

Supporting Information

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Synthesis of new fatty acid derivatives of oleanane and ursane triterpenoids and investigation of their *in vitro* cytotoxic effects on 3T3 fibroblast and PC3 prostate cancer cell lines

**Halil Şenol^{1,*}, Kübra Çokuludağ², Asude Sena Aktaş²,
Sezen Atasoy³, Aydan Dağ¹ and Gülaçtı Topçu⁴**

¹*Bezmiâlem Vakıf University Faculty of Pharmacy Department of Pharmaceutical Chemistry, Fatih, 34093, İstanbul, Türkiye*

²*Bezmiâlem Vakıf University Faculty of Pharmacy, Fatih, 34093, İstanbul, Türkiye*

³*Bezmiâlem Vakıf University Faculty of Pharmacy Department of Biochemistry, Fatih, 34093, İstanbul, Türkiye*

⁴*Bezmiâlem Vakıf University Faculty of Pharmacy Department of Pharmacognosy Fatih 34093, İstanbul, Türkiye*

* Corresponding author:

Halil Şenol; E-Mail: hsenol@bezmialem.edu.tr, Phone: + 90 212 523 2288-3364; Fax: + 90 212 533 2326

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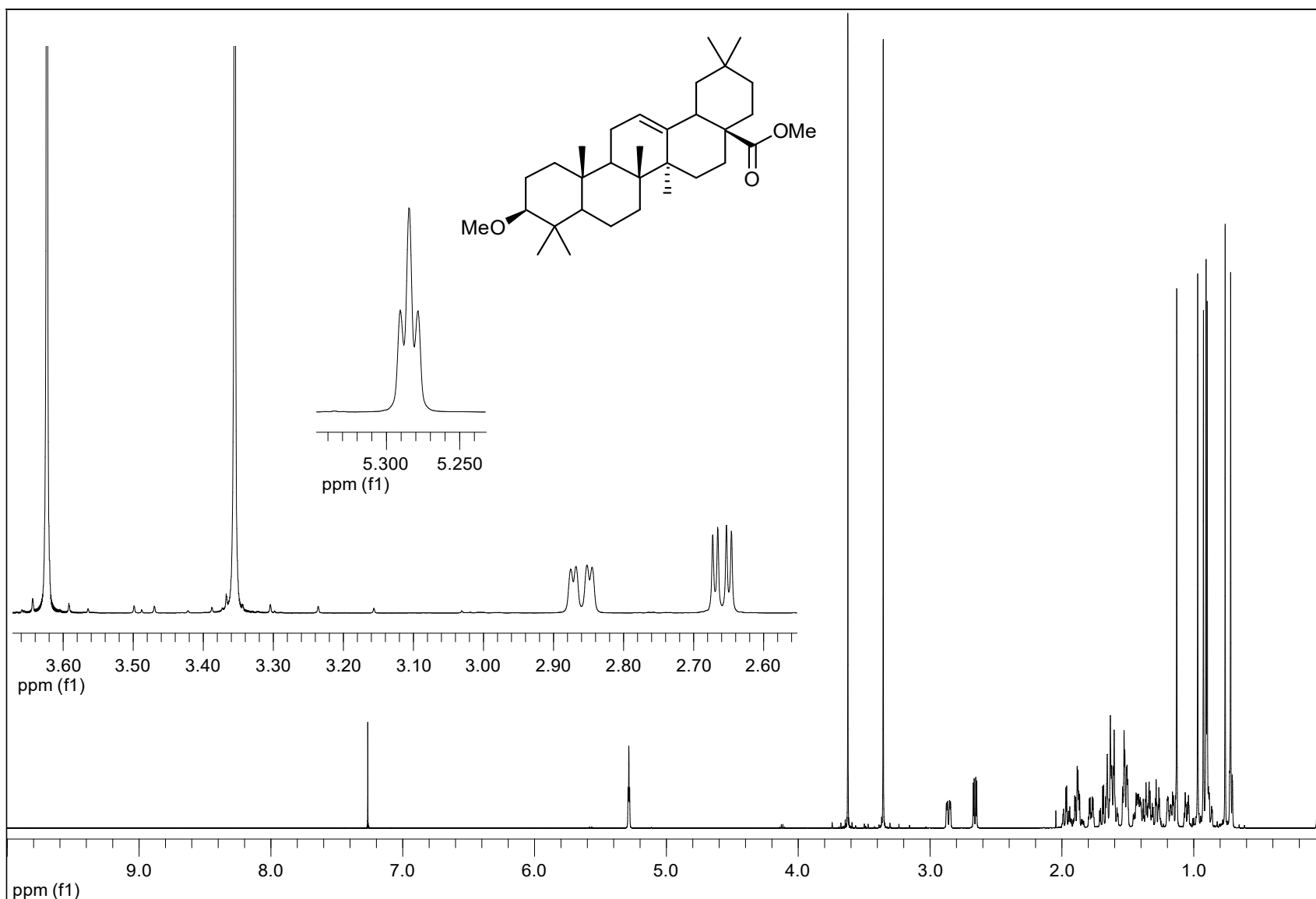


Figure 1: ¹H-NMR Spectrum of Compound 3 (CDCl₃, 500 MHz)

