

Cationic Iridium(III) Complexes Bearing Bis(triazole) Ancillary Ligands

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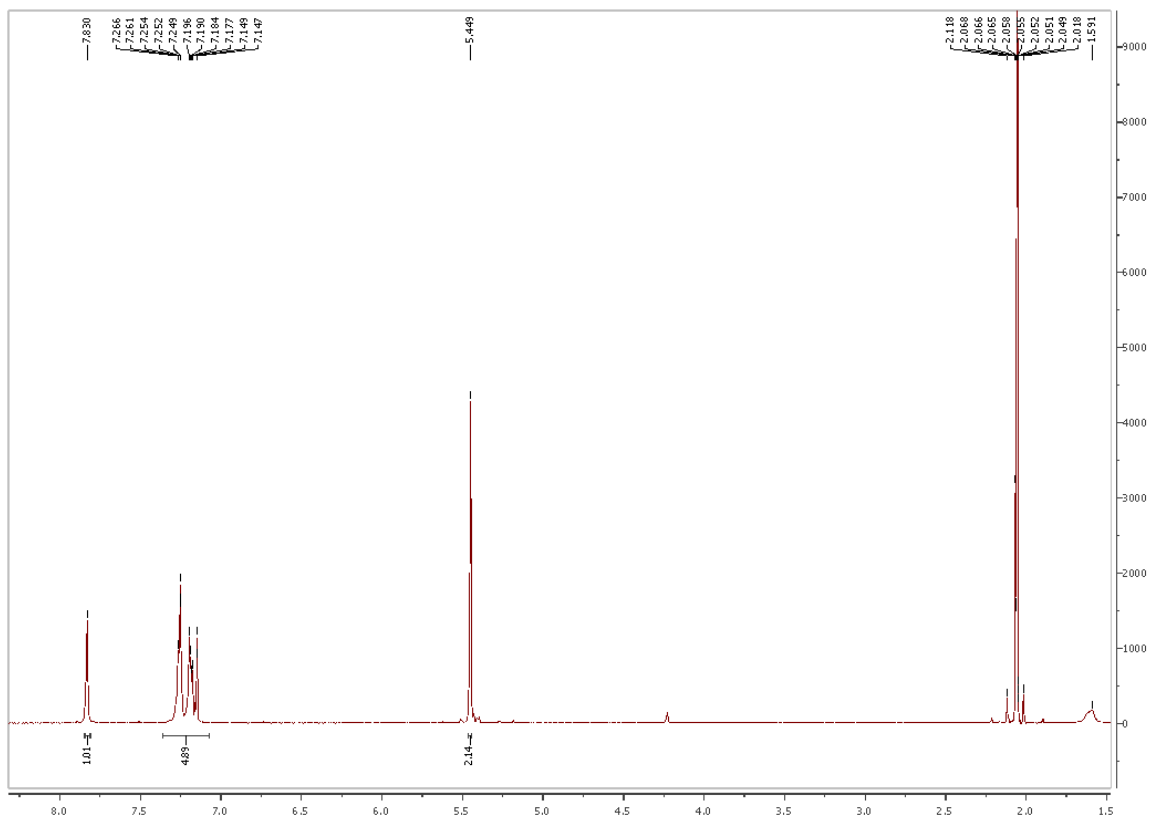
SUPPORTING INFORMATION

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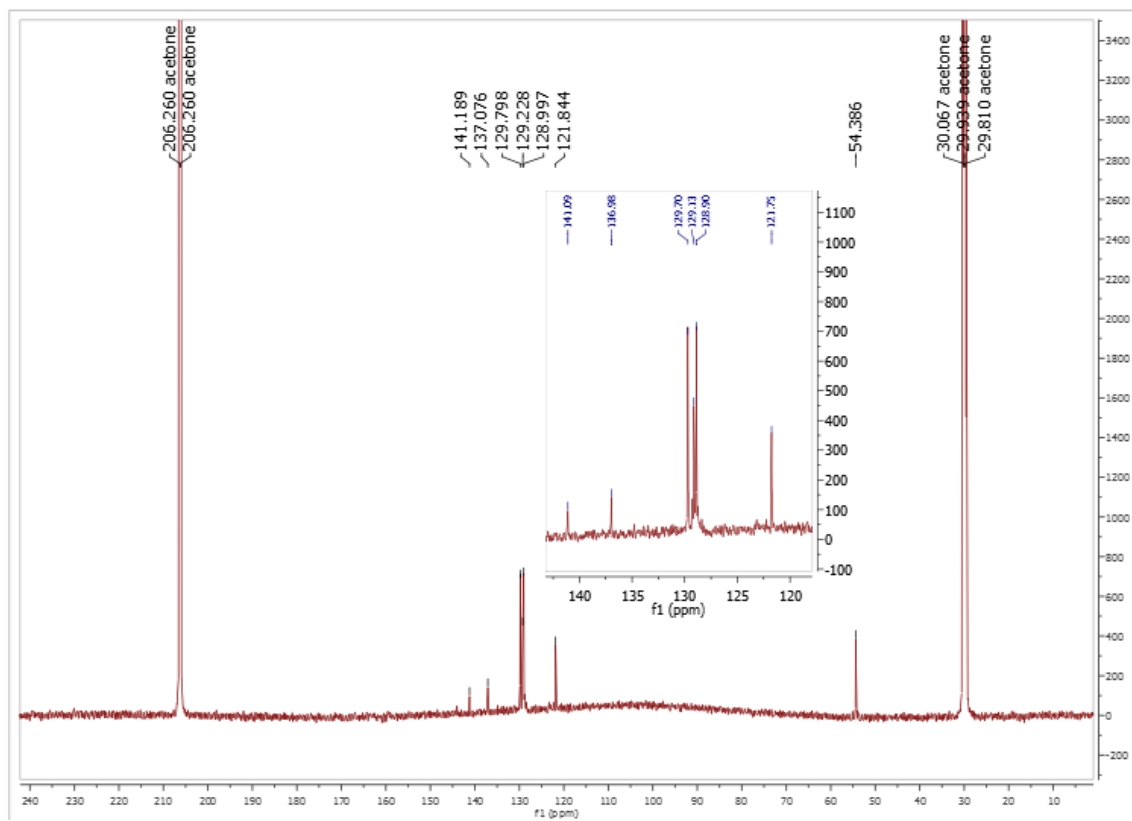
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NMR Spectra

