

Figure 1: IR spectra of 1-cyclopentyl-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazolium chloride (2a)

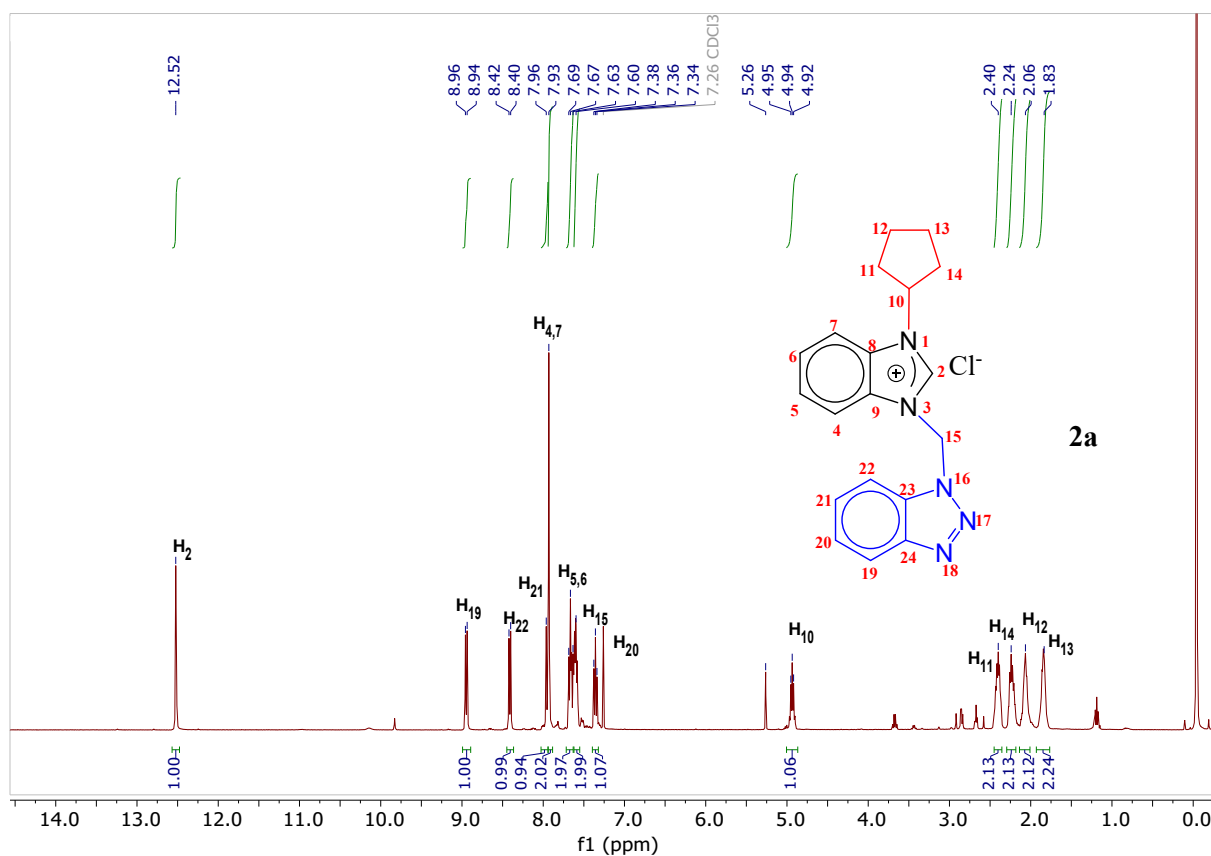


Figure 2: ¹H NMR spectra of 1-cyclopentyl-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazolium chloride (2a)

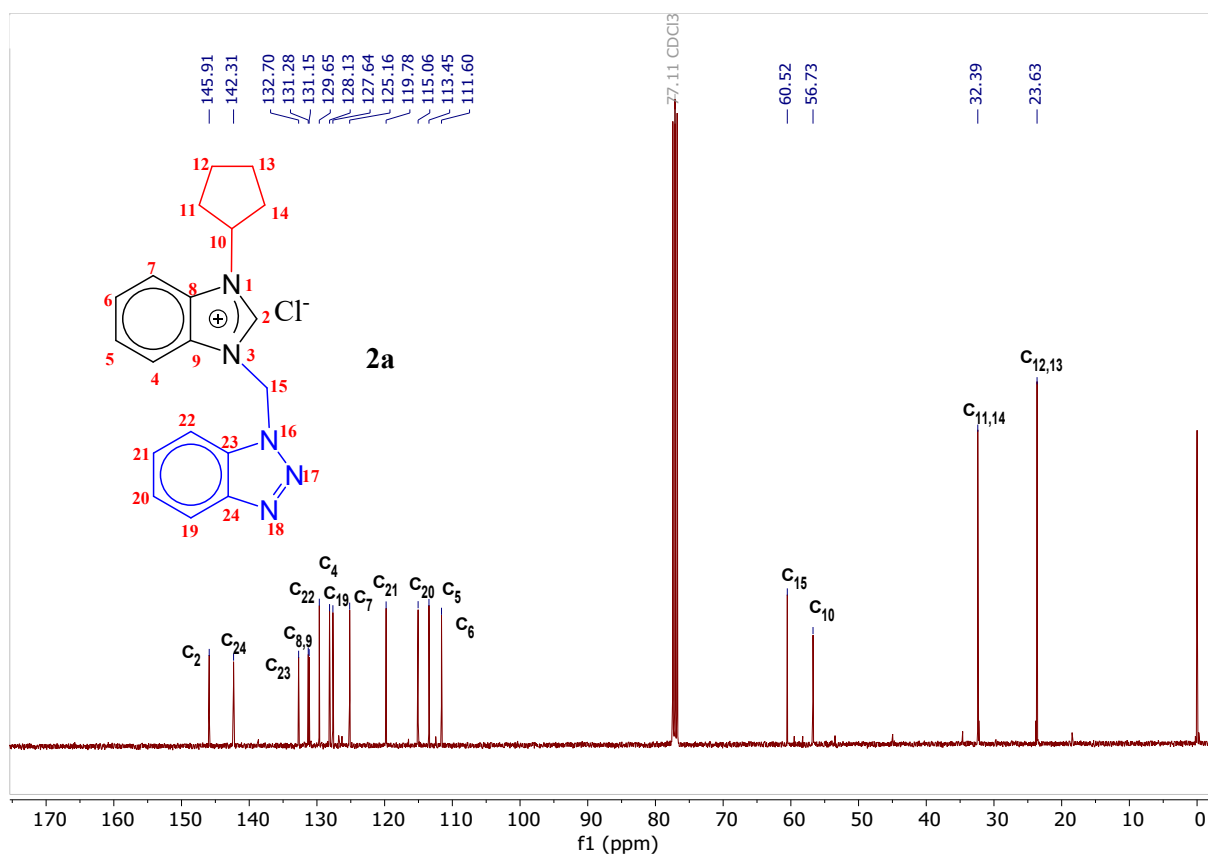


Figure 3 : ¹³C NMR spectra of 1-cyclopentyl-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazolium chloride (2a).

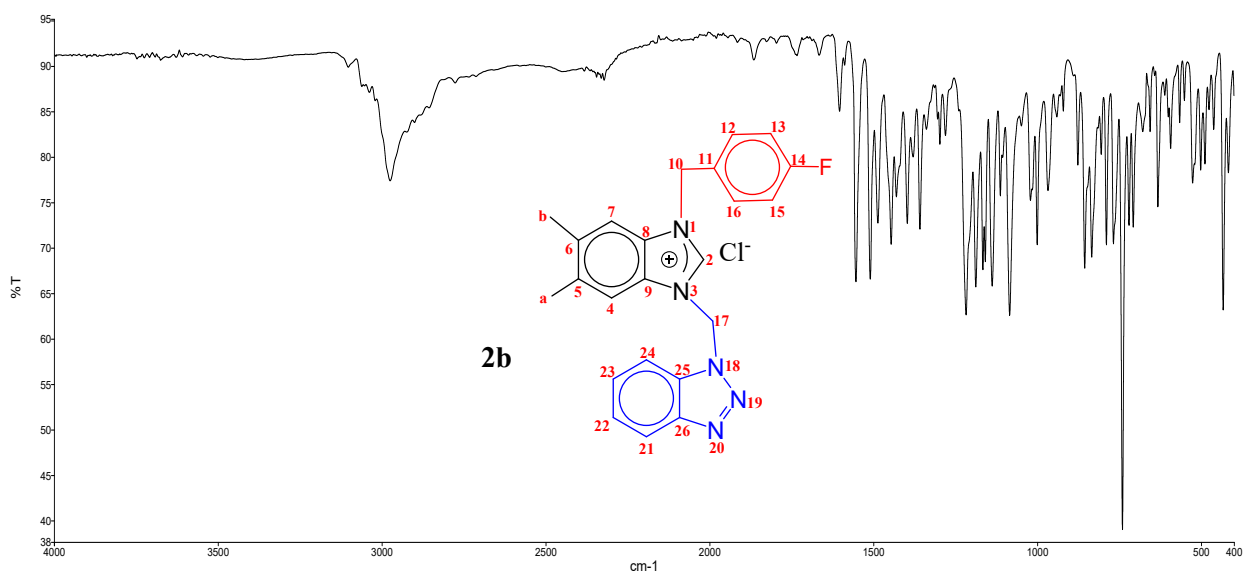


Figure 4: IR spectra of 1-(4-fluorobenzyl)-3-(1-methylbenzo-1,2,3-triazolyl)-5,6-dimethylbenzimidazolium chloride (2b).

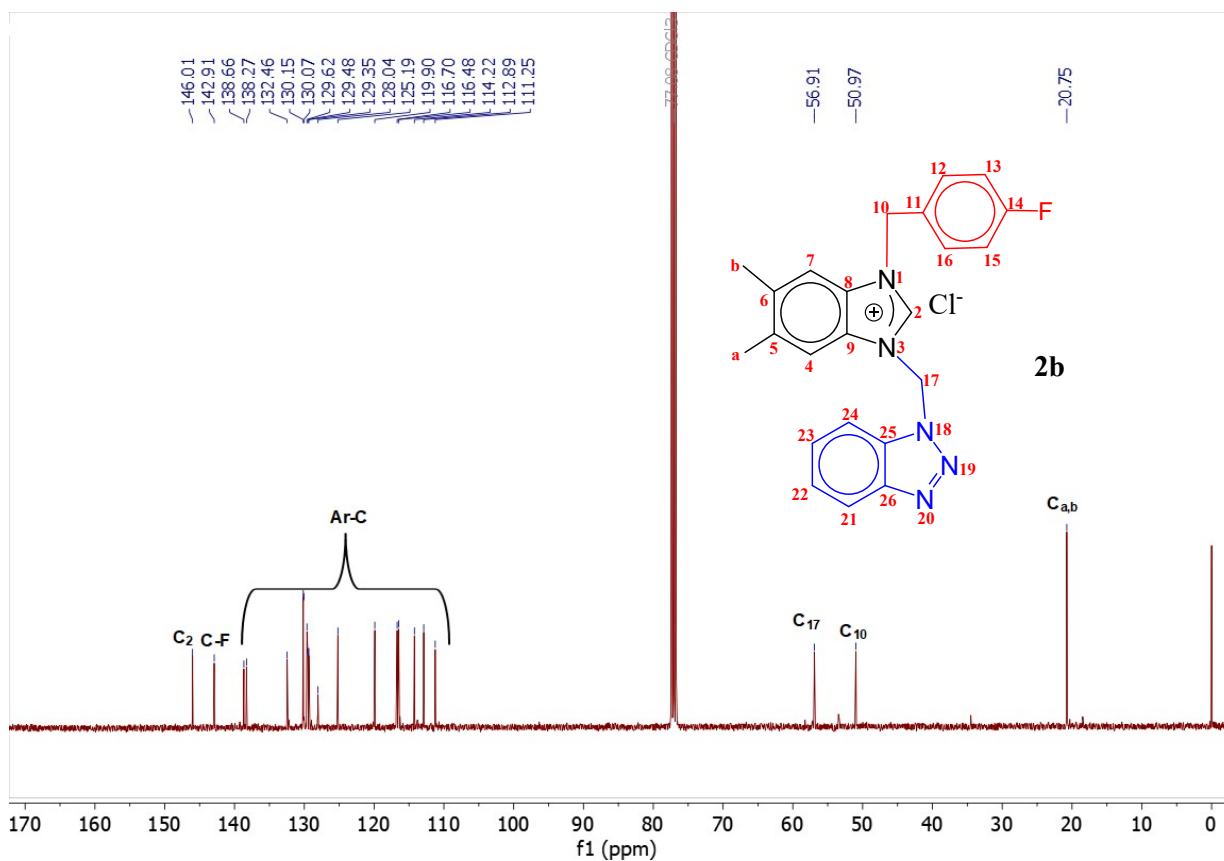
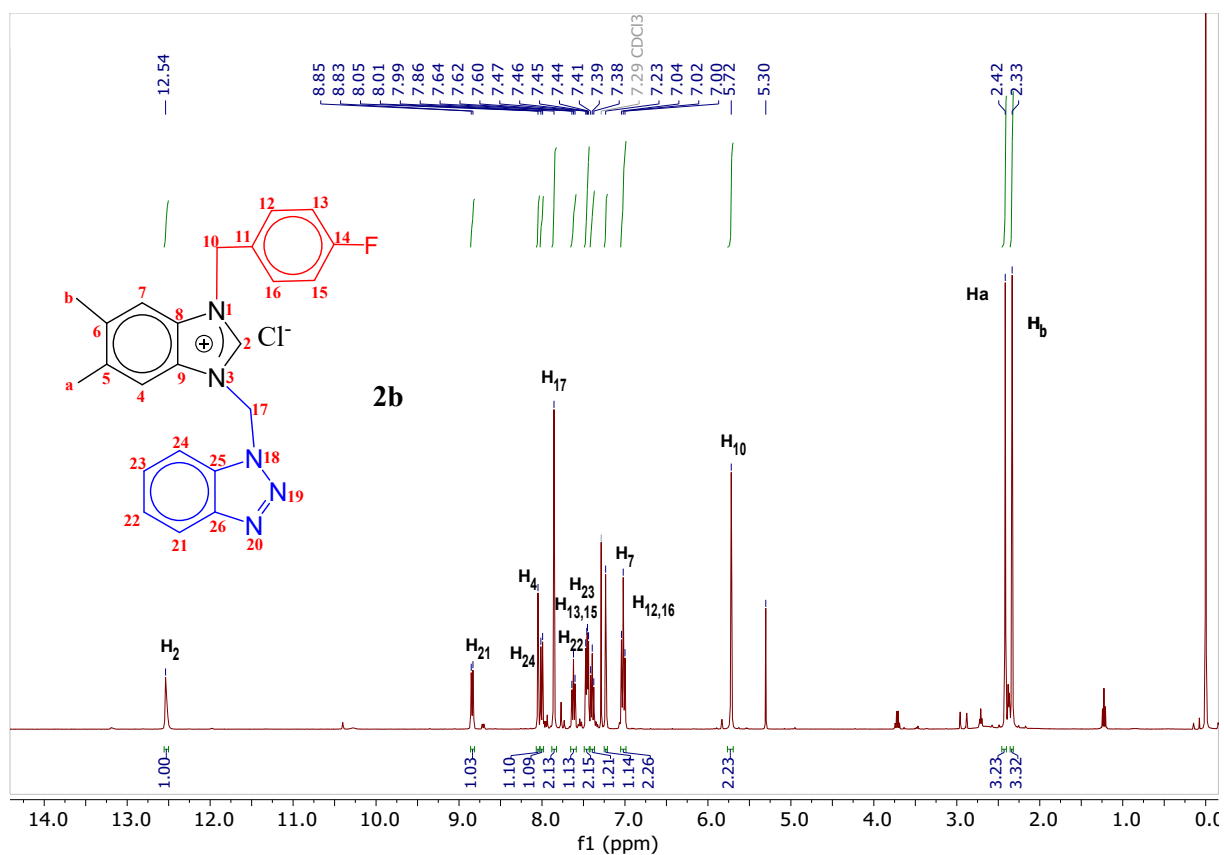


Figure 6 : ^{13}C NMR spectra of 1-(4-fluorobenzyl)-3-(1-methylbenzo-1,2,3-triazolyl)-5,6-dimethylbenzimidazolium chloride (2b).

