

Transition Metal-Free C-H/C-Li Coupling of Non-Aromatic 2*H*-Imidazole 1-oxides with Pentafluorophenyl Lithium in the Design of Novel Fluorophores with Intramolecular Charge Transfer (ICT) Effect

Electronic Supplementary Information (ESI)

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[‡] Institute of Organic Synthesis, Ural Branch of the Russian Academy of Sciences, 22 S.
Kovalevskaya Str., 620041 Ekaterinburg, Russia

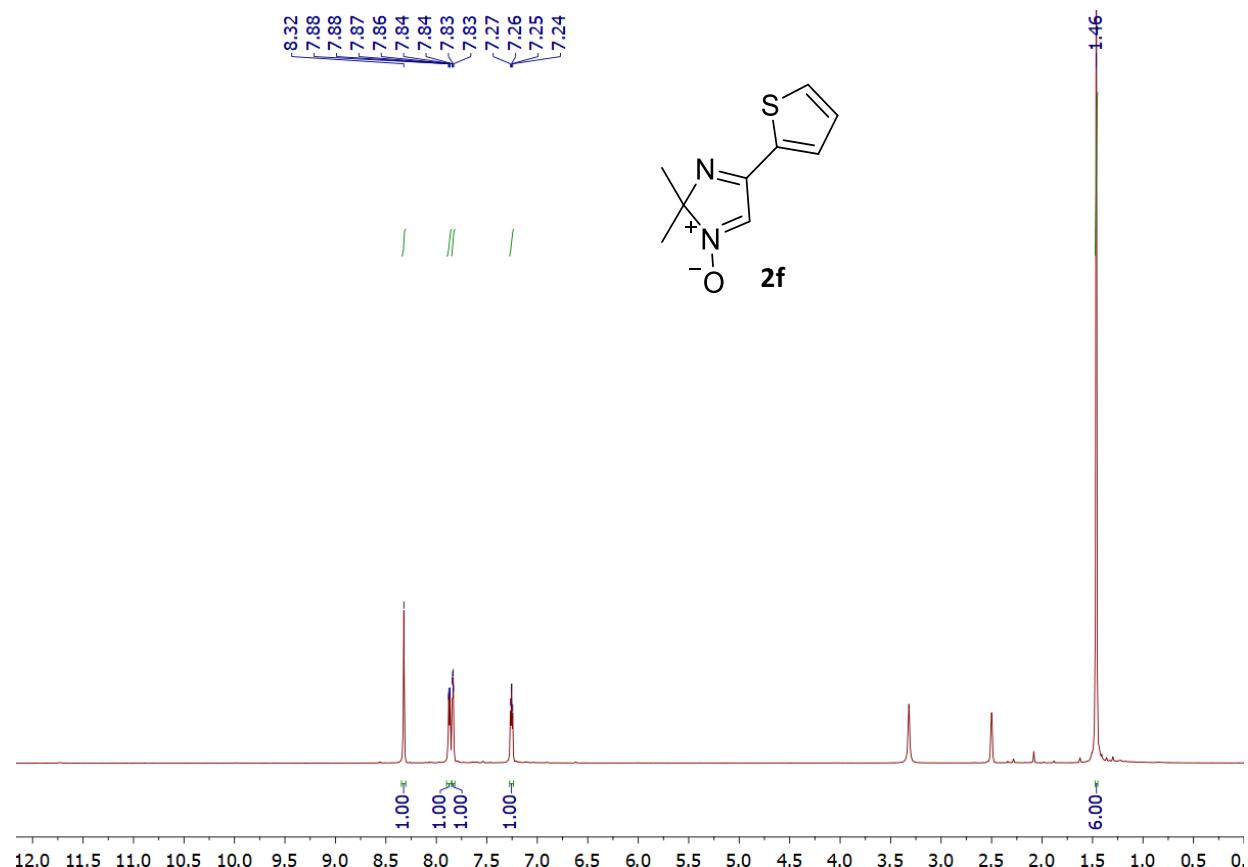
*E-mail: chupakhin@ios.uran.ru

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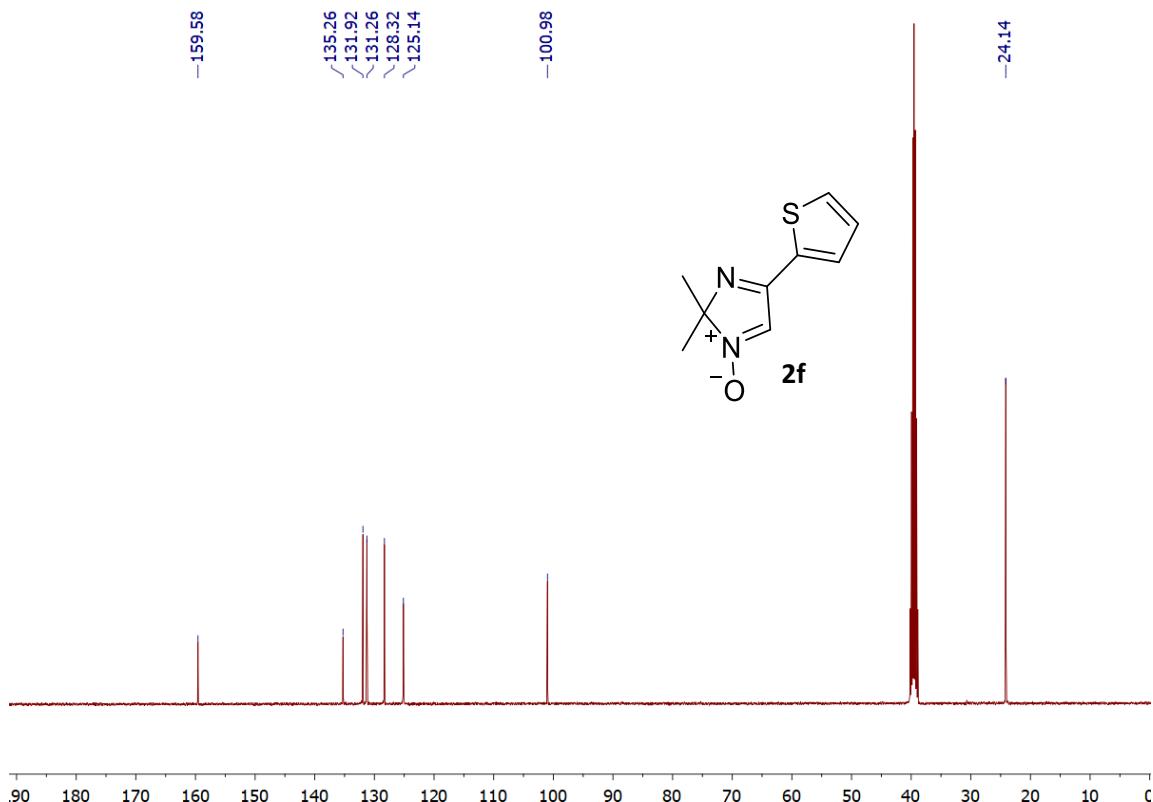
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1. Copies of ^1H , ^{13}C , ^{19}F NMR spectra of 2*H*-imidazole 1-oxides 2f,g,i,j,k,l

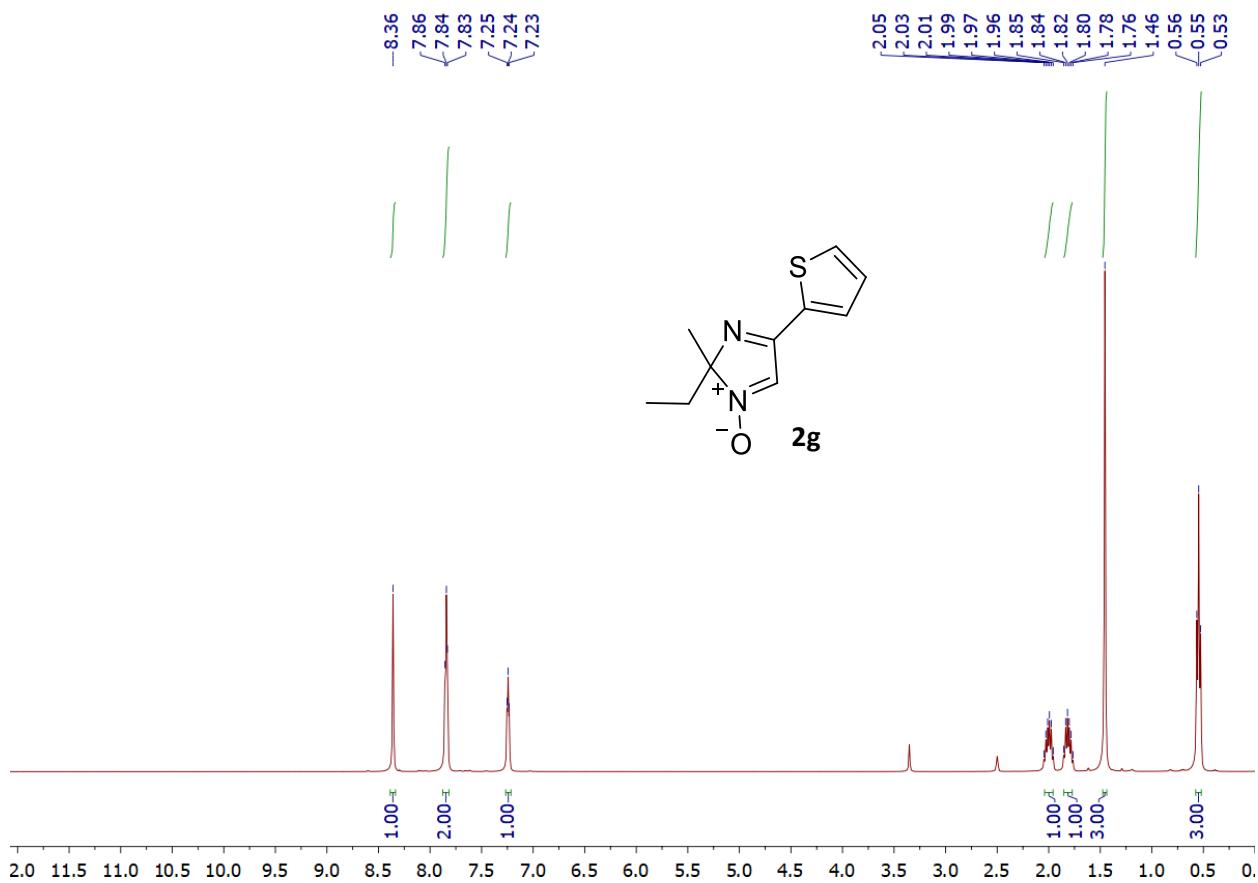
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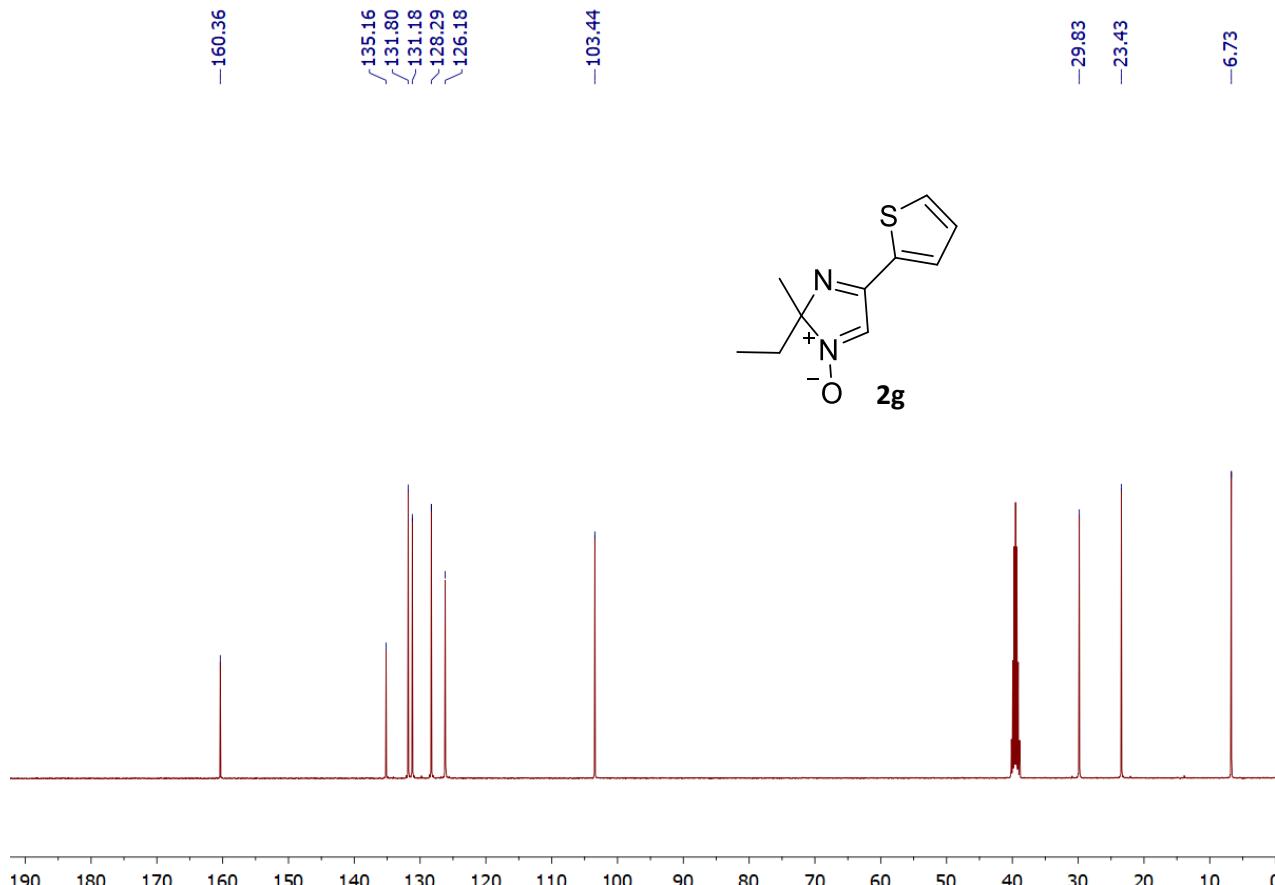
^{13}C { ^1H } NMR (101 MHz, DMSO-d₆)



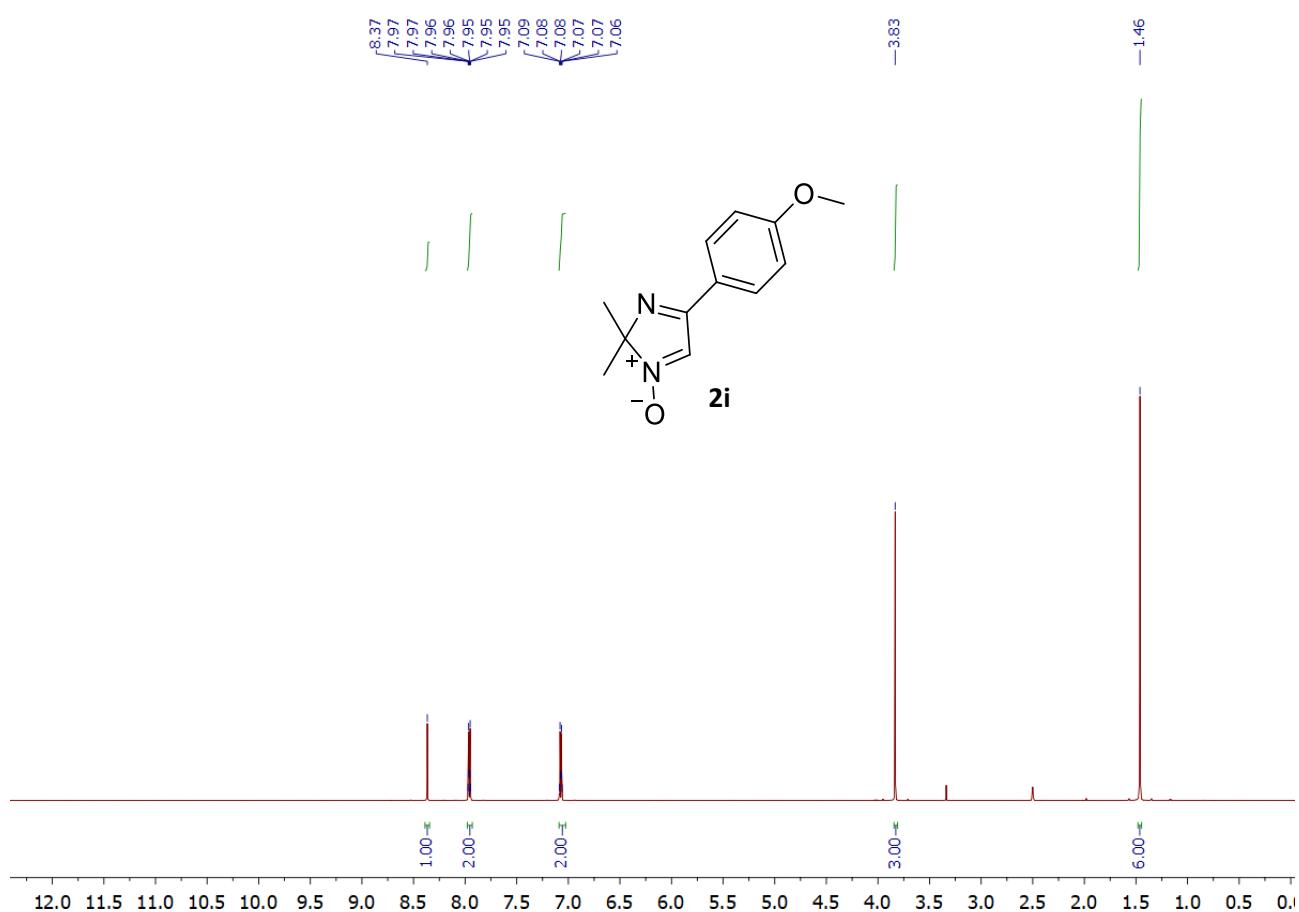
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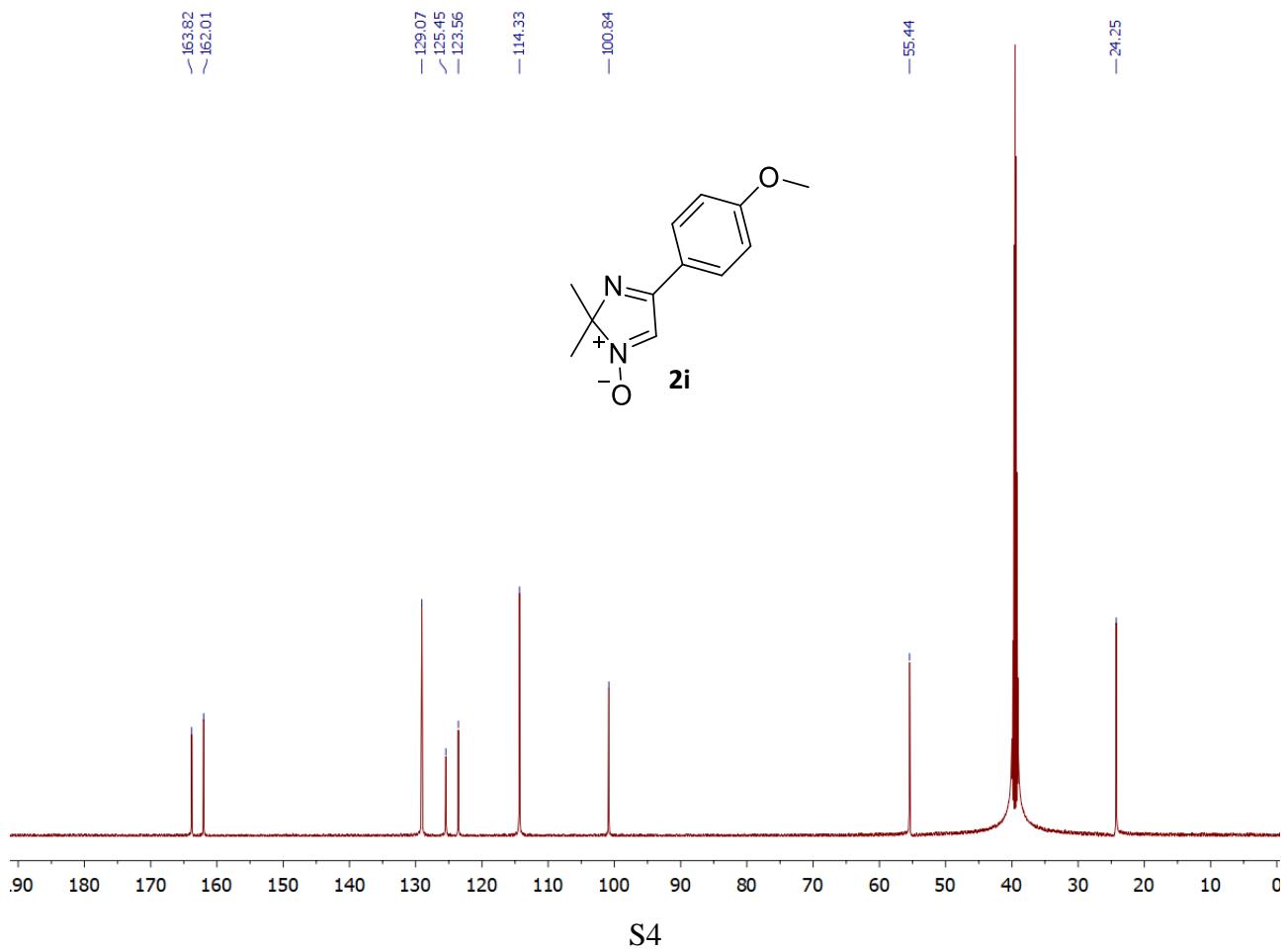
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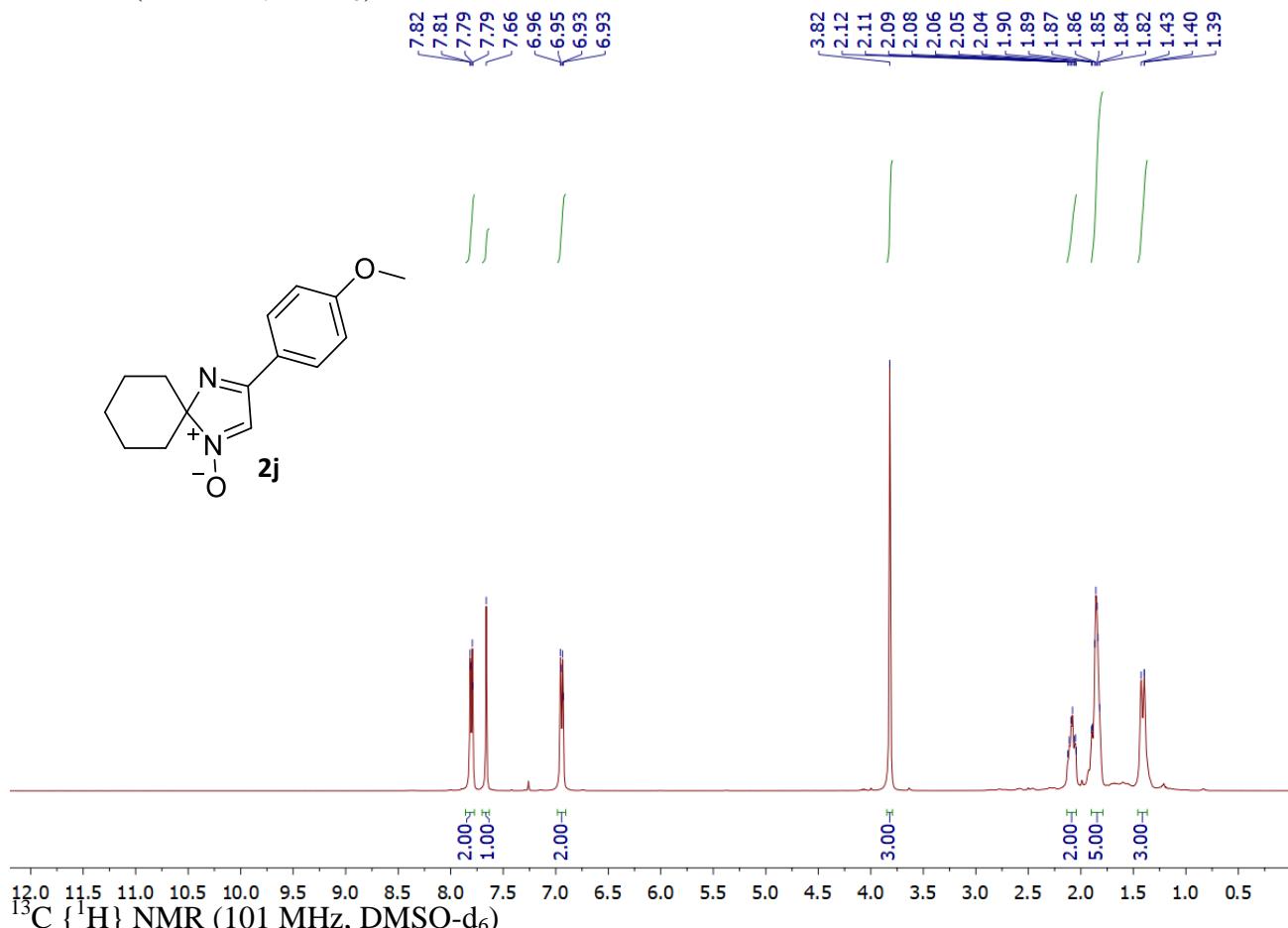
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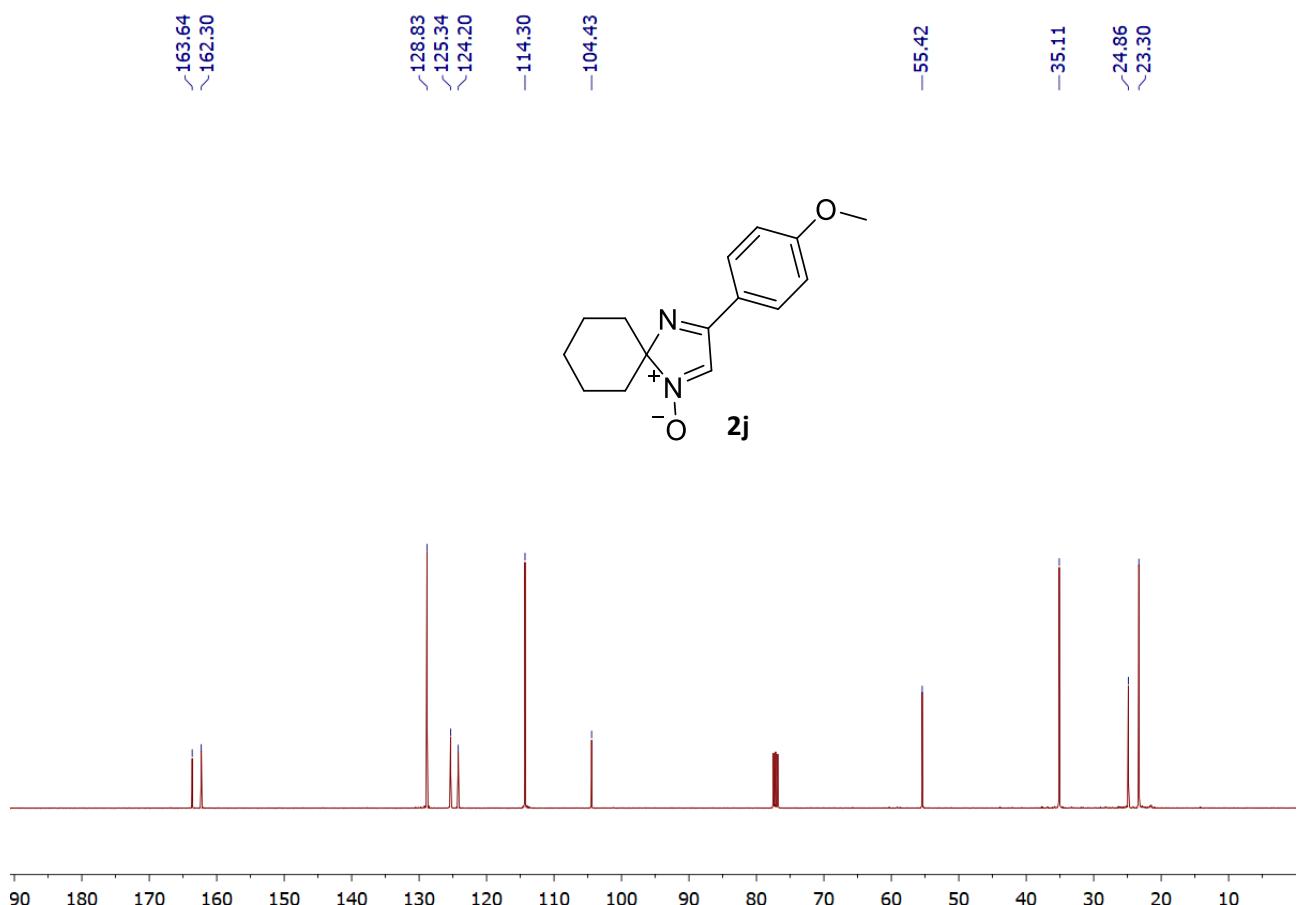
$^{13}\text{C} \{^1\text{H}\}$ NMR (101 MHz, DMSO-d₆)



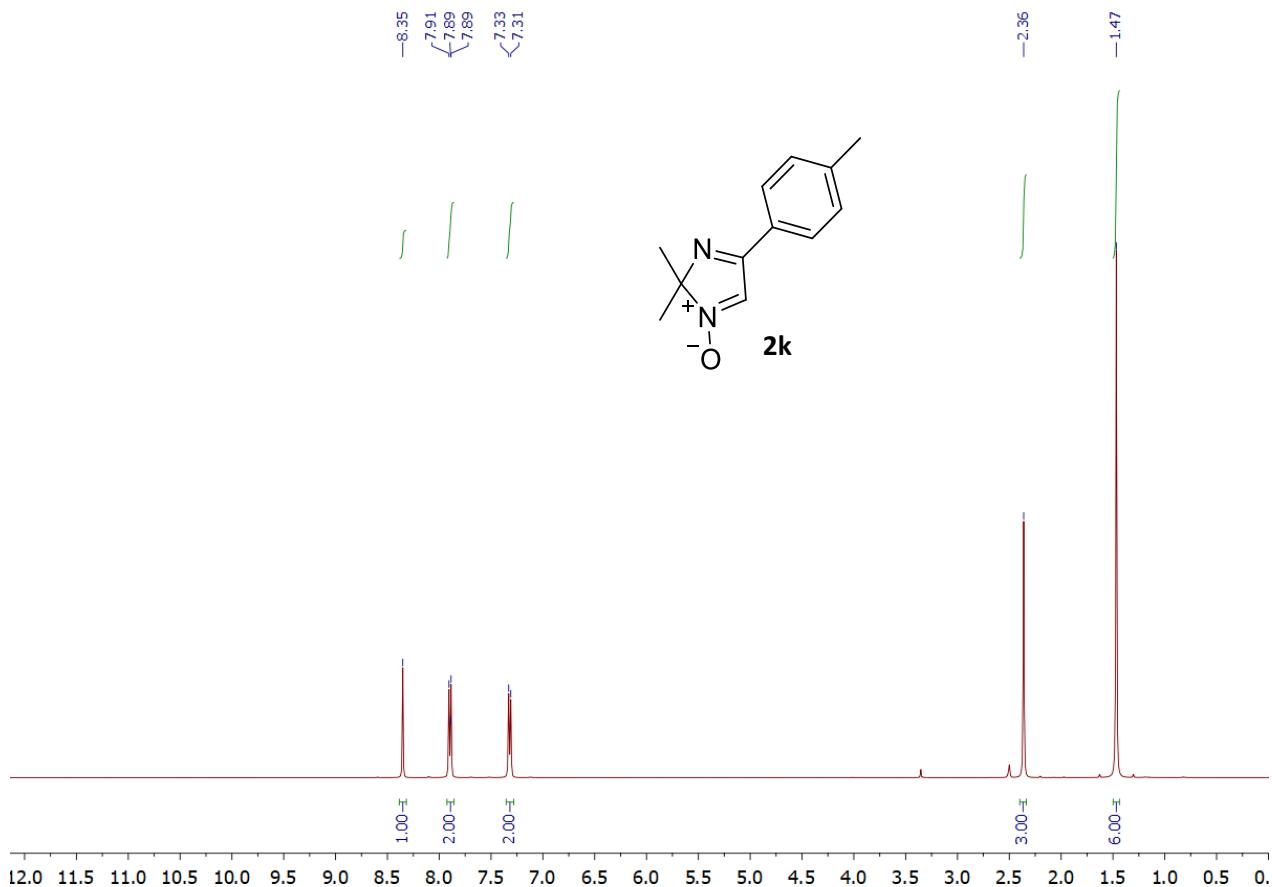
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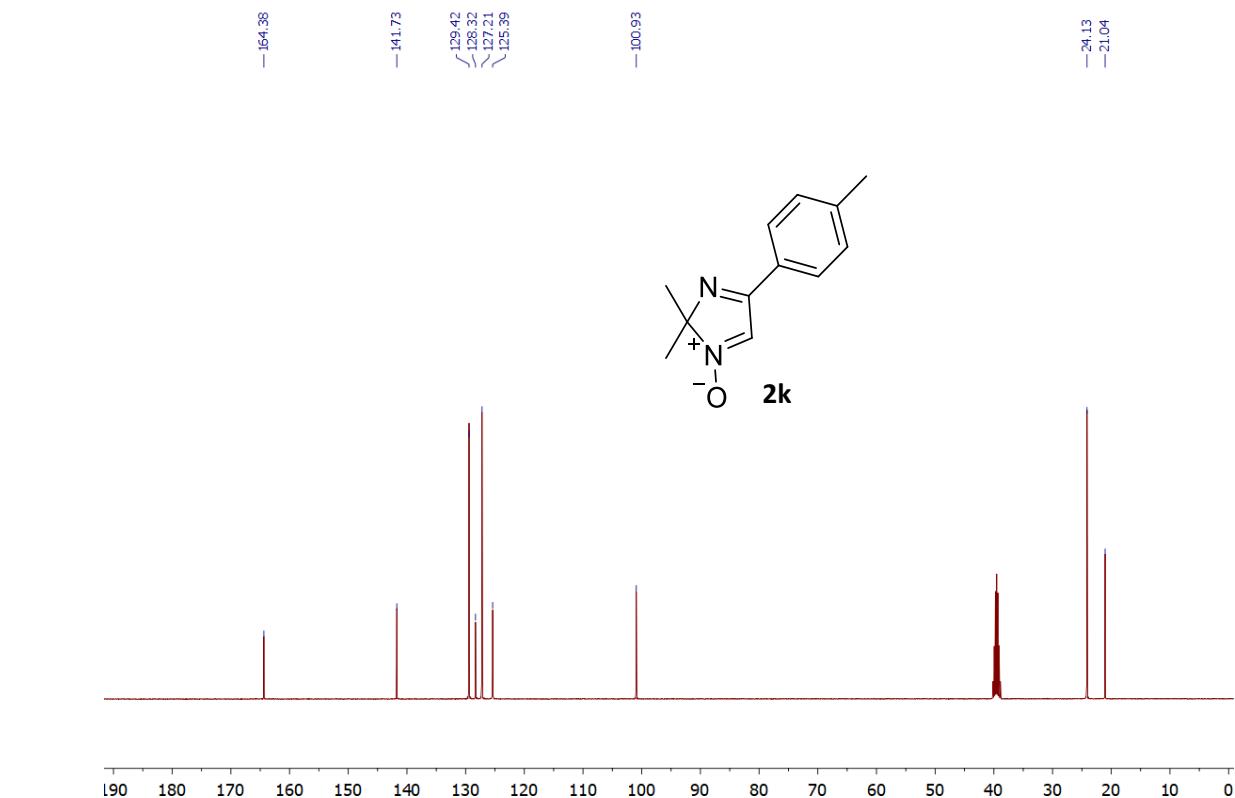
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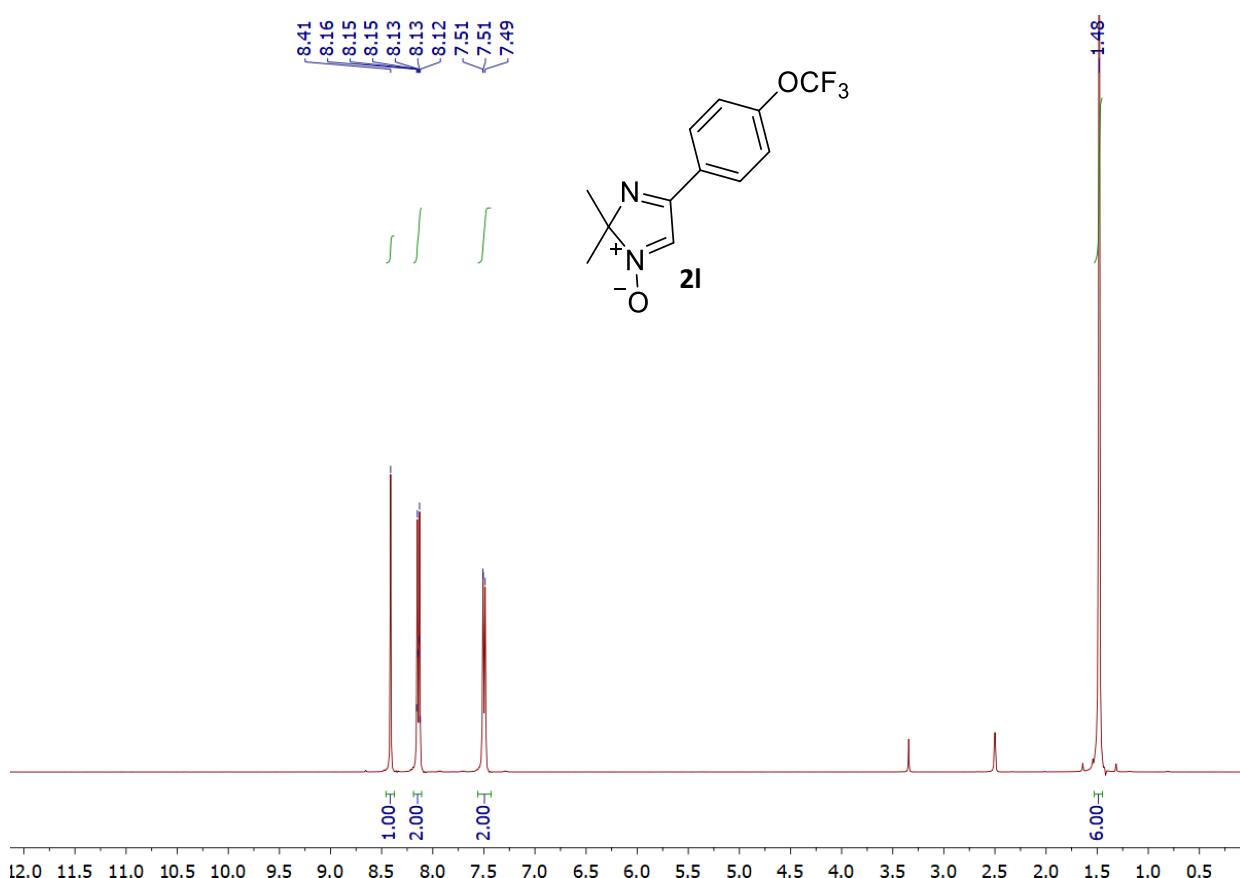
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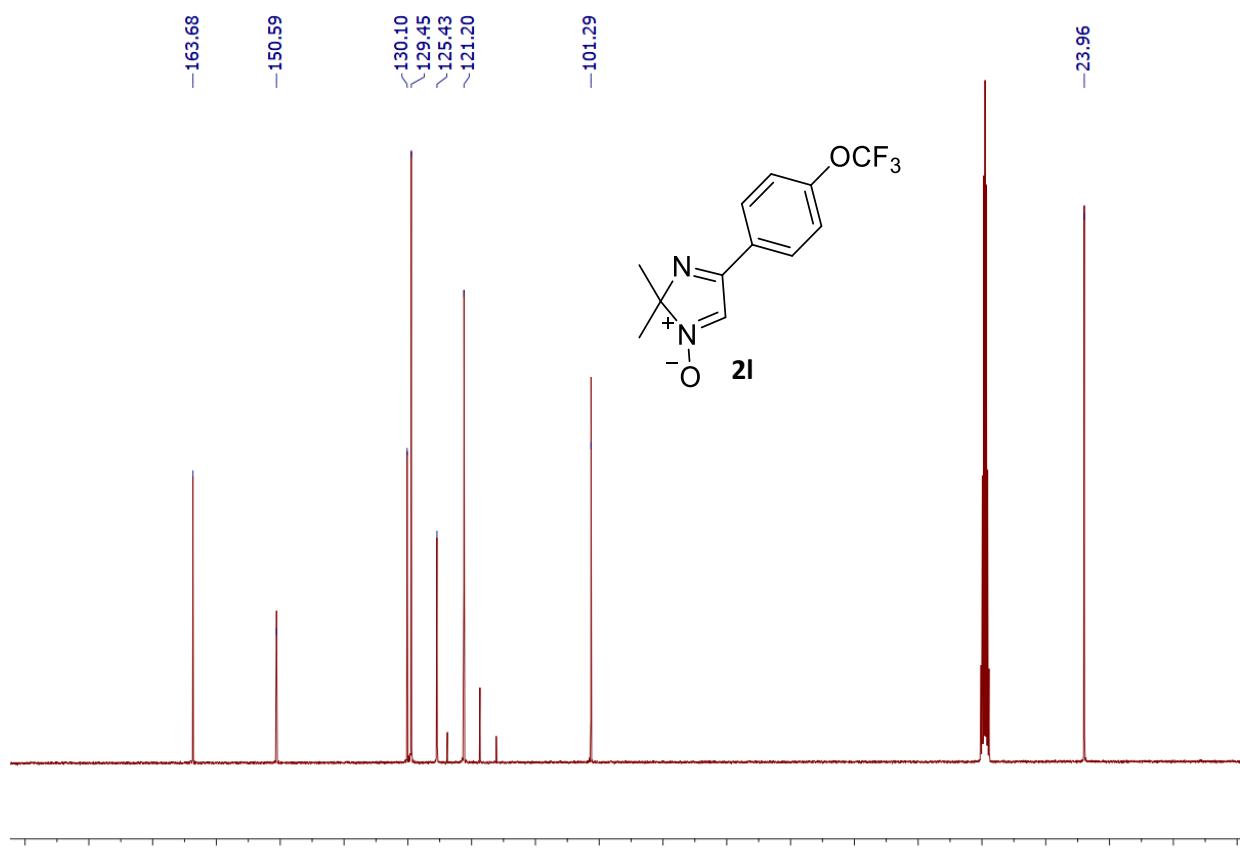
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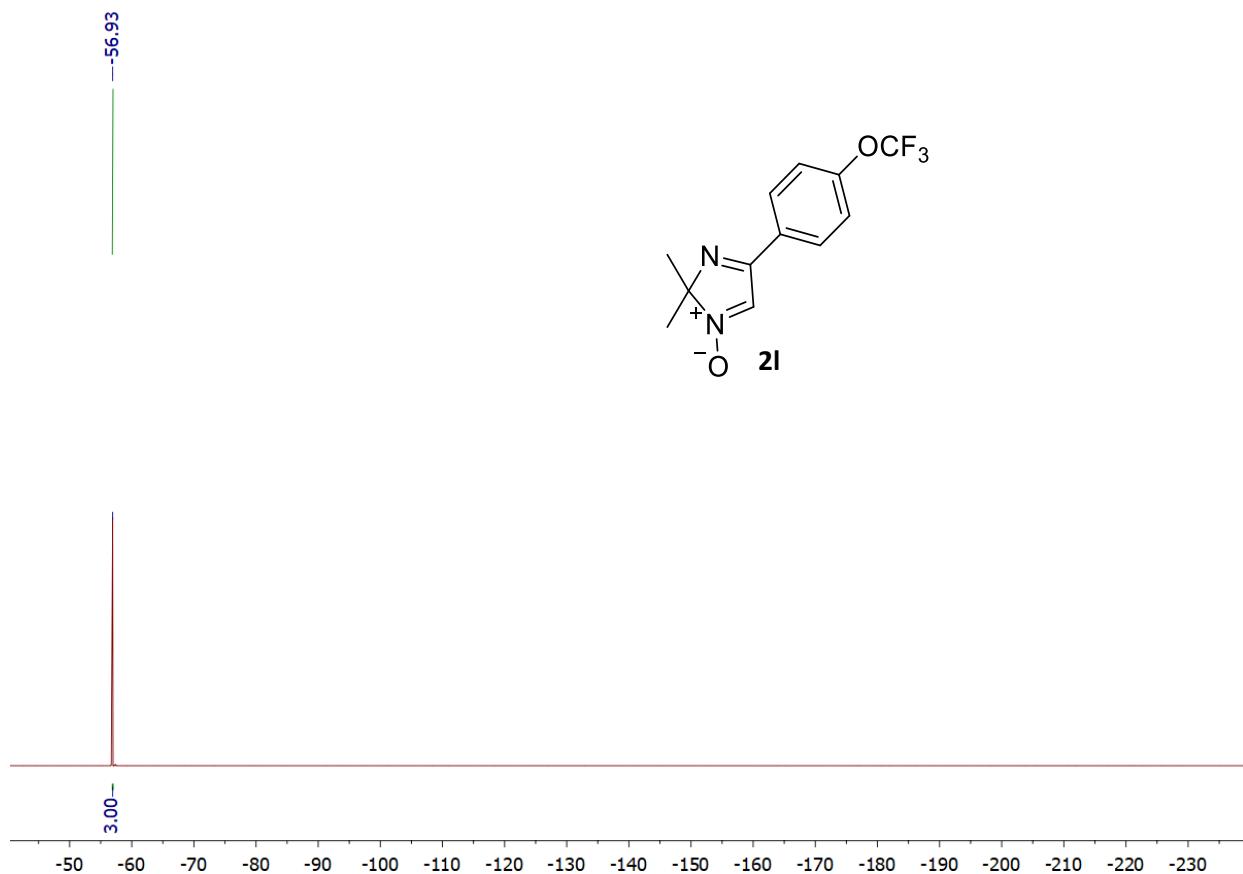
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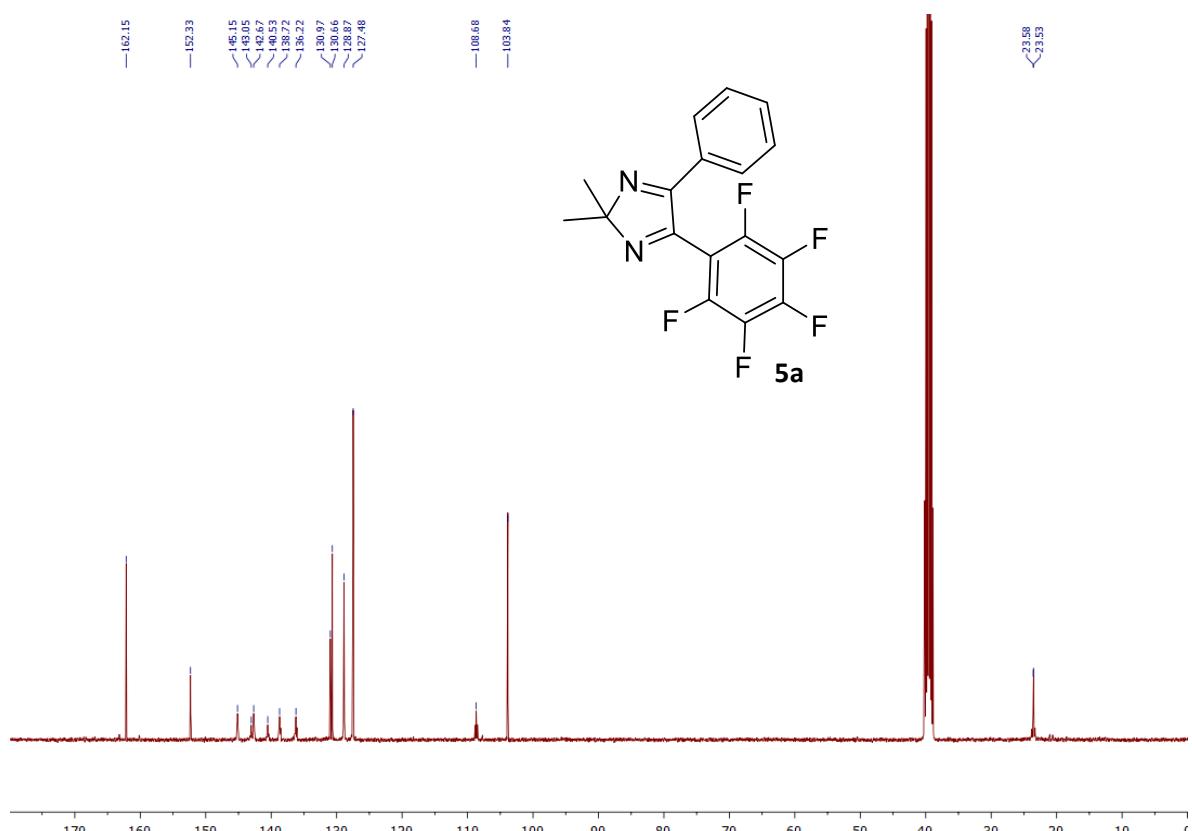
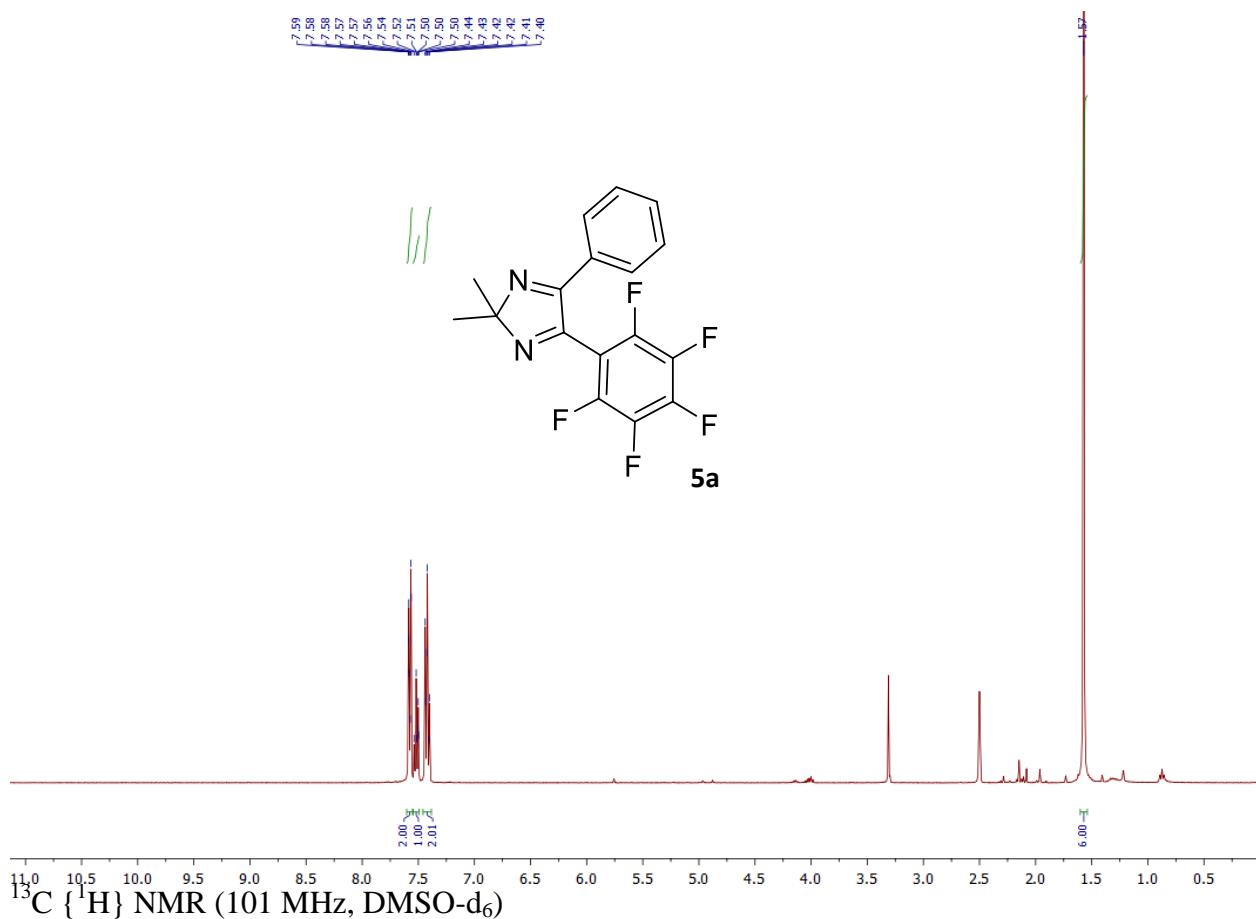


