

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

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

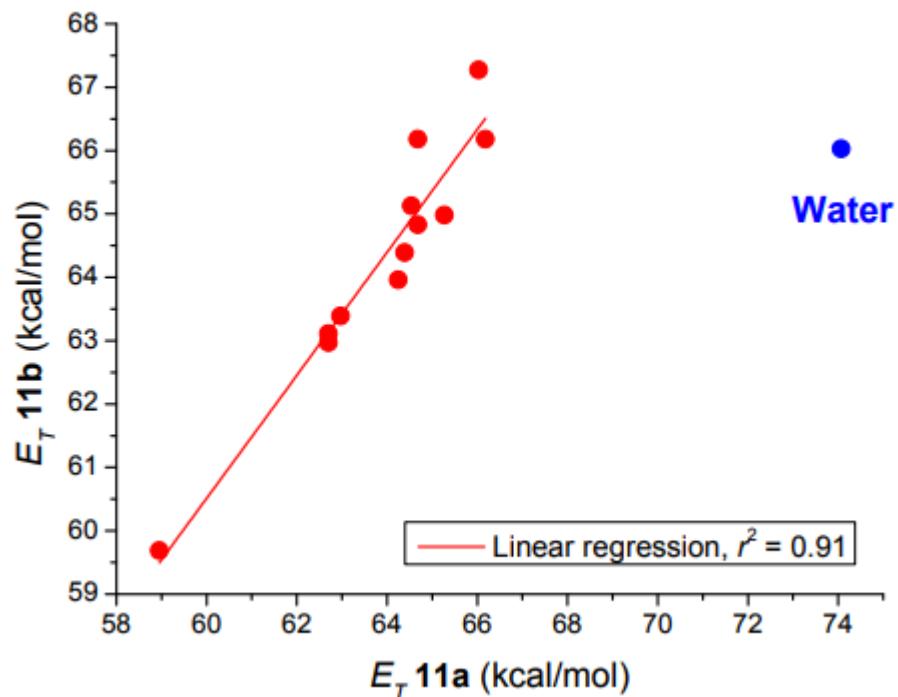


Figure 1: Linear plots of  $E_{T2}$  (11b) against  $E_{T2}$  (11a), in thirteen solvents, with values taken from Table 1 (main manuscript).

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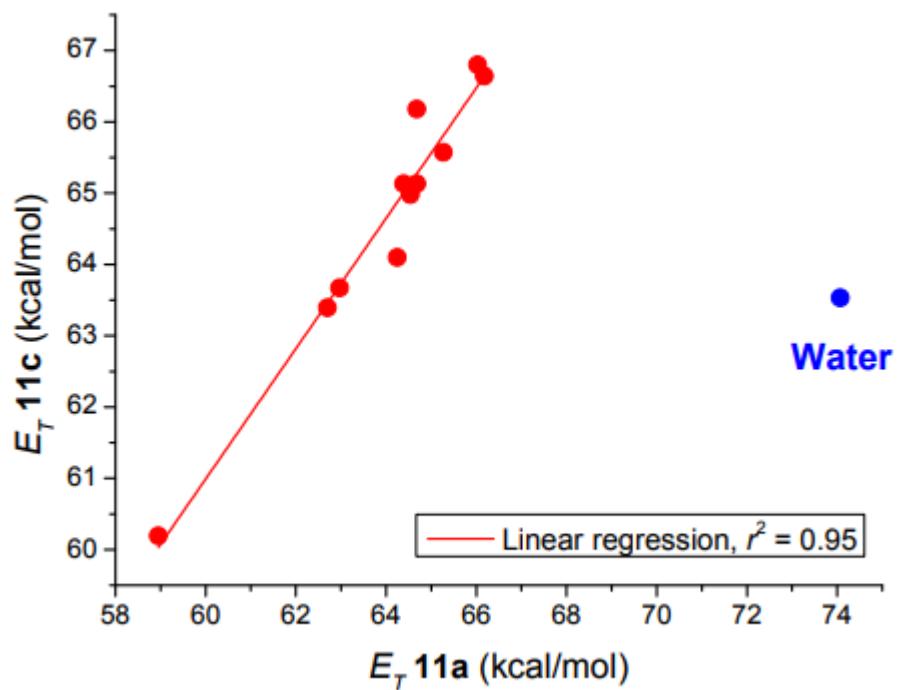
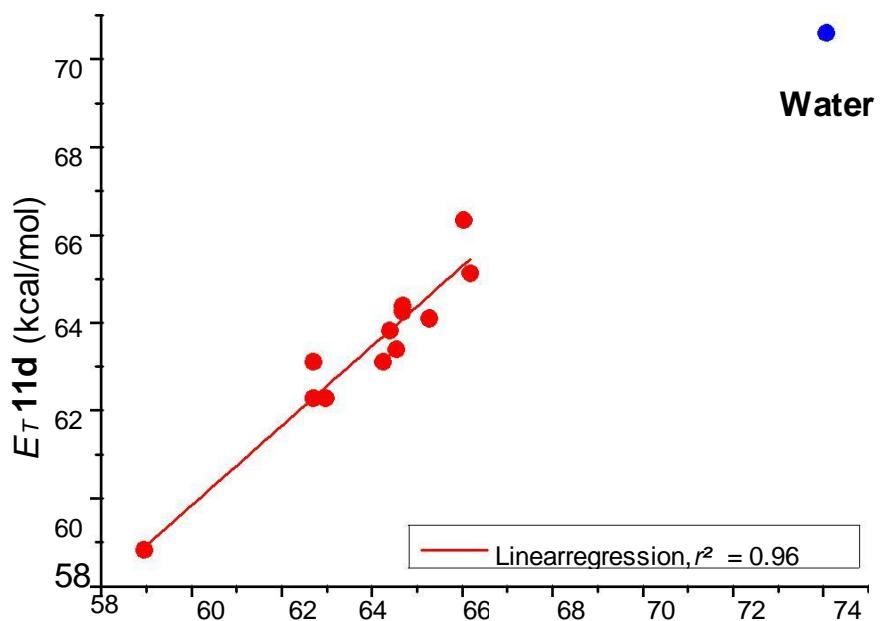


Figure 2: Linear plots of  $E_{T2}$  (11c) against  $E_{T2}$  (11a), in thirteen solvents, with values taken from Table 1 (main manuscript).



$E_T$  11a (kcal/mol)

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

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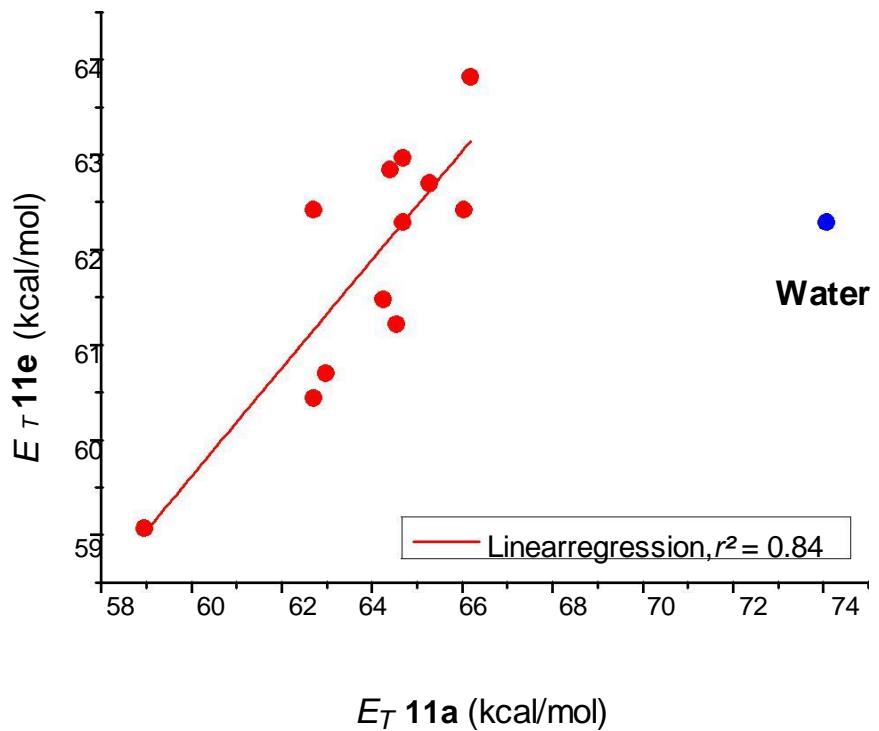


Figure 4: Linear plots of  $E_{T2}$  (11e) against  $E_{T2}$  (11a), in thirteen solvents, with values taken from Table 1 (main manuscript).

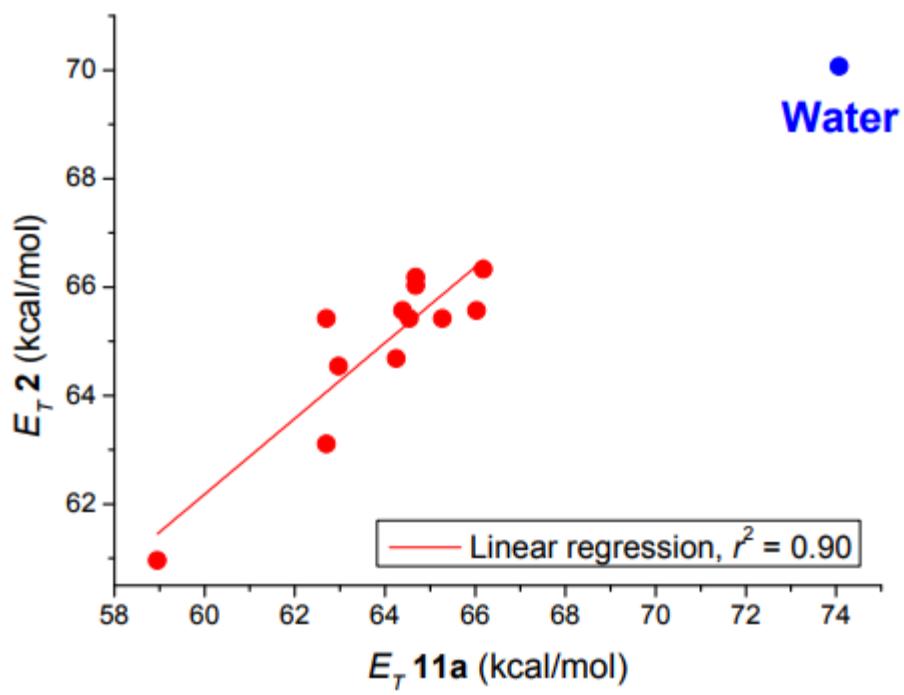


Figure 5: Linear plots of  $E_T$  2 (2) against  $E_T$  2 (11a), in thirteen solvents, with values taken from Table 1 (main manuscript).

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

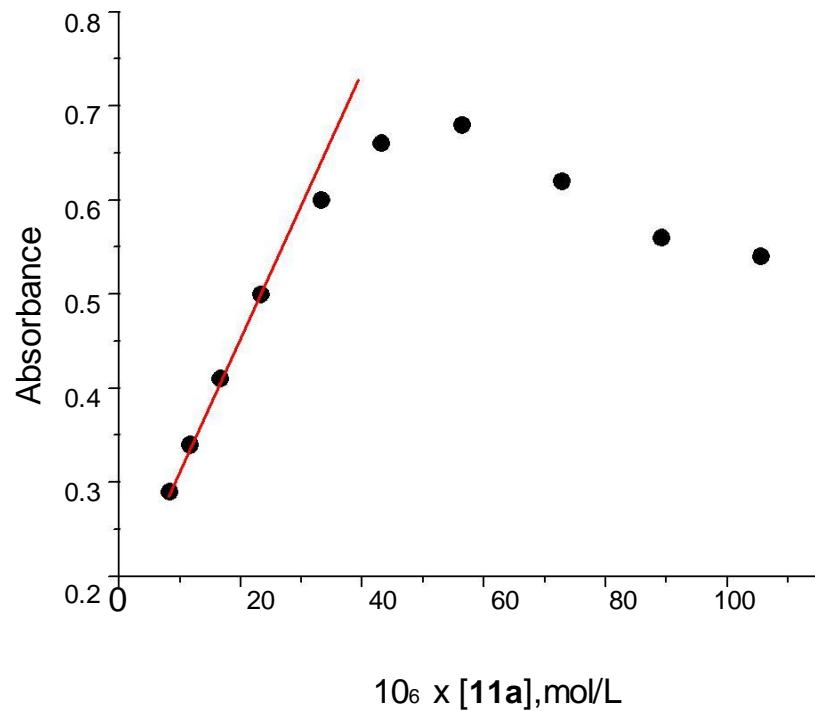


Figure 6: Non-linear Lambert-Beer plots of absorbance readings at 386 nm for increasing concentrations of dye 11a in water, as evidence of dye aggregation in this solvent.

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### 3 Calculated $E_T$ of dyes 2 and 11a

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

Solvent	$E_T^{\text{IV}}$	$E_{T1}$ (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 -Dimethylformamide	0.386	51.05	85.83	52.10	85.56
Dichloromethane	0.309	51.51	86.61	52.25	85.62

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

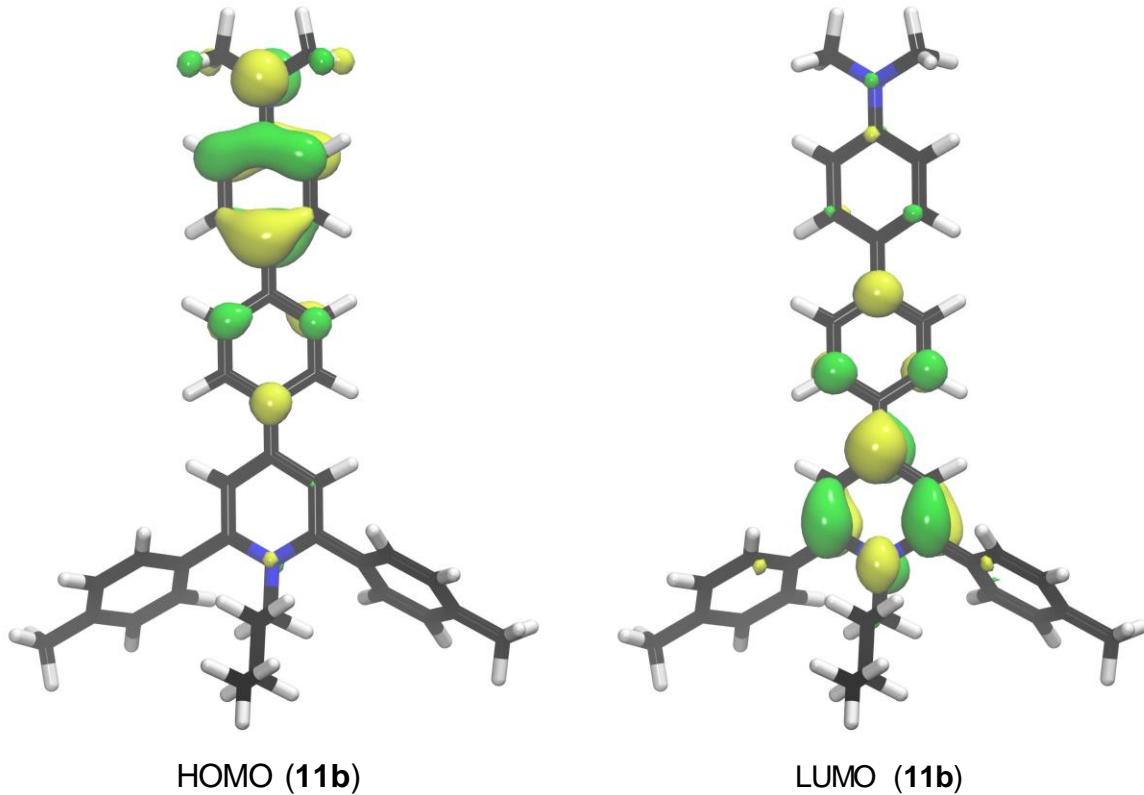


Figure 7: HOMO and LUMO orbitals of dye 11b calculated at B3LYP/6-31+G(d,p) level of theory in gas phase.

