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Solvatochromism of conjugated 4-*N,N*-dimethylaminophenyl-pyridinium donor-acceptor pairs

Mat as Vidal, Marcos C. Rezende, Camila Pastene and Carolina Aliaga, Moises Dom nguez

Facultad de Qu mica y Biolog a, Universidad de Santiago de Chile, Av. Libertador Bernardo O'Higgins 3363, Santiago, Chile

E{mail: moises.dominguez@usach.cl

Contents

List of Figures

1 Solvatochromic comparison of dyes 2 and 11b-e with dye 11a as reference.

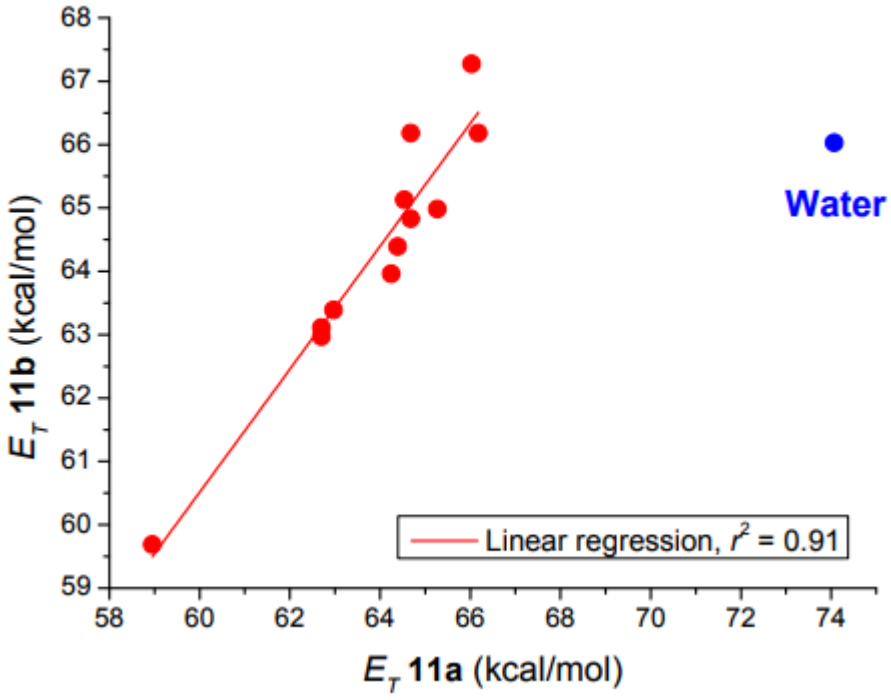


Figure 1: Linear plots of E_{T2} (11b) against E_{T2} (11a), in thirteen solvents, with values taken from Table 1 (main manuscript).

Back to List of Figures section

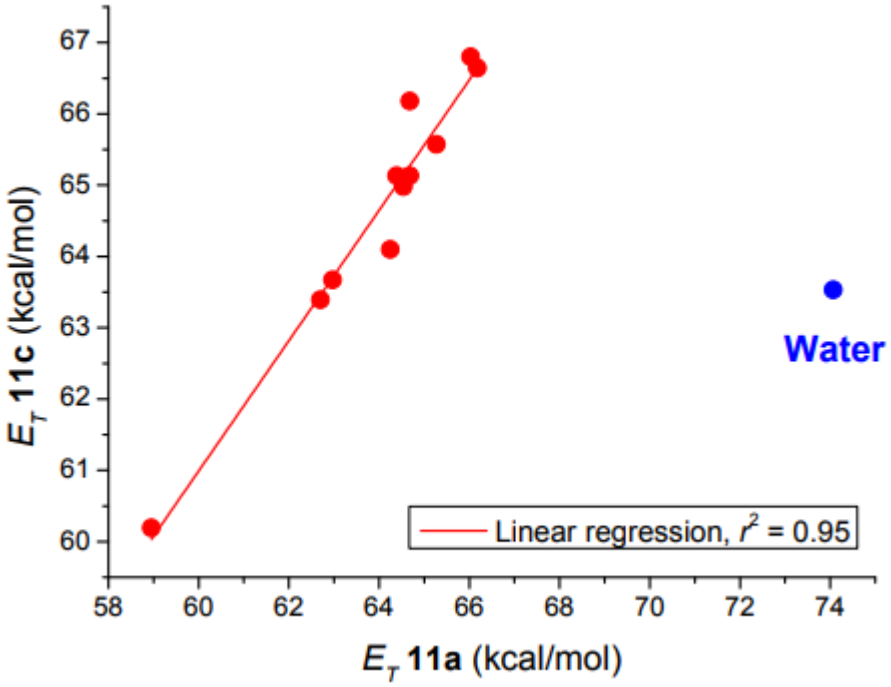


Figure 2: Linear plots of E_{T2} (11c) against E_{T2} (11a), in thirteen solvents, with values taken from Table 1 (main manuscript).

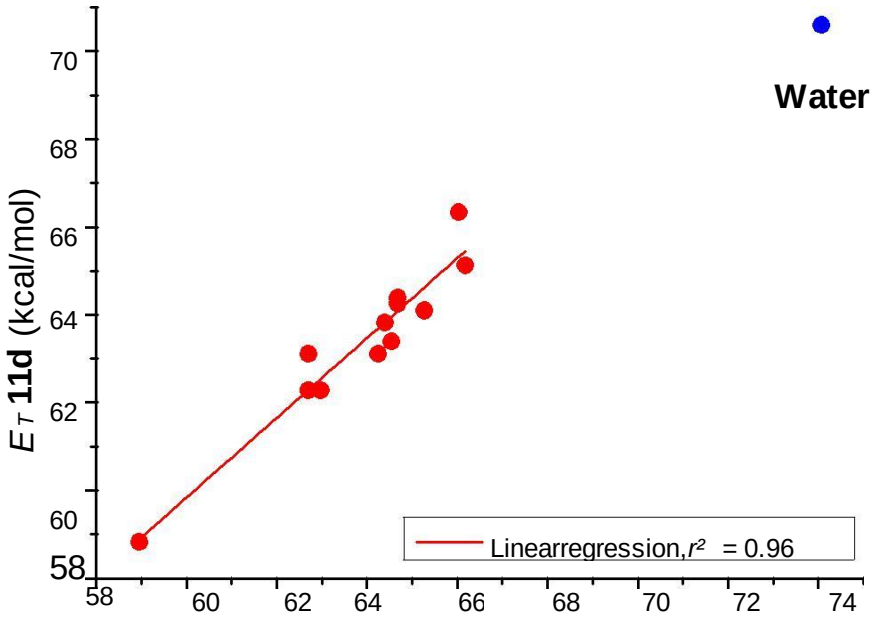


Figure 3: Linear plots of E_{T2} (11d) against E_{T2} (11a), in thirteen solvents, with values taken from Table 1 (main manuscript).

Back to List of Figures section

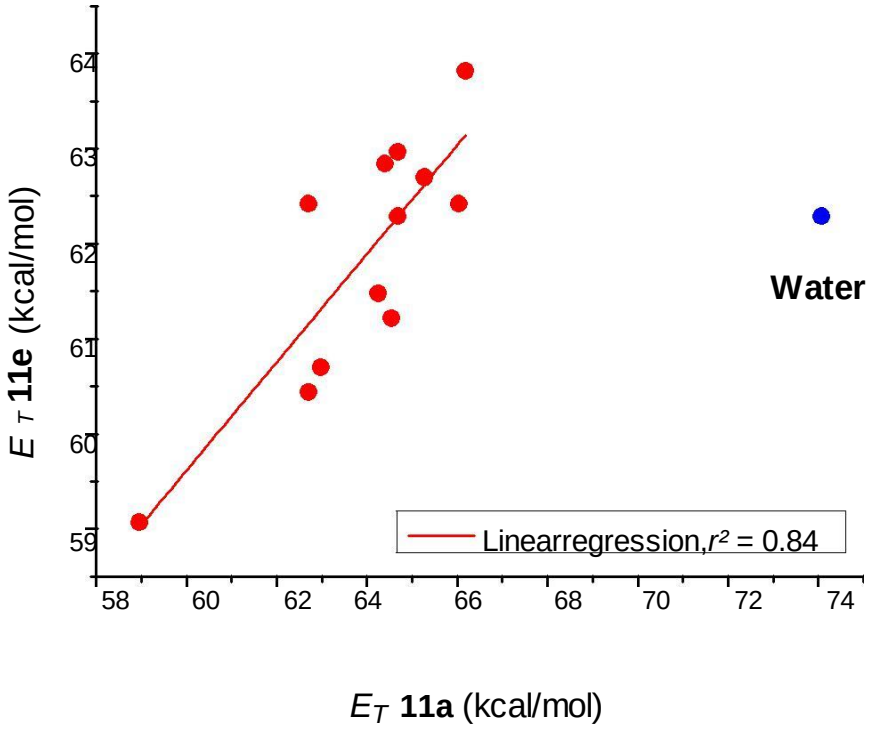


Figure 4: Linear plots of E_{T2} (11e) against E_{T2} (11a), in thirteen solvents, with values taken from Table 1 (main manuscript).

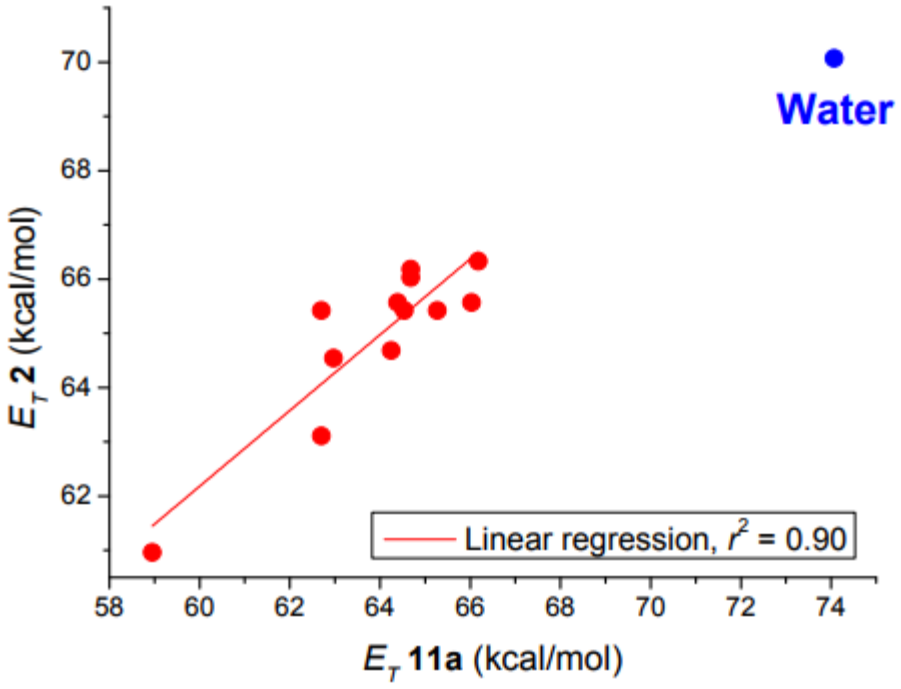


Figure 5: Linear plots of E_{T2} (2) against E_{T2} (11a), in thirteen solvents, with values taken from Table 1 (main manuscript).

Back to List of Figures section

2 Lambert-Beer plot of dye 11a in water solution.

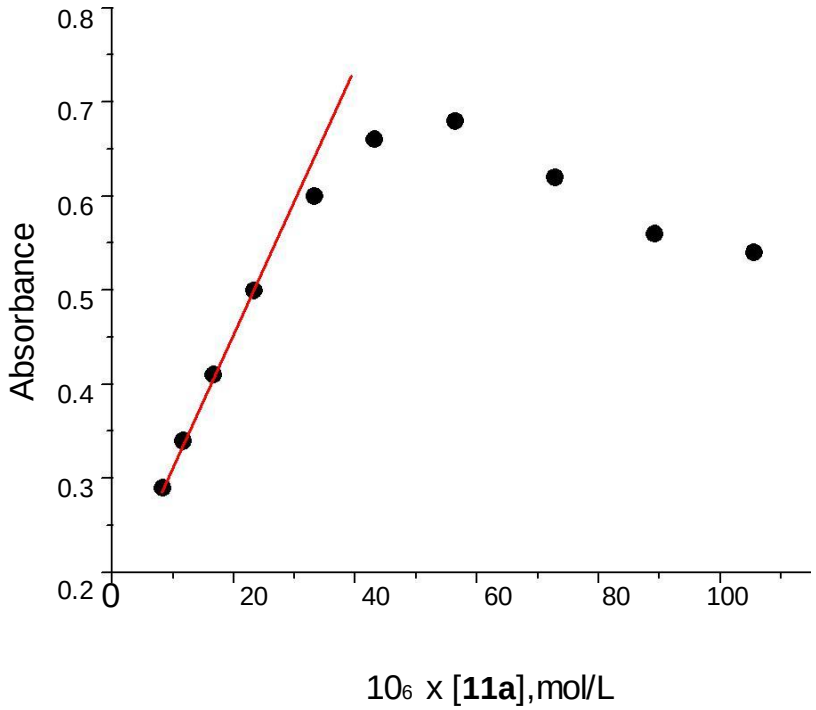


Figure 6: Non-linear Lambert-Beer plots of absorbance readings at 386 nm for increasing concentrations of dye 11a in water, as evidence of dye aggregation in this solvent.

Back to List of Figures section

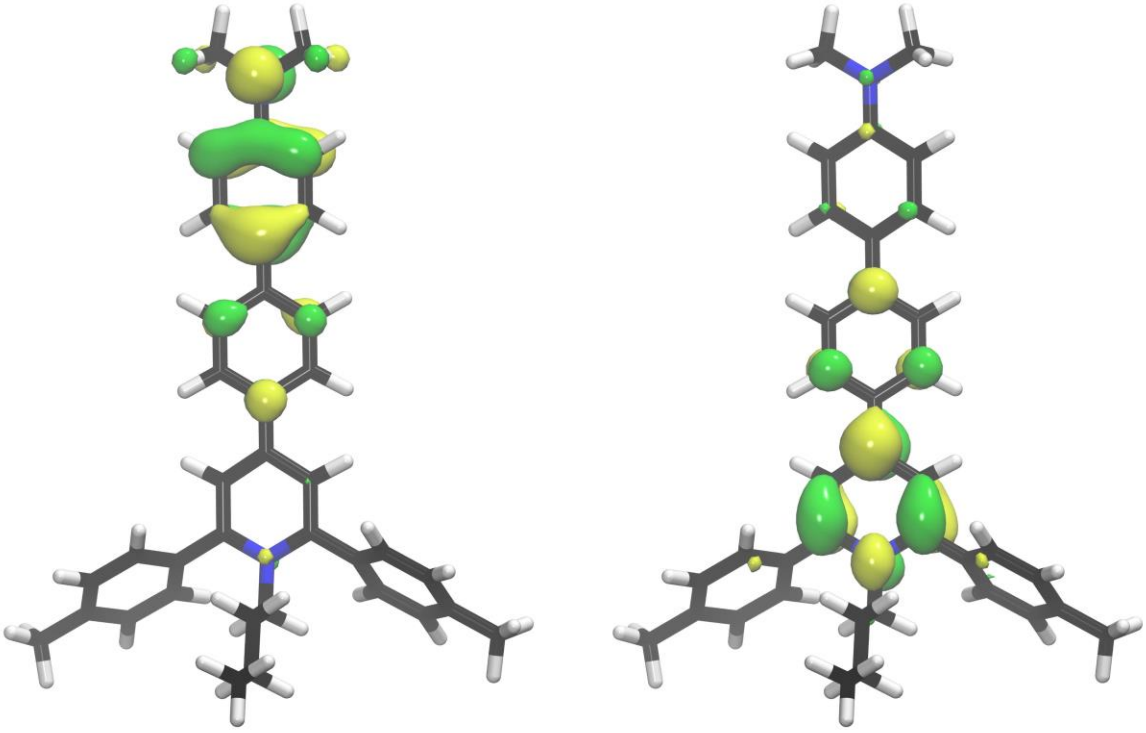
3 Calculated E_T of dyes 2 and 11a

Table 1: Calculated E_T values (kcal.mol-1) of dyes 2 and 11a with theTDDFT method at the B3LYP/6-31+G(d,p) SCRF=PCM level of theory.