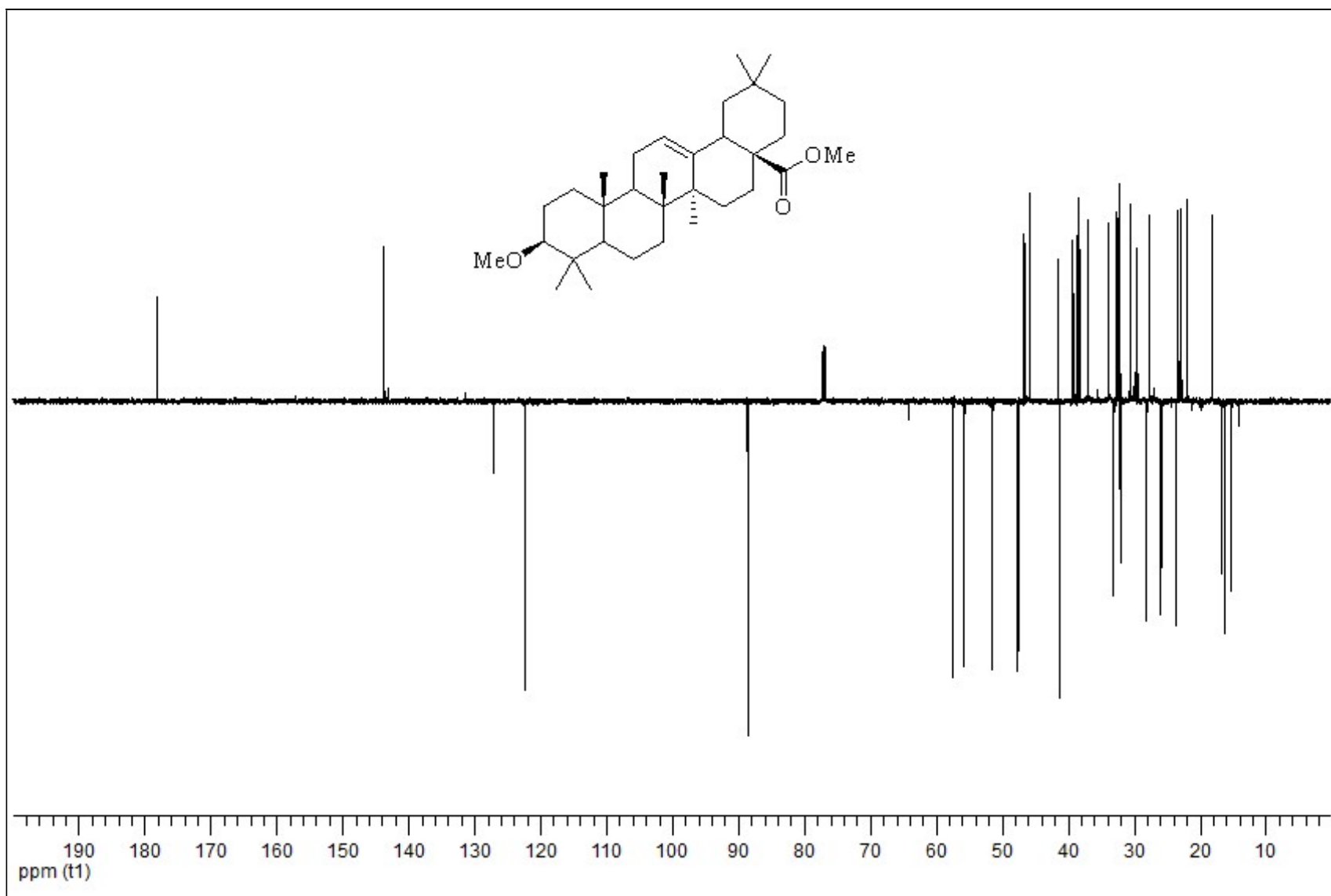


Figure 2: ^{13}C -NMR Spectrum of Compound 3 (CDCl_3 , 125 MHz)

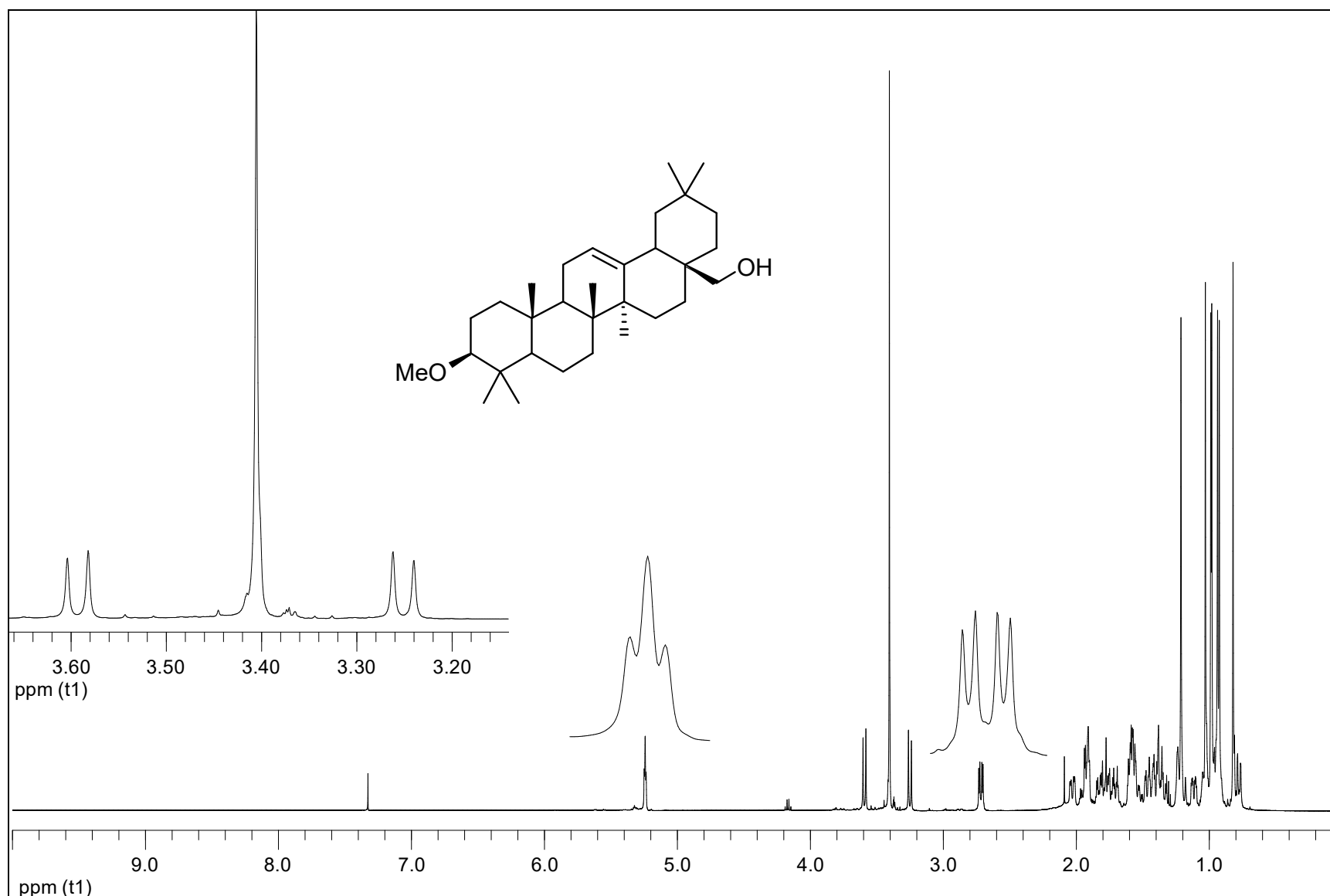


Figure 3: ¹H-NMR Spectrum of Compound 4 (CDCl₃, 500 MHz)