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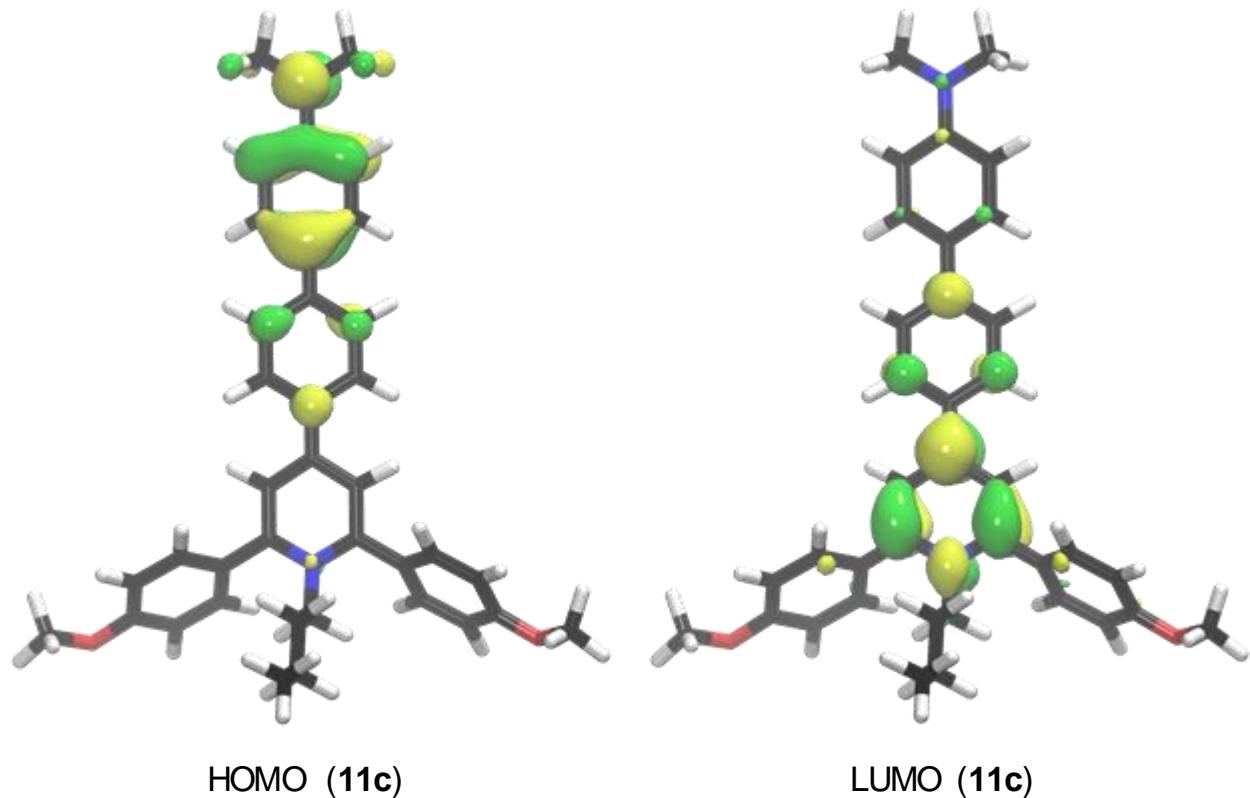


Figure 8: HOMO and LUMO orbitals of dye 11c calculated at B3LYP/6-31+G(d,p) level of theory in gas phase.

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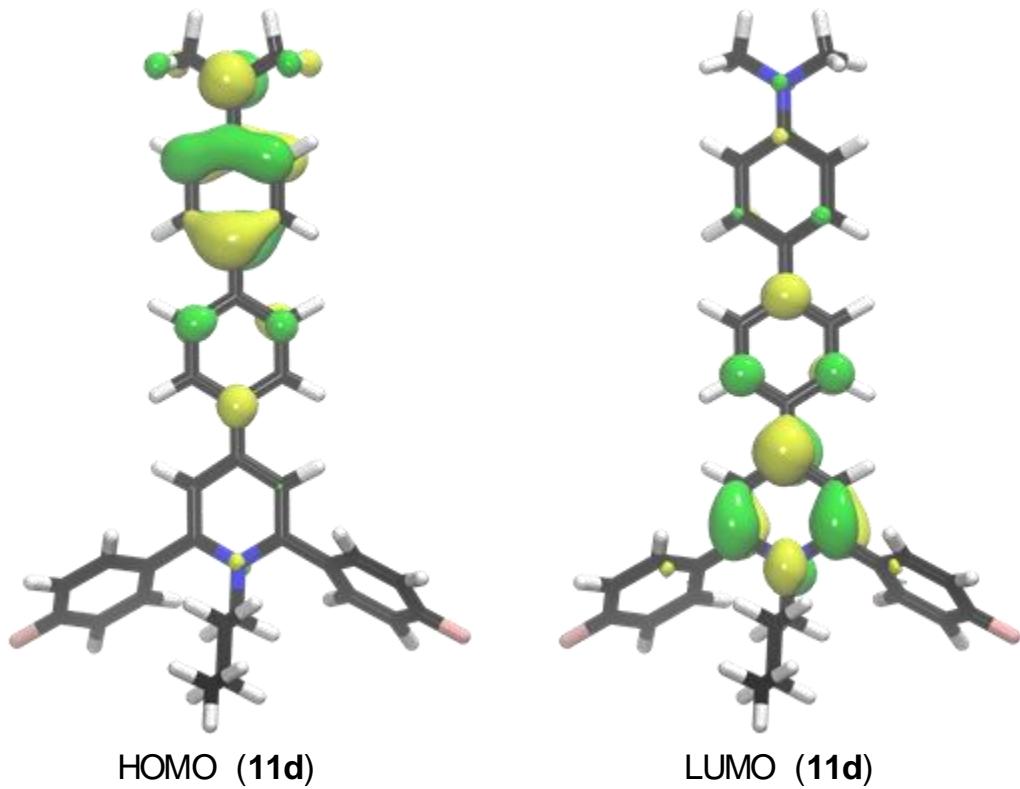


Figure 9: HOMO and LUMO orbitals of dye 11d calculated at B3LYP/6-31+G(d,p) level of theory in gas phase.

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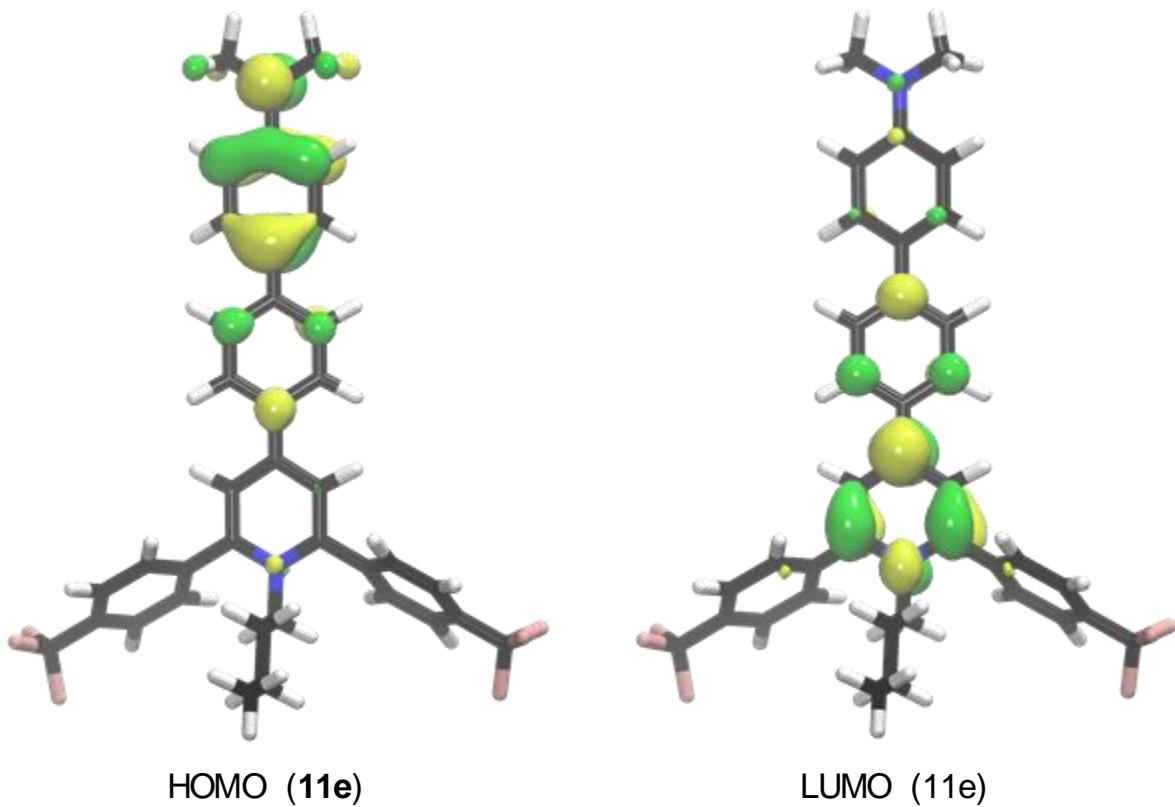
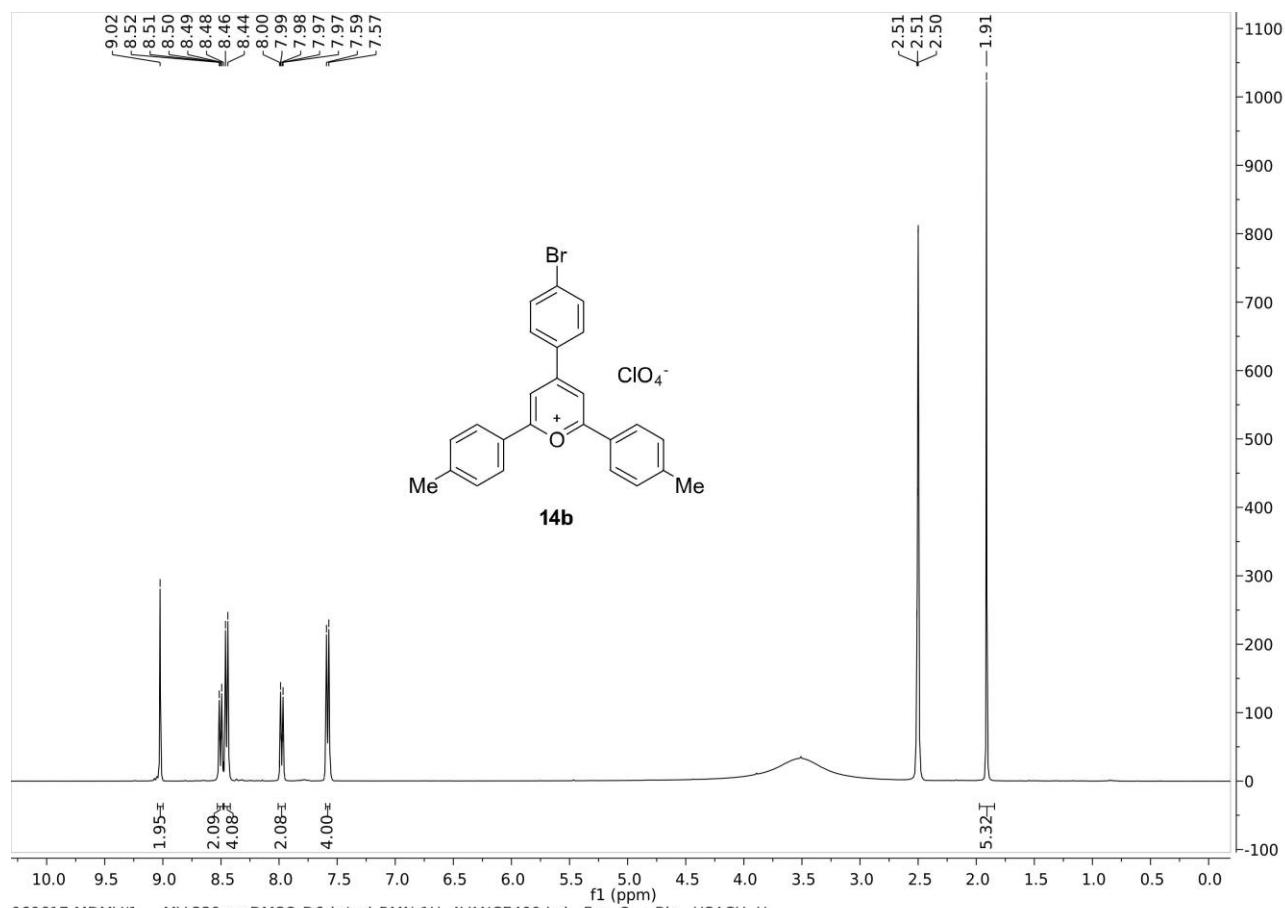


Figure 10: HOMO and LUMO orbitals of dye 11e calculated at B3LYP/6-31+G(d,p) level of theory in gas phase.

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5  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR of new compounds 14b-e, 15a-e and 11a-e.



060617-MDMV/1 — MV-339 en DMSO-D6 (c/pp) RMN-1H, AVANCE400 Lab. Fac. Q. y Bio., USACH. H

Figure 11:  $^1\text{H}$  NMR spectrum of compound 14b in DMSO-d6.  
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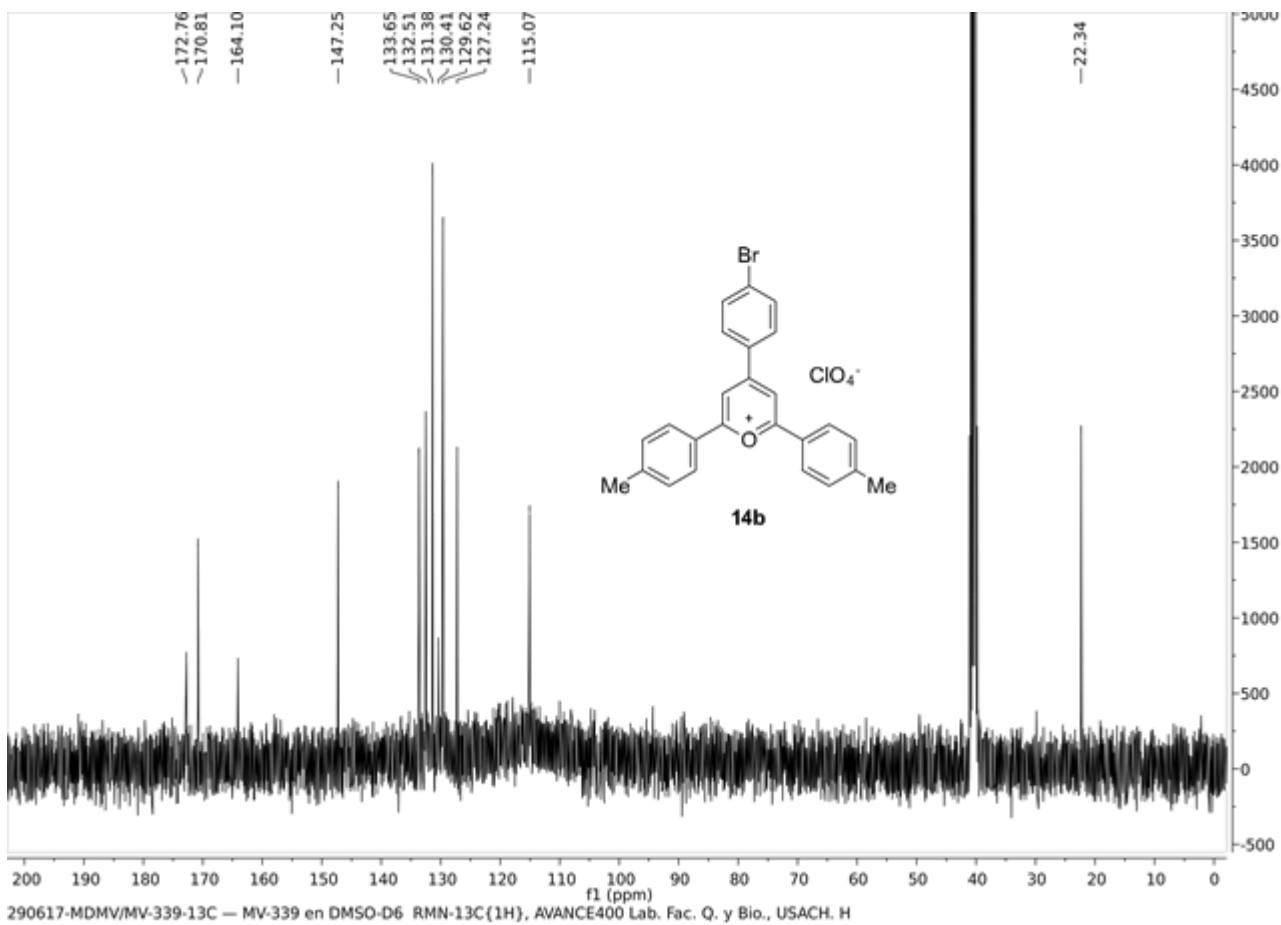


