Supporting Information

Synthesis of NNN Chiral Ruthenium Complexes and their Cytotoxicity Studies.

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1. X-ray Analysis

Justification of alerts observed in the check_cif file of ($^{RR\text{-}MeBu^2}$NNN)$RuCl_2(PPh_3)_3$

Alert level A

RINTA01 ALERT 3 A **The value of Rint is greater than 0.25 Rint given 0.293**

Author response: The data quality is poor due to sensitive and unstable nature of crystal that decreased the crystal quality. Crystals diffracted extremely weakly and disintegrated during the data collection. Multiple attempts were made to grow better diffracting crystals, however, upon mounting, all yielded serious problems due to high instability of crystal. This resulted in weak diffraction and disorder in the solvent atom positions. These factors resulted in high Rint value.

PLAT020 ALERT 3 A **The Value of Rint is greater than 0.12 …… 0.293 Report**

Author response: The data quality is poor due to sensitive and unstable nature of crystal that decreased the crystal quality. Crystals diffracted extremely weakly and disintegrated during the data collection. Multiple attempts were made to grow better diffracting crystals, however, upon mounting, all yielded serious problems due to high instability of crystal. This resulted in weak diffraction and disorder in the solvent atom positions. These factors resulted in high Rint value.

Alert level B

PLAT242 ALERT 2 B **Low 'MainMol' Ueq as Compared to Neighbors of C1B Check**

Author response: ISOR restraints were applied to some of the atoms to avoid atoms becoming flat /Non positive definite's due to poor quality data. Some of these atoms are still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.

PLAT342 ALERT 3 B **Low Bond Precision on C-C Bonds ..... 0.02984 Ang.**

Author response: Extremely poor-quality crystal owing to its unstable nature resulted in observation of streaky diffused Bragg peaks giving poor data, overall poor model and hence low bond precision. However, this does not indicate an incorrect atom type assignment.

.**Table S1:** The crystallographic data of **1c**

Name	(^{R2}NNN)RuCl2(PPh_3) **(1c)**
Empirical formula	$C_{35}H_{42}Cl_2N_3PRu$
Formula weight	707.65
Crystal size (mm^3)	0.32 × 0.24 × 0.22
Crystal system	Monoclinic
Space group	$P2_1$
a (Å)	19.9311 (14)
b (Å)	17.9214 (13)
c (Å)	32.457 (2)
α (deg)	90
β (deg)	102.269 (3)
γ (deg)	90
V ($Å^3$)	11328.6 (14)
Z	12
ρ_{calc} (g cm^{-3})	1.245
μ (M_0 Kα) (mm^{-1})	0.624
F (000)	4392.0
T(K)	296 (2)
Range of indices (h; k; l)	$-23 \le h \le 24$, $-21 \le k \le 21$, $-39 \le l \le 39$
Number of reflections collected	457176
Unique reflection	41737
Completeness to 2θ	1.284 to 51.038
R_{int}	0.2933
Data / restraints / parameters	41737/115/2305
goodness-of-fit	1.008
$R_1[I \ge 2\sigma(I)]$	0.0863
$wR_2[I \ge 2\sigma(I)]$	0.1607
R_1 (all data)	0.1551
wR_2 (all data)	0.1917
Δ_r (max, min) e $Å^{-3}$	0.55/-0.53
Flack parameter	-0.01 (3)

Table S2: Selected bond distances (Å) and angles (°) for the complex **1c**

	(^{R2}NNN)Ru(PPh_3) **(1c)**
Ru–N(pyridine)	1.939 (13)
Ru–N(imine)	2.074 (12)
	2.110 (13)
Ru–Cl	2.431 (5)
	2.466 (5)
Ru–P	2.317 (5)
C=N(imine)	1.30 (2)
	1.29 (2)
(im)N–Ru–N(im)	157.0 (6)
Cl–Ru–Cl	87.9 (2)
P–Ru–Cl (*trans* to PPh_3)	178.65 (19)
P–Ru–Cl (*cis* to PPh_3)	93.45(19)

