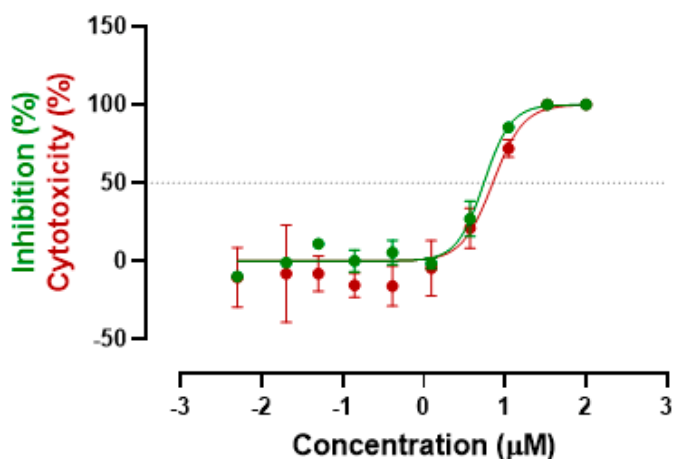


# Exploring the HIV-1 Rev Recognition Element (RRE)-Rev inhibitory capacity and antiretroviral action of benfluron analogs

## Supplementary Materials

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### Supplementary Figures



**Figure S1.** Antiretroviral activity and cellular toxicity of benfluron in PBMC. In this cell type this agent had an antiretroviral EC<sub>50</sub> of 5.50 μM (95% confidence interval 4.65-6.54 μM, R<sup>2</sup>=0.9781) and a toxic concentration CC<sub>50</sub> of 7.09 μM (4.81-10.3 μM, R<sup>2</sup>=0.9147), making for a selectivity index of 1.3.

# $^1\text{H}$ and $^{13}\text{C}$ NMR spectra and HR ESI-MS of benfluron analogs 2-6

## Compound 2

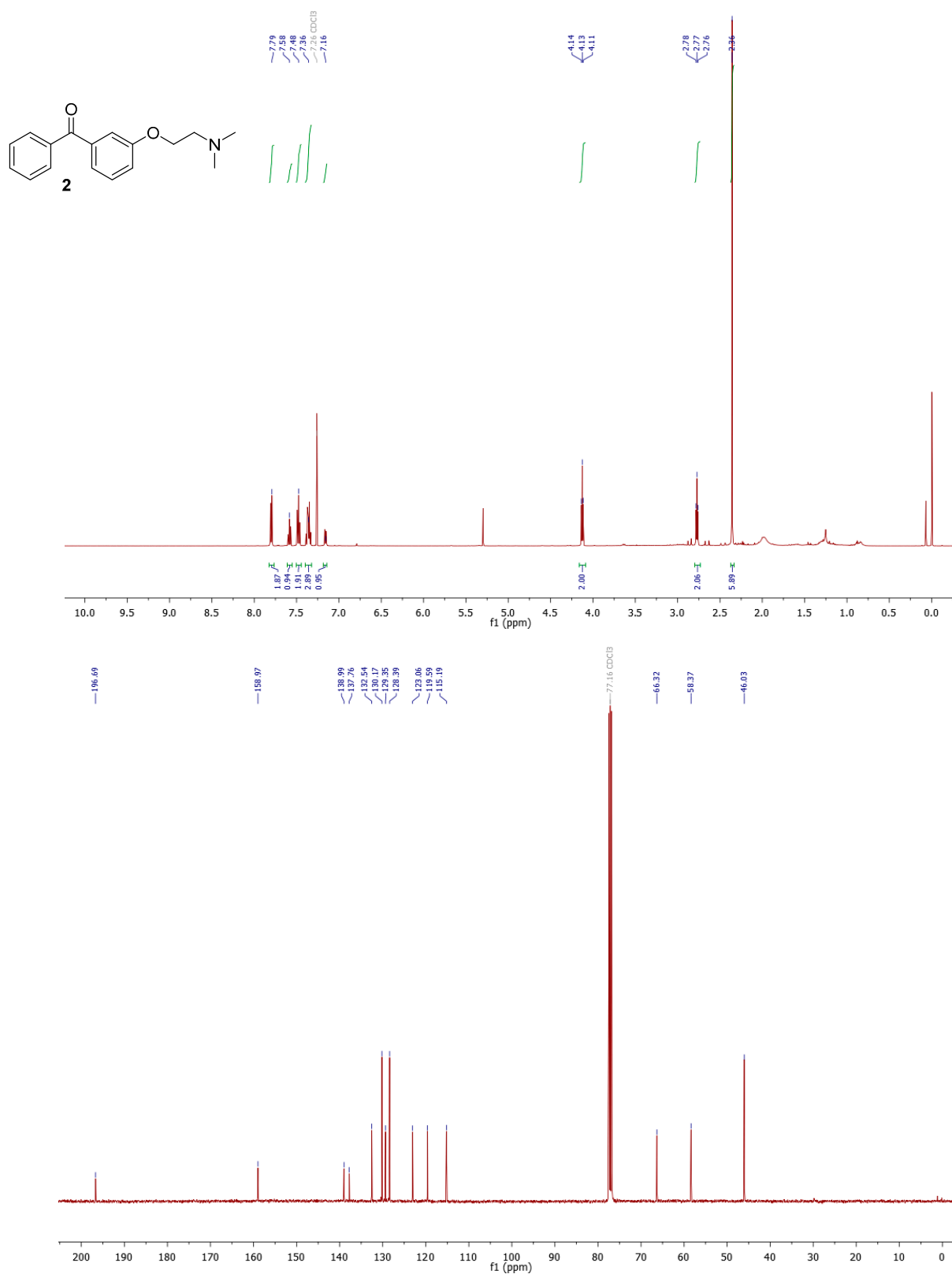
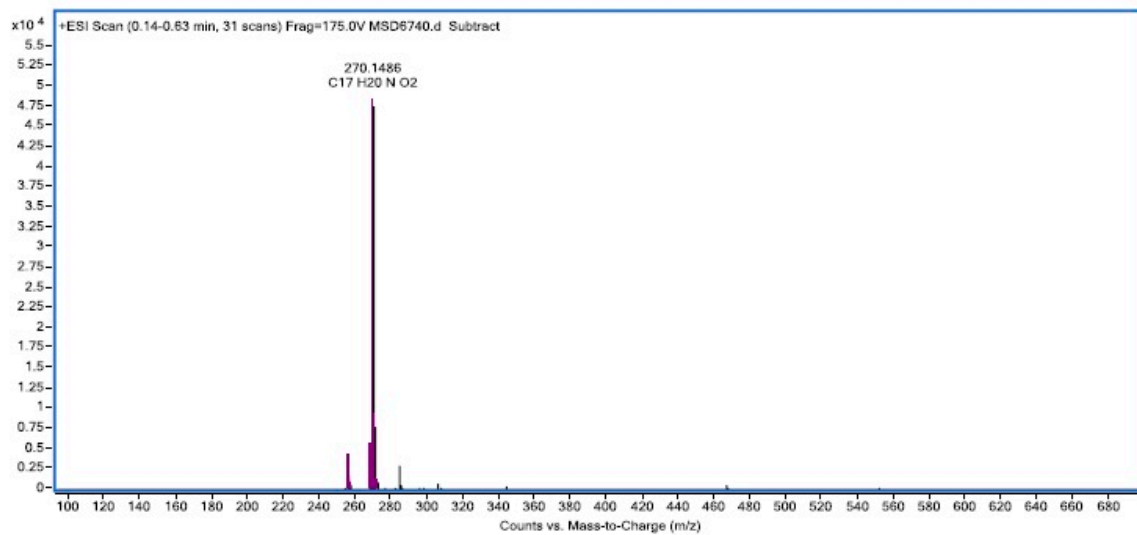
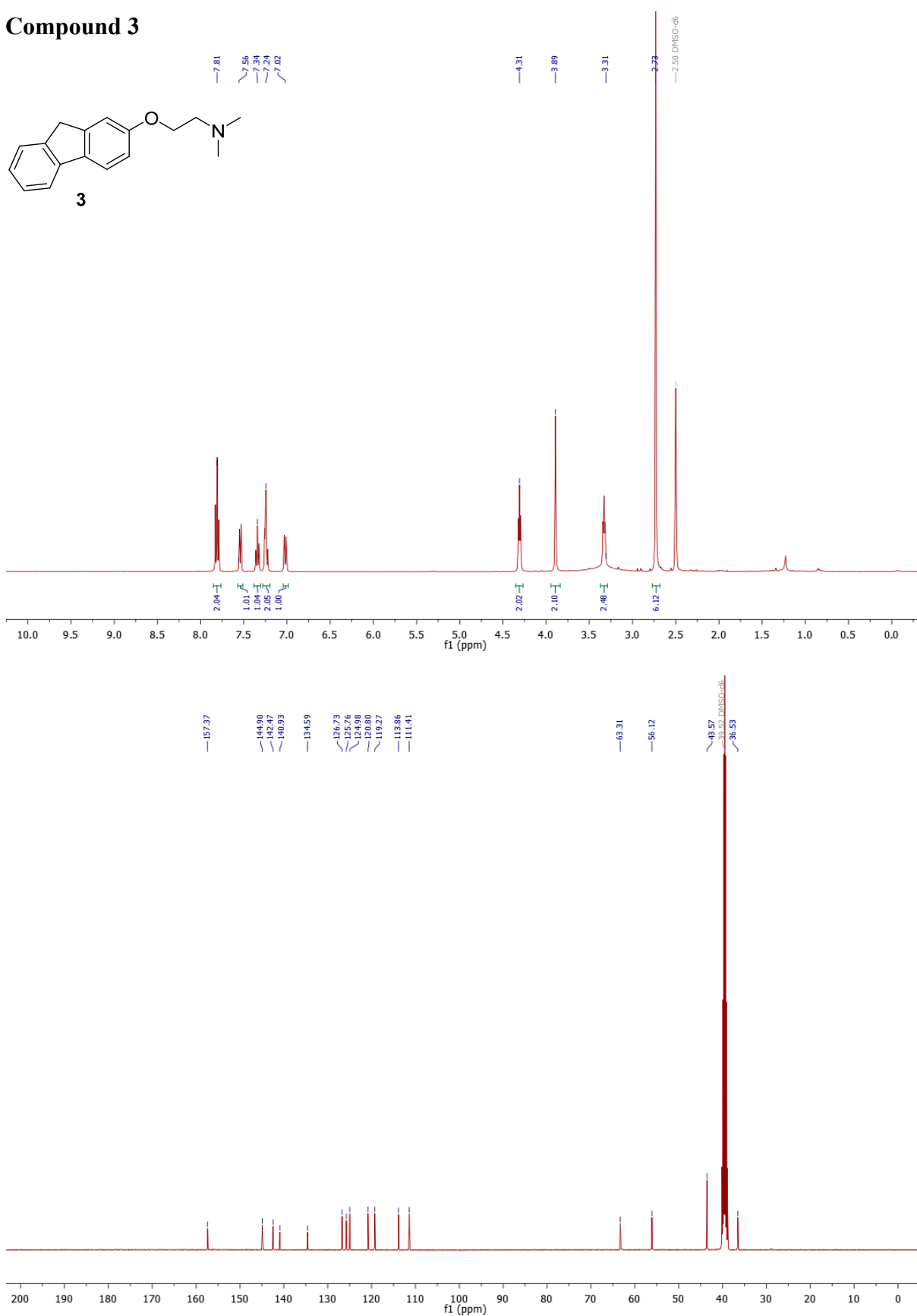


Figure S2.  $^1\text{H}$  (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) spectra of compound 2 in  $\text{CDCl}_3$ .