Figure 12:  $^{13}\text{C}$  NMR spectrum of compound **14b** in DMSO-d6.  
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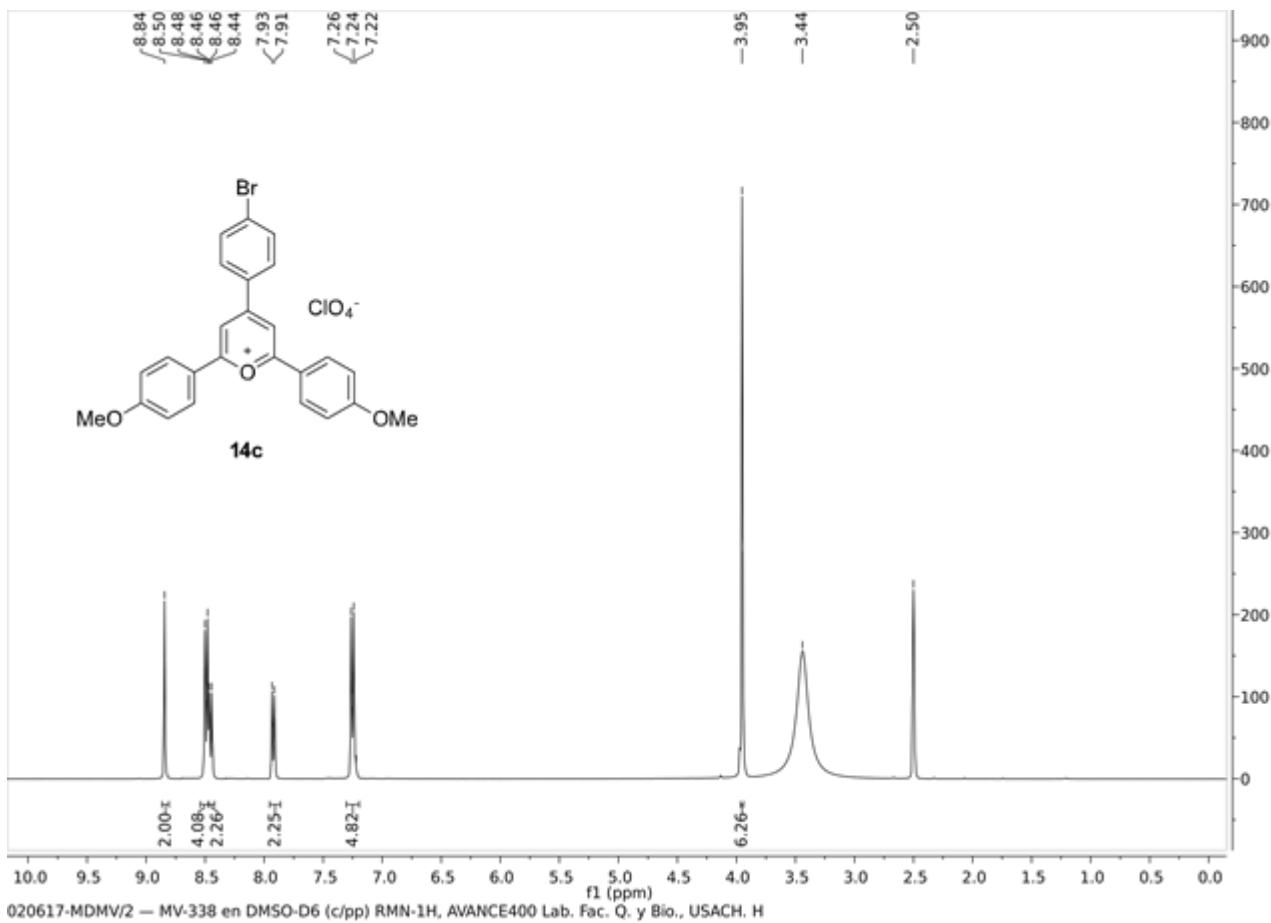


Figure 13:  $^1\text{H}$  NMR spectrum of compound 14c in DMSO-d6.  
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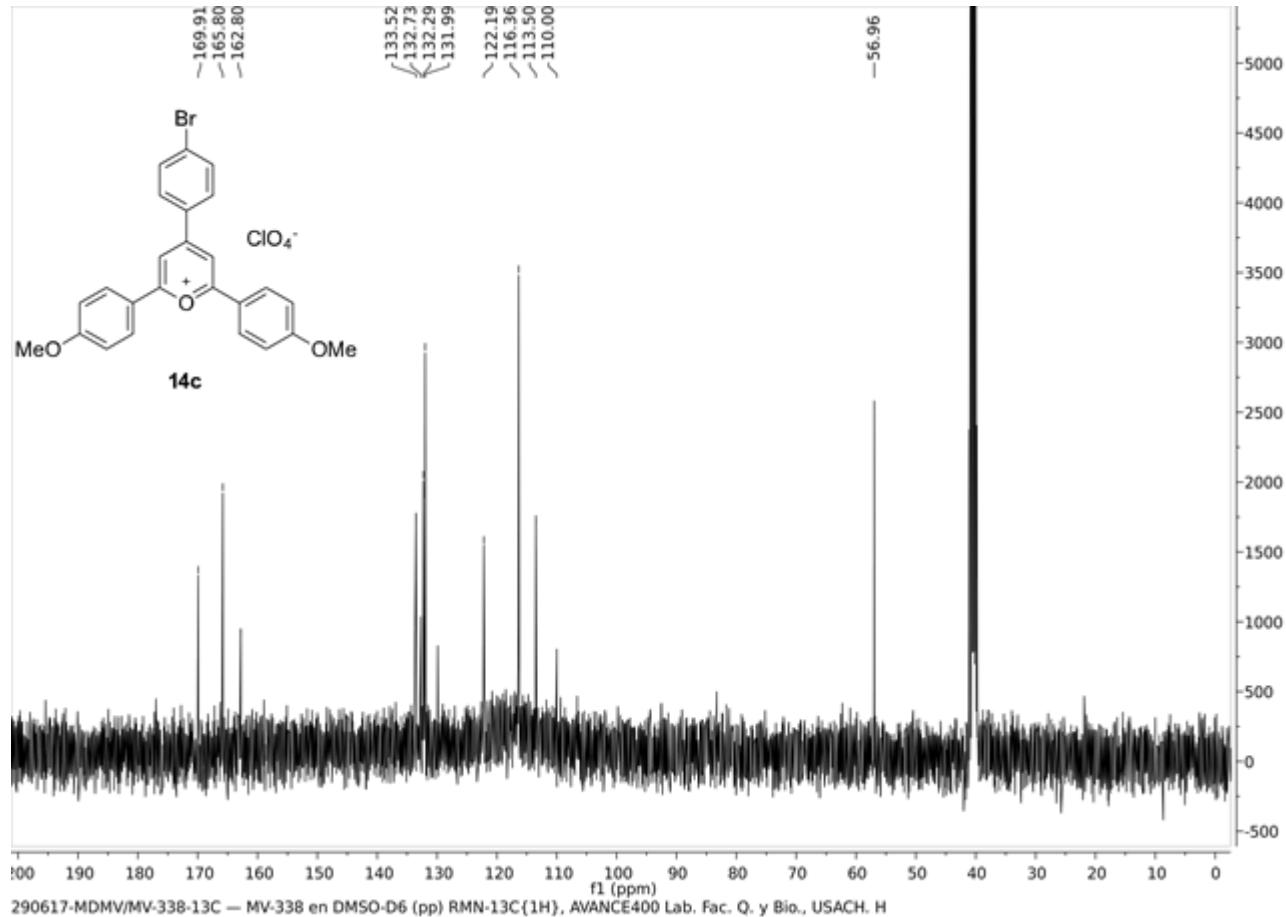


Figure 14:  $^{13}\text{C}$  NMR spectrum of compound **14c** in DMSO-d<sub>6</sub>.  
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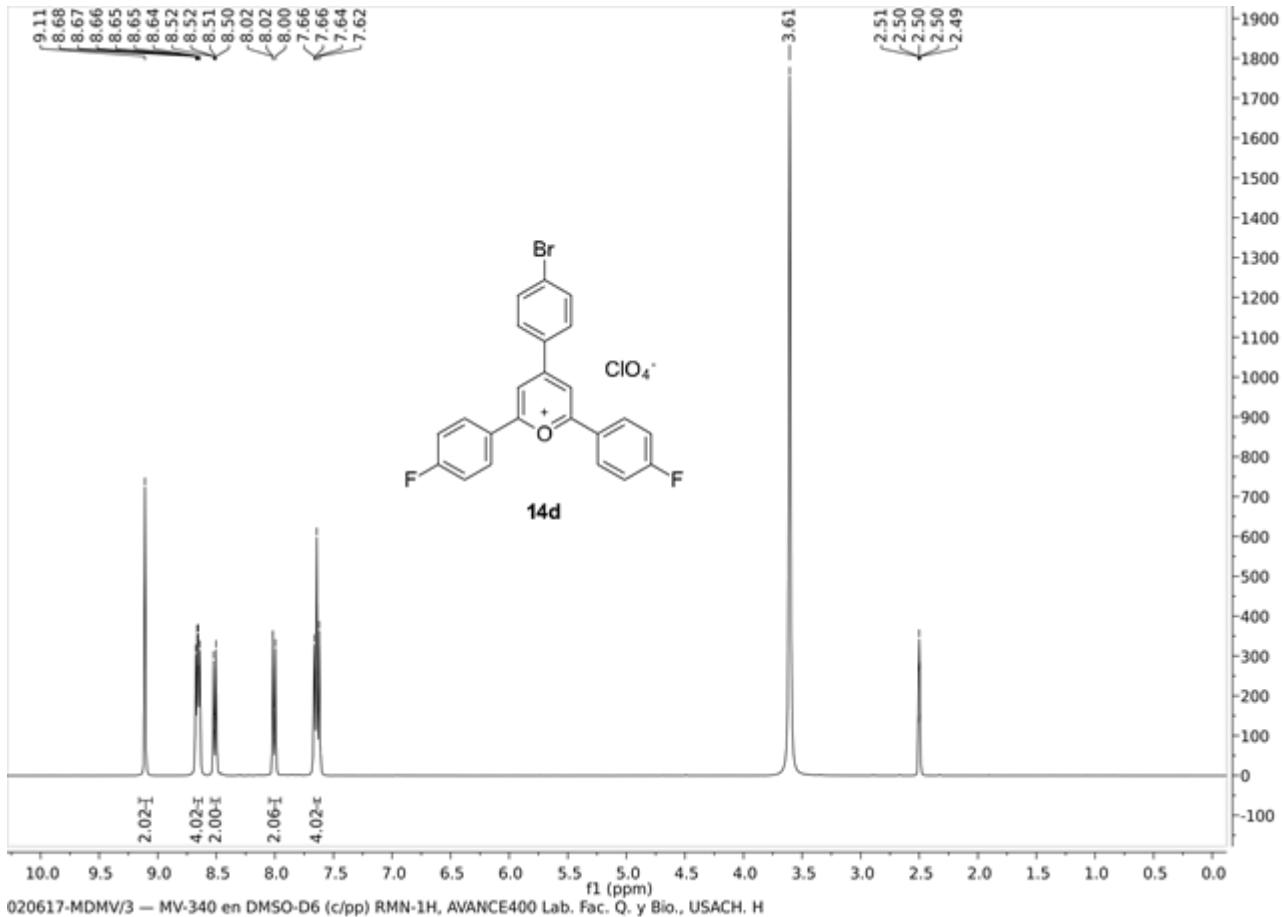


Figure 15: <sup>1</sup>H NMR spectrum of compound 14d in DMSO-d6.  
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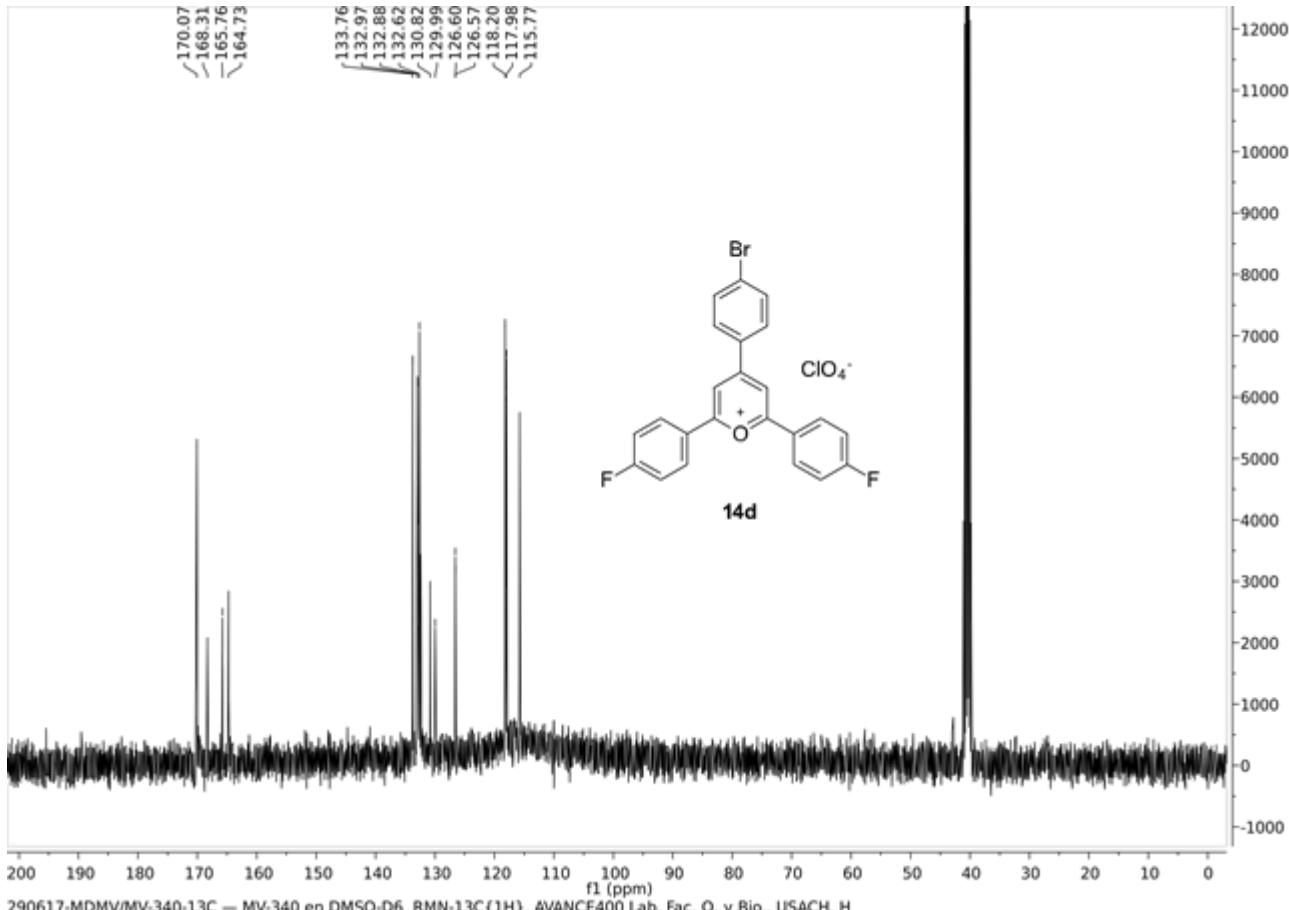


