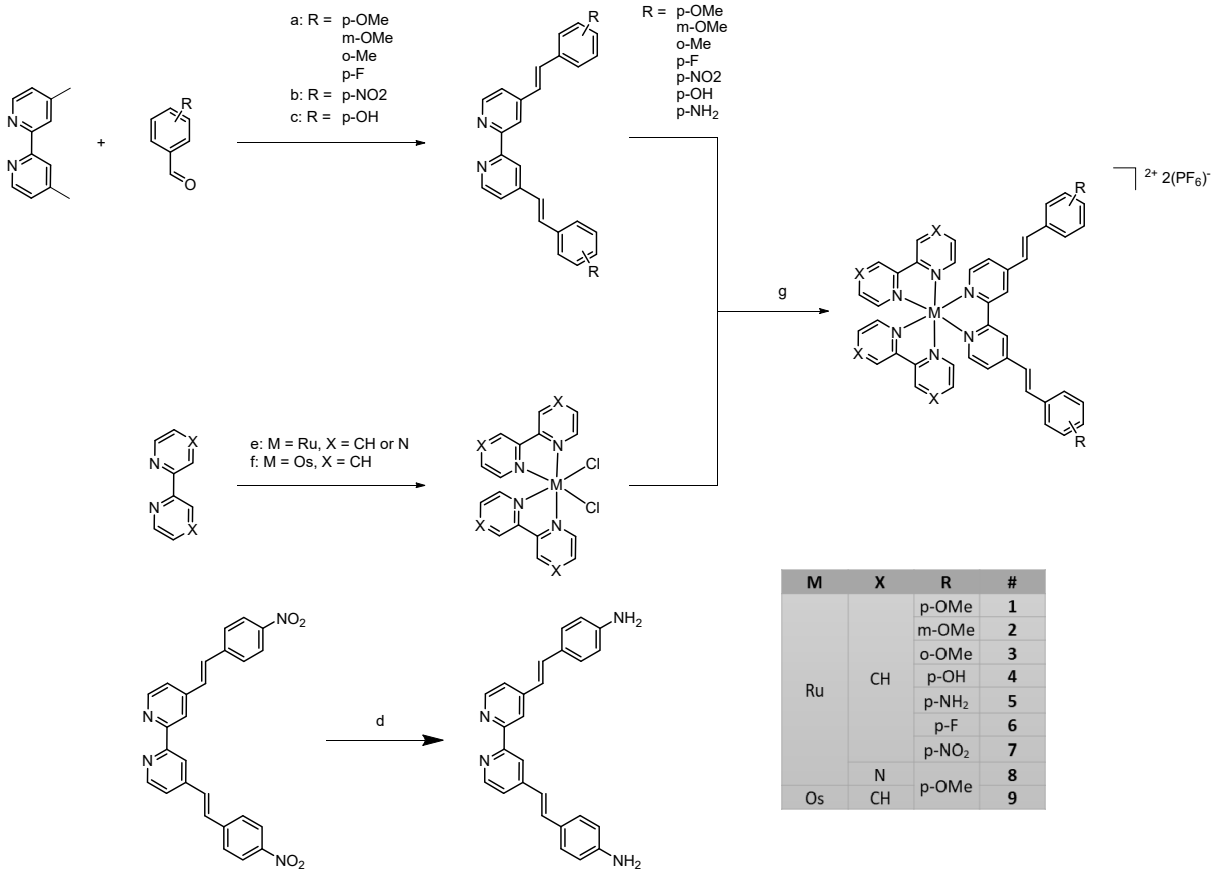
Electronic Supplementary Material (ESI) for Dalton Transactions.


# Supporting information:

# Physical, Spectroscopic, and Biological Properties of Ruthenium and Osmium Photosensitizers Bearing Diversely Substituted 4,4'-di(styryl)-2,2'-bipyridine Ligands

*Robin Vinck,[a] Johannes Karges,[a] Mickaël Tharaud,[b] Kevin Cariou,[a] and Gilles Gasser[a,]**




| M | X | R | # |
|---|---|---|---|
| Ru | CH | p-OMe | 1 |
| | | m-OMe | 2 |
| | | o-OMe | 3 |
| | | p-OH | 4 |
| | | p-$NH_2$ | 5 |
| | | p-F | 6 |
| | | p-$NO_2$ | 7 |
| | N | p-OMe | 8 |
| Os | CH | | 9 |

**Scheme S1**. Synthesis of complexes 1-9. a) KOtBu, DMF, r.t., 16 h; b) Acetic anhydride, reflux, 48 h; c) Acetic anhydride, KOAc, $I_{2\ (cat)}$, reflux, 48 h and then NaOH, MeOH, 64 °C, 1 h; d) $Na_2S_2O_4$, DMSO/$H_2O$ (10:1), 90 °C, 15 h; e) $Ru(dmso)_4Cl_2$, LiCl, DMF, 130 °C, 16 h; f) $Os(NH_4)_2Cl_6$, ethylene glycol, 130 °C, 1 h; g) Ethylene glycol, 130 °C, 24 h for **4**, and **7-9**, EtOH, 80 °C, 6 h for the others.