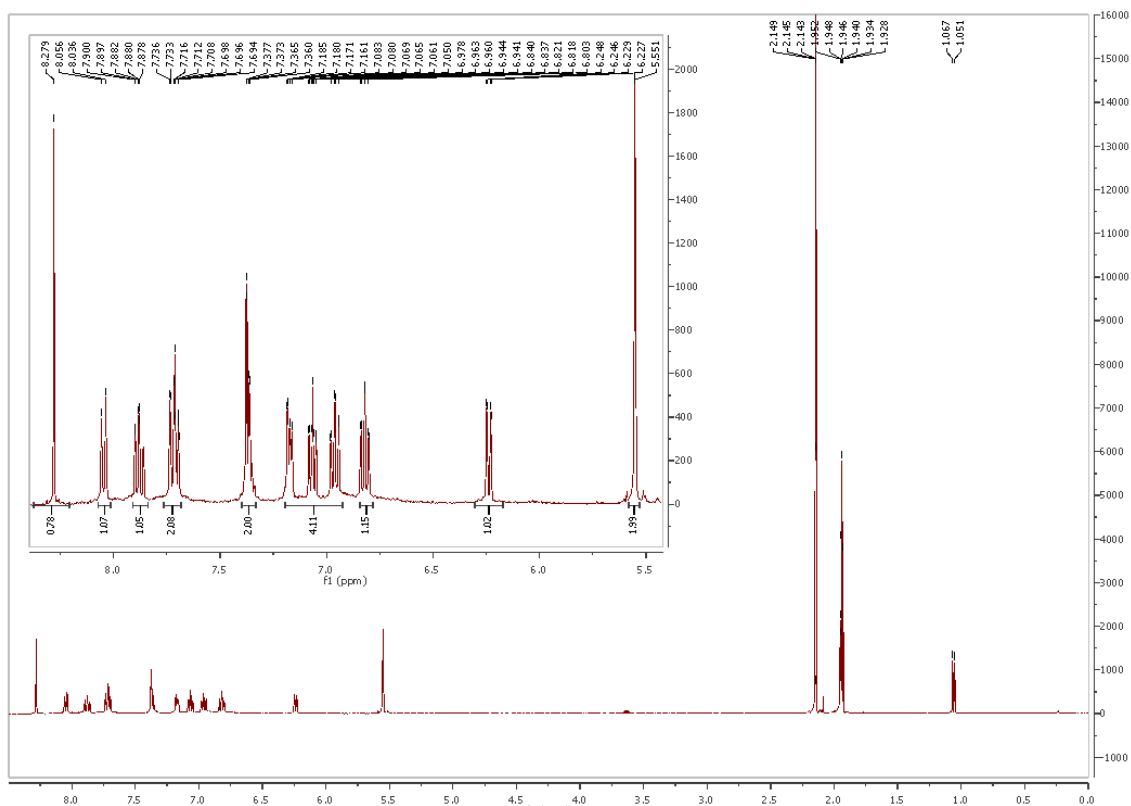
¹H NMR data of 4,4'-Bi-1*H*-1,2,3-triazole, 1,1'-bis(phenylmethyl) in CD₃CN:



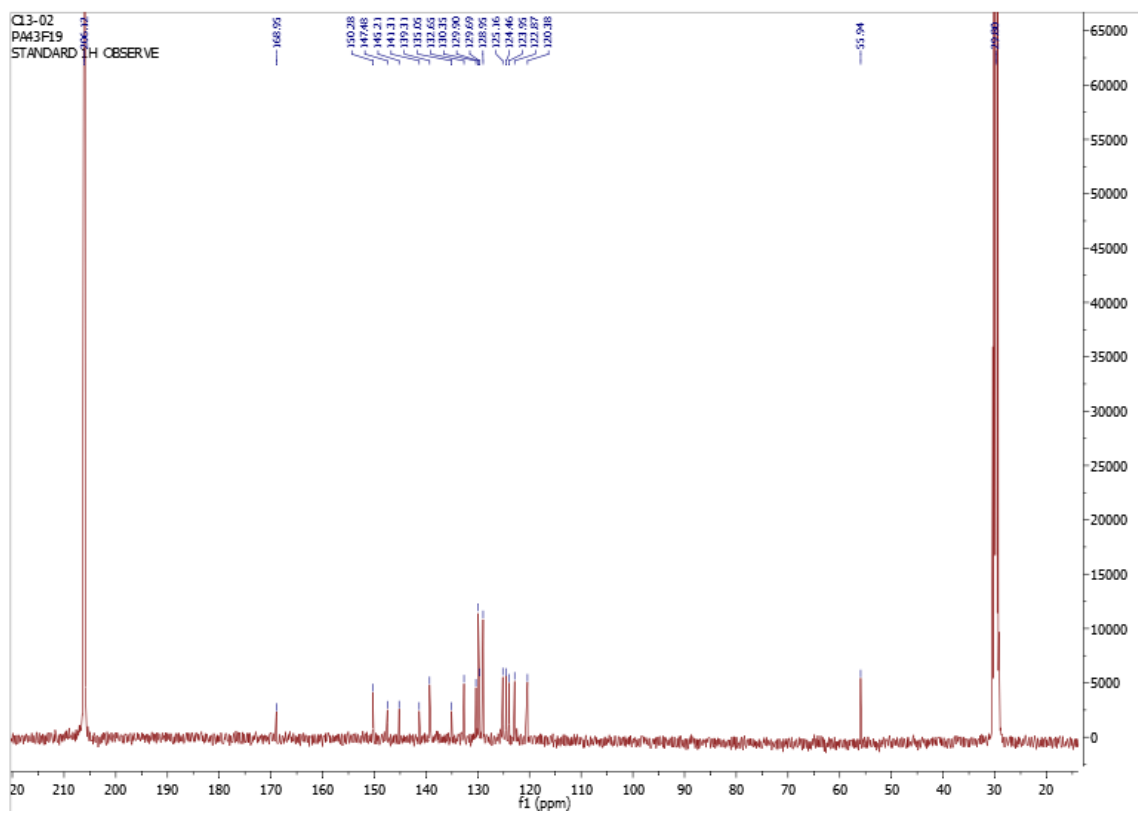
^{13}C NMR data of 4,4'-Bi-1*H*-1,2,3-triazole, 1,1'-bis(phenylmethyl) in Acetone-*d*₆:



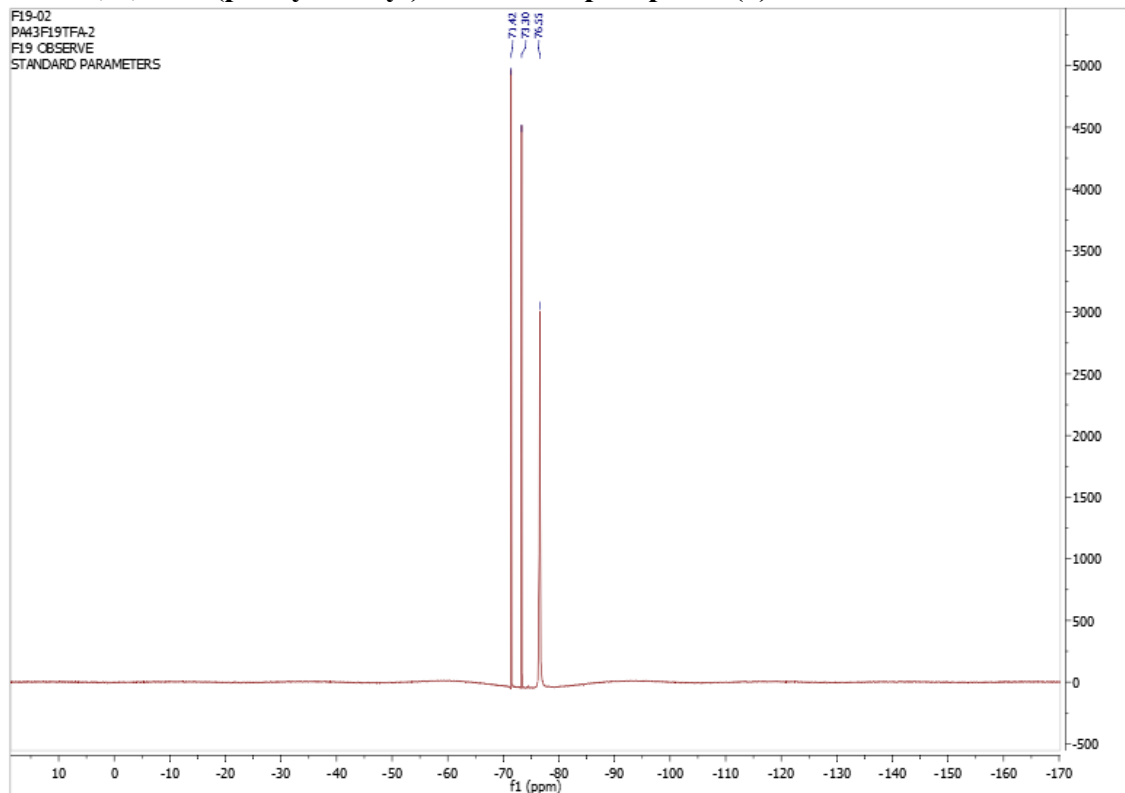
^1H NMR data of Iridium(III) Bis[2-phenylpyridinato- $\text{N},\text{C}2'$]-4,4'-Bi-1*H*-1,2,3-triazole, 1,1'-bis(phenylmethyl) Hexafluorophosphate (1) in CD_3CN :



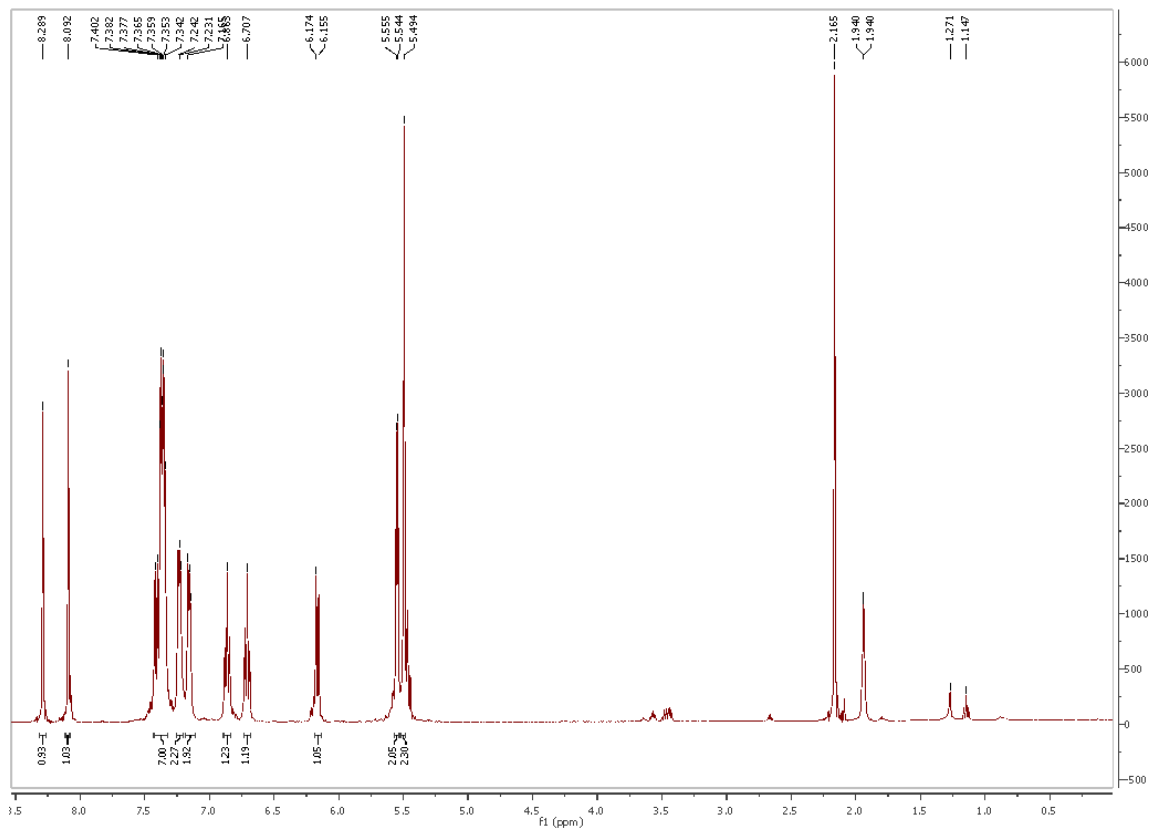
^{13}C NMR data of Iridium(III) Bis[2-phenylpyridinato-N,C2']-4,4'-Bi-1*H*-1,2,3-triazole, 1,1'-bis(phenylmethyl) Hexafluorophosphate (1) in Acetone- d_6 :



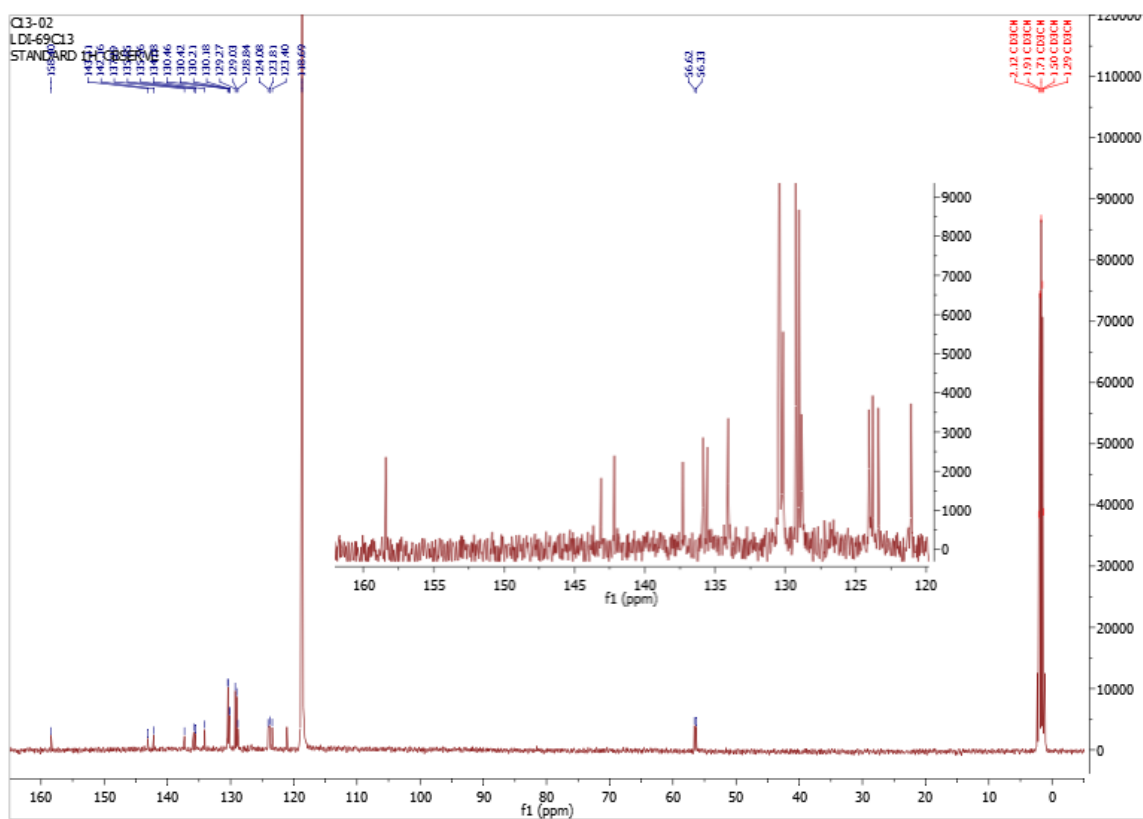
^{19}F NMR data of of Iridium(III) Bis[2-phenylpyridinato-N,C2']-4,4'-Bi-1*H*-1,2,3-triazole, 1,1'-bis(phenylmethyl) Hexafluorophosphate (1):