Figure 16:  $^{13}\text{C}$  NMR spectrum of compound **14d** in DMSO-d6.  
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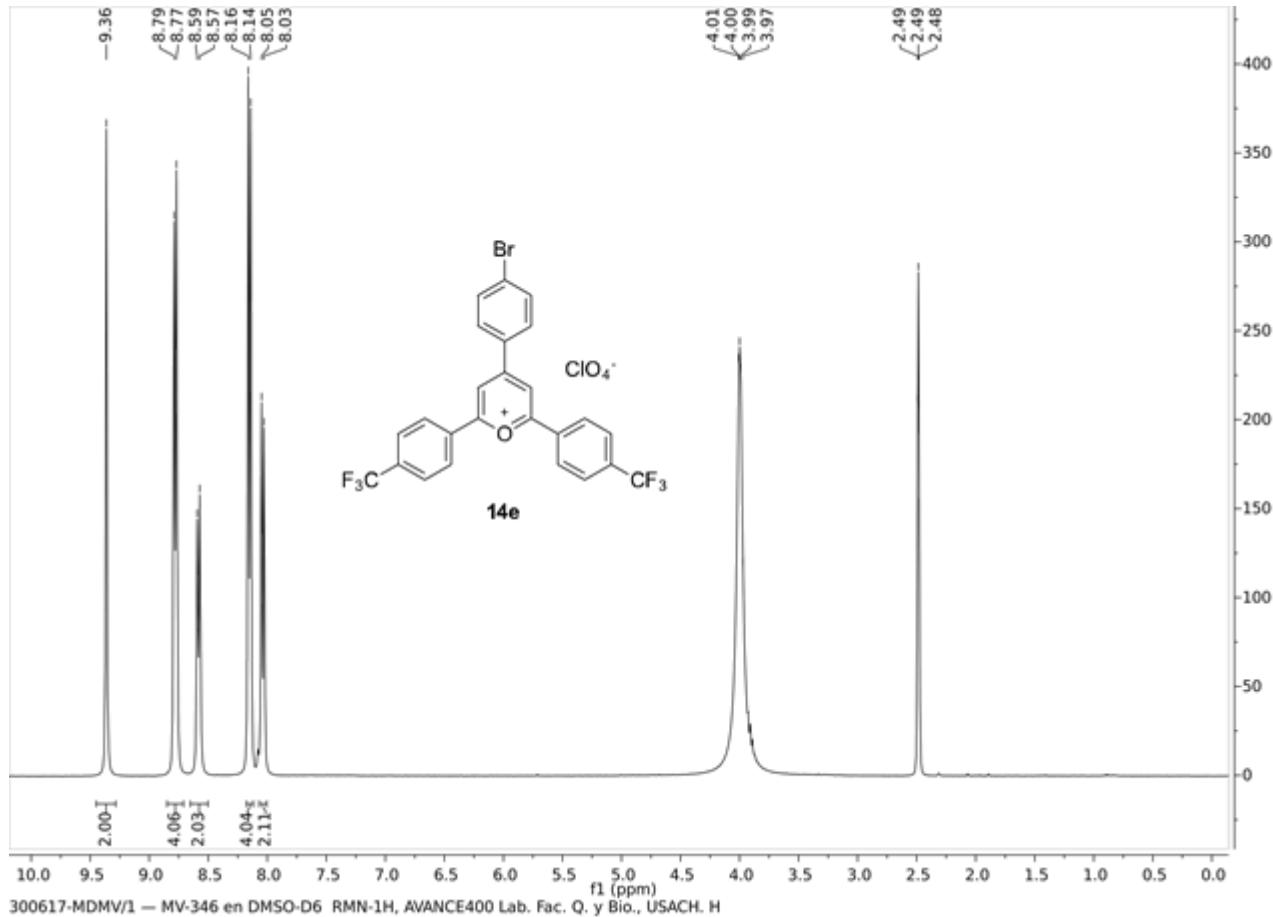


Figure 17:  $^1\text{H}$  NMR spectrum of compound 14e in DMSO-d6.  
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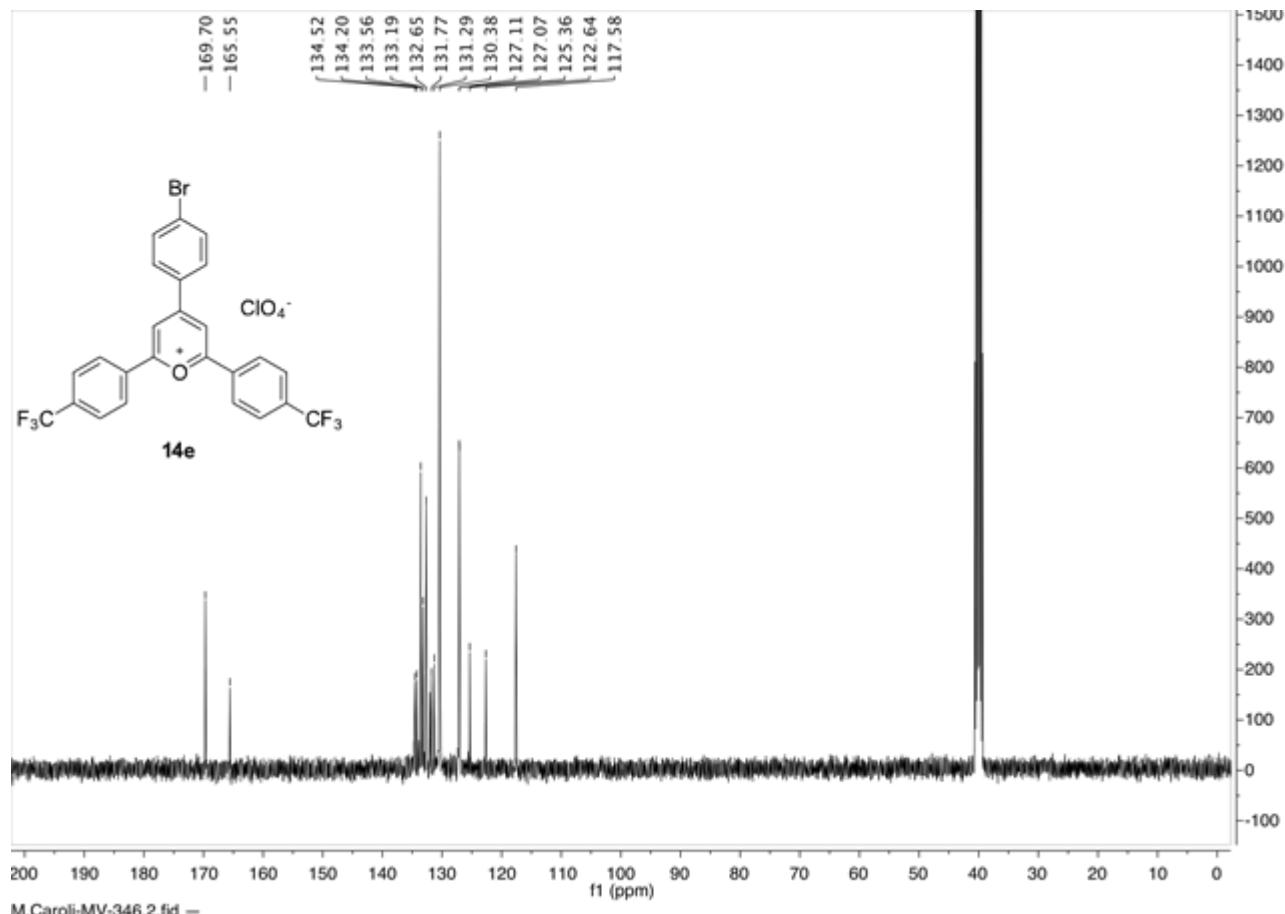


Figure 18:  $^{13}\text{C}$  NMR spectrum of compound 14e in  $\text{DMSO-d}_6$ .  
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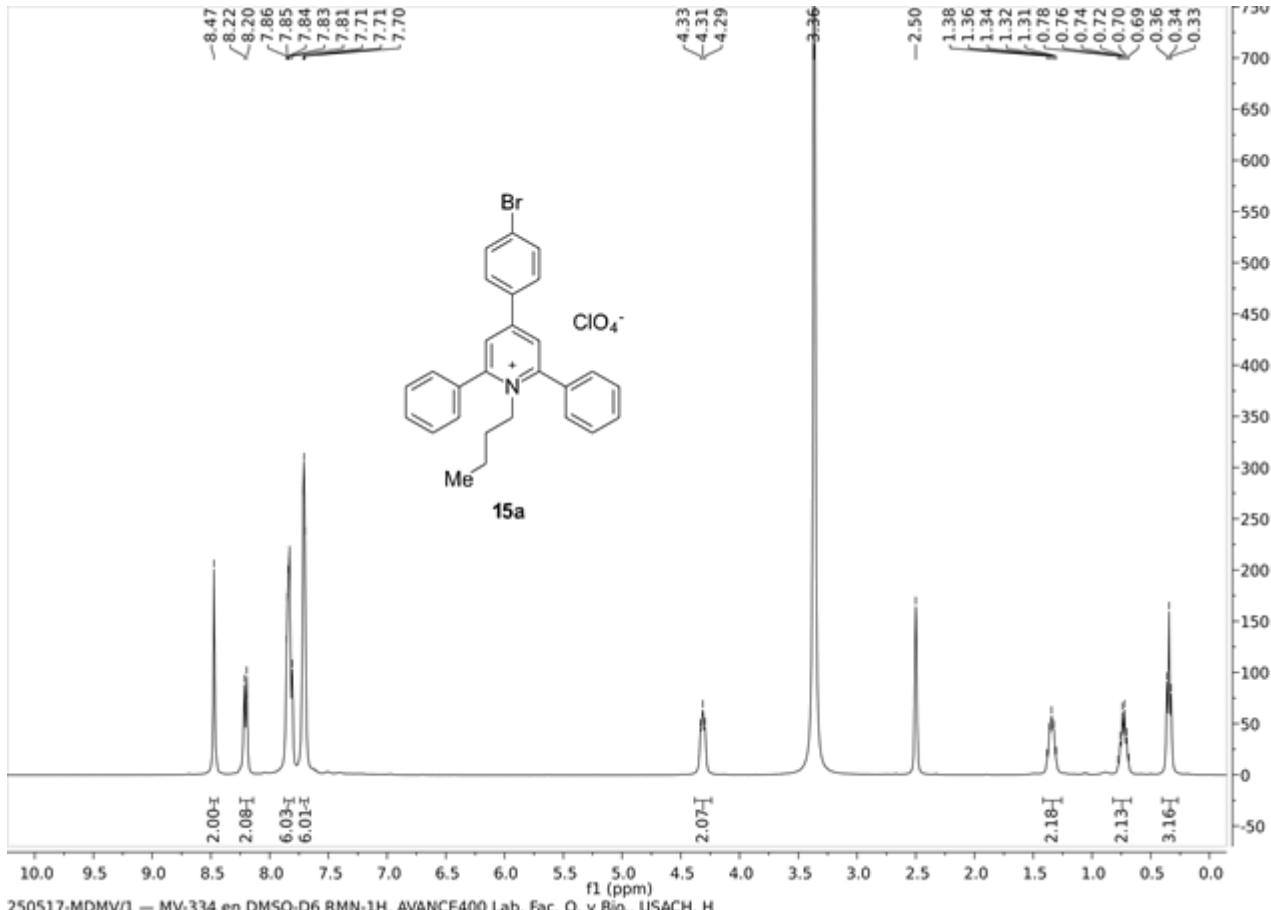


Figure 19:  $^1\text{H}$  NMR spectrum of compound 15a in DMSO-d6.  
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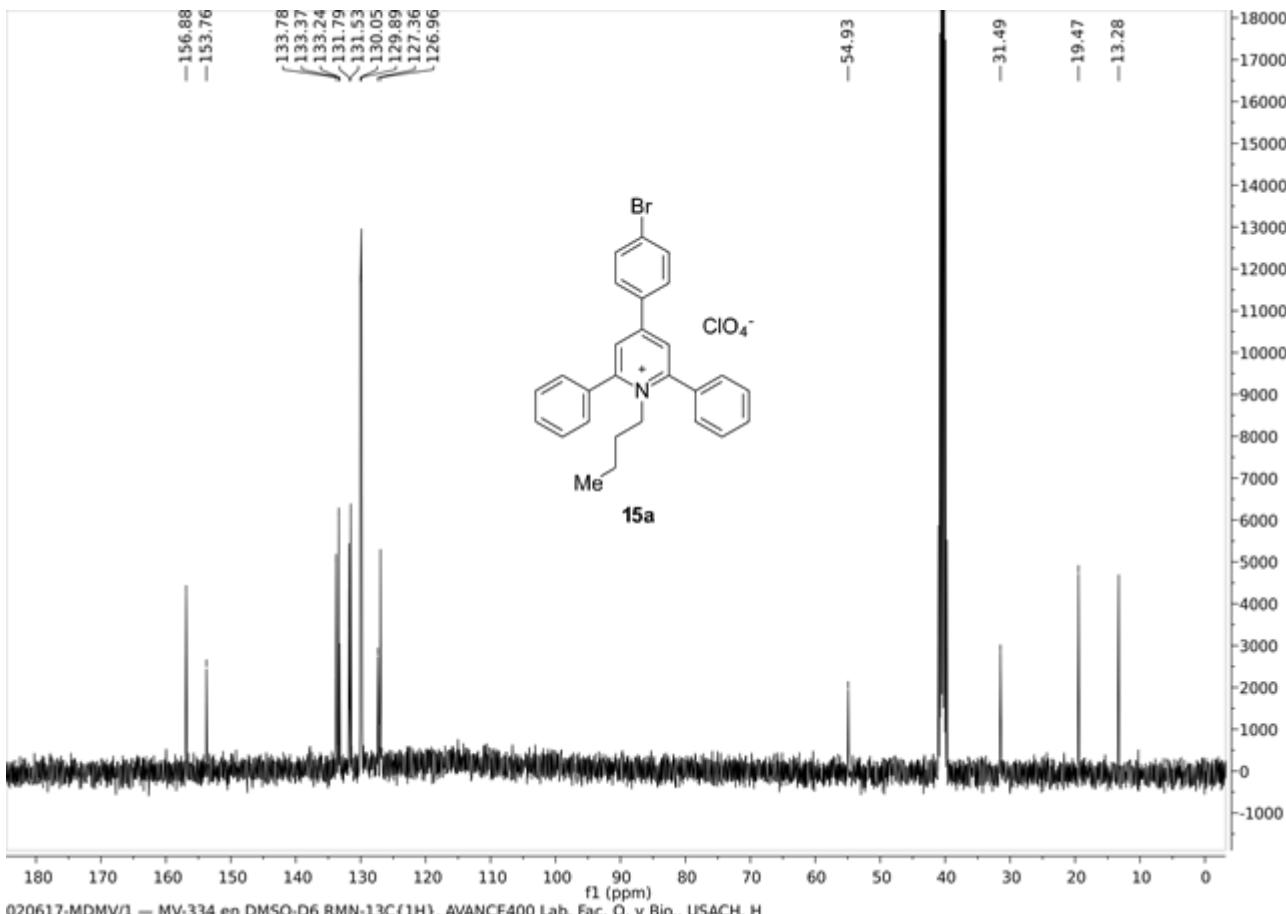


Figure 20:  $^{13}\text{C}$  NMR spectrum of compound **14b** in DMSO-d6.  
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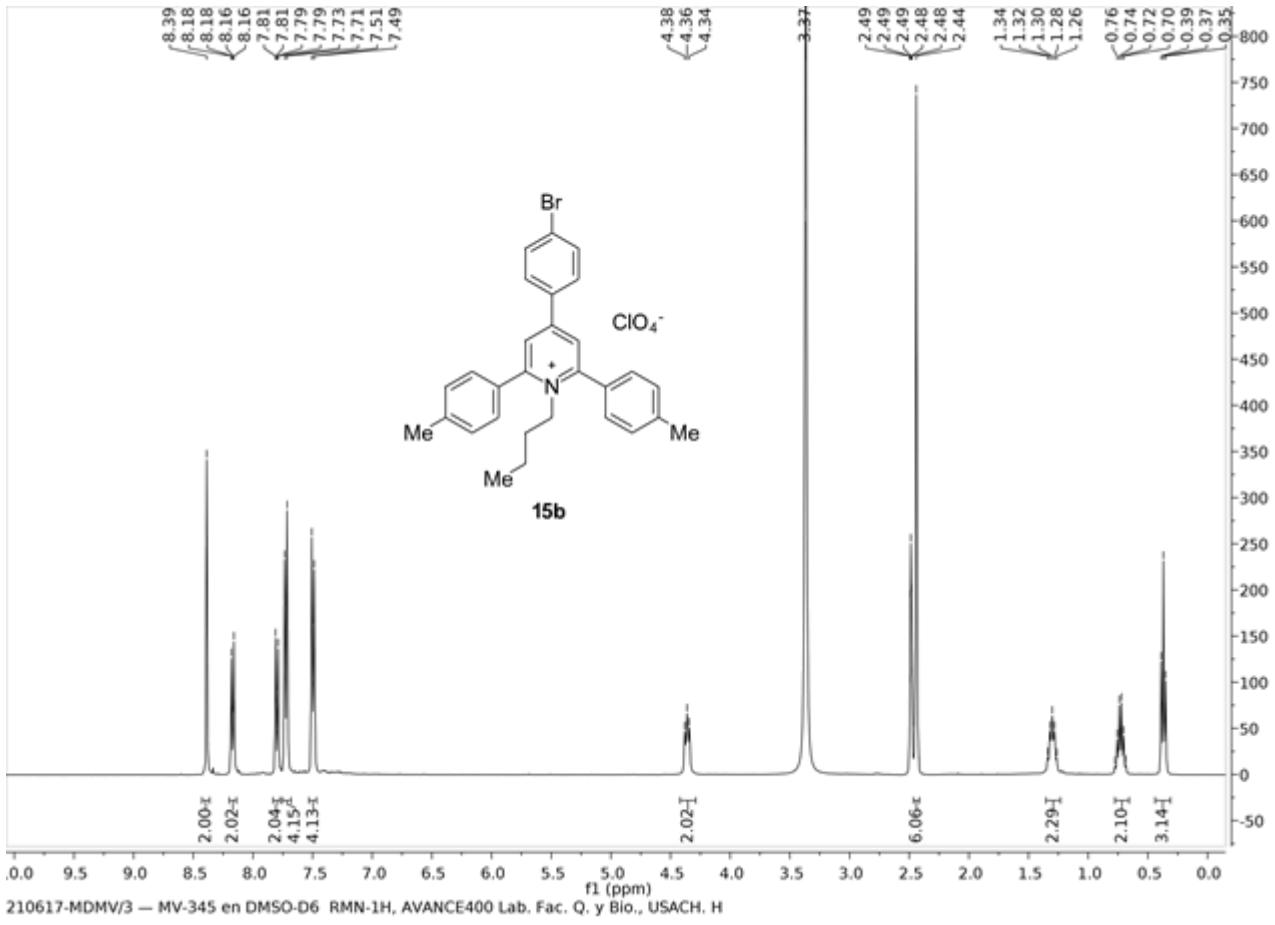


