

Supplementary Material 2

Ru (II)-N-Heterocyclic Carbene Complexes: Synthesis, Characterization, Transfer Hydrogenation Reactions and Biological determination

Lamia Boubakri ^a, A. Chakchouk-Mtibaa^b, L. Mansour^c, L. Mellouli^b, I. Özdemir^d, S. Yasar^d and Naceur Hamdi^{a,c}

1,3-Bis-(3,5-dimethylbenzyl)-5,6-dimethylbenzimidazolium bromide, 1a

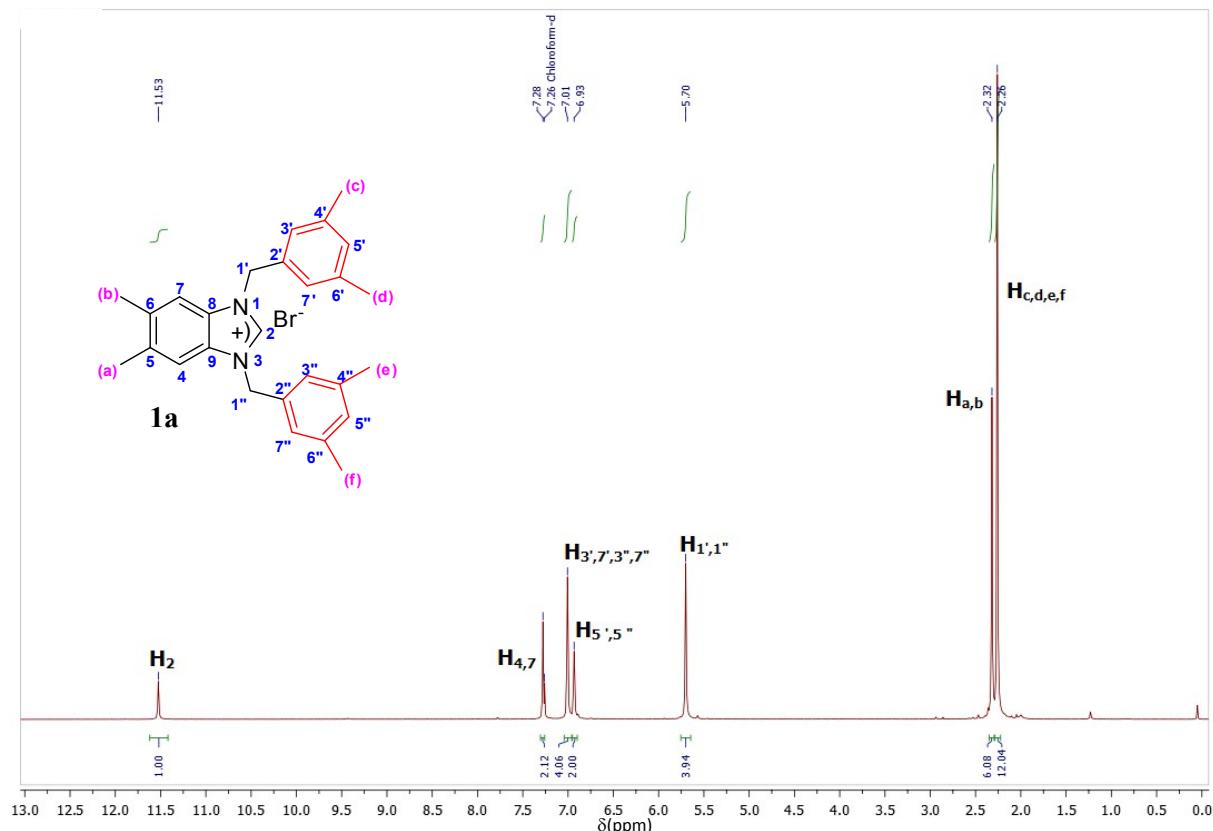


Figure S1: ¹HNMR spectra of benzimidazolium salt 1a (CDCl₃, 300MHz).

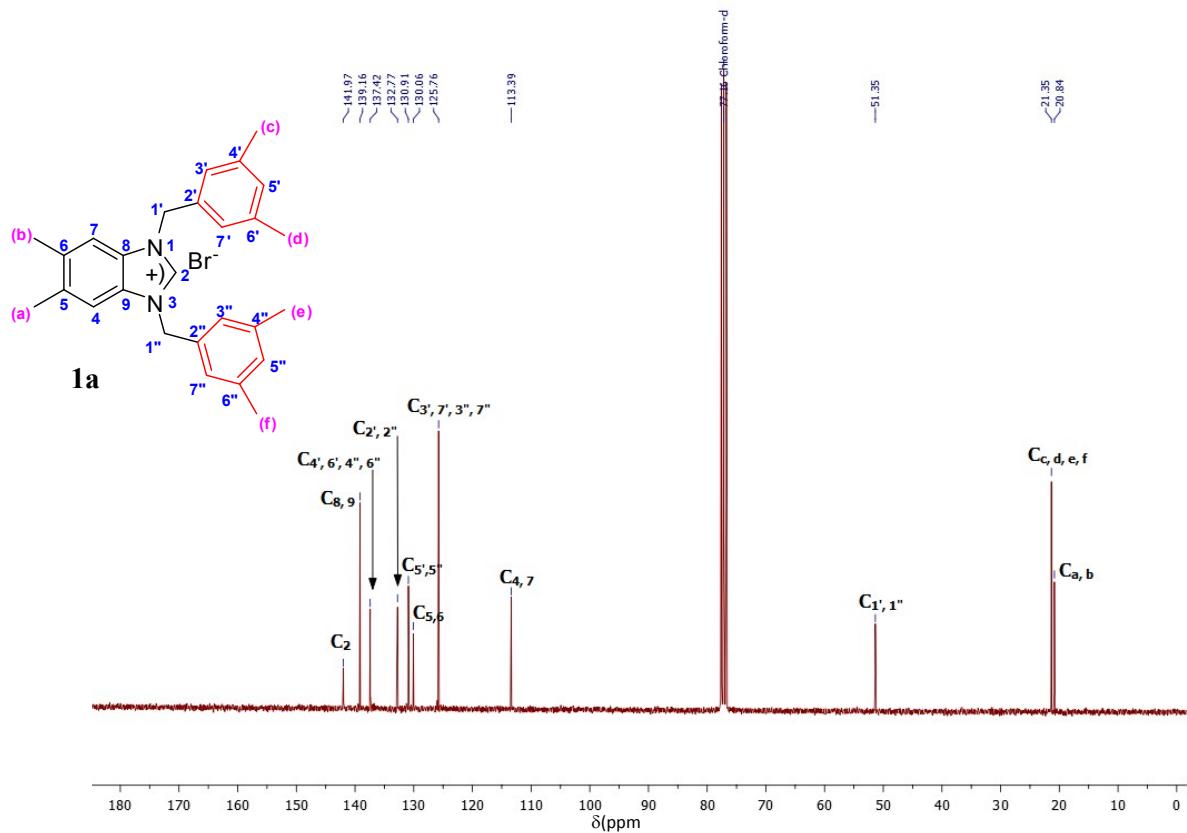


Figure S2: ^{13}C NMR spectra of benzimidazolium salt **1a** (CDCl_3 , 75MHz).

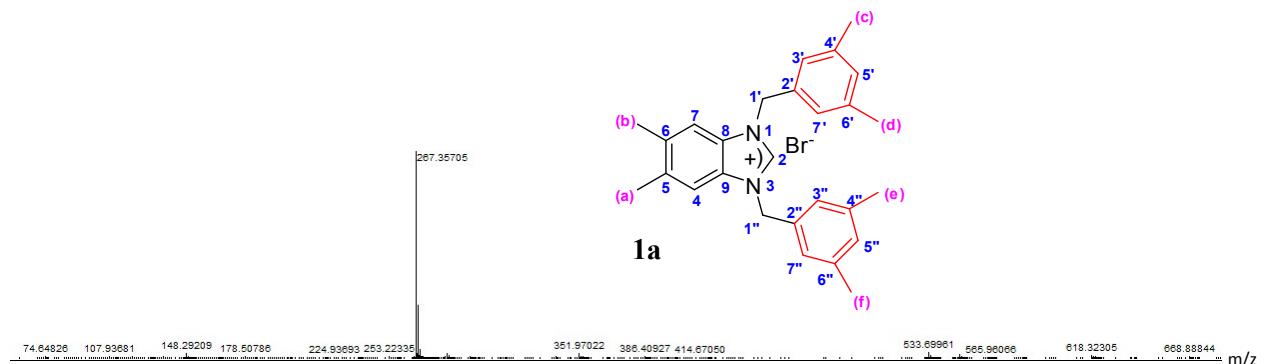


Figure S3: DART-TOF-MS of benzimidazolium salt **1a**.

1, 3-Bis (4-methylbenzyl)-5,6-dimethyl benzimidazoliumbromide, 1b

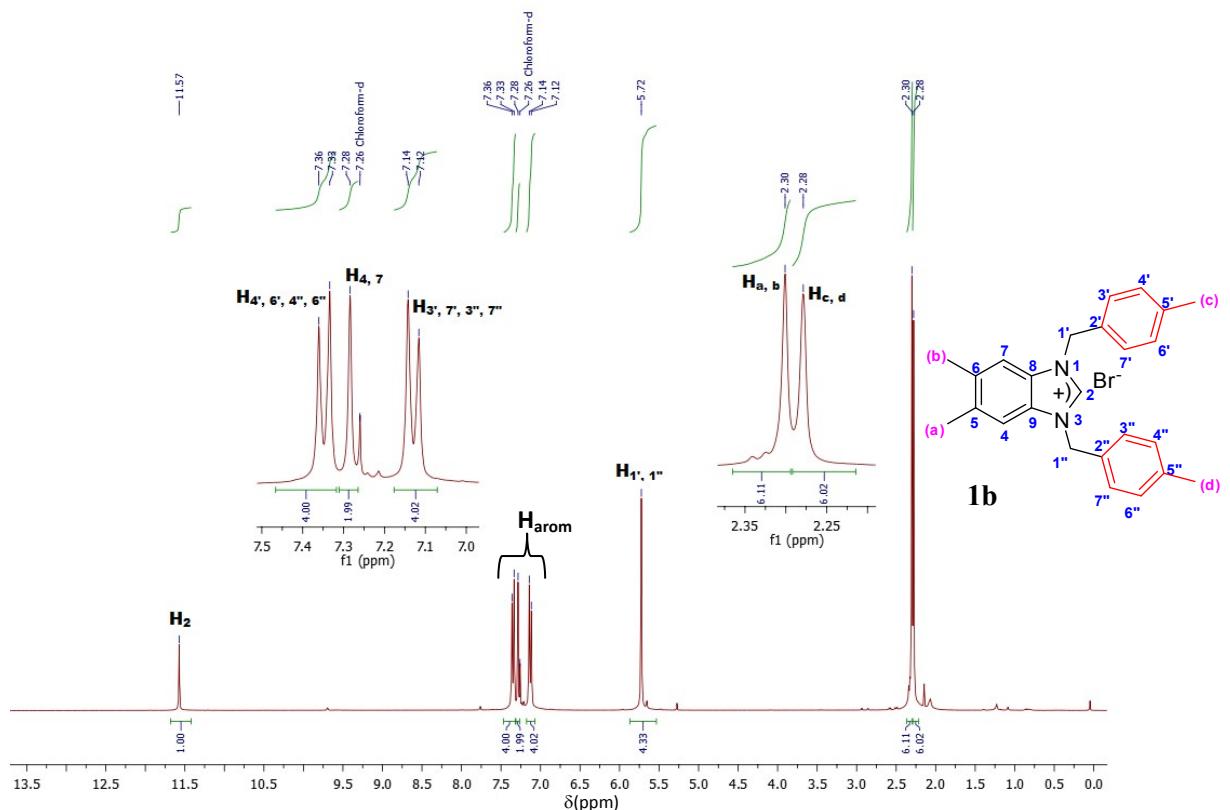


Figure S4: ^1H NMR spectra of benzimidazolium salt **1b** (CDCl_3 , 300MHz).

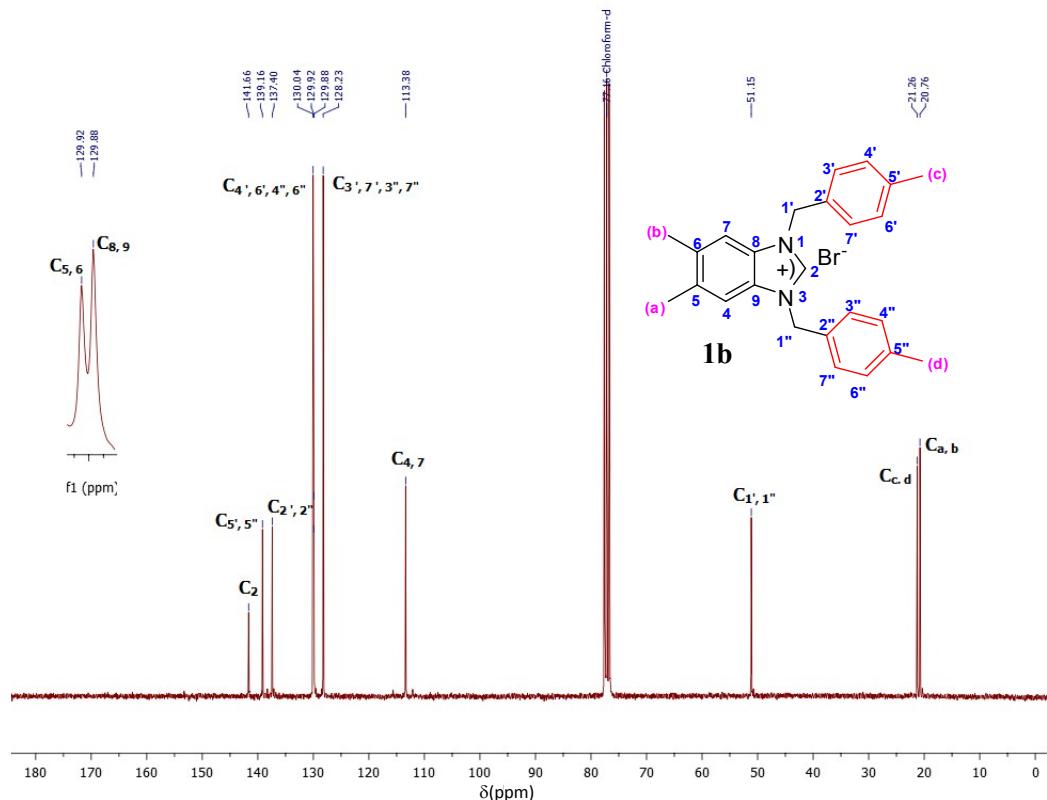
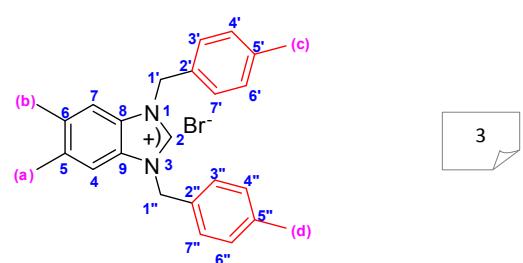


Figure S5: ^{13}C NMR spectra of benzimidazolium salt **1b** (CDCl_3 , 75MHz).



