

## Supporting Information

# Asymmetric synthesis of methoxylated ether lipids: Total synthesis of polyunsaturated C18:3 omega-3 and omega-6 MEL triene derivatives

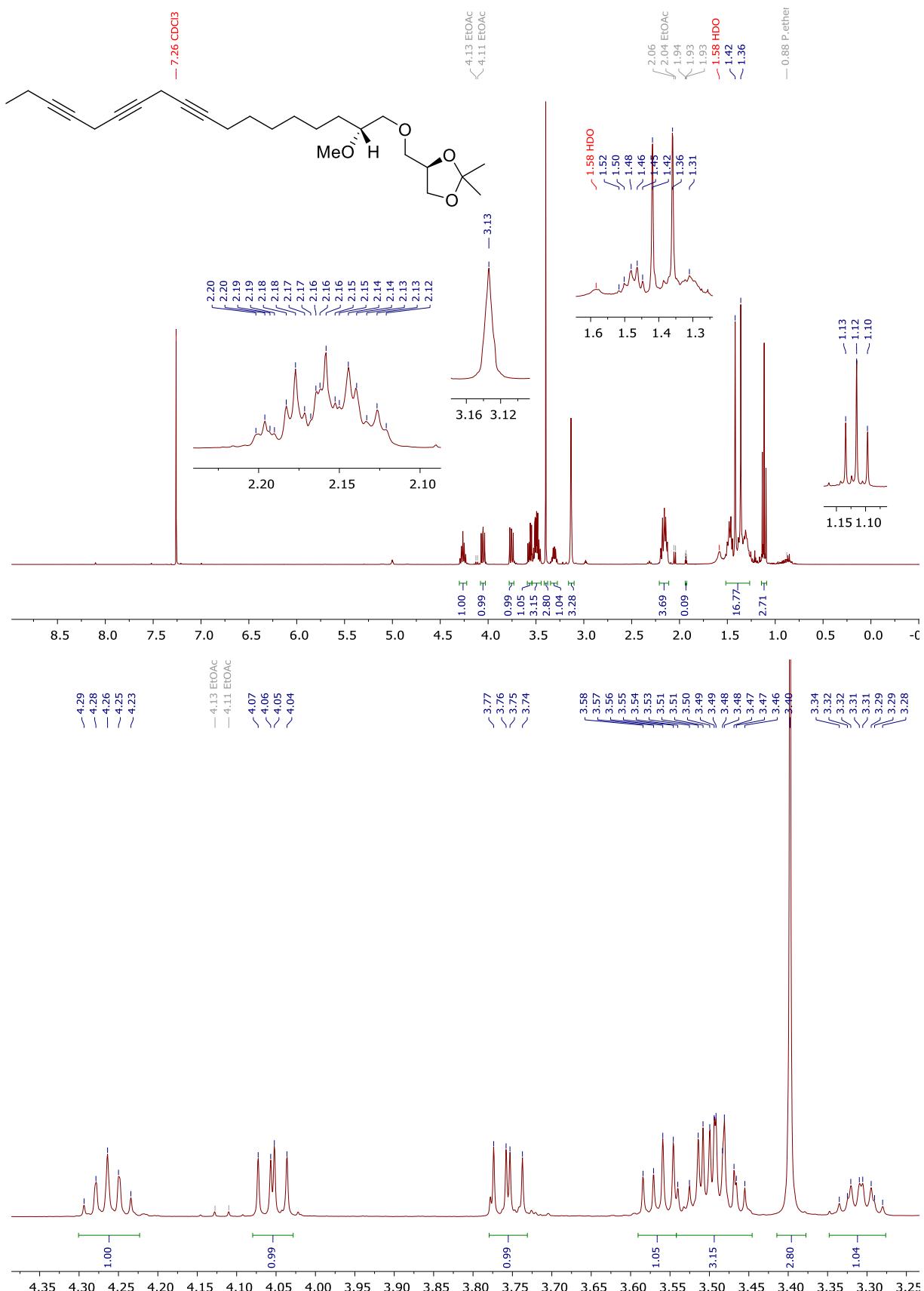
Svanur Sigurjónsson and Guðmundur G. Haraldsson\*

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Iceland

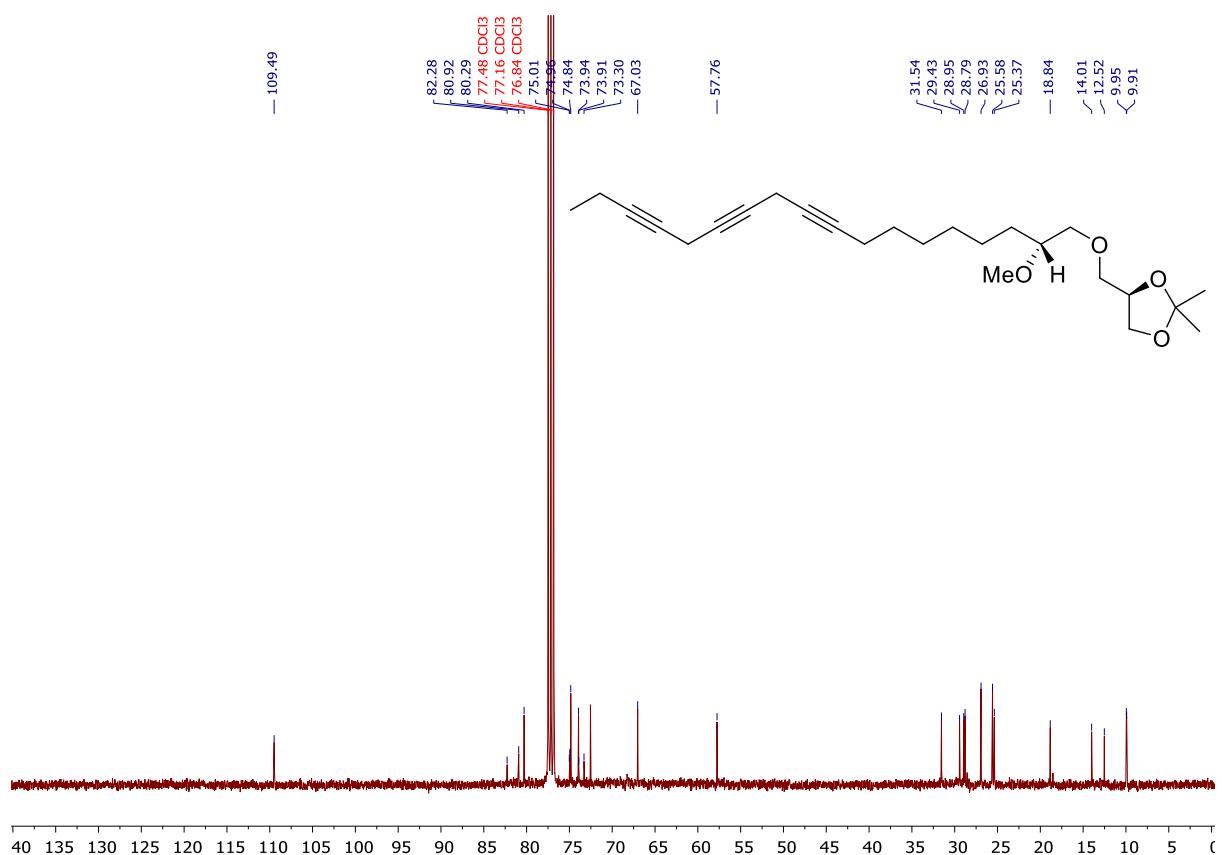
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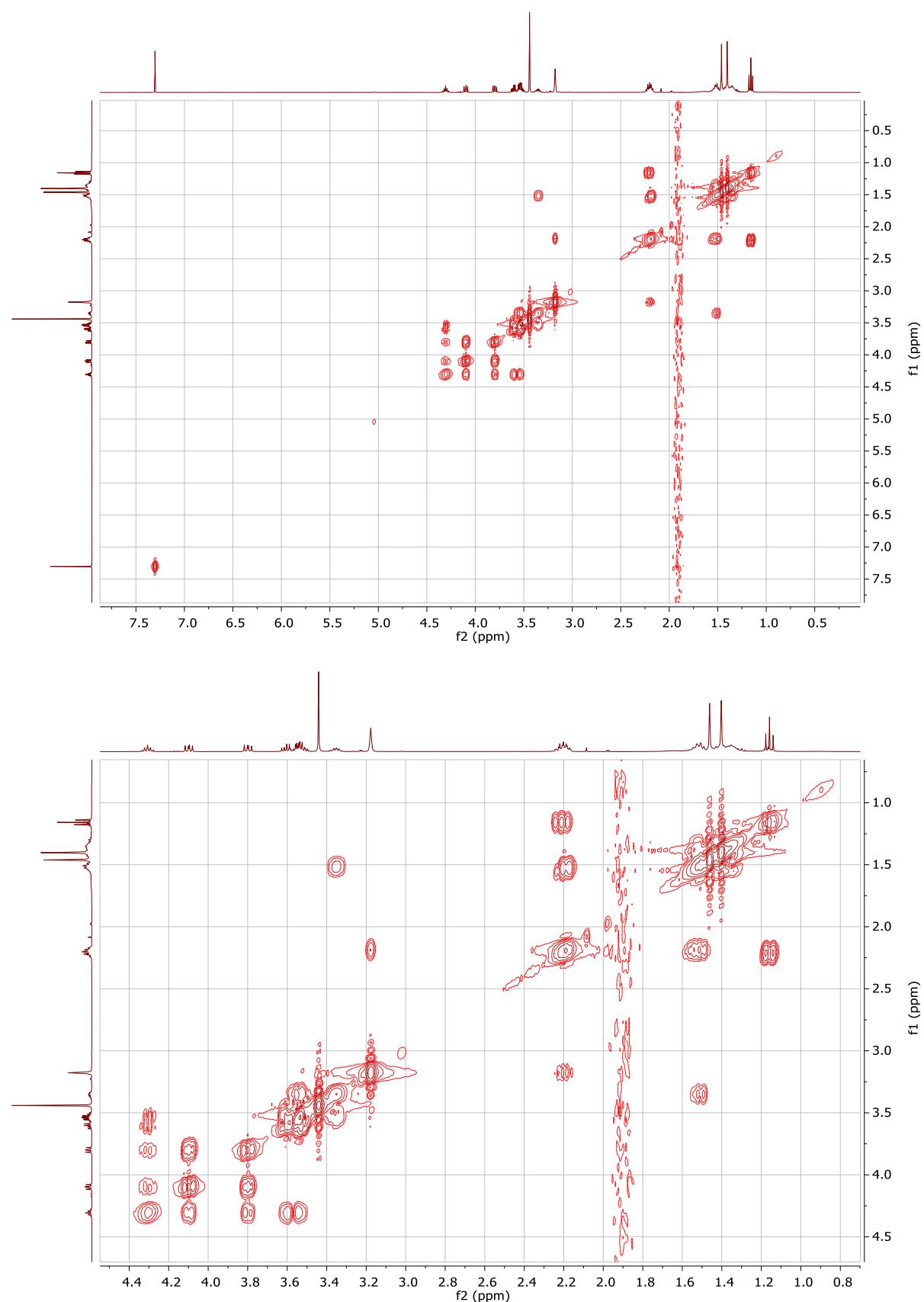
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **12**



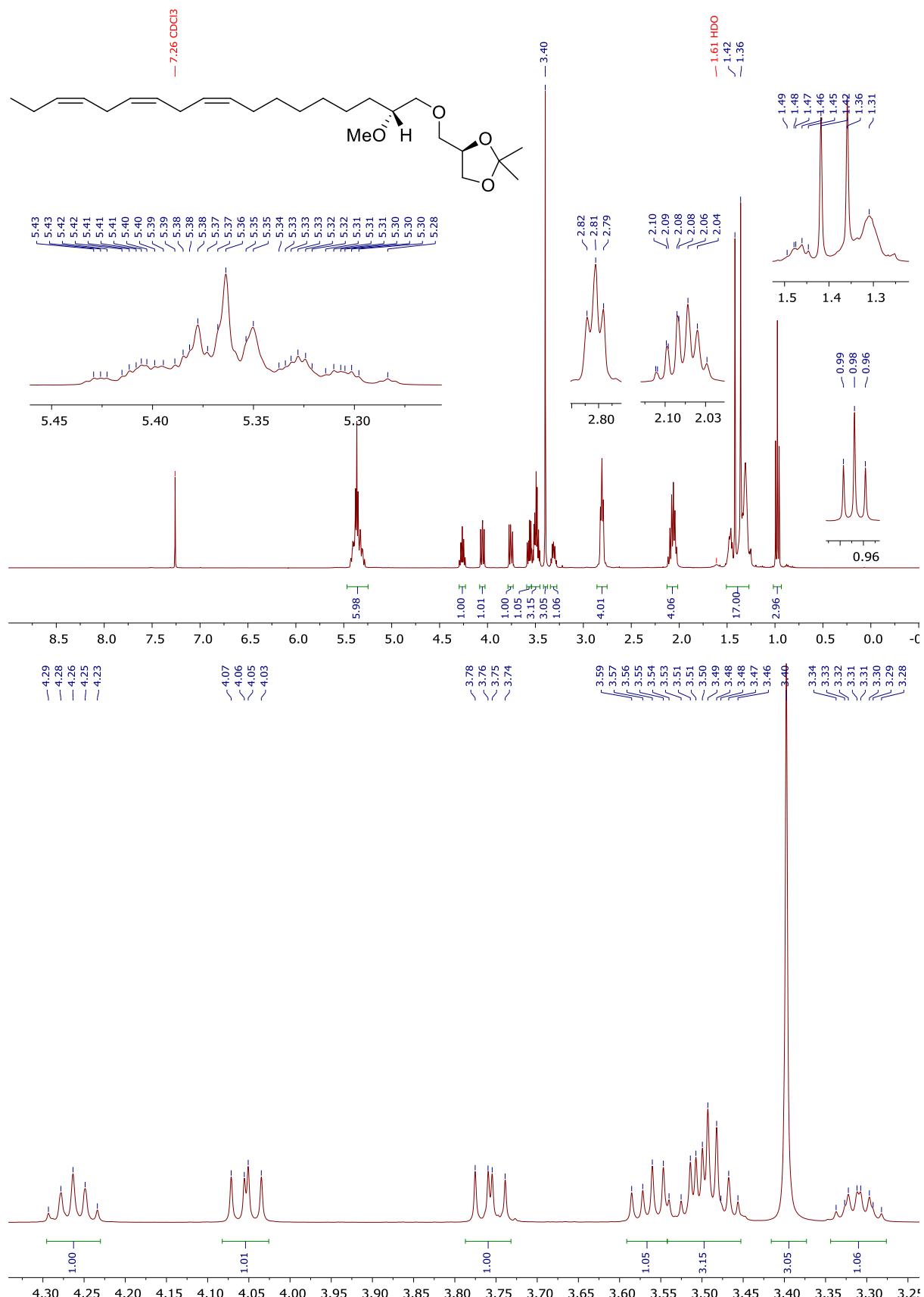
<sup>13</sup>C{H} NMR (101 MHz, CDCl<sub>3</sub>) of compound **12**



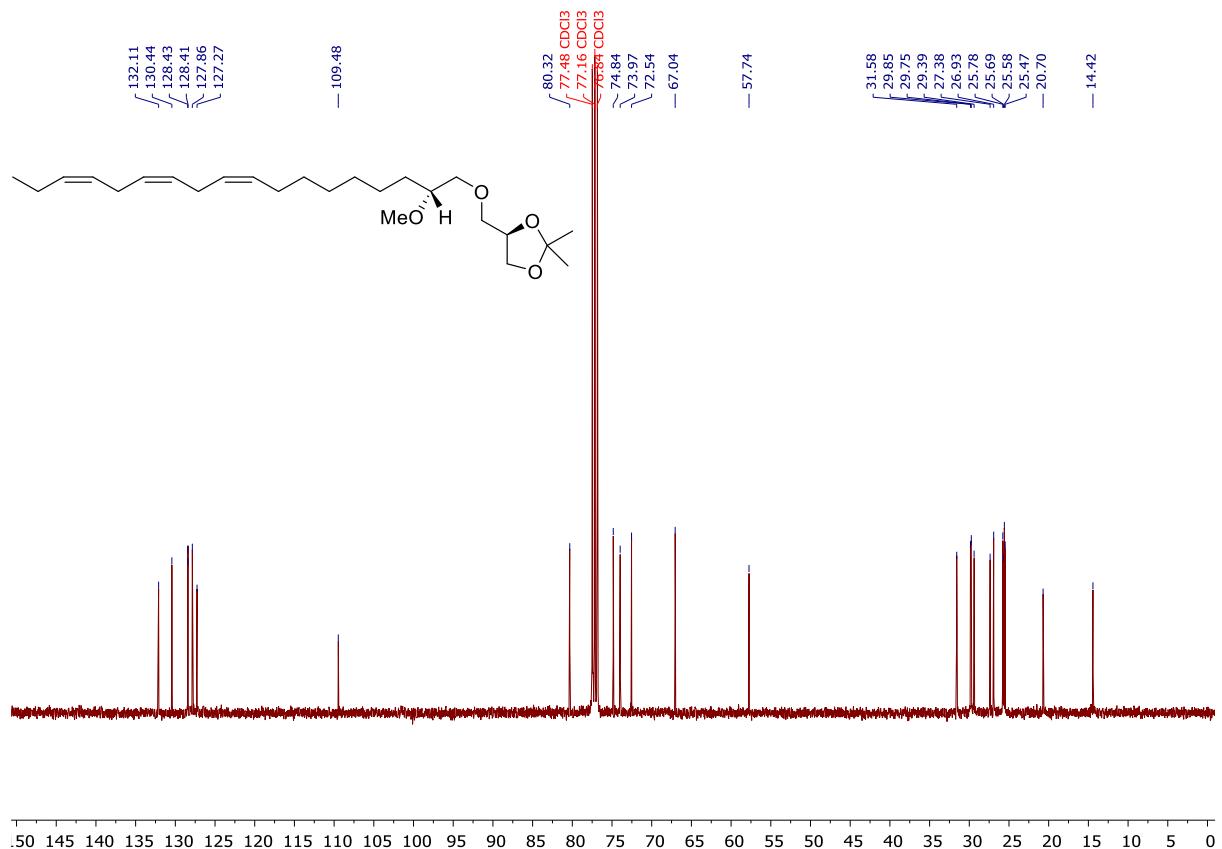
$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **12**



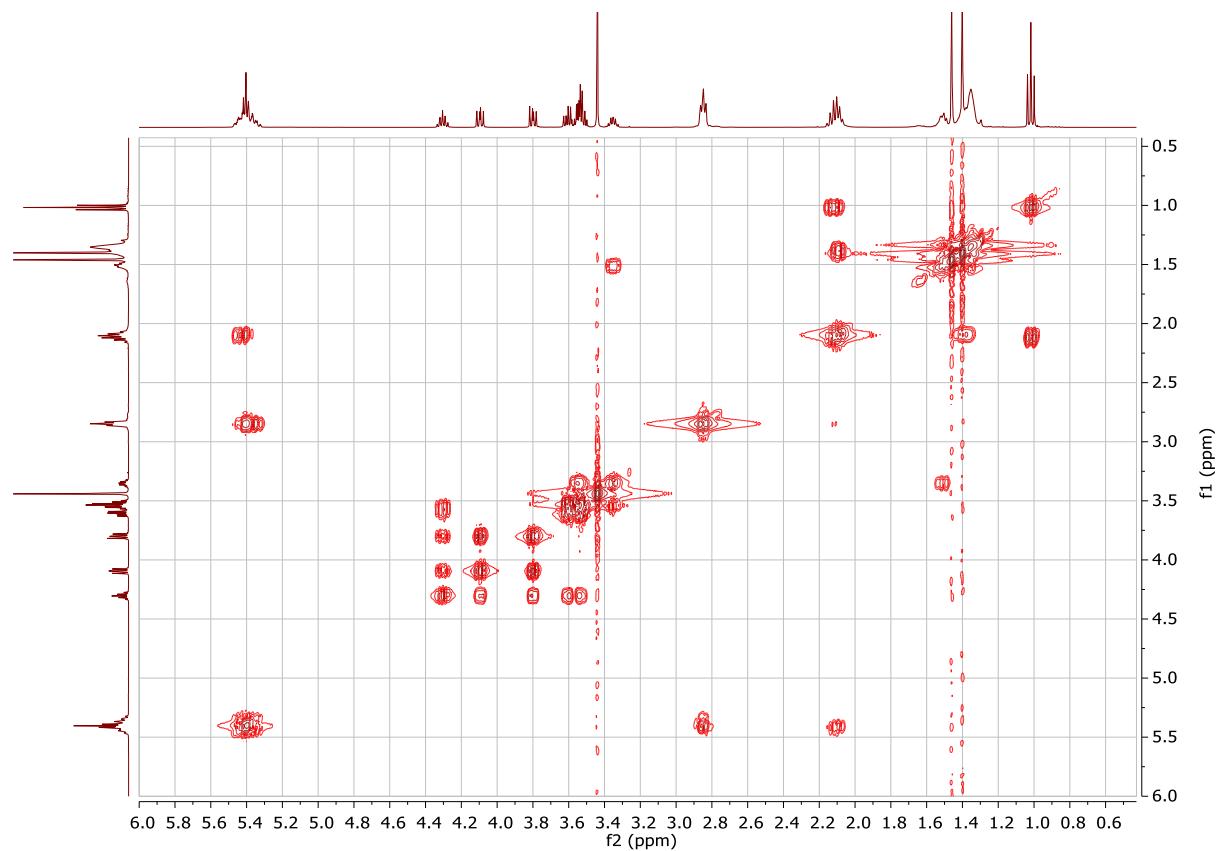
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **13**



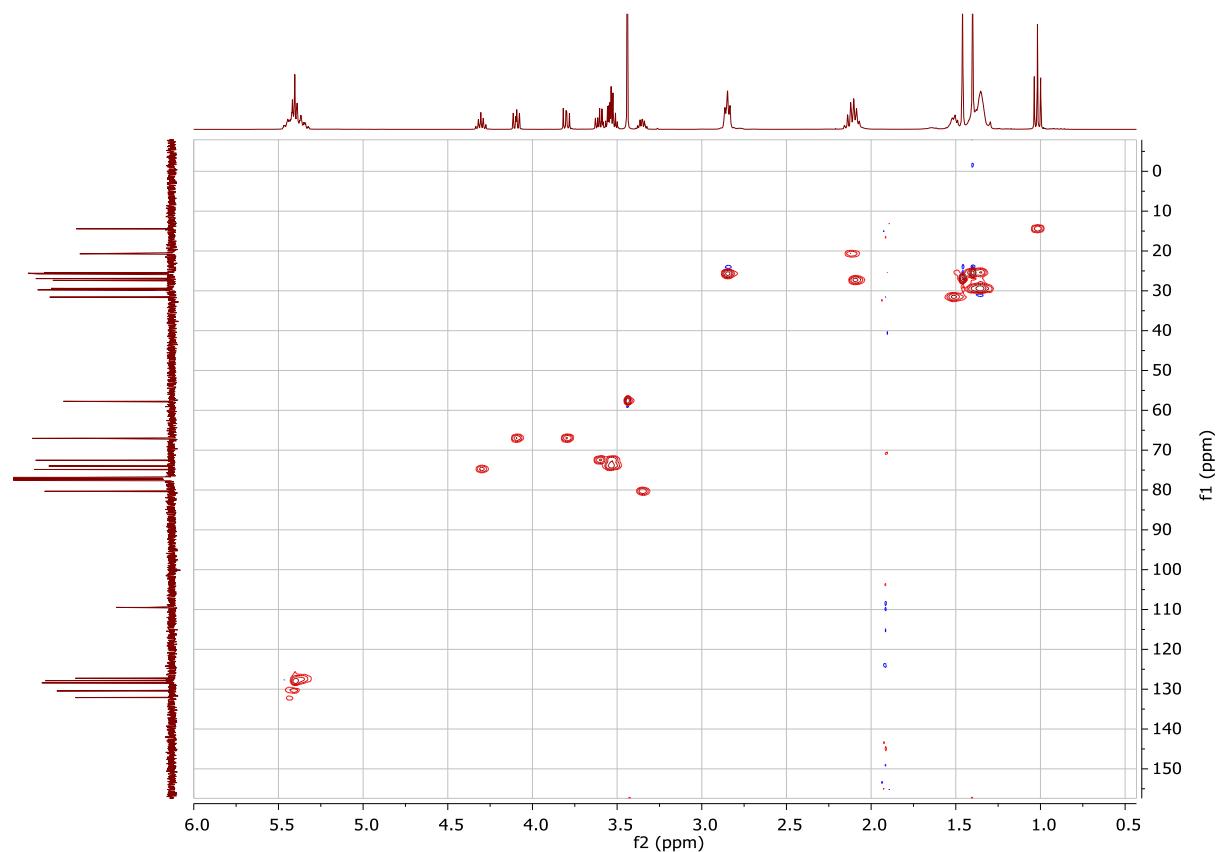
<sup>13</sup>C{H} NMR (101 MHz, CDCl<sub>3</sub>) of compound **13**



