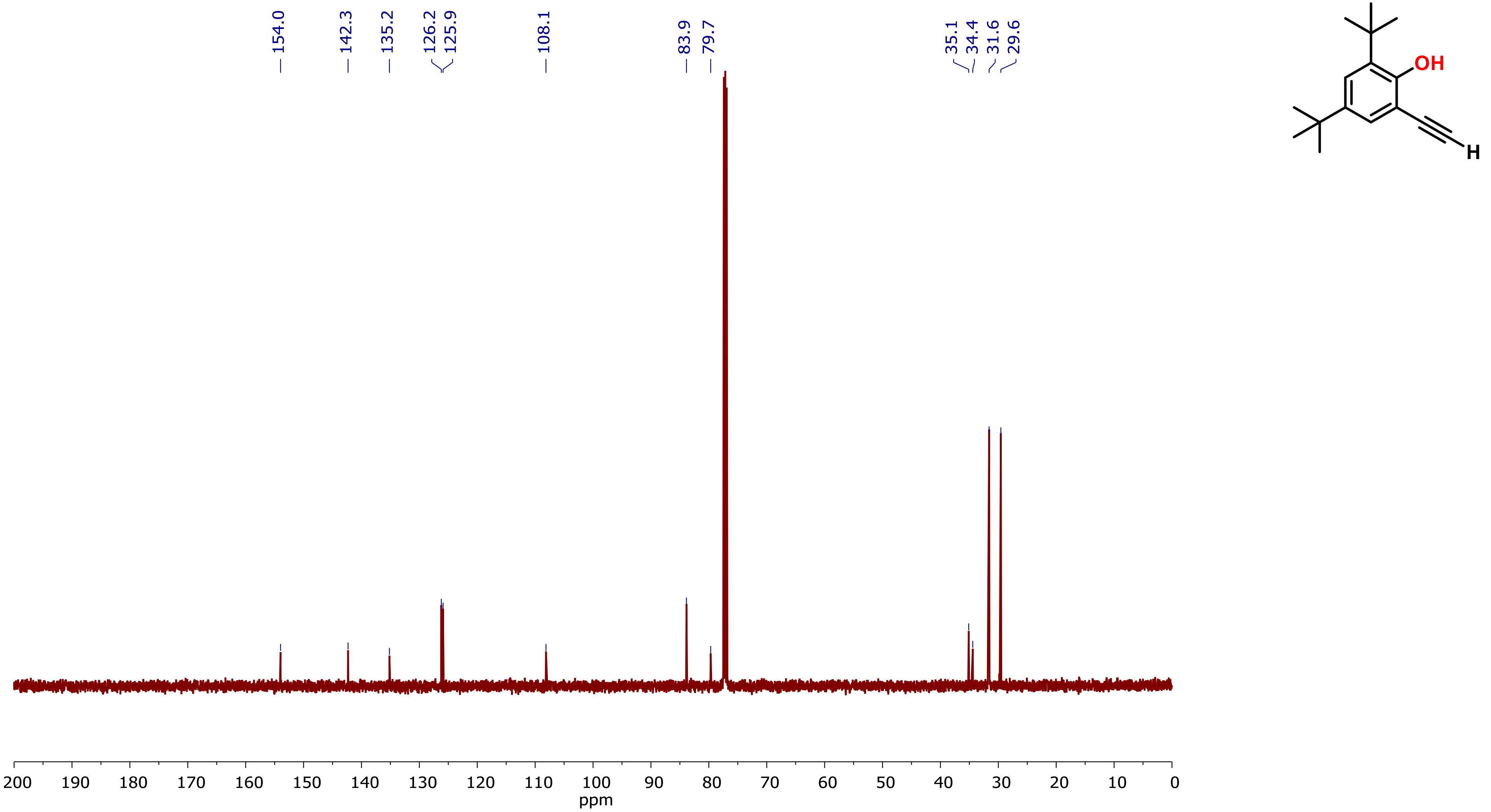


Figure S 6: ^{13}C-NMR of **C** in $CDCl_3$

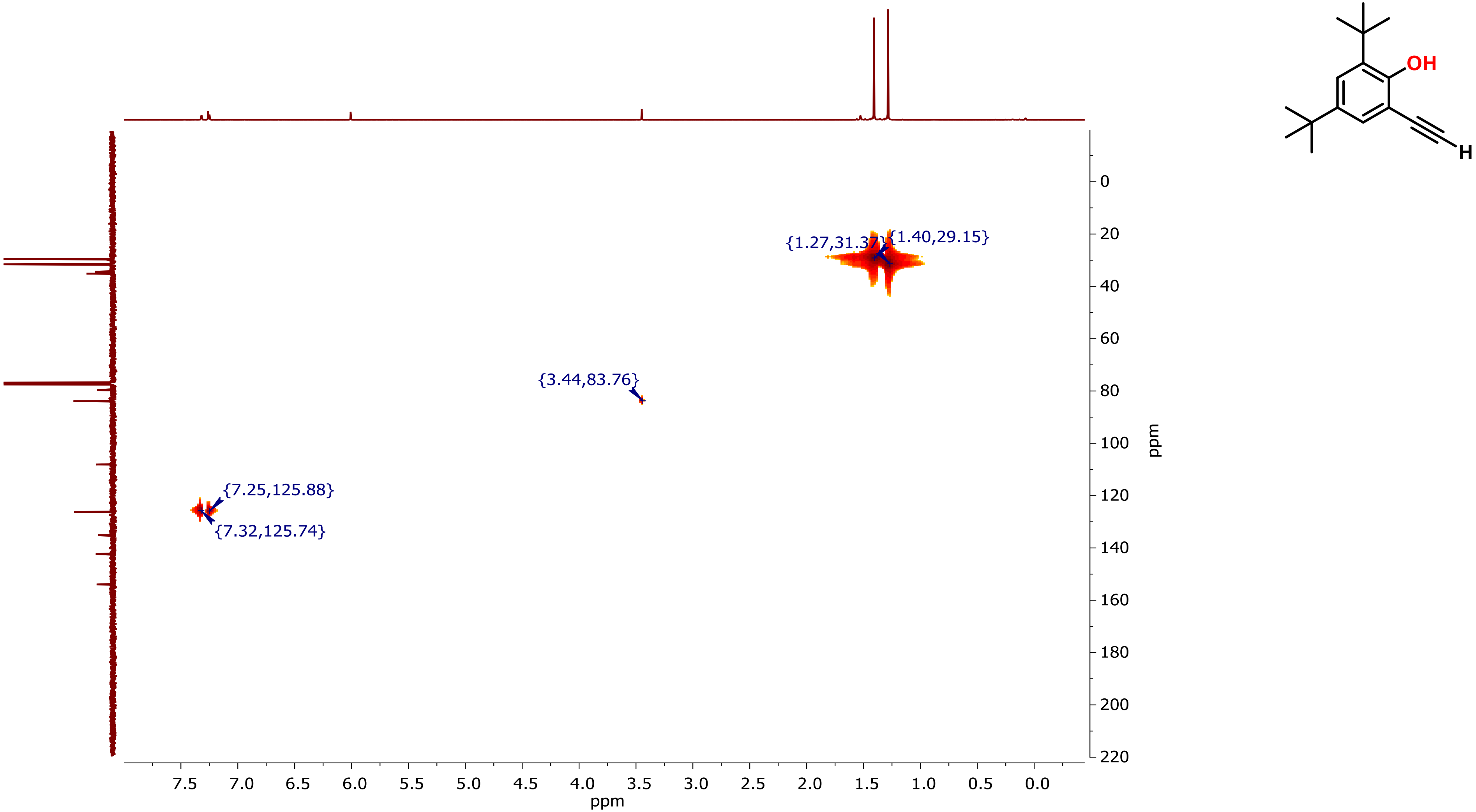


Figure S 7: ^{1}H-^{13}C HSQC of **C** in $CDCl_3$

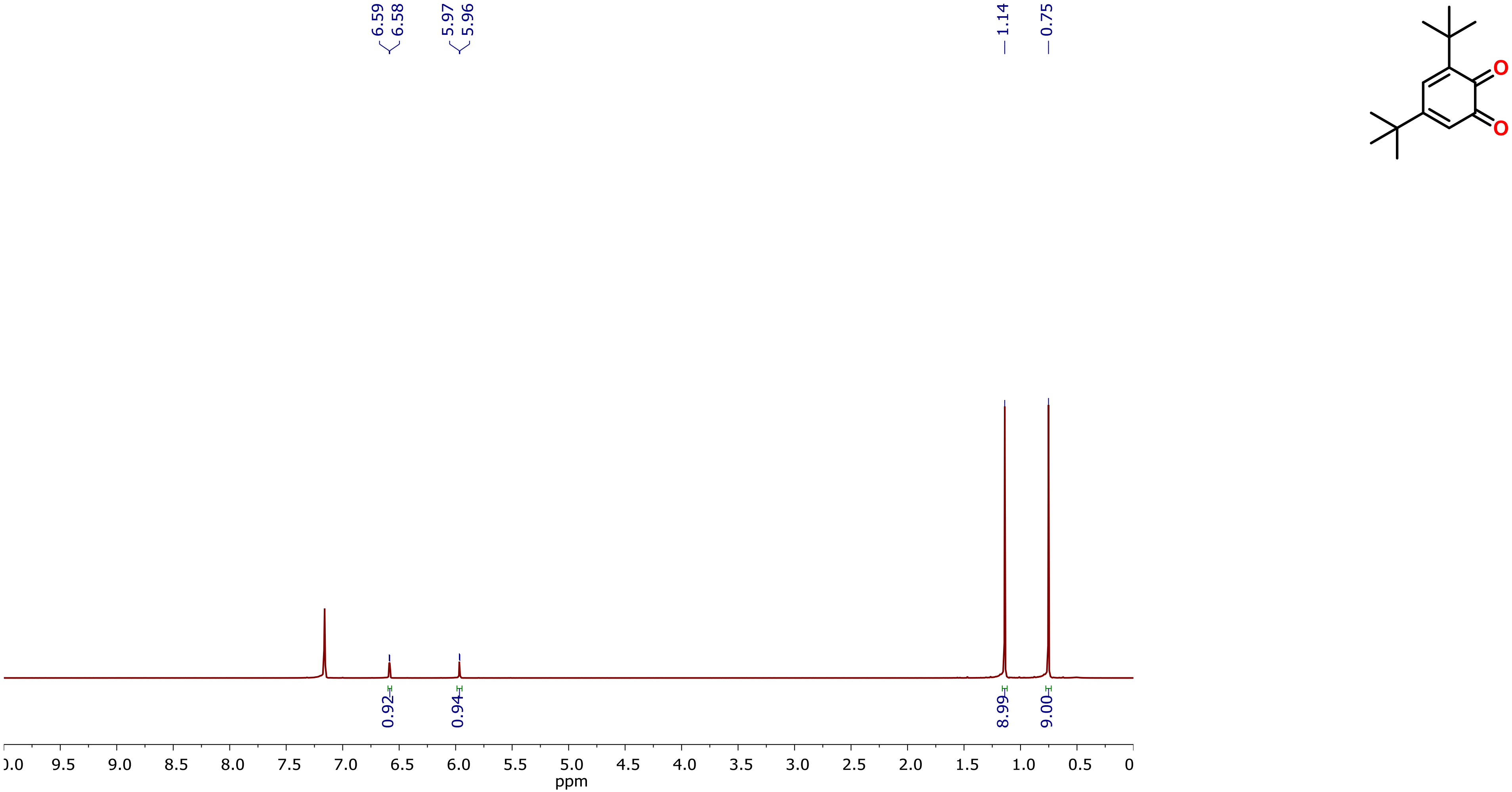


Figure S 8: ^{1}H-NMR of **E** in C_6D_6

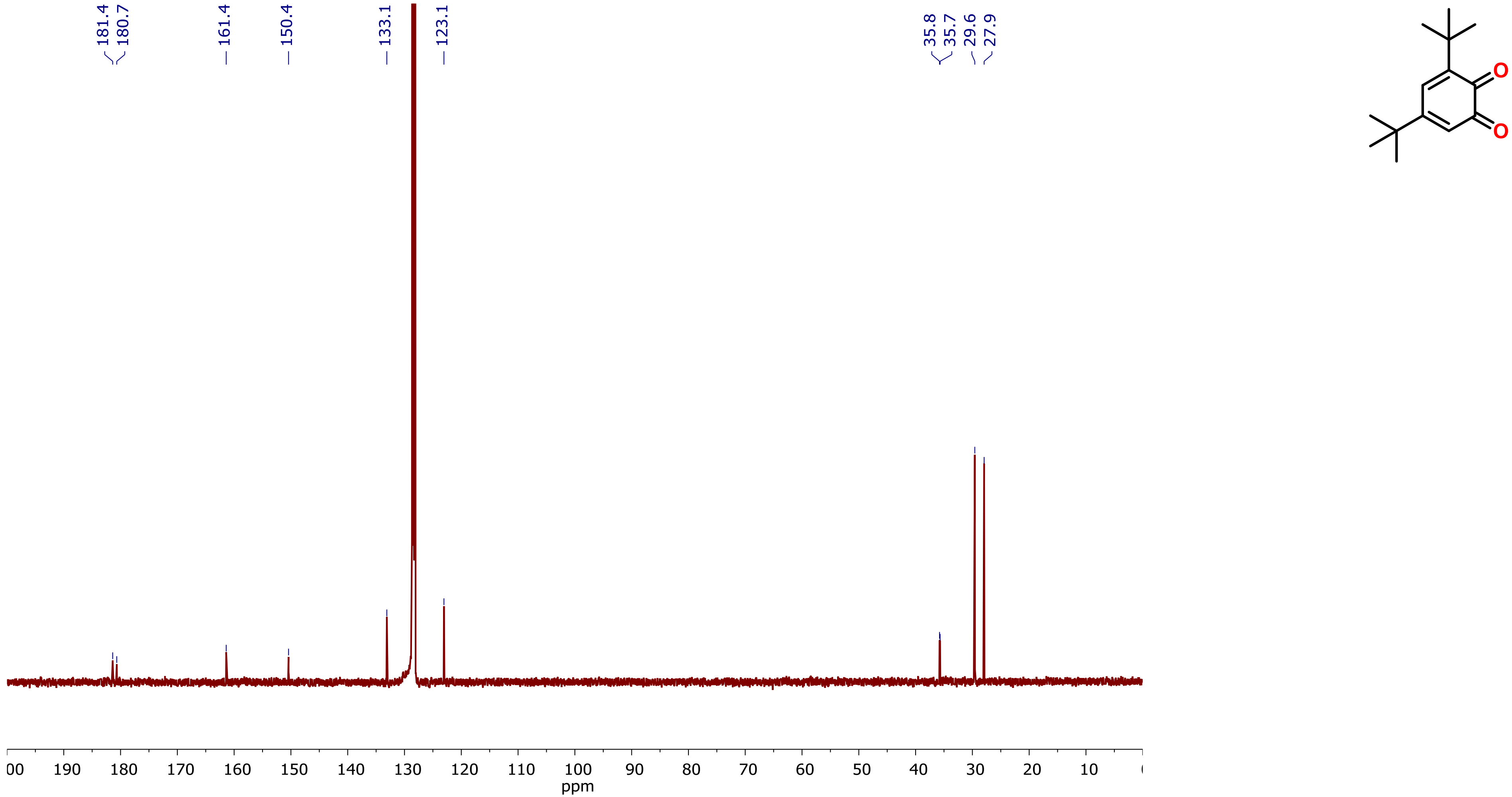


Figure S 9: ^{13}C-NMR of **E** in C_6D_6

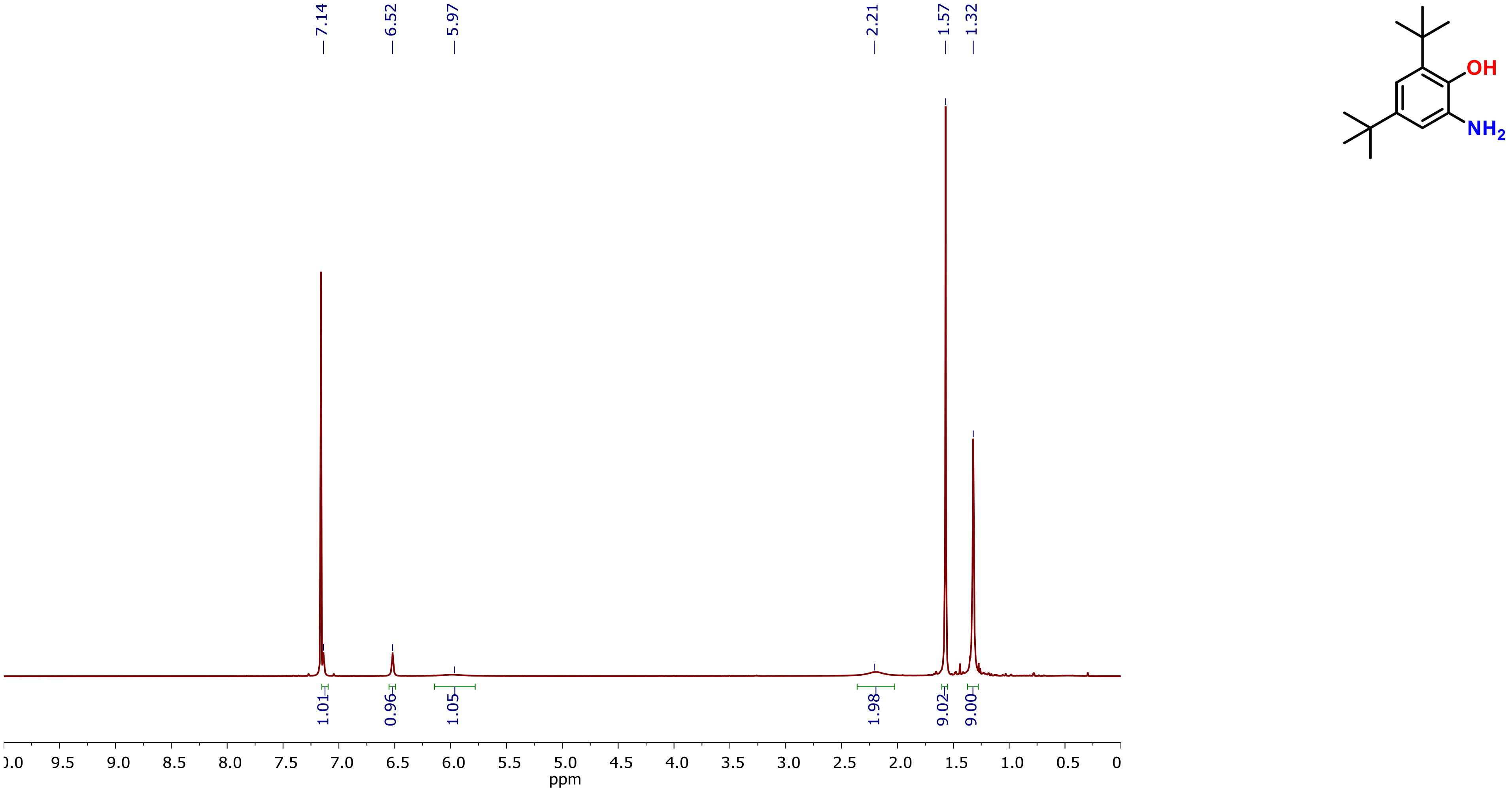


Figure S 10: ^{1}H-NMR of **F** in C_6D_6

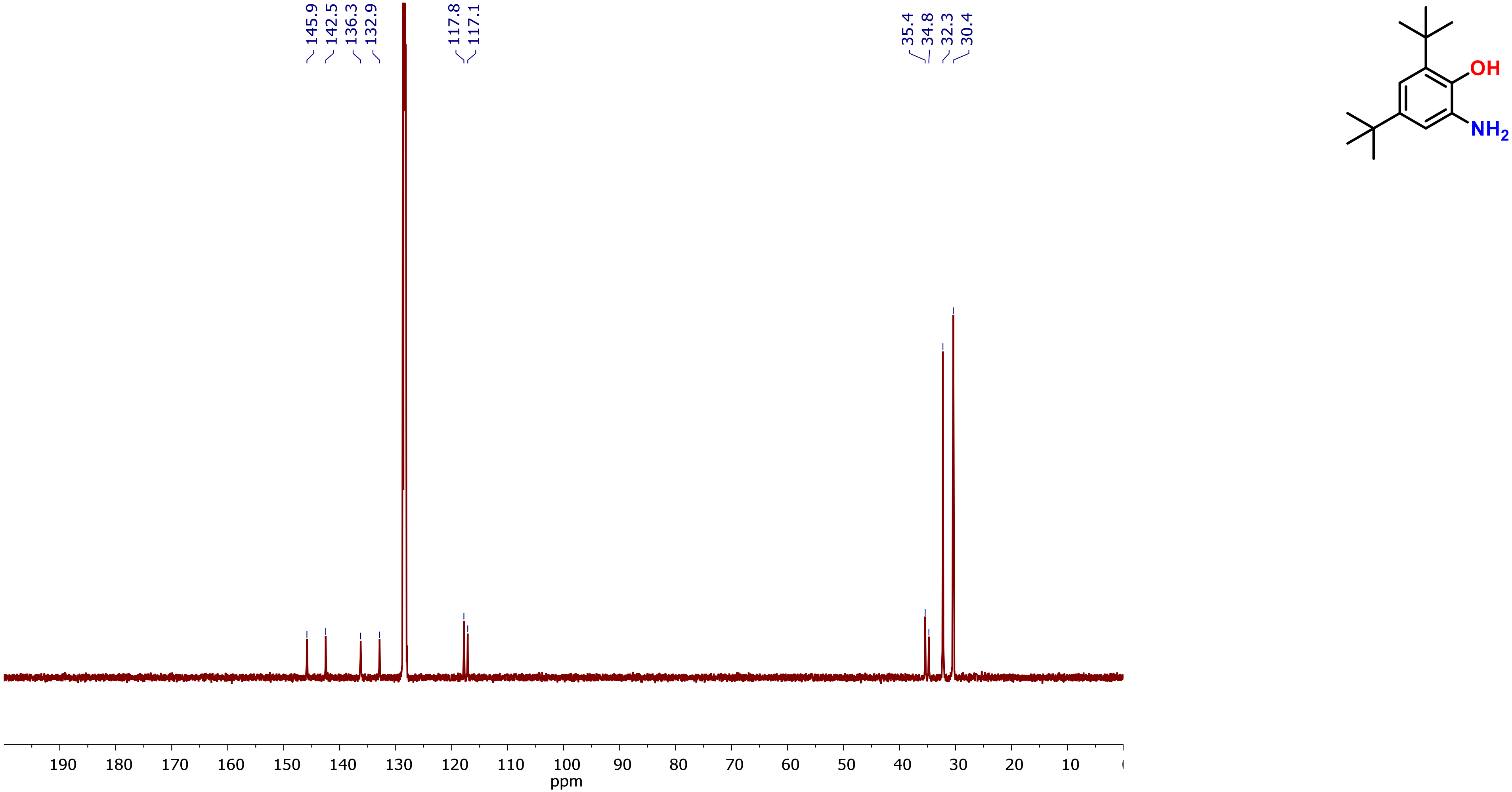


Figure S 11: ^{13}C-NMR of **F** in C_6D_6