2. NMR and ESI-MS Spectra

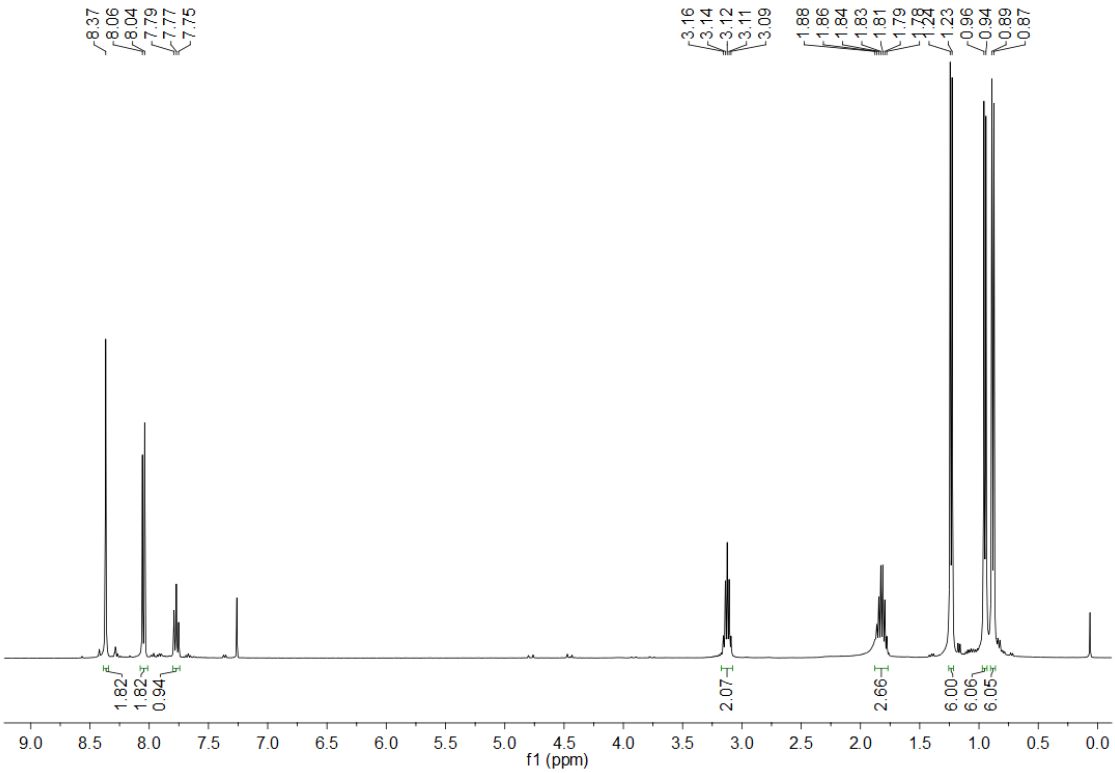

Figure S1: ^{1}H NMR Spectra of **4** in $CDCl_3$

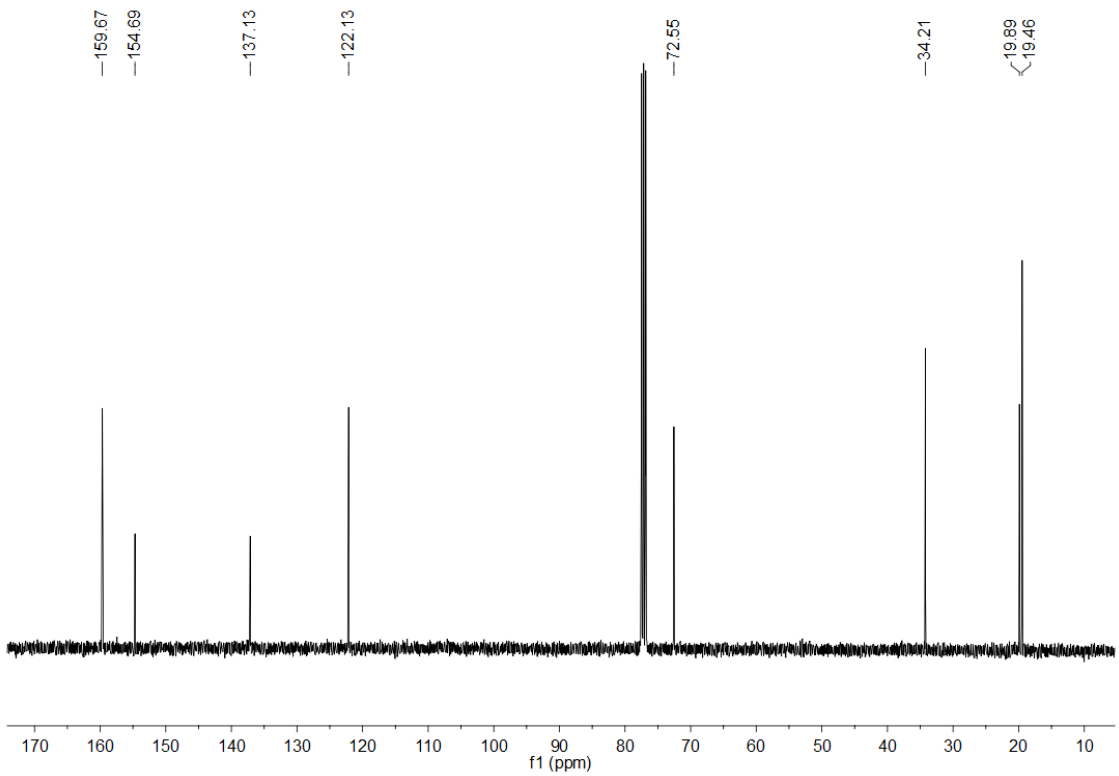

Figure S2: $^{13}C\{^{1}H\}$ NMR Spectra of **4** in $CDCl_3$

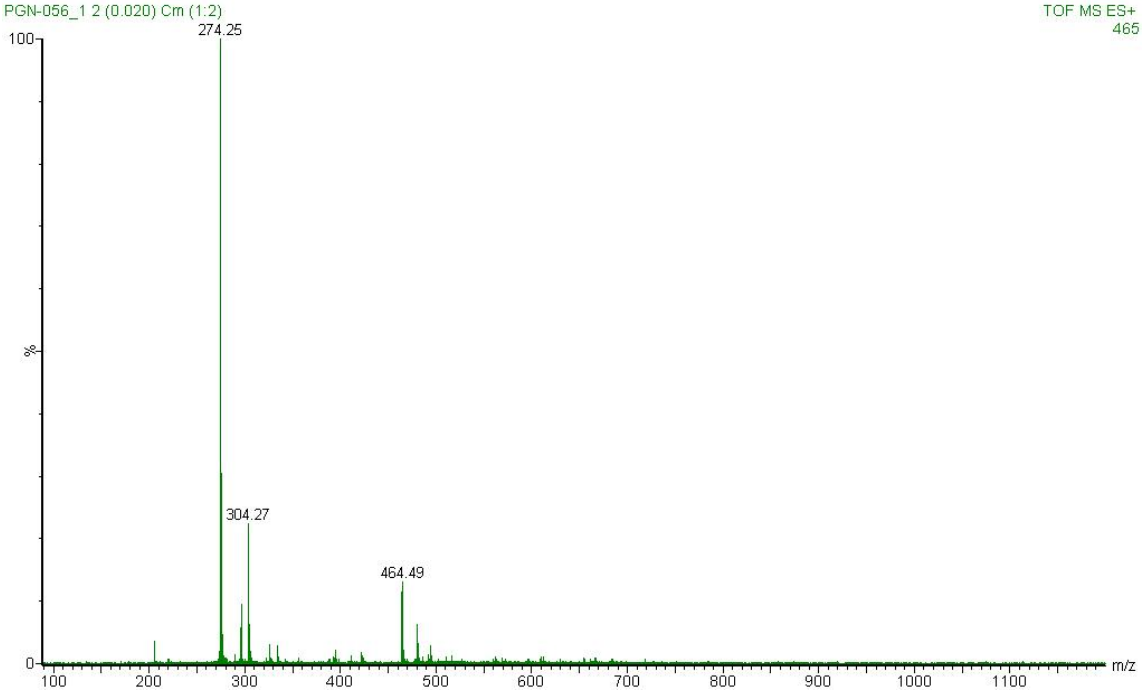

Figure S3: ESI-MS Spectra of **4** in CH_3OH

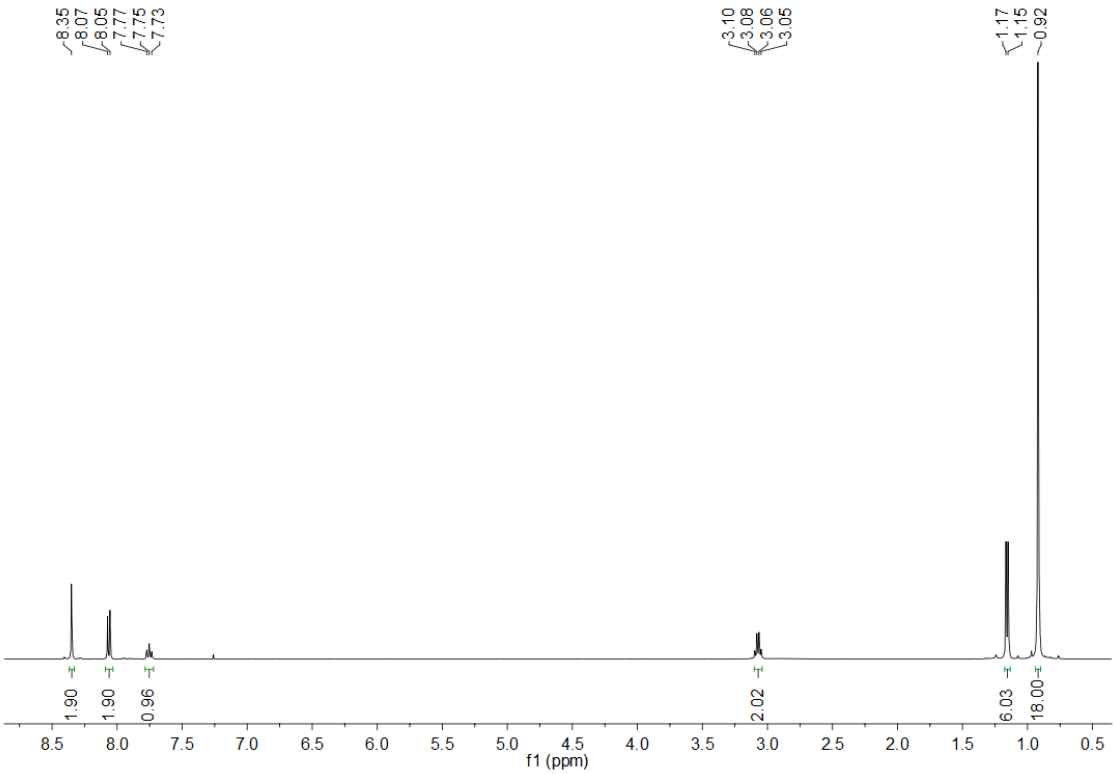

Figure S4: ^{1}H NMR Spectra of **6** in $CDCl_3$

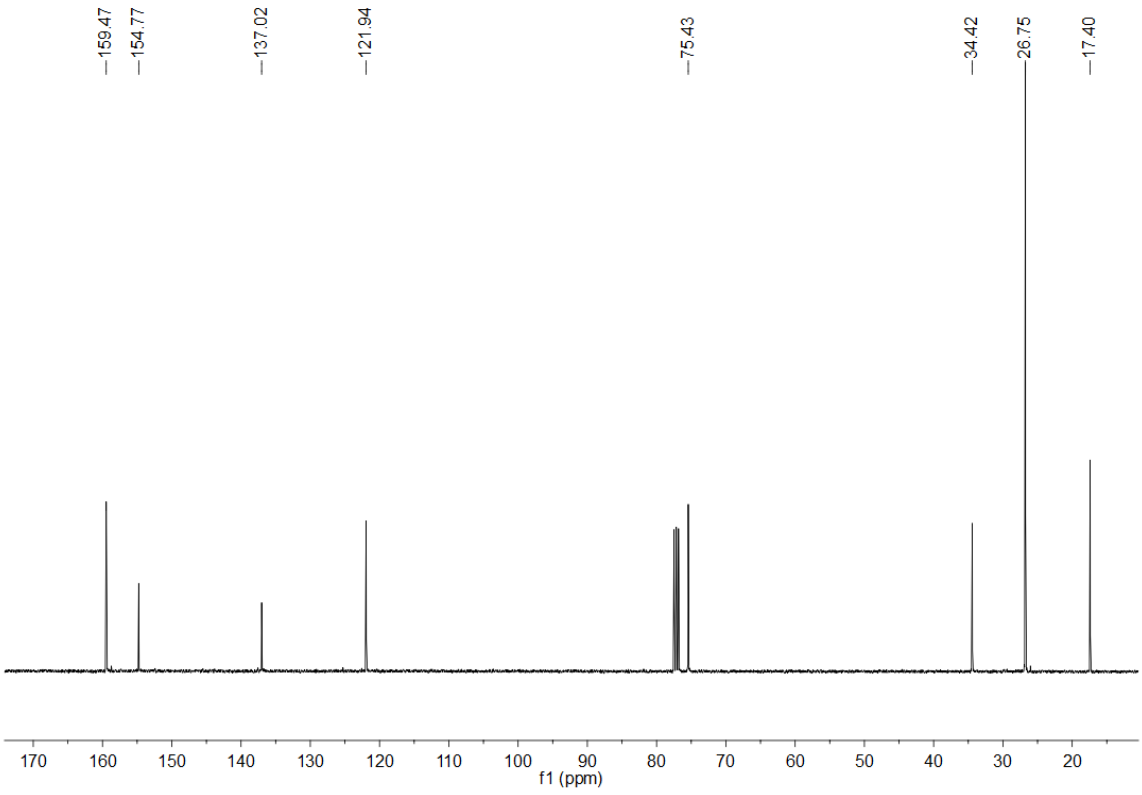

Figure S5: $^{13}C\{^{1}H\}$ NMR Spectra of **6** in $CDCl_3$

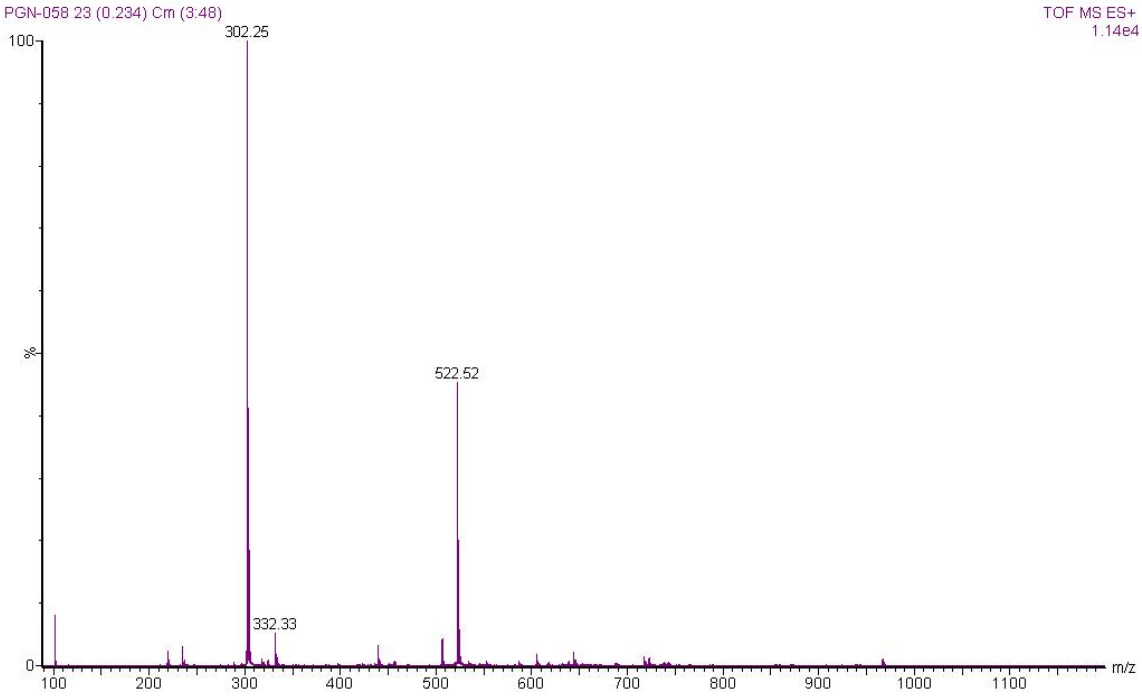

Figure S6: ESI-MS Spectra of **6** in CH_3OH

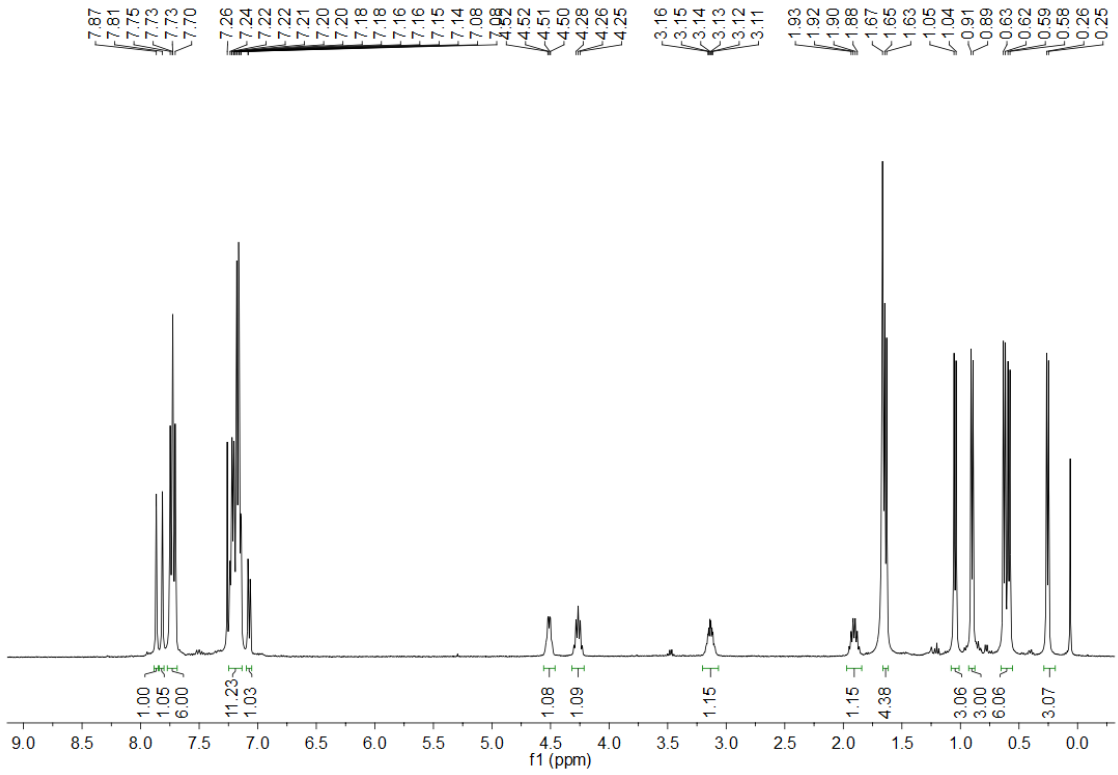