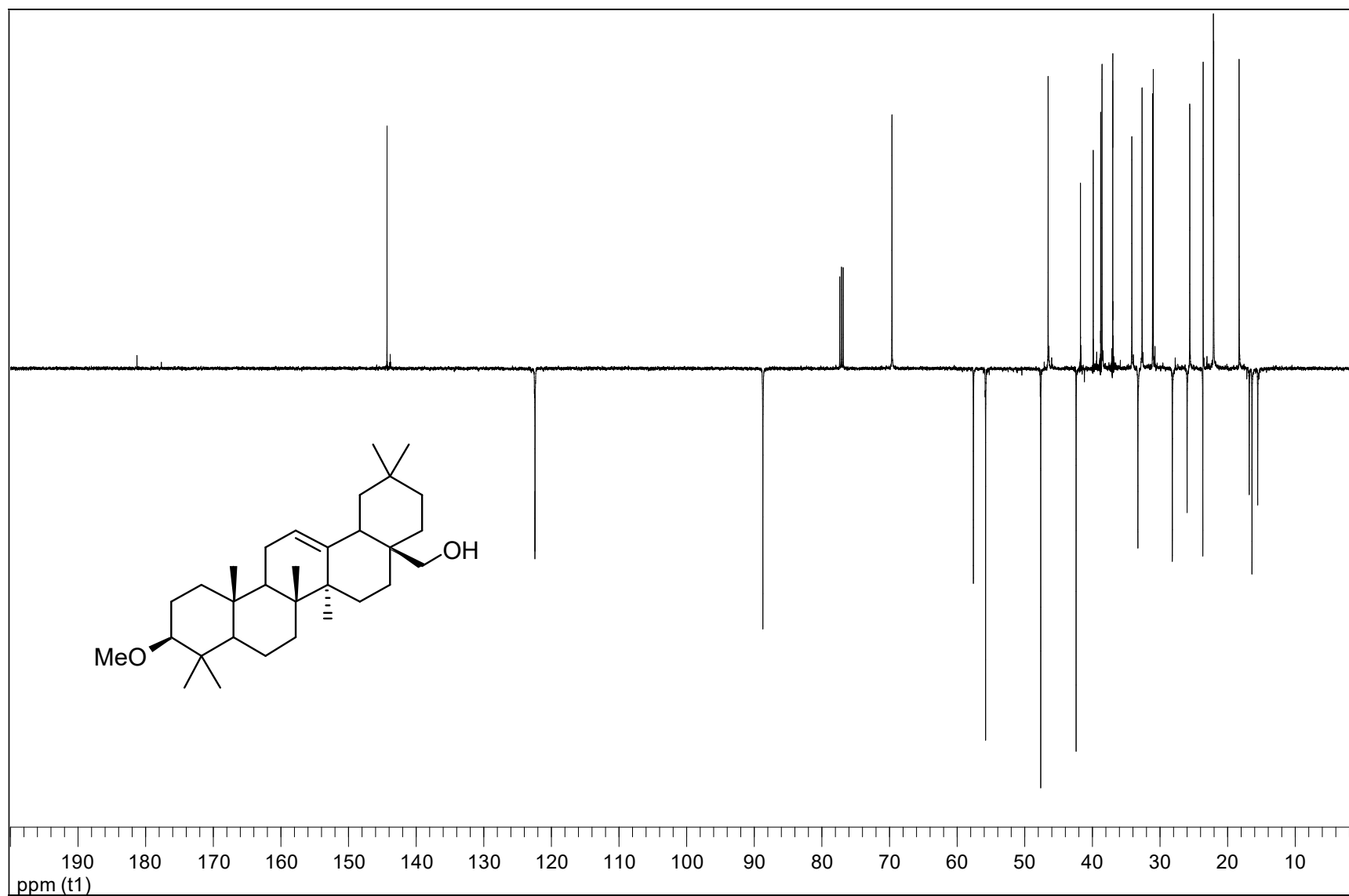


Figure 4: ^{13}C -APT NMR Spectrum of Compound 4 (CDCl_3 , 125 MHz)

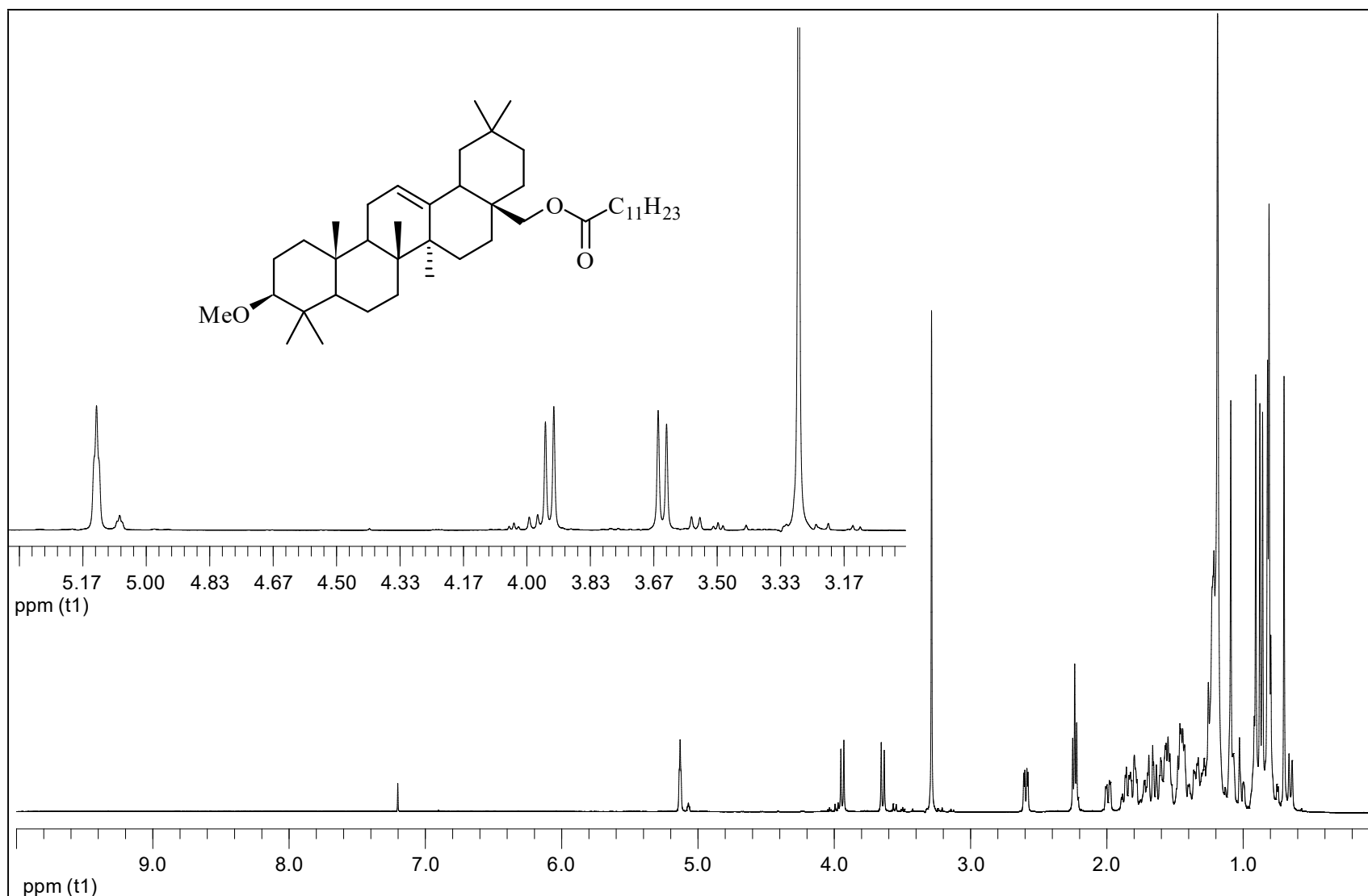


Figure 5: ¹H-NMR Spectrum of Compound 5a (CDCl₃, 500 MHz)