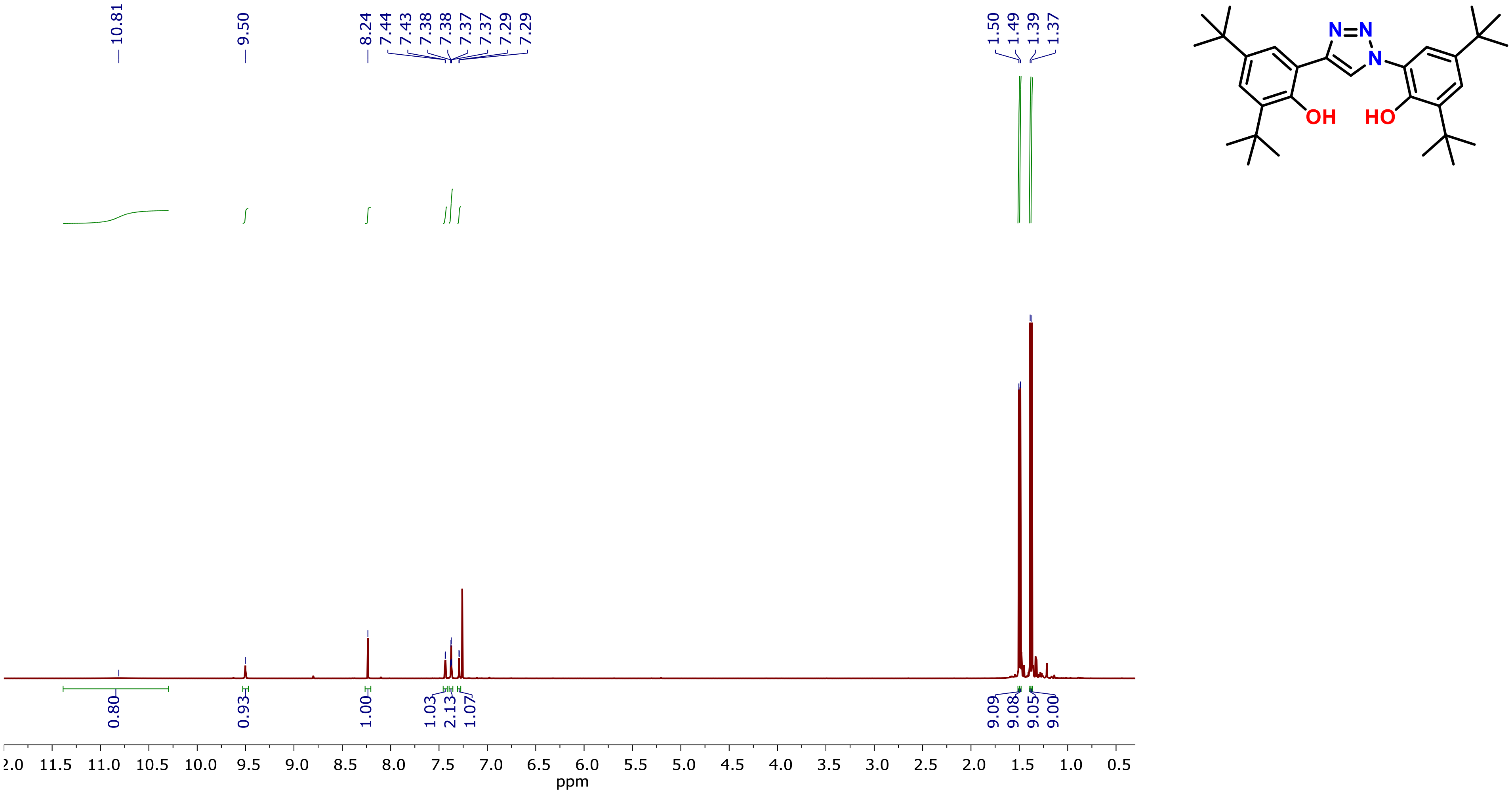


Figure S 12: ^{1}H-NMR of **1** in $CDCl_3$

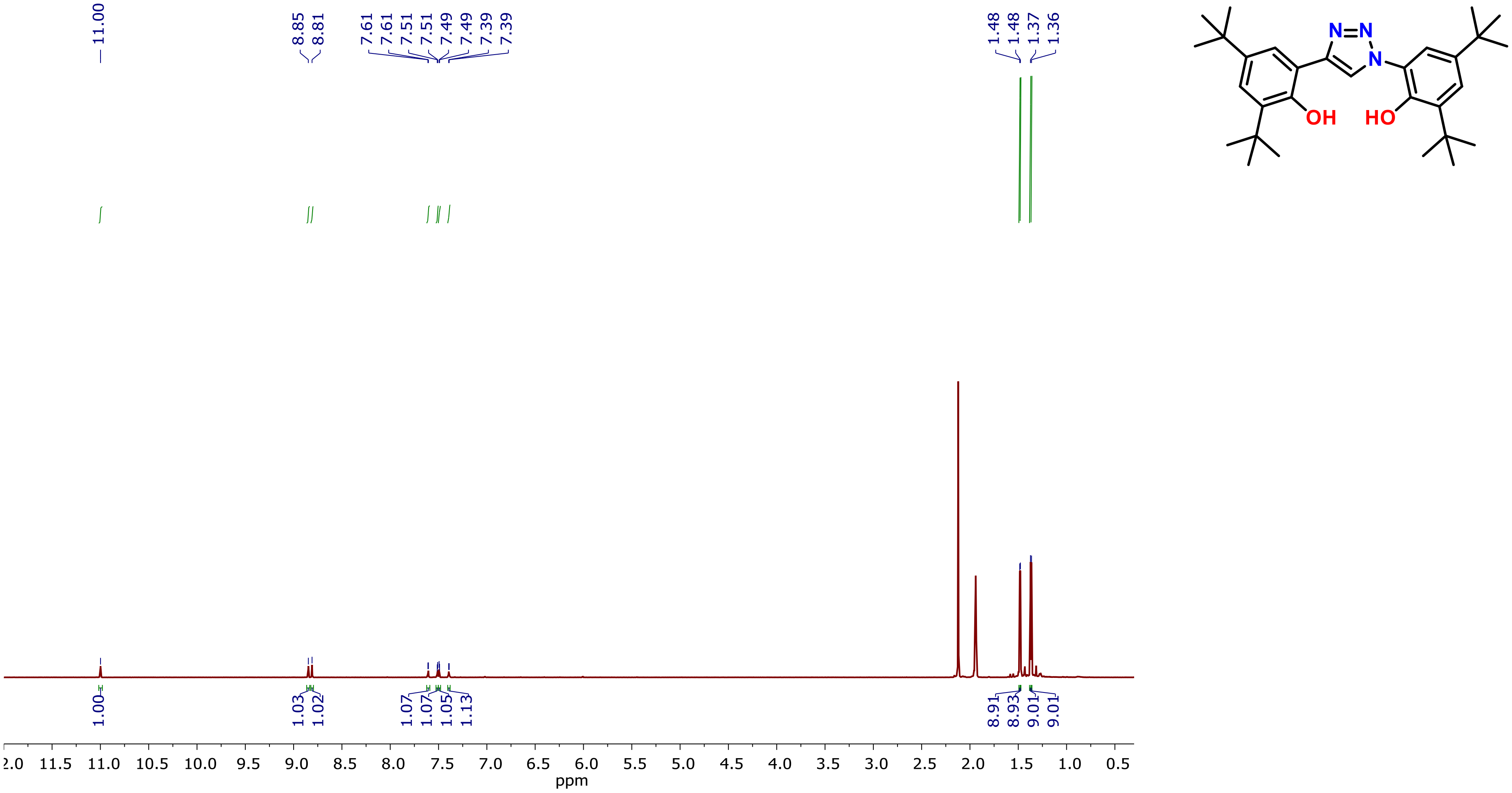


Figure S 13: ^{1}H-NMR of **1** in CD_3CN

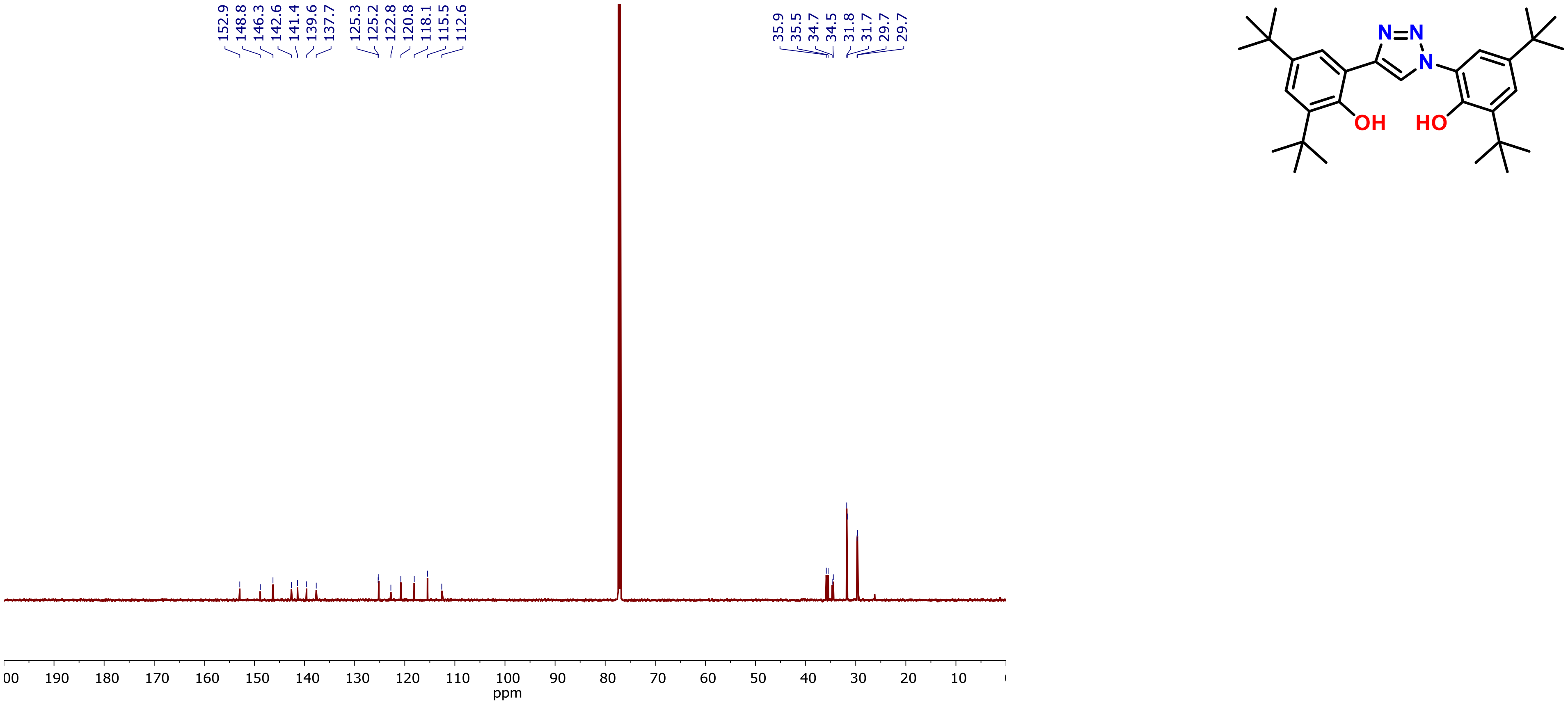


Figure S 14: ^{13}C-NMR of **1** in $CDCl_3$

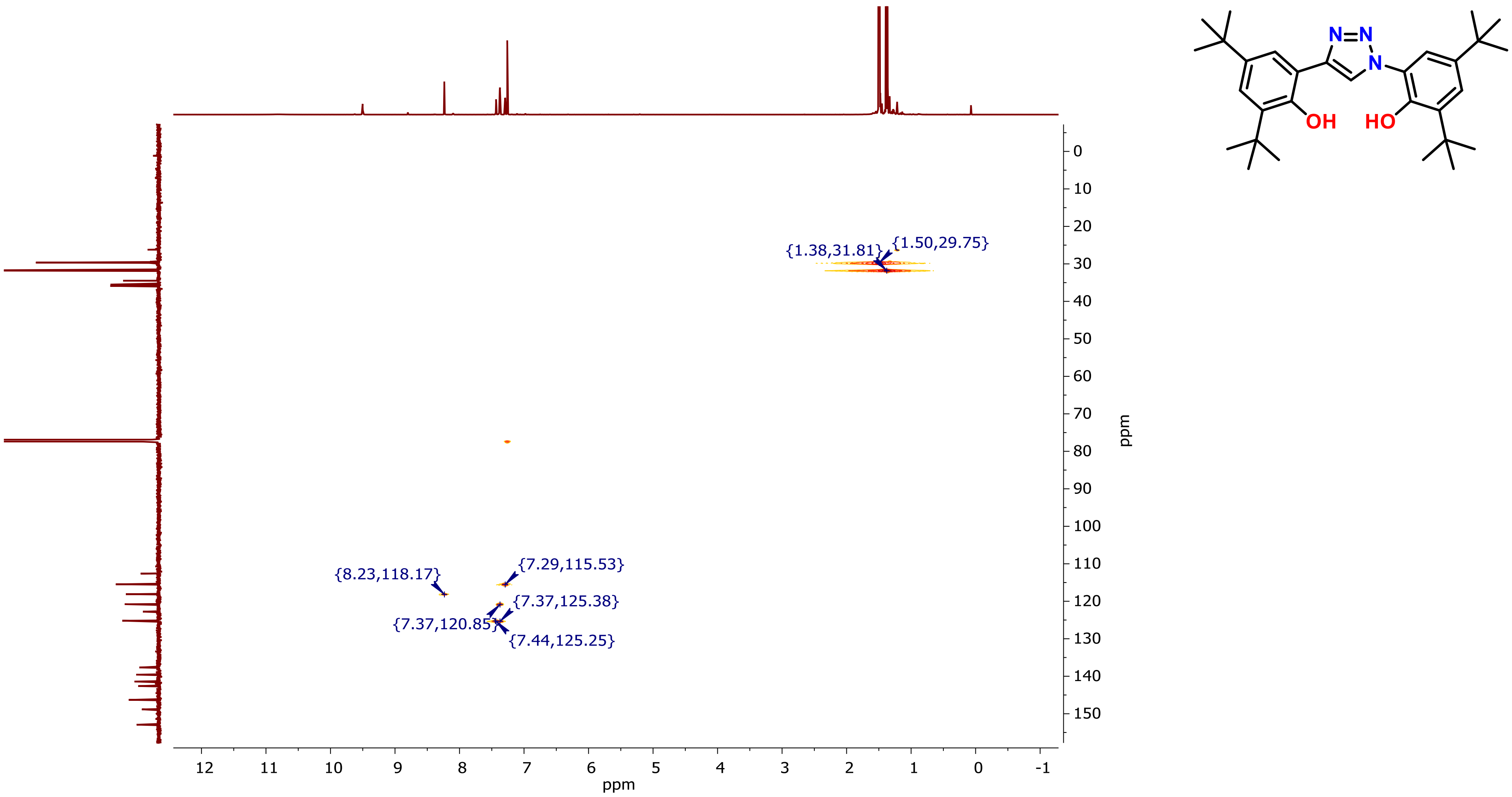


Figure S 15: ^1H-^{13}C HSQC of **1** in $CDCl_3$

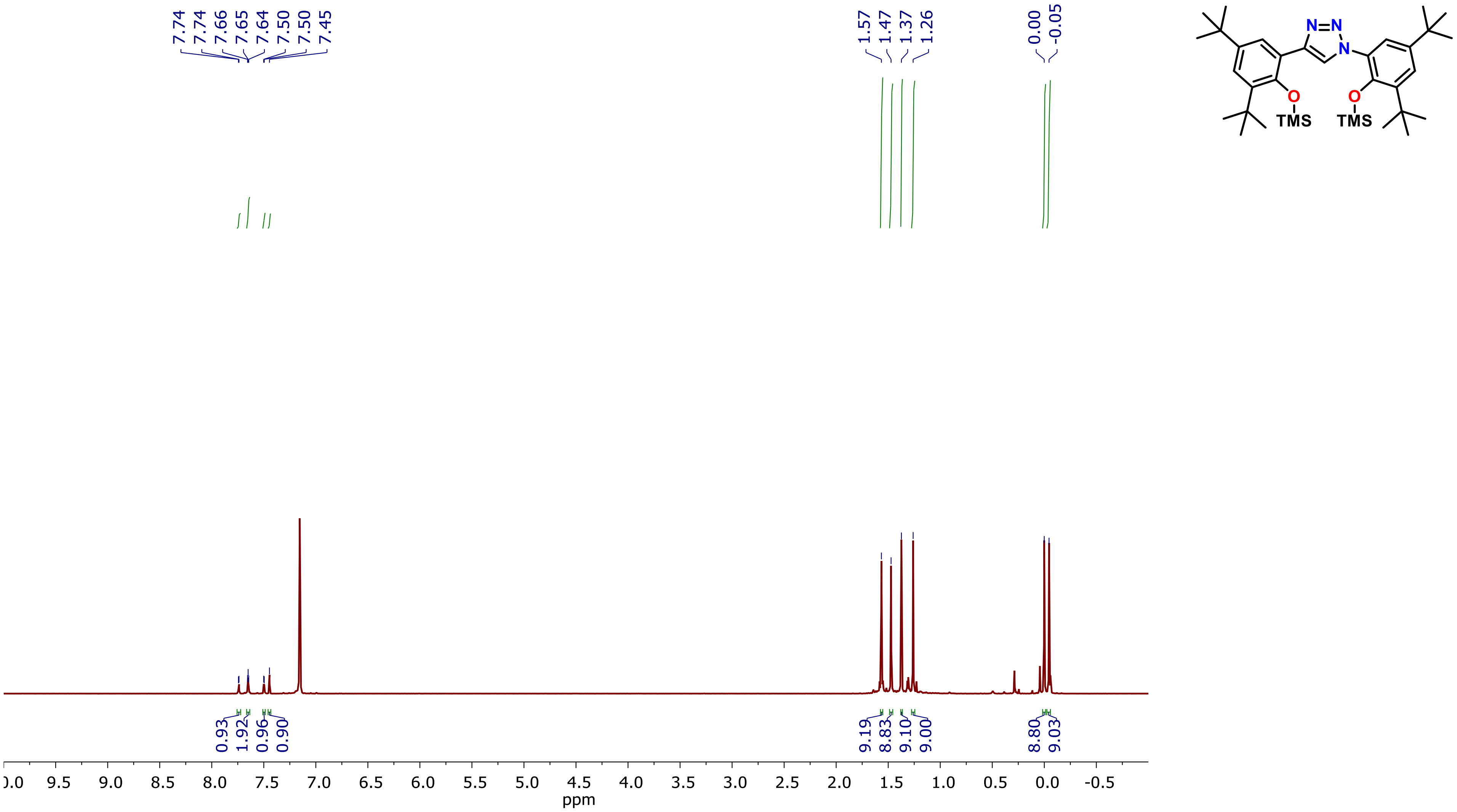


Figure S 16: ^{1}H-NMR of **2** in C_6D_6

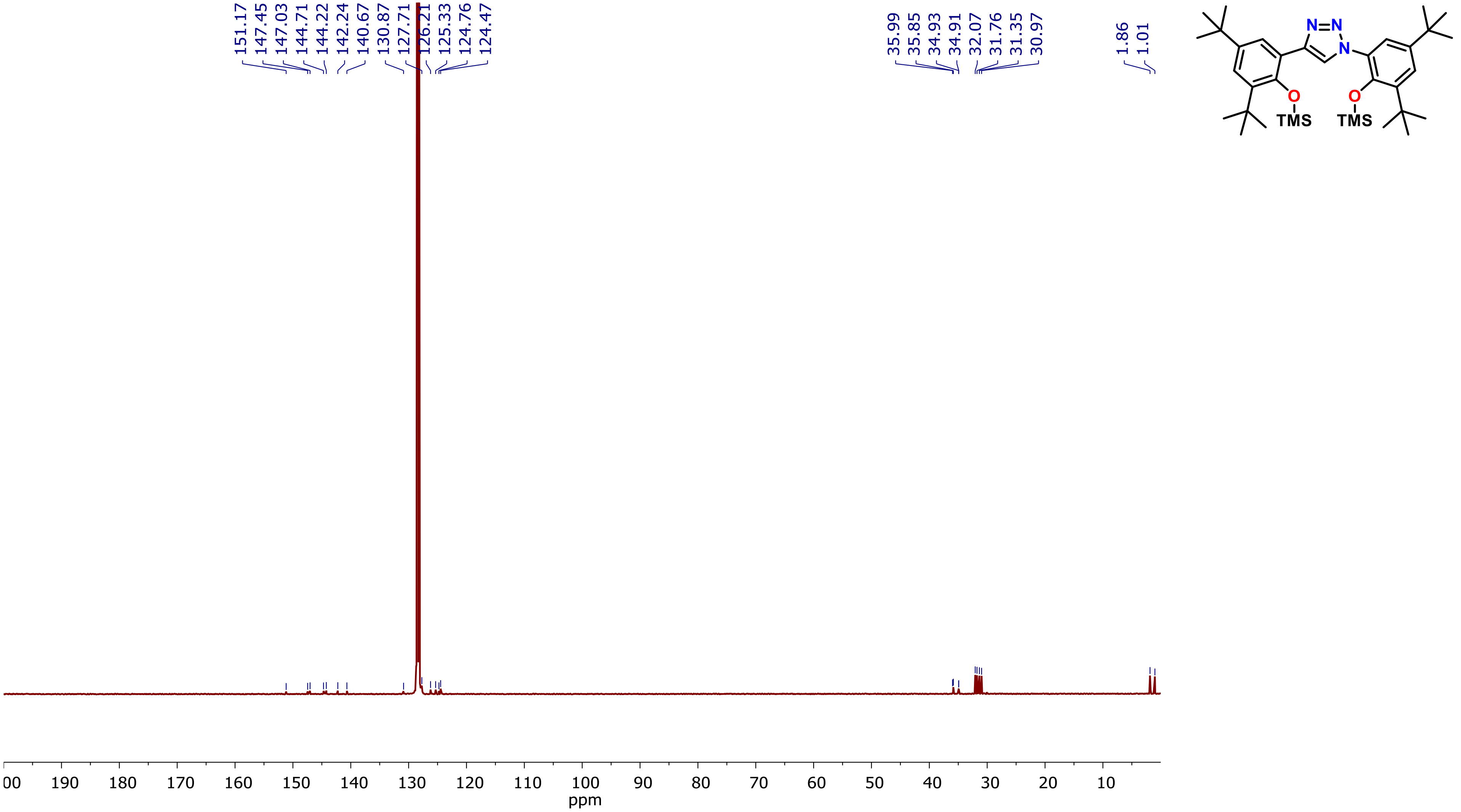
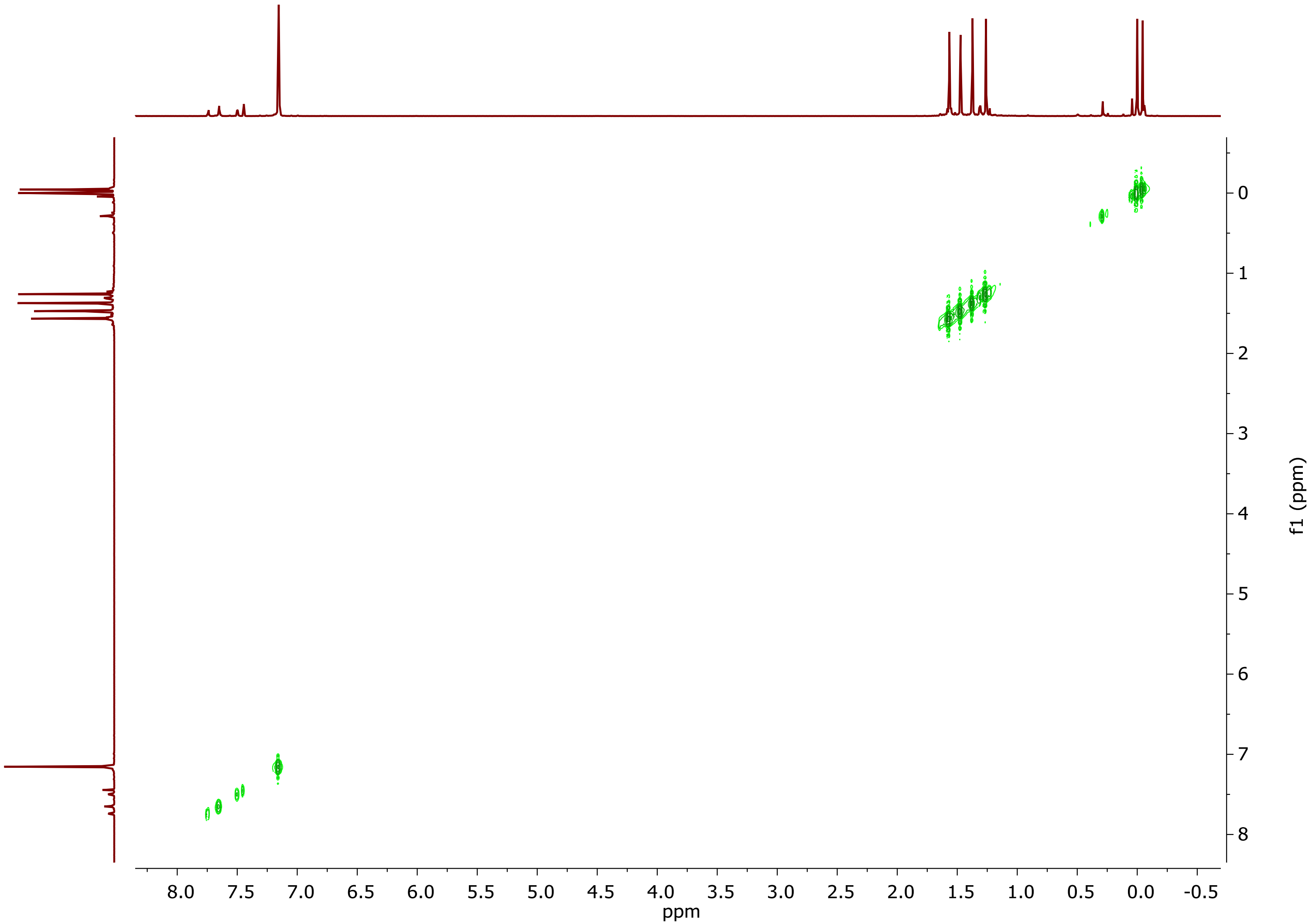