Figure S7: ^1H NMR Spectra of **1c** in $CDCl_3$

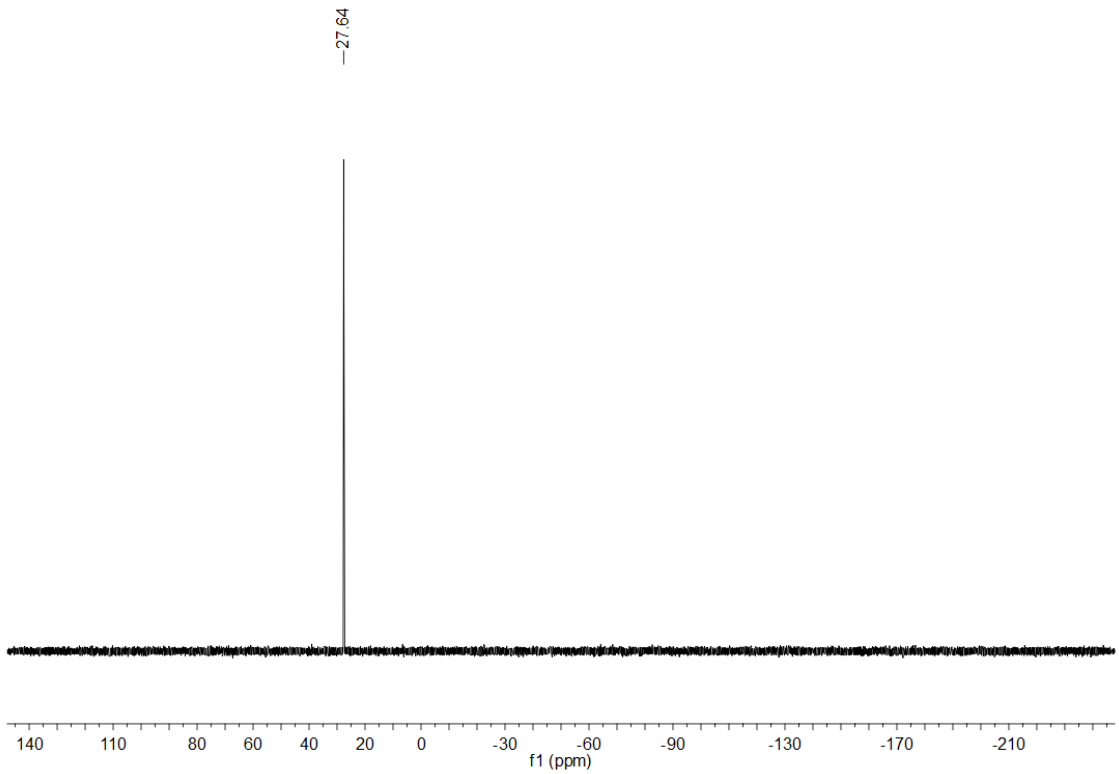

Figure S8: $^{31}P\{^{1}H\}$ NMR Spectra of **1c** in $CDCl_3$

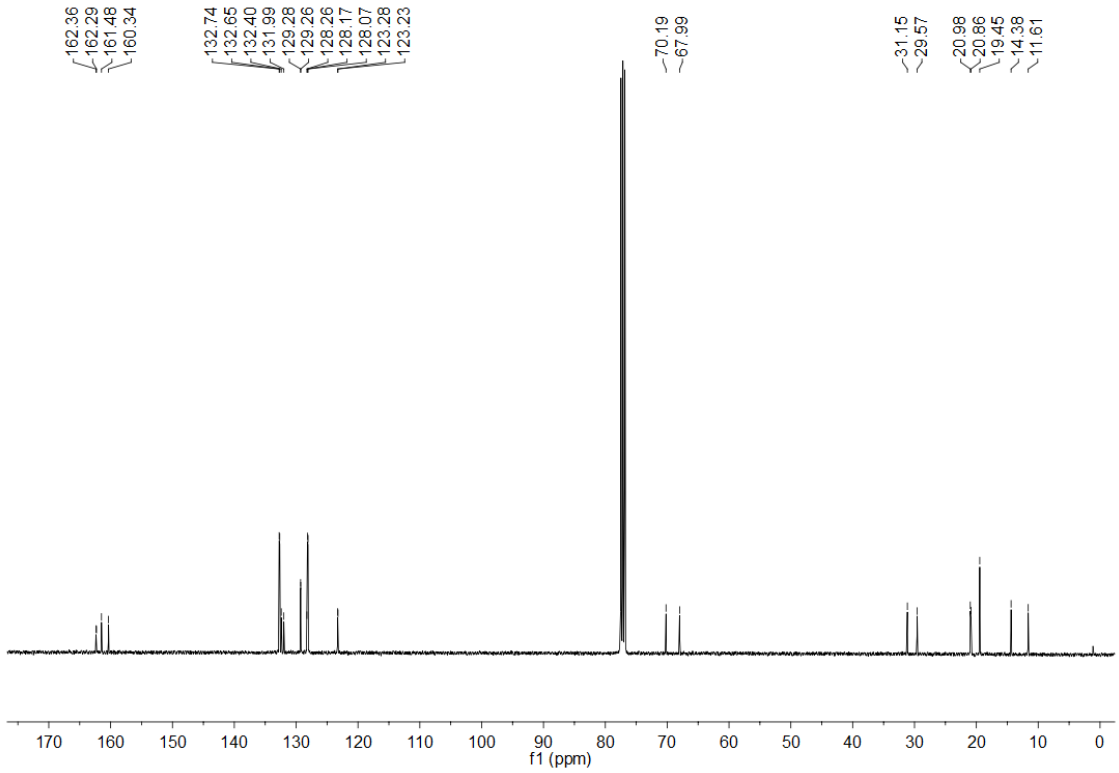

Figure S9: $^{13}C\{^{1}H\}$ NMR Spectra of **1c** in $CDCl_3$

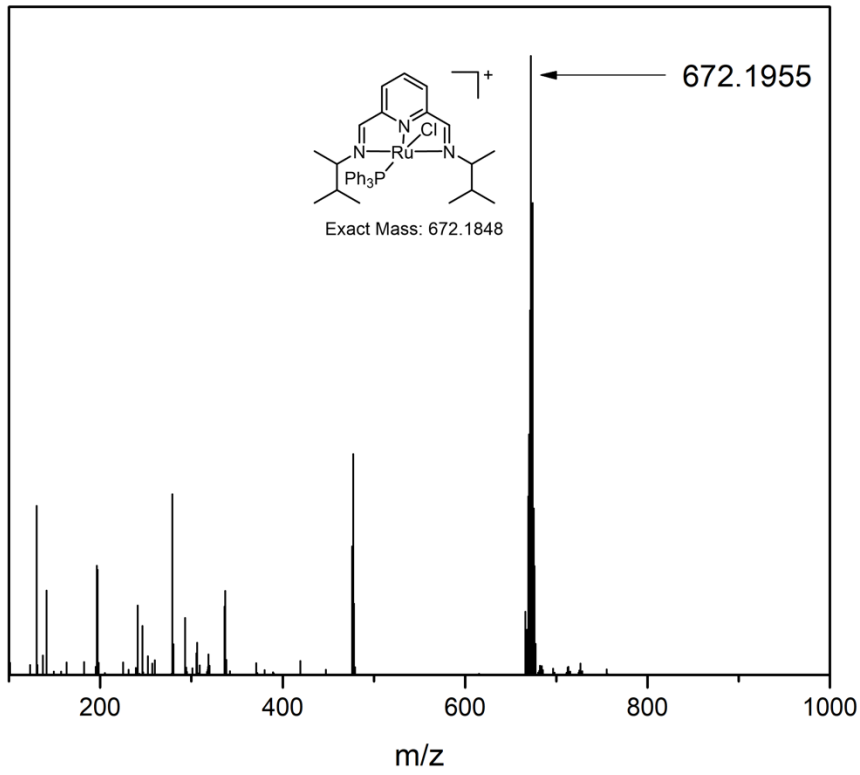

Figure S10: ESI-MS Spectra of **1c** in CH_3OH

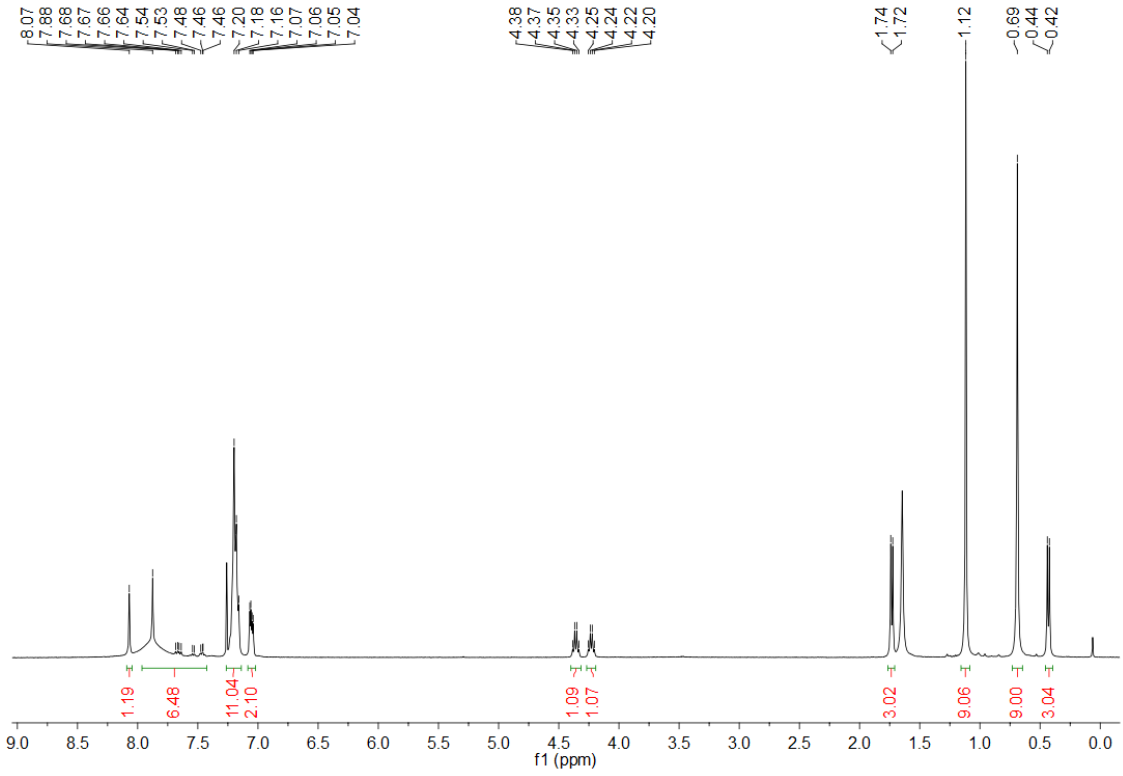

Figure S11: ^1H NMR Spectra of **1d** in $CDCl_3$

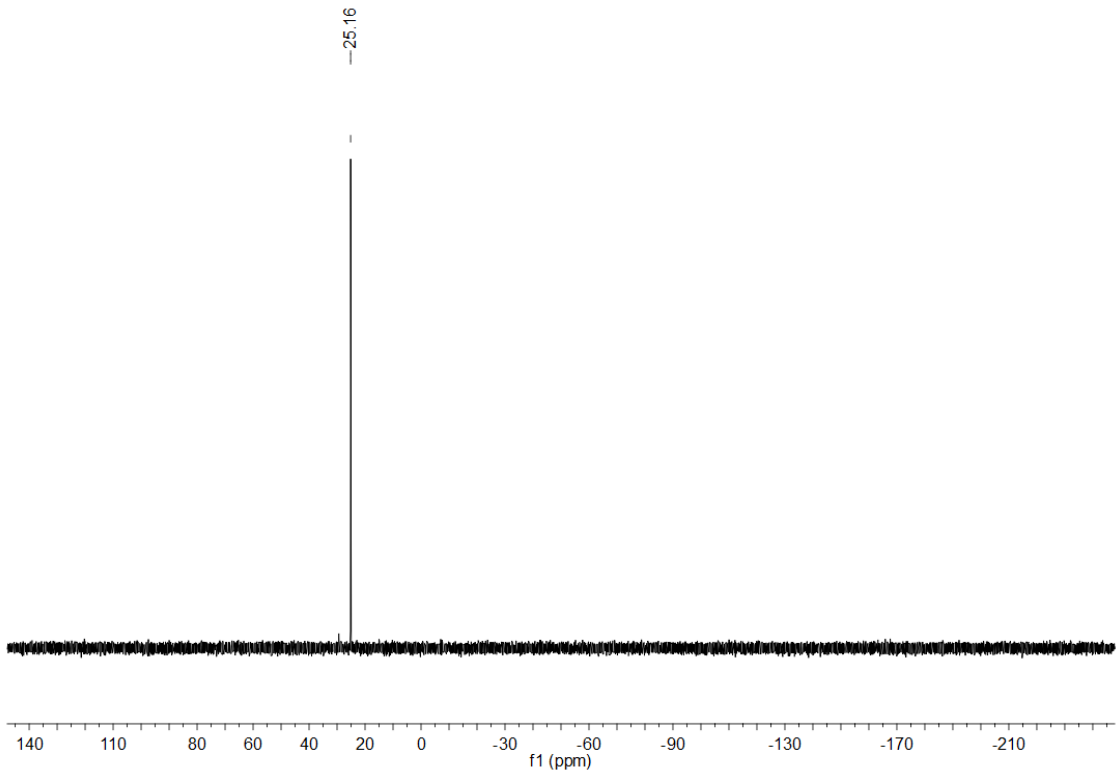

Figure S12: $^{31}P\{^{1}H\}$ NMR Spectra of **1d** in $CDCl_3$

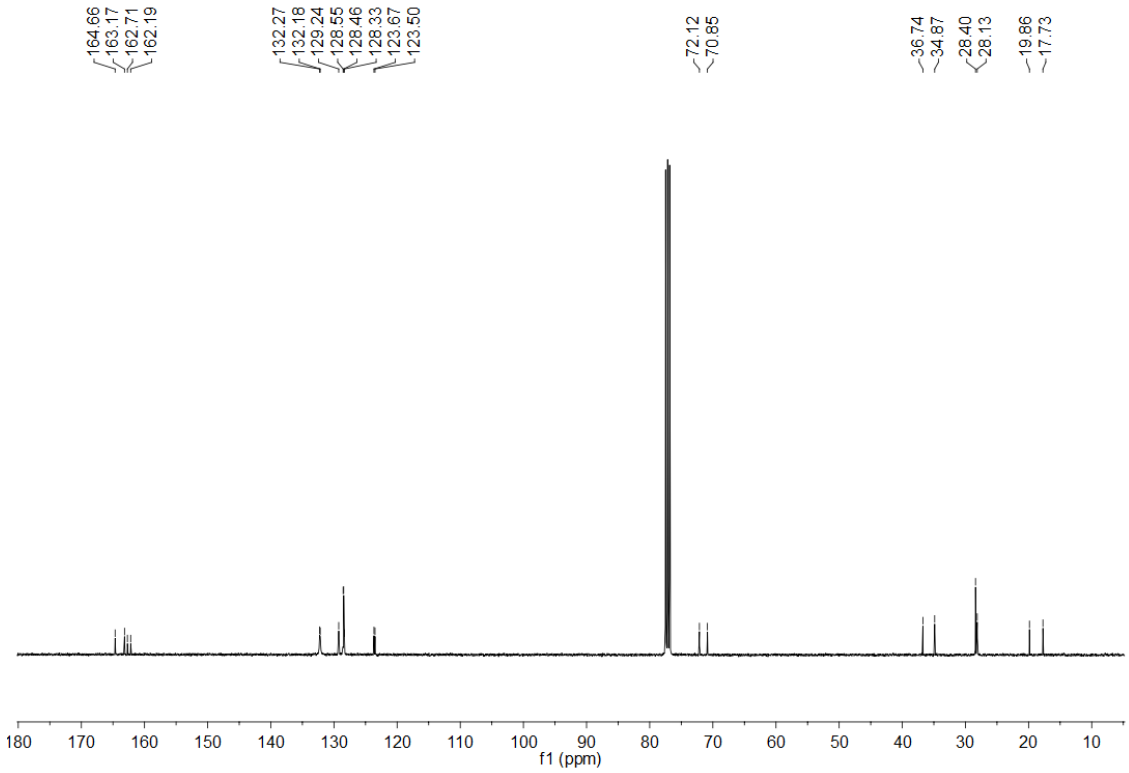

Figure S13: $^{13}C\{^{1}H\}$ NMR Spectra of **1d** in $CDCl_3$

