Supporting Information for

Effect of Bulky Groups in Ruthenium Heteroleptic Sensitizers on Dye Sensitized Solar Cell Performance

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Experimental Details

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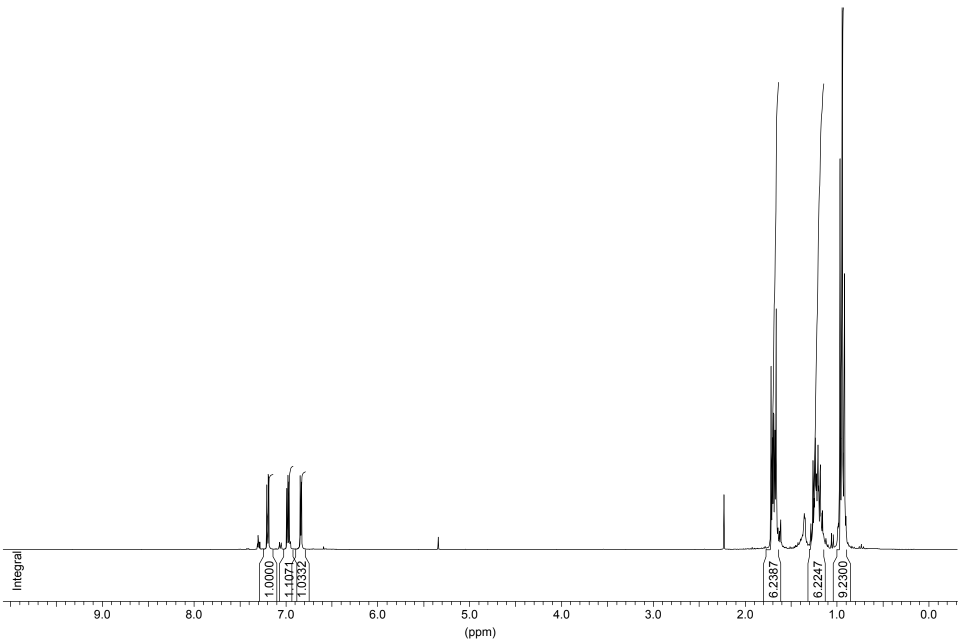
EXPERIMENTAL DETAILS

Chemicals employed all over this work were purchased from Aldrich Chemical Co. and used as received without further purification. Dry solvents were purchased from SDS in *anhydrous grade* and further dried over activated molecular sieves. The monitoring of the reactions was carried out by TLC, employing aluminum sheets coated with silica gel 60 F_{254} (normal phase) or with LiChroprep RP-18 $F_{254\text{-}S}$ (reverse phase), both purchased from Merck. Purification of compounds was performed by flash column chromatography using silica gel Merck-60 (230-400 mesh, 0.040-0.063 mm) or Aldrich Sephadex LH-20. EI-MS spectra were determined on a VG AutoSpec instrument, MALDI-TOF MS and HRMS spectra were recorded with a Bruker Reflex III spectrometer. NMR spectra were recorded with a Bruker AC-300 instrument with a laser beam operating at 337 nm. Dithranol (1,8,9-anthracenetriol) and PEGNa1000 poly(ethylenglycol)-1000 were used as matrix and internal reference, respectively. The logarithm of the absorption coefficient (ε) is indicated in brackets for each maximum. FT-IR spectra were recorded on a Bruker Vector 22 spectrophotometer from solid samples embedded in pressed disks of KBr.

Figure S1: ^{1}H-NMR and ^{13}C-NMR spectra of compound 1



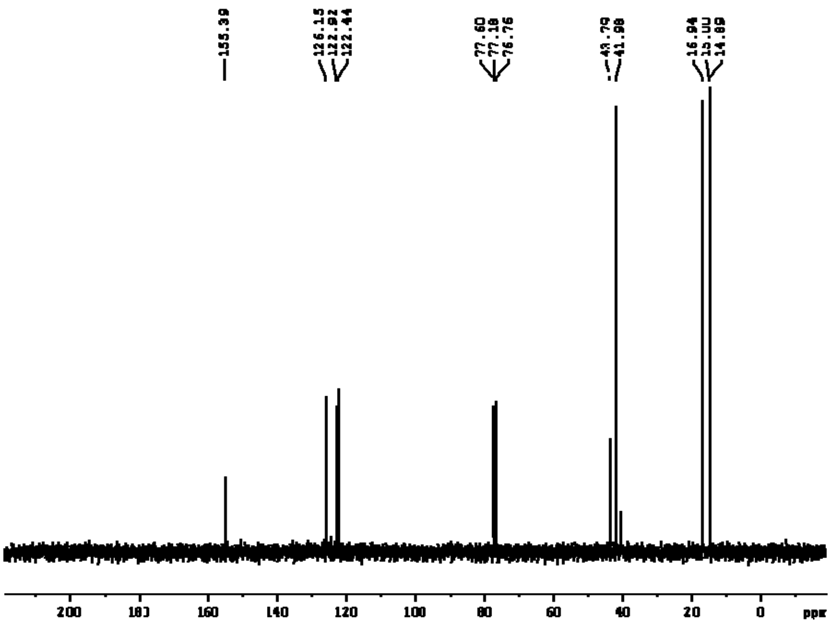
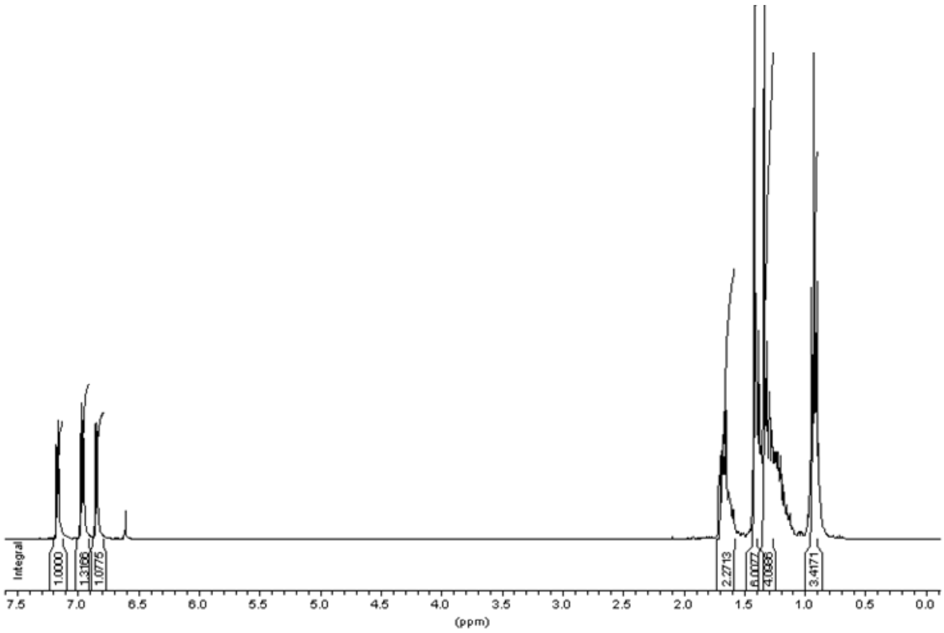