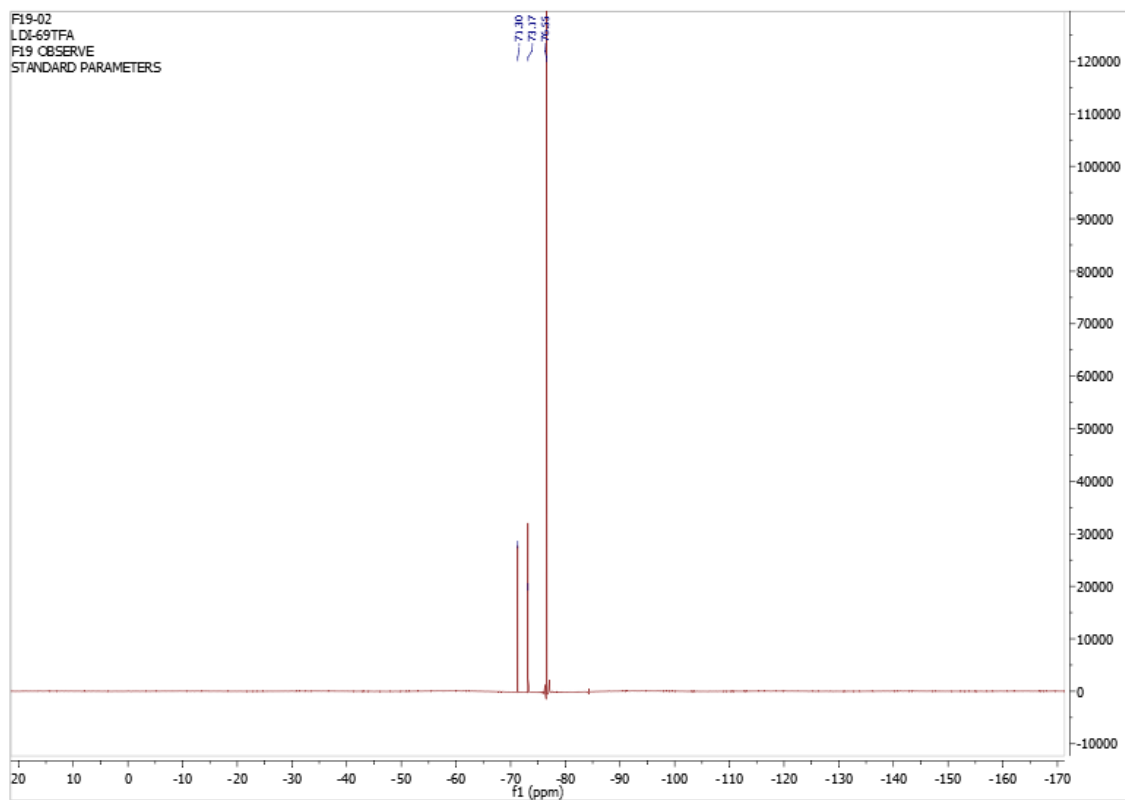
¹H NMR data of Iridium(III) Bis[(1'-phenyl)1,2,3-triazolato-N,C^{2'}]-4,4'-Bi-1H-1,2,3-triazole, 1,1'-bis(phenylmethyl) Hexafluorophosphate (2) in CD₃CN:



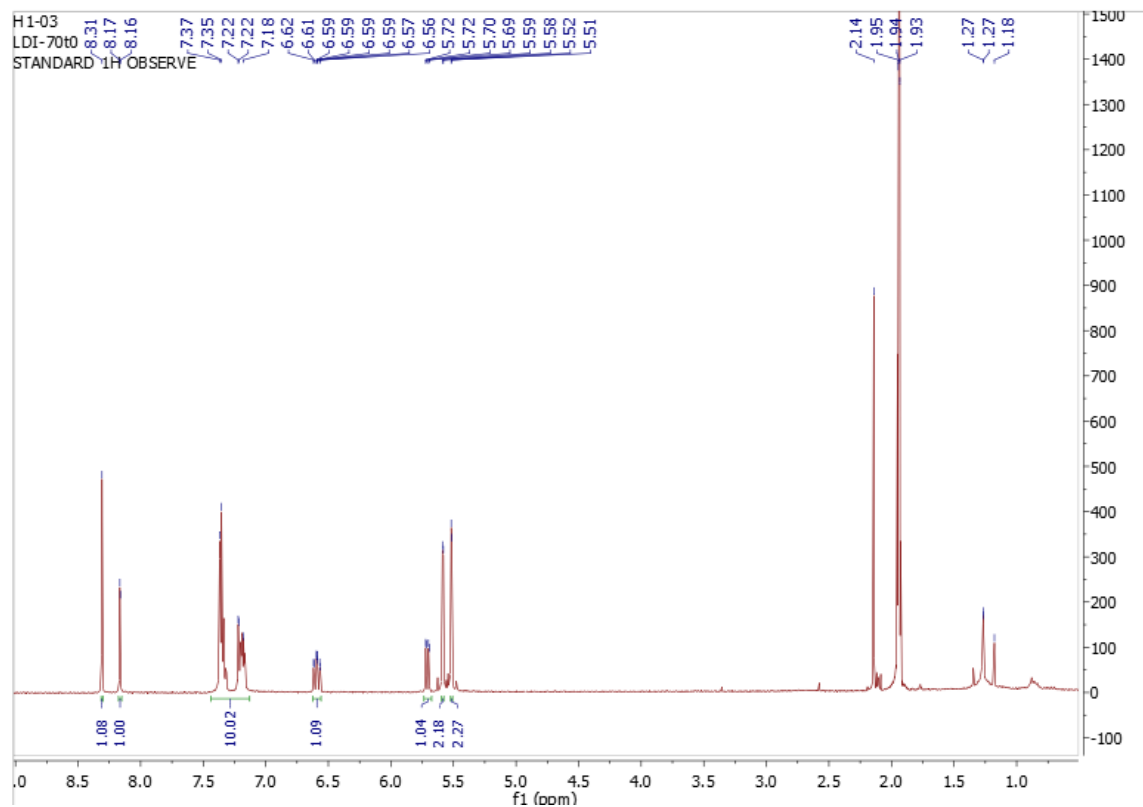
^{13}C NMR data of Iridium(III) Bis[(1'-phenyl)1,2,3-triazolato-N,C $^{2'}$]-4,4'-Bi-1H-1,2,3-triazole, 1,1'-bis(phenylmethyl) Hexafluorophosphate (2) in CD_3CN :