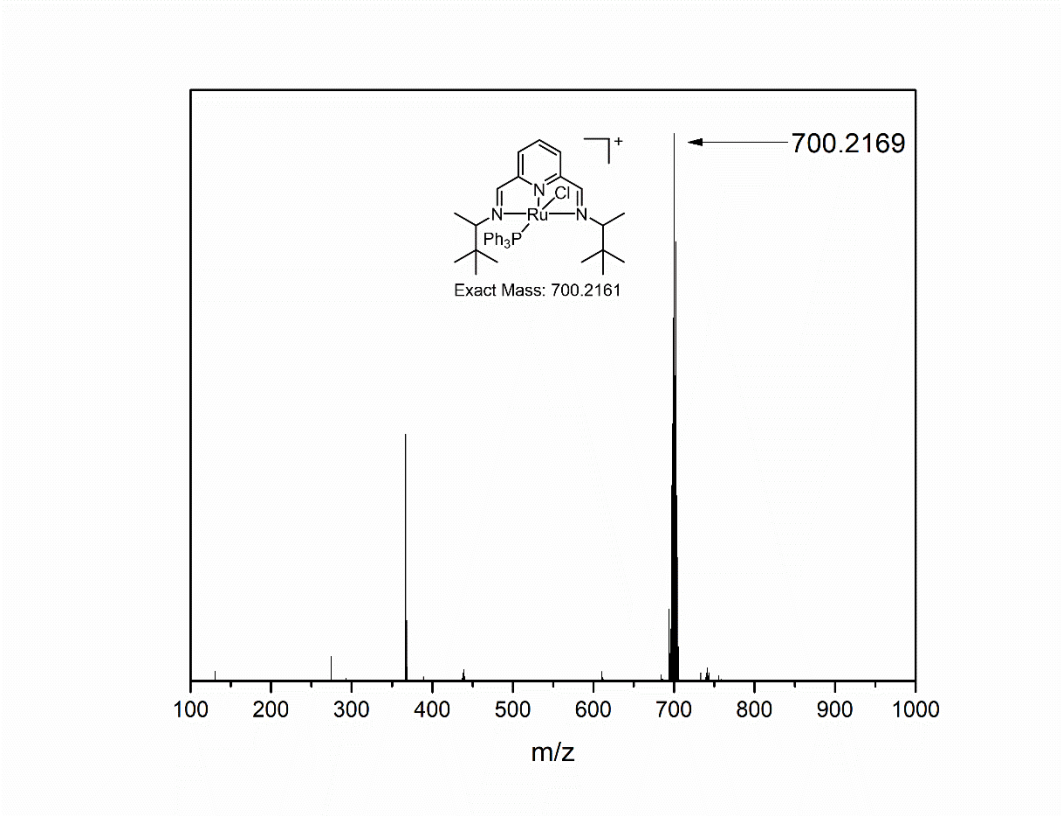

Figure S14: ESI-MS Spectra of **1d** in CH_3OH

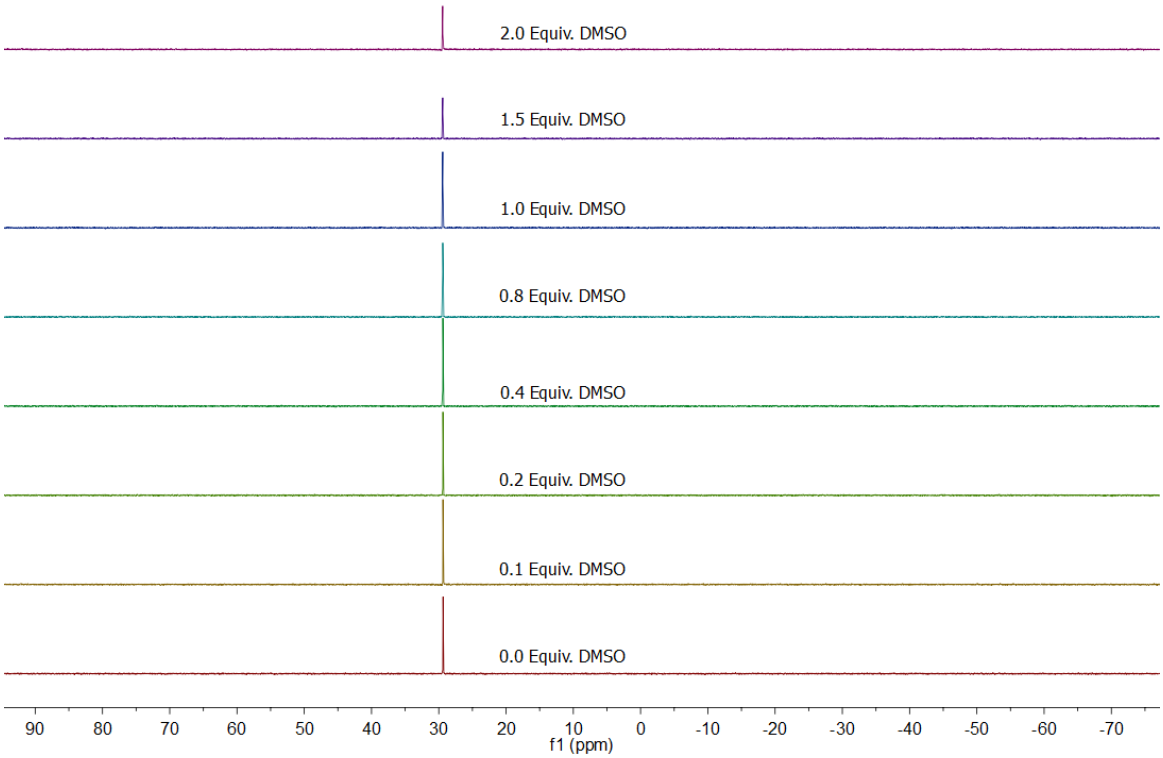

Figure S15: $^{31}P\{^{1}H\}$ NMR stacked plot of **1a** in $CDCl_3$ with adding various amount of DMSO

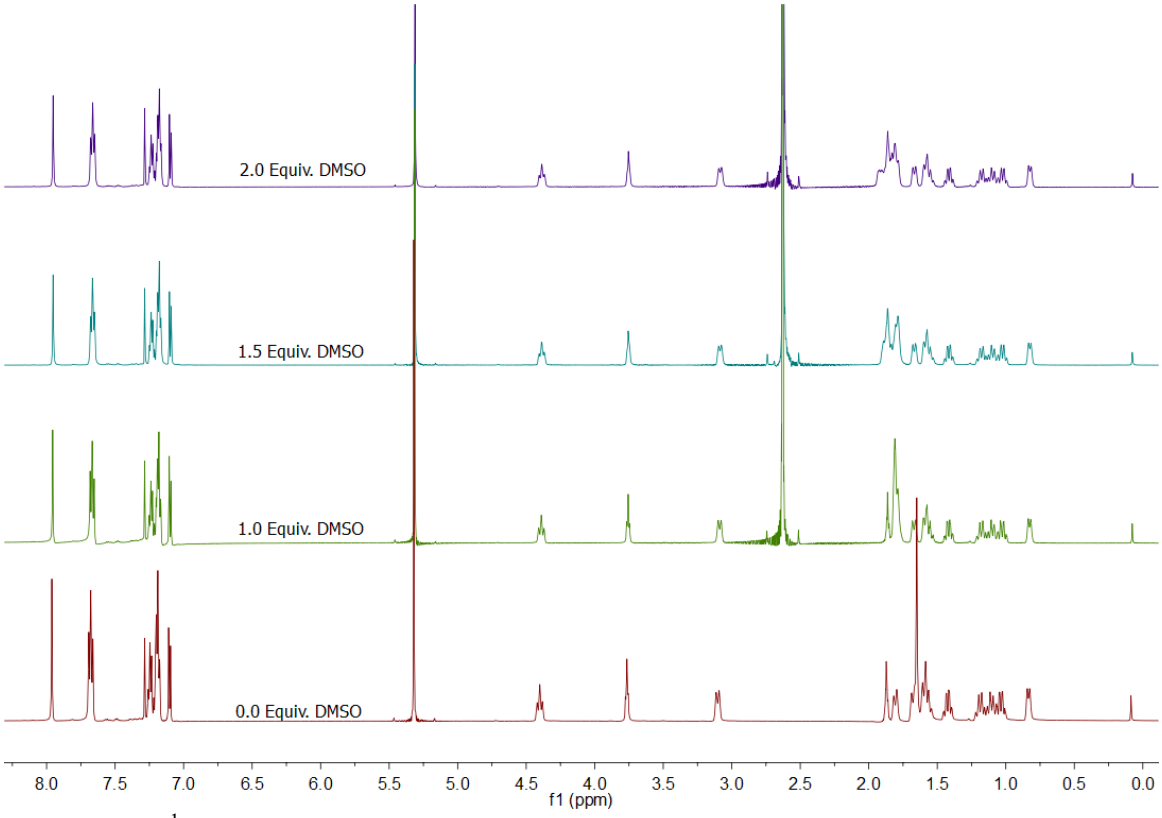

Figure S16: ^{1}H NMR stacked plot of **1a** in $CDCl_3$ with adding various amount of DMSO

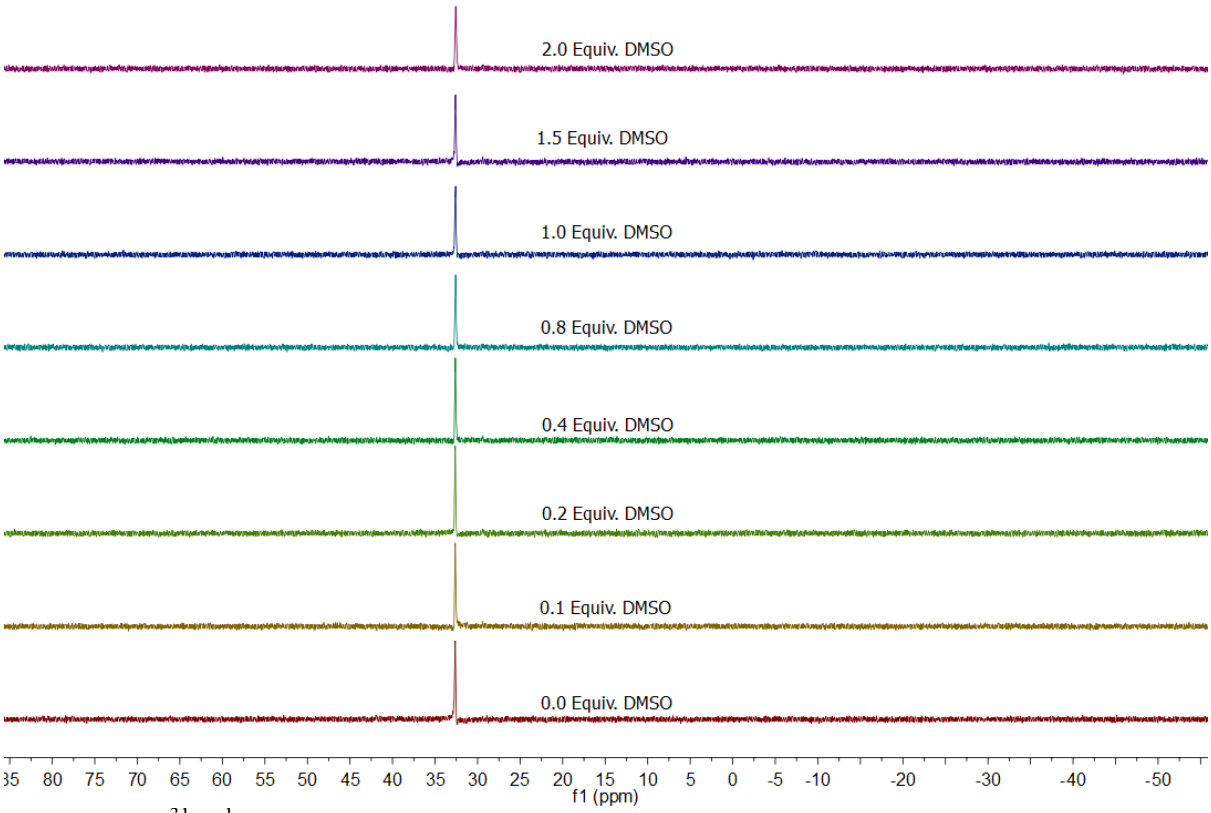

Figure S17: $^{31}P\{^{1}H\}$ NMR stacked plot of **1b** in $CDCl_3$ with adding various amount of DMSO

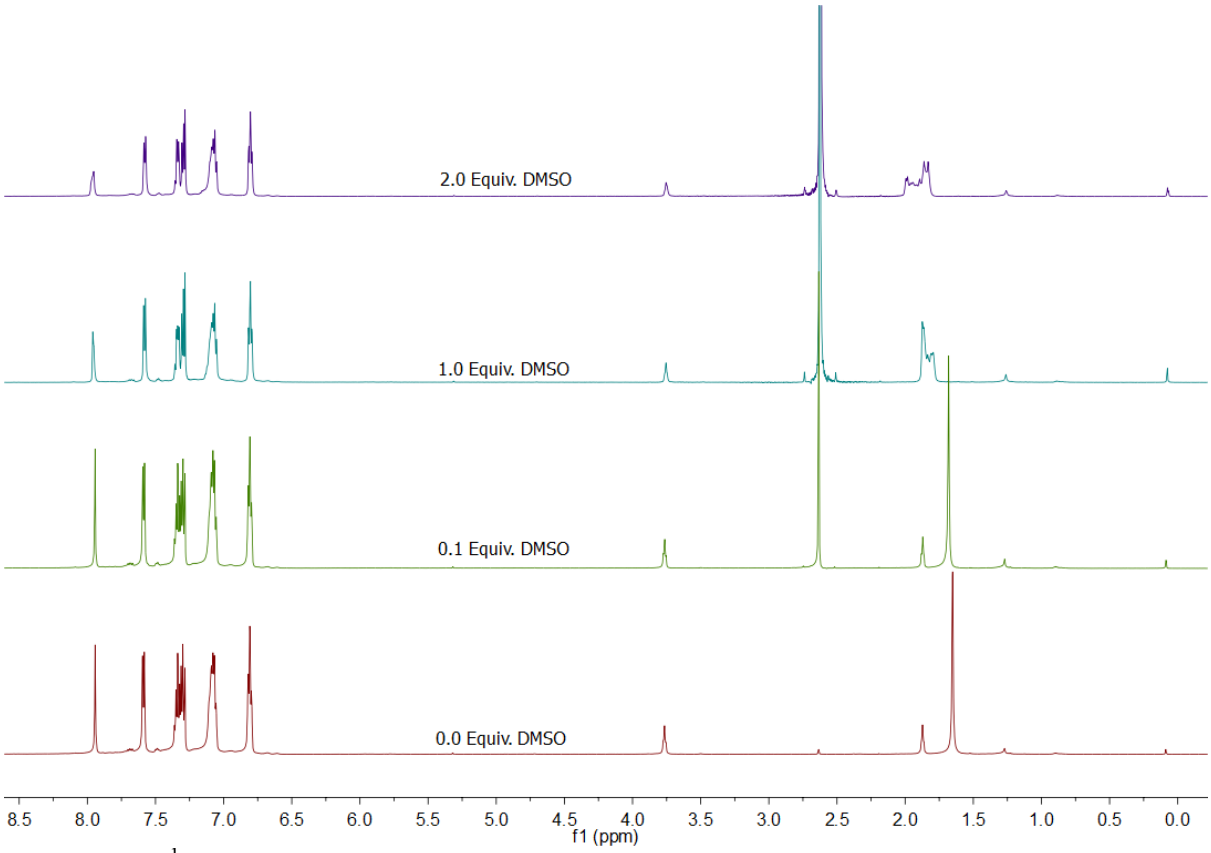

Figure S18: ^{1}H NMR stacked plot of **1b** in $CDCl_3$ with adding various amount of DMSO