Figure S2: ^{1}H-NMR and ^{13}C-NMR spectra of compound 2



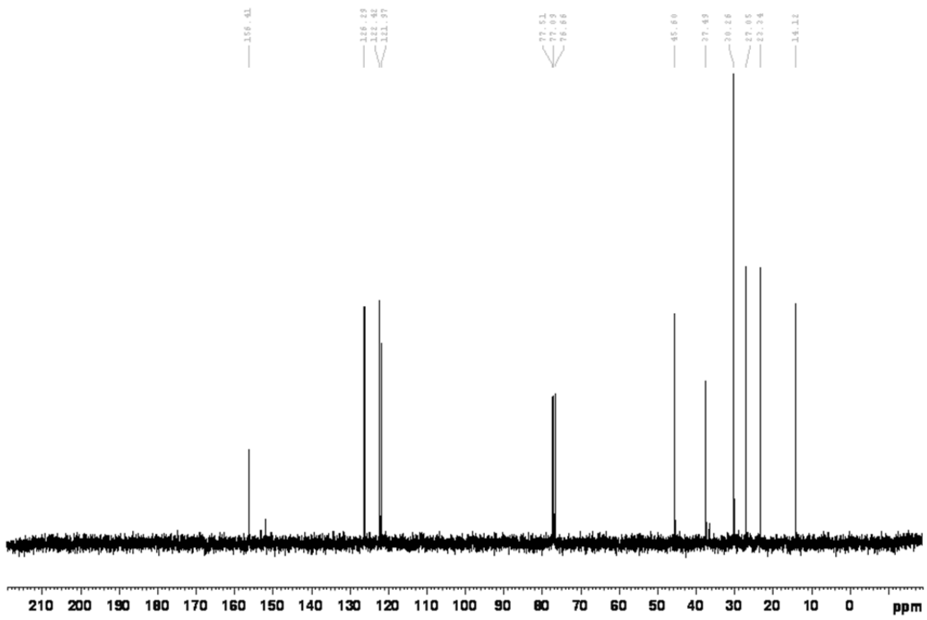


Figure S3: ^{1}H-NMR