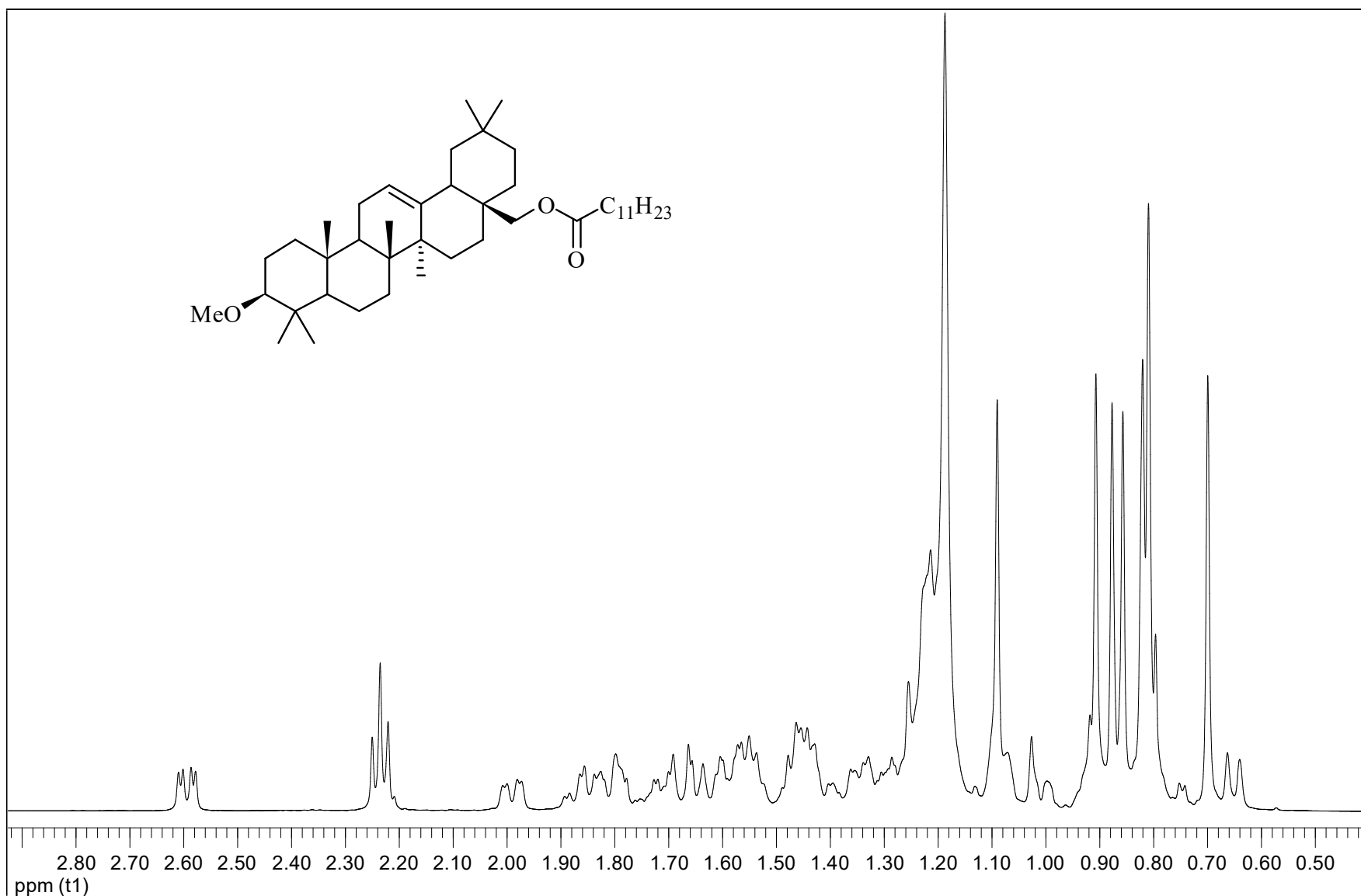


Figure 6: ¹H-NMR Spectrum of Compound **5a** (Extended) (CDCl₃, 500 MHz)

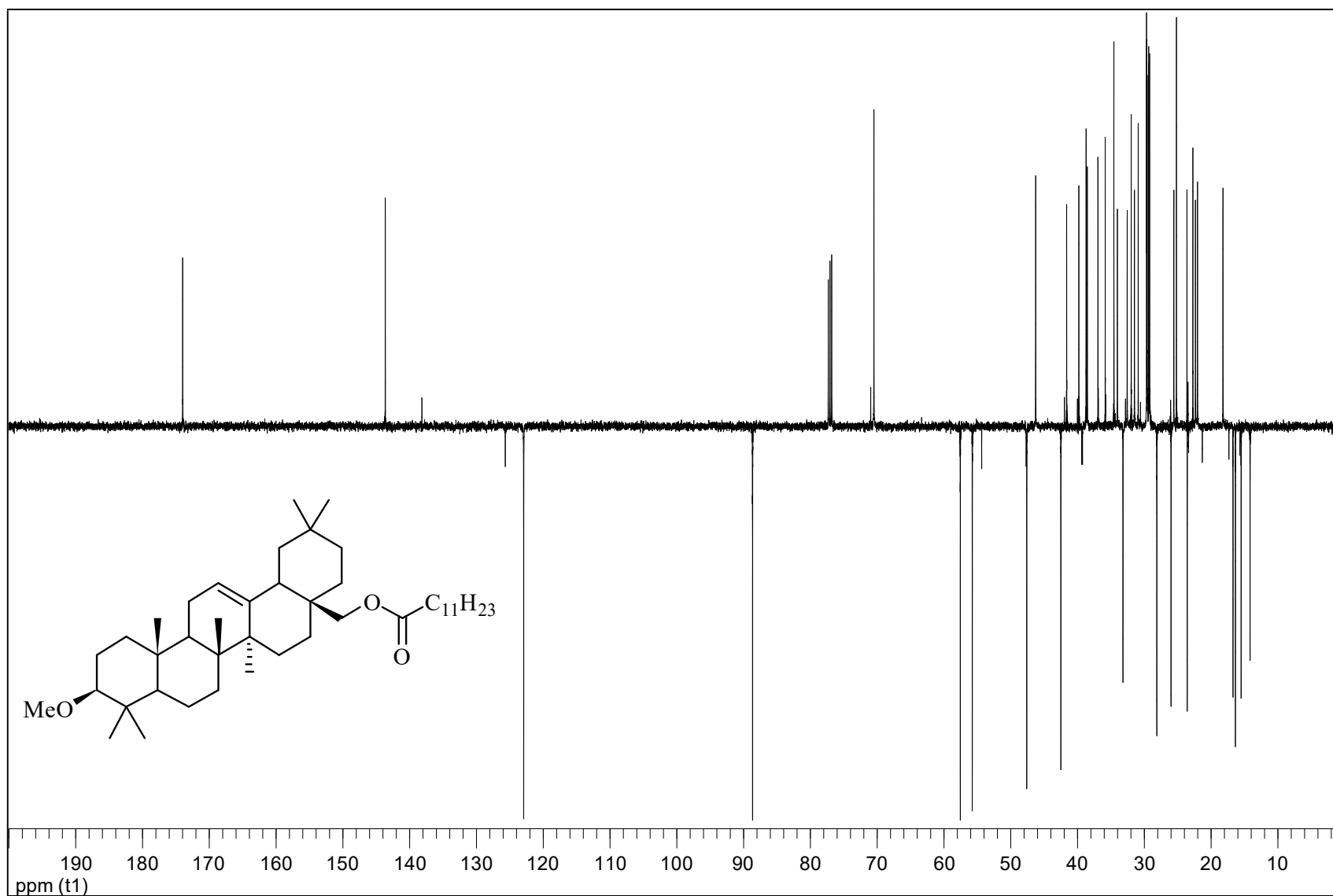


Figure 7: ^{13}C -APT NMR Spectrum of Compound **5a** (CDCl_3 , 125 MHz)