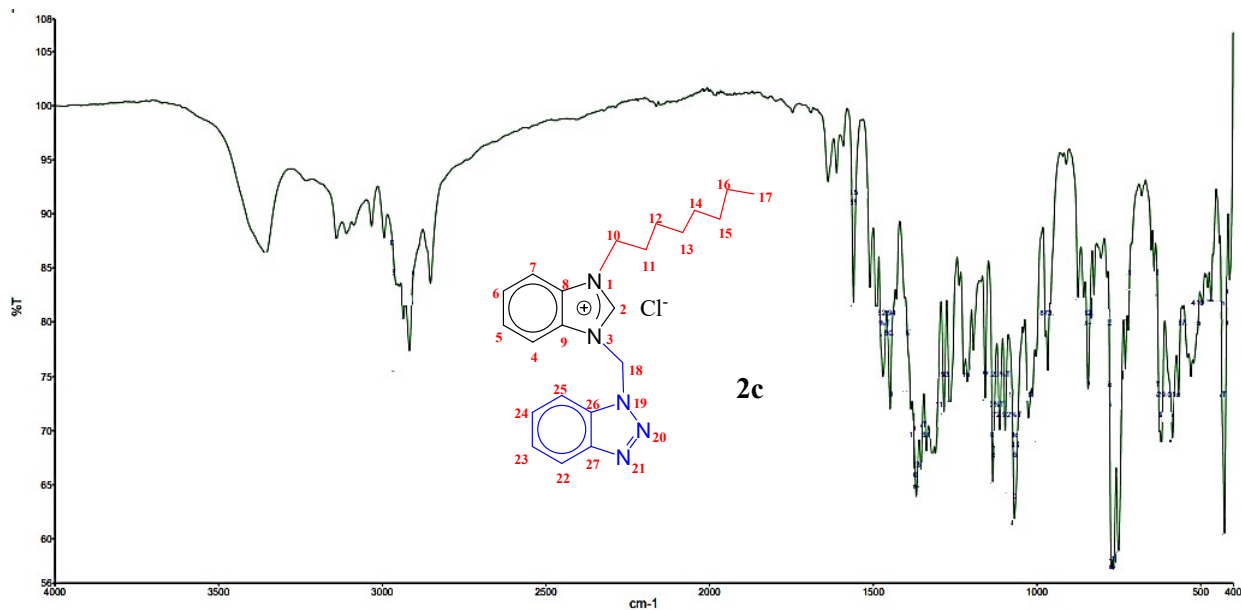


Figure 7: IR spectra of 1-octyl-3-(1-methylbenzo-1,2,3-triazolyl)-5,6-dimethylbenzimidazolium chloride (2c).

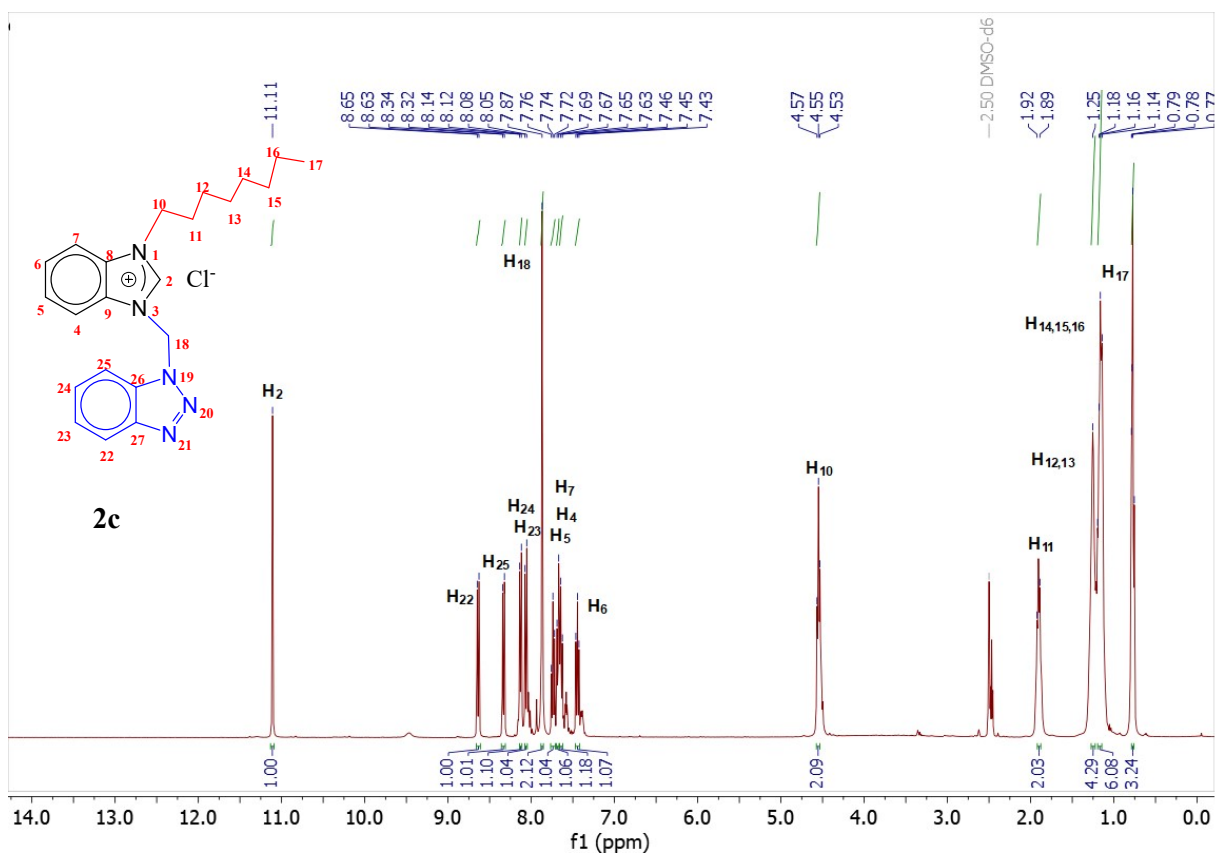


Figure 8 : ^1H NMR spectra of 1-octyl-3-(1-methylbenzo-1,2,3-triazolyl)-5,6-dimethylbenzimidazolium chloride (2c)

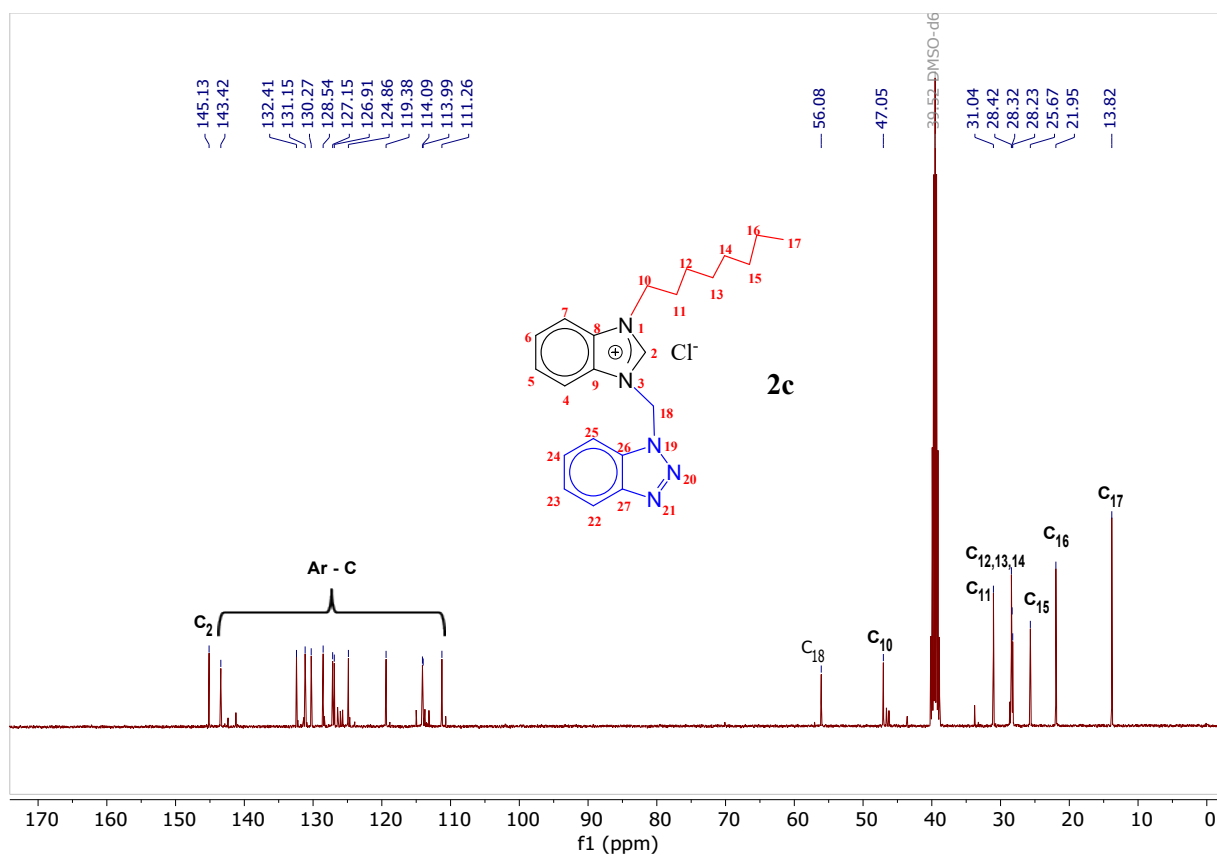


Figure 9 : ¹³C NMR spectra of 1-octyl-3-(1-methylbenzo-1,2,3-triazolyl)-5,6-dimethylbenzimidazolium chloride (2c).

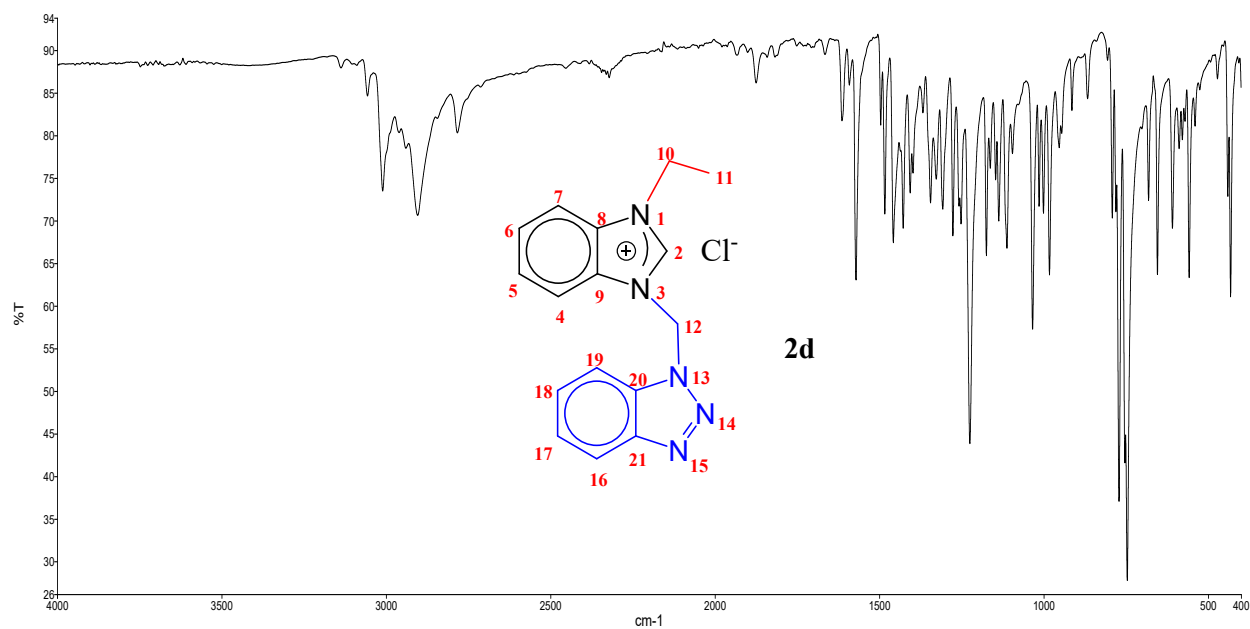


Figure 10: IR spectra of 1-Ethyl-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazolium chloride (2d).