and ^{13}C-NMR spectra of compound 3

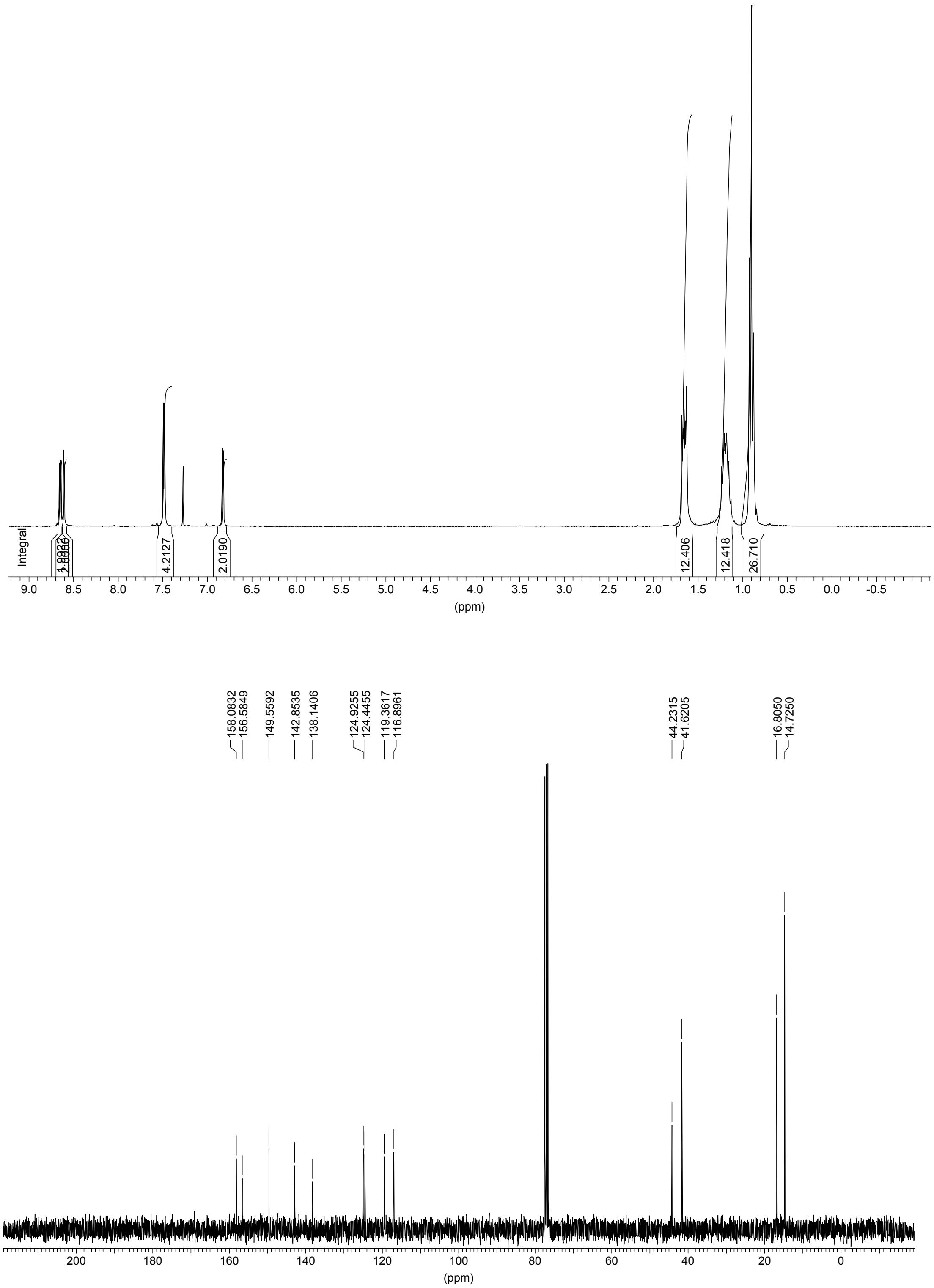
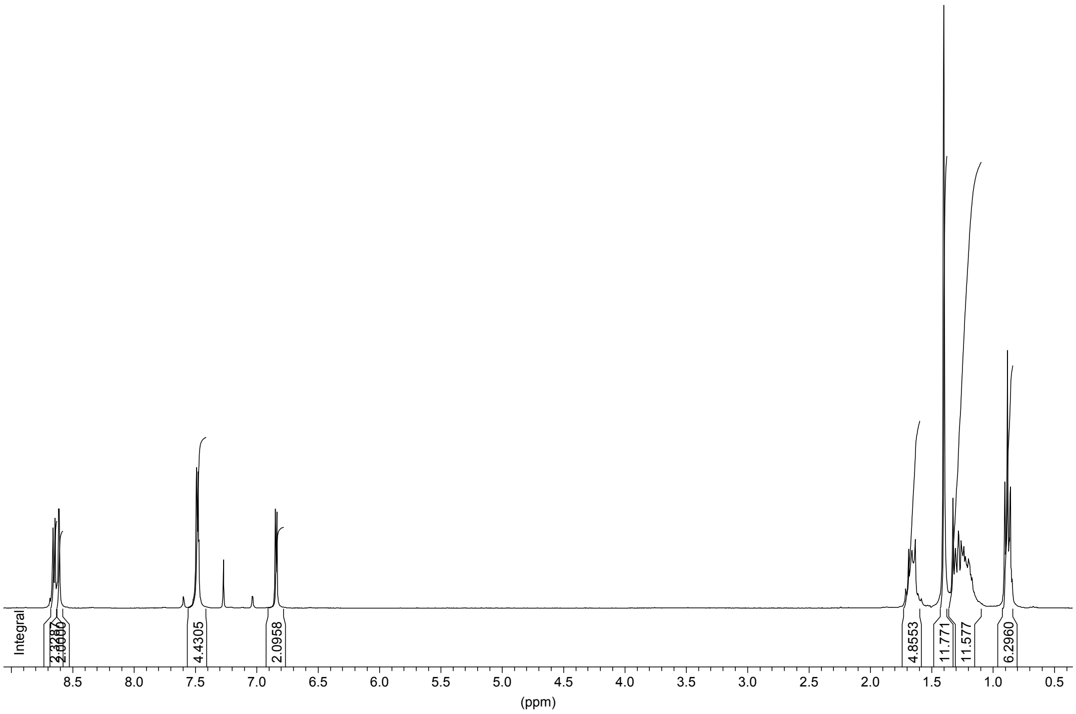