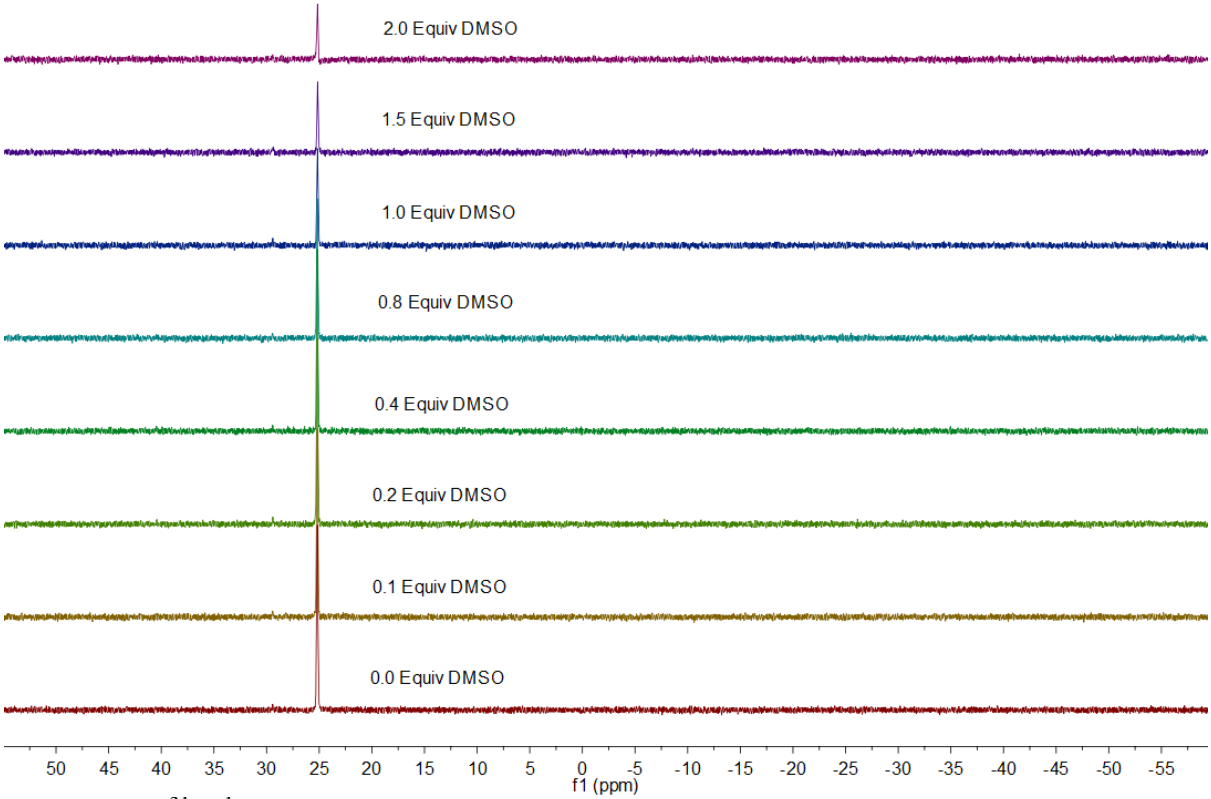

Figure S19: $^{31}P\{^{1}H\}$ NMR stacked plot of **1d** in $CDCl_3$ with adding various amount of DMSO

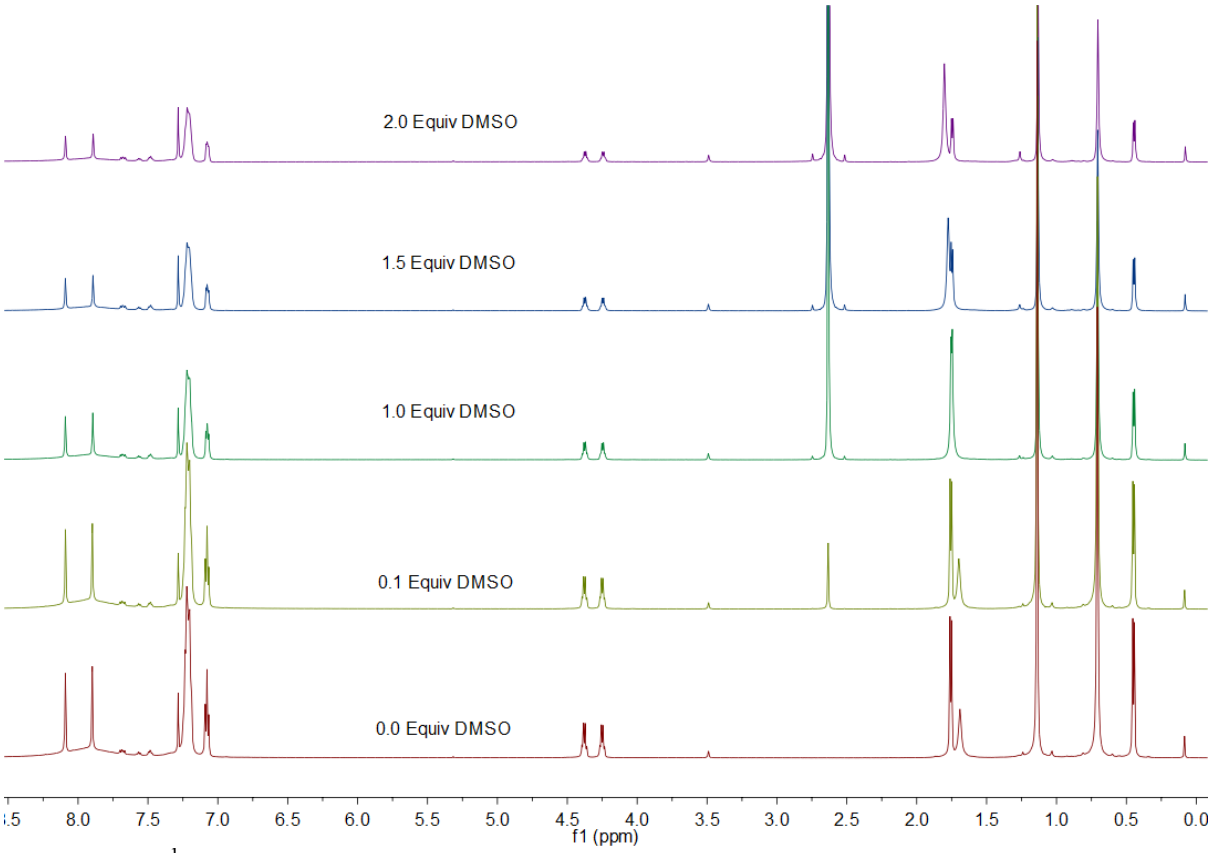

Figure S20: ^{1}H NMR stacked plot of **1d** in $CDCl_3$ with adding various amount of DMSO