Solvent	E_T^N	E_{T1} (2)	E_{T2} (2)	E_{T1} (11a)	E_{T2} (11a)
Water	1.000	51.63	86.24	52.35	85.87
Methanol	0.762	51.21	85.91	52.09	85.58
Ethanol	0.654	50.88	85.69	51.95	85.40
1-Propanol	0.617	50.63	85.51	51.83	85.27
1-Butanol	0.586	50.39	85.33	51.71	85.14
1-Octanol	0.537	49.40	84.60	51.25	84.62
Acetonitrile	0.460	51.21	85.93	52.12	85.61
Dimethylsulfoxide	0.444	51.22	85.95	52.19	85.66
N,N -Dimthylformamide	0.386	51.05	85.83	52.10	85.56
Dichloromethane	0.309	51.51	86.61	52.25	85.62

Back to List of Figures section

4 Frontier molecular orbitals images of dyes 11b-e in gas phase

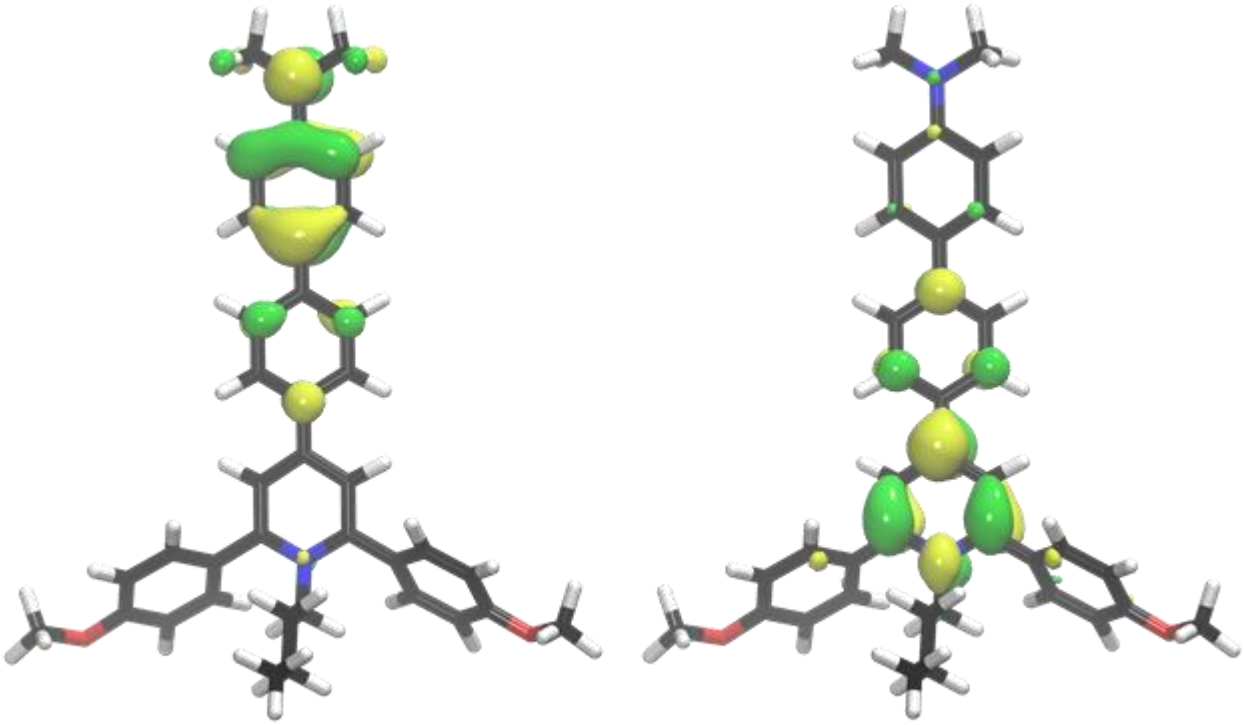


HOMO (**11b**) LUMO (**11b**)

Figure 7: HOMO and LUMO orbitals of dye 11b calculated at B3LYP/6-31+G(d,p) level of theory in gas phase.

Back to List of Figures section

Back to Contents section

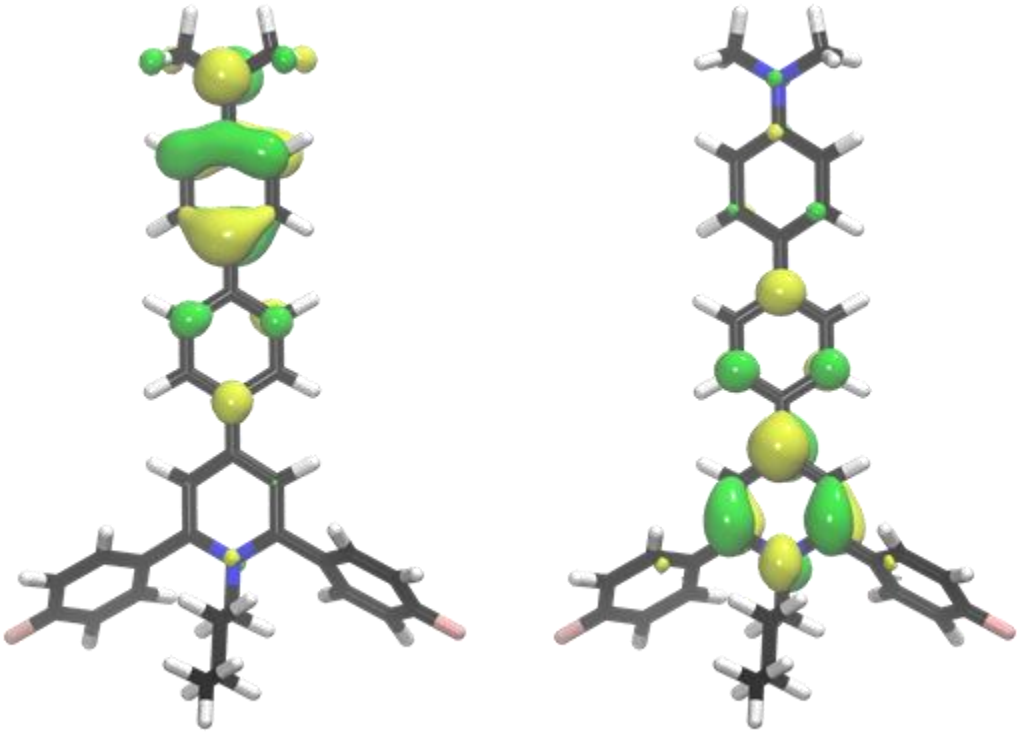


HOMO (**11c**) LUMO (**11c**)

Figure 8: HOMO and LUMO orbitals of dye 11c calculated at B3LYP/6-31+G(d,p) level of theory in gas phase.

Back to List of Figures section

Back to Contents section

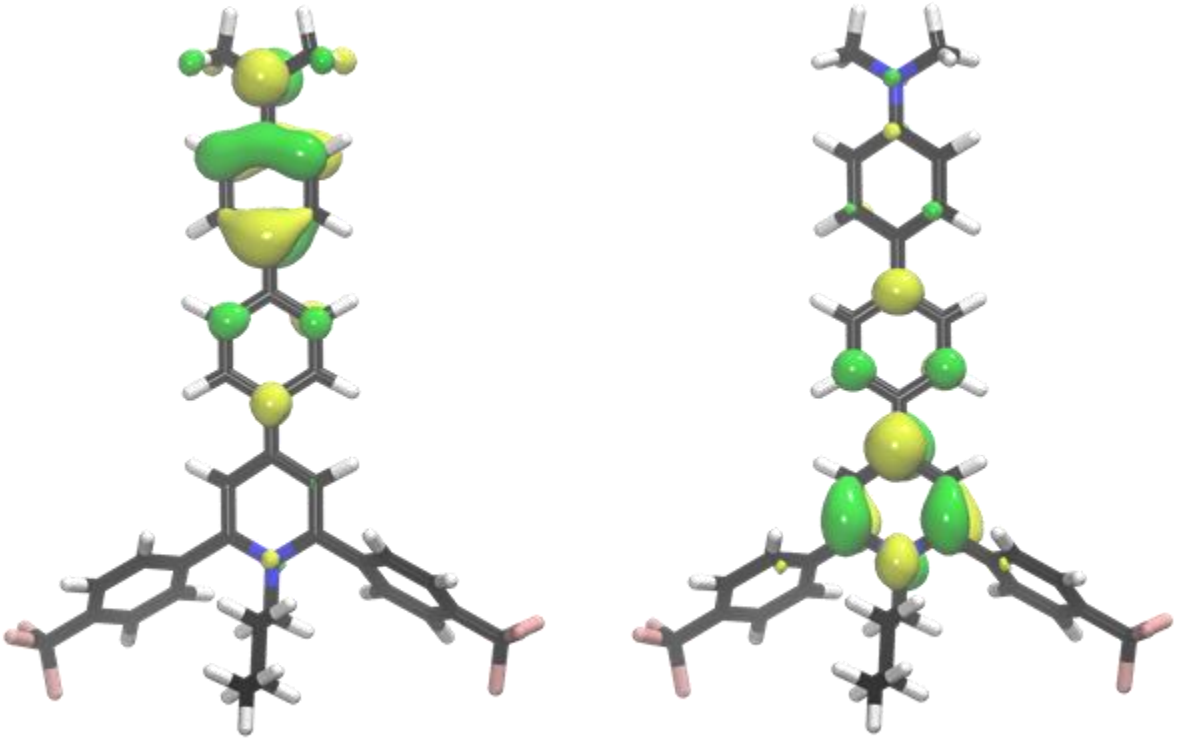


HOMO (**11d**) LUMO (**11d**)

Figure 9: HOMO and LUMO orbitals of dye 11d calculated at B3LYP/6-31+G(d,p) level of theory in gas phase.

Back to List of Figures section

Back to Contents section



HOMO (**11e**) LUMO (11e)

Figure 10: HOMO and LUMO orbitals of dye 11e calculated at B3LYP/6-31+G(d,p) level of theory in gas phase.

Back to List of Figures section

Back to Contents section

^{1}H NMR and ^{13}C NMR of new compounds 14b-e, 15a-e and 11a-e.

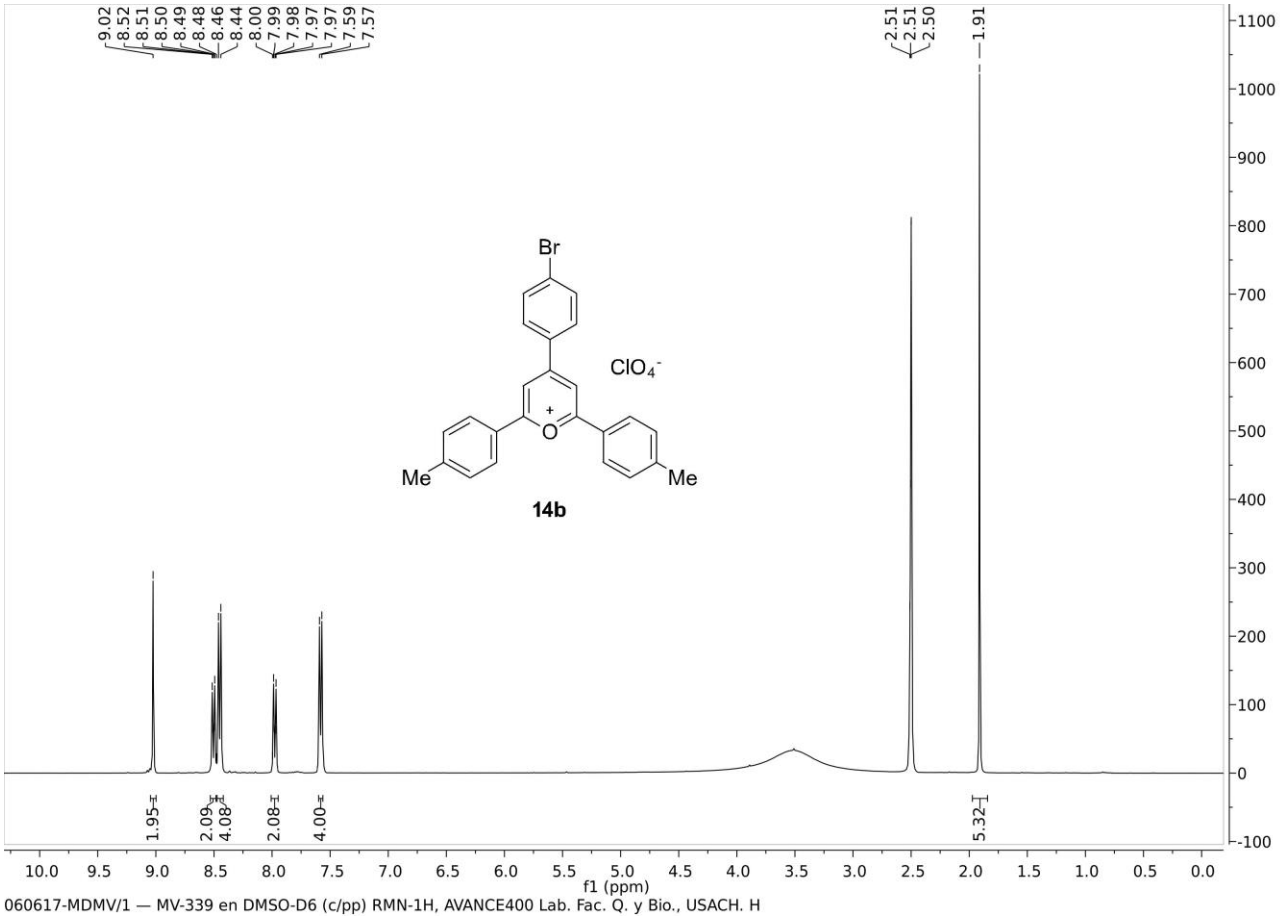


Figure 11: ^{1}H NMR spectrum of compound 14b in DMSO-d6.
Back to List of Figures section

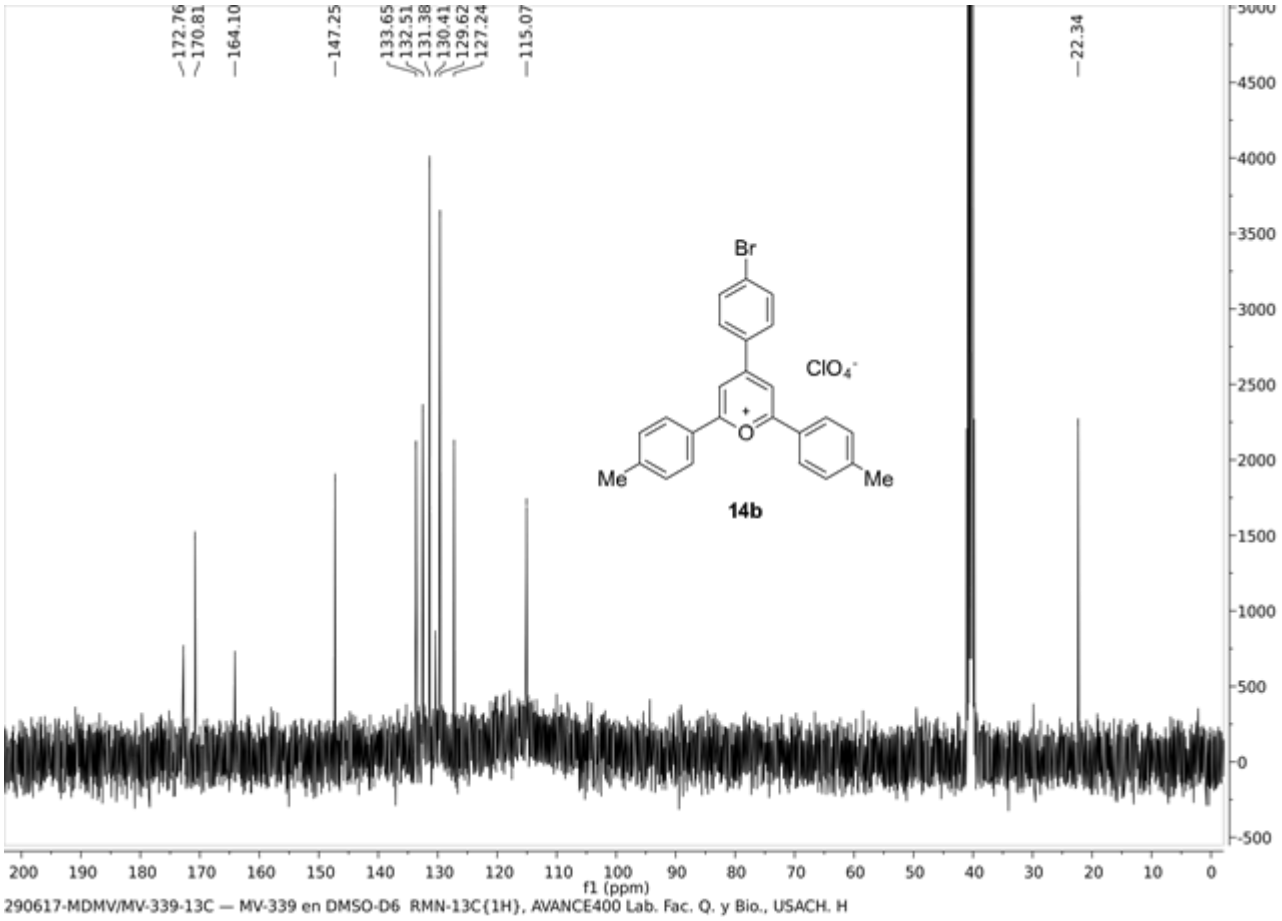


Figure 12: ^{13}C NMR spectrum of compound 14b in DMSO-d6.
Back to List of Figures section