Figure S4: ^{1}H-NMR and ^{13}C-NMR spectra of compound 4



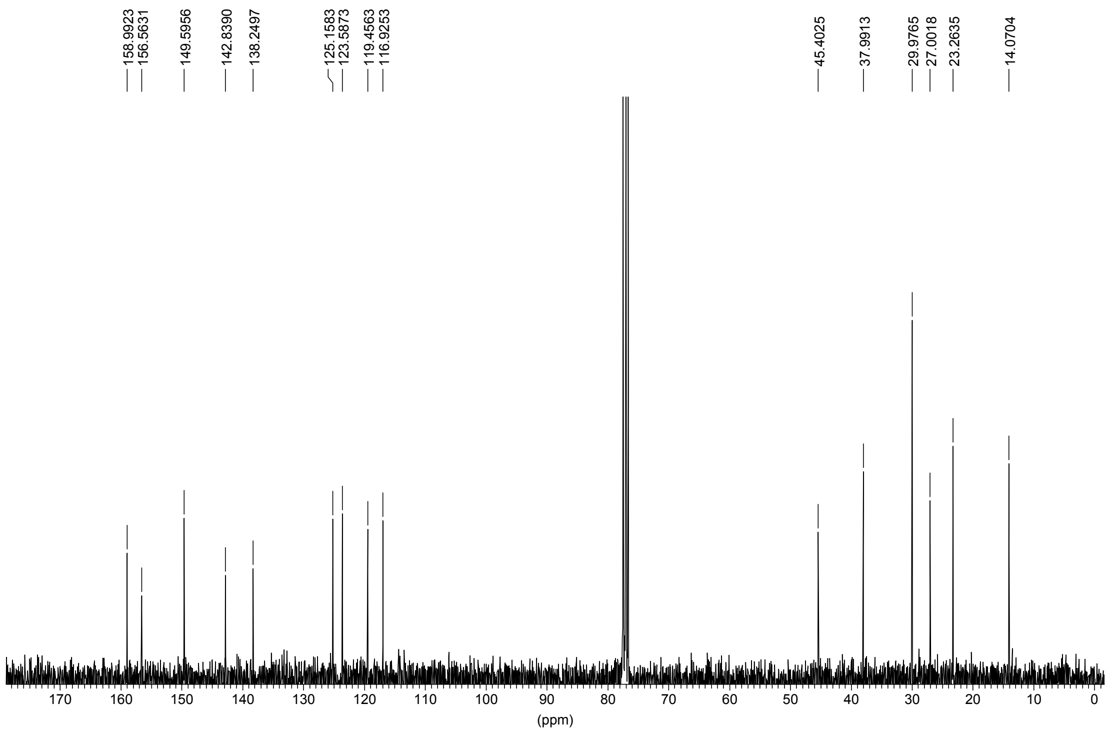


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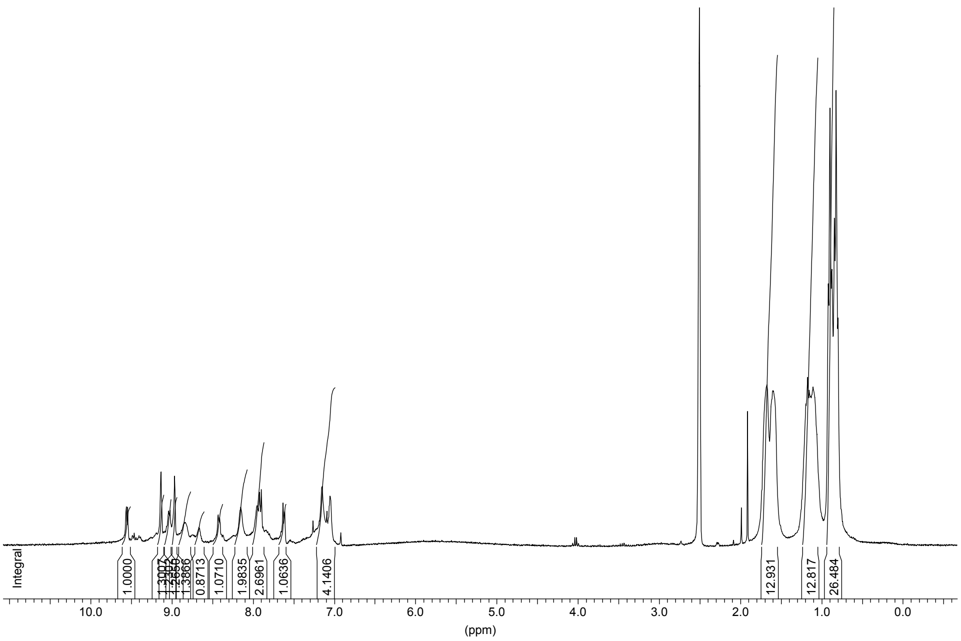
Figure S5: ^{1}H-NMR and UV-vis spectra of TT204



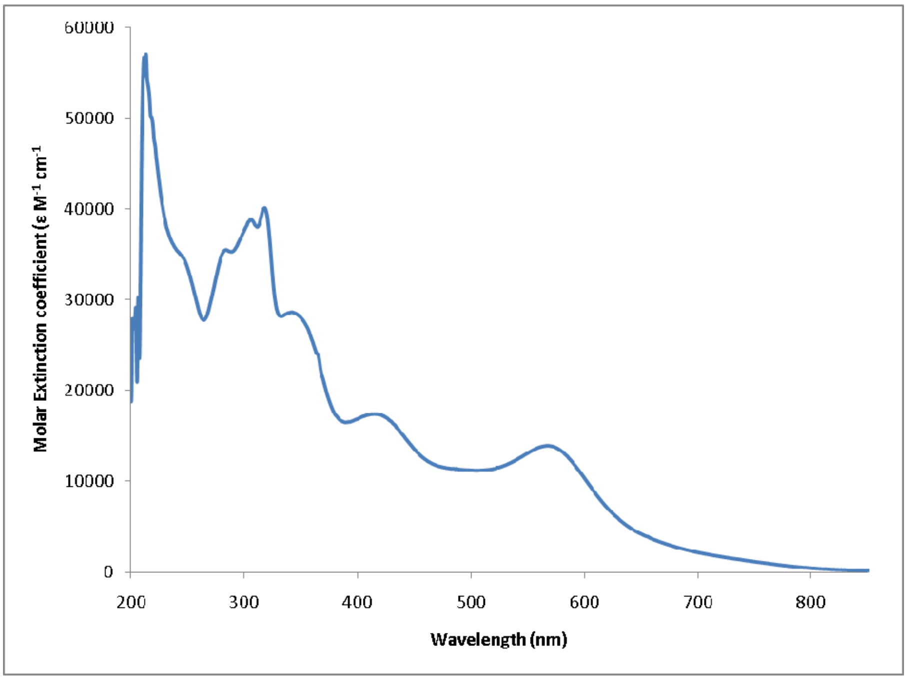


Figure S6: FT-IR and MALDI-TOF spectra of TT204.