Figure S 17: ^{13}C-NMR of **2** in C_6D_6



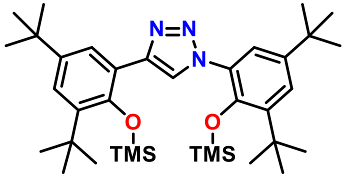


Figure S 18: ^1H-^1H-COSY of **2** in C_6D_6

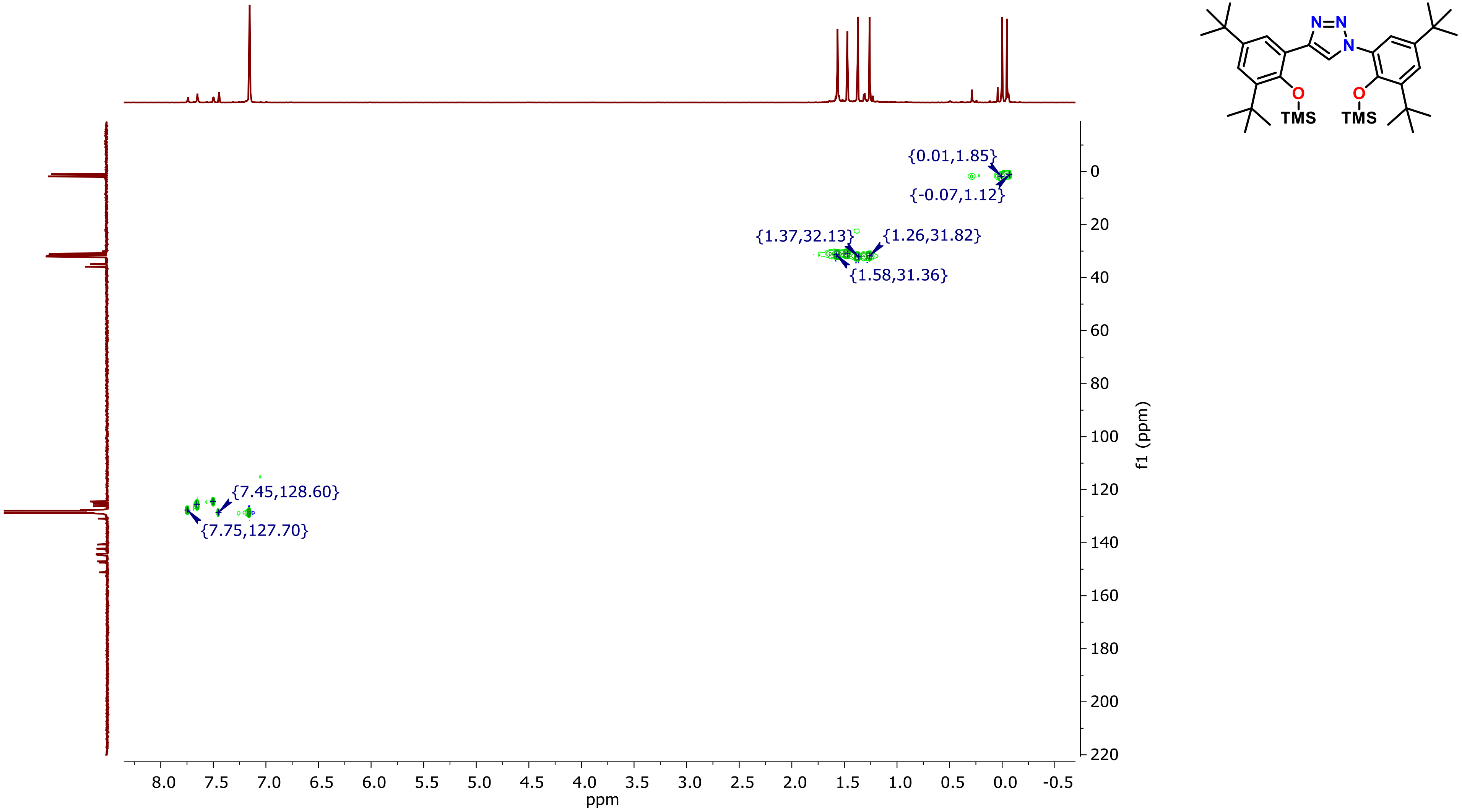


Figure S 19: ^{1}H-^{13}C-HSQC of **2** in C_6D_6

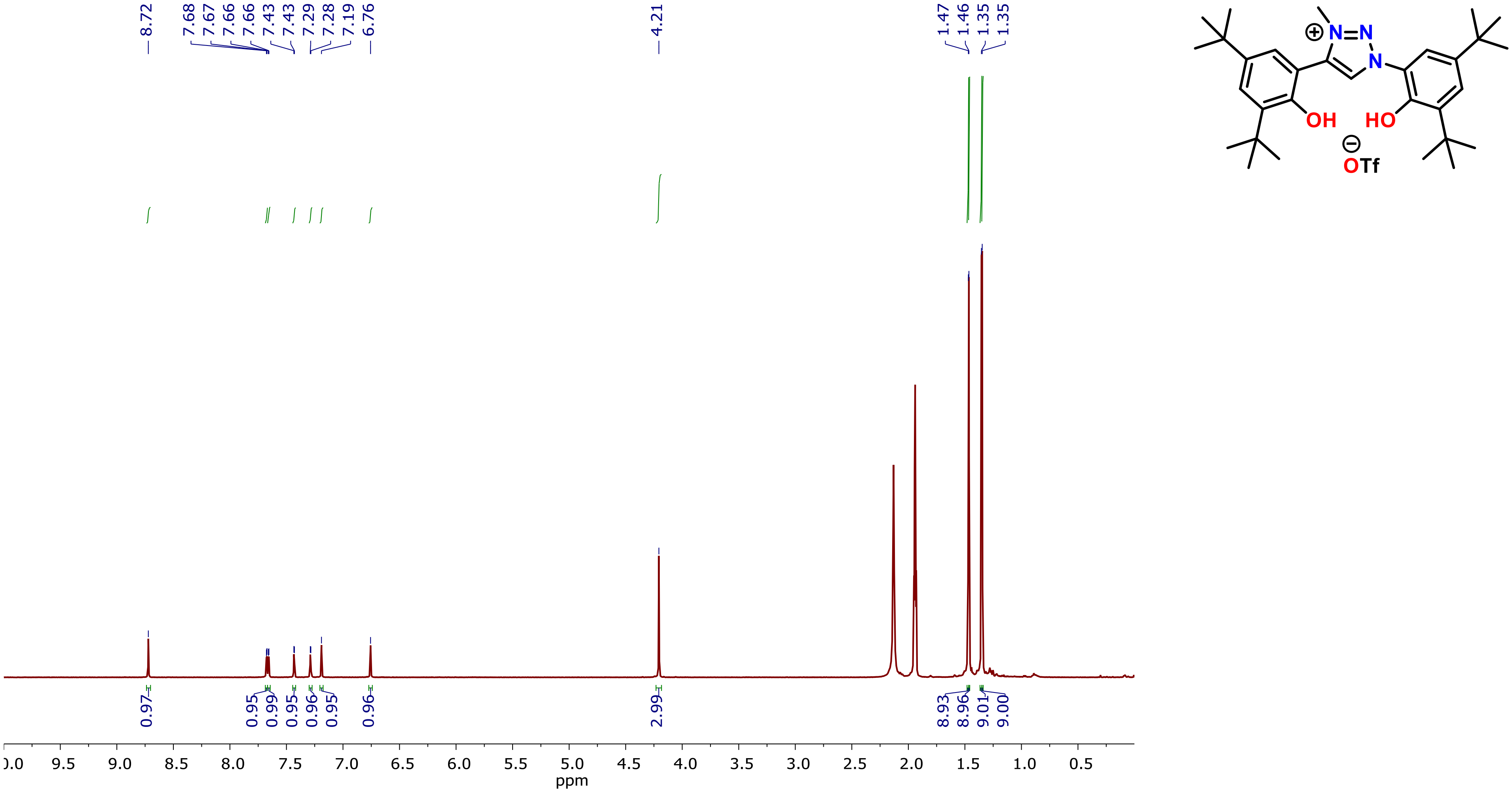


Figure S 20: ^{1}H-NMR of **H_3L[OTf]** in CD_3CN

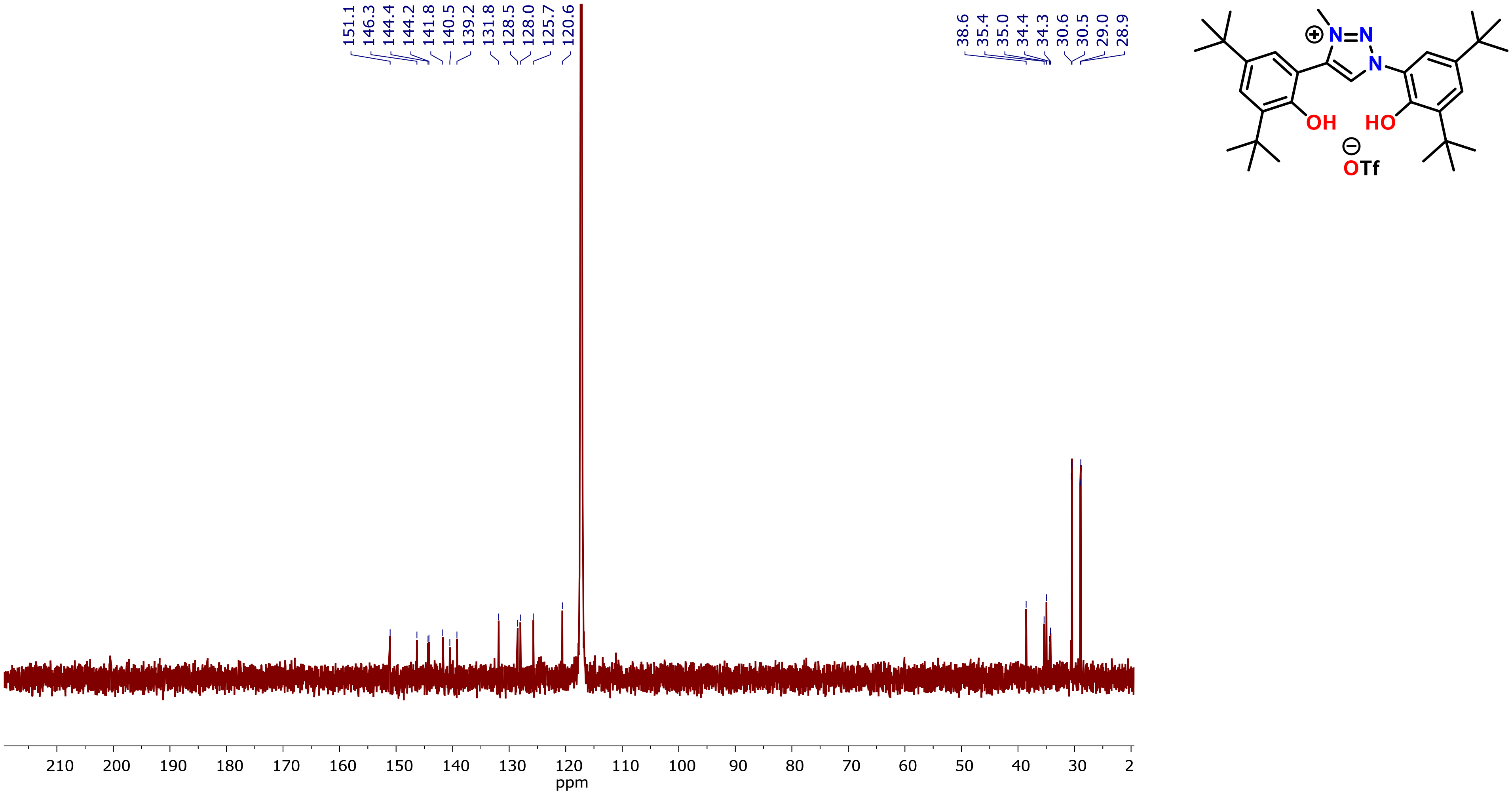


Figure S 21: ^{13}C-NMR of **H$_3$L[OTf]** in CD$_3$CN

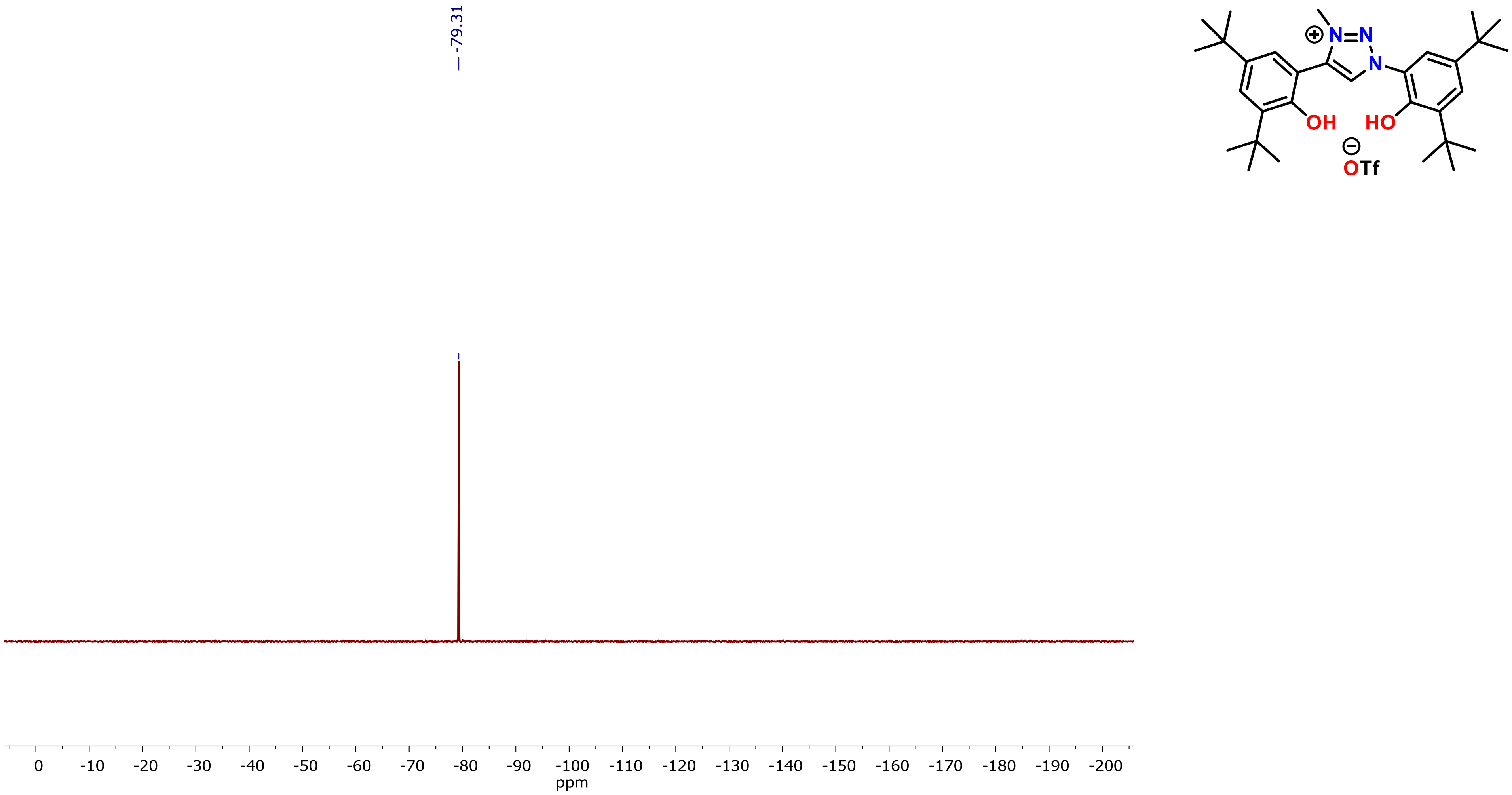


Figure S 22: ^{19}F-NMR of **H_3L[OTf]** in CD_3CN

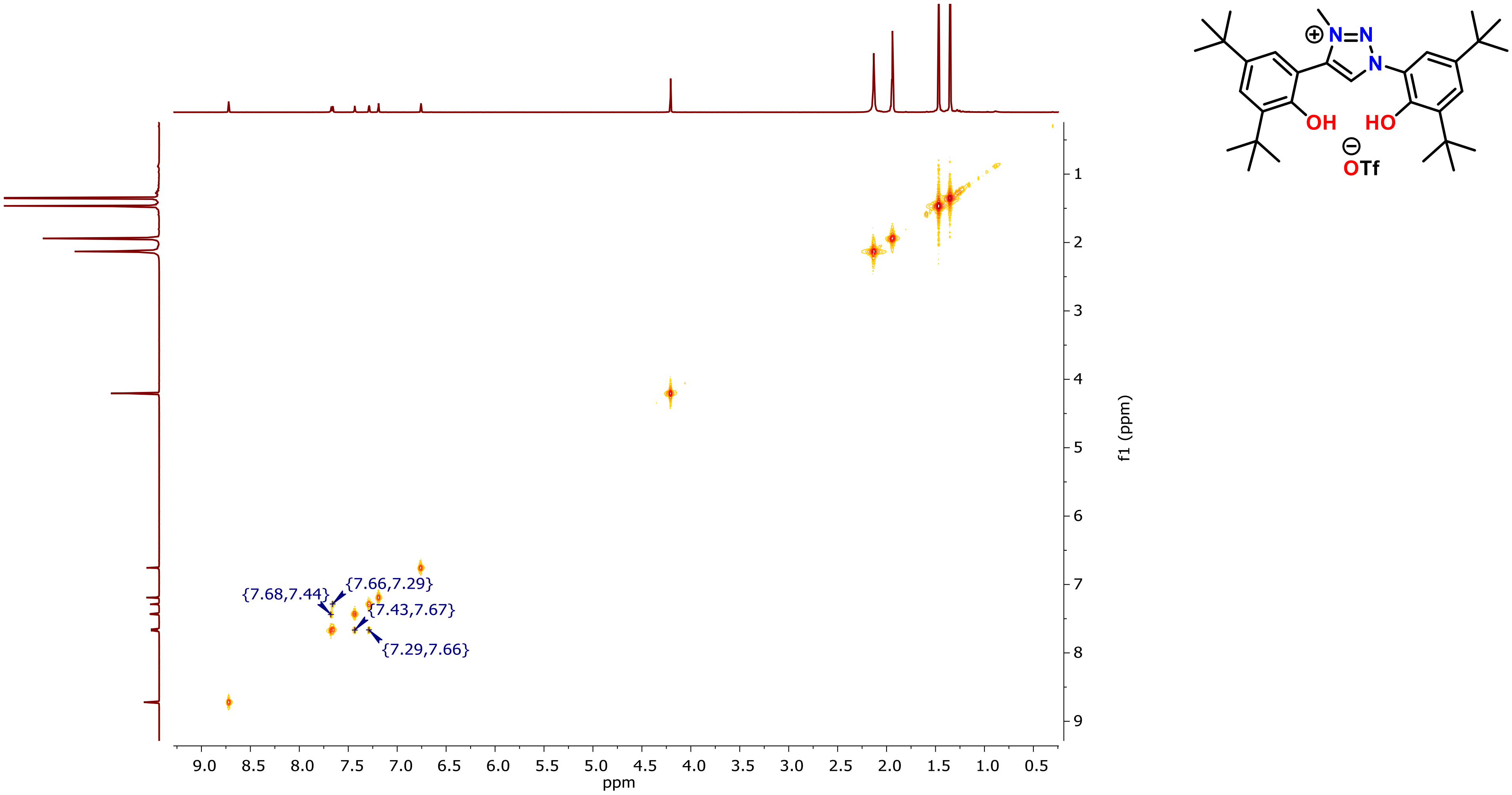


Figure S 23: ^{1}H-^{1}H-COSY of **H_3L[OTf]** in CD_3CN

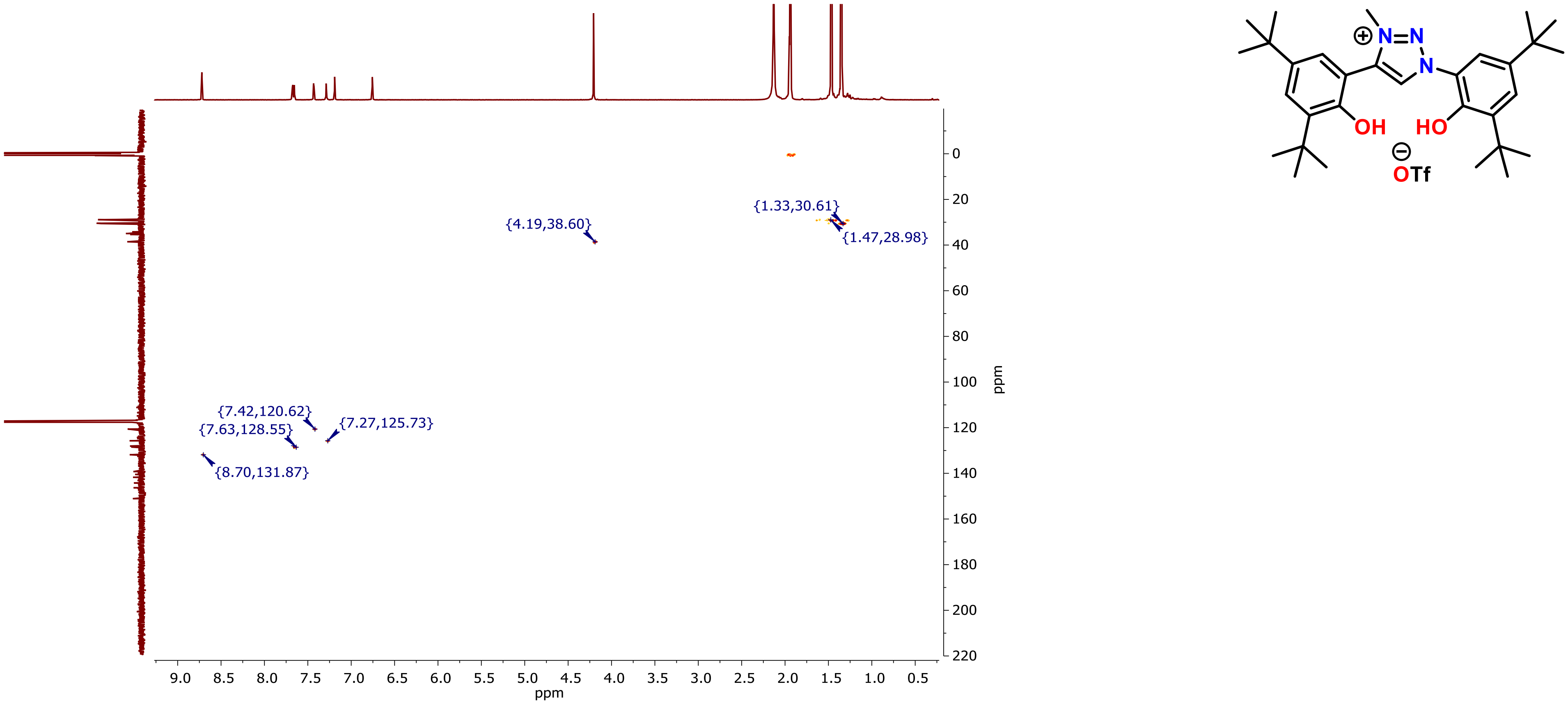


Figure S 24: ^{1}H-^{13}C HSQC NMR of **$H_3L[OTf]$** in CD_3CN

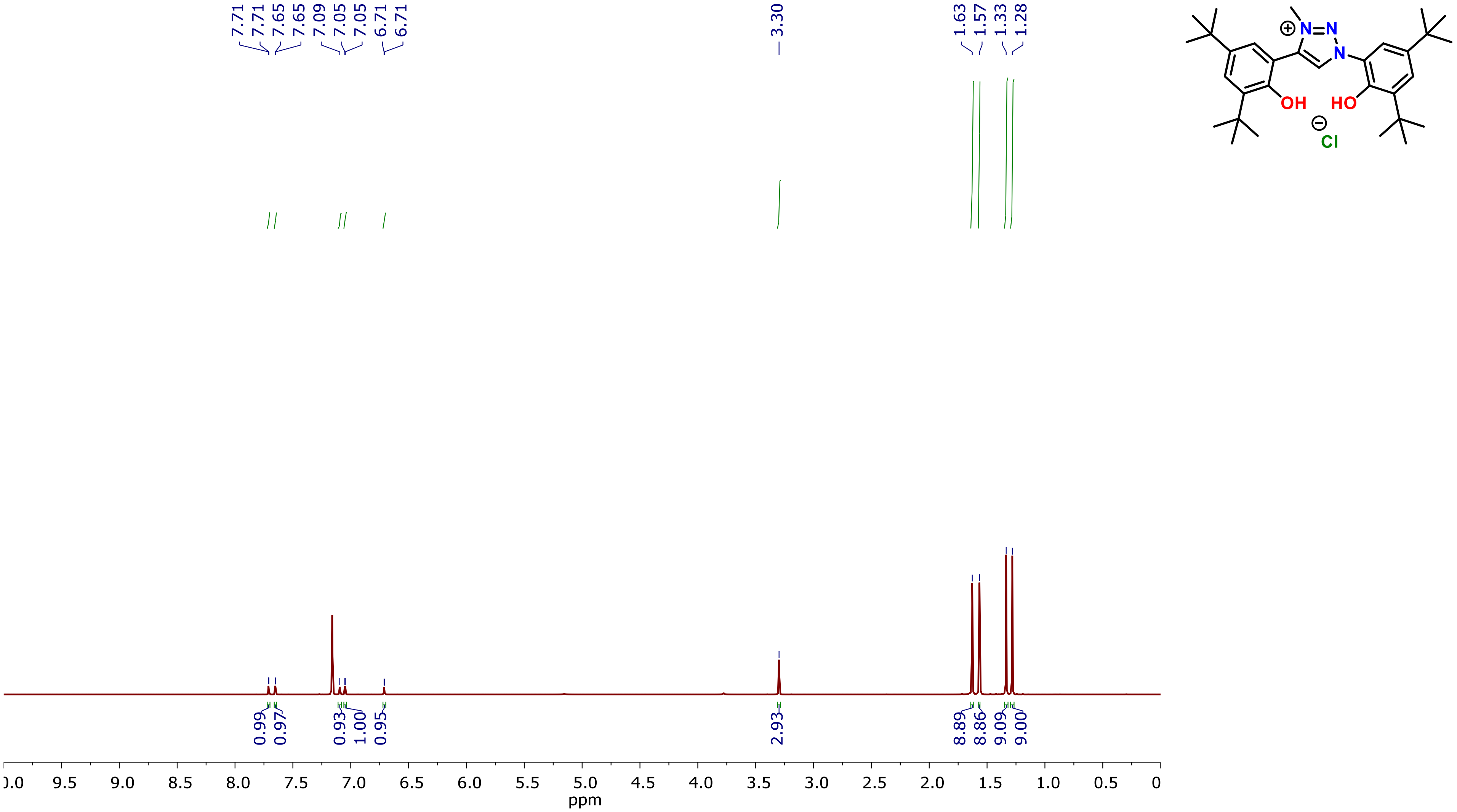


Figure S 25: ^{1}H-NMR of **H_3L[Cl]** in C_6D_6

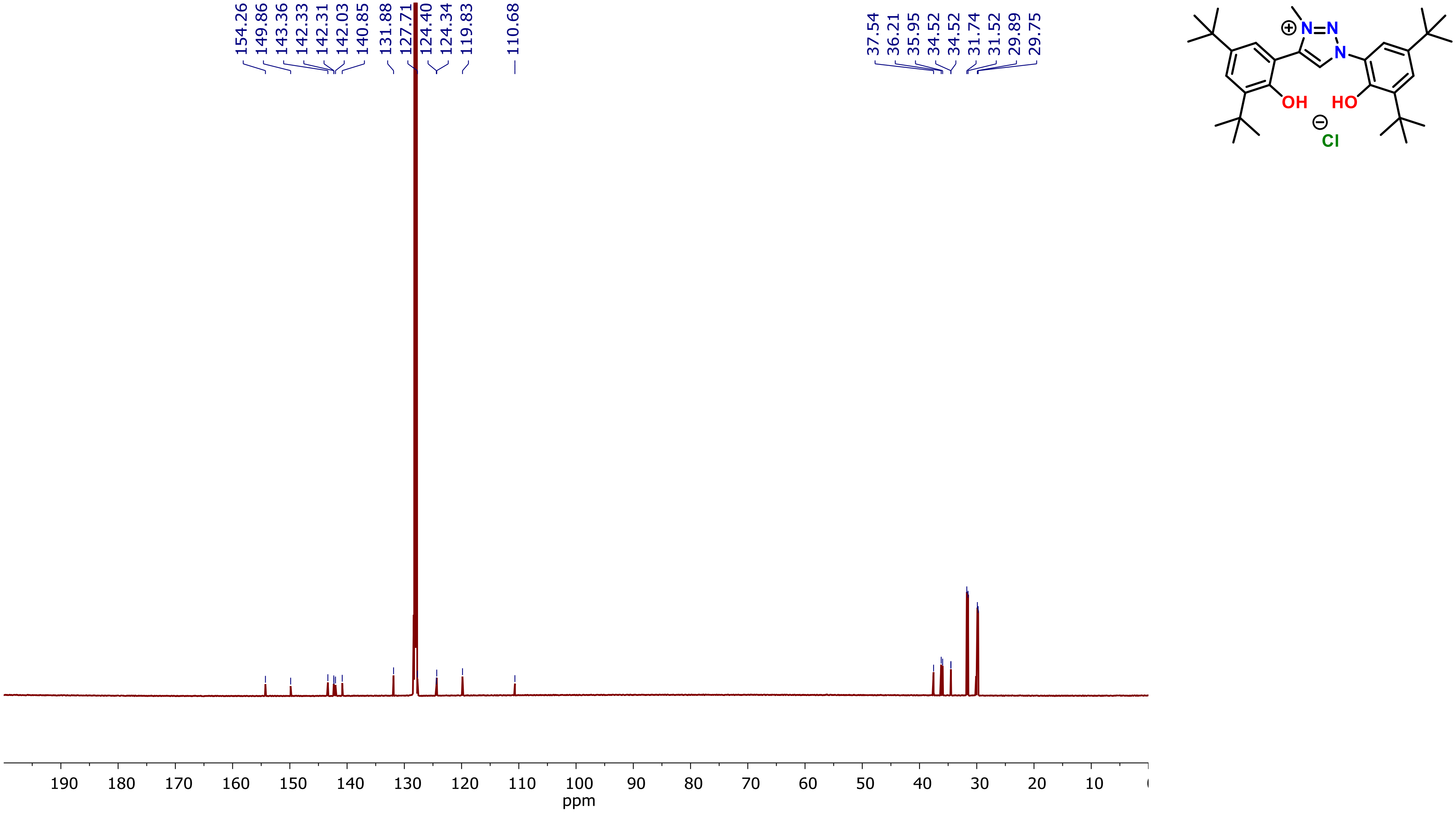


Figure S 26: ^{13}C-NMR of **H_3L[Cl]** in C_6D_6

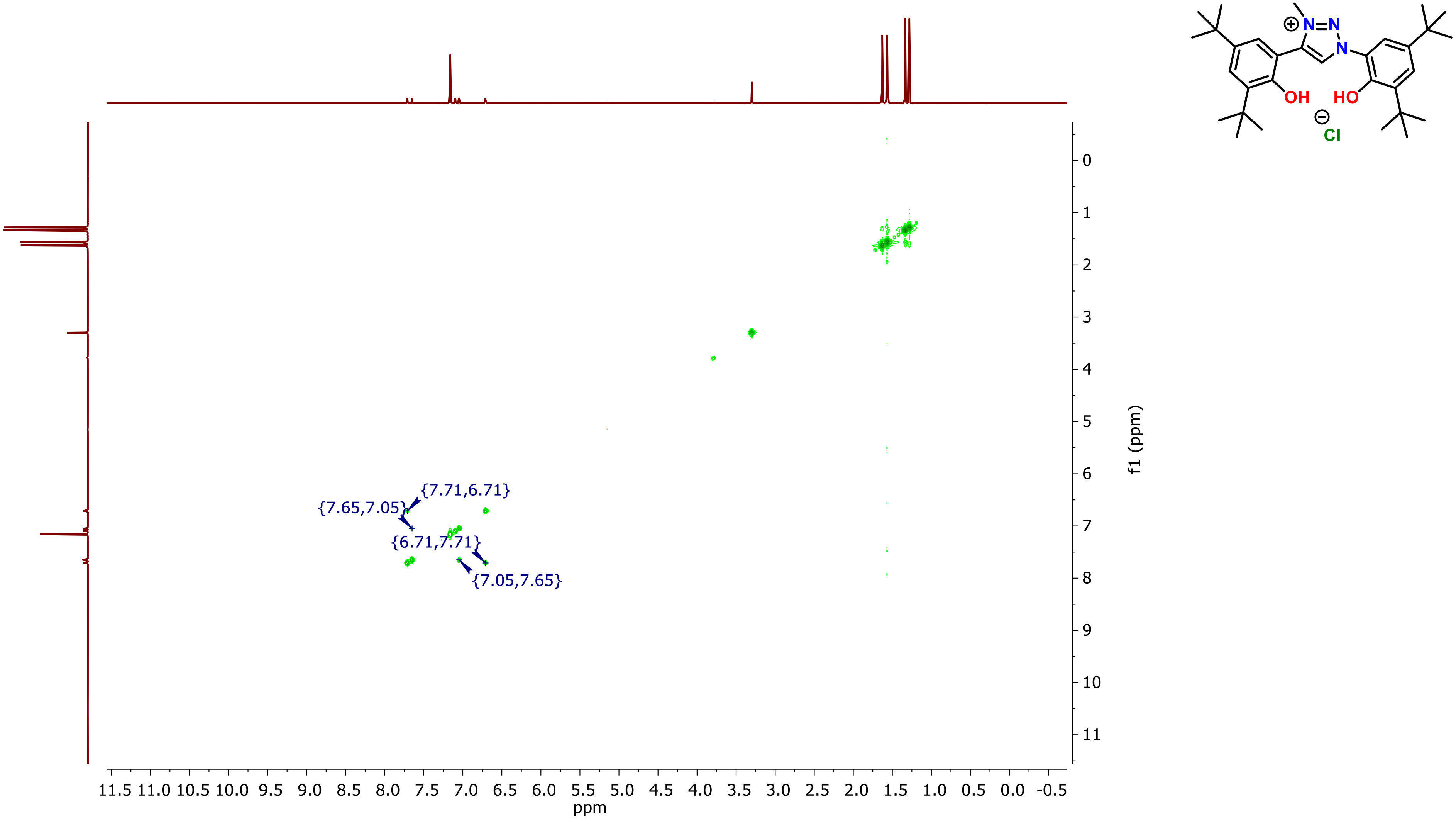
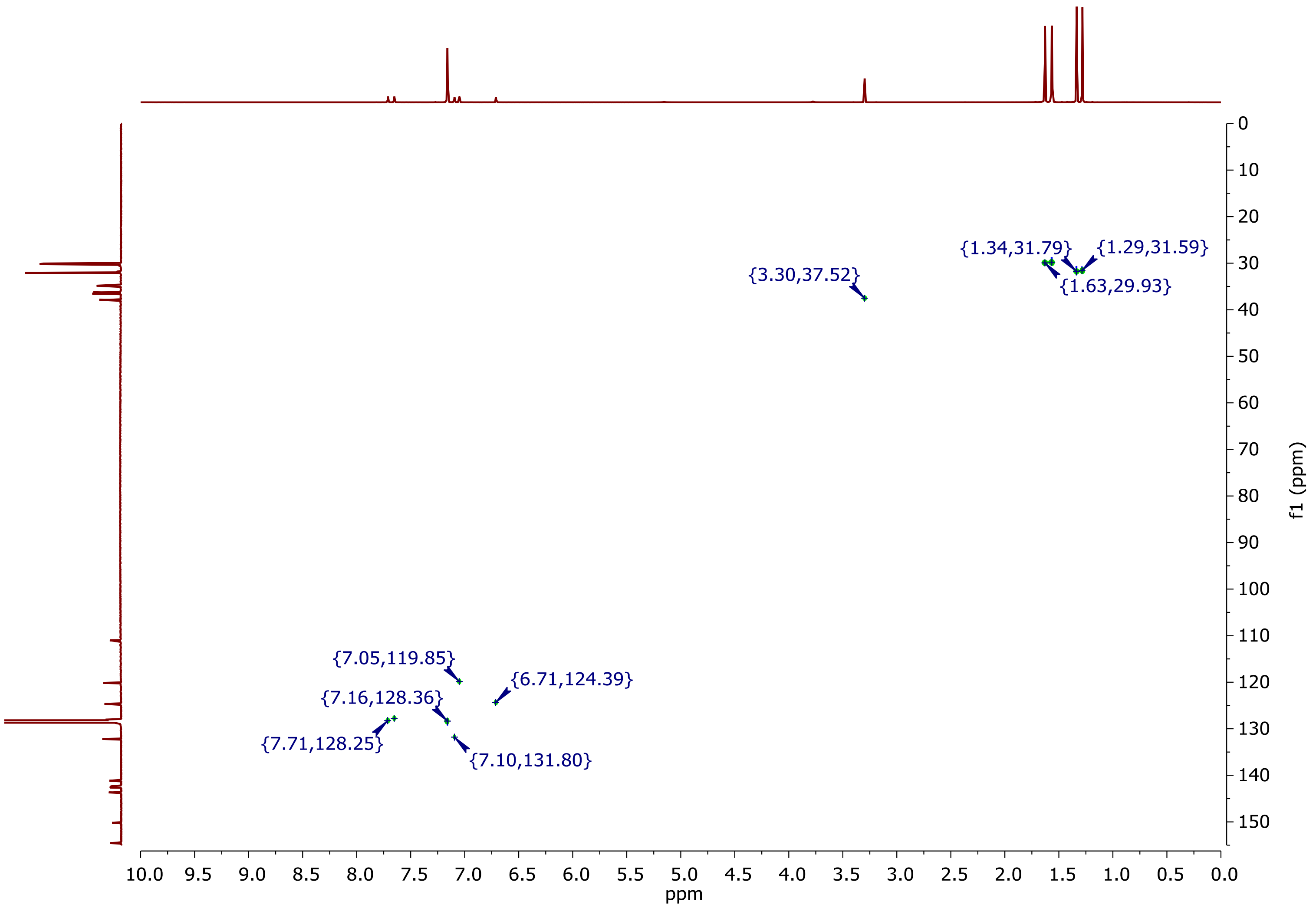