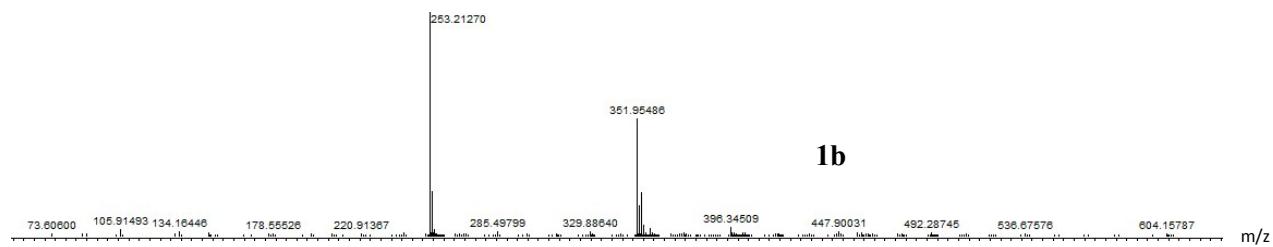


Figure S6: DART-TOF-MS of benzimidazolium salt **1b**.

1, 3-Bis (4-tet-butylbenzyl) - 5,6-dimethyl benzimidazolium bromide, 1c

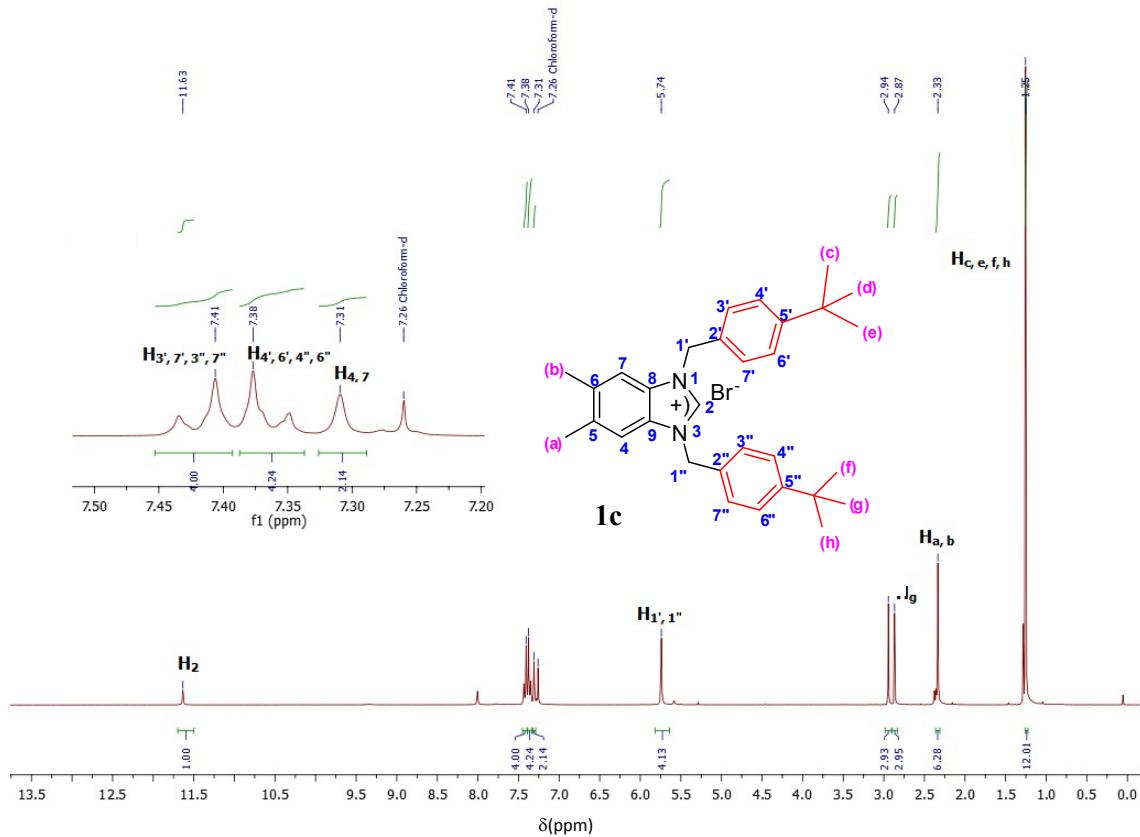


Figure S7: ^1H NMR spectra of benzimidazolium salt **1c** (CDCl_3 , 300MHz).

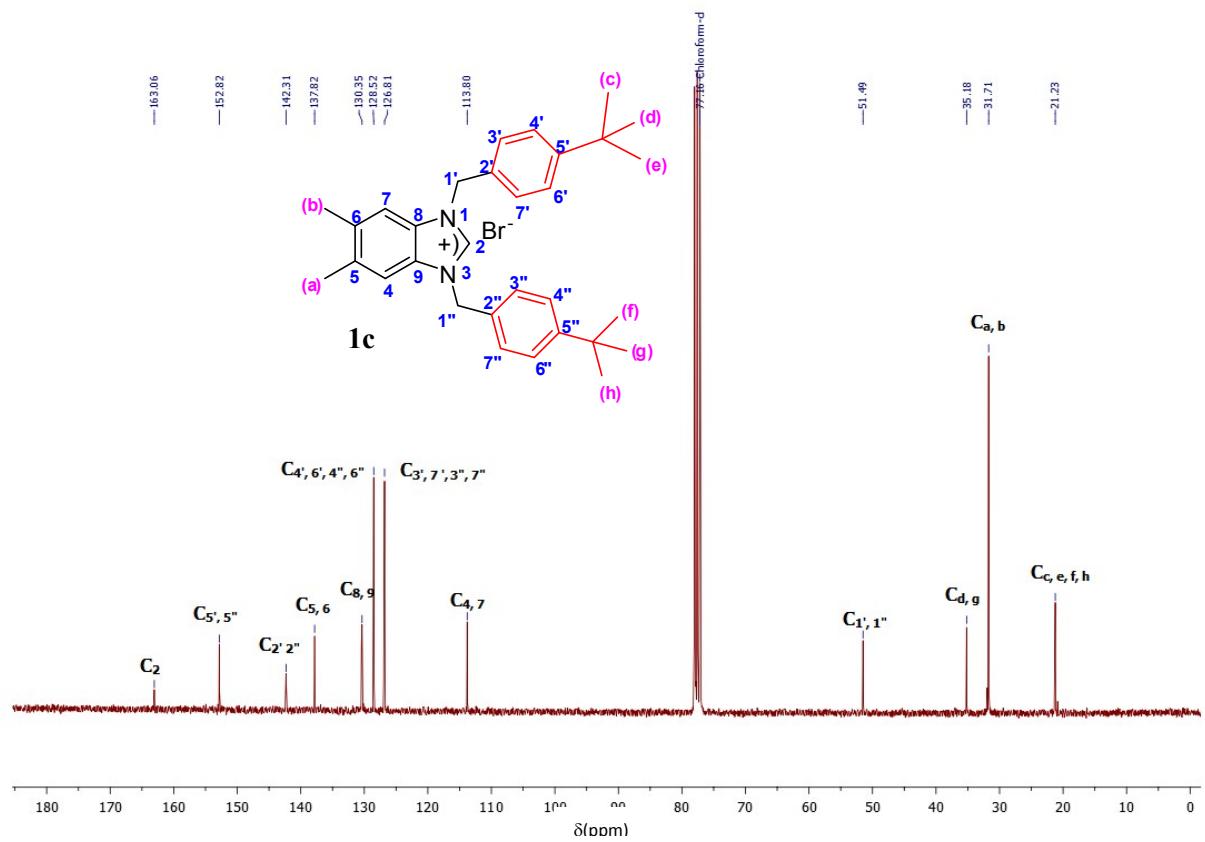


Figure S8: ^{13}C NMR spectra of benzimidazolium salt **1c** (CDCl_3 , 75MHz).

1-(3,5-dimethylbenzyl)-3-(2,3,5,6-tetramethylbenzyl)-5,6-dimethylbenzimidazolium chloride, **1d**

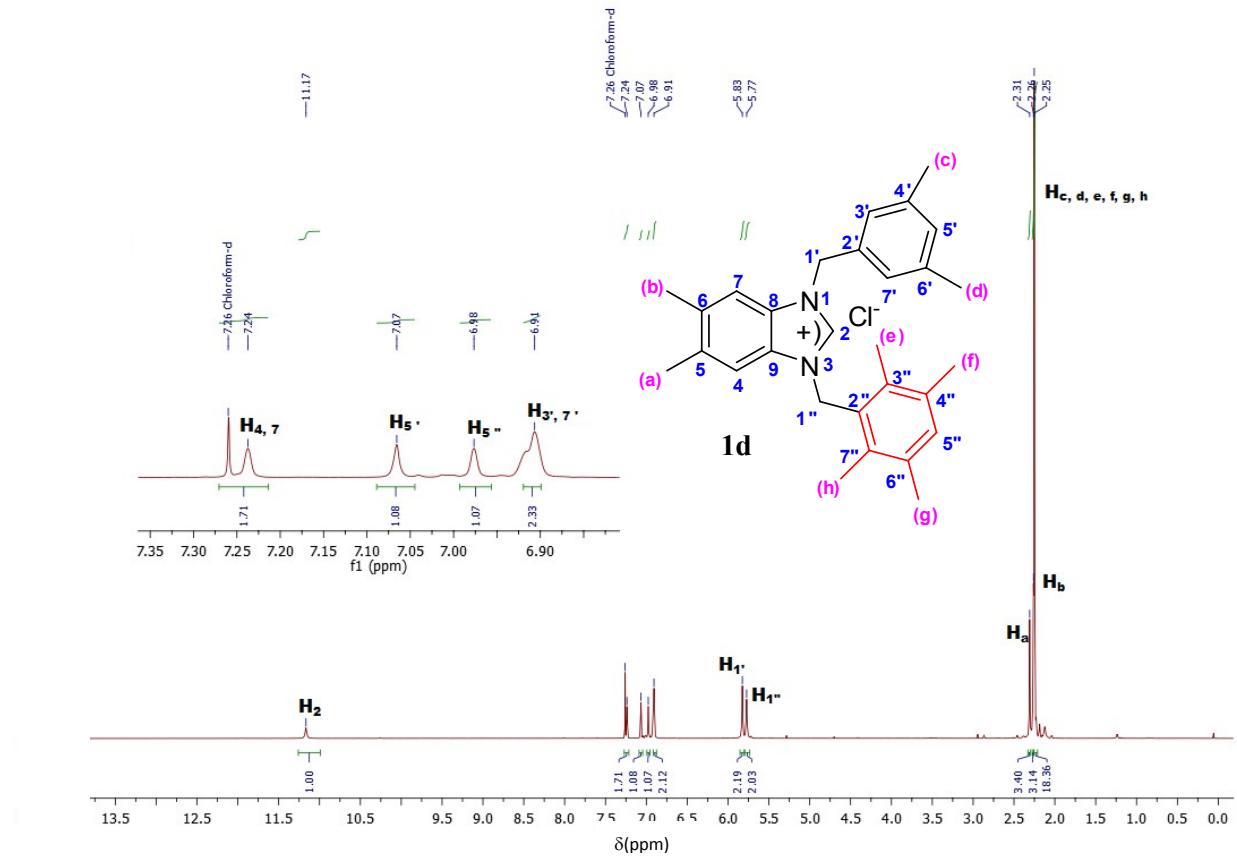


Figure S9: ^1H NMR spectra of benzimidazolium salt **1d** (CDCl_3 , 300MHz).

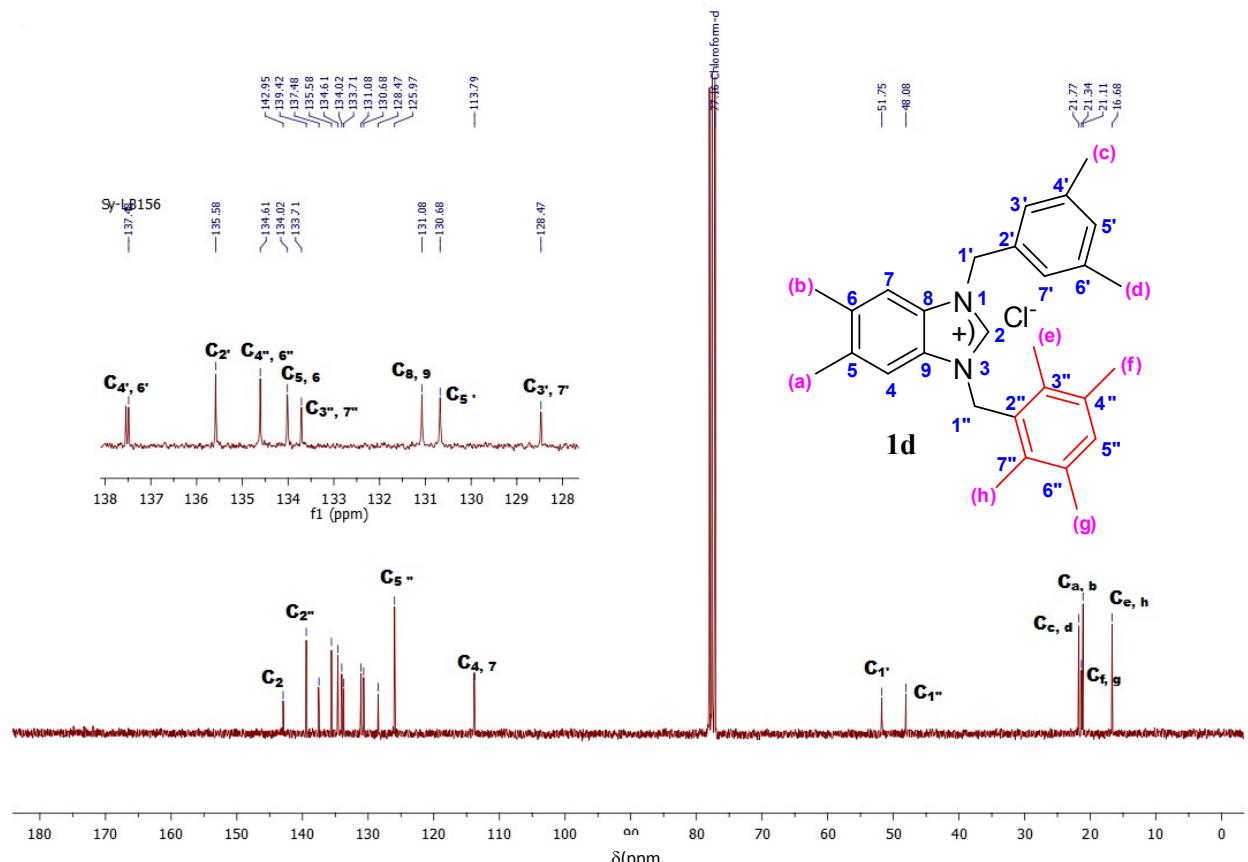


Figure S10: ^{13}C NMR spectra of benzimidazolium salt **1d** (CDCl_3 , 75MHz).