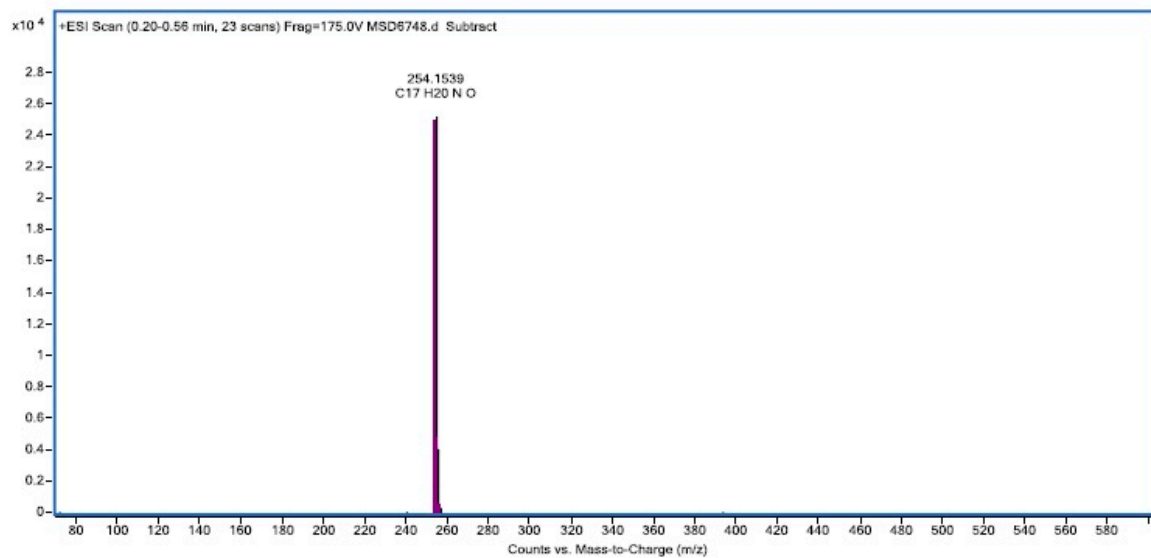


**Figure S3.** HR ESI-MS spectrum of compound **2** in MeOH.

### Compound 3

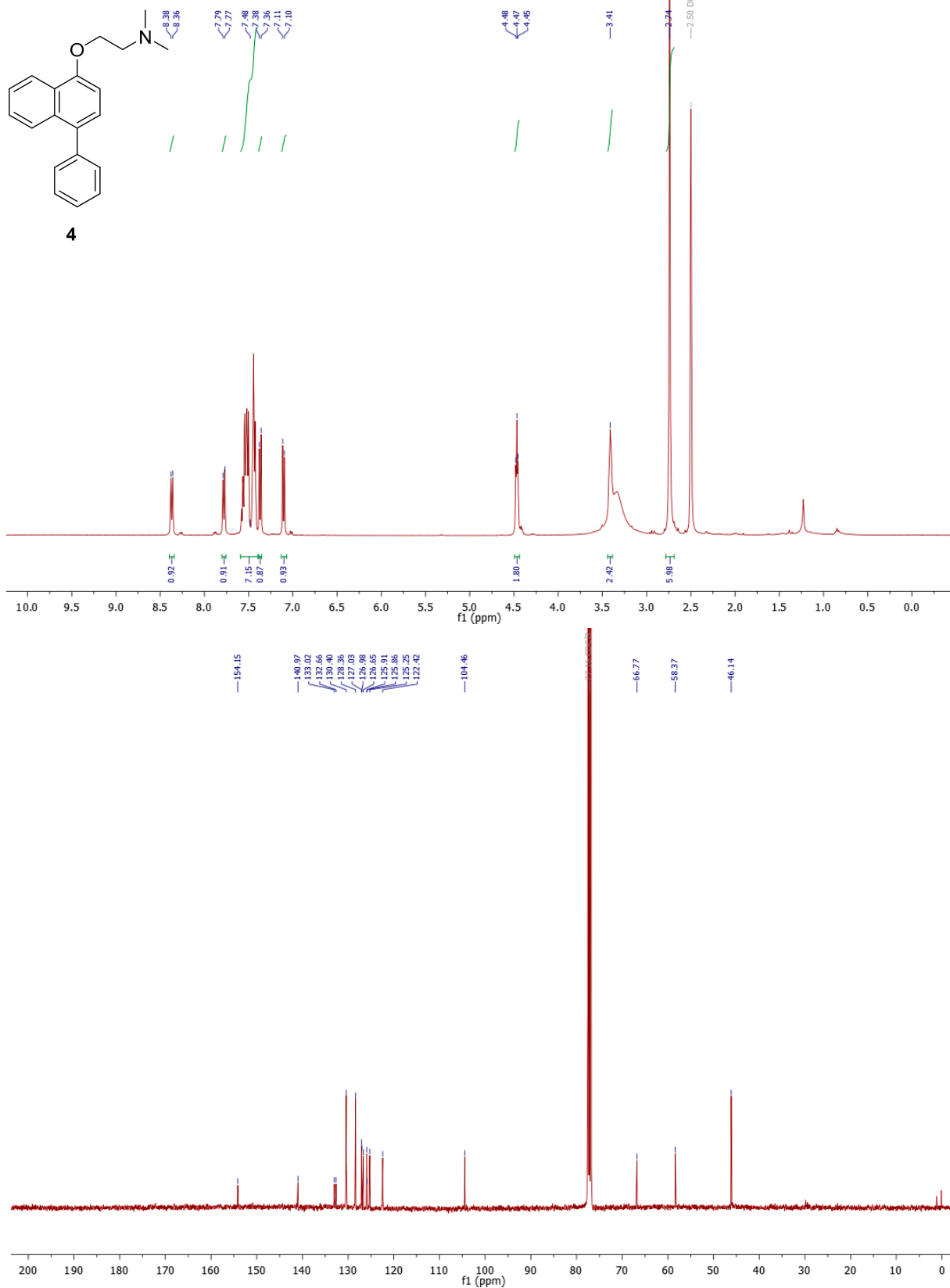


**Figure S4.** <sup>1</sup>H (400 MHz) and <sup>13</sup>C NMR (101 MHz) spectra of compound **3** in DMSO-d<sub>6</sub>.

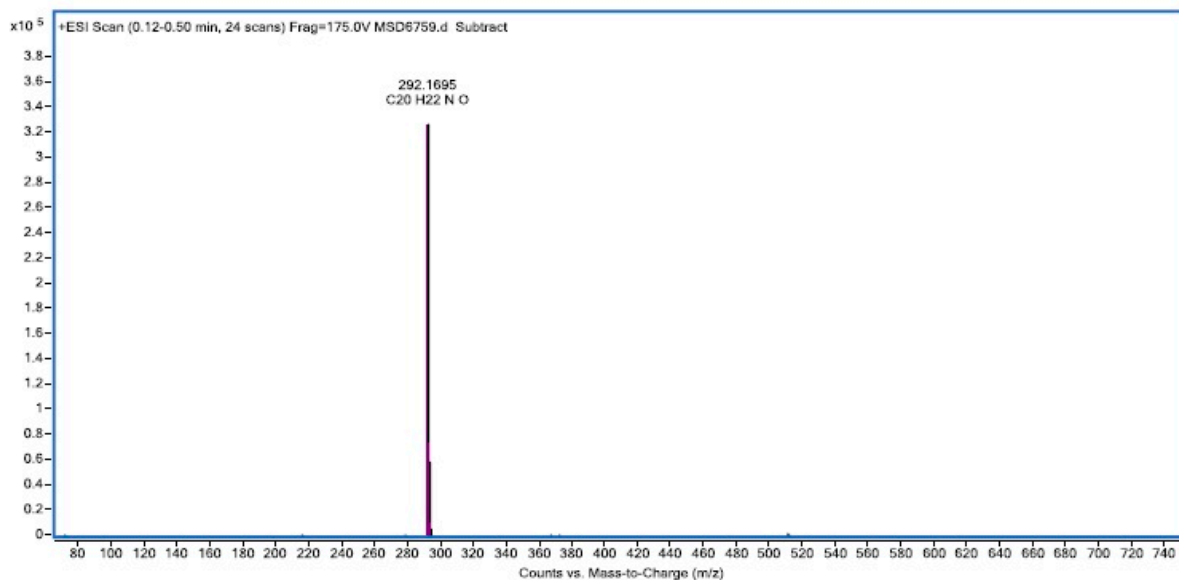


**Figure S5.** HR ESI-MS spectrum of compound **3** in MeOH.

# Compound 4



**Figure S6.** <sup>1</sup>H (DMSO-*d*<sub>6</sub>, 400 MHz) and <sup>13</sup>C NMR (CDCl<sub>3</sub>, 101 MHz) spectra of **4**.