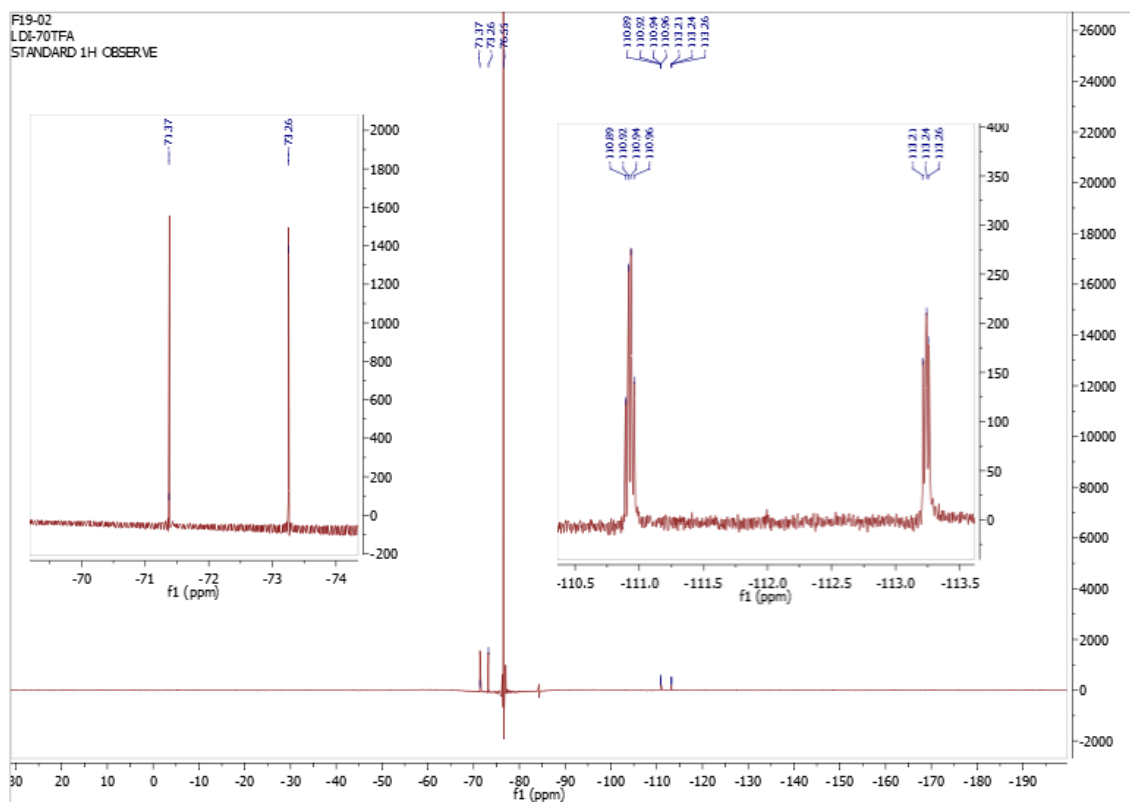
^{19}F NMR data of Iridium(III) Bis[(1'-phenyl)1,2,3-triazolato-N,C^{2'}]-4,4'-Bi-1H-1,2,3-triazole, 1,1'-bis(phenylmethyl) Hexafluorophosphate (2):



**^1H NMR data of Iridium(III) Bis[1'-(4',6'-difluorophenyl)1,2,3-triazolato-N,C 21]-
4,4'-Bi-1H-1,2,3-triazole, 1,1'-bis(phenylmethyl) Hexafluorophosphate (3) in
 CD_3CN :**



**^{19}F NMR data of Iridium(III) Bis[1'-(4',6'-difluorophenyl)1,2,3-triazolato-N,C $^{2'}$]-
4,4'-Bi-1H-1,2,3-triazole, 1,1'-bis(phenylmethyl) Hexafluorophosphate (3):**