1-(3,5-dimethylbenzyl) -3-(4-tet-butylbenzyl)-5,6-dimethylbenzimidazolium bromide, 1e

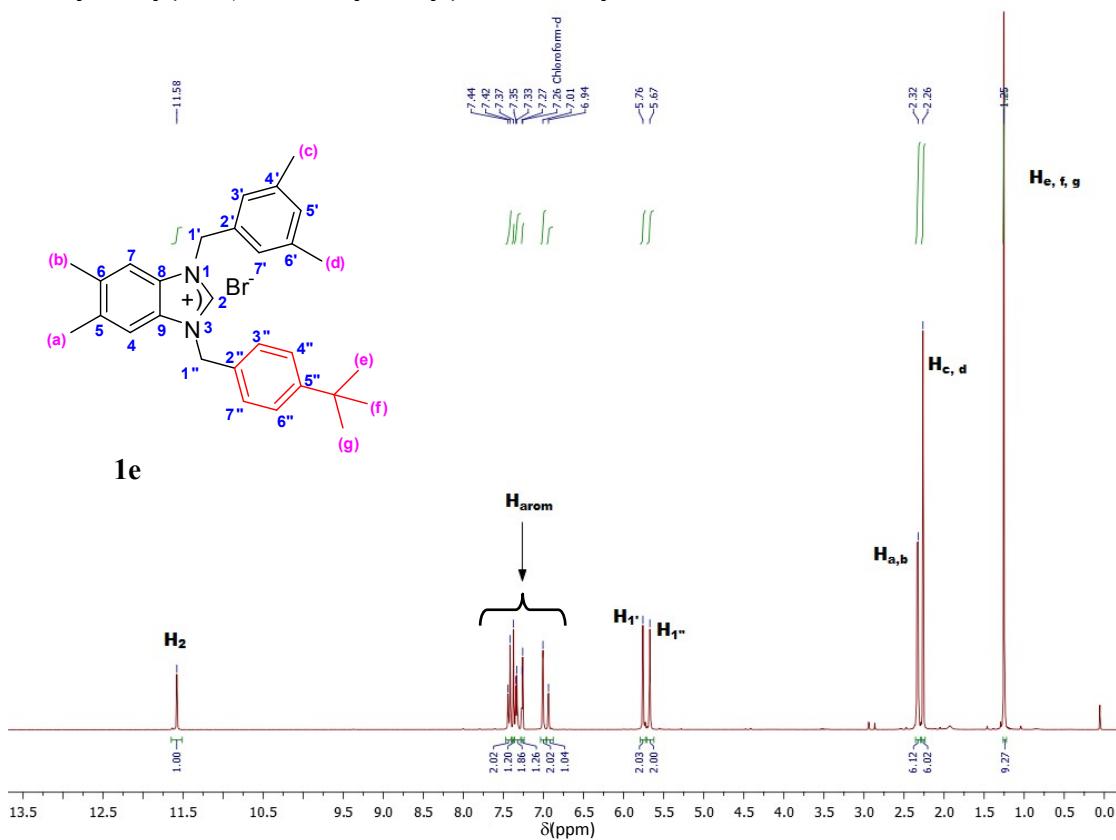


Figure S11: ^1H NMR spectra of benzimidazolium salt **1e** (CDCl_3 , 300MHz).

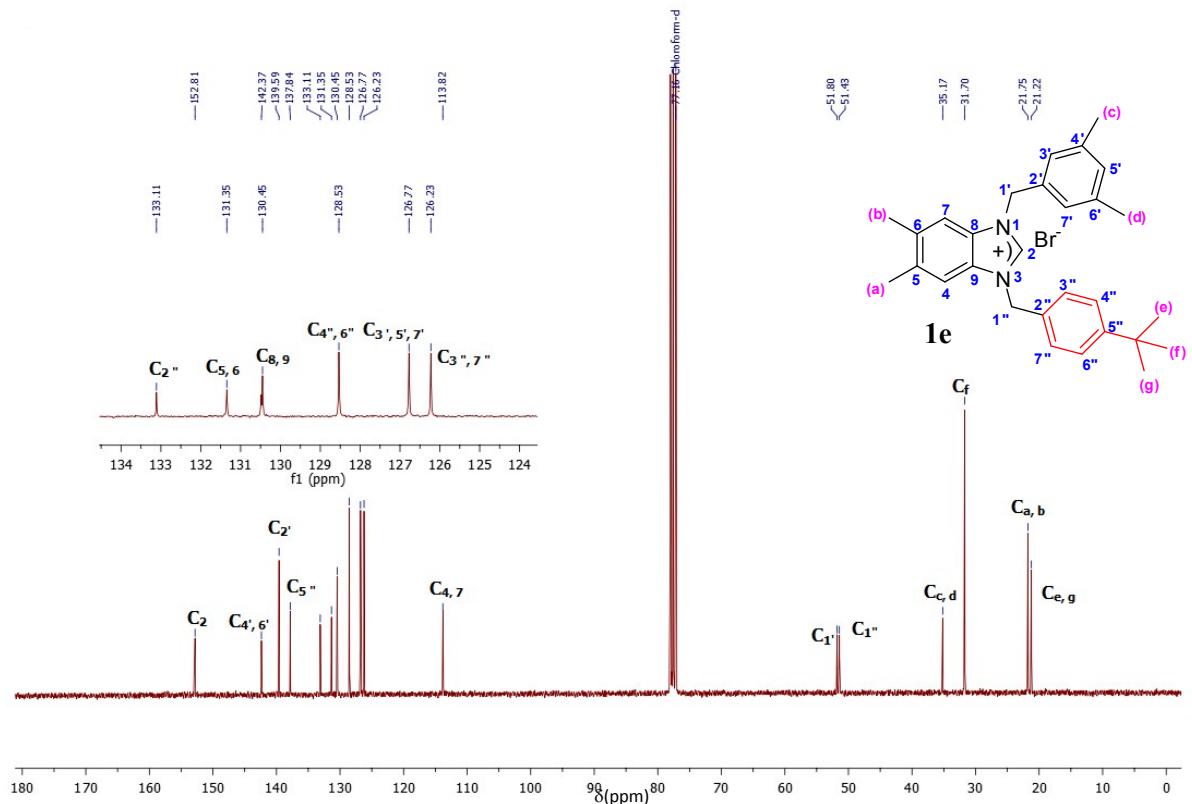


Figure S12: ^{13}C NMR spectra of benzimidazolium salt **1e** (CDCl_3 , 75MHz).

1-(3,5-dimethylbenzyl)-3-(4-methylbenzyl)-5,6-dimethyl benzimidazolium bromide, **1f**

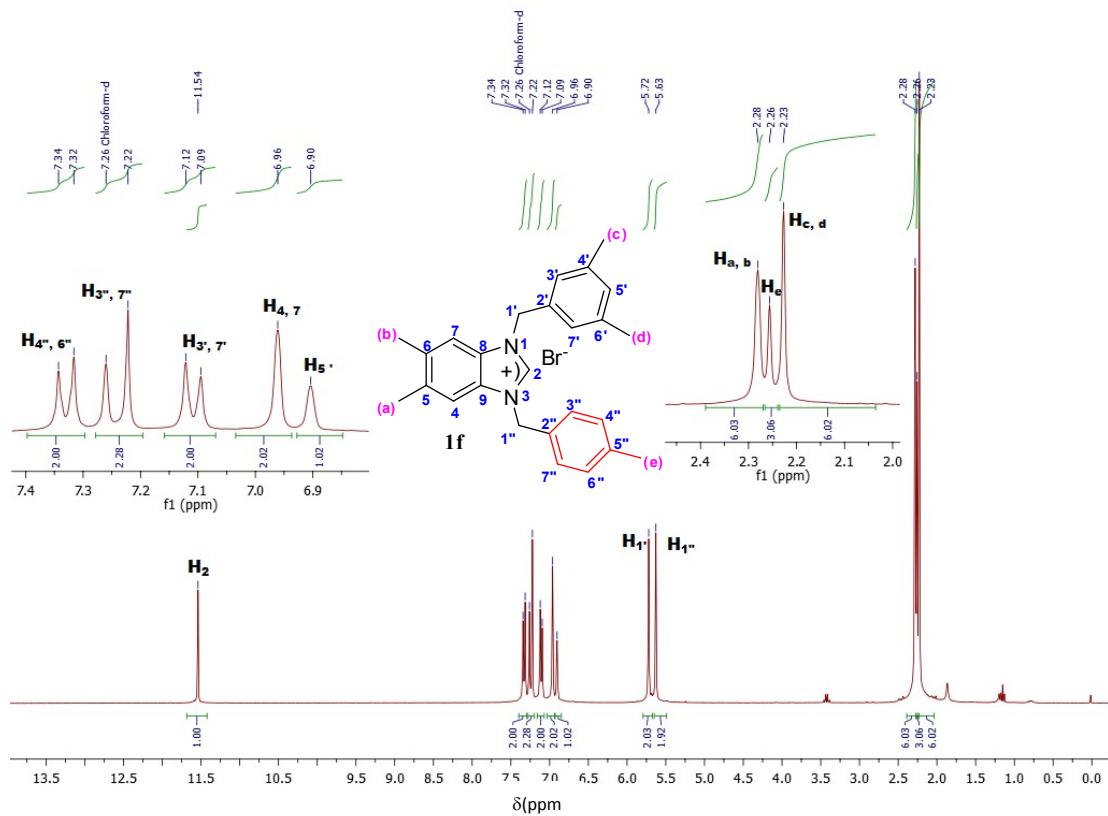


Figure S13: ^1H NMR spectra of benzimidazolium salt **1f** (CDCl_3 , 300MHz).

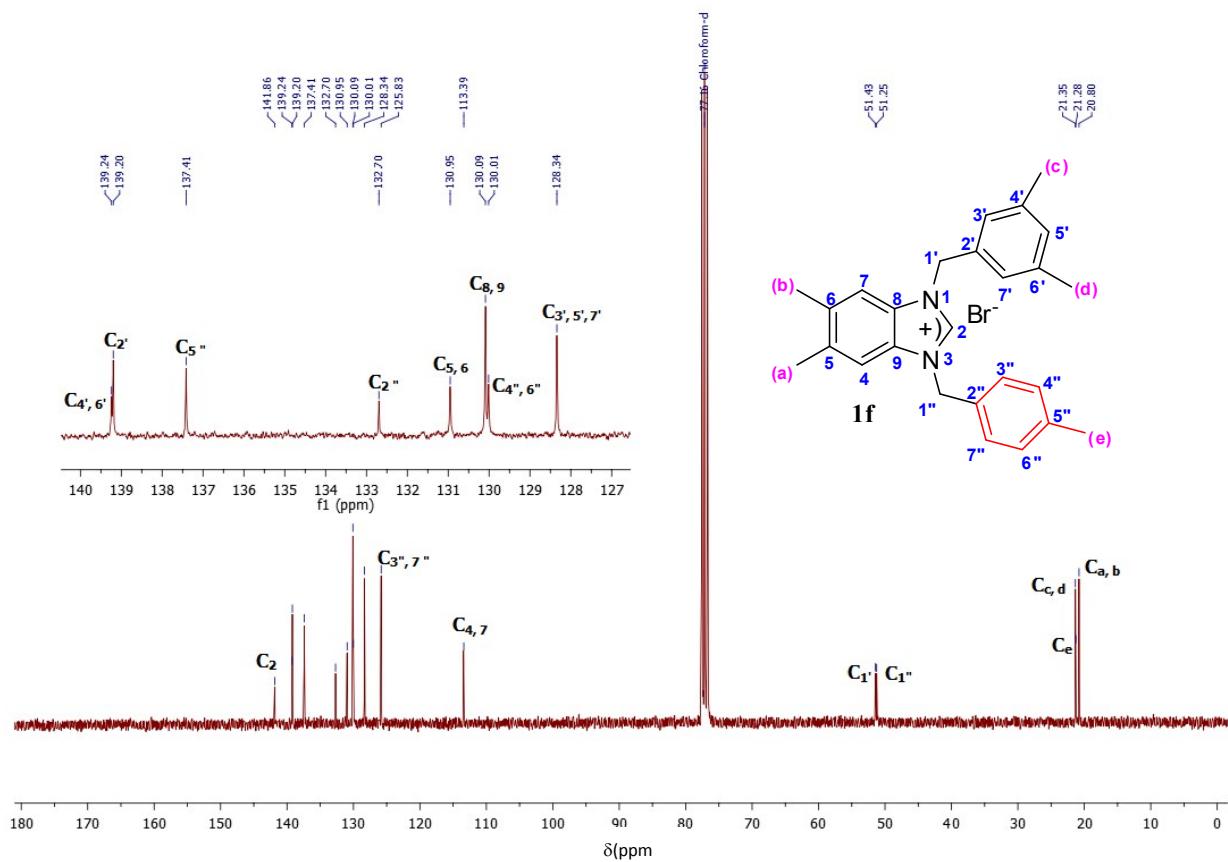


Figure S14: ^{13}C NMR spectra of benzimidazolium salt **1f** (CDCl_3 , 75MHz).