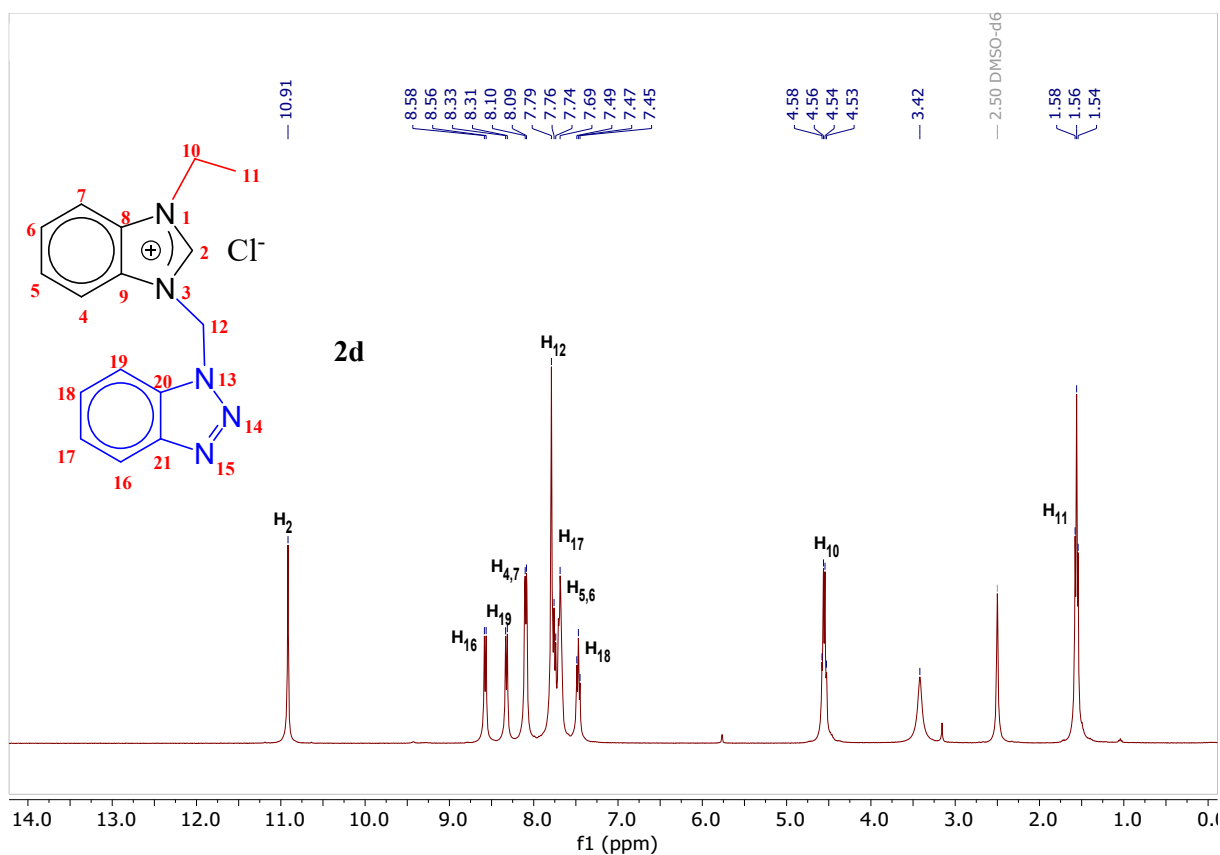


Figure 11 : ^1H NMR spectra of 1-Ethyl-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazolium chloride (2d).

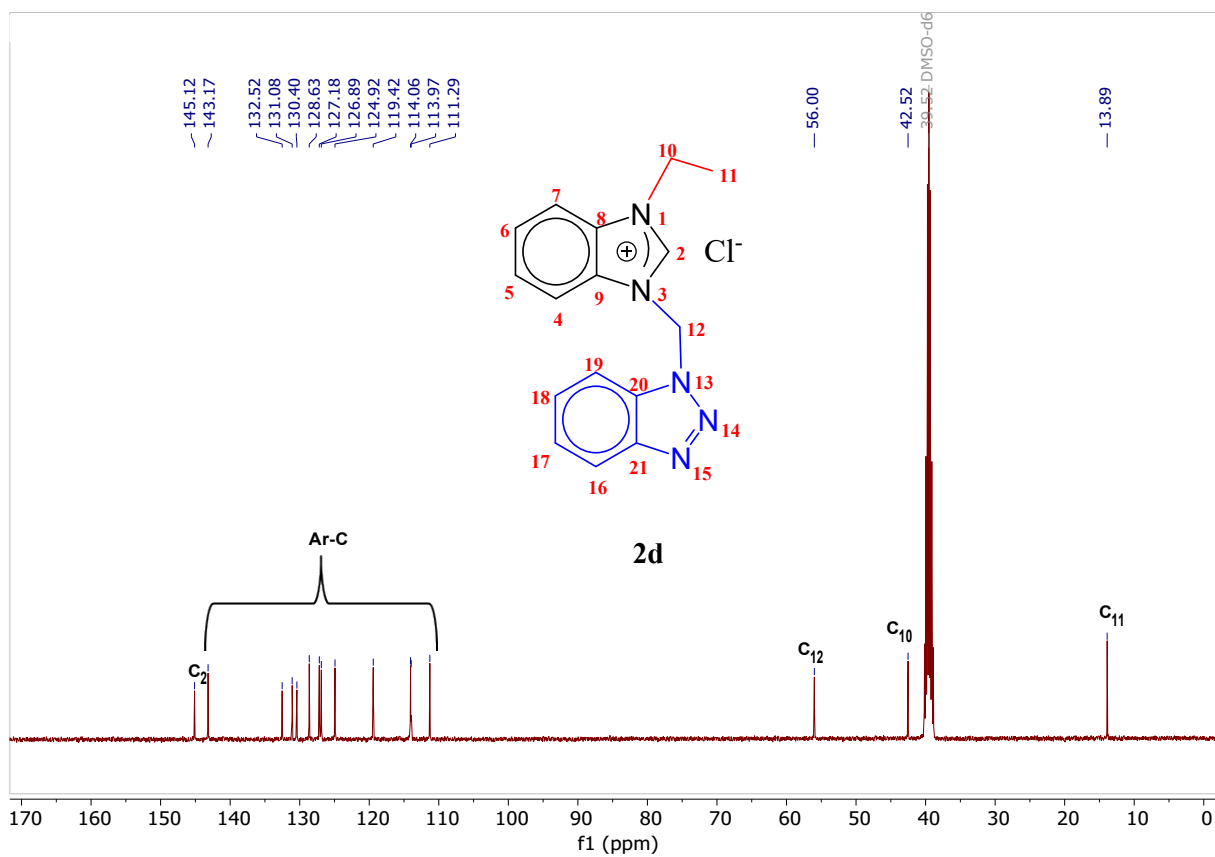


Figure 12 : ^{13}C NMR spectra of 1-Ethyl-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazolium chloride (2d).

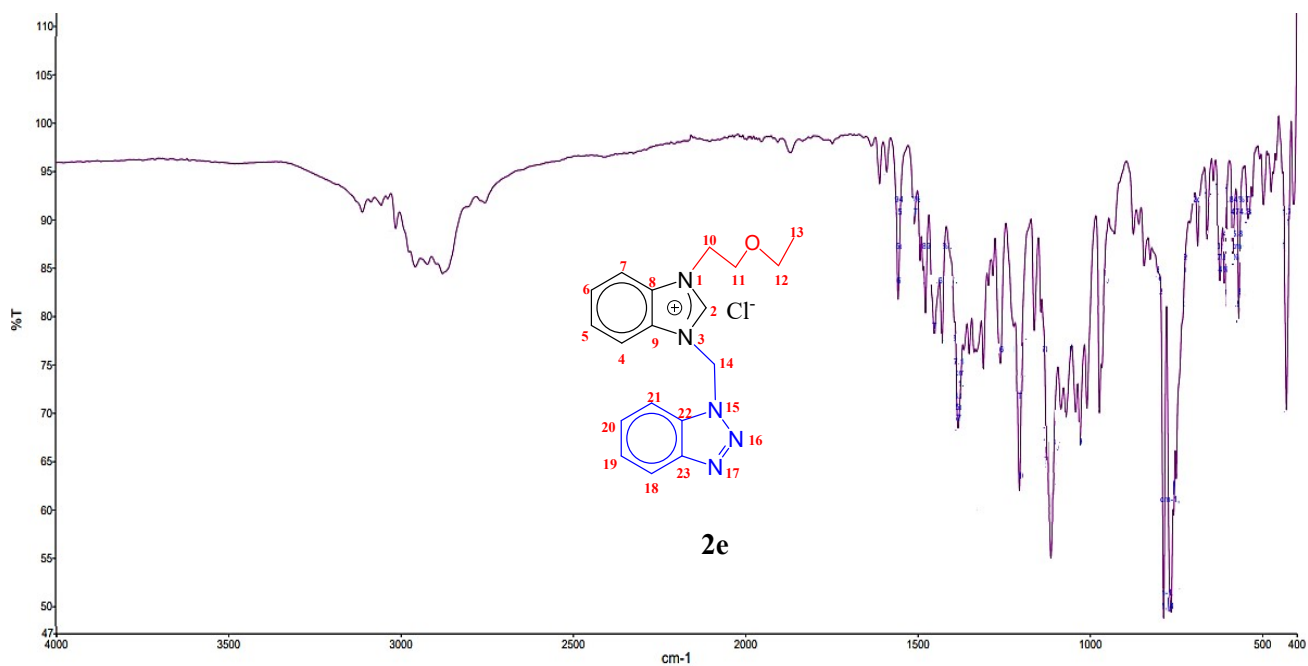


Figure 13: IR spectra of 1-(2-ethoxyethyl)-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazolium chloride (2e)

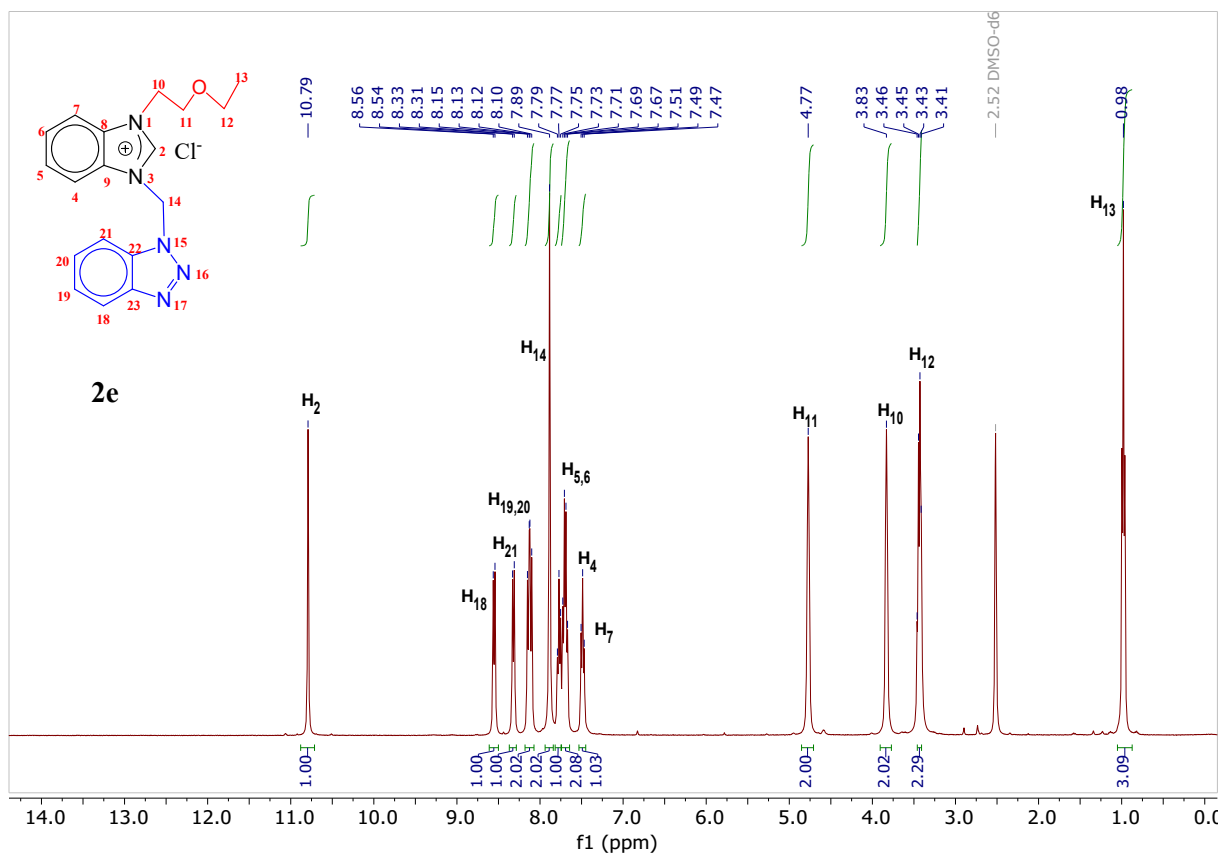


Figure 14 : ^1H NMR spectra of 1-(2-ethoxyethyl)-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazolium chloride (2e).

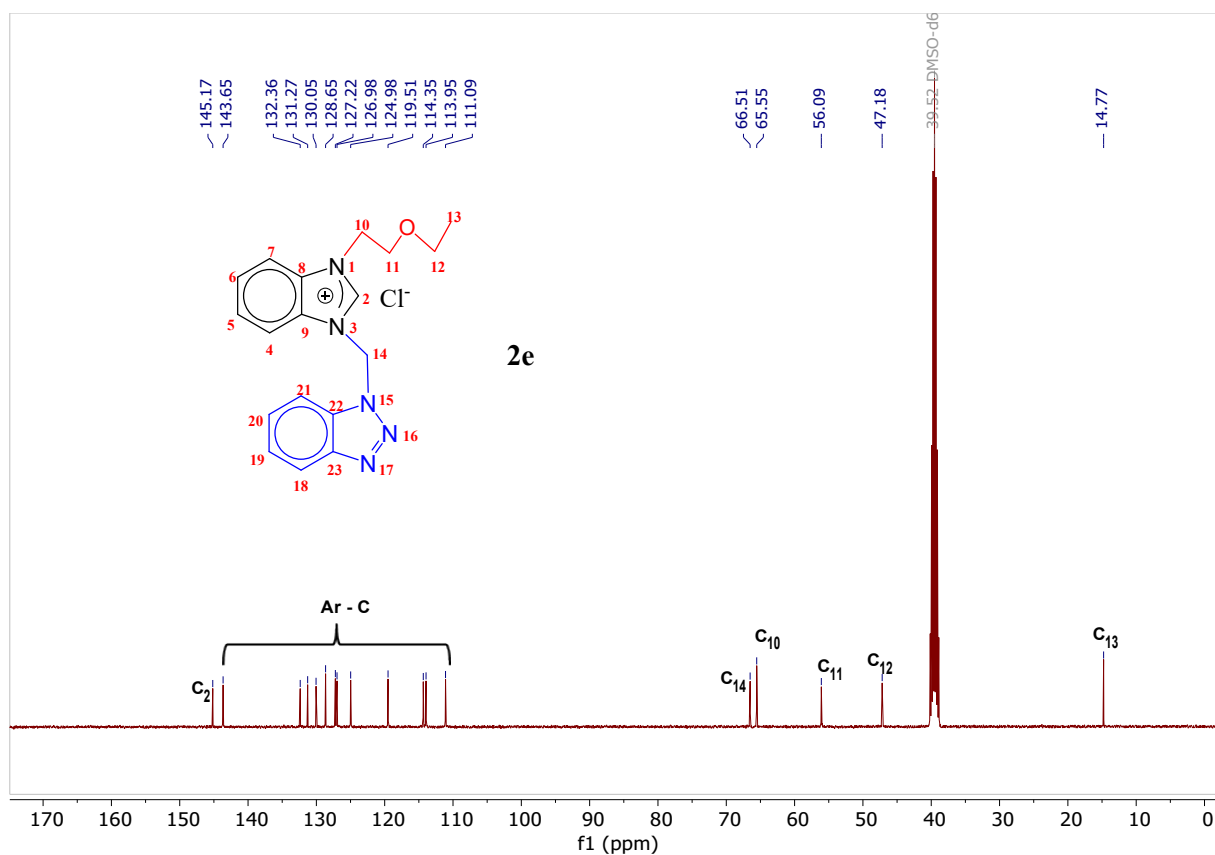


Figure 15 : ¹³CNMR spectra of 1-(2-ethoxyethyl)-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazolium chloride (2e).