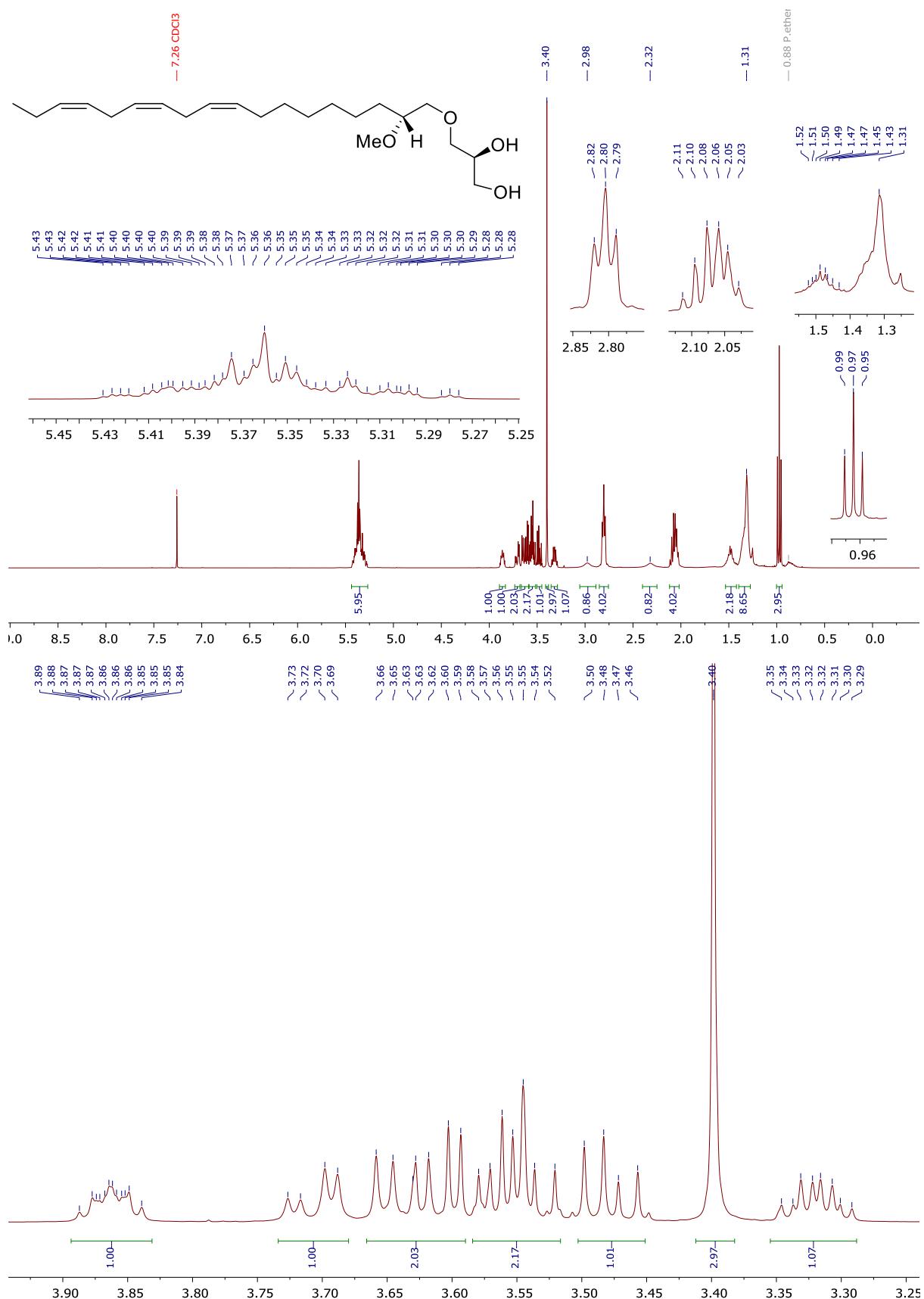
$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **13**



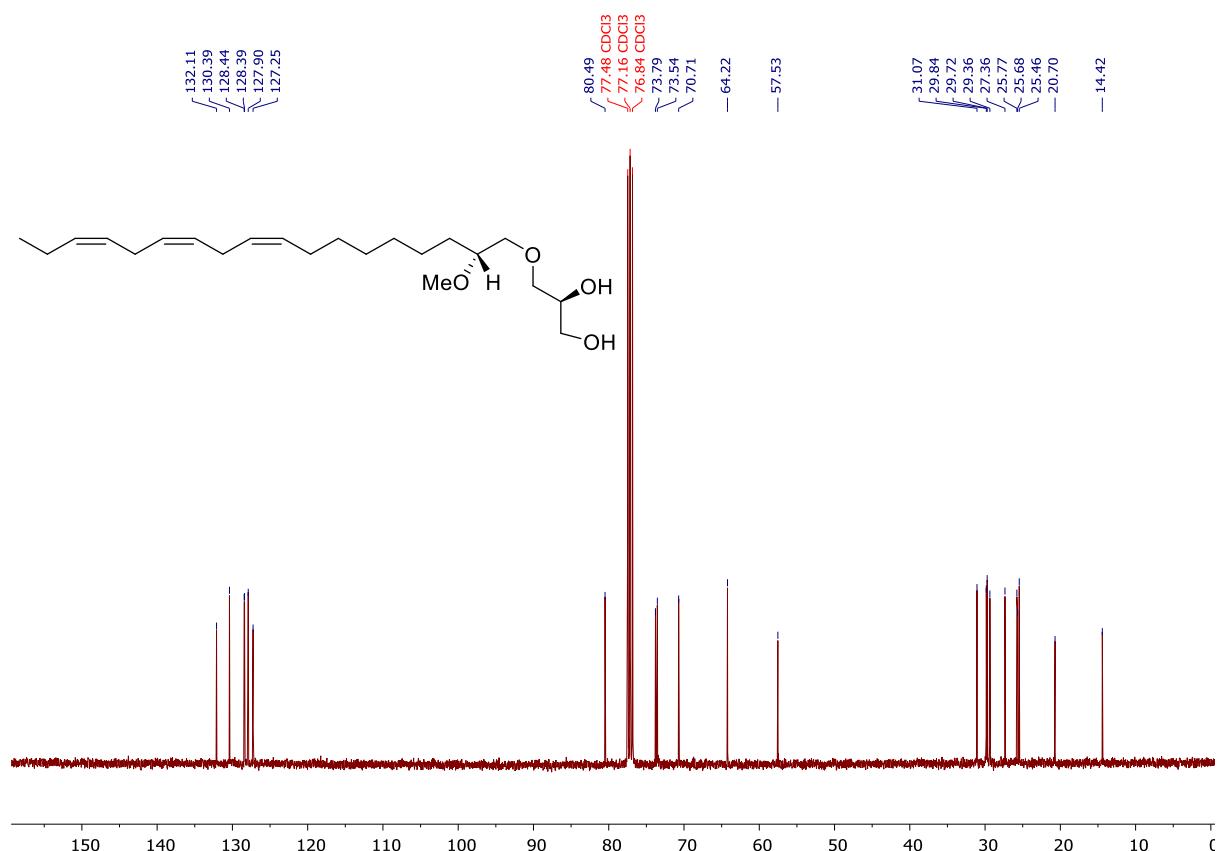
$^{13}\text{C}$ - $^1\text{H}$  HSQC spectrum of compound **13**



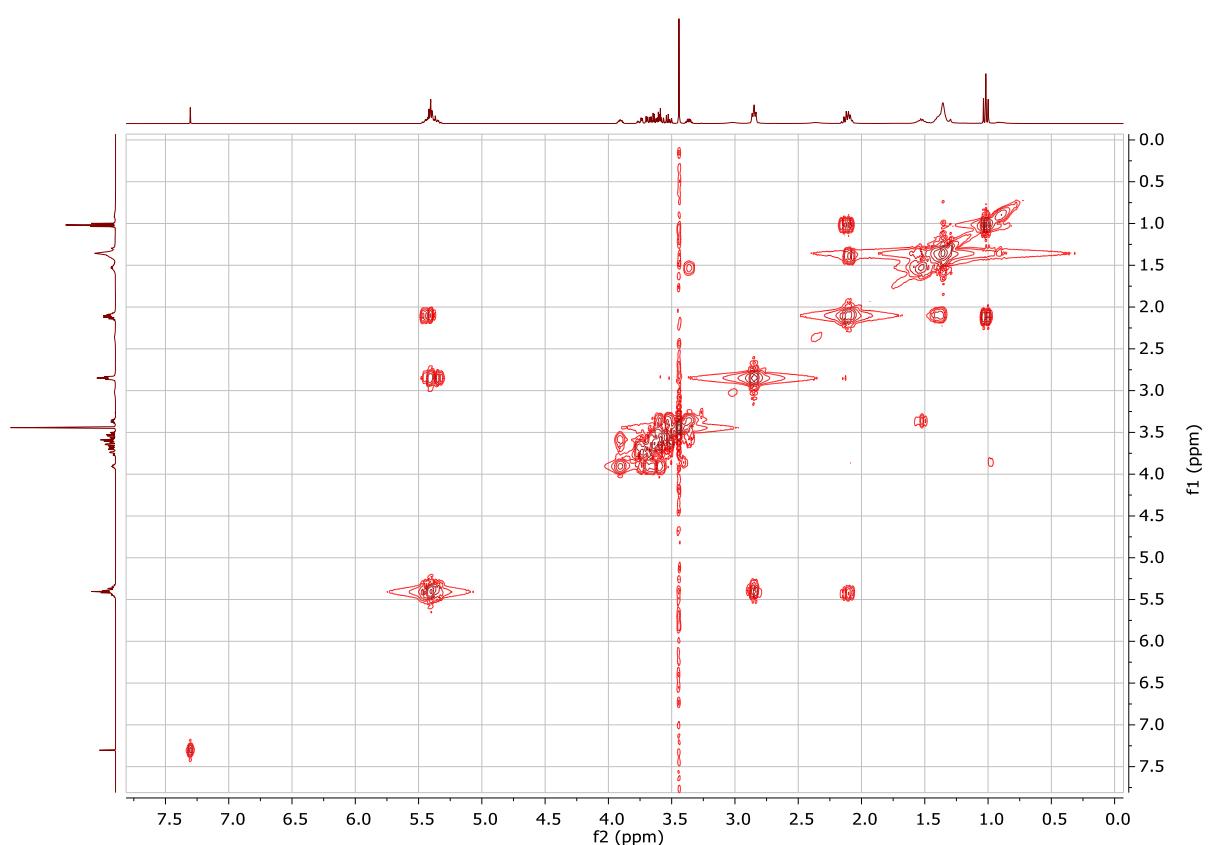
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of MEL 5

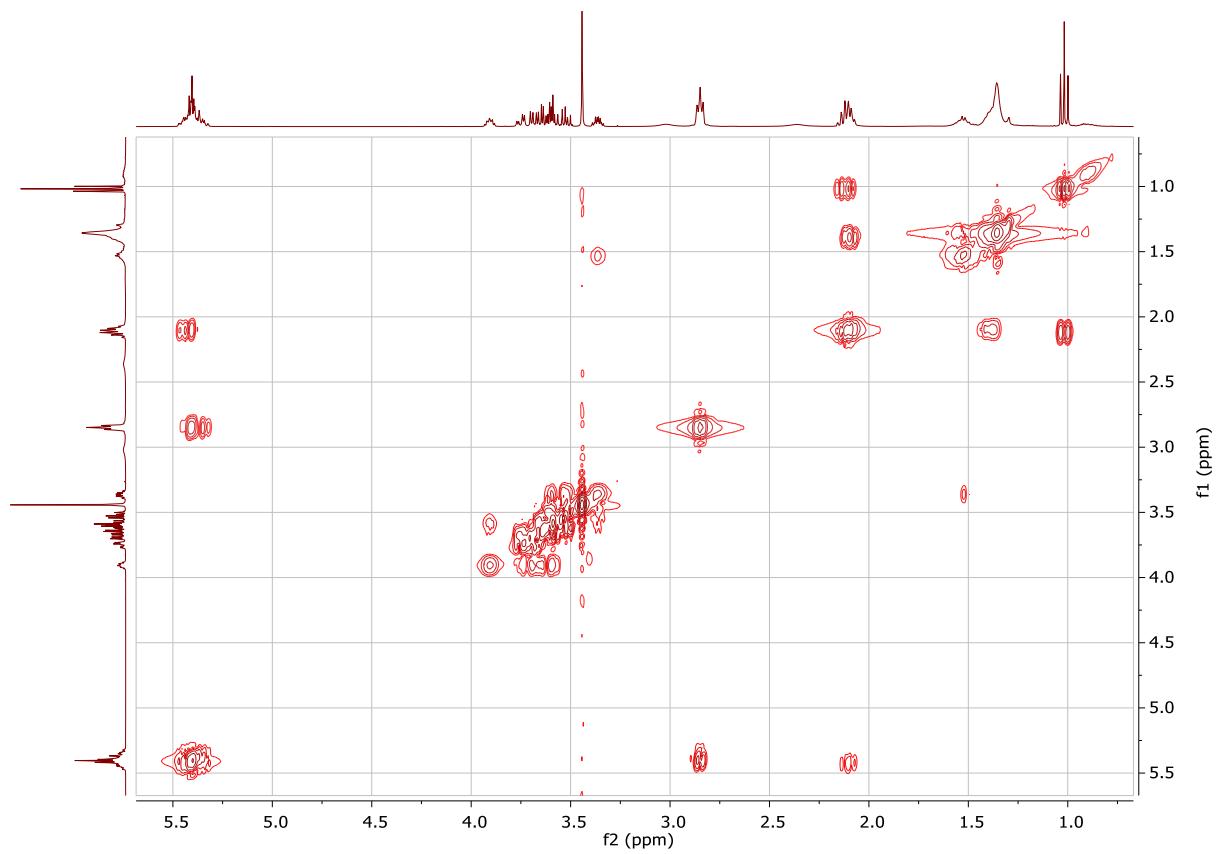


$^{13}\text{C}\{\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ ) of MEL 5

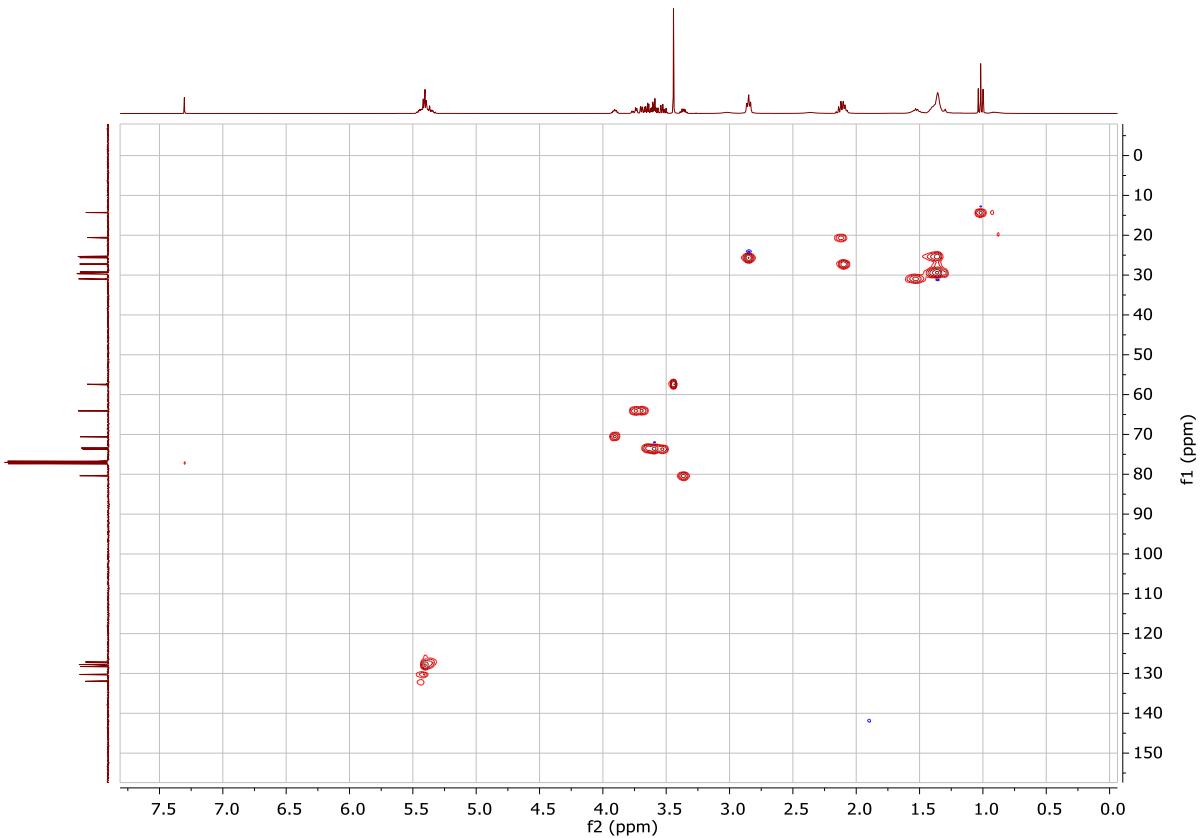


$^1\text{H}$ - $^1\text{H}$  COSY spectrum of MEL 5

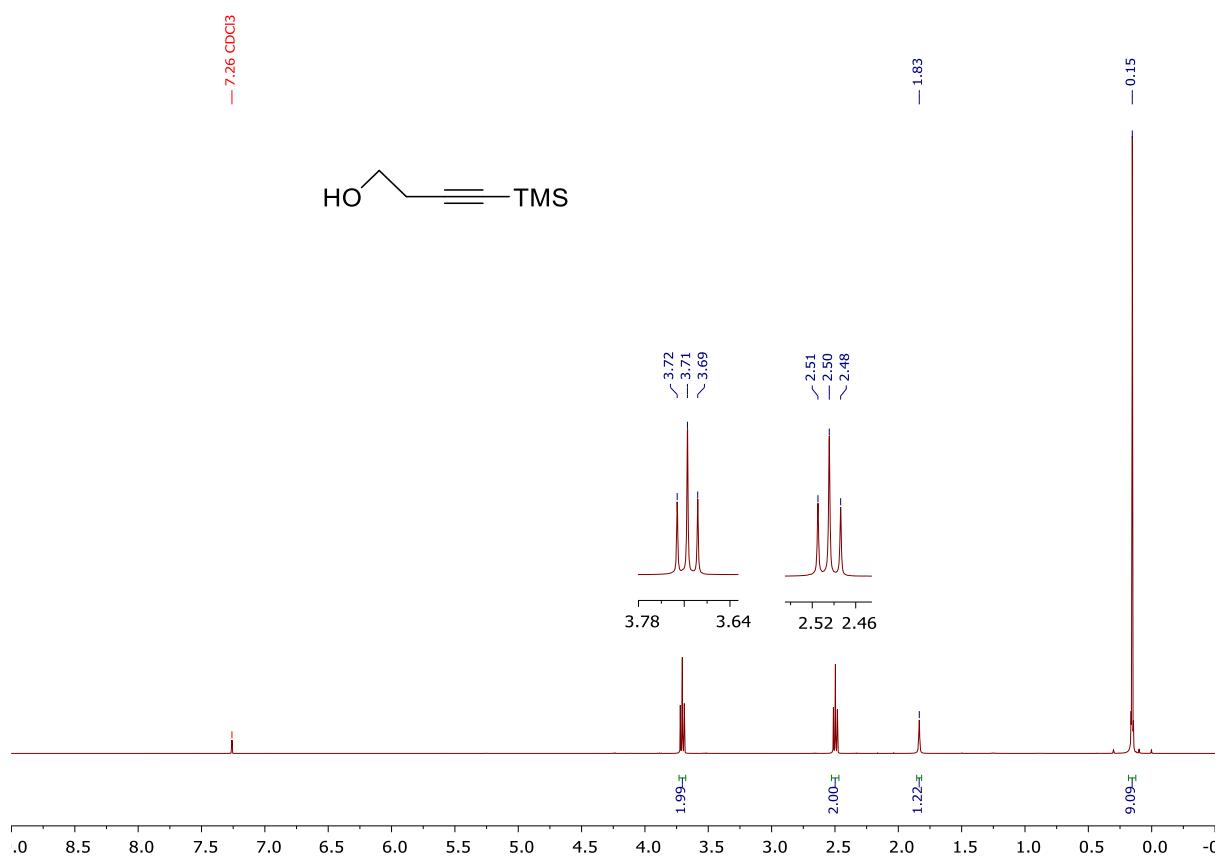




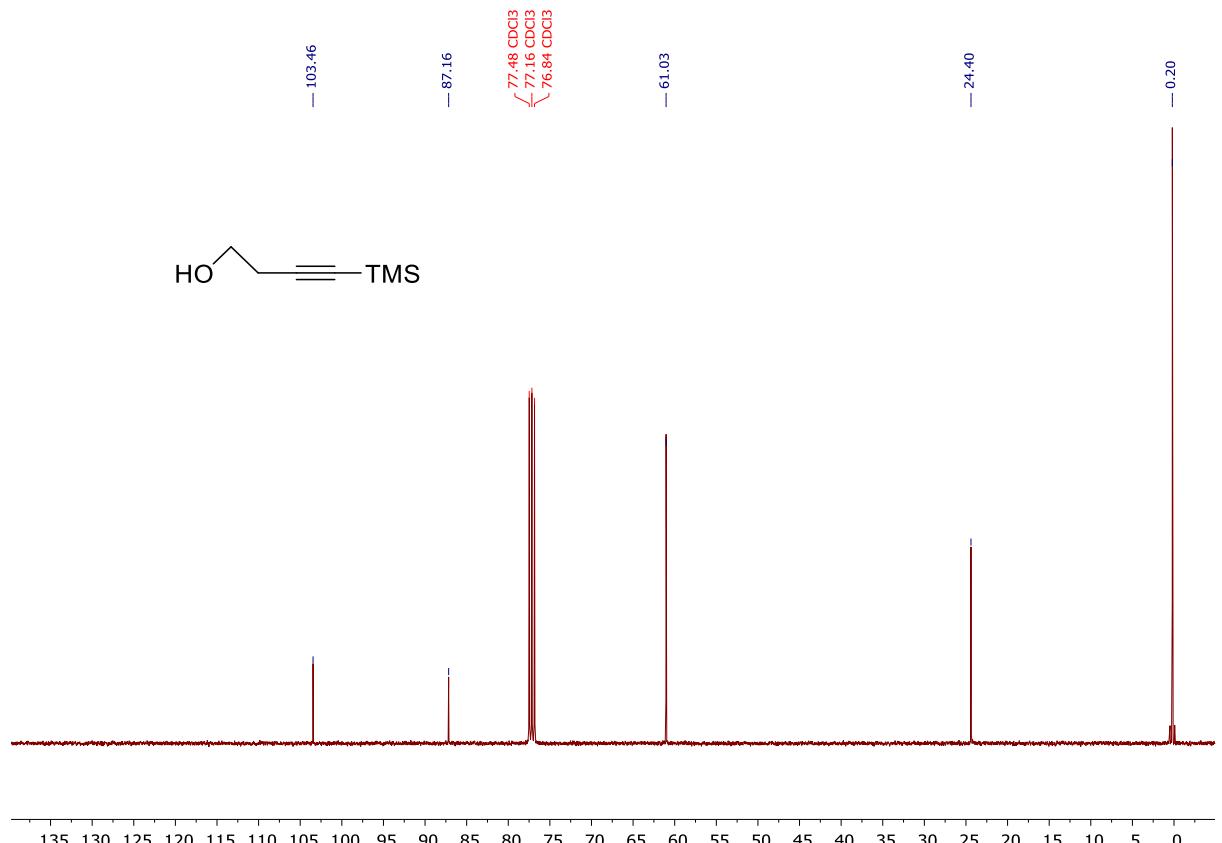
$^{13}\text{C}$ - $^1\text{H}$  HSQC spectrum of MEL 5