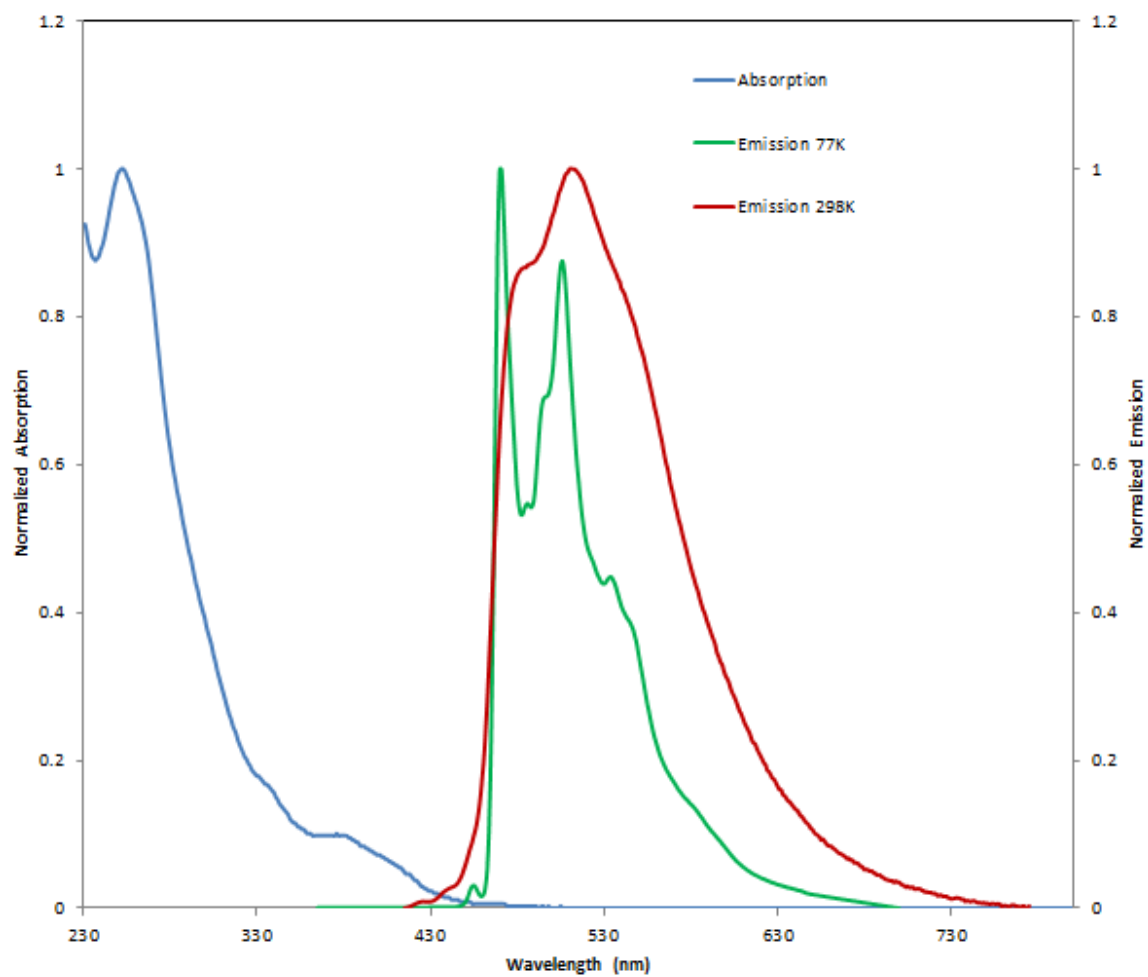


Figure S1: Absorption, 77 K and 298 K emission spectra for **1** ($\lambda_{\text{exc}} = 400\text{nm}$):

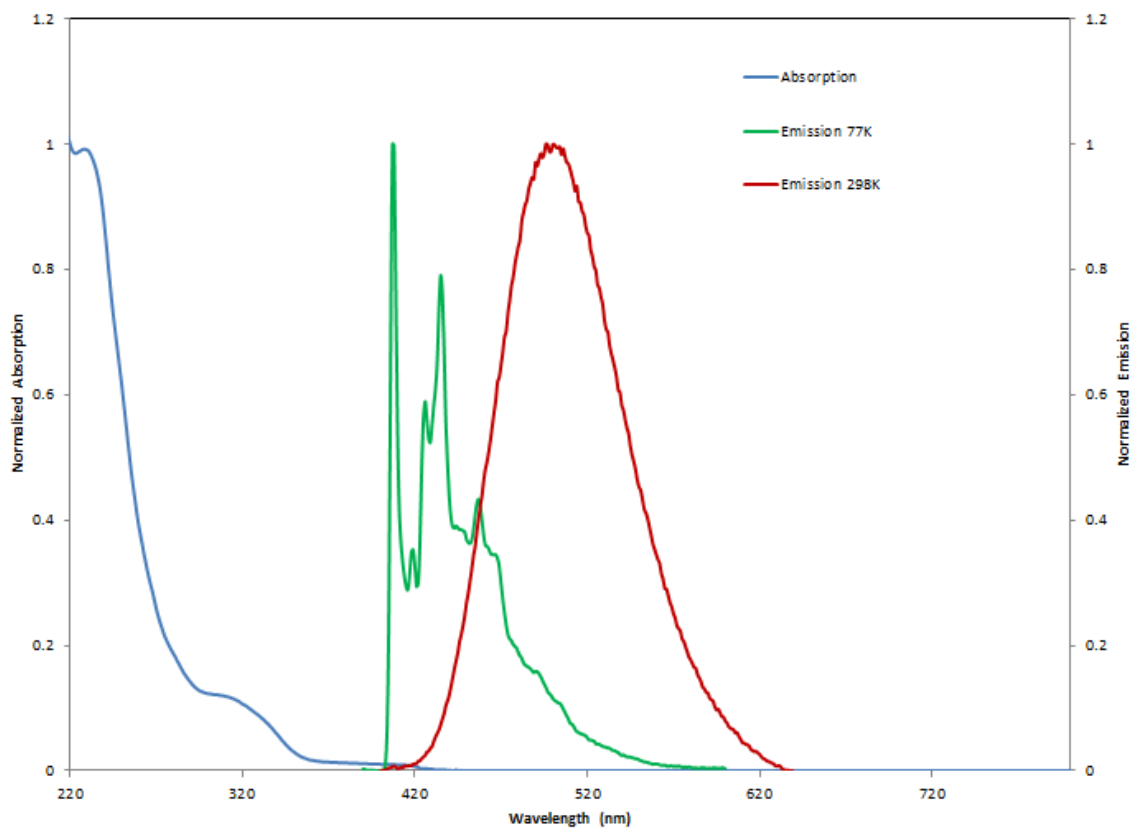


Figure S2: Absorption, 77 K and 298 K emission spectra for **2** ($\lambda_{\text{exc}} = 300\text{nm}$):

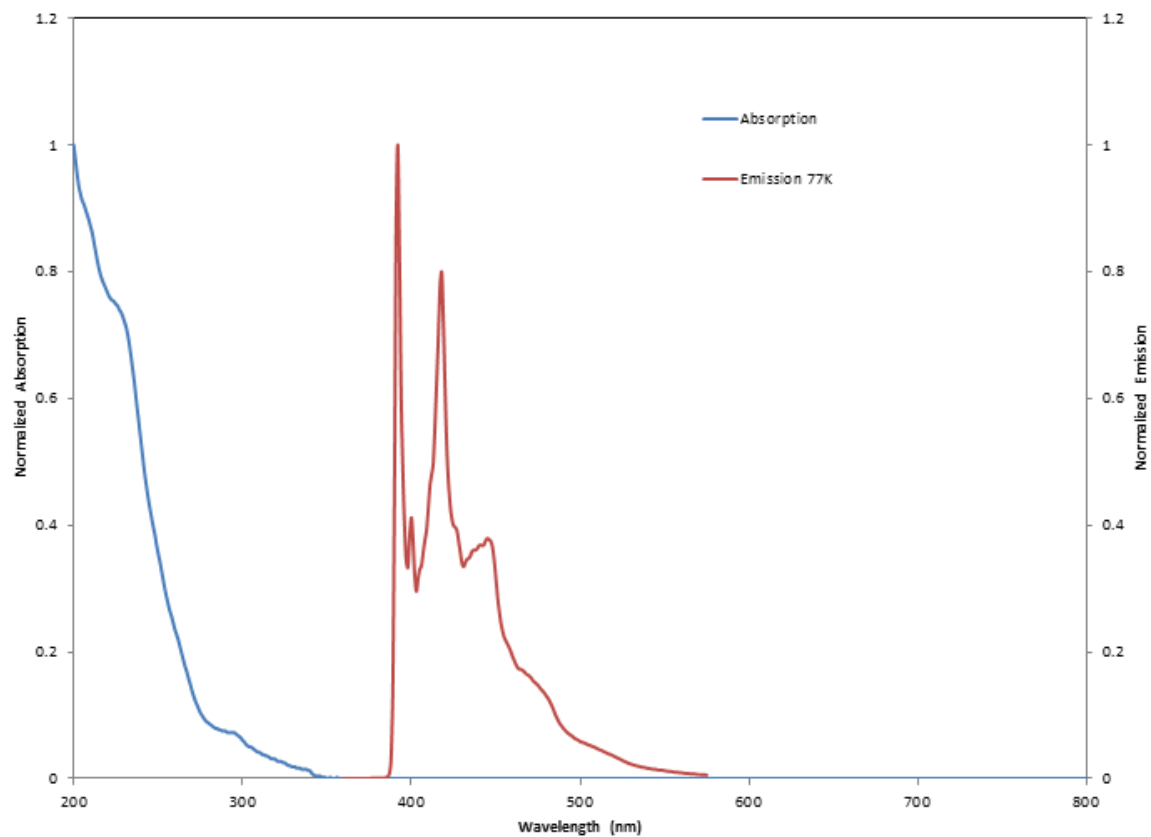


Figure S3: Absorption and 77 K emission spectra for **3** ($\lambda_{\text{exc}} = 290\text{nm}$):