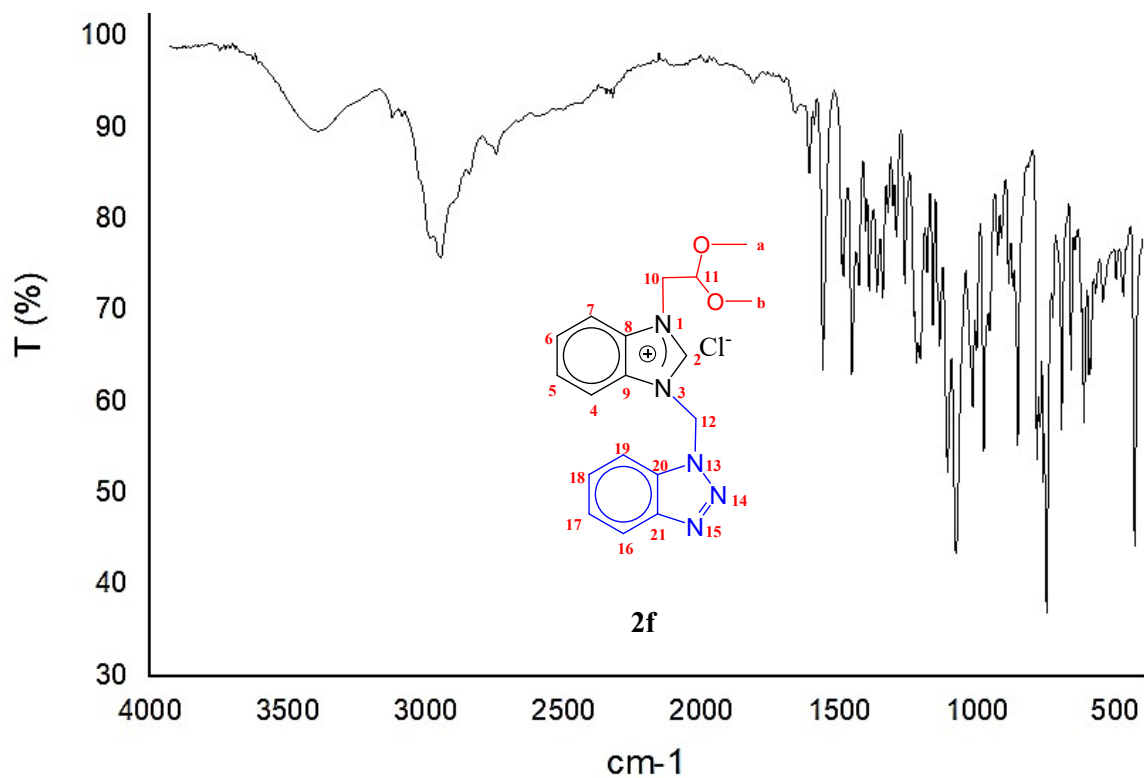


Figure 16: IR spectra of 1-(2,2-dimethoxyethyl)-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazolium chloride (2f).

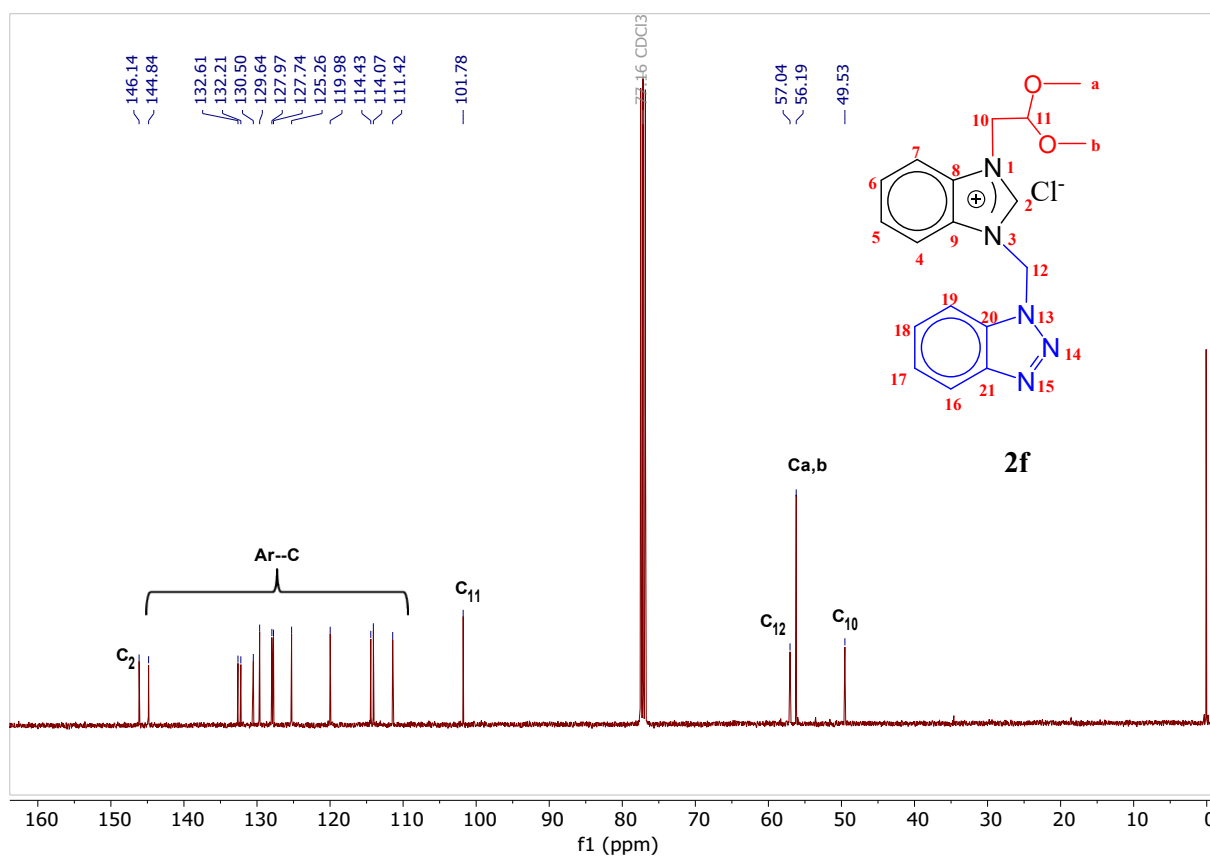
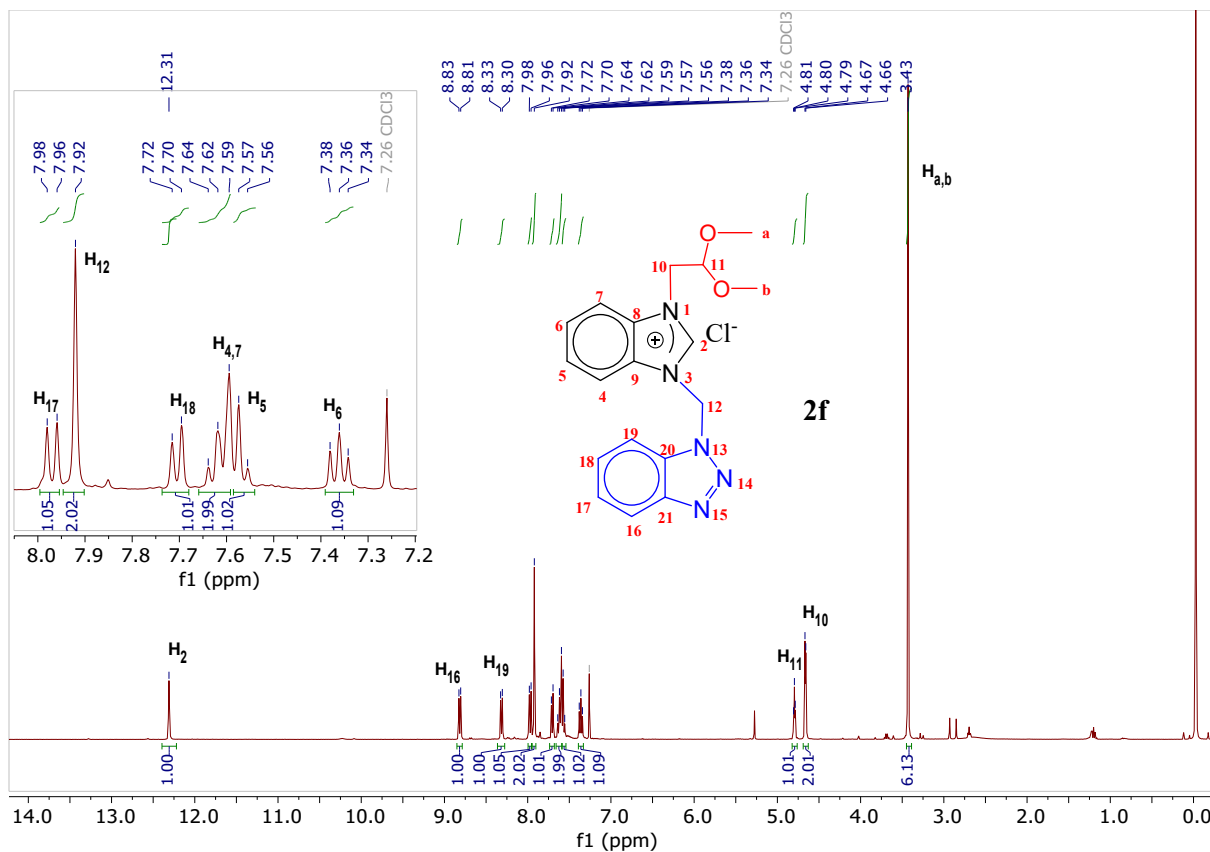


Figure 18 : ^{13}C NMR spectra of 1-(2,2-dimethoxyethyl)-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazolium chloride (2f).

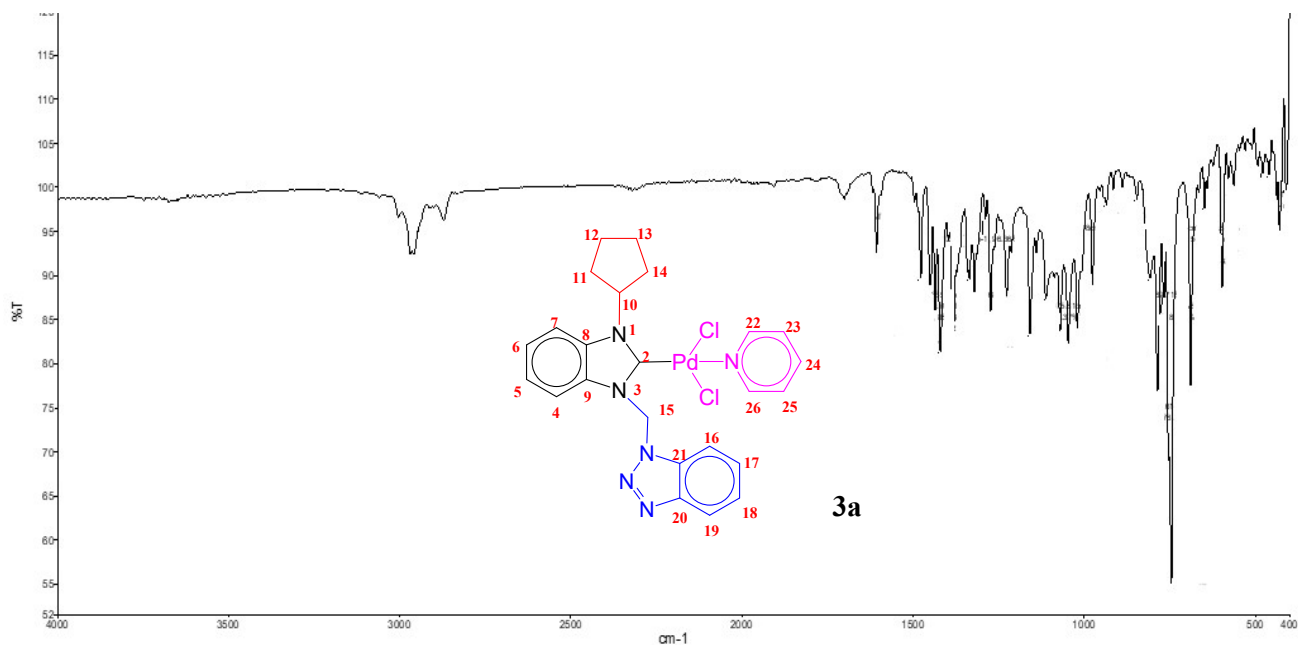


Figure 19: IR spectra of Dichloro[1-cyclopentyl-3-(1-methylbenzo-1,2,3-triazolyl) benzimidazole-2-ylidene] pyridine palladium(II) (3a)