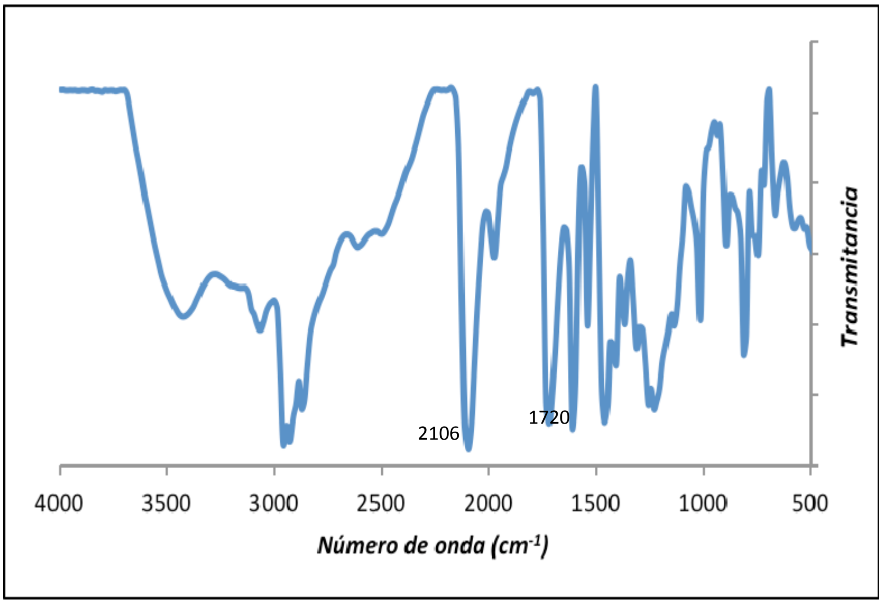


Figure S7: FiMALDI-TOF spectra of TT204

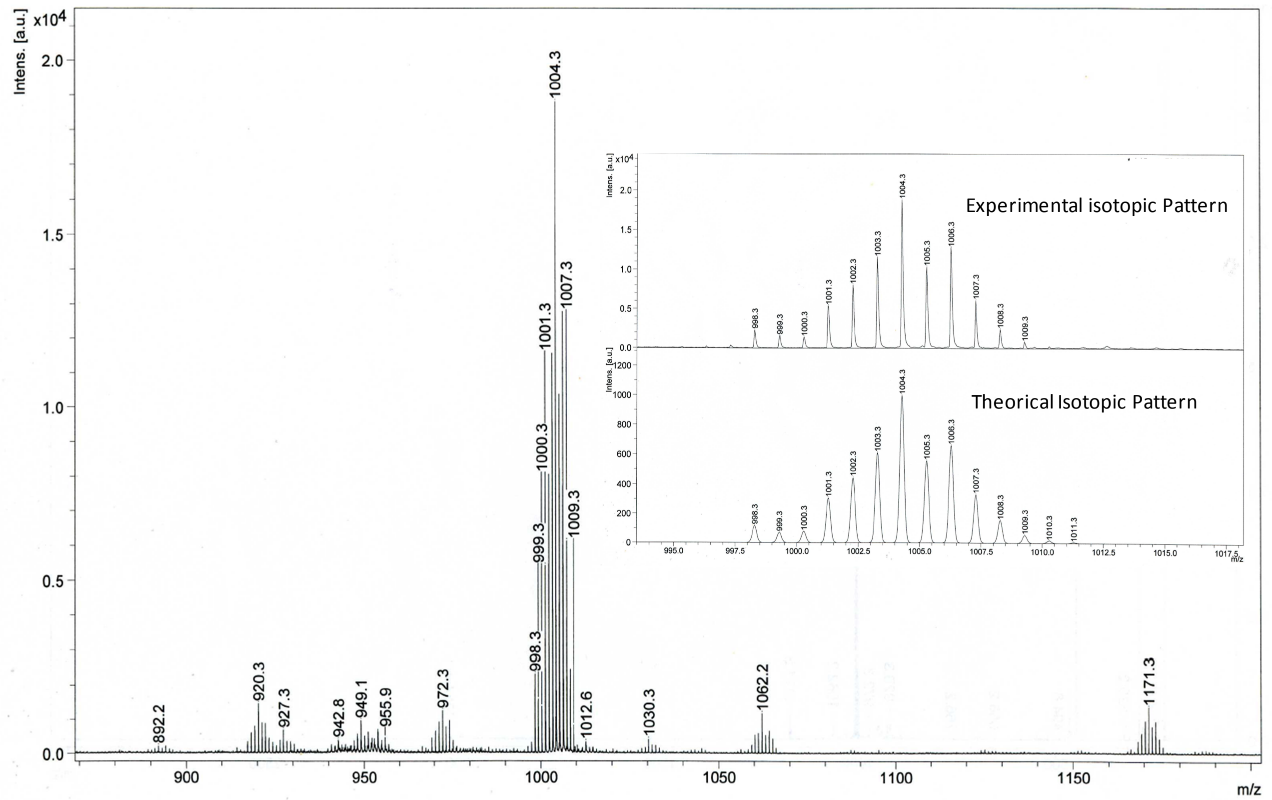
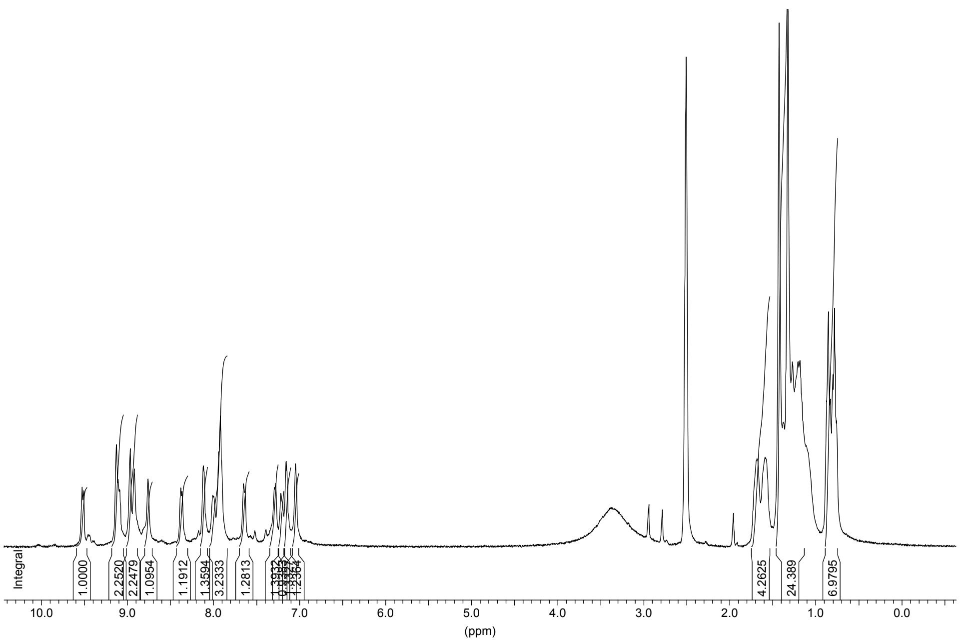