Bromo-[1,3-Bis (3,5-dimethylbenzyl) benzimidazole-2-ylidene] silver (I), 2a

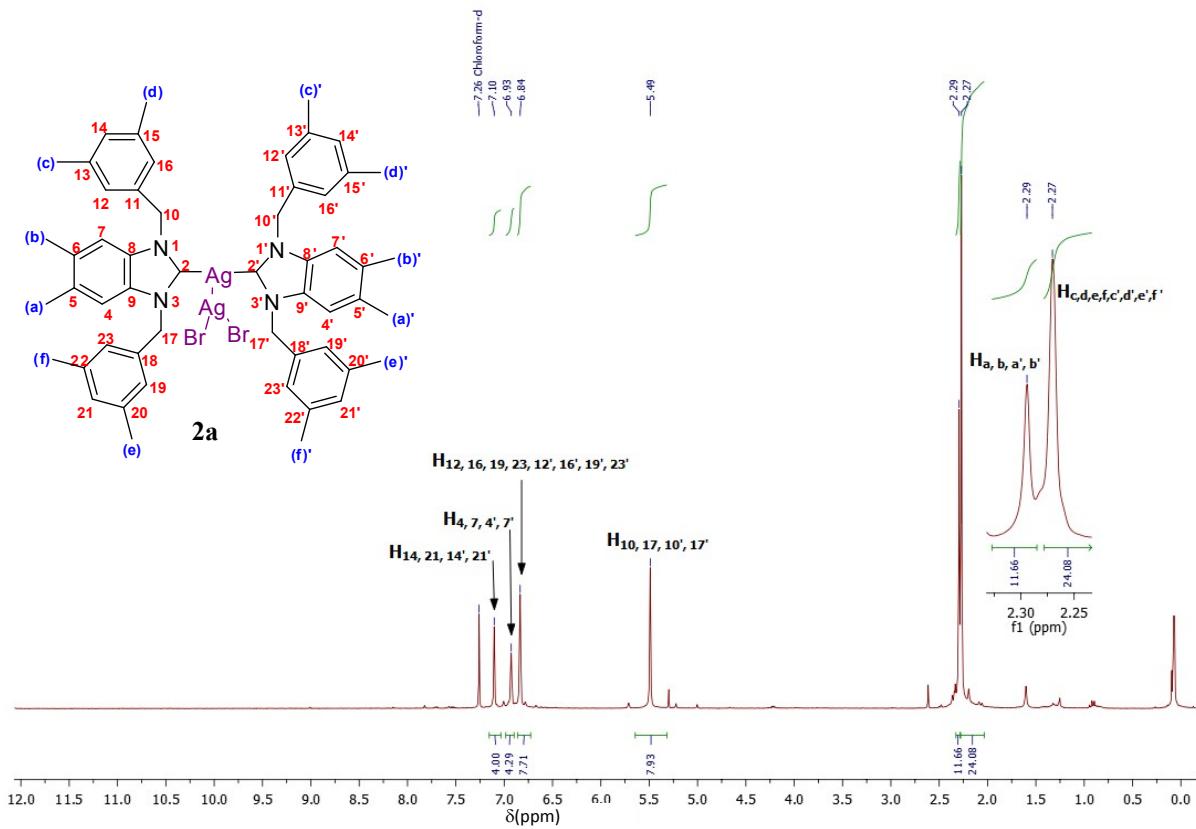


Figure S15: ^1H NMR spectra of Ag(I)-N-Heterocyclic Carbene complexes **2a**(CDCl_3 , 300MHz).

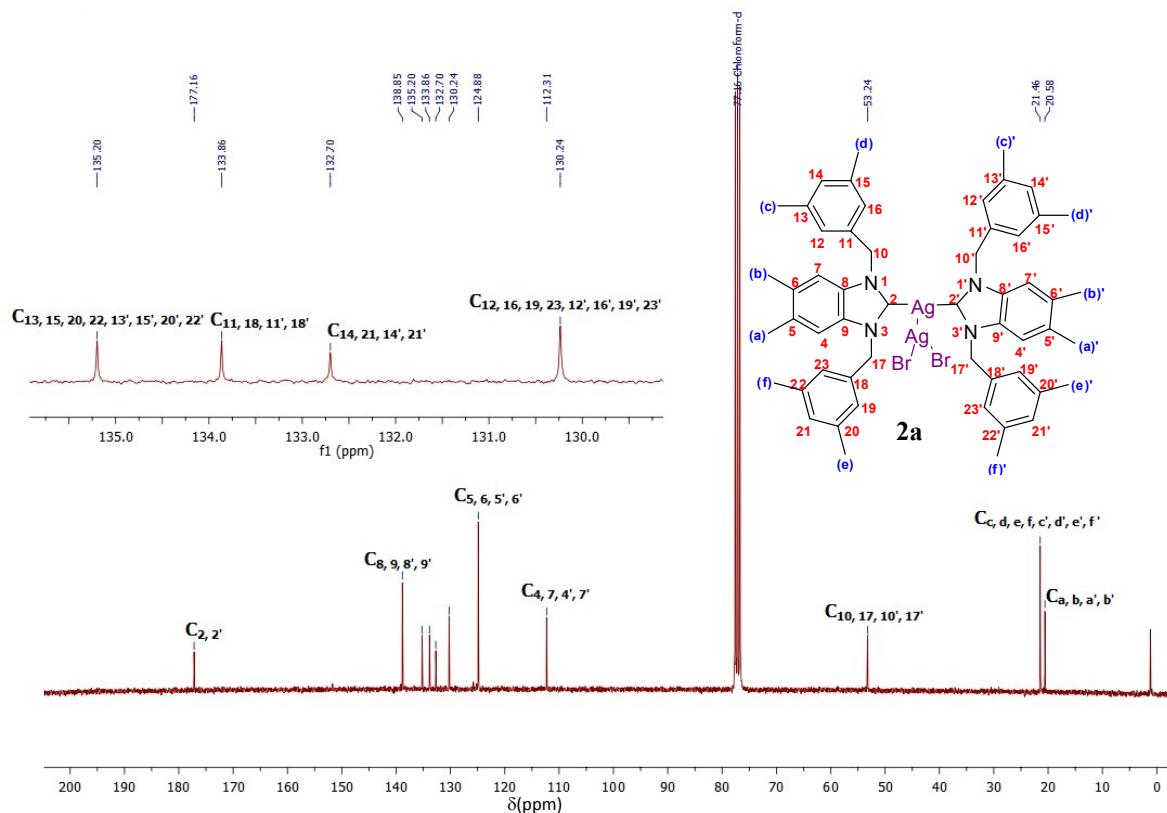


Figure S16: ^{13}C NMR spectra of Ag(I)-N-Heterocyclic Carbene complexes **2a**(CDCl_3 , 75MHz).

Bromo-[1,3-Bis (4-methylbenzyl) benzimidazole-2-ylidene] silver (I), 2b

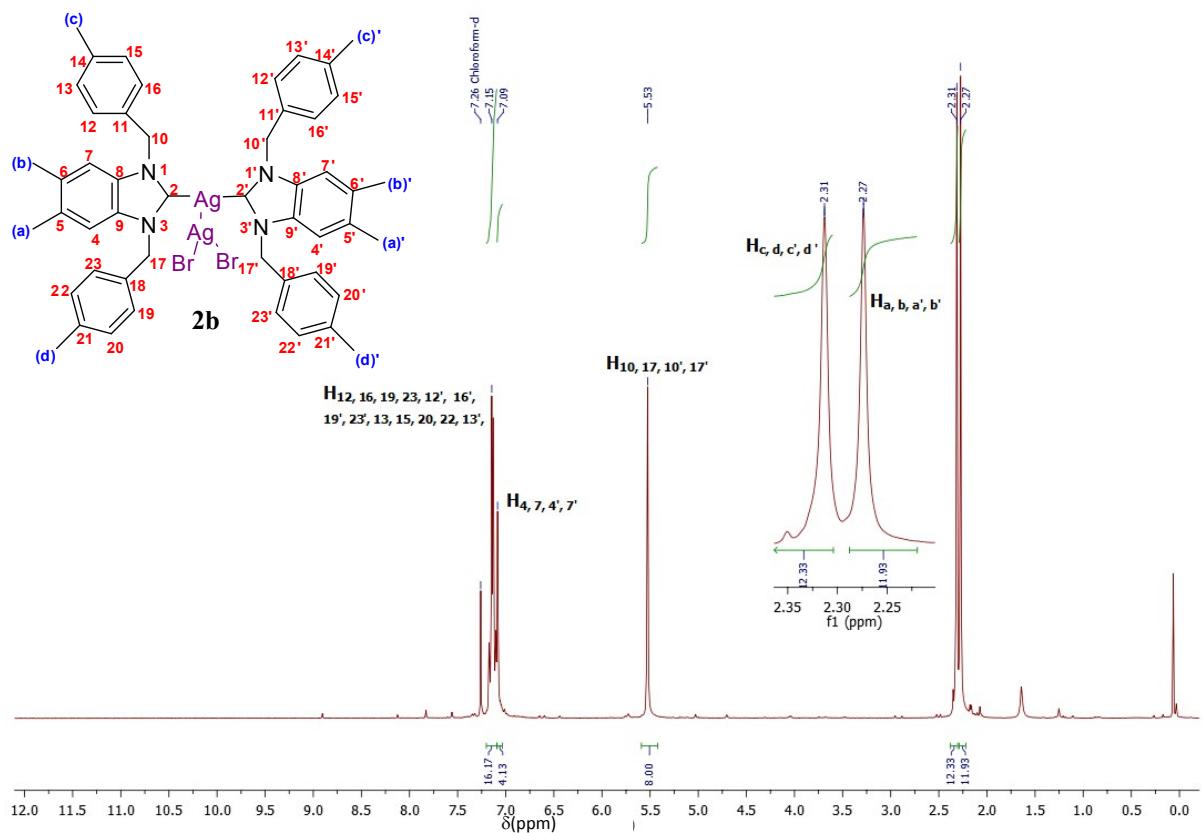


Figure S17: ¹H NMR spectra of Ag(I)-N-Heterocyclic Carbene complexes **2b** (CDCl₃, 300MHz).

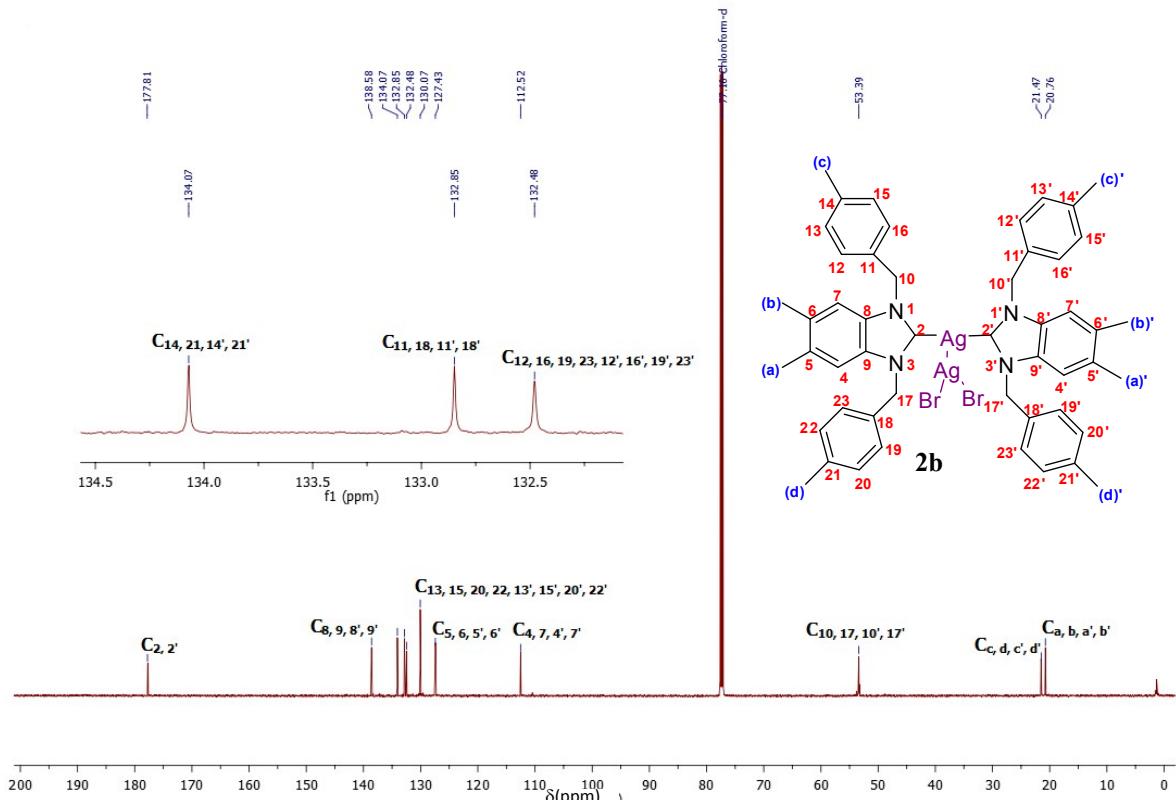


Figure S18: ¹³C NMR spectra of Ag(I)-N-Heterocyclic Carbene complexes **2b** (CDCl₃, 75MHz).

Bromo-[1, 3- Bis-(4-tert-butylbenzyl) benzimidazole-2-ylidene] silver (I**), **2c****

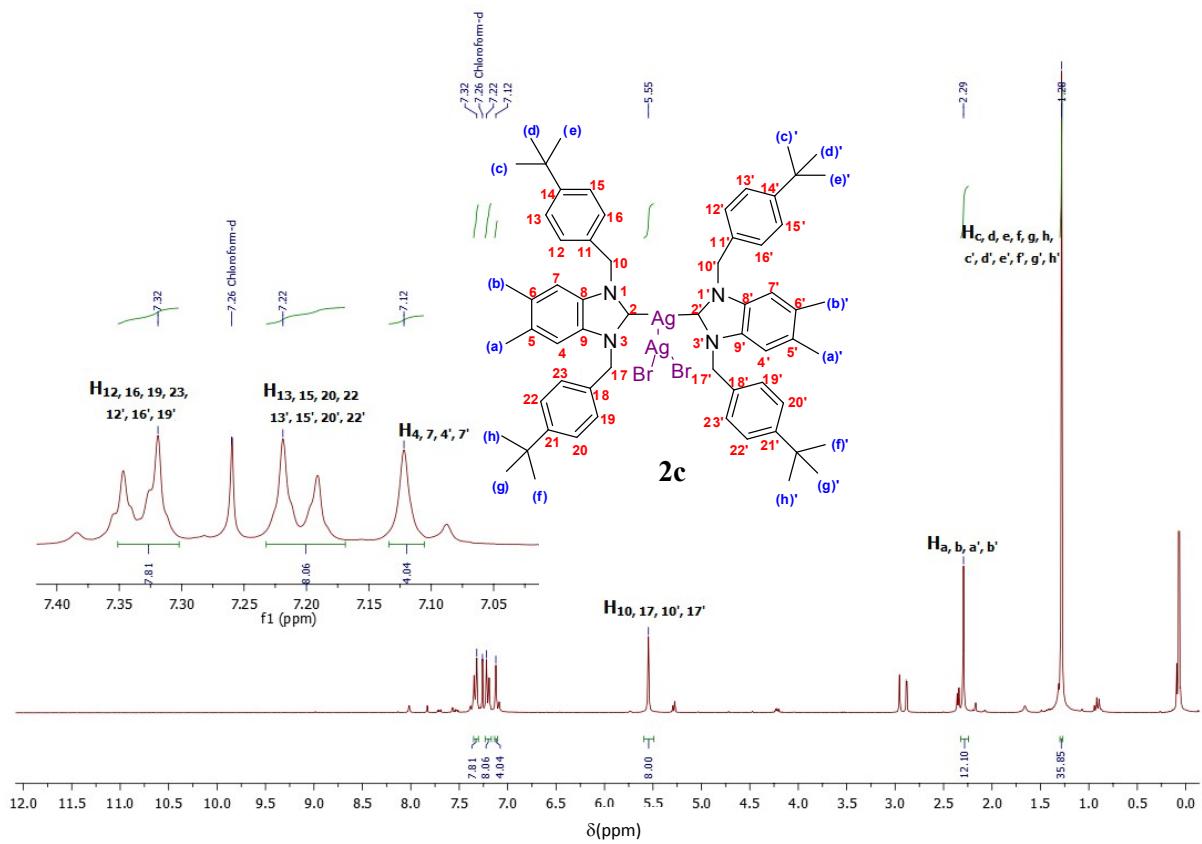


Figure S19: ¹HNMR spectra of Ag(I)-N-Heterocyclic Carbene complexes **2c** (CDCl_3 , 300MHz).