**Figure S7.** HR ESI-MS spectrum of compound 4 in MeOH.

# Compound 5

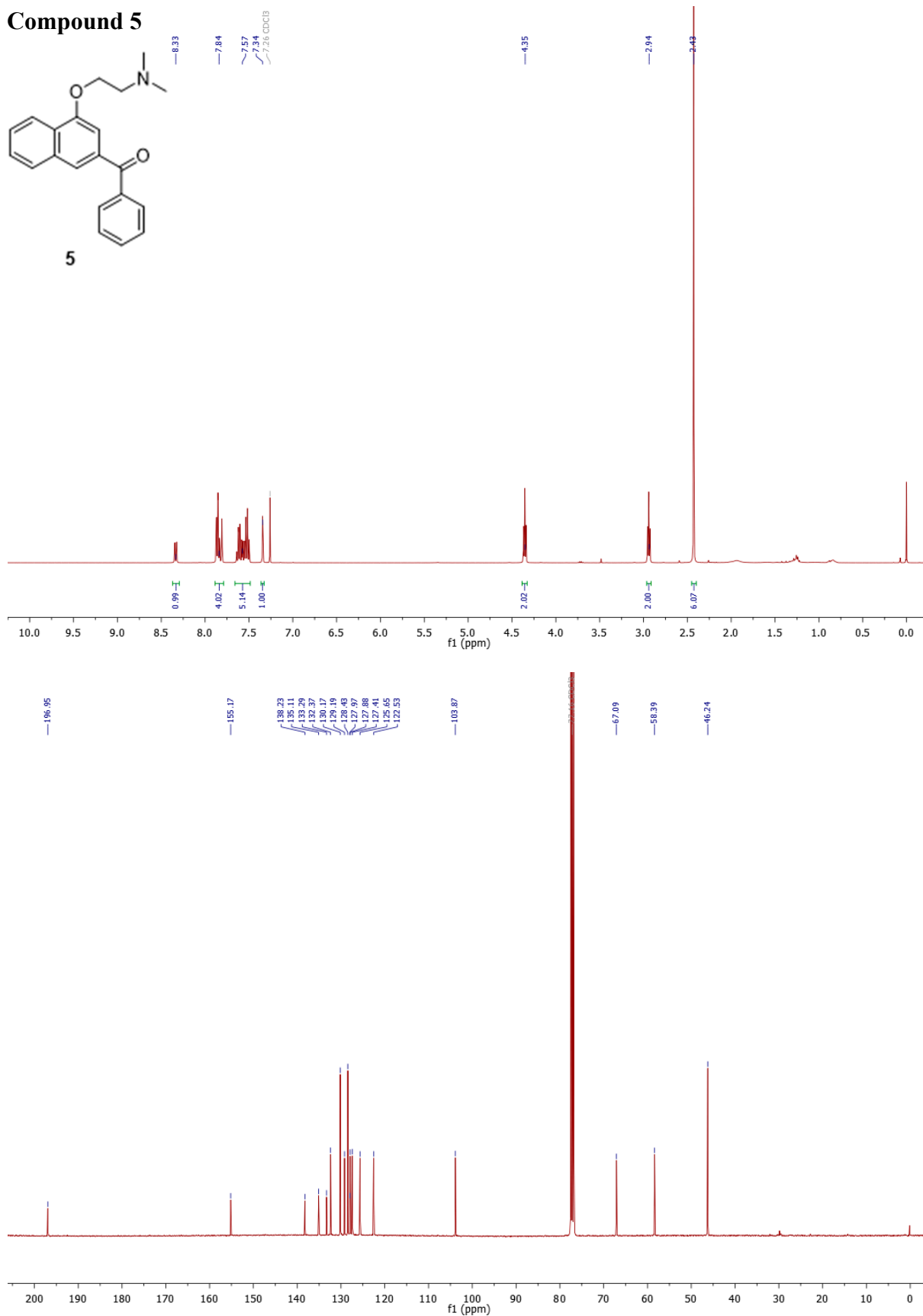
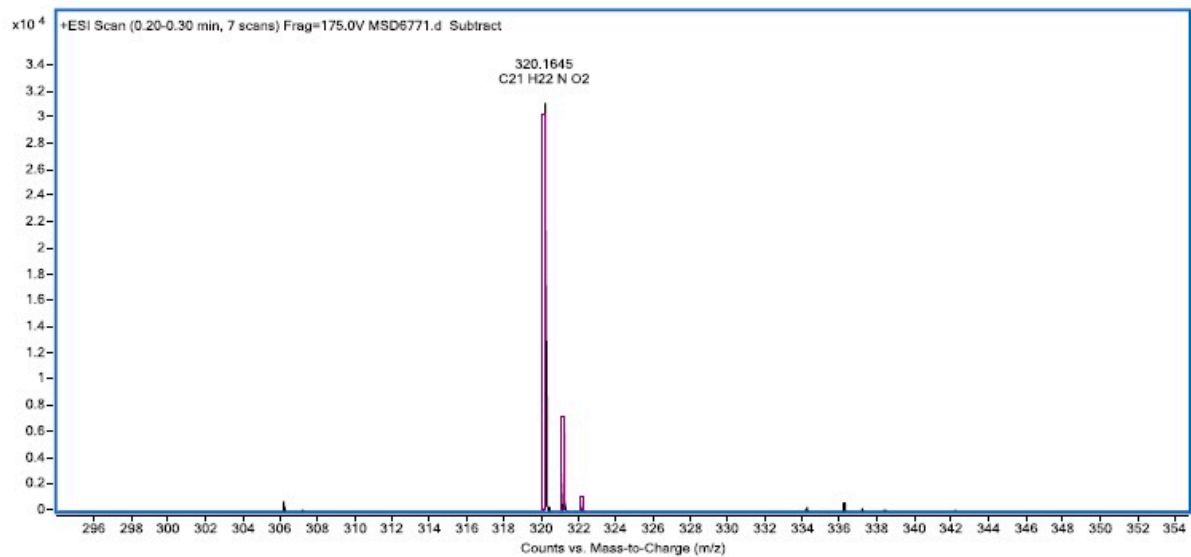


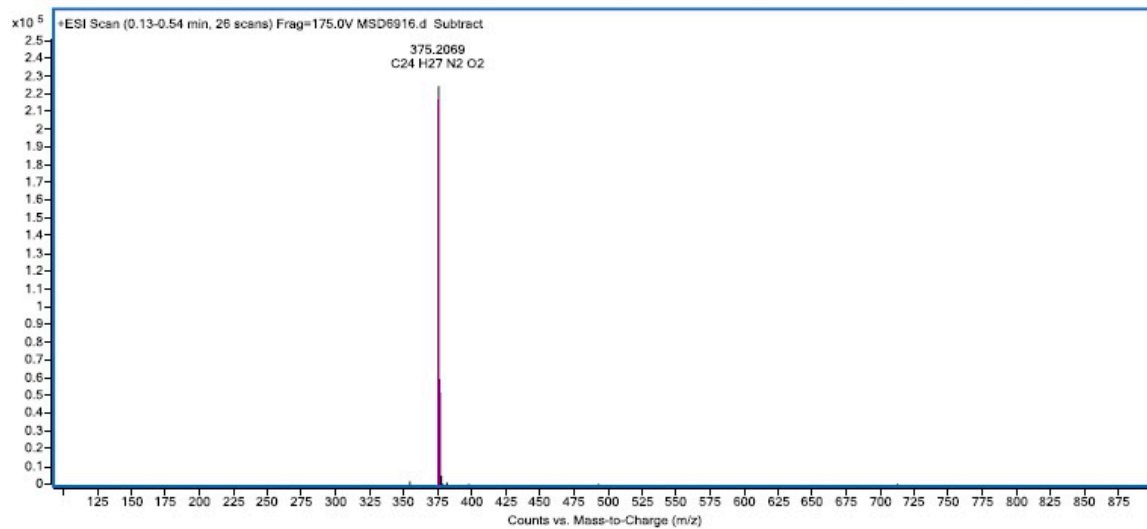
Figure S8. <sup>1</sup>H (400 MHz) and <sup>13</sup>C NMR (101 MHz) spectra of compound 5 in CDCl<sub>3</sub>.





**Figure S9.** HR ESI-MS spectrum of compound **5** in MeOH.





**Figure S11.** HR ESI-MS spectrum of compound **6** in MeOH.

## Reversed-phase HPLC analysis of benfluron analogs (2-6):

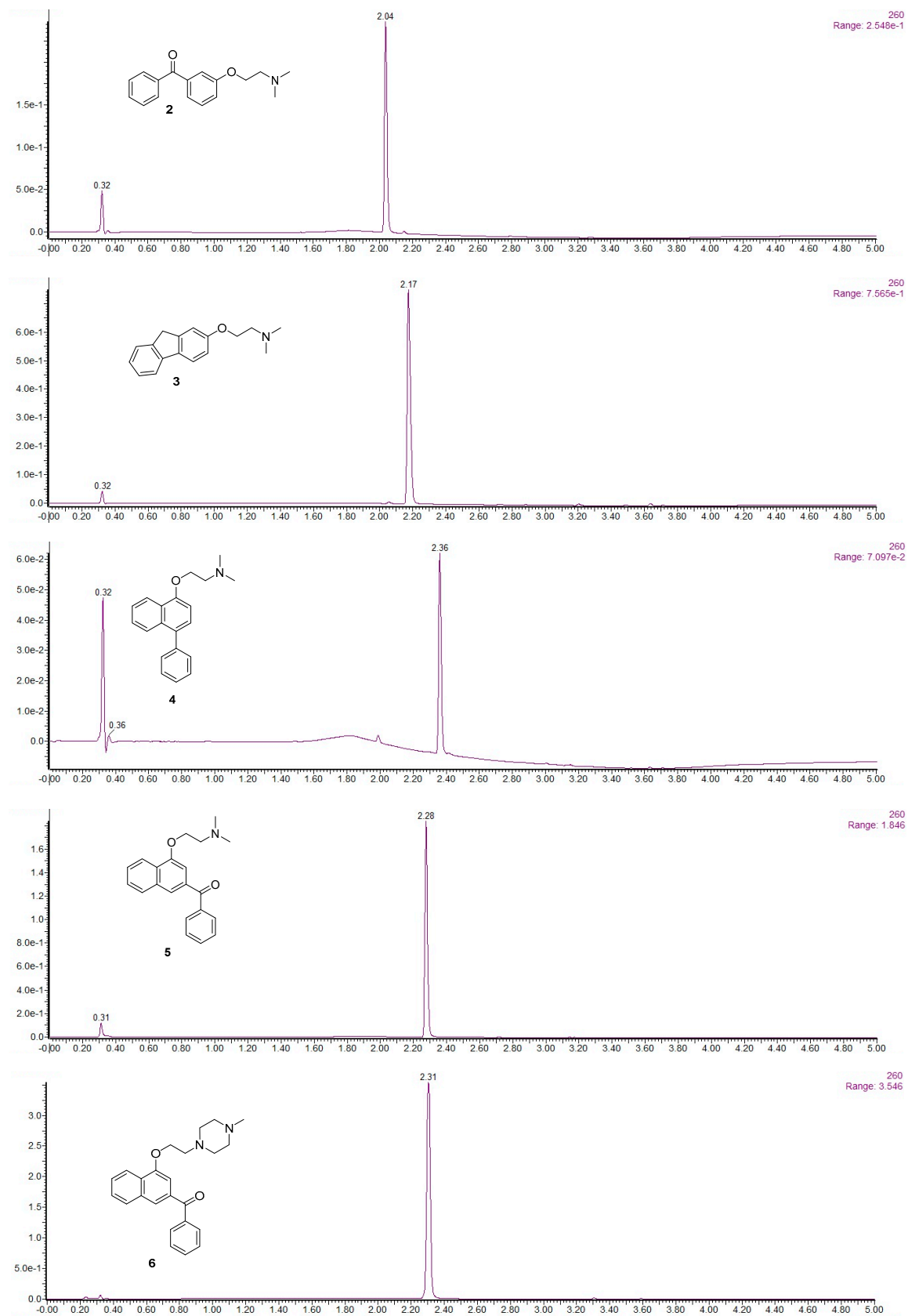


Figure S12. Reversed-phase HPLC chromatograms of benfluron analogs 2-6.