Figure S8: ^{1}H-NMR and UV-vis spectra of TT205



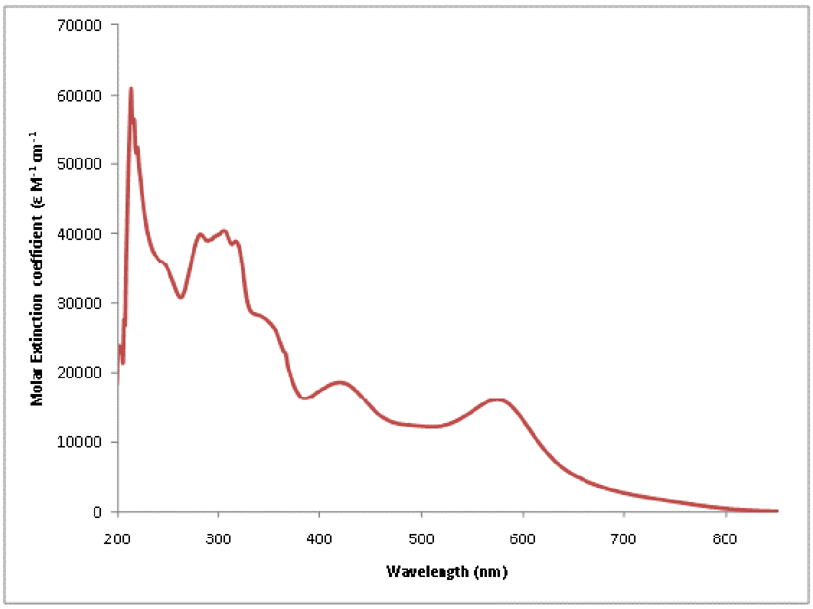


Figure S8: ^{13}C-NMR spectrum of TT205