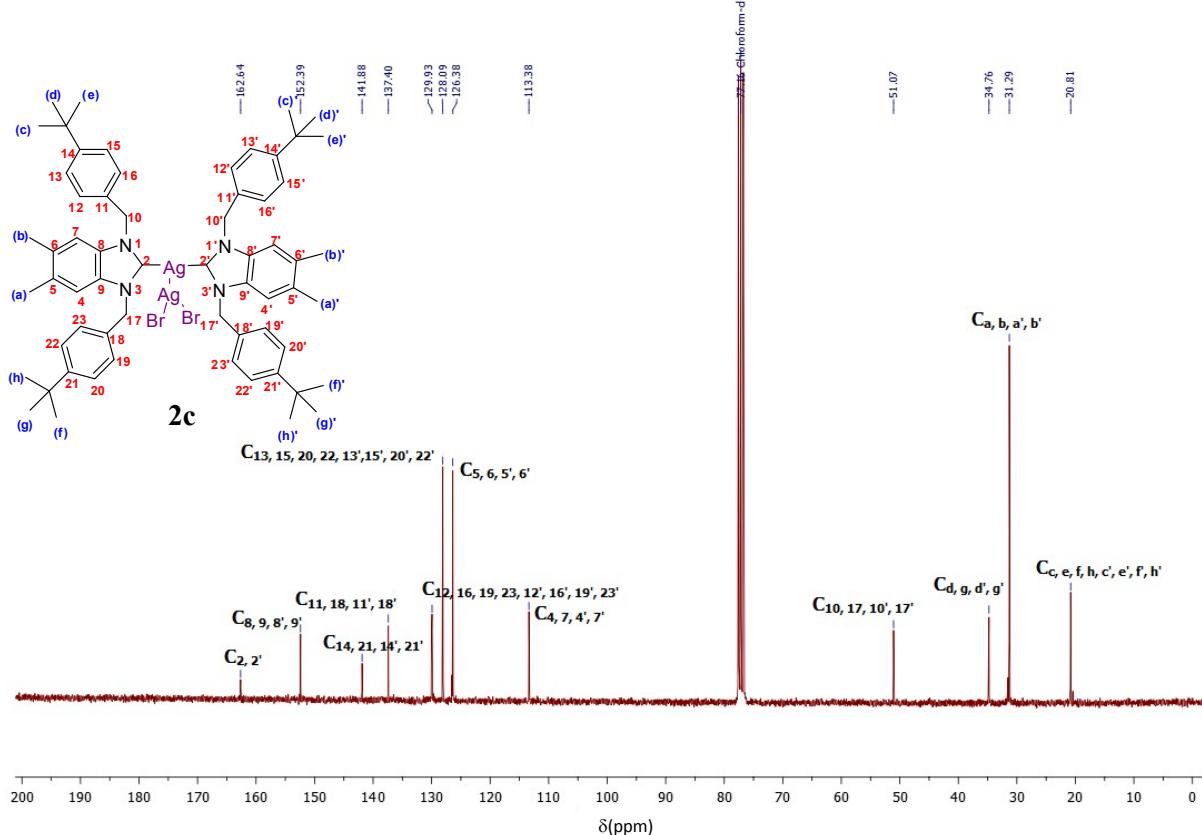


Figure S20: ¹³CNMR spectra of Ag(I)-N-Heterocyclic Carbene complexes **2c** (CDCl_3 , 75MHz).

Chloro-[1-(3,5-dimethylbenzyl)-3-(2,3,5,6-tetramethylbenzyl) benzimidazole-2-ylidene] silver (I), 2d

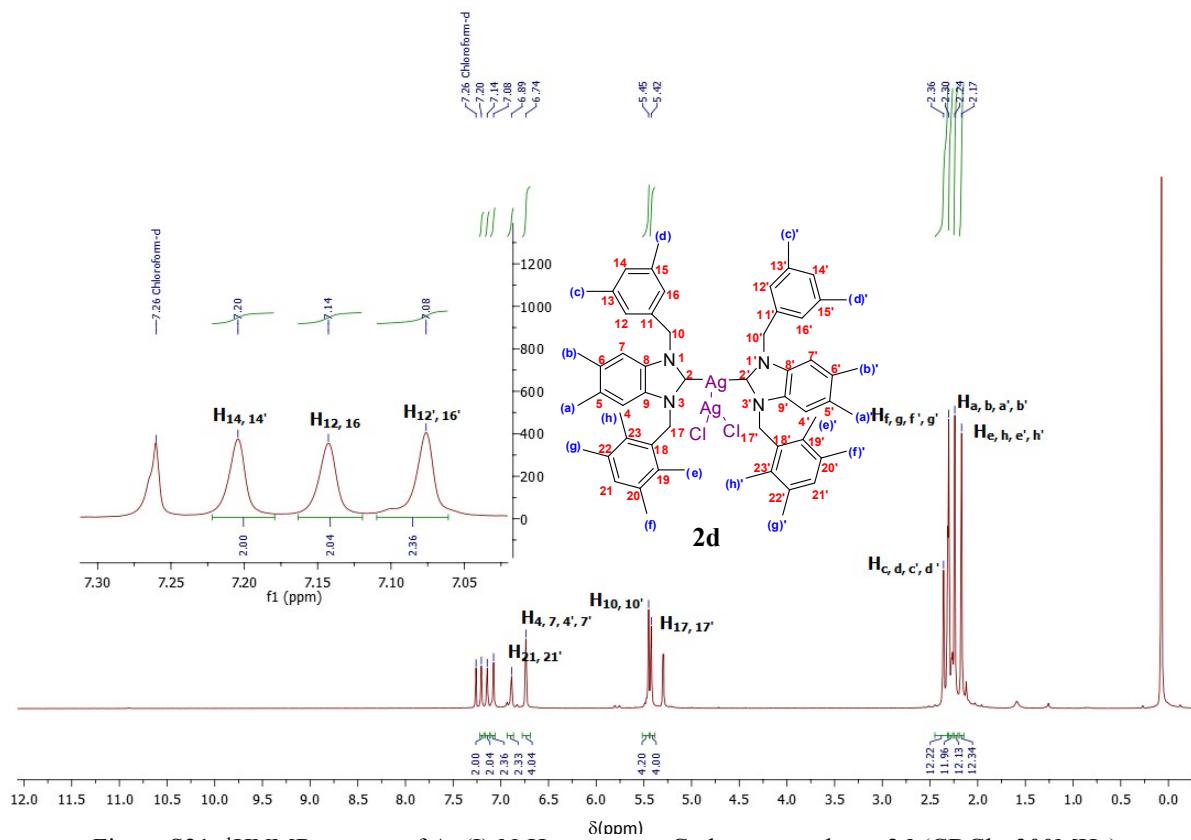


Figure S21: ^1H NMR spectra of Ag(I)-N-Heterocyclic Carbene complexes **2d** (CDCl_3 , 300MHz).

Bromo-[1-(3,5-dimethylbenzyl)-3-(4-tert-butylbenzyl) benzimidazole-2-ylidene] silver (I), 2e

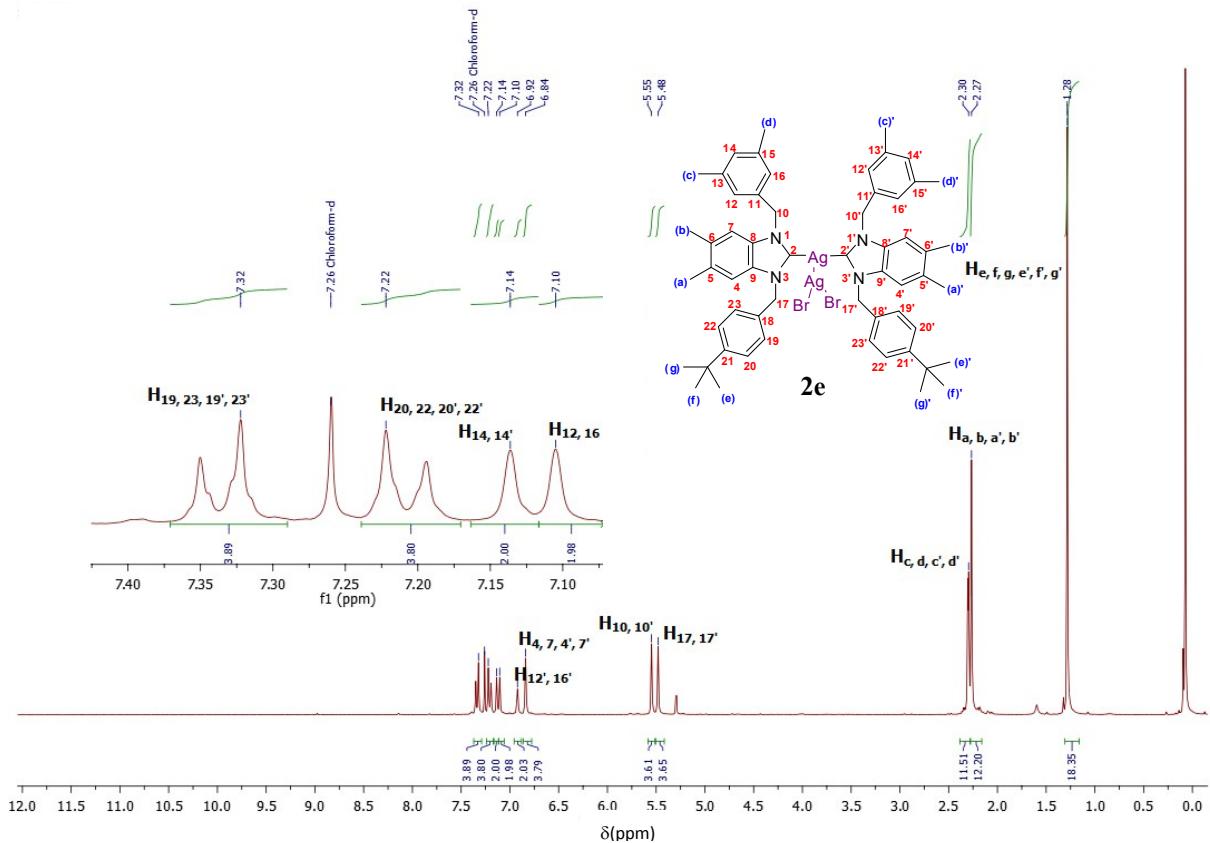


Figure S22: ^1H NMR spectra of Ag(I)-N-Heterocyclic Carbene complexes **2e** (CDCl_3 , 300MHz).

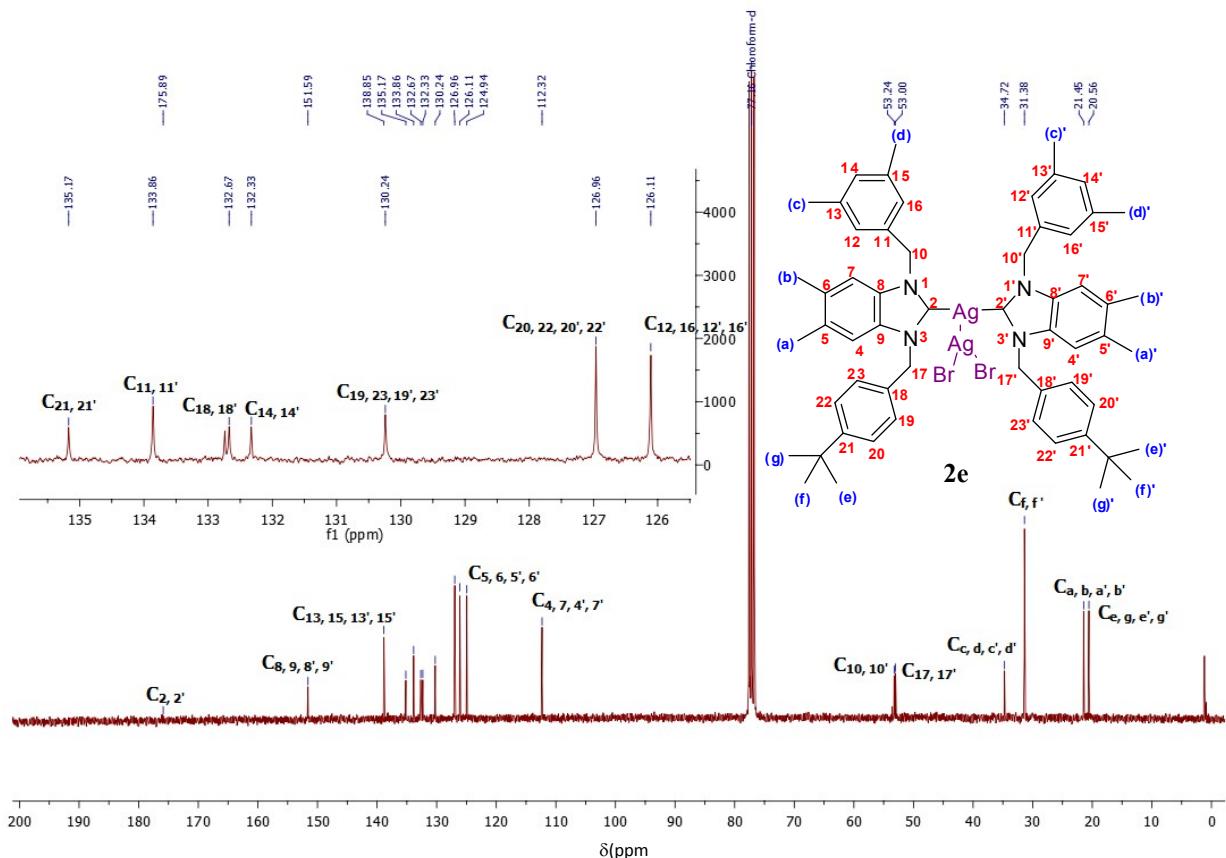


Figure S23: ^{13}C NMR spectra of Ag(I)-N-Heterocyclic Carbene complexes **2e**(CDCl_3 , 75MHz).