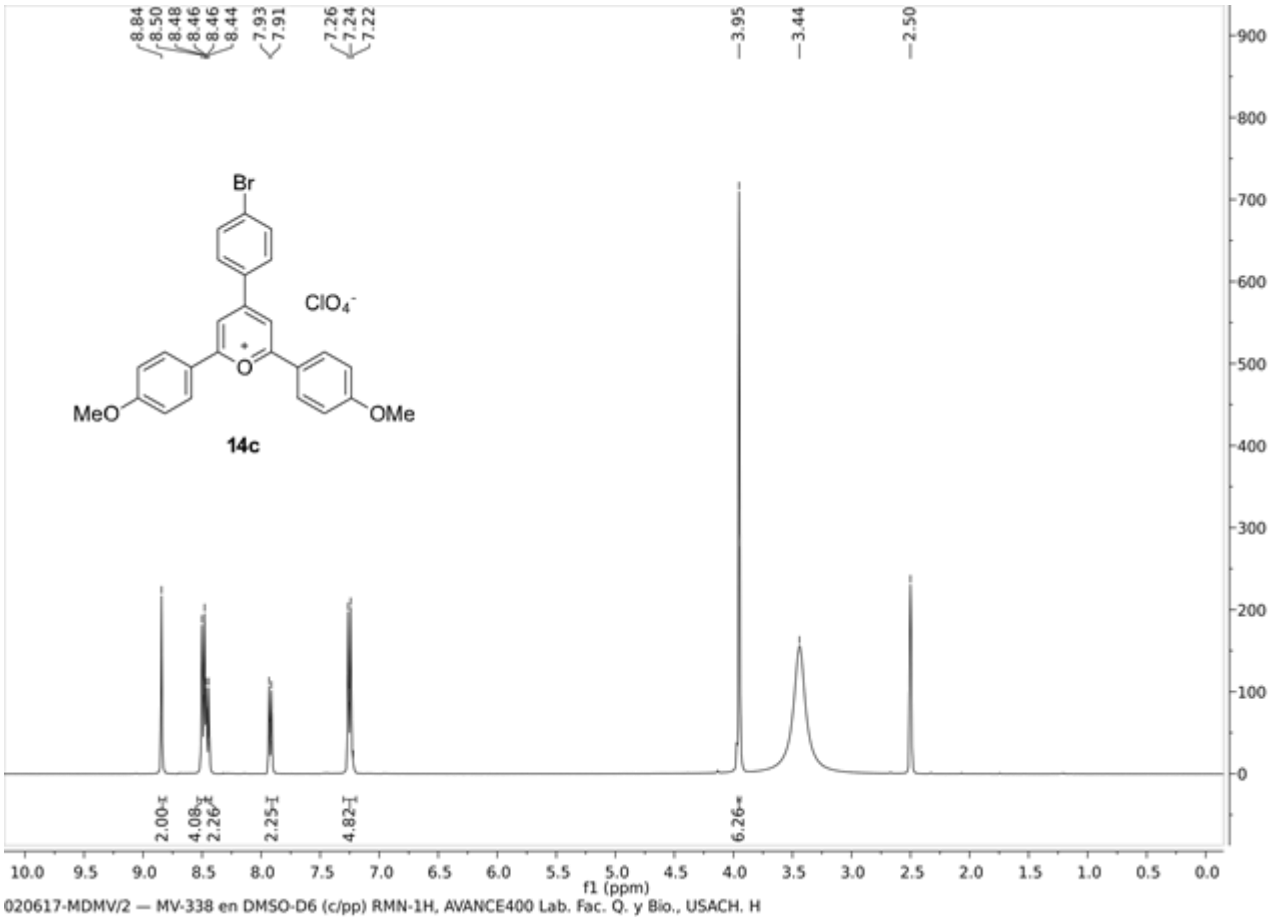


Figure 13: ^{1}H NMR spectrum of compound 14c in DMSO-d6.
Back to List of Figures section

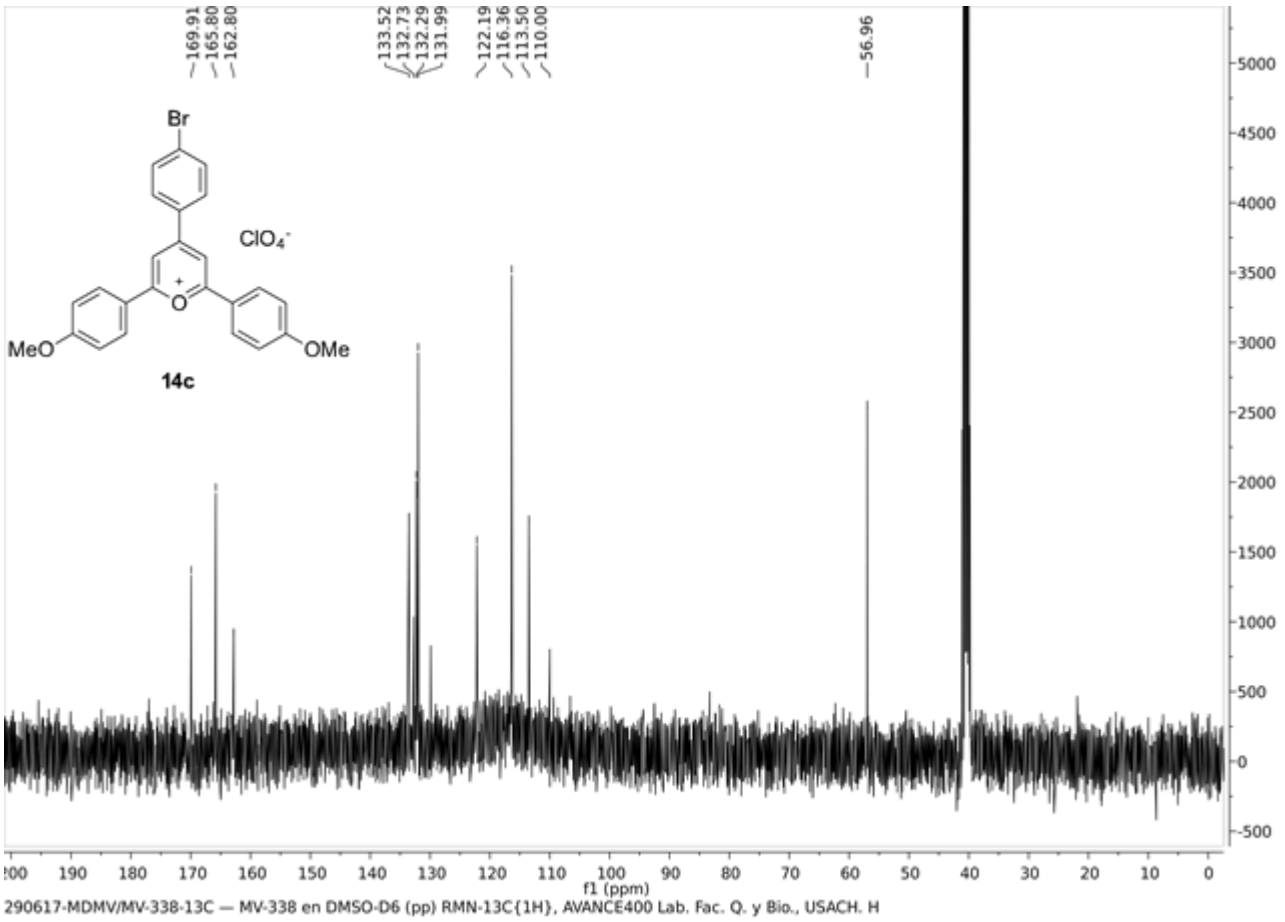


Figure 14: ^{13}C NMR spectrum of compound 14c in DMSO-d6.
Back to List of Figures section

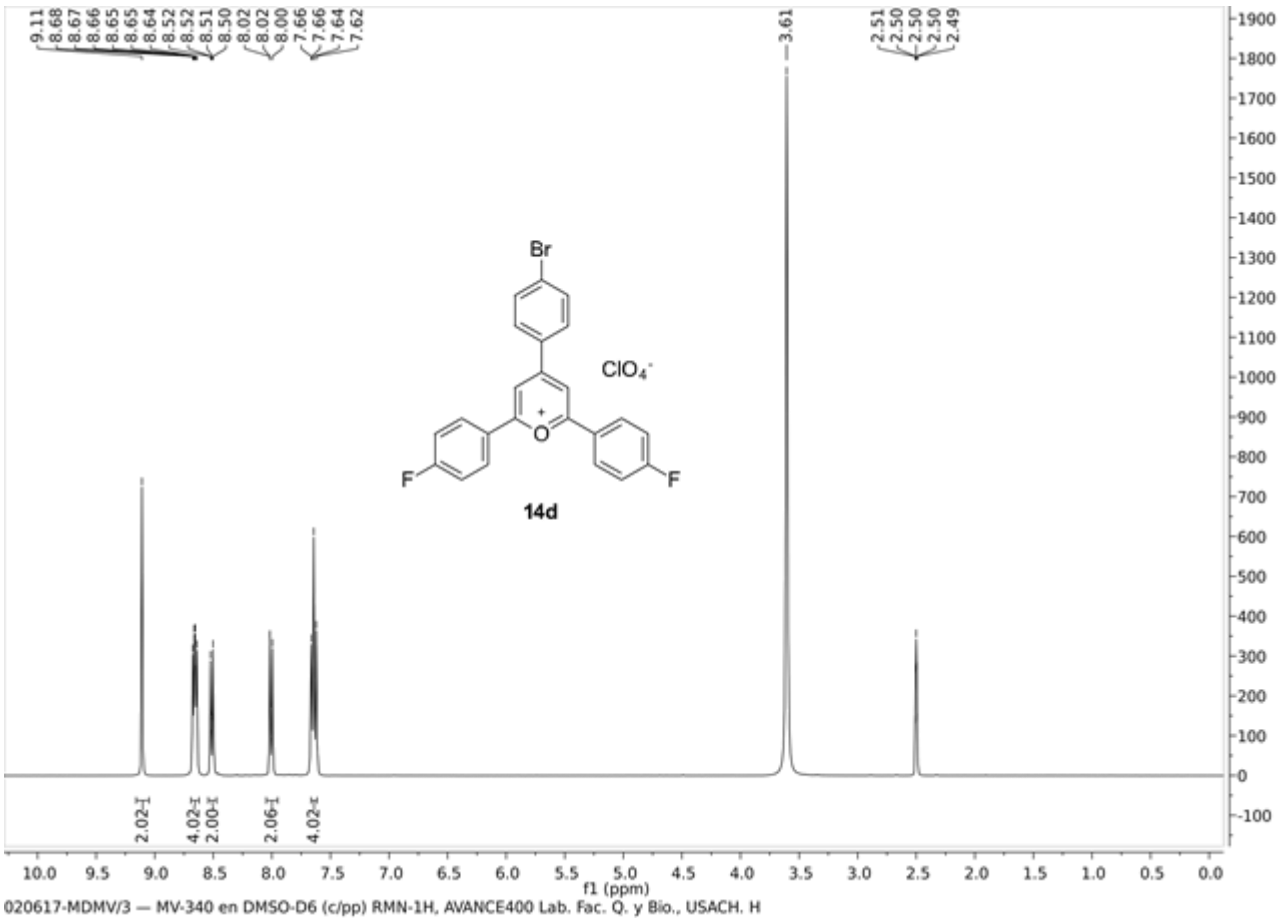


Figure 15: ^{1}H NMR spectrum of compound 14d in DMSO-d6.
Back to List of Figures section

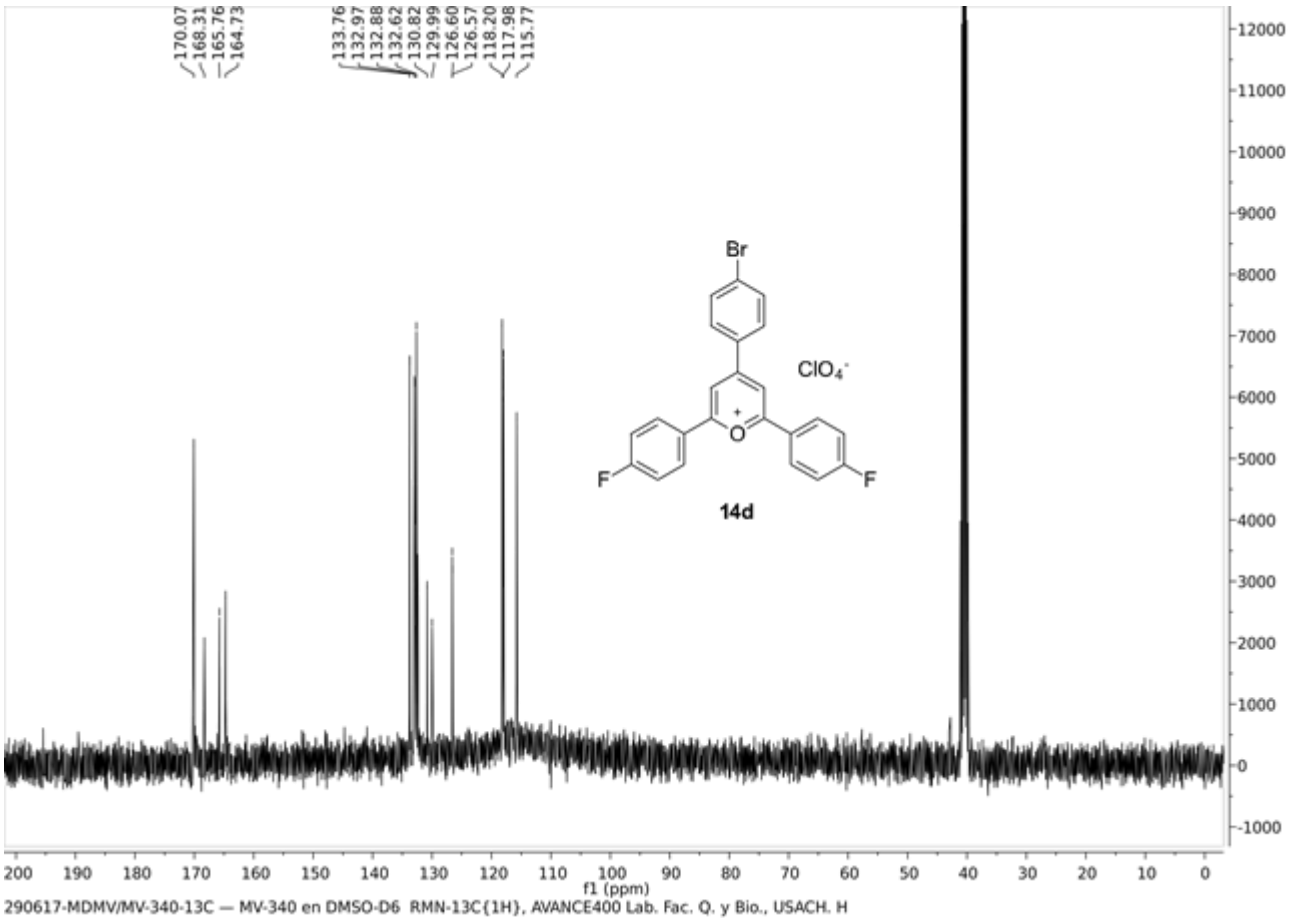


Figure 16: ^{13}C NMR spectrum of compound 14d in DMSO-d6.