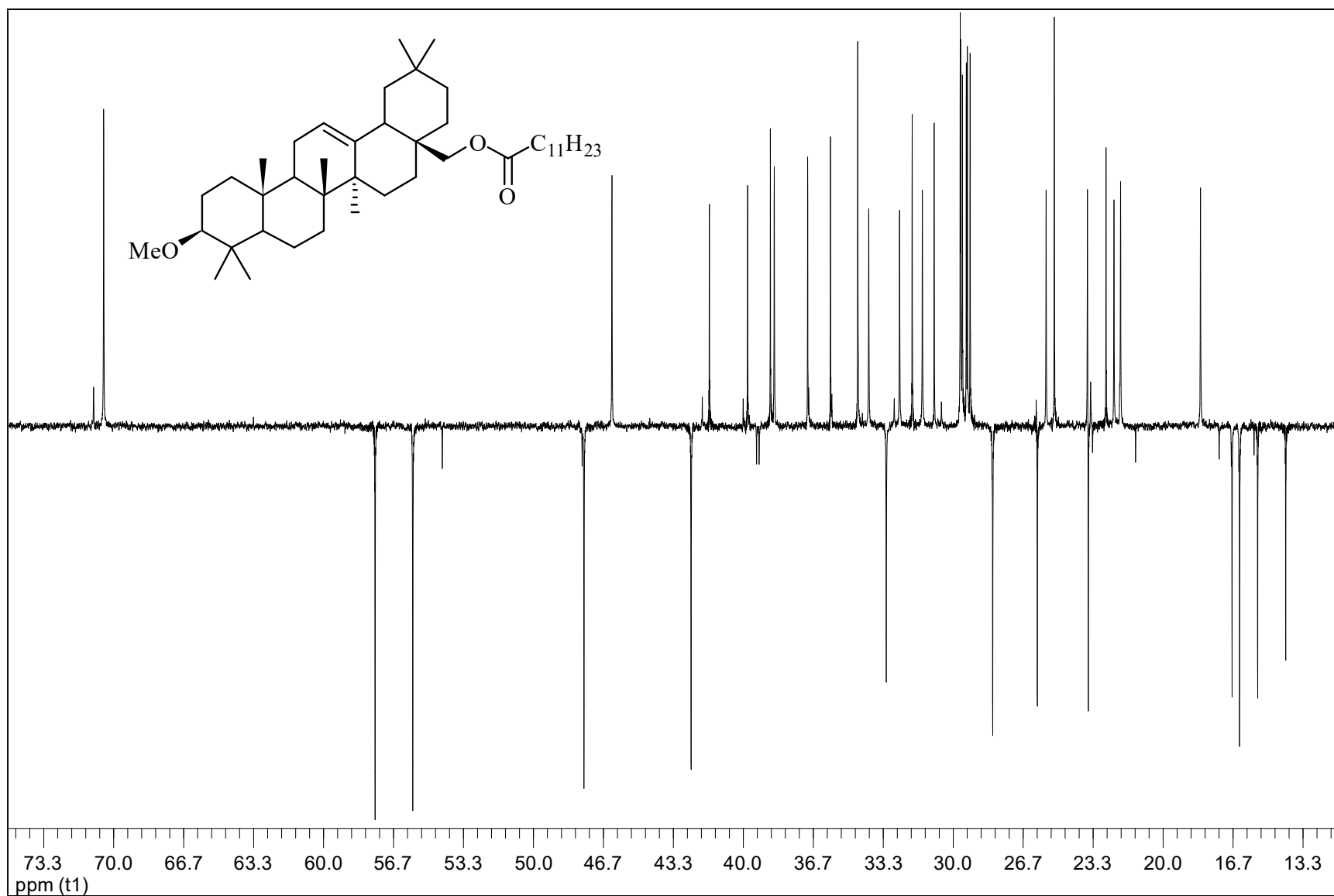


Figure 8: ¹³C-APT NMR Spectrum of Compound **5a** (Extended) (CDCl₃, 125 MHz)

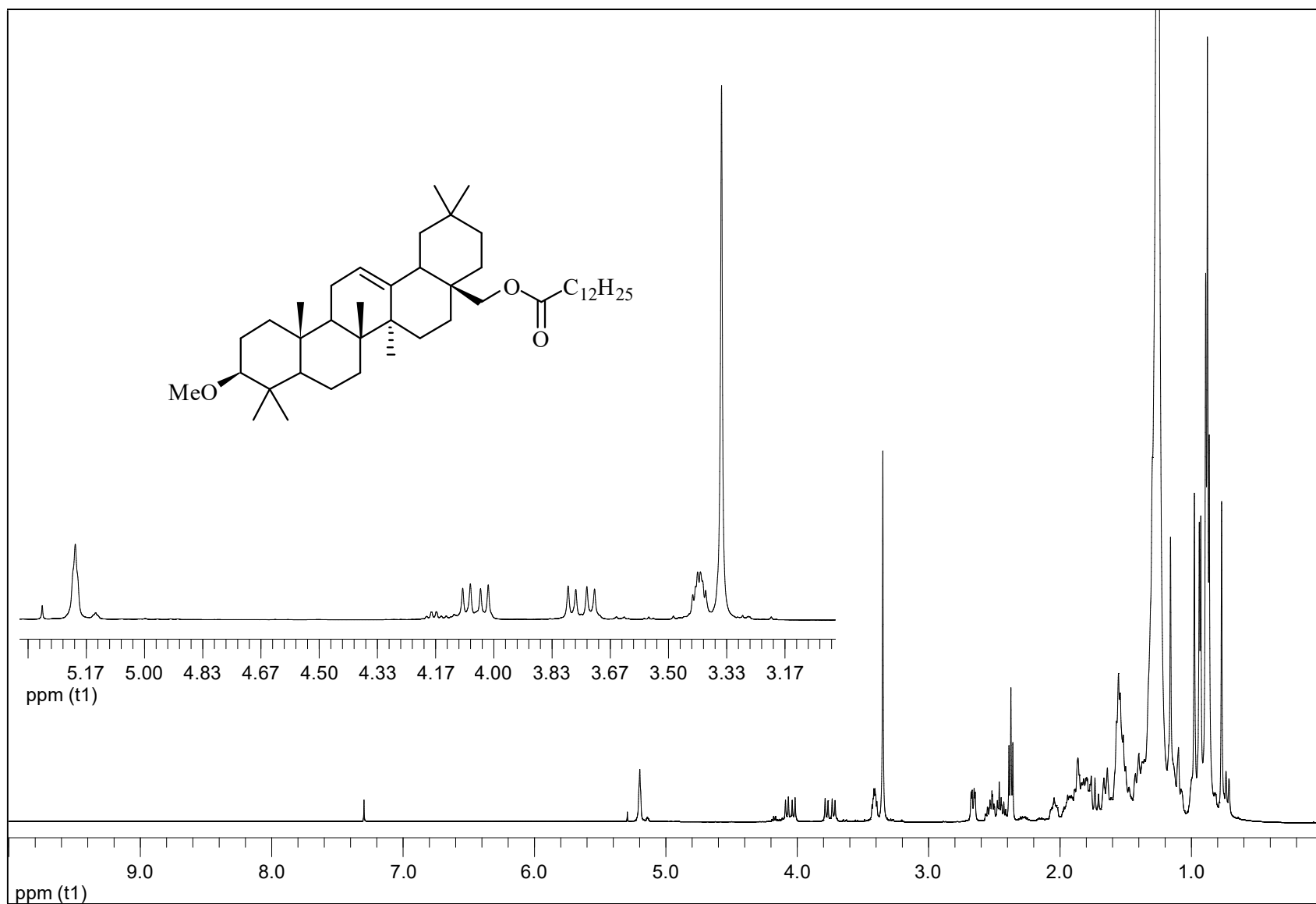


Figure 9: $^1\text{H-NMR}$ Spectrum of Compound **5b** (CDCl_3 , 500 MHz)