Bromo-[1-(3,5-dimethylbenzyl)-3-(4-methylbenzyl) benzimidazole-2-ylidene]silver (**I**), **2f**

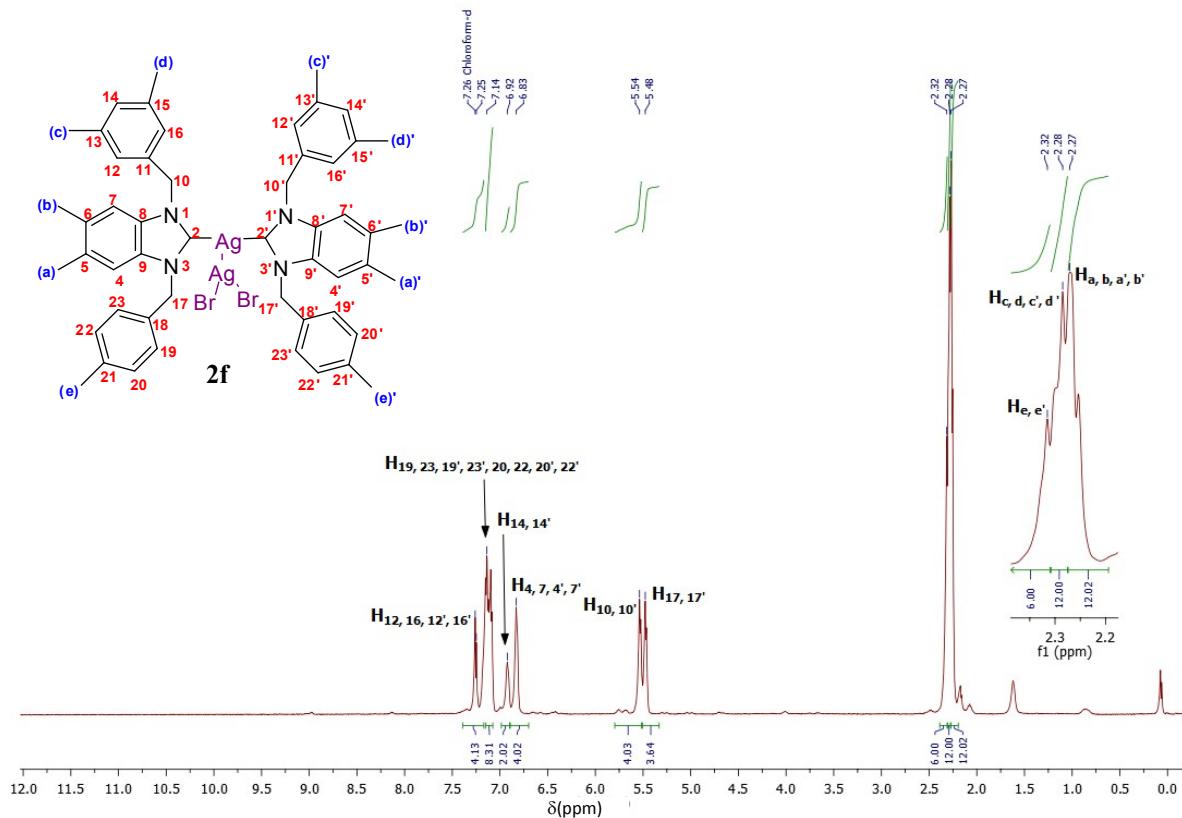


Figure S24: ^1H NMR spectra of Ag(I)-N-Heterocyclic Carbene complexes **2f** (CDCl_3 , 300MHz).

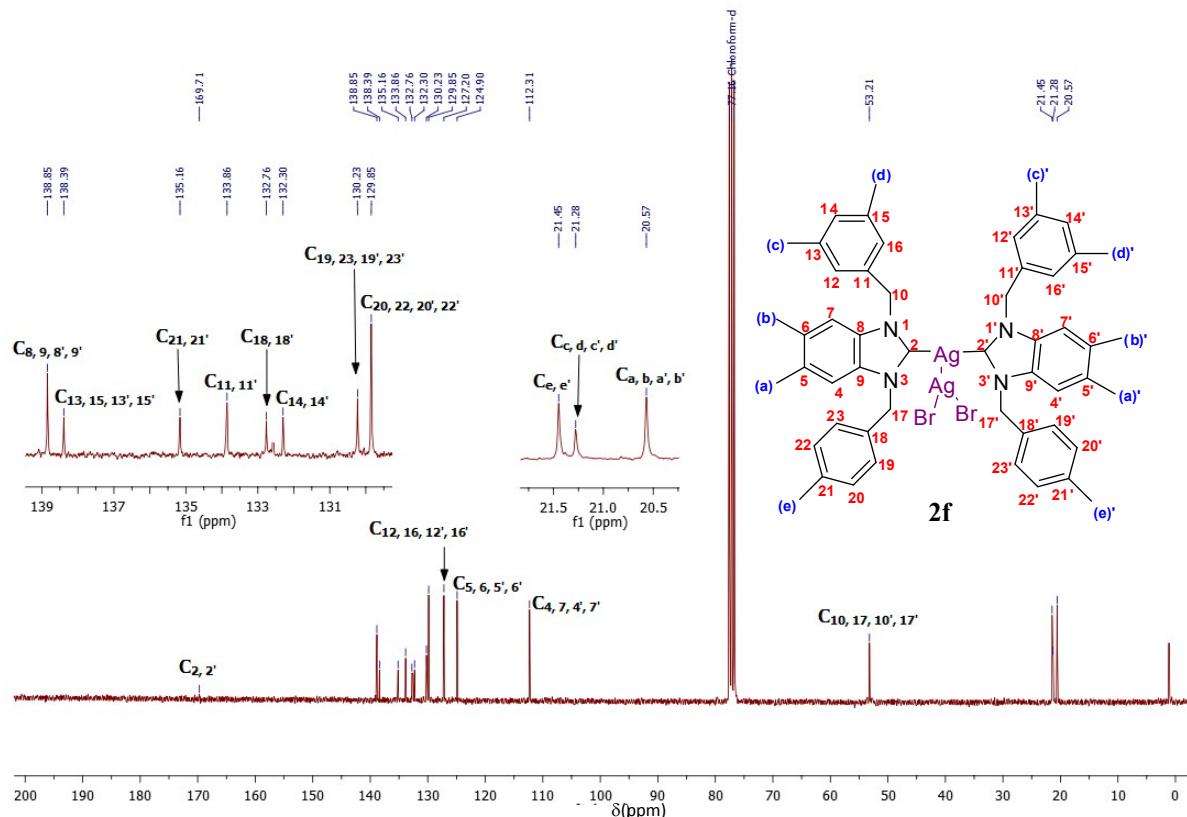


Figure S25: ^{13}C NMR spectra of Ag(I)-N-Heterocyclic Carbene complexes **2f** (CDCl_3 , 75MHz).

Dichloro-[1,3-bis(4-methylbenzyl)benzimidazol-2-ylidene](*p*-cymene)-ruthenium(II), **3b**

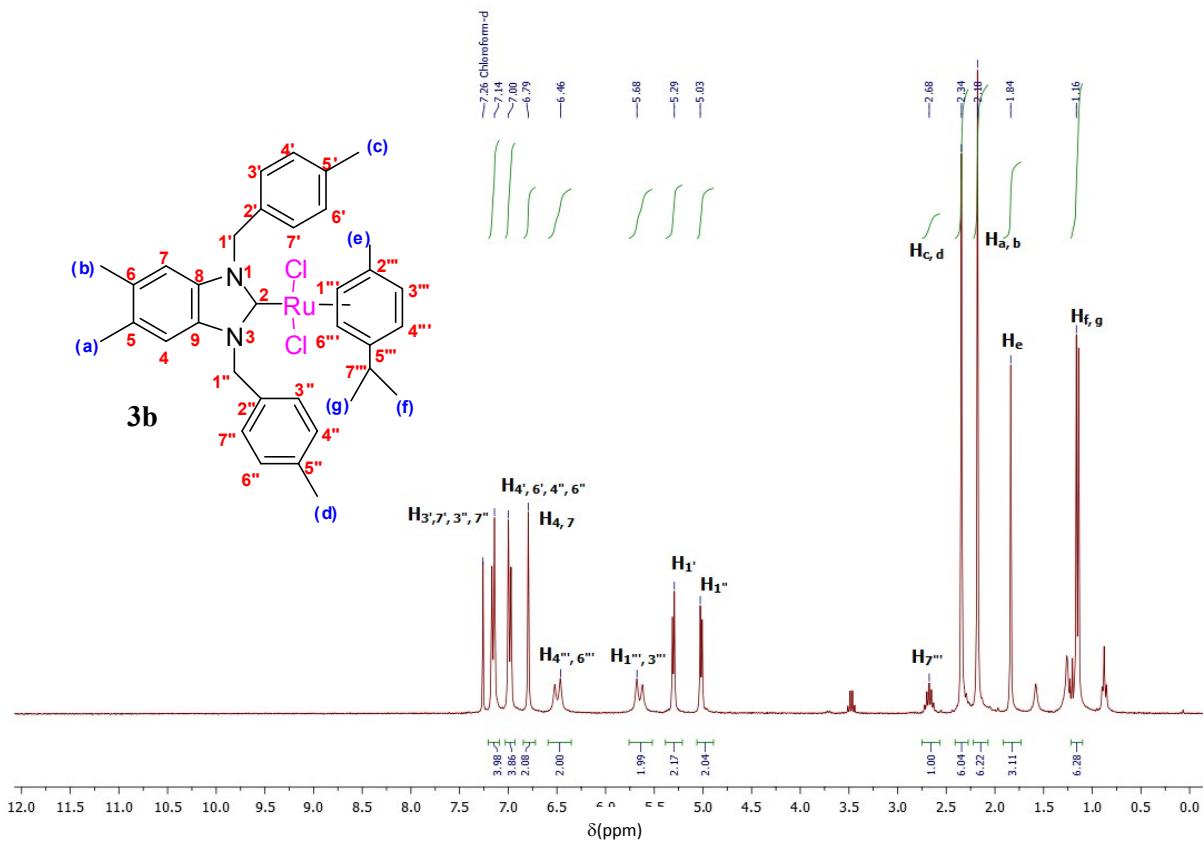


Figure S29: ^1H NMR spectra of Ru(II)-N-Heterocyclic Carbene complexes **3b** (CDCl_3 , 300MHz).

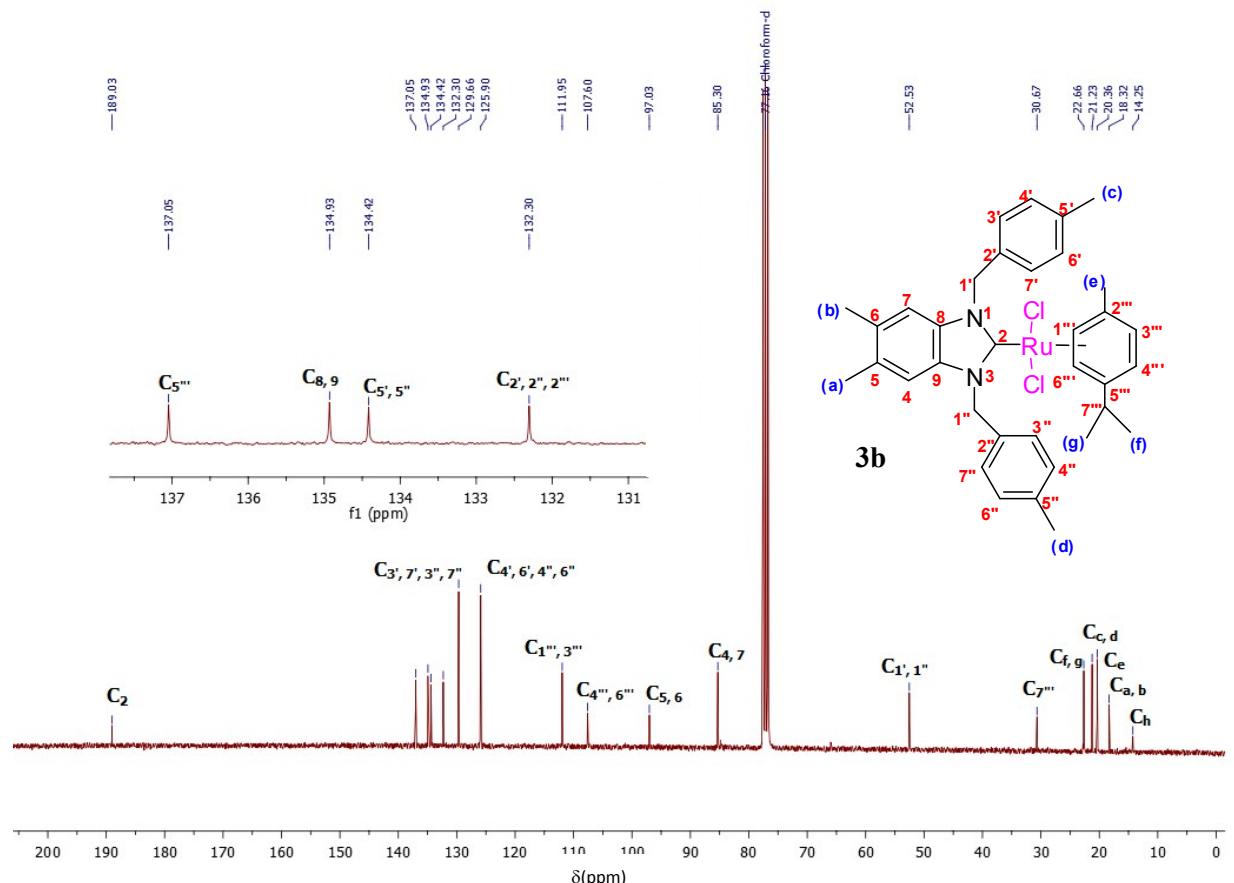


Figure S30: ^{13}C NMR spectra of Ru(II)-N-Heterocyclic Carbene complexes **3b** (CDCl_3 , 75MHz).