Figure 21:  $^1\text{H}$  NMR spectrum of compound 15b in DMSO-d<sub>6</sub>.  
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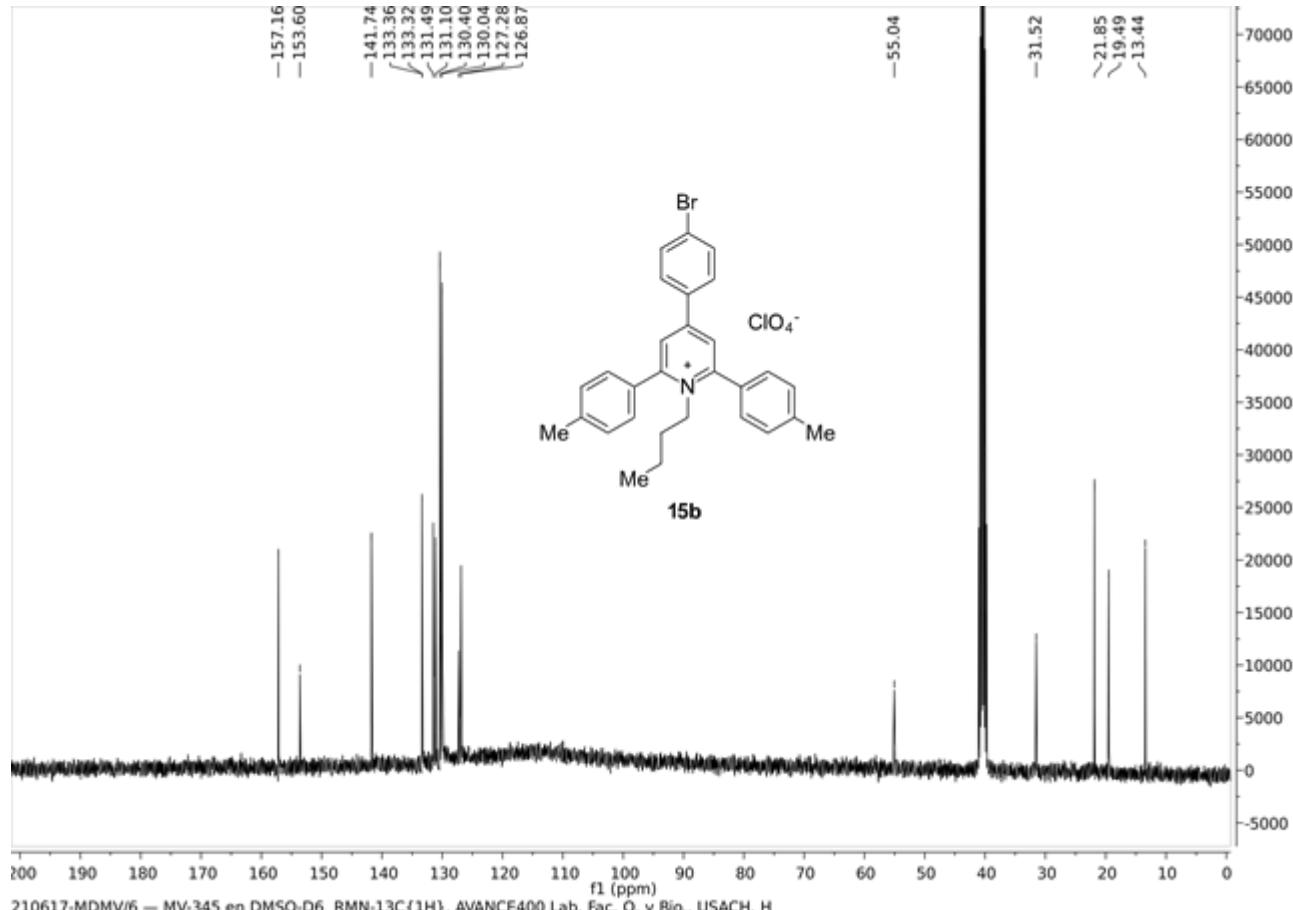


Figure 22:  $^{13}\text{C}$  NMR spectrum of compound 15b in DMSO-d6.  
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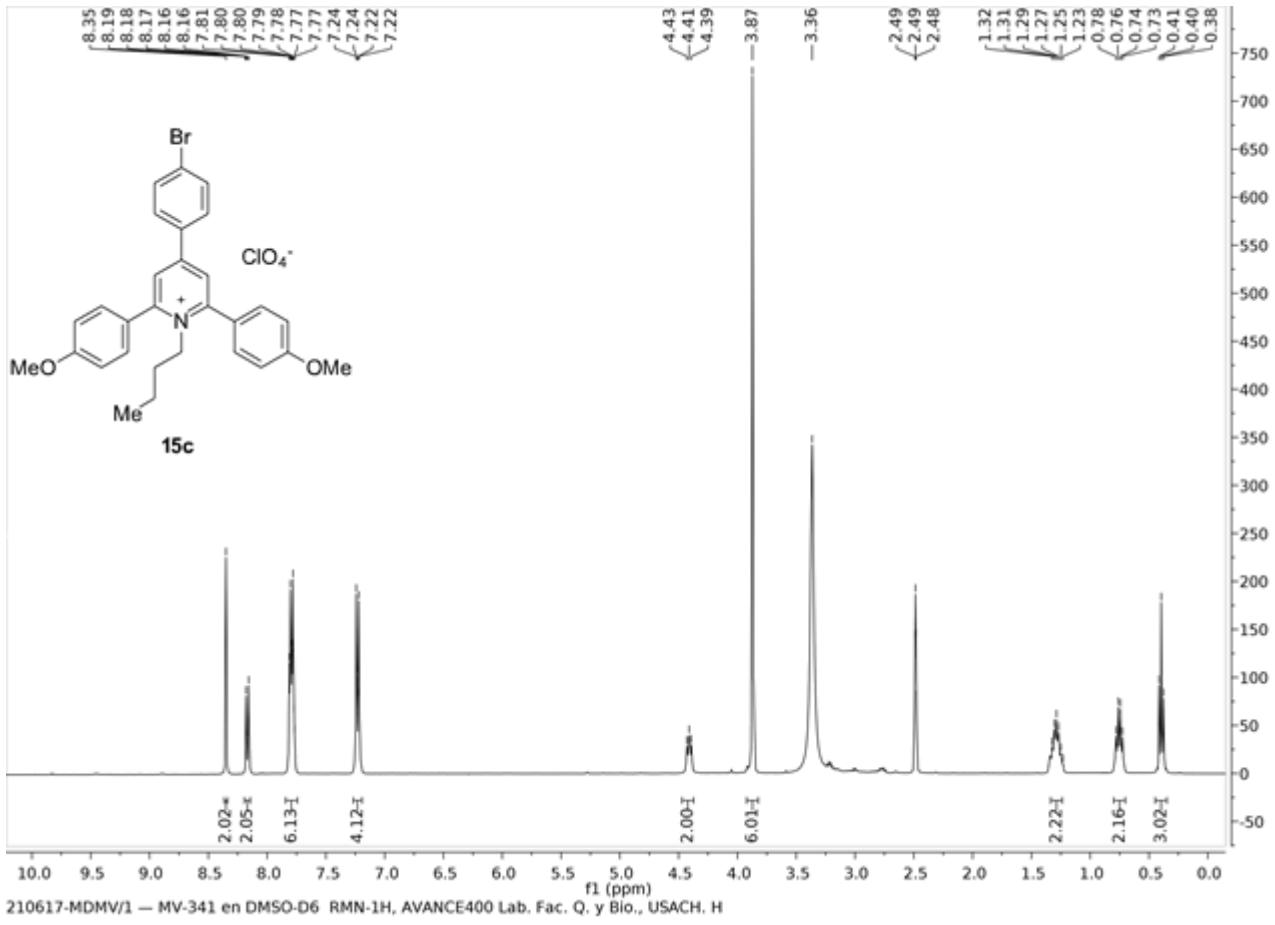


Figure 23:  $^1\text{H}$  NMR spectrum of compound 15c in DMSO-d6.  
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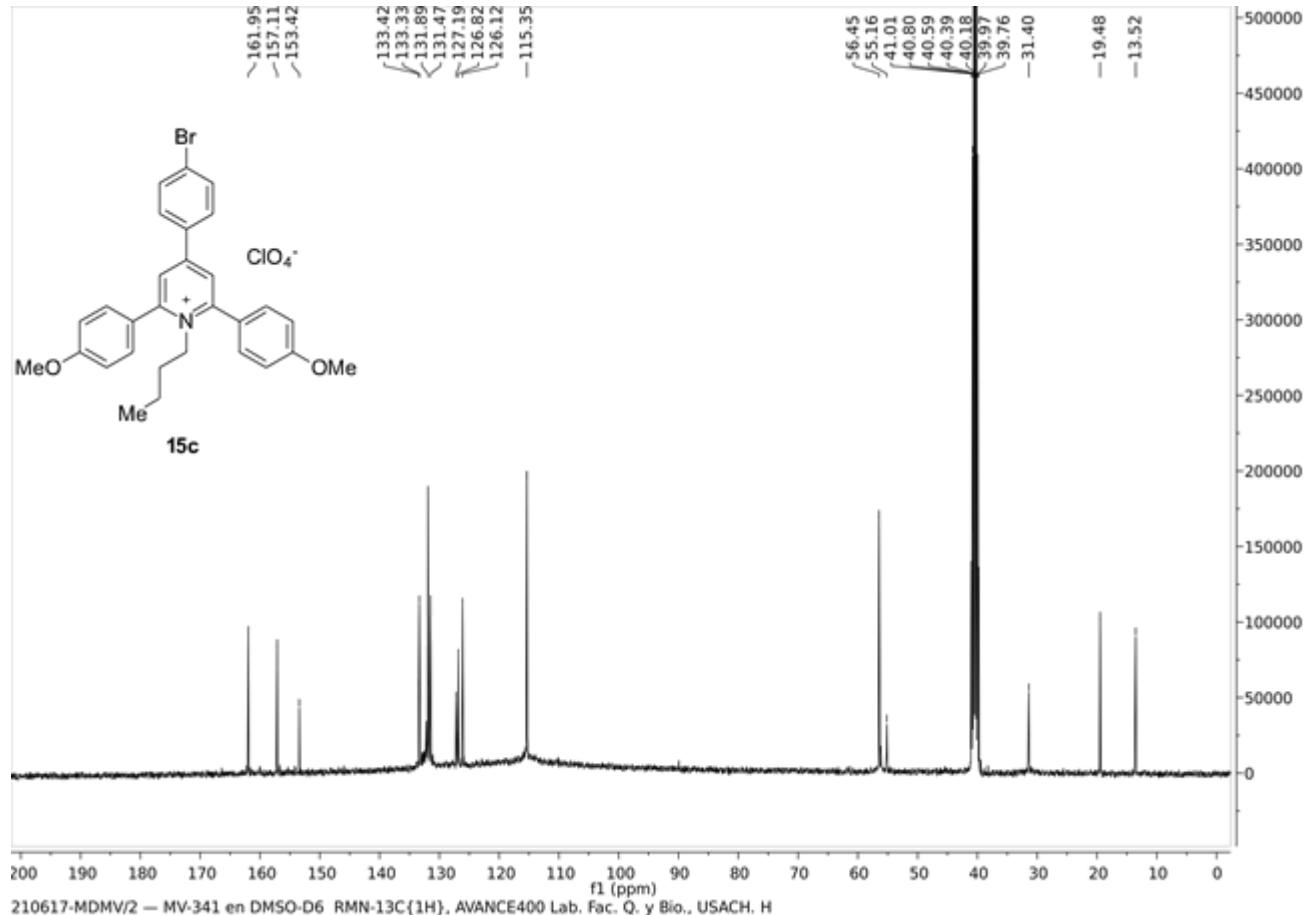


Figure 24:  $^{13}\text{C}$  NMR spectrum of compound 15c in DMSO-d6.  
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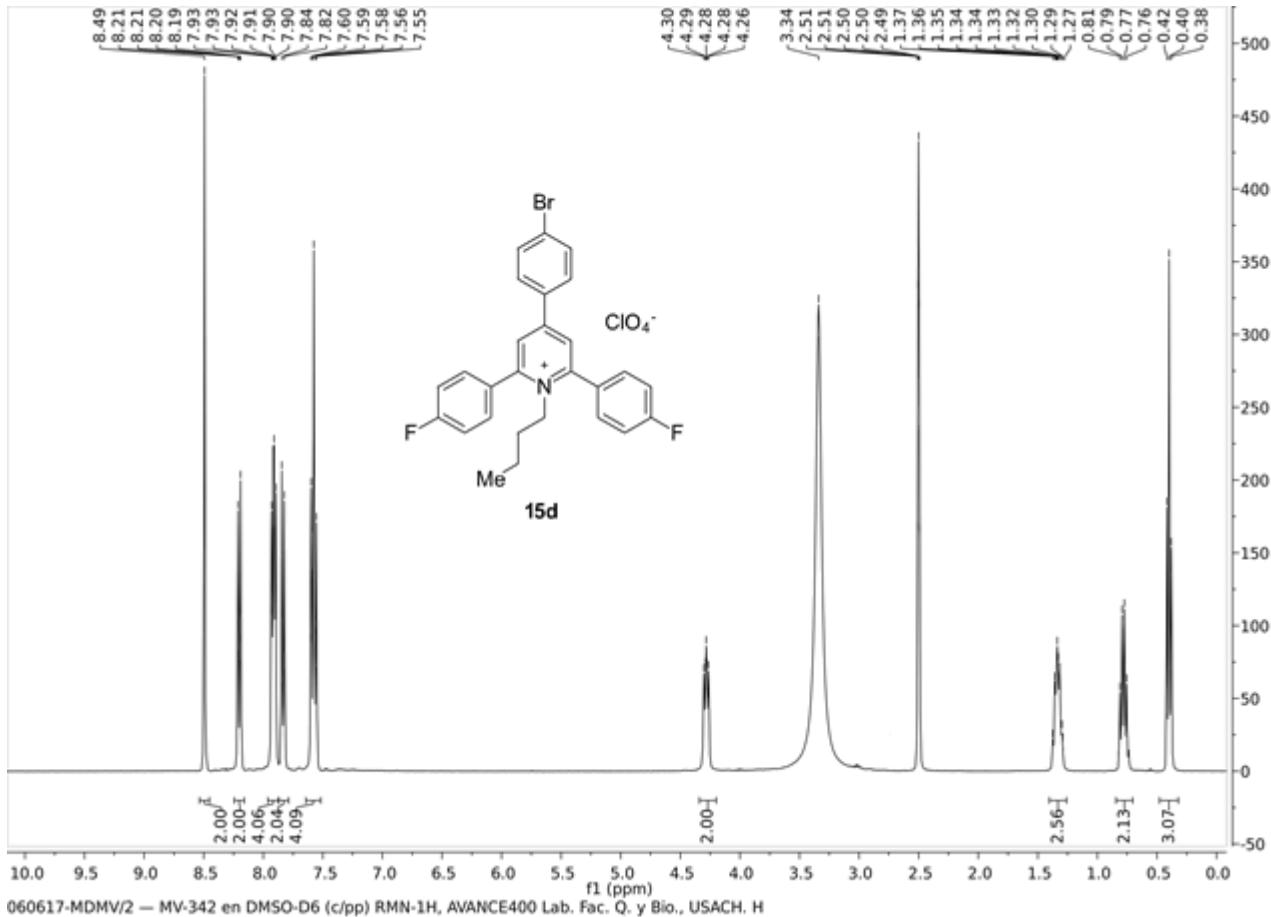