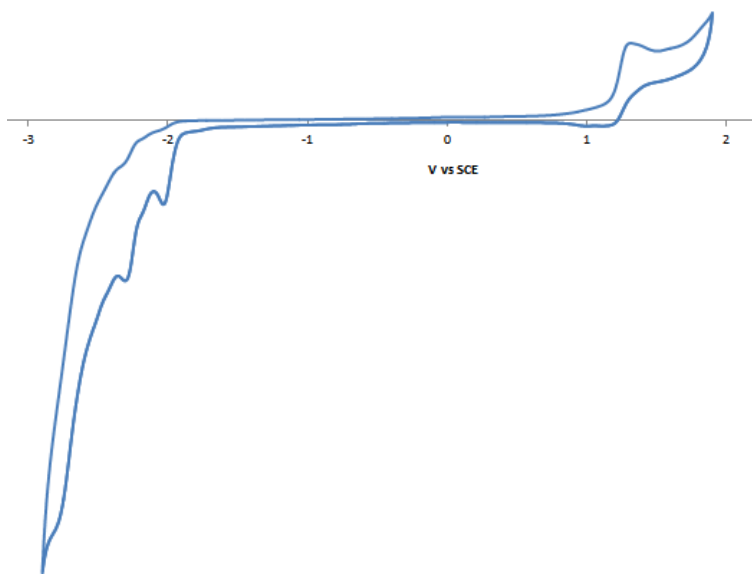


Figure S4: Cyclic voltammogram of **1** in ACN with 0.1 M TBAPF₆.

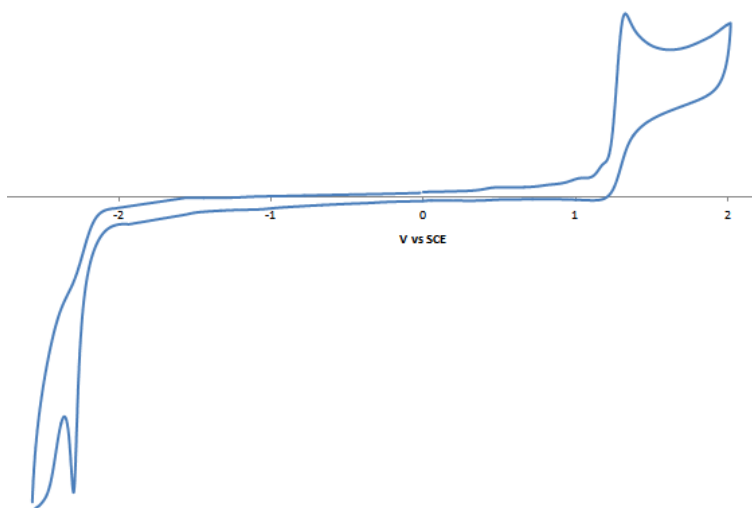


Figure S5: Cyclic voltammogram of **2** in ACN with 0.1 M TBAPF₆.

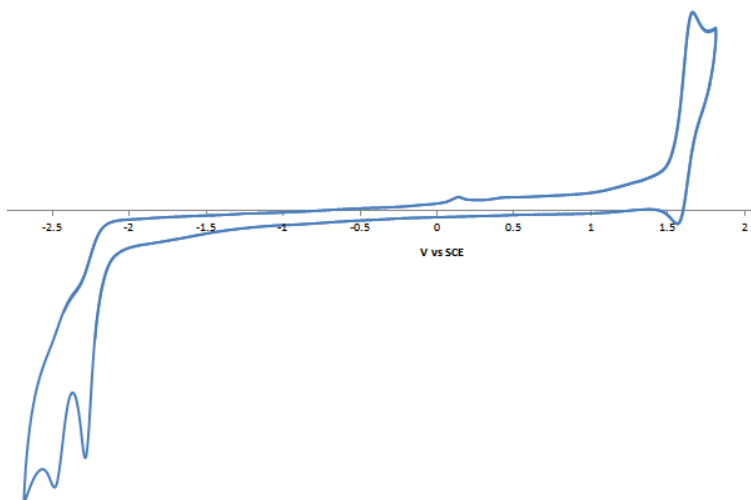


Figure S6: Cyclic voltammogram of **3** in ACN with 0.1 M TBAPF₆.

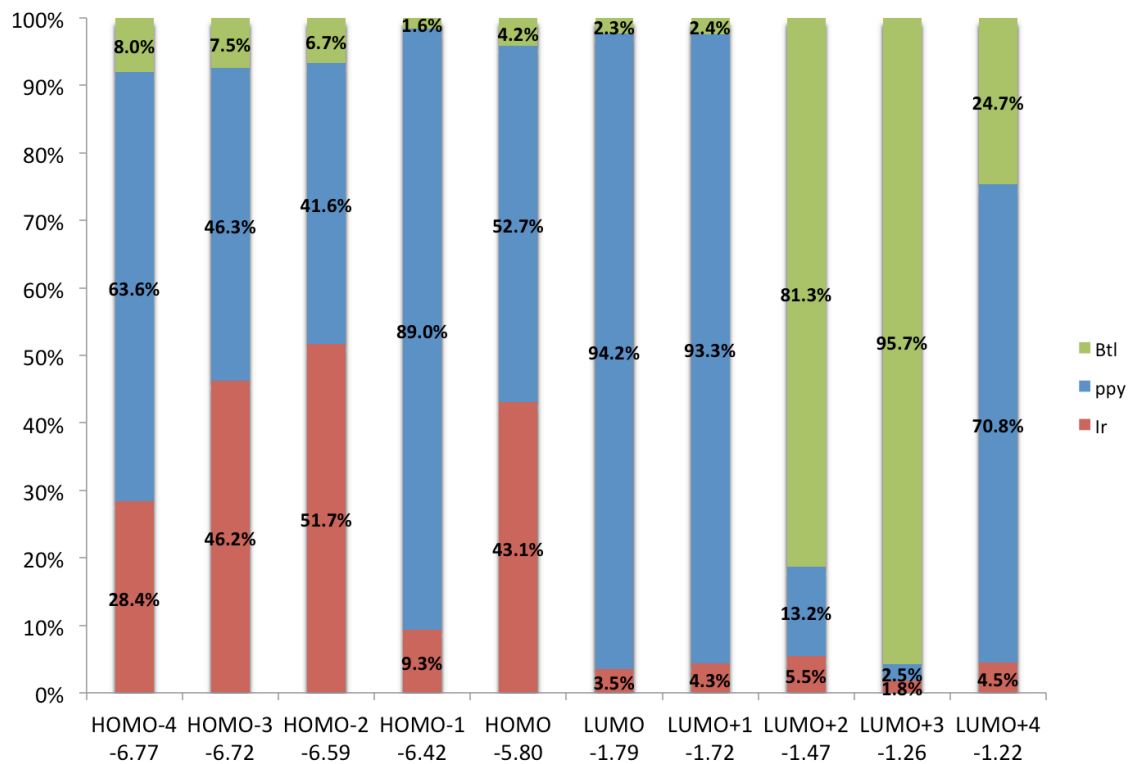


Figure S7: MO quantification of **1**.