Dichloro-[1,3-bis(4-tertbutylbenzyl)benzimidazol-2-ylidene]-(*p*-cymene)-ruthenium(II), **3c**

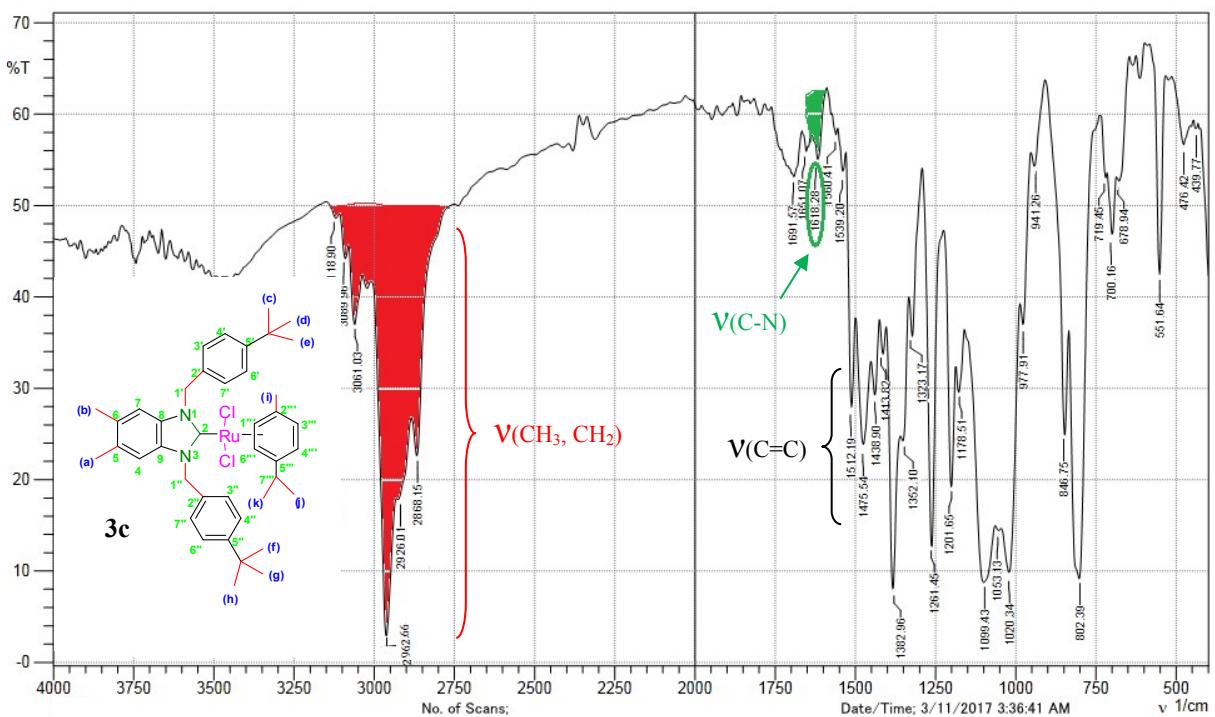


Figure S31: FT-IR spectra of Ru(II)-N-Heterocyclic Carbene complexes **3c**.

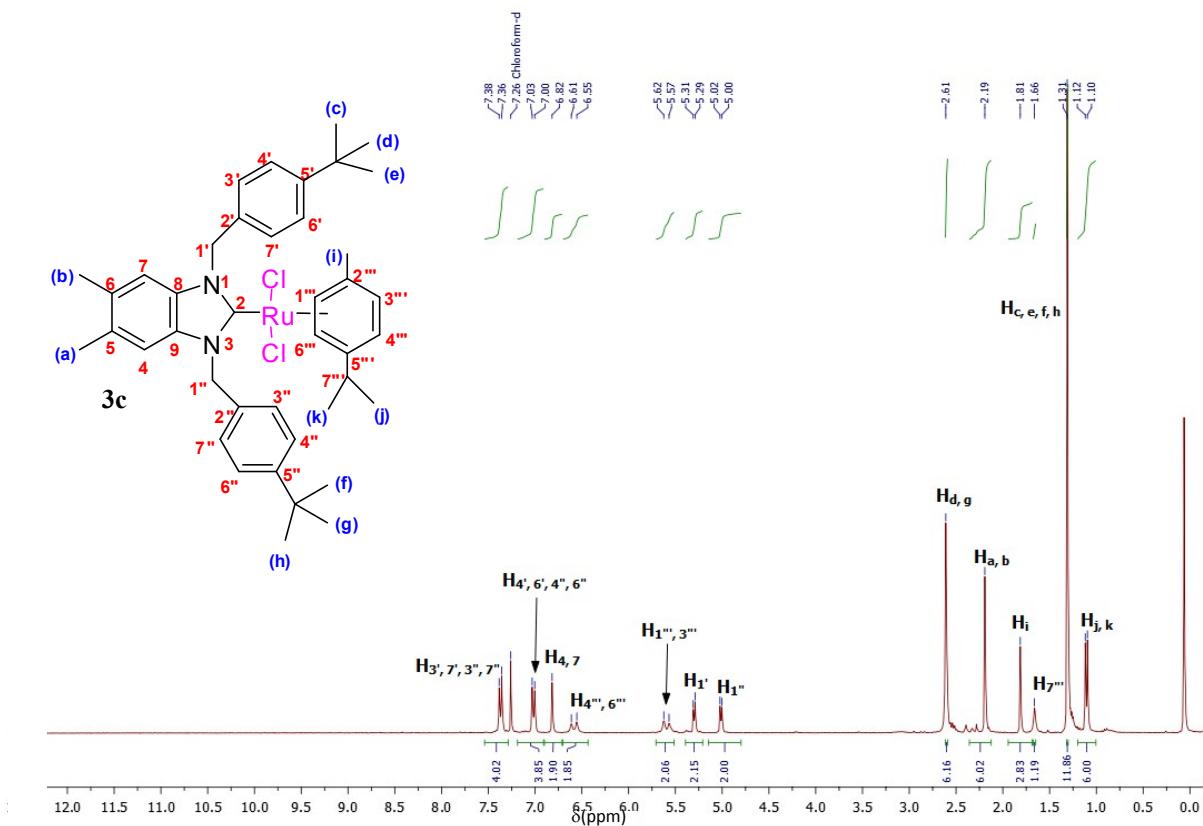


Figure S32: ¹H NMR spectra of Ru(II)-N-Heterocyclic Carbene complexes **3c** (CDCl₃, 300MHz).

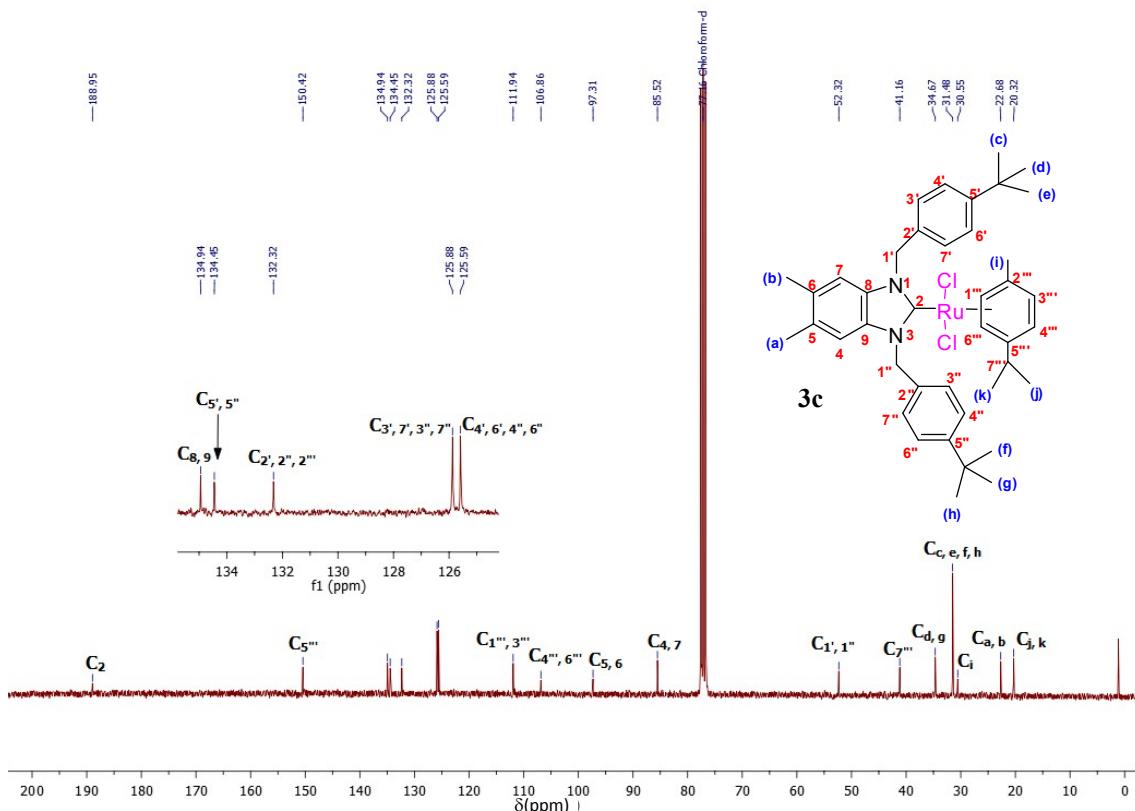


Figure S32: ¹³C NMR spectra of Ru(II)-N-Heterocyclic Carbene complexes **3c** (CDCl₃, 75MHz).

*Dichloro-[1-(3,5-dimethylbenzyl)-3- (2,3,5,6-tetramethylbenzyl)benzimidazol-2-ylidene](*p*-cymene)ruthenium(II), 3d*

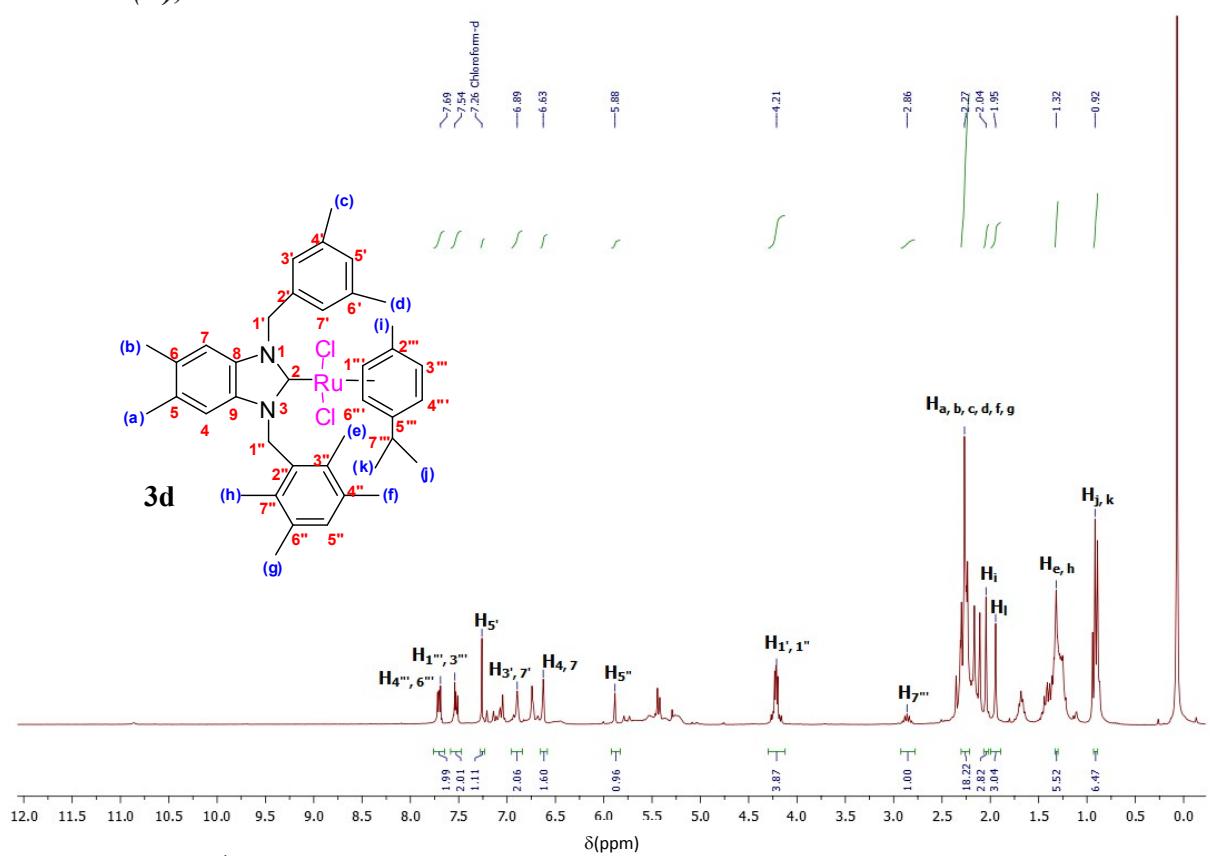


Figure S33: ¹H NMR spectra of Ru(II)-N-Heterocyclic Carbene complexes **3d** (CDCl₃, 300MHz).

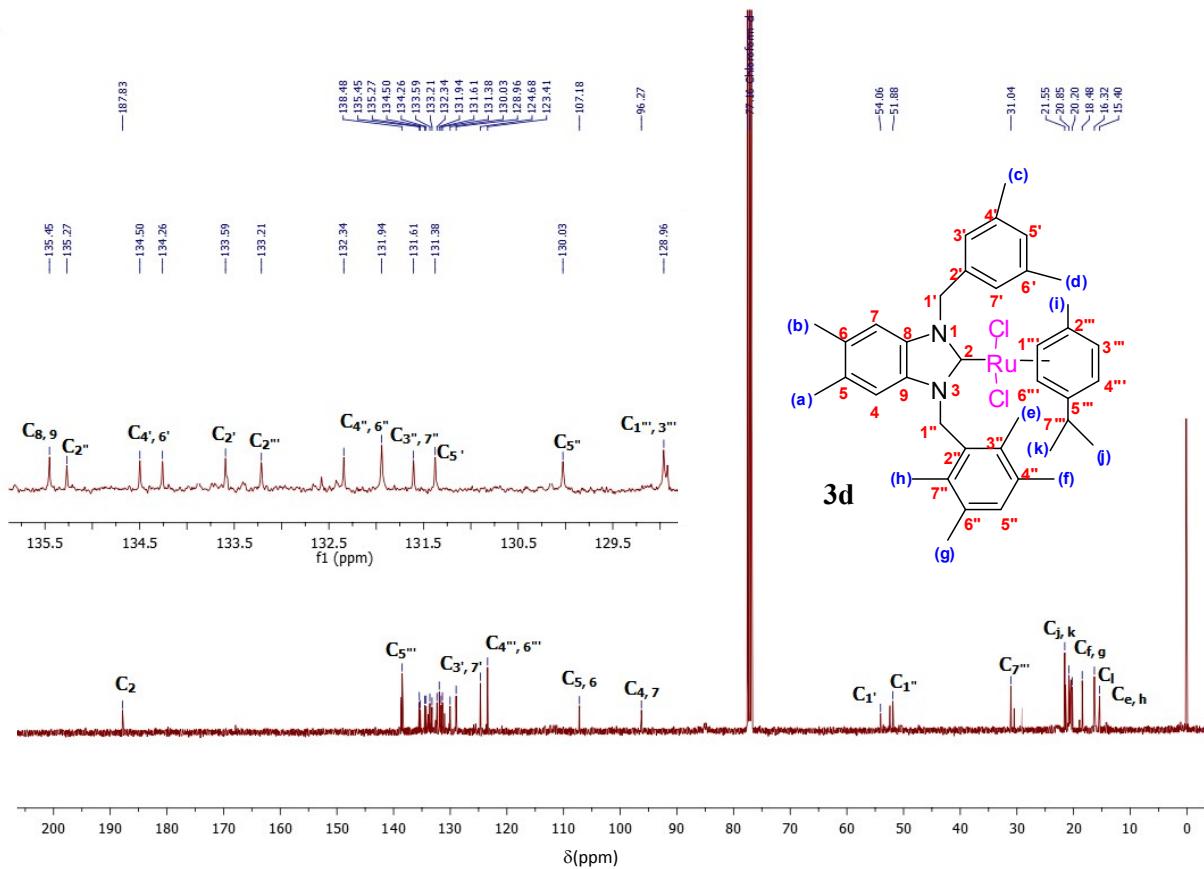


Figure S34: $^{13}\text{CNMR}$ spectra of Ru(II)-N-Heterocyclic Carbene complexes **3d** (CDCl_3 , 75MHz).