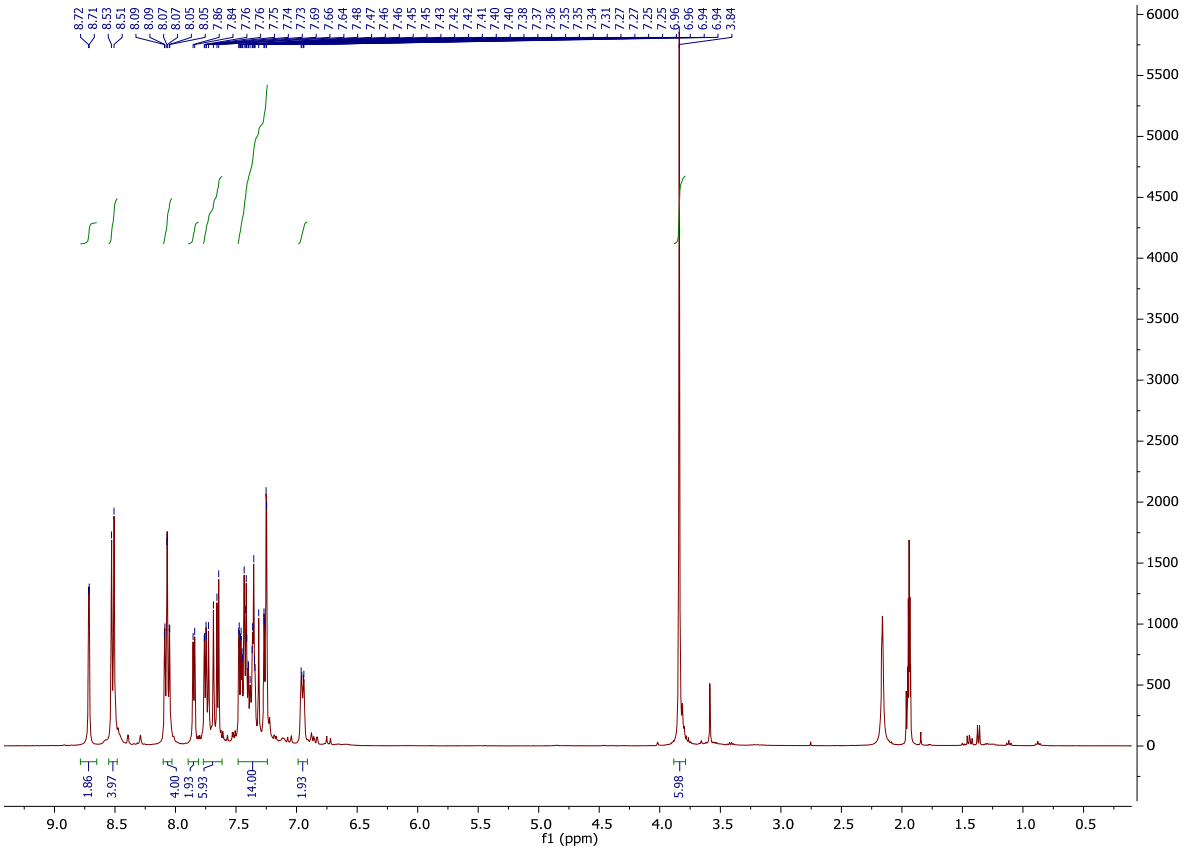



**Figure S1.** $^{1}$H-NMR spectrum of **2** in $CD_3CN$, 400 MHz

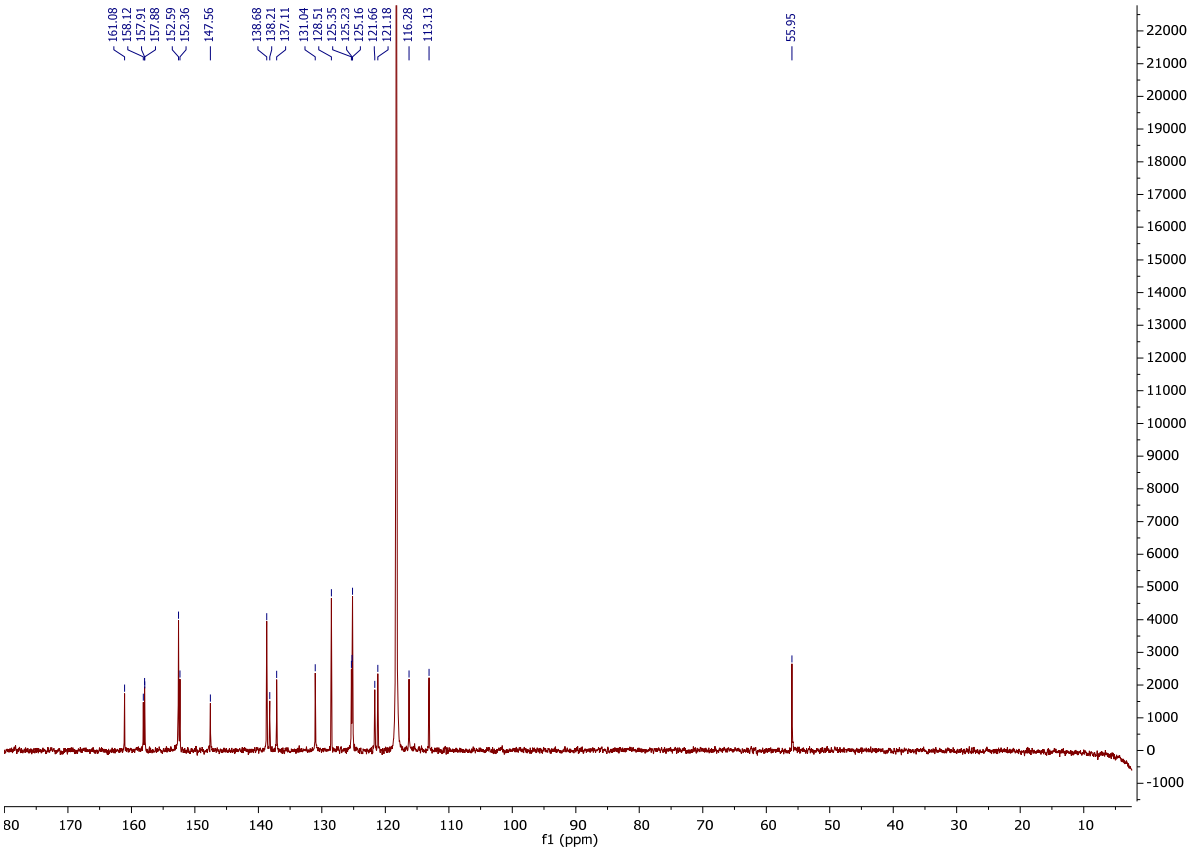



**Figure S2**. $^{13}$C-NMR spectrum of **2** in $CD_3CN$, 100 MHz

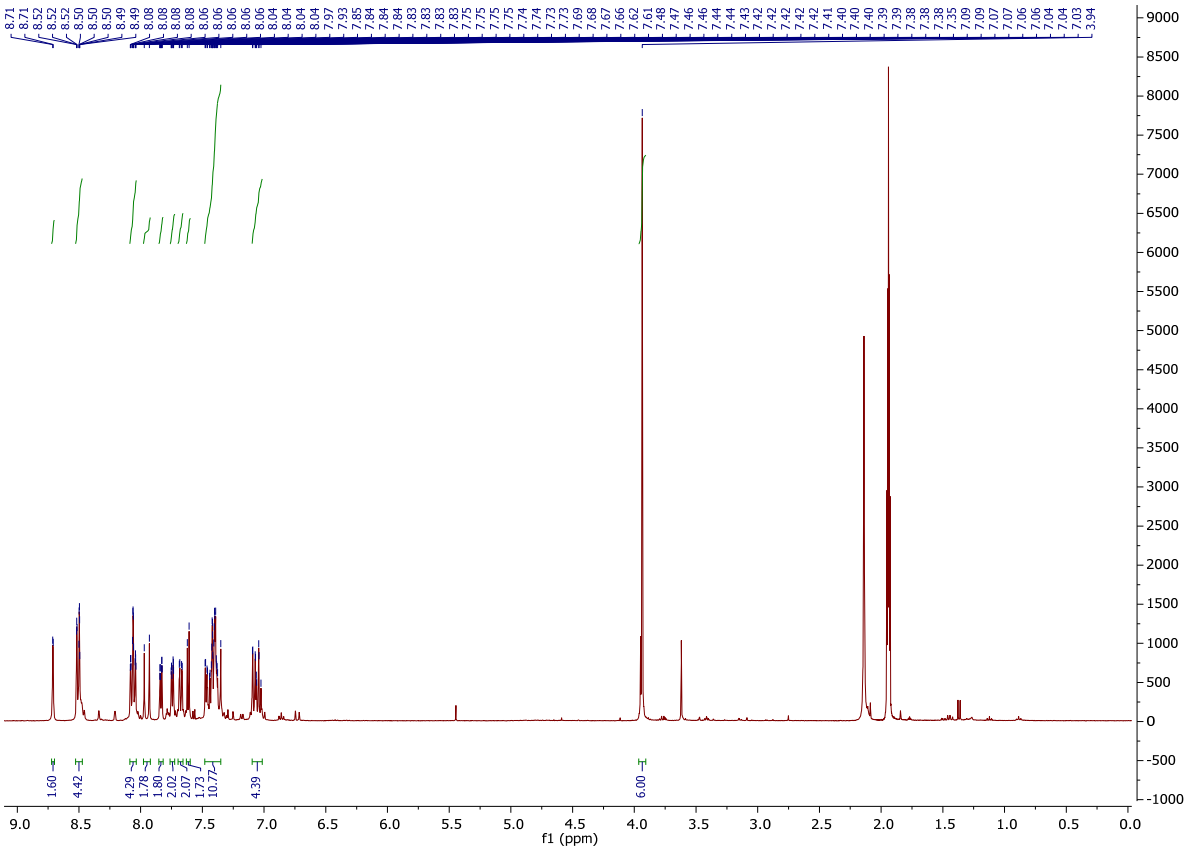


**Figure S3**. $^{1}$H-NMR spectrum of **3** in $CD_3CN$, 400 MHz

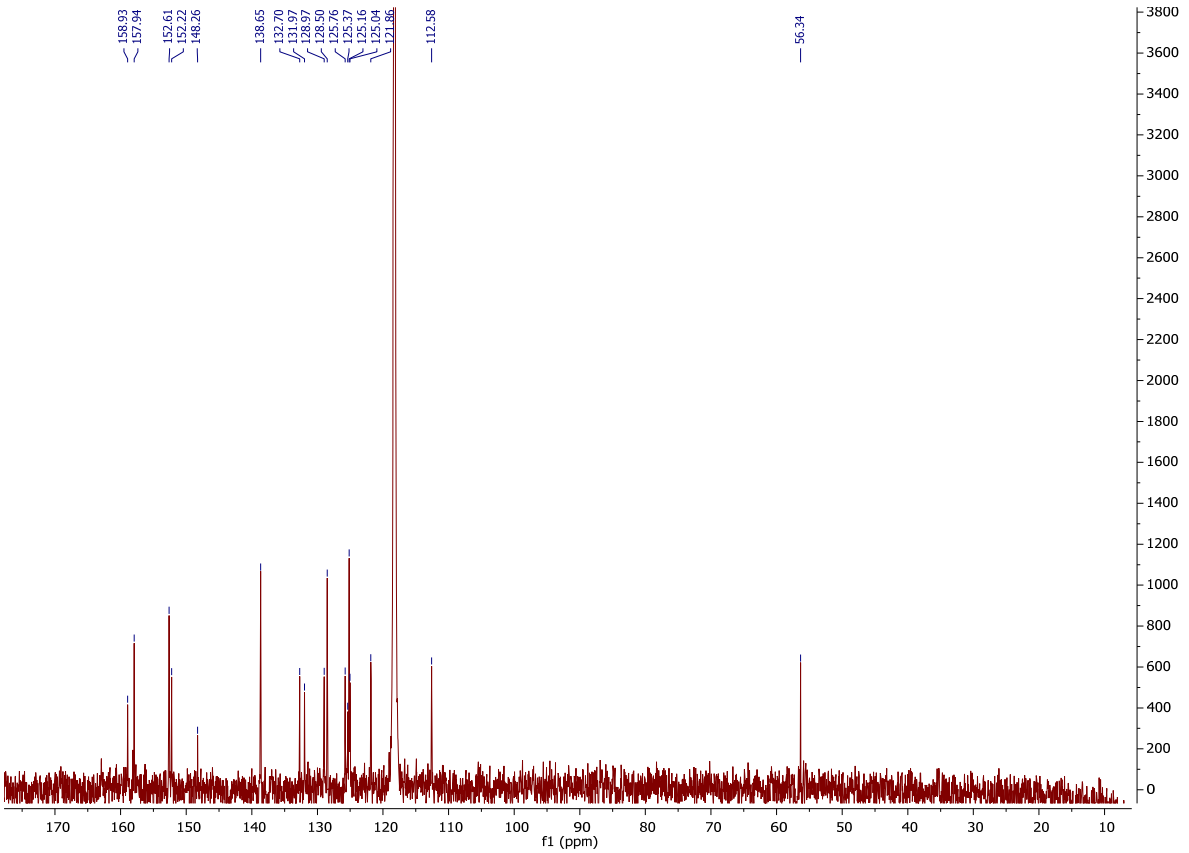