# $^1\text{H}$ and $^{13}\text{C}$ NMR spectra and HR ESI-MS of compounds 2b-5b

## Compound 2b

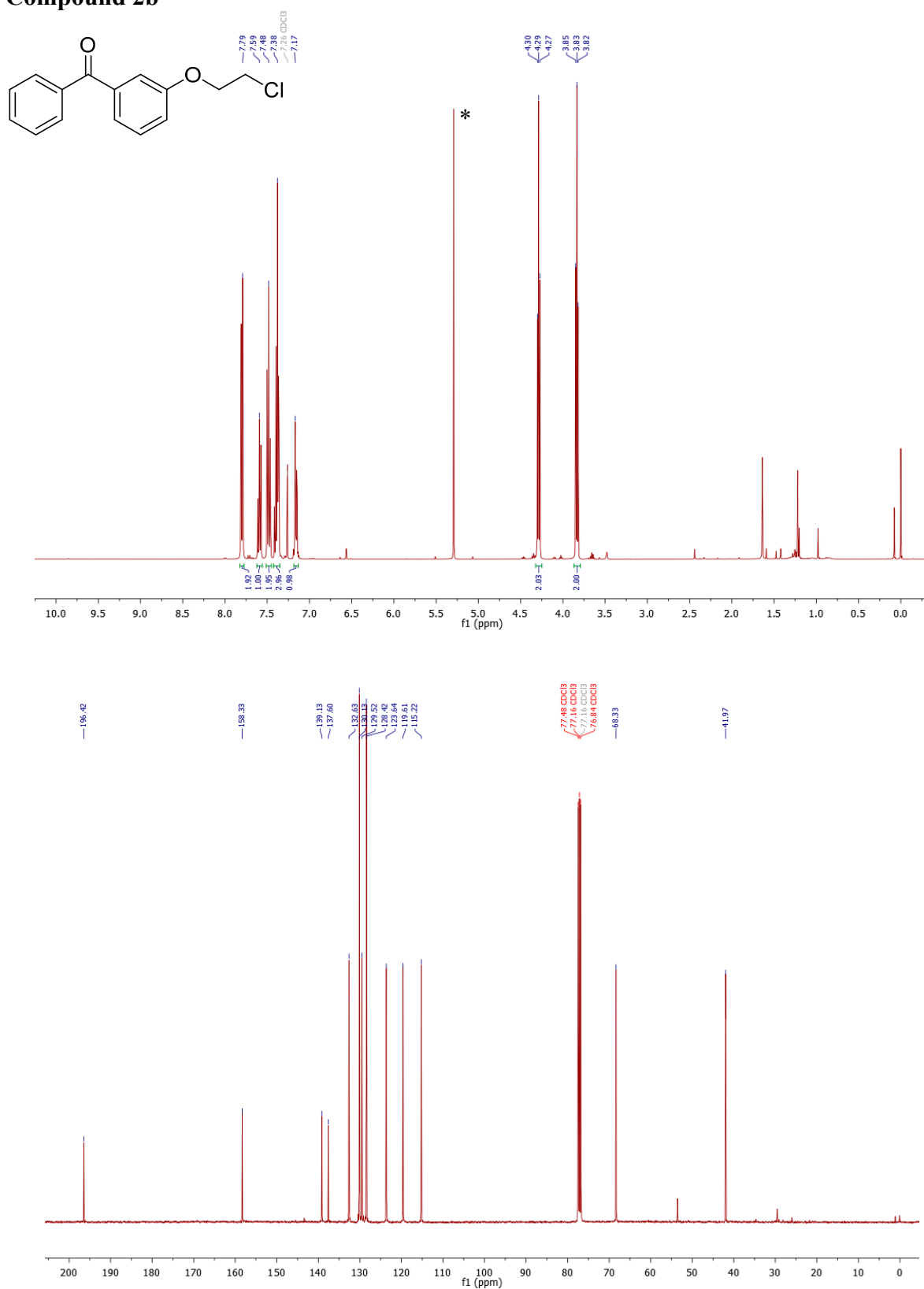
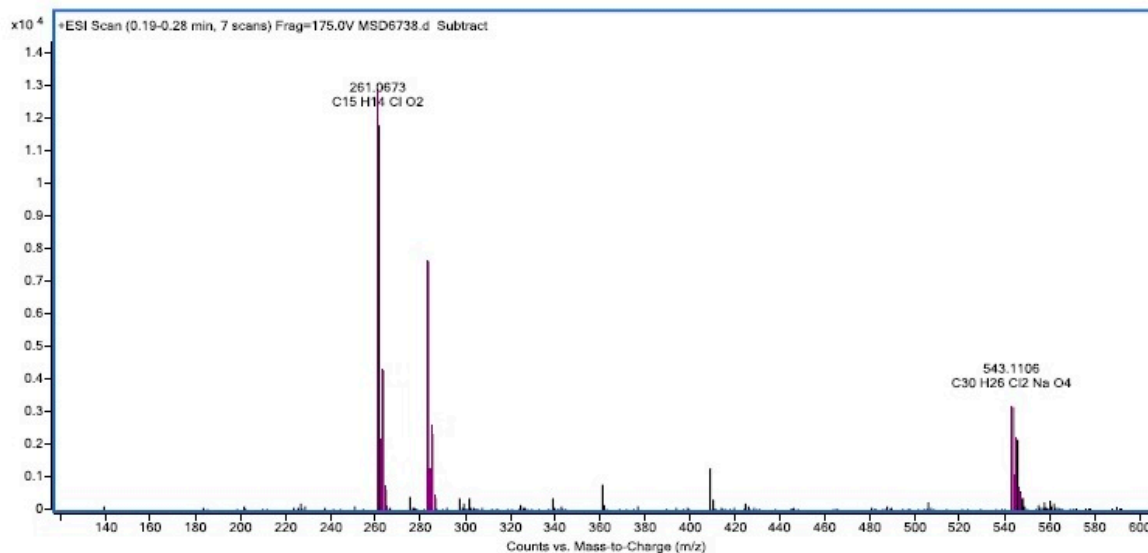
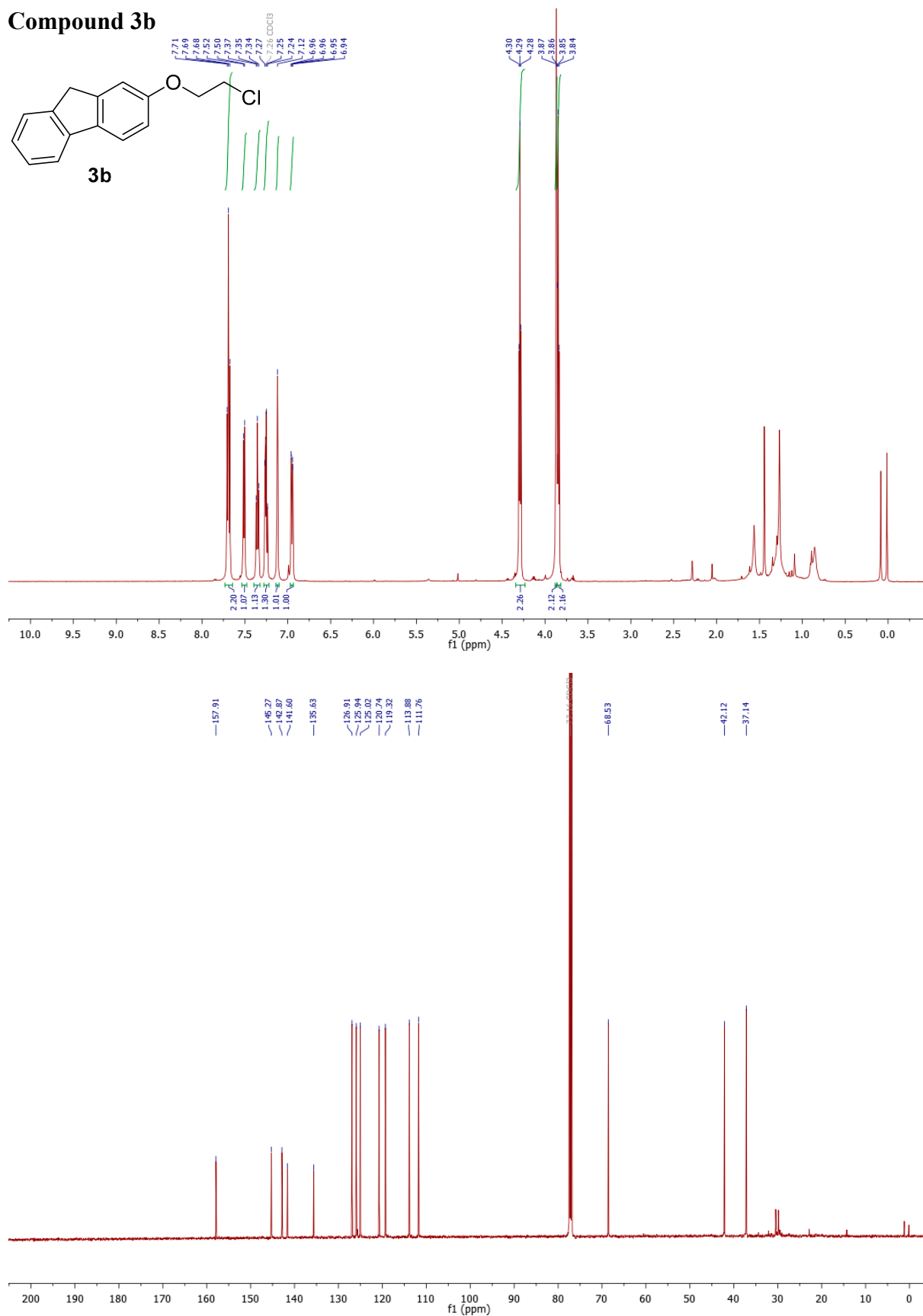


Figure S13.  $^1\text{H}$  (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) spectra of compound 2b in  $\text{CDCl}_3$ .

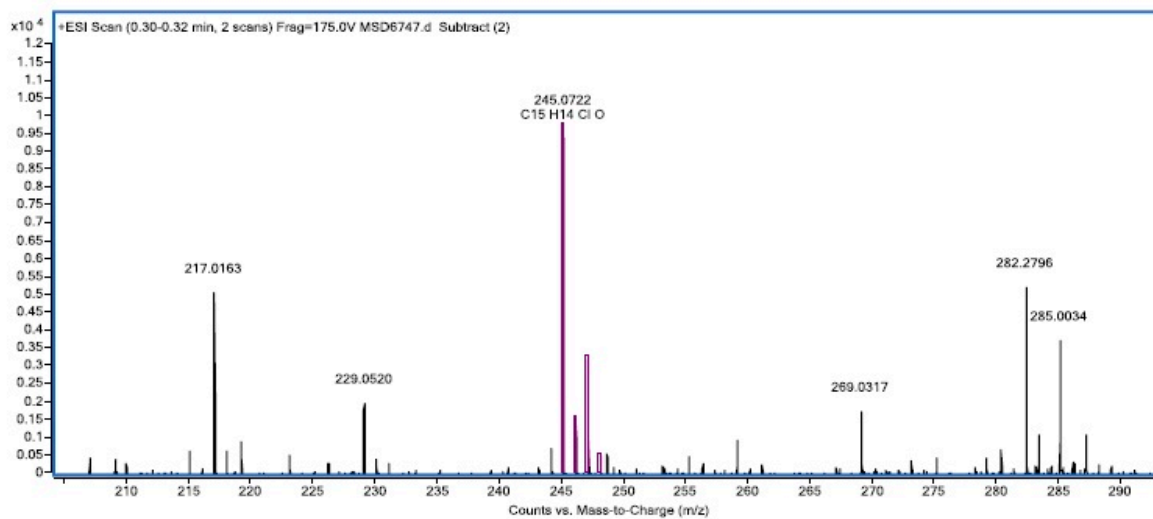
\* DCM residue signal.