Back to List of Figures section

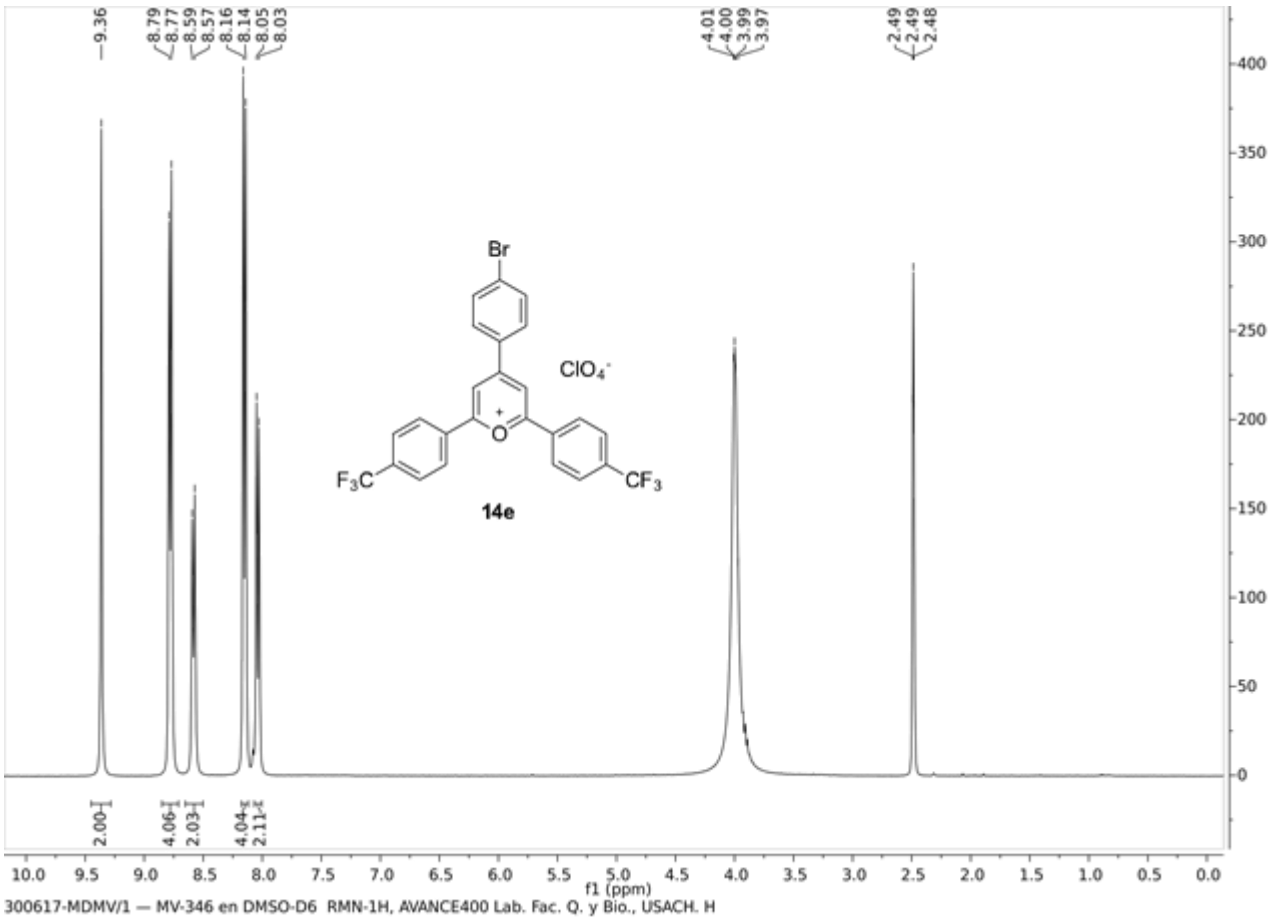


Figure 17: ^{1}H NMR spectrum of compound 14e in DMSO-d6.
Back to List of Figures section

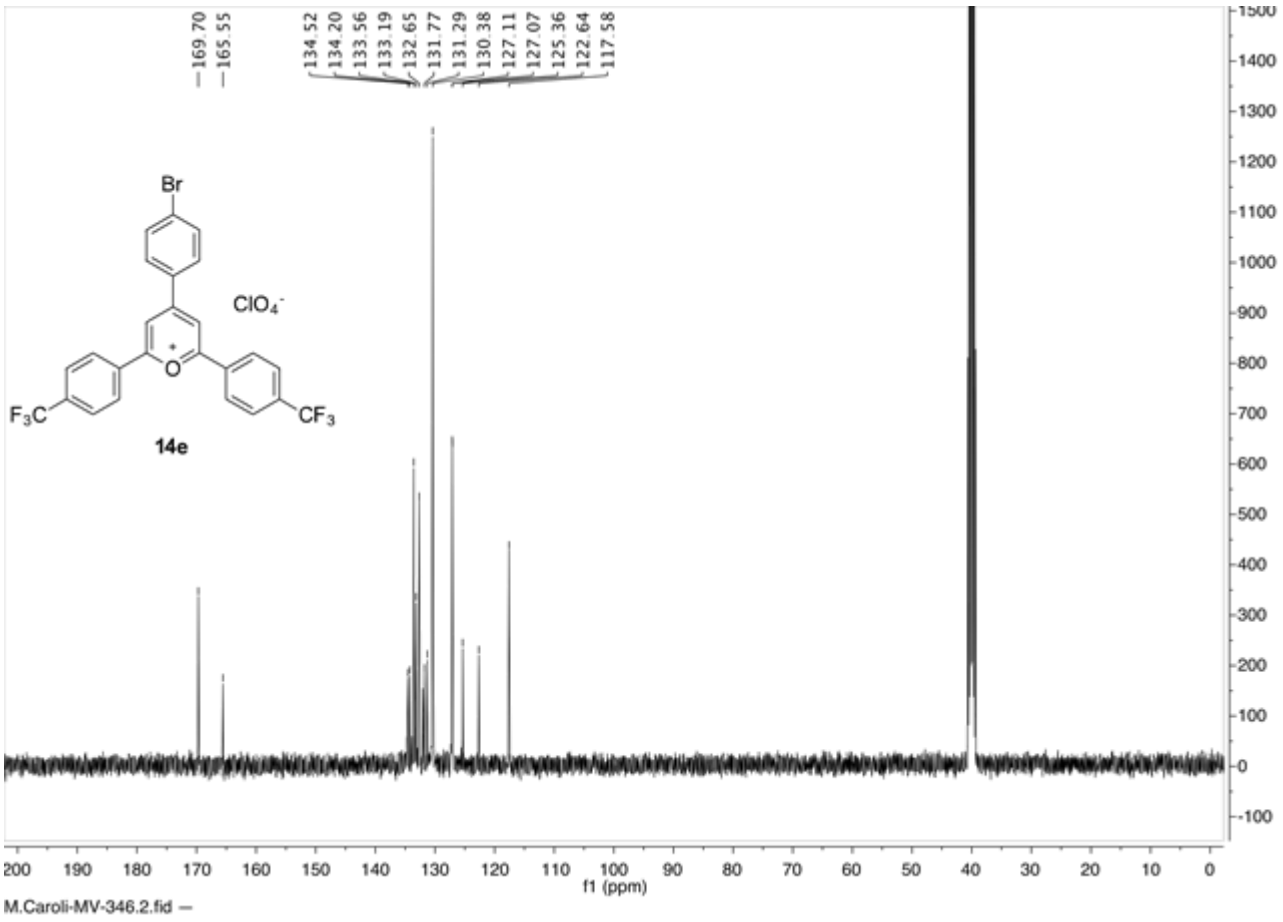


Figure 18: ^{13}C NMR spectrum of compound 14e in DMSO-d6.
Back to List of Figures section

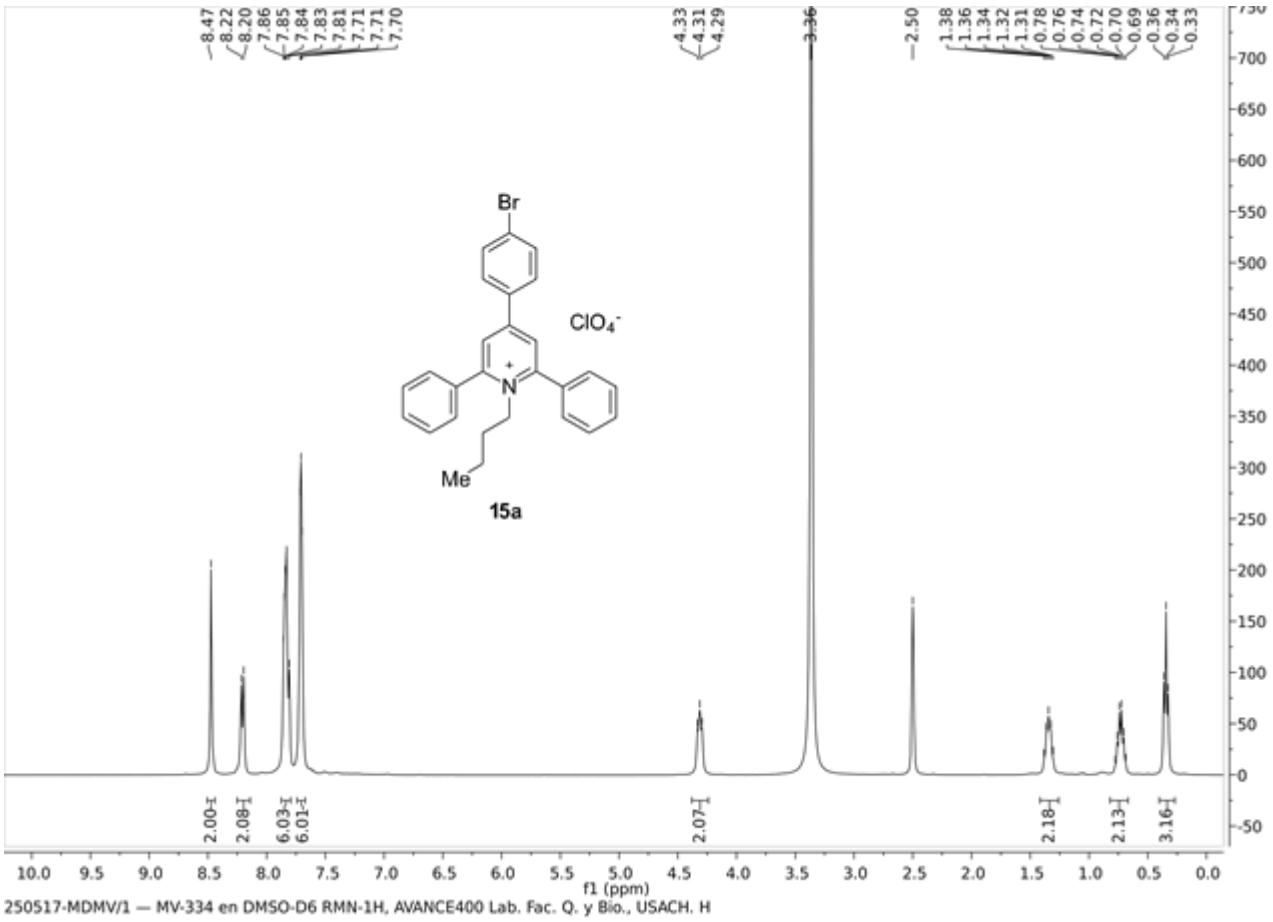


Figure 19: ^{1}H NMR spectrum of compound 15a in DMSO-d6.
Back to List of Figures section

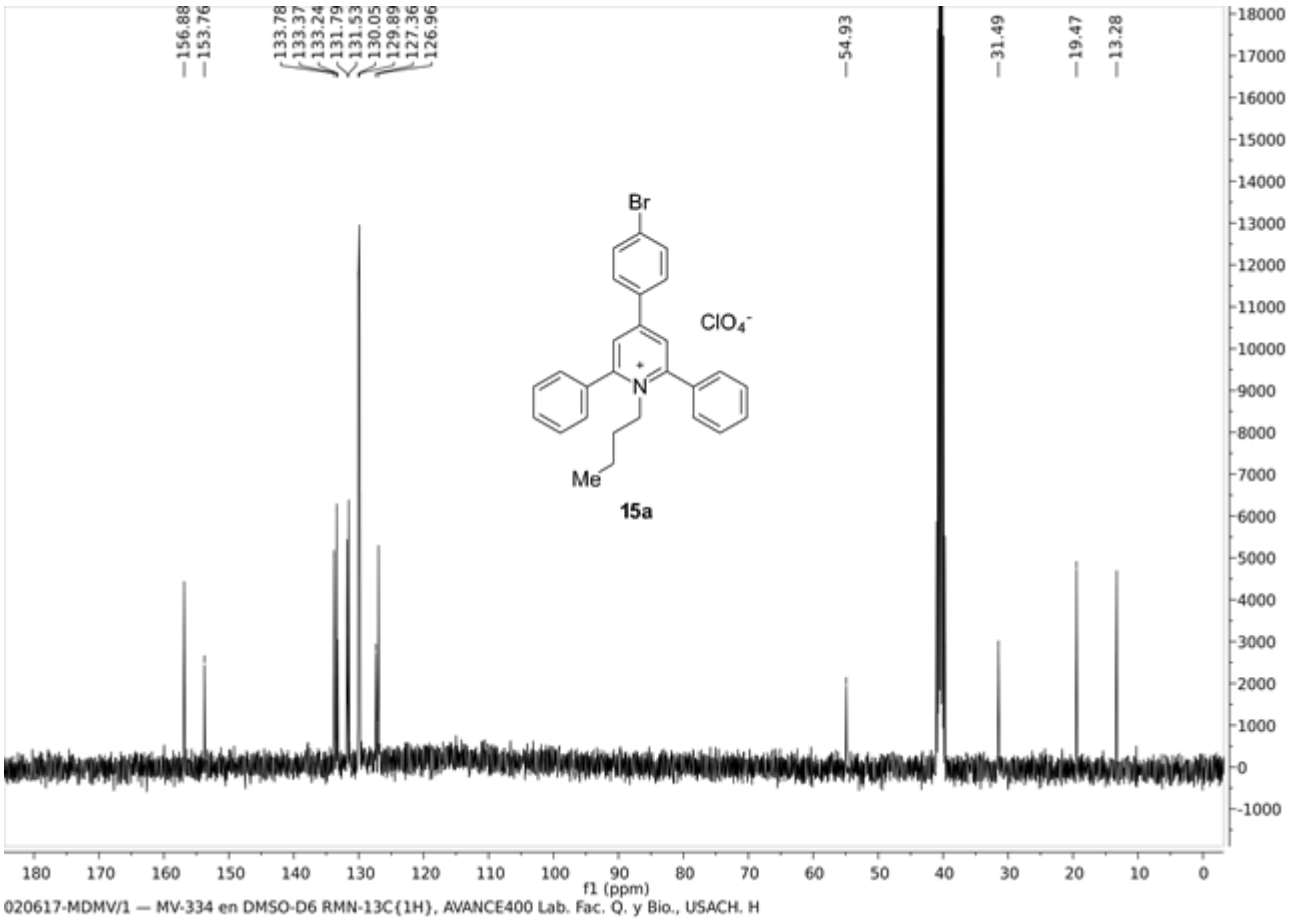


Figure 20: ^{13}C NMR spectrum of compound 14b in DMSO-d6.
Back to List of Figures section

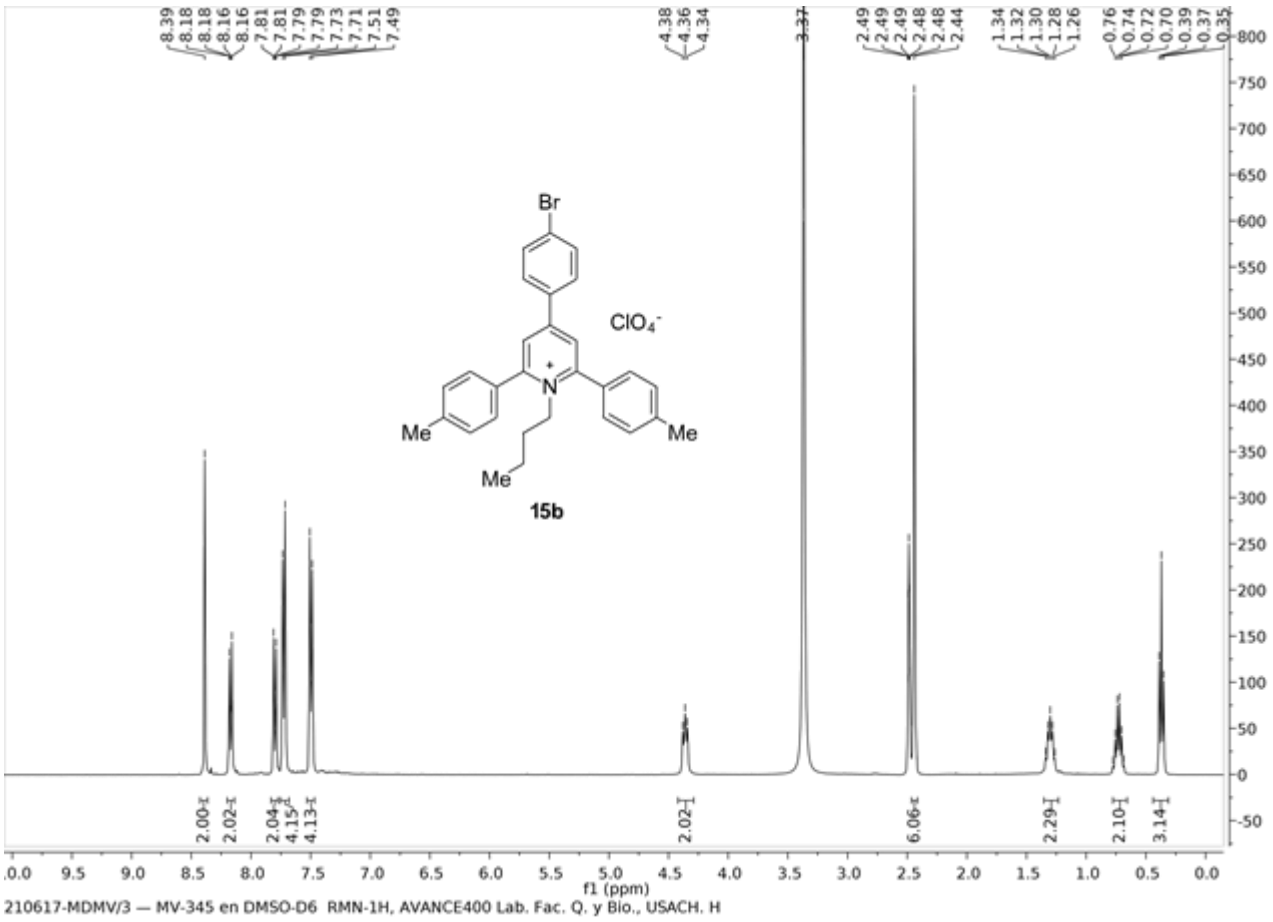


Figure 21: ^{1}H NMR spectrum of compound 15b in DMSO-d6.
Back to List of Figures section