**Figure S4**. $^{13}$C-NMR spectrum of **3** in $CD_3CN$, 100 MHz

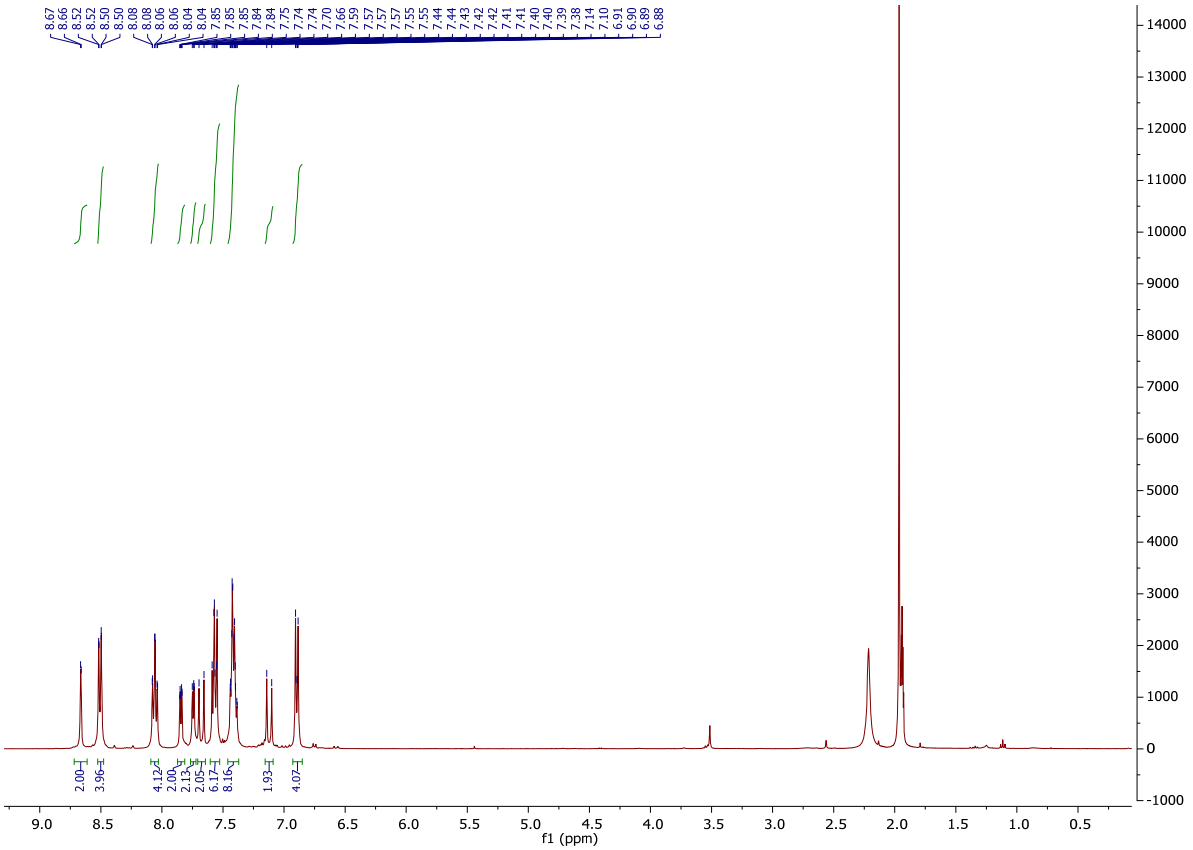



**Figure S5**. $^{1}$H-NMR spectrum of **4** in $CD_3CN$, 400 MHz

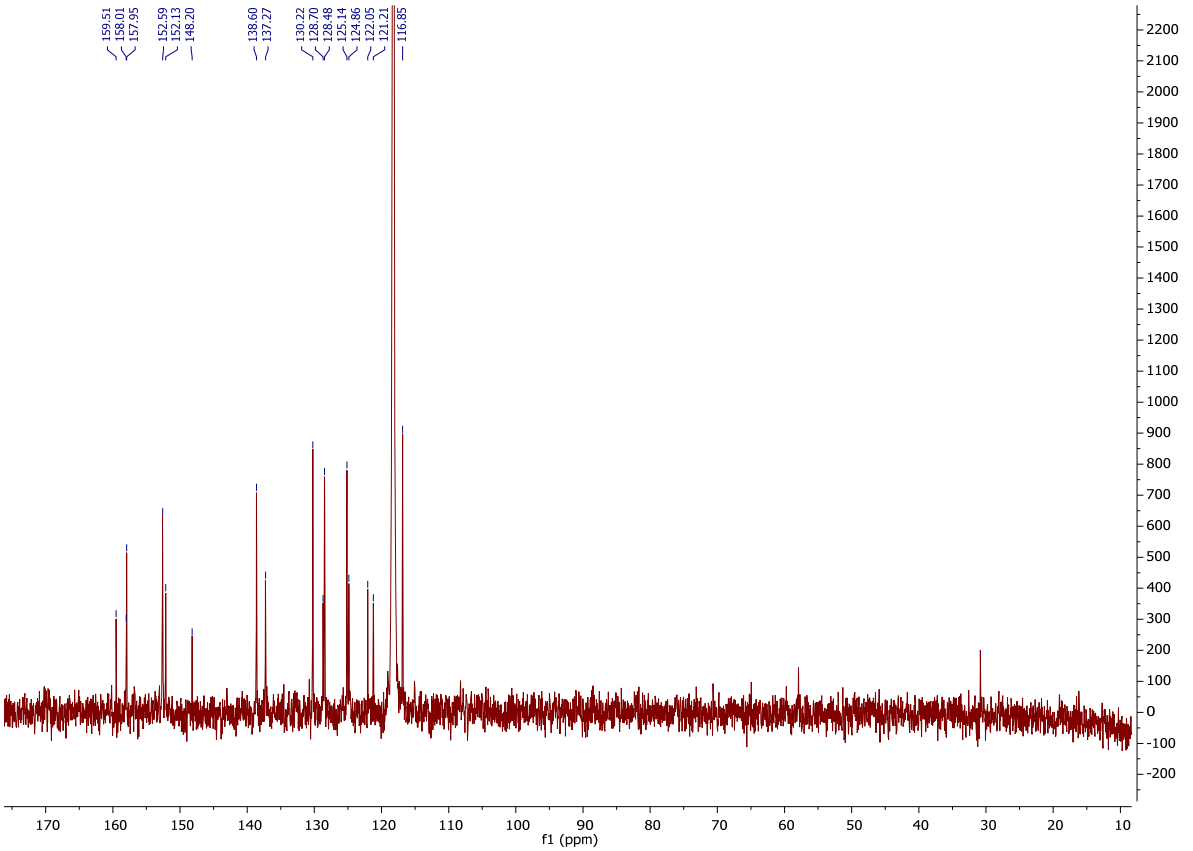



**Figure S6**. $^{13}$C-NMR spectrum of **4** in $CD_3CN$, 100 MHz

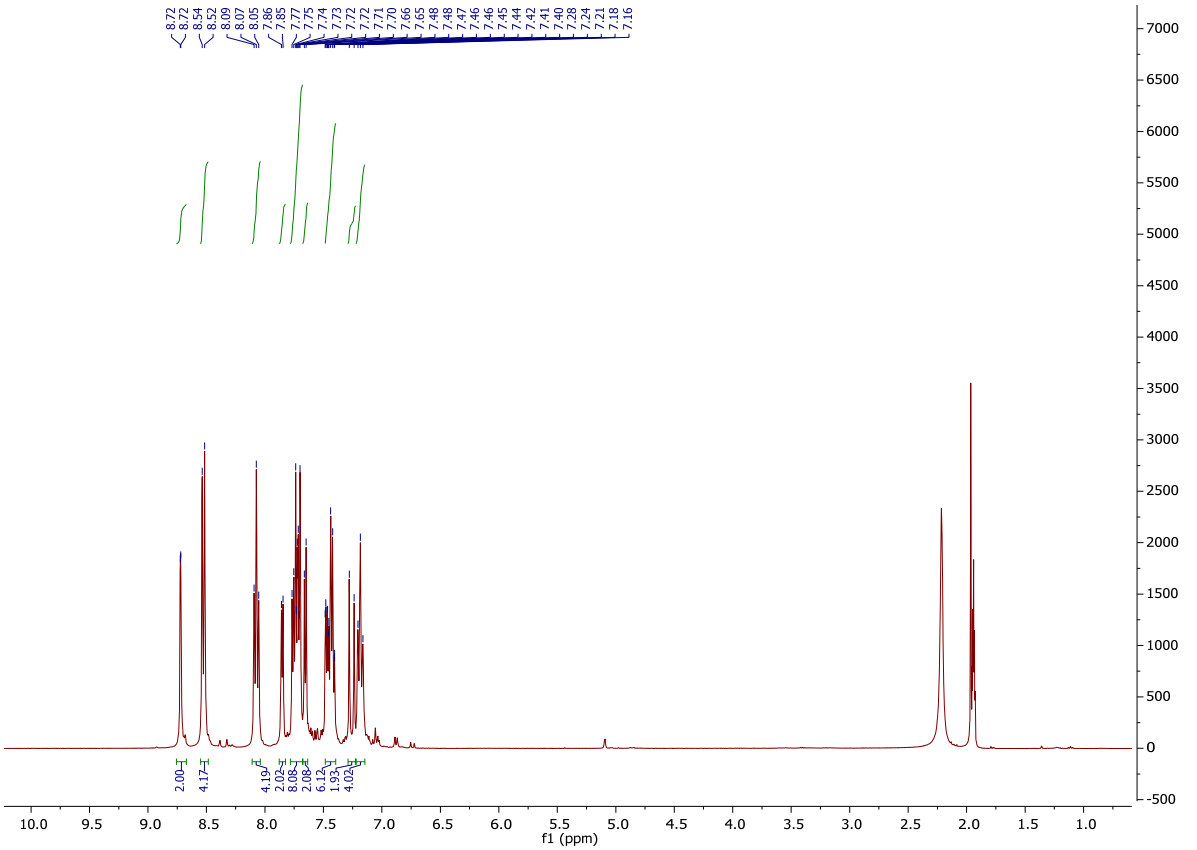



**Figure S7**. $^{1}$H-NMR spectrum of **6** in $CD_3CN$, 400 MHz

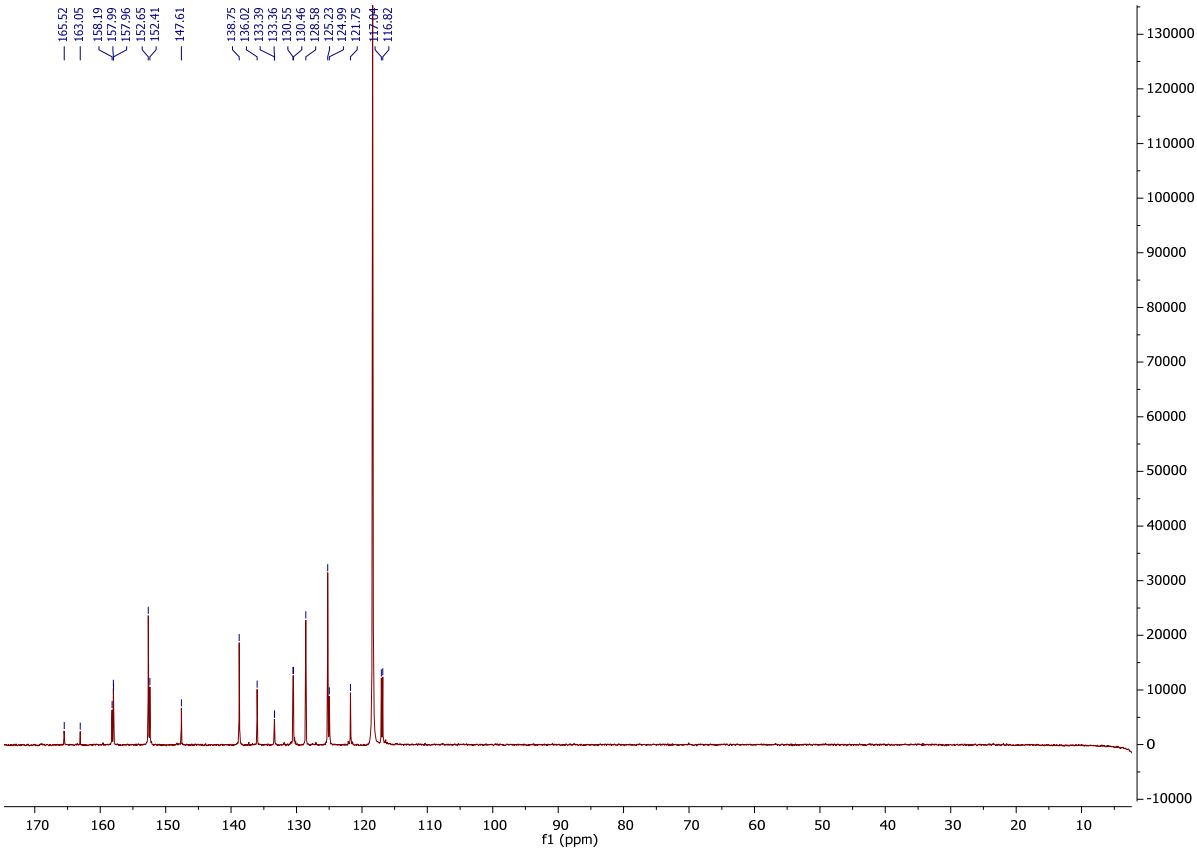