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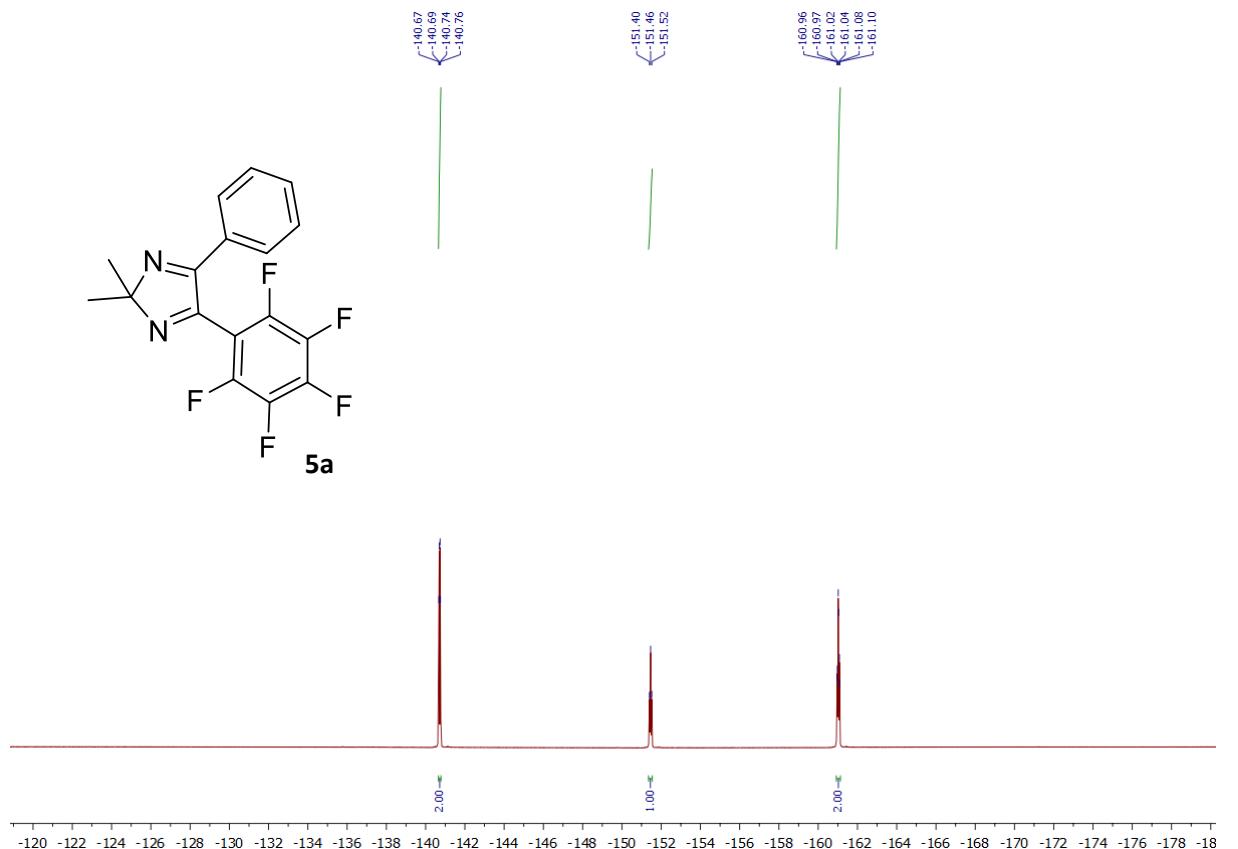


2. Copies of ^1H , ^{13}C , ^{19}F NMR spectra of 4-(perfluorophenyl)-substituted 2*H*-imidazole 5a-l

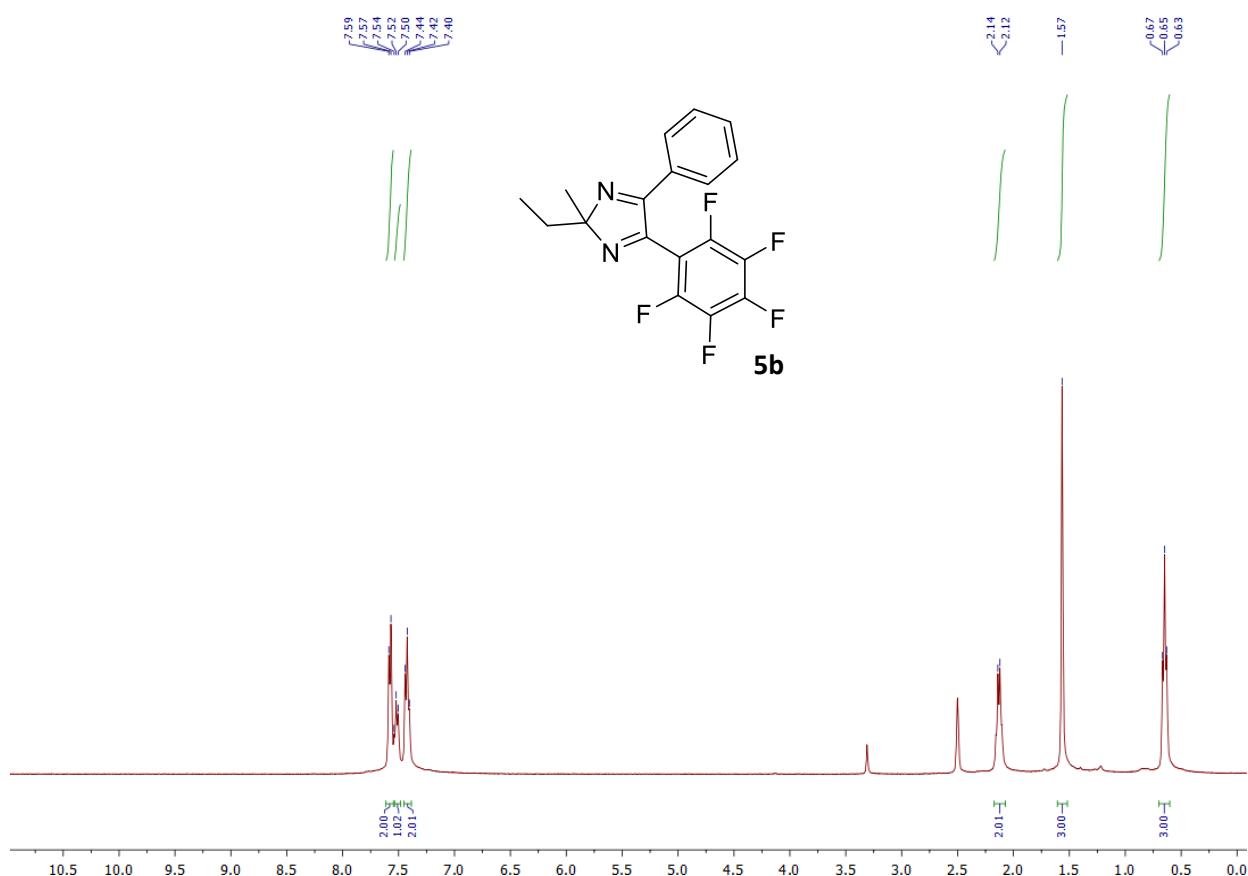
^1H NMR (400 MHz, DMSO-d₆)



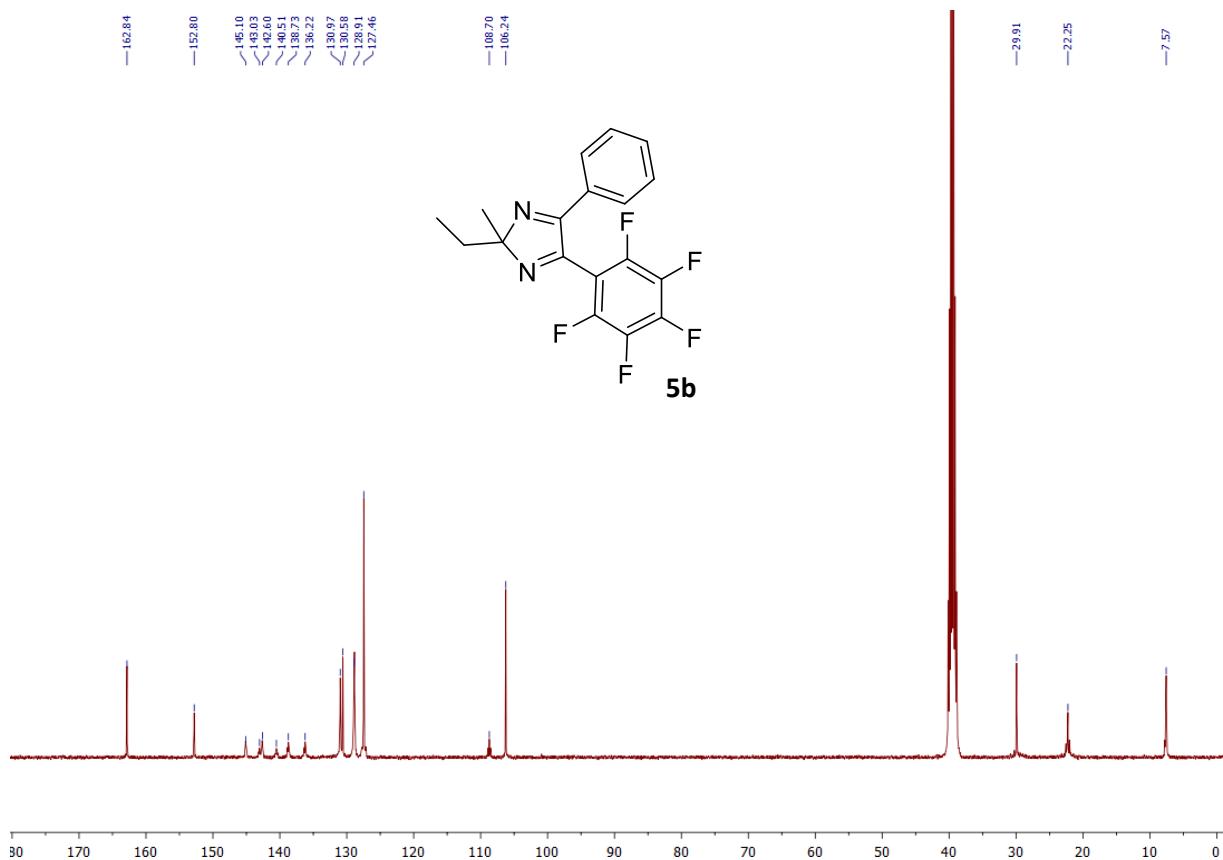
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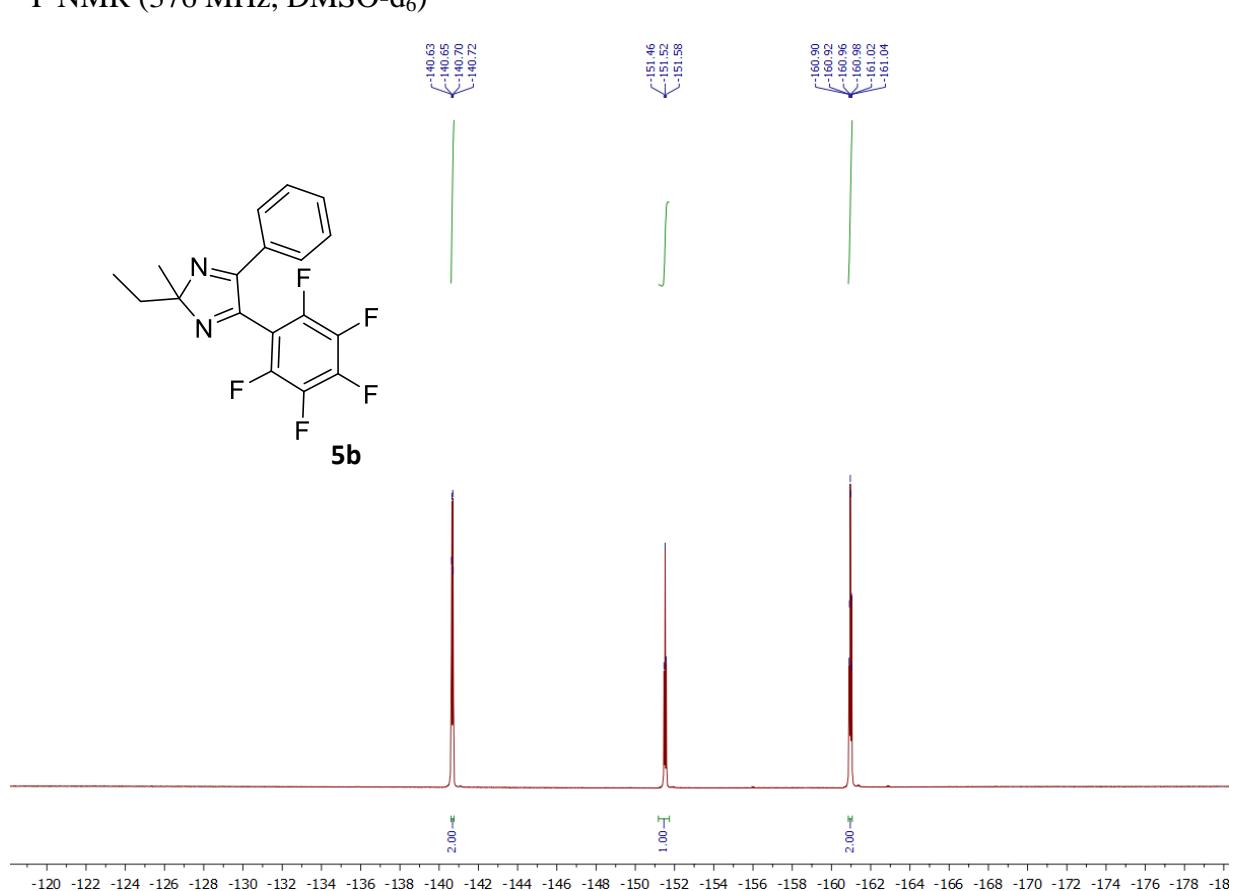
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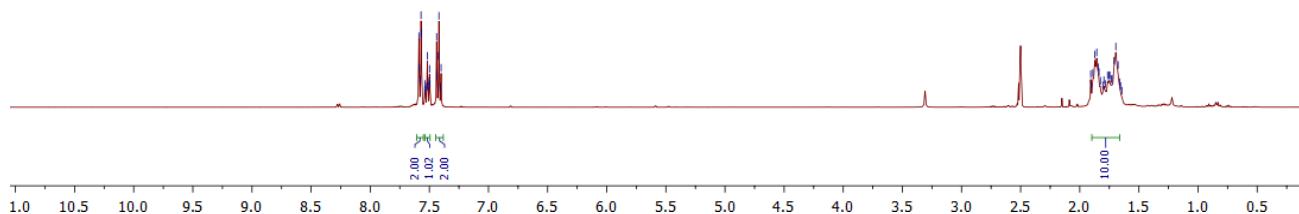
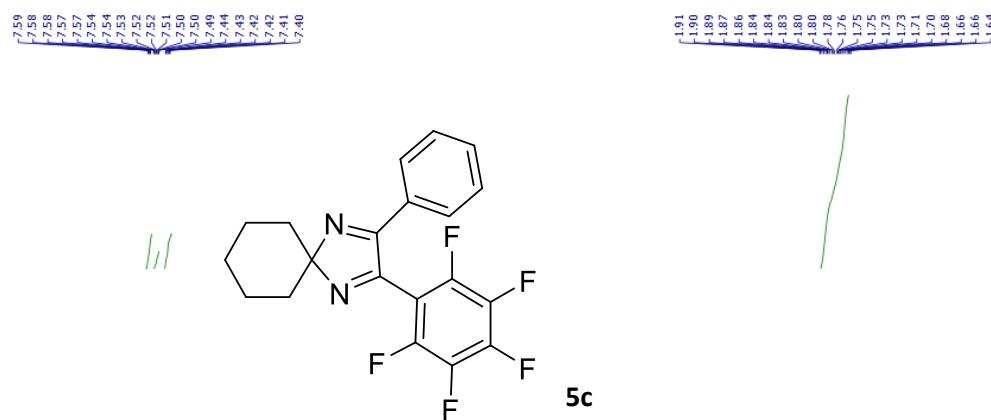
^{13}C { ^1H } NMR (101 MHz, DMSO-d₆)



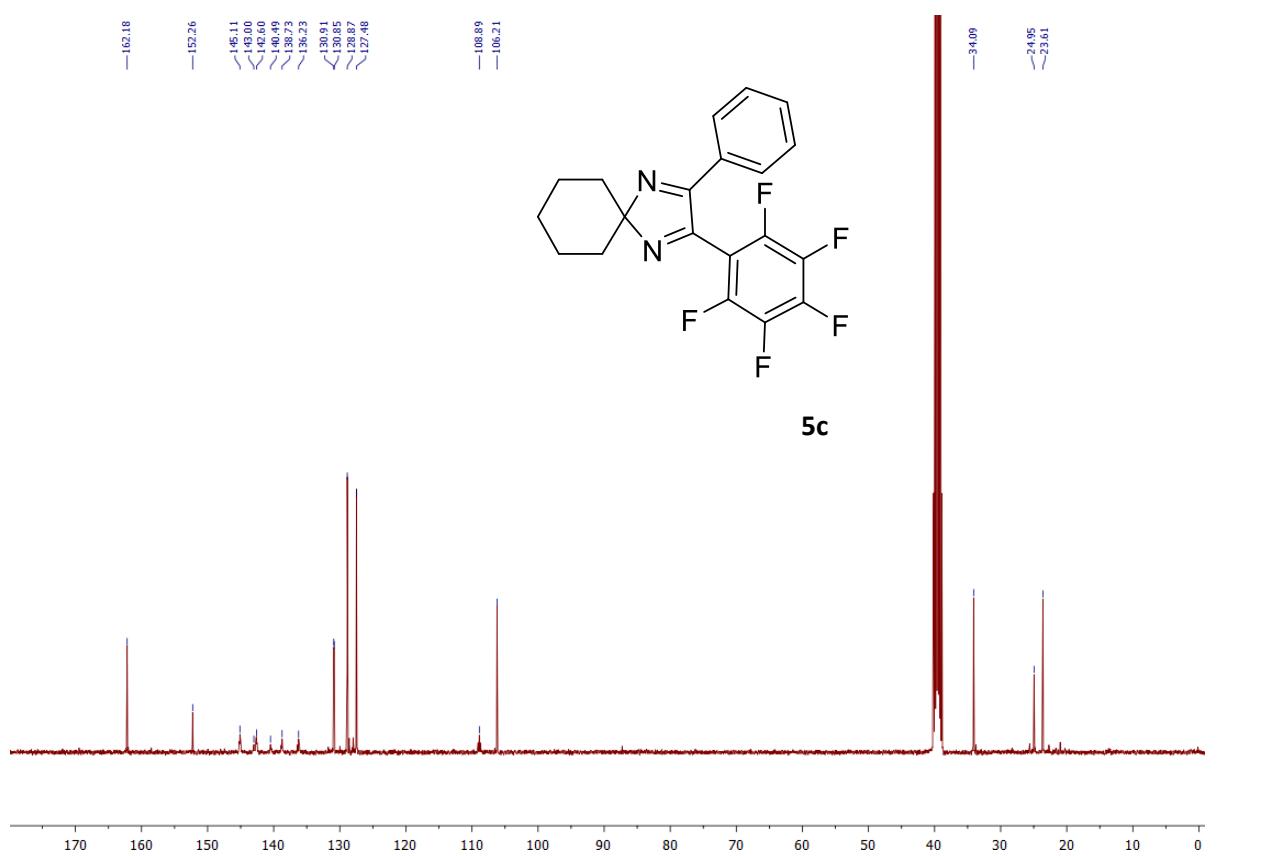
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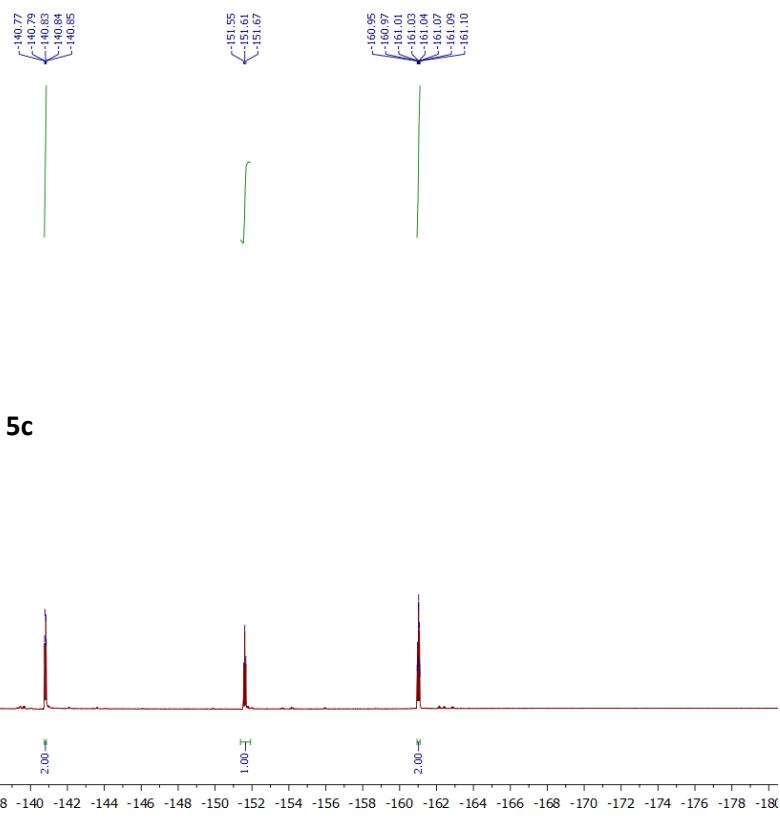
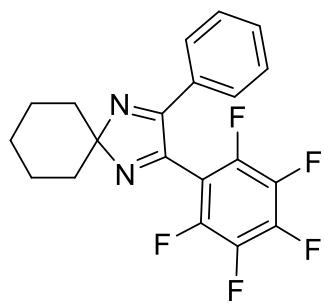
¹H NMR (400 MHz, DMSO-d₆)