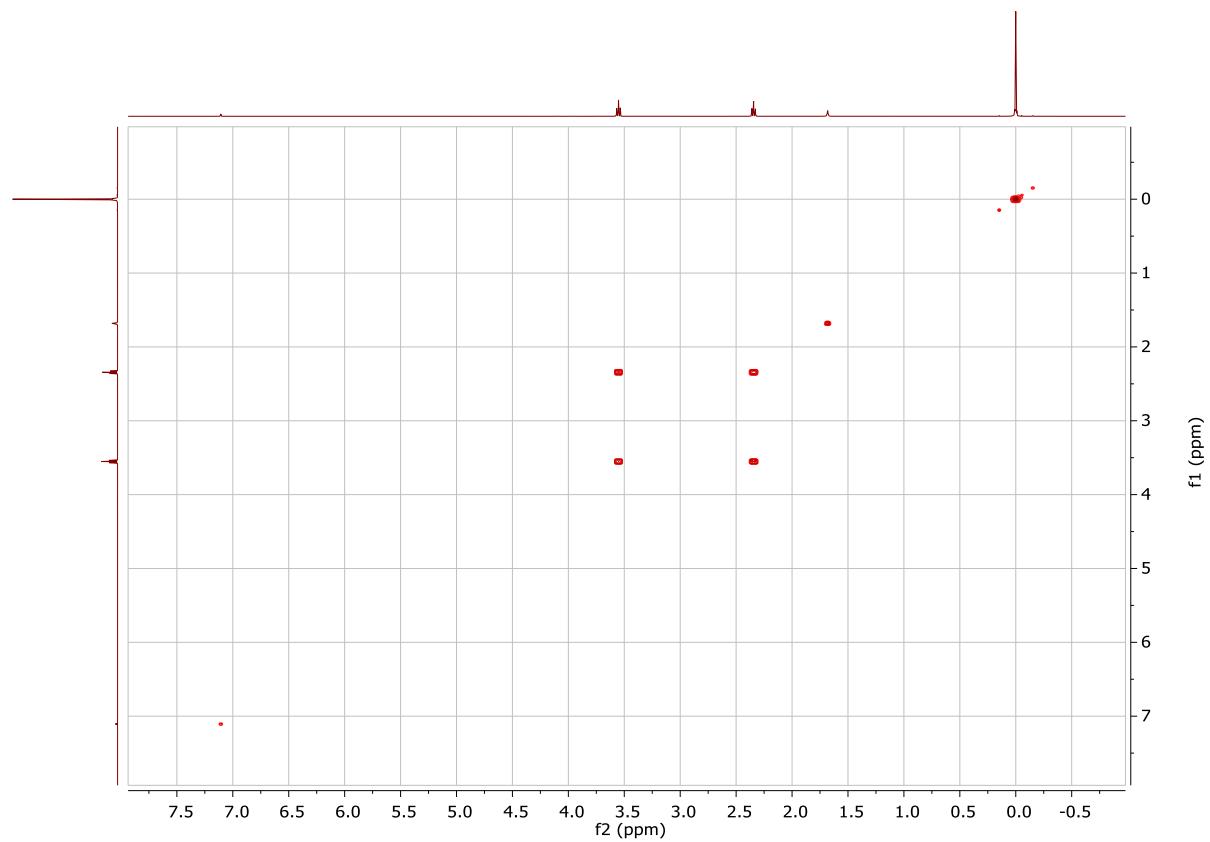
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **14**



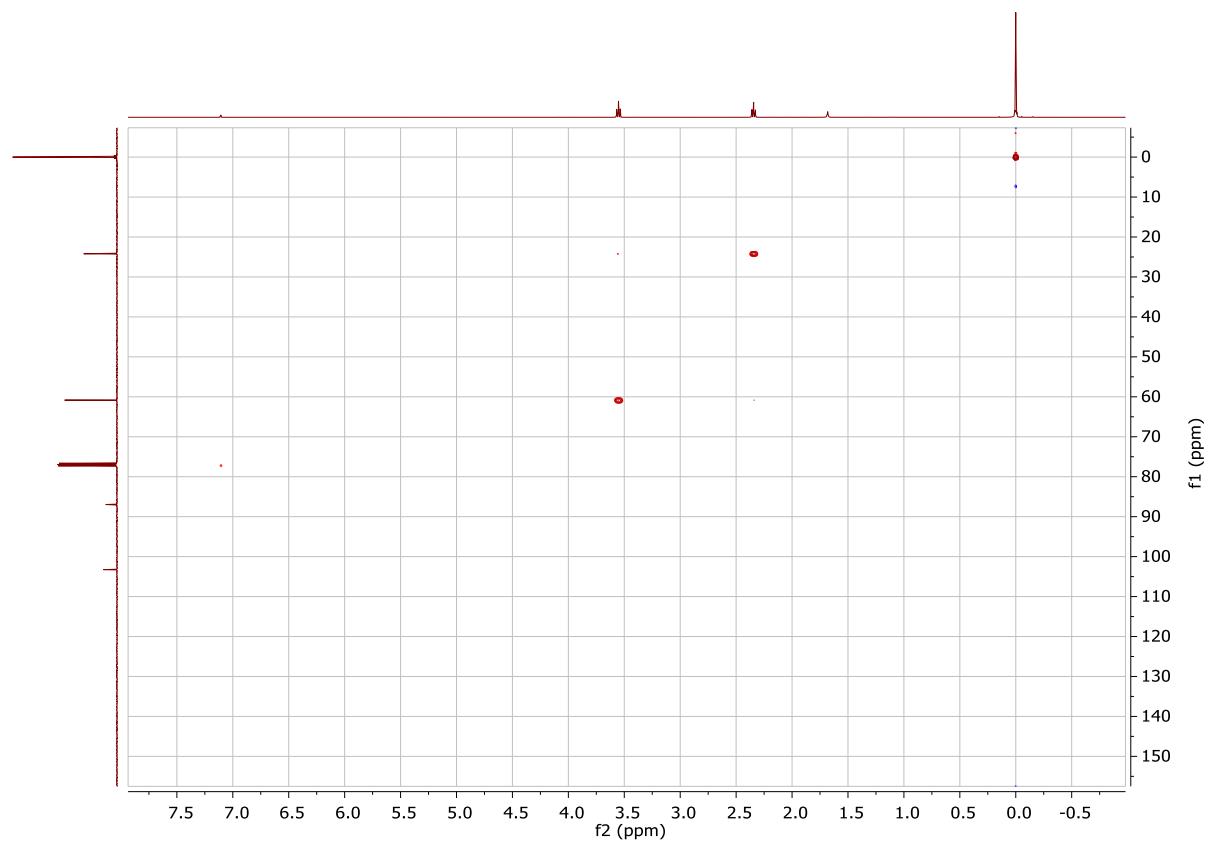
<sup>13</sup>C{H} NMR (101 MHz, CDCl<sub>3</sub>) of compound **14**



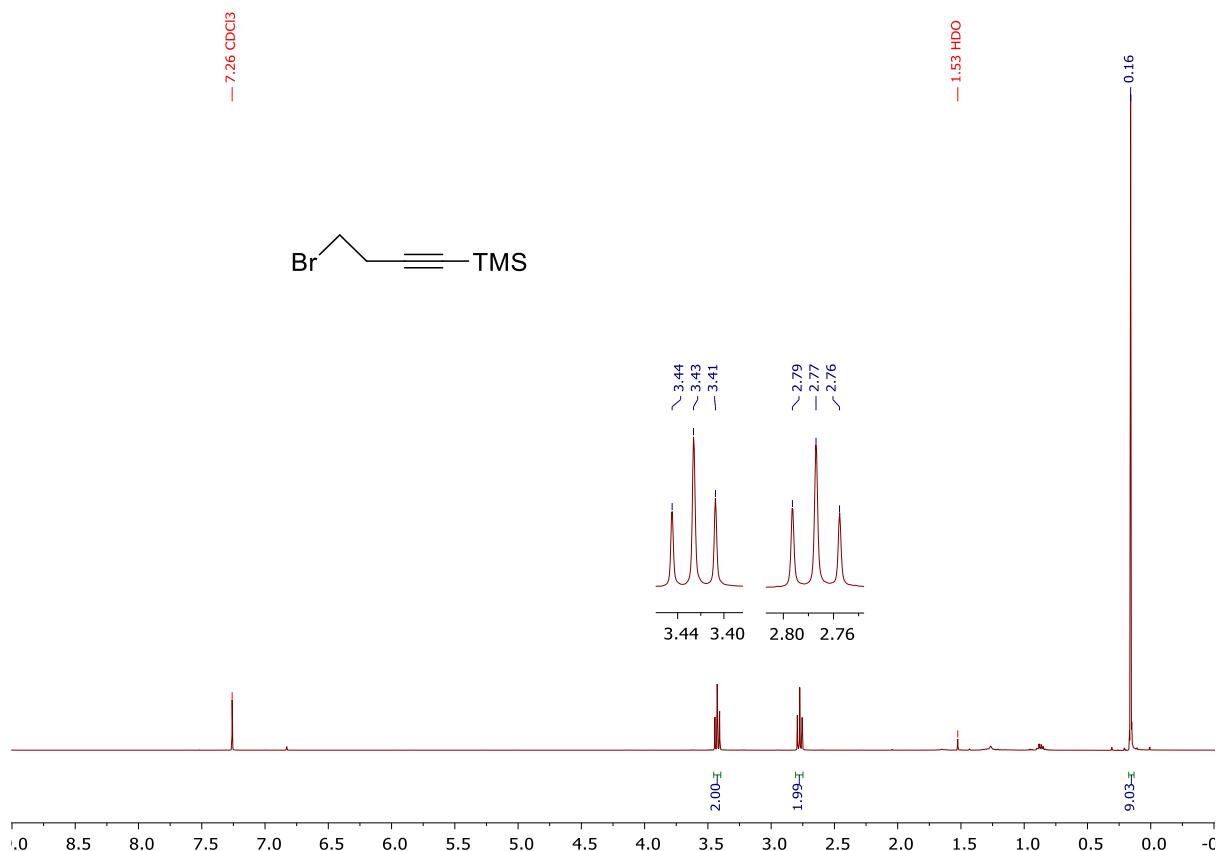
$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **14**



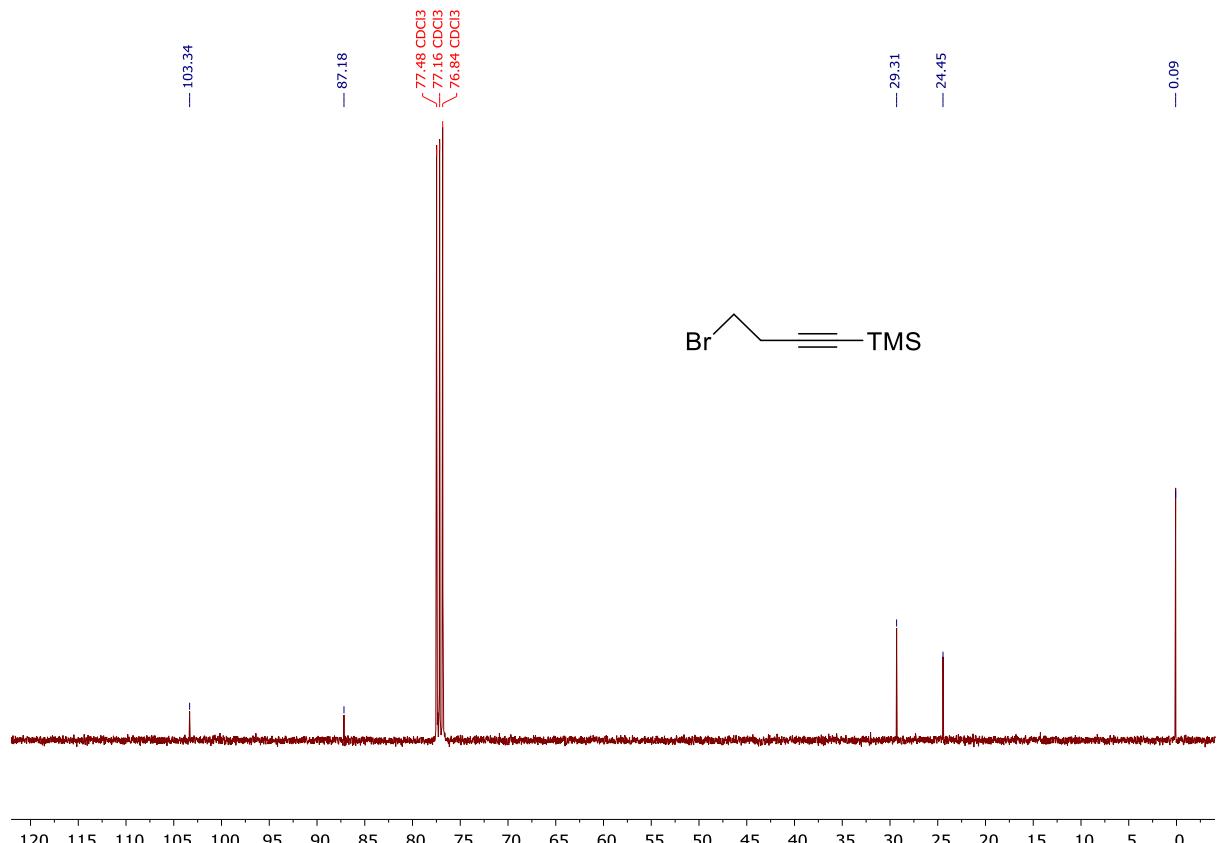
$^{13}\text{C}$ - $^1\text{H}$  HSQC spectrum of compound **14**



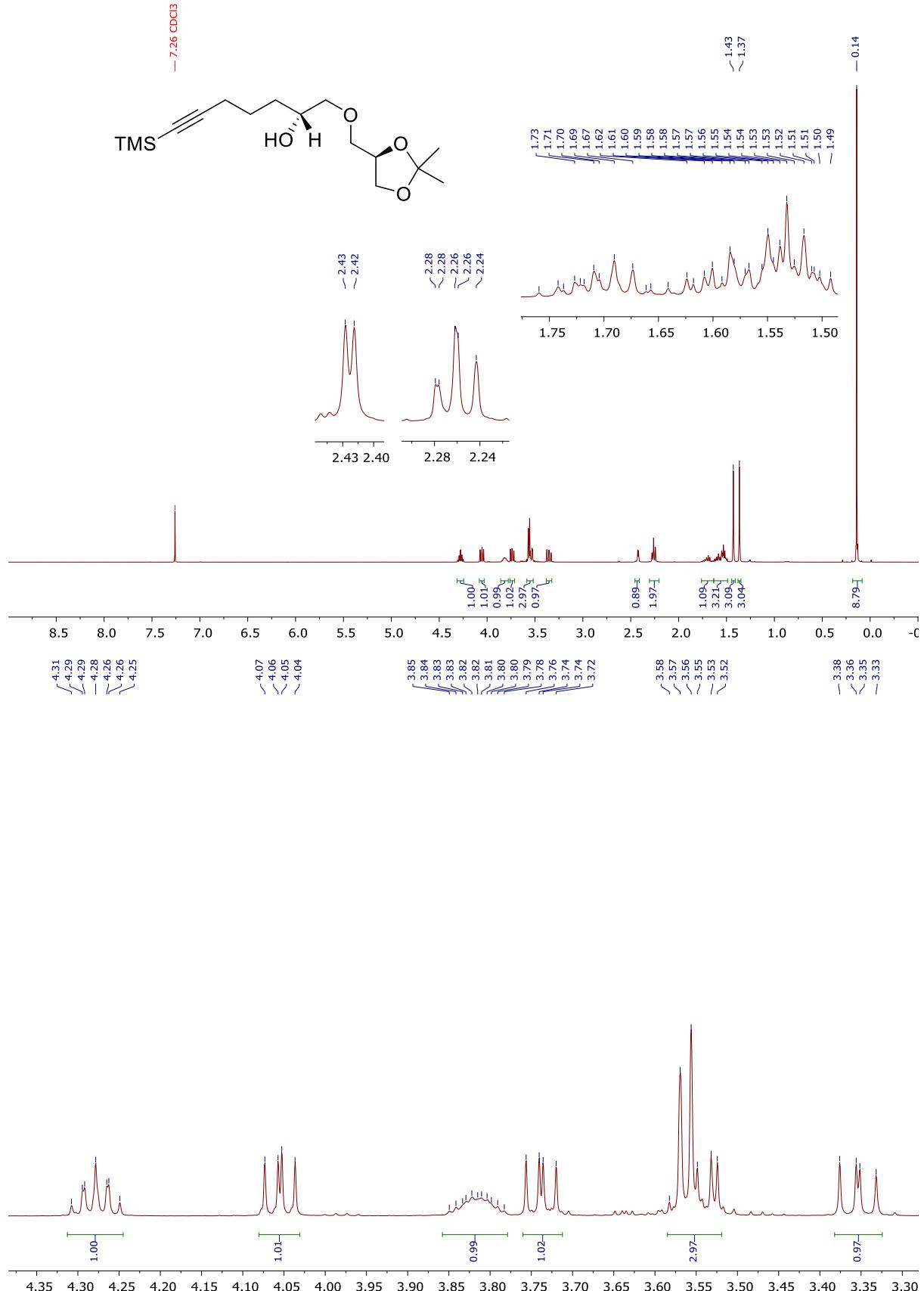
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **15**



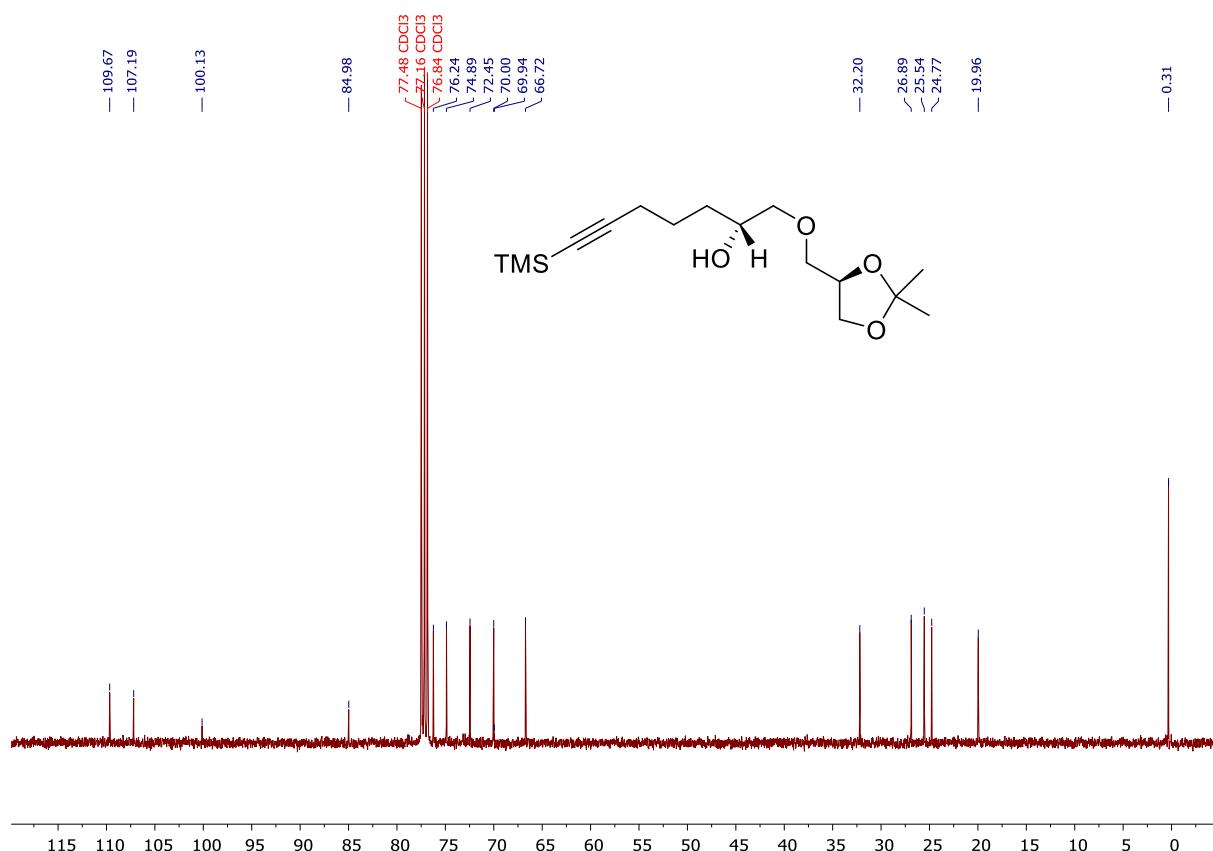
<sup>13</sup>C{H} NMR (101 MHz, CDCl<sub>3</sub>) of compound **15**