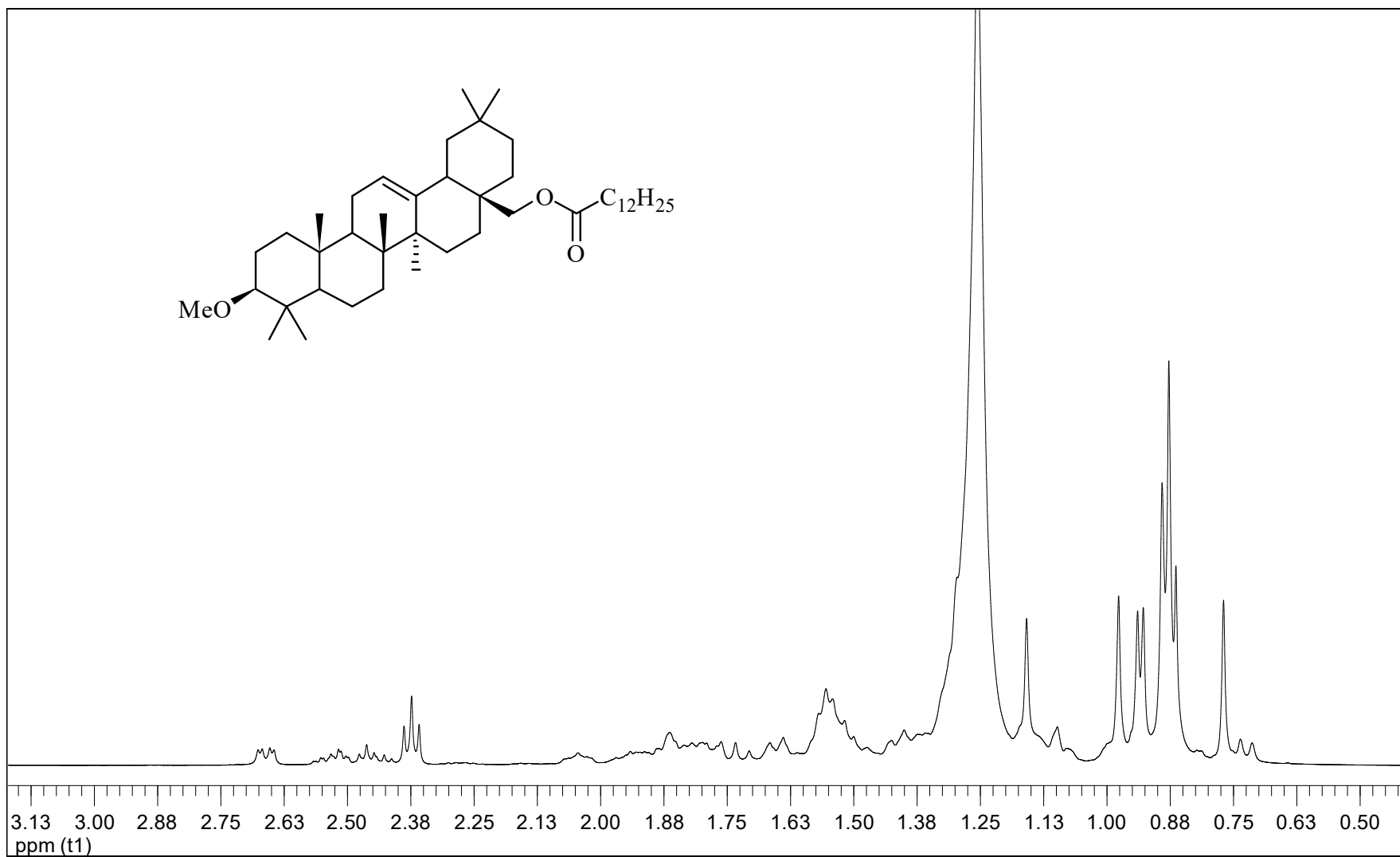


Figure 10: ¹H-NMR Spectrum of Compound **5b** (Extended) (CDCl₃, 500 MHz)

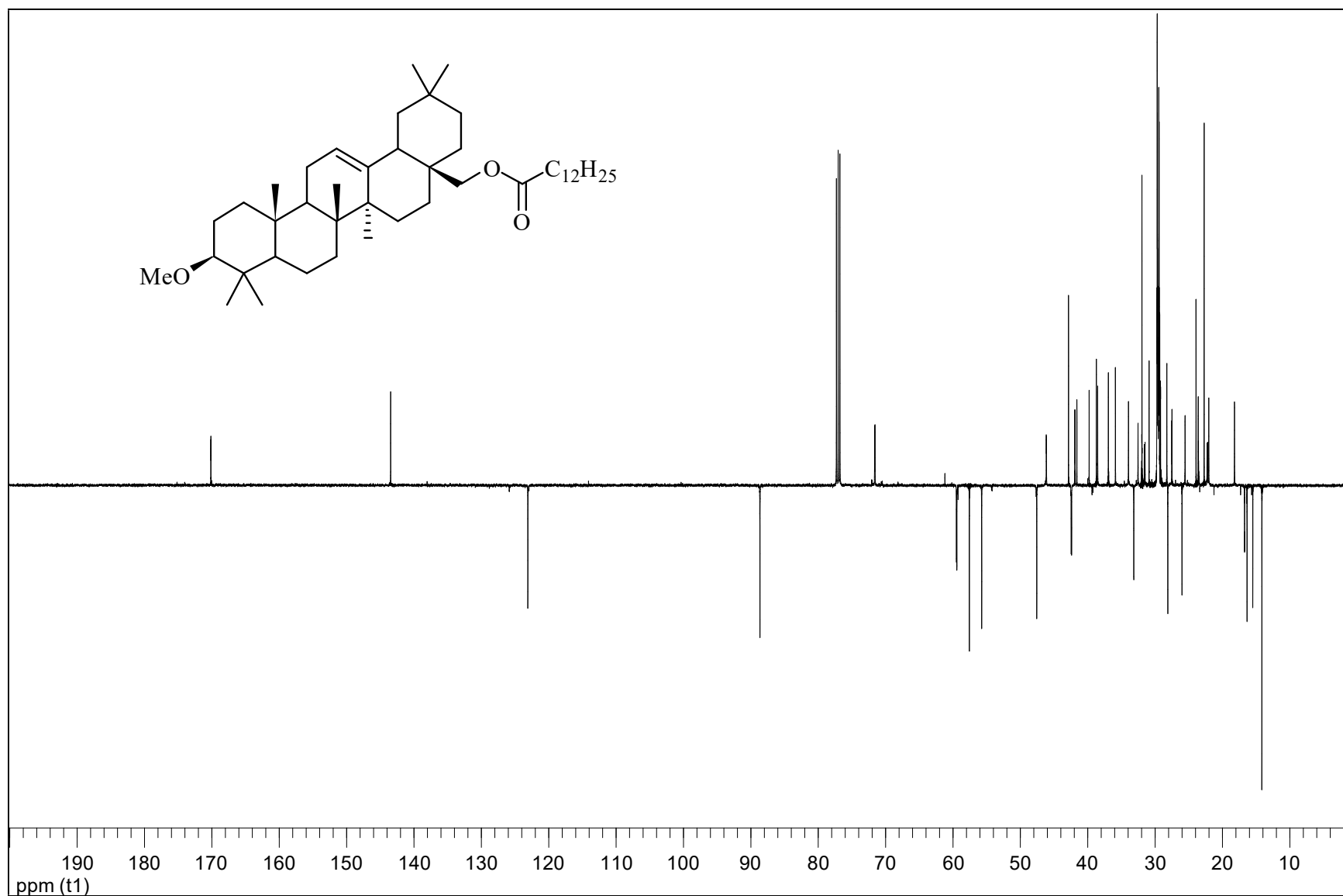


Figure 11: ^{13}C -APT NMR Spectrum of Compound 5b (CDCl_3 , 125 MHz)