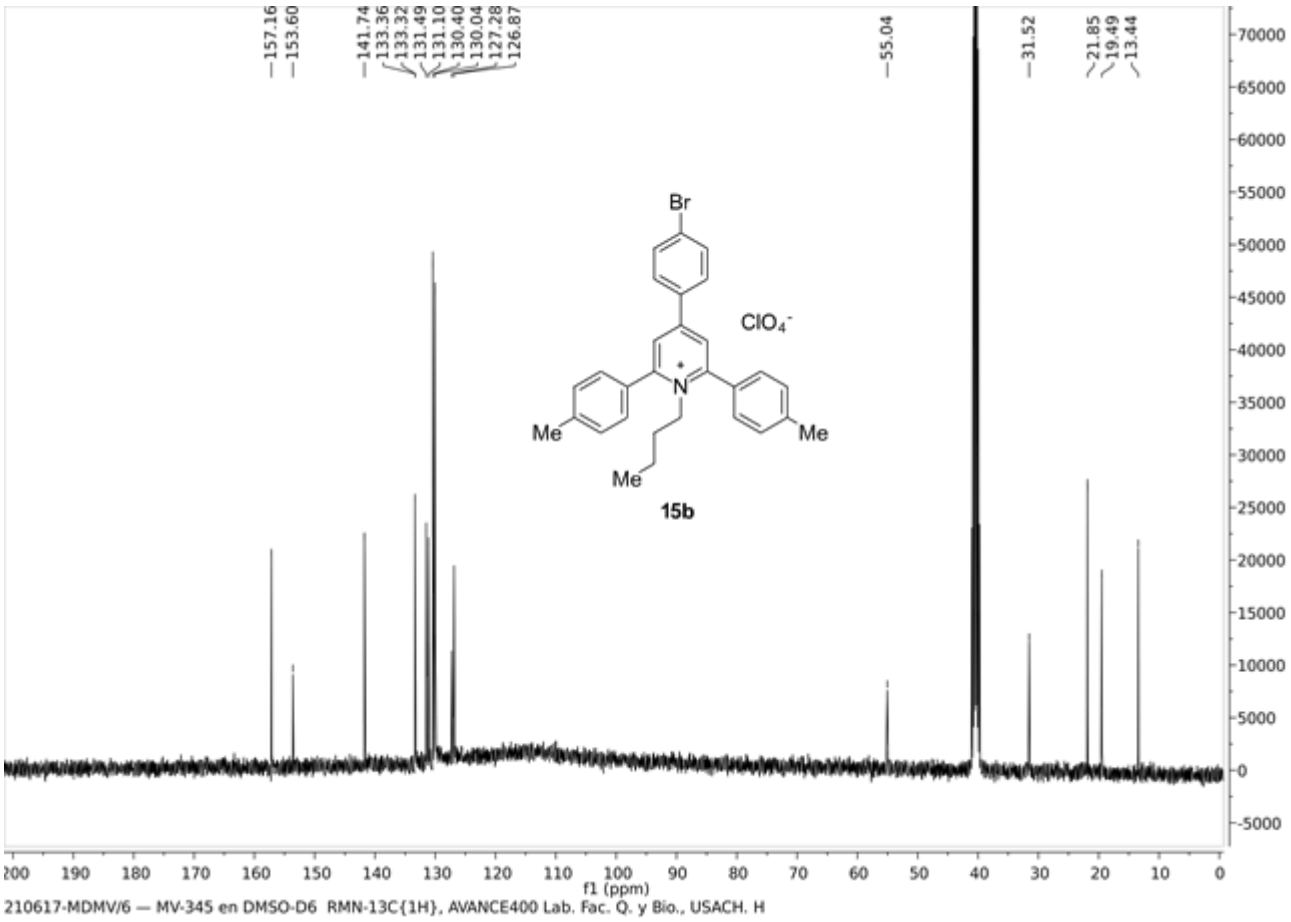


Figure 22: ^{13}C NMR spectrum of compound 15b in DMSO-d6.

Back to List of Figures section

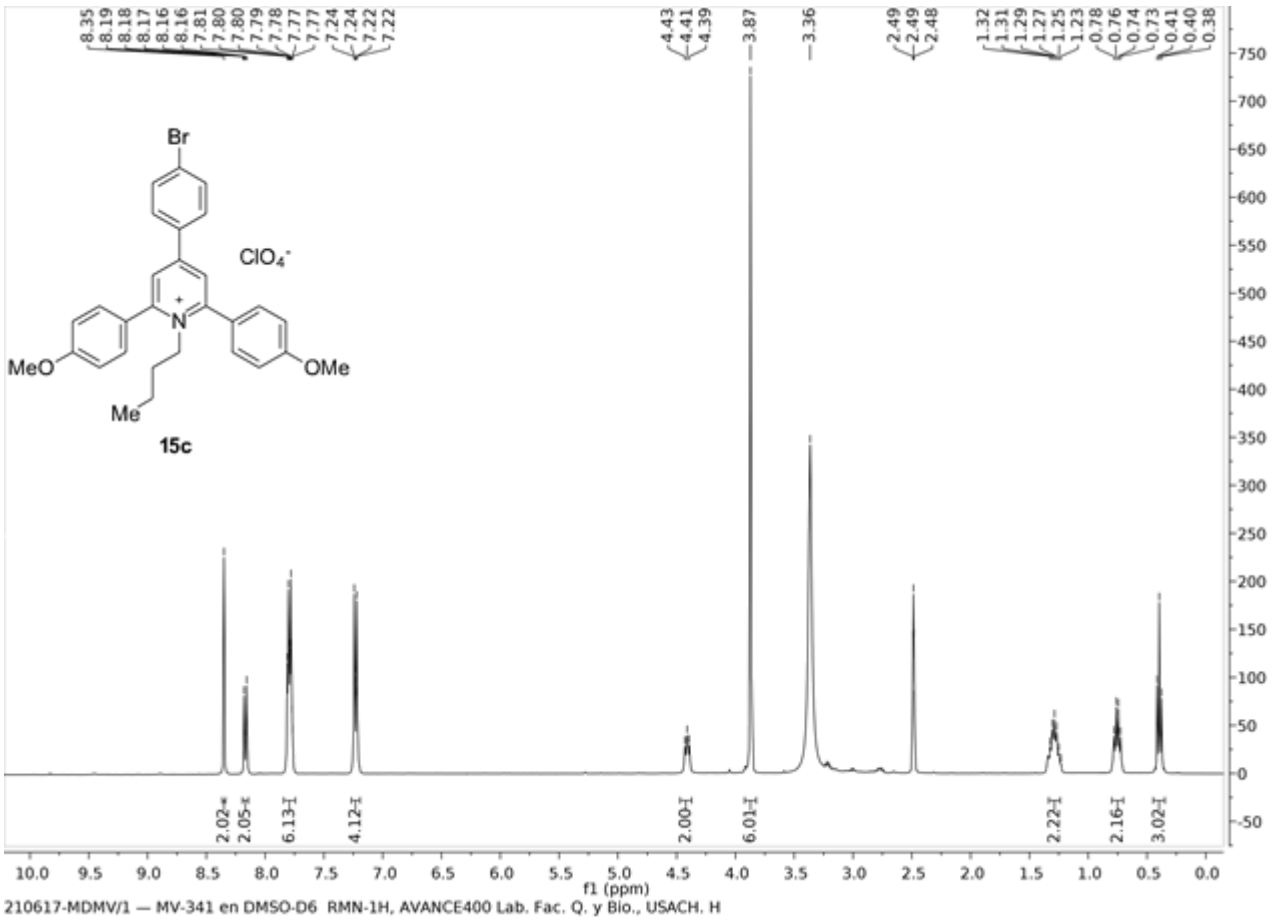


Figure 23: ^{1}H NMR spectrum of compound 15c in DMSO-d6.
Back to List of Figures section

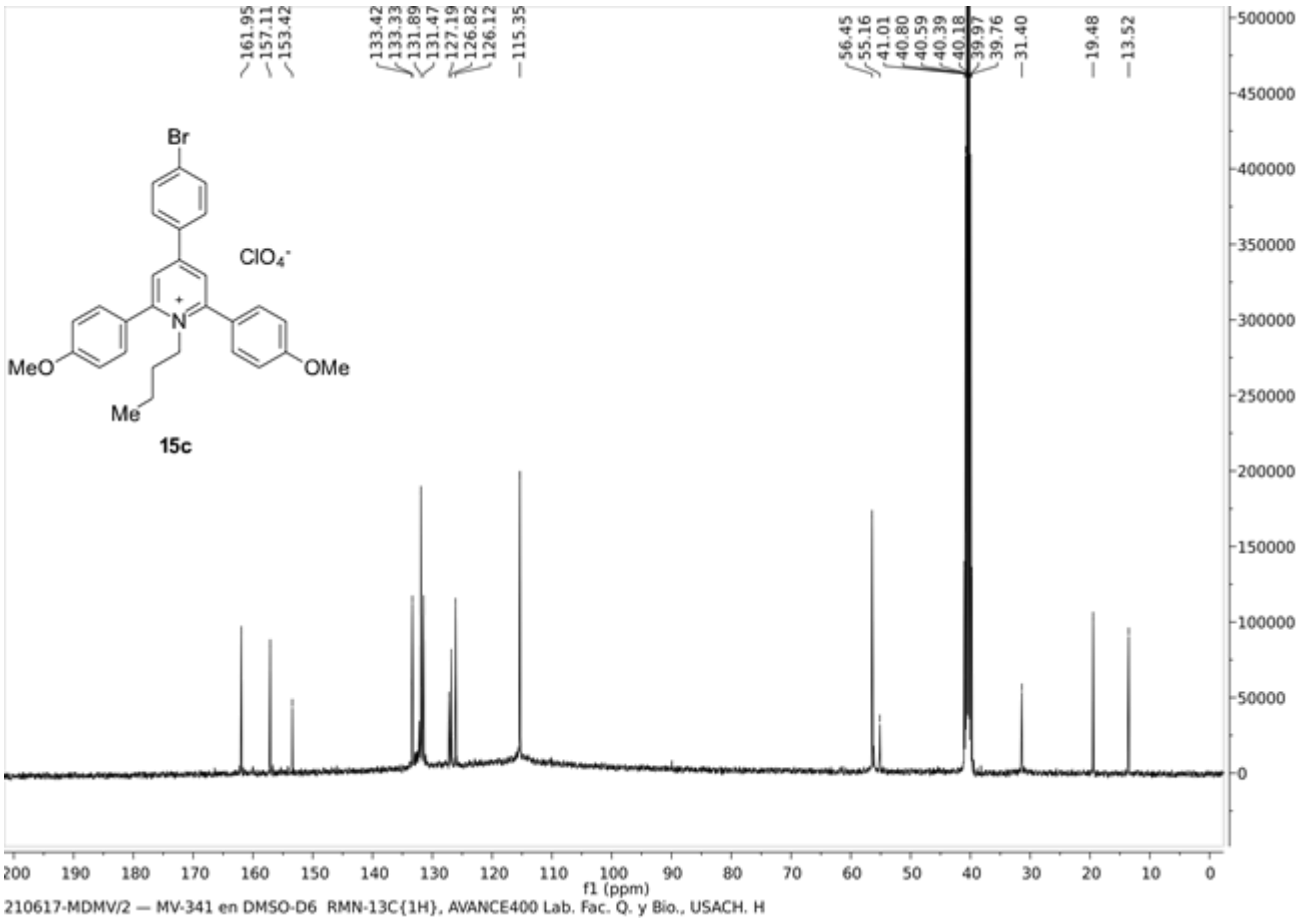


Figure 24: ^{13}C NMR spectrum of compound 15c in DMSO-d6.
Back to List of Figures section

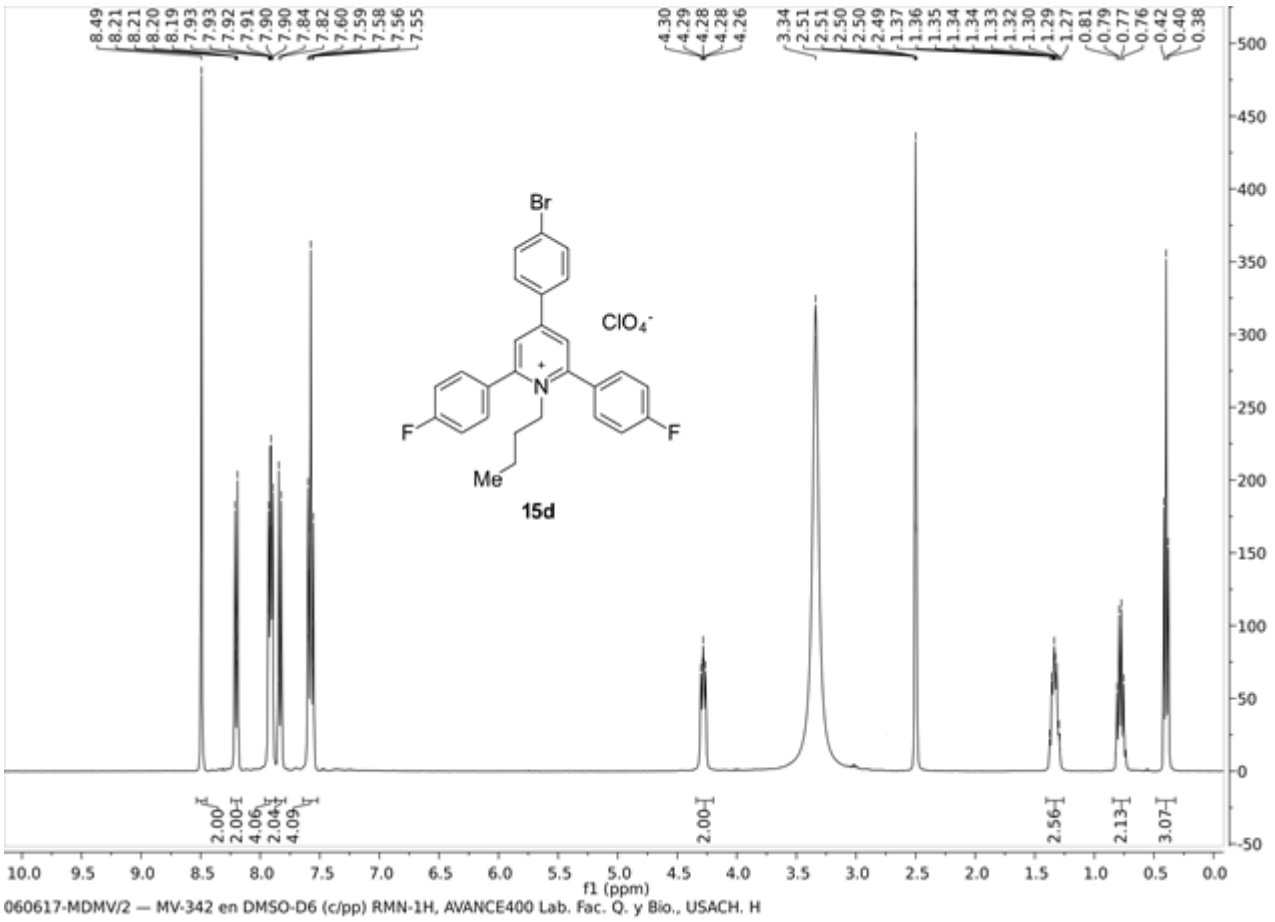


Figure 25: ^{1}H NMR spectrum of compound 15d in DMSO-d6.
Back to List of Figures section