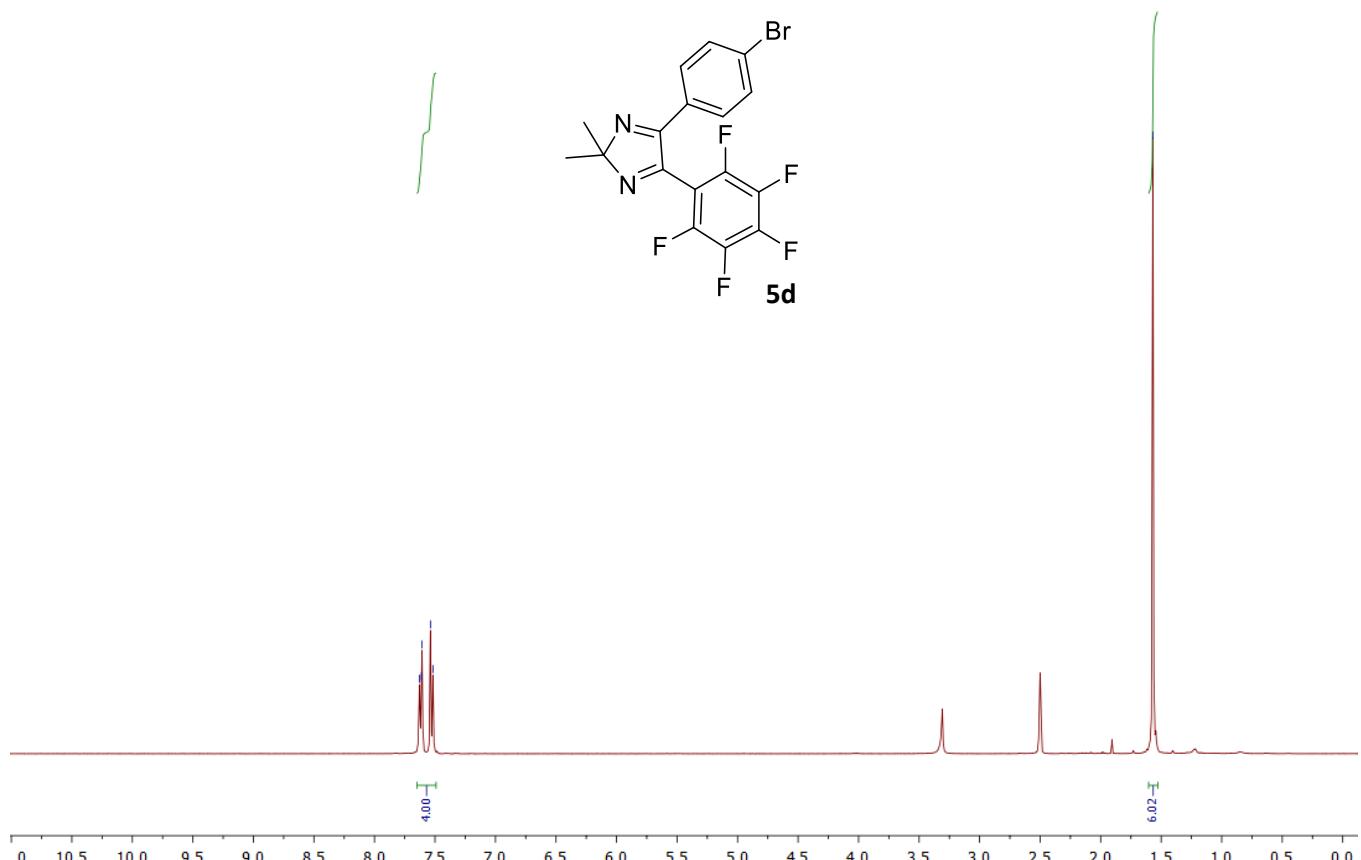
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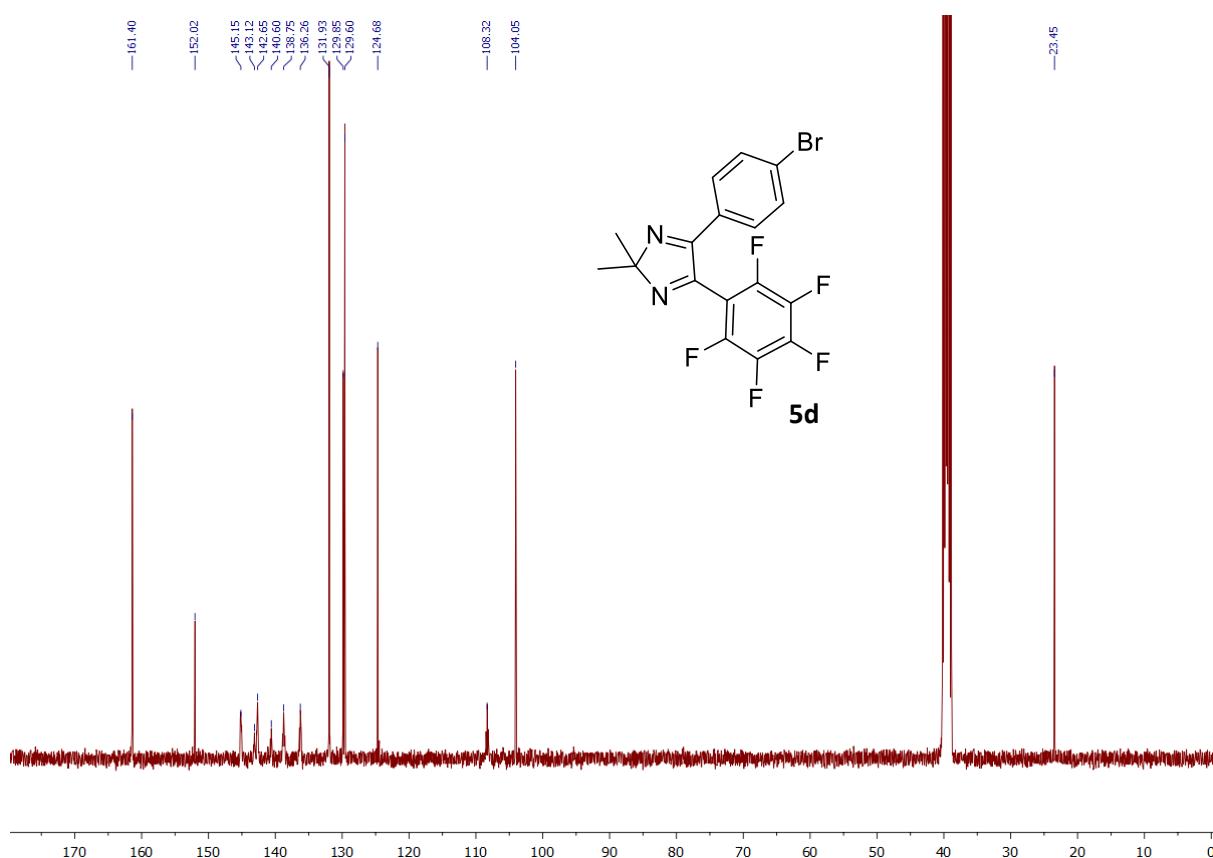
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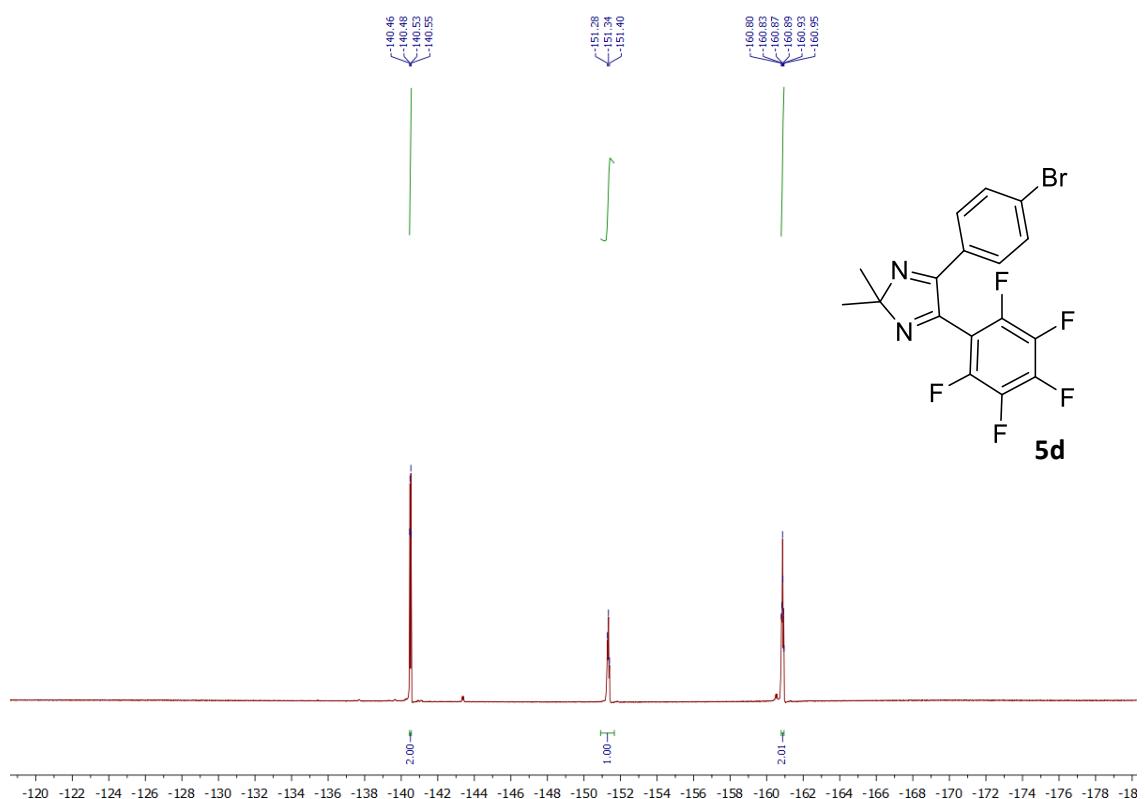
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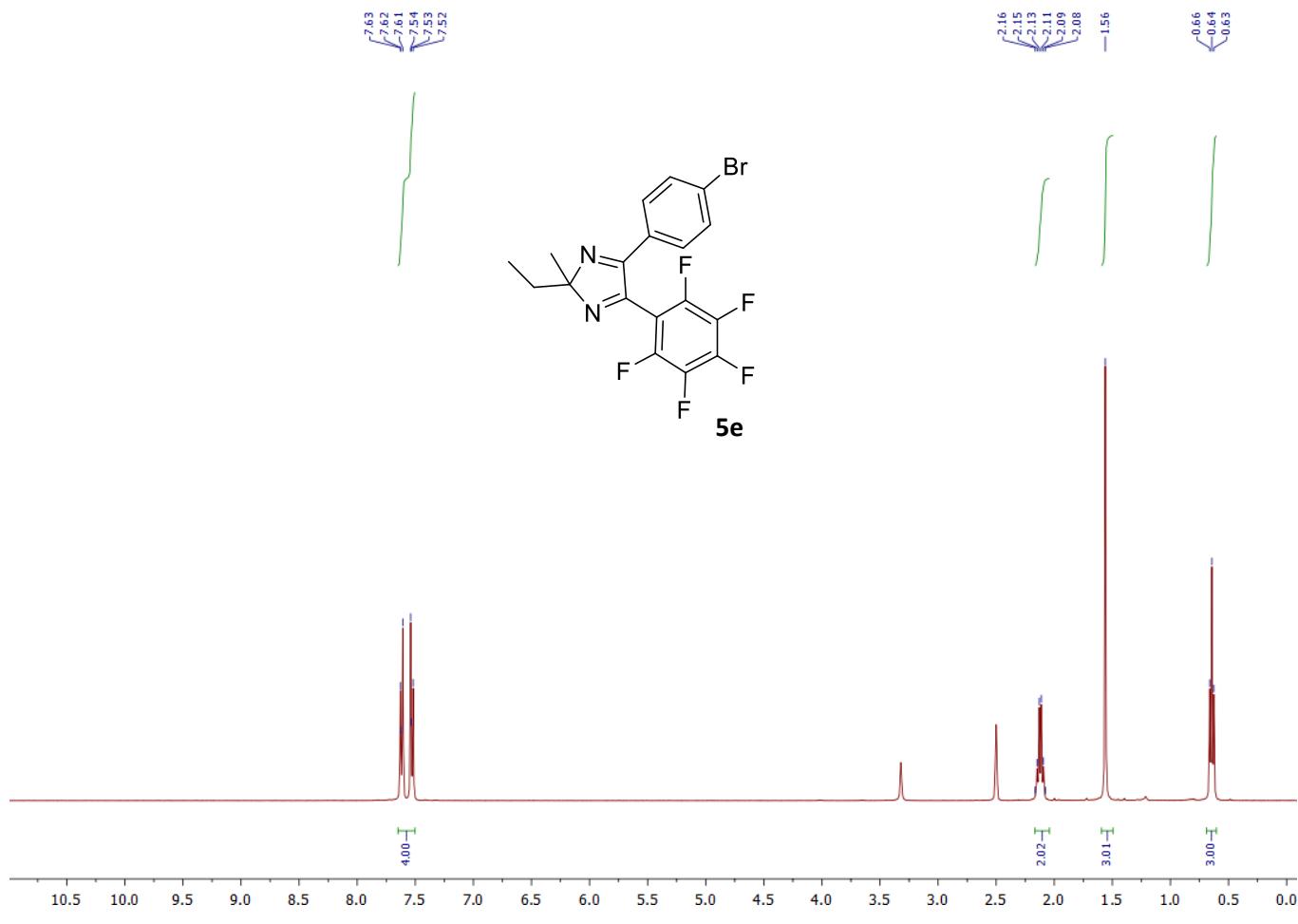
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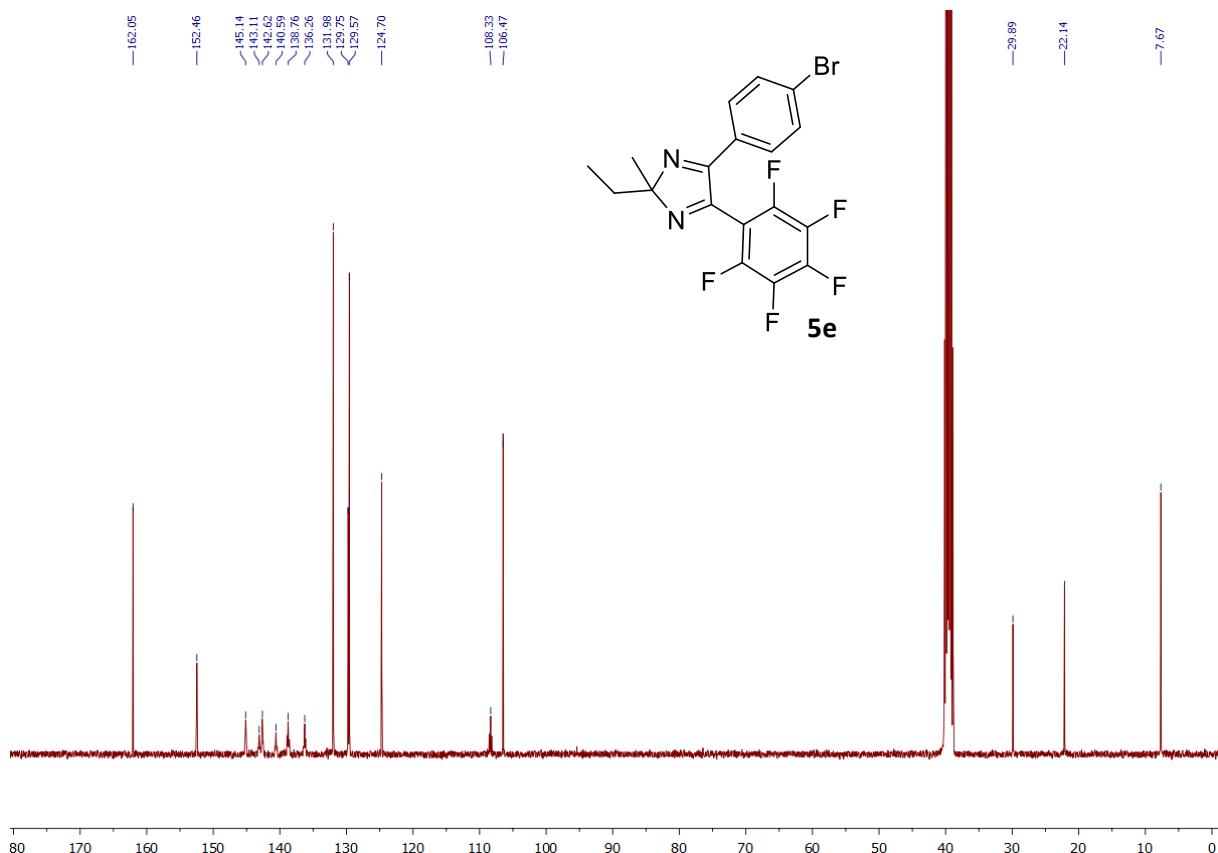
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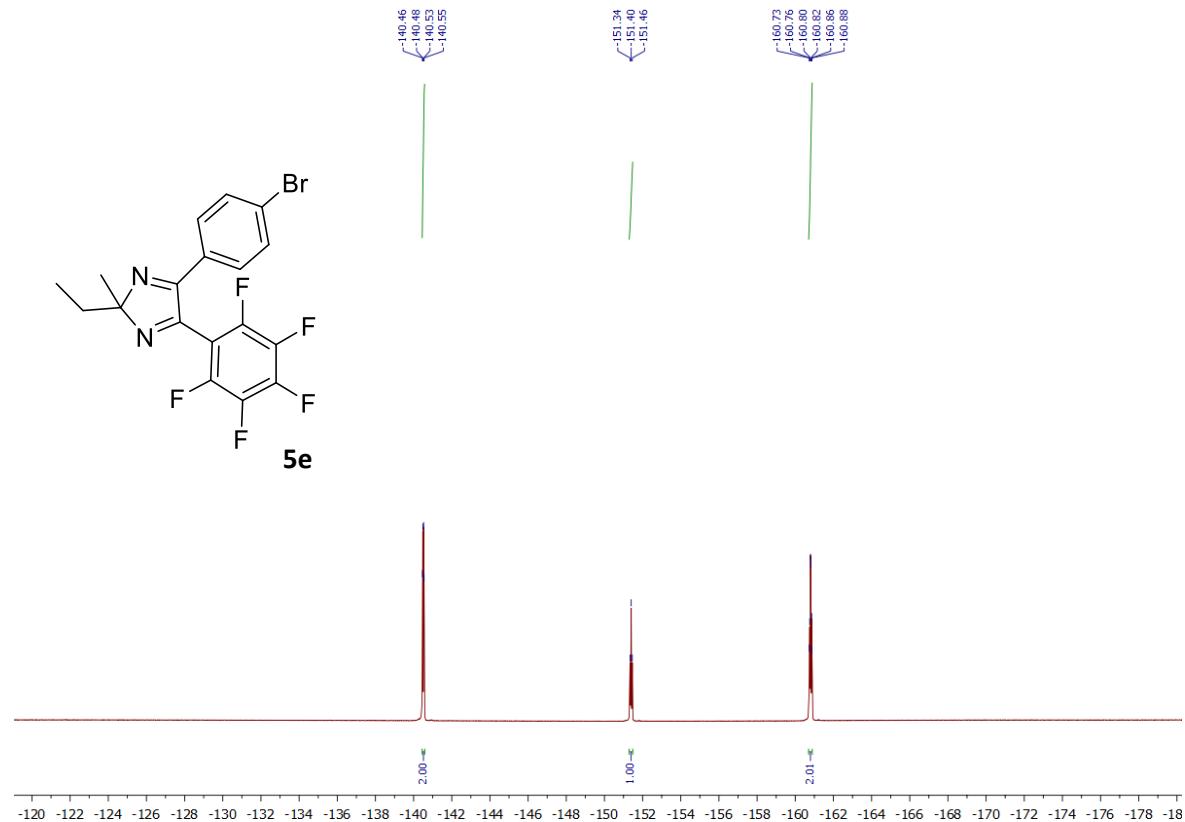
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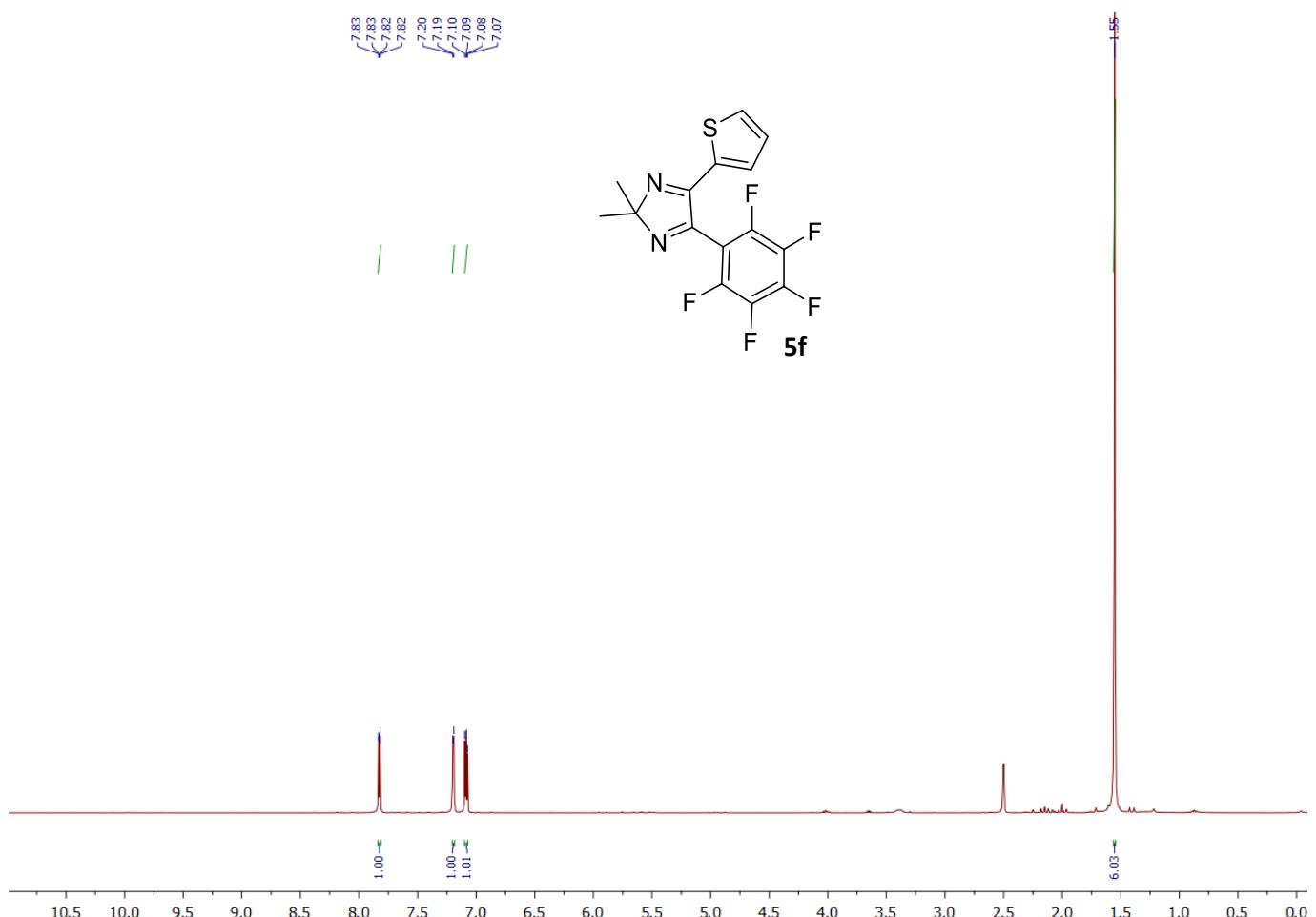
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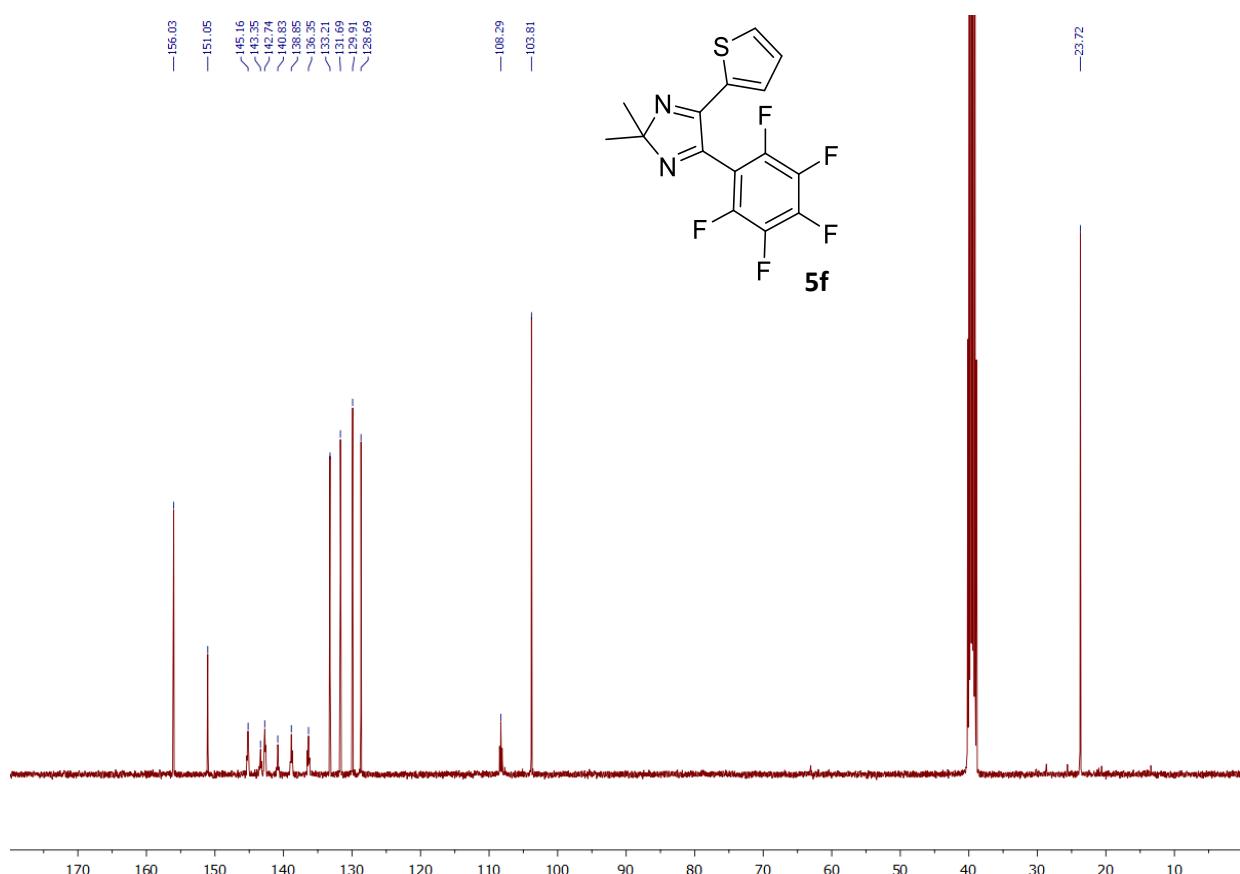
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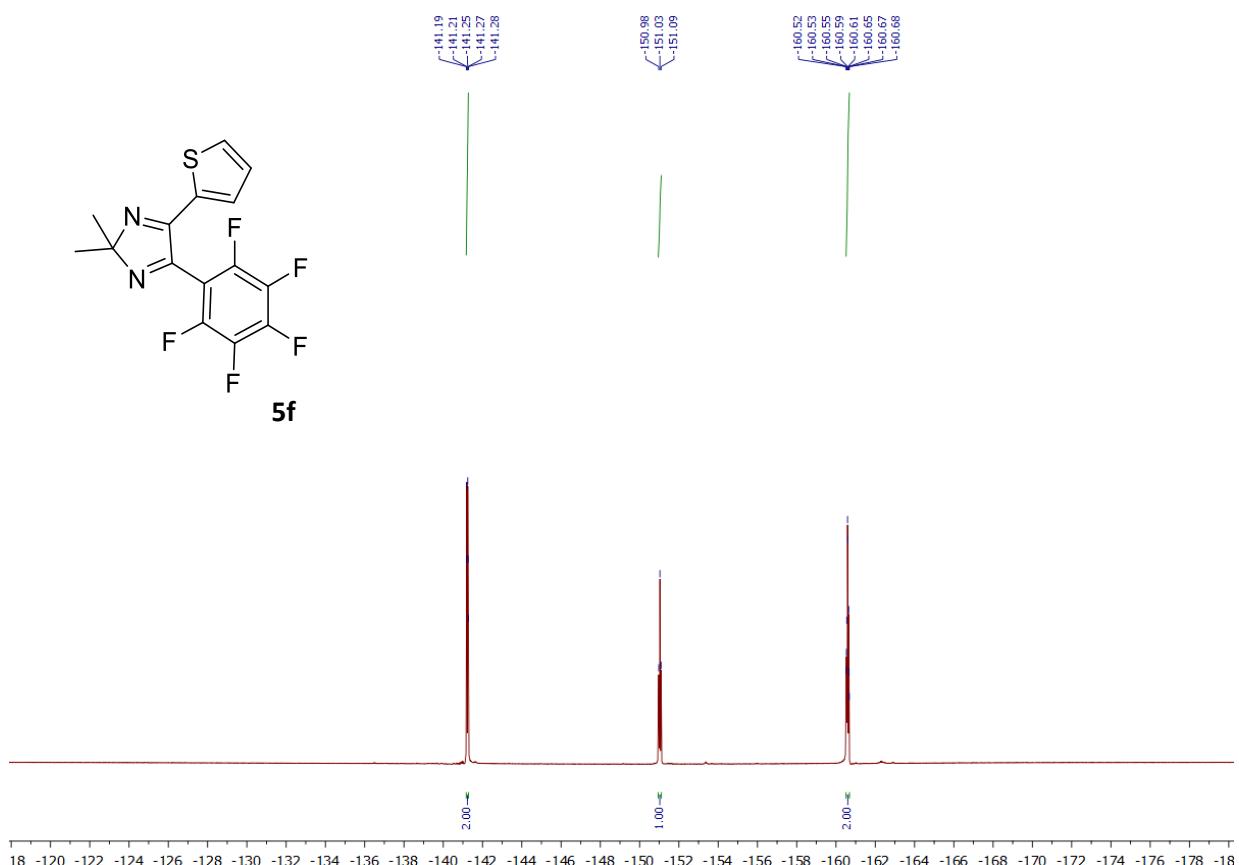
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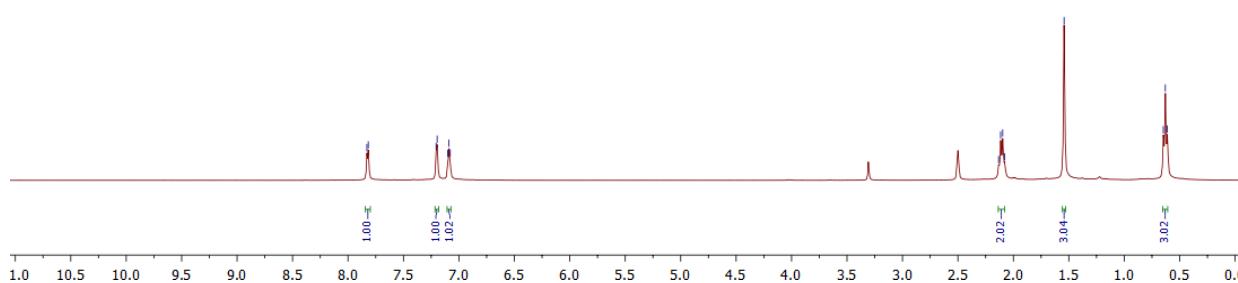
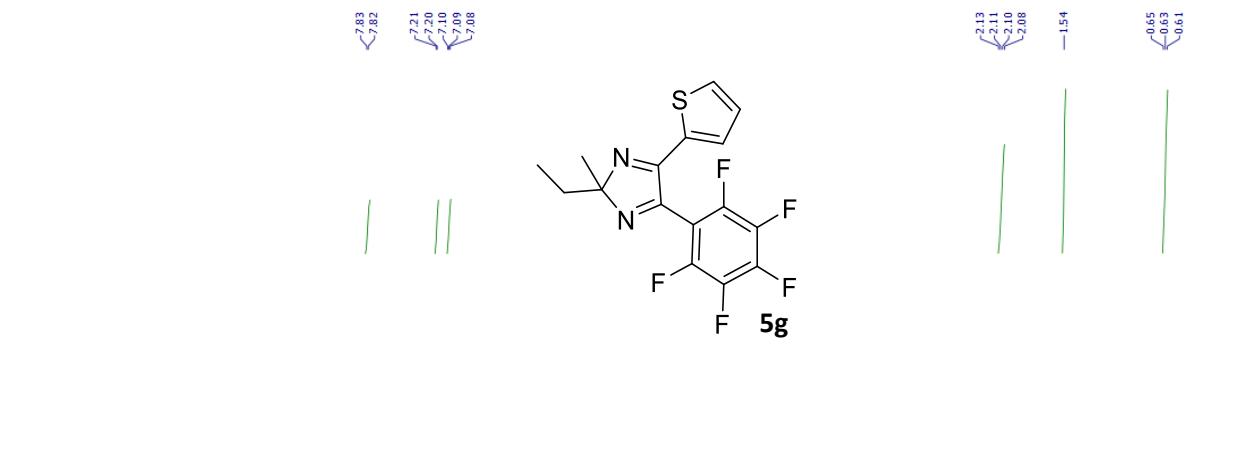
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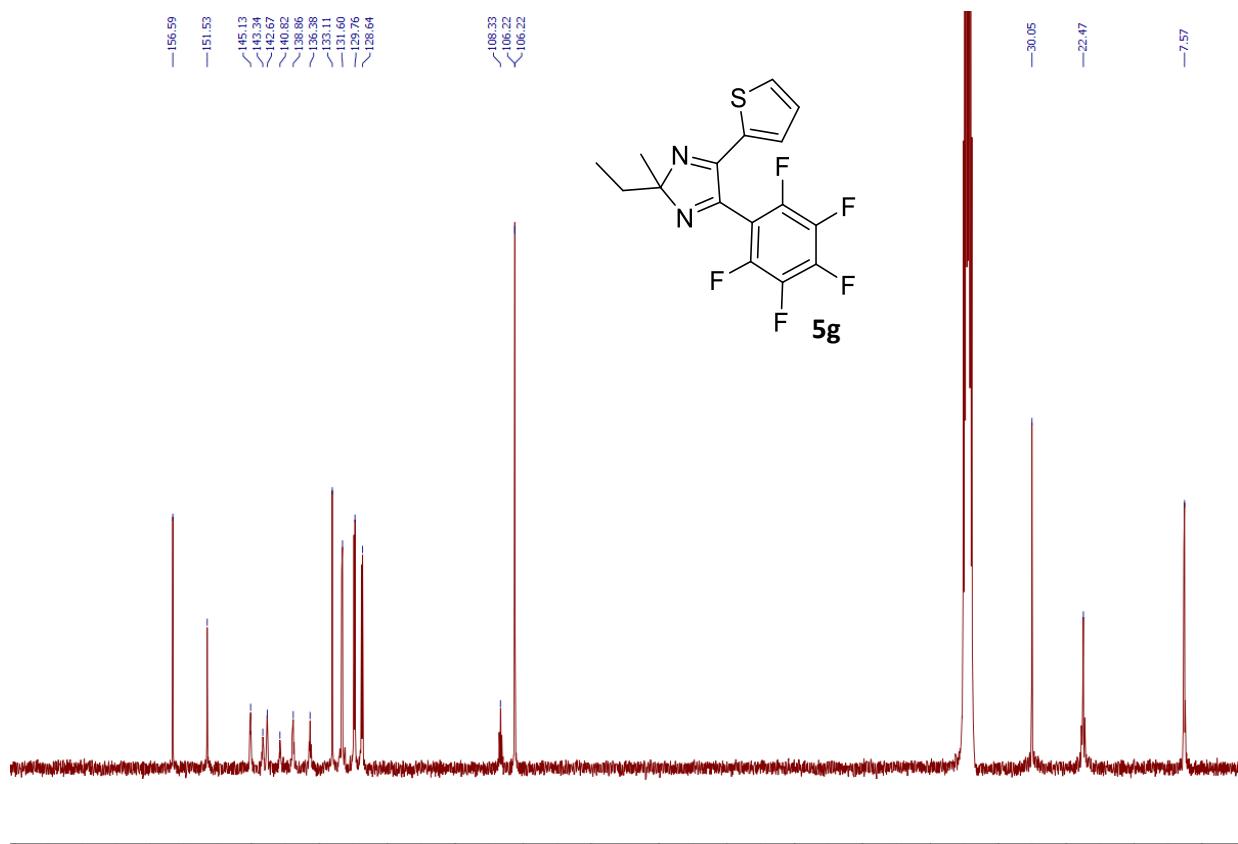
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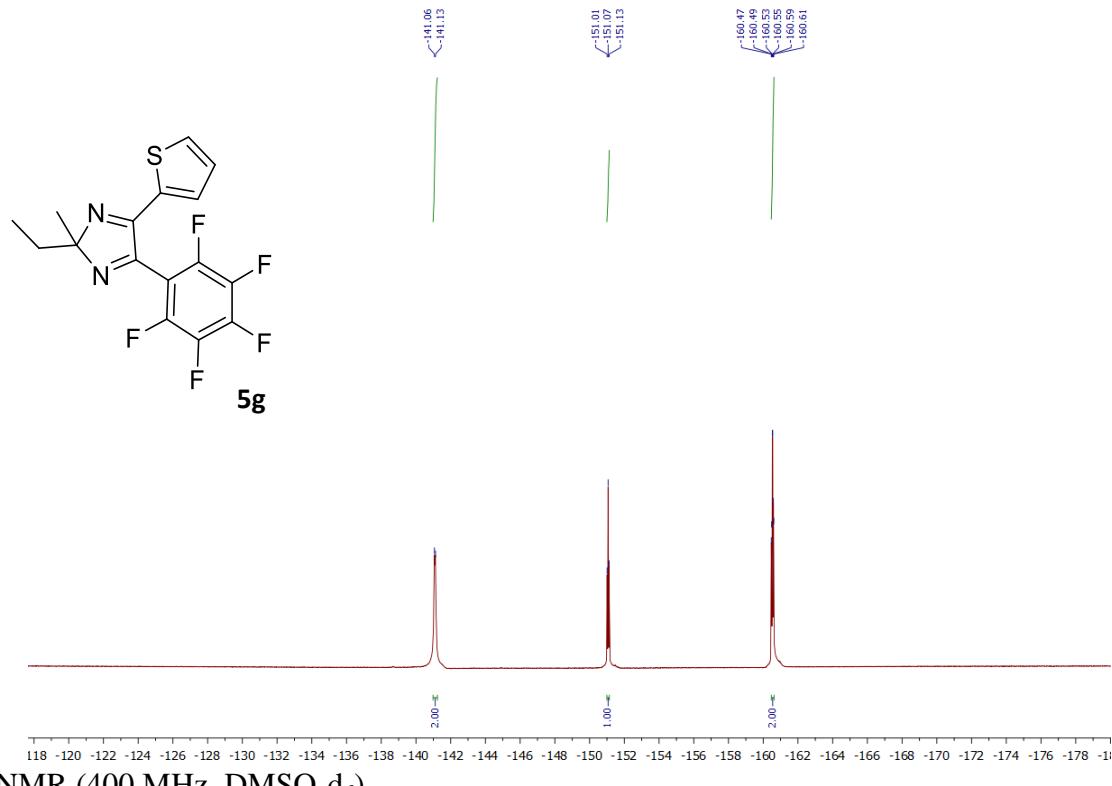
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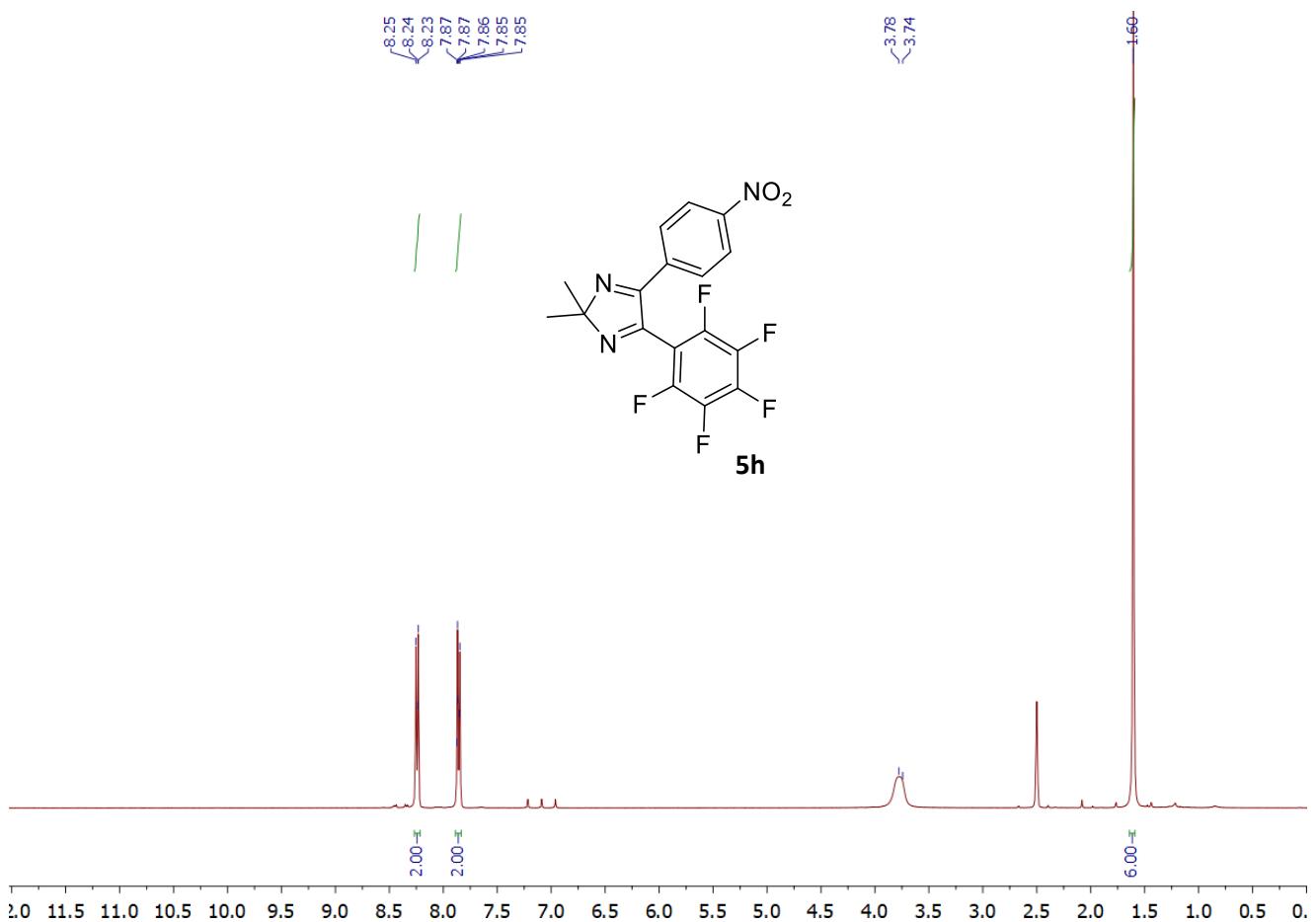
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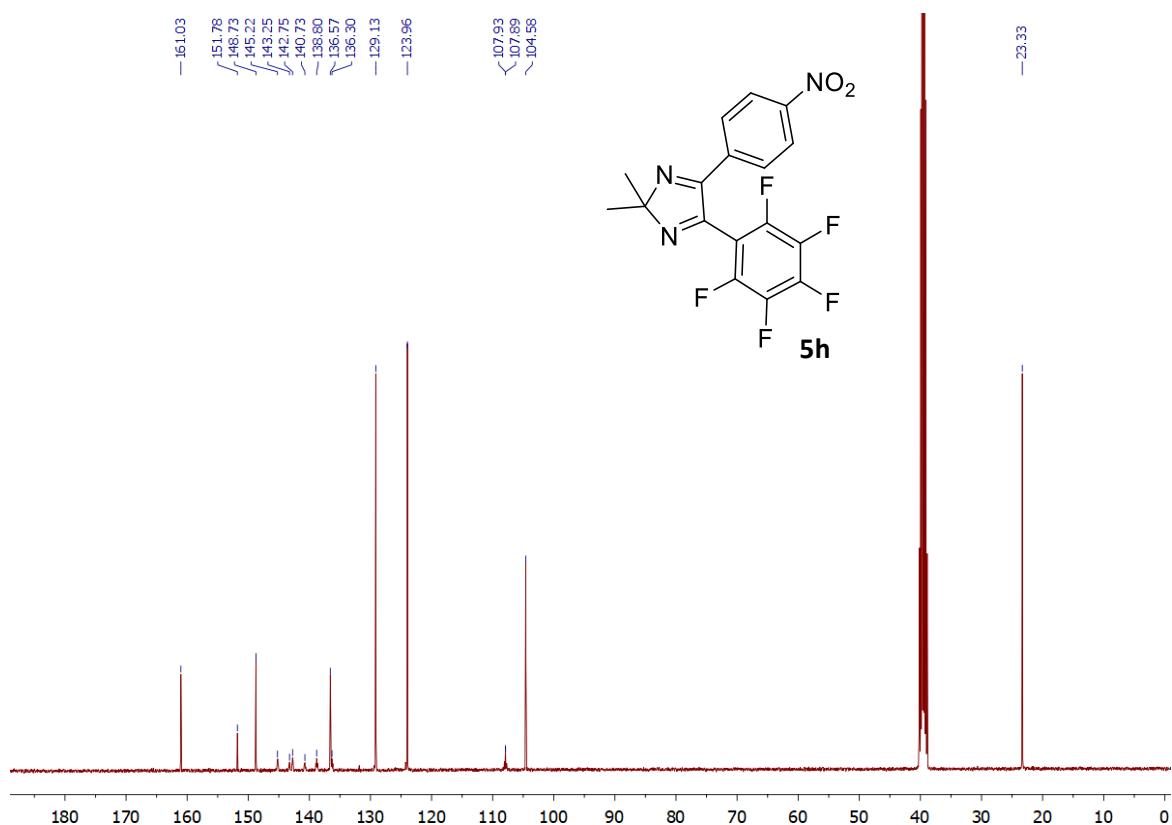
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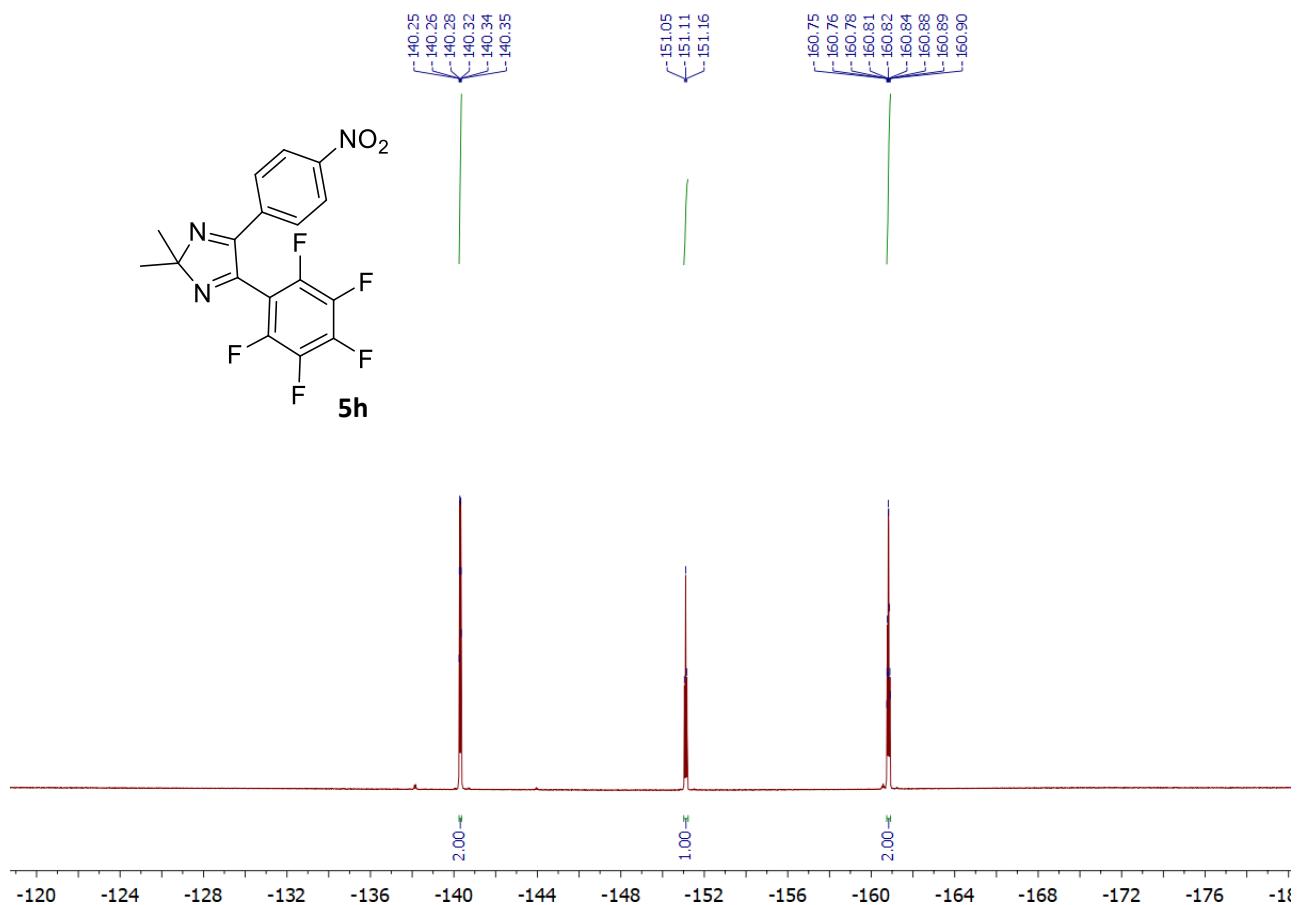
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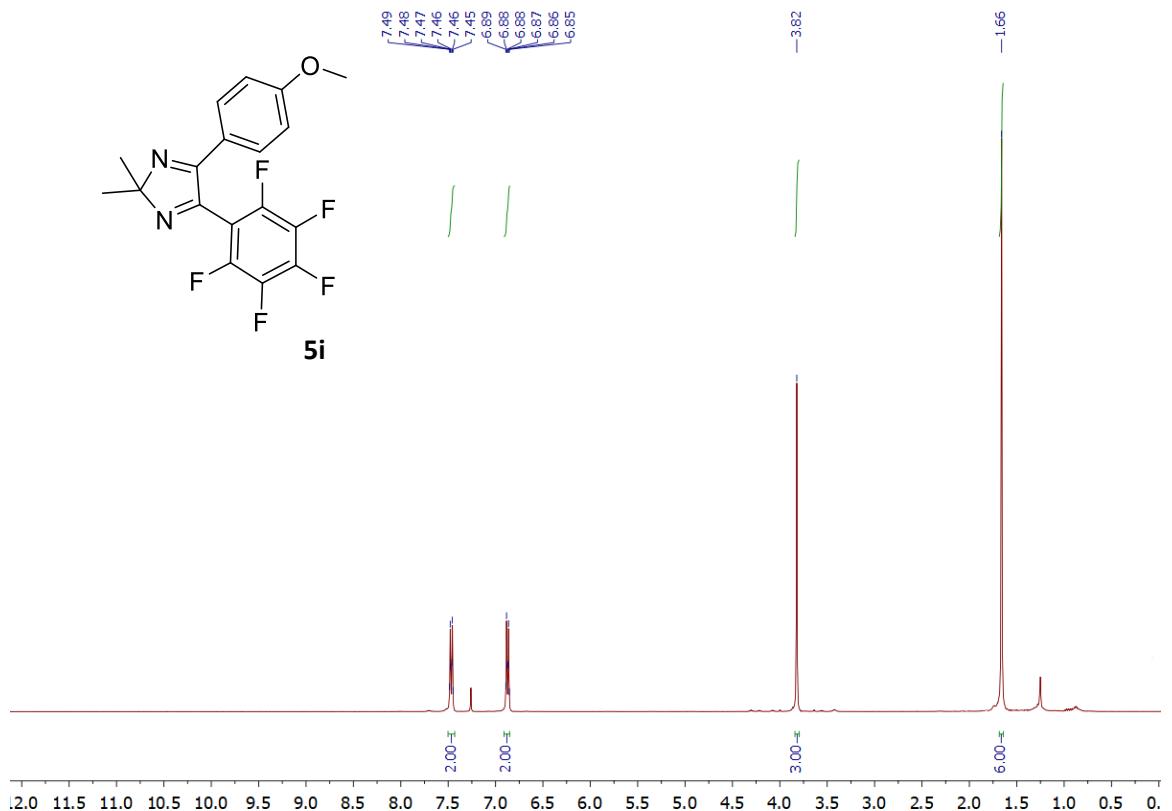
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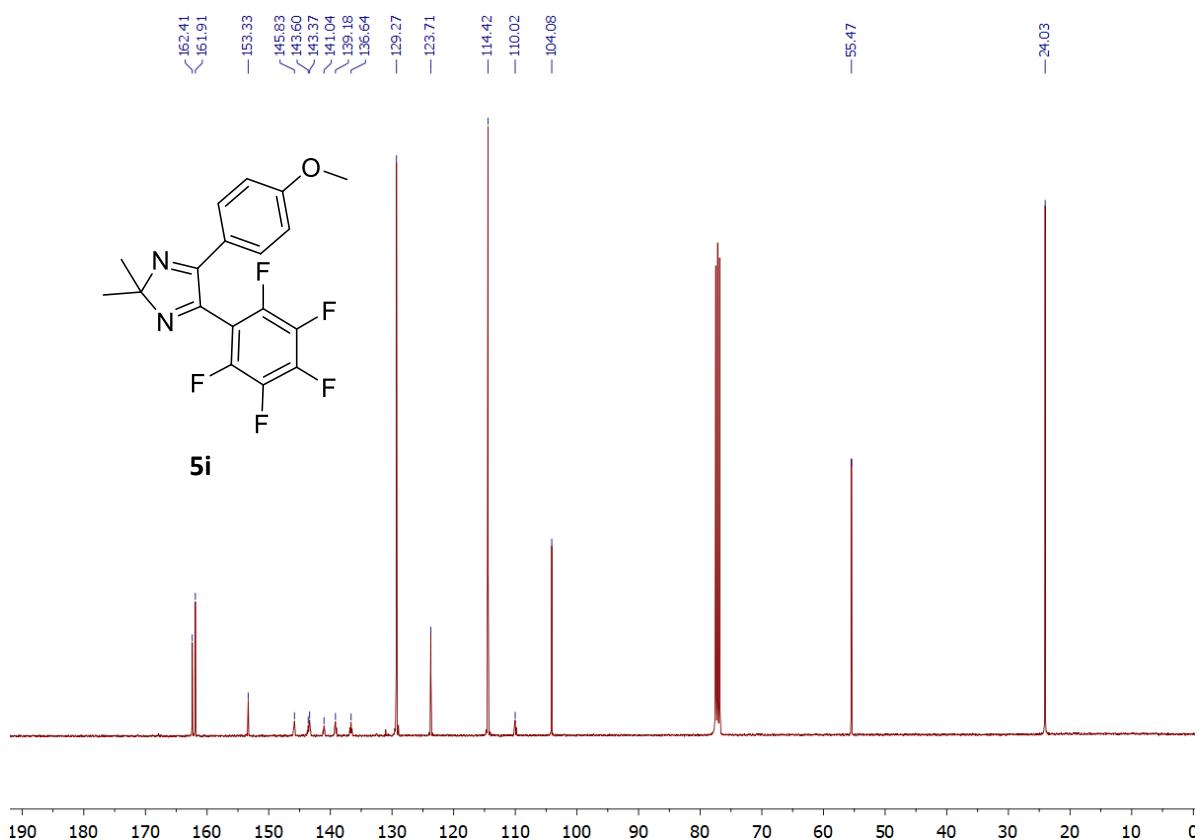
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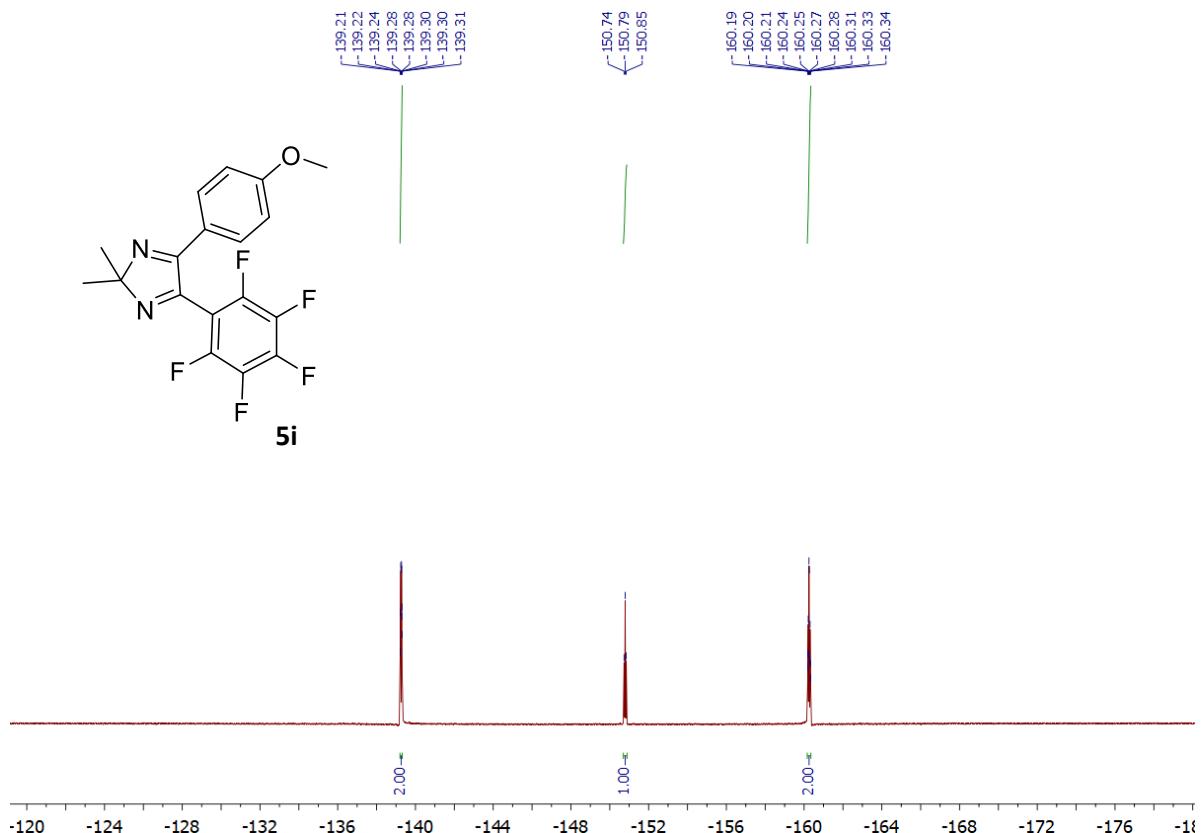
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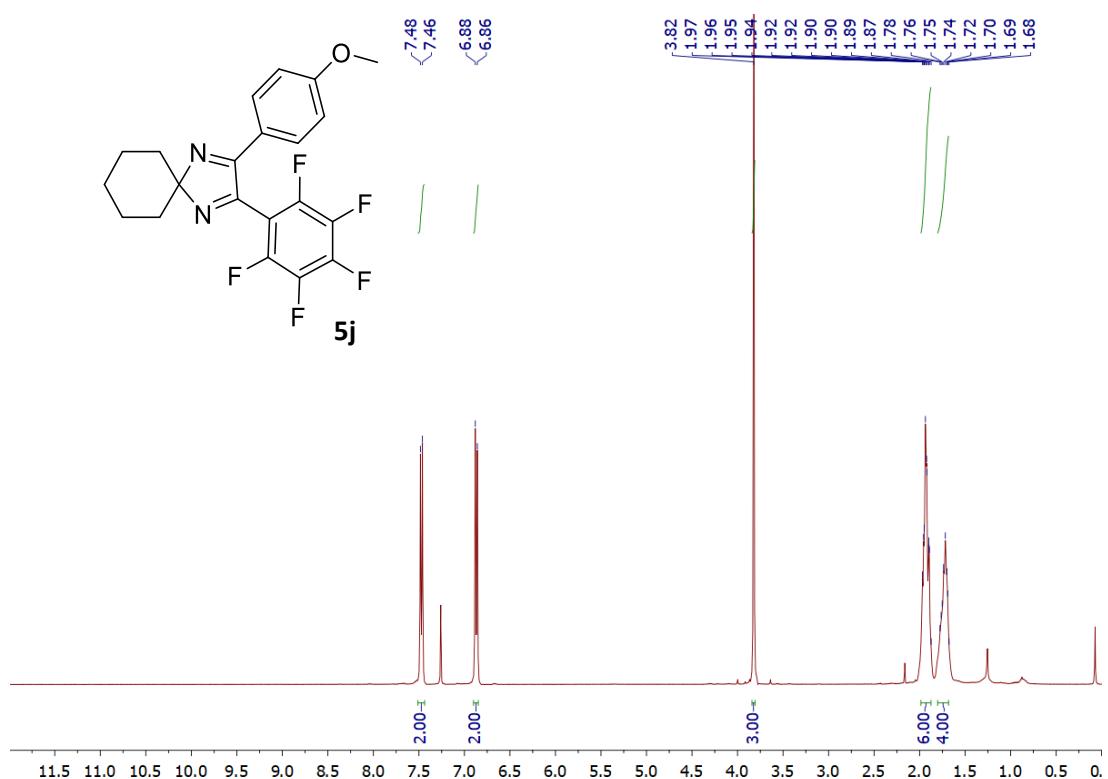
$^{13}\text{C} \{^1\text{H}\}$ NMR (101 MHz, DCCl_3)