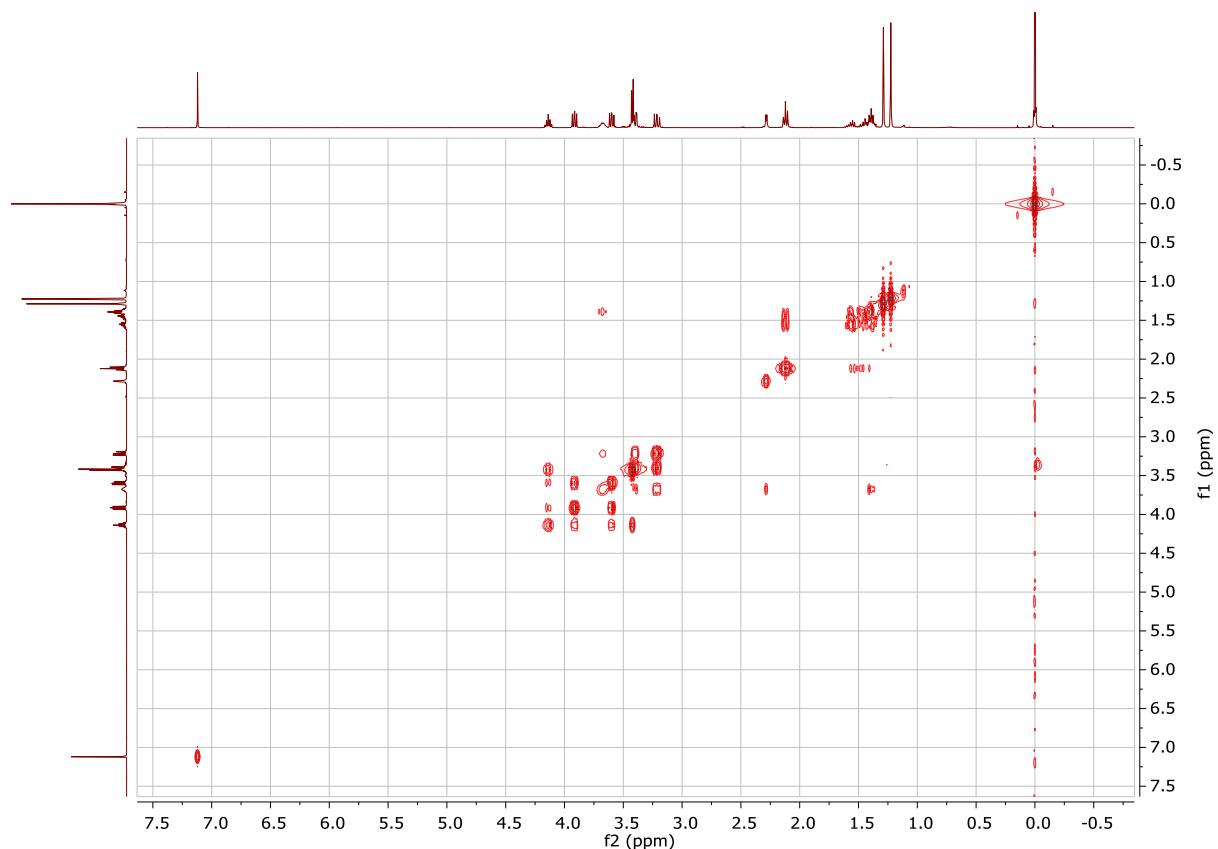
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **16**

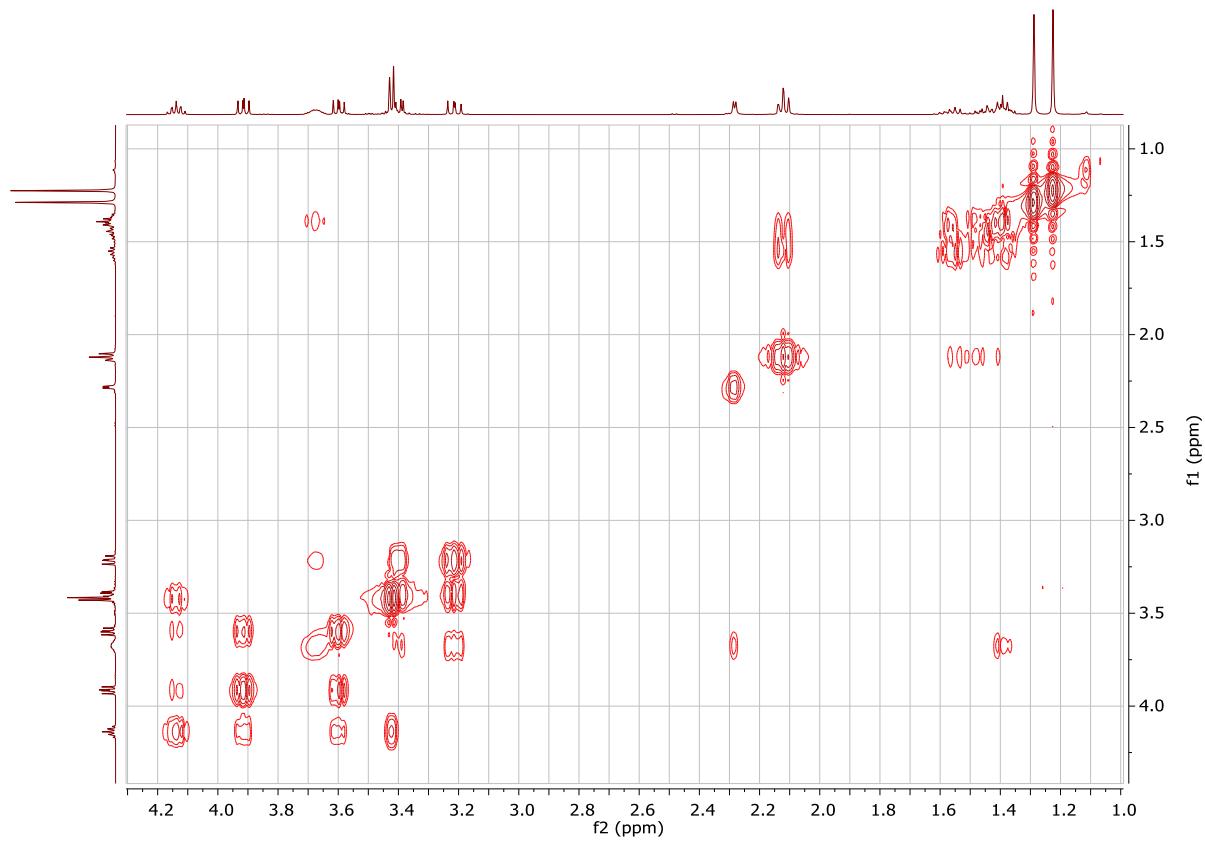


$^{13}\text{C}\{\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ ) of compound **16**

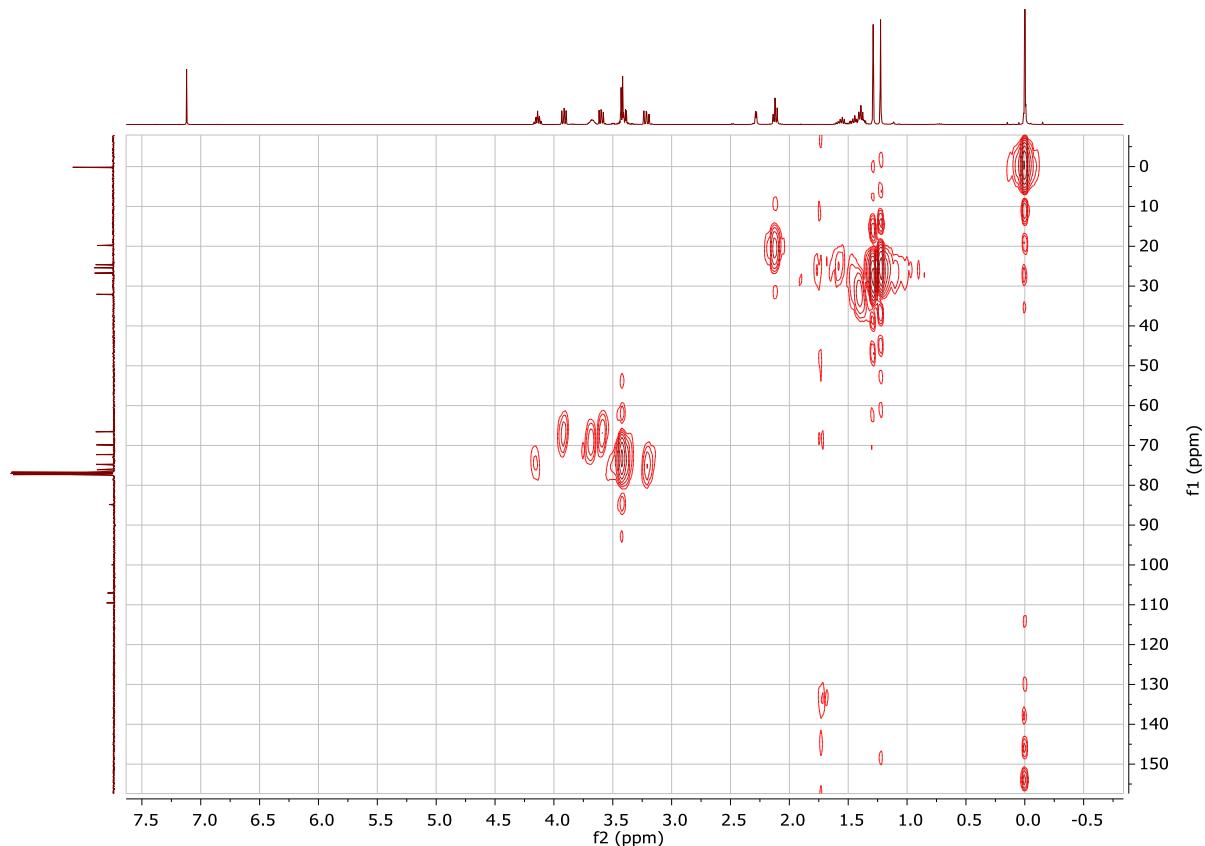


$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **16**

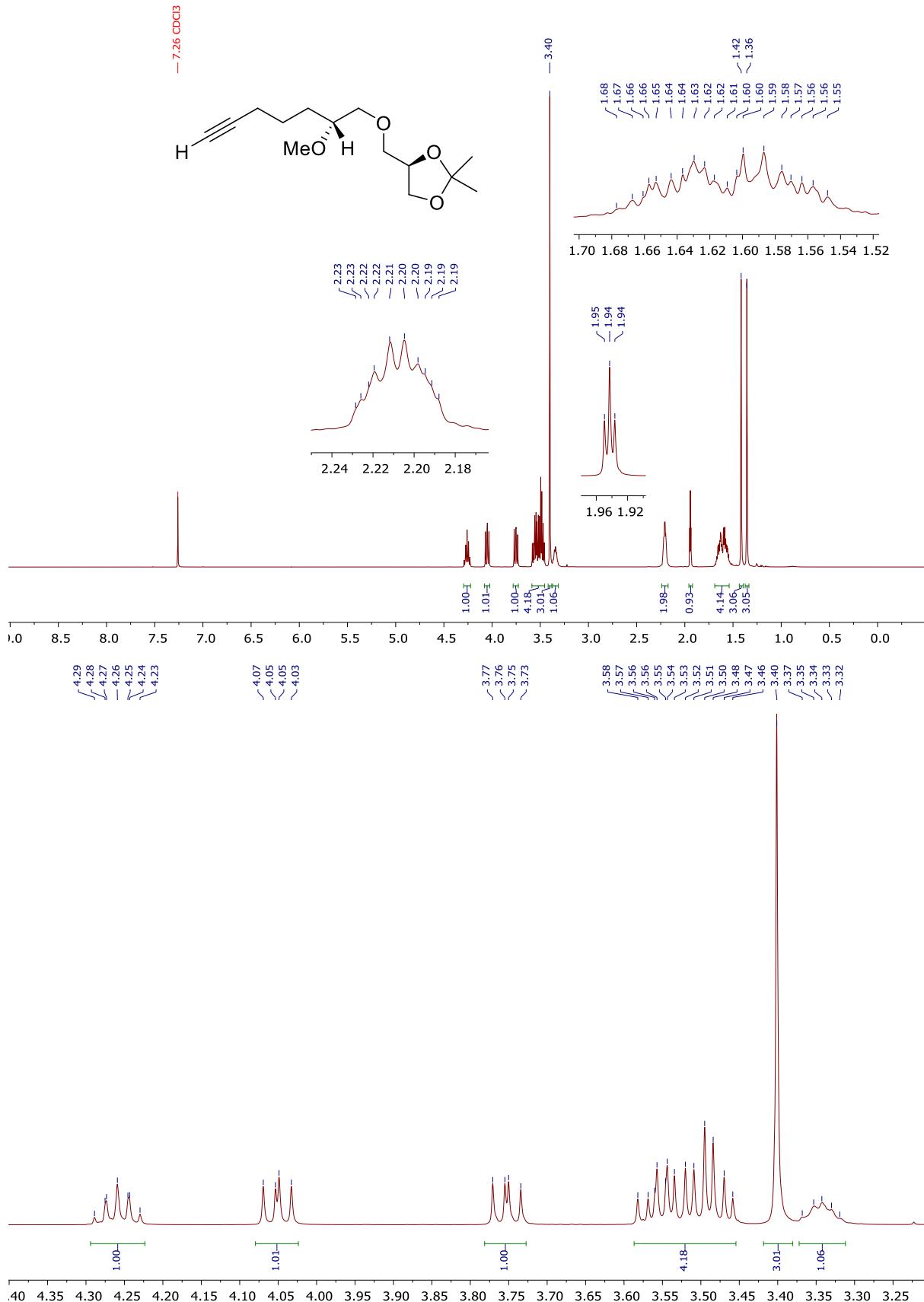




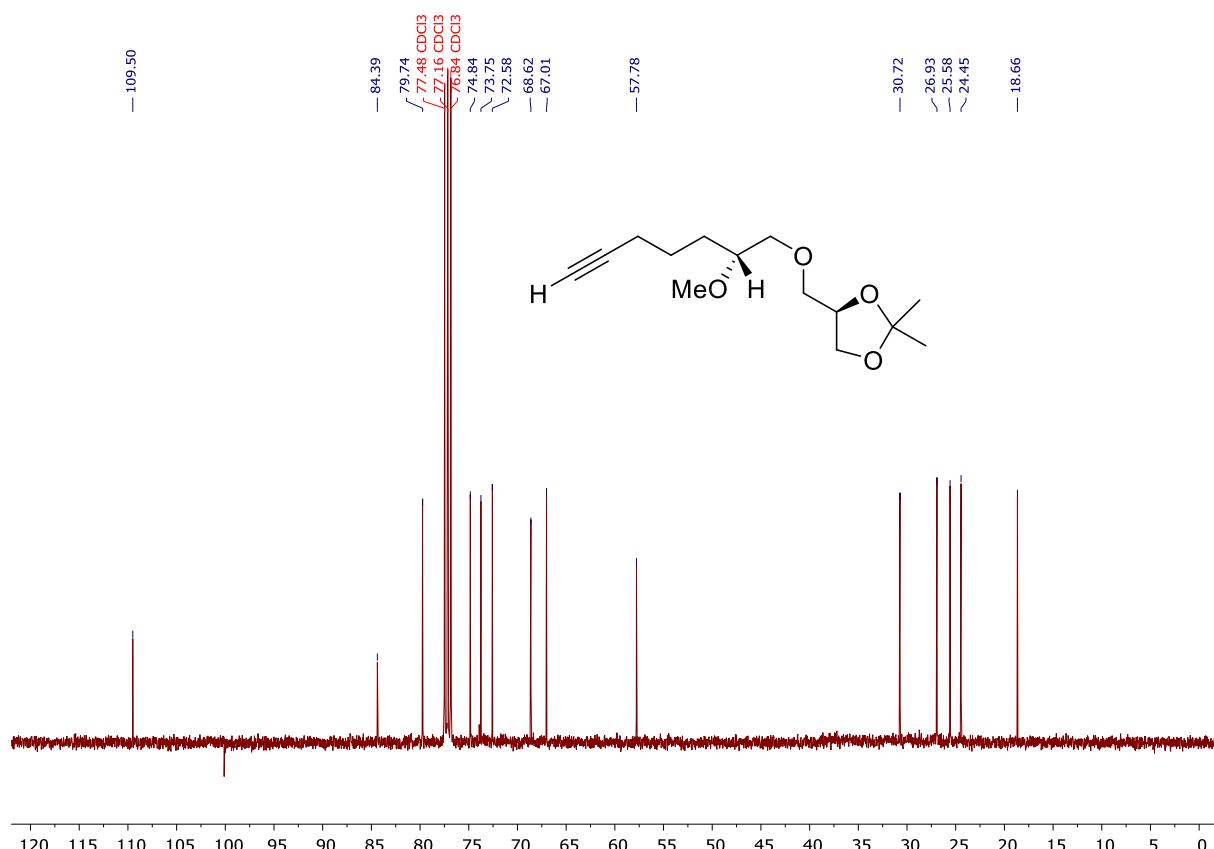
<sup>13</sup>C-<sup>1</sup>H HSQC spectrum of compound **16**



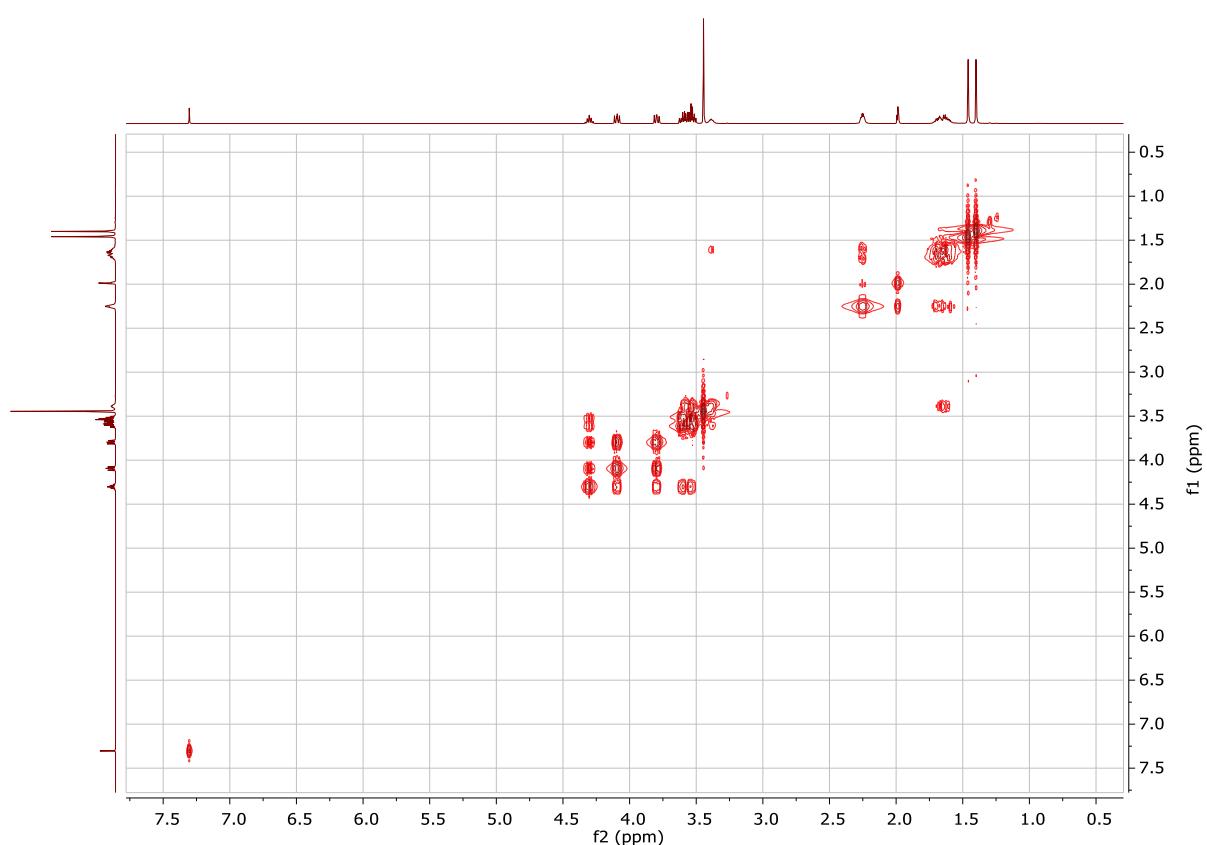
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **17**

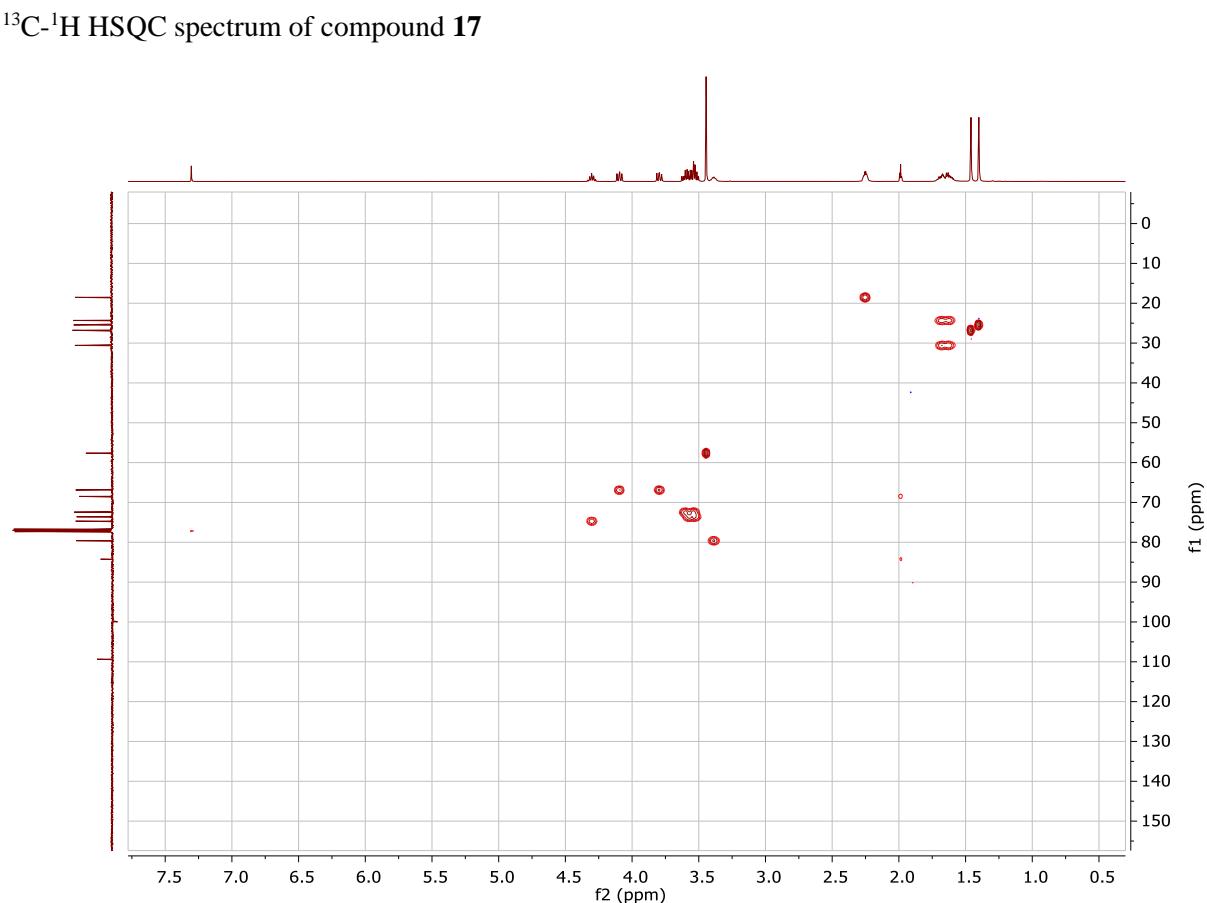
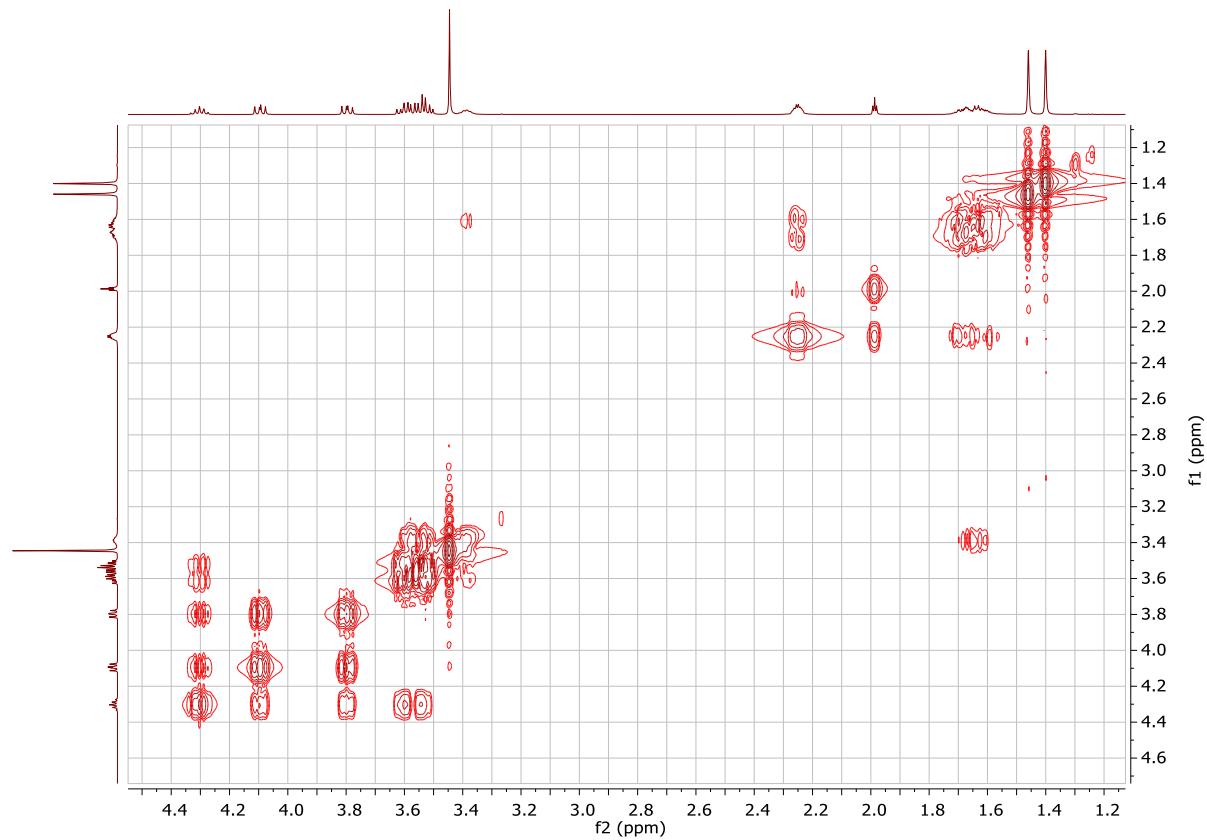