3. UV-Visible spectra

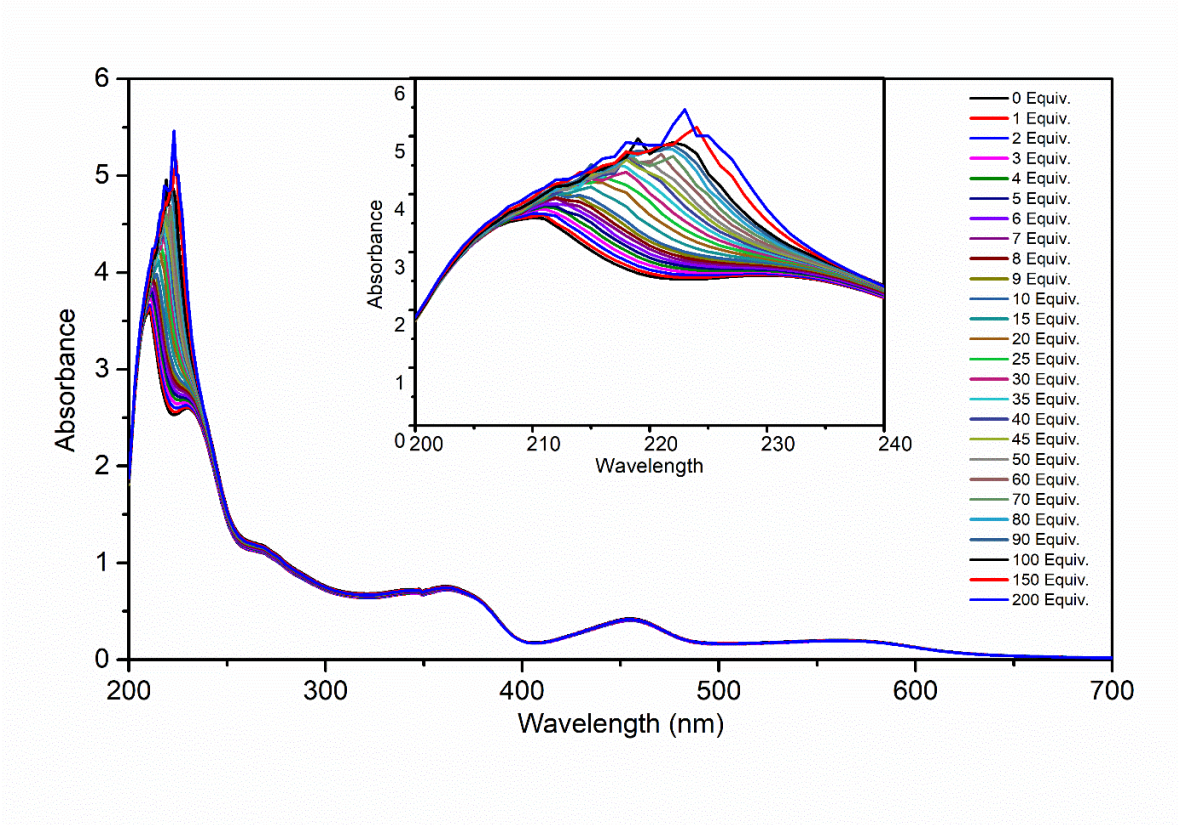

Figure S21: UV-Vis spectrum of **1a** in methanol with gradient addition of DMSO

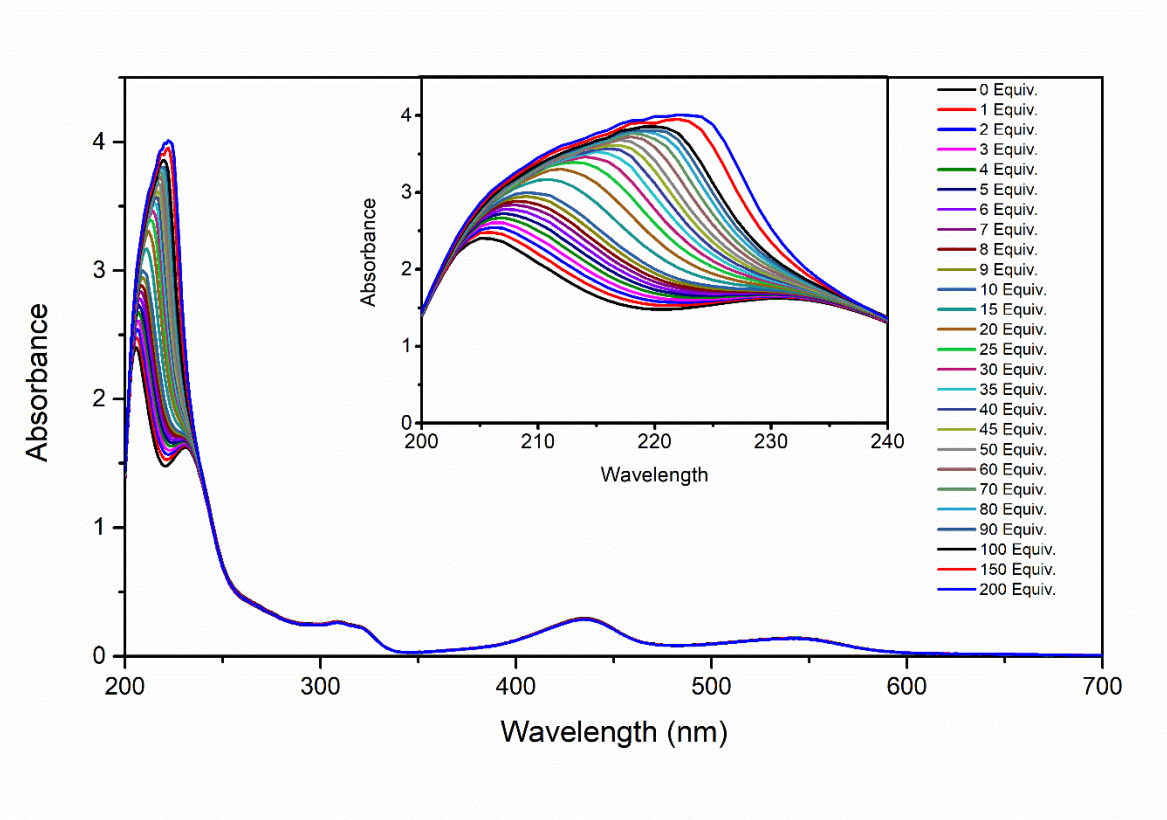

Figure S22: UV-Vis spectrum of **1b** in methanol with gradient addition of DMSO

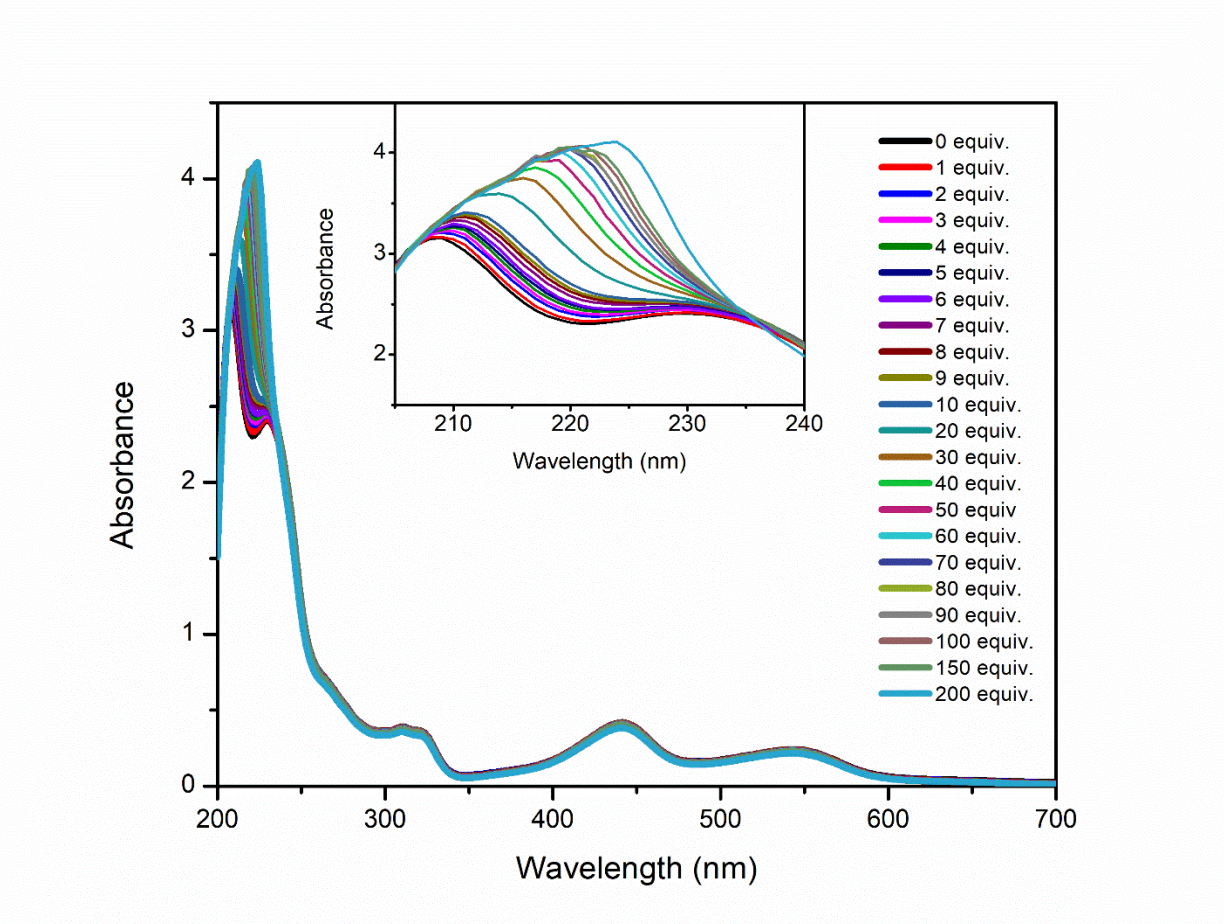

Figure S23: UV-Vis spectrum of **1d** in methanol with gradient addition of DMSO

4. Cyclic voltammetry

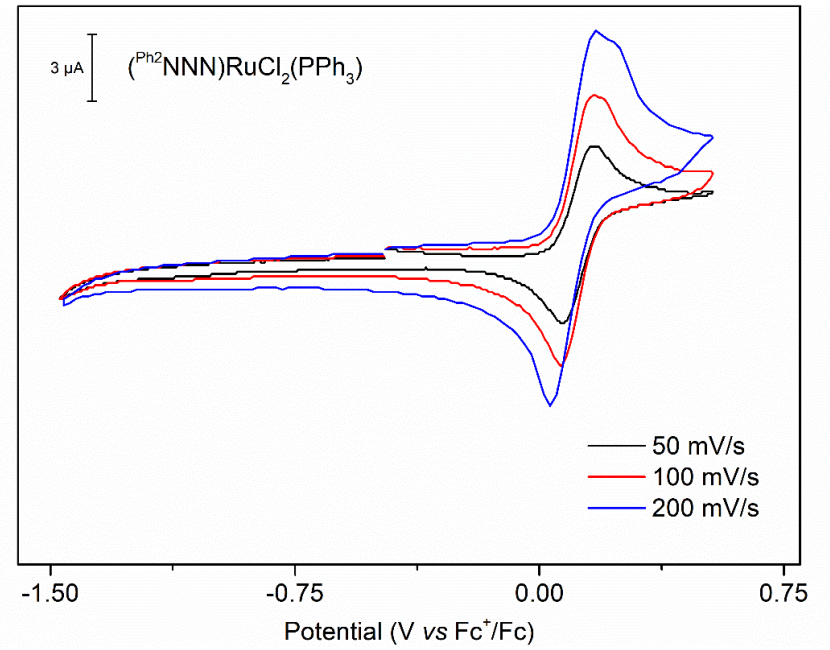

Figure S24: Cyclic voltammogram of **1a** in dichloromethane at different scan rates.

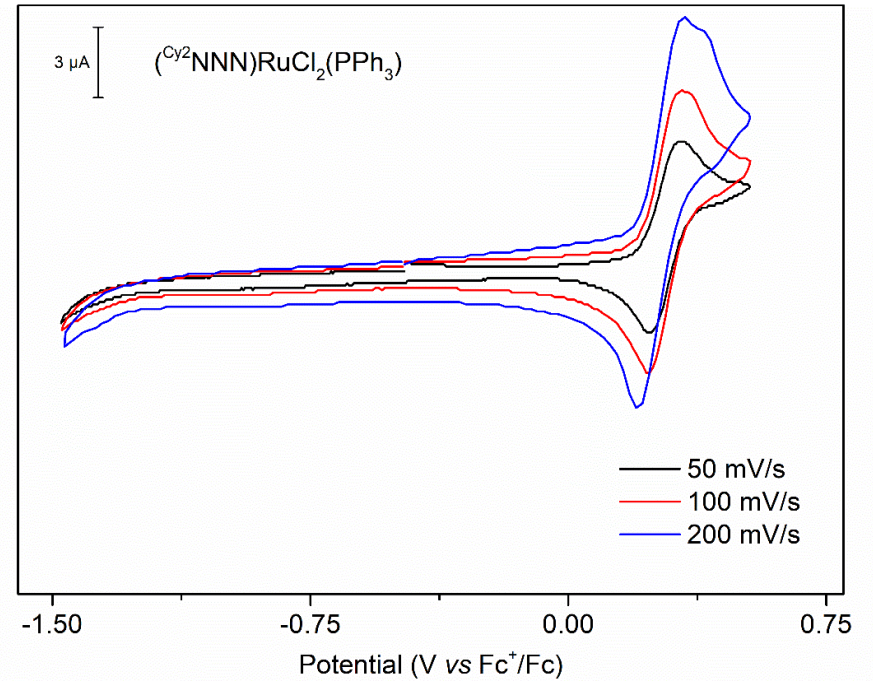

Figure S25: Cyclic voltammogram of **1b** in dichloromethane at different scan rates.

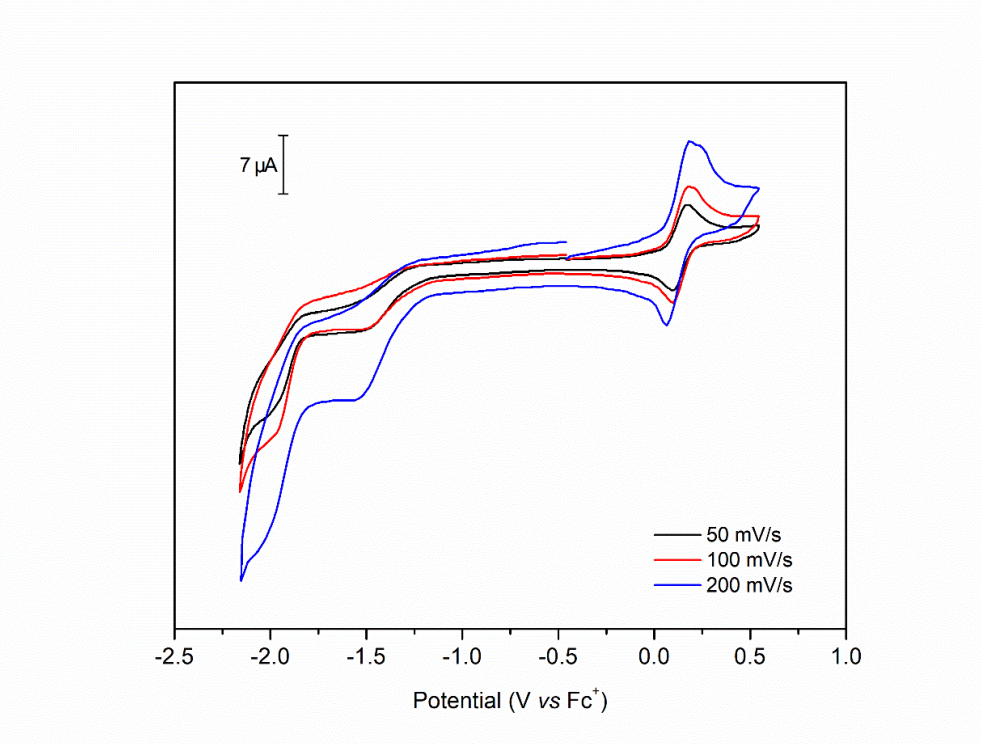

Figure S26: Cyclic voltammogram of **1c** in dichloromethane at different scan rates.

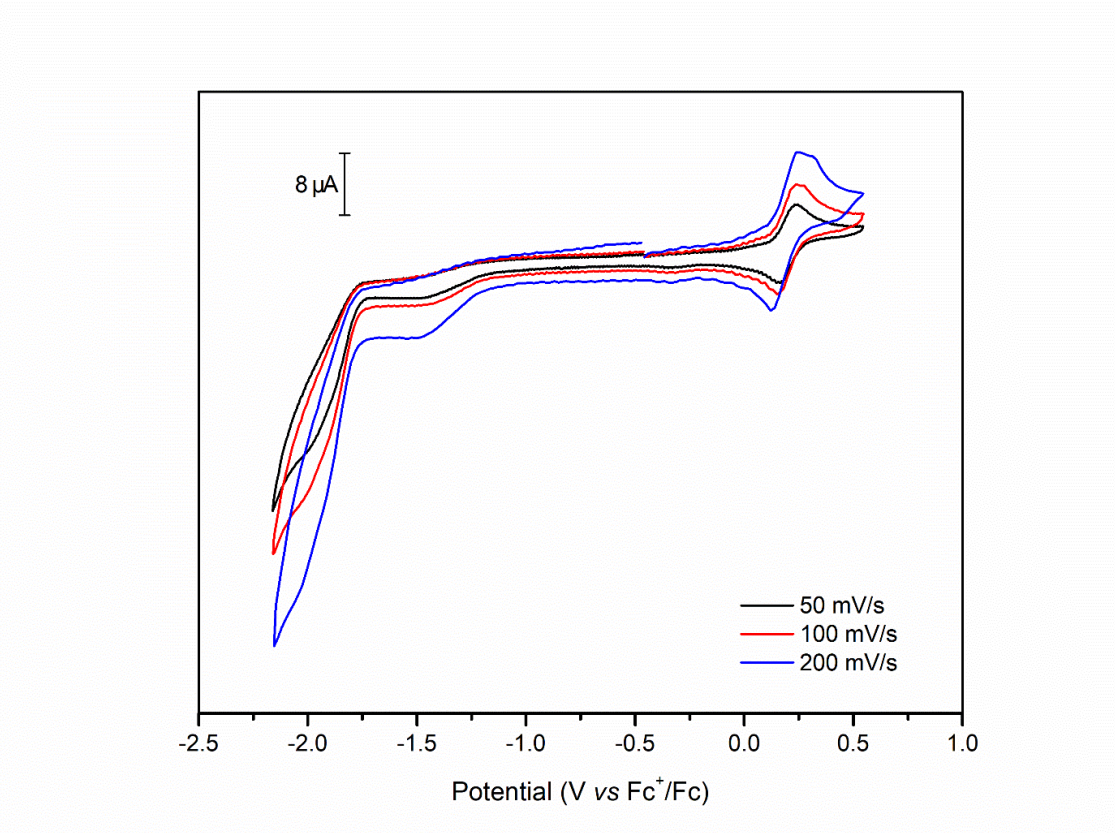

Figure S27: Cyclic voltammogram of **1d** in dichloromethane at different scan rates.