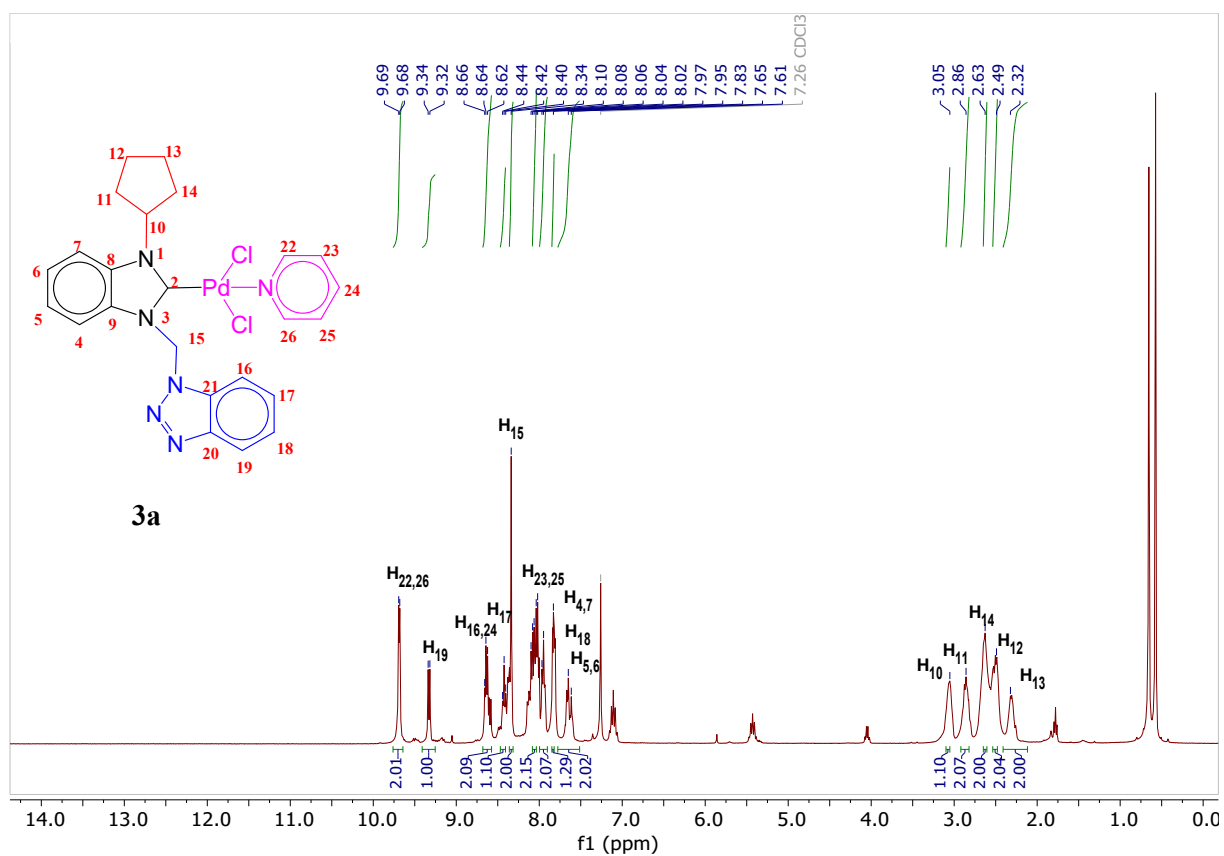
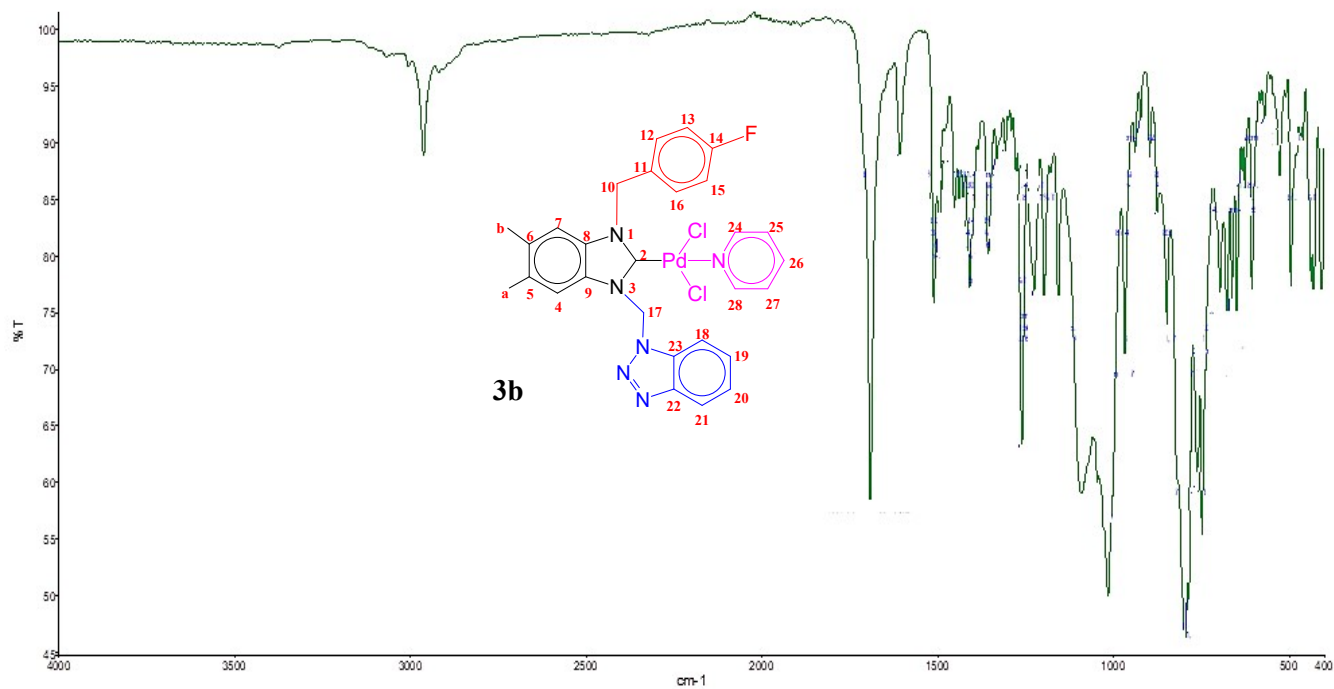
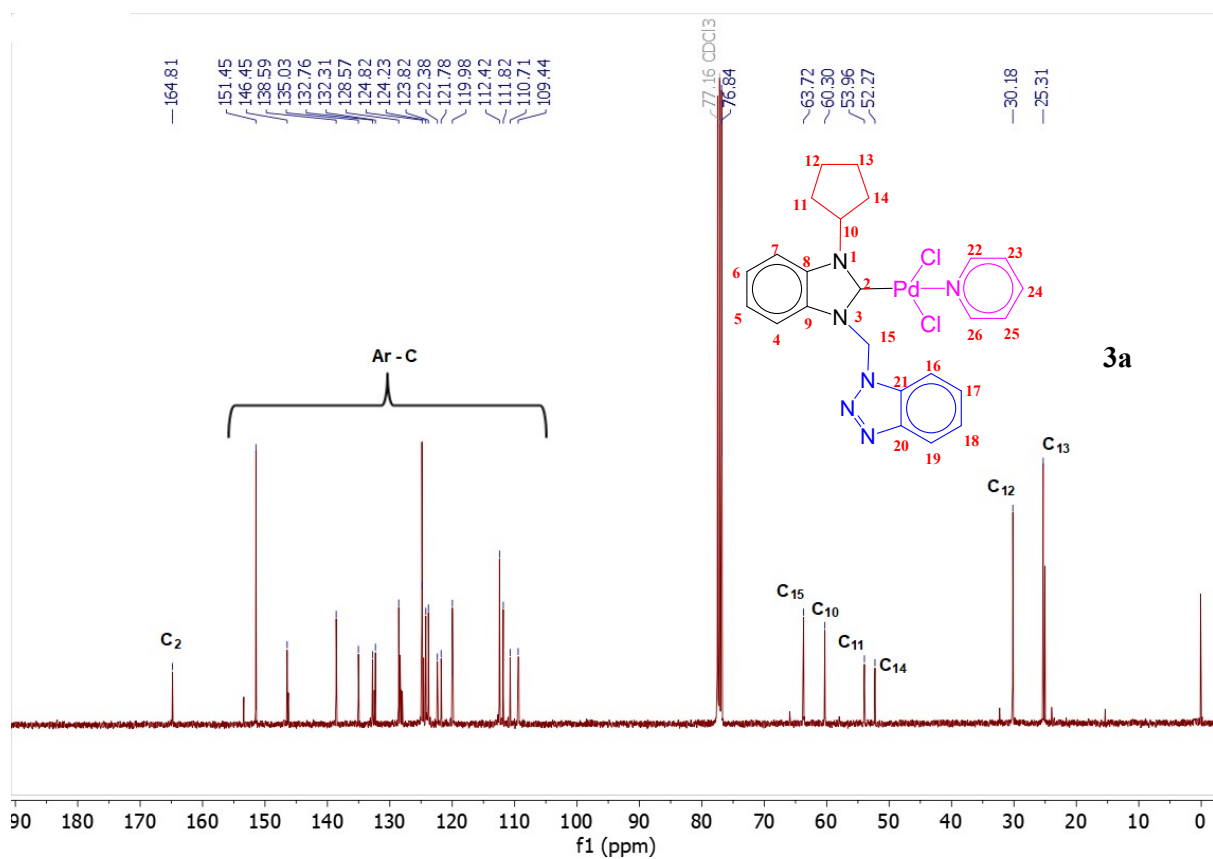


Figure 20: ^1H NMR spectra of Dichloro[1-cyclopentyl-3-(1-methylbenzo-1,2,3-triazolyl) benzimidazole-2-ylidene] pyridine palladium(II) (3a)



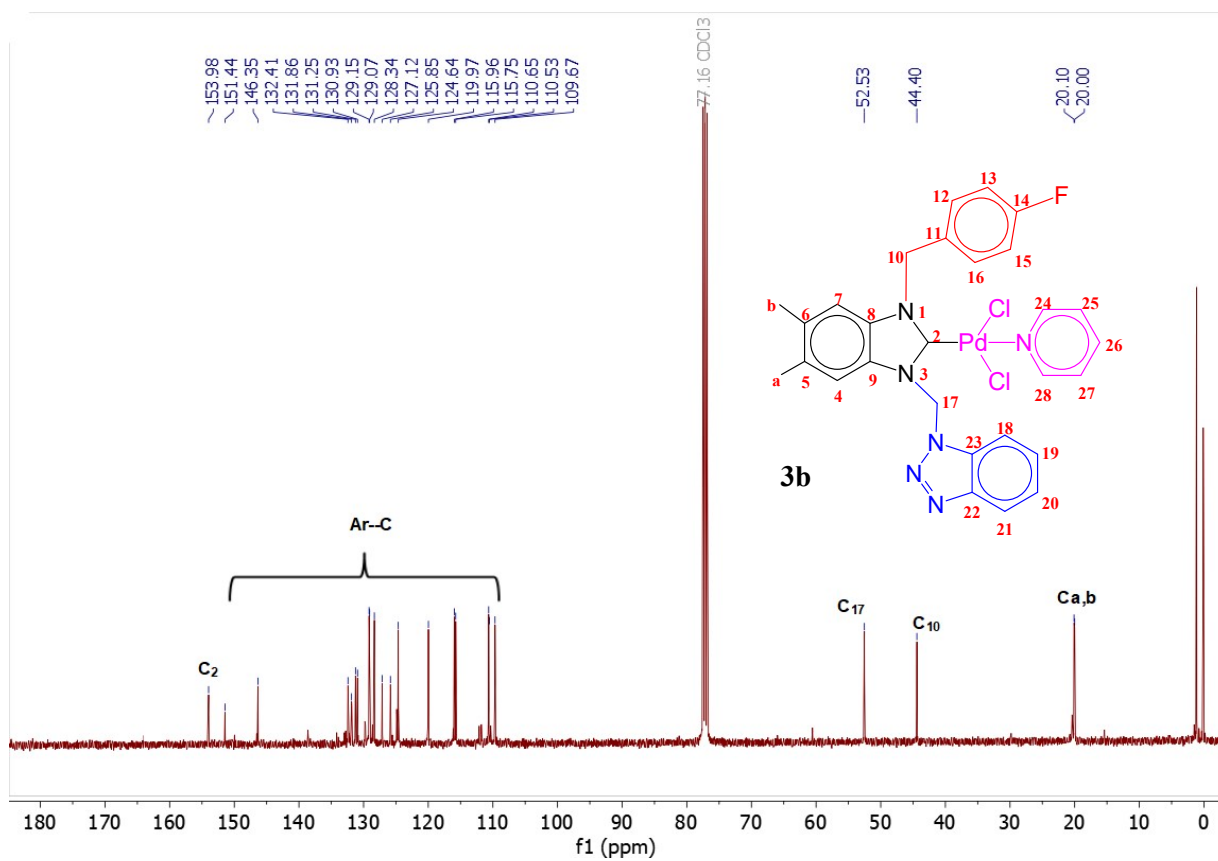
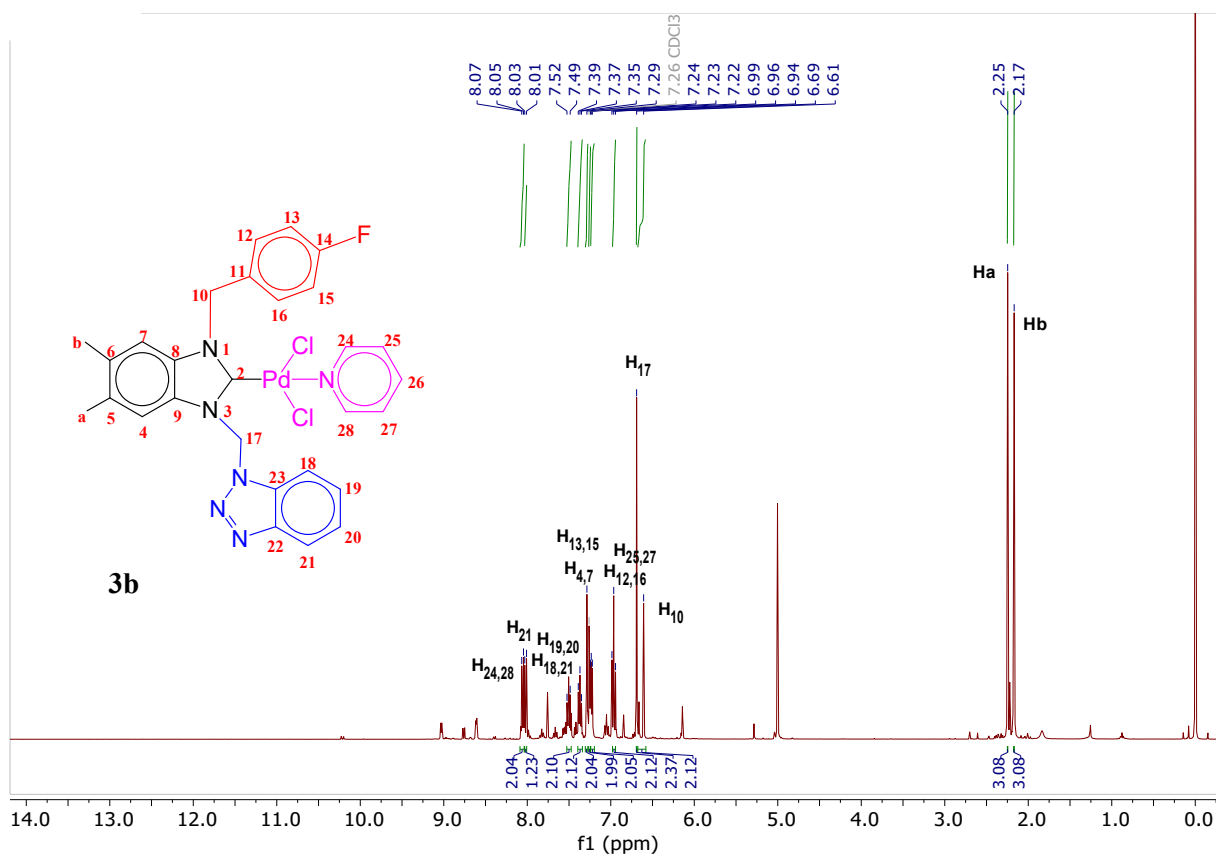


Figure 24 : ^{13}C NMR spectra of Dichloro[1-(4-fluorobenzyl)-3-(1-methylbenzo-1,2,3-triazolyl)-5,6-dimethyl benzimidazole-2-ylidene] pyridine palladium (3b)