Figure S 27: ^1H-^1H-COSY of **$H_3L[Cl]$** in C_6D_6



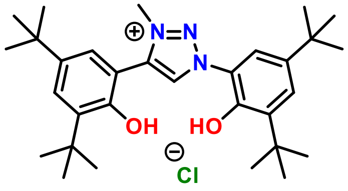


Figure S 28: ^{1}H-^{13}C-HSQC of **H$_3$L[Cl]** in C_6D_6

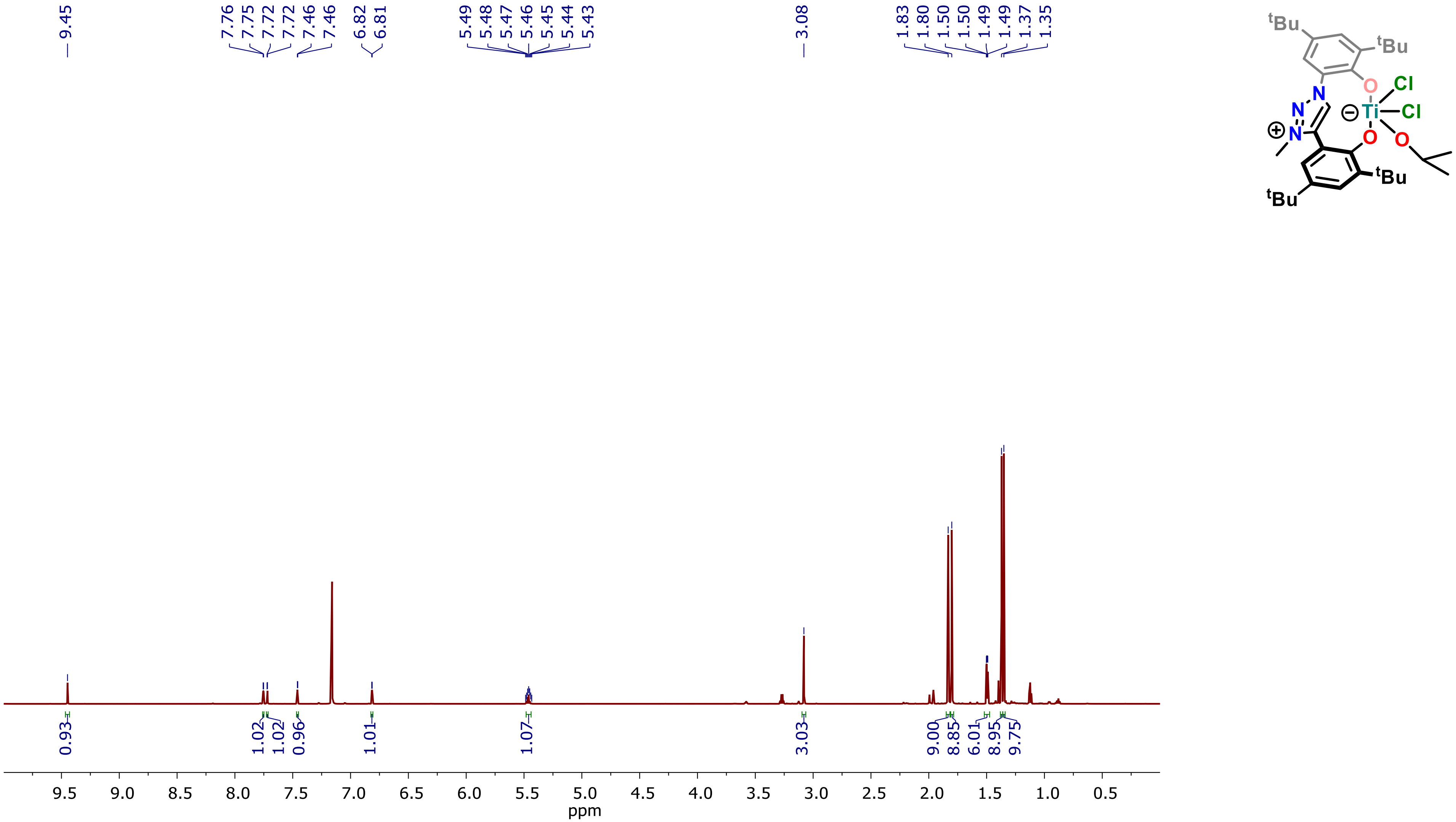


Figure S 29: ^{1}H-NMR of **3** in C_6D_6

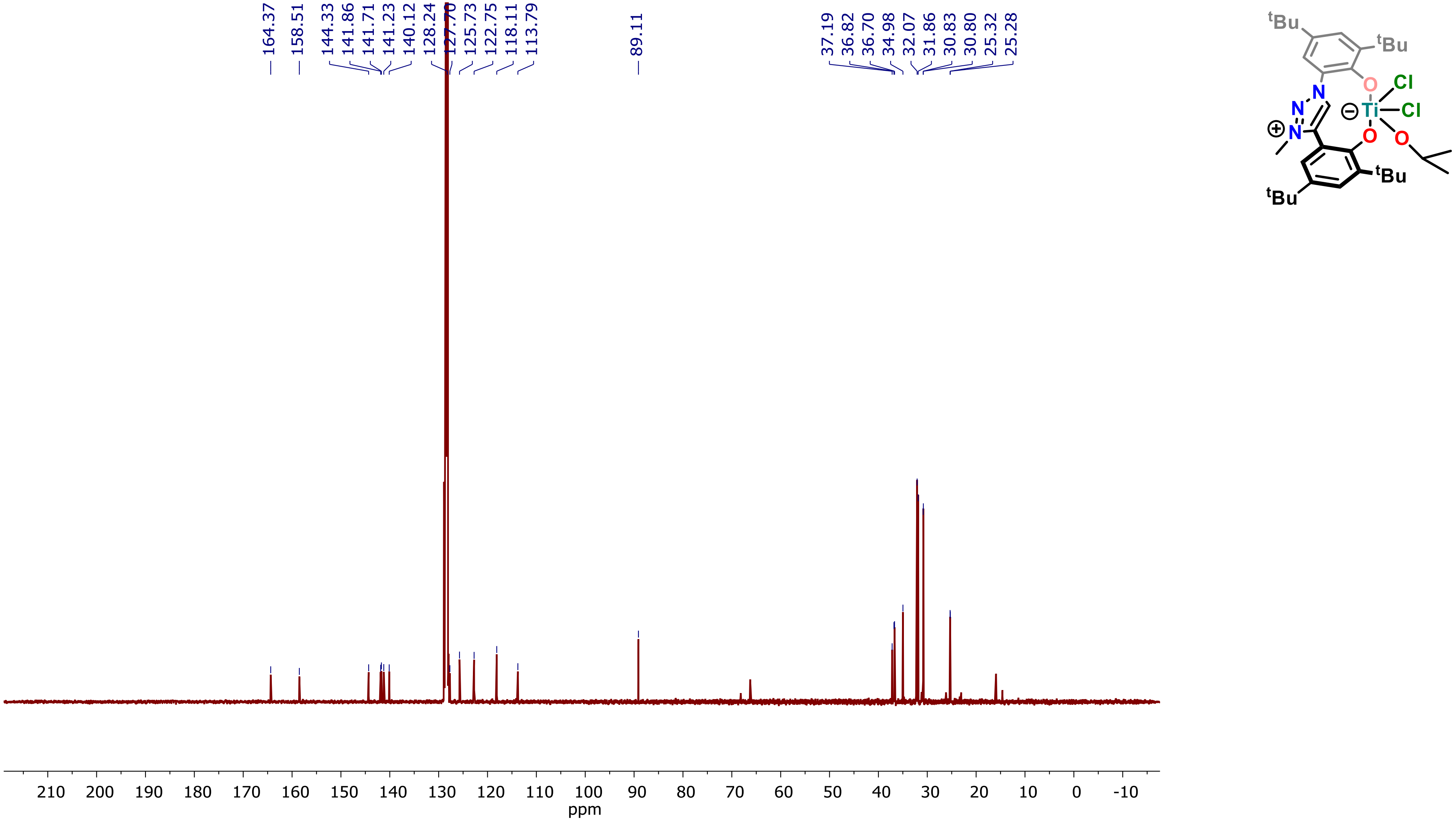


Figure S 30: ^{13}C-NMR of **3** in C_6D_6

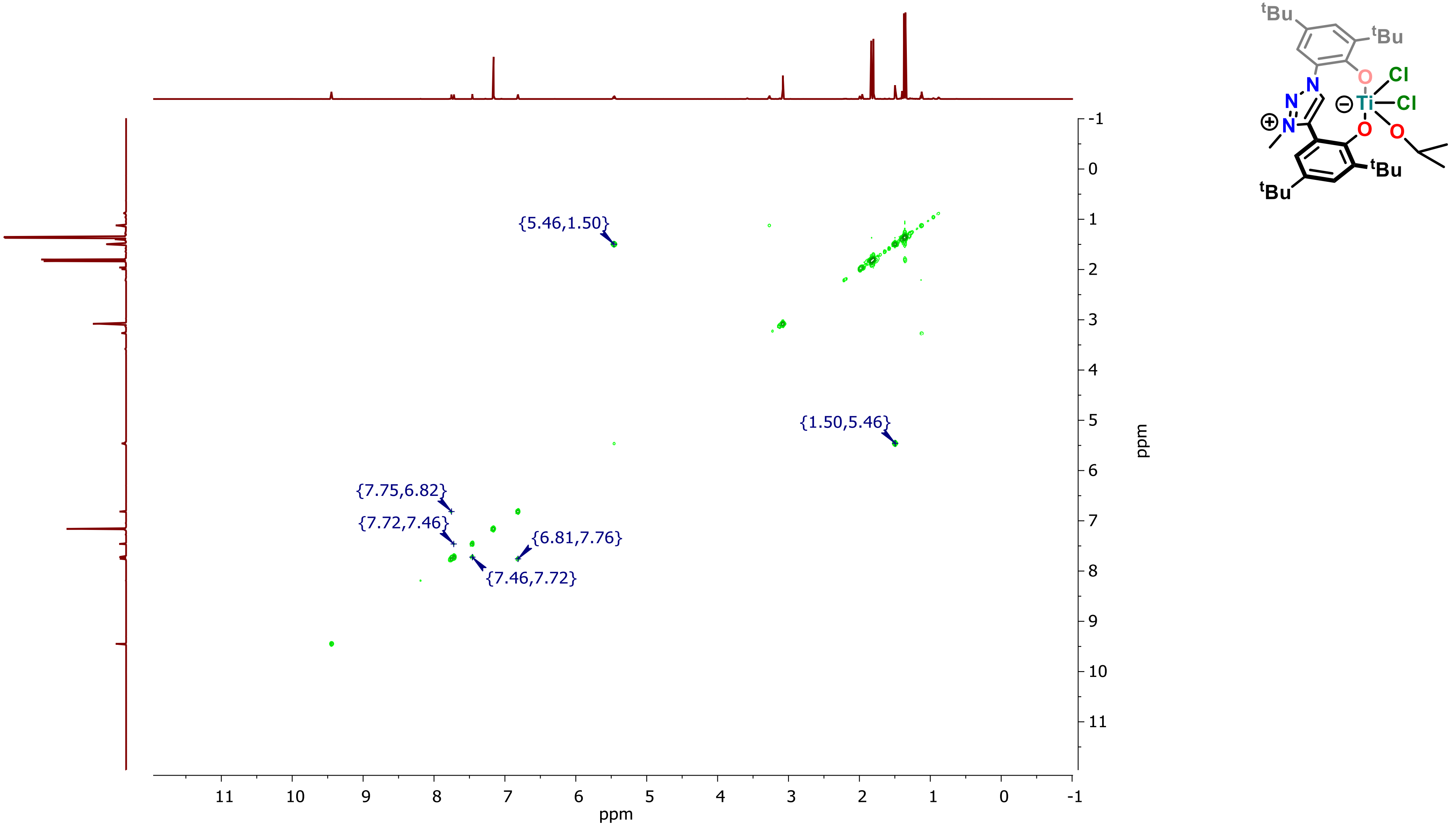


Figure S 31: ^1H-^1H COSY of **3** in C_6D_6

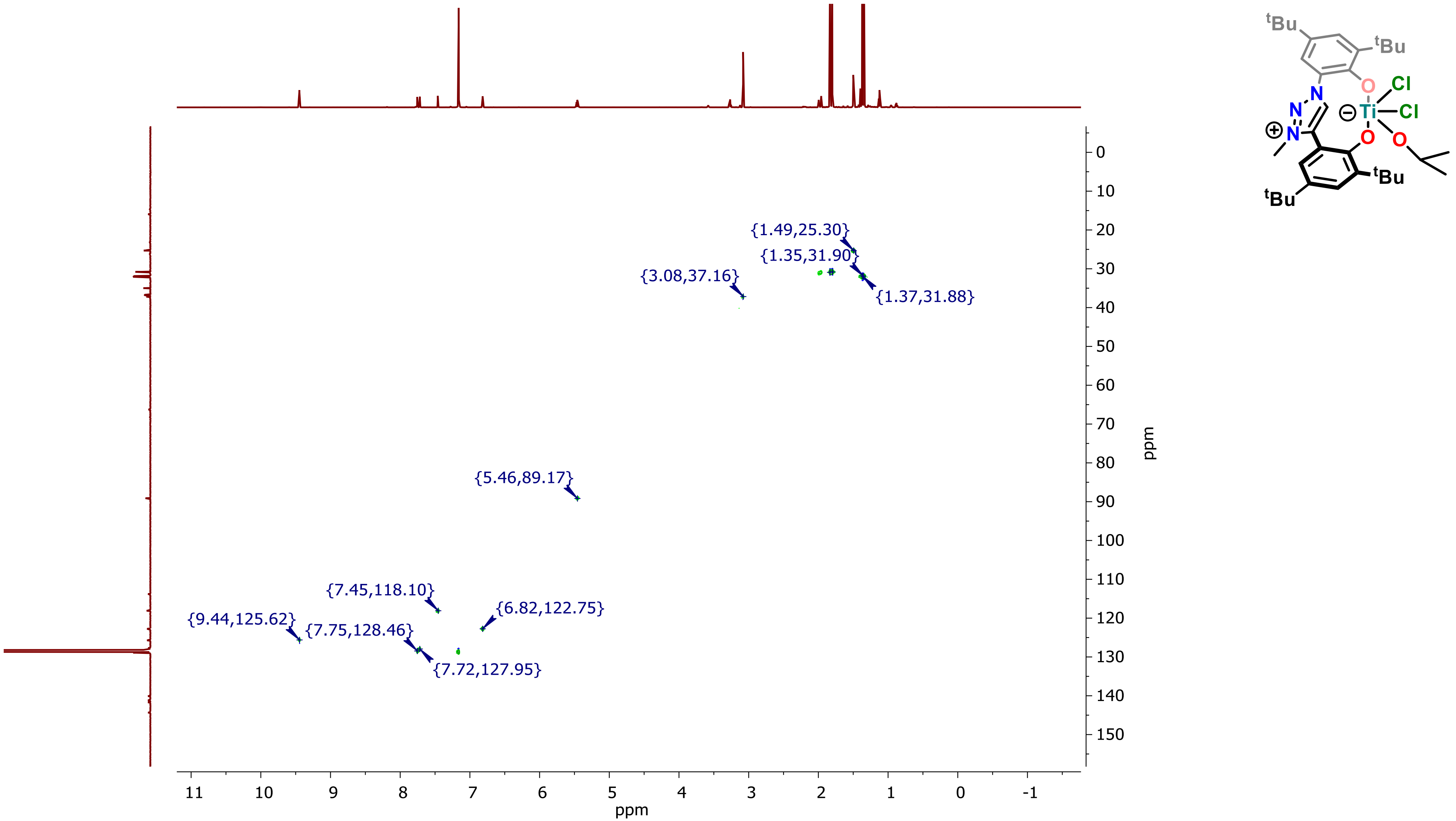
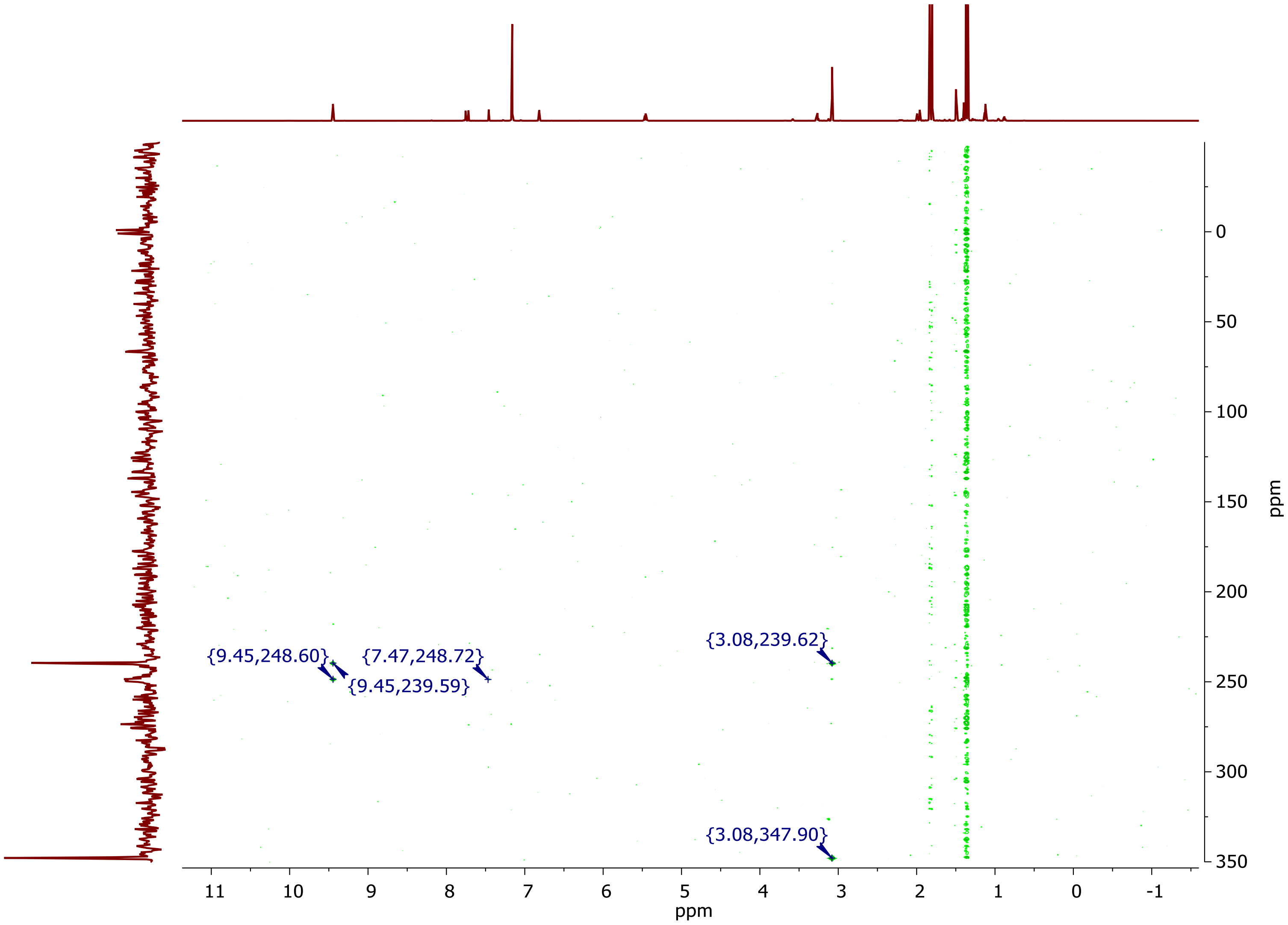