$^{13}\text{C}\{\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ ) of compound **17**

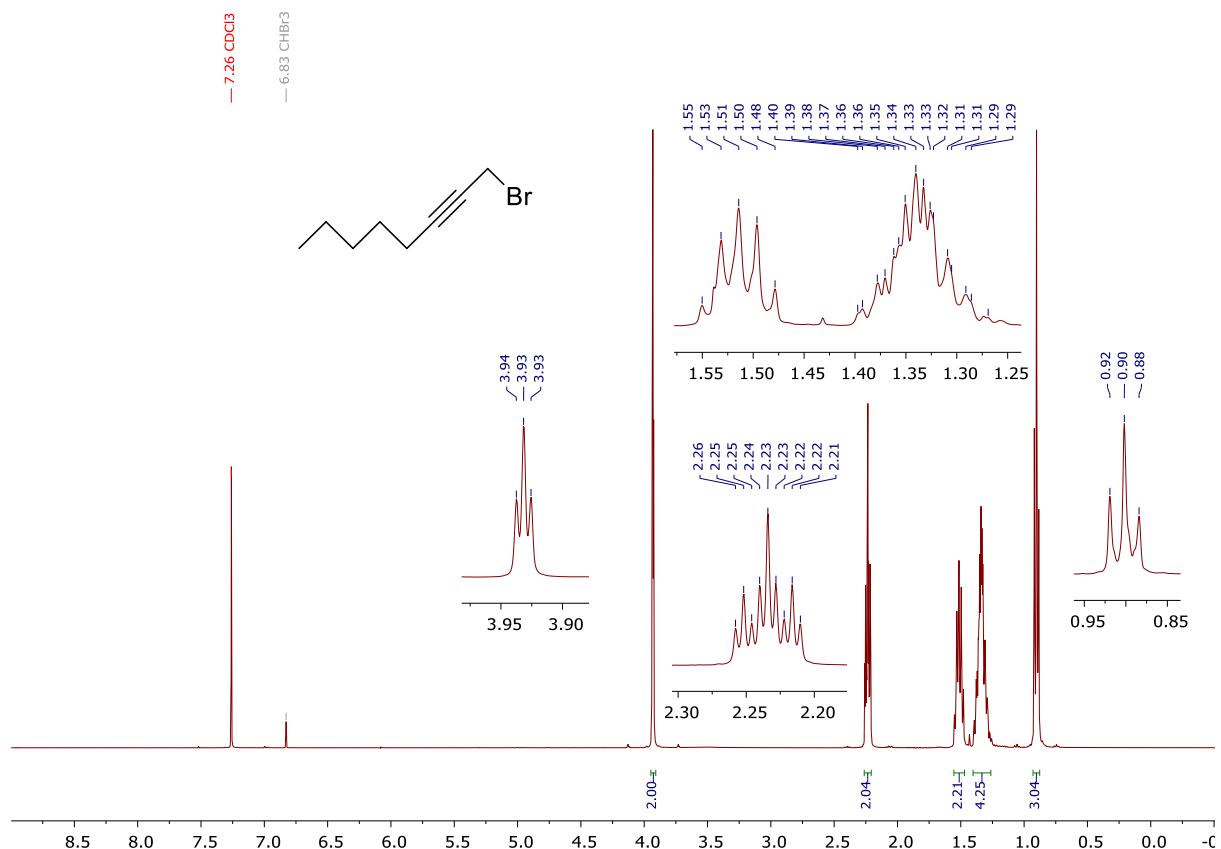


$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **17**

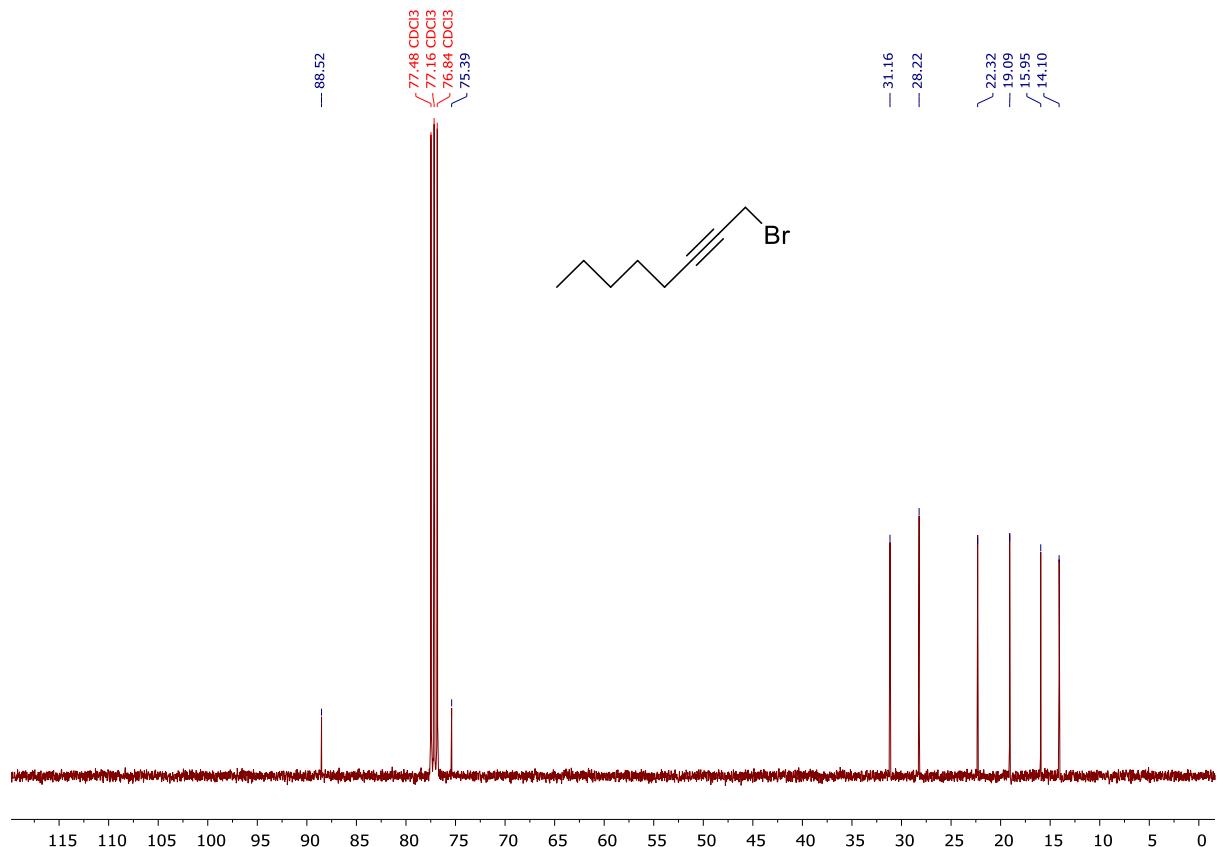




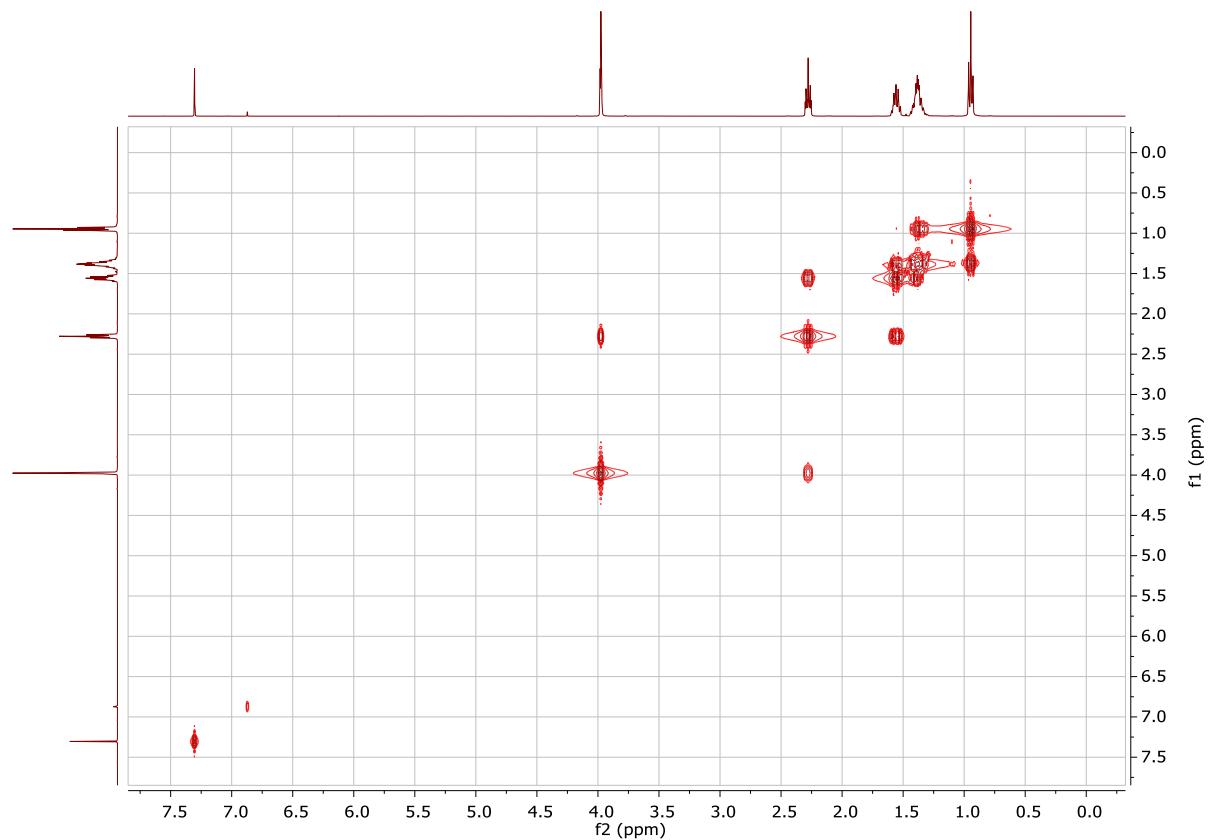
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **18**



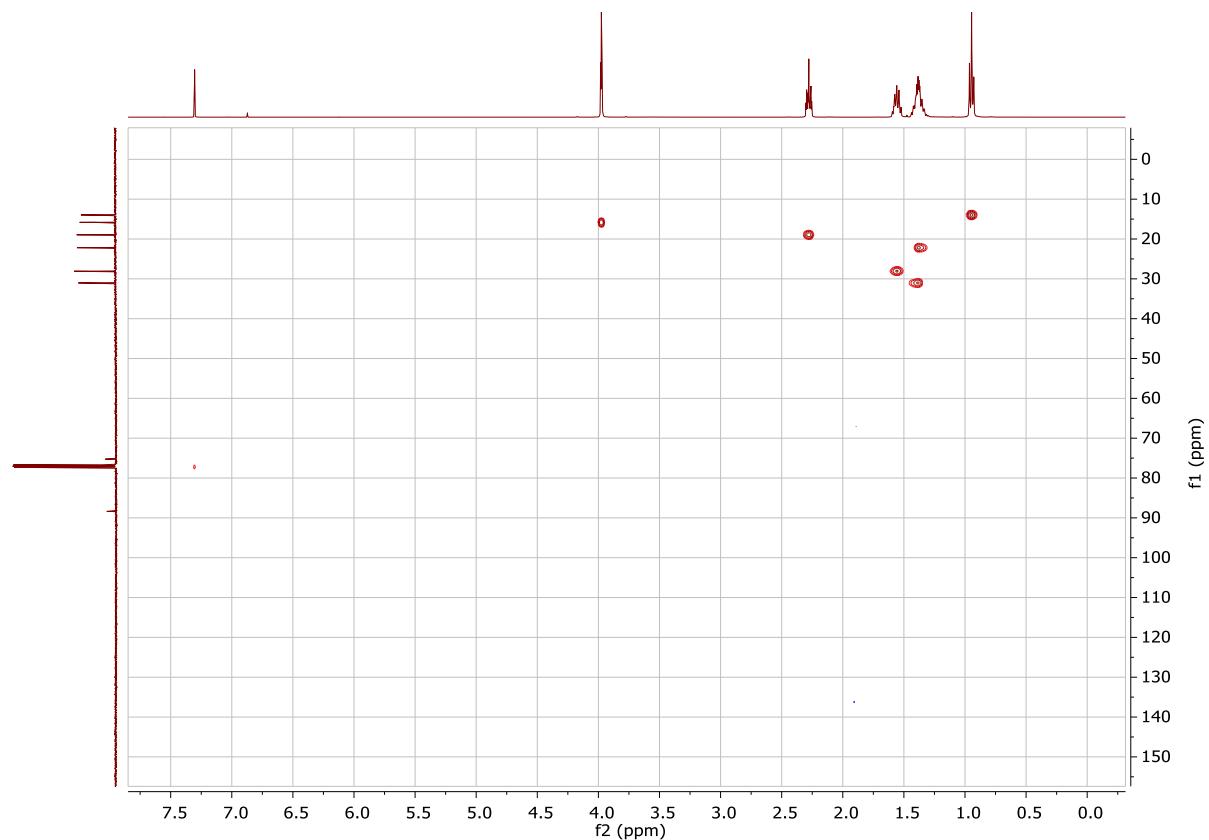
<sup>13</sup>C{H} NMR (101 MHz, CDCl<sub>3</sub>) of compound **18**



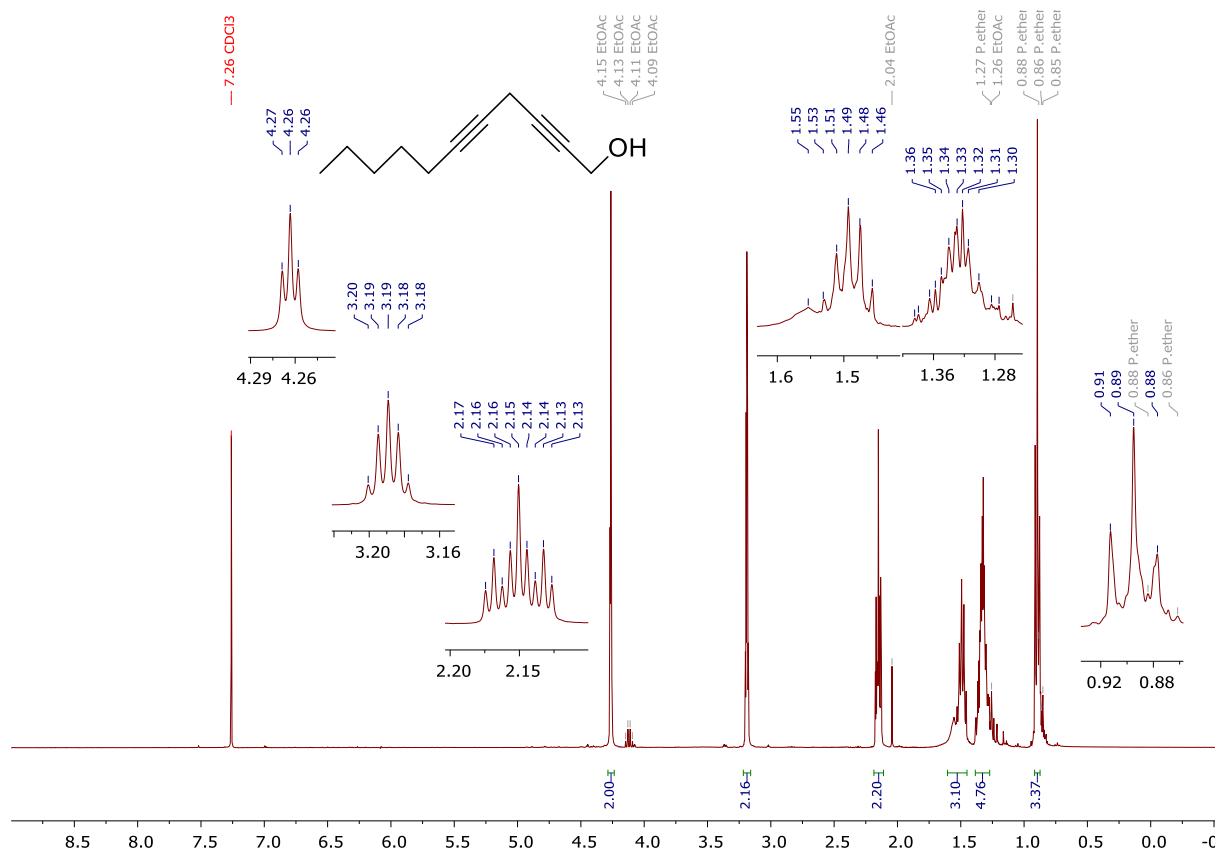
$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **18**



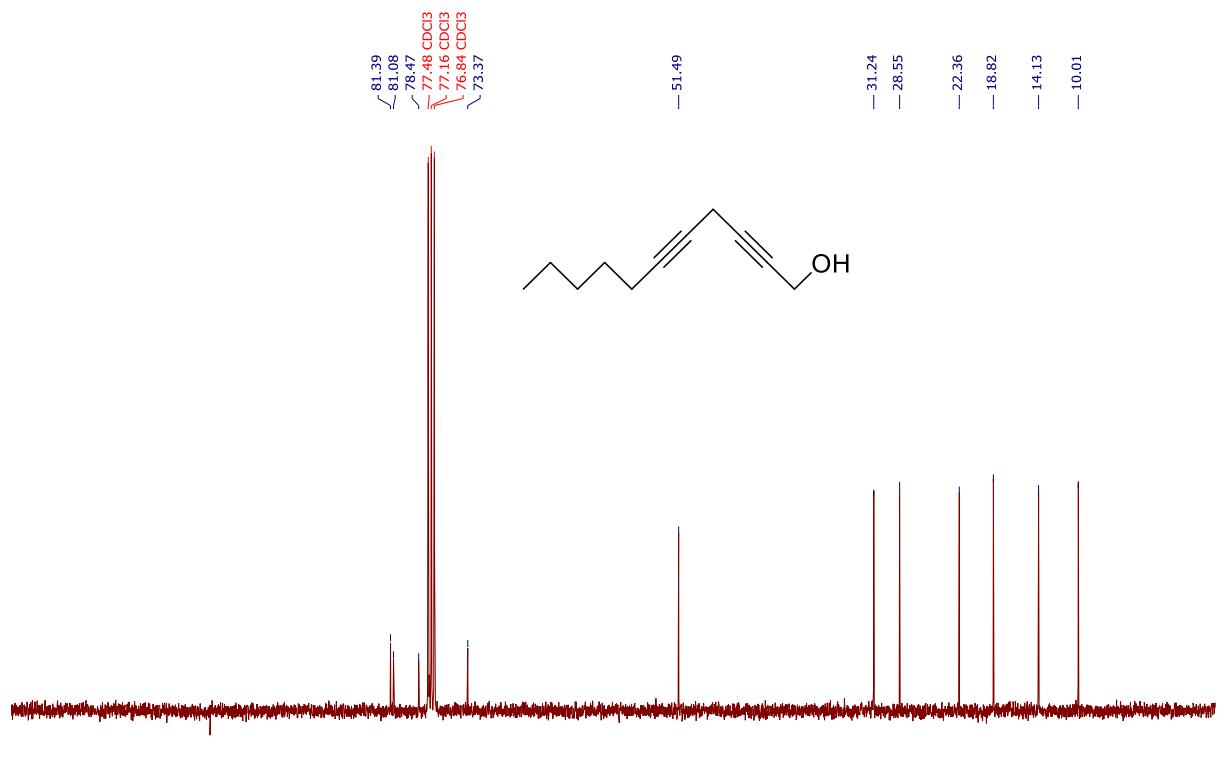
$^{13}\text{C}$ - $^1\text{H}$  HSQC spectrum of compound **18**