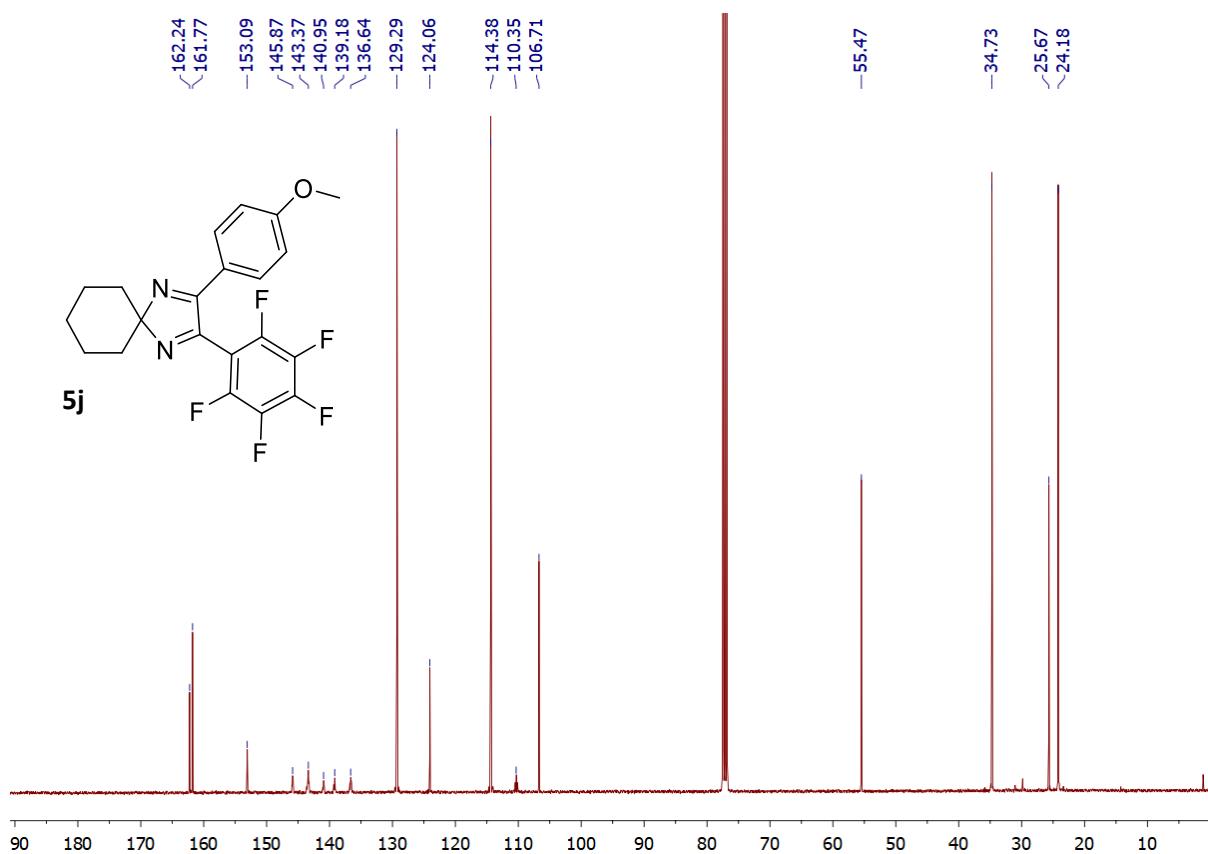
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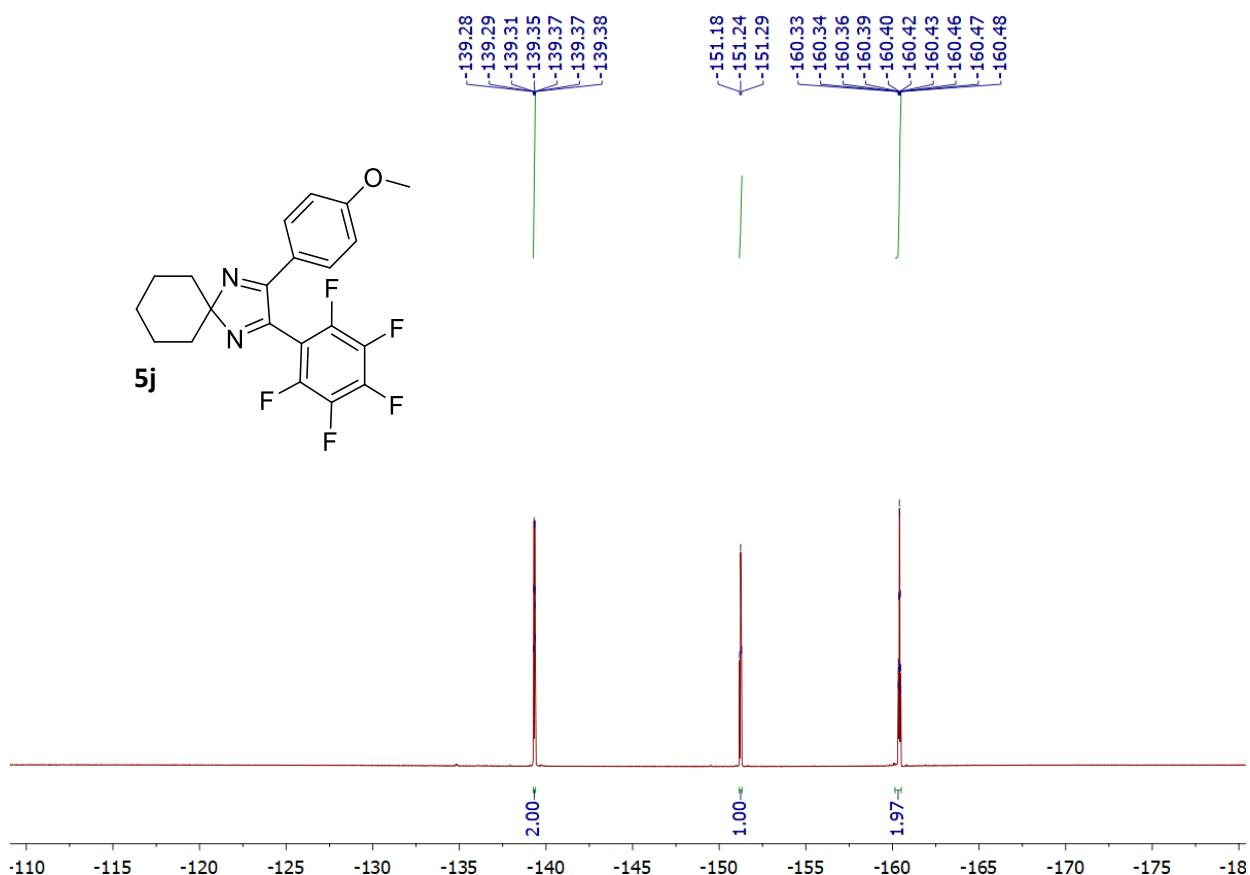
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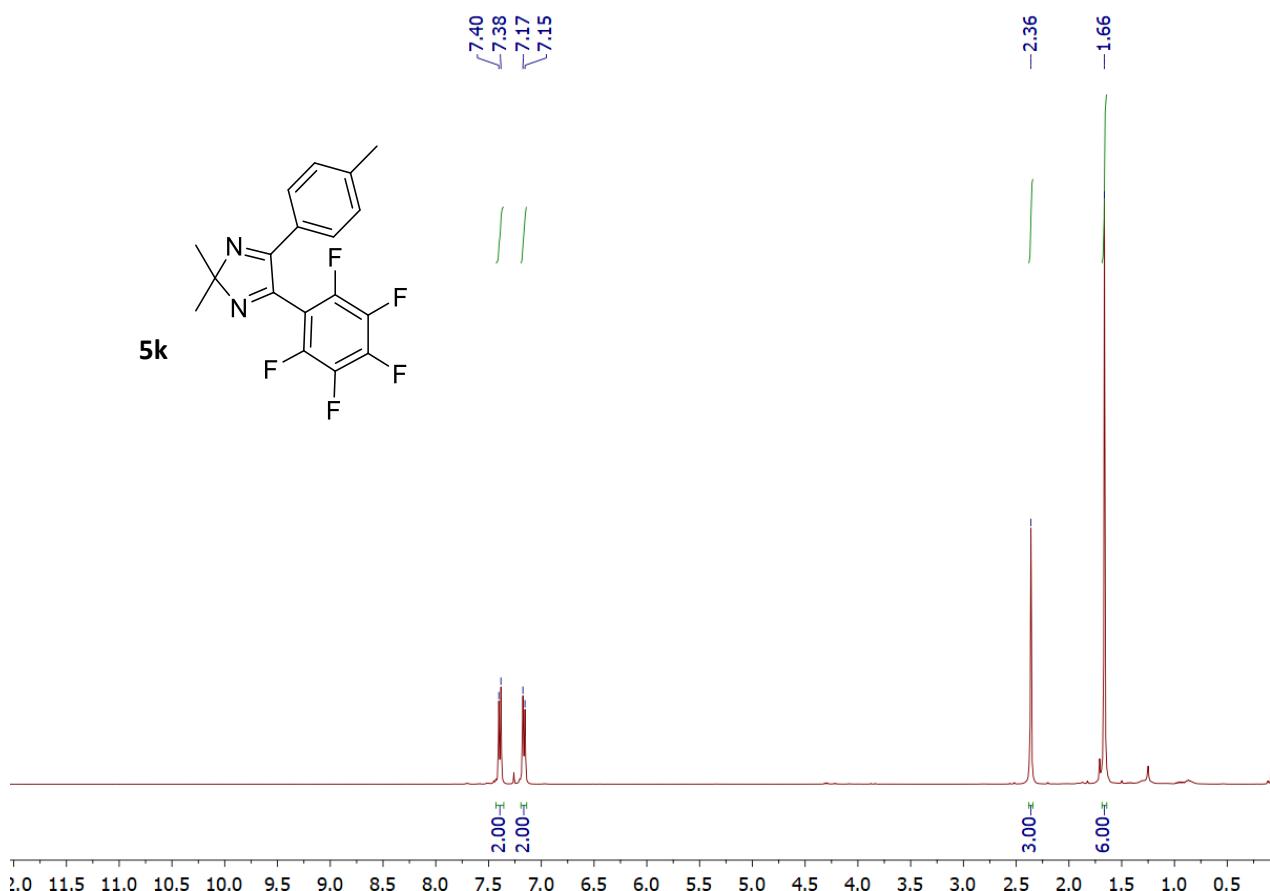
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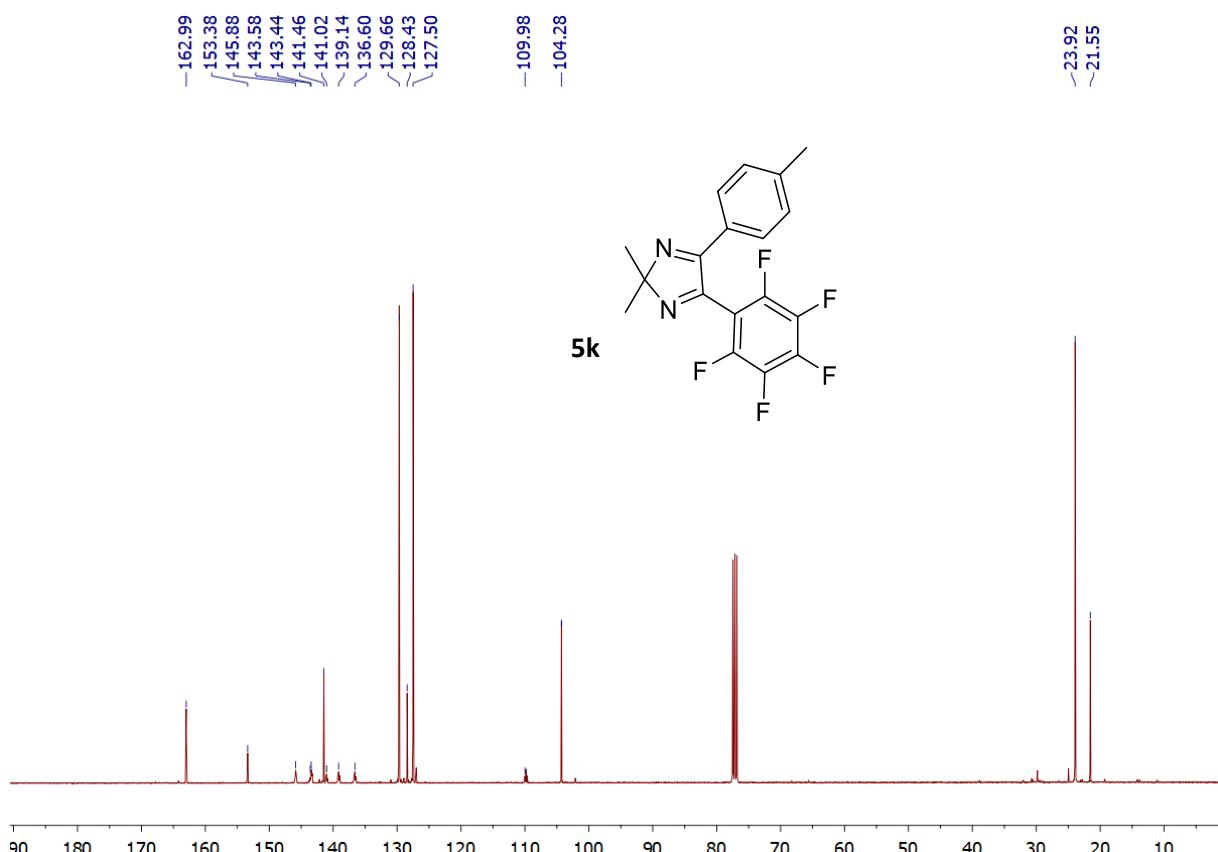
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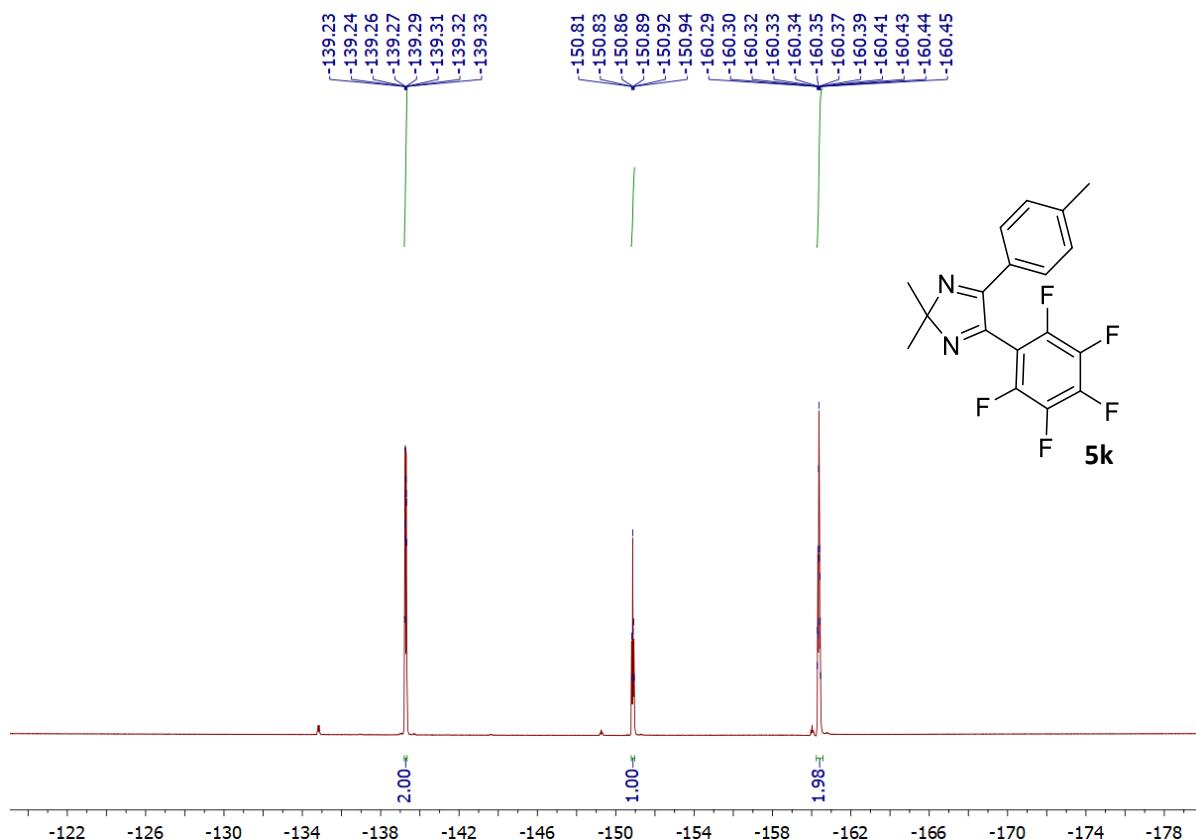
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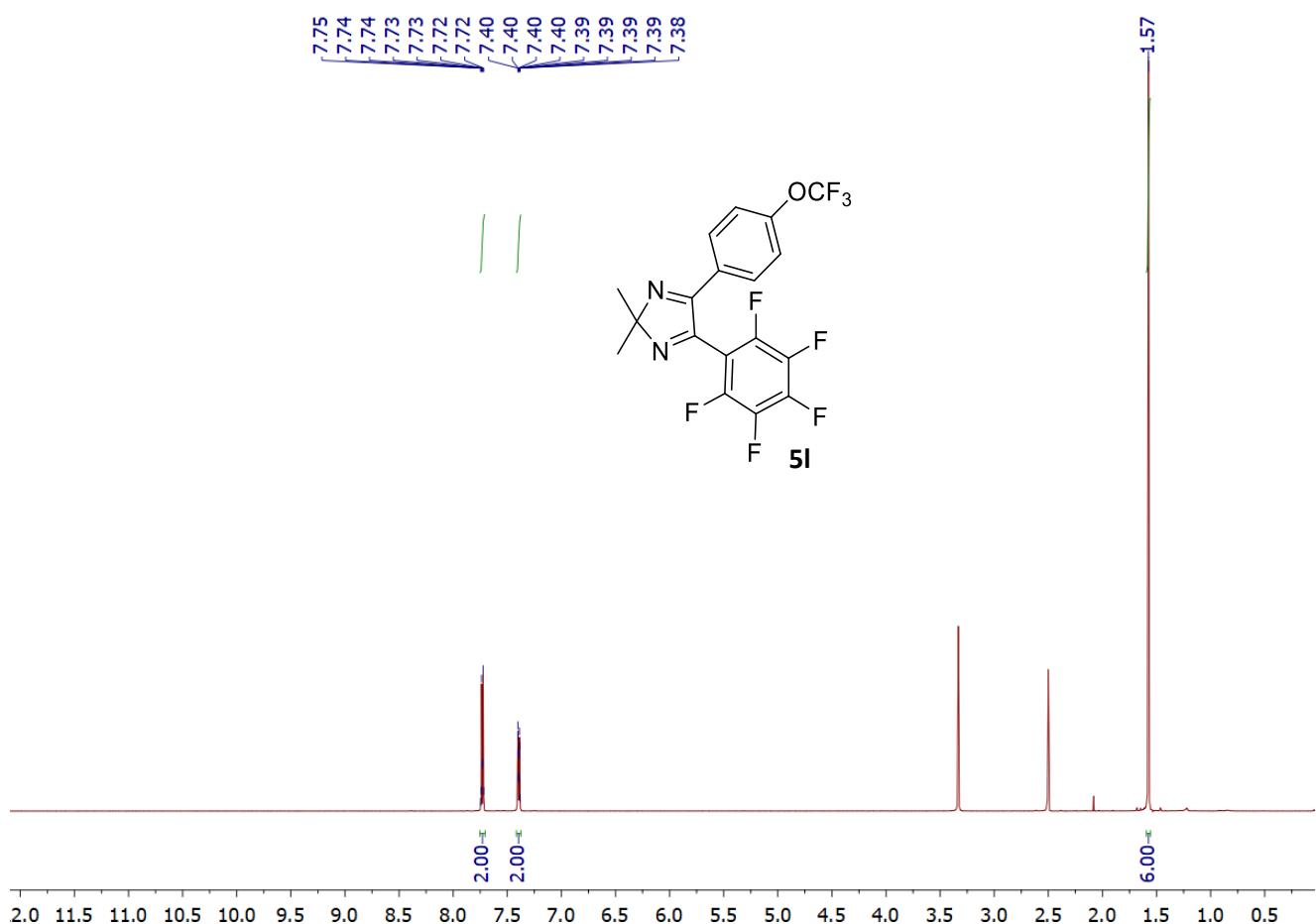
$^{13}\text{C} \{^1\text{H}\}$ NMR (101 MHz, DCCl_3)



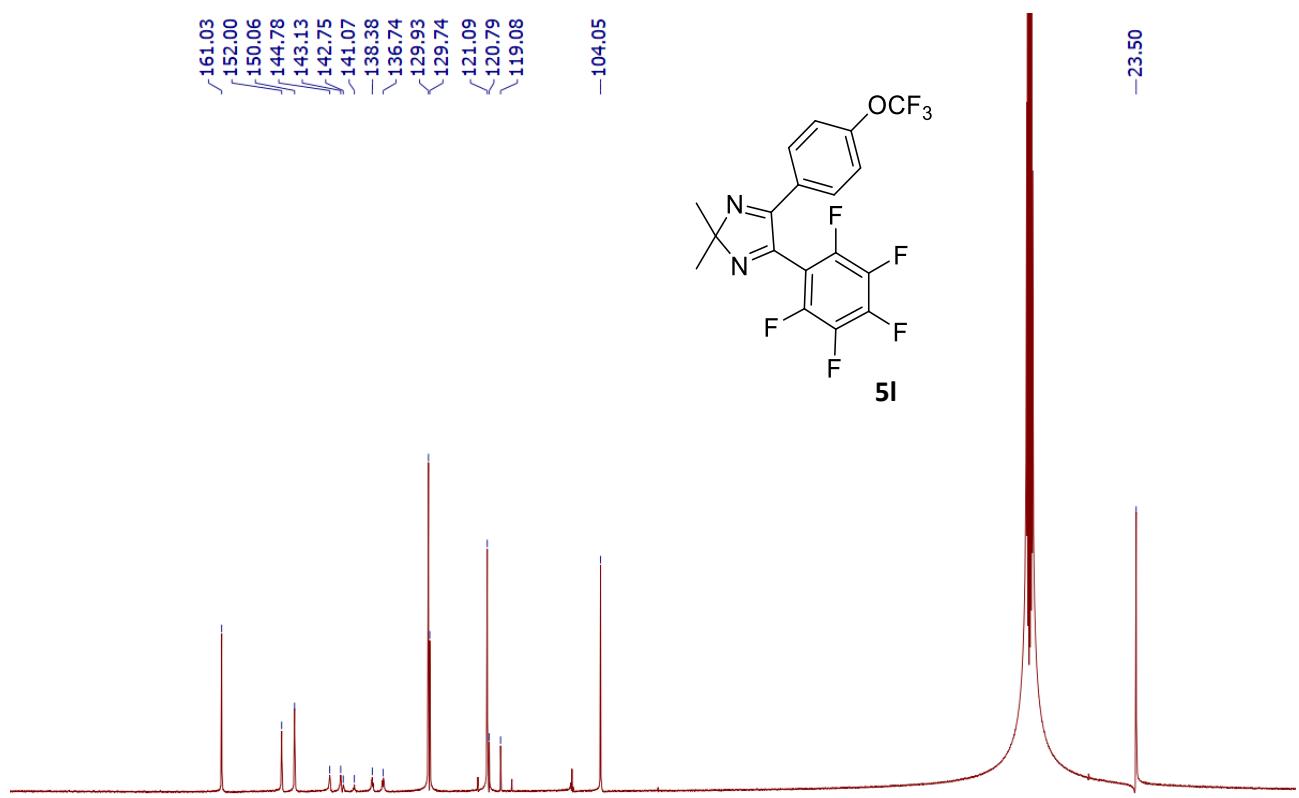
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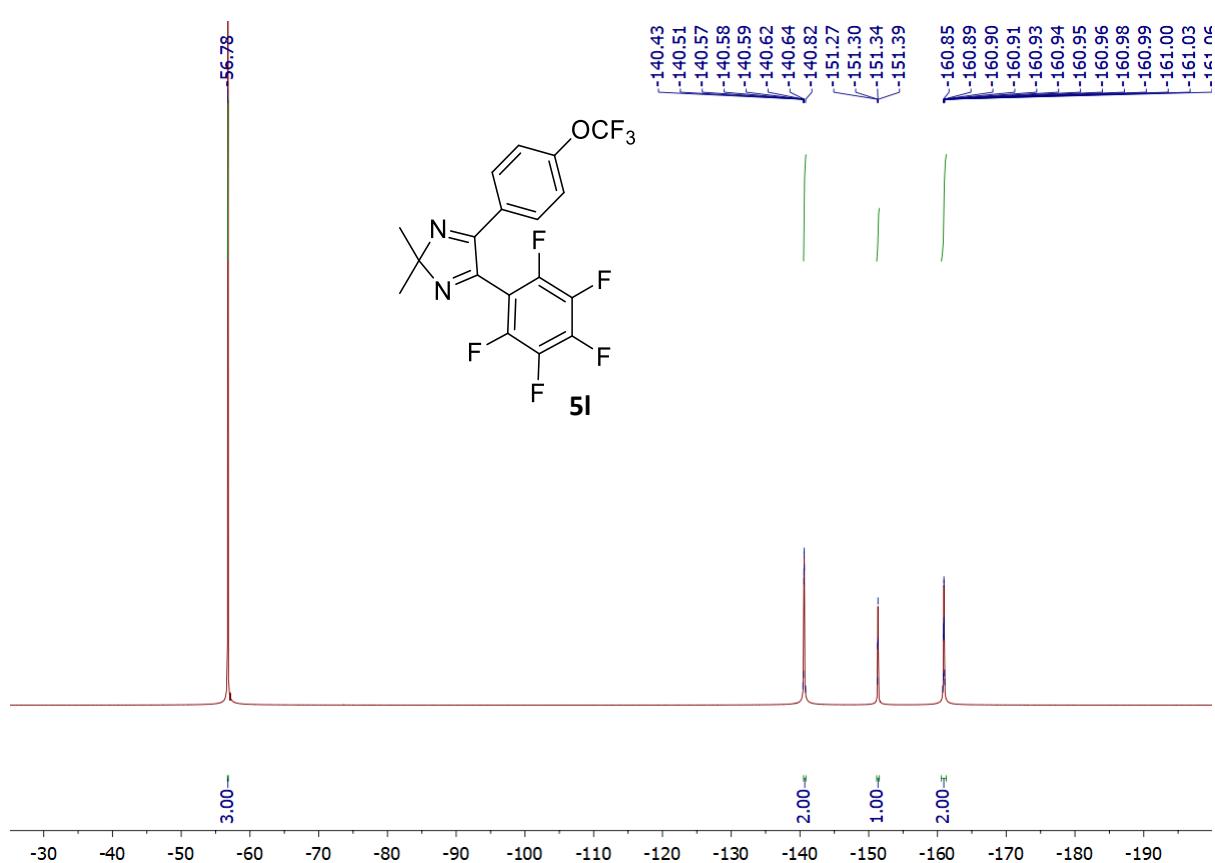
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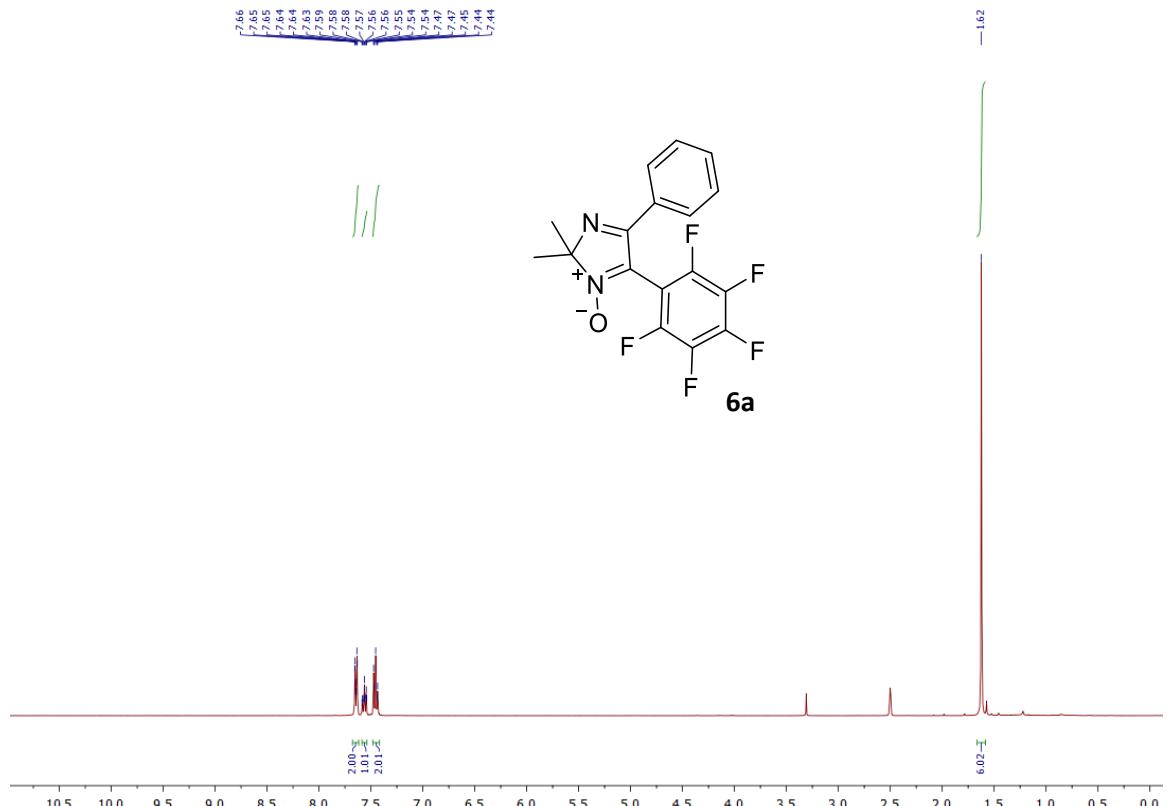


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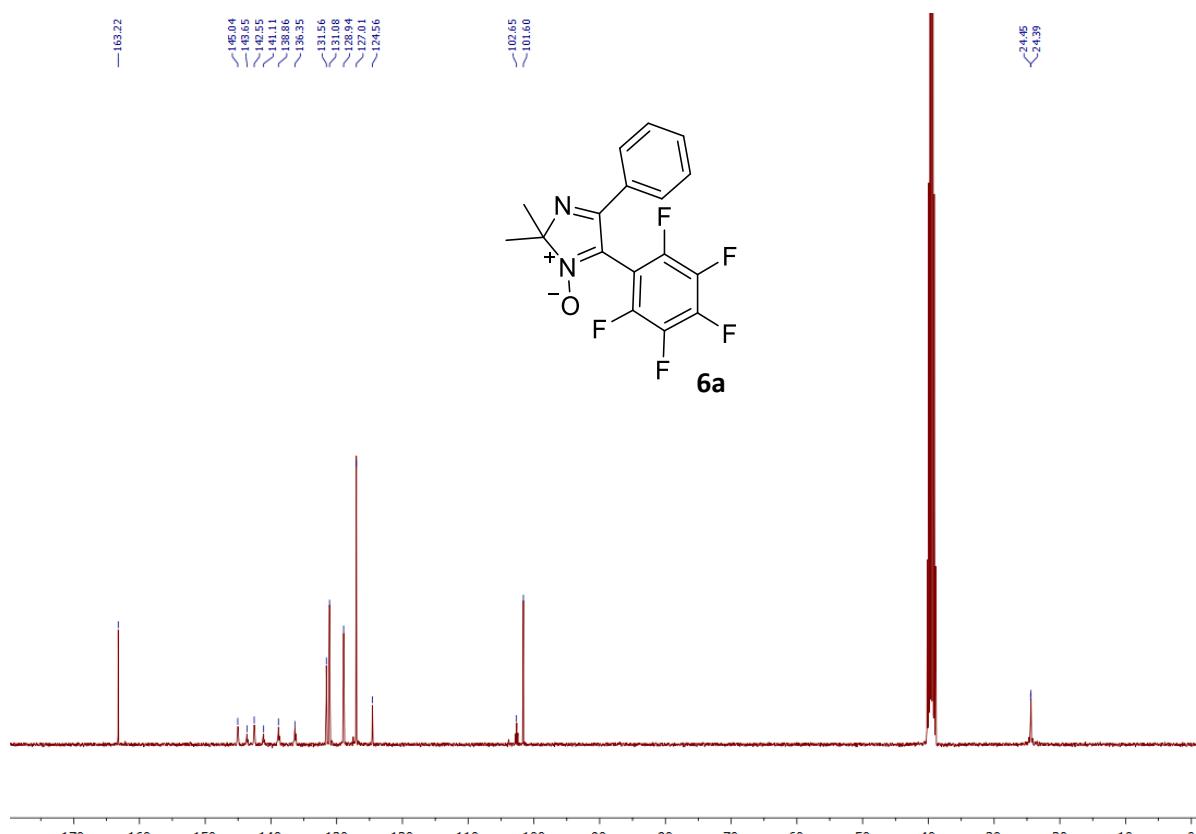


3. Copies of ^1H , ^{13}C , ^{19}F NMR spectra of 5-(perfluorophenyl)- substituted 2*H*-imidazole 1-oxide 6a-l

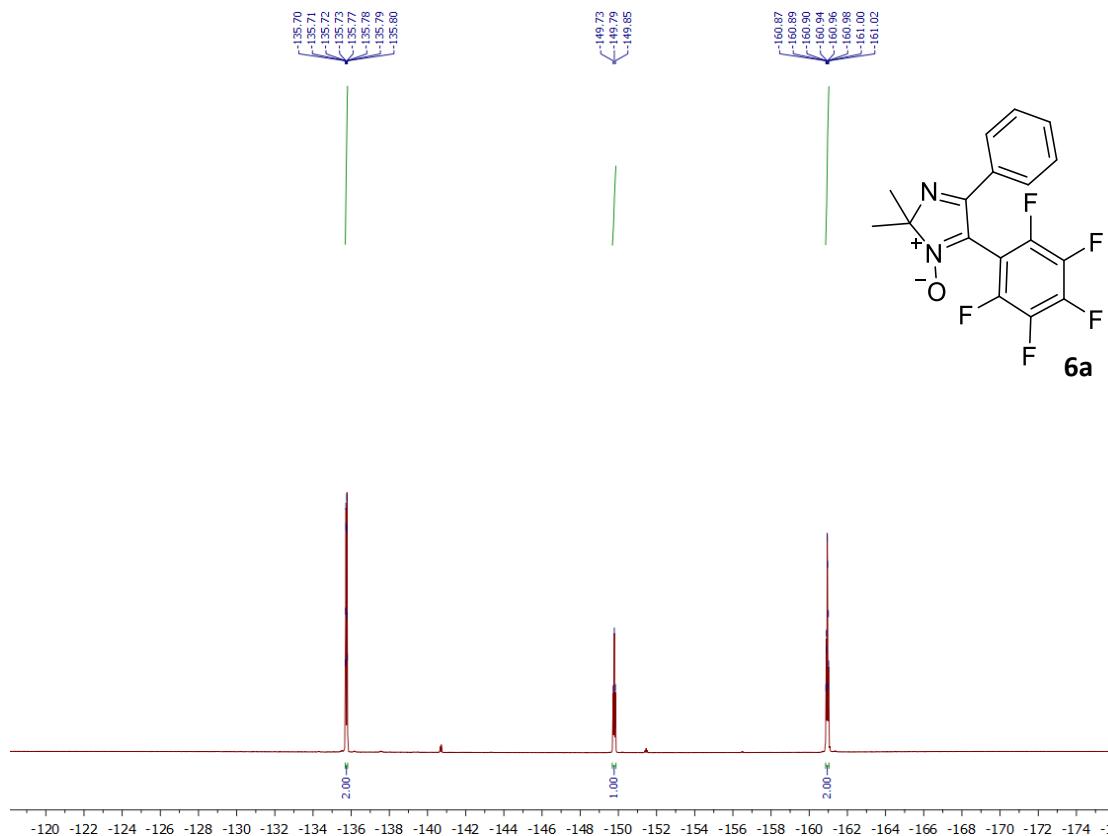
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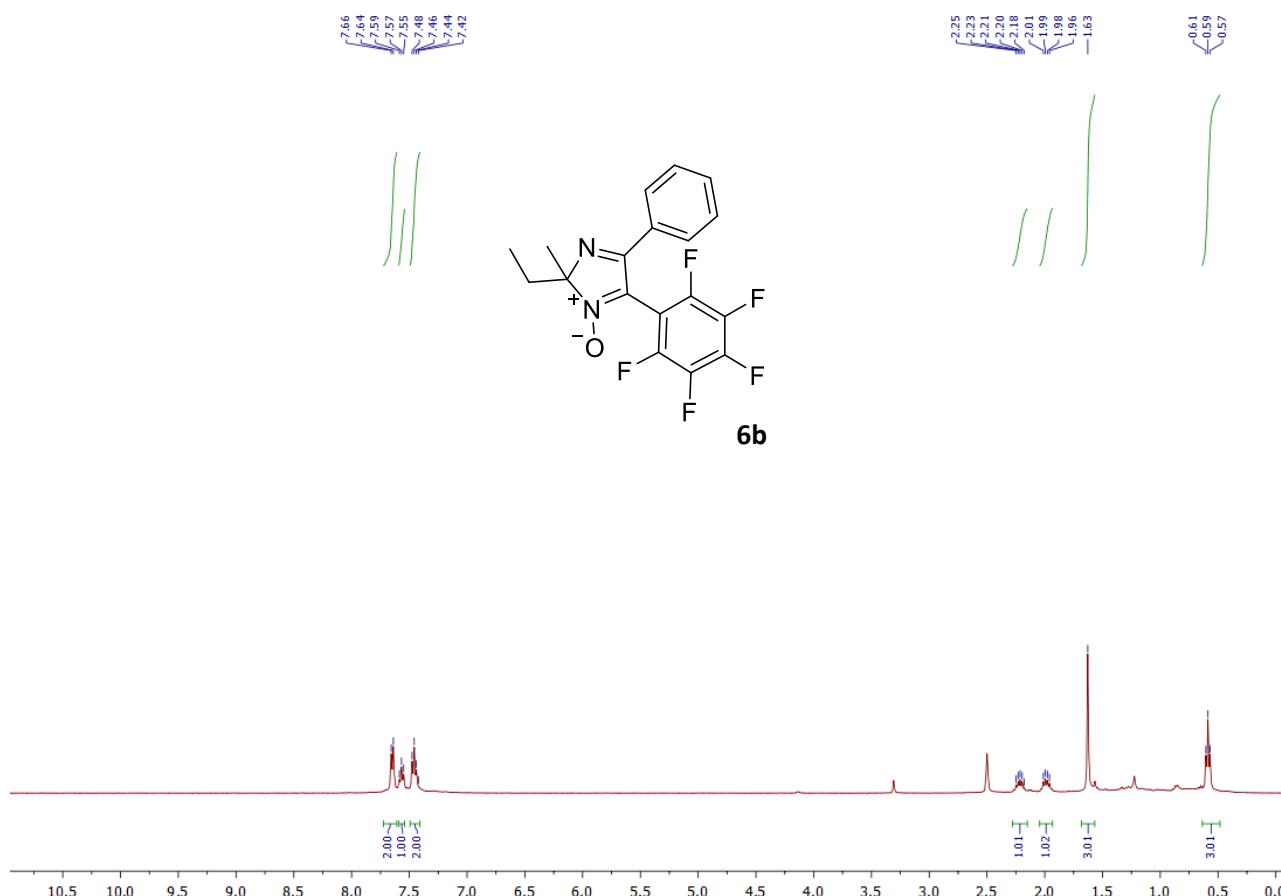
^{13}C { ^1H } NMR (101 MHz, DMSO-d₆)



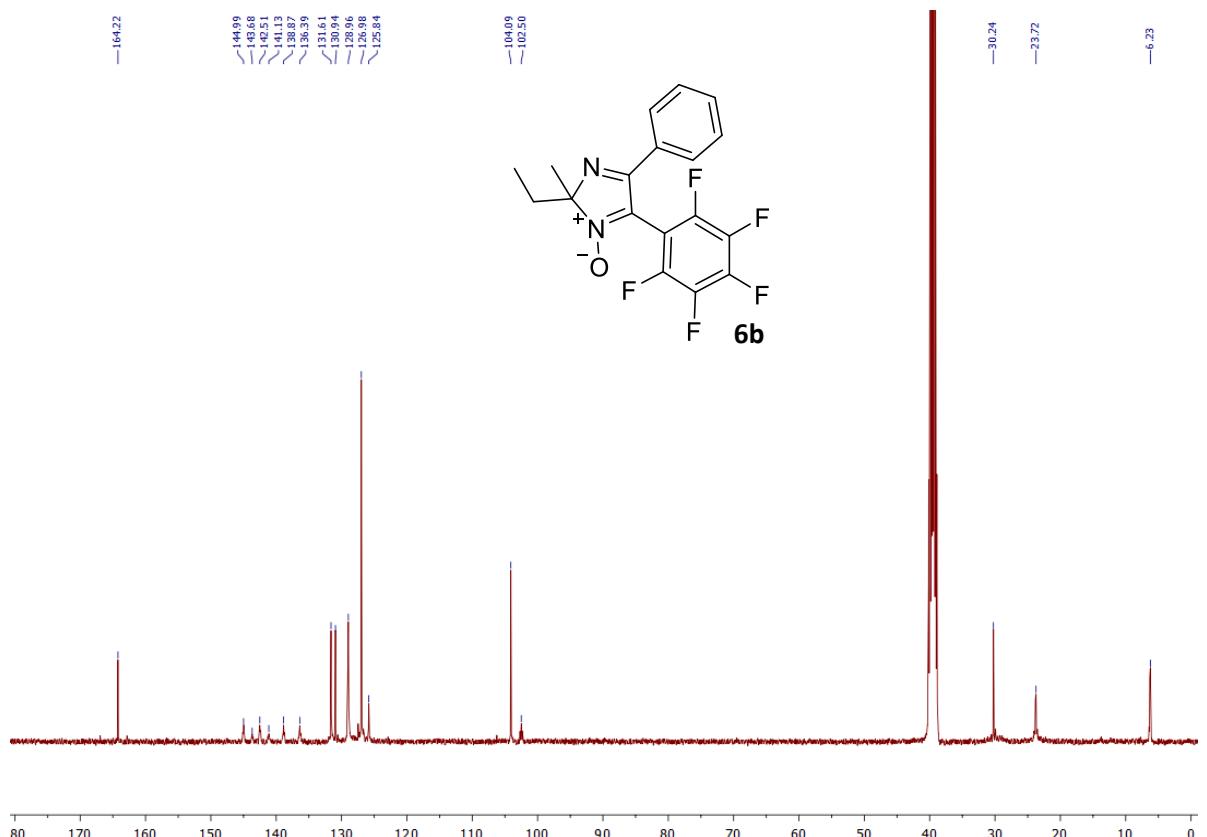
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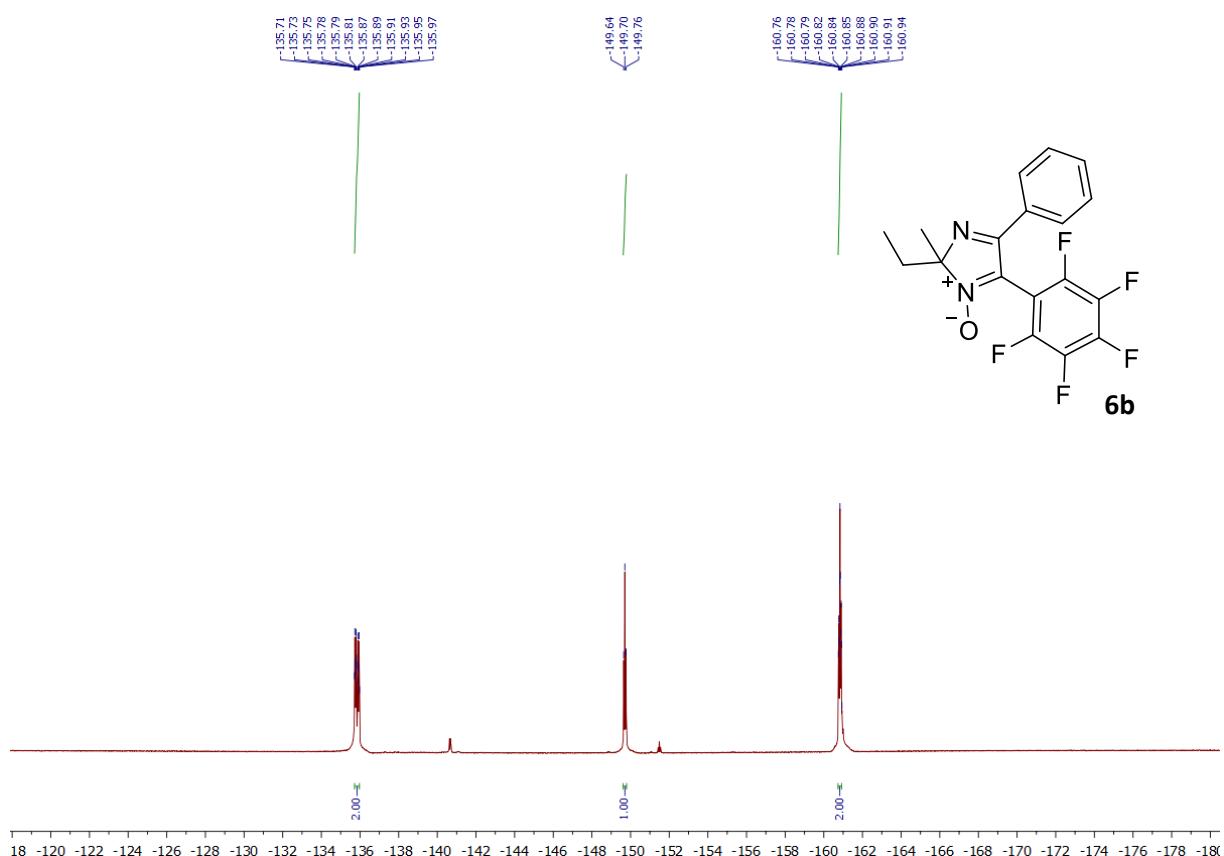
¹H NMR (400 MHz, DMSO-d₆)



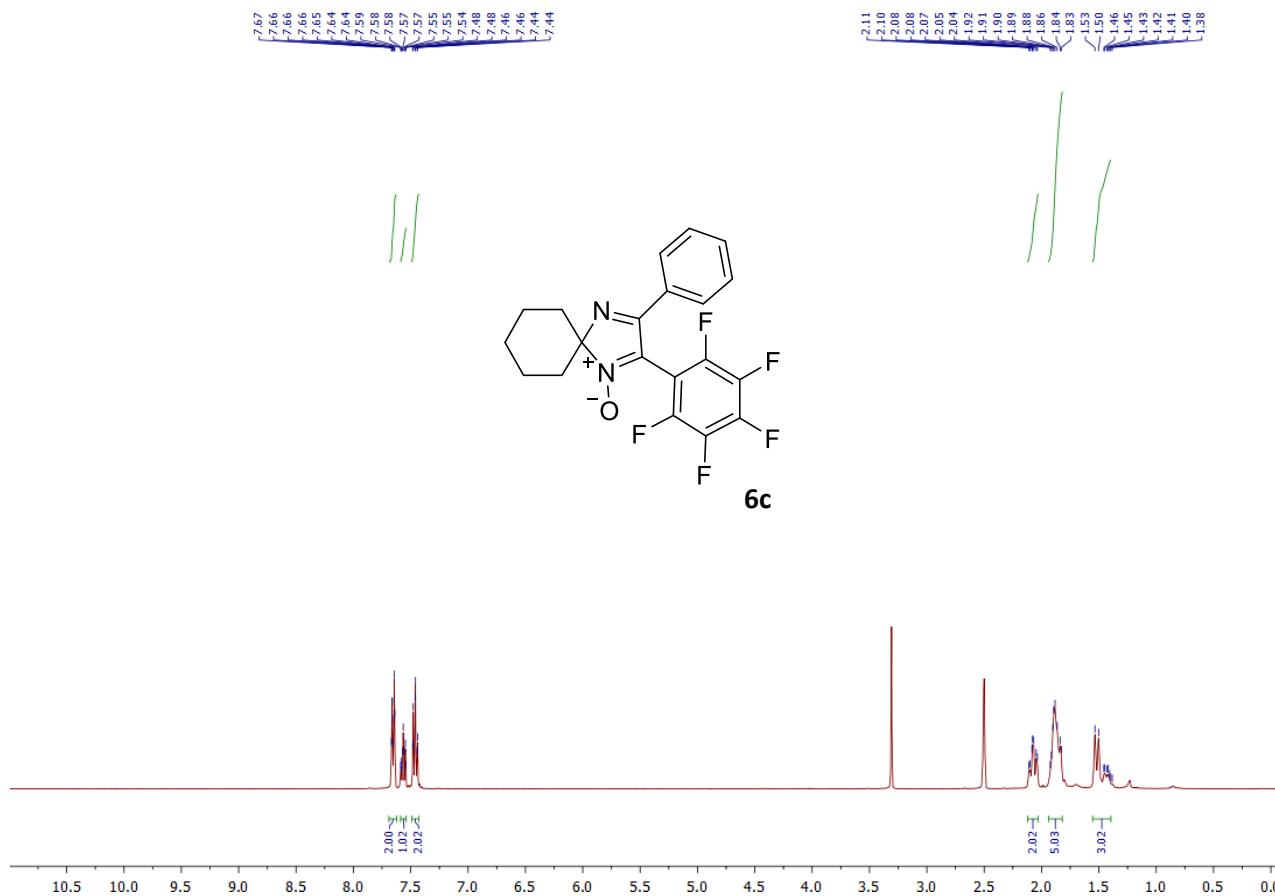
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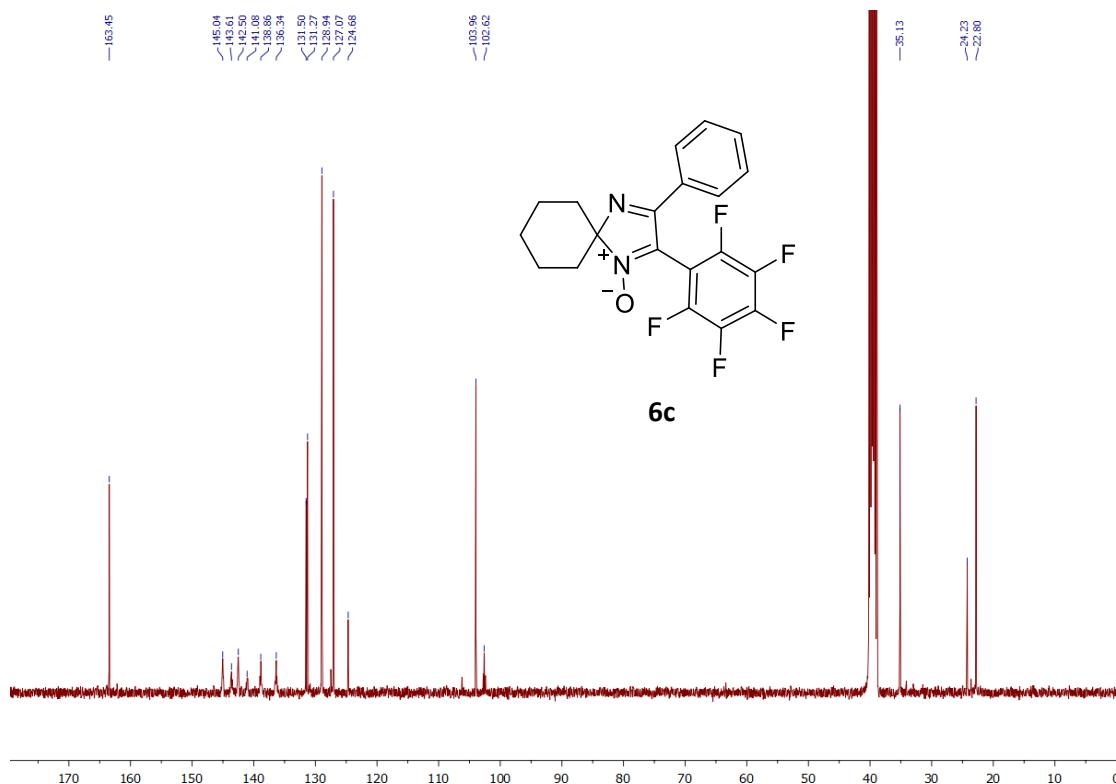
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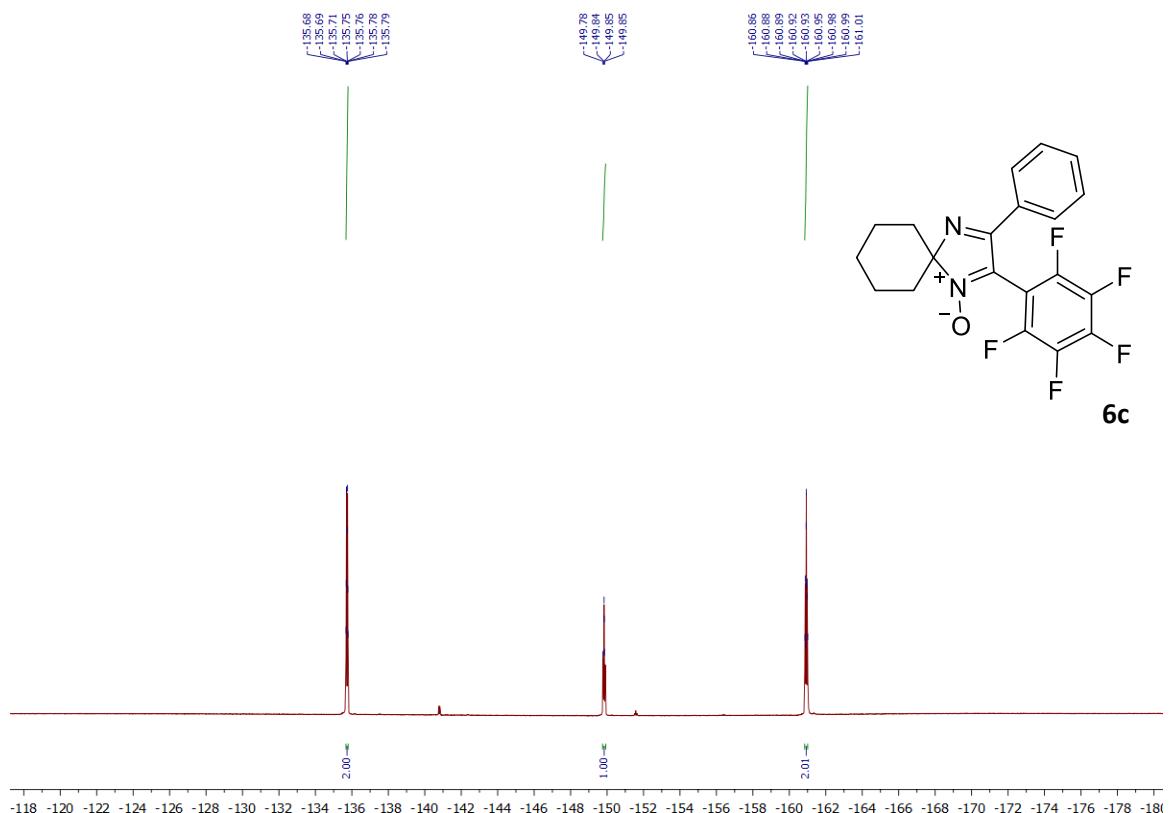
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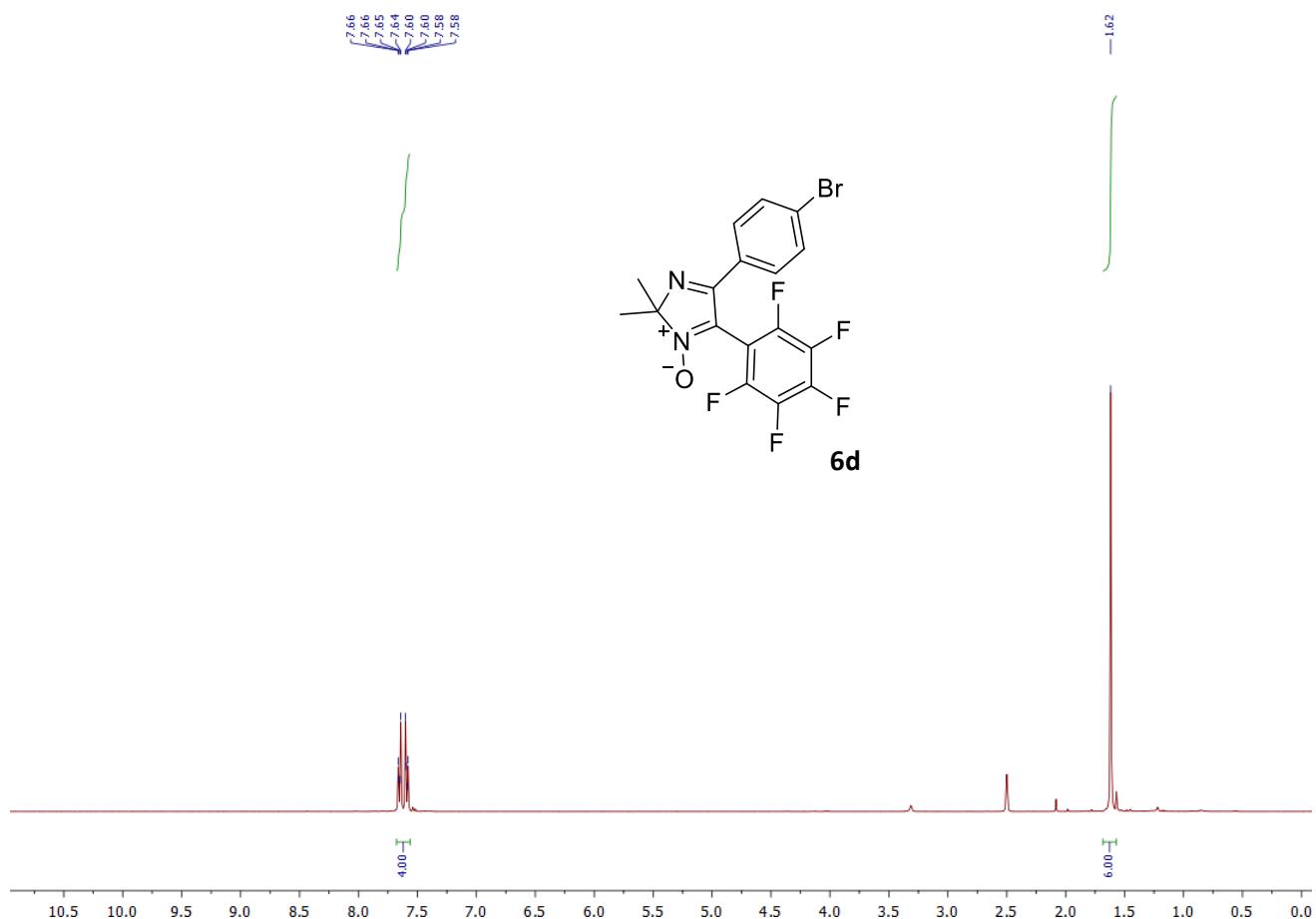
¹³C {¹H} NMR (101 MHz, DMSO-d₆)