Figure S 32: ^{1}H-^{13}C- HSQC of **3** in C_6D_6



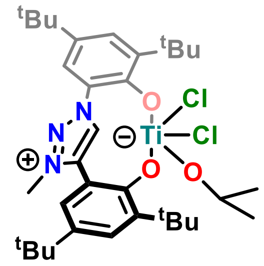


Figure S 33: ^{1}H-^{15}N HMBC of **3** in C_6D_6

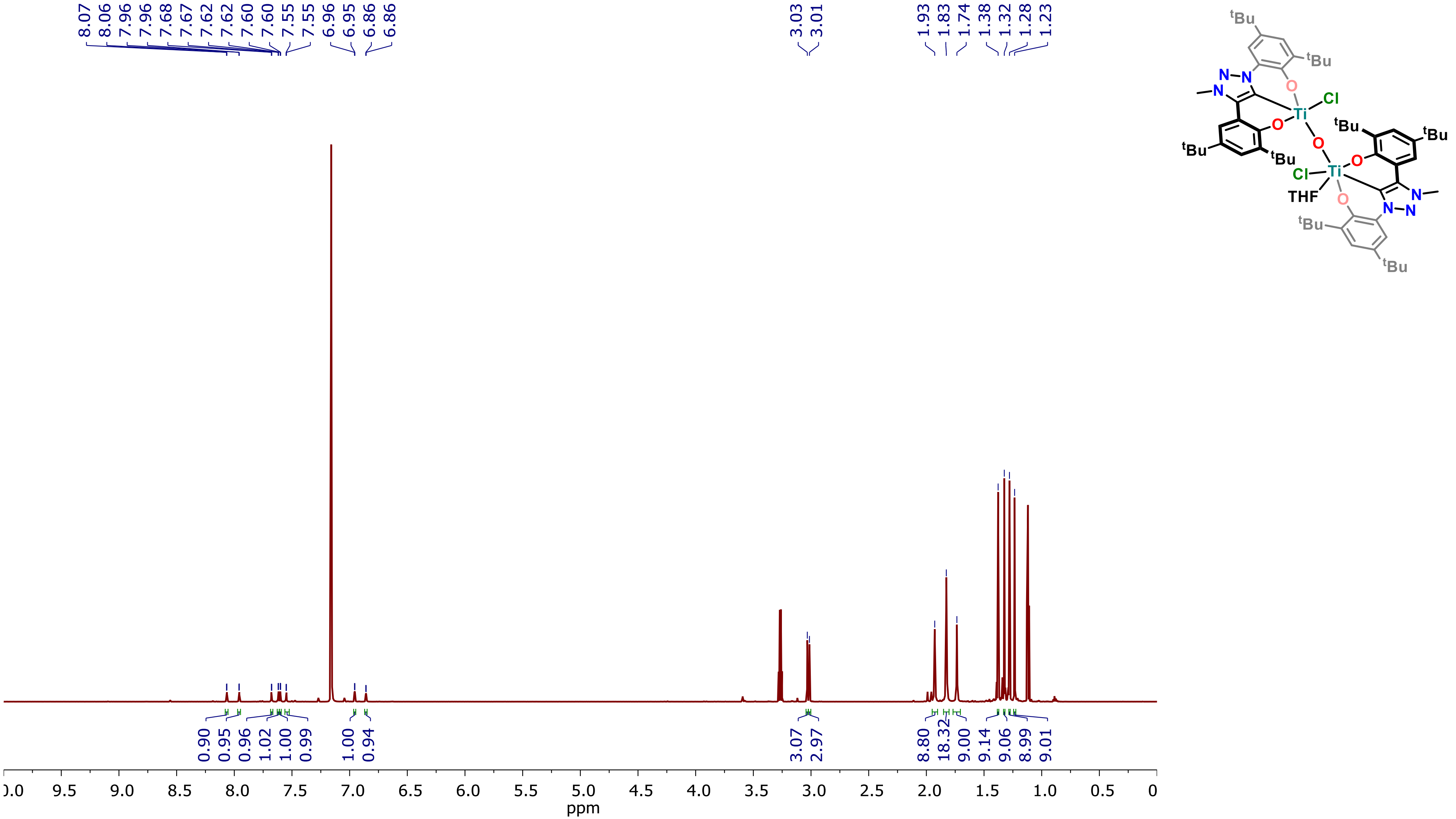


Figure S 34: ^{1}H-NMR of **4** in C_6D_6

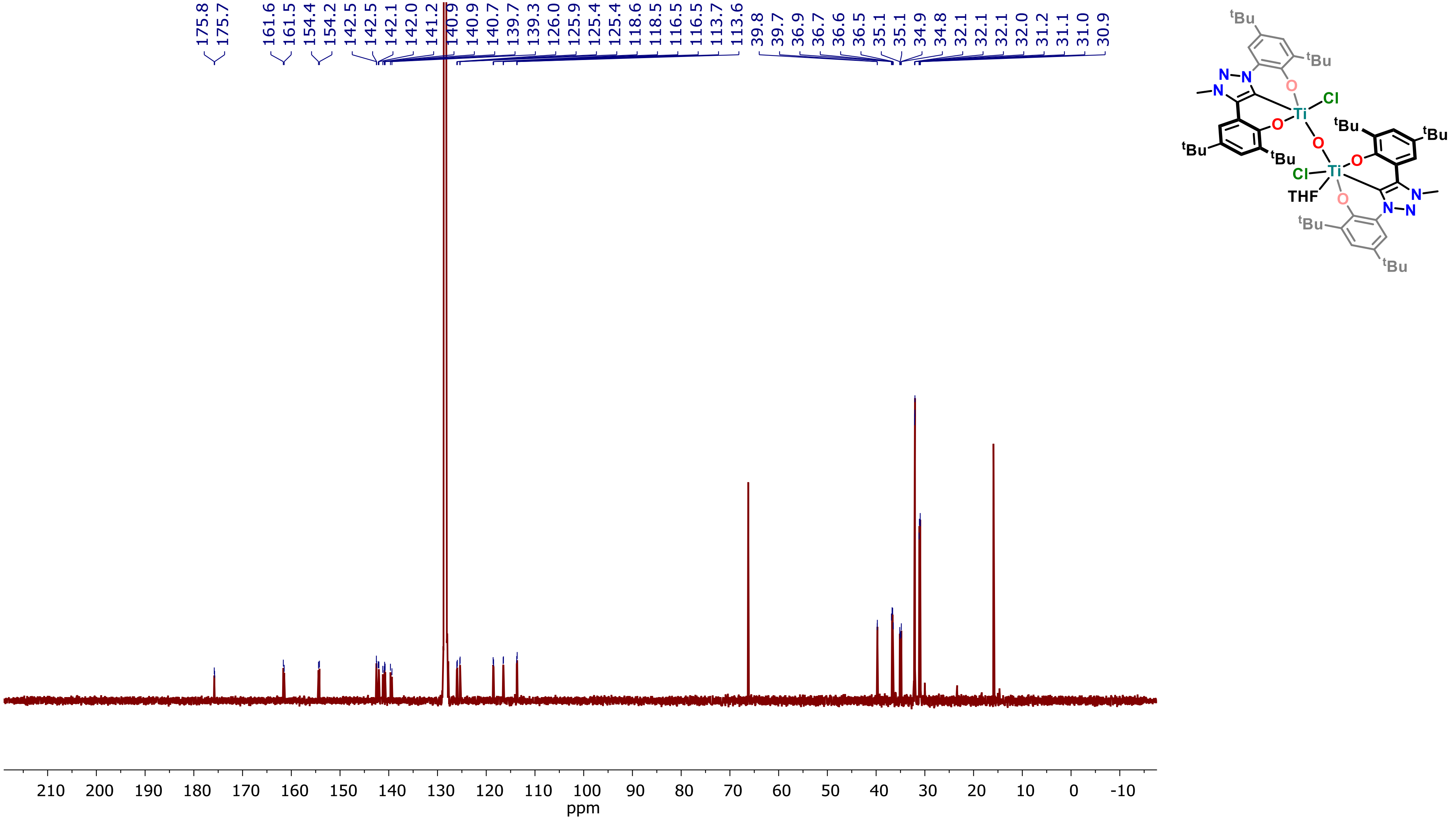


Figure S 35: ^{13}C-NMR of **4** in C_6D_6

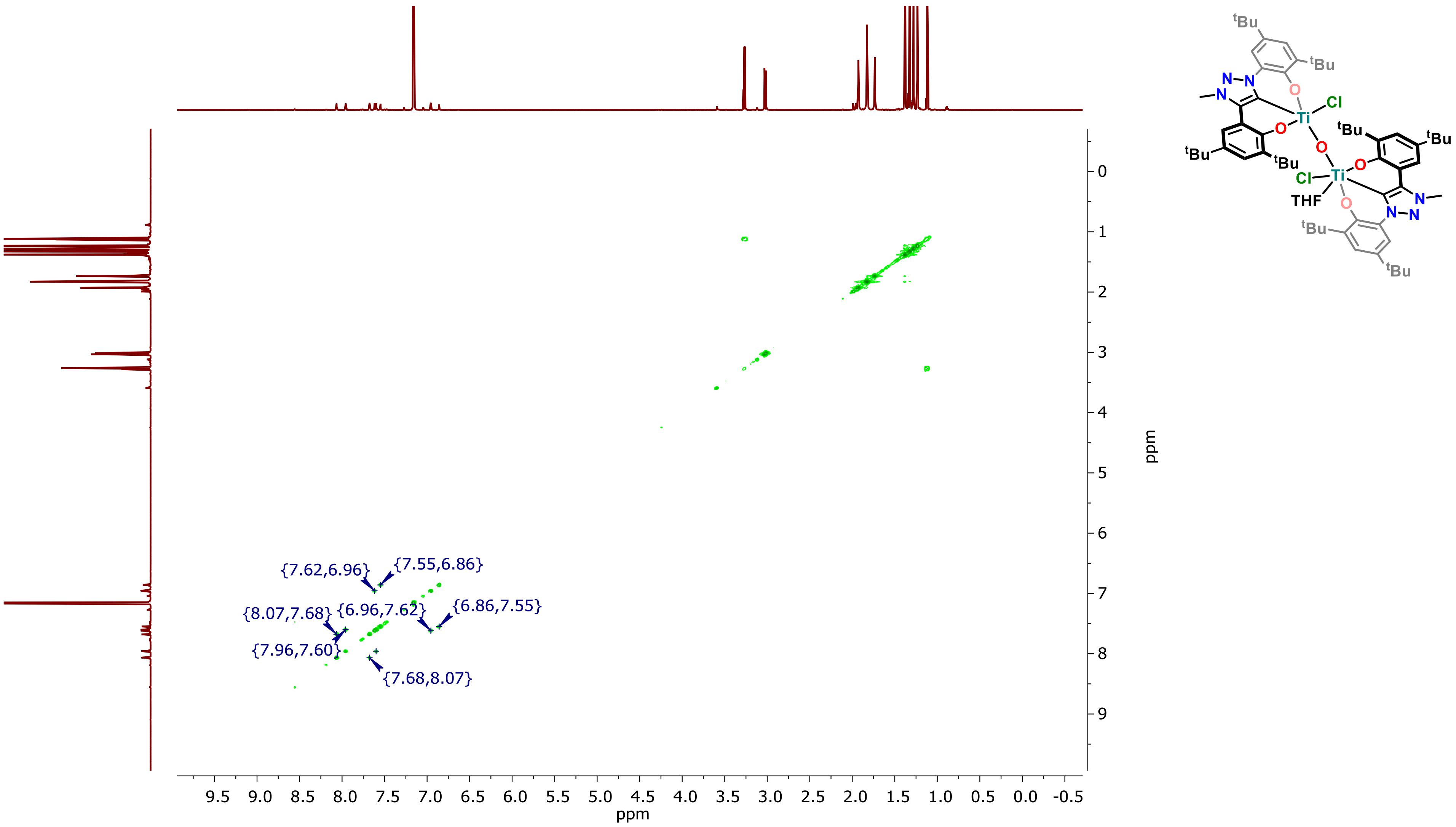


Figure S 36: ^{1}H-^{1}H COSY of **4** in C_6D_6

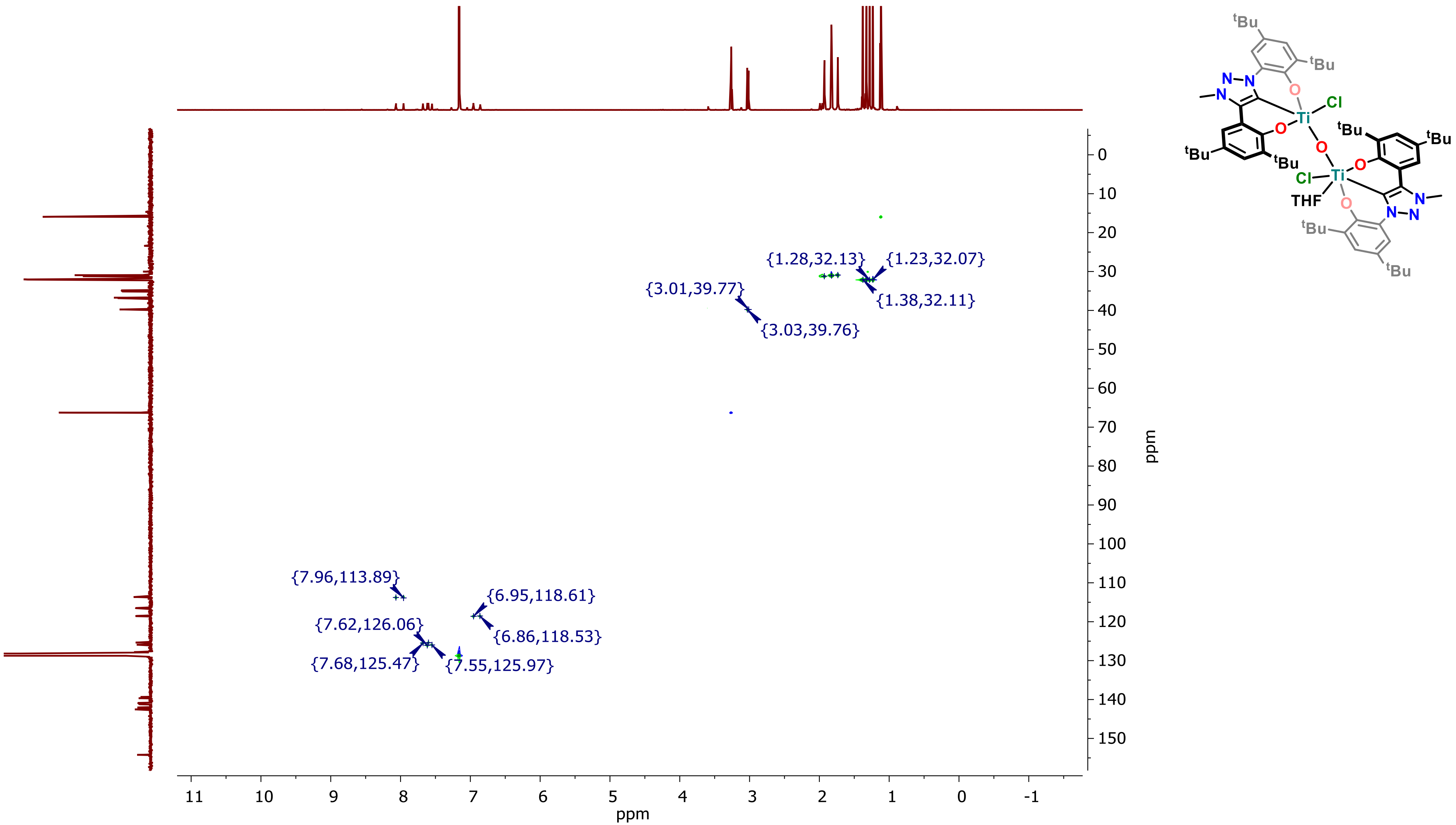


Figure S 37: ^{1}H-^{13}C HSQC of **4** in C_6D_6

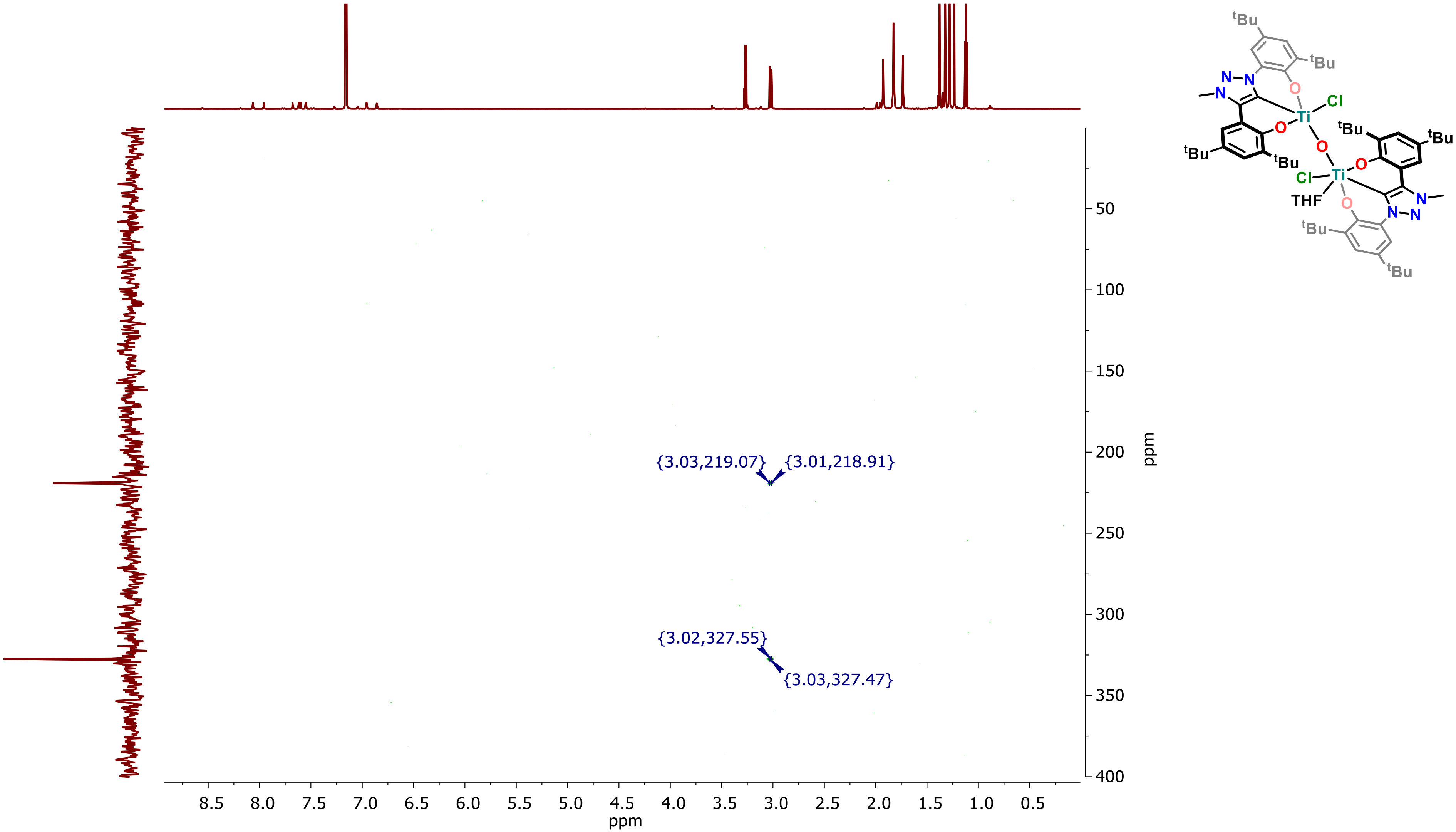


Figure S 38: ^1H-^{15}N HMBC of **4** in C_6D_6

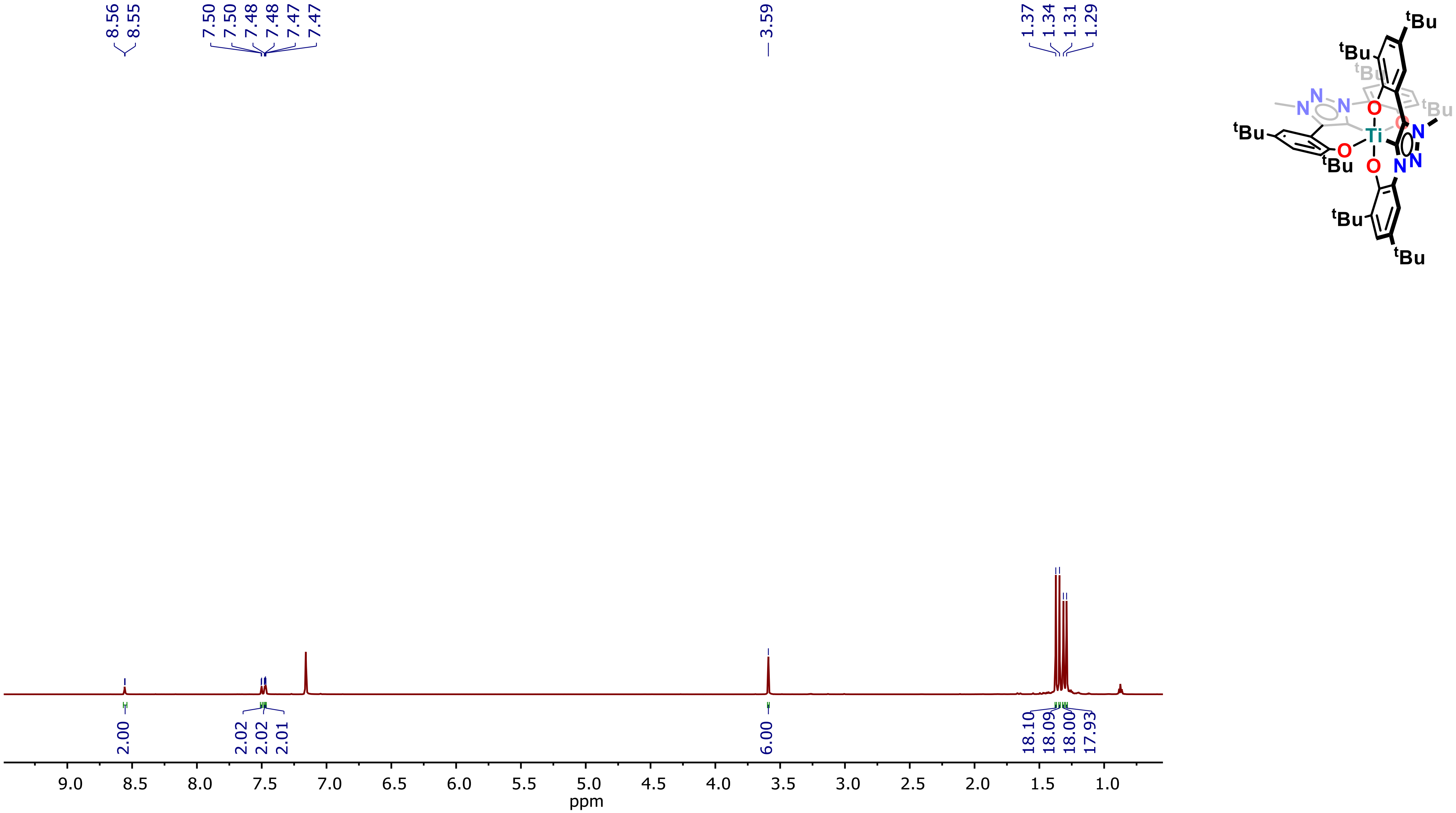


Figure S 39: ^{1}H-NMR of **5** in C_6D_6

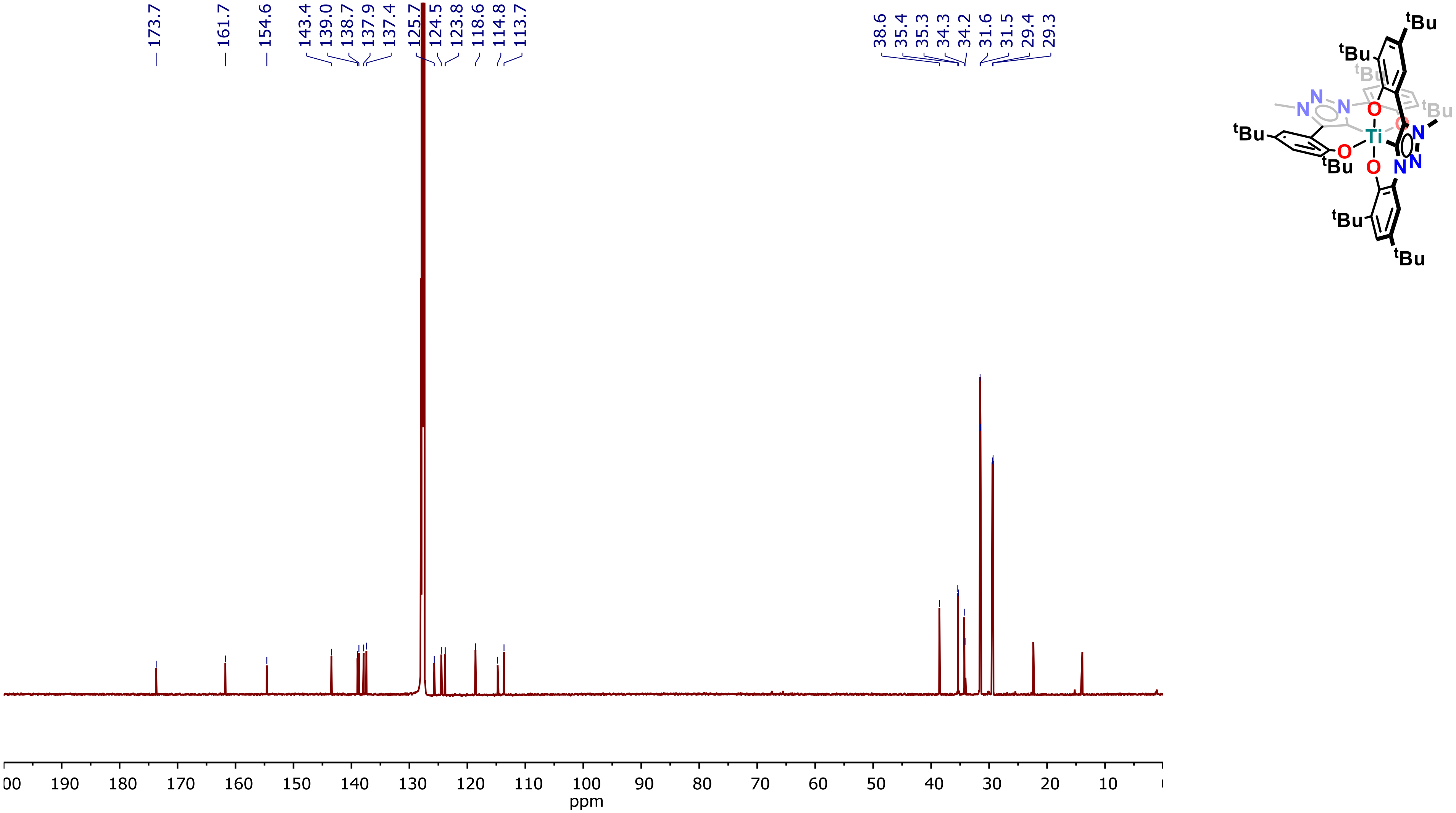


Figure S 40: ^{13}C-NMR of **5** in C_6D_6

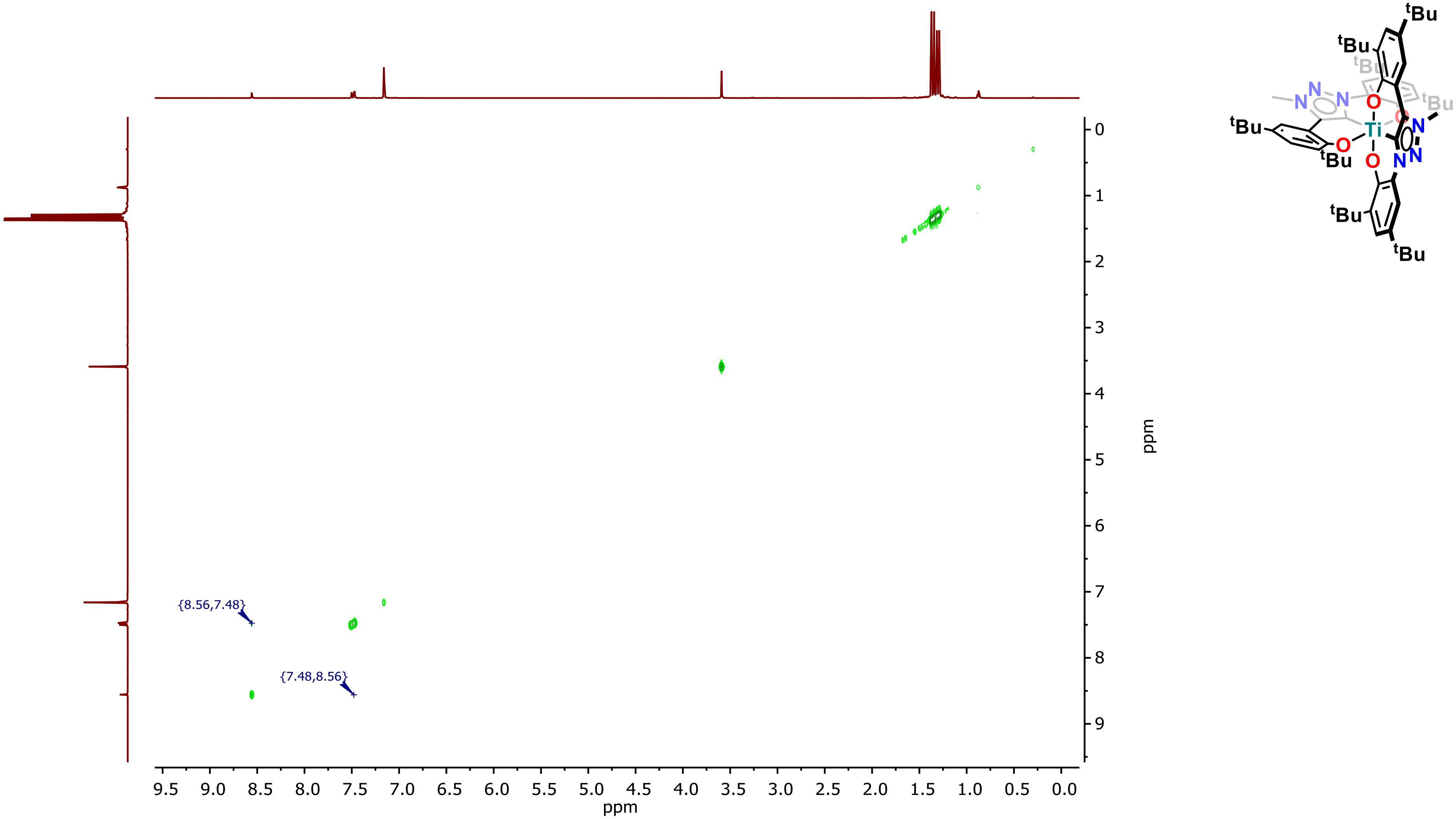
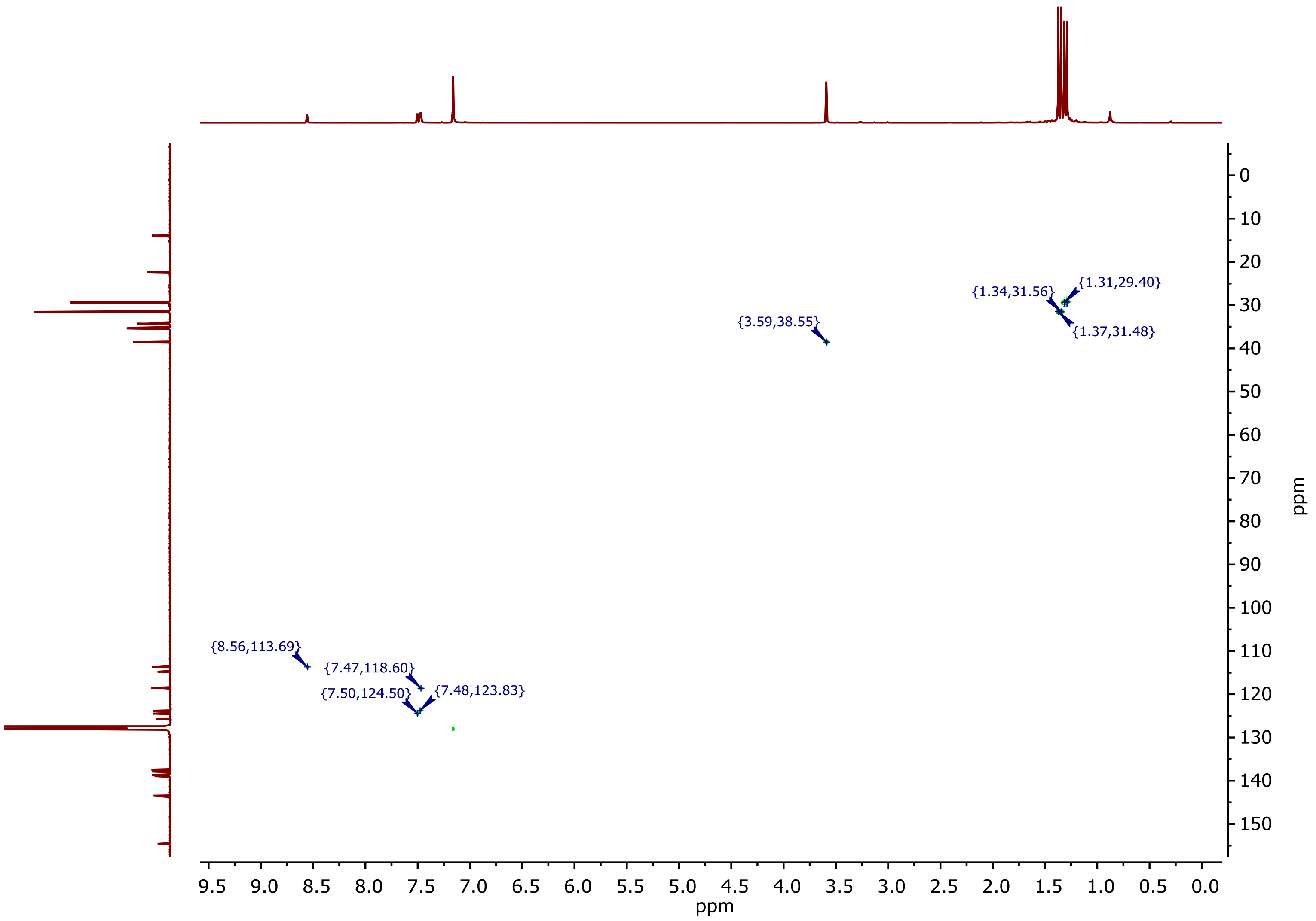


Figure S 41: ^{1}H-^{1}H COSY NMR of **5** in C_6D_6



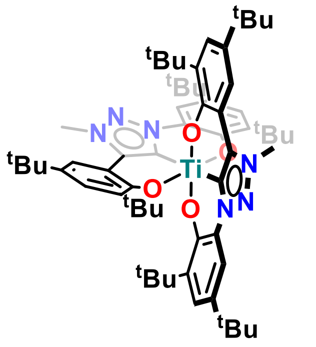
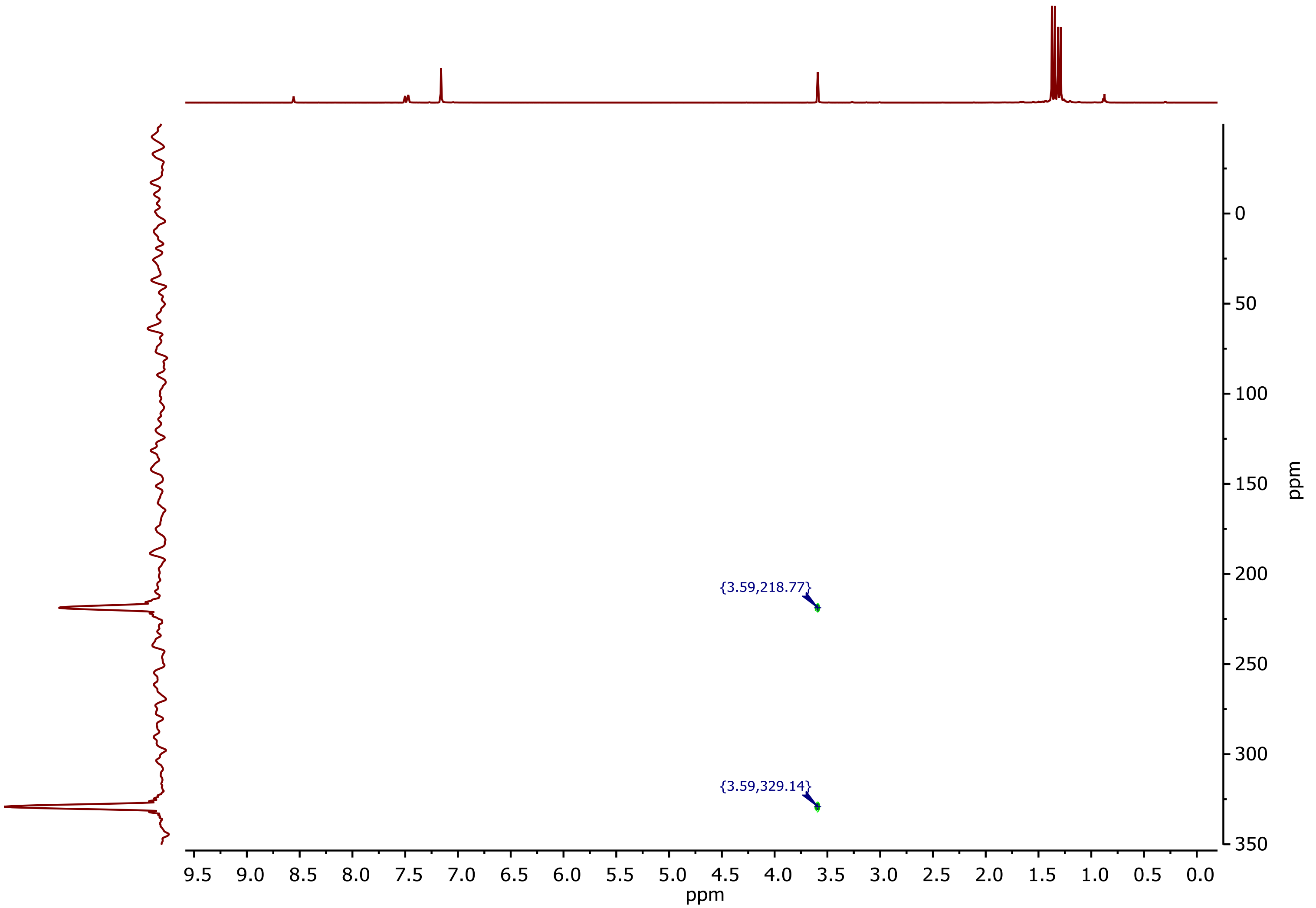