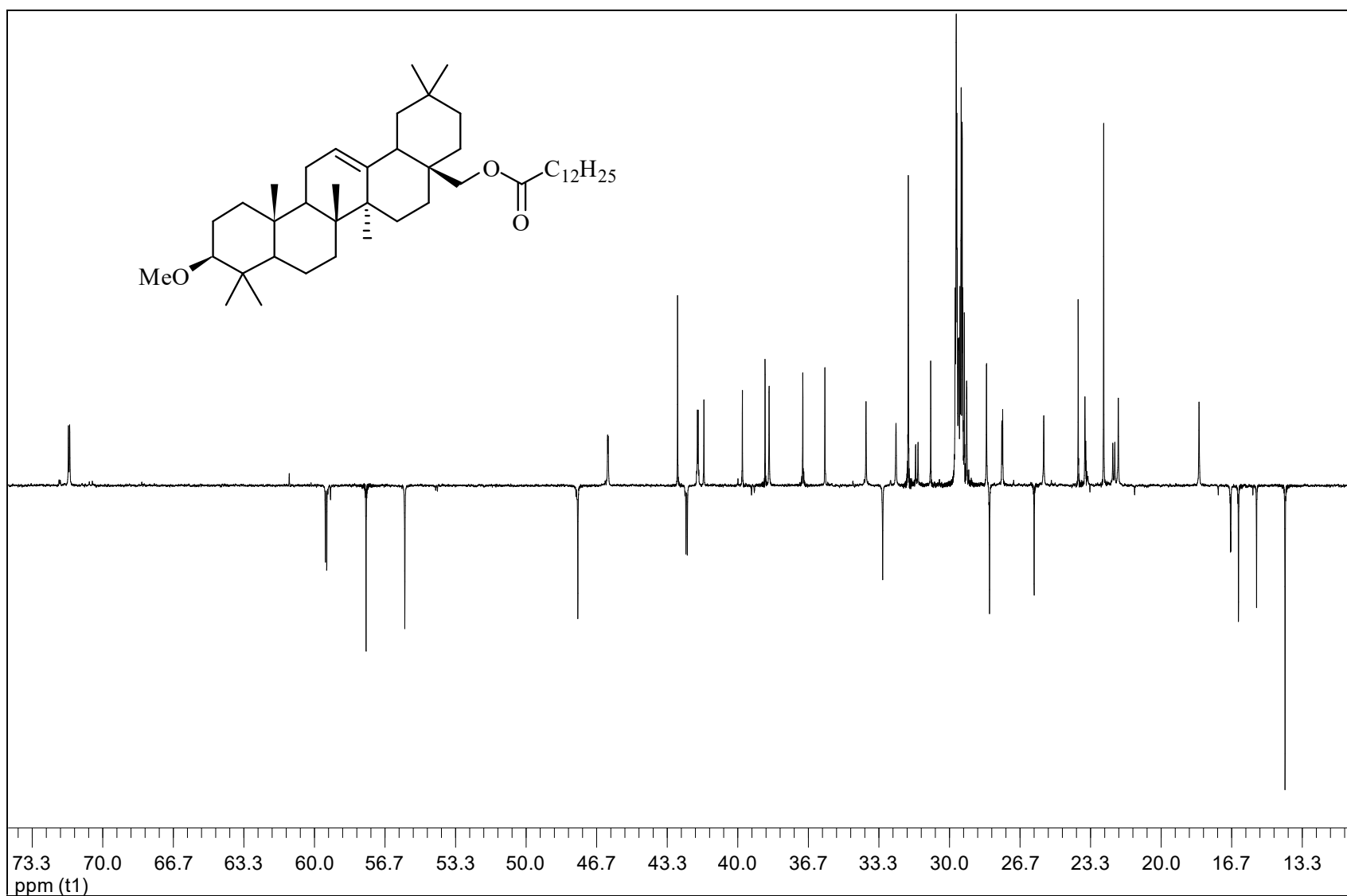


Figure 12: ¹³C-APT NMR Spectrum of Compound **5b** (Extended) (CDCl₃, 125 MHz)

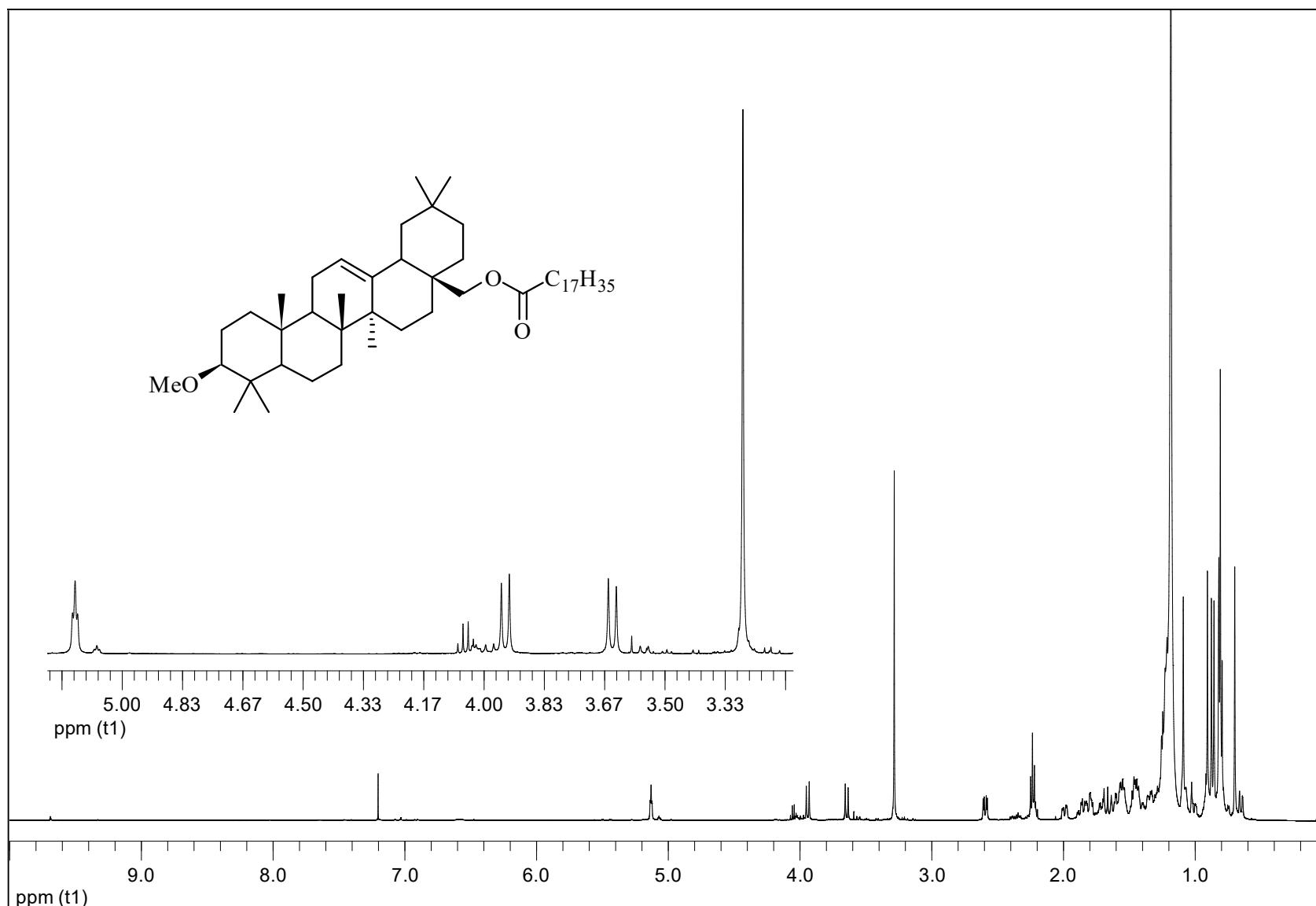


Figure 13: ¹H-NMR Spectrum of Compound 5c (CDCl₃, 500 MHz)