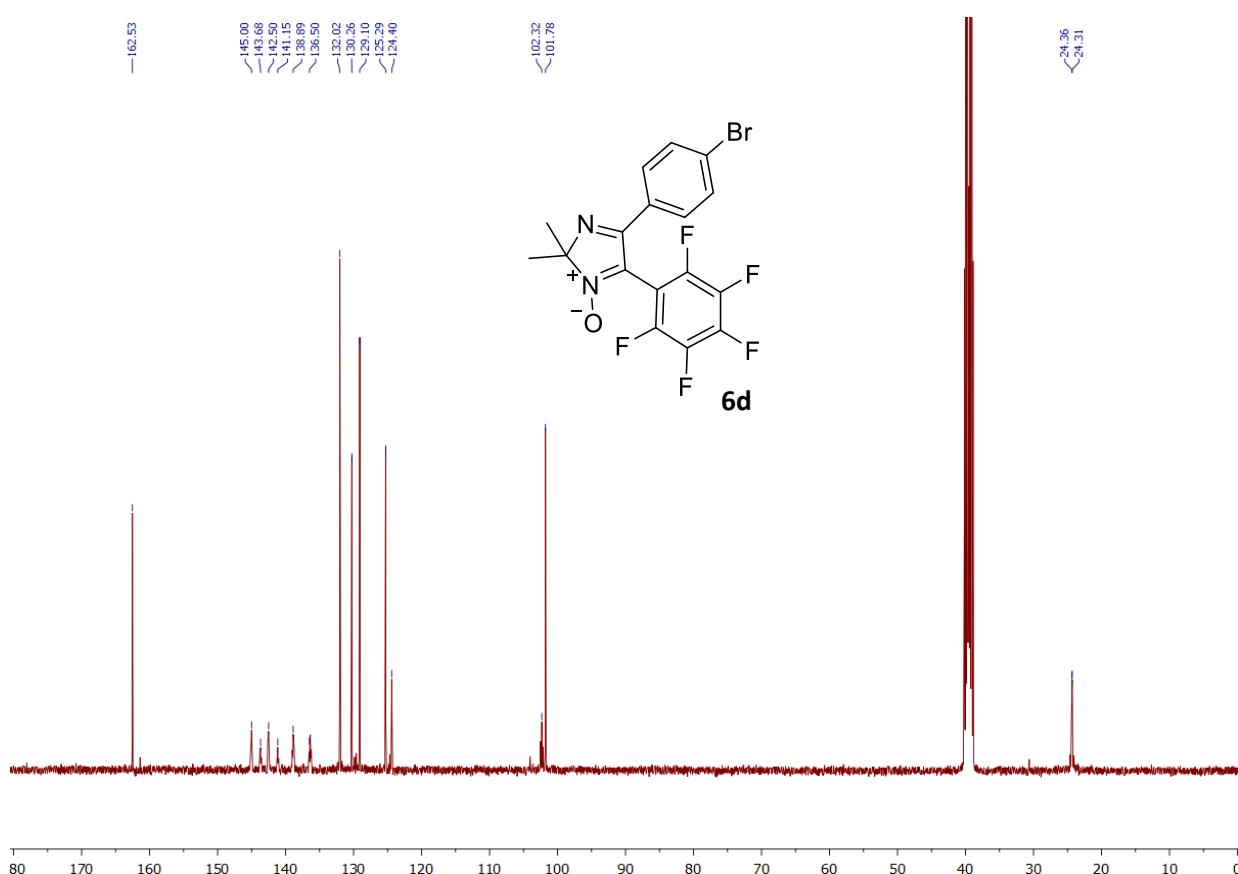
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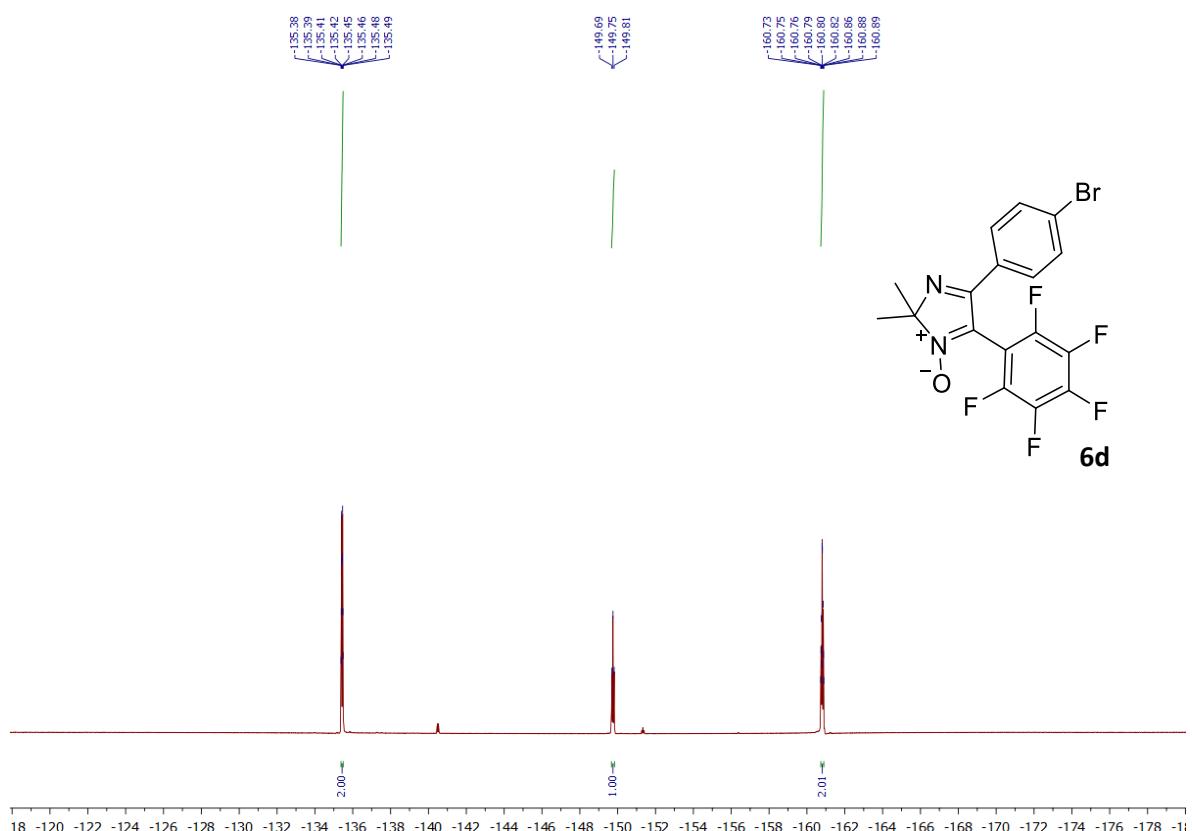
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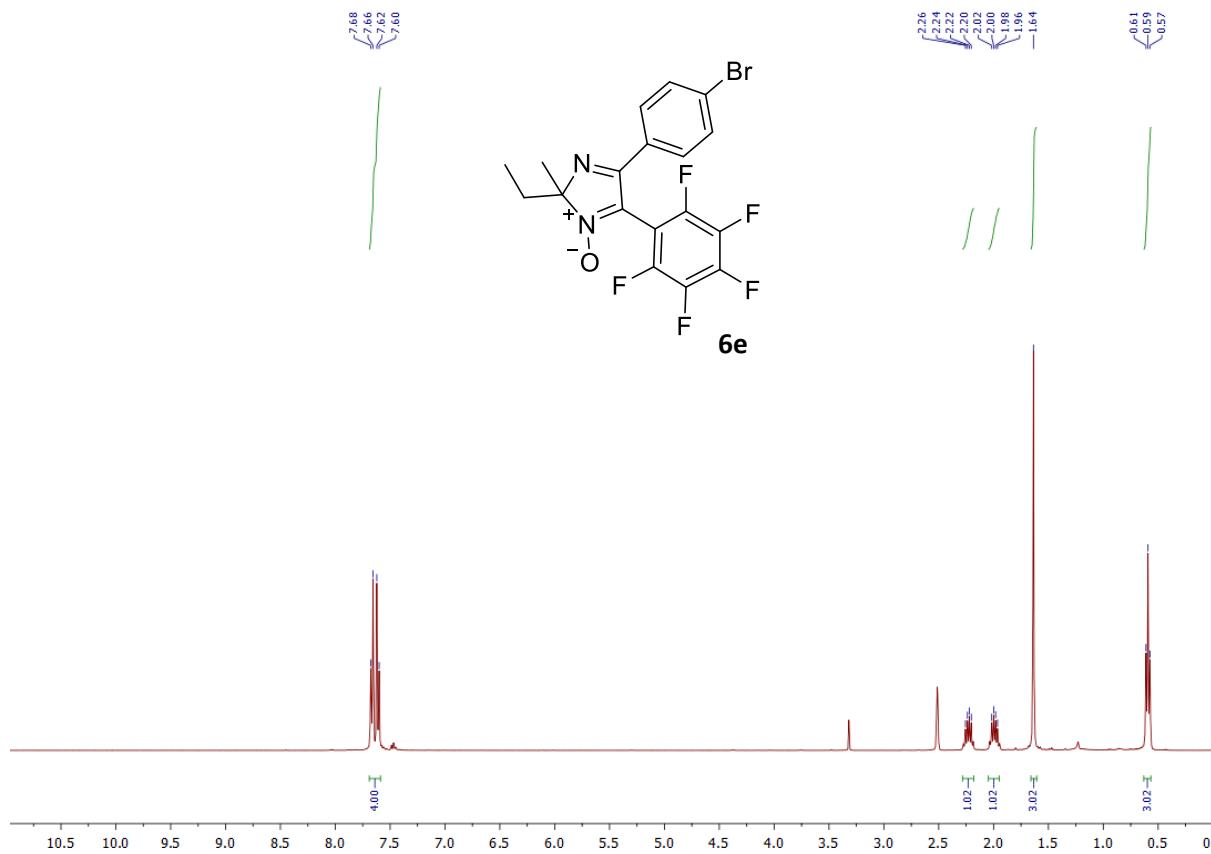
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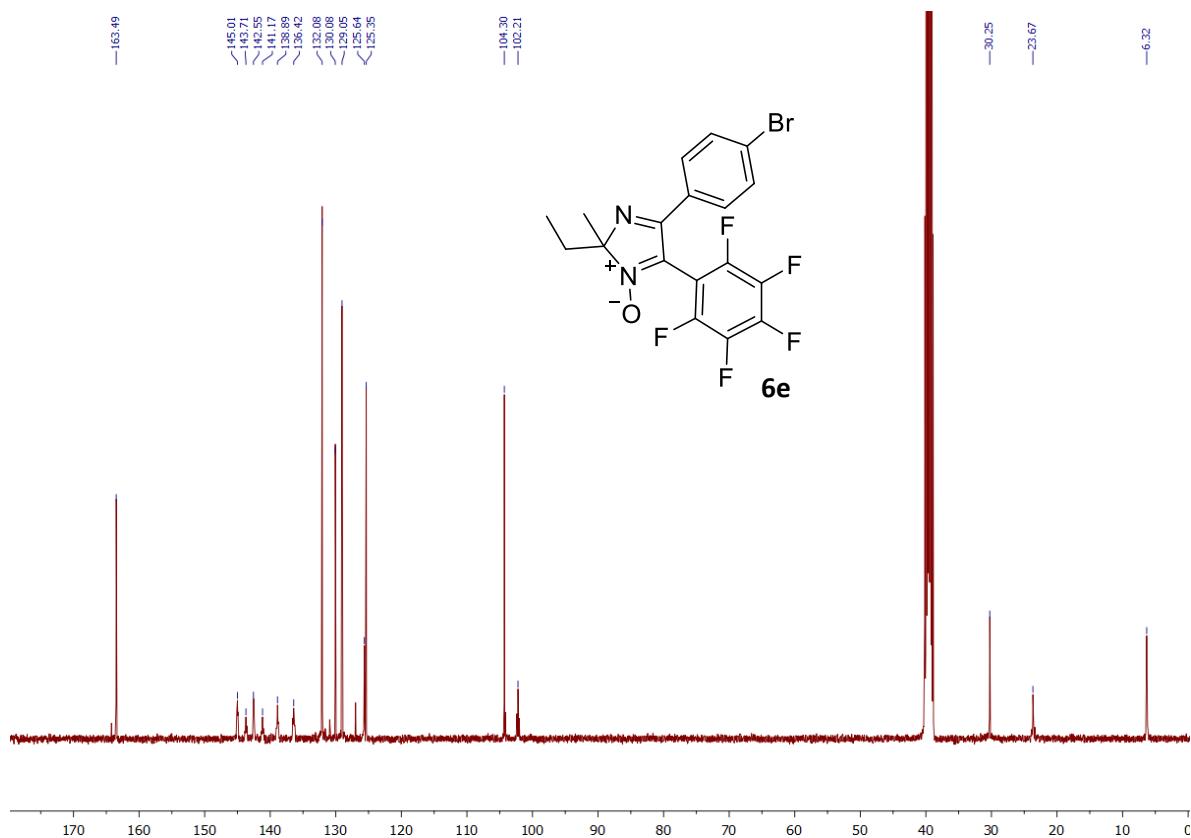
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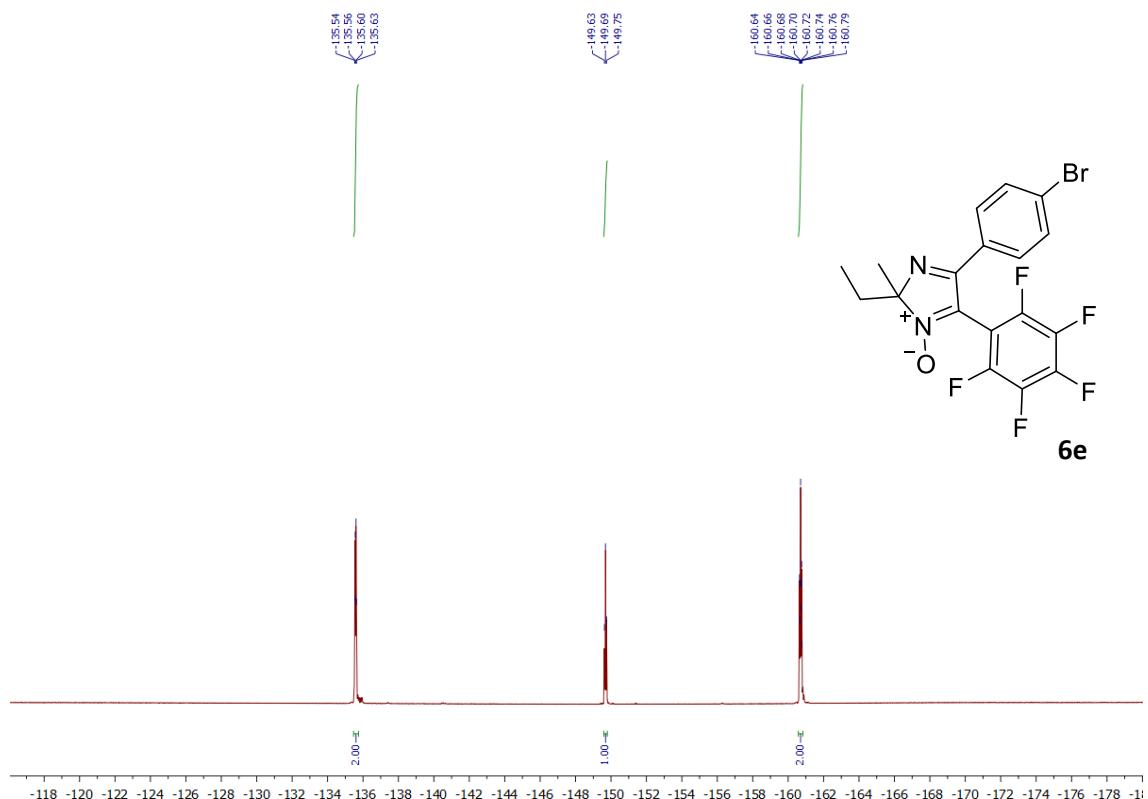
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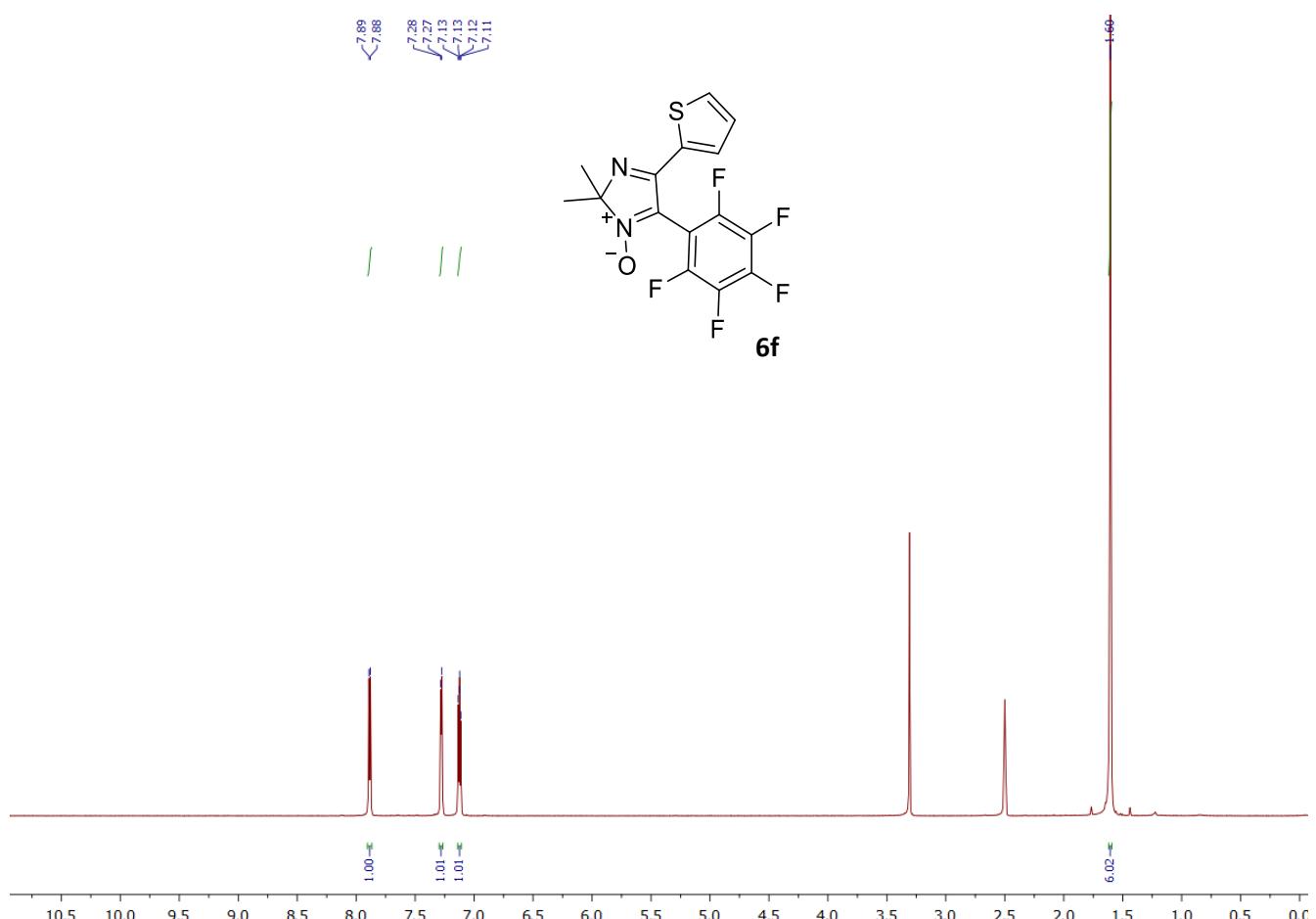
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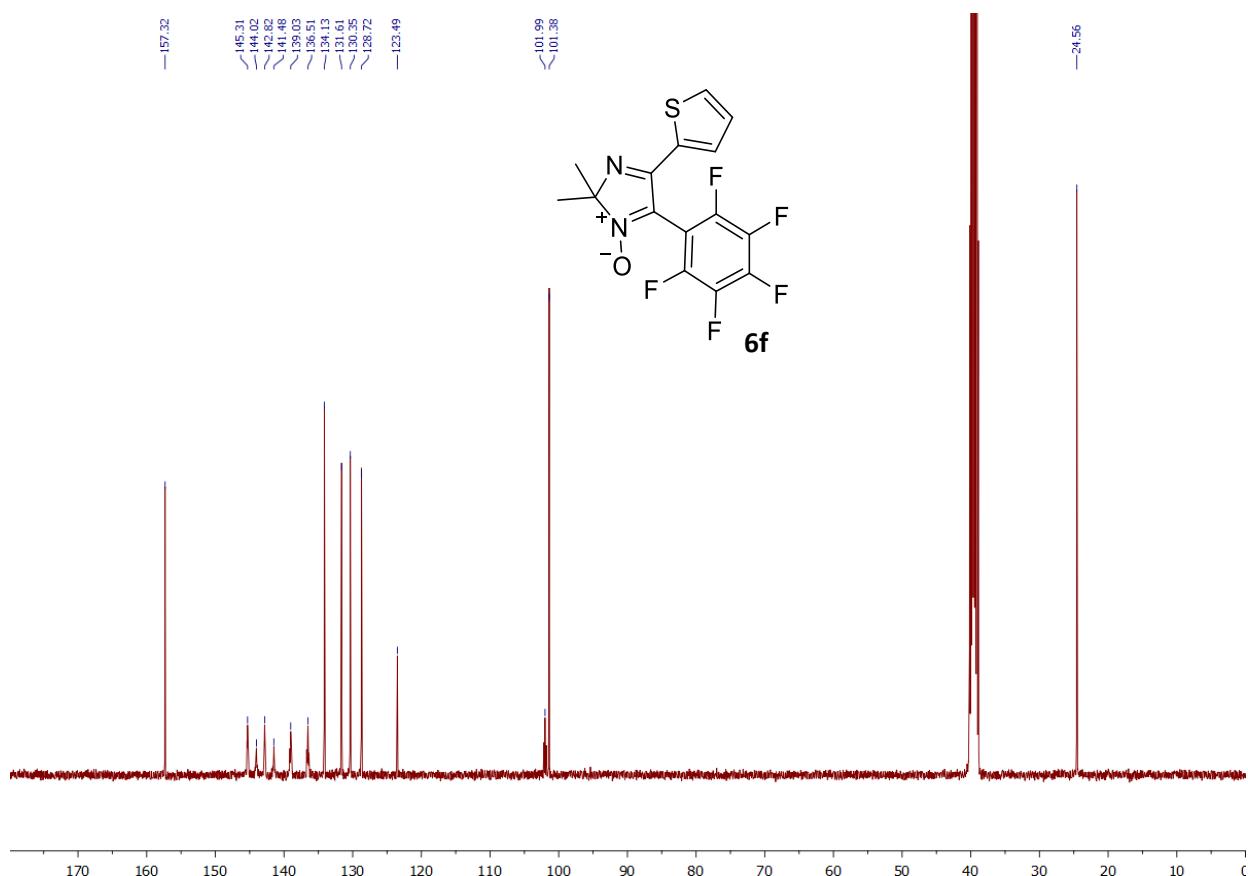
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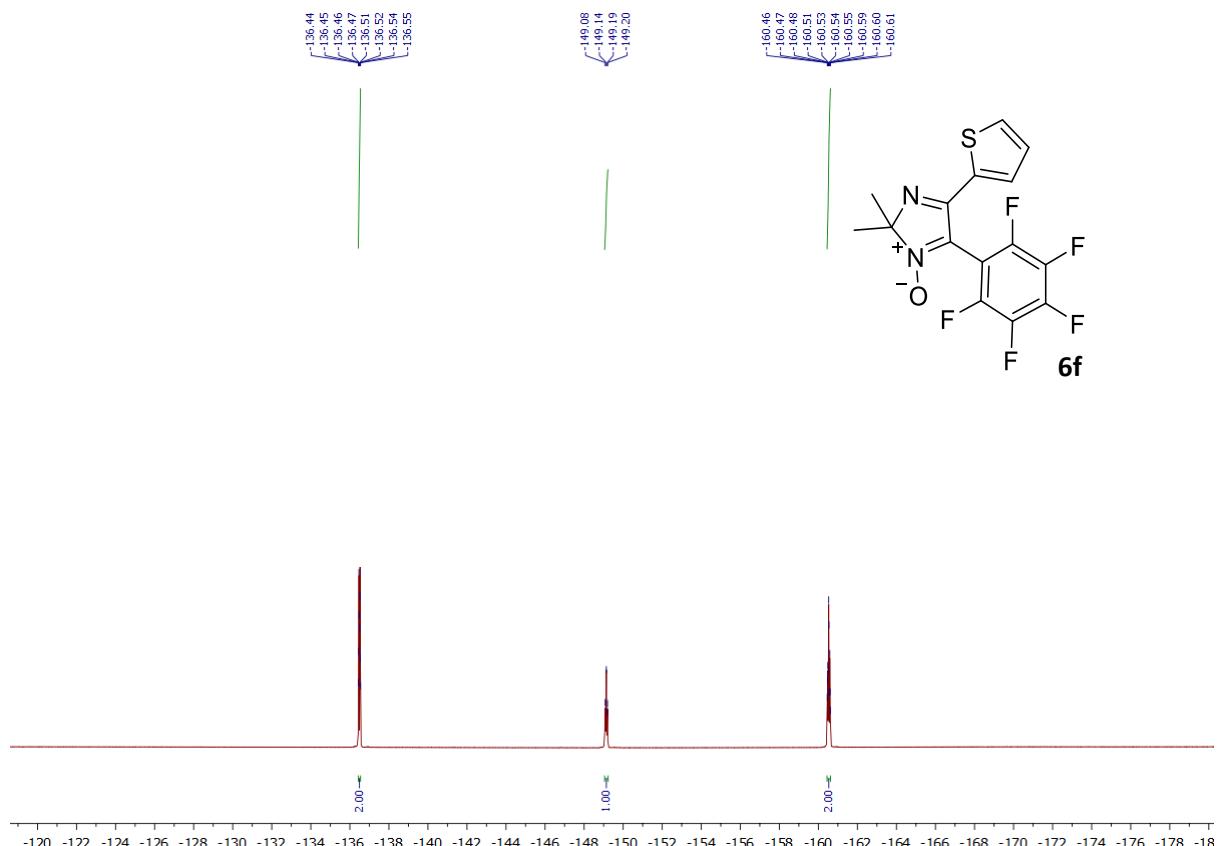
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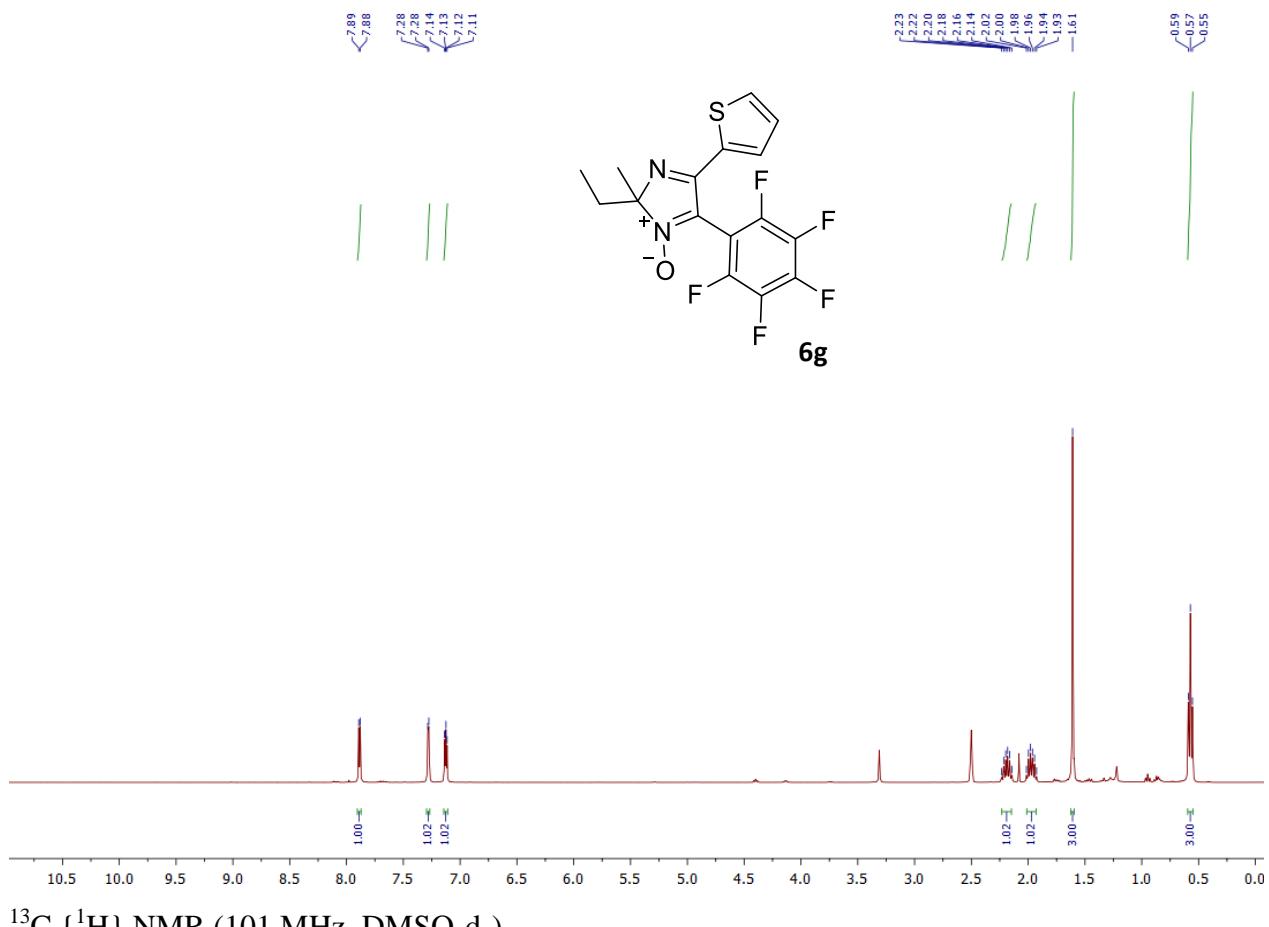
^{13}C { ^1H } NMR (101 MHz, DMSO-d₆)



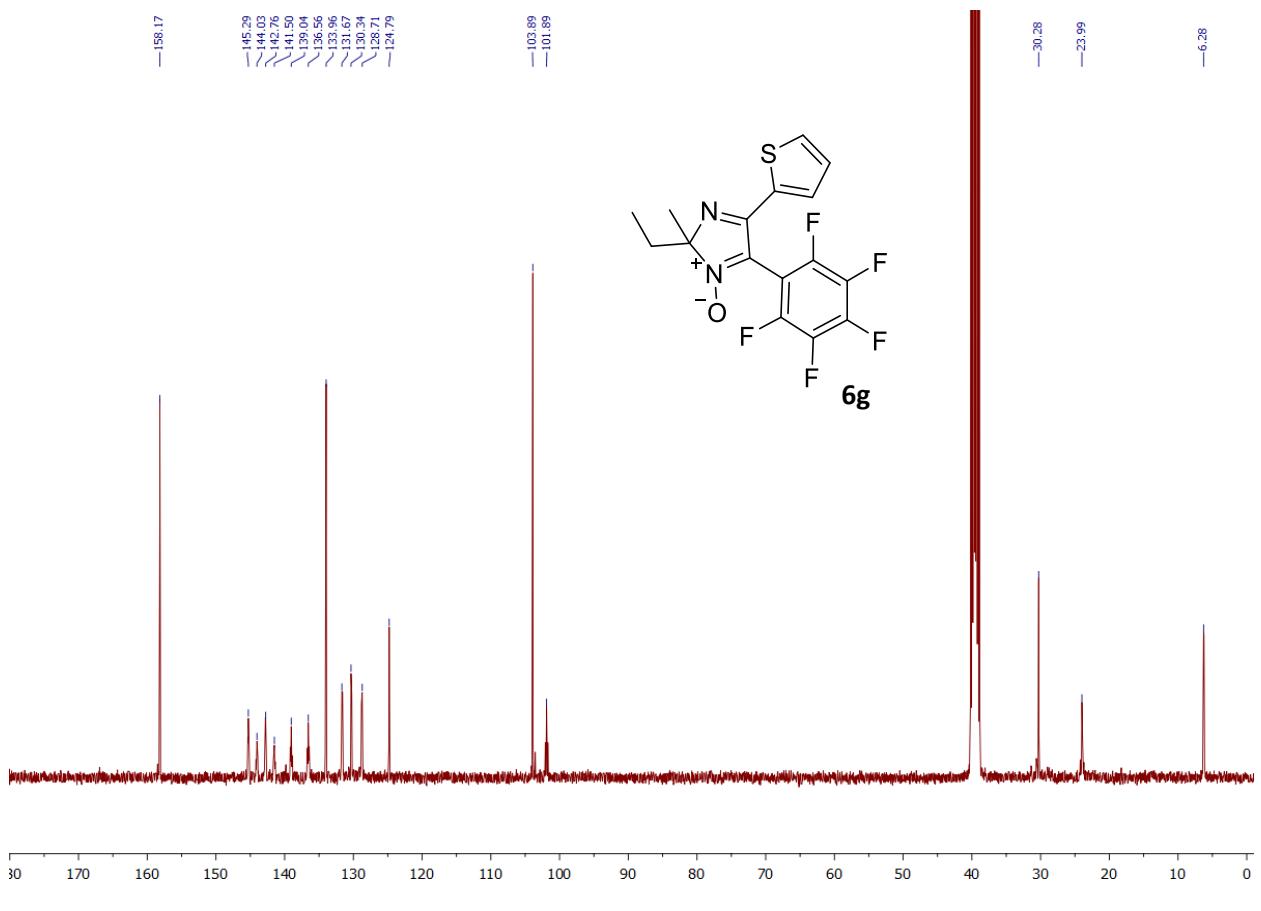
^{19}F NMR (376 MHz, DMSO-d₆)



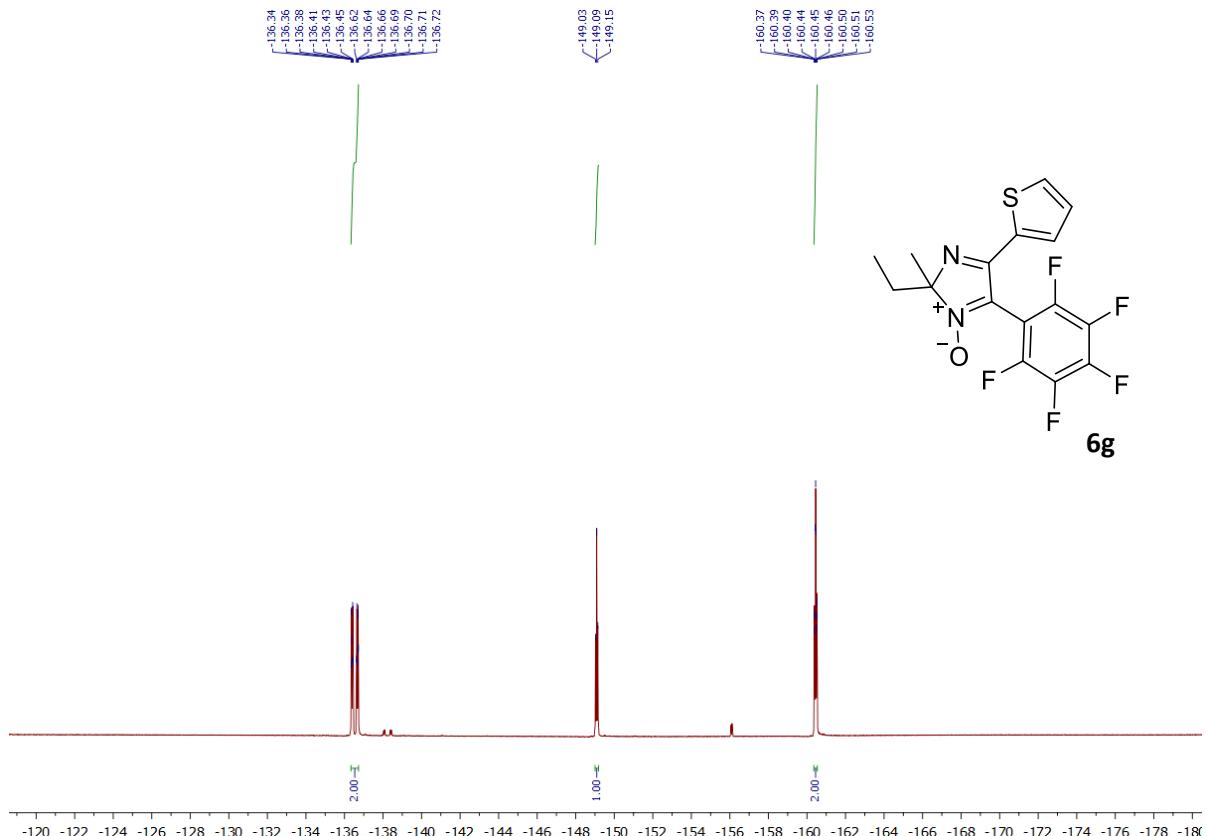
¹H NMR (400 MHz, DMSO-d₆)



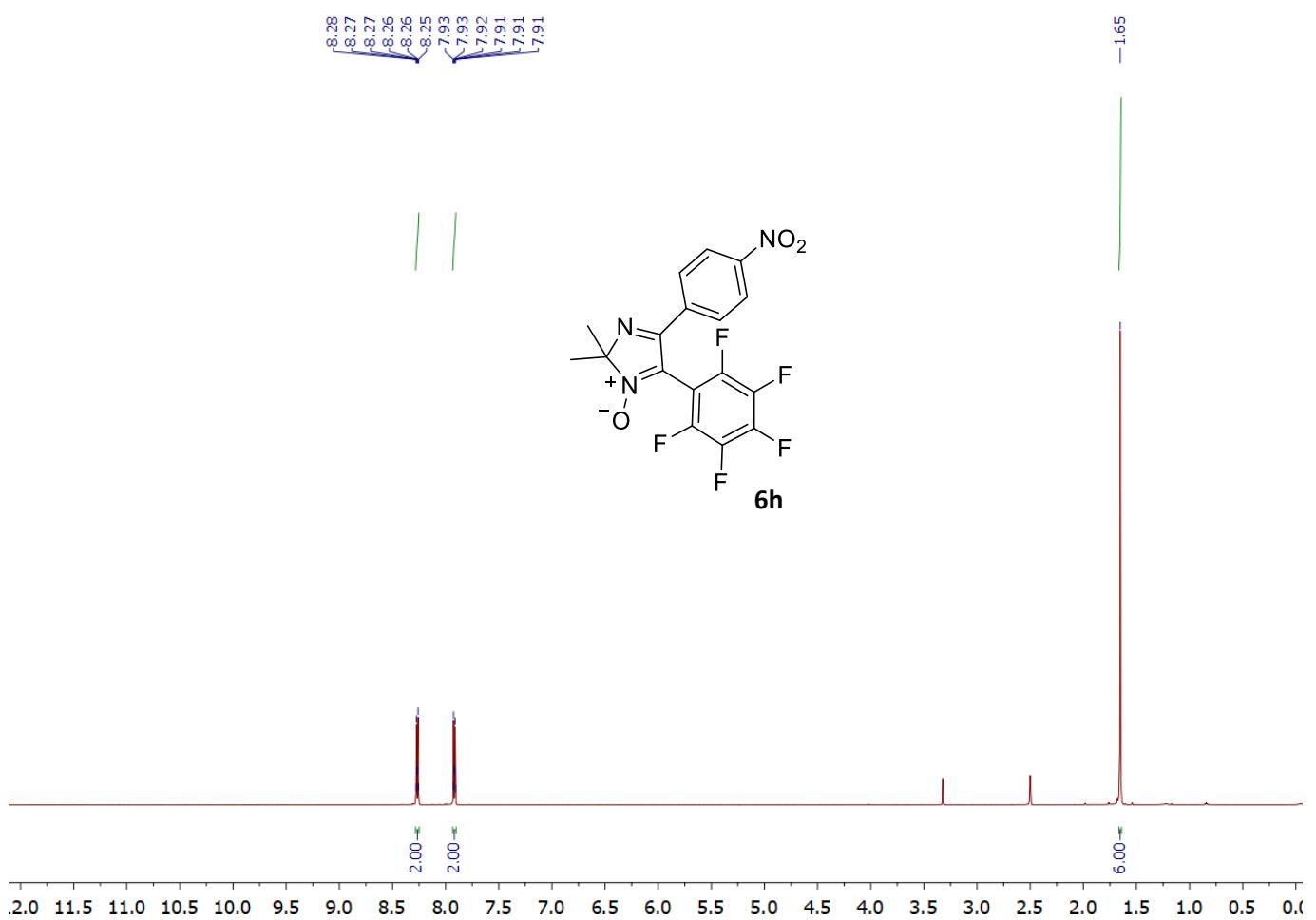
¹³C {¹H} NMR (101 MHz, DMSO-d₆)



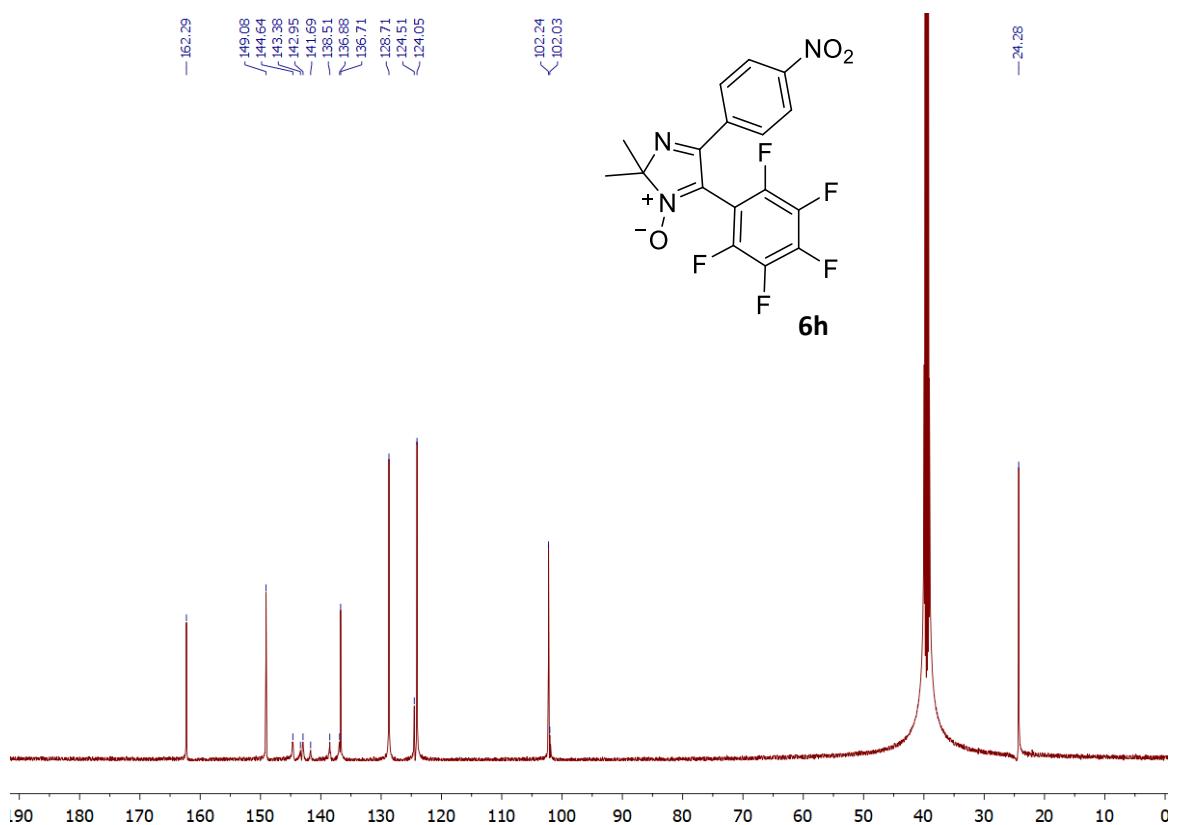
¹⁹F NMR (376 MHz, DMSO-d₆)