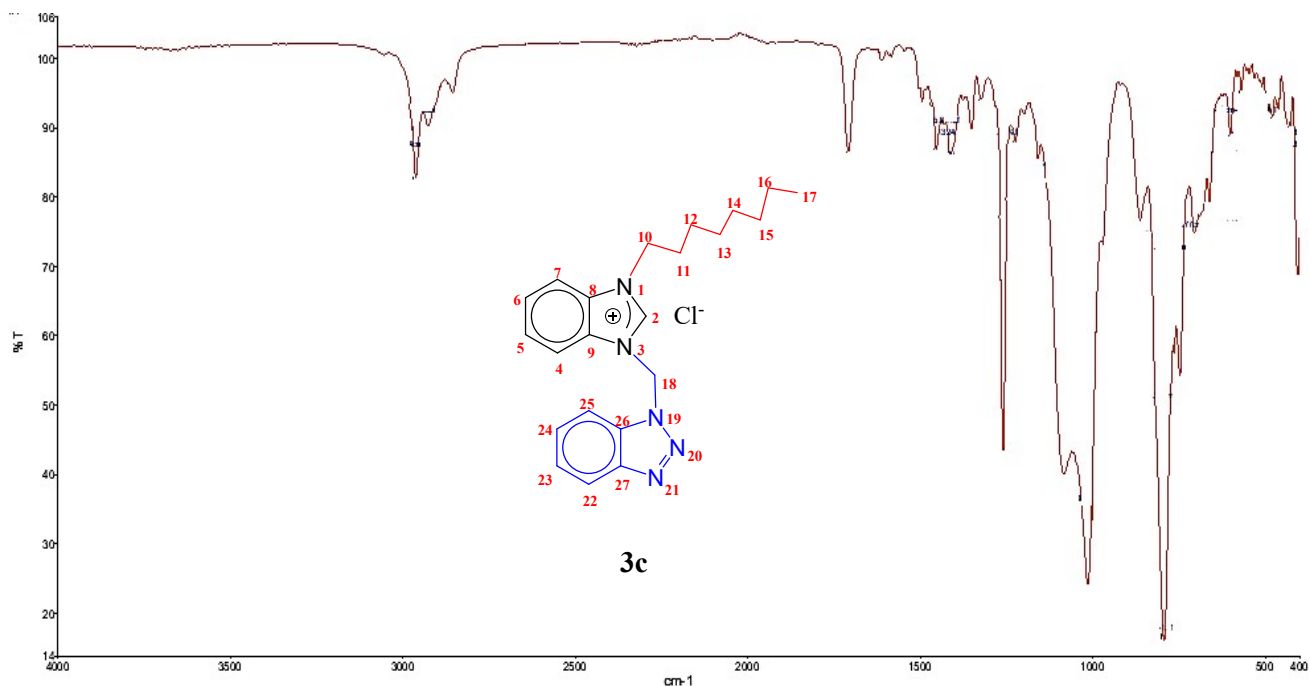


Figure 25: IR spectra of Dichloro[1-octyl-3-(1-methylbenzo-1,2,3-triazolyl) benzimidazole-2-ylidene] pyridine palladium(II) (3c)

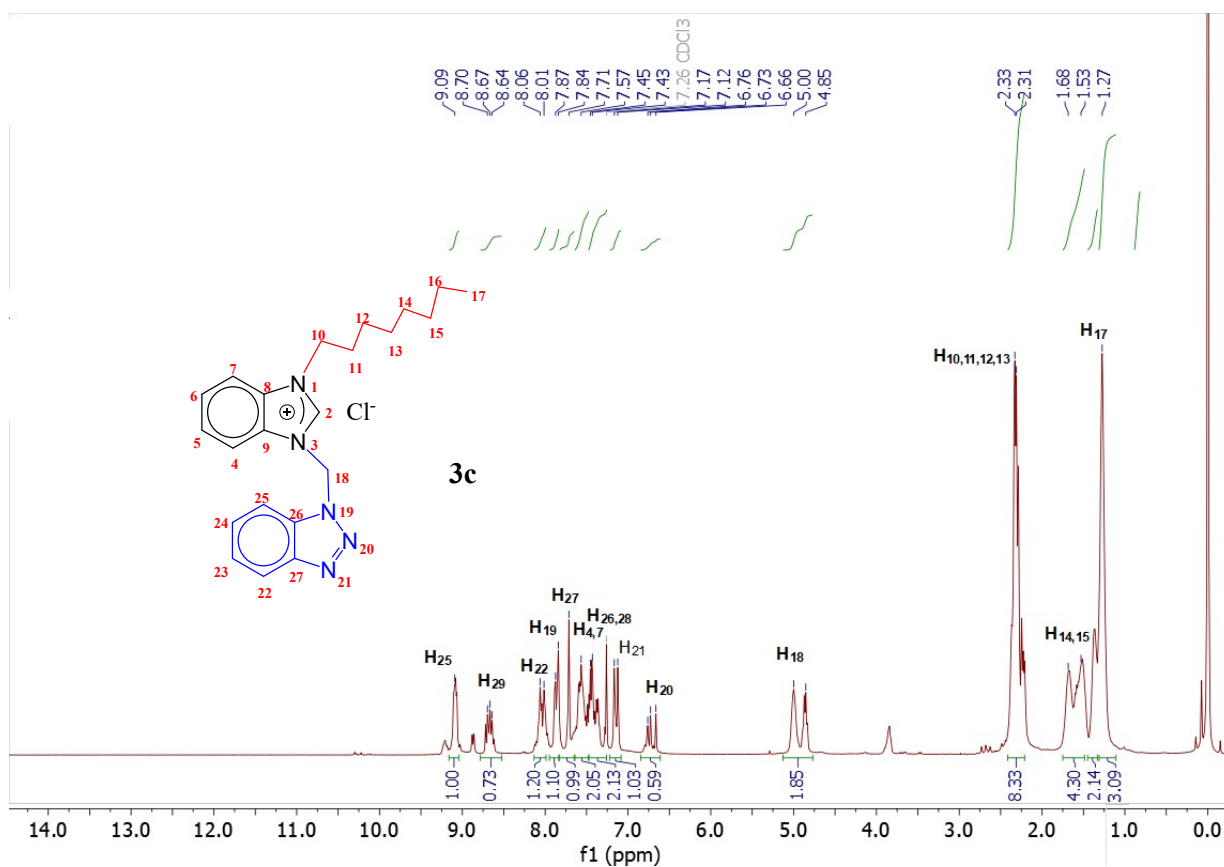


Figure 26 : ^1H NMR spectra of Dichloro[1-octyl-3-(1-methylbenzo-1,2,3-triazolyl) benzimidazole-2-ylidene] pyridine palladium(II) (3c)

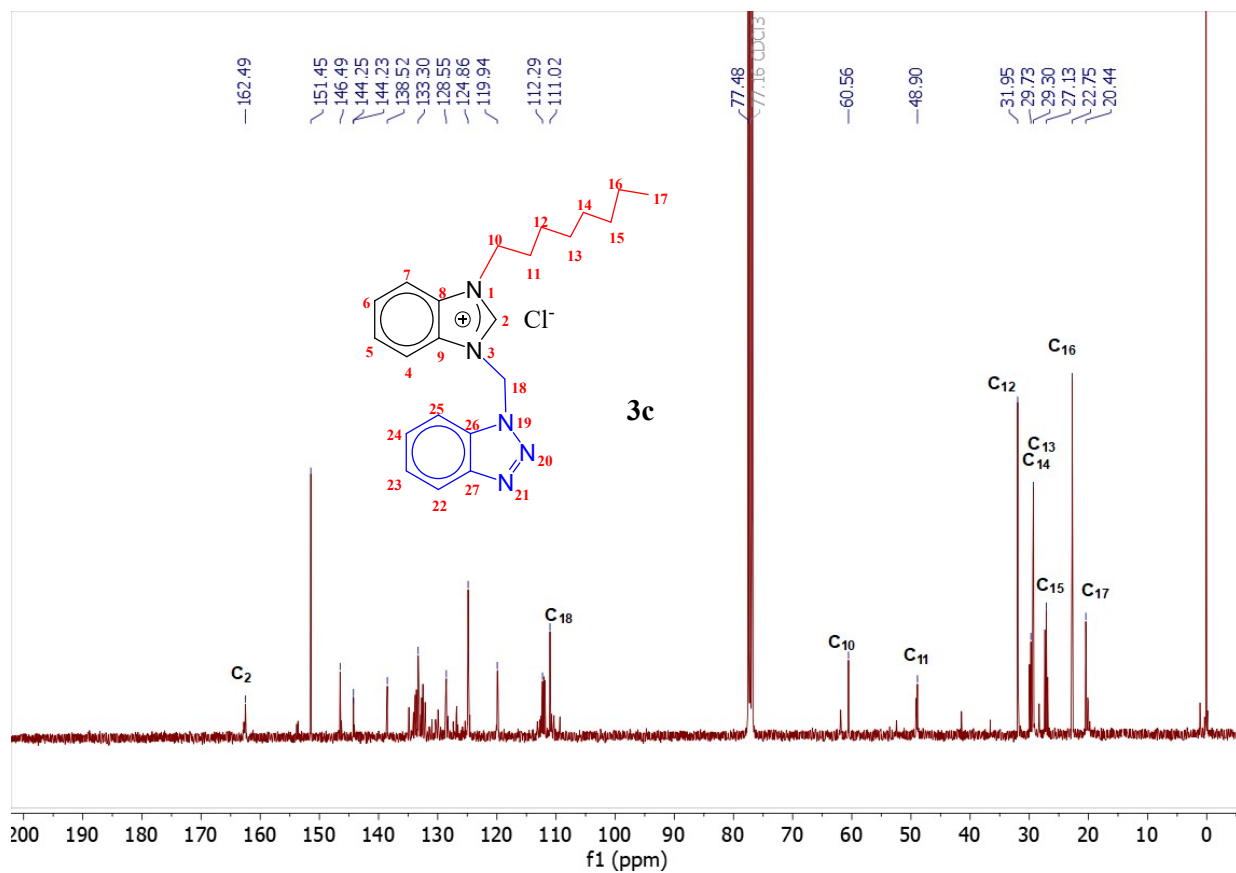


Figure 27 : ^{13}C NMR spectra of Dichloro[1-octyl-3-(1-methylbenzo-1,2,3-triazolyl) benzimidazole-2-ylidene] pyridine palladium(II) (3c).

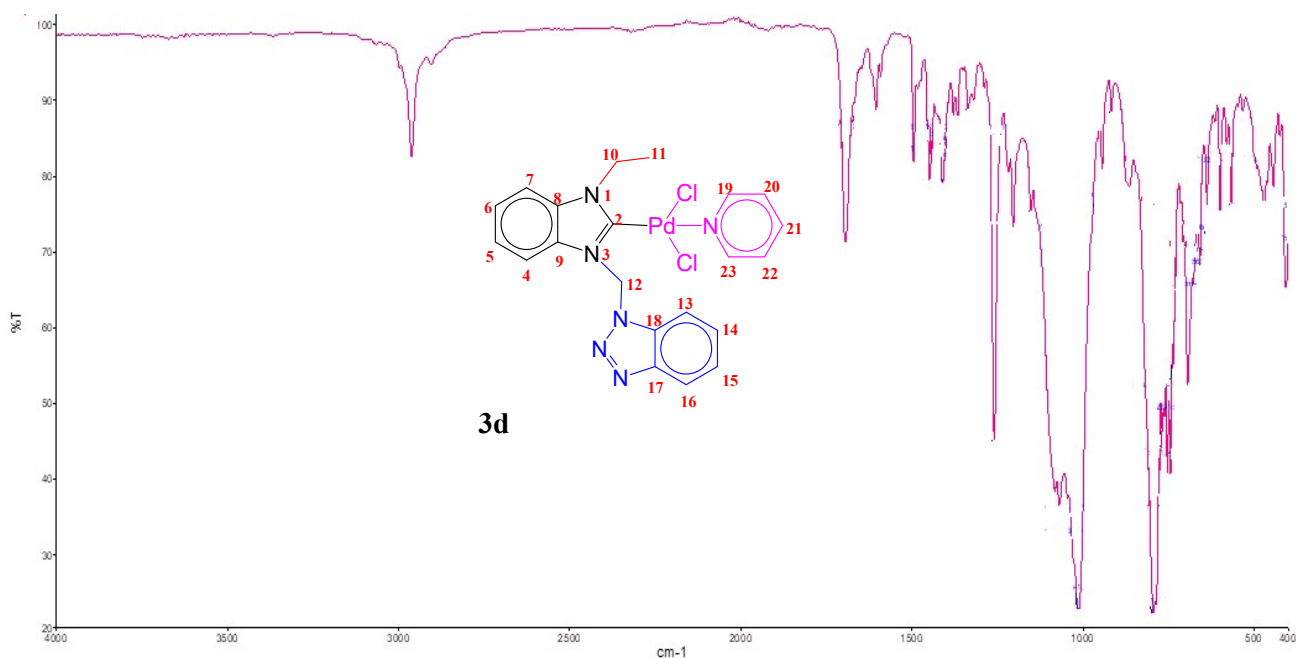


Figure 28: IR spectra of Dichloro[1-Ethyl-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazole-2-ylidene] pyridine palladium(II) (3d)

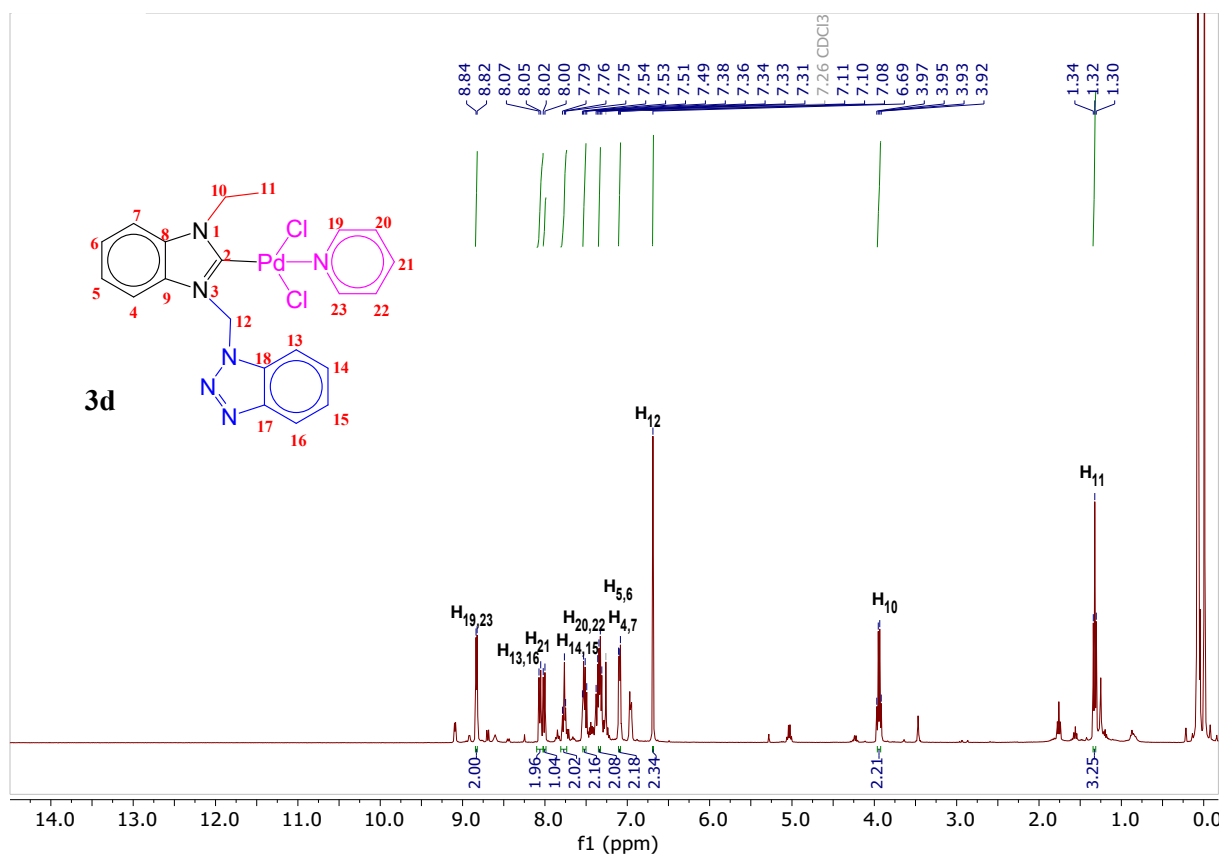


Figure 29 : ¹H NMR spectra of Dichloro[1-Ethyl-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazole-2-ylidene] pyridine palladium(II) (3d)