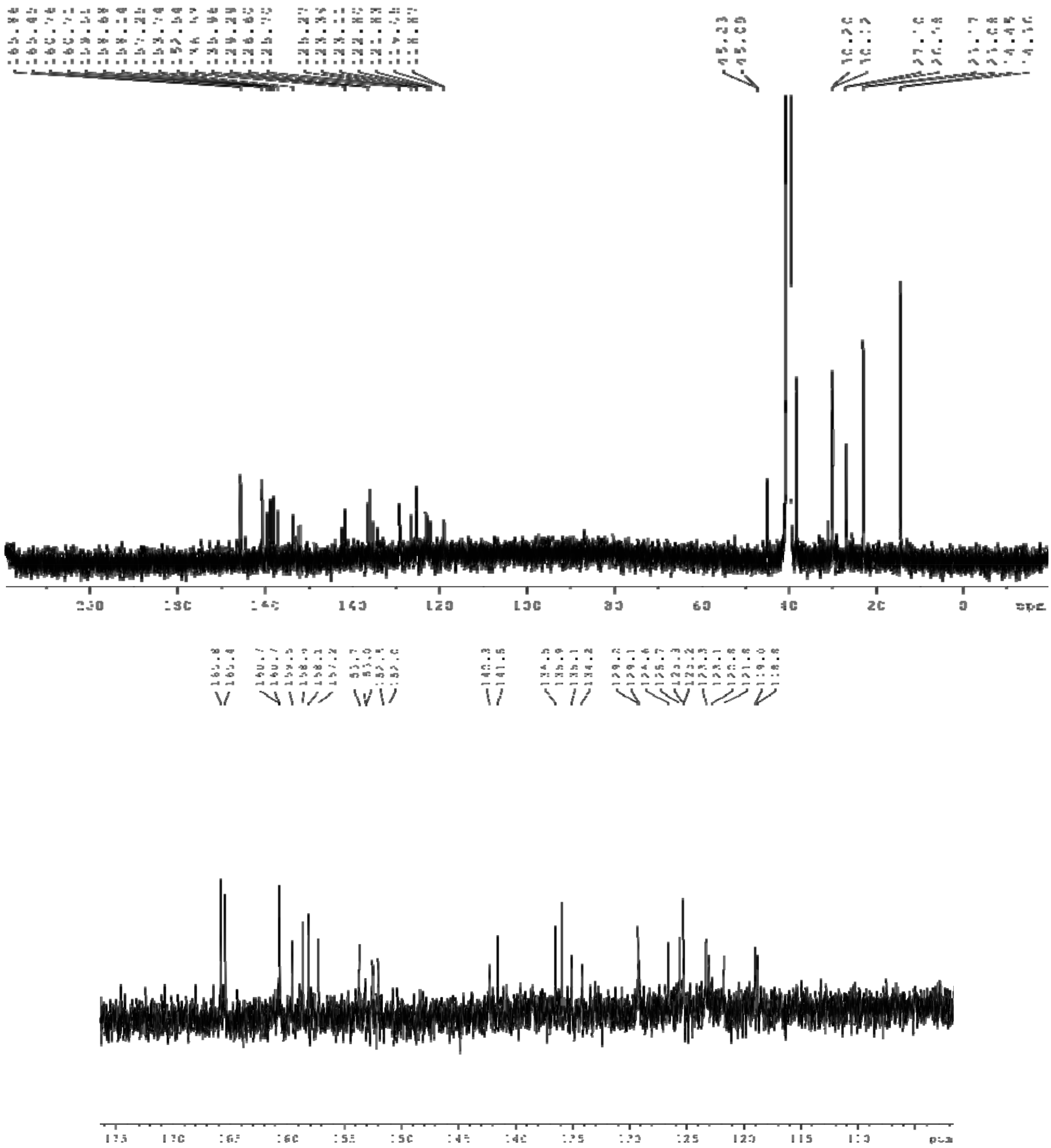
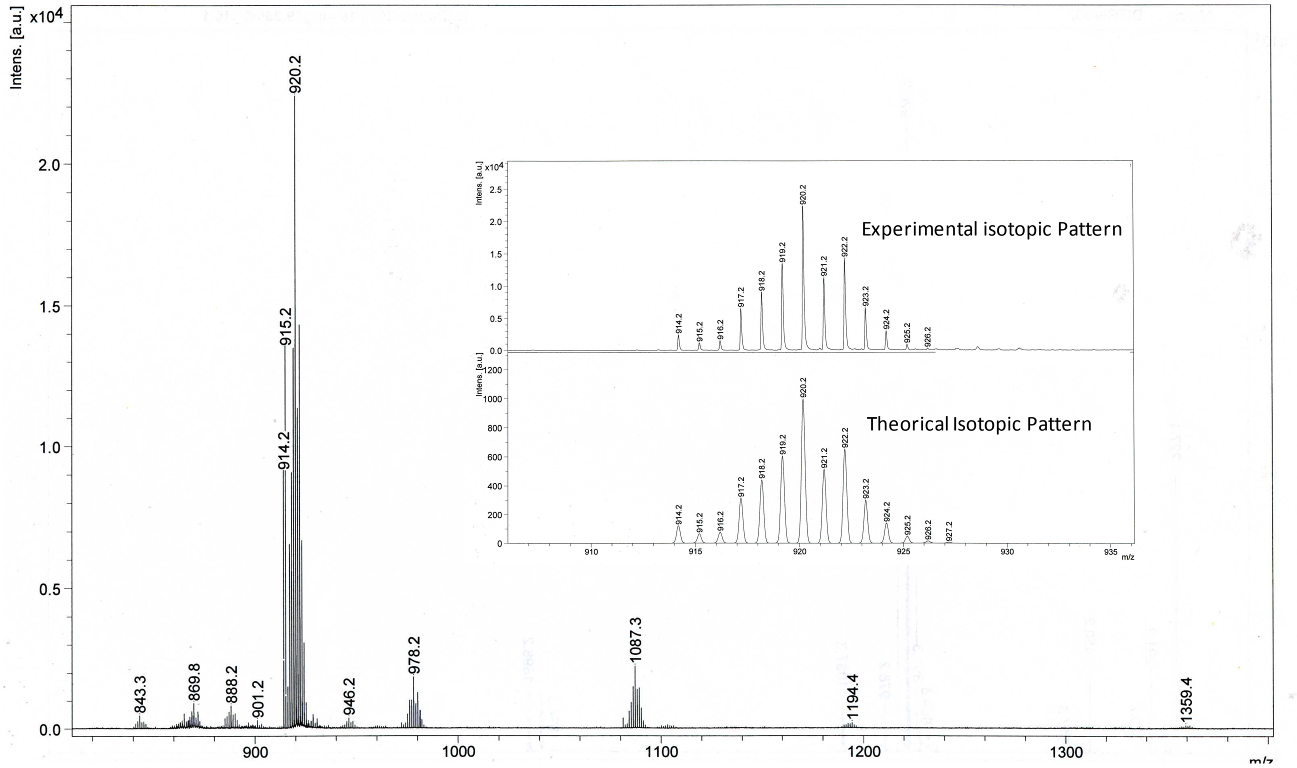
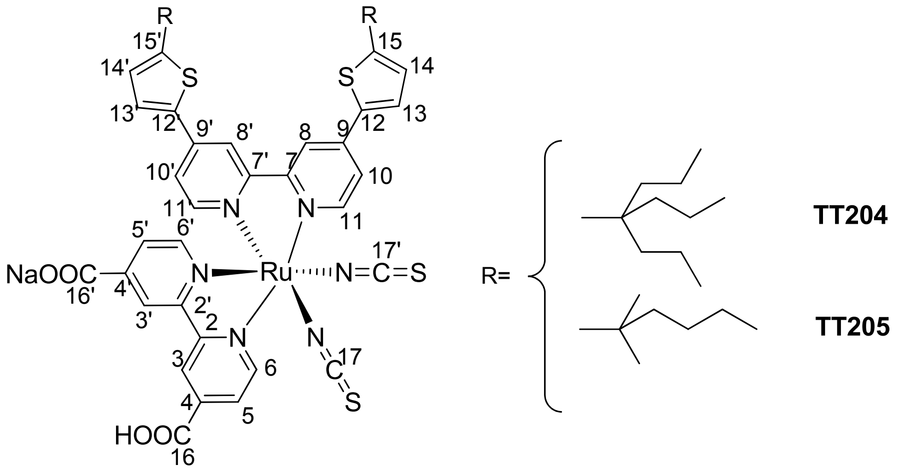