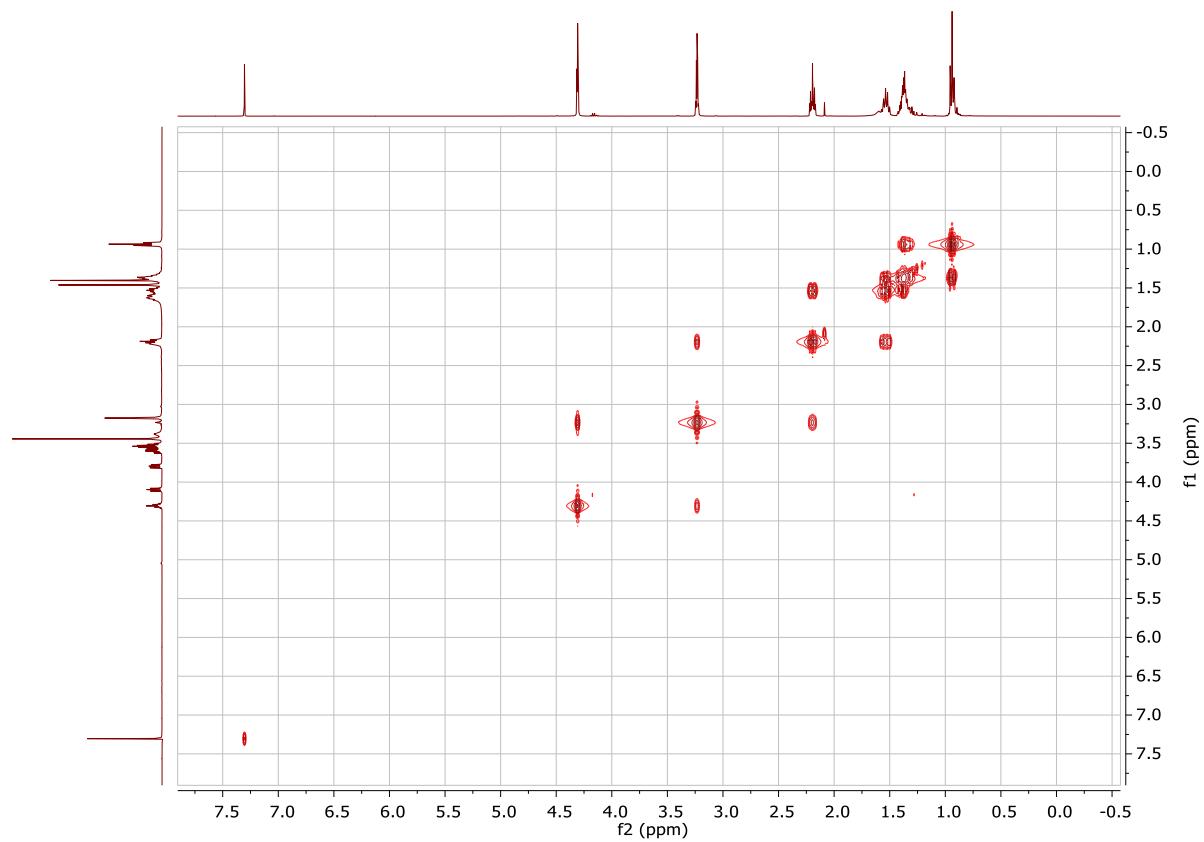
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **19**



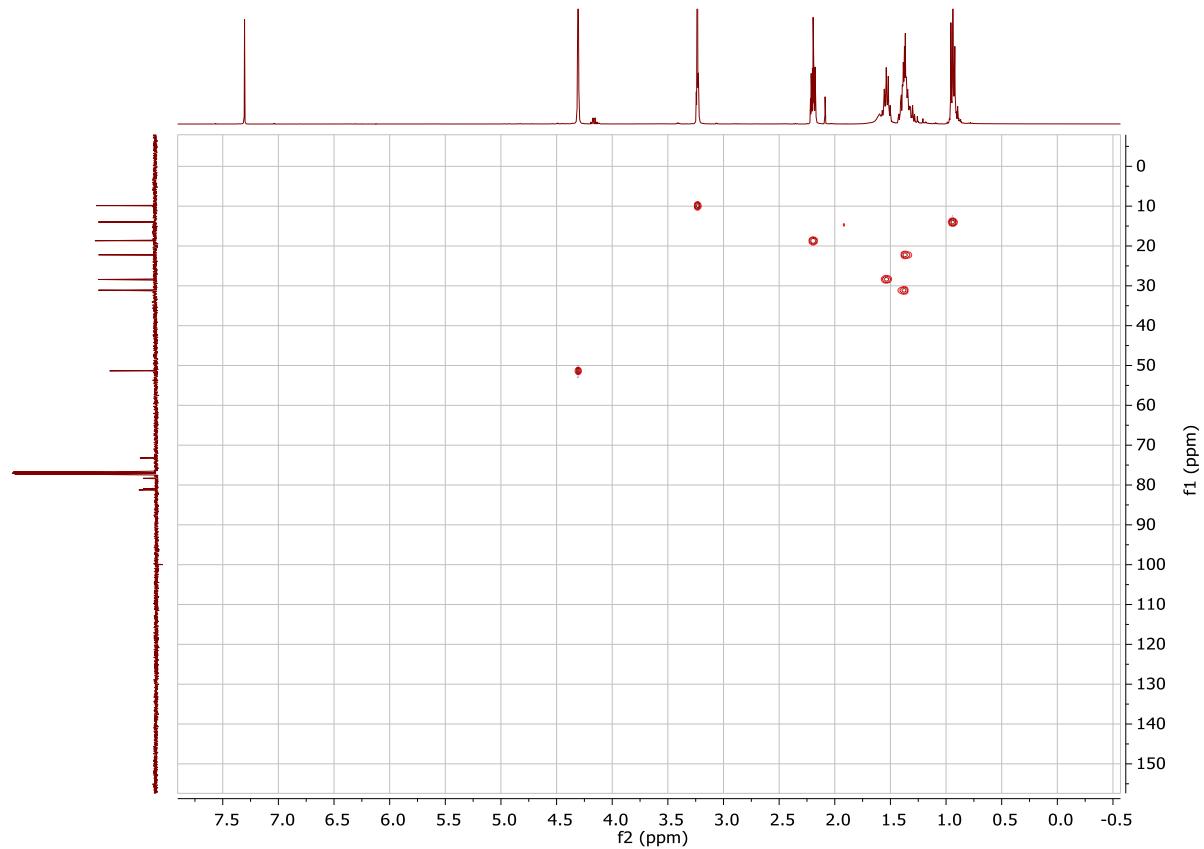
<sup>13</sup>C{H} NMR (101 MHz, CDCl<sub>3</sub>) of compound **19**



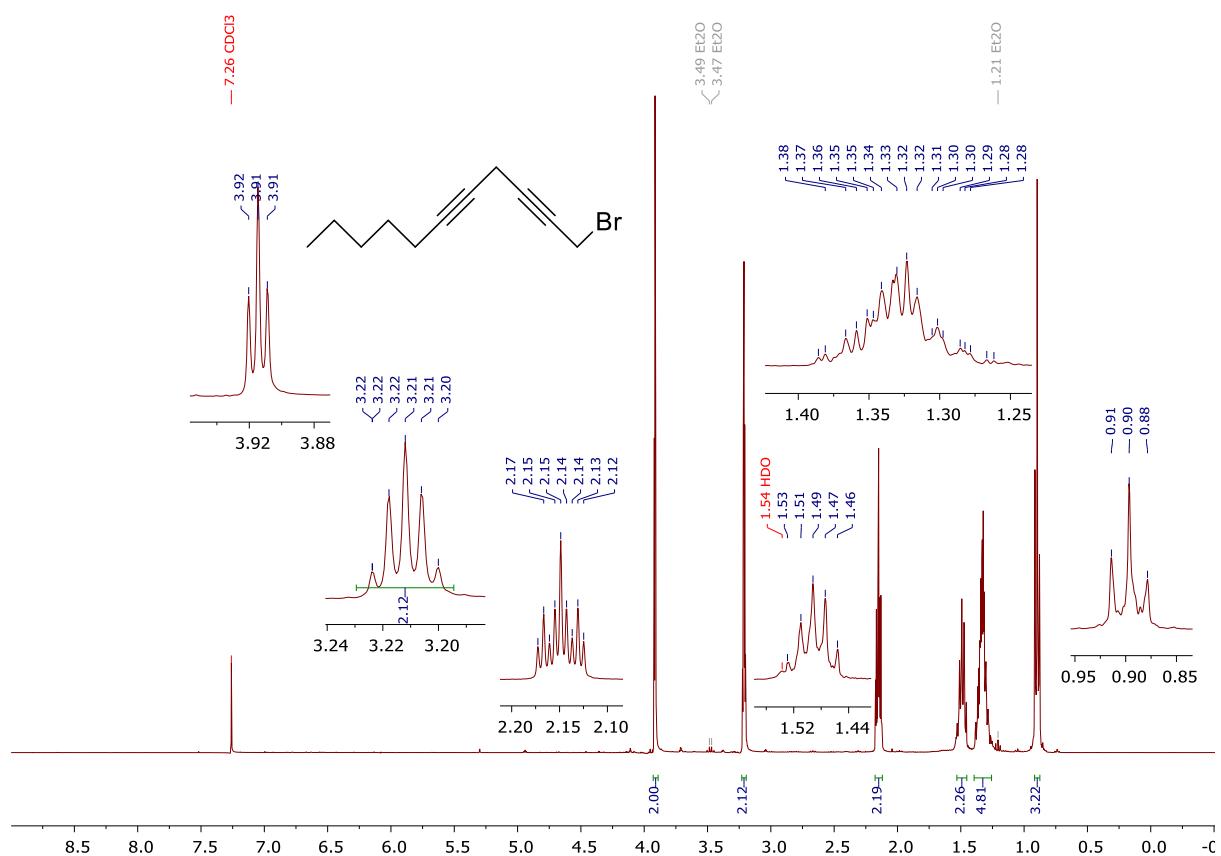
$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **19**



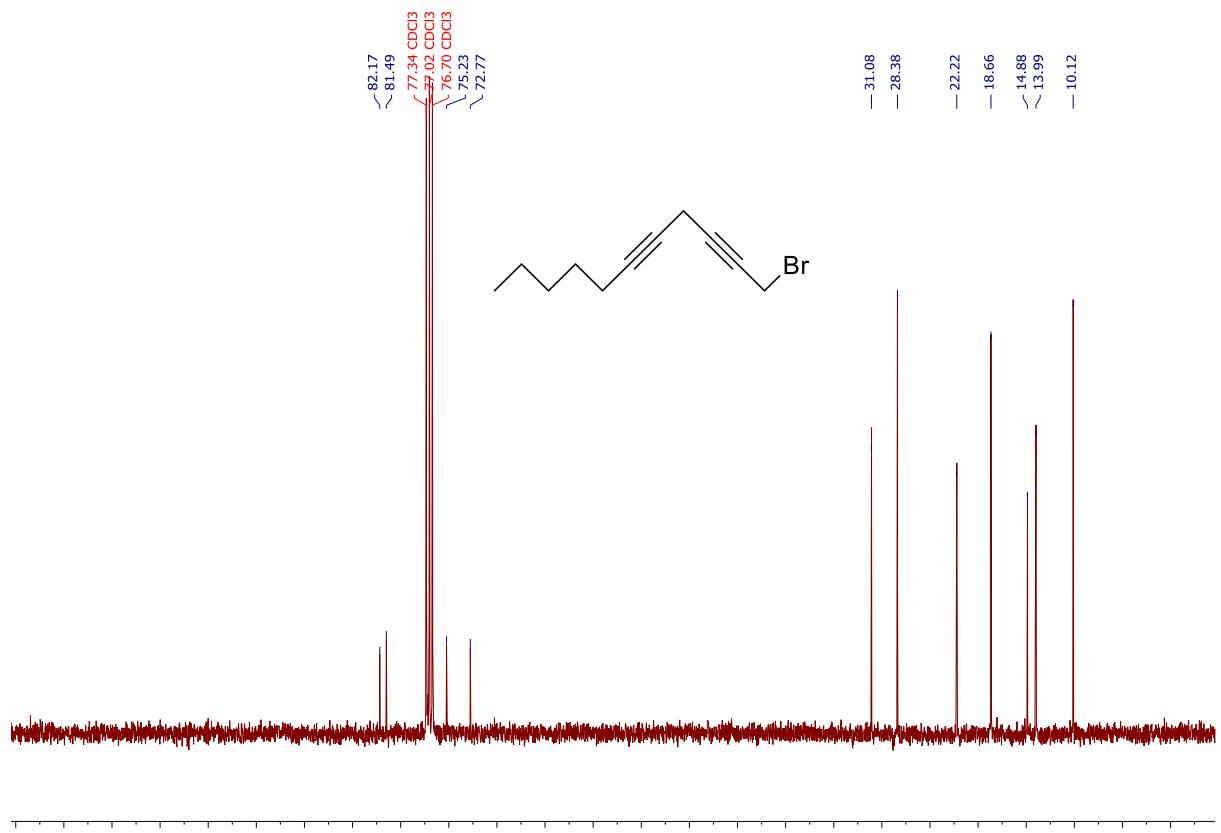
$^{13}\text{C}$ - $^1\text{H}$  HSQC spectrum of compound **19**



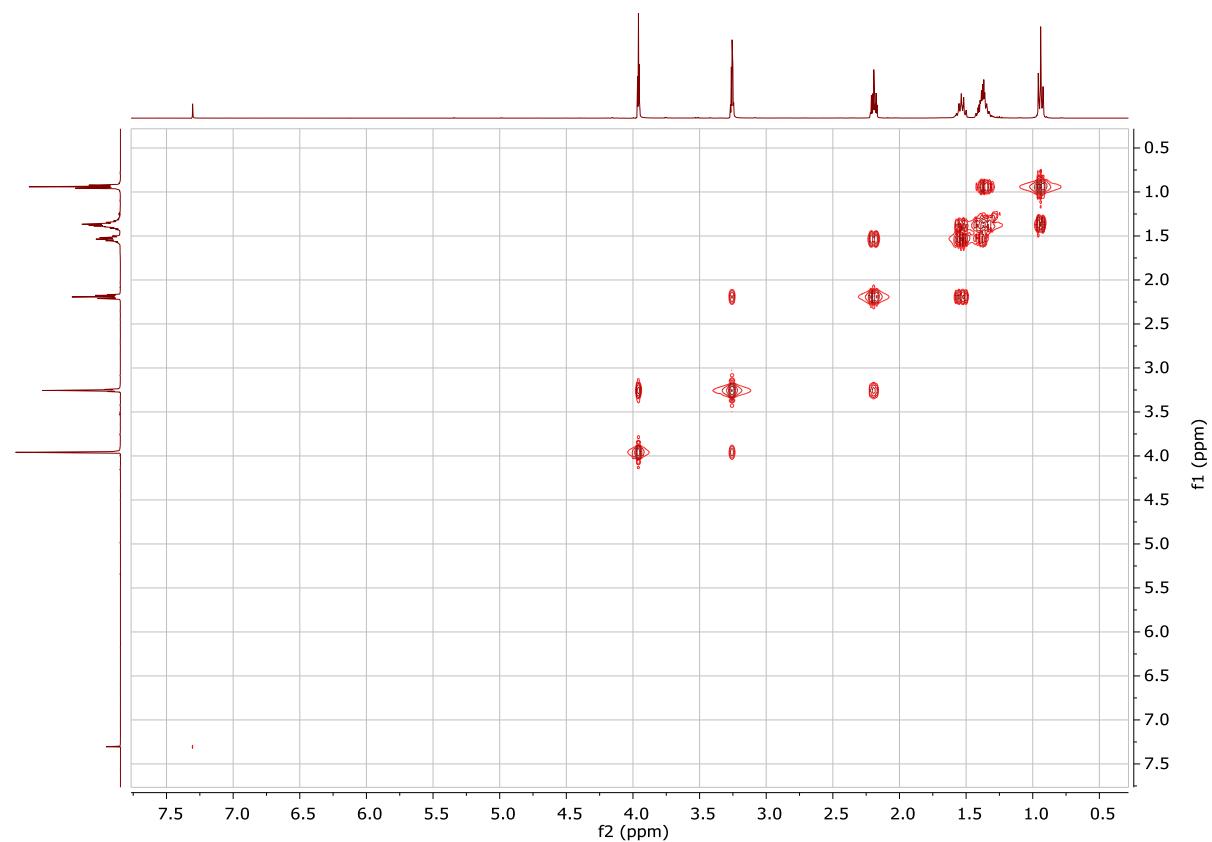
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **20**



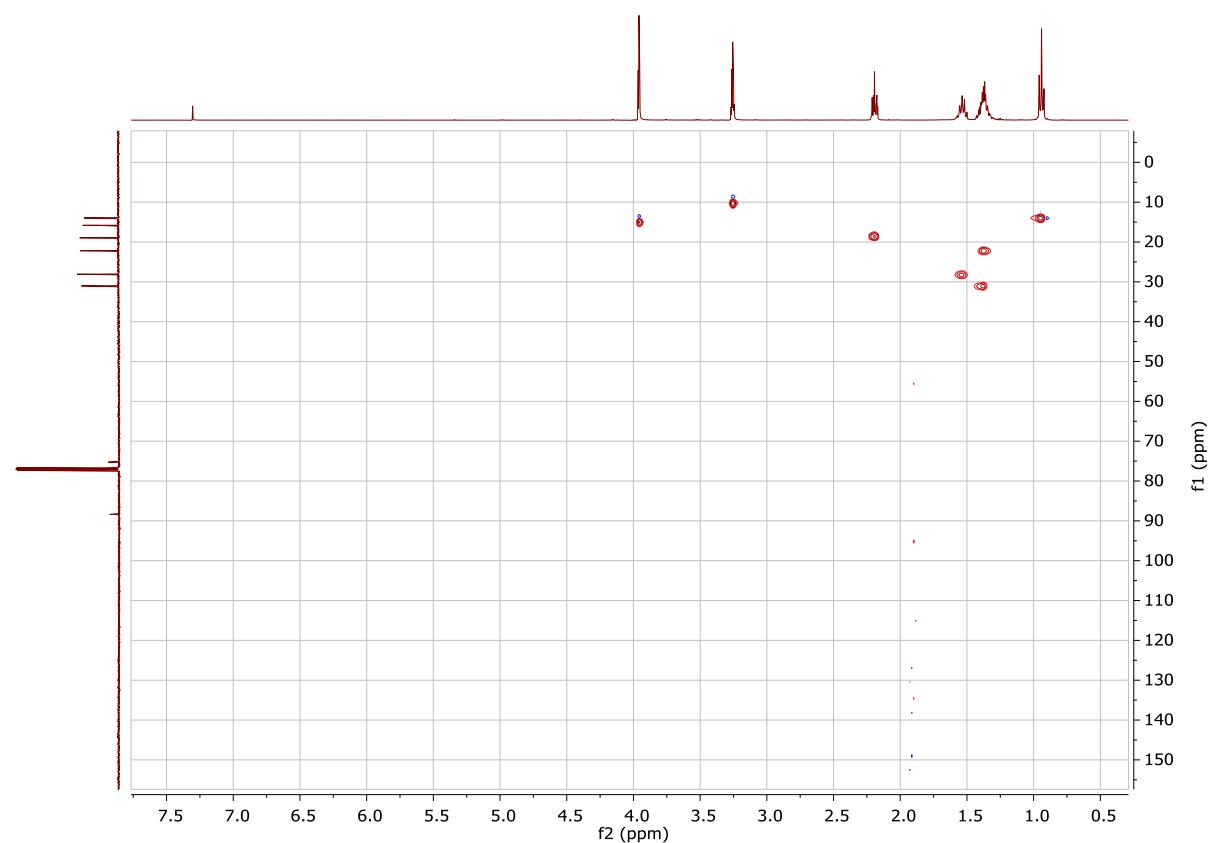
<sup>13</sup>C{H} NMR (101 MHz, CDCl<sub>3</sub>) of compound **20**



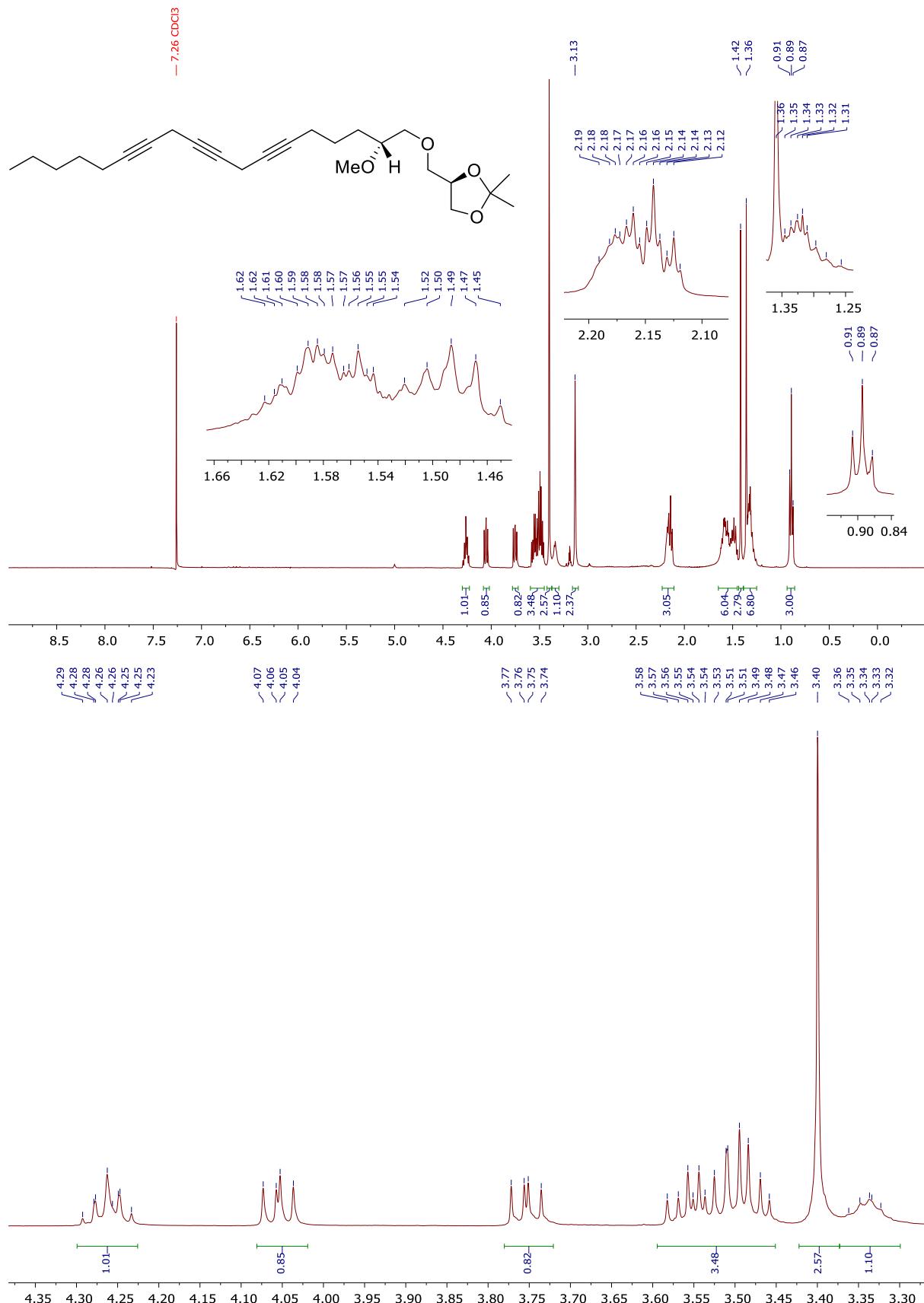
$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **20**