5. Circular dichroism spectra

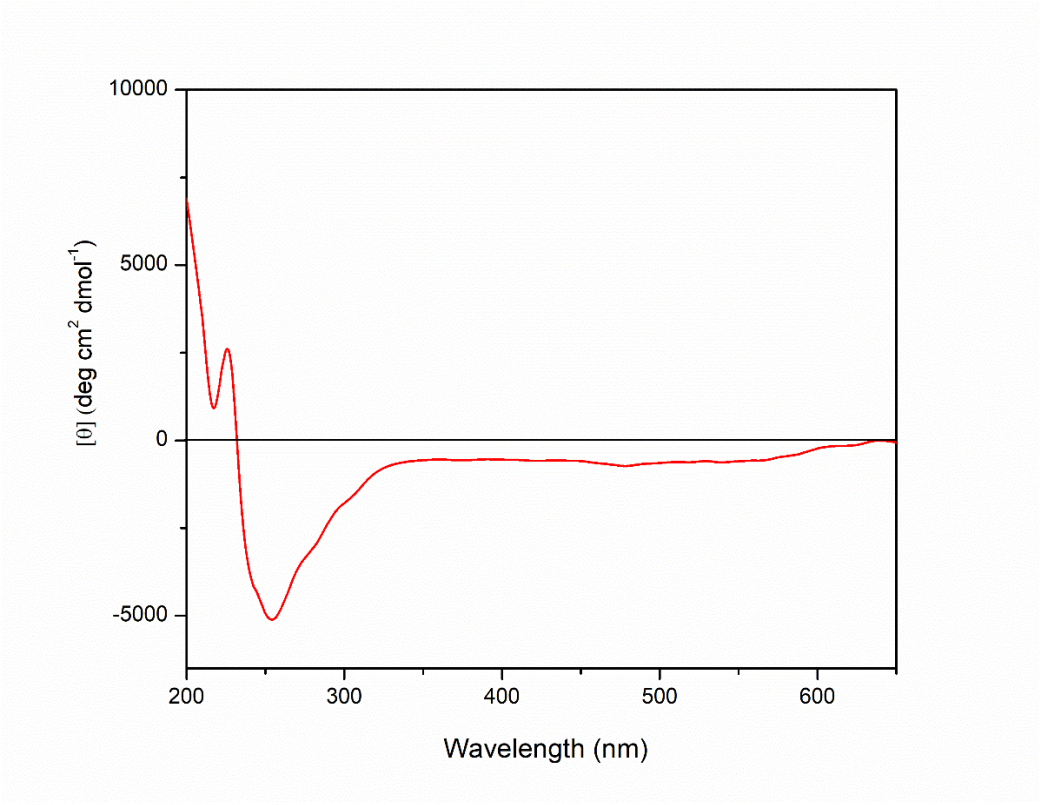

Figure S28: Circular Dichroism (CD) spectra of **4** in methanol

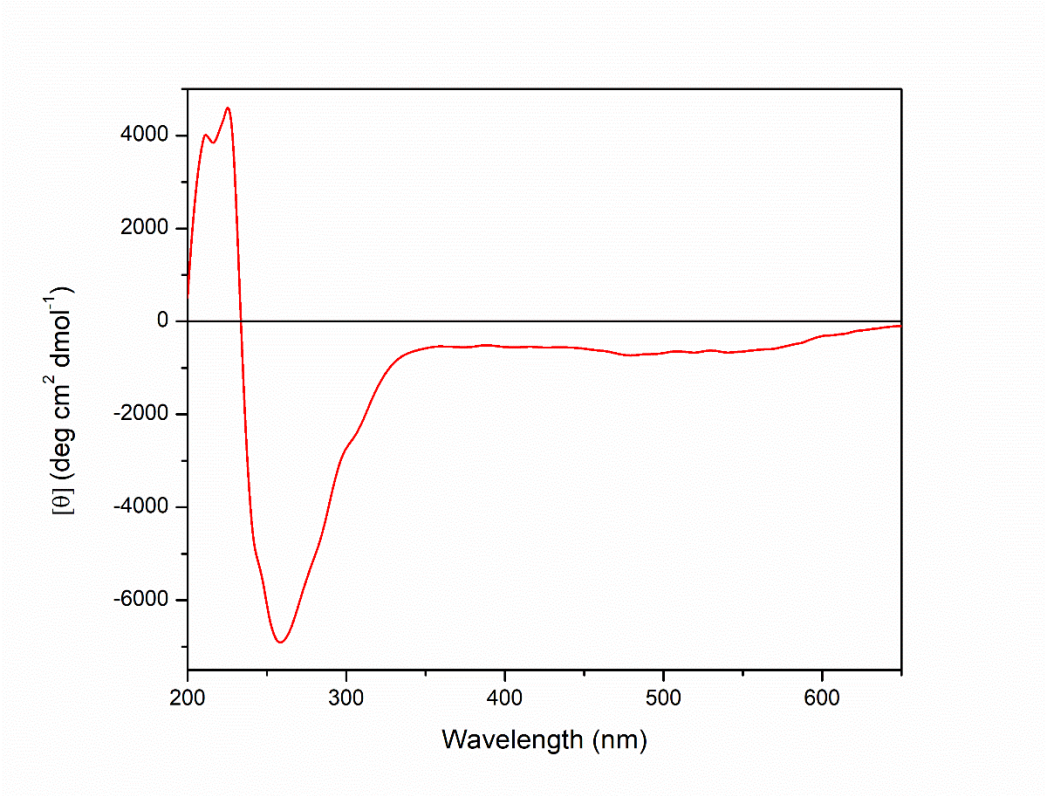

Figure S29: Circular Dichroism (CD) spectra of **6** in methanol

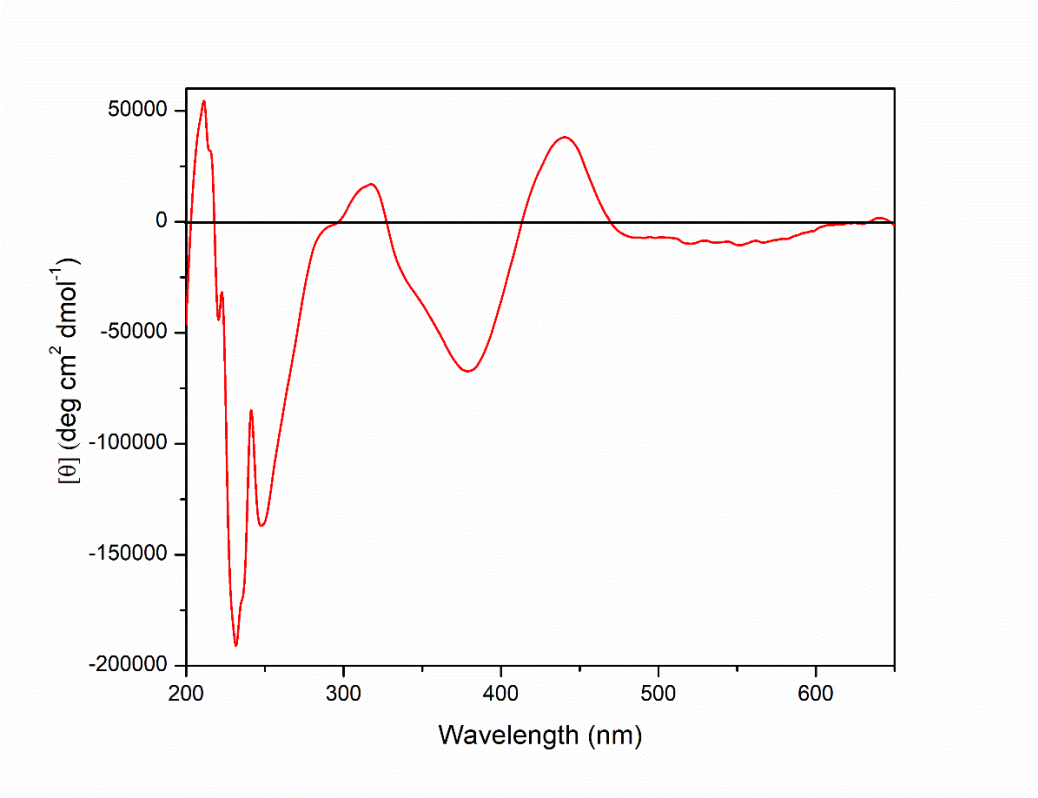

Figure S30 Circular Dichroism (CD) spectra of **1c** in methanol

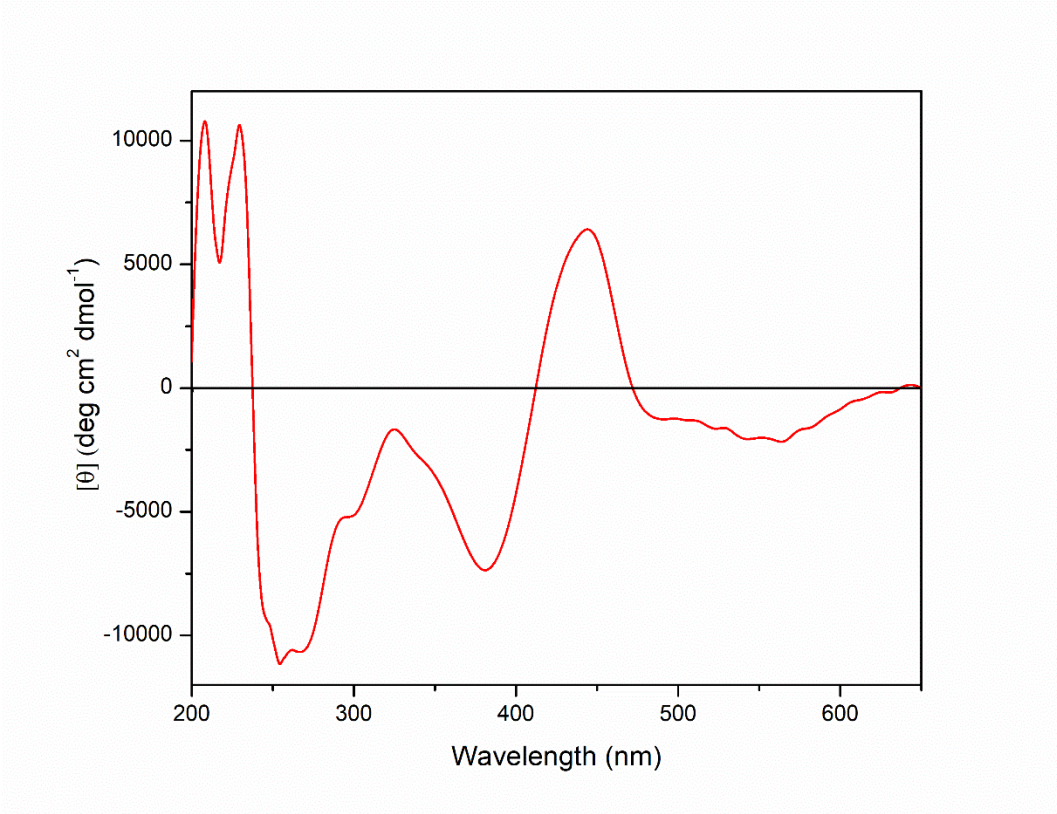

Figure S31: Circular Dichroism (CD) spectra of **1d** in methanol

6. ESI-MS spectra in the presence of DMSO

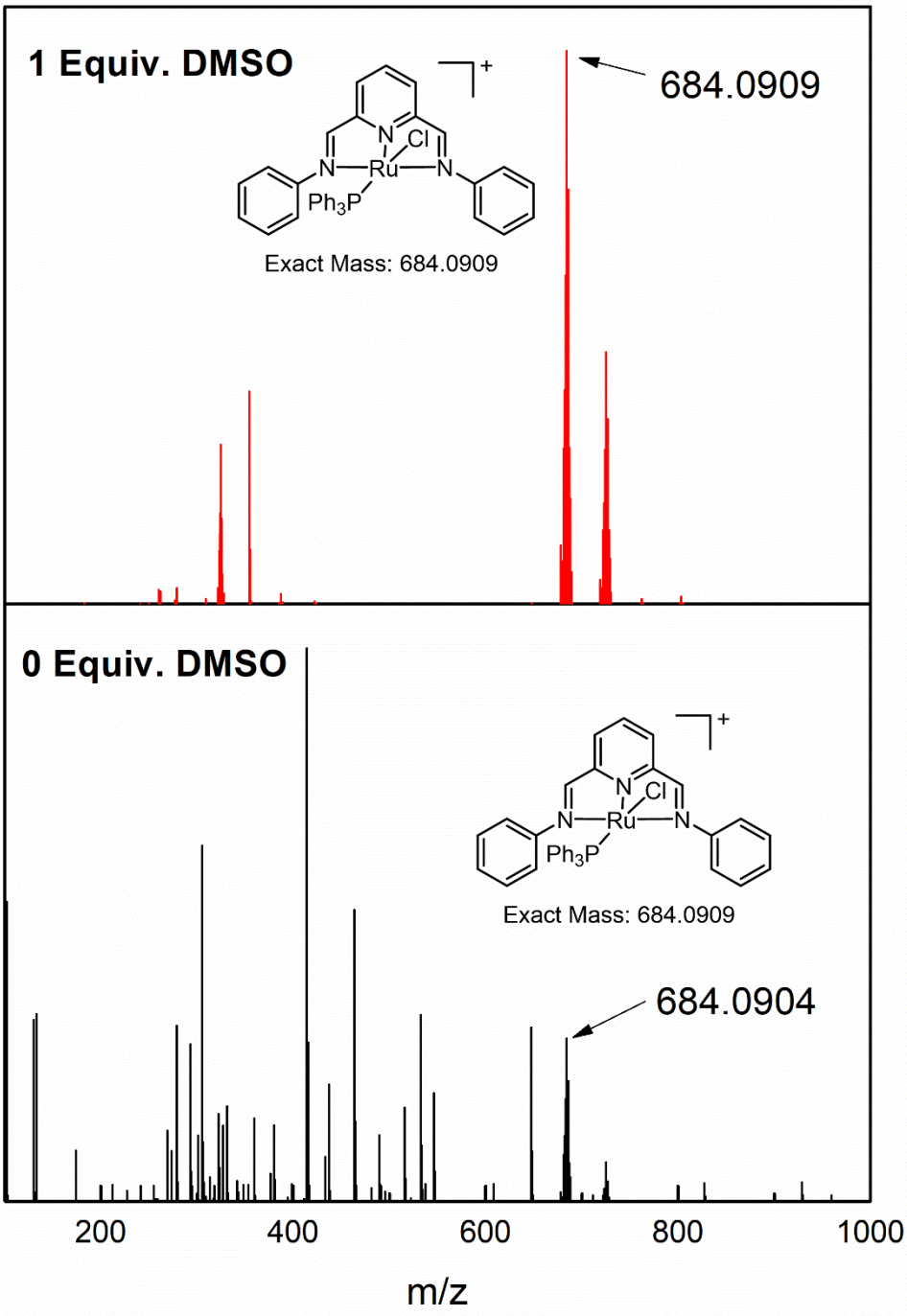

Figure S32: ESI-MS Spectra of **1a** in presence and in absence of DMSO in methanol