**Figure S14.** HR ESI-MS spectrum of compound **2b** in MeOH.

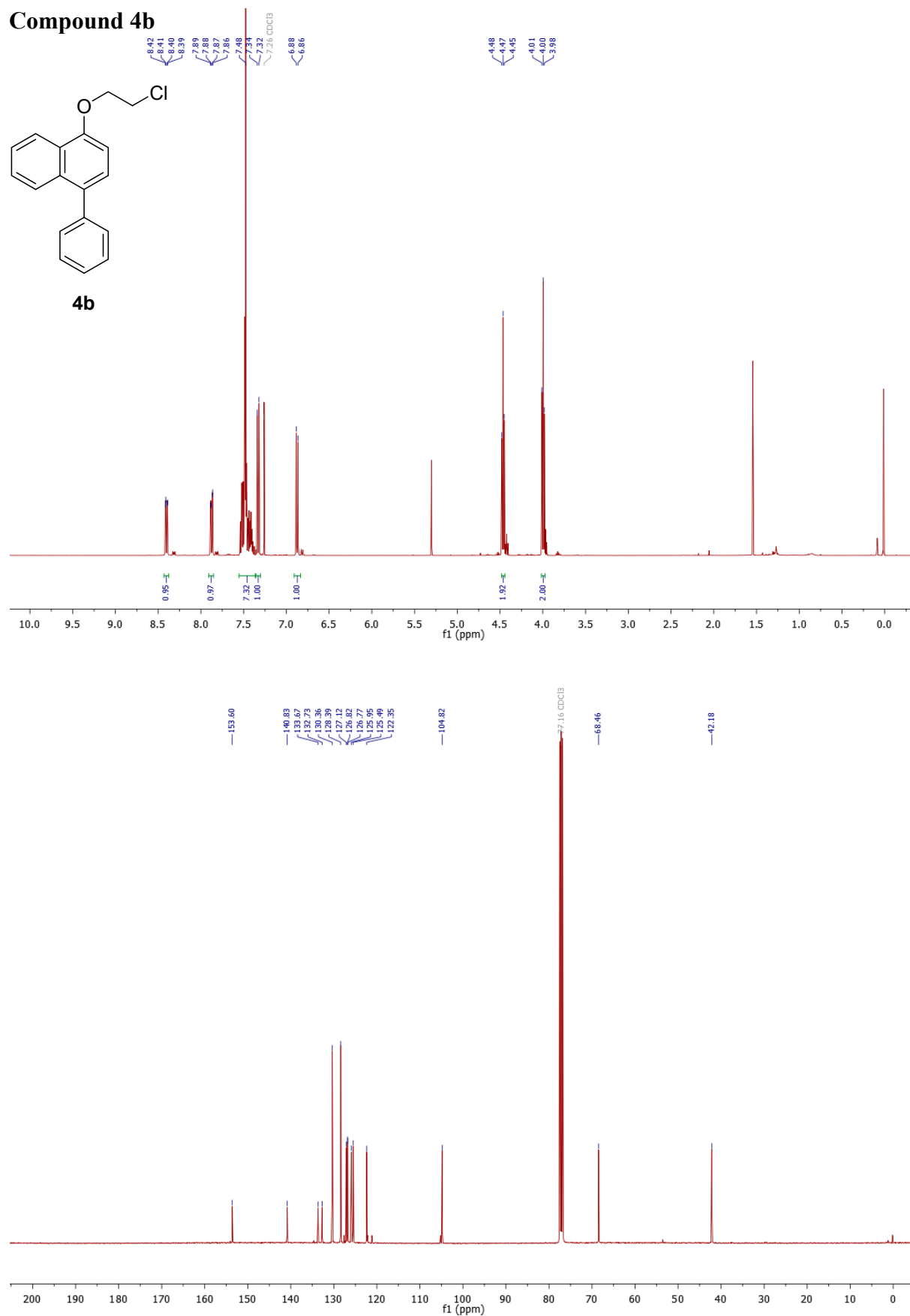


**Figure S15.** <sup>1</sup>H (400 MHz) and <sup>13</sup>C NMR (101 MHz) spectra of compound **3b** in CDCl<sub>3</sub>.

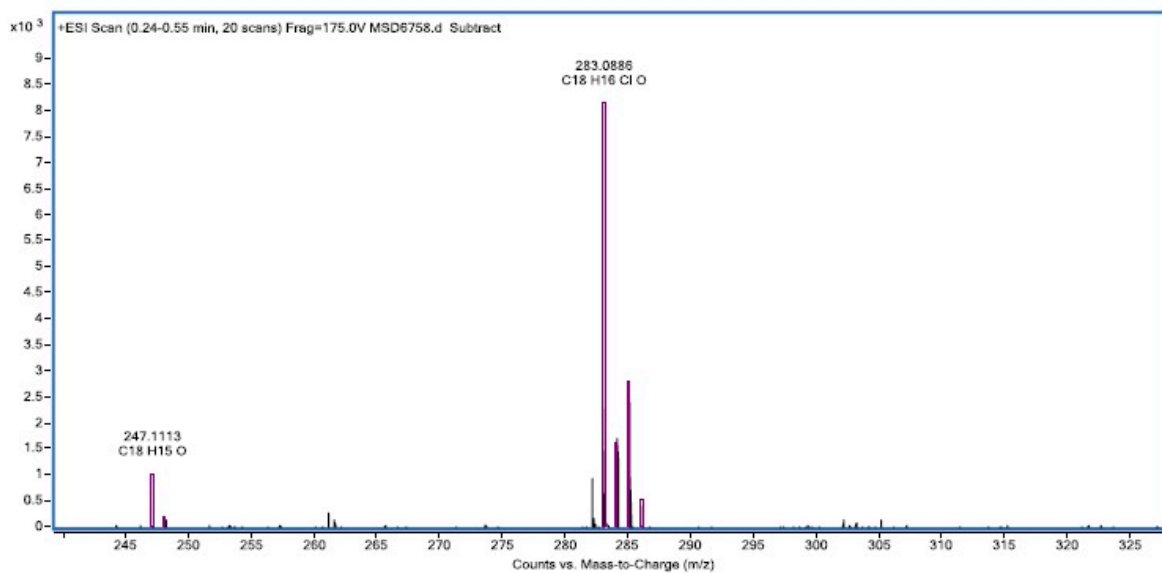


**Figure S16.** HR ESI-MS spectrum of compound **3b** in MeOH.





**Figure S17.** <sup>1</sup>H (400 MHz) and <sup>13</sup>C NMR (101 MHz) spectra of compound **4b** in CDCl<sub>3</sub>.



**Figure S18.** HR ESI-MS spectrum of compound **4b** in MeOH.

### Compound 5b

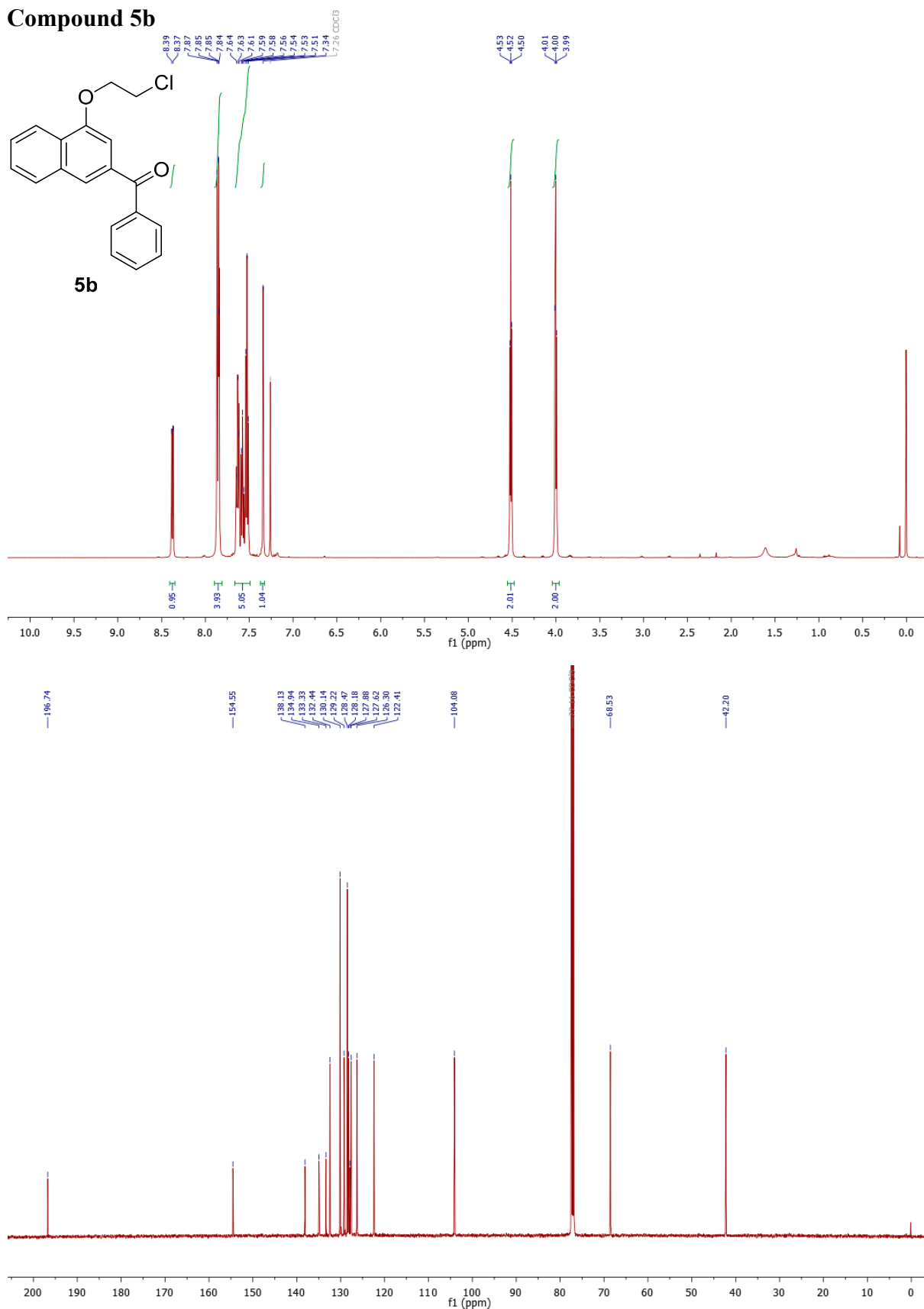