**Figure S8**. $^{13}$C-NMR spectrum of **6** in $CD_3CN$, 100 MHz

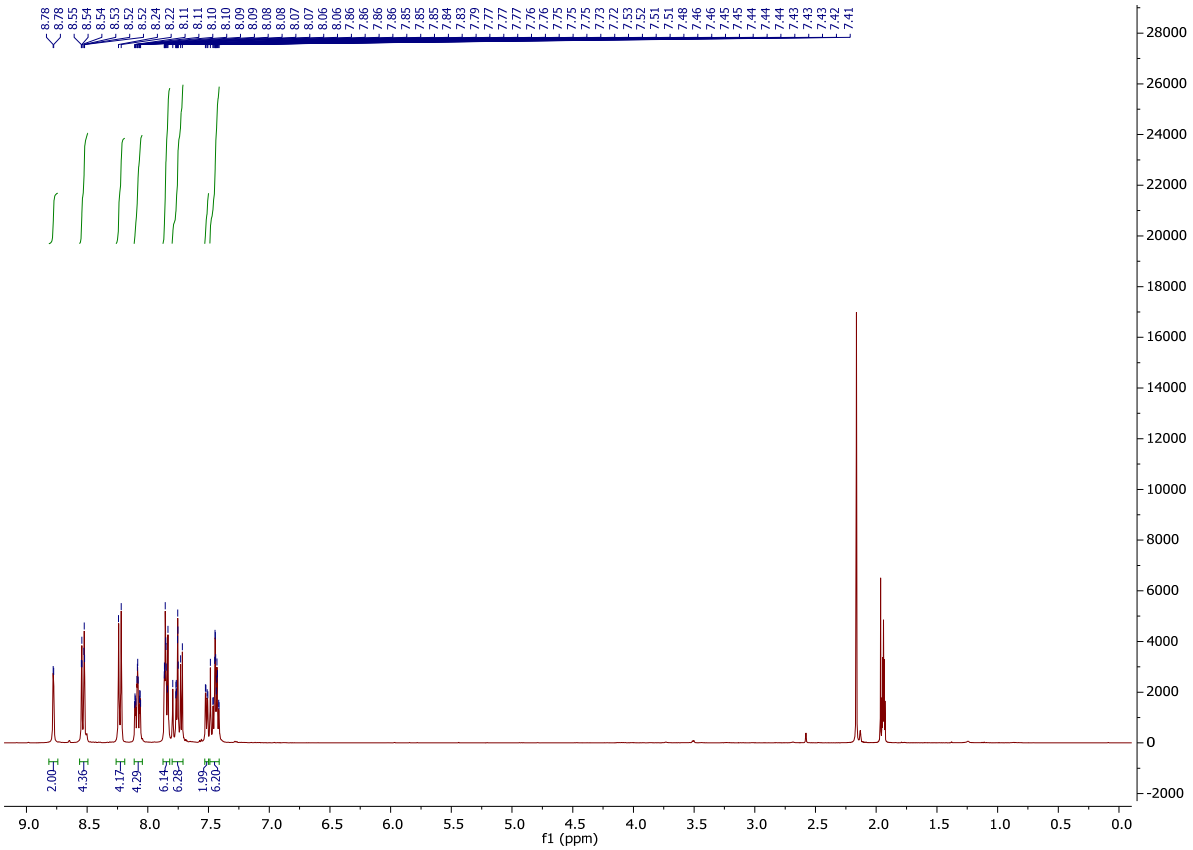



**Figure S9**. $^{1}$H-NMR spectrum of **7** in $CD_3CN$, 400 MHz

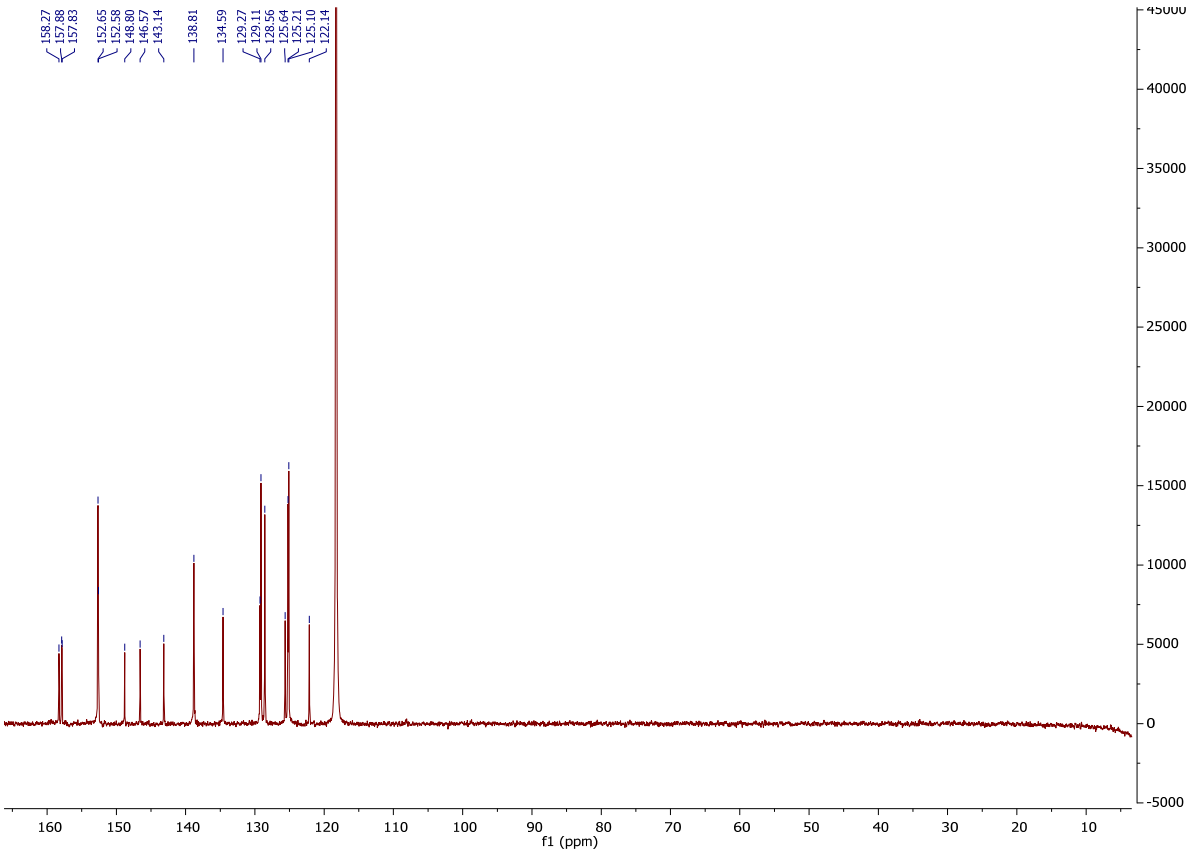



**Figure S10**. $^{13}$C-NMR spectrum of **7** in $CD_3CN$, 100 MHz

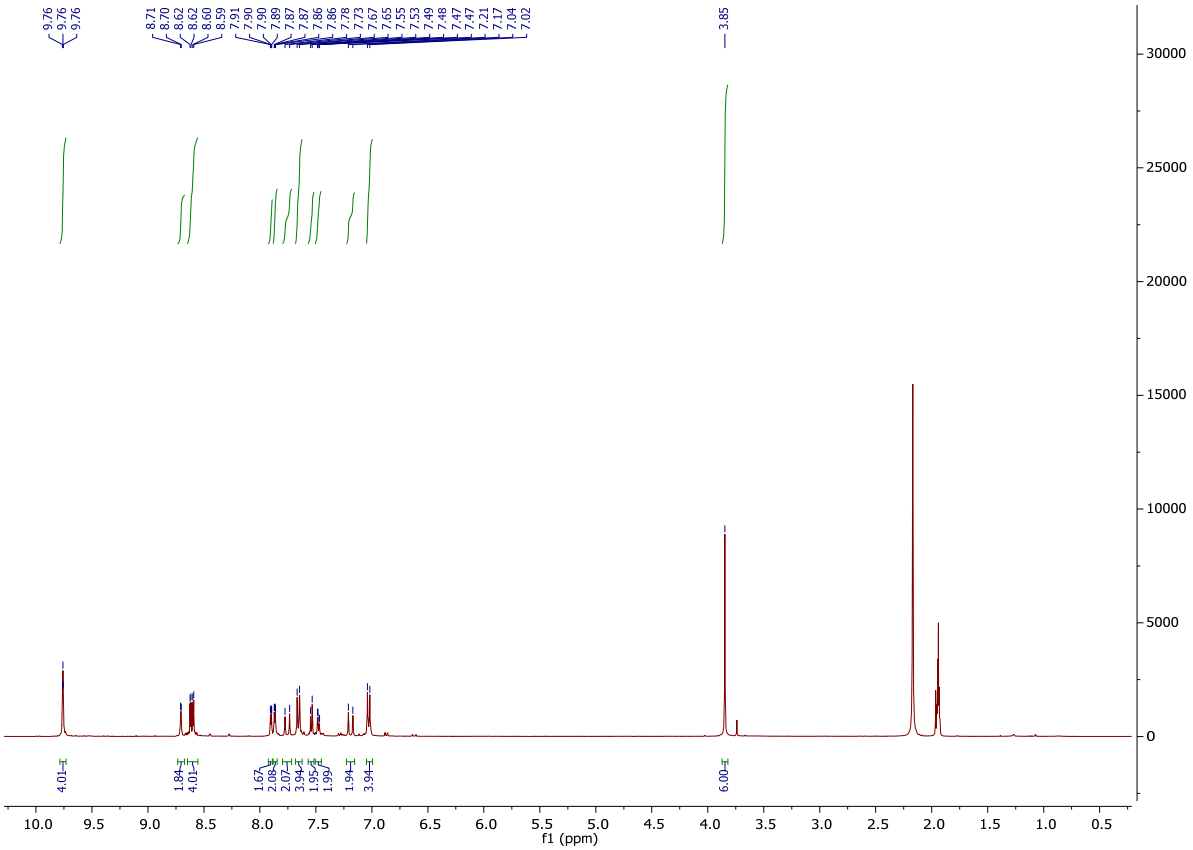