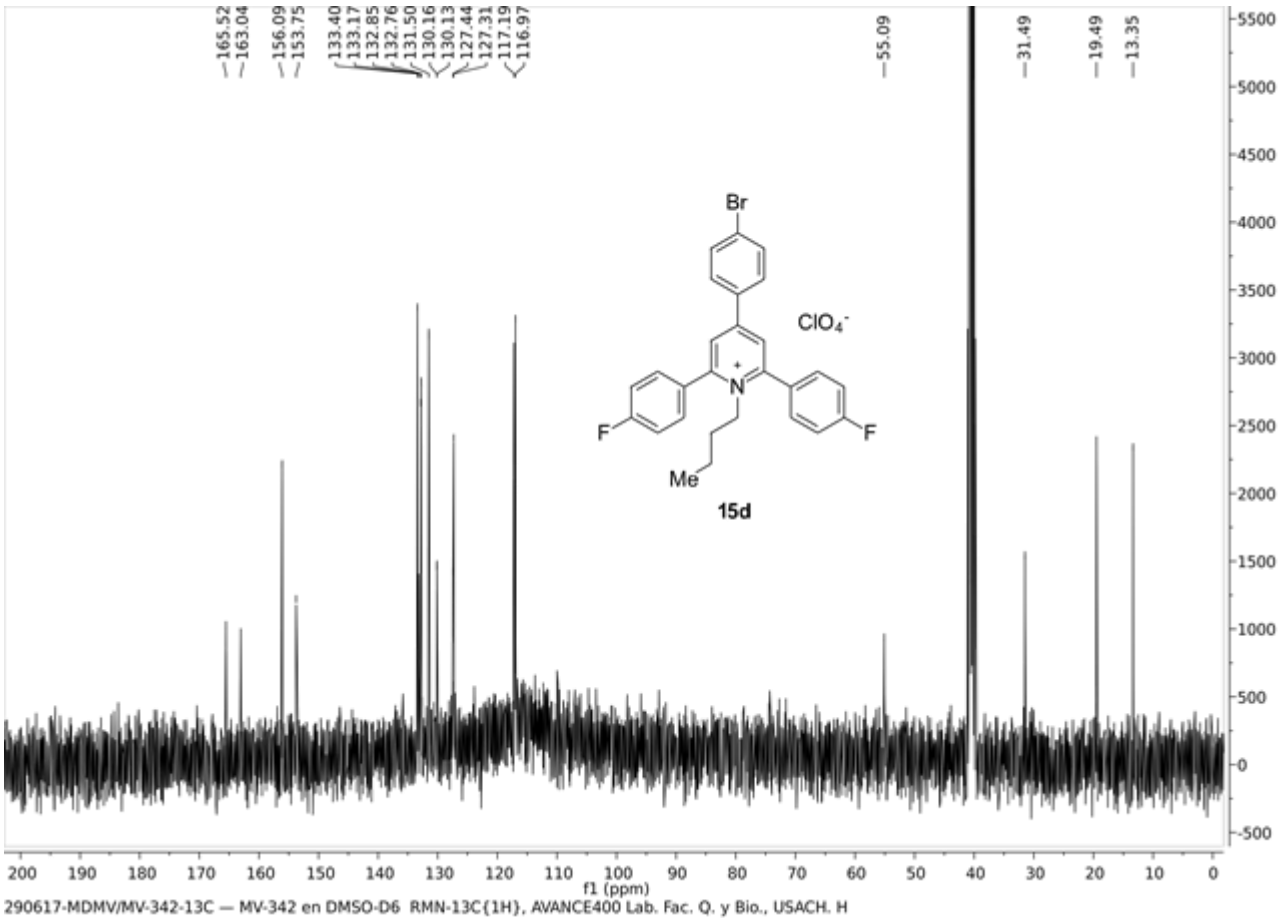


Figure 26: ^{13}C NMR spectrum of compound 15d in DMSO-d6.

Back to List of Figures section

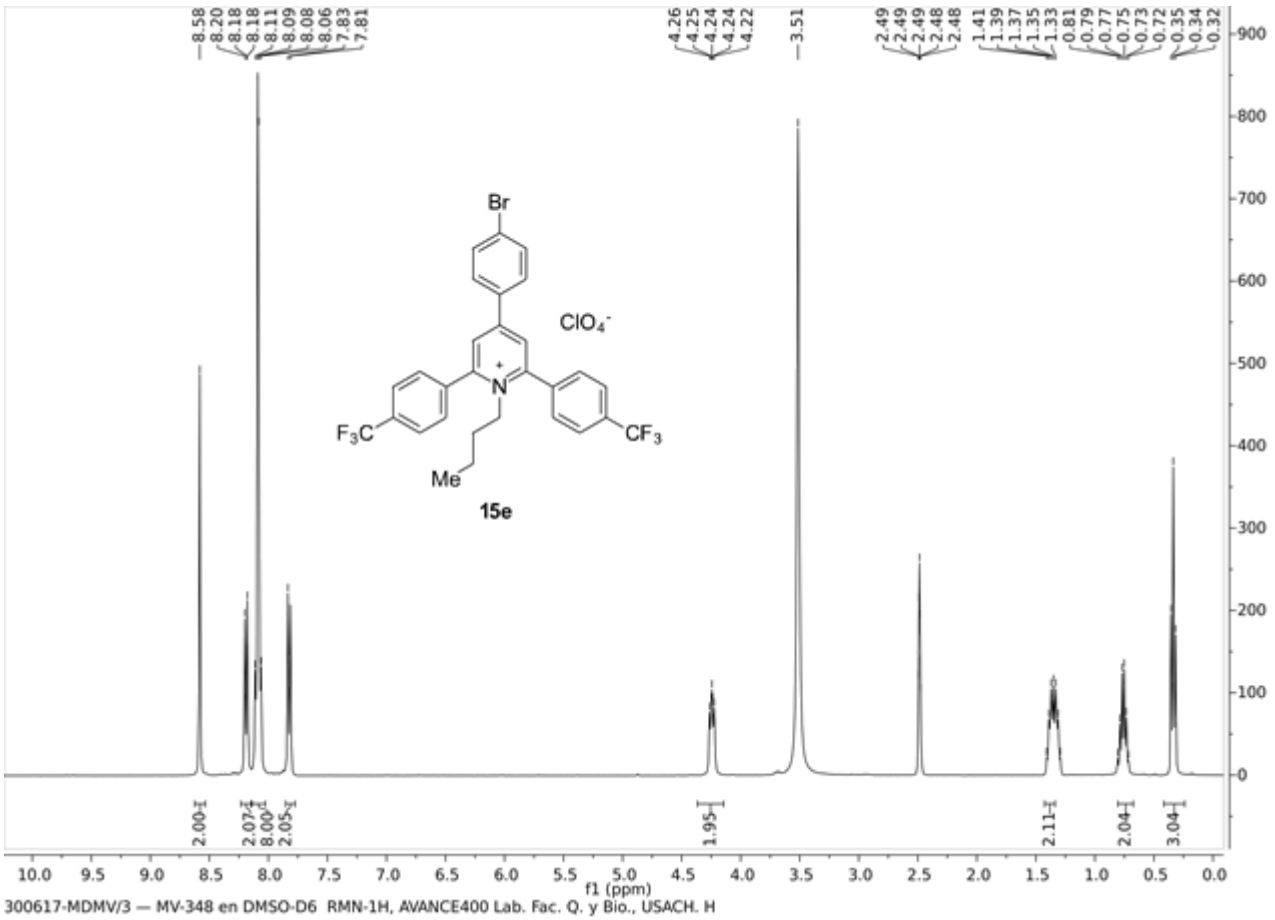


Figure 27: ^{1}H NMR spectrum of compound 15e in DMSO-d6.
Back to List of Figures section

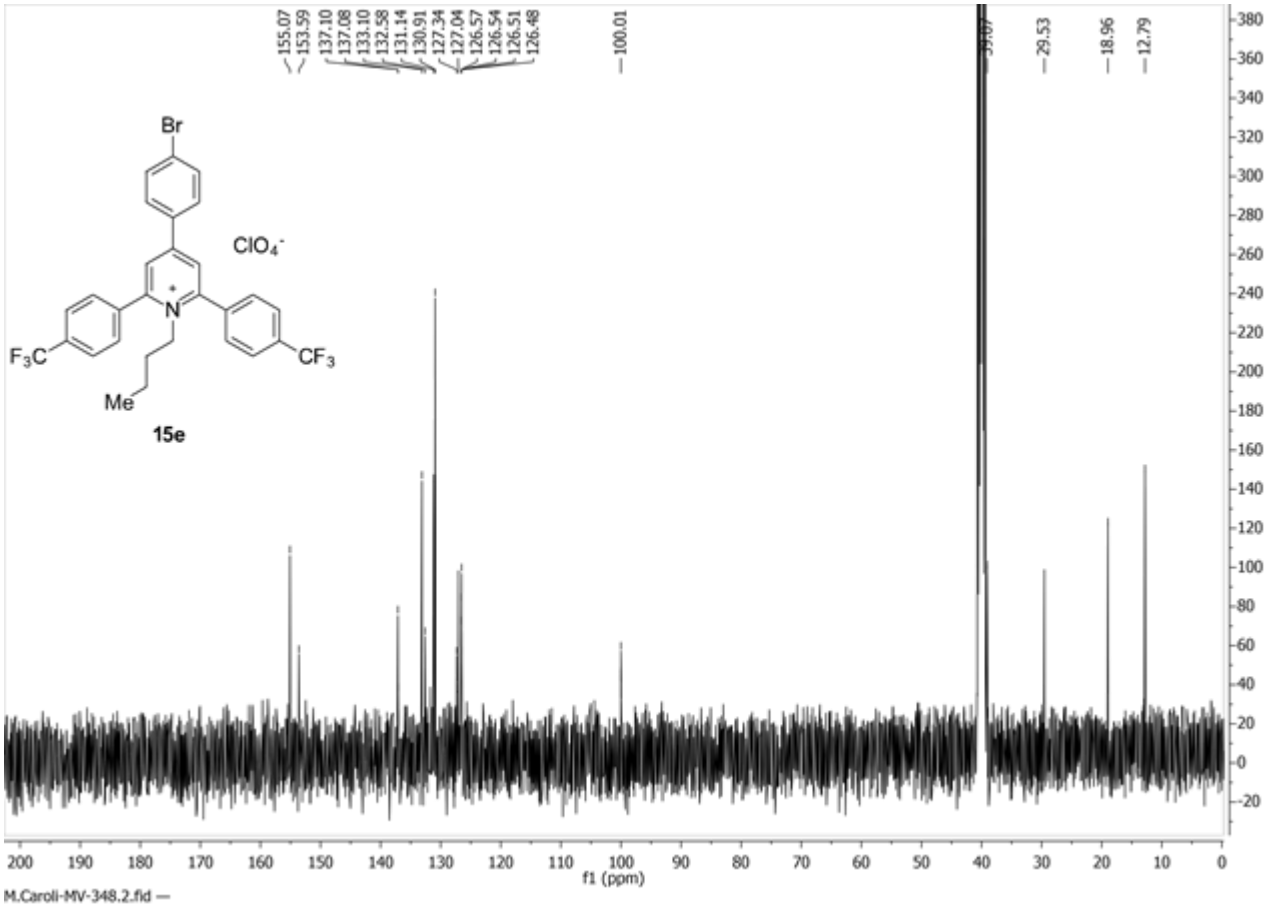


Figure 28: ^{13}C NMR spectrum of compound 15e in DMSO-d6.

Back to List of Figures section

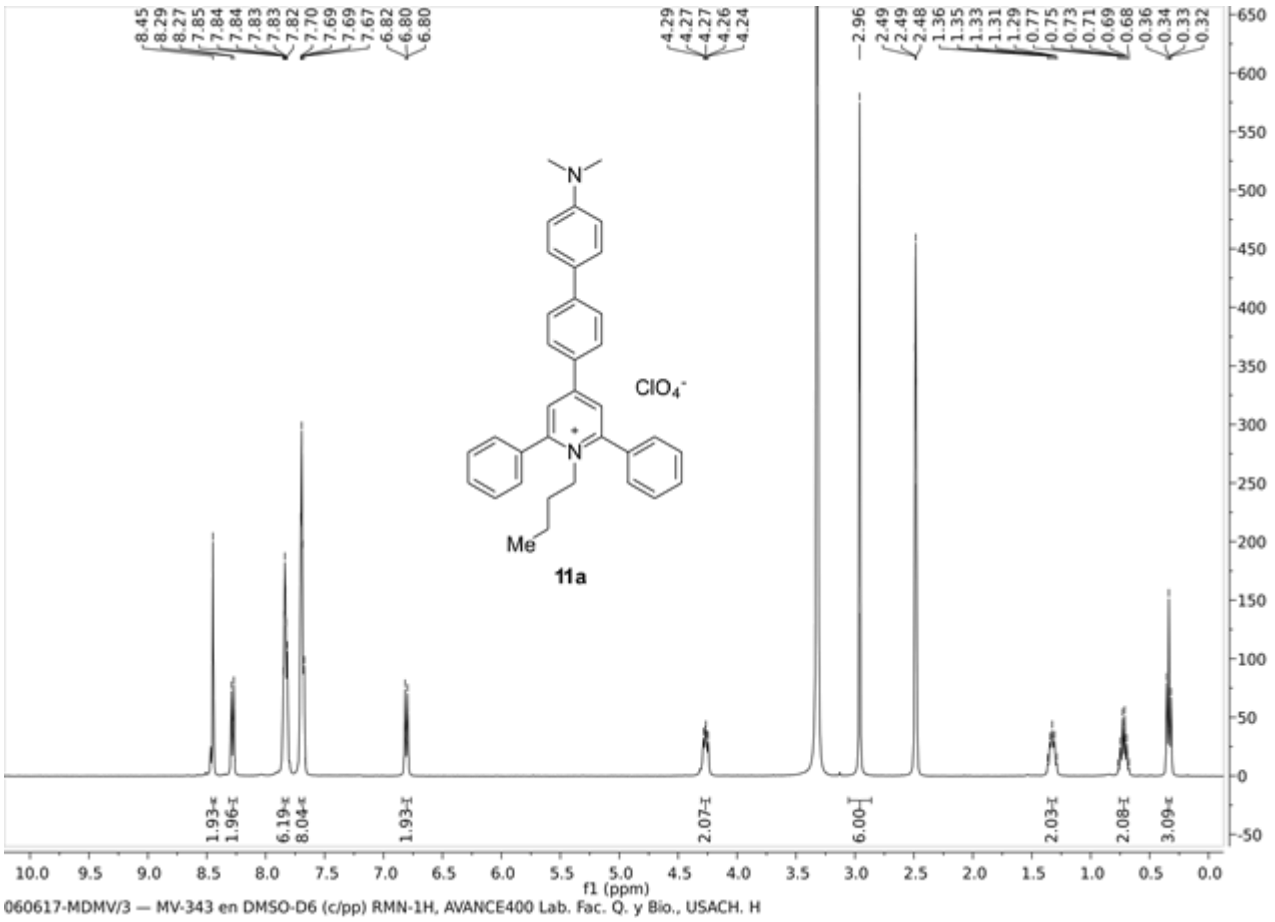


Figure 29: ^{1}H NMR spectrum of compound 11a in DMSO-d6.
Back to List of Figures section