Figure 25:  $^1\text{H}$  NMR spectrum of compound 15d in DMSO-d6.  
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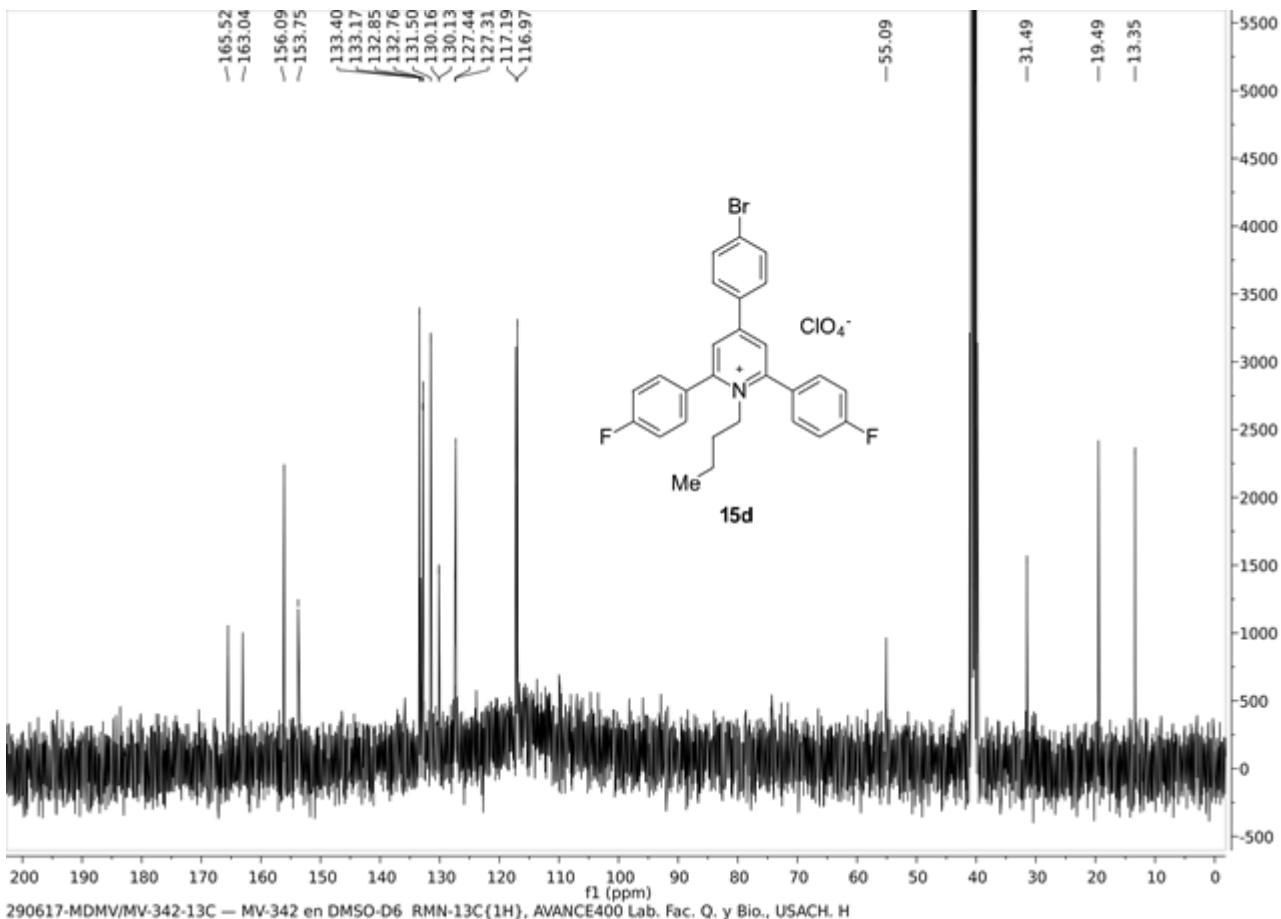


Figure 26:  $^{13}\text{C}$  NMR spectrum of compound 15d in DMSO-d<sub>6</sub>.  
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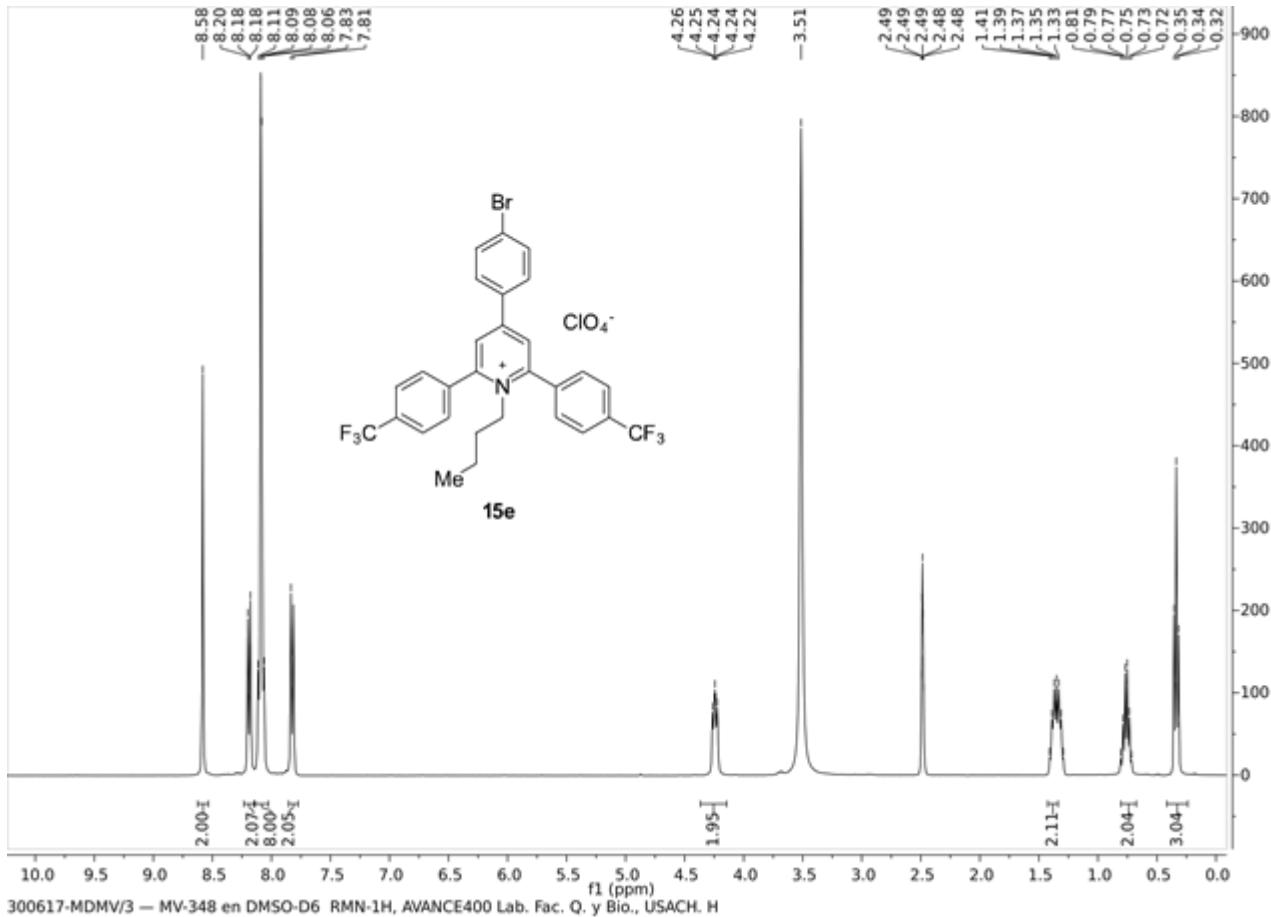


Figure 27:  $^1\text{H}$  NMR spectrum of compound 15e in DMSO-d6.  
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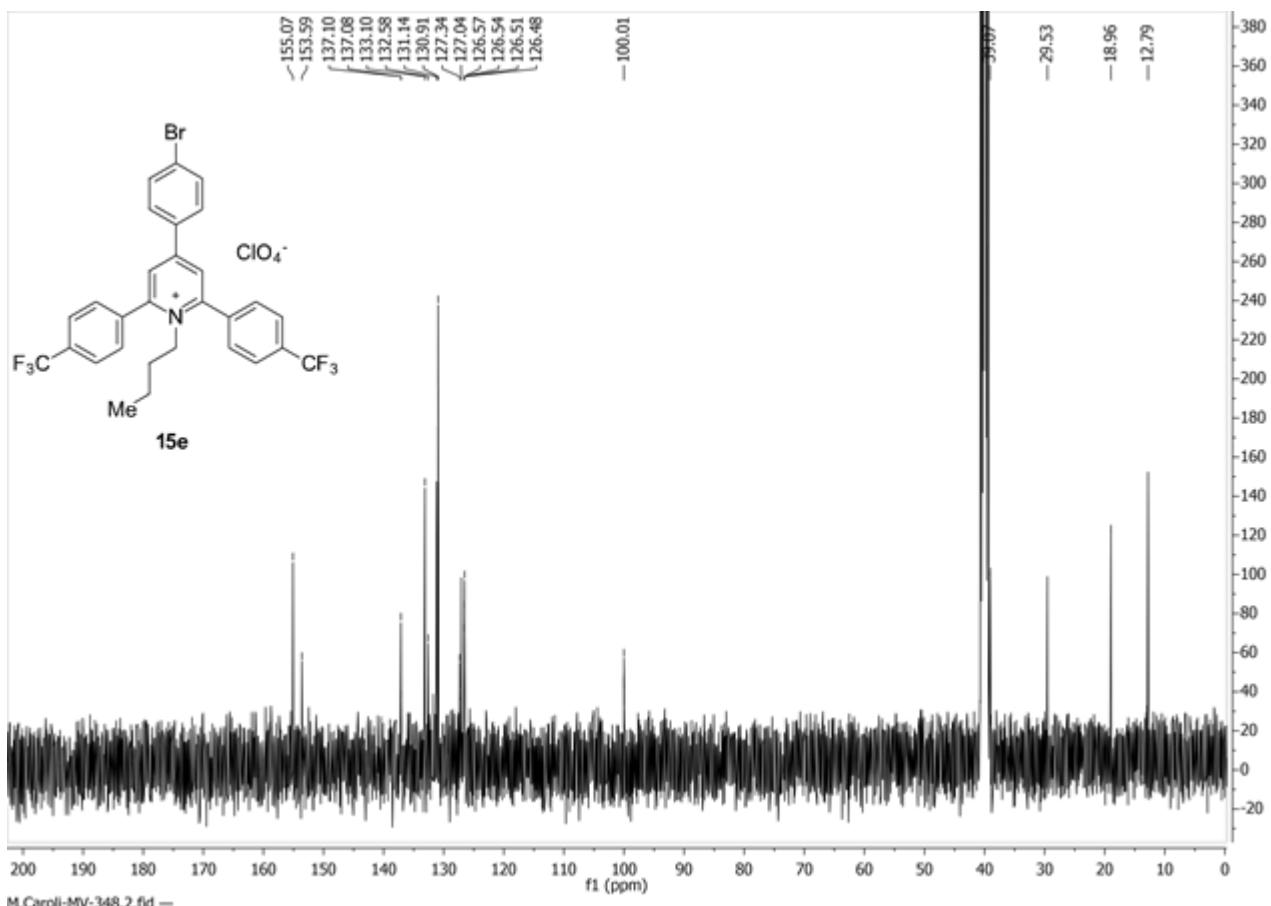


Figure 28:  $^{13}\text{C}$  NMR spectrum of compound 15e in  $\text{DMSO-d}_6$ .  
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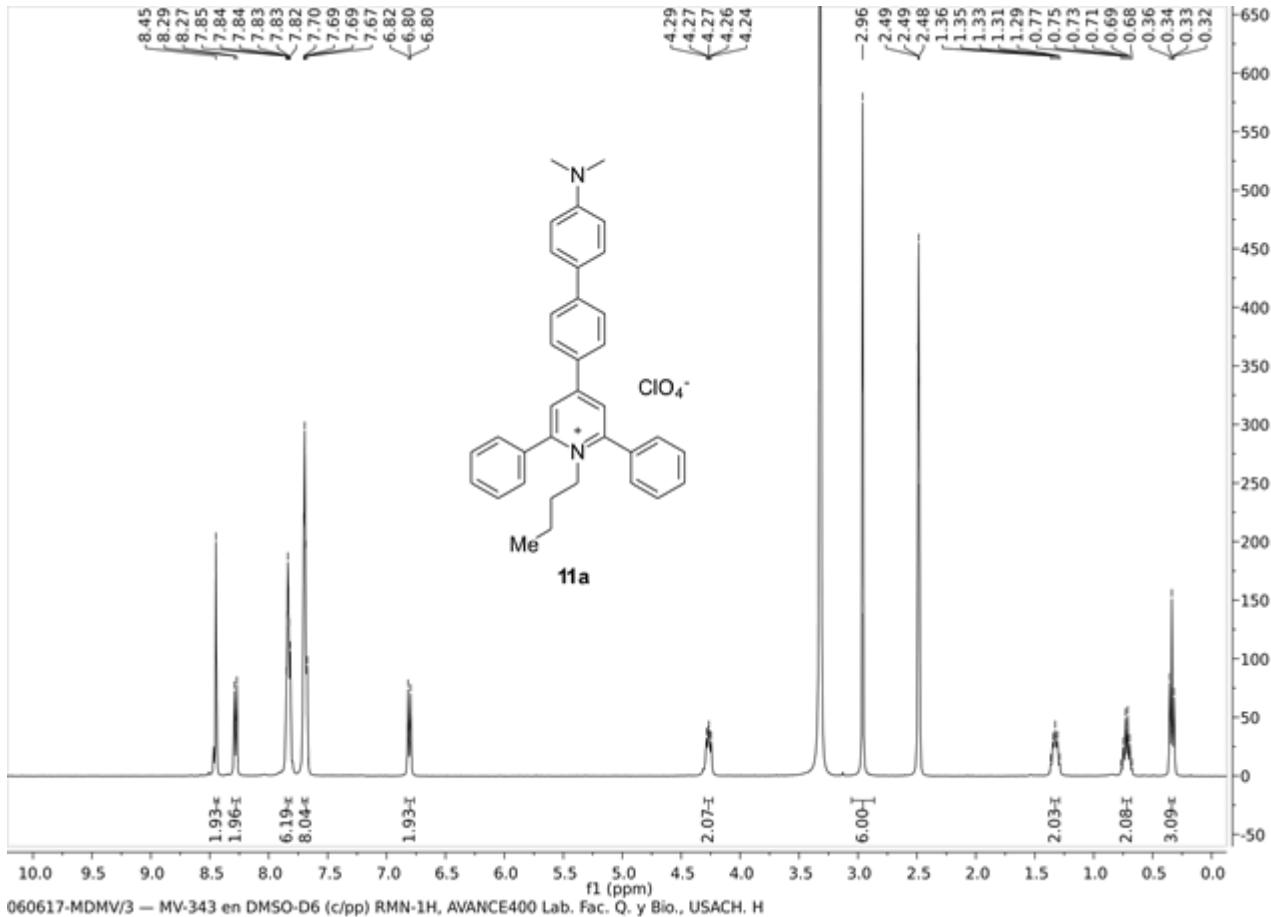
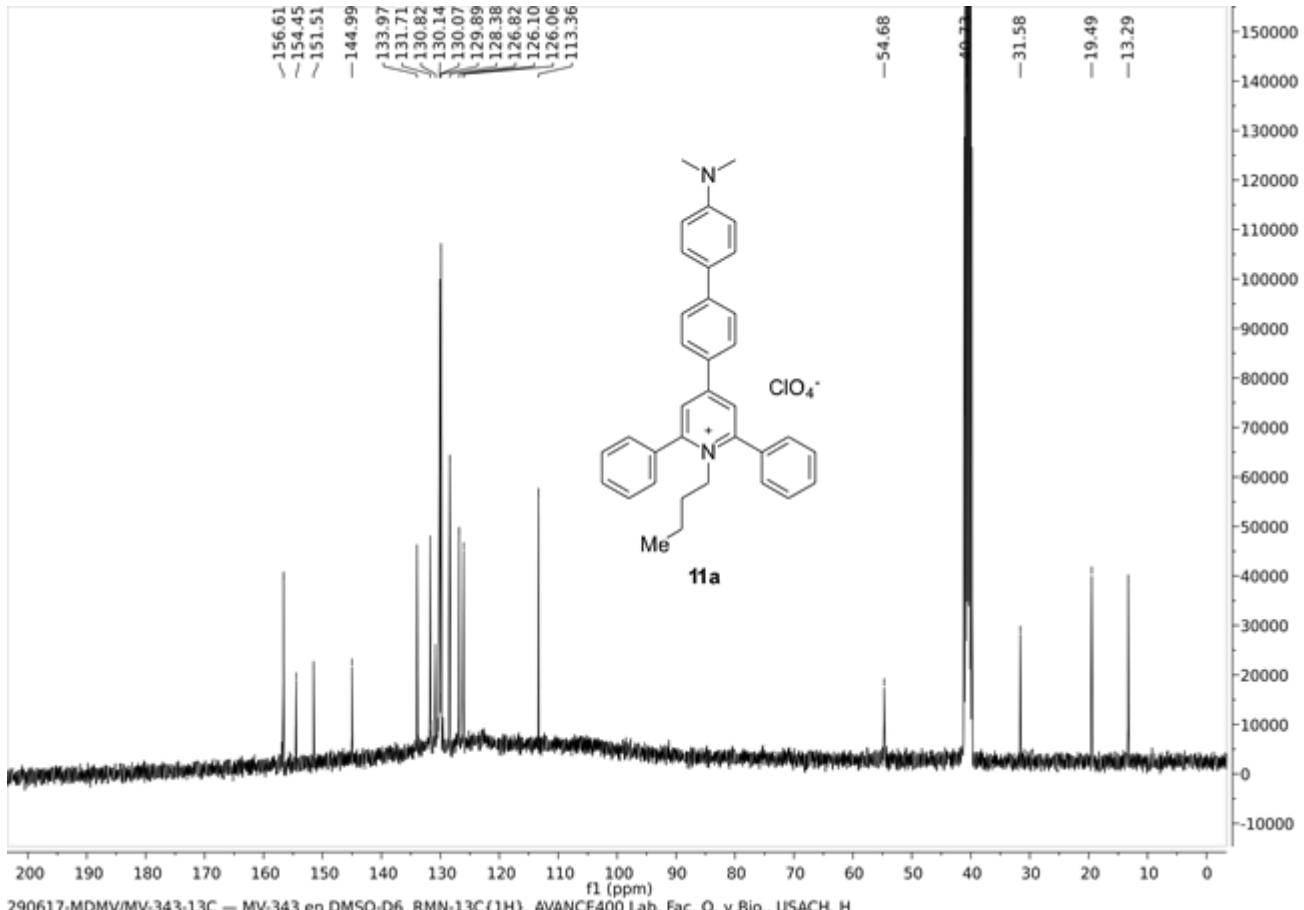