*Dichloro-[1-(3,5-dimethylbenzyl)-3-(4-tertbutylbenzyl)benzimidazol-2-ylidene](*p*-cymene)ruthenium(II), **3e***

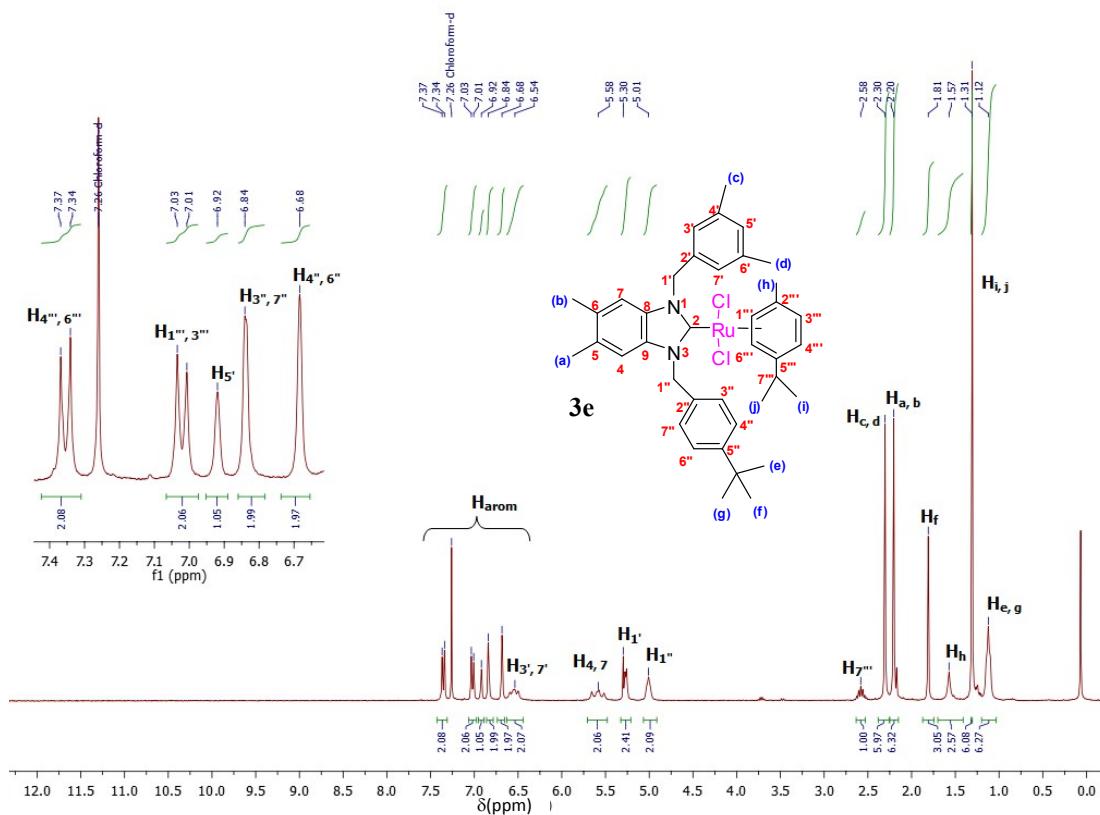


Figure S35: $^1\text{HNMR}$ spectra of Ru(II)-N-Heterocyclic Carbene complexes **3e** (CDCl_3 , 300MHz).

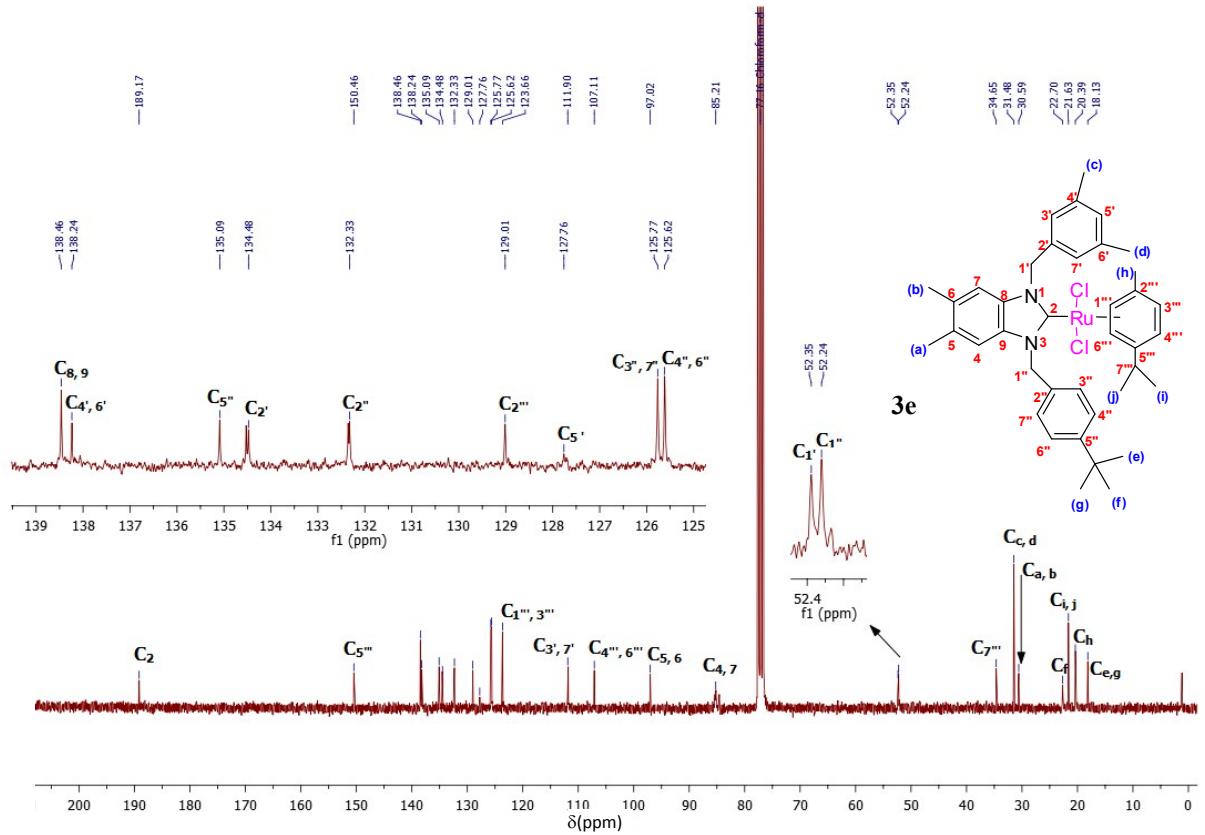


Figure S36: ¹³C NMR spectra of Ru(II)-N-Heterocyclic Carbene complexes **3e** (CDCl_3 , 75MHz).

Dichloro-[1-(3,5-dimethylbenzyl)-3- (4-methylbenzyl)benzimidazol-2-ylidene](*p*-cymene)-ruthenium(II), 3f

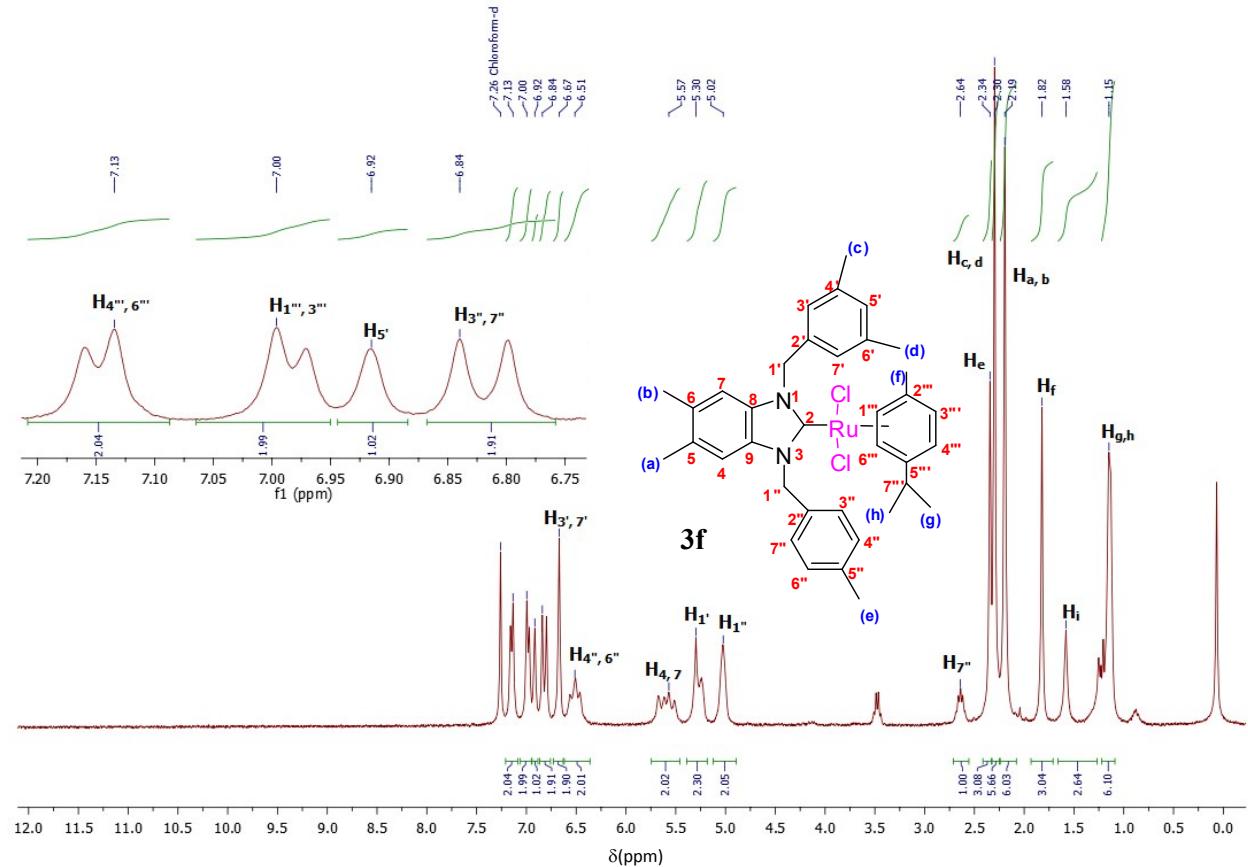


Figure S37: ^1H NMR spectra of Ru(II)-N-Heterocyclic Carbene complexes **3f** (CDCl_3 , 300MHz).

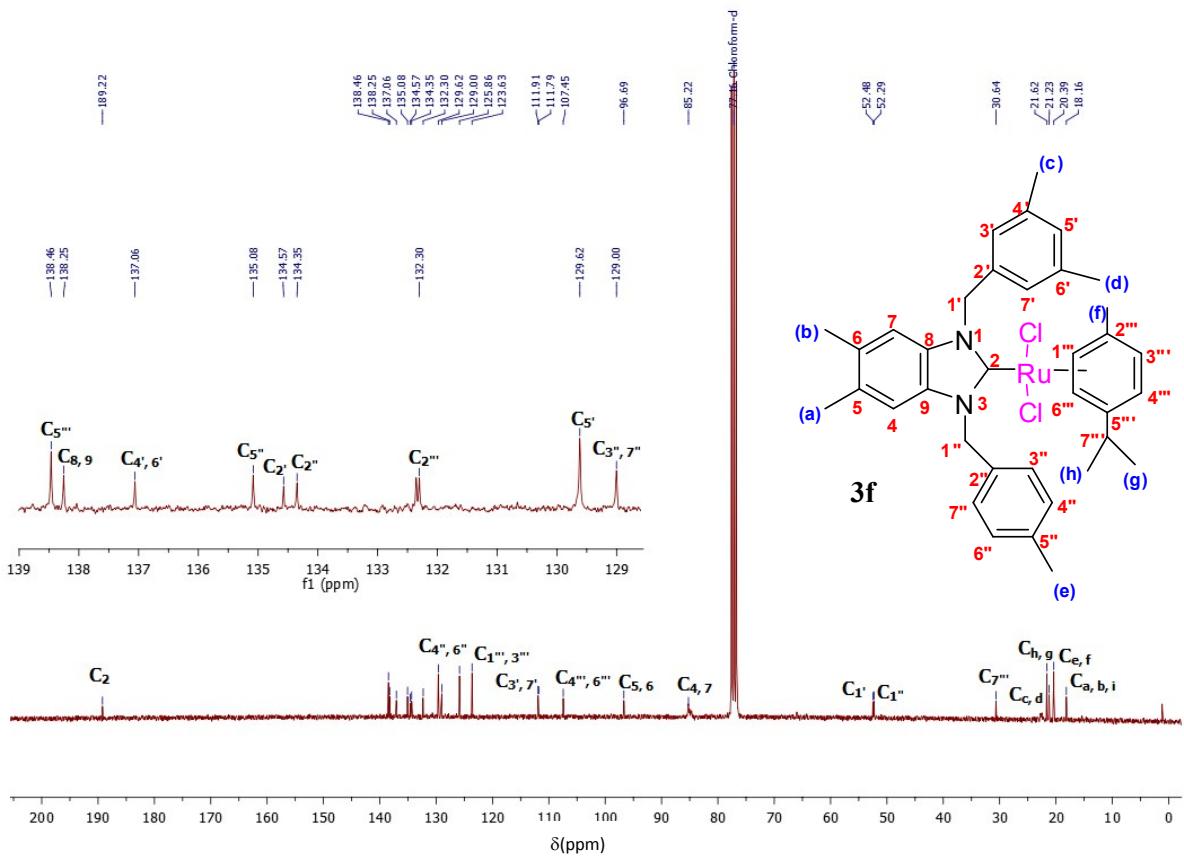


Figure S38: ¹³C NMR spectra of Ru(II)-N-Heterocyclic Carbene complexes **3f** (CDCl₃, 75MHz).