**Figure S11**. $^{1}$H-NMR spectrum of **8** in $CD_3CN$, 400 MHz

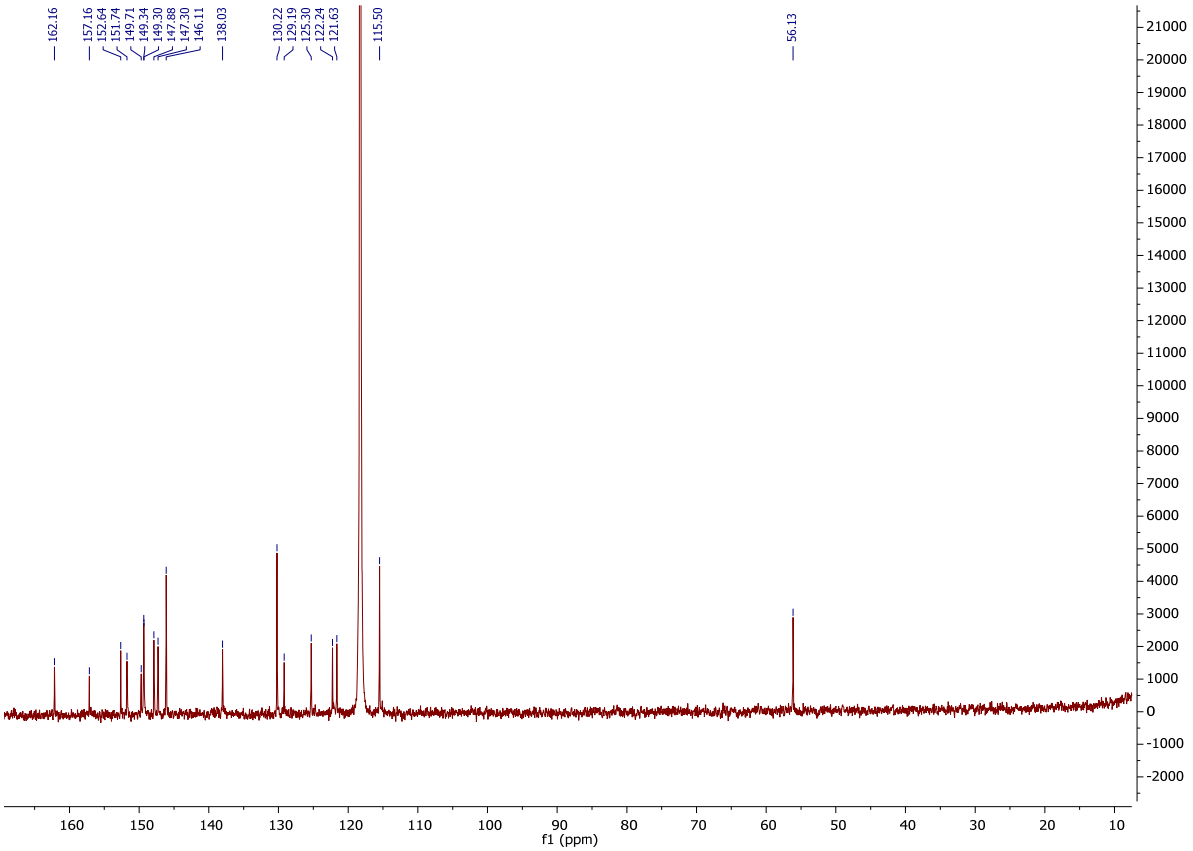



**Figure S12**. $^{13}$C-NMR spectrum of **8** in $CD_3CN$, 100 MHz

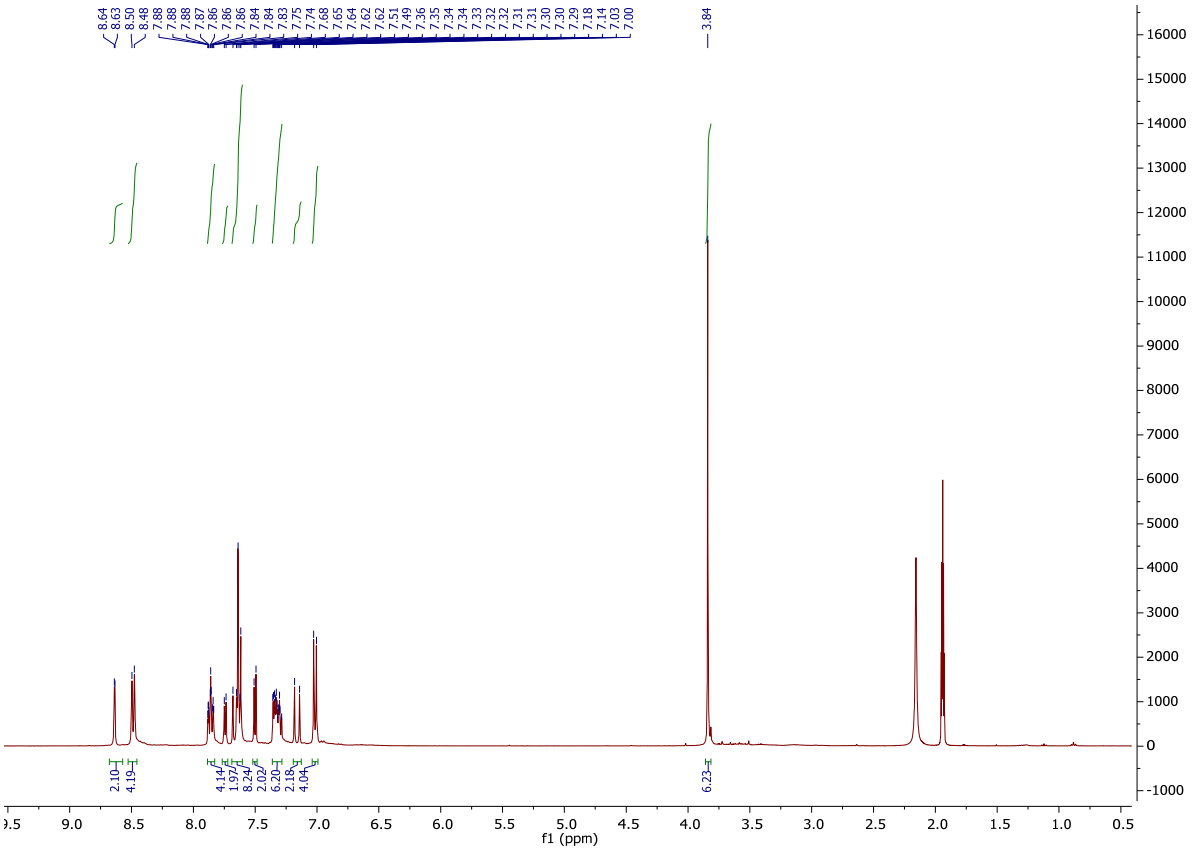



**Figure S13**. $^{1}$H-NMR spectrum of **9** in $CD_3CN$, 400 MHz

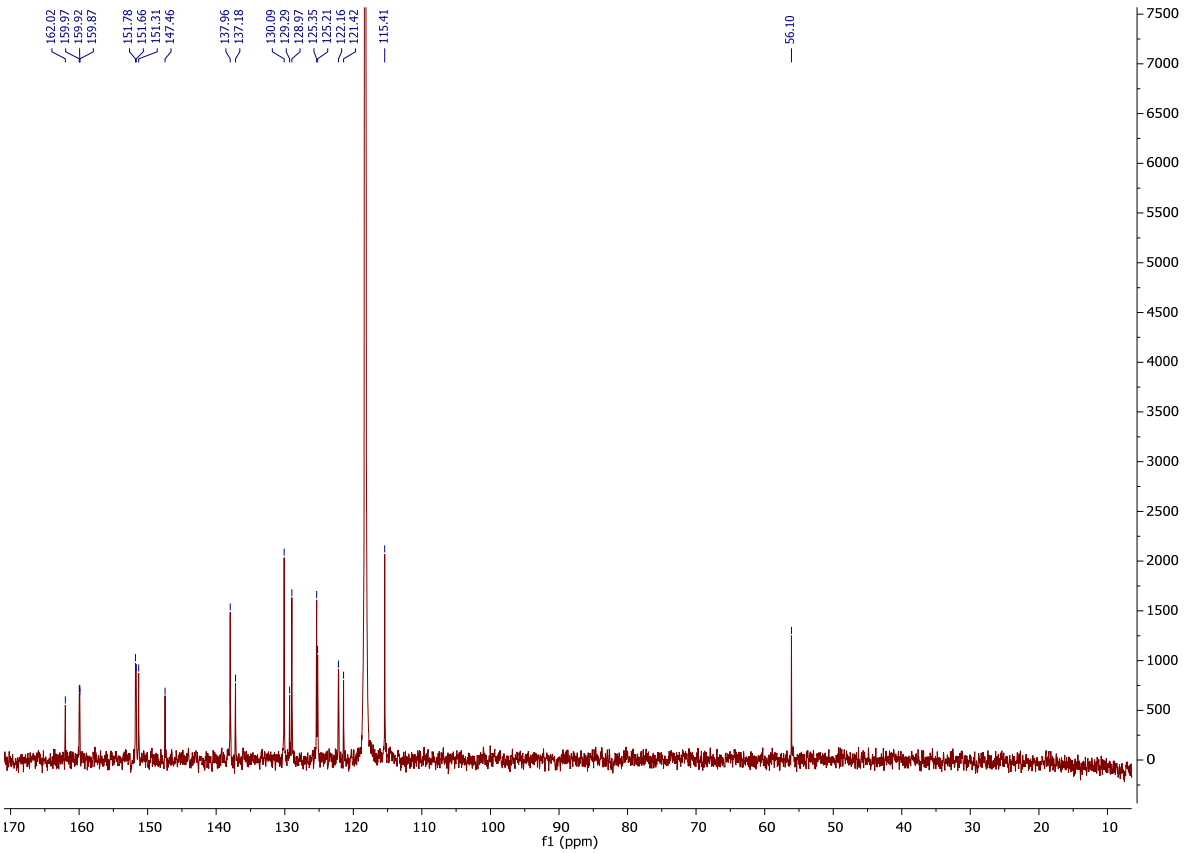



**Figure S14**. $^{13}$C-NMR spectrum of **9** in $CD_3CN$, 100 MHz

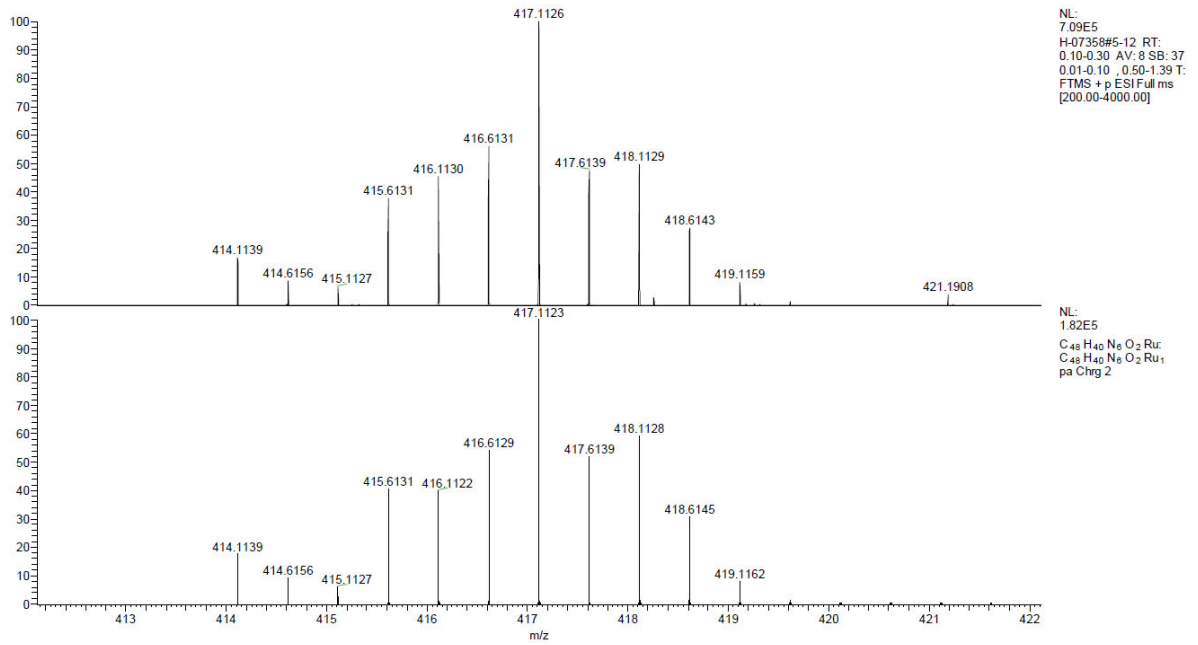