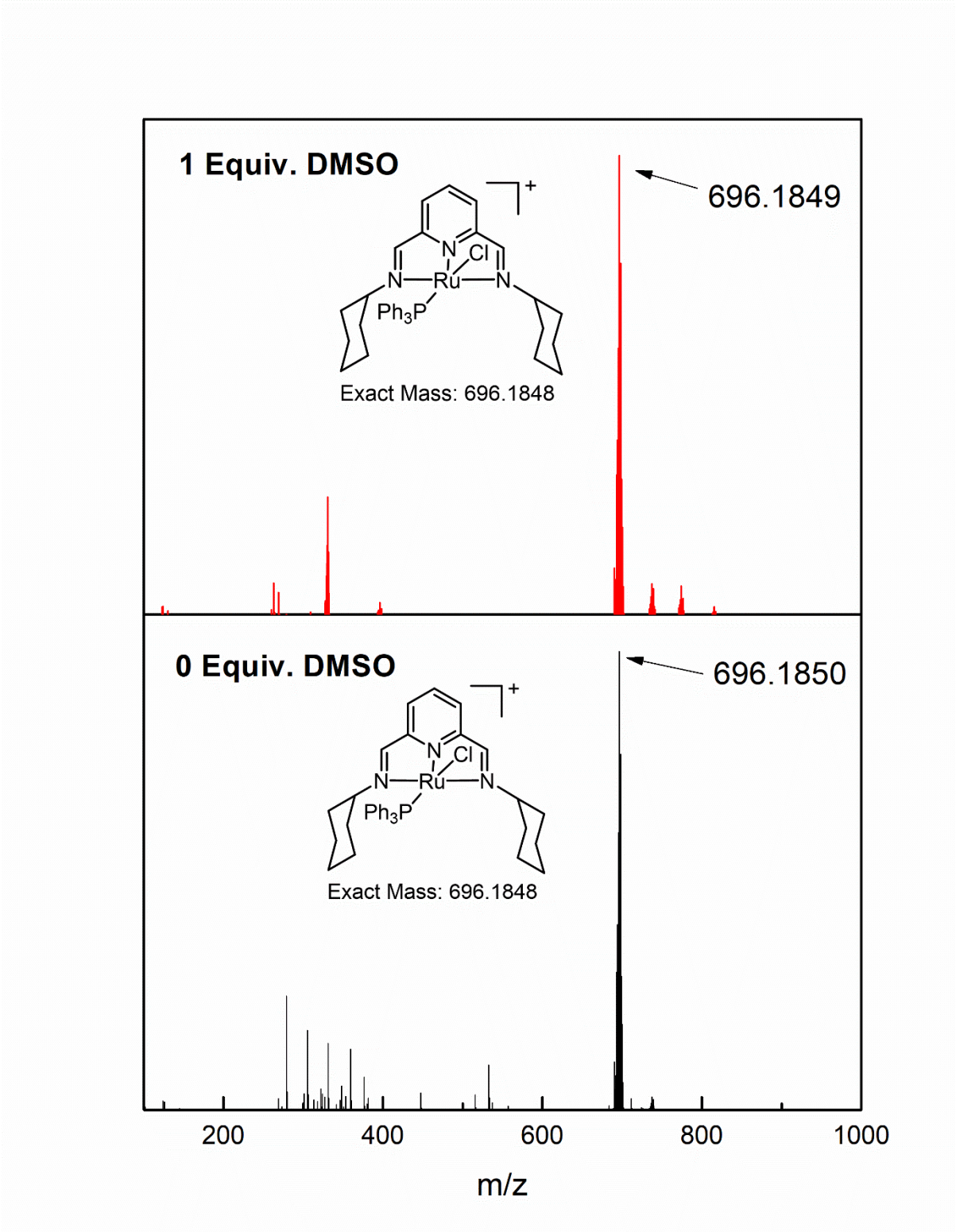

Figure S33: ESI-MS Spectra of **1b** in presence and in absence of DMSO in methanol

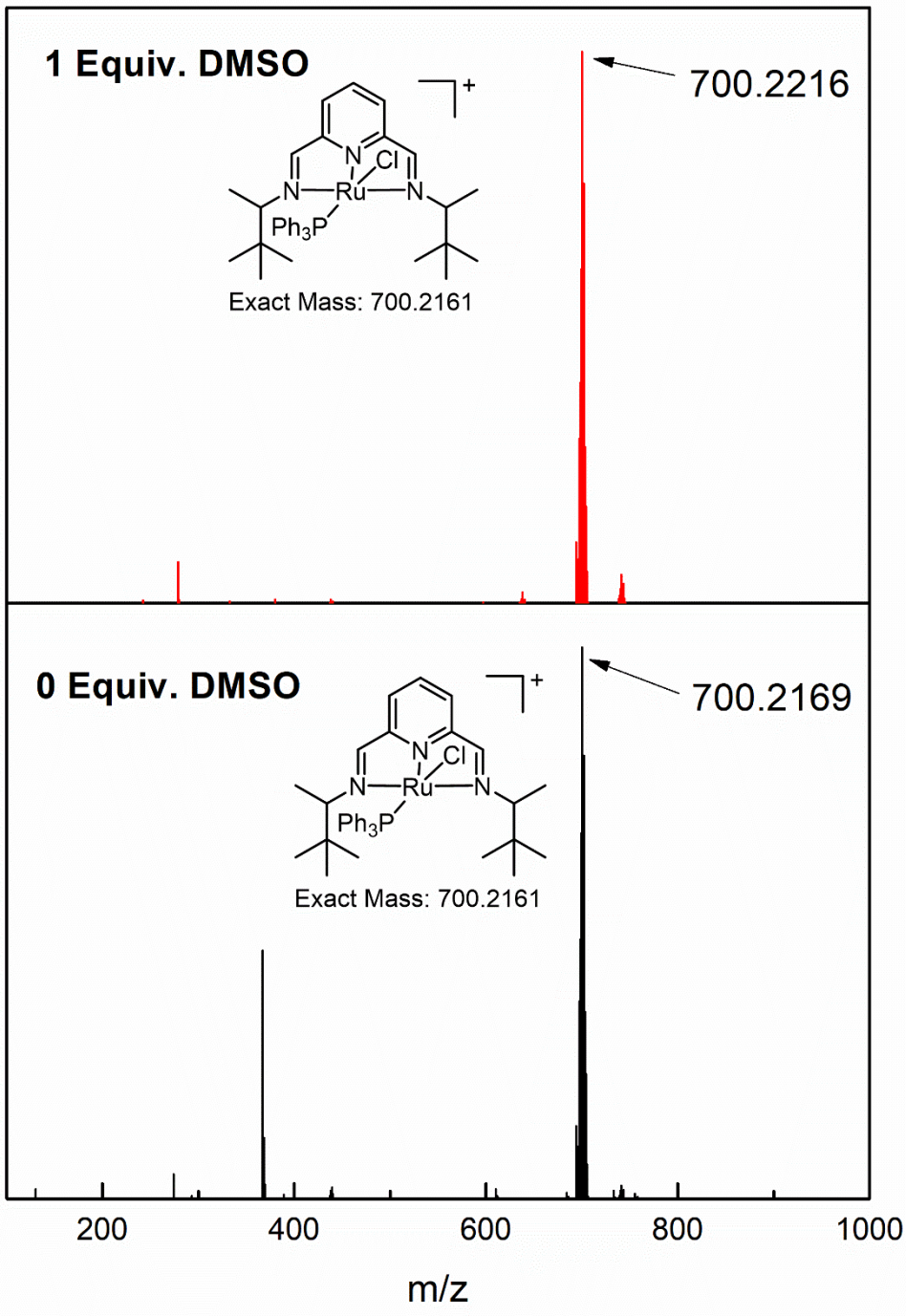

Figure S34: ESI-MS Spectra of **1d** in presence and in absence of DMSO in methanol

7. Fluorescence studies of the complexes in presence of DMSO

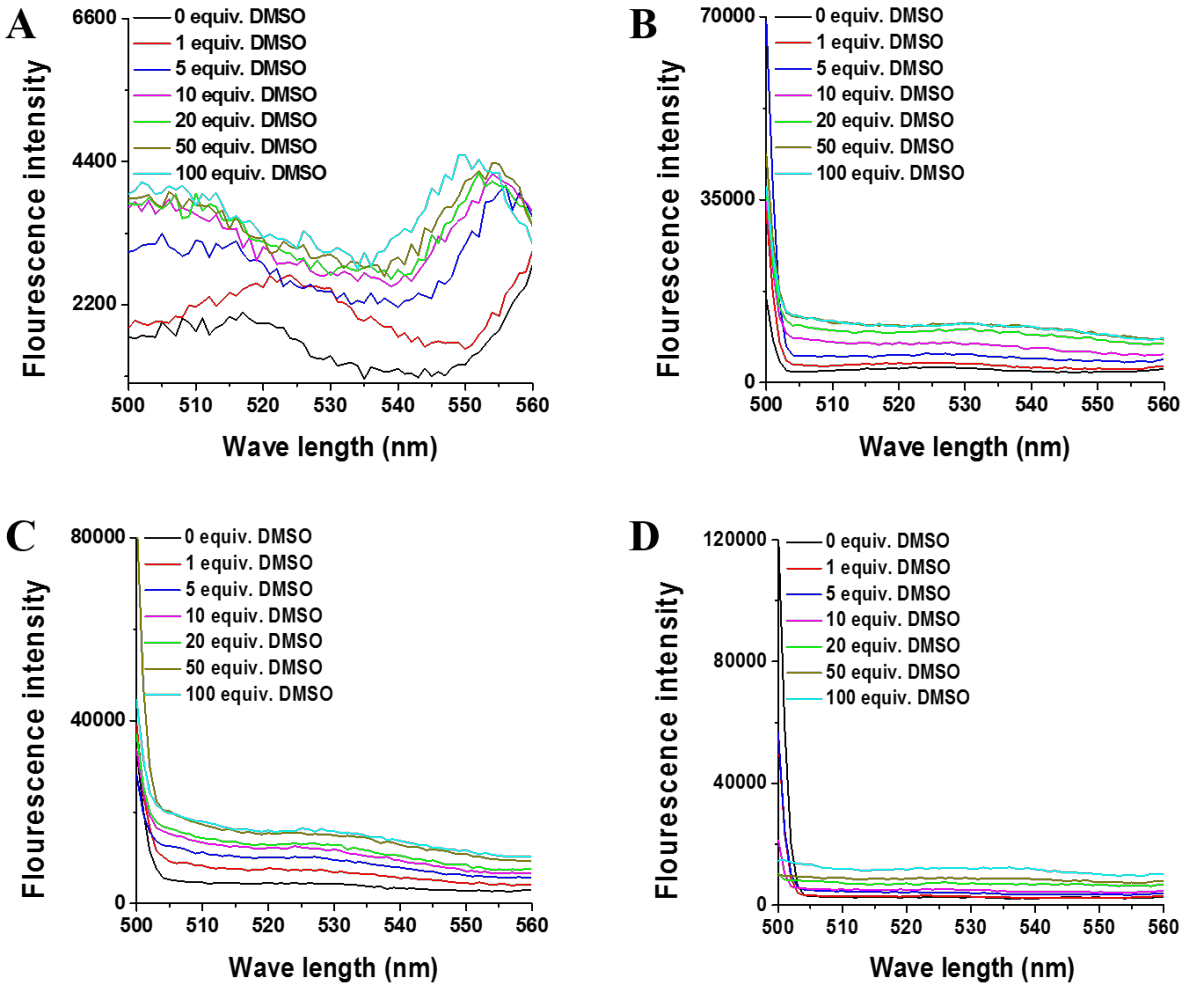

Figure S35: The fluorescence spectral profiles of (A) 1a, (B) 1b, (C) 1c, and (D) 1d complexes in DMSO were recorded from 500-560 nm when excited at 488 nm.