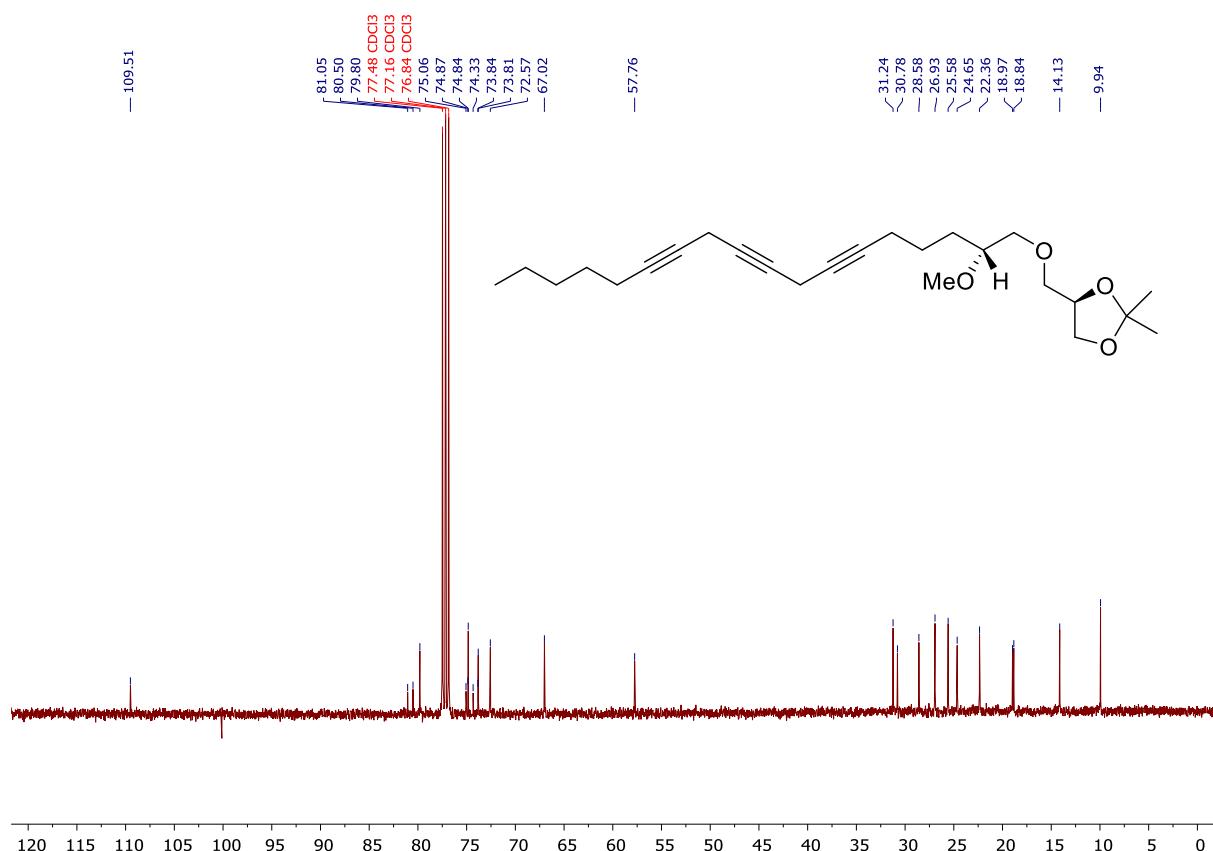
$^{13}\text{C}$ - $^1\text{H}$  HSQC spectrum of compound **20**



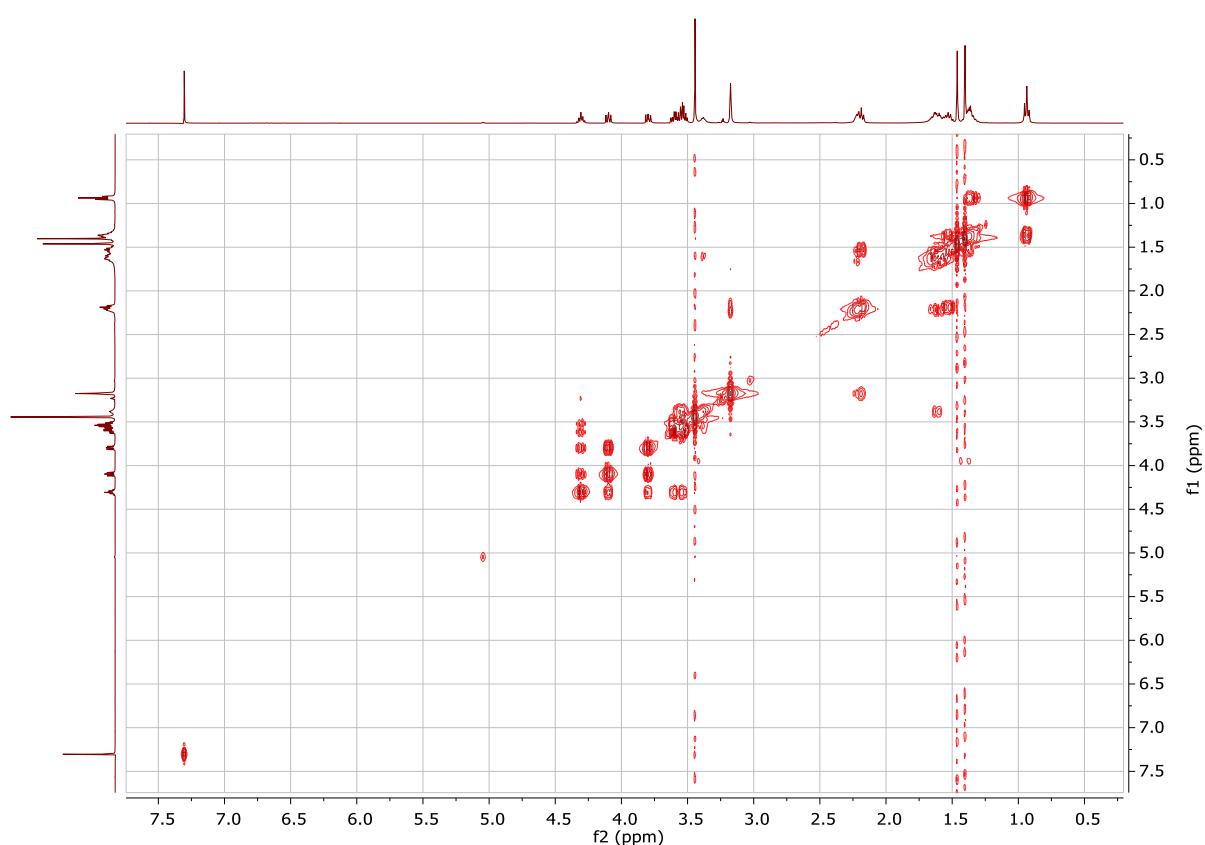
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **21**

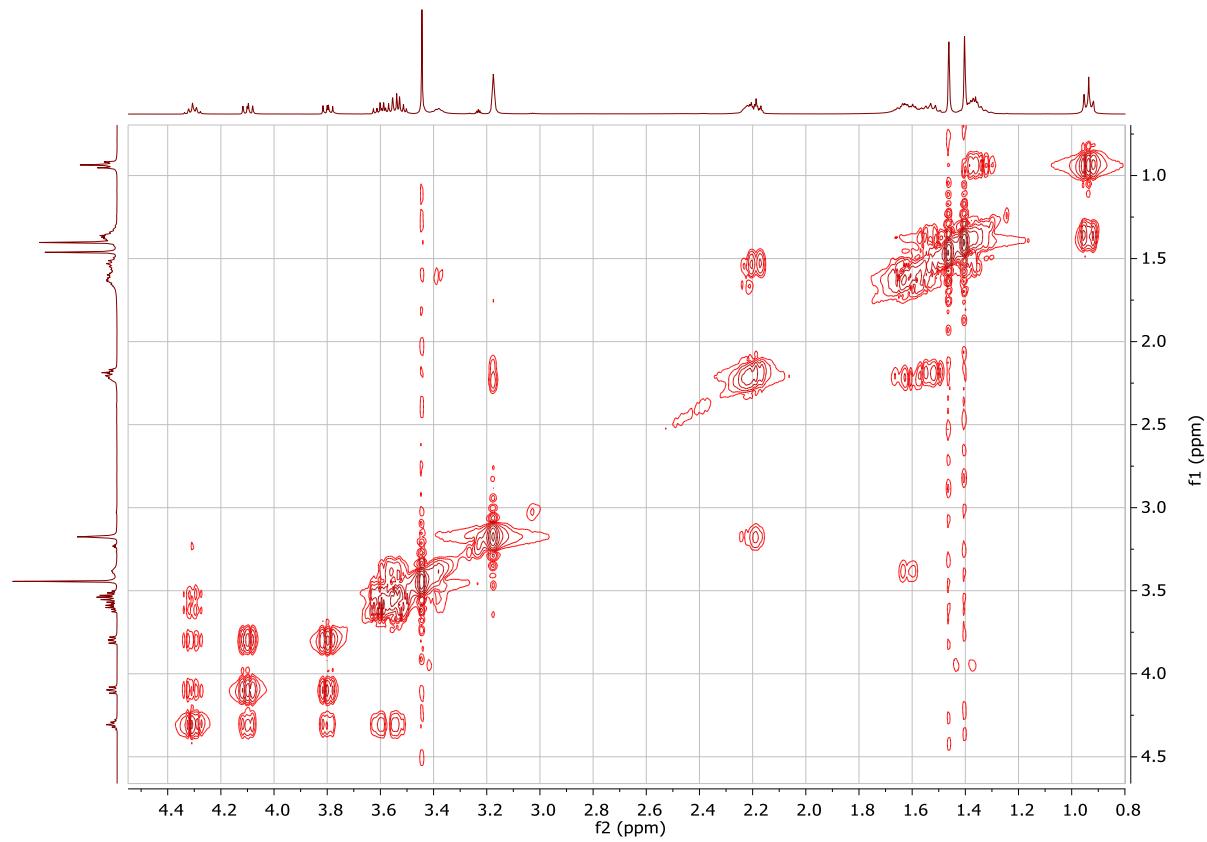


$^{13}\text{C}\{\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ ) of compound **21**

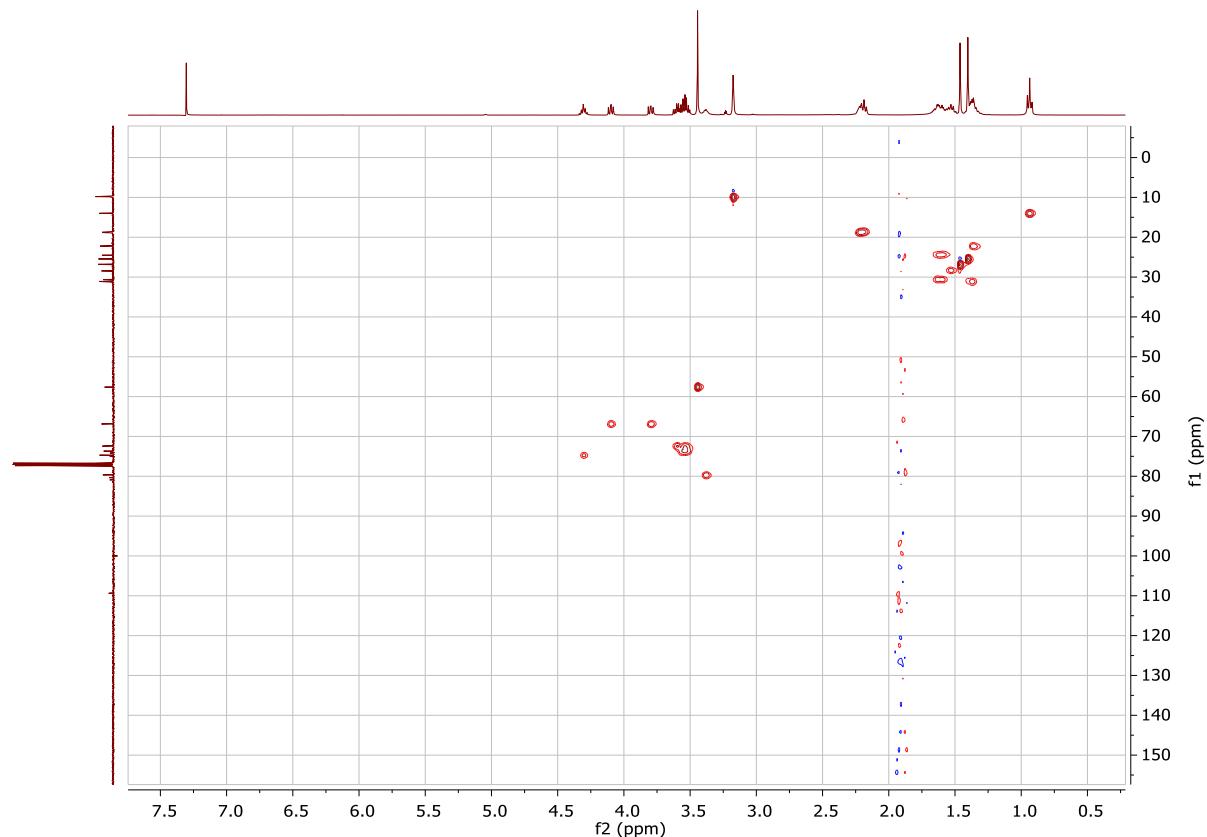


$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **21**

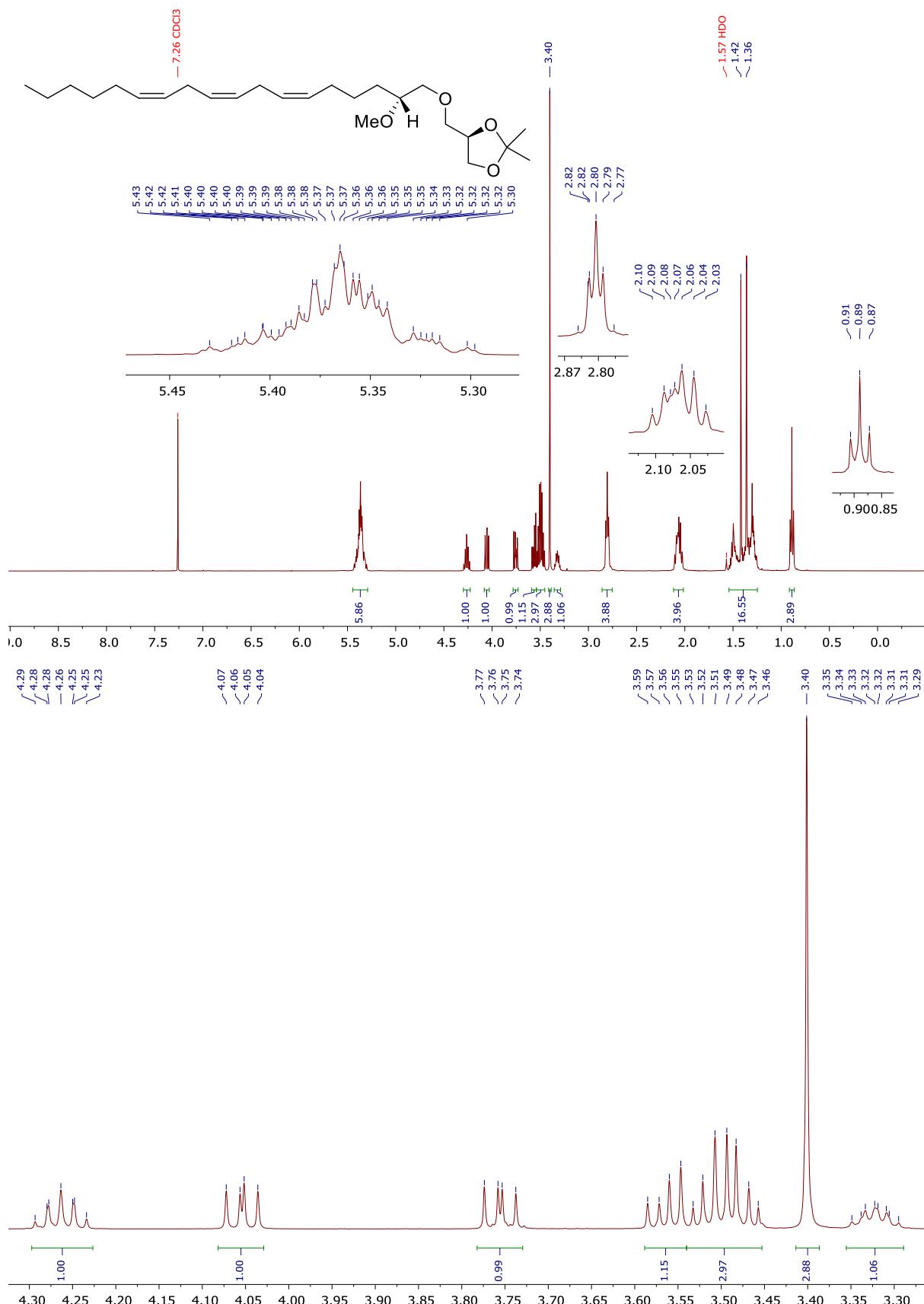




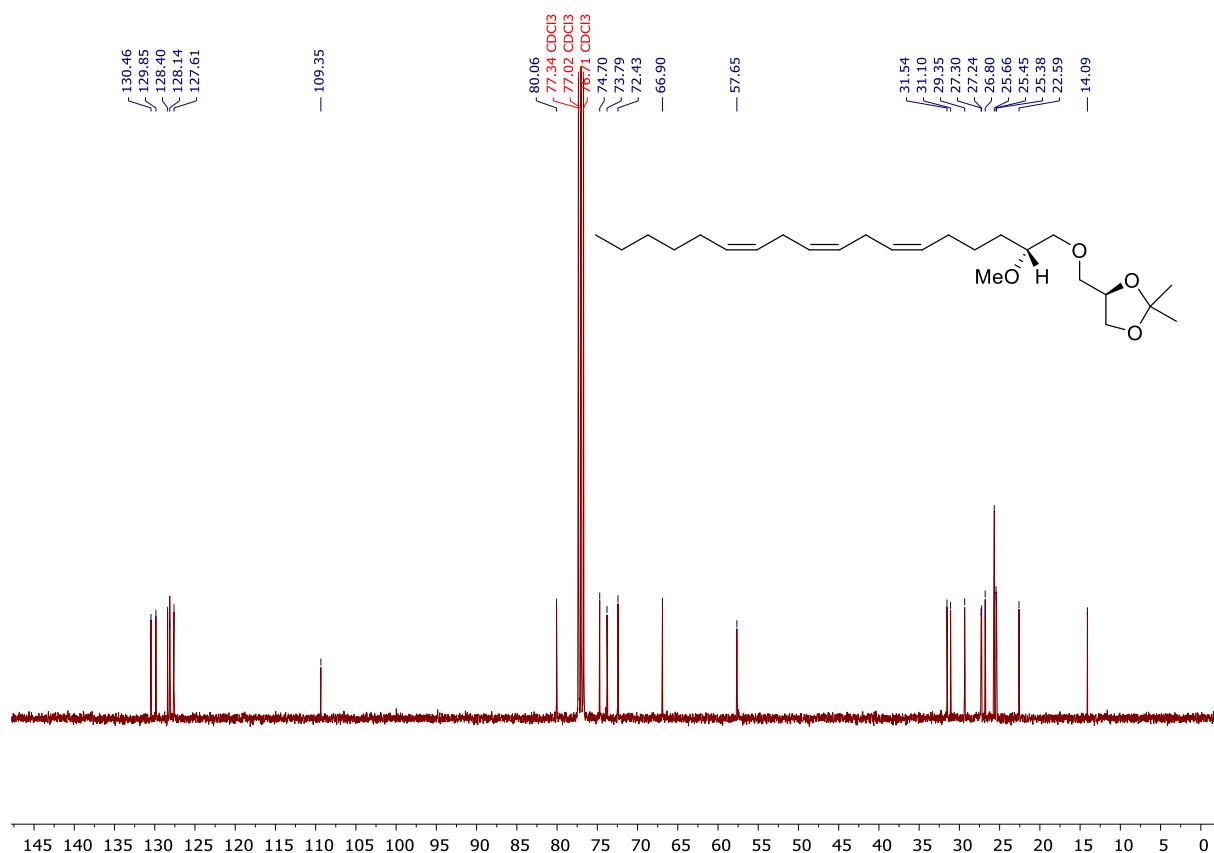
<sup>13</sup>C-<sup>1</sup>H HSQC spectrum of compound **21**



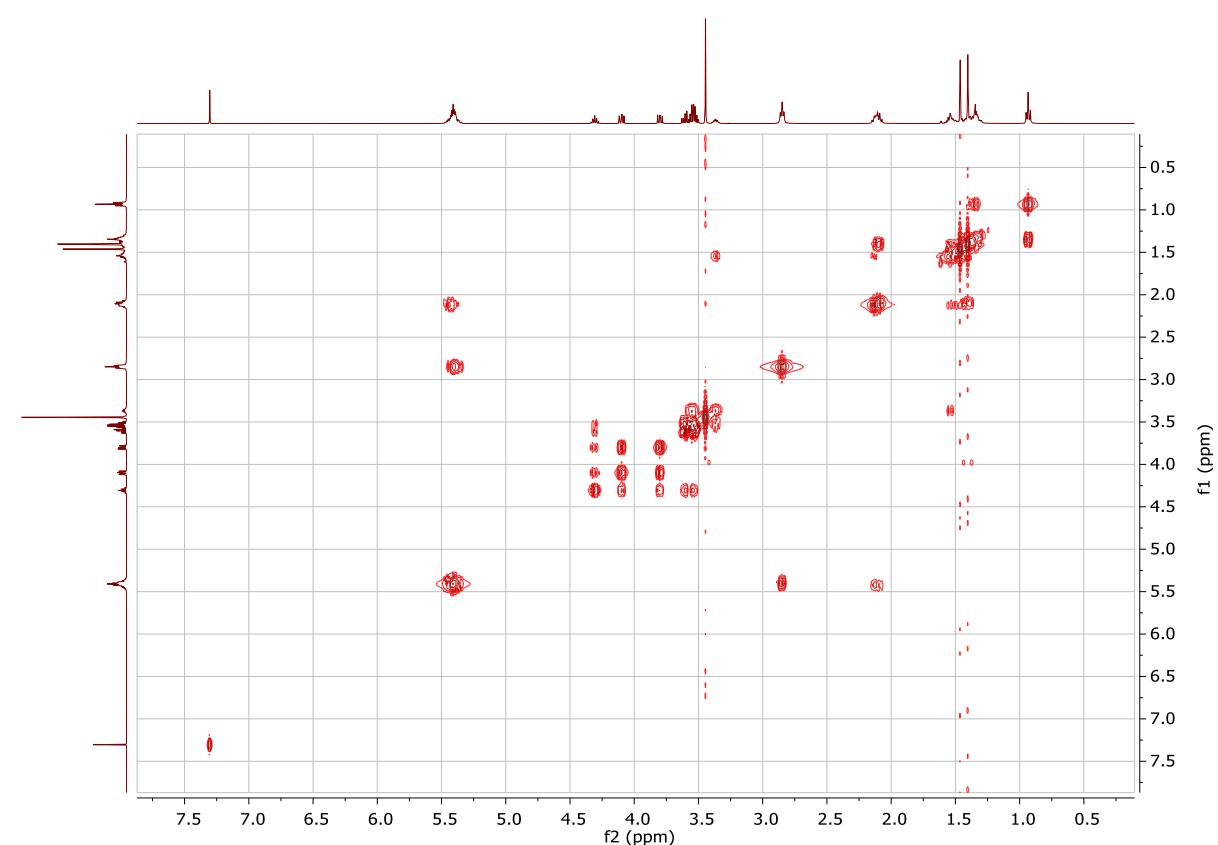
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound 22