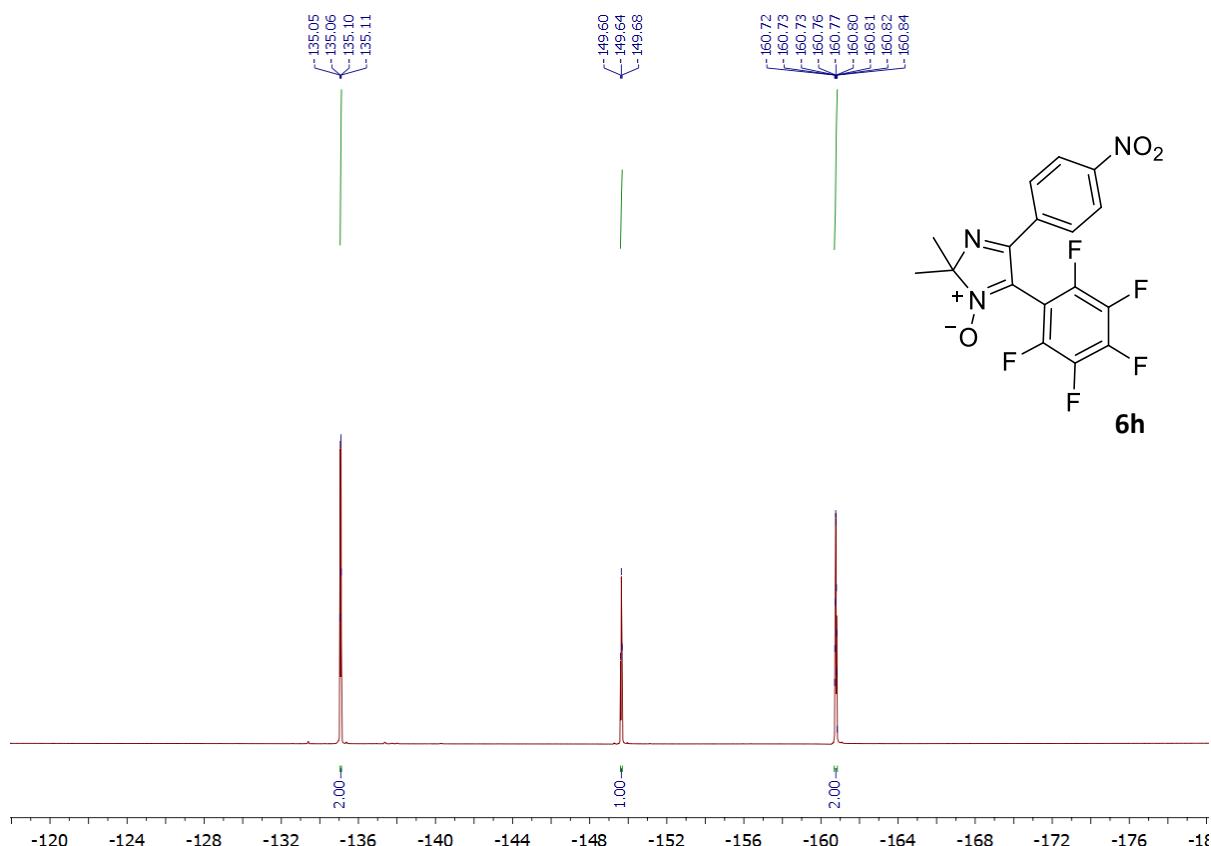
¹H NMR (600 MHz, DMSO-d₆)



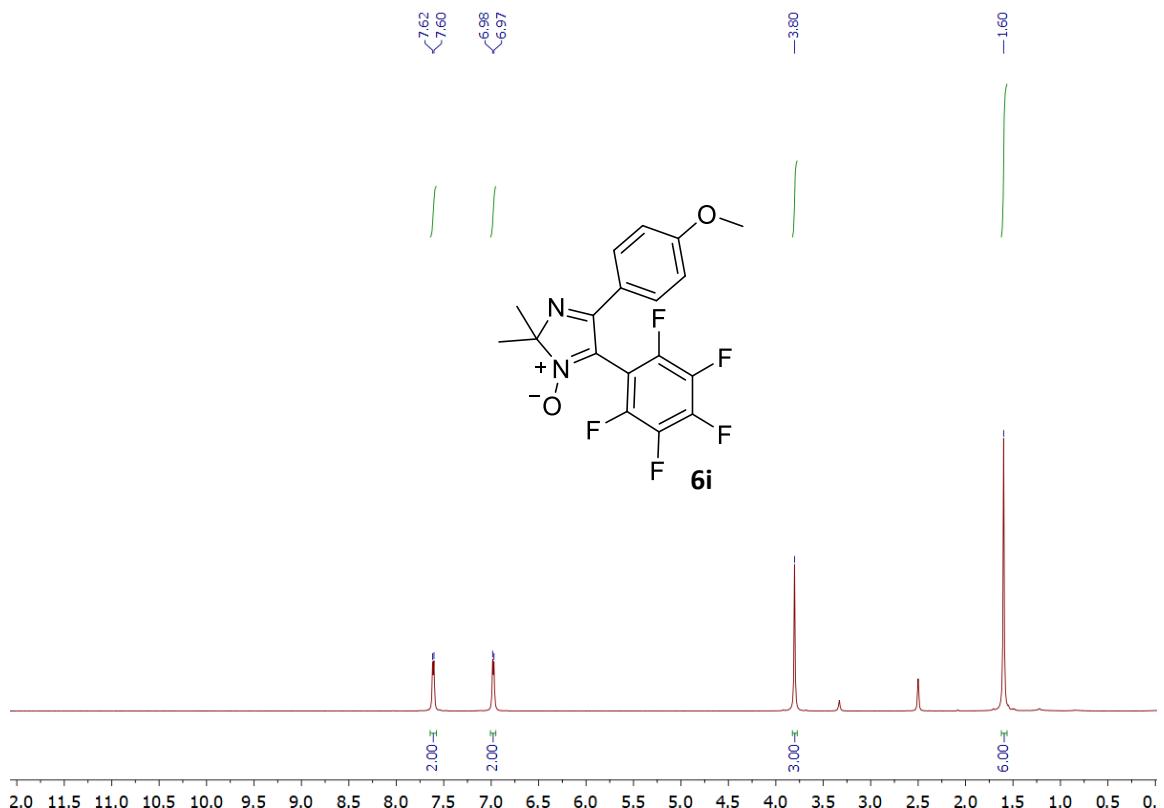
^{13}C { ^1H } NMR (101 MHz, DMSO-d₆)



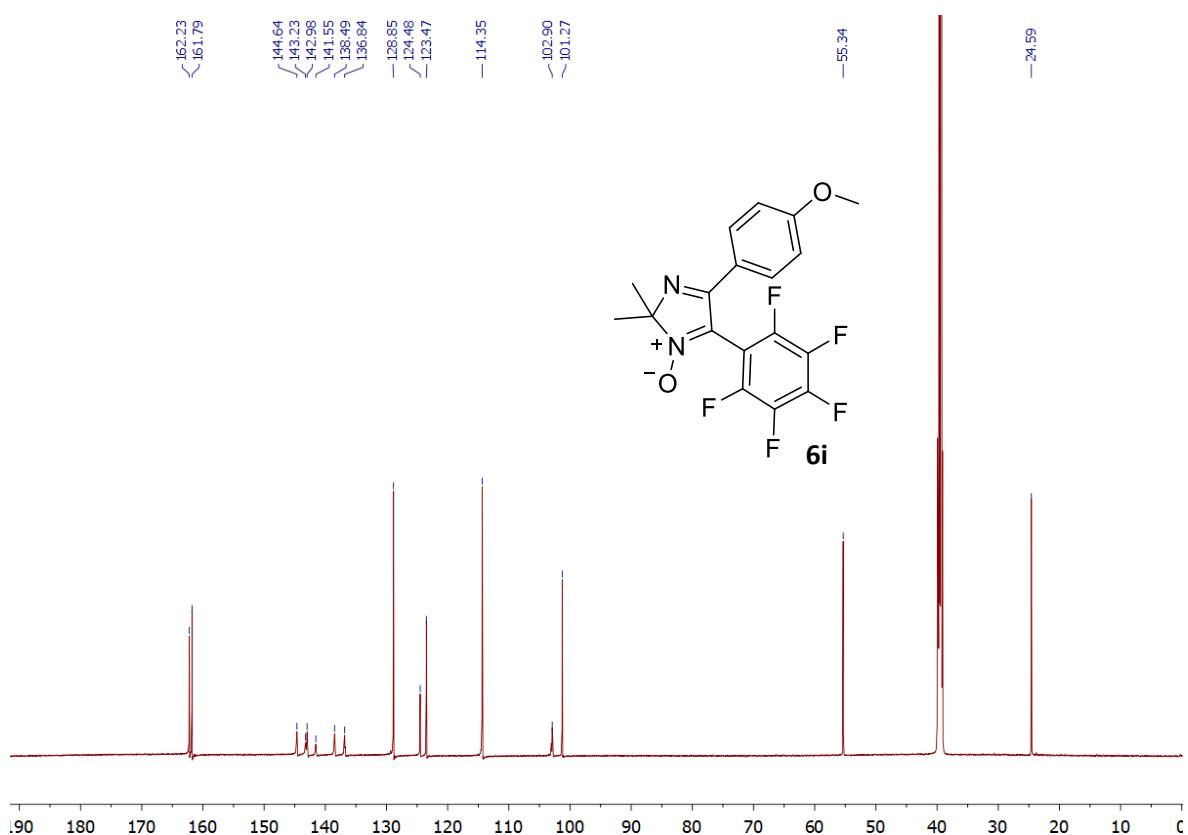
^{19}F NMR (376 MHz, DMSO-d₆)



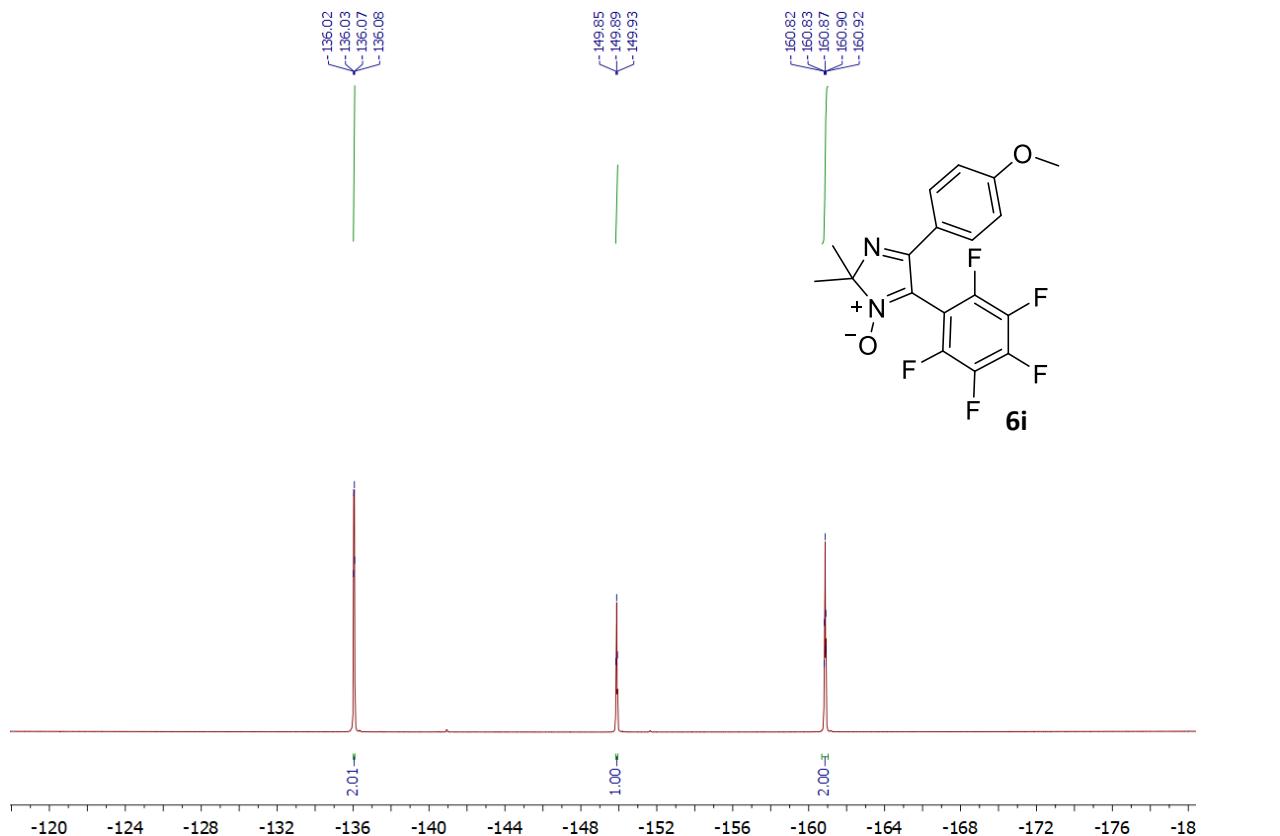
¹H NMR (600 MHz, DMSO-d₆)



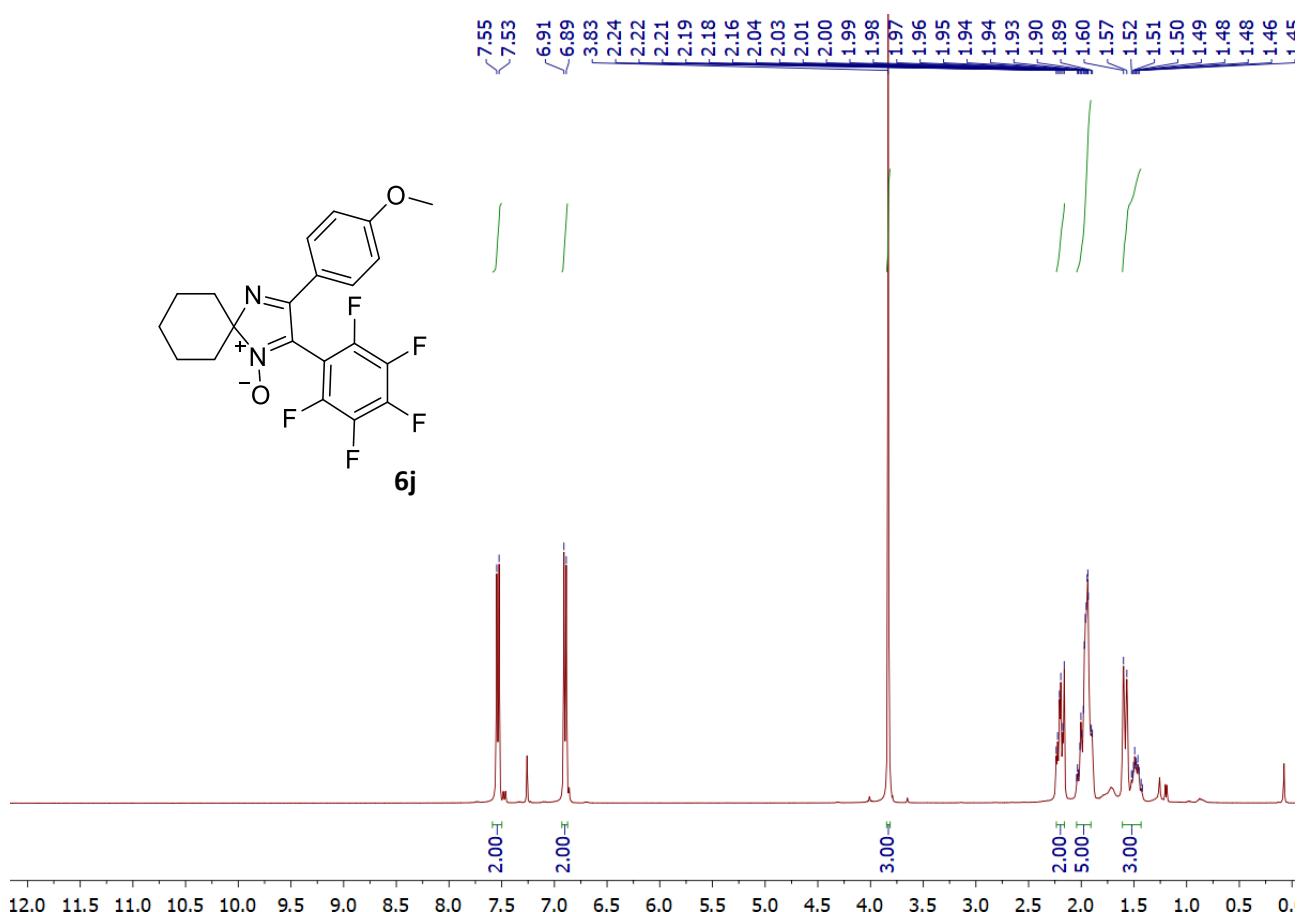
¹³C {¹H} NMR (101 MHz, DMSO-d₆)



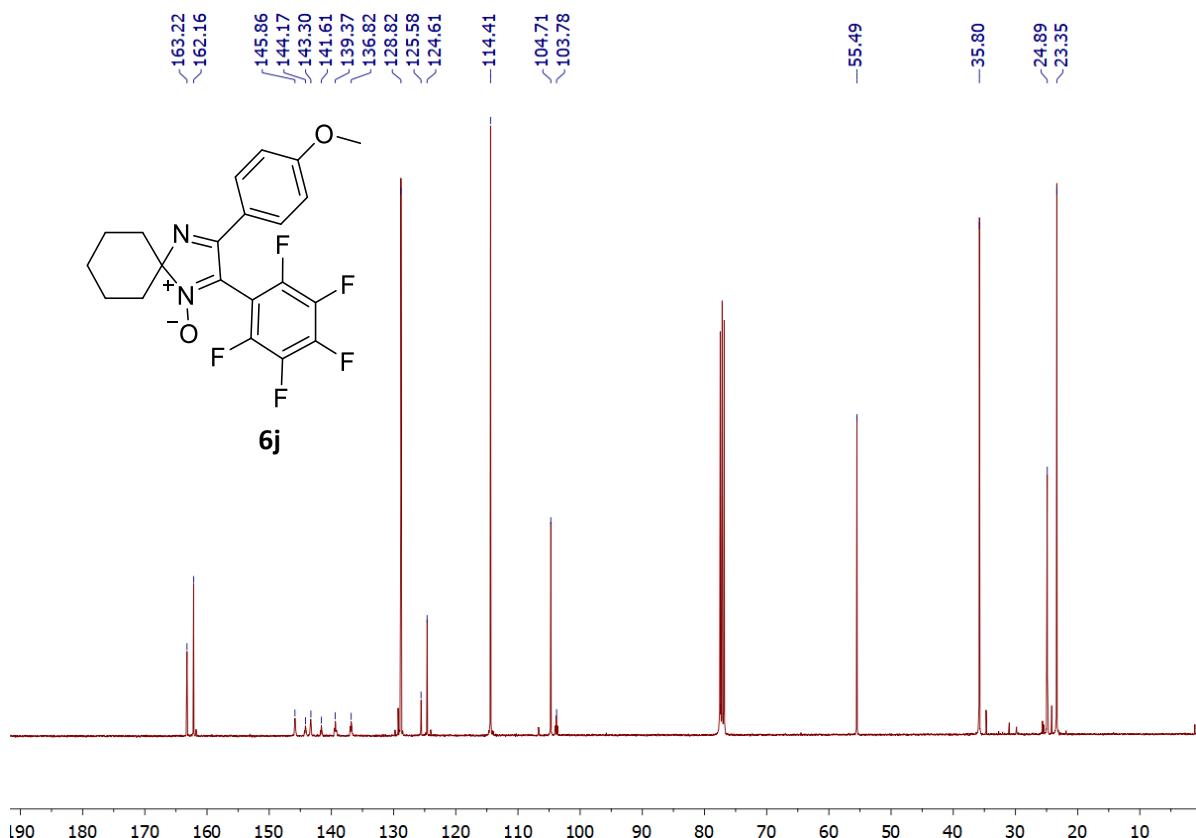
¹⁹F NMR (376 MHz, DMSO-d₆)



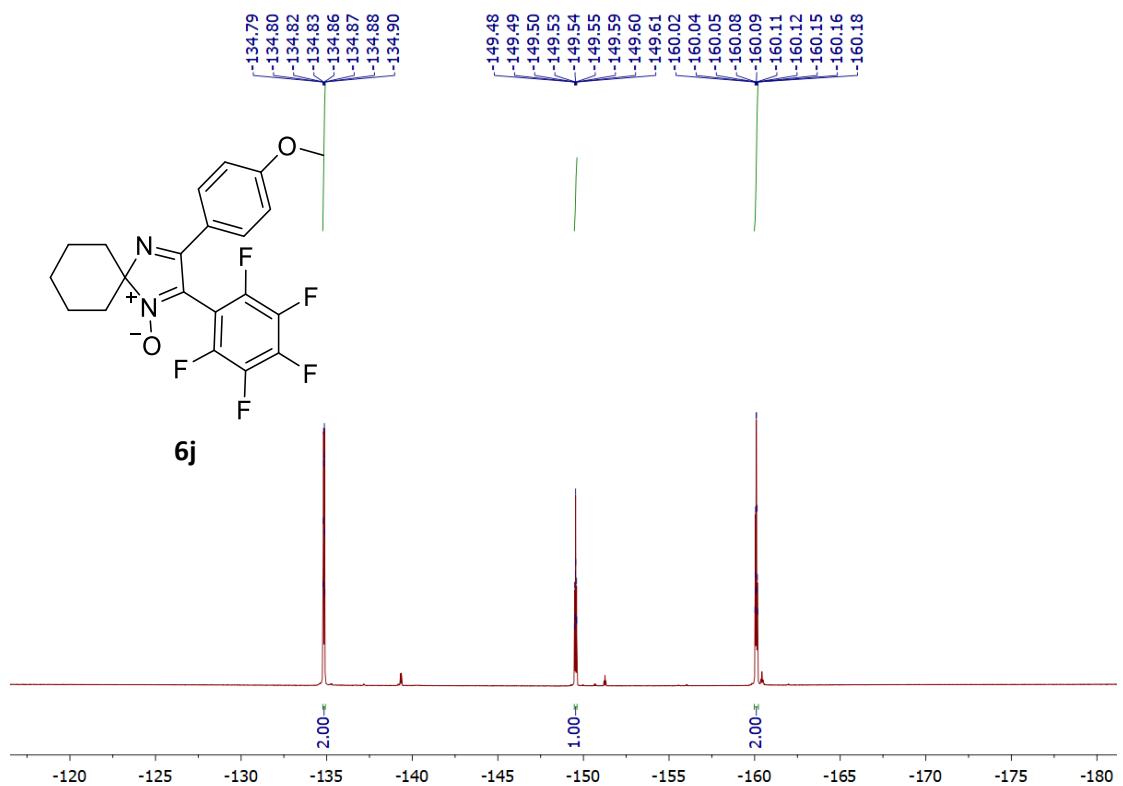
¹H NMR (400 MHz, CDCl₃)



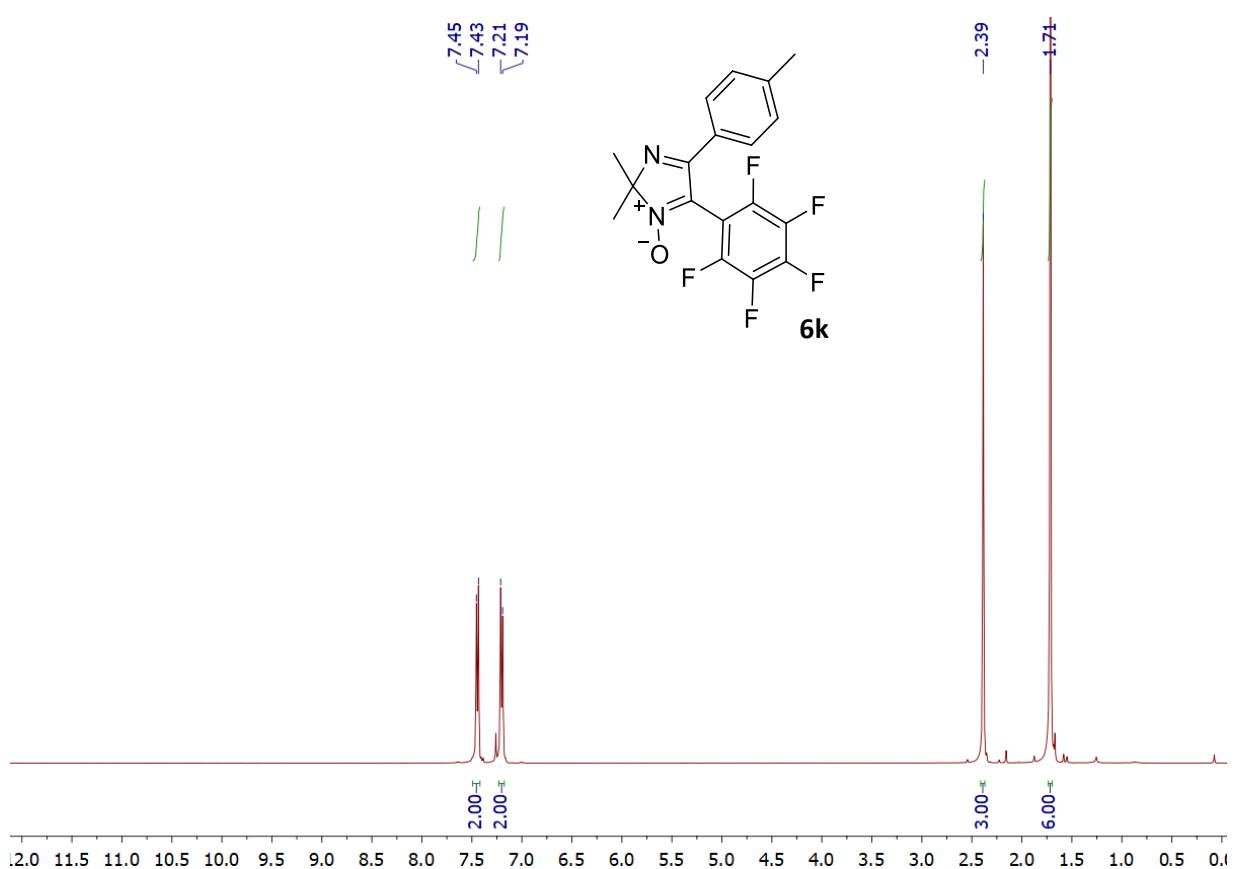
^{13}C { ^1H } NMR (101 MHz, DCCl_3)



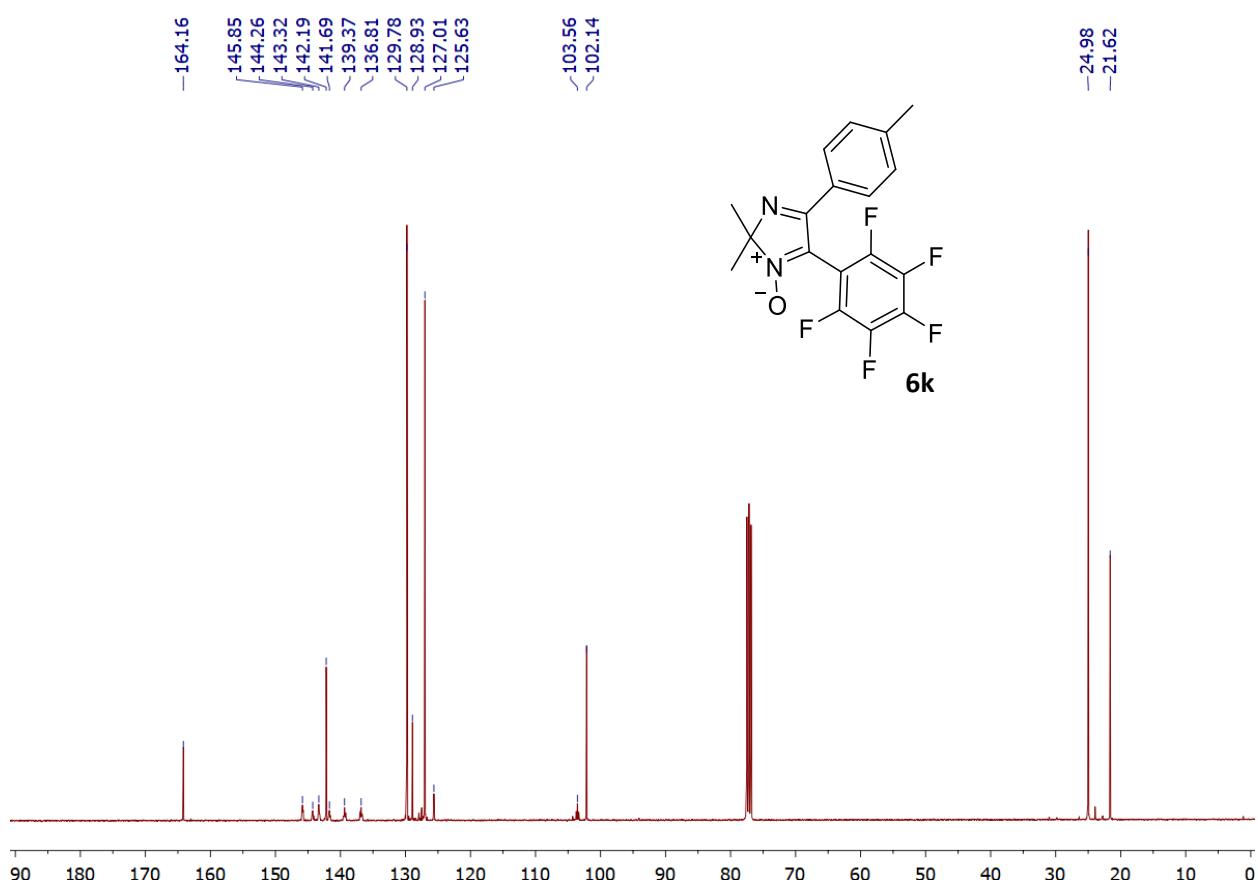
^{19}F NMR (376 MHz, DCCl_3)



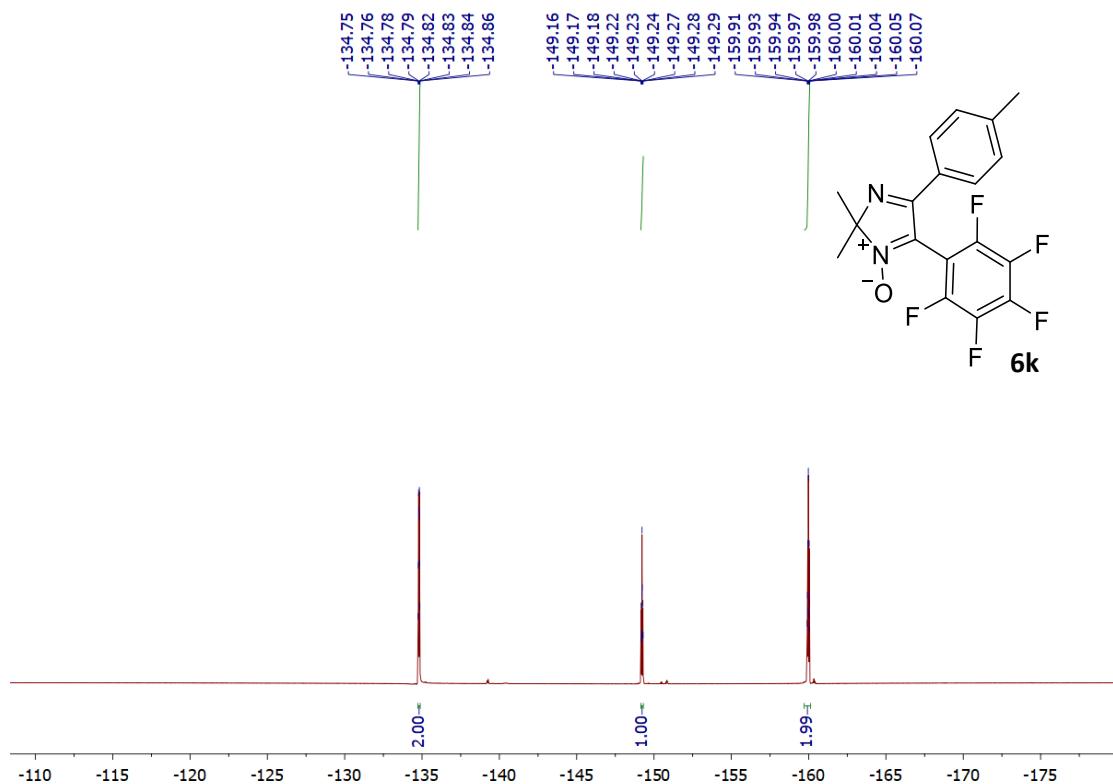
¹H NMR (400 MHz, DCCl₃)



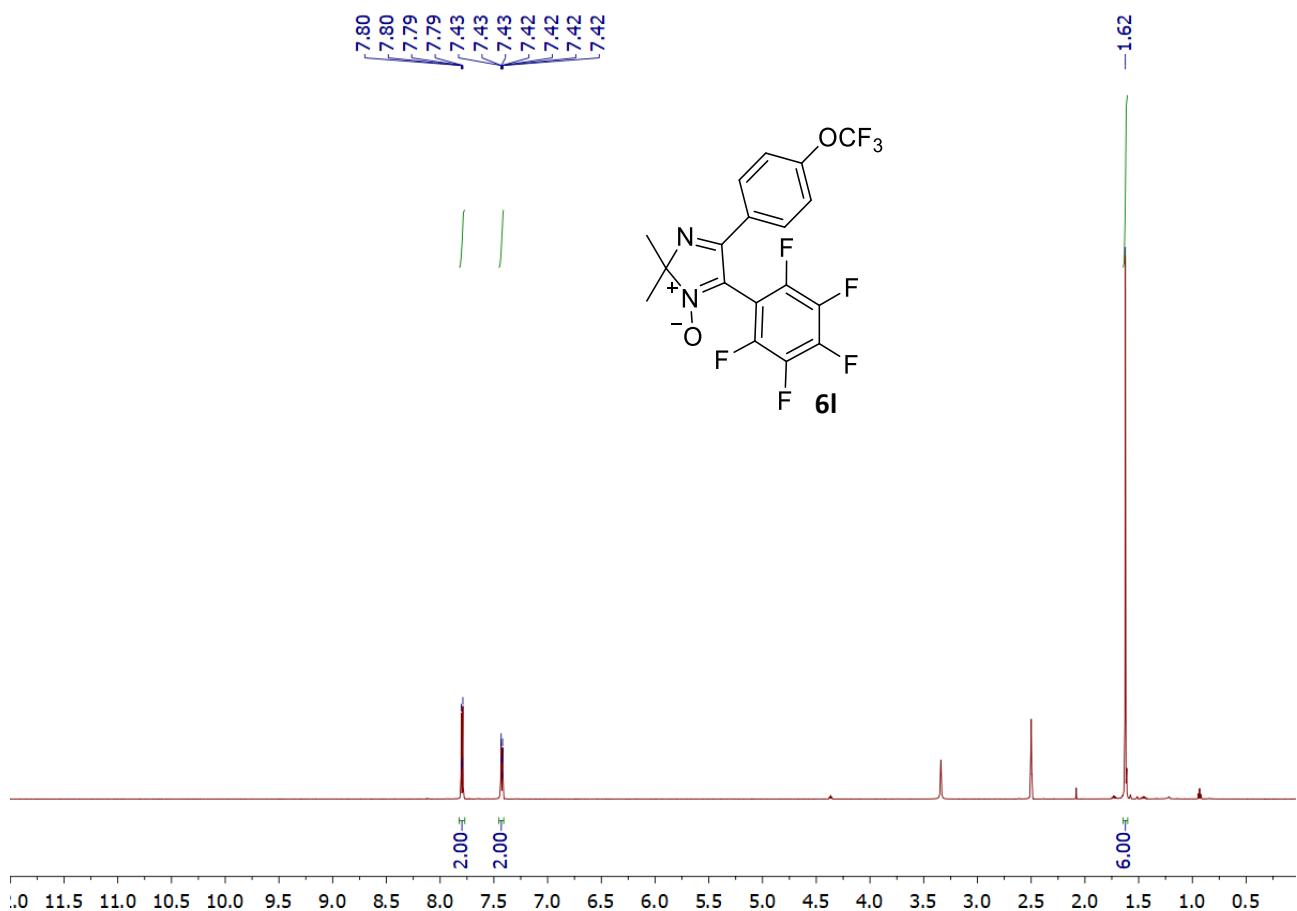
¹³C {¹H} NMR (101 MHz, DCCl₃)



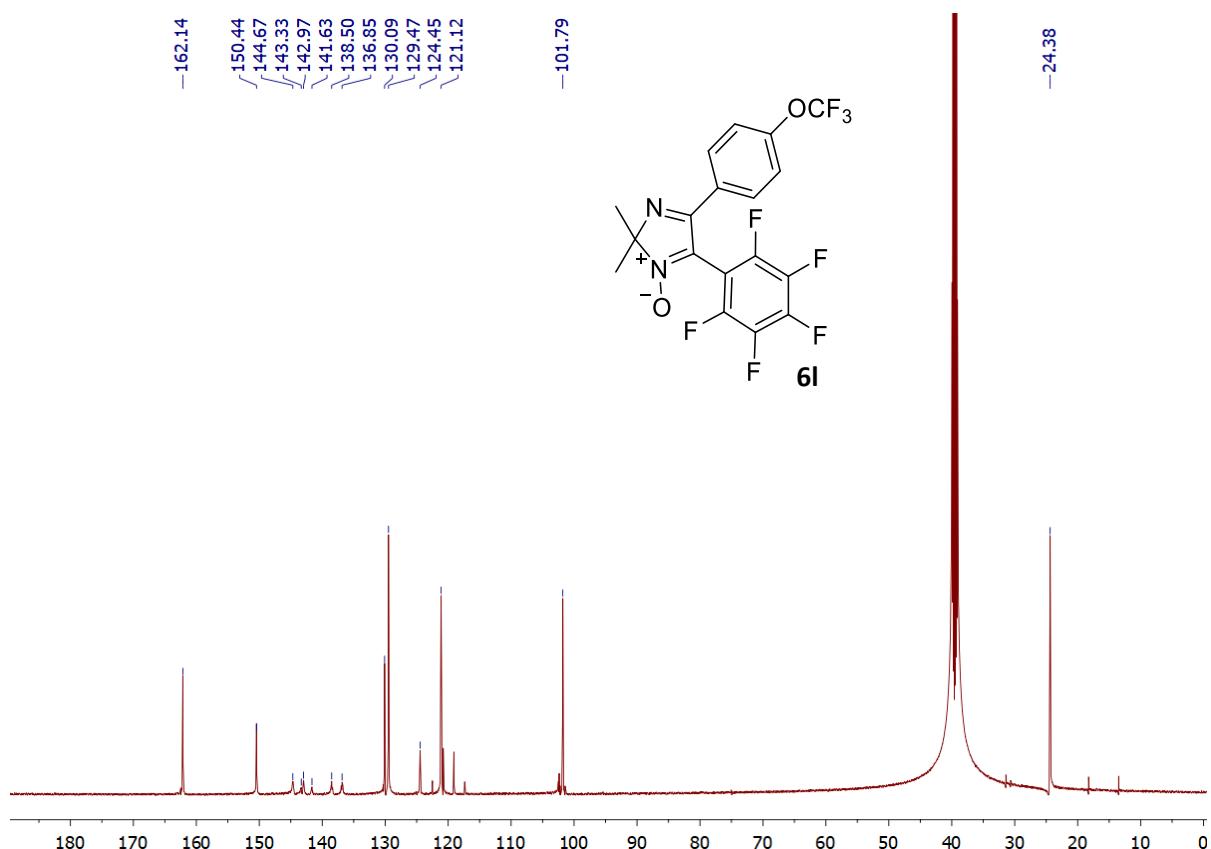
¹⁹F NMR (376 MHz, DCCl_3)



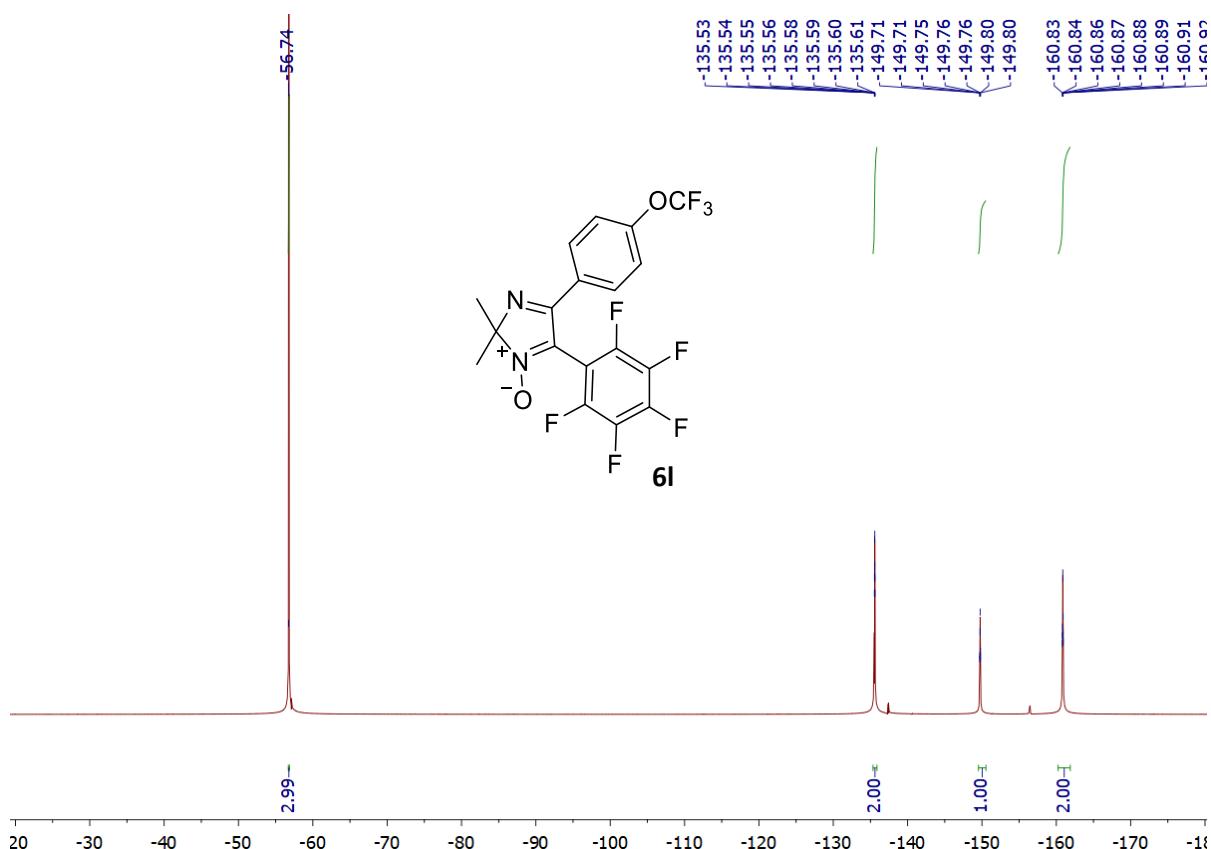
¹H NMR (400 MHz, DCCl_3)



^{13}C { ^1H } NMR (101 MHz, DCCl_3)



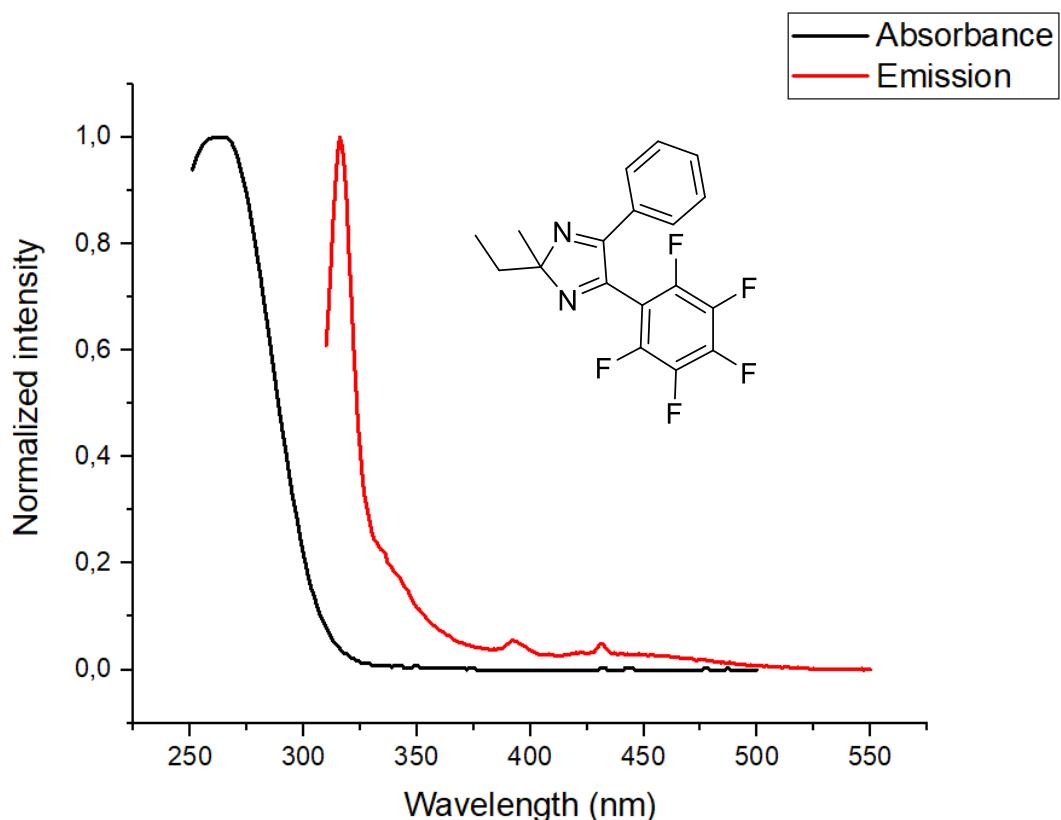
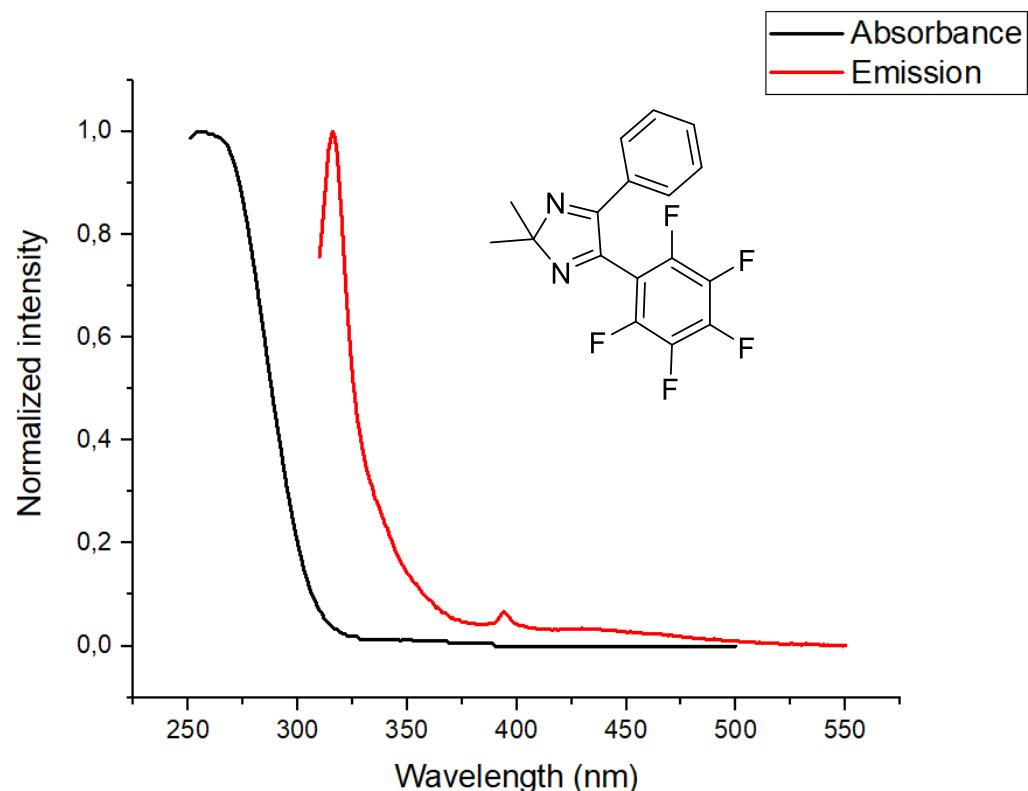
^{19}F NMR (376 MHz, DCCl_3)