Figure S9: MALDI-TOF spectra of TT205


Intens. [a.u.]
x10^4
920.2
915.2
914.2
843.3
869.8
888.2
901.2
946.2
978.2
1087.3
1194.4
1359.4
m/z
Experimental isotopic Pattern
Theorical Isotopic Pattern



Ru complex **TT204**. ^{1}H-RMN (300 MHz, $CDCl_3$), δ (ppm): 9.58 (d, *J* = 5.7 Hz, 1H, H-6), 9.18 (s (br), 1H, H-3), 9.07 (d, *J* = 5.7 Hz, 1H, H-6’), 9.0 (s (br), 1H, H-3’), 8.83 (s (br), 1H, H-8), 8.68 (s (br), 1H, H-8’), 8.41 (d, *J* = 5.7 Hz, 1H, H-5), 8.15 (m, 2H, H-5’), 7.63 (d, *J* = 6.1 Hz, 1H, H-10), 7.2-6.9 (m, 4H, H-11’, H-10’, H-14, H-14’), 1.8-1.5 (m, 12H, C-$\underline{CH_2}$-CH_2-CH_3, C’-$\underline{CH_2}$’-CH_2’-CH_3’), 1.3-1.0 (m, 12H, C-CH_2-$\underline{CH_2}$-CH_3, C’-CH_2’-$\underline{CH_2}$’-CH_3’), 1.0-0.8 (m, 27H, CH_3, CH_3’).

Ru complex **TT205**. ^{1}H-RMN (300 MHz, $CDCl_3$), δ (ppm): 9.52 (d, *J* = 5.9 Hz, 1H, H-6), 9.12 (m, 2H, H-6’, H-3), 8.90 (s, 1H, H-3’), 8.78 (s, 1H, H-8), 8.70 (s, 1H, H-8’), 8.39 (d, *J* = 5.7 Hz, 1H, H-5), 8.10 (s, 1H, H-13),8.03 (s, 1H, H-5’) 7.96 (m, 2H, H-13’), 7.68 (s (br), 1H, H-10), 7.30 (d, *J* = 6.2 Hz, 1H, H-11’), 7.19 (s (br), 1H, H-10’), 7.13 (s (br), 1H, H-14), 7.04 (s (br), 1H, H-14’), 1.57 (m, 4H, $C(CH_3)_2$-$\underline{CH_2}$-$(CH_2)_2$-CH_3, $C(CH_3)_2$’-$\underline{CH_2}$’-$(CH_2)_2$’-CH_3’), 1.50 (s, 6H, C($\underline{CH_3}$)$_2$-CH_2-$(CH_2)_2$-CH_3), 1.48 (s, 6H, C’($\underline{CH_3}$)$_2$’-CH_2’-$(CH_2)_2$’-CH_3’), 1.5-1.0 (m, 8H, $C(CH_3)_2$-CH_2-($\underline{CH_2}$)$_2$-CH_3, $C(CH_3)_2$’-CH_2’-($\underline{CH_2}$)$_2$’-CH_3’), 0.74 (t, *J* = 7.1 Hz, 3H, $C(CH_3)_2$-CH_2-$(CH_2)_2$-$\underline{CH_3}$), 0.70 (t, *J* = 7.1 Hz, 3H, $C(CH_3)_2$’-CH_2’-$(CH_2)_2$’-$\underline{CH_3}$’). ^{13}C-RMN (75.5 MHz, $CDCl_3$), δ (ppm): 165.8 (C-17), 165.4 (C-17’), 160.75 (C-2), 160.71 (C-2’), 159.5 (C-7), 158.6 (C-7’), 158.1 (C-11), 157.2 (C-11’), 153.7 (C-6), 153.0,153.08 (C-4, C-4’), 152.5 (C-6’),, 152.0 (C-9, C-9’), 142.3 (C-12), 141.5 (C-12’), 136.5 (C-15), 135.9 (C-15’), 135.1 (C-17), 134.2 (C-17’), 129.2, 129.1 (C13, C13’), 126.6 (C-5), 125.6 (C-10), 125.3 (C-14, C-14’), 122.3 (C-5’), 123.2 (C-3’), 122.8 (C-8), 121.8 (C10’), 119.0 (C-3’), 118.8 (C-8’), 45.2, 45.0 (-$\underline{C}(CH_3)_2$-

CH_2-$(CH_2)_2$-CH_3, C$(CH_3)_2$'-CH_2'-$(CH_2)_2$'-CH_3'), 38.3, 38,2 (C$(CH_3)_2$-CH_2-$(CH_2)_2$-CH_3, C$(CH_3)_2$'-CH_2'-$(CH_2)_2$'-CH_3'), 30.2, 30.0 (C$(CH_3)_2$-CH_2-$(CH_2)_2$-CH_3, C'$(CH_3)_2$'-CH_2'-$(CH_2)_2$'-CH_3'), 27.1, 26.9, 23.1, 23.0 C$(CH_3)_2$-CH_2-$(CH_2)_2$-CH_3, C$(CH_3)_2$'-CH_2'-$(CH_2)_2$'-CH_3'), 14.4, 14.3 (C$(CH_3)_2$-CH_2-$(CH_2)_2$-CH_3, C$(CH_3)_2$'-CH_2'-$(CH_2)_2$'-CH_3').