**Figure S15**. (Experimental/Theoretical) ESI-HRMS spectrum of **2** (positive detection mode)

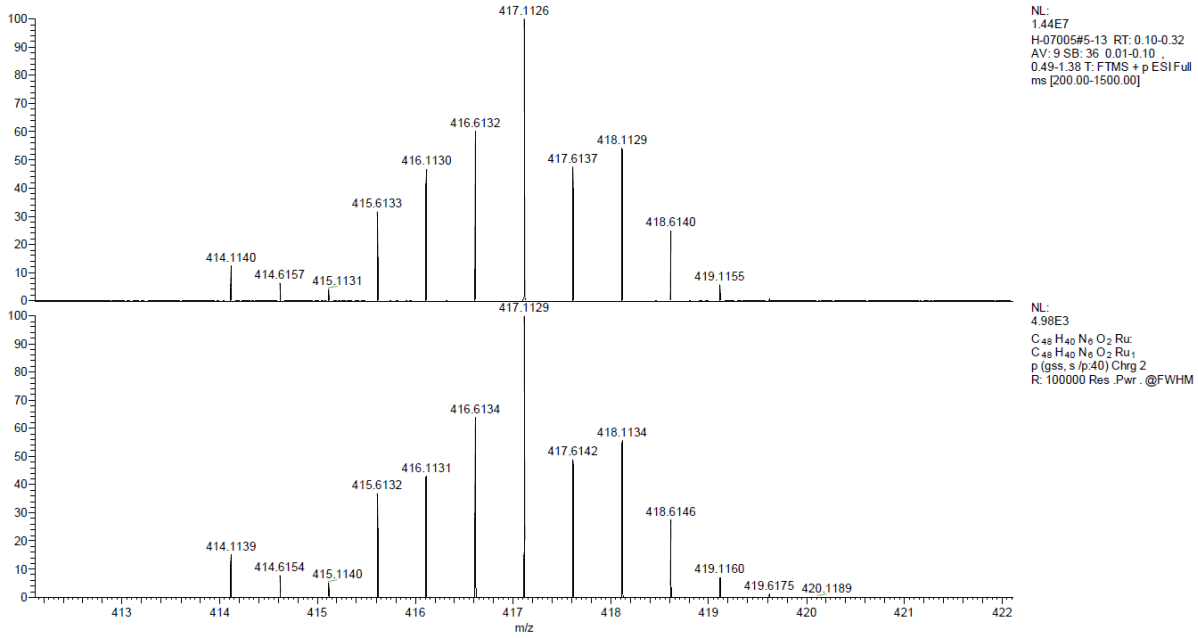



**Figure S16**. (Experimental/Theoretical) ESI-HRMS spectrum of **3** (positive detection mode)

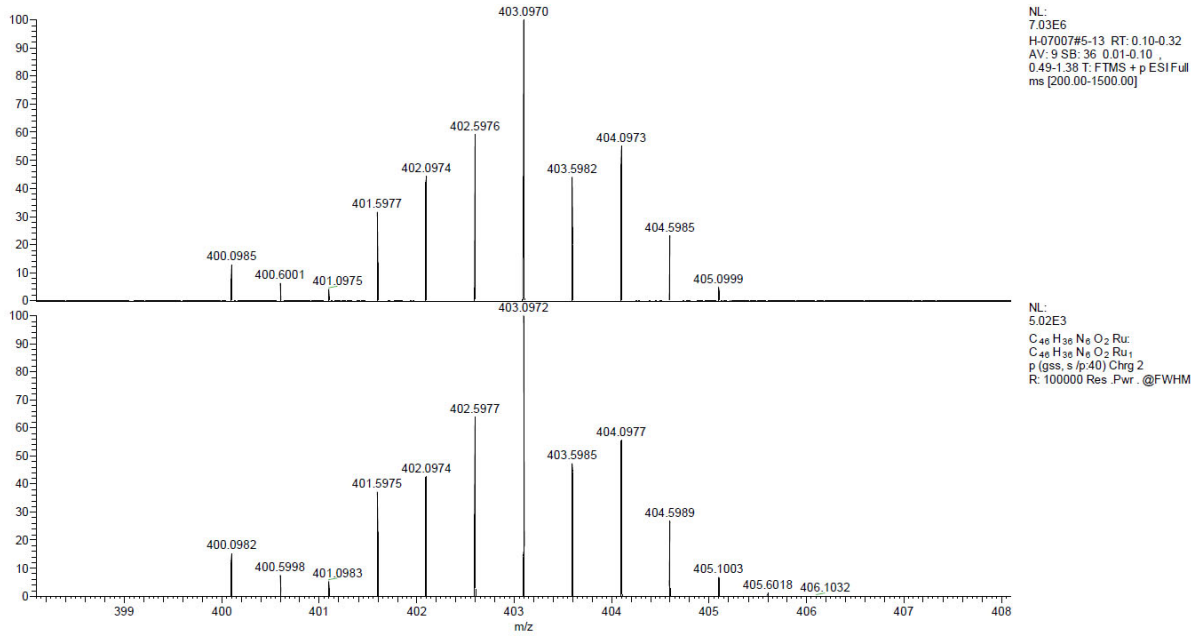



**Figure S17**. (Experimental/Theoretical) ESI-HRMS spectrum