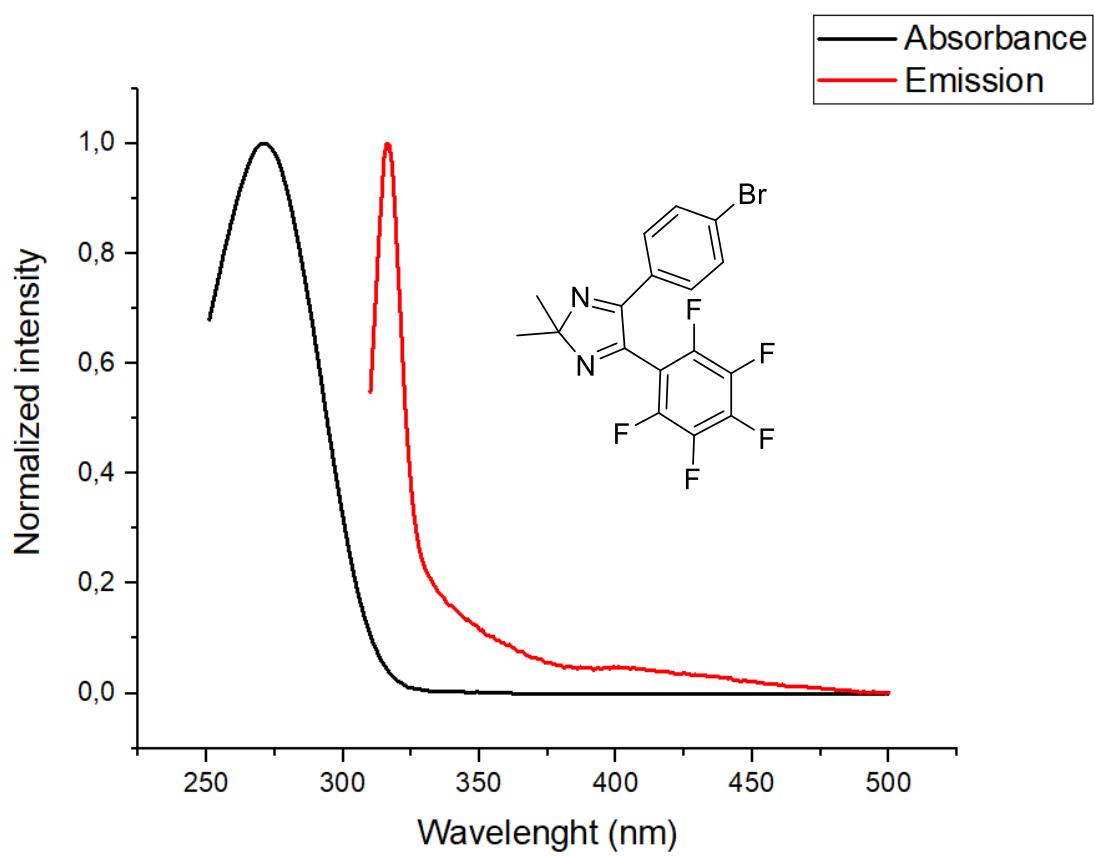
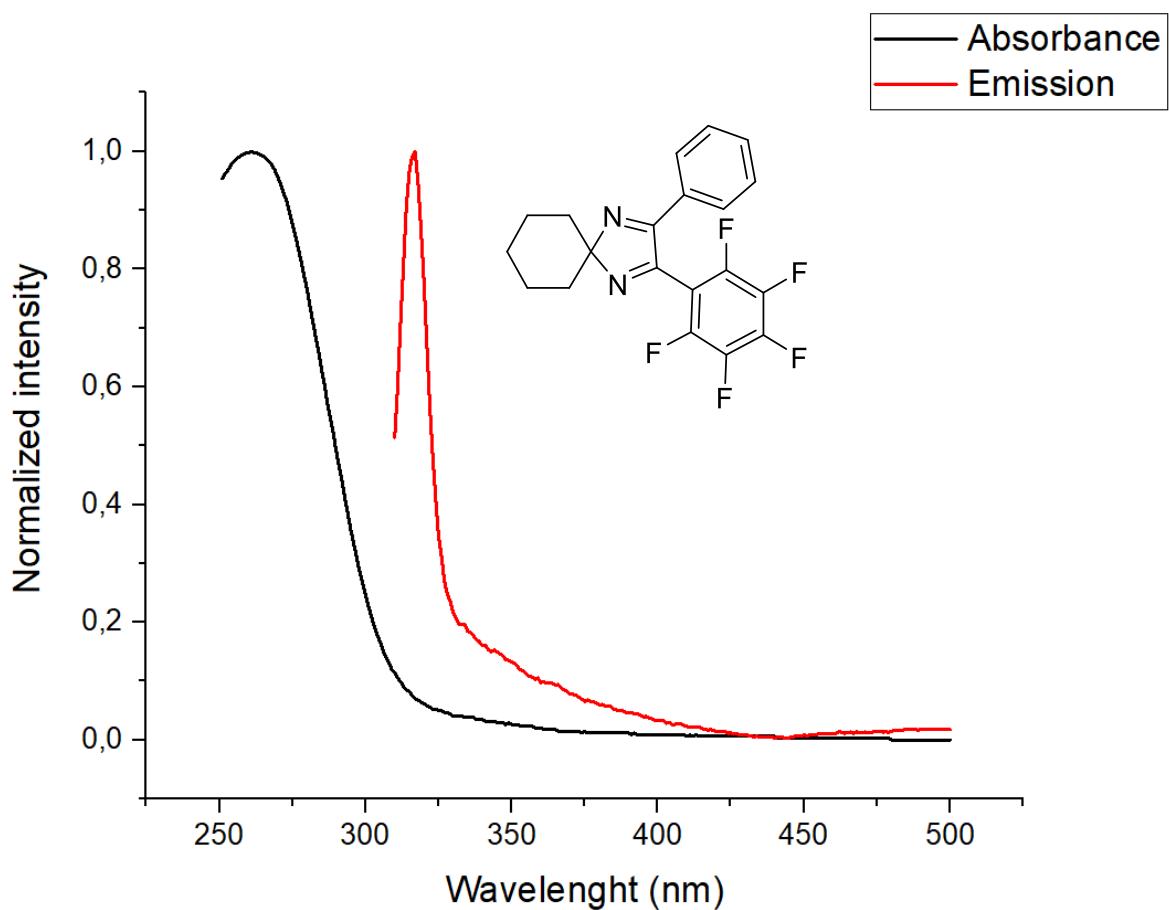


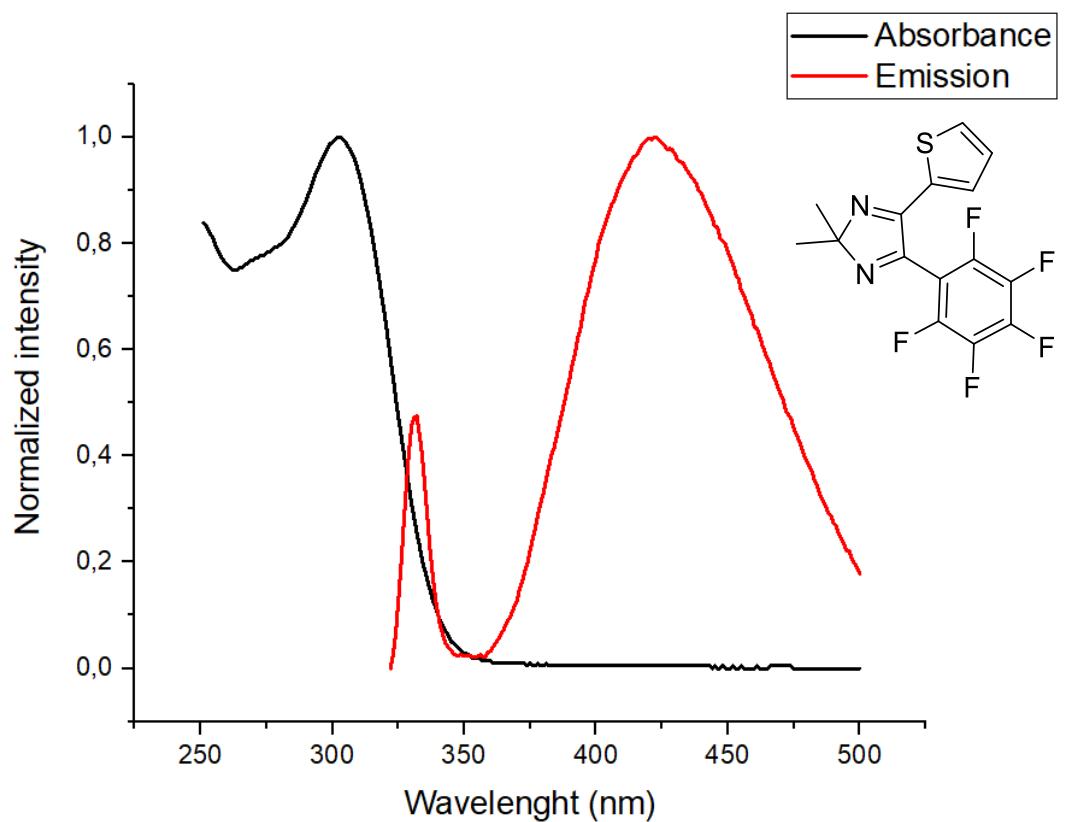
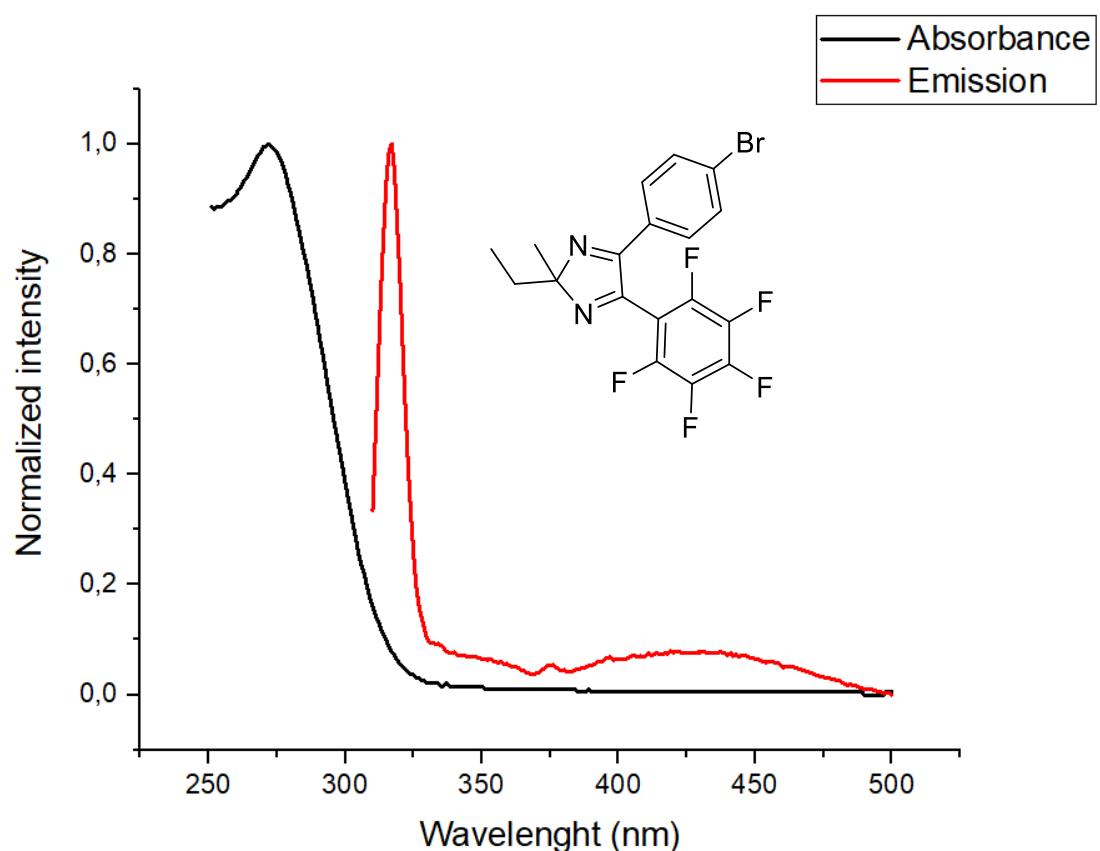
4. Photophysical studies

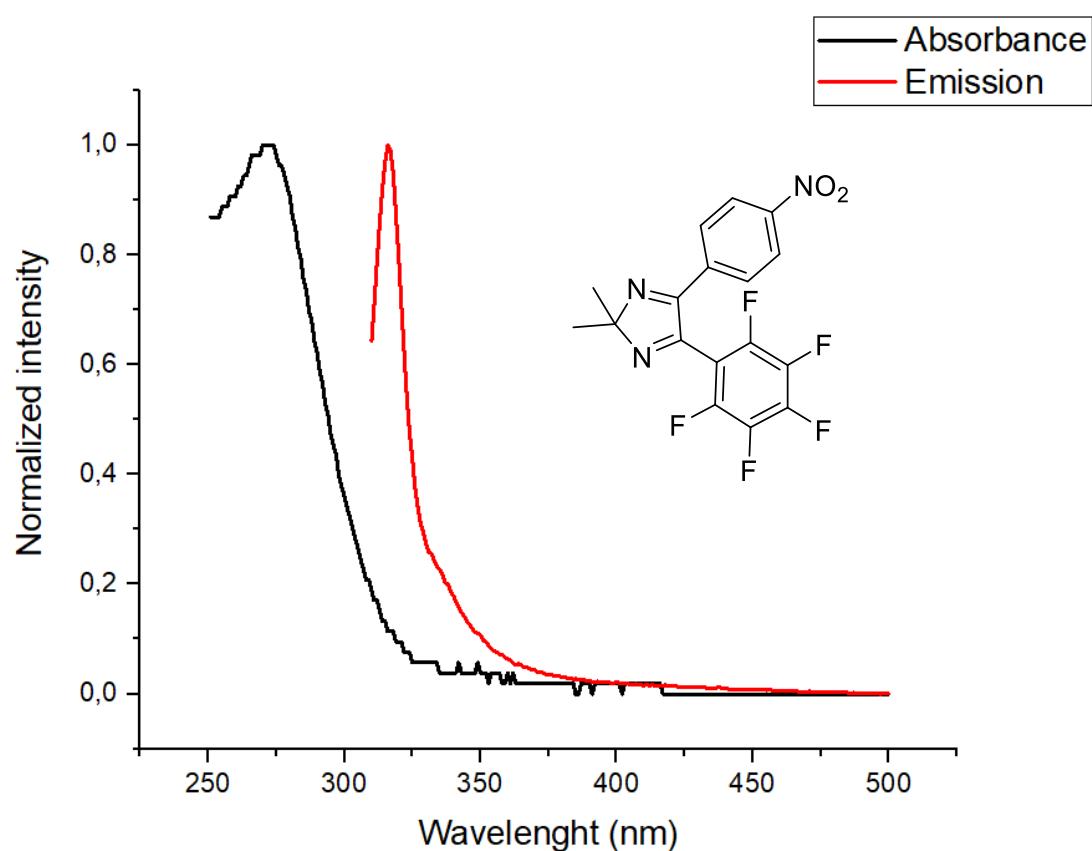
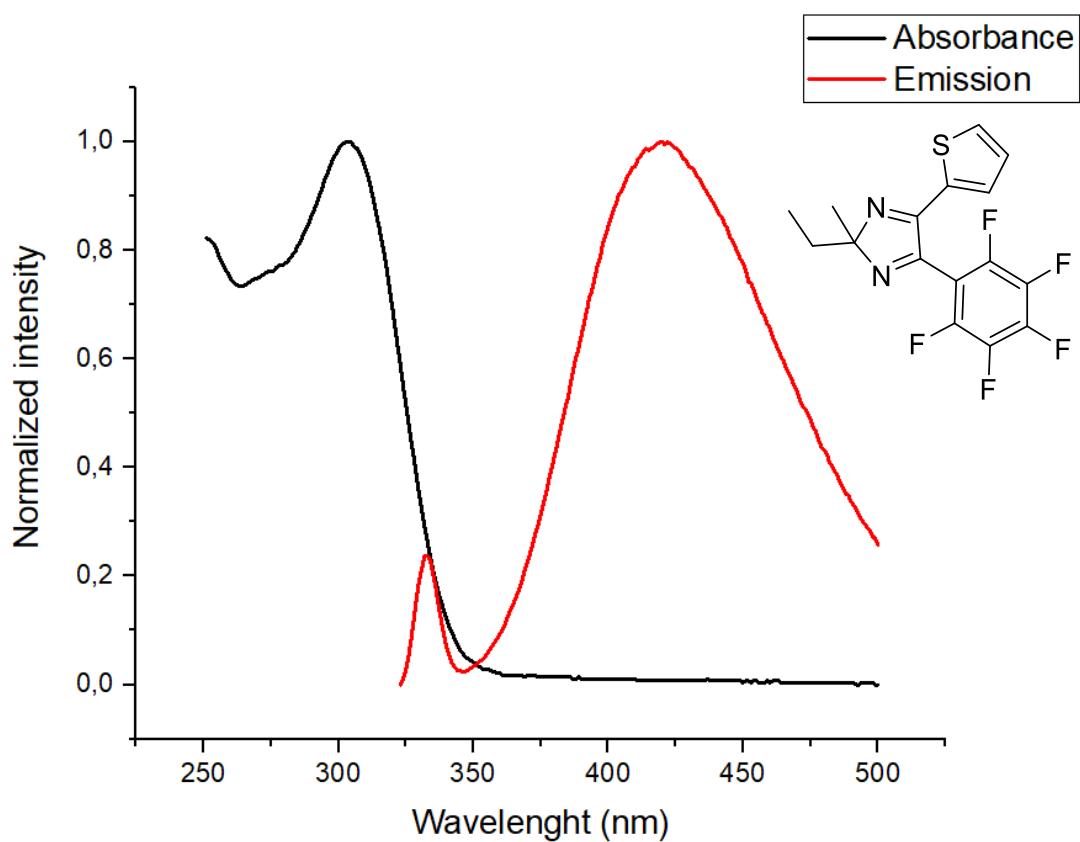
4.1. Spectra for 4-(perfluorophenyl)-substituted 2*H*-imidazole 5(a-l)

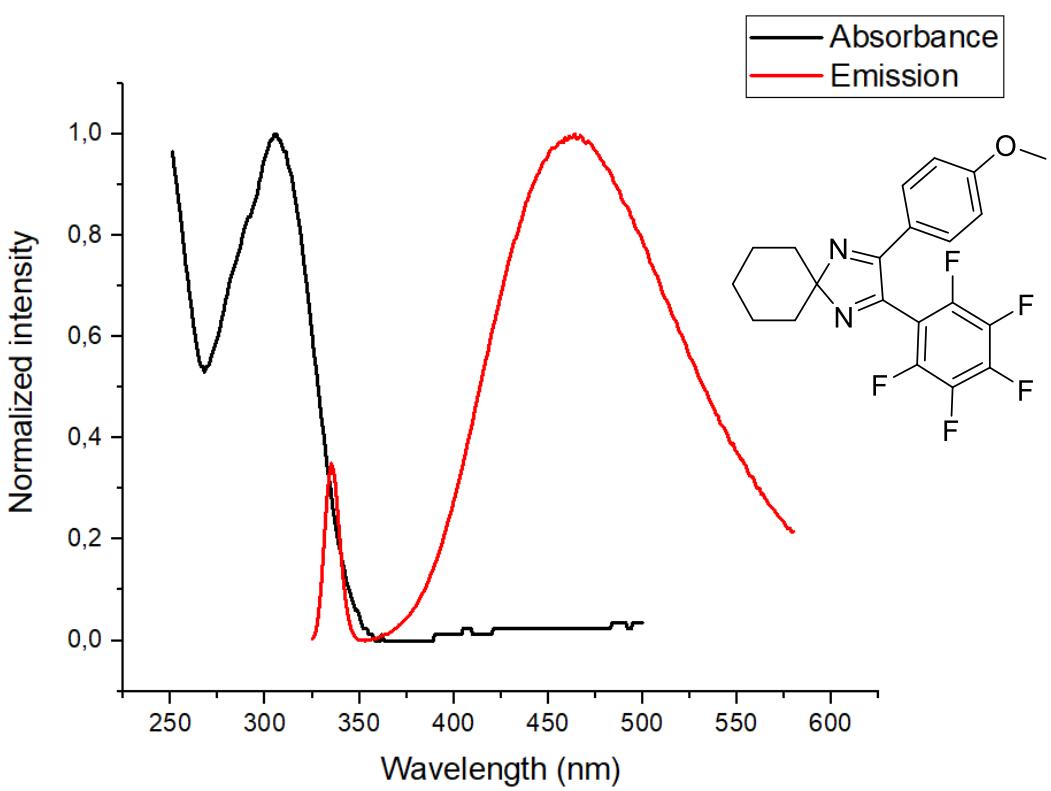
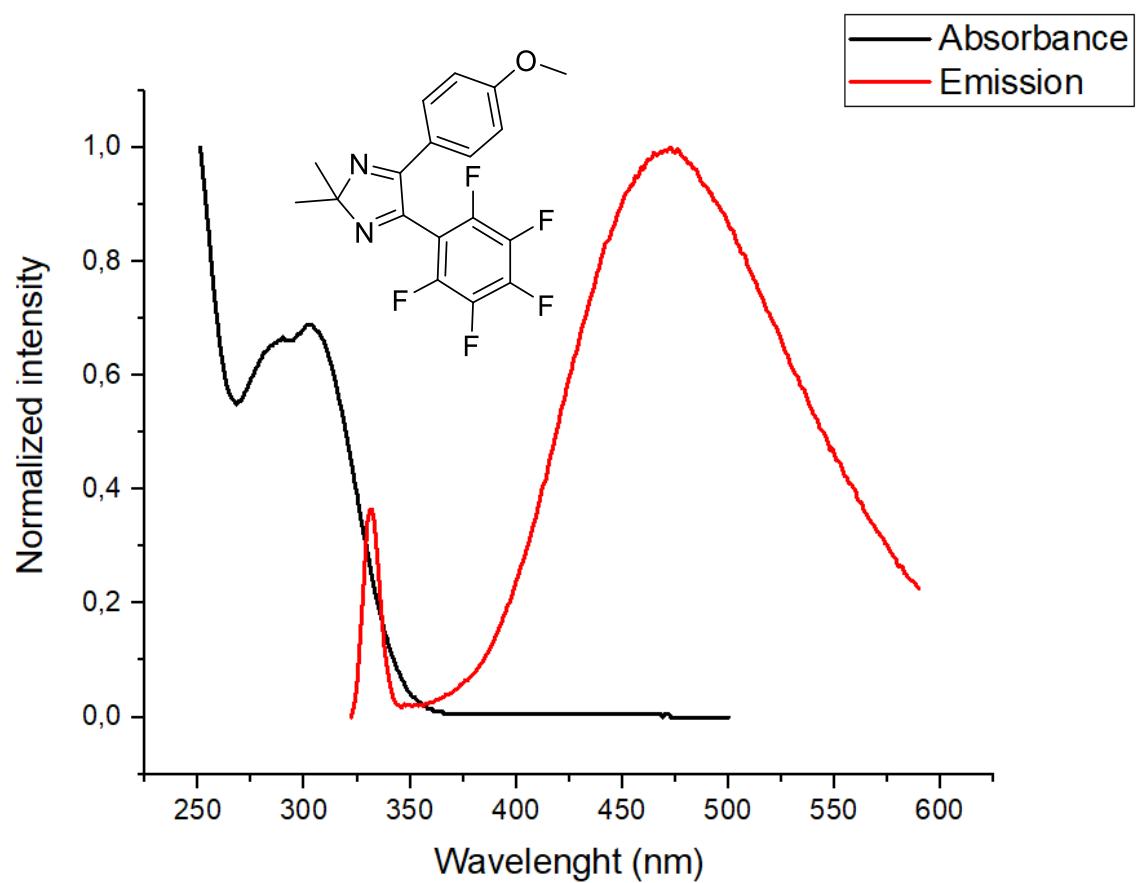
Absorbance and emission spectra were measured at concentrations approximately $C = 1 \times 10^{-5}$ M in MeOH

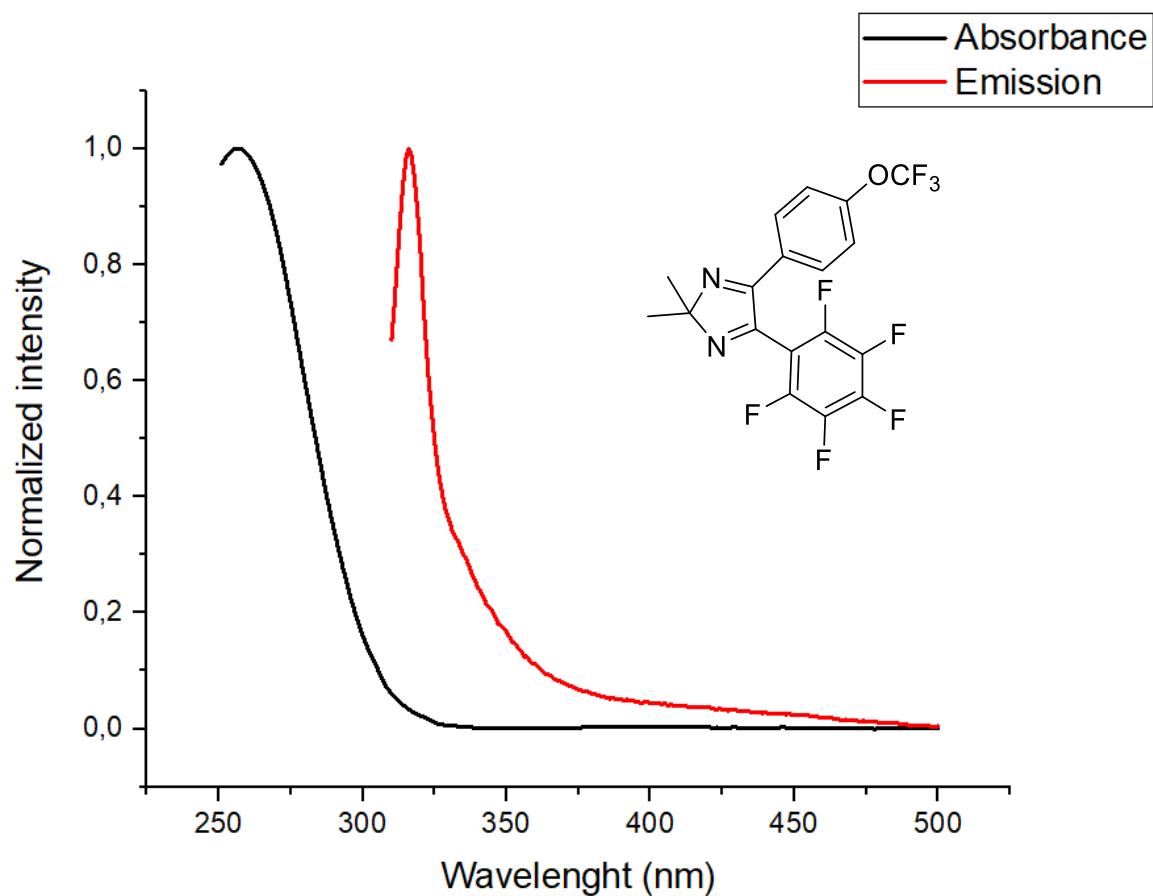
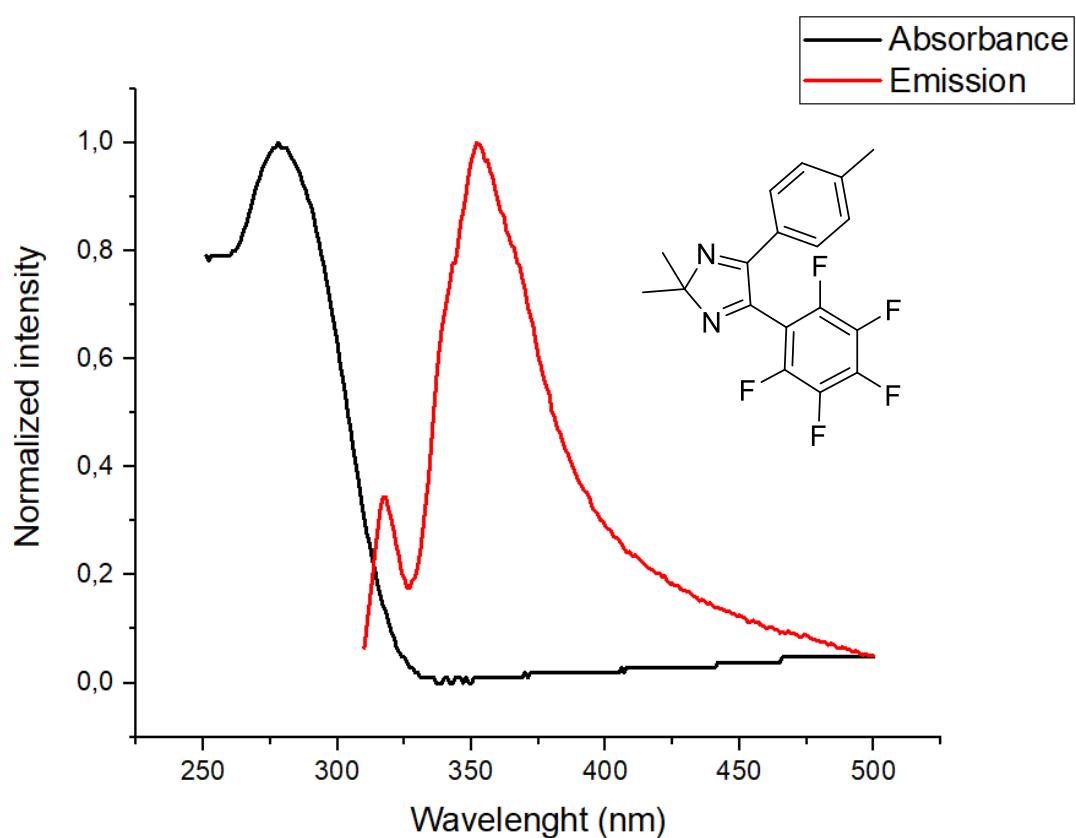




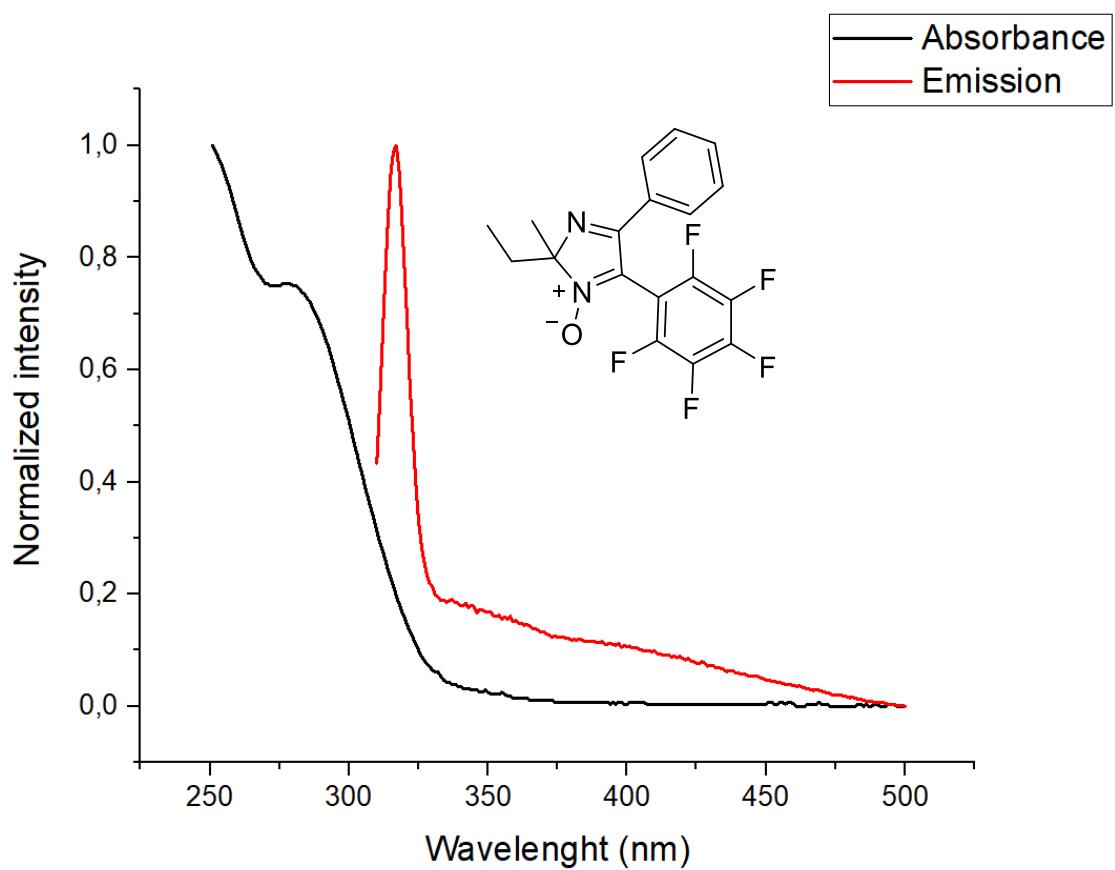
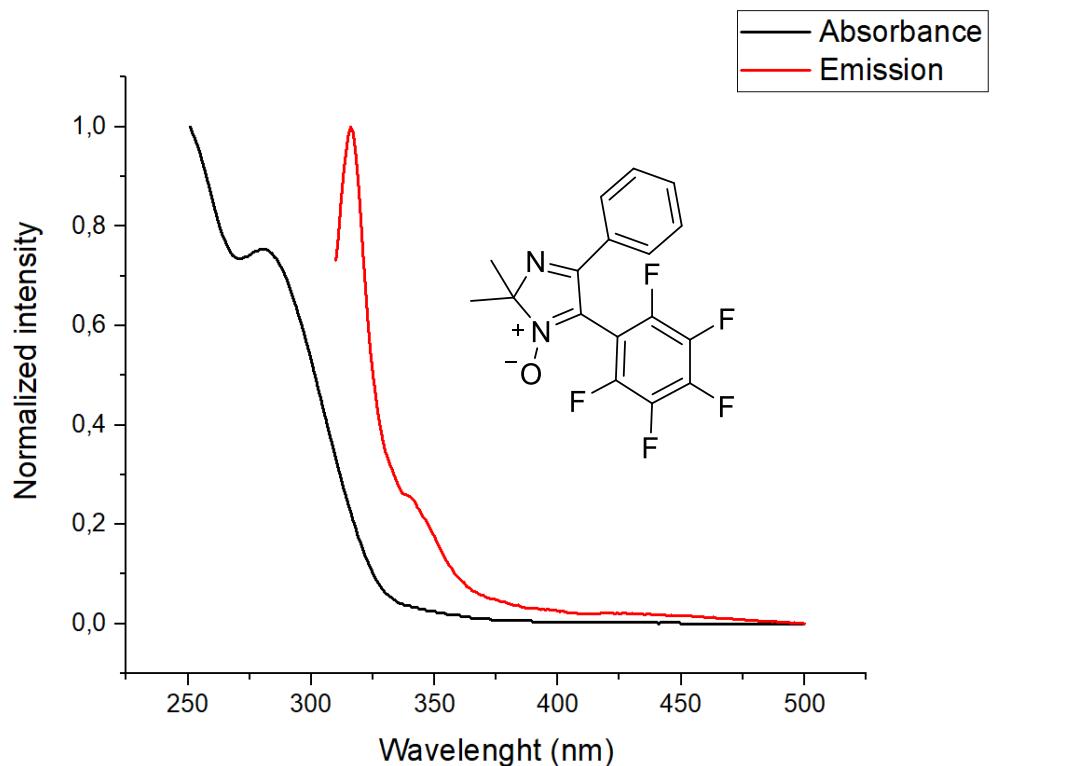


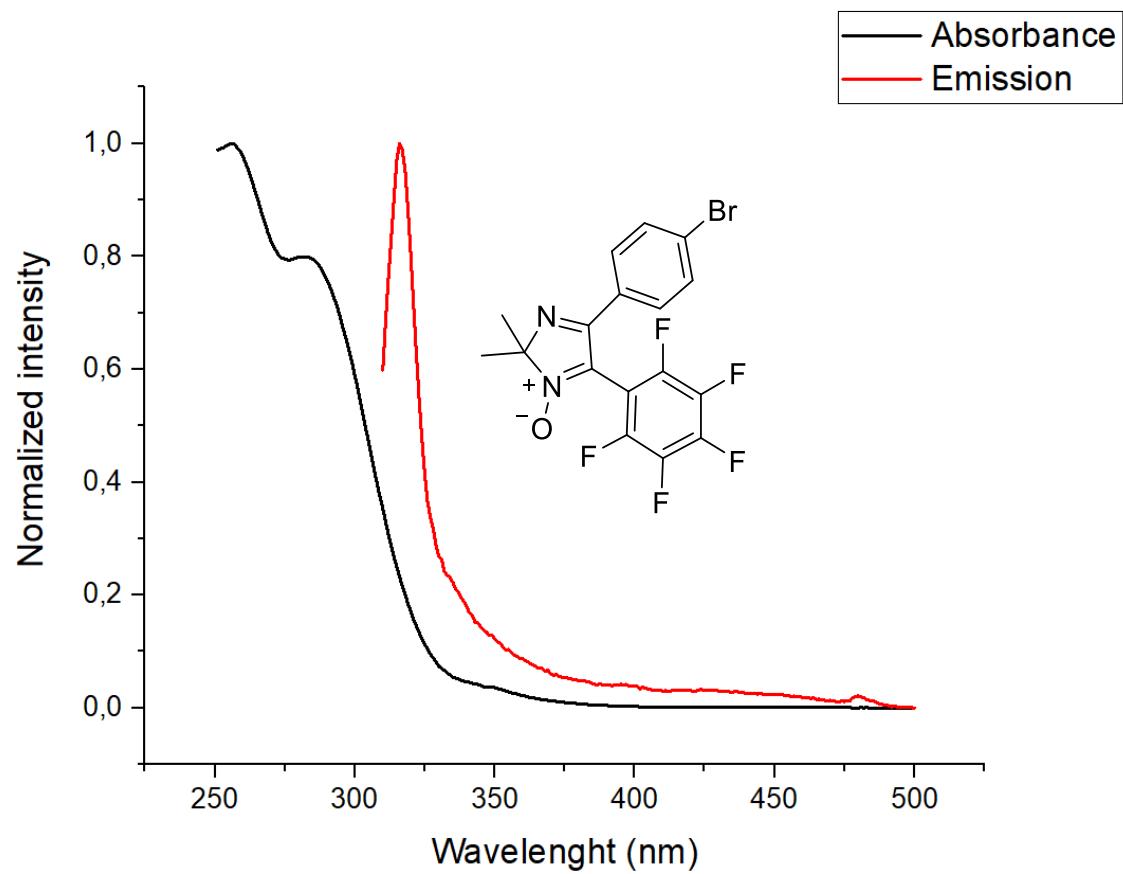
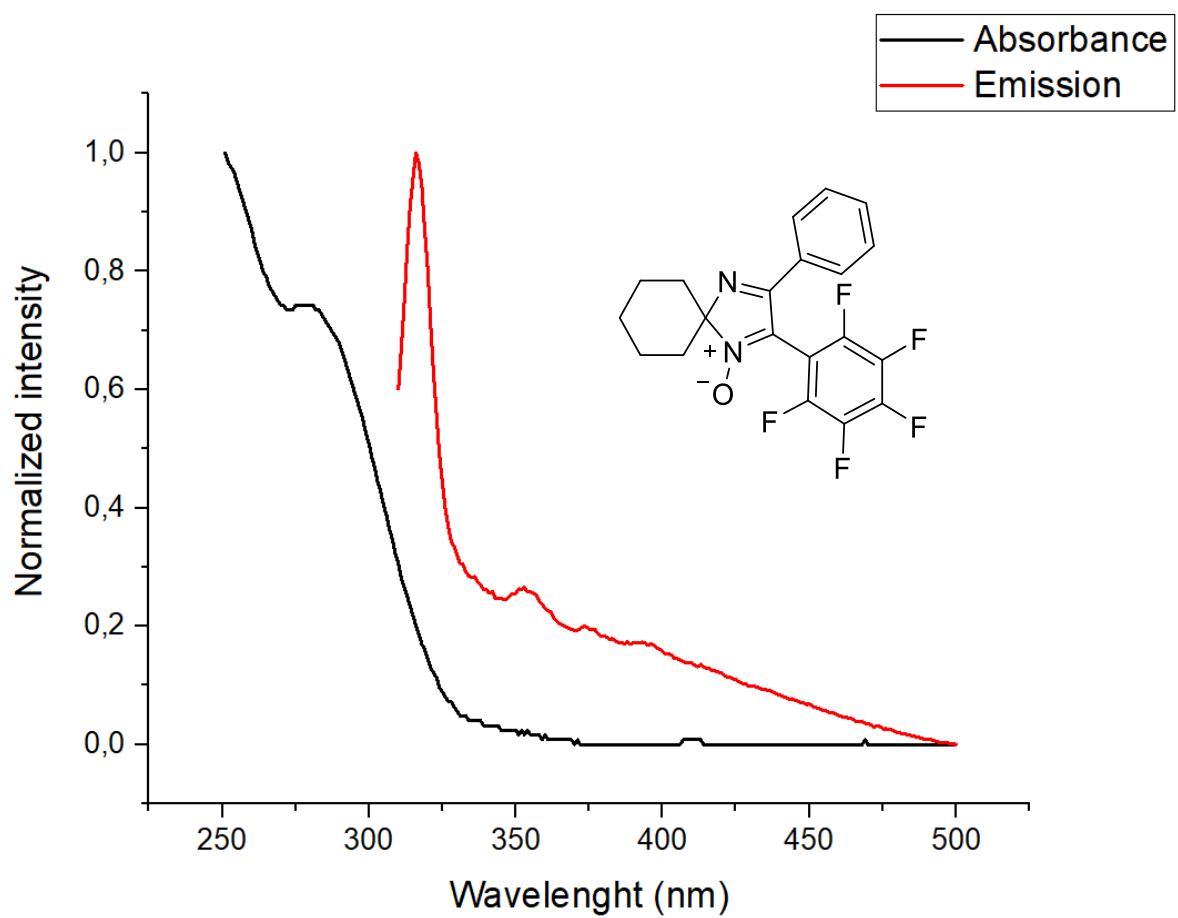


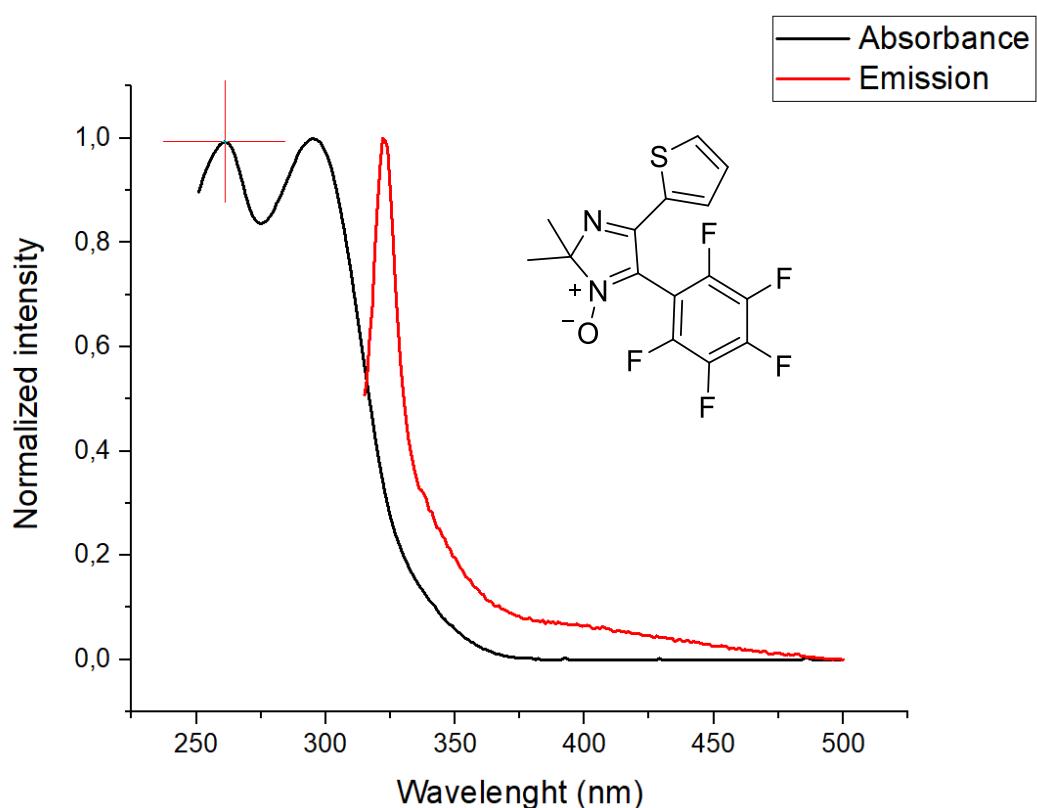
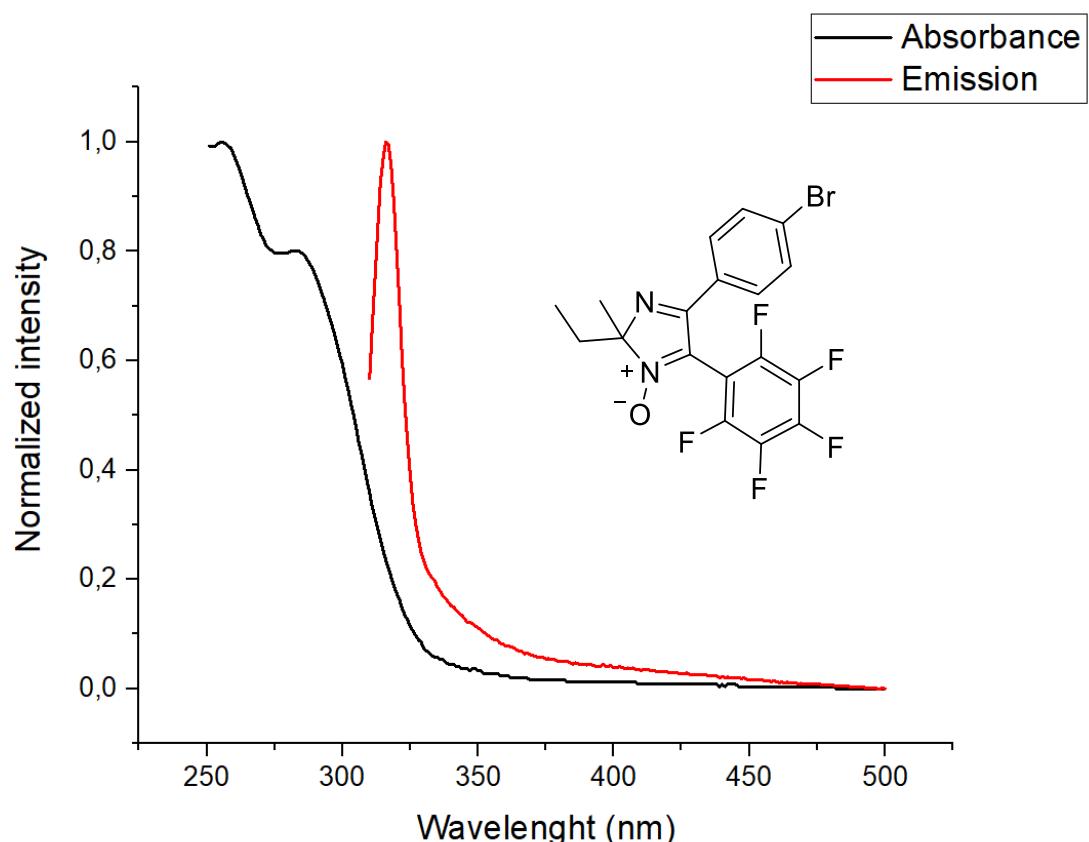