Figure 29:  $^1\text{H}$  NMR spectrum of compound 11a in DMSO-d6.  
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290617-MDMV/MV-343-13C — MV-343 en DMSO-D6 RMN-13C(1H), AVANCE400 Lab. Fac. Q. y Bio., USACH. H

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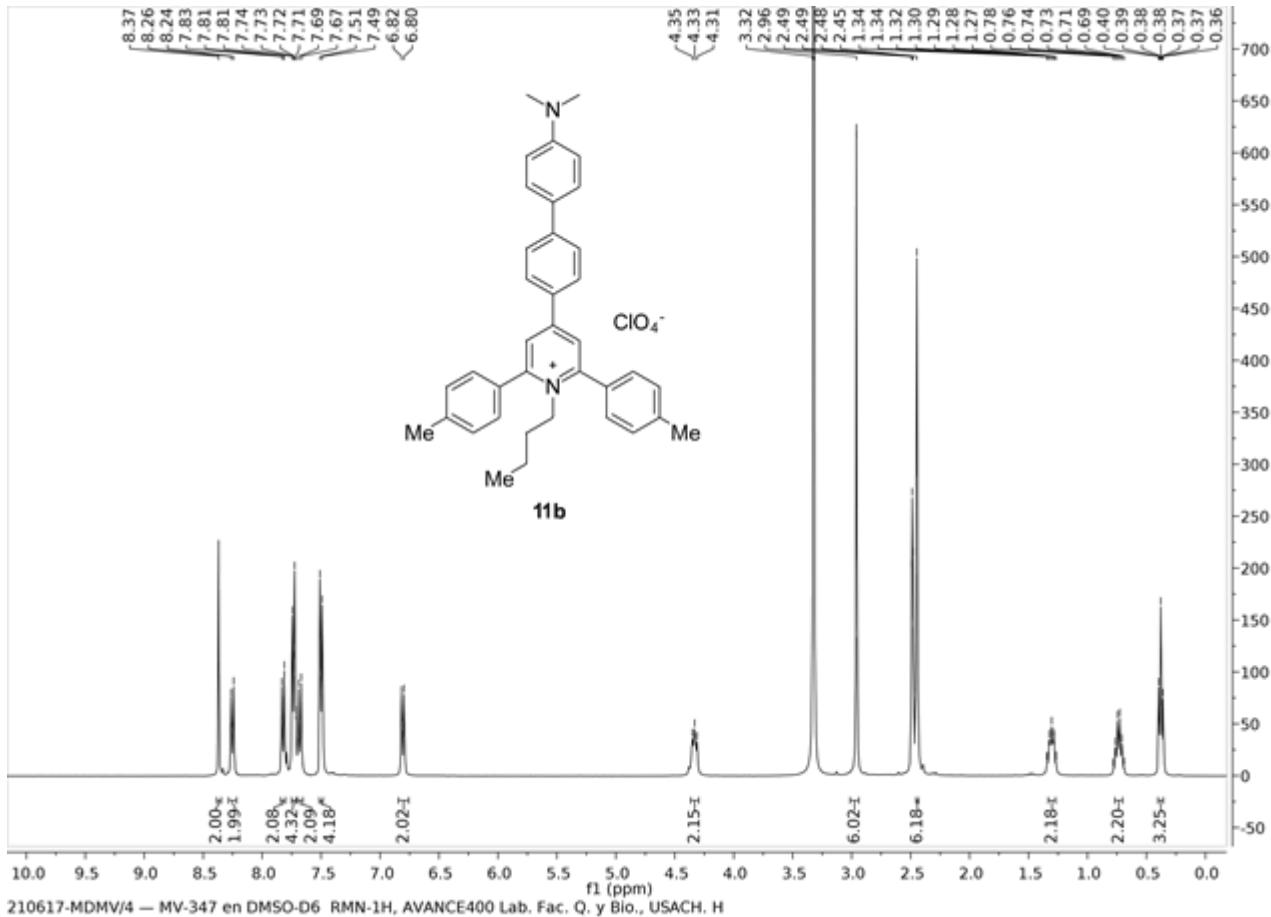


Figure 31:  $^1\text{H}$  NMR spectrum of compound **11b** in DMSO-d6.  
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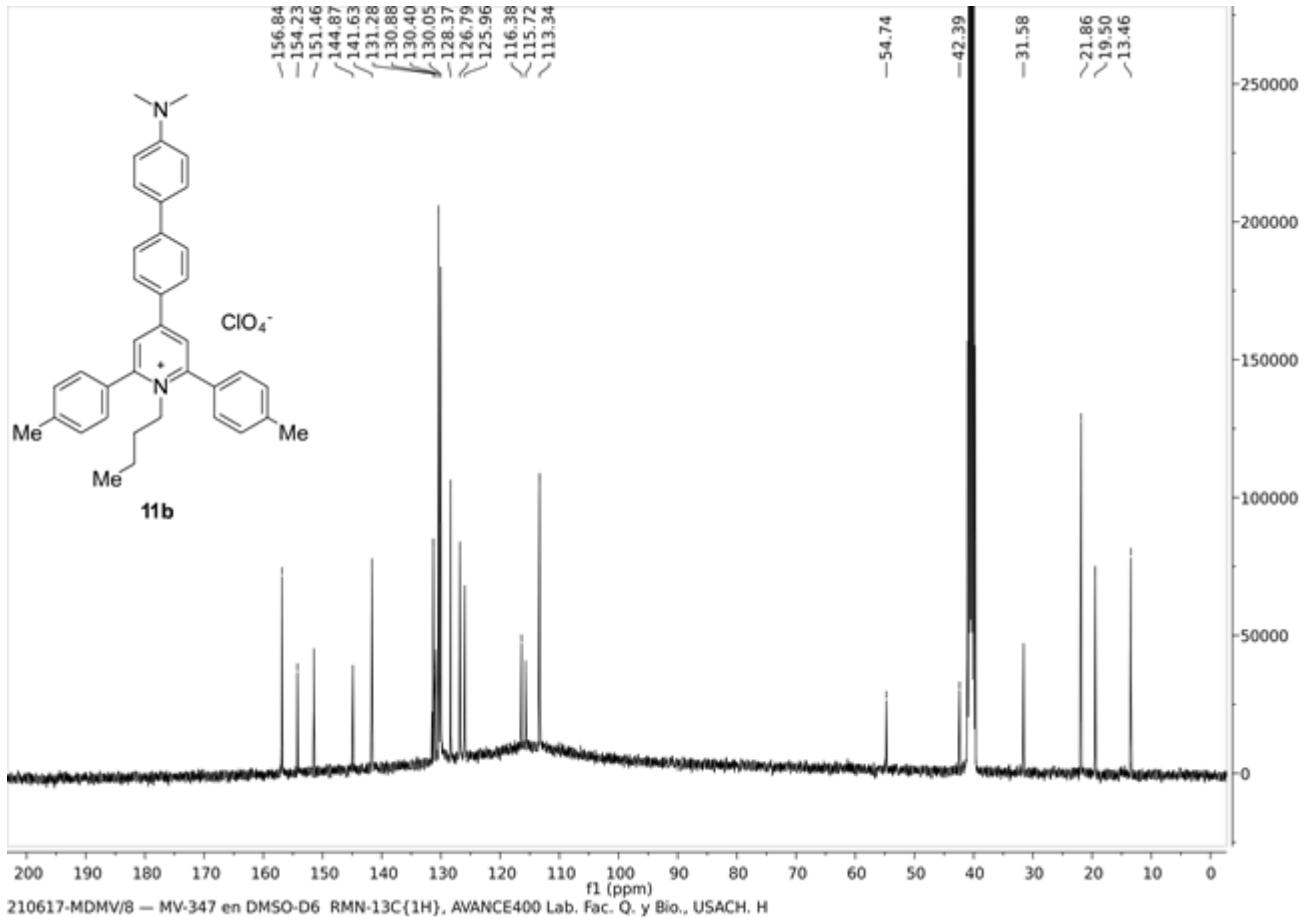


Figure 32:  $^{13}\text{C}$  NMR spectrum of compound 11b in DMSO-d6.  
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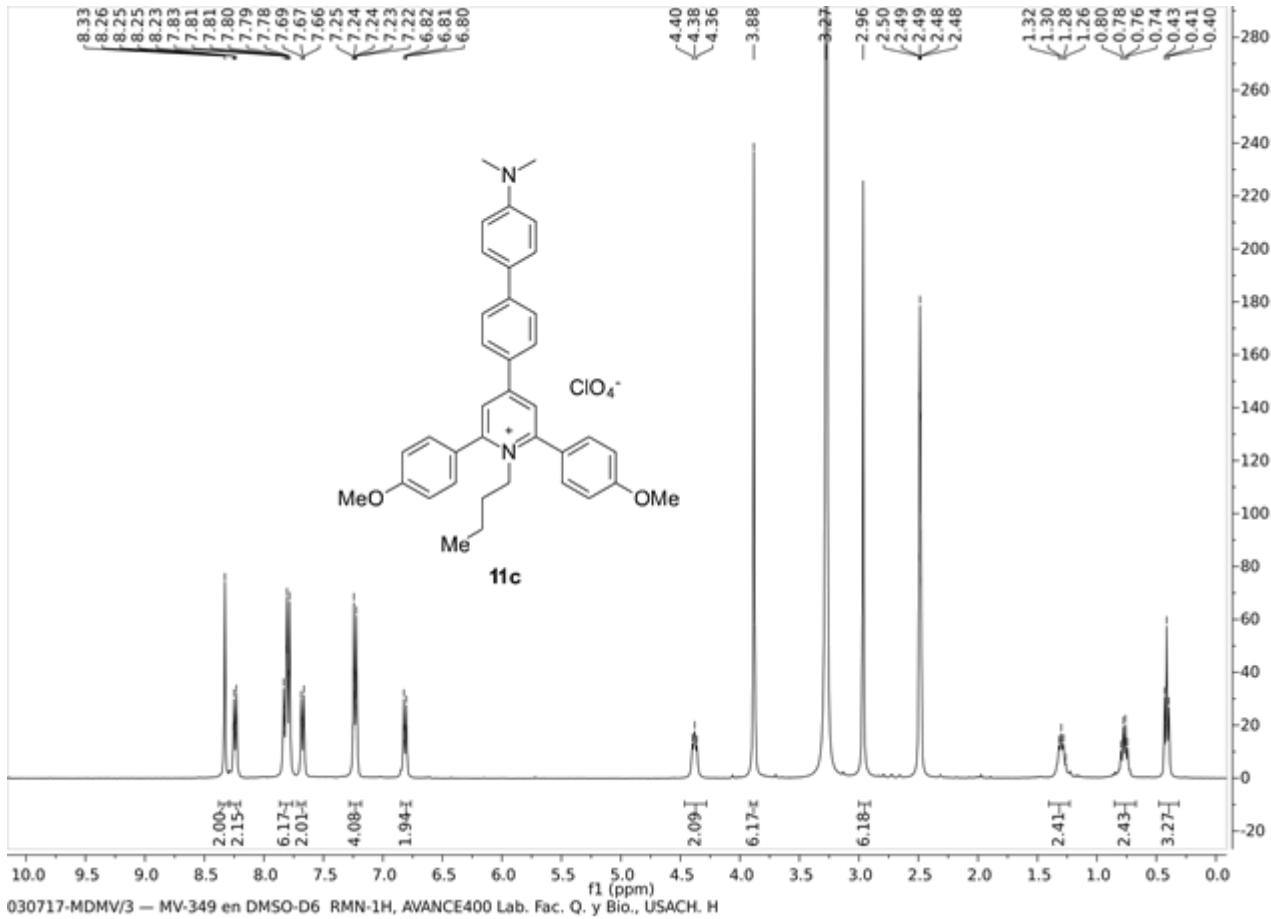


Figure 33:  $^1\text{H}$  NMR spectrum of compound **11c** in DMSO-d6.  
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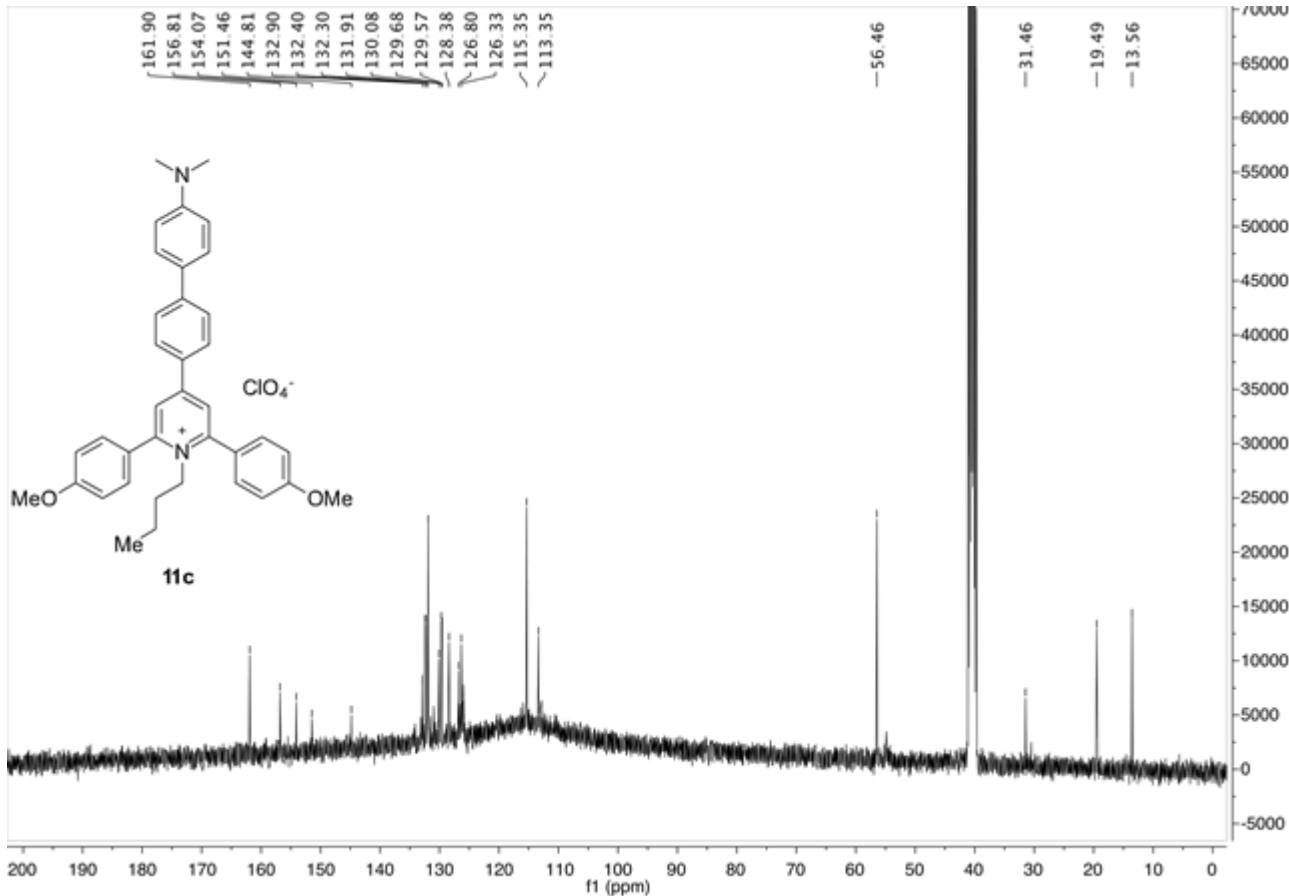