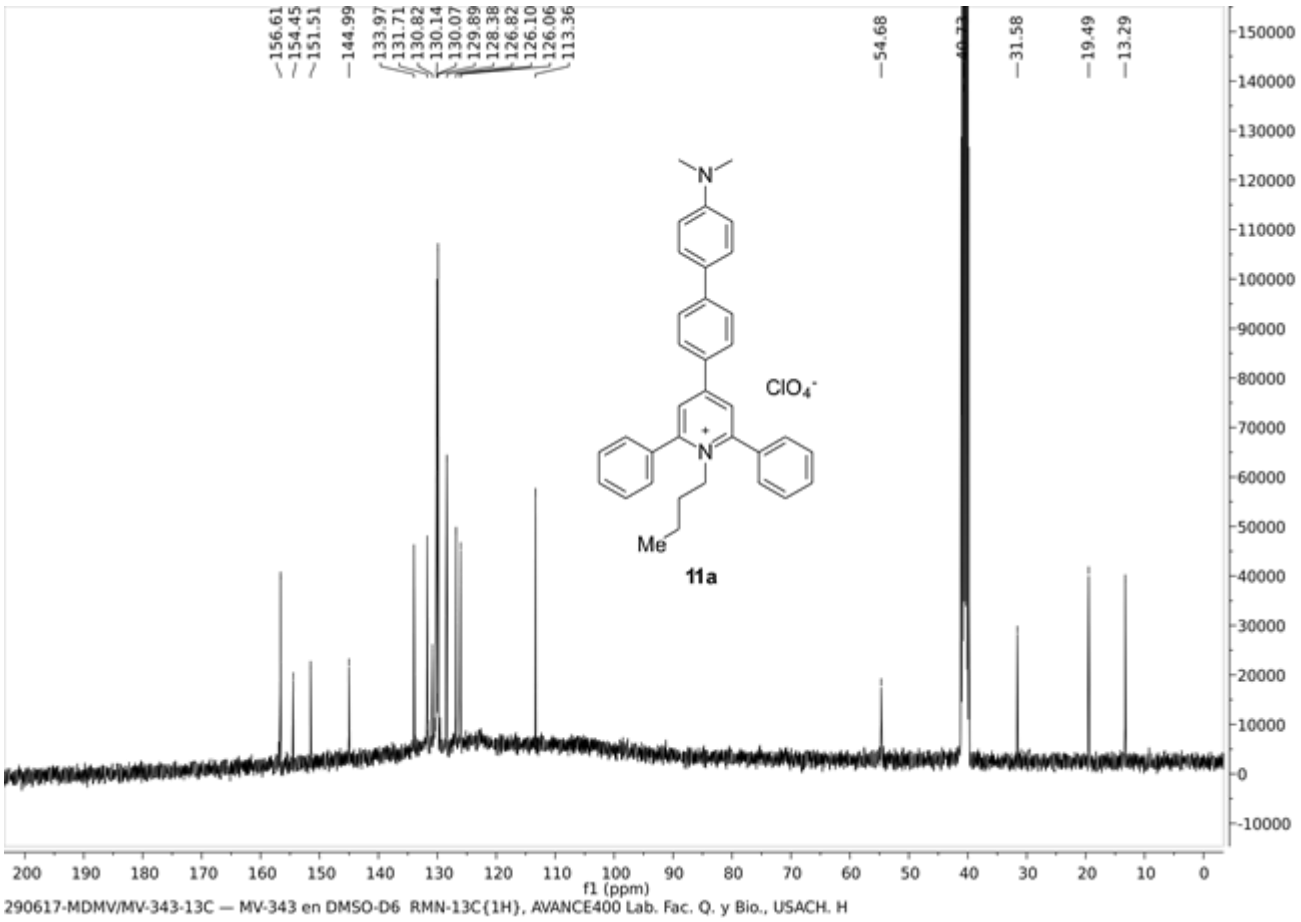


Figure 30: ^{13}C NMR spectrum of compound 11a in DMSO-d6.

Back to List of Figures section

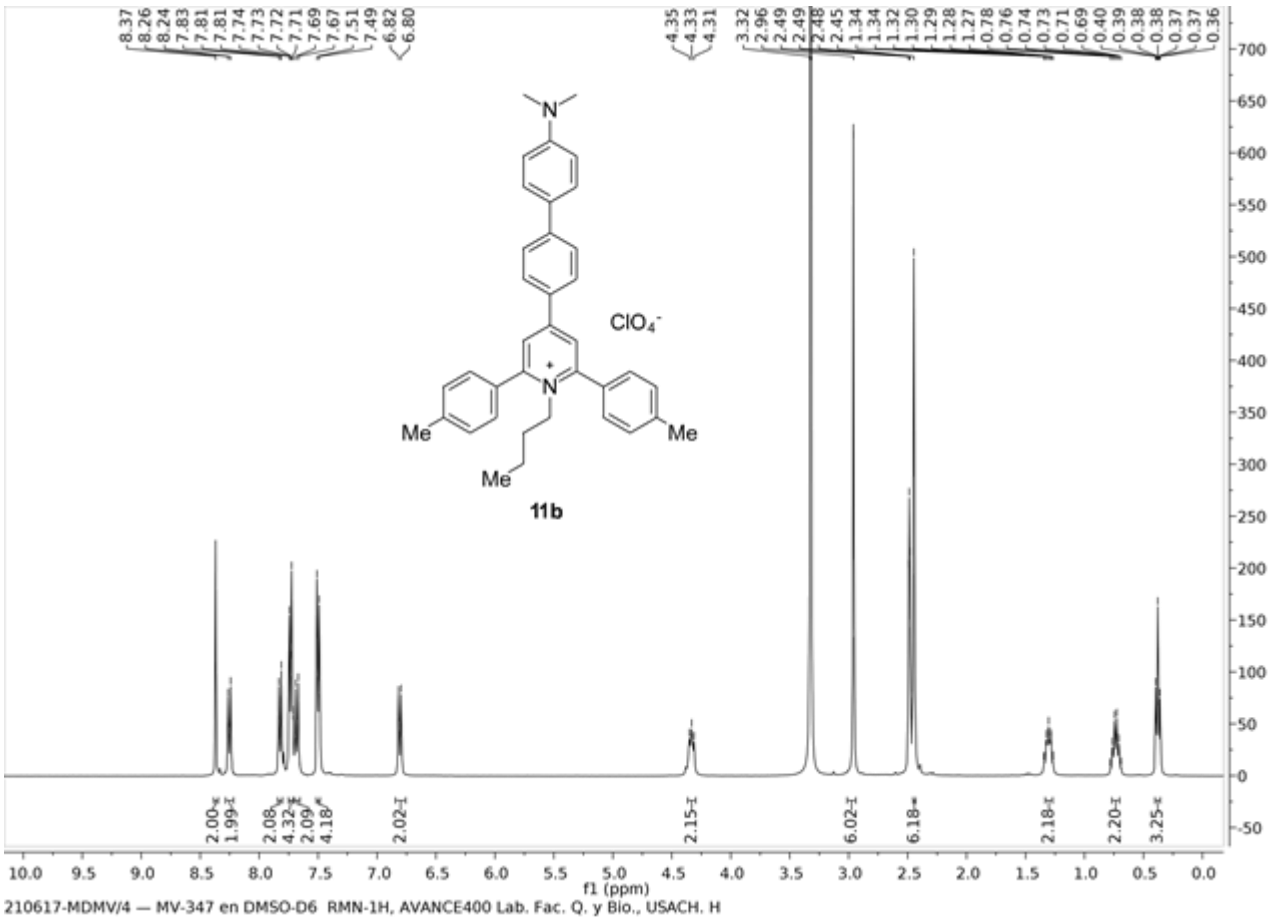


Figure 31: ^{1}H NMR spectrum of compound 11b in DMSO-d6.
Back to List of Figures section

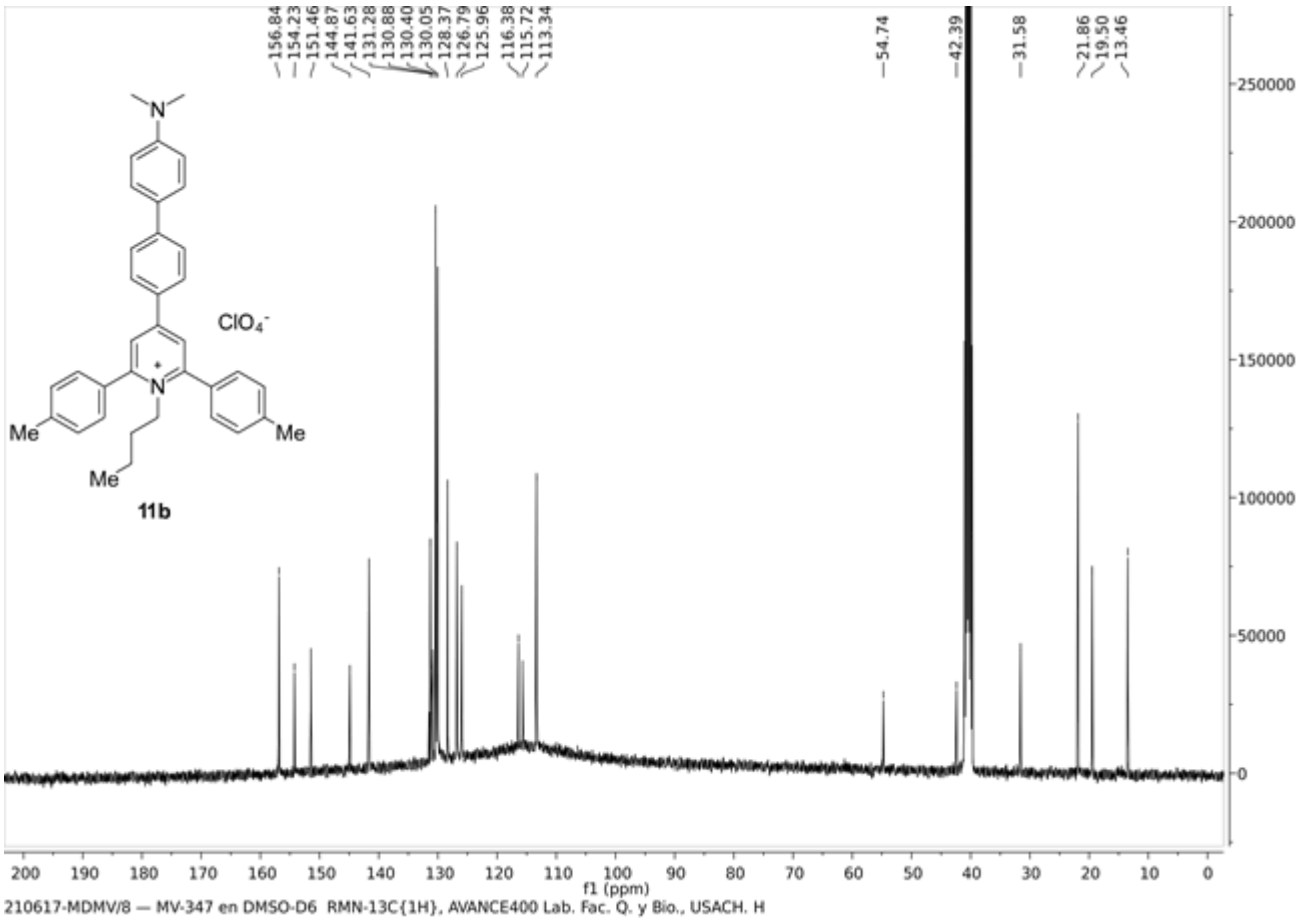


Figure 32: ^{13}C NMR spectrum of compound 11b in DMSO-d6.
Back to List of Figures section

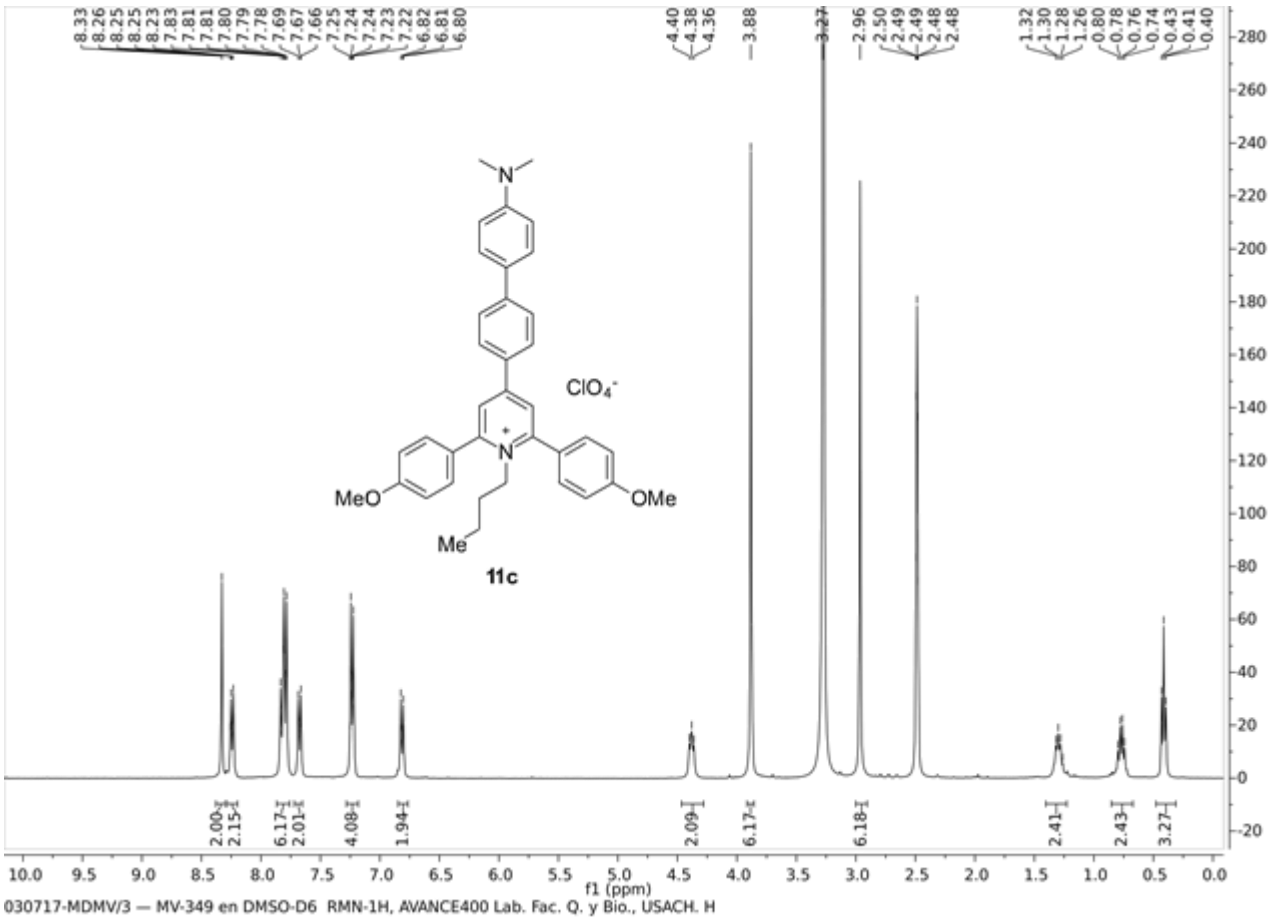


Figure 33: ^{1}H NMR spectrum of compound 11c in DMSO-d6.
Back to List of Figures section

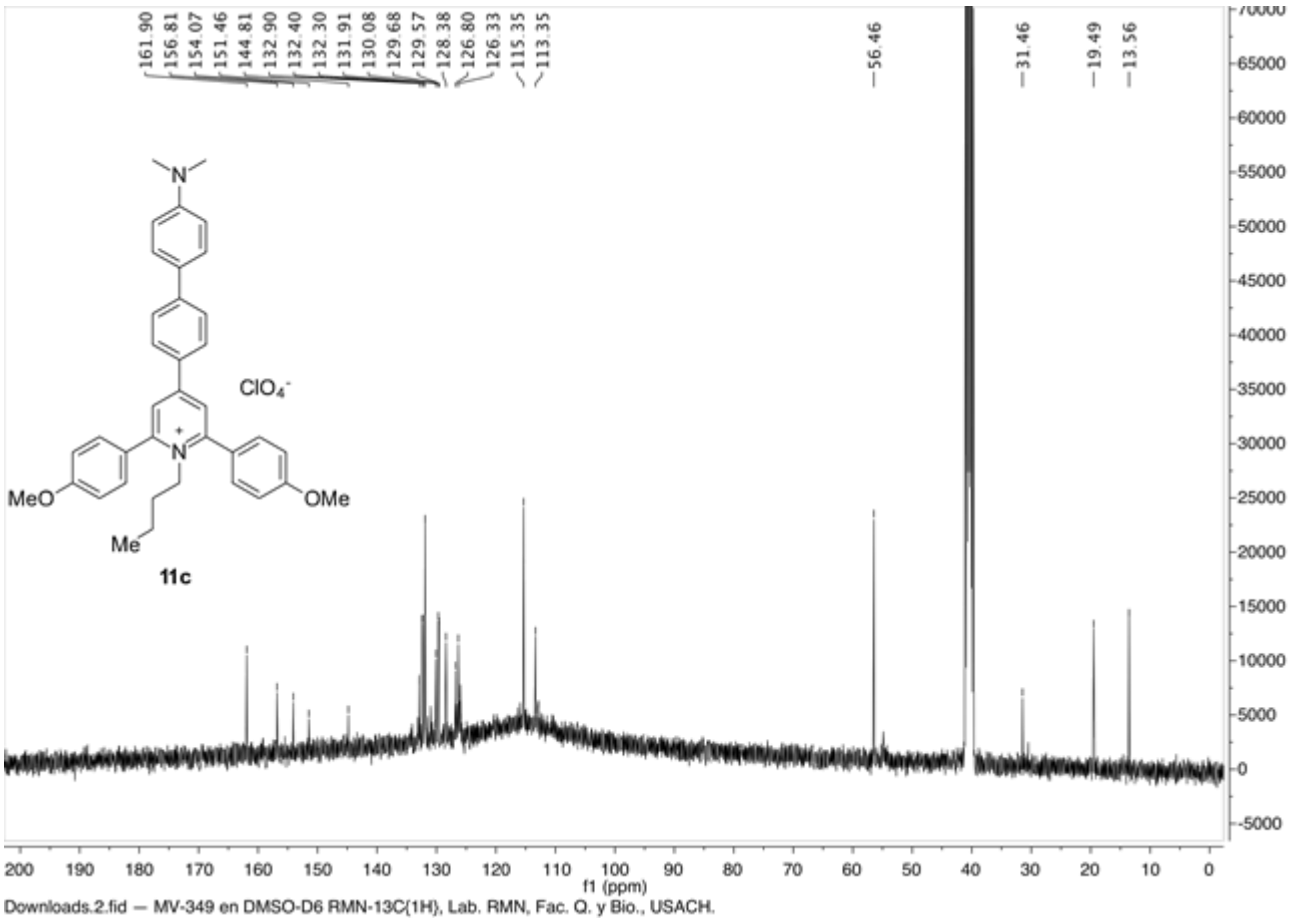


Figure 34: ^{13}C NMR spectrum of compound 11c in DMSO-d6.
Back to List of Figures section