Figure S 42: ^{1}H-^{13}C HSQC NMR of **5** in C_6D_6



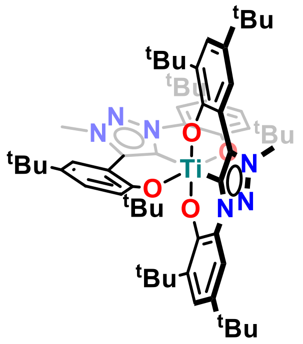


Figure S 43: ^{1}H-^{15}N HMBC NMR of **5** in C_6D_6

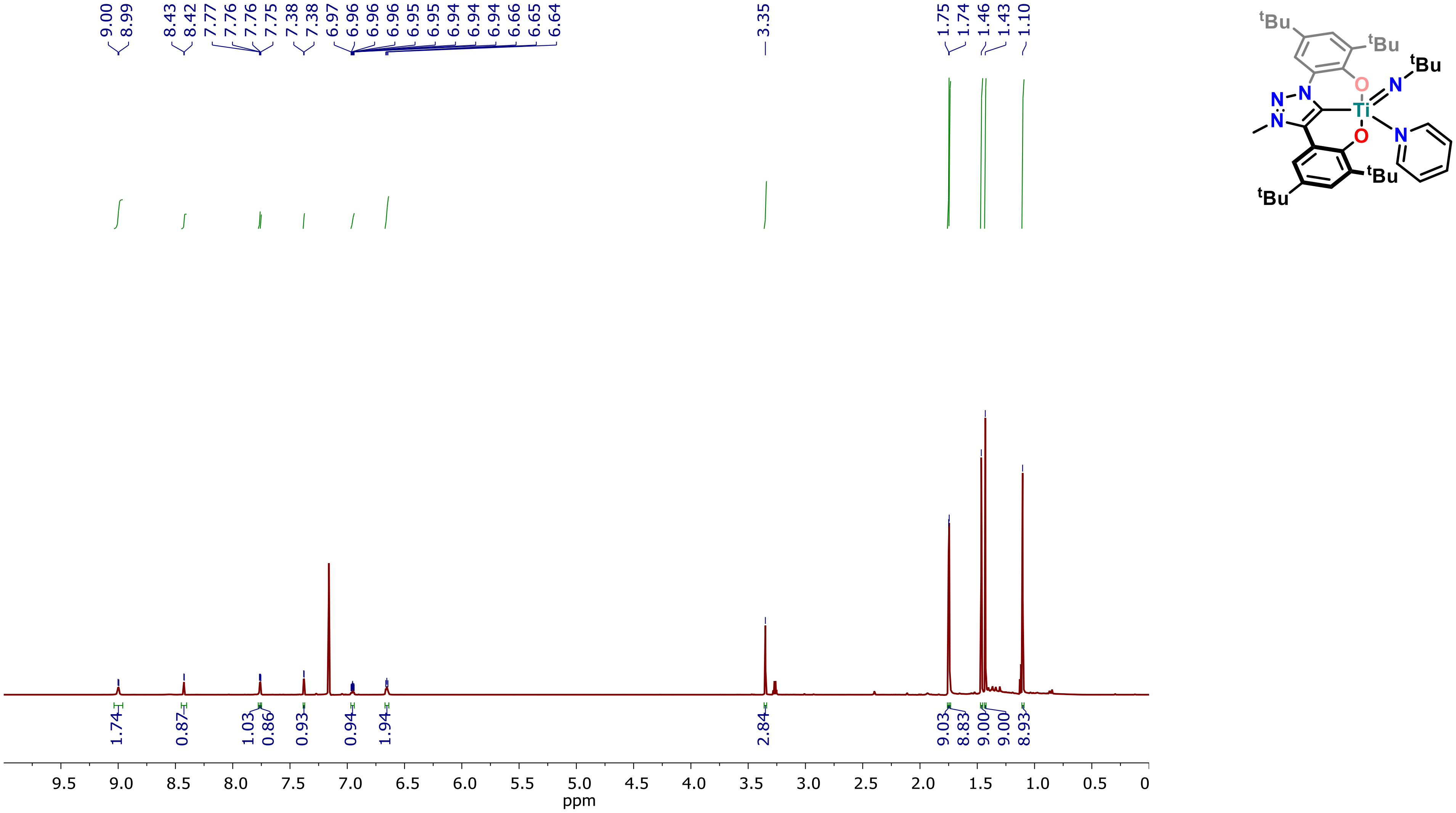


Figure S 44: ^{1}H-NMR of **6** in C_6D_6

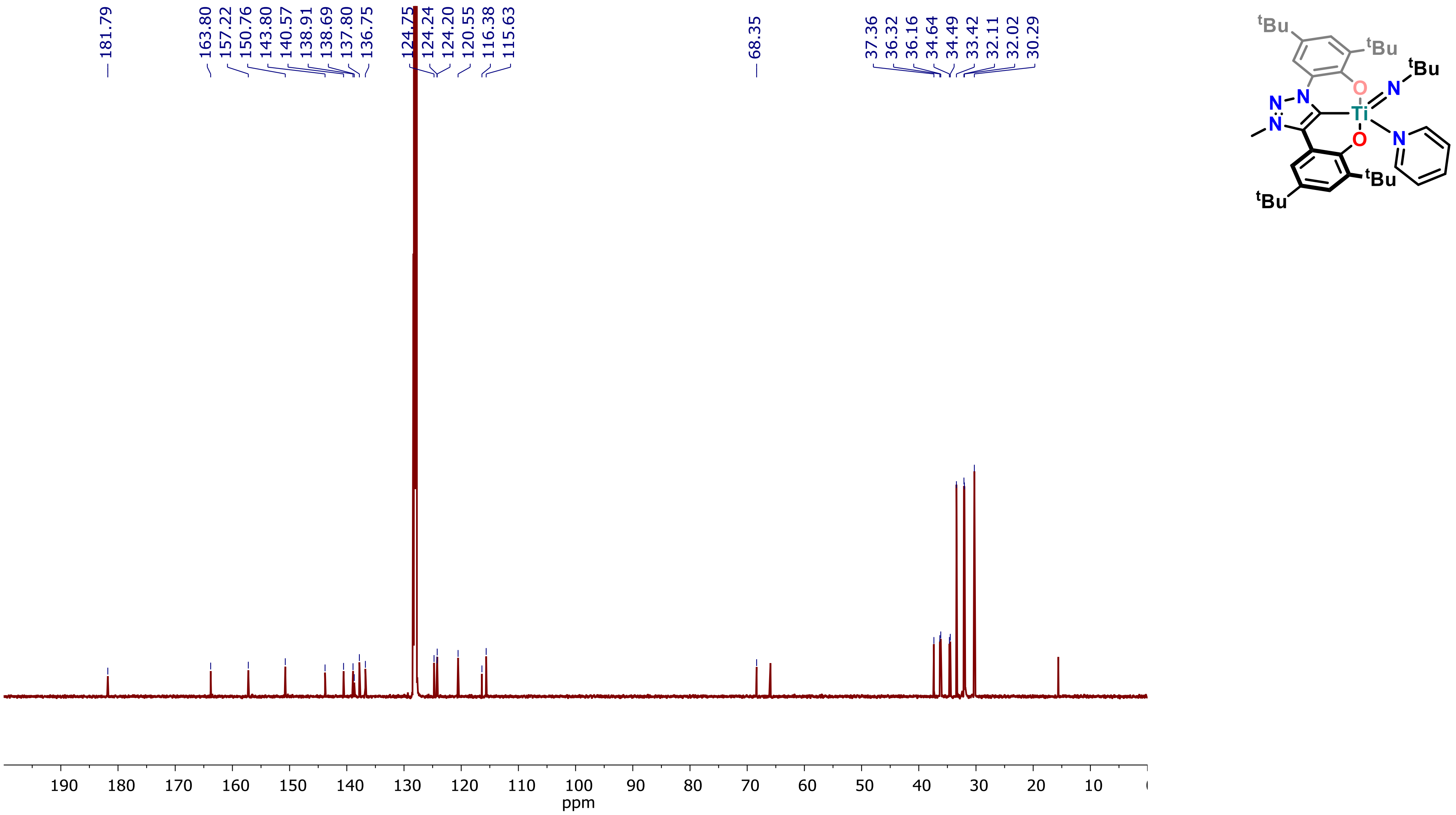


Figure S 45: ^{13}C-NMR of **6** in C_6D_6

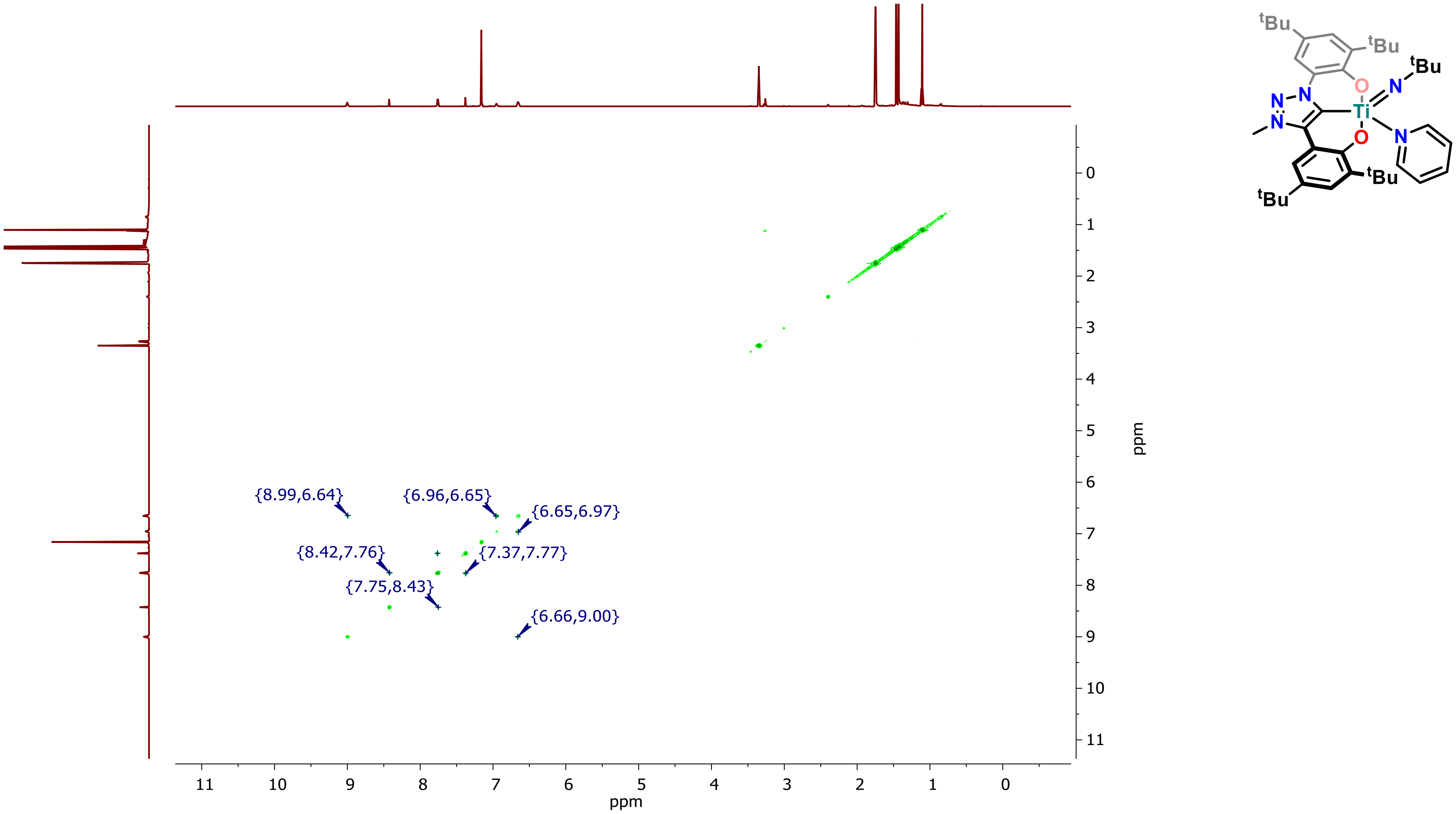
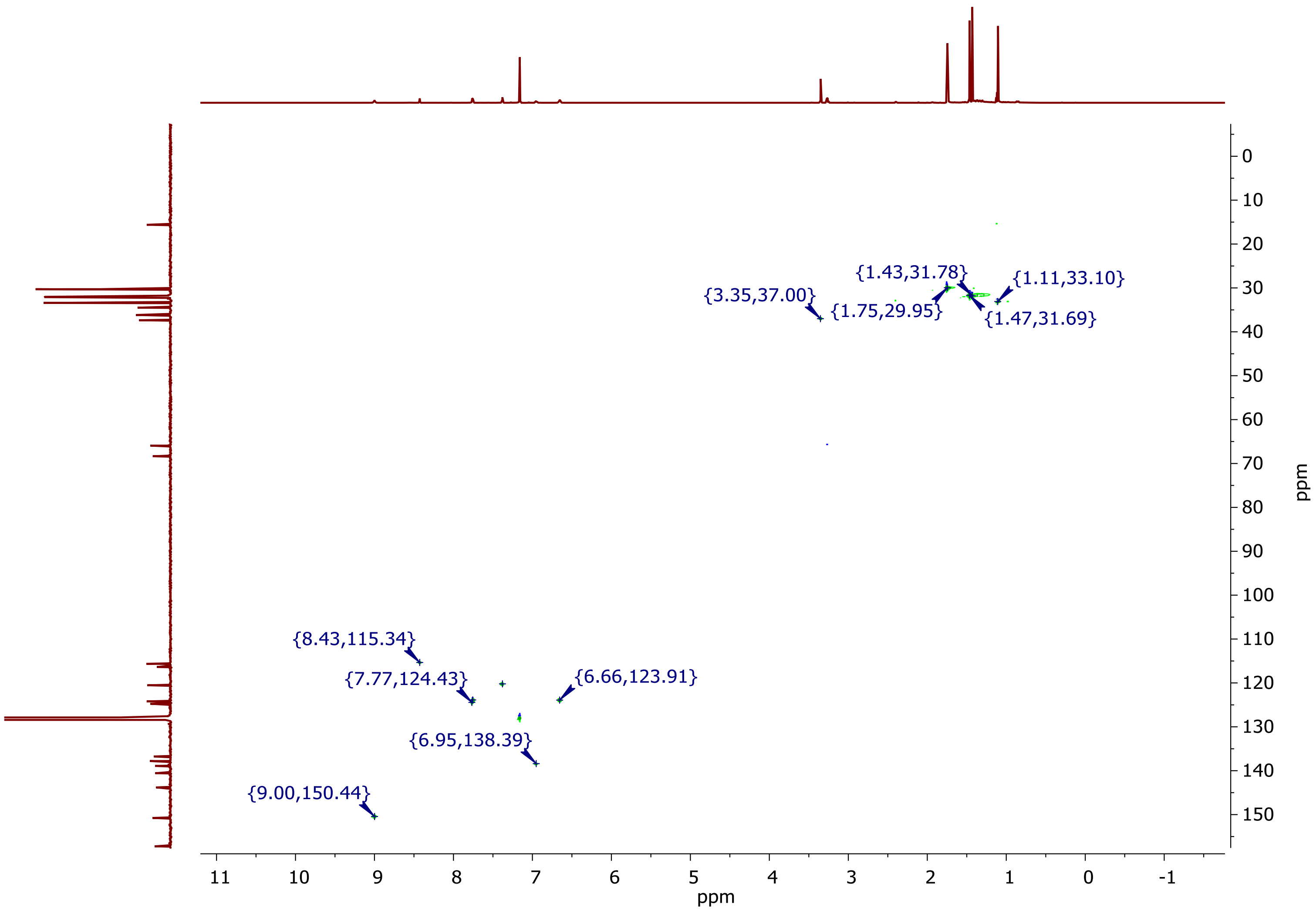


Figure S 46: ^{1}H-^{1}H-COSY of **6** in C_6D_6



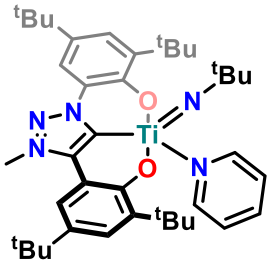
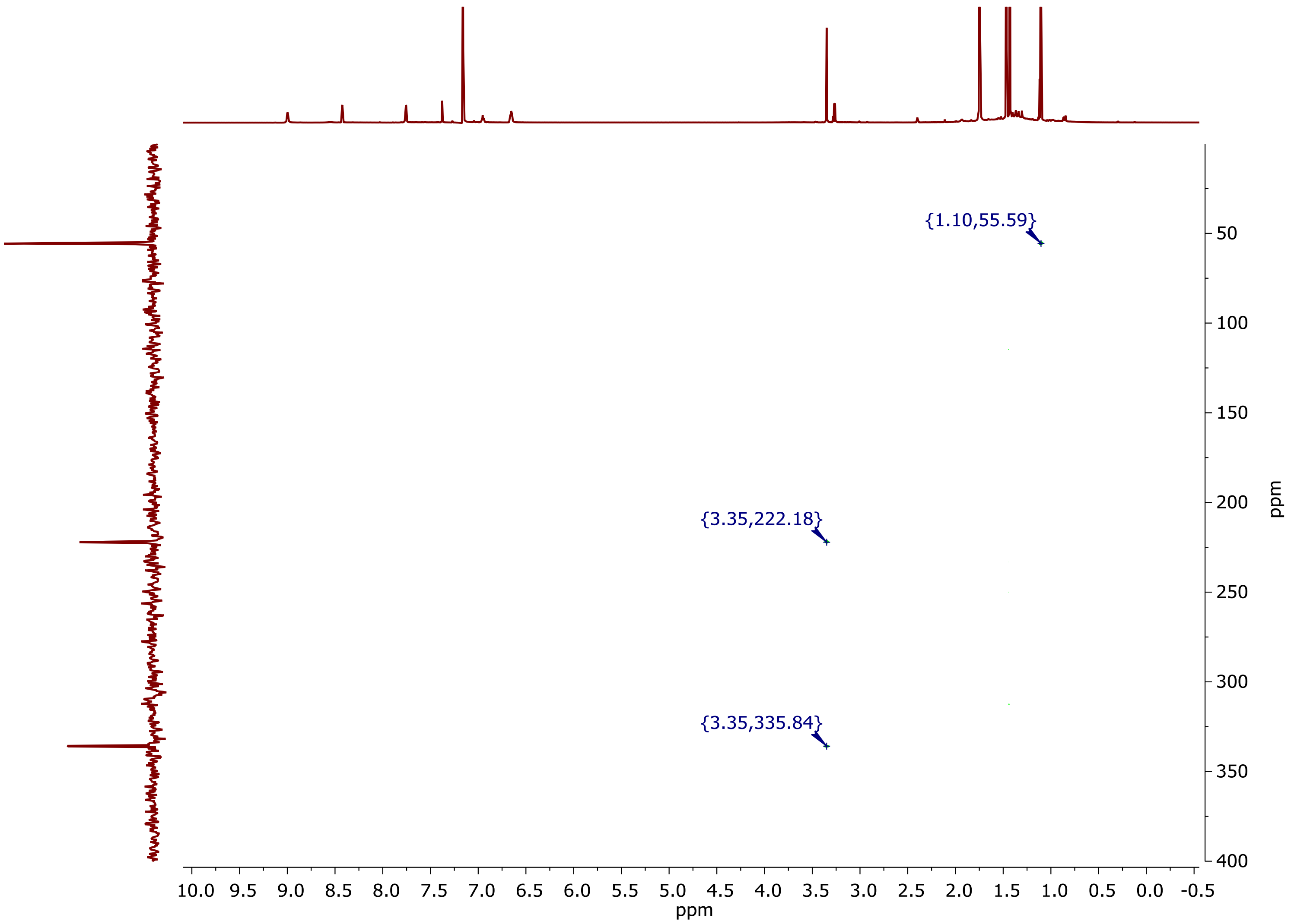


Figure S 47: ^{1}H-^{13}C-HSQC of **6** in C_6D_6



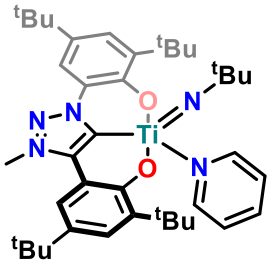


Figure S 48: ^{1}H-^{15}N-HMBC of **6** in C_6D_6

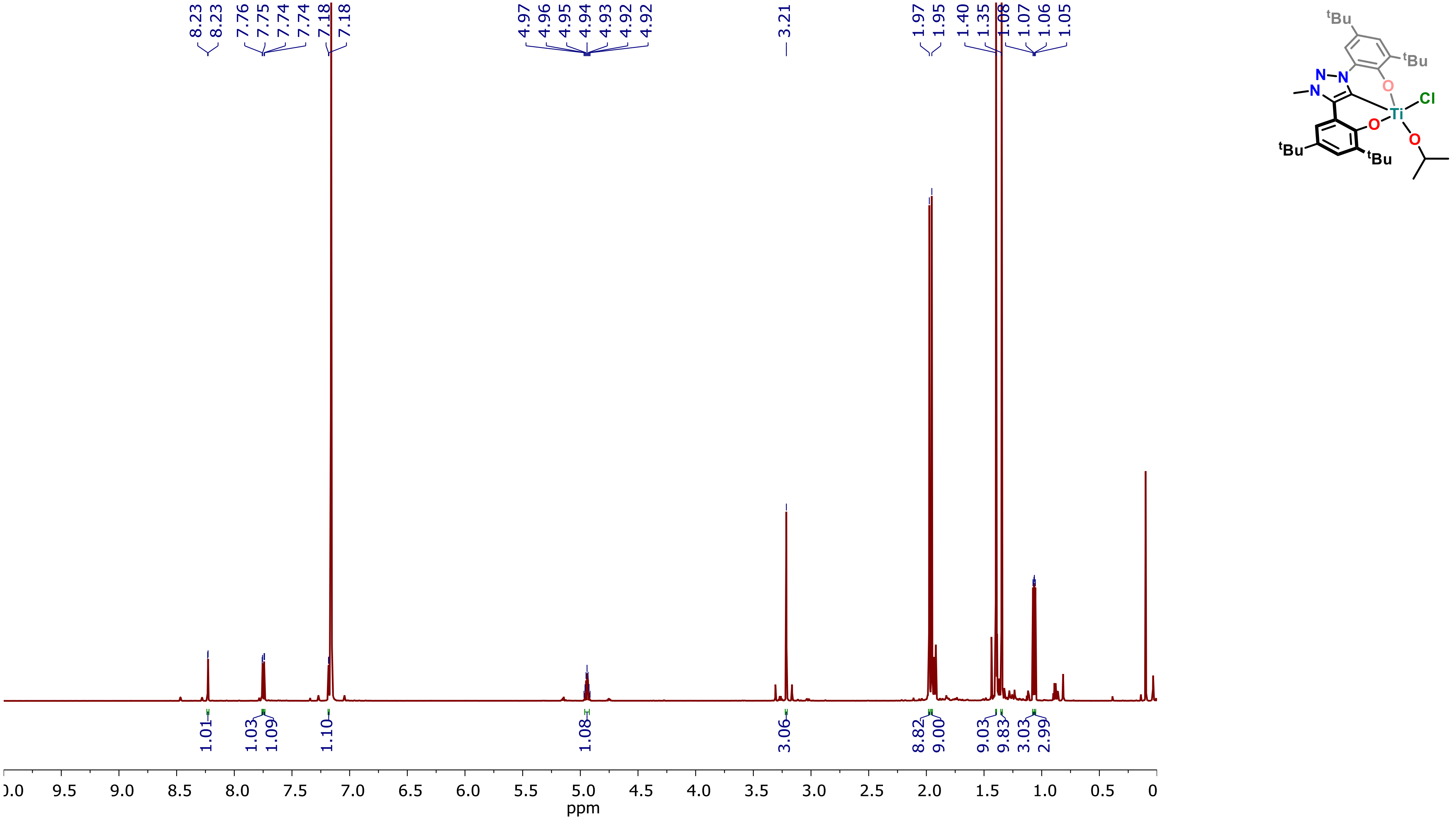


Figure S 49: ^{1}H-NMR of **7** in C_6D_6

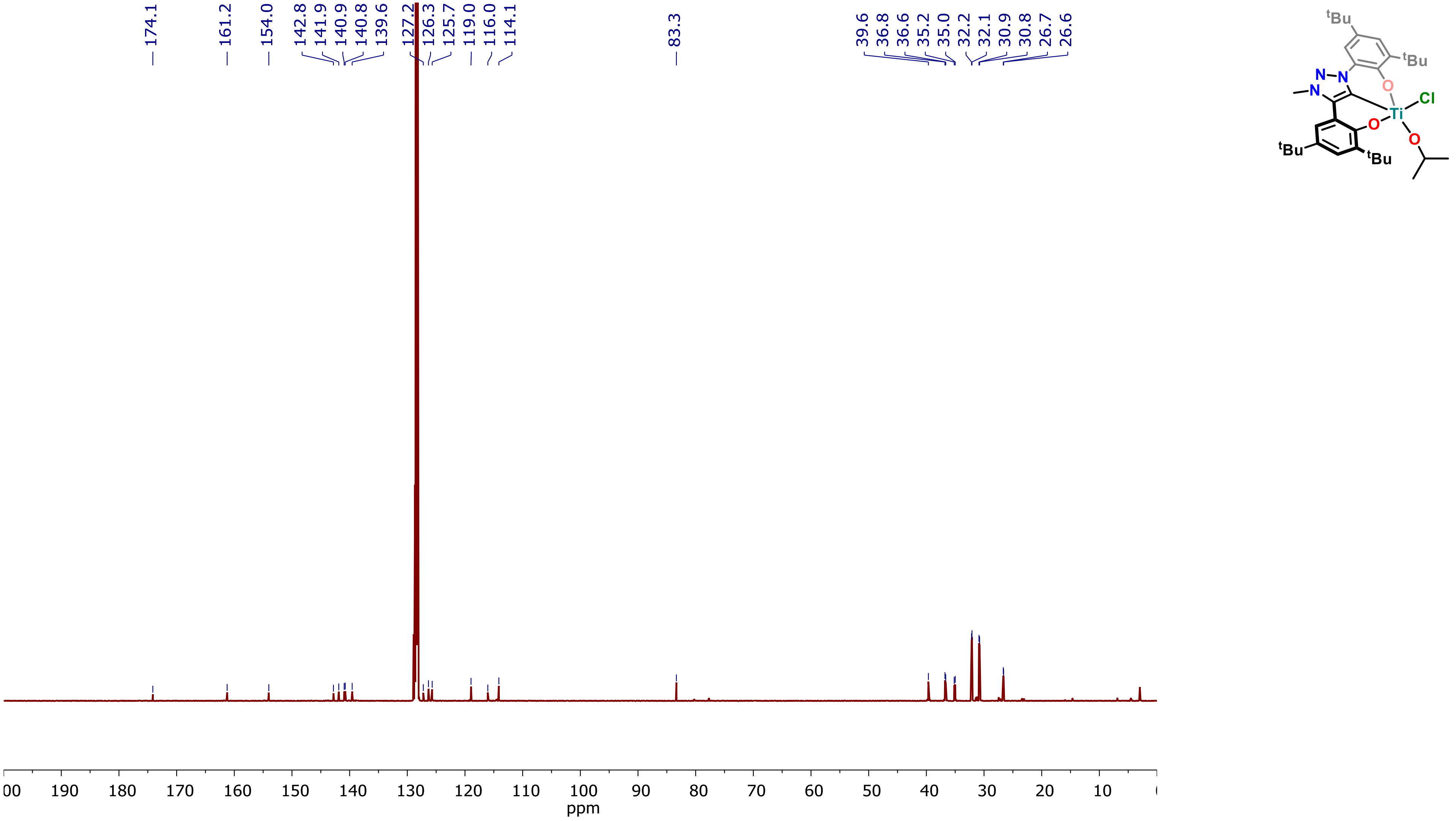


Figure S 50: ^{13}C-NMR of **7** in C_6D_6

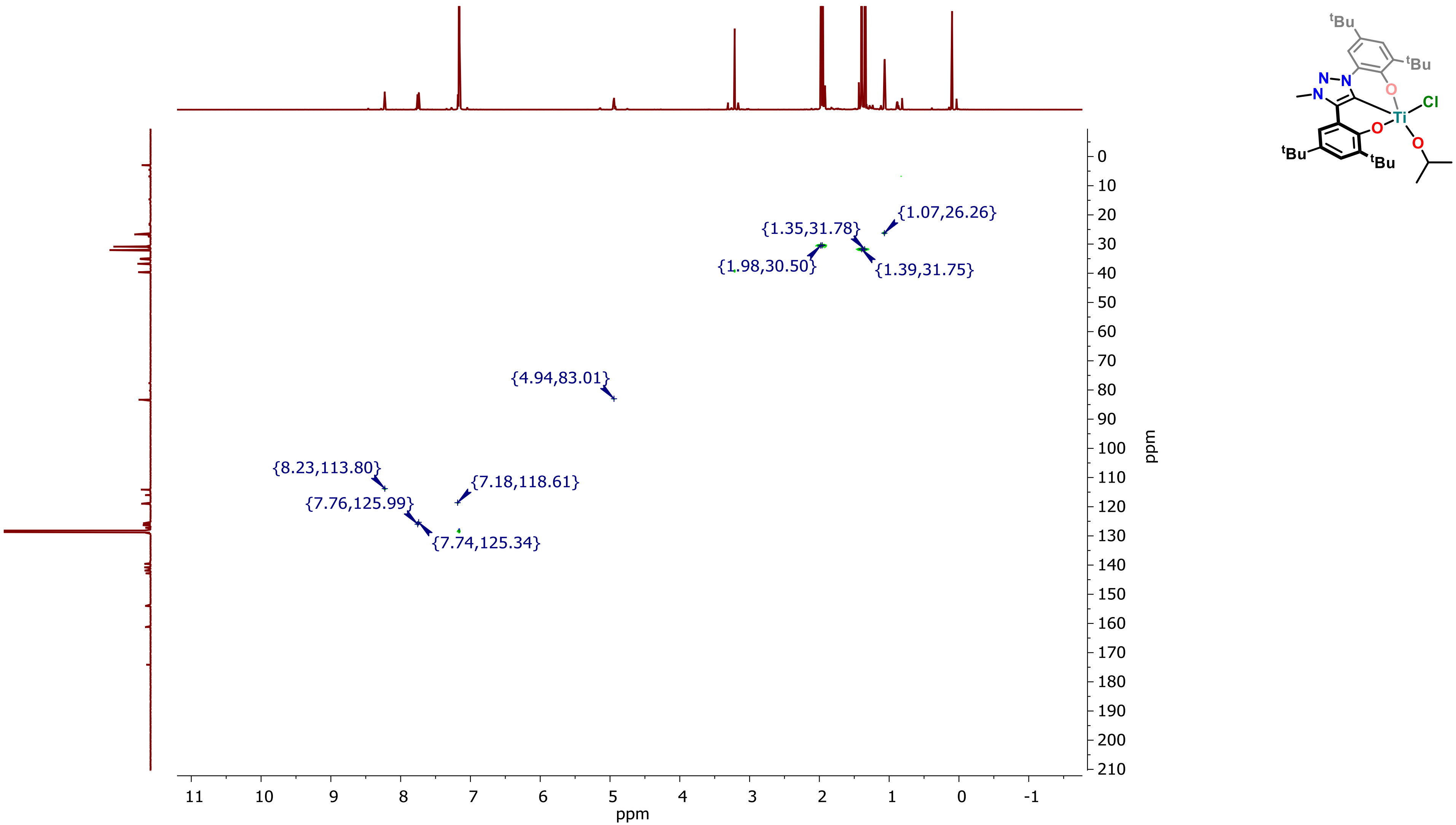
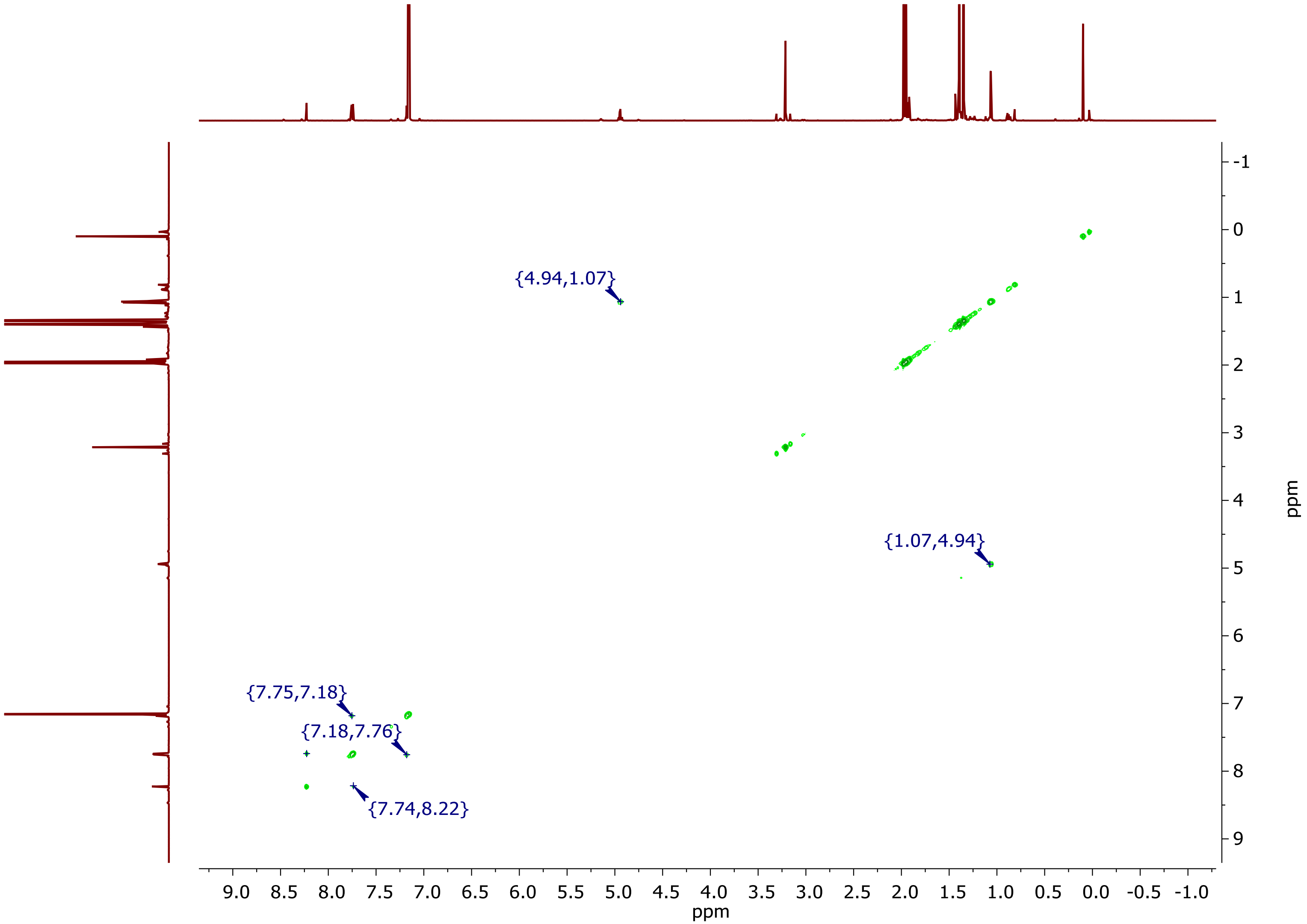