of **4** (positive detection mode)

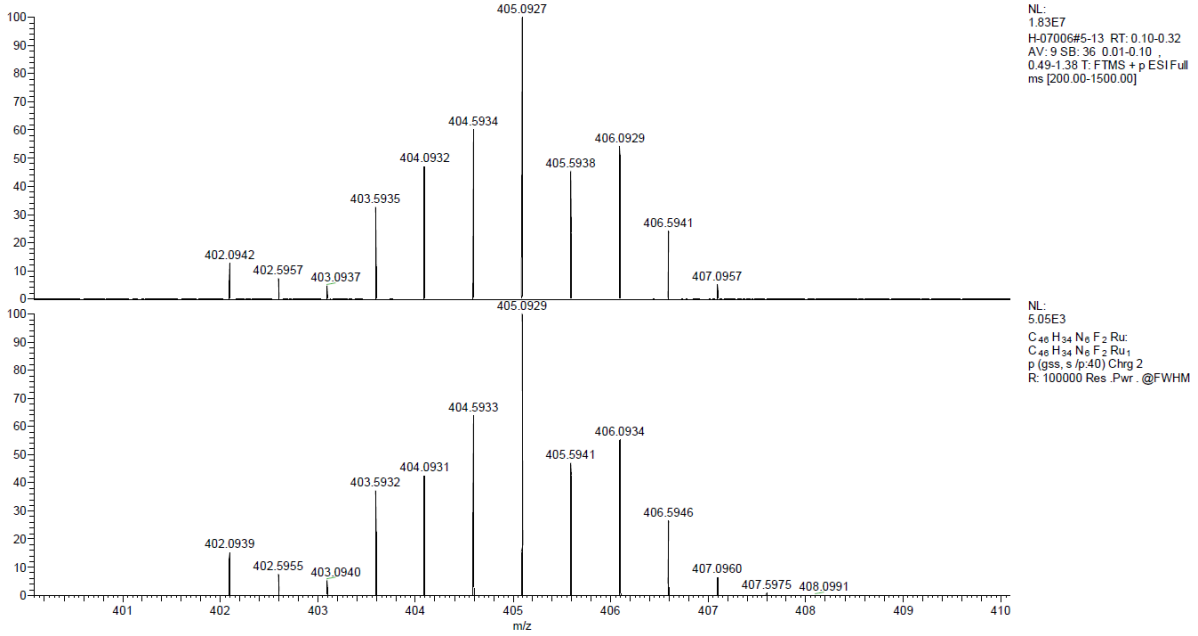



**Figure S18**. (Experimental/Theoretical) ESI-HRMS spectrum of **6** (positive detection mode)

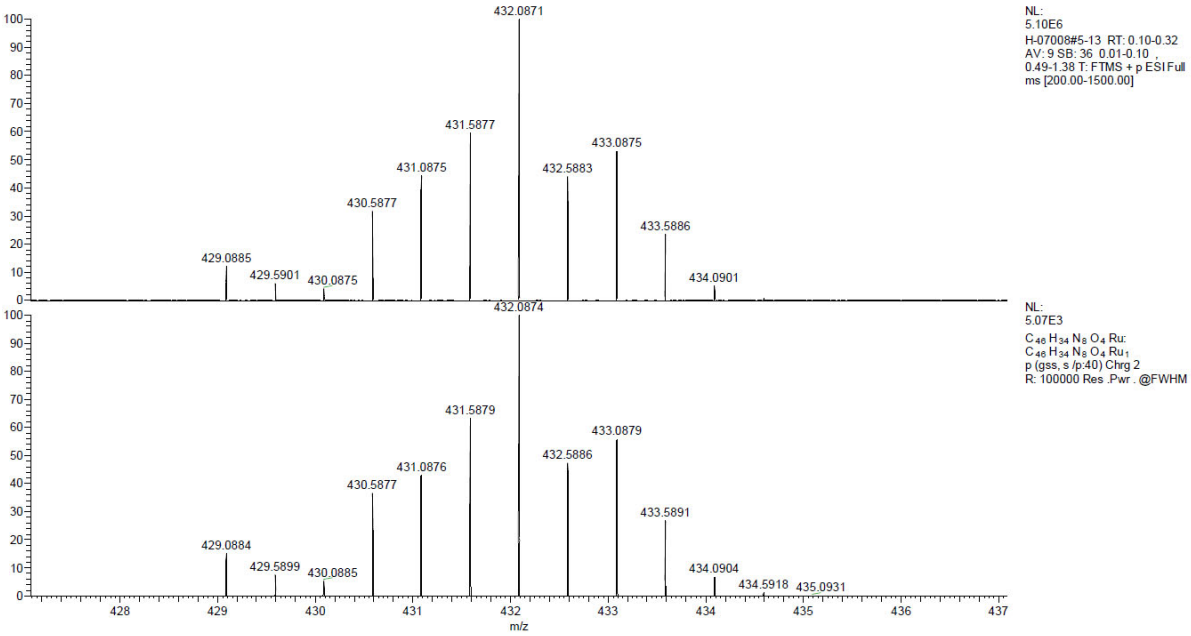



**Figure S19**. (Experimental/Theoretical) ESI-HRMS spectrum of **7** (positive detection mode)

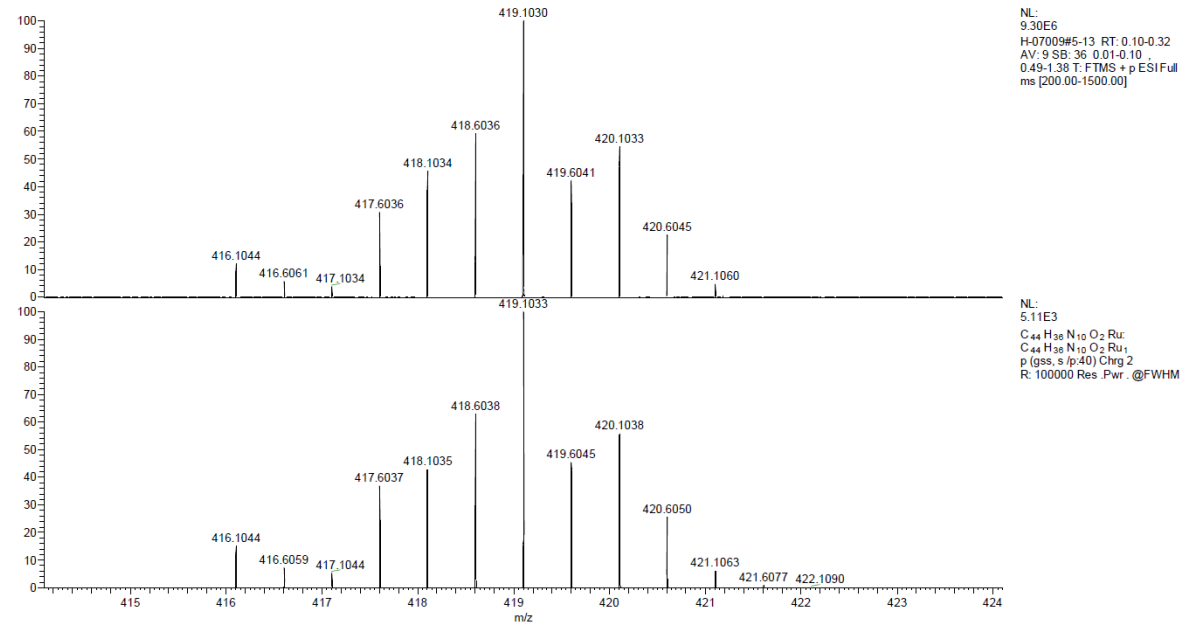