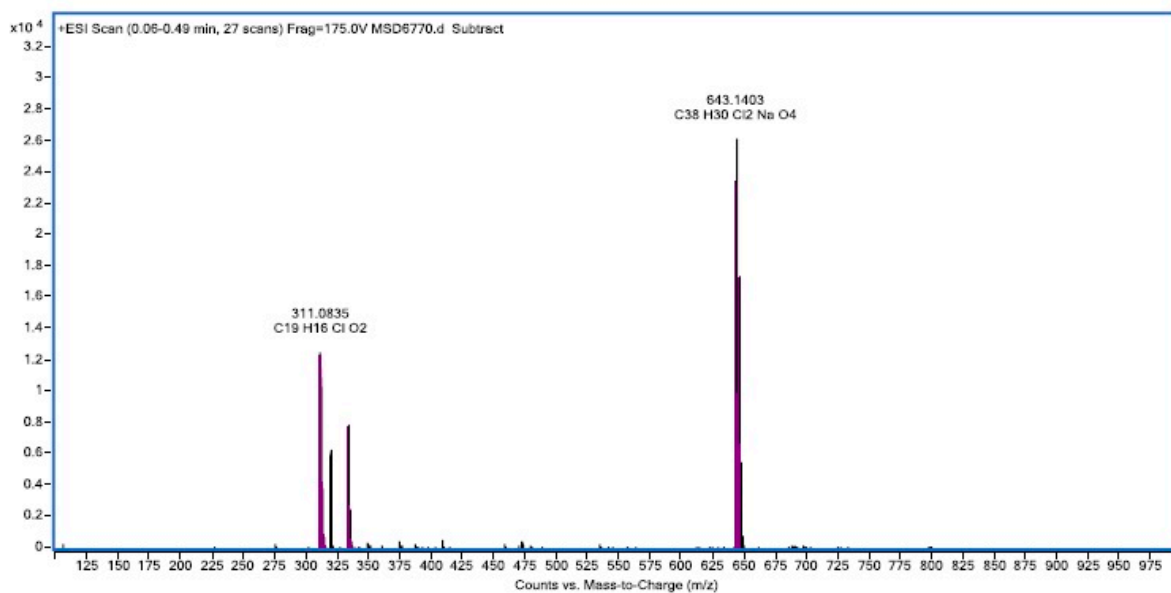
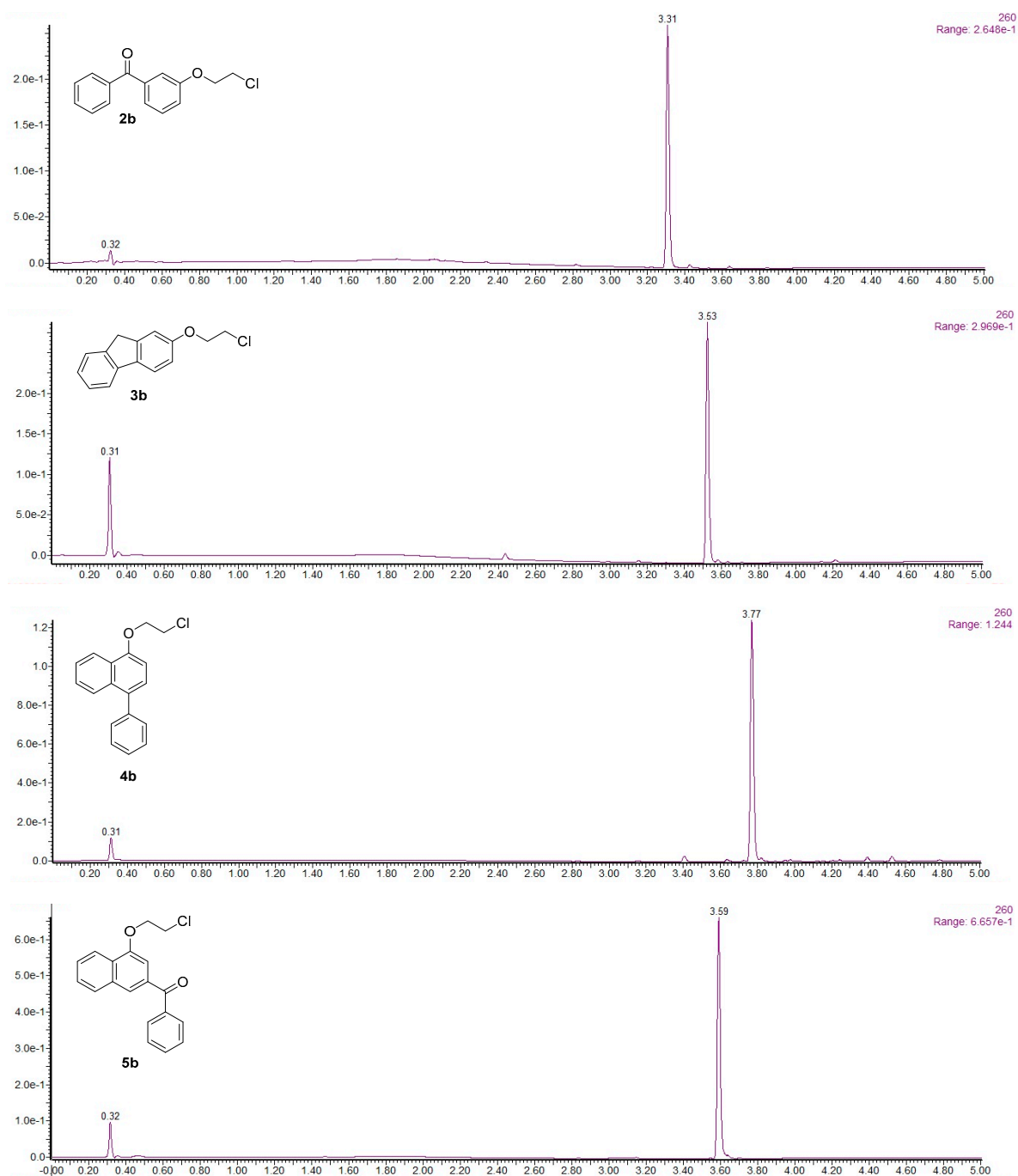


Figure S19.  $^1\text{H}$  (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) spectra of compound **5b** in  $\text{CDCl}_3$ .



**Figure S20.** HR ESI-MS spectrum of compound **5b** in MeOH.

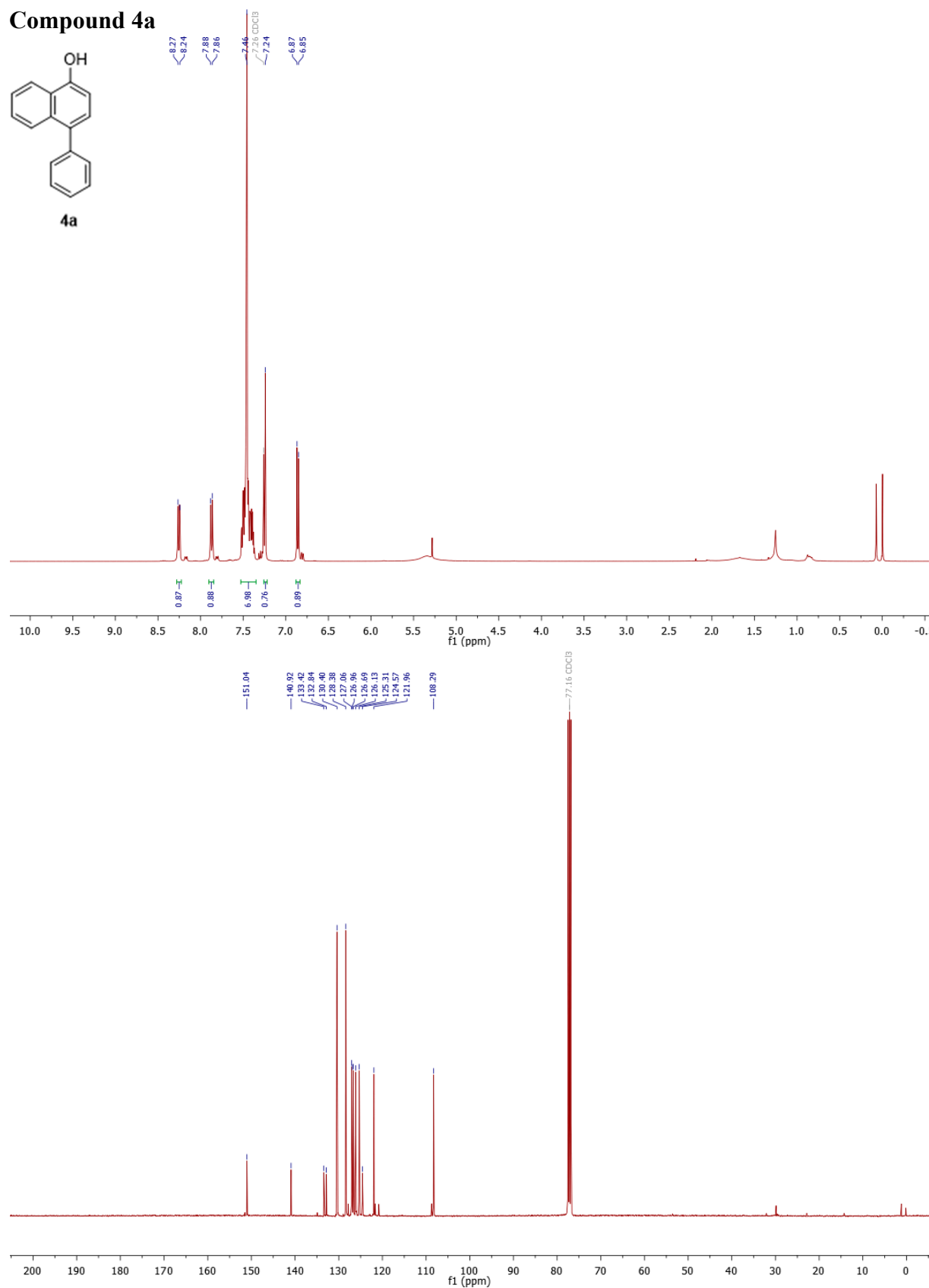
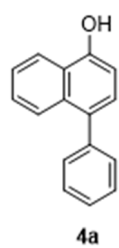
## Reversed-phase HPLC analysis of compounds 2b-5b



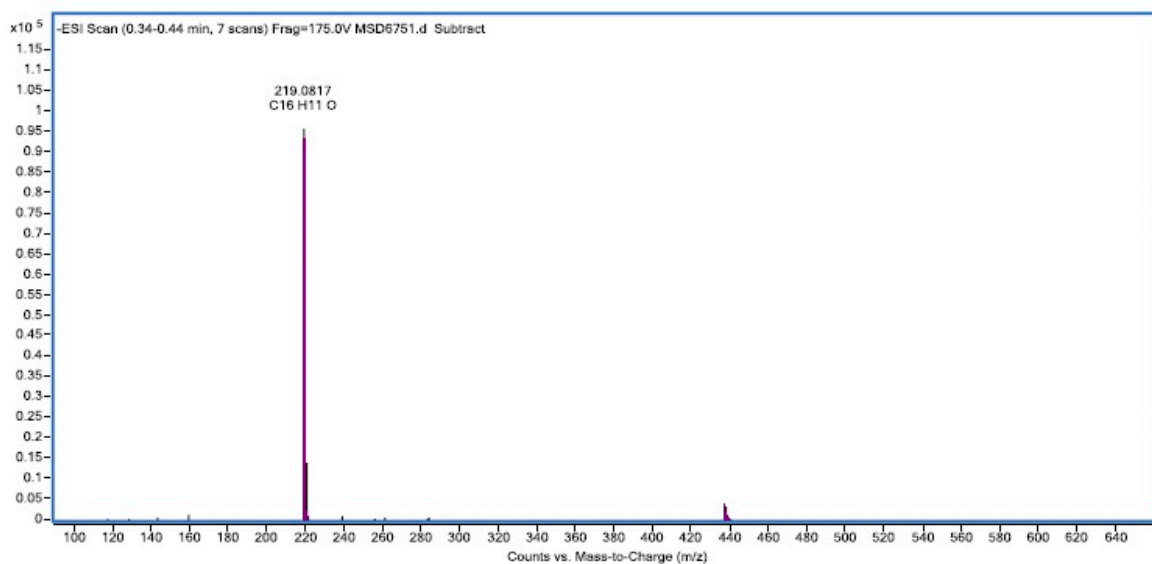
**Figure S21.** Reversed-phase HPLC chromatograms of compounds 2b-5b.