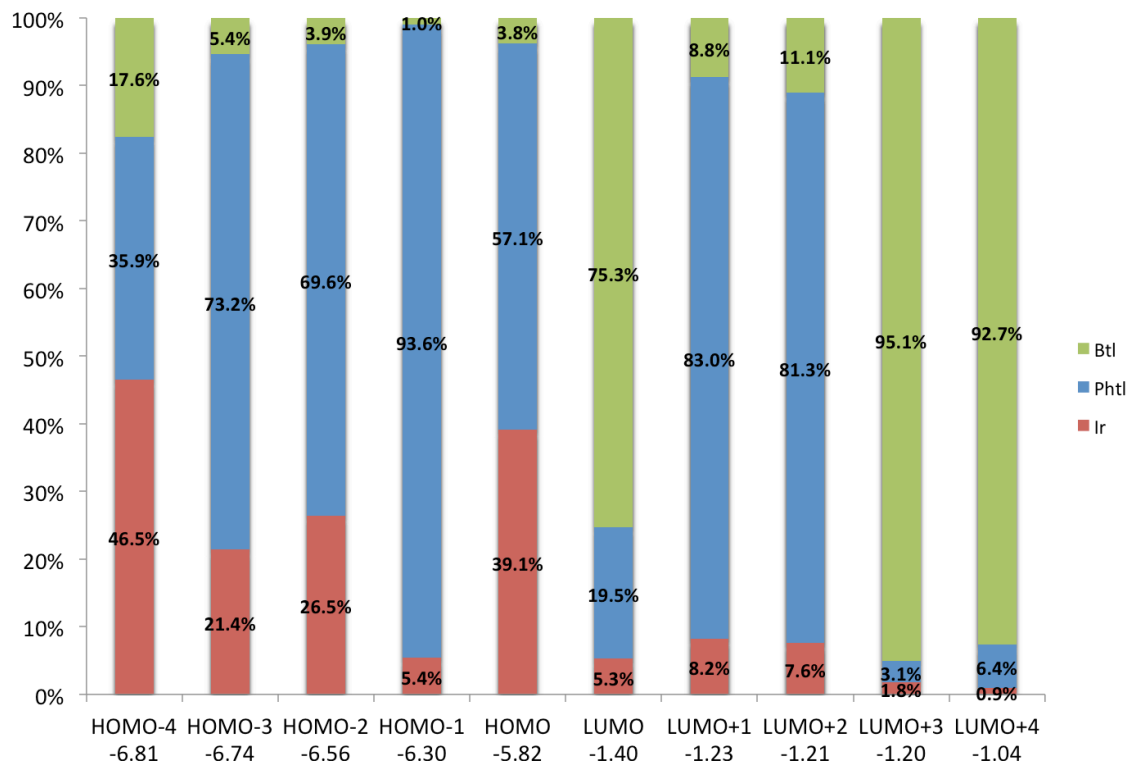


Figure S8: MO quantification of 2.

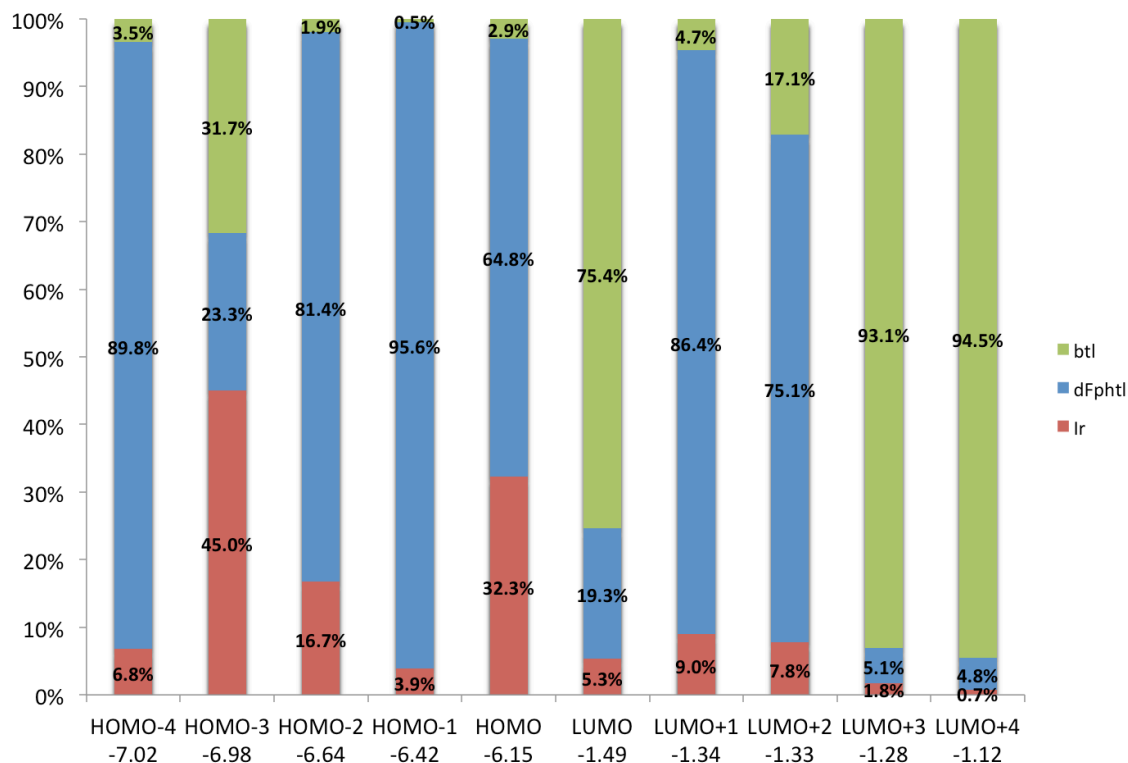


Figure S9: MO quantification of **3**.

	Singlet State (S_0)	Triplet State (T_1)
Scaling Factor	0.5	0.5
Magnitude of dipole (D)	13.5919	12.1886

Figure S10: Dipole moment predictions for **1**.

	Singlet State (S_0)	Triplet State (T_1)
Scaling Factor	1	1
Magnitude of dipole (D)	11.5785	8.3573

Figure S11: Dipole moment predictions for **2**.

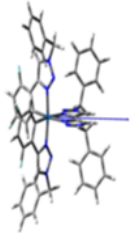
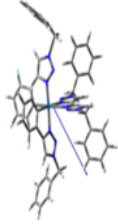
	Singlet State (S_0)	Triplet State (T_1)
		
Scaling Factor	0.5	0.3
Magnitude of dipole (D)	16.5459	24.3718

Figure S12: Dipole moment predictions for **3**.