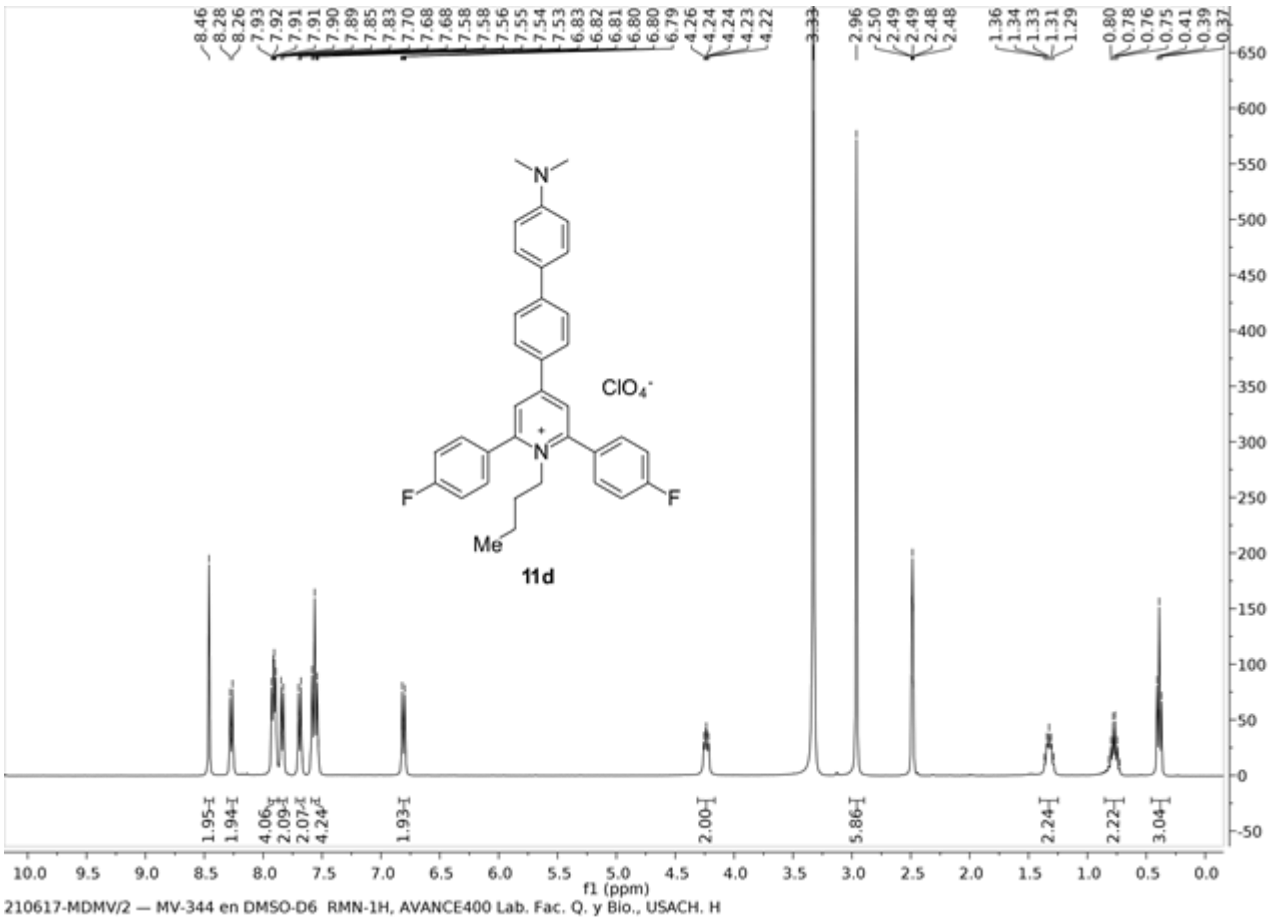


Figure 35: ^{1}H NMR spectrum of compound 11d in DMSO-d6.
Back to List of Figures section

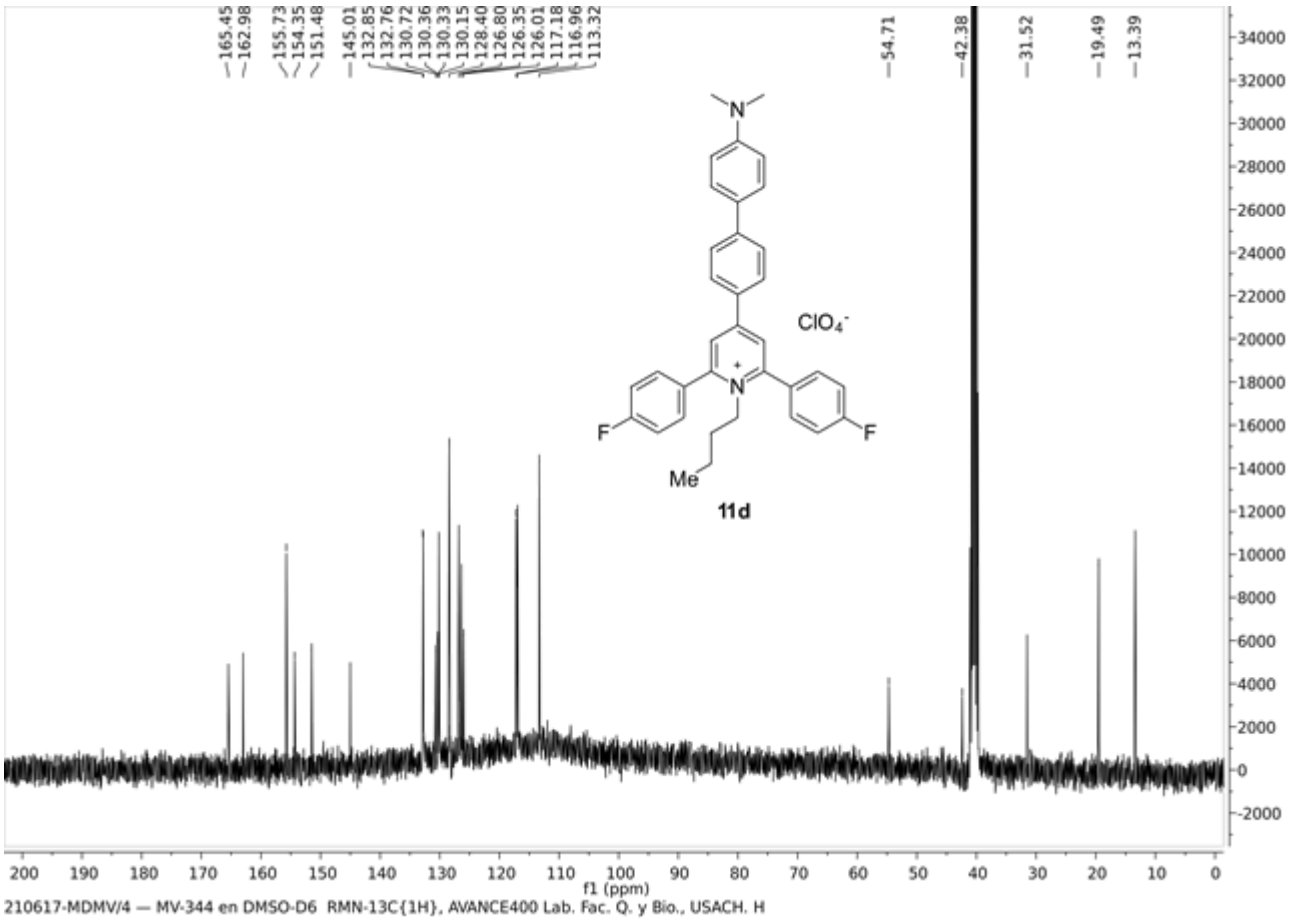


Figure 36: ^{13}C NMR spectrum of compound 11d in DMSO-d6.

Back to List of Figures section

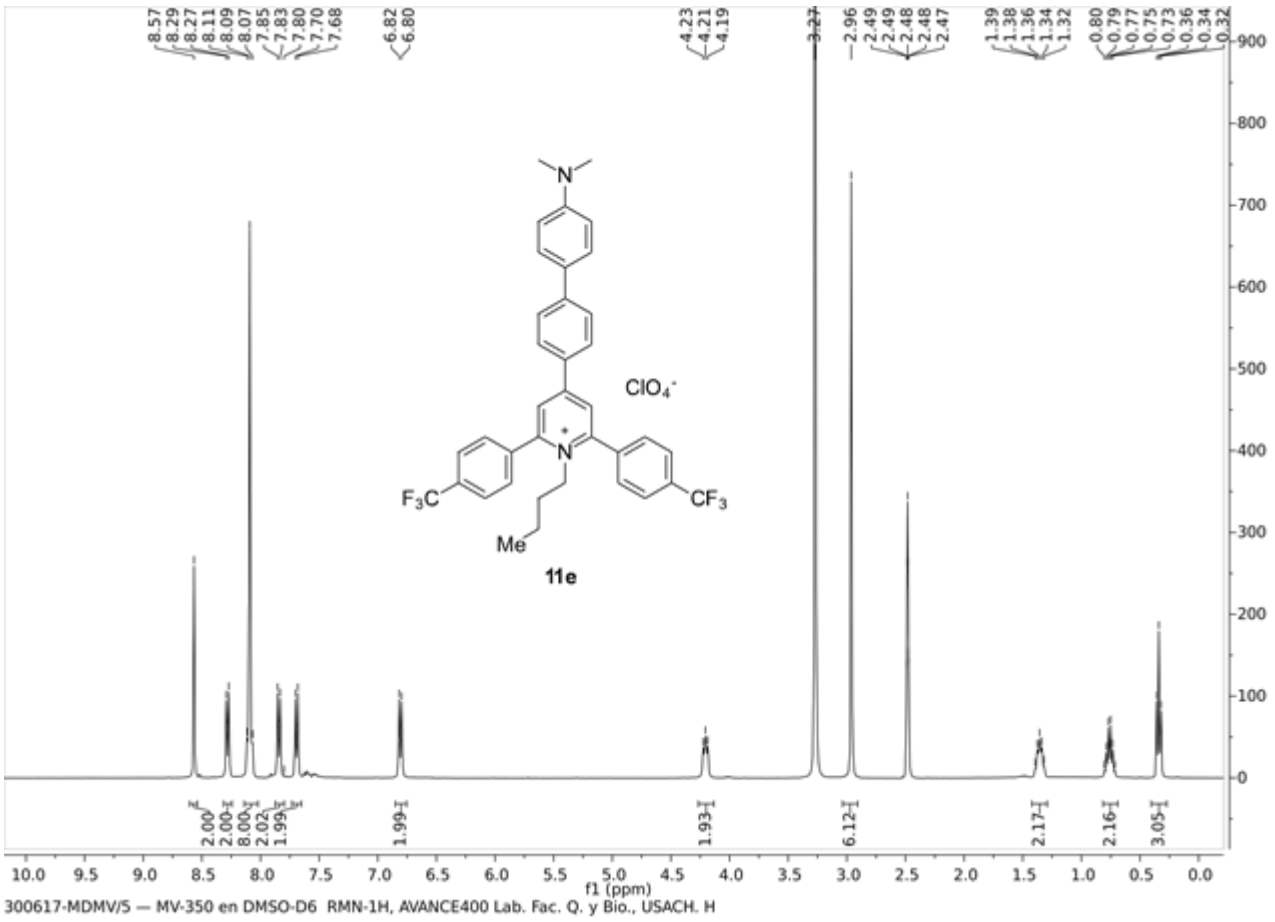


Figure 37: ^{1}H NMR spectrum of compound 11e in DMSO-d6.
Back to List of Figures section

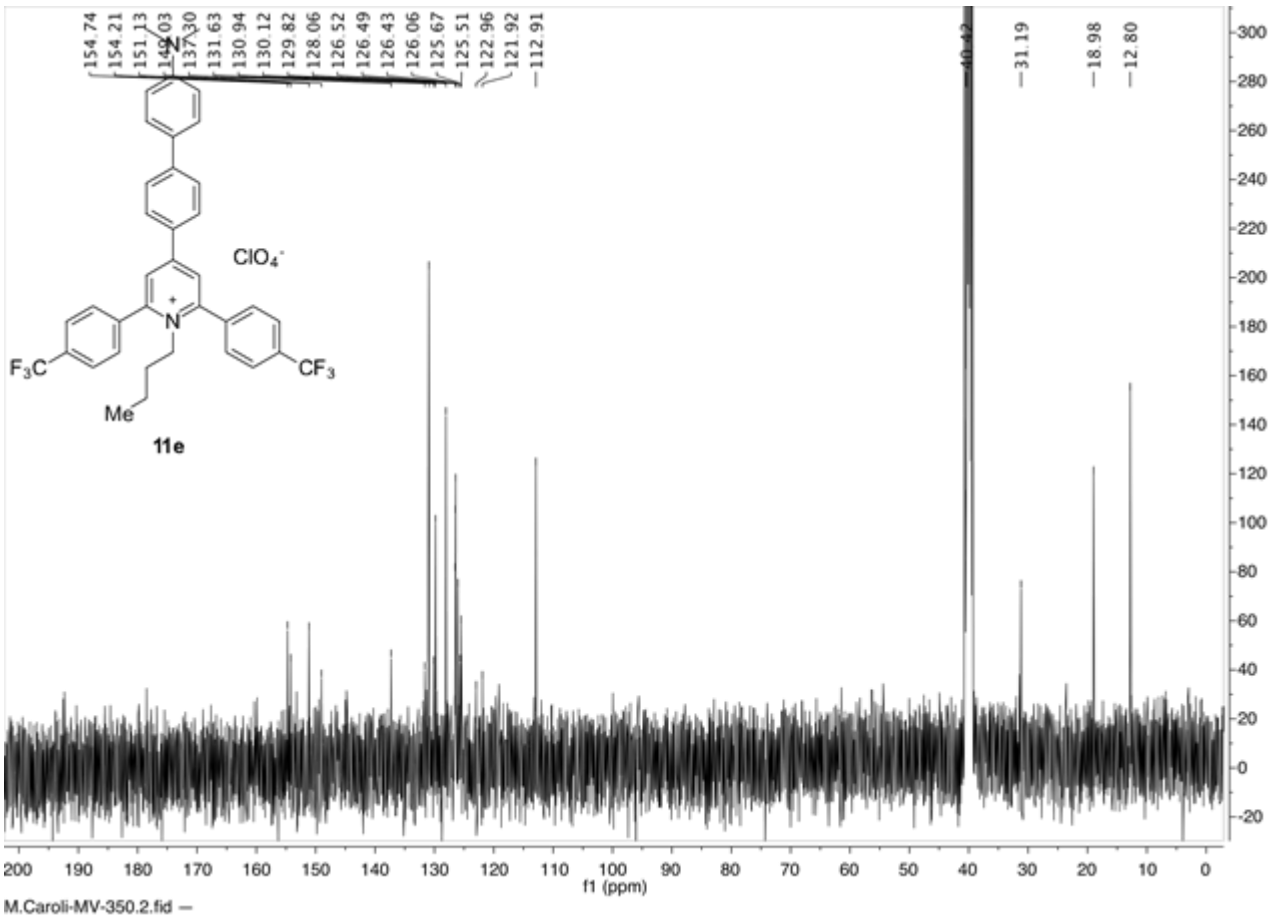


Figure 38: ^{13}C NMR spectrum of compound 11e in DMSO-d6.

Back to List of Figures section