# $^1\text{H}$ and $^{13}\text{C}$ NMR spectra, HR ESI-MS and HPLC analysis of compounds 4a-5a

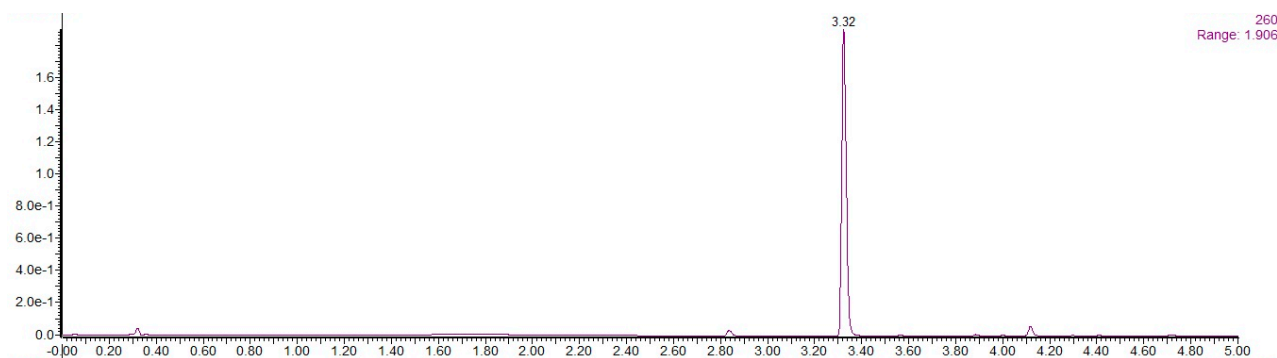
## Compound 4a



**Figure S22.**  $^1\text{H}$  (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) spectra of compound **4a** in  $\text{CDCl}_3$ .

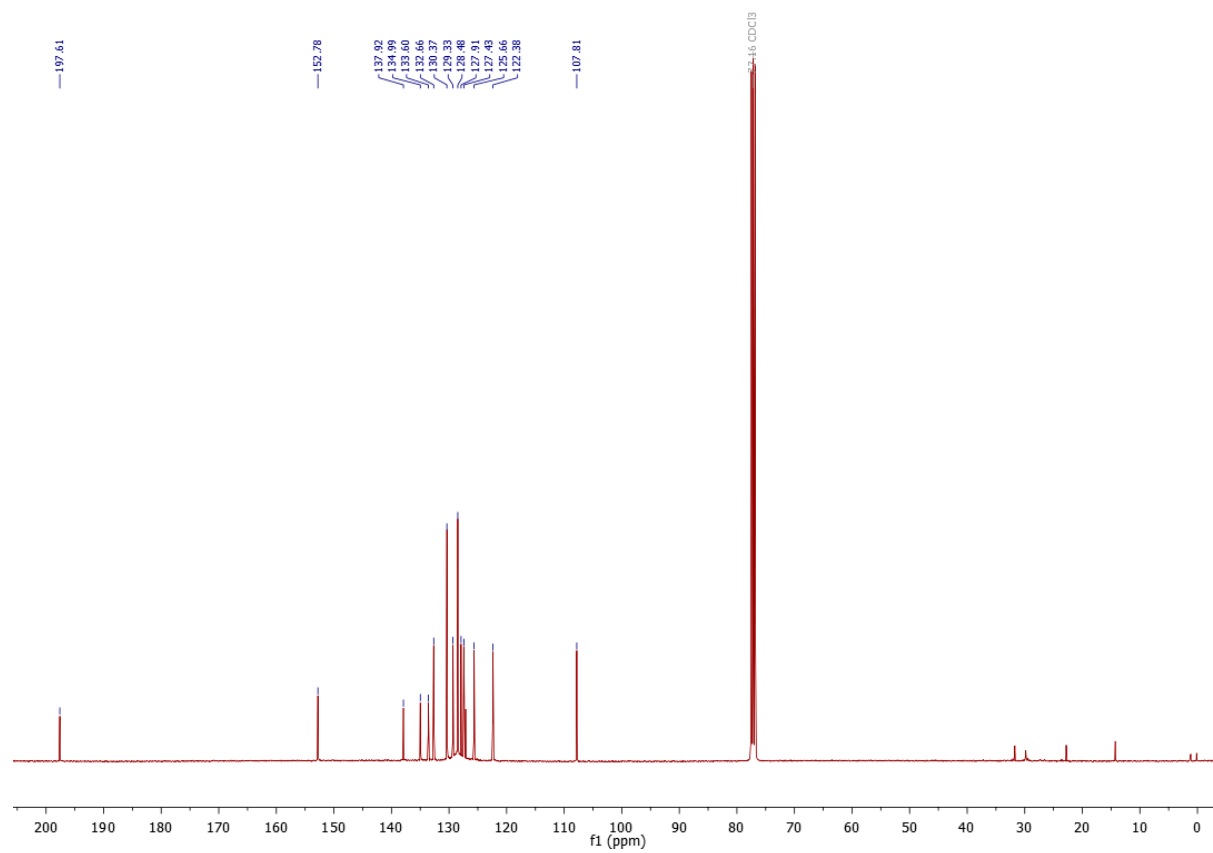
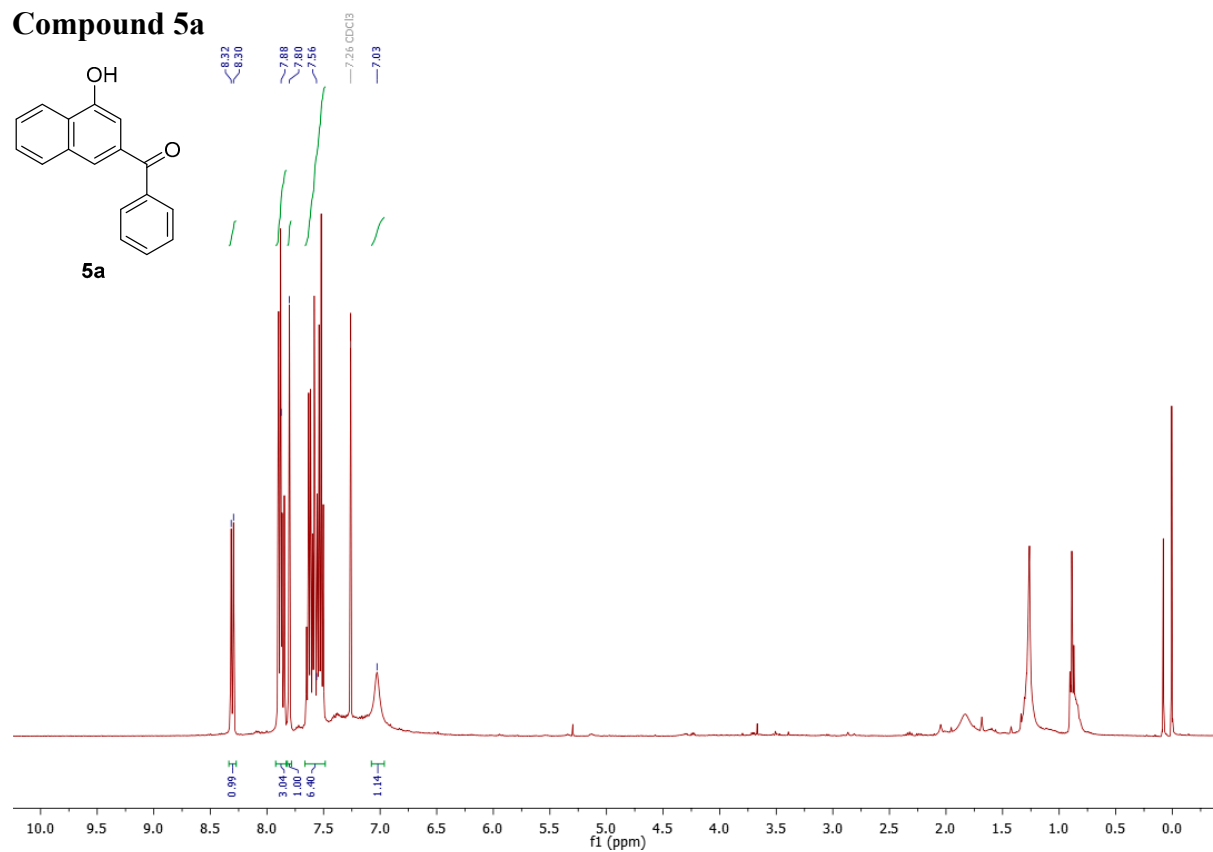
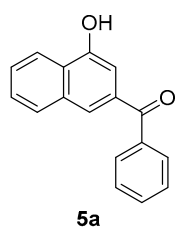


**Figure S23.** HR ESI-MS spectrum of compound **4a** in MeOH.



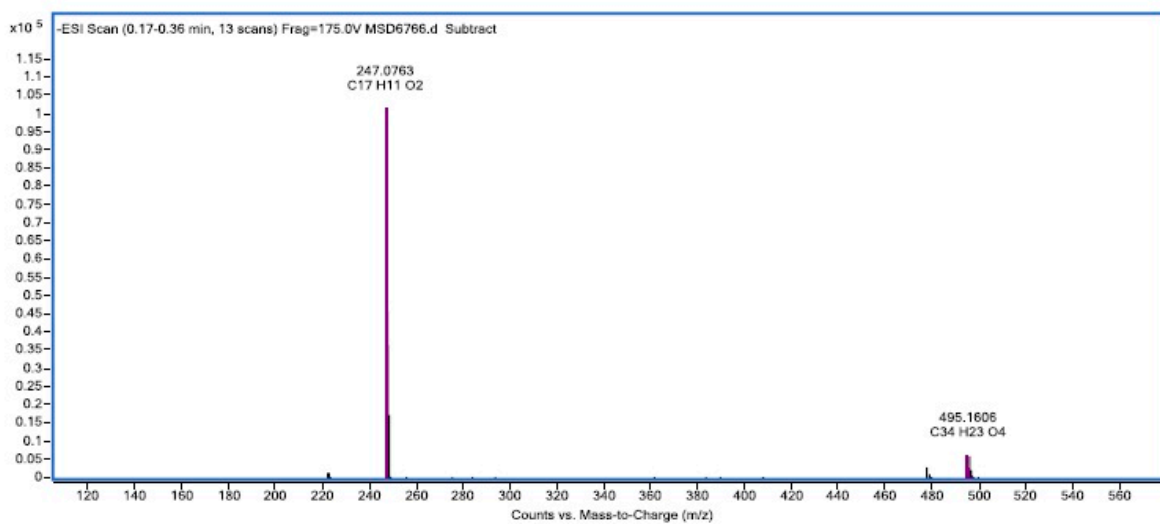
**Figure S24.** Reversed-phase HPLC chromatogram of compound **4a**.