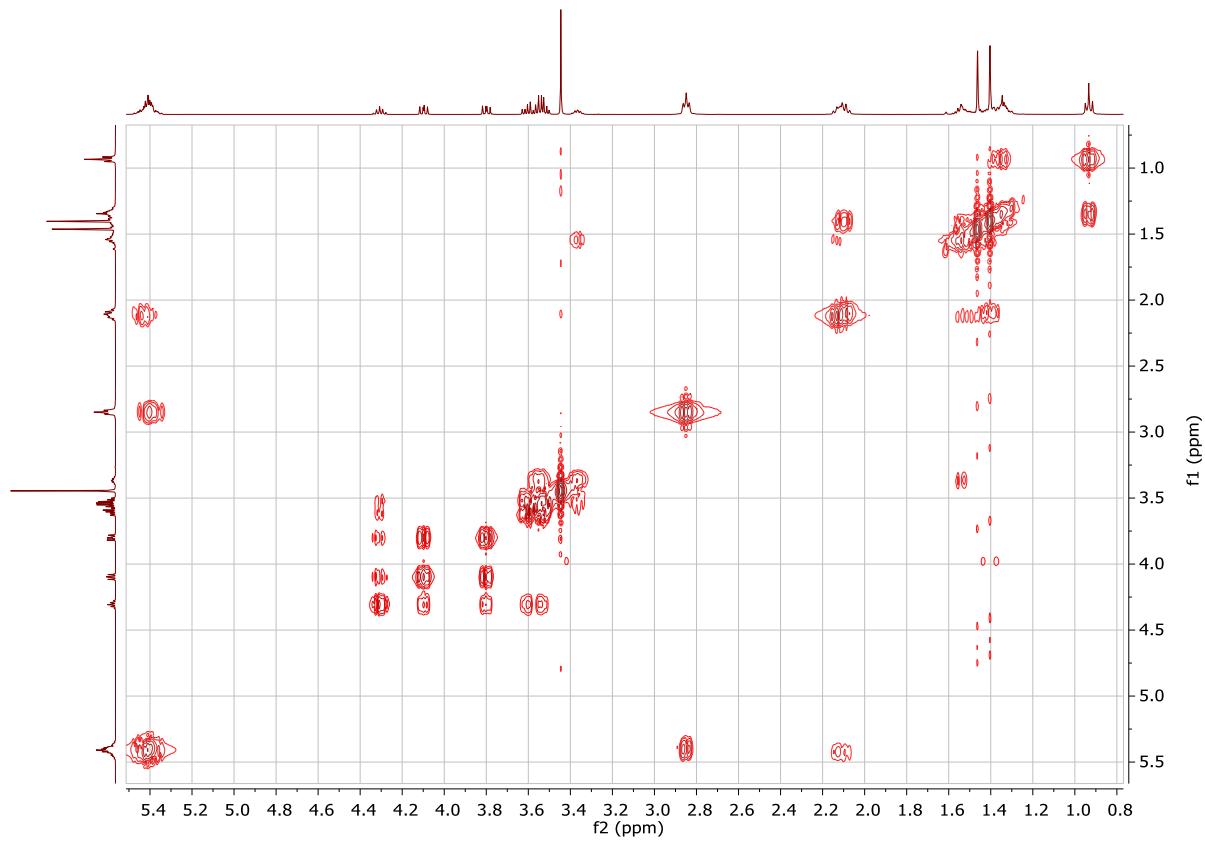


$^{13}\text{C}\{\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ ) of compound 22

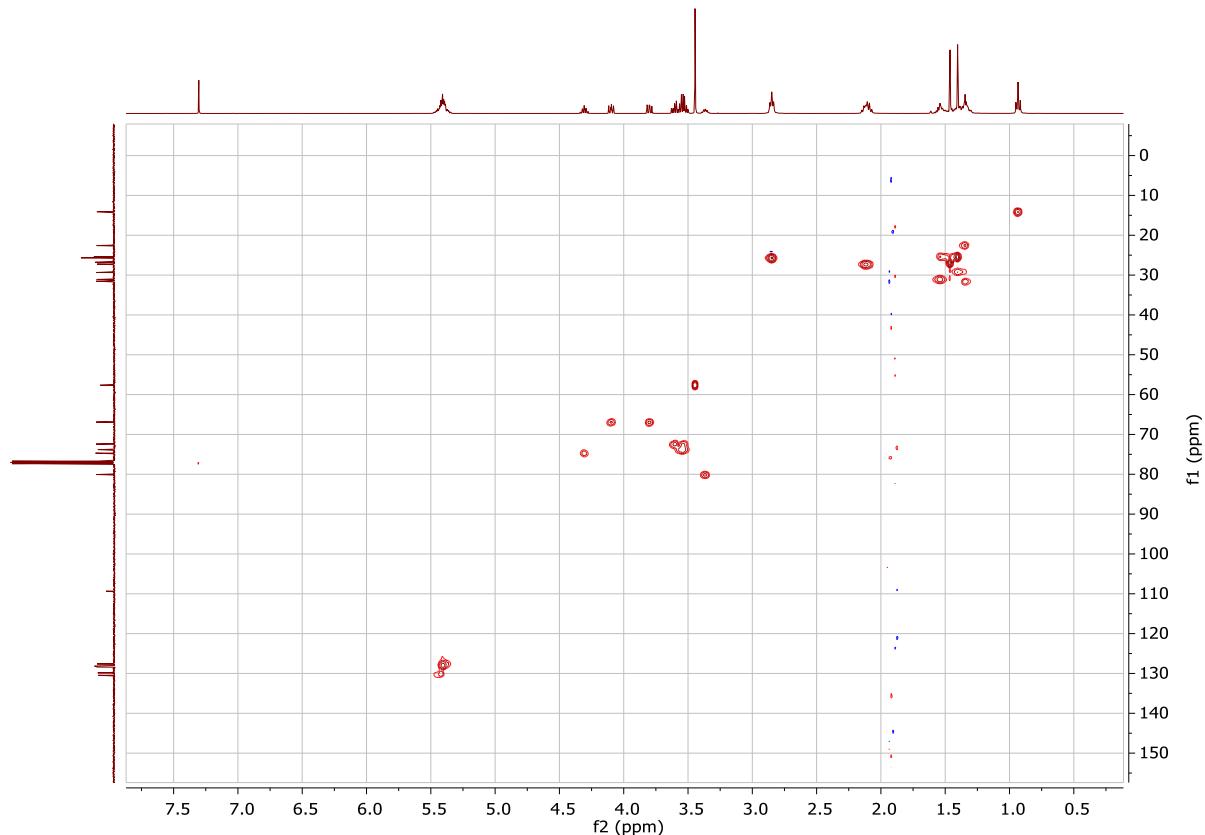


$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 22

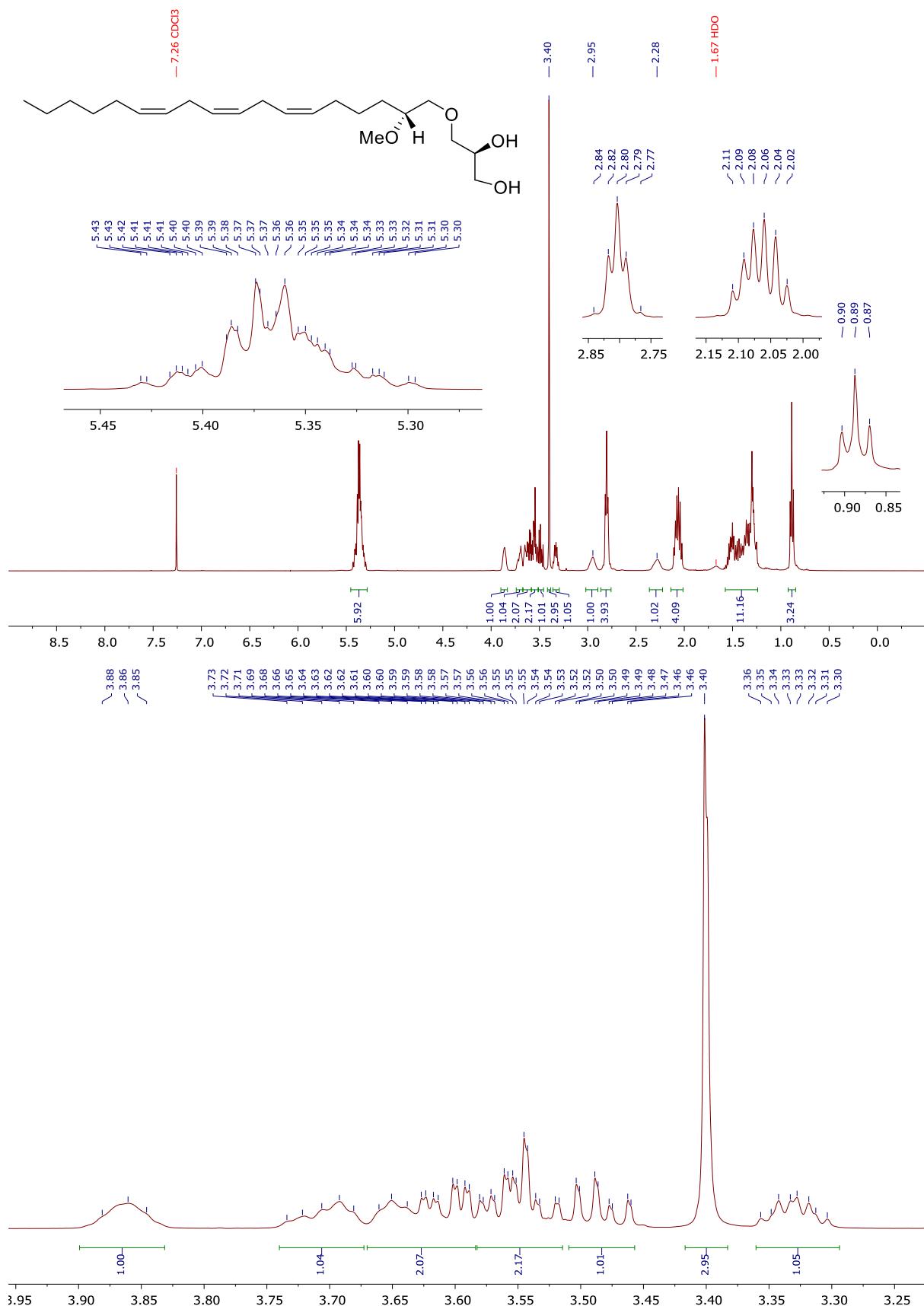




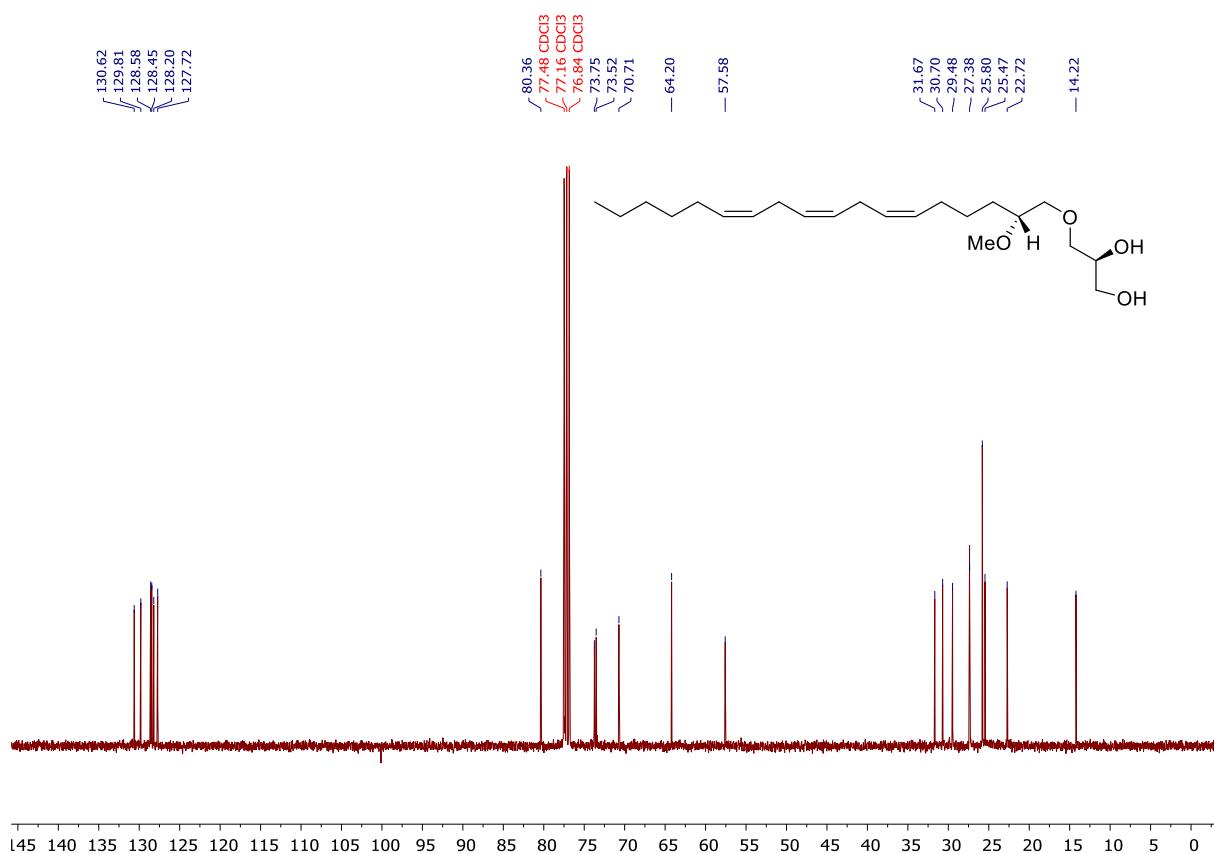
<sup>13</sup>C-<sup>1</sup>H HSQC spectrum of compound 22



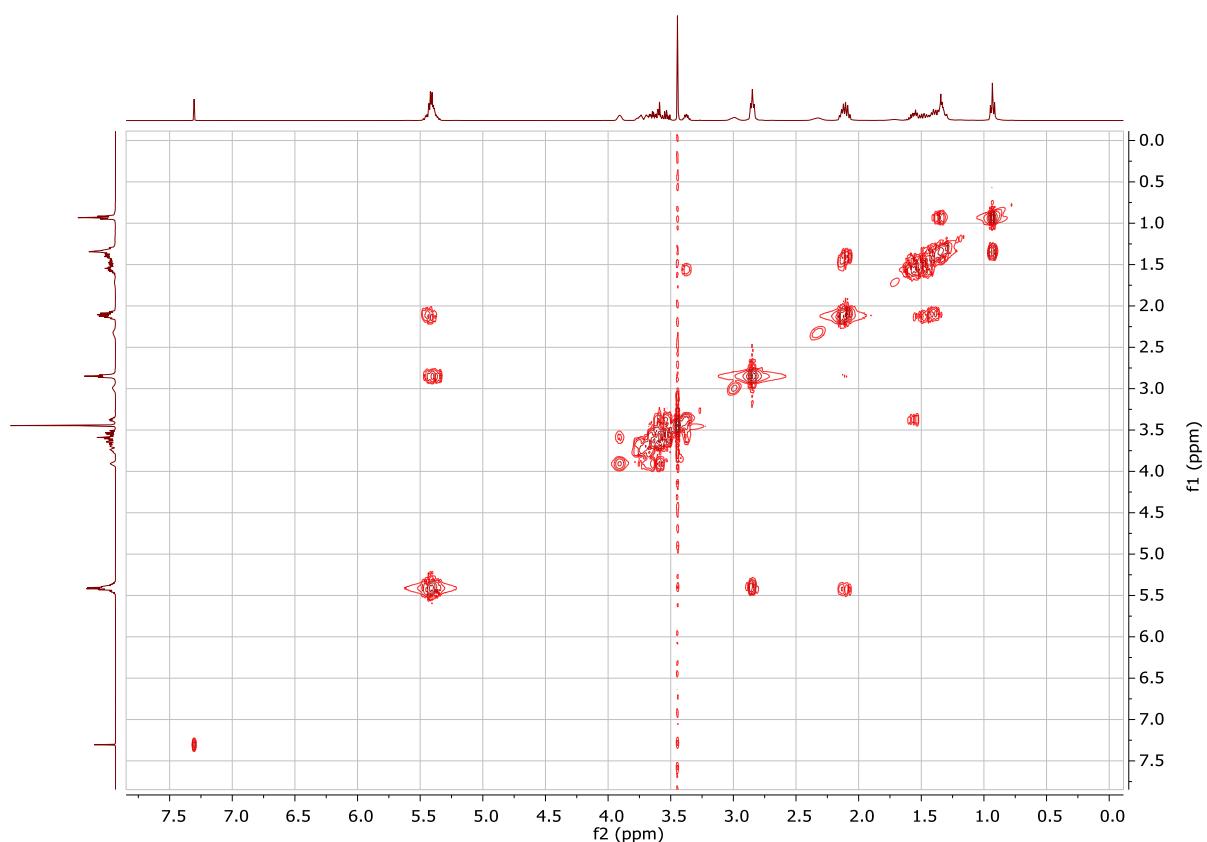
<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of MEL **6**



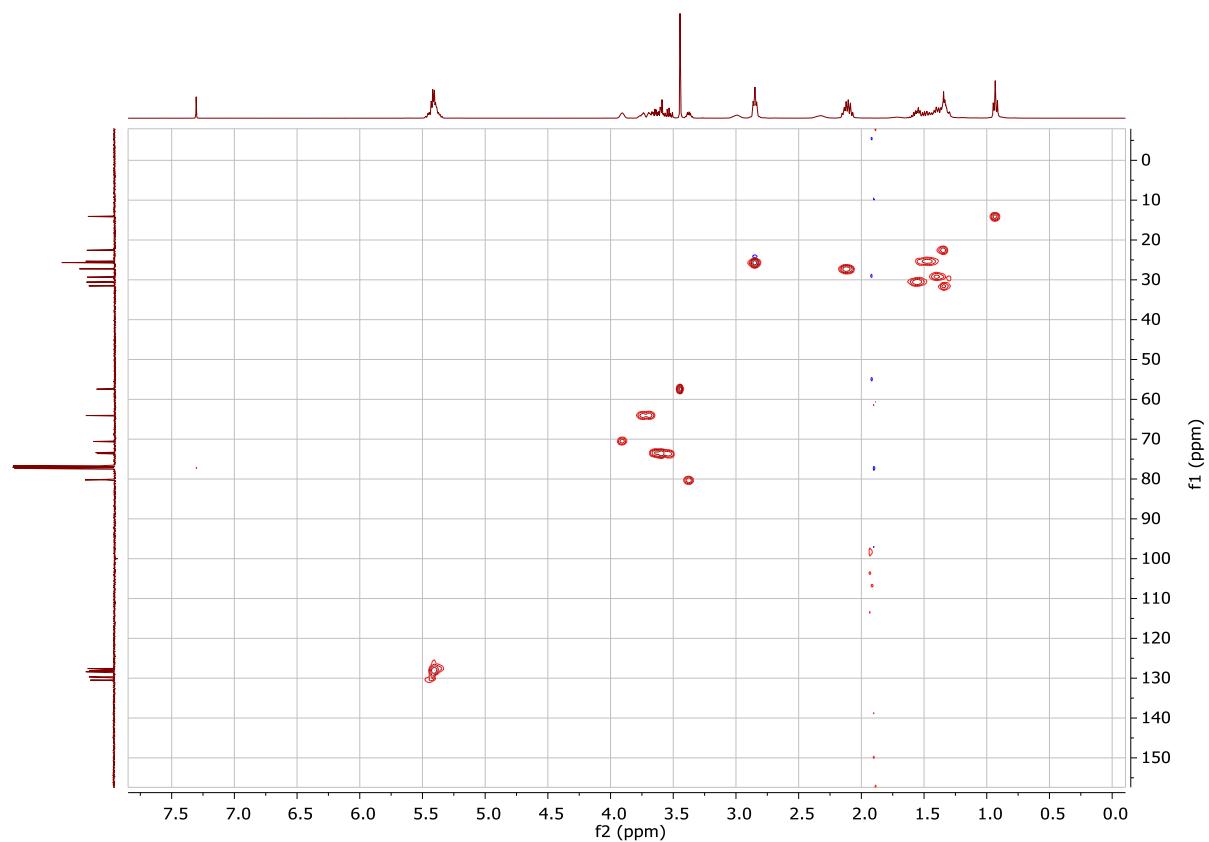
$^{13}\text{C}\{\text{H}\}$  NMR (101 MHz,  $\text{CDCl}_3$ ) of MEL **6**

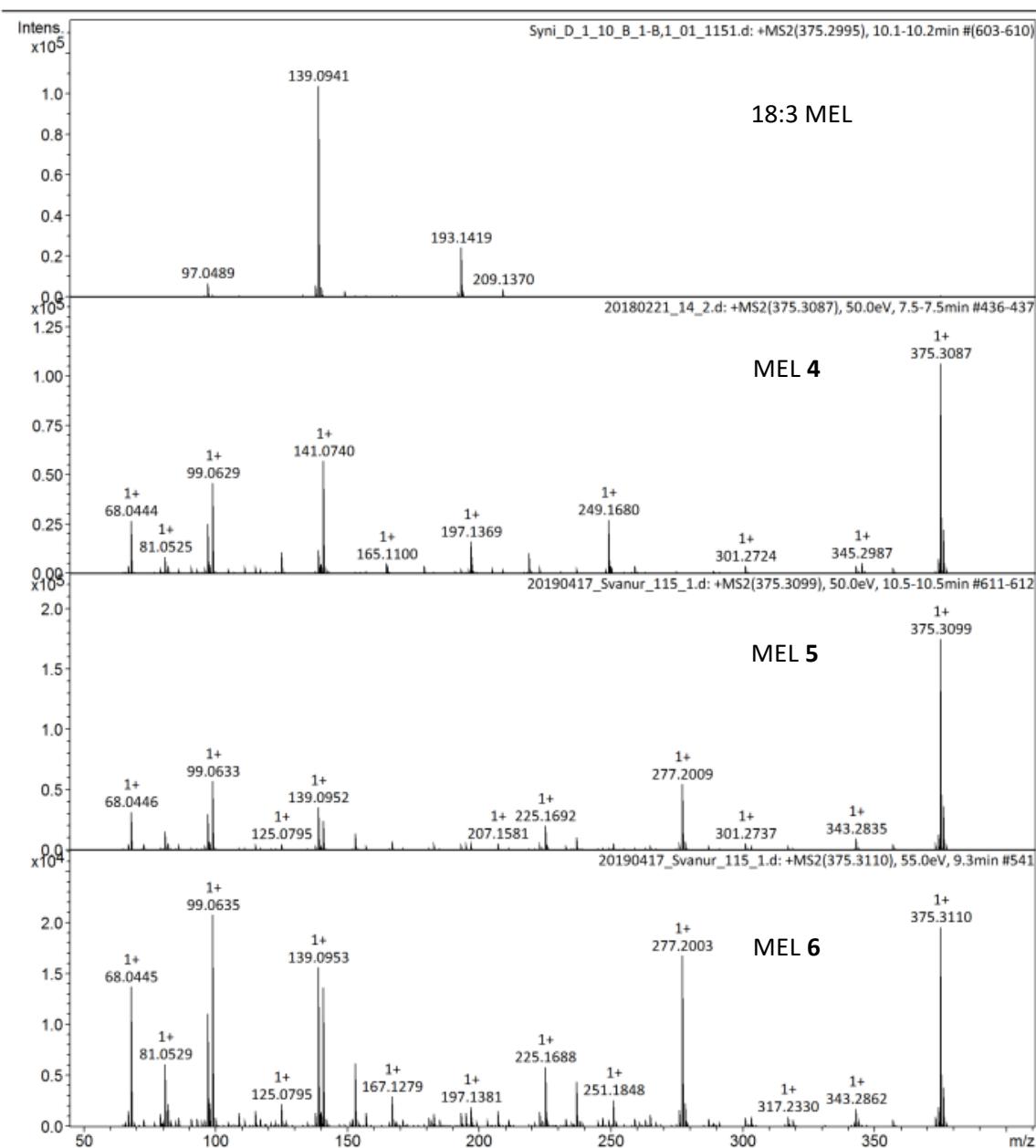


$^1\text{H}$ - $^1\text{H}$  COSY spectrum of MEL **6**



$^{13}\text{C}$ - $^1\text{H}$  HSQC spectrum of MEL 6





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**Figure 1S.** Comparison of the  $[M+Li]^+$  MS/MS fragmentation spectra of the synthesized MELs **4**, **5**, and the 18:3 MEL found in the shark and dogfish liver oil sample (top).