Figure S 51: ^{1}H-^{13}C-HSQC of **7** in C_6D_6



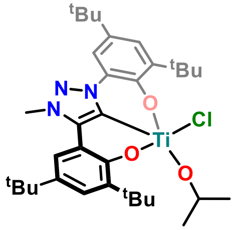


Figure S 52: ^{1}H-^{1}H-COSY of **7** in C_6D_6

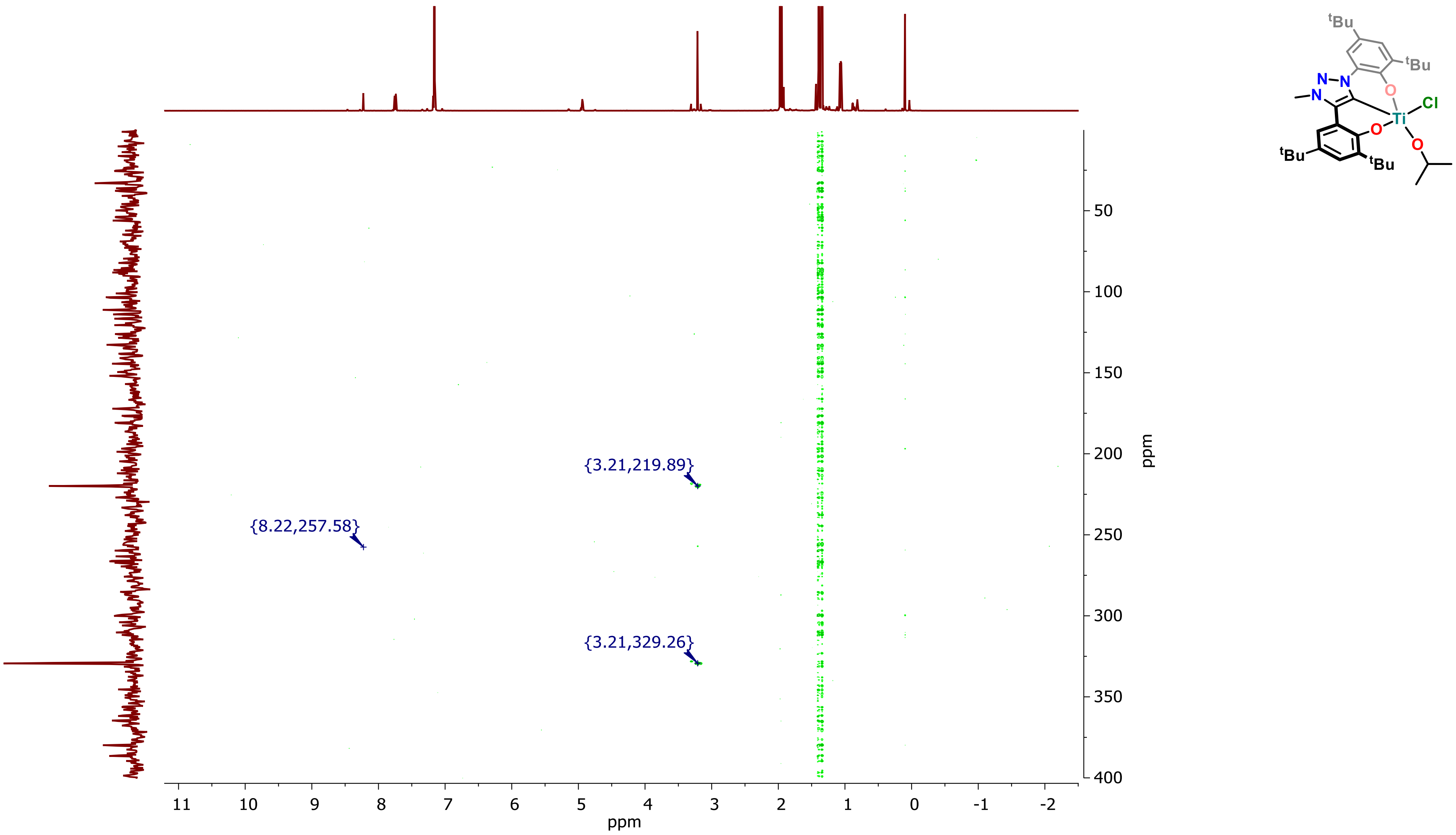


Figure S 53: ^{1}H-^{15}N-HMBC of **7** in C_6D_6

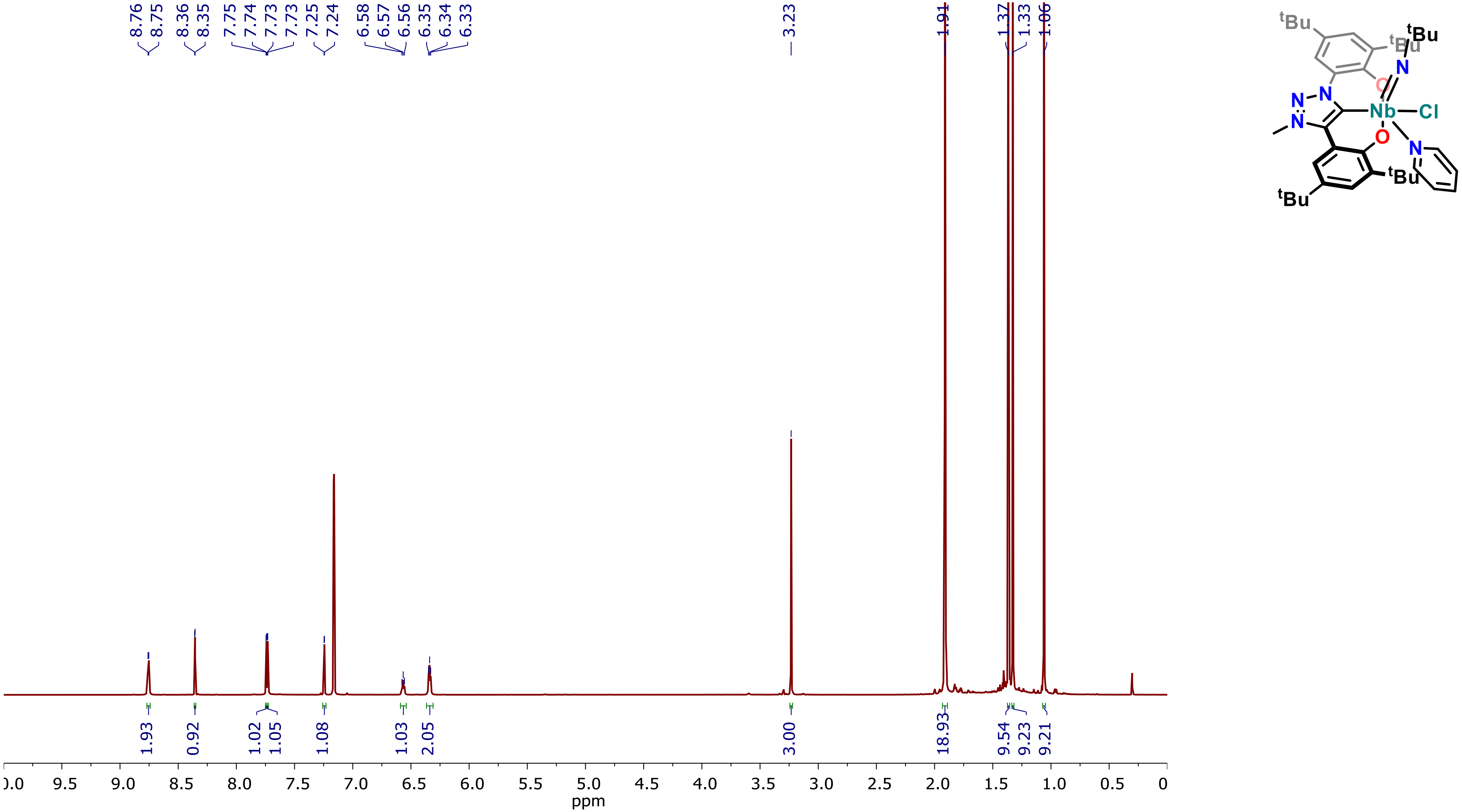


Figure S 54: ^{1}H-NMR of **9** in C_6D_6

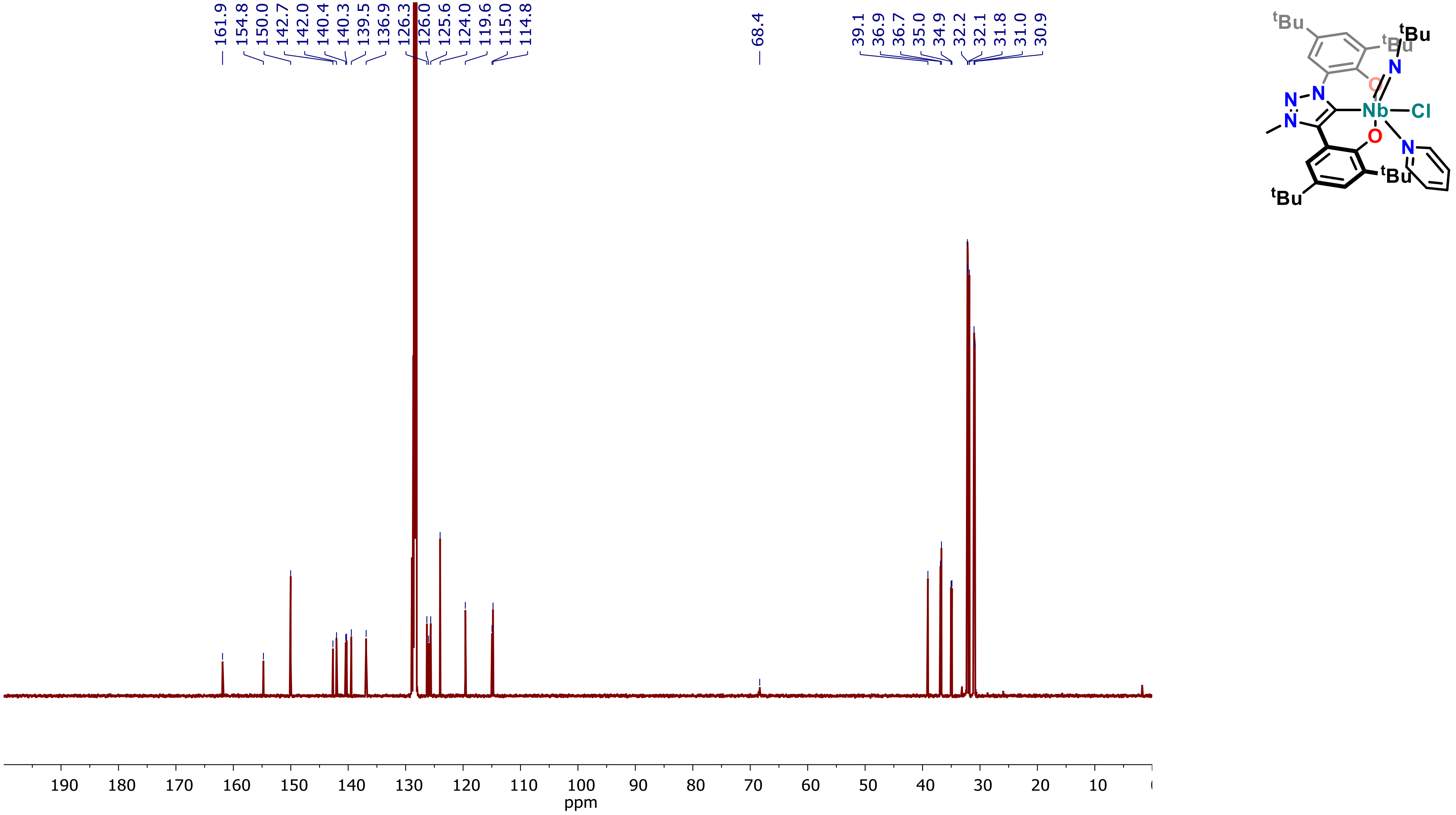
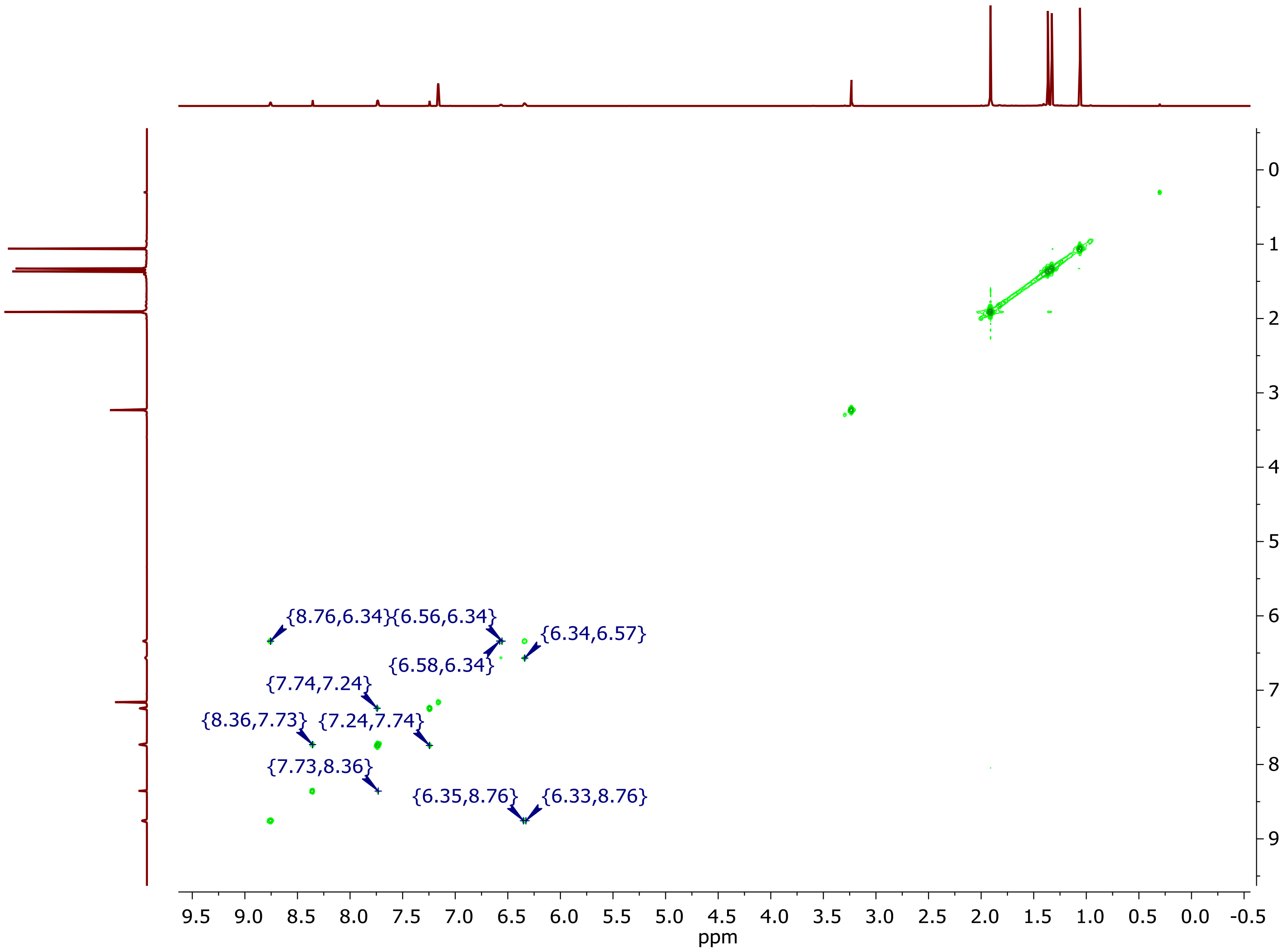


Figure S 55: ^{13}C-NMR of **9** in C_6D_6



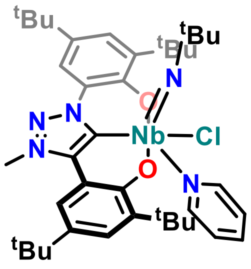


Figure S 56: ^{1}H-^{1}H-COSY of **9** in C_6D_6

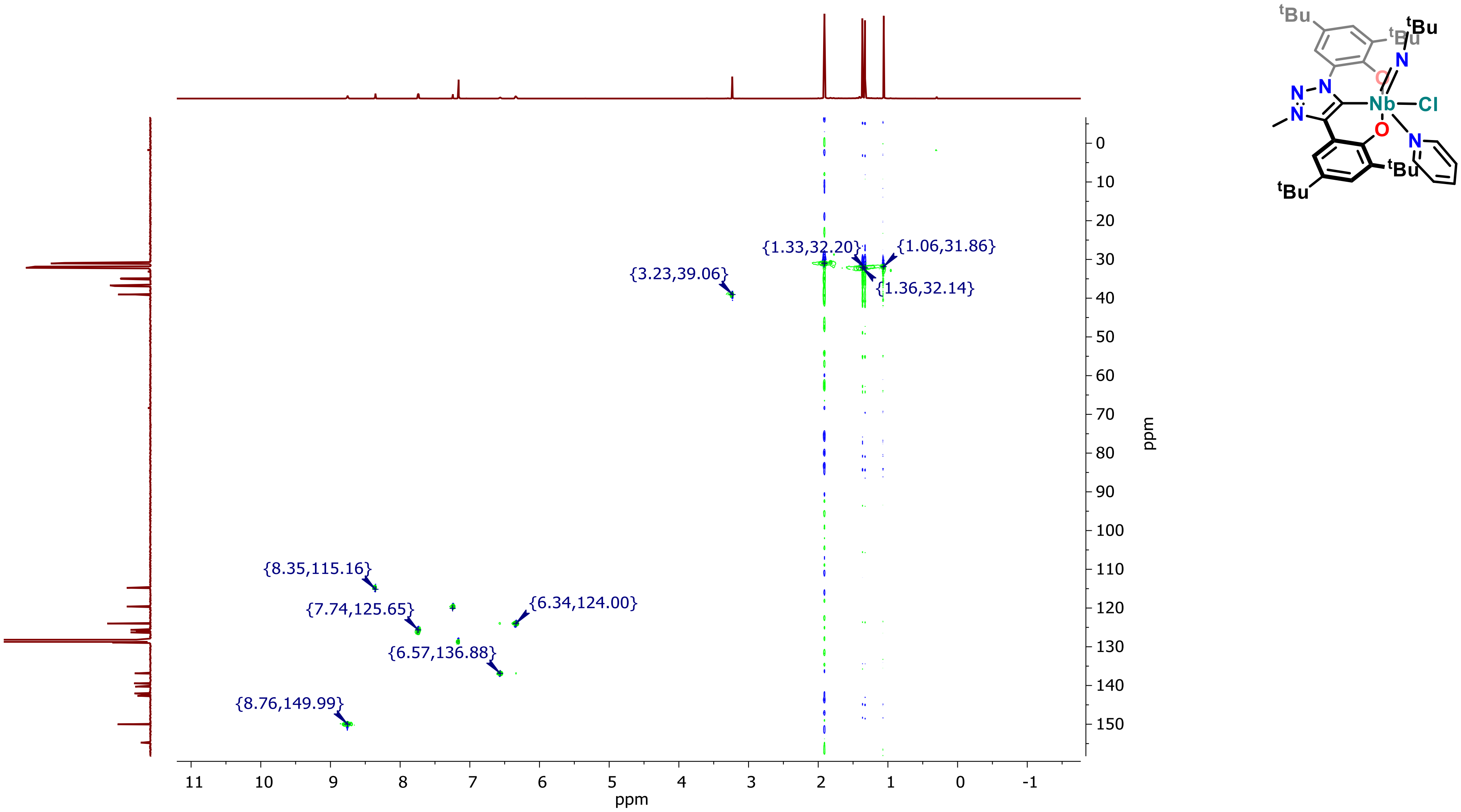
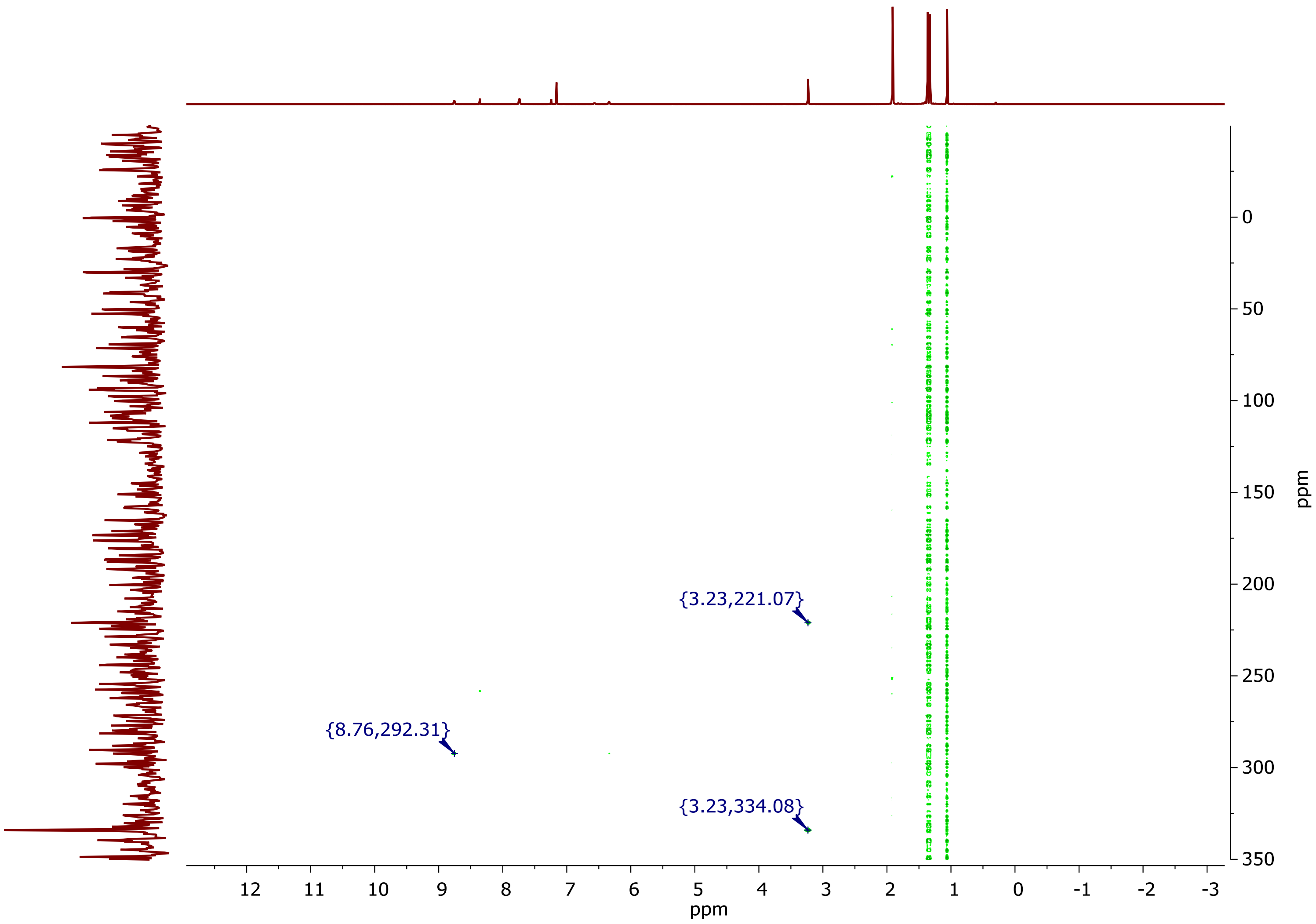


Figure S 57: ^{1}H-^{13}C-HSQC of **9** in C_6D_6



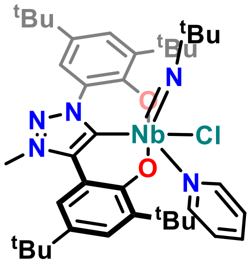


Figure S 58: ^{1}H-^{15}N-HMBC of **9** in C_6D_6

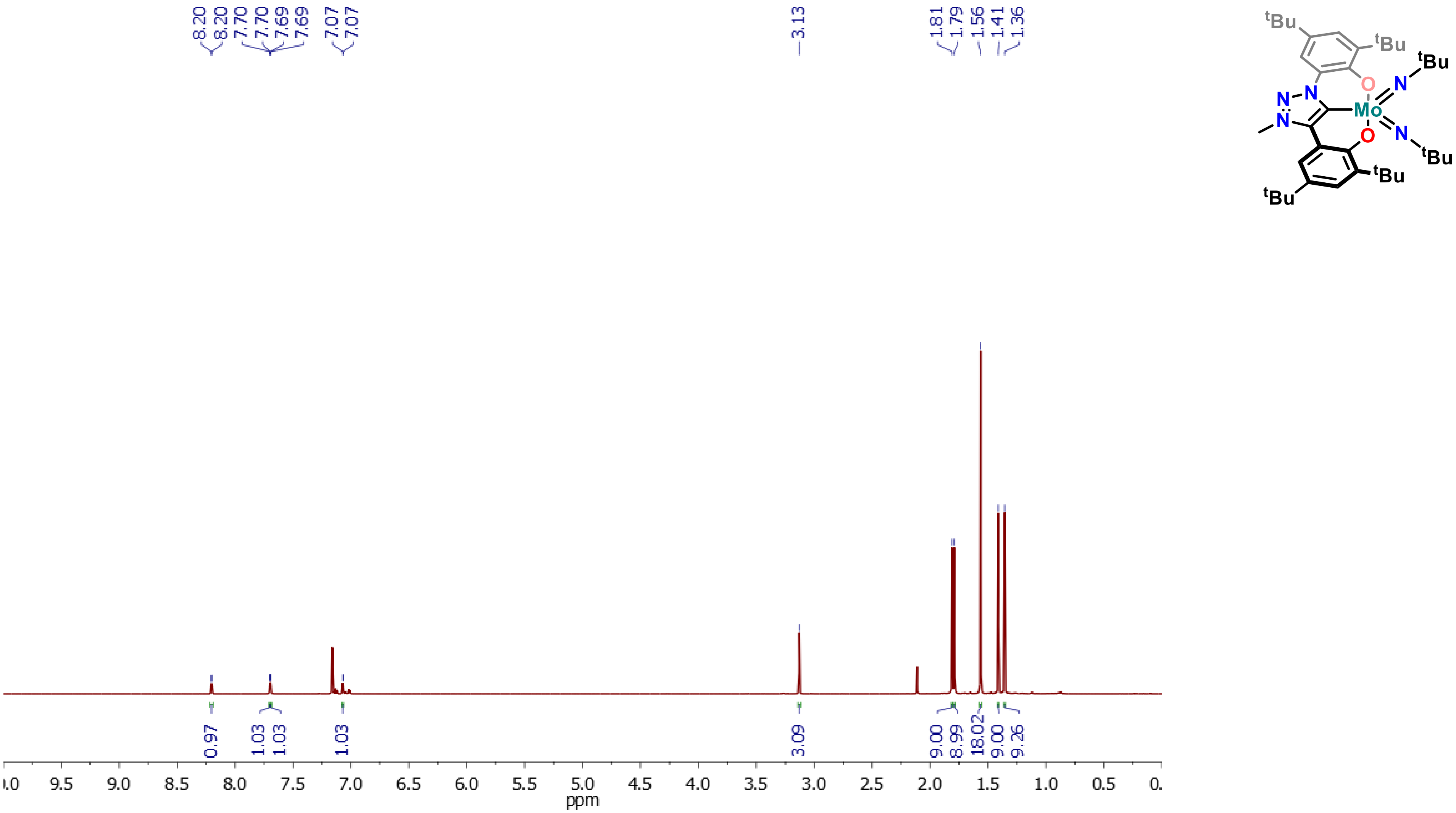


Figure S 59: ^{1}H-NMR of **10** in C_6D_6

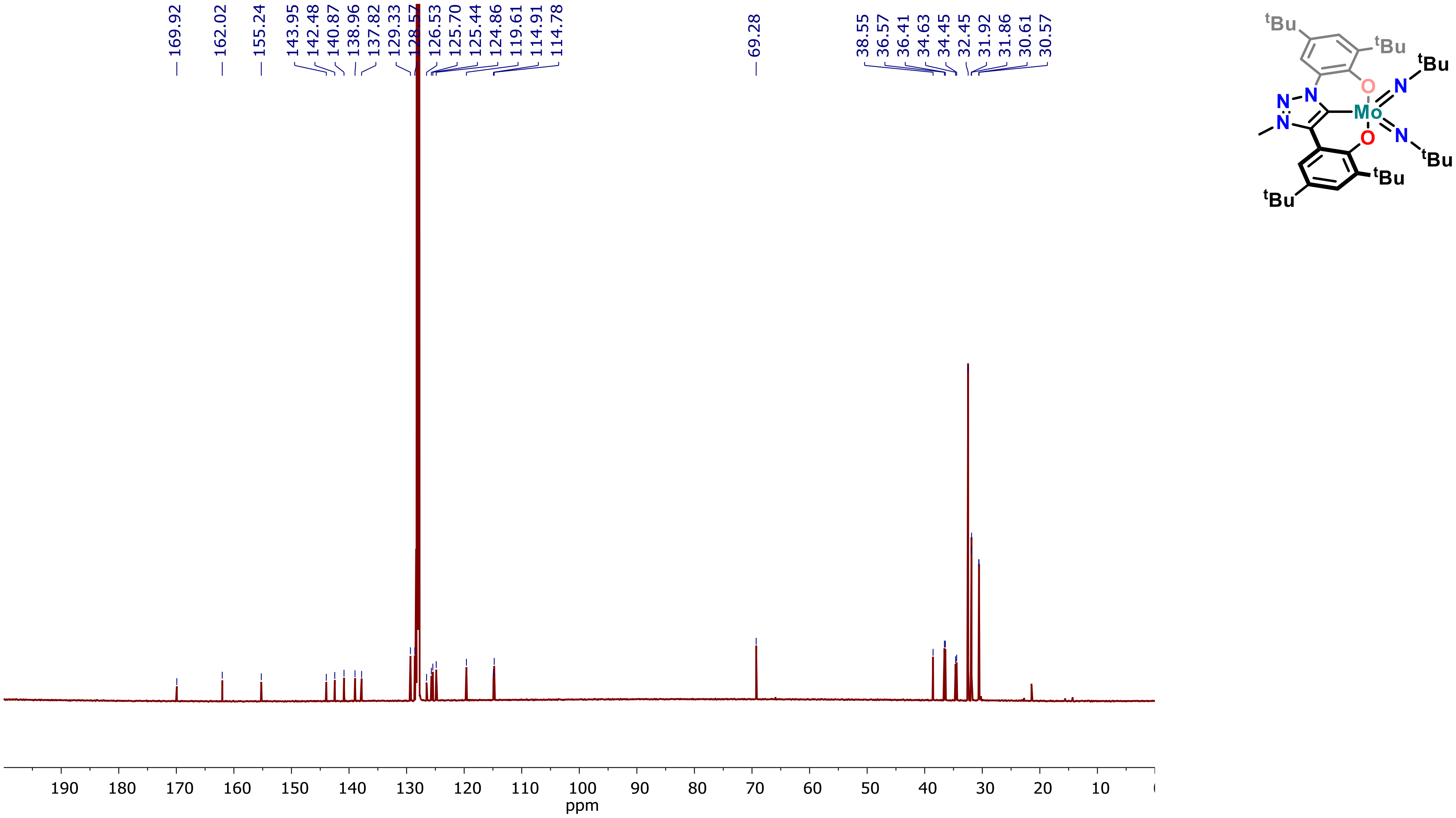
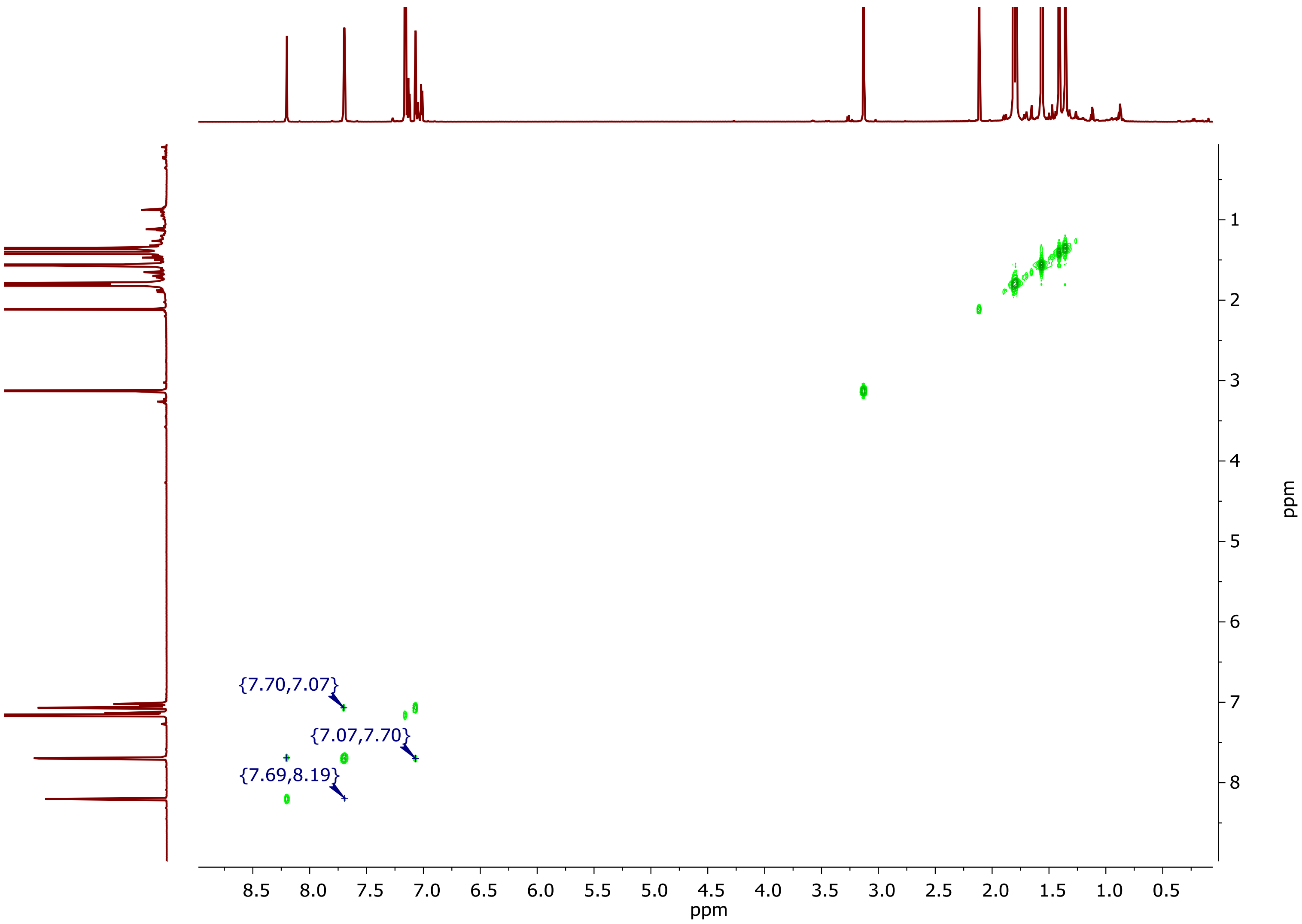