Figure 34:  $^{13}\text{C}$  NMR spectrum of compound **11c** in DMSO-d6.  
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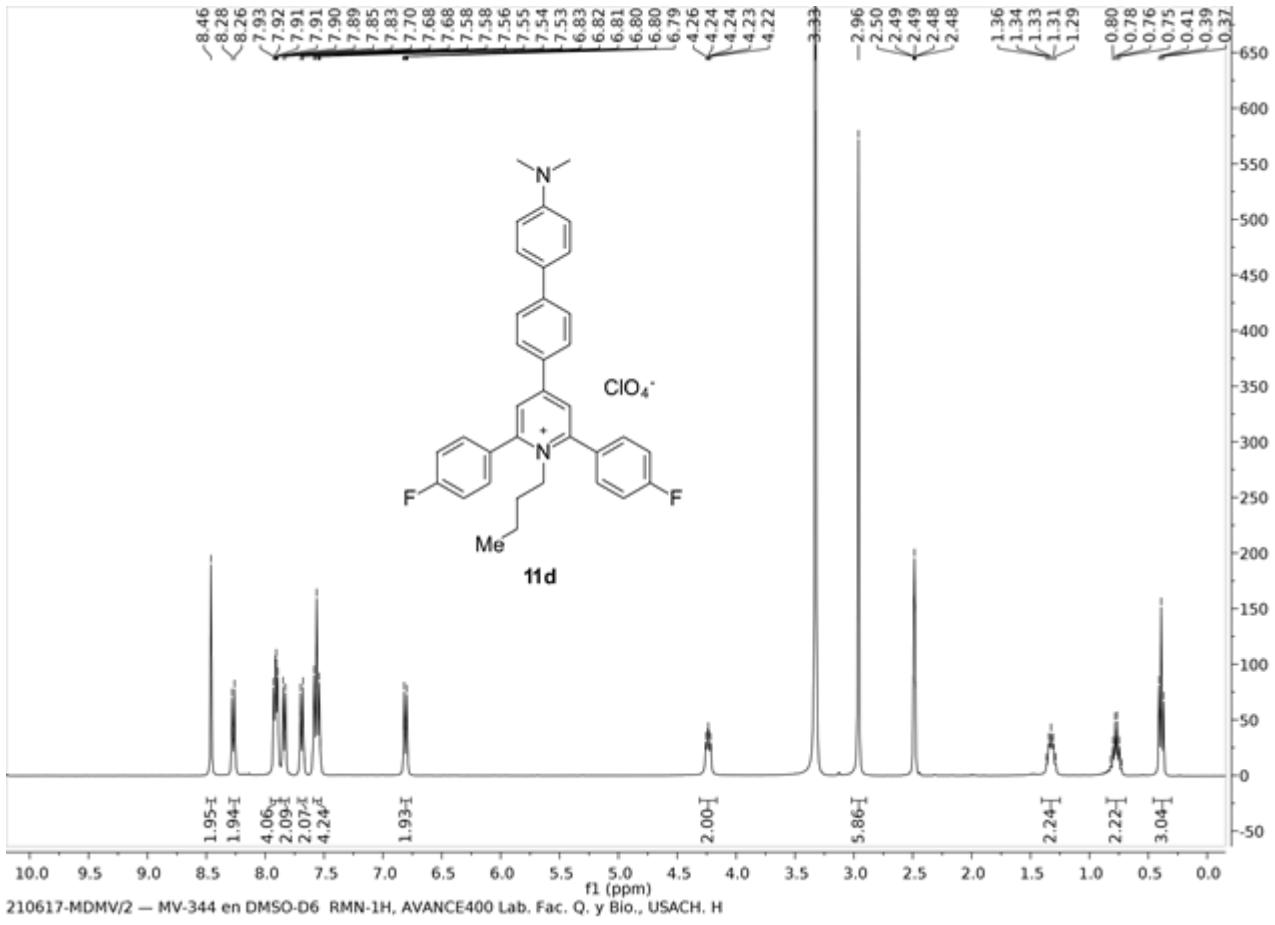


Figure 35:  $^1\text{H}$  NMR spectrum of compound 11d in DMSO-d<sub>6</sub>.  
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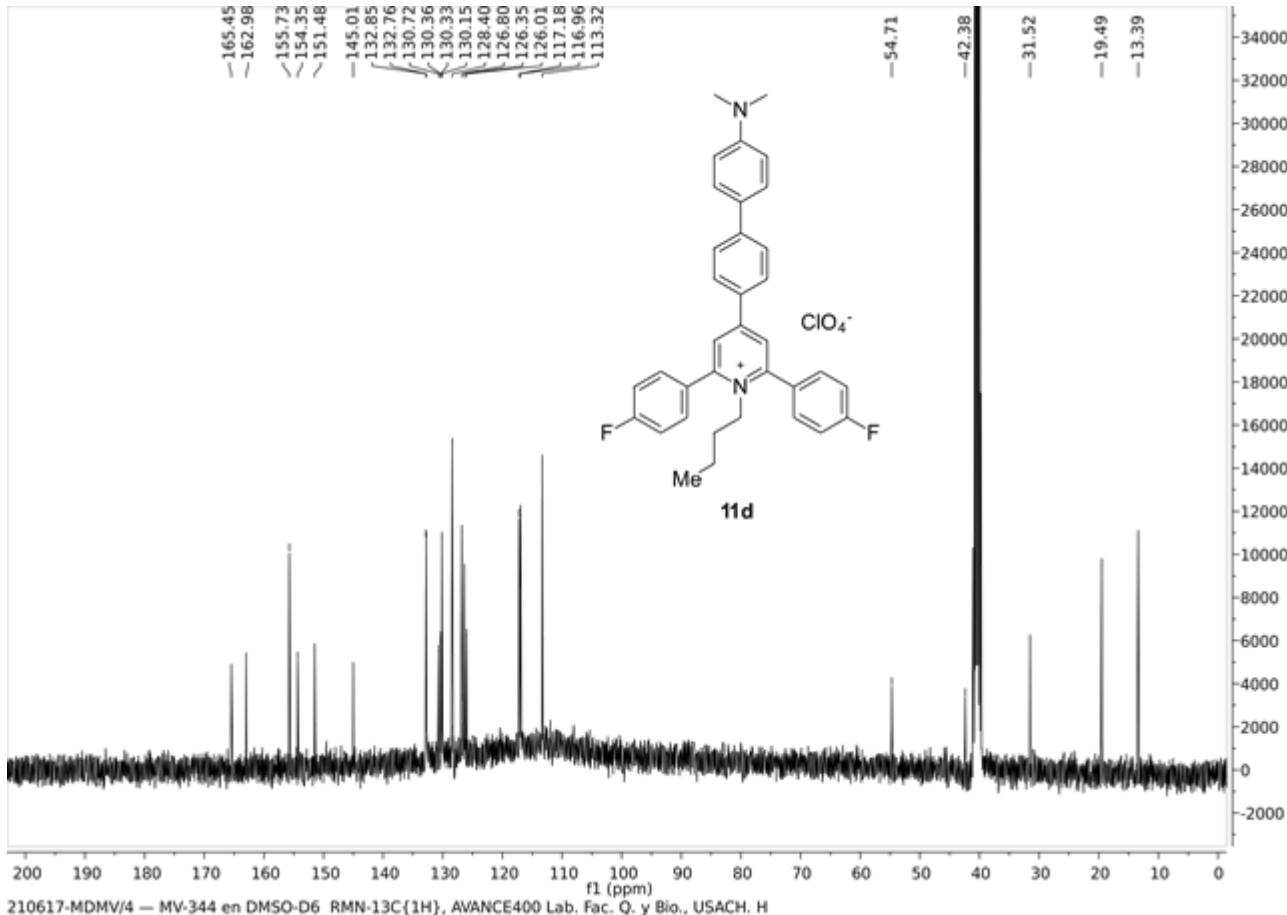


Figure 36:  $^{13}\text{C}$  NMR spectrum of compound **11d** in DMSO-d6.  
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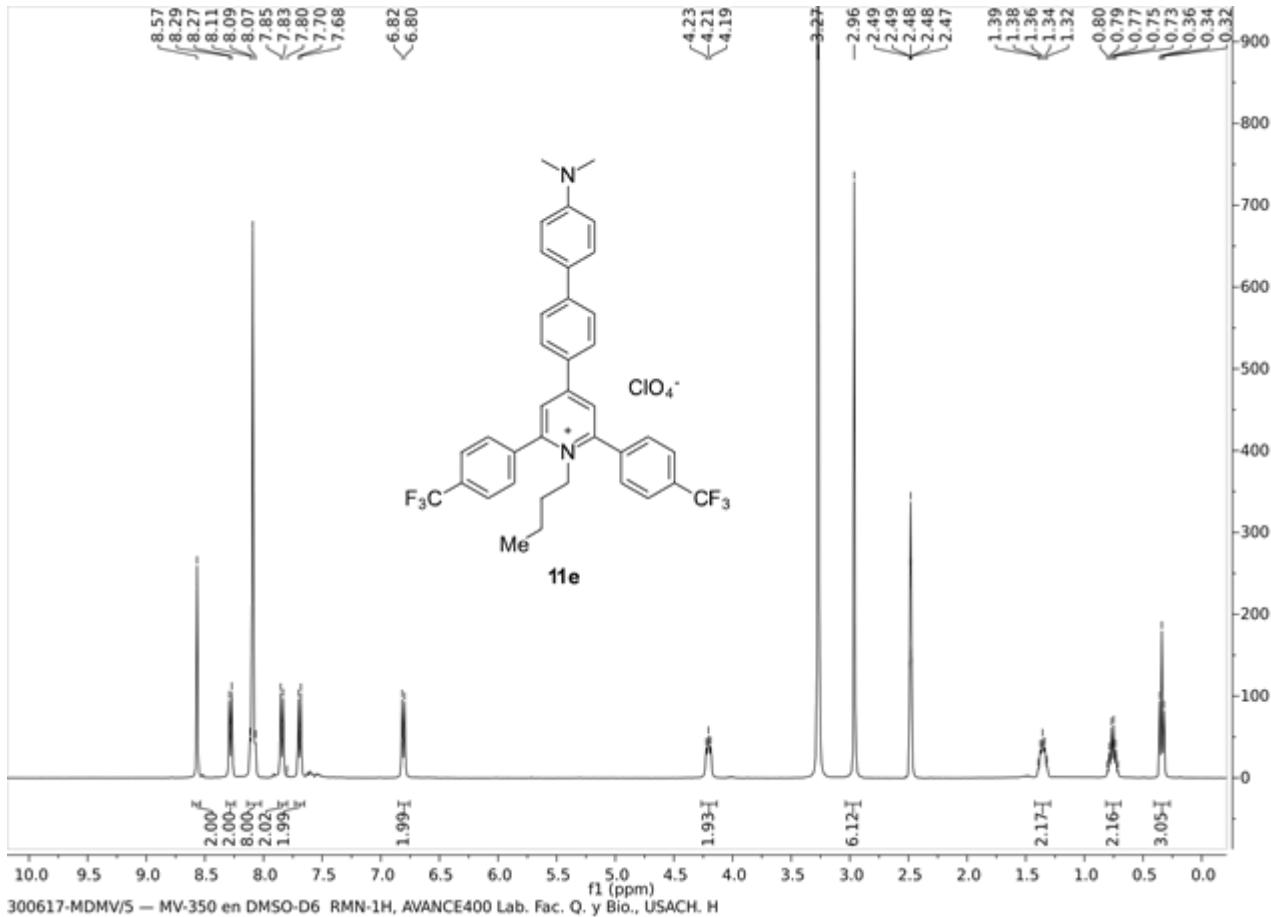


Figure 37:  $^1\text{H}$  NMR spectrum of compound 11e in DMSO-d6.  
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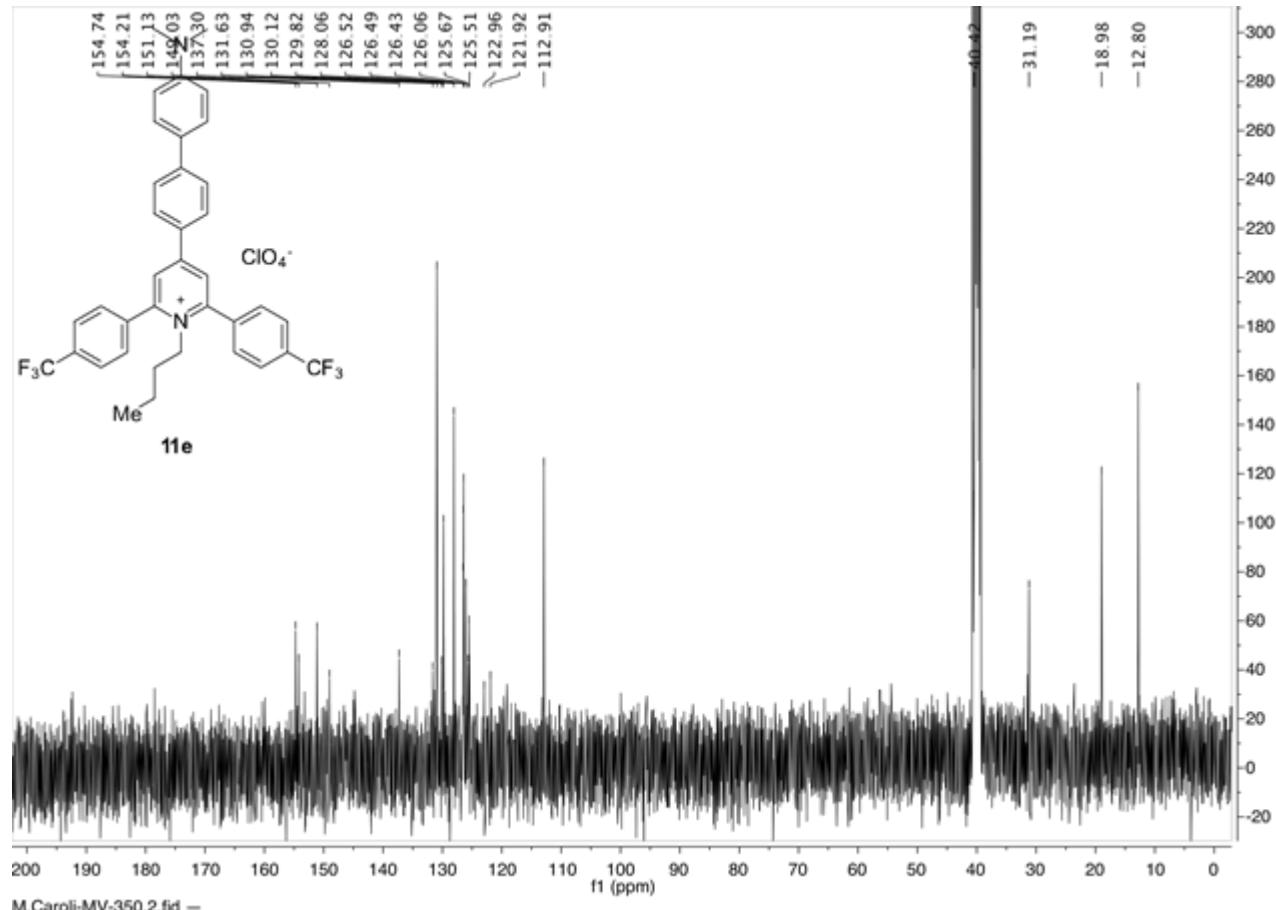


Figure 38:  $^{13}\text{C}$  NMR spectrum of compound 11e in  $\text{DMSO-d}_6$ .  
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