**Figure S20**. (Experimental/Theoretical) ESI-HRMS spectrum of **8** (positive detection mode)

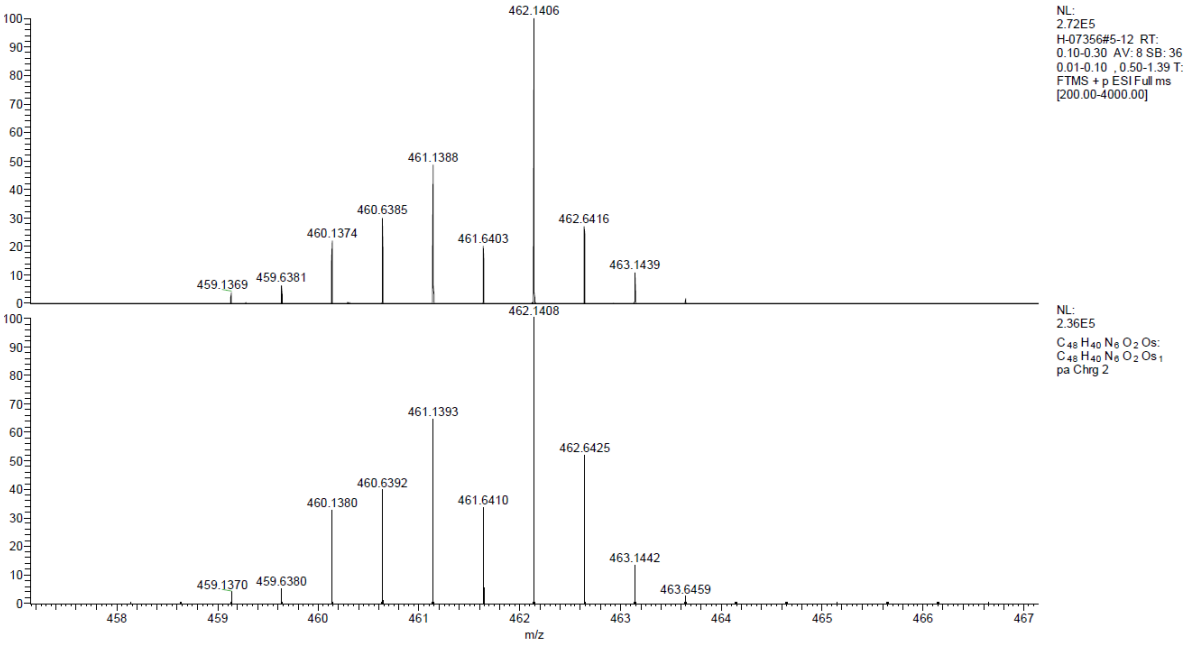



**Figure S21**. (Experimental/Theoretical) ESI-HRMS spectrum of **9** (positive detection mode)

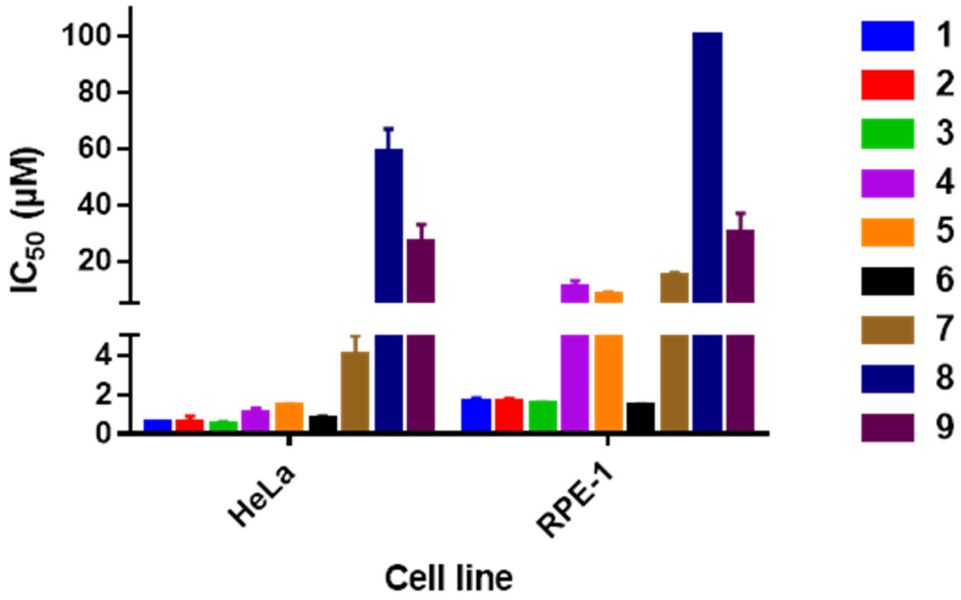



**Figure S22**. Comparative representation of complexes 1-9 phototoxicity upon irradiation at 480 nm for 10 min in HeLa and RPE-1 cells.