### Compound 5a

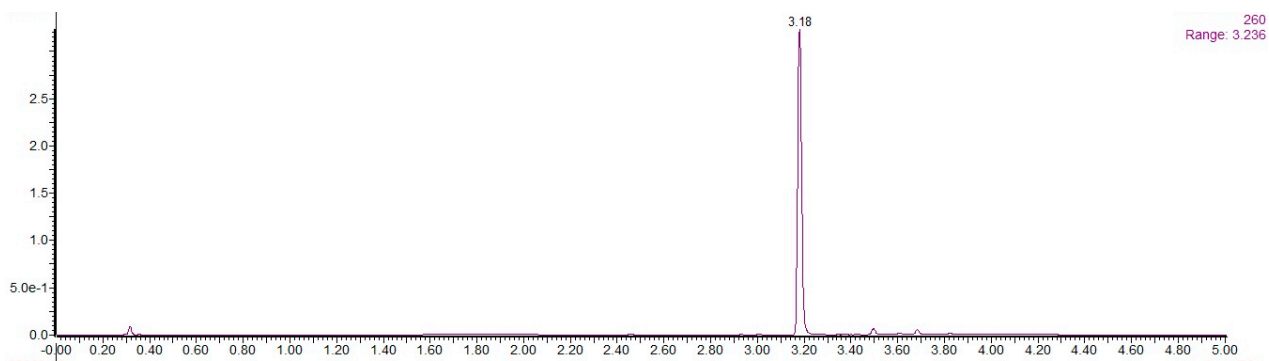


**Figure S25.**  $^1\text{H}$  (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) spectra of compound **5a** in  $\text{CDCl}_3$ .



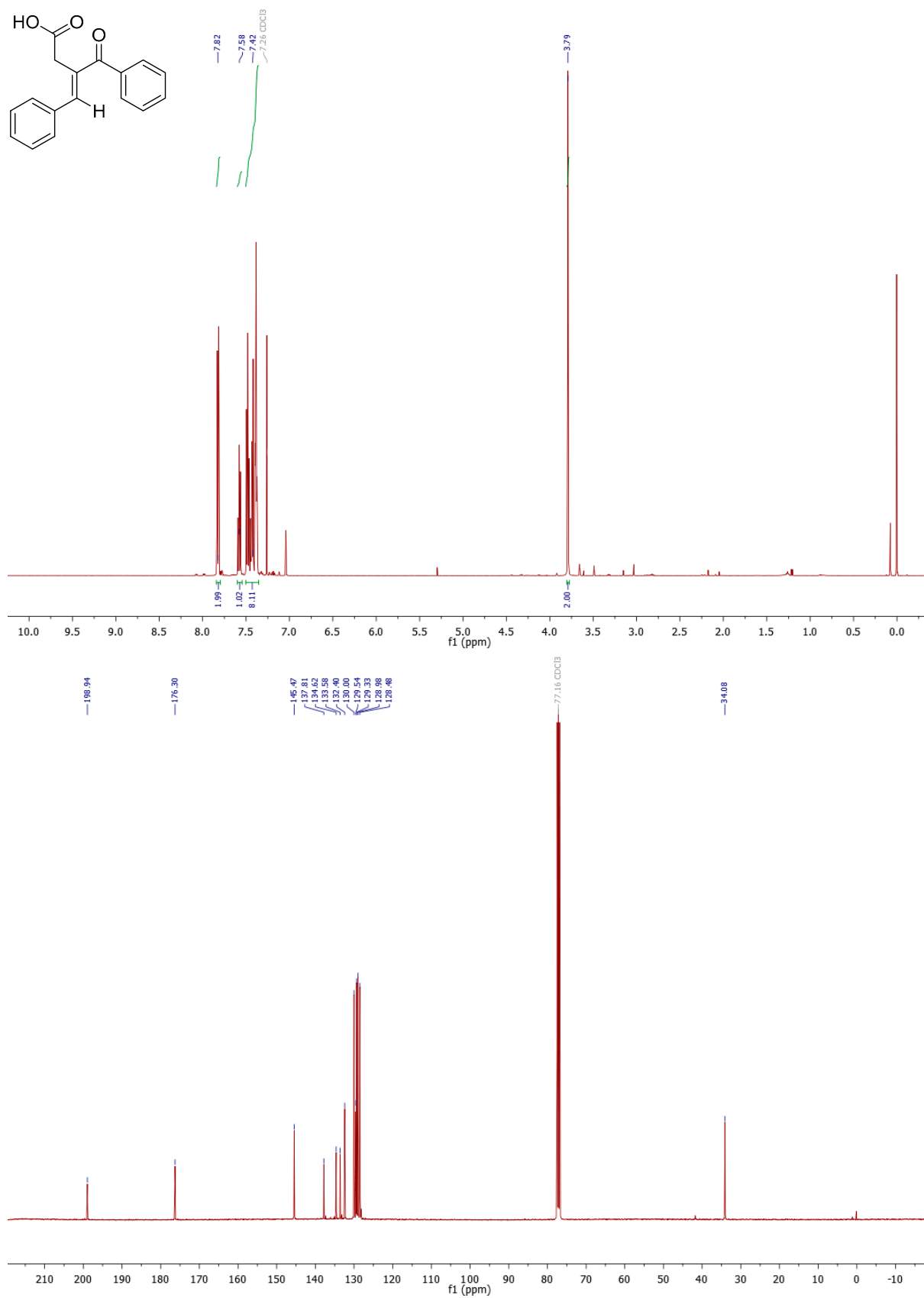


**Figure S26.** HR ESI-MS spectrum of compound **5a** in MeOH.



**Figure S27.** Reversed-phase HPLC chromatogram of compound **5a**.

**$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra, HR ESI-MS and HPLC analysis of compound 7.**



**Figure S28.**  $^1\text{H}$  (400 MHz) and  $^{13}\text{C}$  NMR (101 MHz) spectra of compound 7 in  $\text{CDCl}_3$ .

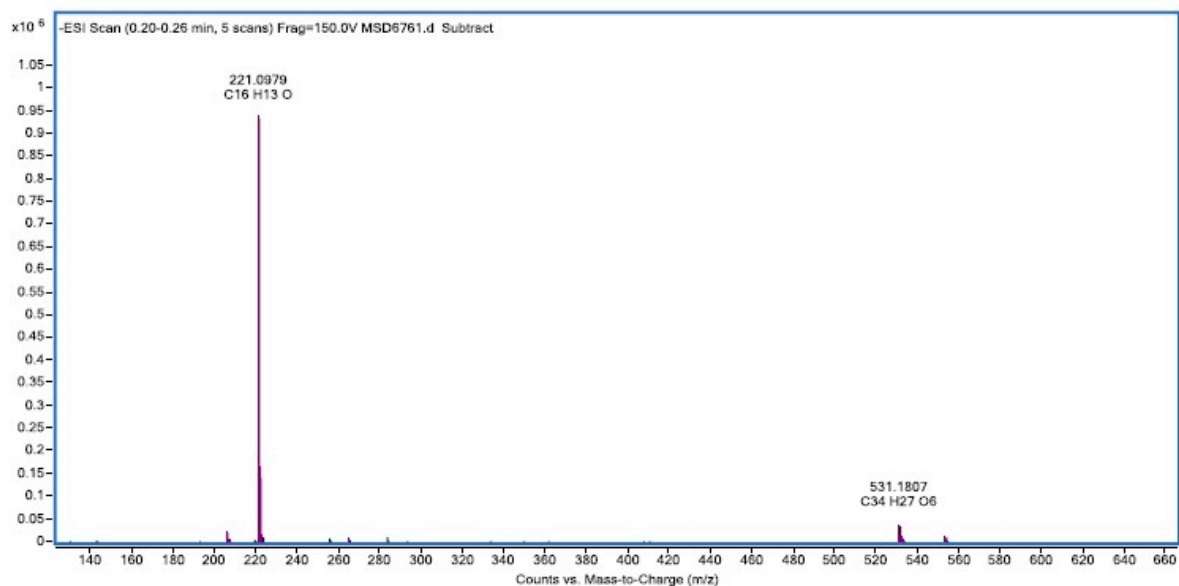


Figure S29. HR ESI-MS spectrum of compound 7 in MeOH.

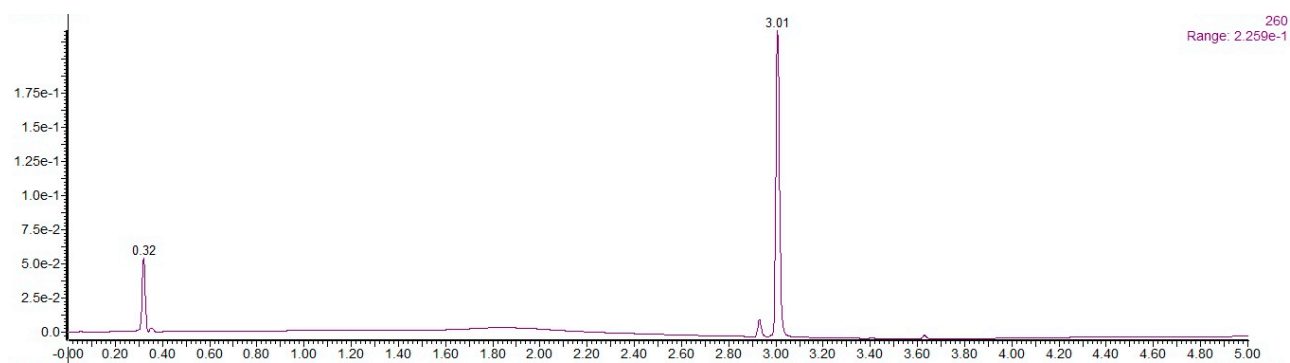


Figure S30. Reversed-phase HPLC chromatogram of compound 7.