Figure S 60: ^{13}C-NMR of **10** in C_6D_6



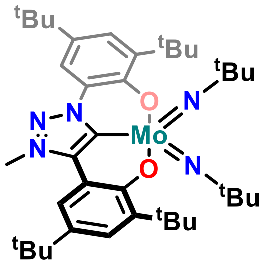


Figure S 61: ^{1}H-^{1}H-COSY of **10** in C_6D_6

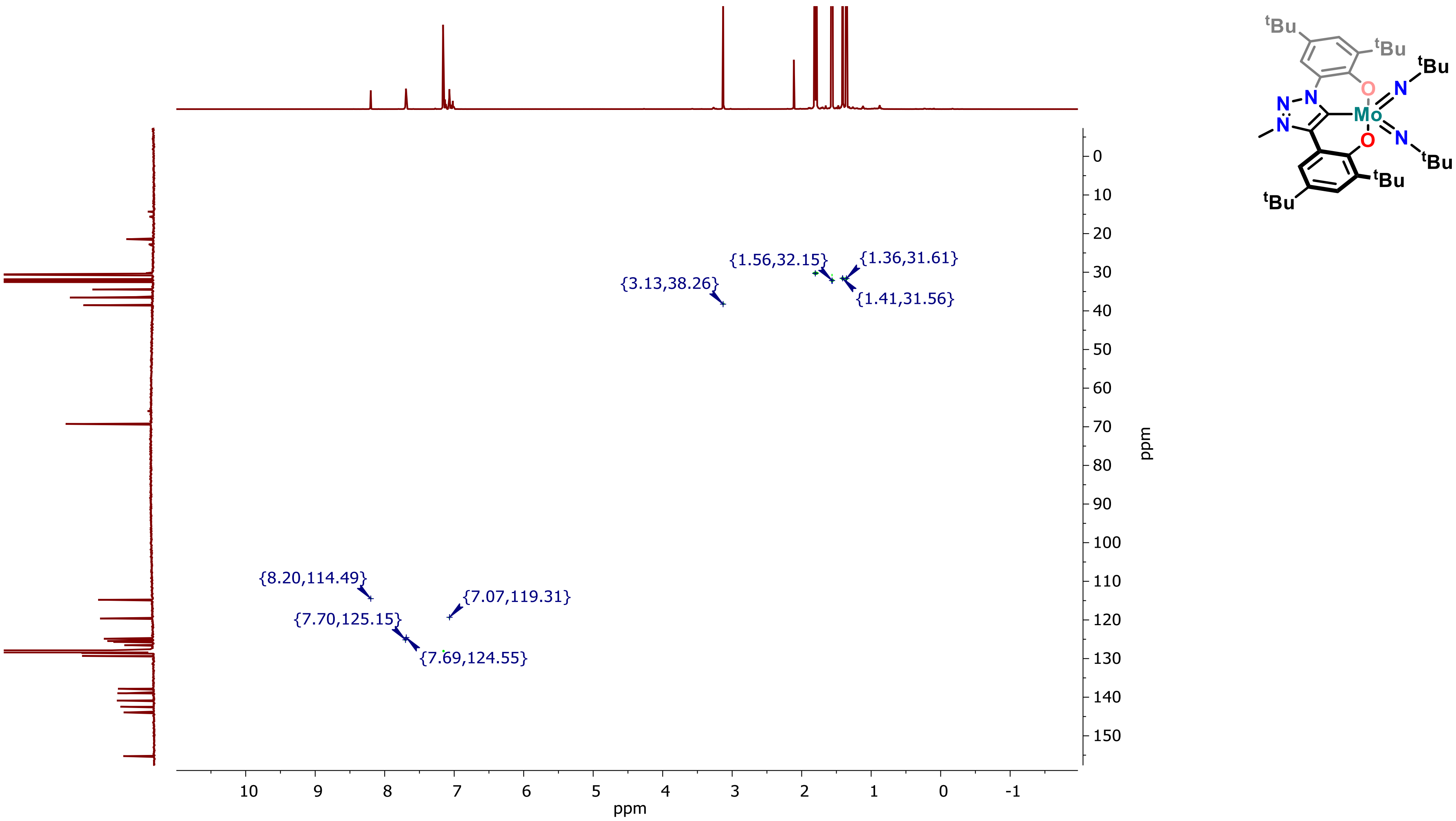
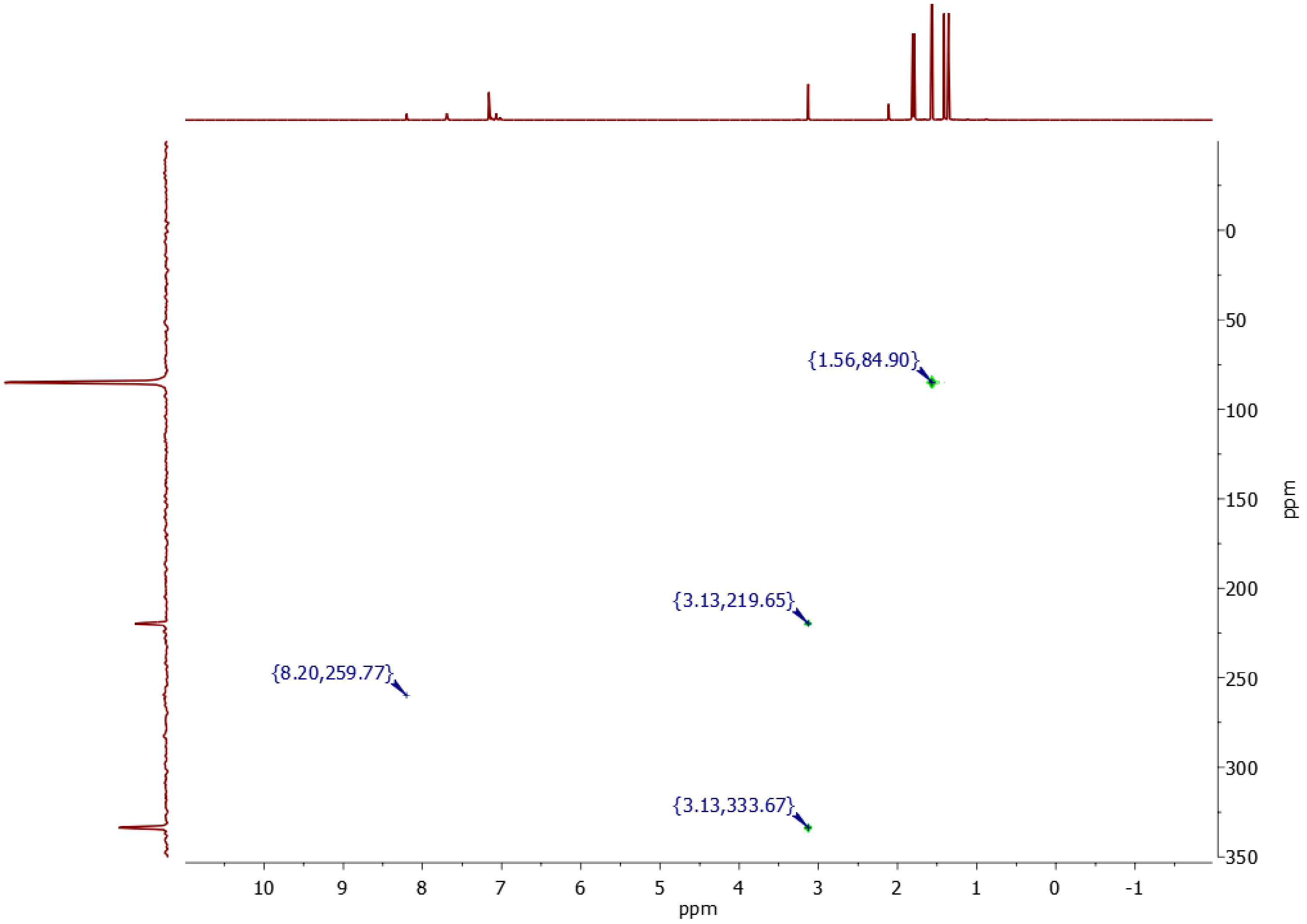


Figure S 62: ^{1}H-^{13}C-HSQC of **10** in C_6D_6



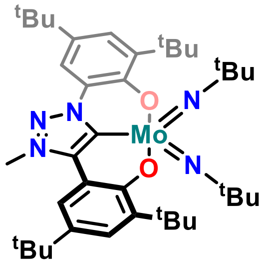
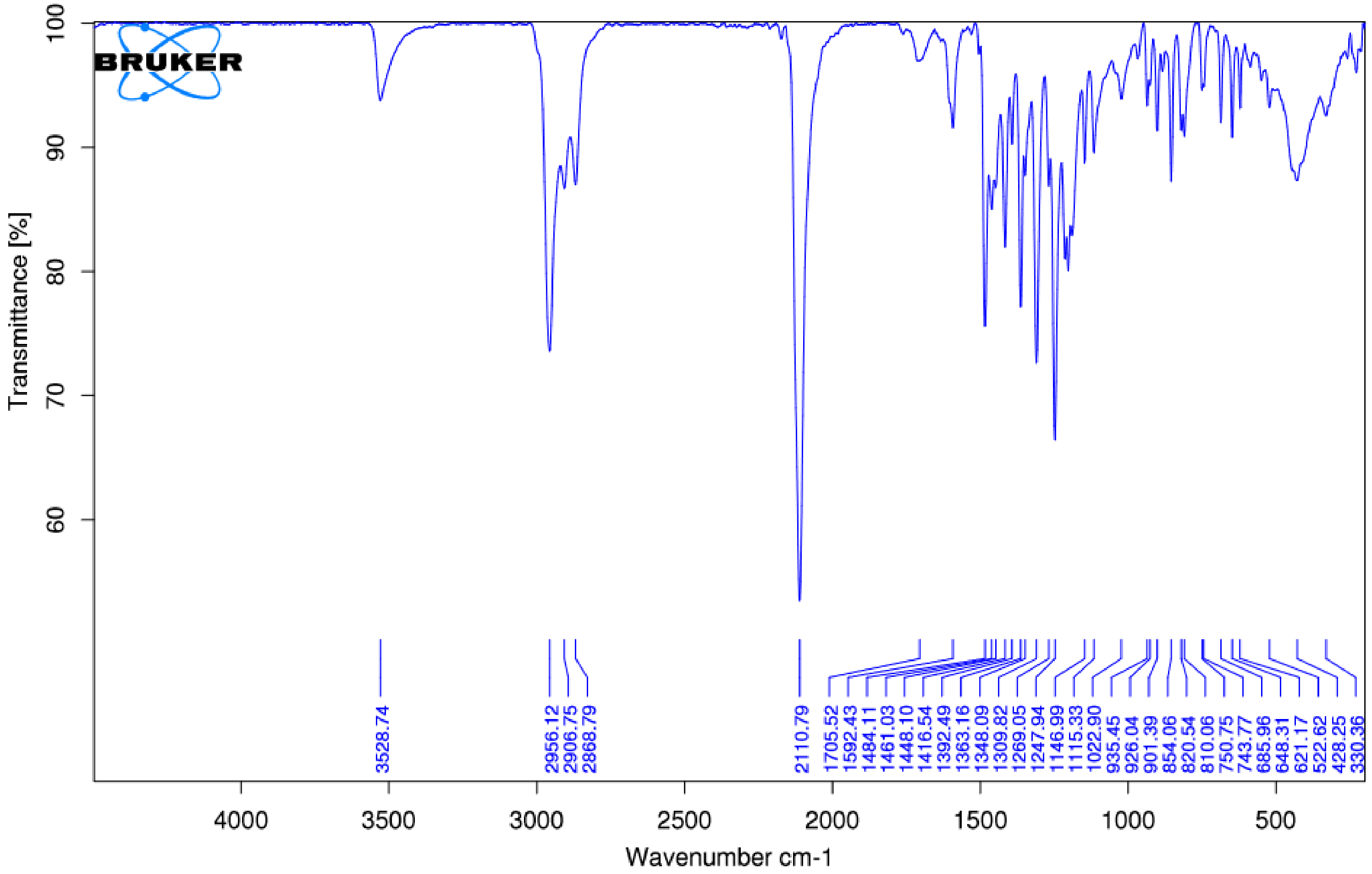


Figure S 63: ^{1}H-^{15}N-HMBC of **10** in C_6D_6

3. IR-Spectra



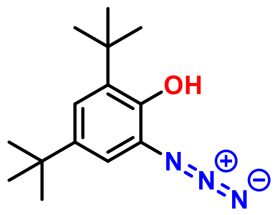


Figure S 64: IR Spectra of **G** taken at room temperature. Band at 2111 cm^{-1} belongs the azide stretch, at 3528 cm^{-1} to the OH stretch.

4. Crystallographic details

Table S 1: Crystallographic details

	1	**$H_3L[OTf]$**	**$[H_2L]_2$***	**3****	**4***	**6**	**9**	**10***
Chemical formula	$C_{30}H_{43}N_3O_2$	$C_{31}H_{46}N_3O_2$ CF_3SO_3 $(C_6H_6)_{0.5}$	$C_{62}H_{90}N_6O_4$	$C_{34}H_{51}N_3O_2Cl_2Ti_1$	$C_{66}H_{94}N_6O_6Cl_2Ti_2$	$C_{40}H_{57}N_5O_2Ti_1$	$C_{40}H_{57}N_5O_2Nb_1$ $C_4H_{10}O$	$C_{39}H_{61}N_5O_2Mo_1$
M_r	477.67	680.83	983.39	668.57	1234.17	687.80	842.38	727.86
Crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic	Trigonal
Space group	$C2/c$	$P2_1$/c	*P*-1	$P2_1$	$C2/c$	$P2_1/n$	*P*-1	*R*-3
a (Å)	26.750(5)	16.821(5)	14.116(3)	9.096(2)	37.210(2)	9.374(3)	11.009(2)	39.69(1)
b (Å)	10.170(2)	12.129(3)	15.693(3)	19.166(4)	16.687(1)	16.810(5)	15.840(2)	39.69(1)
c (Å)	11.170(2)	19.288(5)	16.506(3)	11.5415(2)	27.017(2)	25.014(8)	15.982(2)	14.511(4)
α (°)	90	90	69.462(4)	90	90	90	103.559(3)	90
β (°)	114.10(3)	111.467(5)	82.703(4)	93.40(1)	108.543(5)	90.800(6)	93.800(3)	90
γ (°)	90	90	81.560(4)	90	90	90	108.092(3)	120
V (Å^3)	2775(1)	3662(2)	3375(1)		15905(1)	3941(2)	2545.9(7)	19798(12)
Z	4	4	2		8	4	2	18
Densitiy (g cm^{-3})	1.143	1.235	0.967		1.031	1.159	1.099	1.099
F(000)	1040	1452	1072		5264	1480	896	6984
Radiation Type	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα	MoKα
μ (mm^{-1})	0.071	0.146	0.060		0.312	0.256	0.326	0.332
Crystal size	0.30x0.25x0.15	0.15x0.14x0.11	0.39x0.15x0.10		0.12x0.12x0.11	0.42x0.32x0.15	0.45x0.44x0.32	0.35x0.32x0.09
Meas. Refl.	6109	19822	65353		42122	26363	29018	24804
Indep. Refl.	2532	6767	12374		13941	6902	9465	8090
Obsvd. [$I > 2\sigma(I)$]	1720	3211	8416		9142	4175	7628	4993
R_{int}	0.0422	0.1385	0.0665		0.0302	0.0918	0.0590	0.1092
R [$F^2 > 2\sigma(F^2)$]	0.0535	0.0941	0.0681		0.0780	0.0899	0.0470	0.0664
wR(F^2)	0.1273	0.2904	0.1756		0.2479	0.2468	0.1184	0.1764
S	1.038	0.947	1.031		1.047	1.083	1.031	1.017
$\Delta\rho_{max}$	0.221	1.335	0.514		2.379	1.097	1.299	1.258
$\Delta\rho_{min}$	-0.172	-0.727	-0.474		-0.564	-0.660	-0.875	-1.099
CCDC	1921635	1921636	1921637		1921638	1921639	1921640	1921641

*Due to heavy solvent disorders, solvent molecules have been removed by applying the SQUEEZE technique

** due to the low quality of the crystals, no further crystallographic details can be discussed here.

Table S 2: Selected bond lengths and angles

	1	H$_3$L[OTf]	[H$_2$L]$_2$	3**	$4^{\#*}$	6	9	10
M1-C1	-	-	-		2.111(5) / 2.130(5)	2.112(5)	2.196(3)	2.204(5)
M1-O1	-	-	-		1.861(4) / 1.845(3)	1.968(4)	1.982(2)	2.005(3)
M1-O2	-	-	-		1.845(3) / 1.888(3)	1.948(4)	1.985(2)	2.013(3)
M1-Cl1	-	-	-		2.375(2) / 2.364(2)	-	2.454(1)	-
M1-O10	-	-	-	-	1.905(3) / 1.728(3)	-	-	-
M1-N40	-	-	-		-	1.682(5)	1.756(3)	1.741(4)
M1-N50	-	-	-		-	-	-	1.749(4)
C40-N40	-	-	-		-	1.457(7)	1.449(4)	1.466(7)
C50-N50	-	-	-		-	-	-	1.455(7)
C1-C2	1.352(2)	1.364(6)	1.378(4)		1.379(6)	1.373(7)	1.382(4)	1.399(7)
C2-C5	1.440(2)	1.462(6)	1.457(3)		1.441(7)	1.444(7)	1.460(4)	1.462(7)
C5-C10	1.400(3)	1.381(6)	1.424(4)		1.397(7)	1.408(7)	1.416(4)	1.406(7)
C10-O1	1.374(2)	1.365(6)	1.311(3)		1.344(6)	1.341(6)	1.346(3)	1.353(5)
N1-C11	-	1.447(6)	1.435(3)		1.446(6)	1.435(7)	1.431(4)	1.423(6)
C11-C16	-	1.379(6)	1.403(4)		1.403(6)	1.404(8)	1.408(4)	1.394(7)
C16-O2	-	1.374(5)	1.310(3)		1.339(5)	1.330(6)	1.331(3)	1.323(6)
C2-C1-N1	106.3(3)	106.8(4)	107.2(2)		104.9(4)	104.0(5)	103.9(2)	103.7(4)
M1-N40-C40	-	-	-	-	-	170.0(4)	171.8(2)	151.9(4)
M1-N50-C50	-	-	-	-	-	-	-	174.1(4)
M1-O10-M2	-	-	-	-	158.5(2)	-	-	-

[#] left values correspond to the 6-fold coordinated titanium center Ti1, right values to the 5-fold coordinated titanium center Ti2

*since the internal bond distances and angles in the ligands do not differ drastically from each other, only the value for the ligand on Ti1 are displayed

** due to the low quality of the crystals no bond distances can be discussed here.

5. Cyclic voltammetry

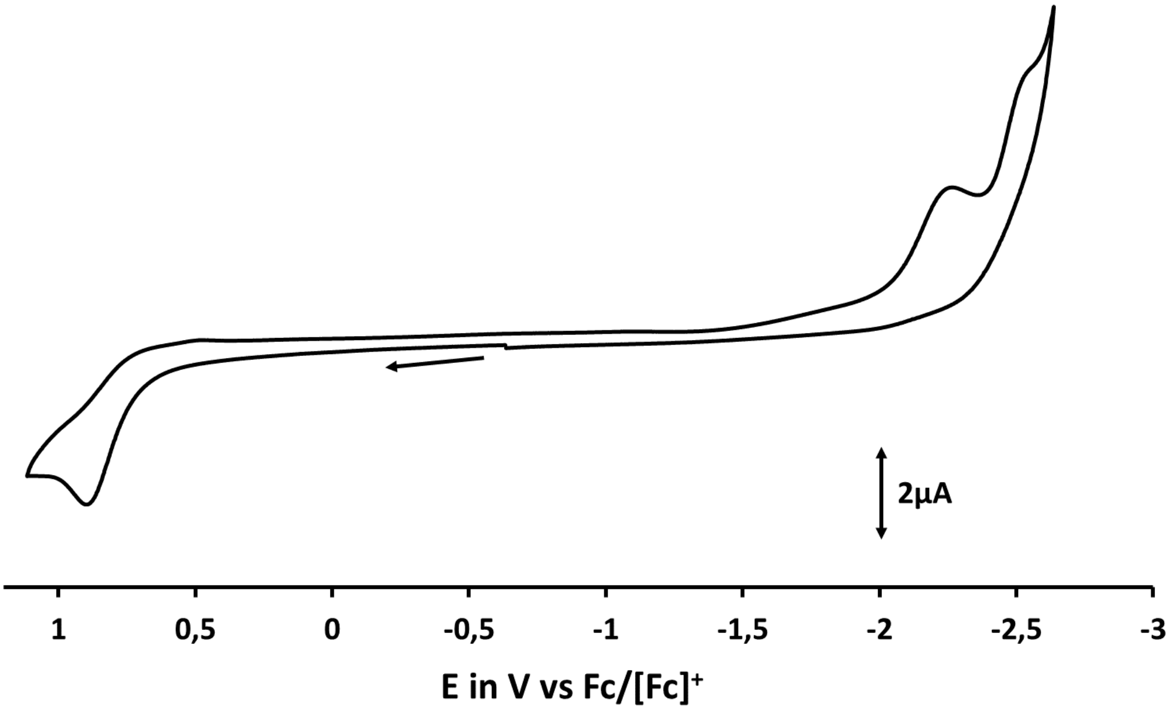


Figure S 65: Cyclic voltammogramm of **$H_3L[Cl]$** recorded in 0.1 M NBu_4PF_6 in dichloromethane at room temperature.

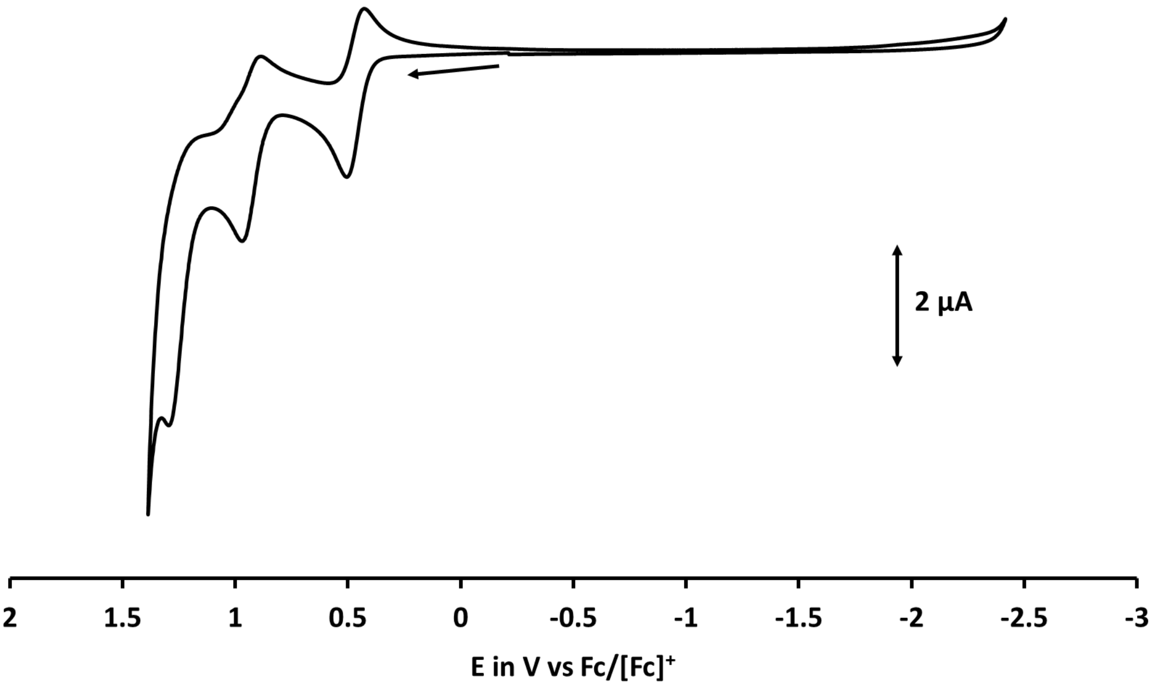


Figure S 66: Cyclic voltammogramm of **5** recorded in 0.1 M NBu_4PF_6 in dichloromethane at room temperature.

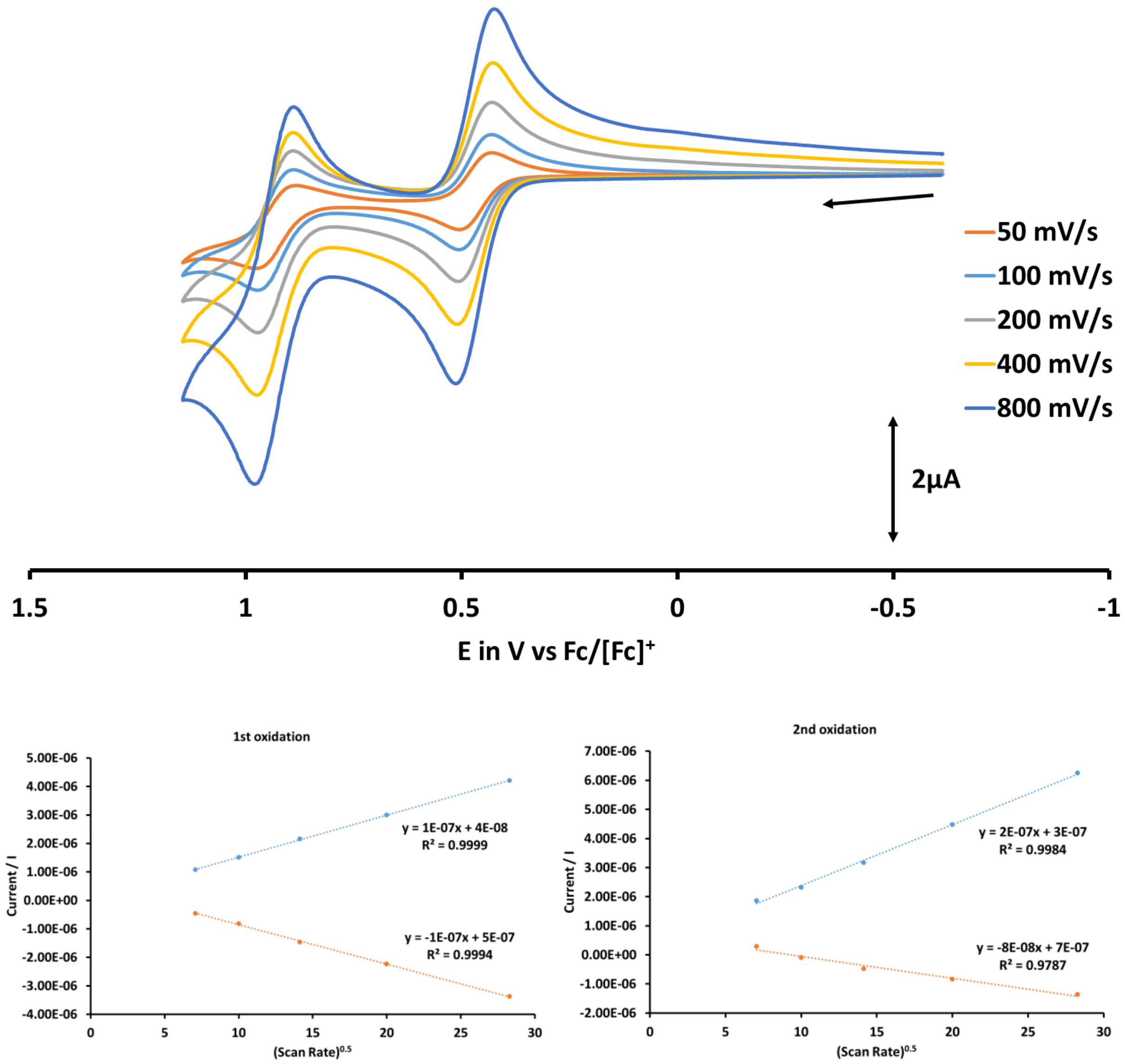


Figure S 67: Cyclic voltammogramm of **5** recorded in 0.1 M NBu_4PF_6 in dichloromethane at room temperature recorded at different scan rates (top). Linear dependency of the current and the square root of the scan rate for the oxidation processes (bottom)

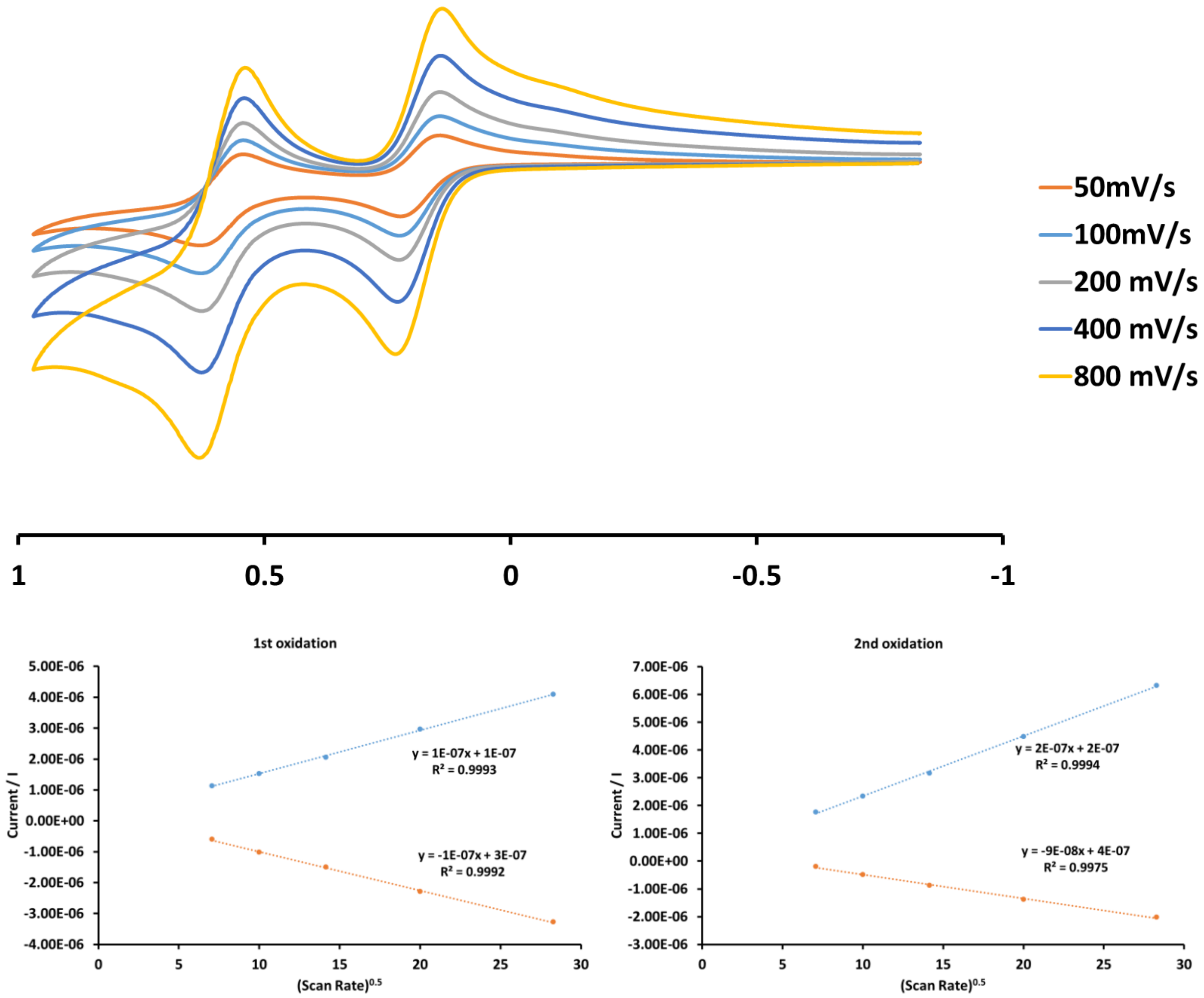


Figure S 68: Cyclic voltammogramm of **11** recorded in 0.1 M NBu_4PF_6 in dichloromethane at room temperature recorded at different scan rates (top). Linear dependency of the current and the square root of the scan rate for the oxidation processes (bottom)

6. Literature

[1] T.M. Khomenko, O.V. Salomatina, S.Y. Kurbakova, I.V. Il'ina, K.P. Volcho, N.I. Komarova, D.V. Korchagina, N.F. Salakhutdinov, A.G. Tolstikov *Russ J Org Chem* **2006**, *42*, 1653.

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Author contributions

The project was designed by SH. Experimental work was carried out by MB, FAW and SH. X-ray measurement and structure solutions were conducted by SH, RS and CW. Cyclic voltammetry experiments were carried out by AGN and SH. The manuscript was written by SH and prove read by all authors.