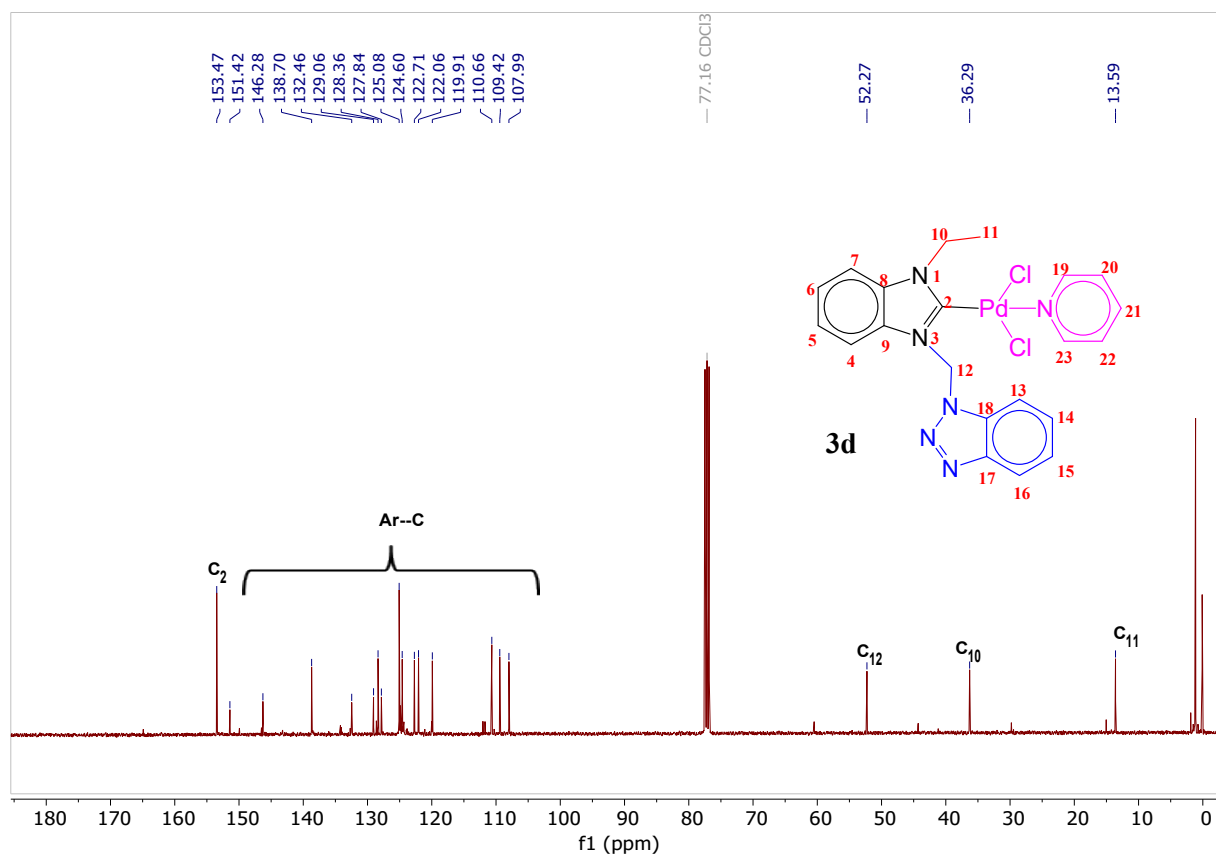


Figure 30 : ^{13}C NMR spectra of Dichloro[1-Ethyl-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazole-2-ylidene] pyridine palladium(II) (3d)

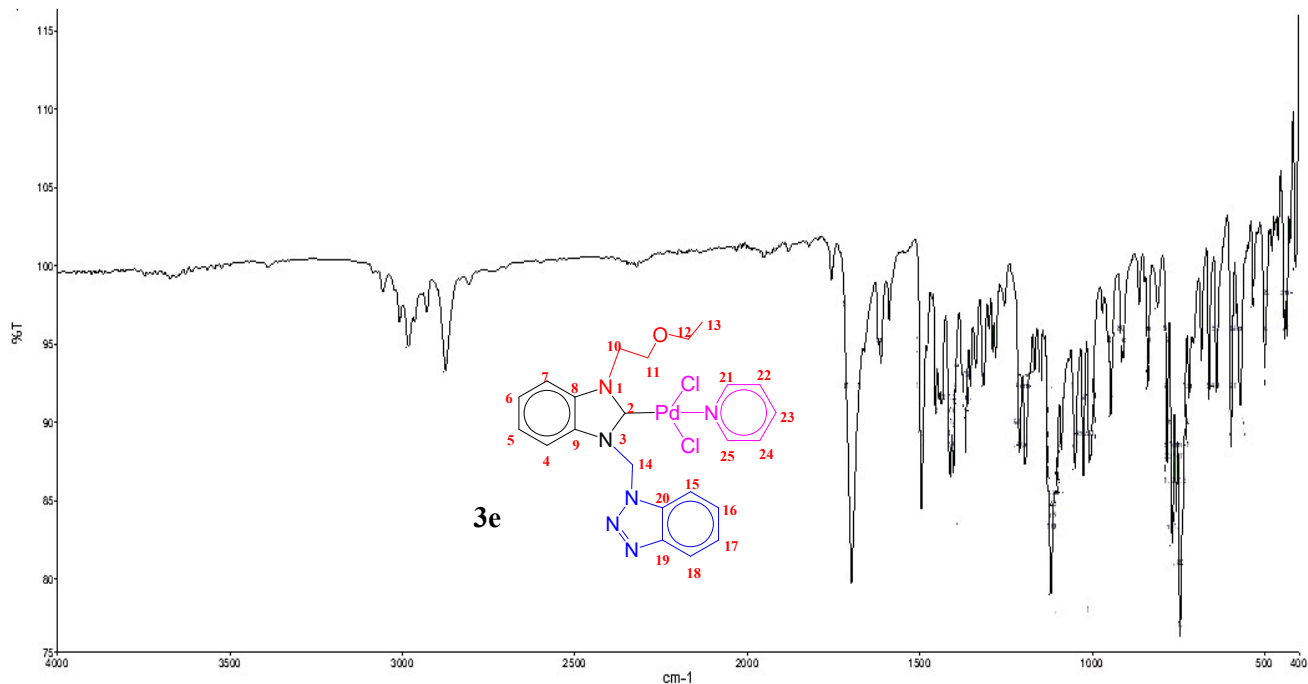


Figure 31: IR spectra of Dichloro[1-(2-ethoxyethyl)-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazole-2-ylidene] pyridine palladium(II) (3e)

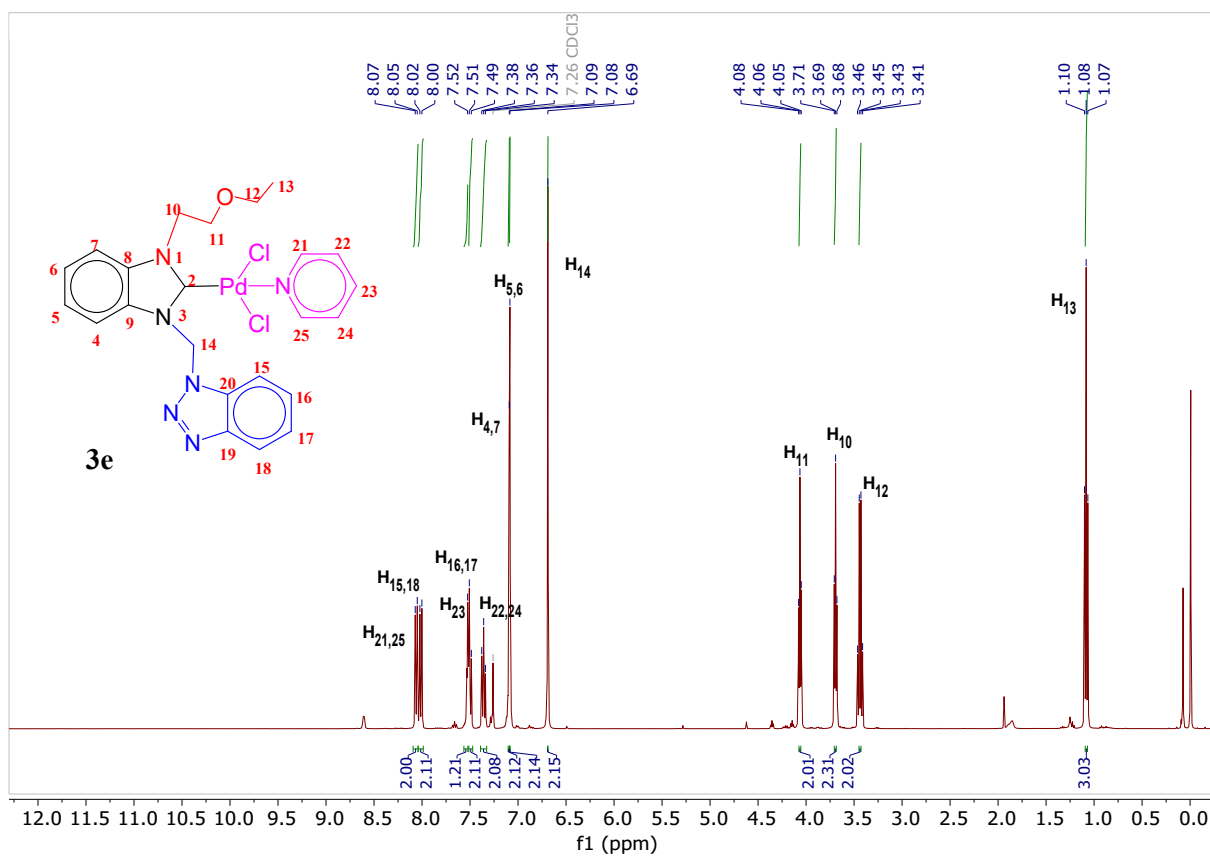


Figure 32 : ^1H NMR spectra of Dichloro[1-(2-ethoxyethyl)-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazole-2-ylidene] pyridine palladium(II) (3e)

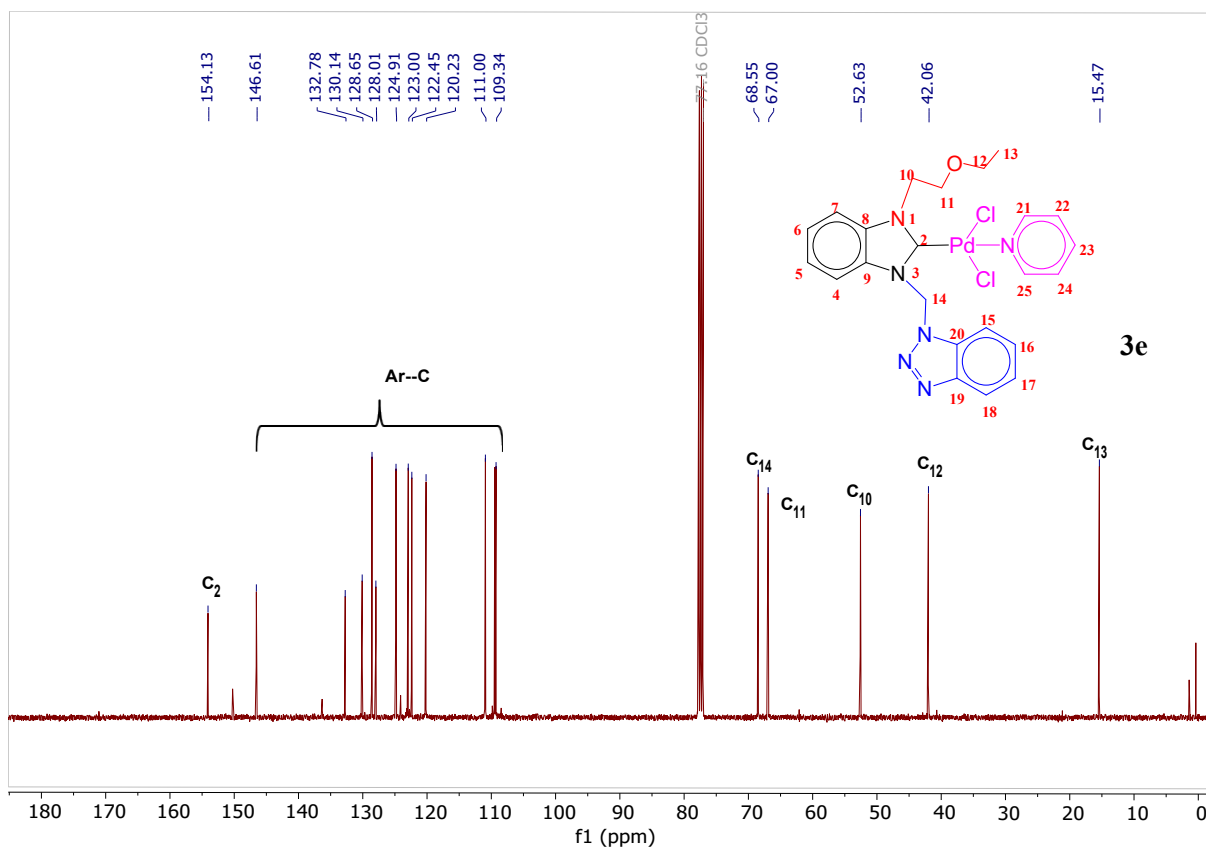


Figure 33 : ^{13}C NMR spectra of Dichloro[1-(2-ethoxyethyl)-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazole-2-ylidene] pyridine palladium(II) (3e).