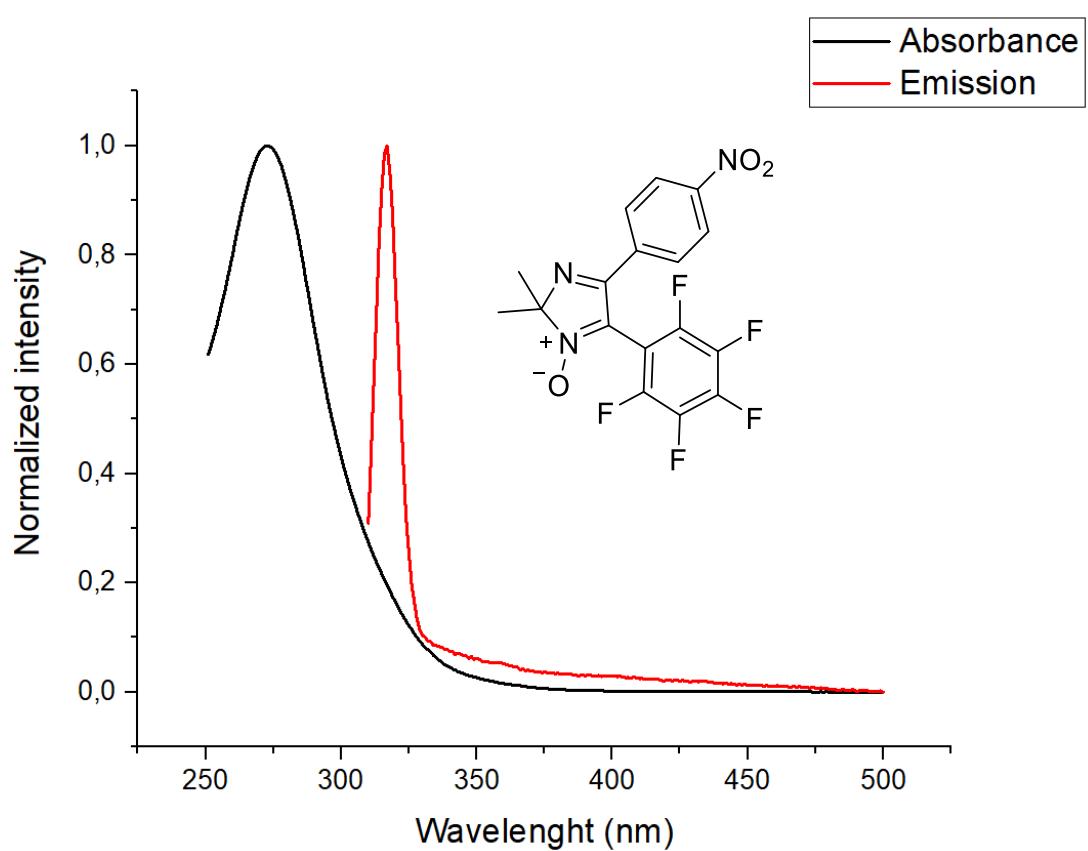
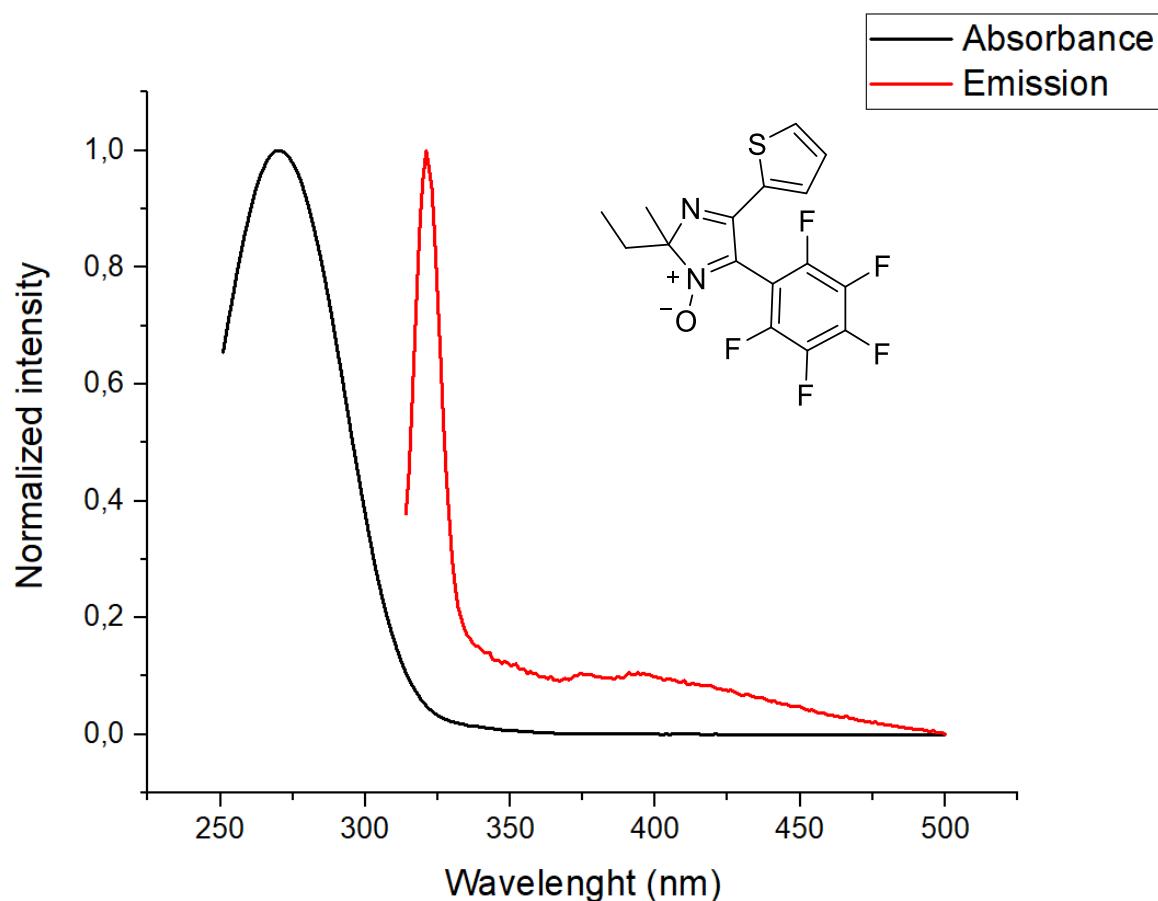


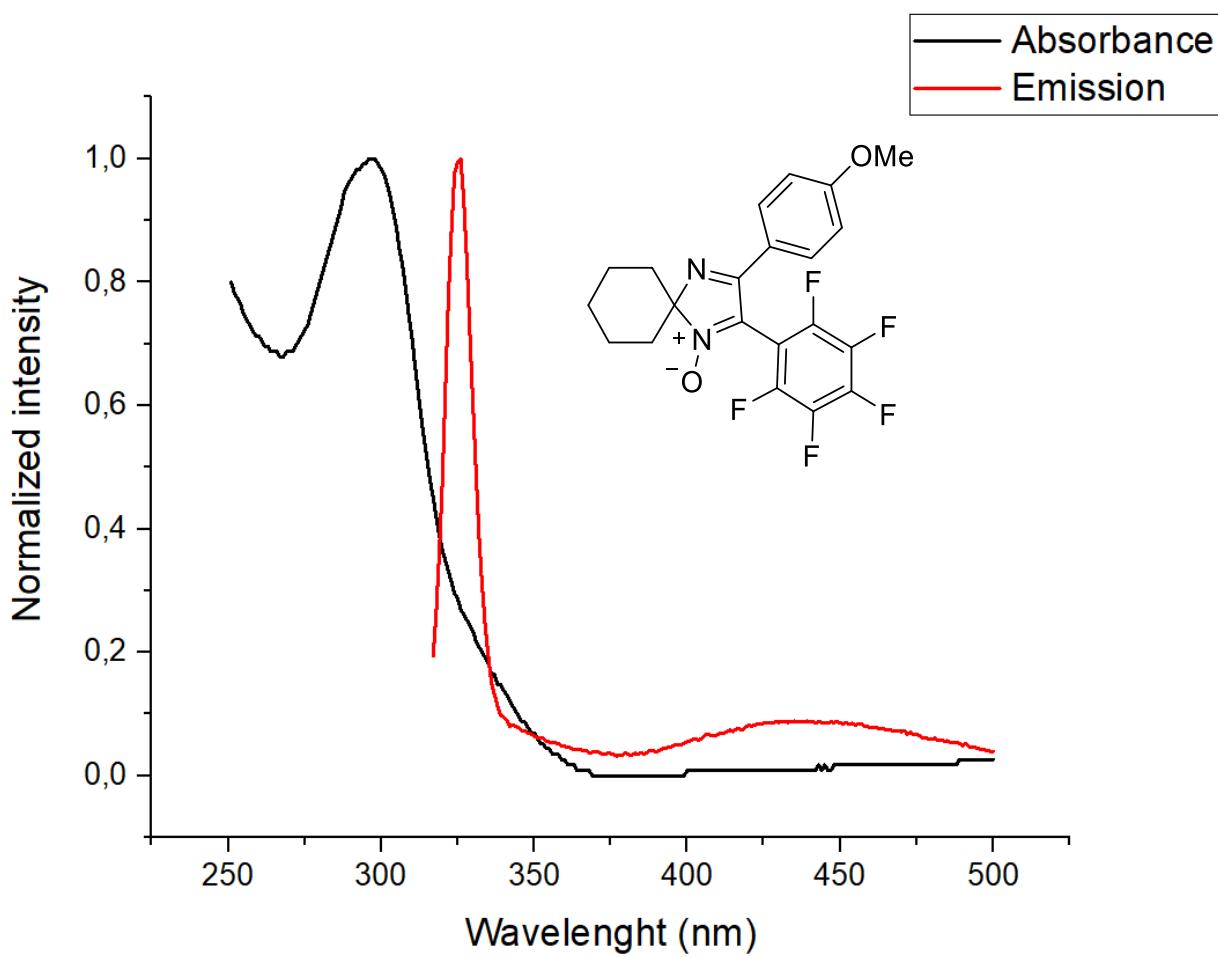
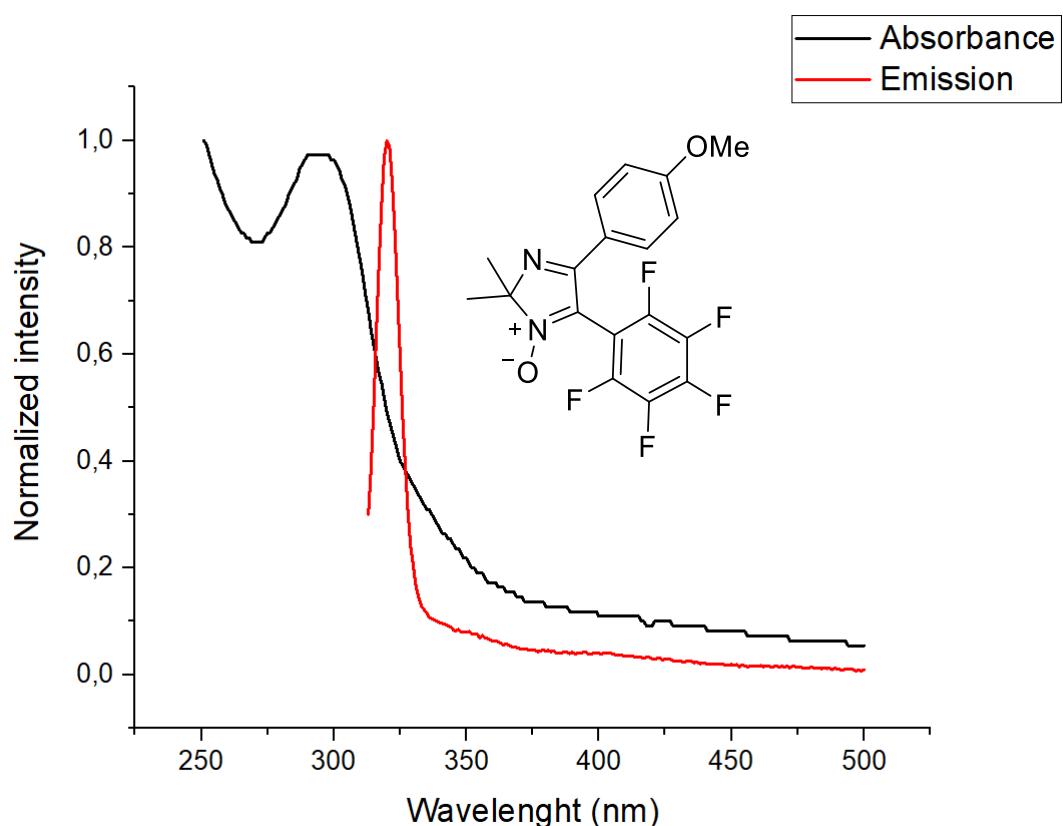
4.2. Spectra for 4-(perfluorophenyl)-substituted 2*H*-imidazole 1-oxides 6(a-l)

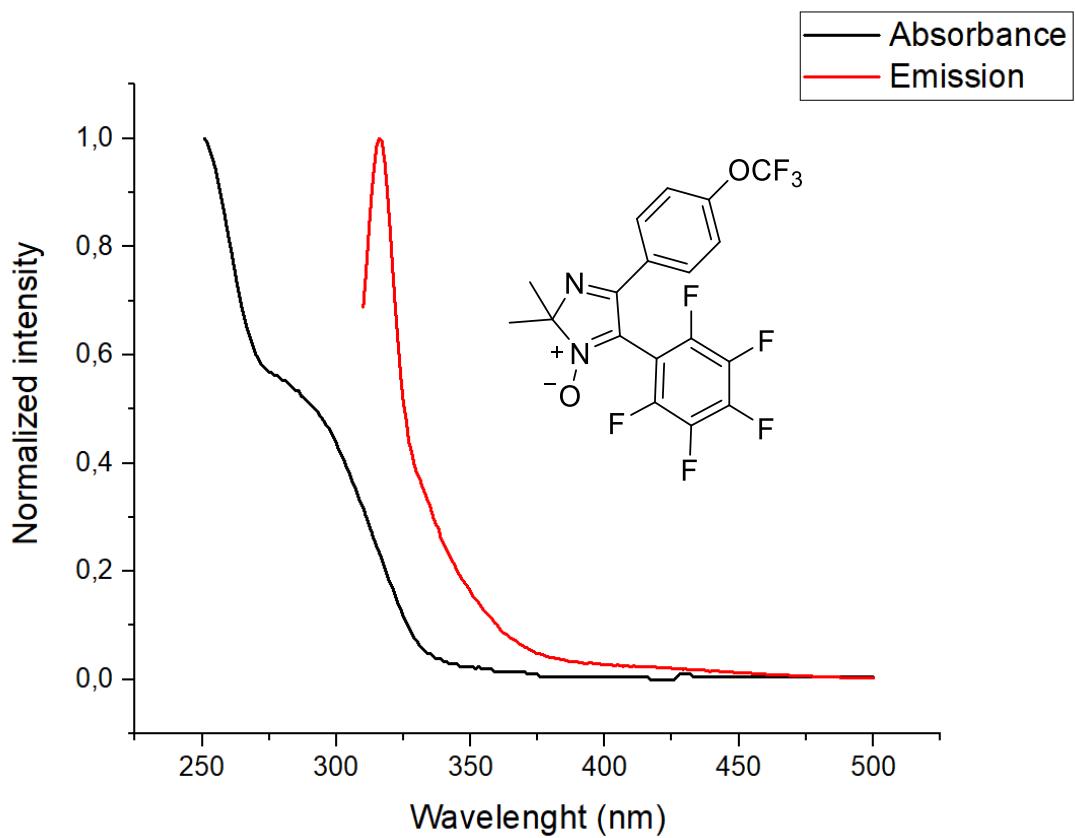
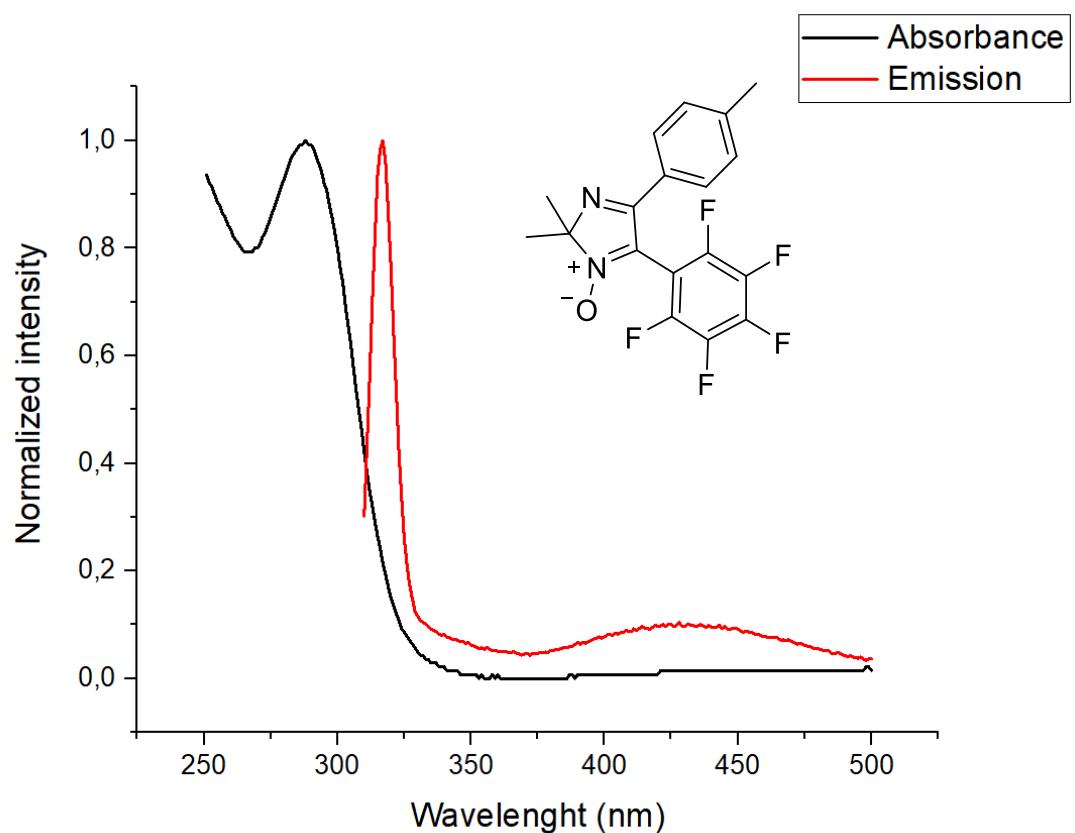






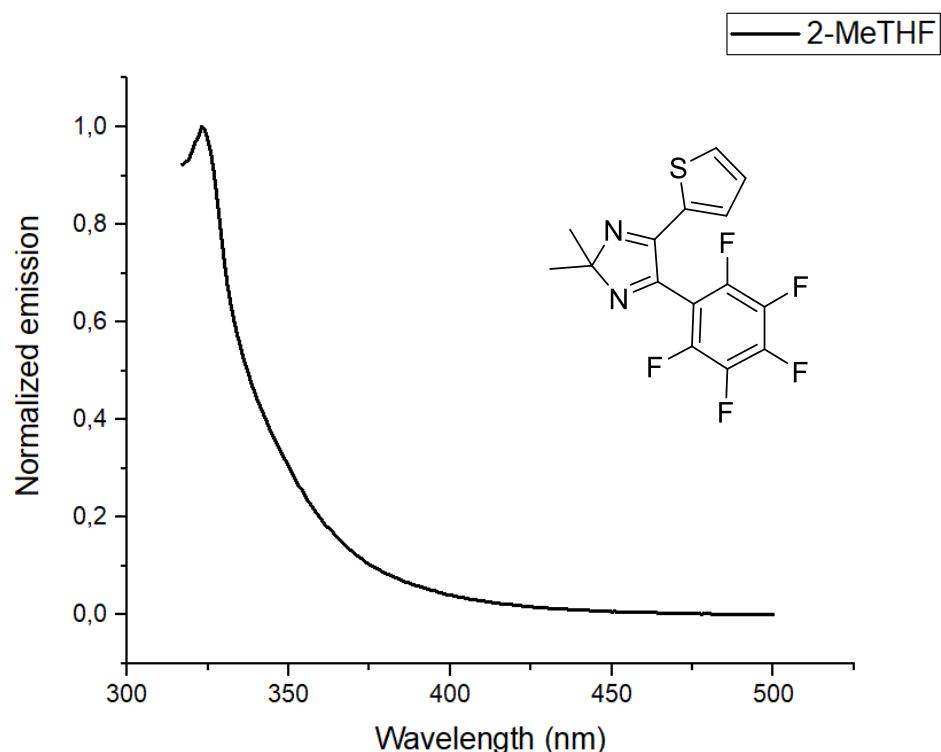




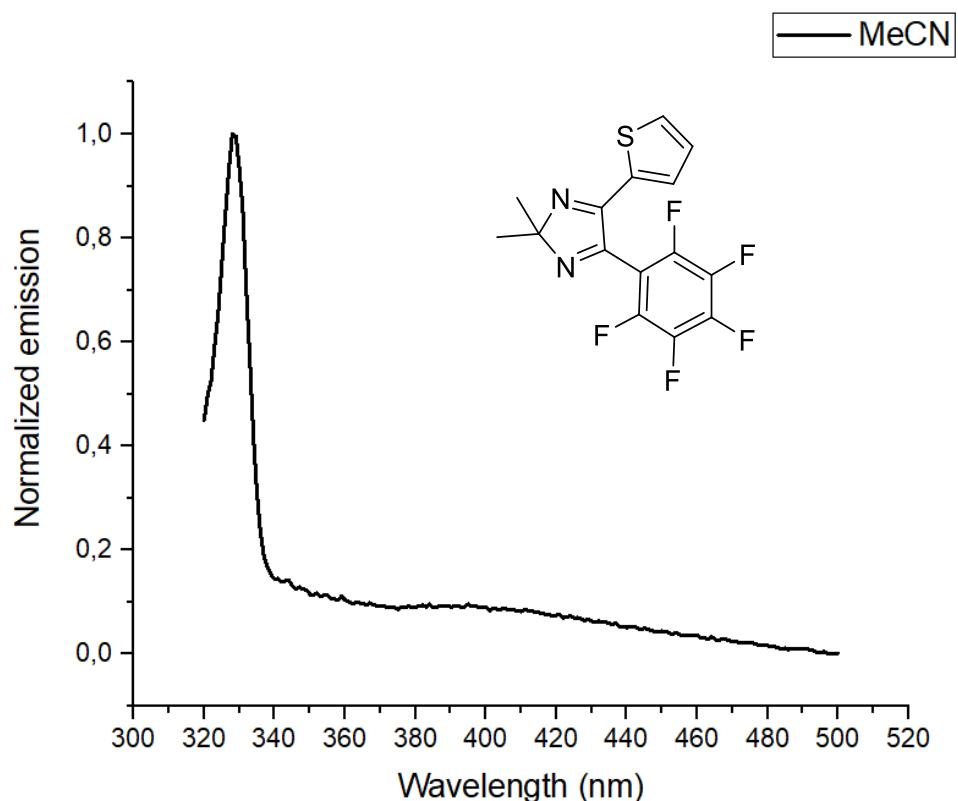


4.3. Solvent effect on emission for 4-(perfluorophenyl)-substituted 2*H*-imidazole **5f**

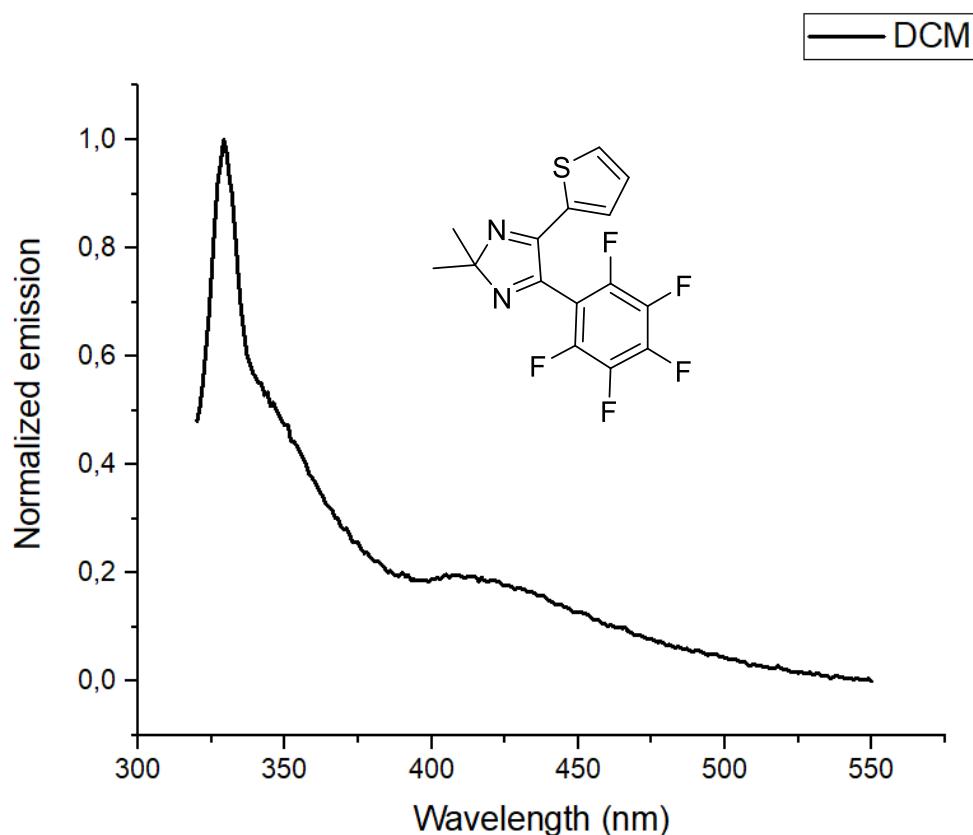
All spectra were measured at approximately compound concentrations C=1* 10-5 M in corresponding solvent



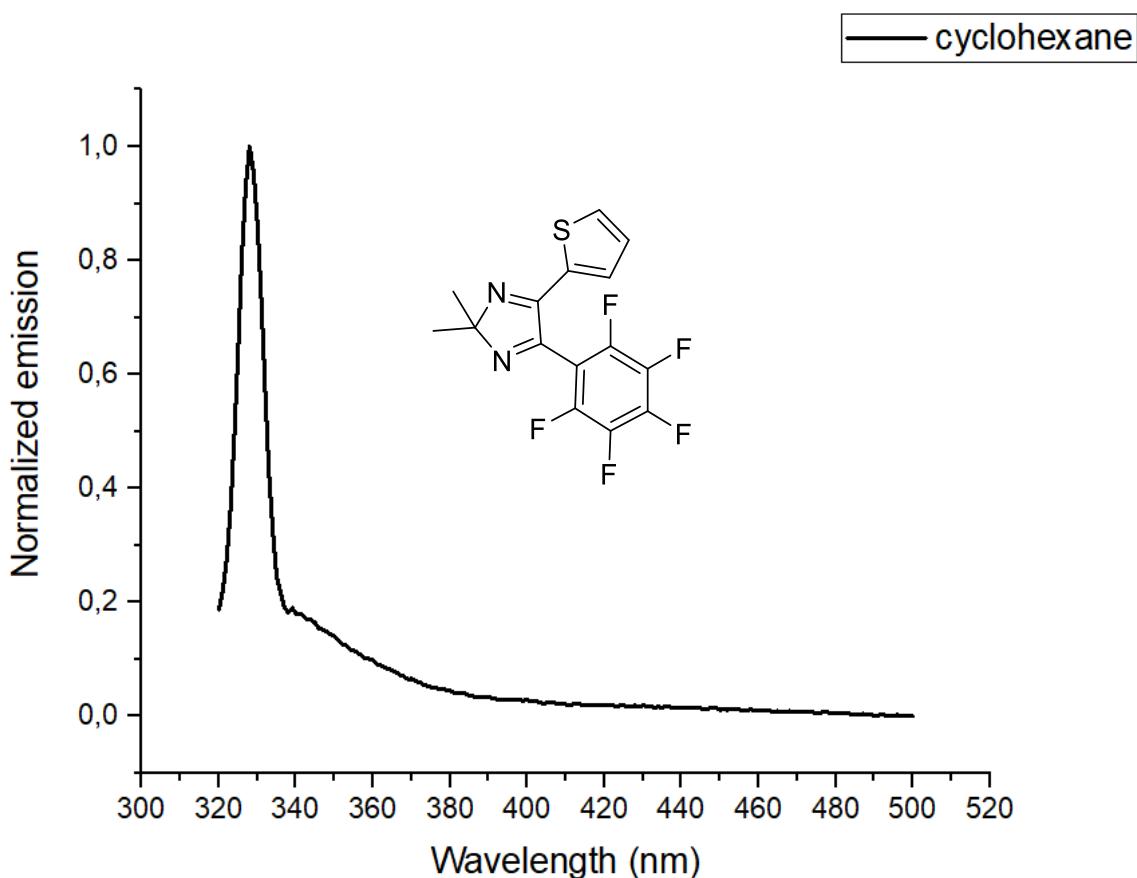
Emission spectra for **5f** in 2-MeTHF ($\lambda_{\text{ex}} = 297 \text{ nm}$)



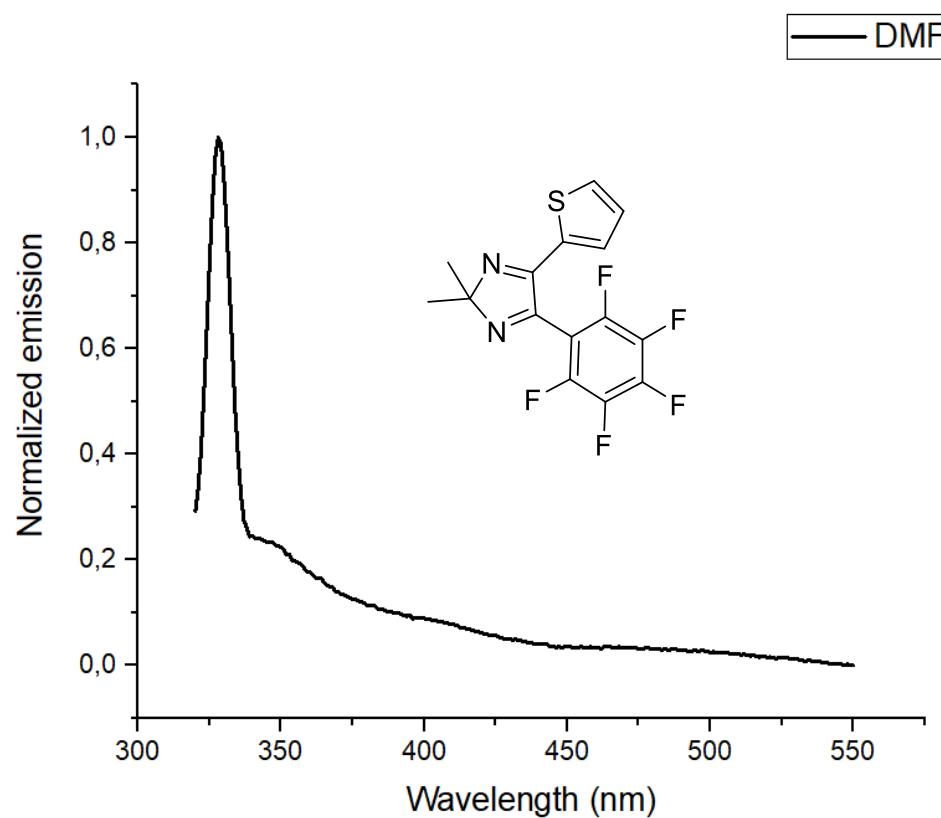
Emission spectra for **5f** in MeCN ($\lambda_{\text{ex}} = 300 \text{ nm}$)



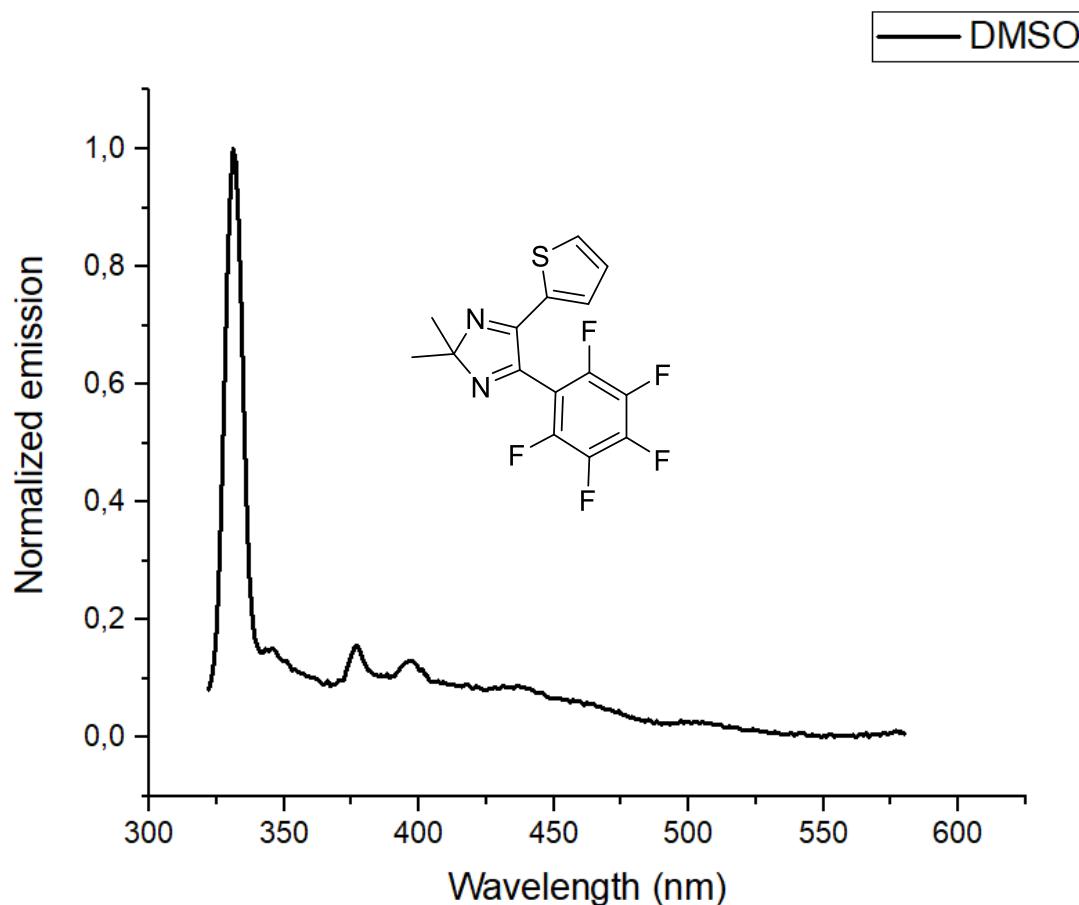
Emission spectra for **5f** in DCM ($\lambda_{\text{ex}} = 300 \text{ nm}$)



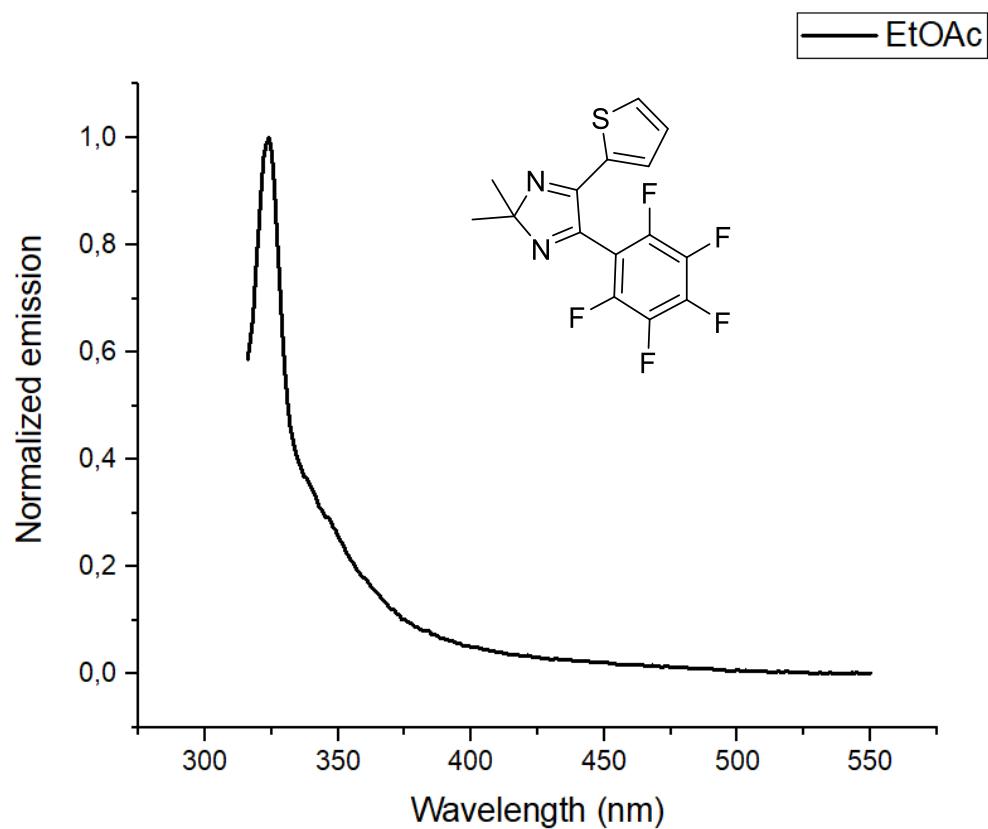
Emission spectra for **5f** in cyclohexane ($\lambda_{\text{ex}} = 300 \text{ nm}$)



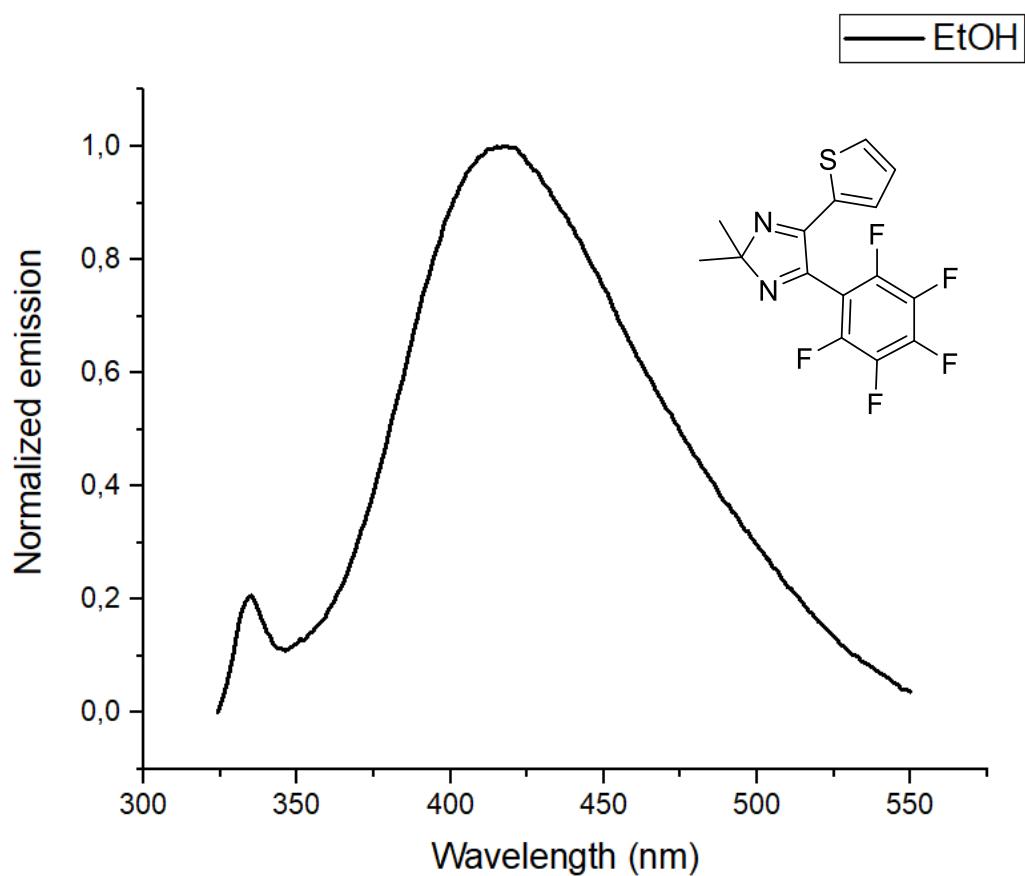
Emission spectra for **5f** in DMF ($\lambda_{\text{ex}} = 300 \text{ nm}$)



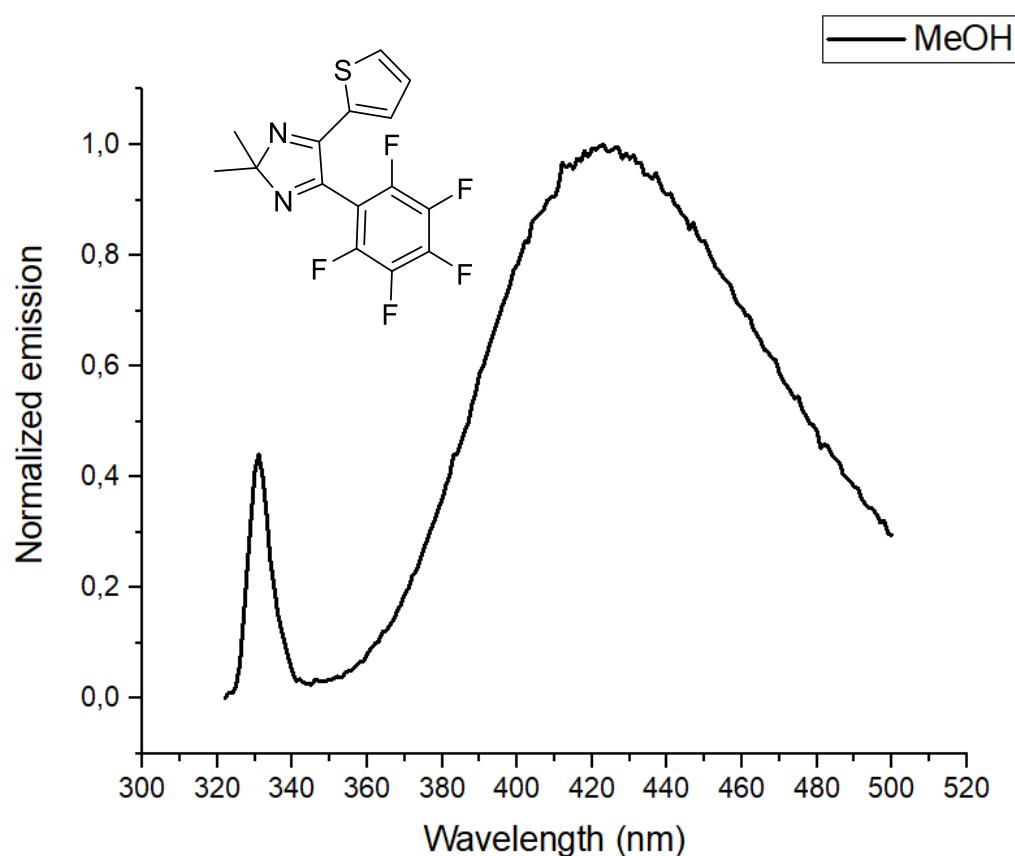
Emission spectra for **5f** in DMSO ($\lambda_{\text{ex}} = 302 \text{ nm}$)



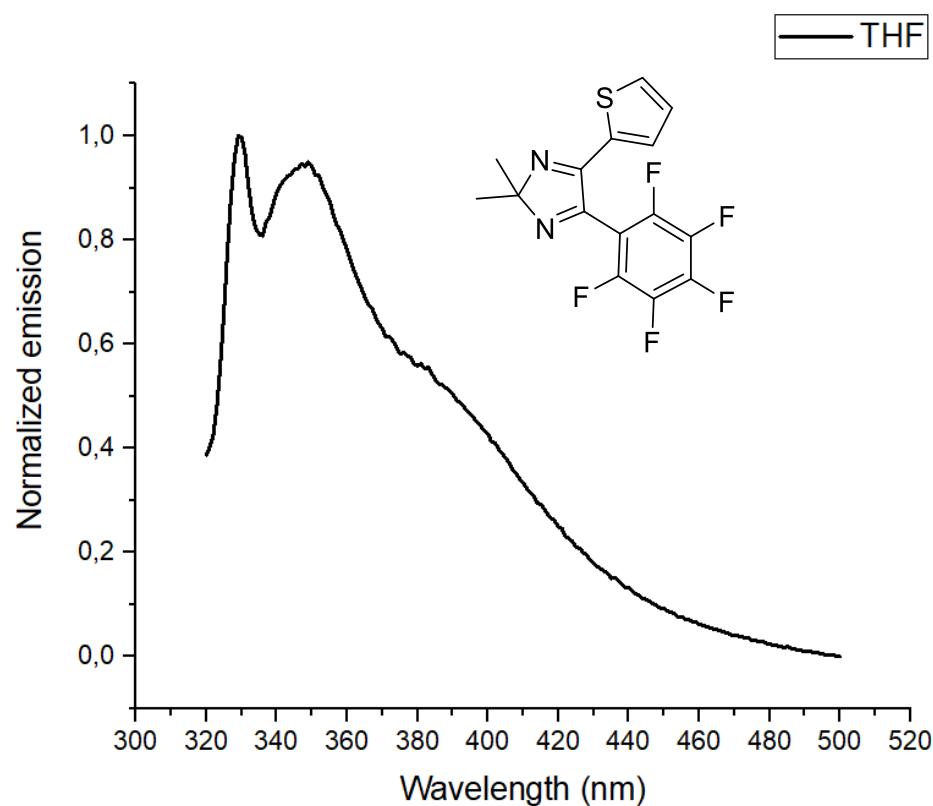
Emission spectra for **5f** in EtOAc ($\lambda_{\text{ex}} = 296 \text{ nm}$)



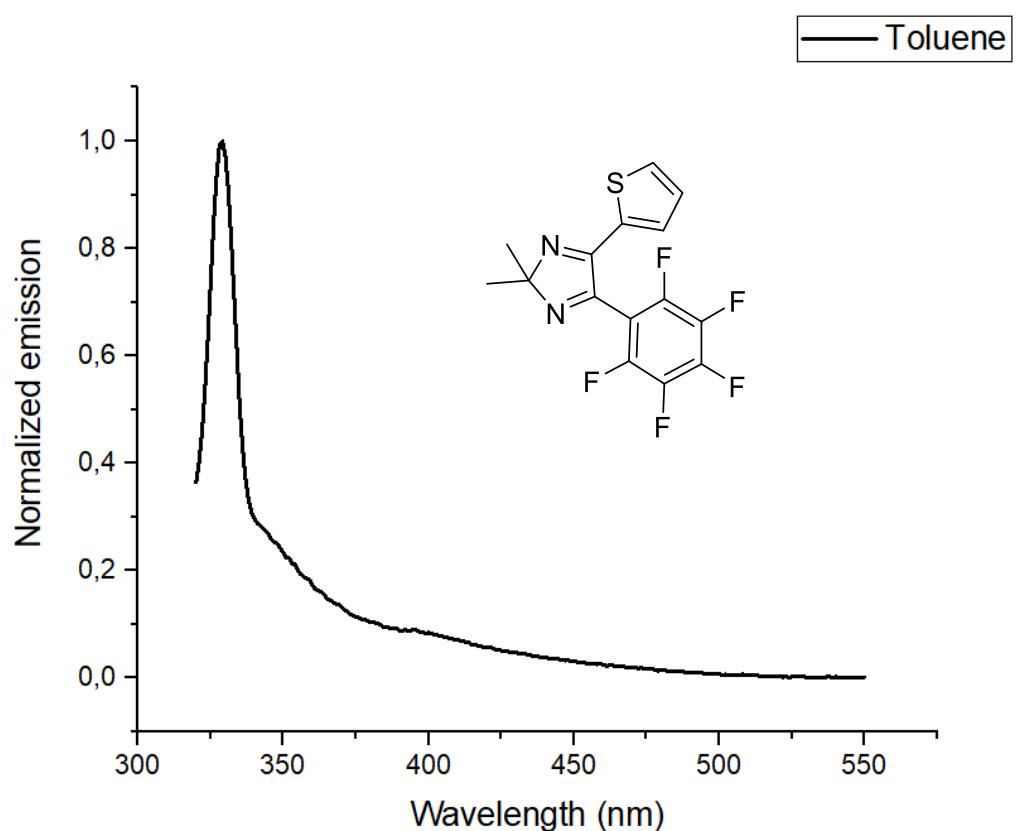
Emission spectra for **5f** in EtOH ($\lambda_{\text{ex}} = 304 \text{ nm}$)



Emission spectra for **5f** in MeOH ($\lambda_{\text{ex}} = 302 \text{ nm}$)



Emission spectra for **5f** in THF ($\lambda_{\text{ex}} = 300 \text{ nm}$)



Emission spectra for **5f** in Toluene ($\lambda_{\text{ex}} = 300 \text{ nm}$)