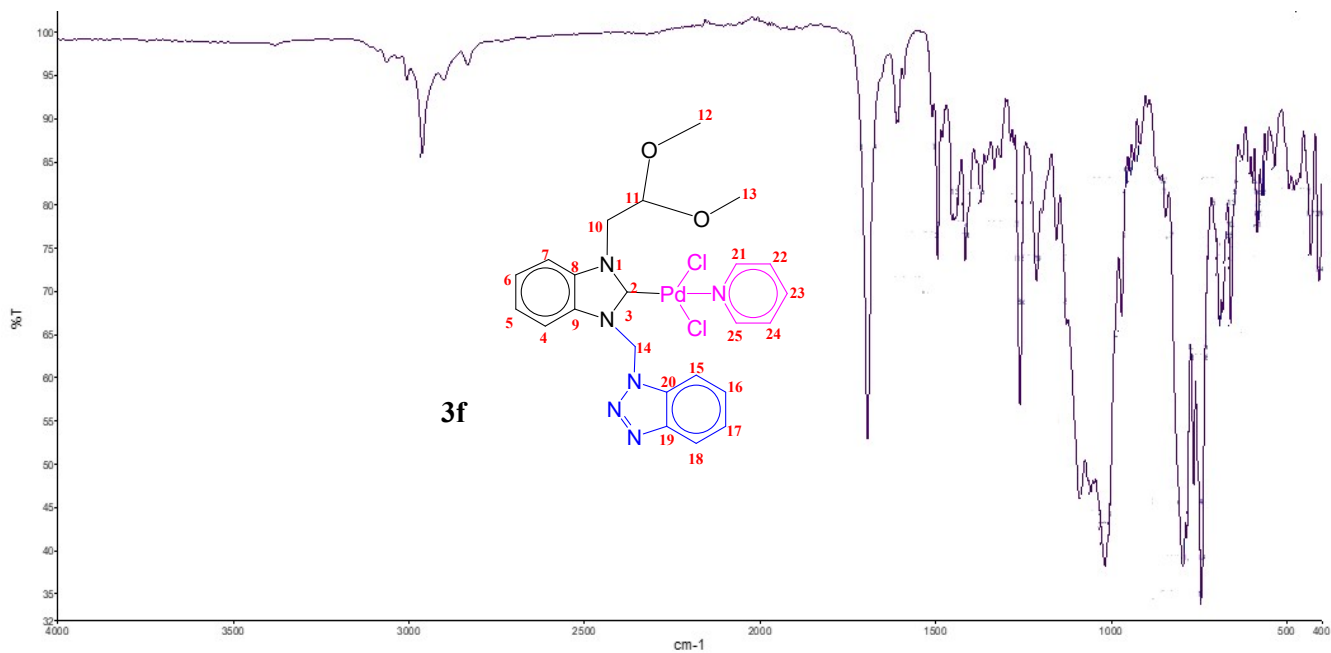


Figure 34: IR spectra of Dichloro[1-(2,2-dimethoxyethyl)-3-(1-methylbenzo-1,2,3-triazolyl)benzimidazole-2-ylidene] pyridine palladium(II) (3f).

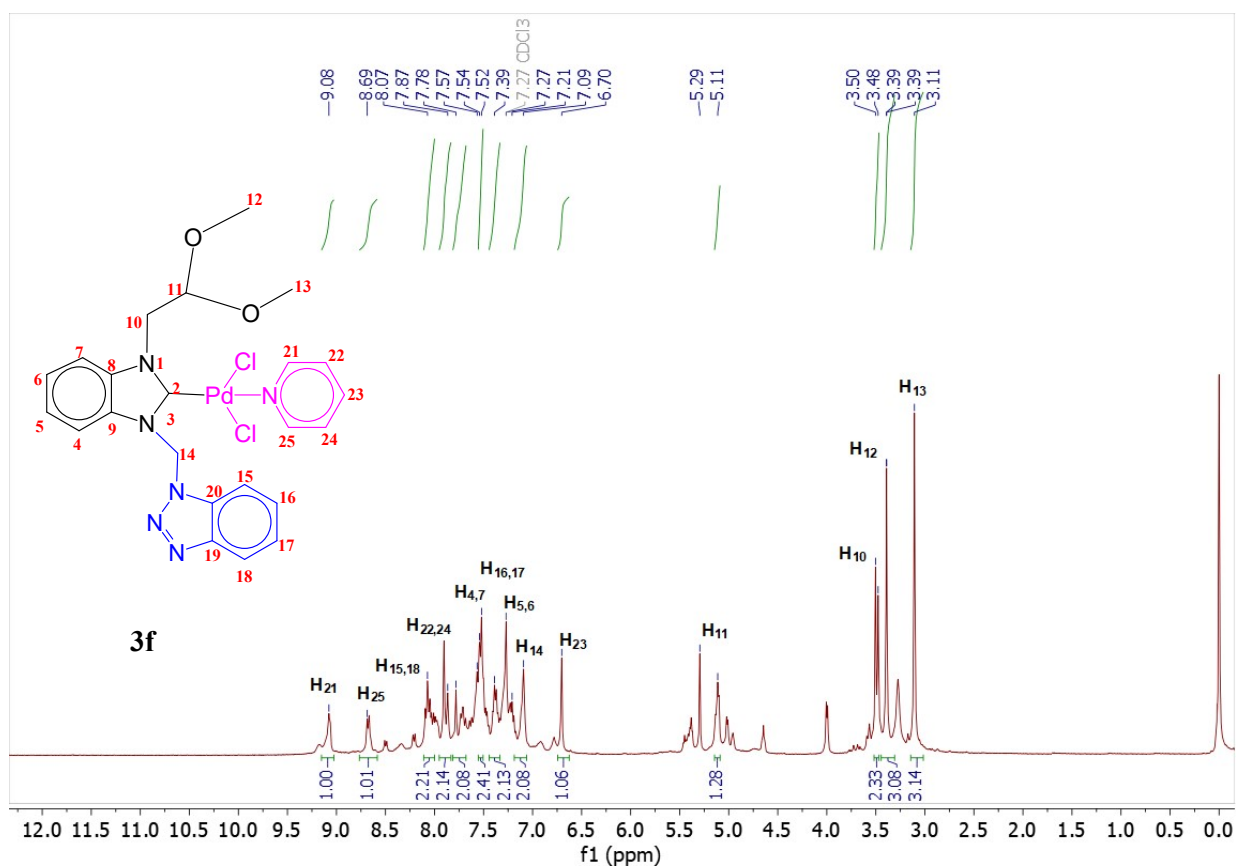


Figure 35 : ^1H NMR spectra of Dichloro[1-(2,2-dimethoxyethyl)-3-(1-methylbenzo-1,2,3-triazoly)benzimidazole-2-ylidene] pyridine palladium(II) (**3f**).

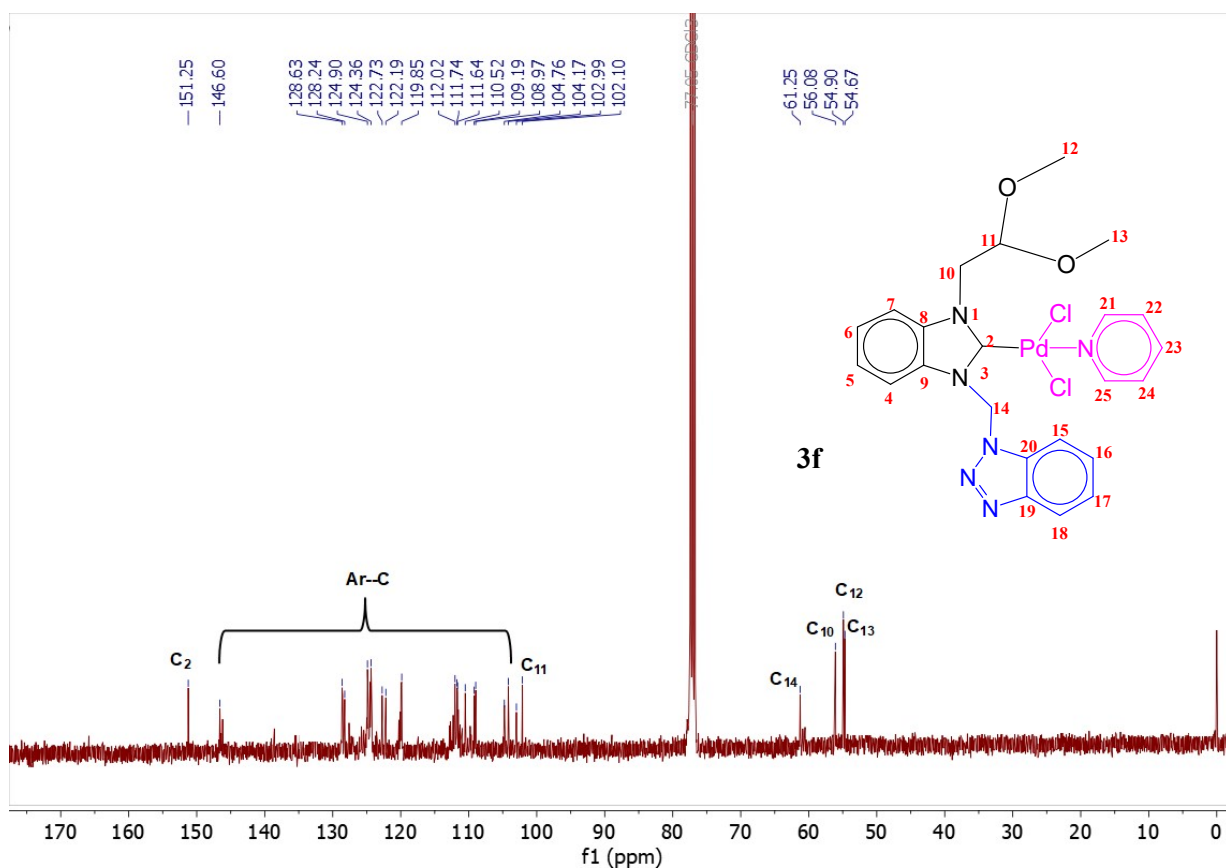


Figure 36 : ^{13}C NMR spectra of Dichloro[1-(2,2-dimethoxyethyl)-3-(1-methylbenzo-1,2,3-triazoly)benzimidazole-2-ylidene] pyridine palladium(II) (3f).

Table S1. Crystallographic data and structure refinement for the title compound

<i>chemical formula</i>	$\text{C}_{23}\text{H}_{24}\text{Cl}_2\text{N}_6\text{O}_2\text{Pd}$
<i>formula weight (g·mol⁻¹)</i>	593.78
<i>T (K) / crystal size (mm³)</i>	100(2) / 0.356 x 0.302 x 0.242
<i>crystal system / space group</i>	Monoclinic / $P2_1/n$
<i>Cell</i>	
<i>a (Å)</i>	13.4331(8)
<i>b (Å)</i>	12.7371(7)
<i>c (Å)</i>	15.3320(11)
<i>α (°)</i>	90
<i>β (°)</i>	111.330(2)
<i>γ (°)</i>	90
<i>V (Å³) / Z</i>	2443.6(3) / 4
<i>density calculated (Mg·m⁻³)</i>	1.614

<i>absorption coefficient (mm⁻¹)</i>	<i>1.011</i>
<i>F(000)</i>	<i>1200</i>
<i>θ range (°) for data collection</i>	<i>2.142- 30.508</i>
<i>index range</i>	<i>-19 ≤ h ≤ 19, -18 ≤ k ≤ 18, -21 ≤ l ≤ 21</i>
<i>reflections collected</i>	<i>72237</i>
<i>independent reflections / R_{int}</i>	<i>7458 / 0.0508</i>
<i>goodness-of-fit on F²</i>	<i>1.073</i>
<i>final R indices [I > 2σ(I)]</i>	<i>R1 = 0.0282, wR2 = 0.0504</i>
<i>CCDC</i>	

Table S2. Selected bond lengths of the title compound

Bonds lengths (Å)	exp.	DFT calc.		
		B3LYP	CAM-B3LYP	M06-2X
Pd(1)-C(1)	1.9645(12))	1.9876	1.977	1.9628
Pd(1)-N(1)	2.0868(11))	2.1799	2.1614	2.2104
Pd(1)-Cl(1)	2.2817(3)	2.3828	2.3575	2.3876
Pd(1)-Cl(2)	2.2997(4)	2.3833	2.3576	2.3909
C(1)-N(2)	1.3466(15))	1.3494	1.3408	1.3402
C(1)-N(3)	1.3601(15))	1.3569	1.3485	1.3481
N(2)-C(2)	1.3941(16))	1.3998	1.3959	1.3947
N(2)-C(13)	1.4559(16))	1.463	1.4563	1.457
C(13)-C(14)	1.5184(18))	1.5342	1.5255	1.5273
C(14)-O(1)	1.3992(16))	1.4058	1.3981	1.3962
C(14)-O(2)	1.4021(15))	1.4114	1.4024	1.3988
O(1)-C(15)	1.4234(19))	1.4289	1.4203	1.4202
O(2)-C(16)	1.4246(19))	1.4275	1.4188	1.4179
C(2)-C(3)	1.3873(17))	1.3915	1.3865	1.3894
C(2)-C(7)	1.3884(17))	1.3998	1.3909	1.3944
C(3)-C(4)	1.3871(18))	1.3914	1.3846	1.387
C(4)-C(5)	1.4102(19))	1.4034	1.399	1.4029
C(5)-C(6)	1.3871(19))	1.3918	1.385	1.3875

C(6)-C(7)	1.3918(17)	1.3931	1.3883	1.3915
C(7)-N(3)	1.3944(16)	1.4011	1.3972	1.3952
N(1)-C(8)	1.3323(18)	1.3446	1.3387	1.3401
N(1)-C(12)	1.3343(18)	1.3444	1.3386	1.3398
C(8)-C(9)	1.382(2)	1.3893	1.3834	1.3875
C(9)-C(10)	1.393(3)	1.3911	1.3853	1.3882
C(10)-C(11)	1.385(2)	1.391	1.3852	1.388
C(11)-C(12)	1.384(2)	1.3893	1.3835	1.3876
N(3)-C(17)	1.4519(16)	1.4606	1.4528	1.4537
C(17)-N(4)	1.4456(16)	1.4447	1.439	1.4389
N(4)-C(18)	1.3626(16)	1.3724	1.3582	1.3553
N(4)-N(5)	1.3640(15)	1.372	1.3668	1.3649
N(5)-N(6)	1.2929(17)	1.2834	1.275	1.2755
N(6)-C(19)	1.3794(18)	1.3801	1.3765	1.38
C(18)-C(19)	1.3964(18)	1.4072	1.3964	1.3985
C(18)-C(23)	1.3985(18)	1.4007	1.3978	1.3999
C(19)-C(20)	1.3982(19)	1.4017	1.3984	1.4014
C(20)-C(21)	1.381(2)	1.3831	1.3752	1.3785
C(21)-C(22)	1.418(2)	1.4146	1.4119	1.4154
C(22)-C(23)	1.3765(19)	1.3856	1.3772	1.3798