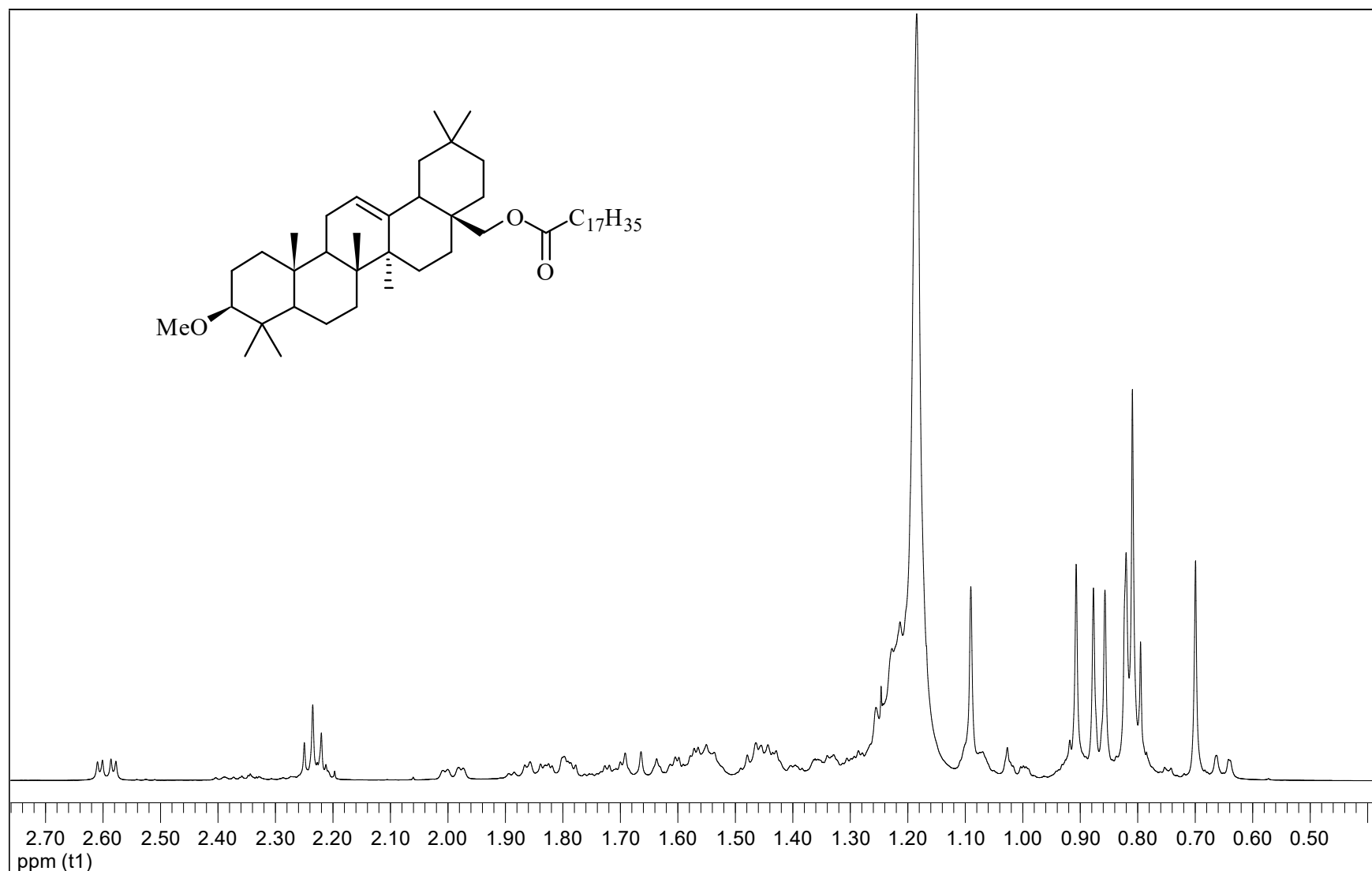


Figure 14: ¹H-NMR Spectrum of Compound 5c (Extended) (CDCl₃, 500 MHz)

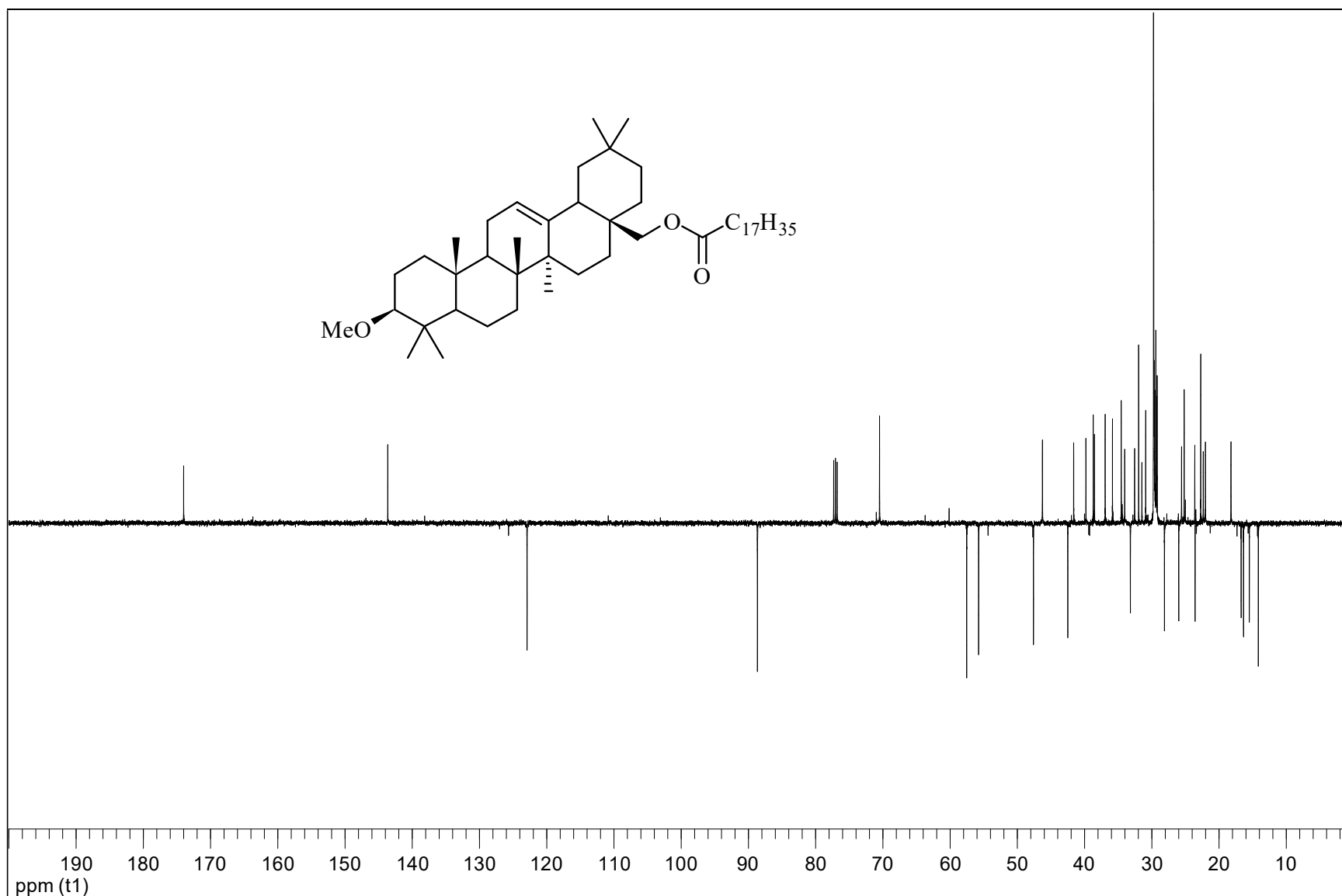


Figure 15: ^{13}C -APT NMR Spectrum of Compound **5c** (CDCl_3 , 125 MHz)

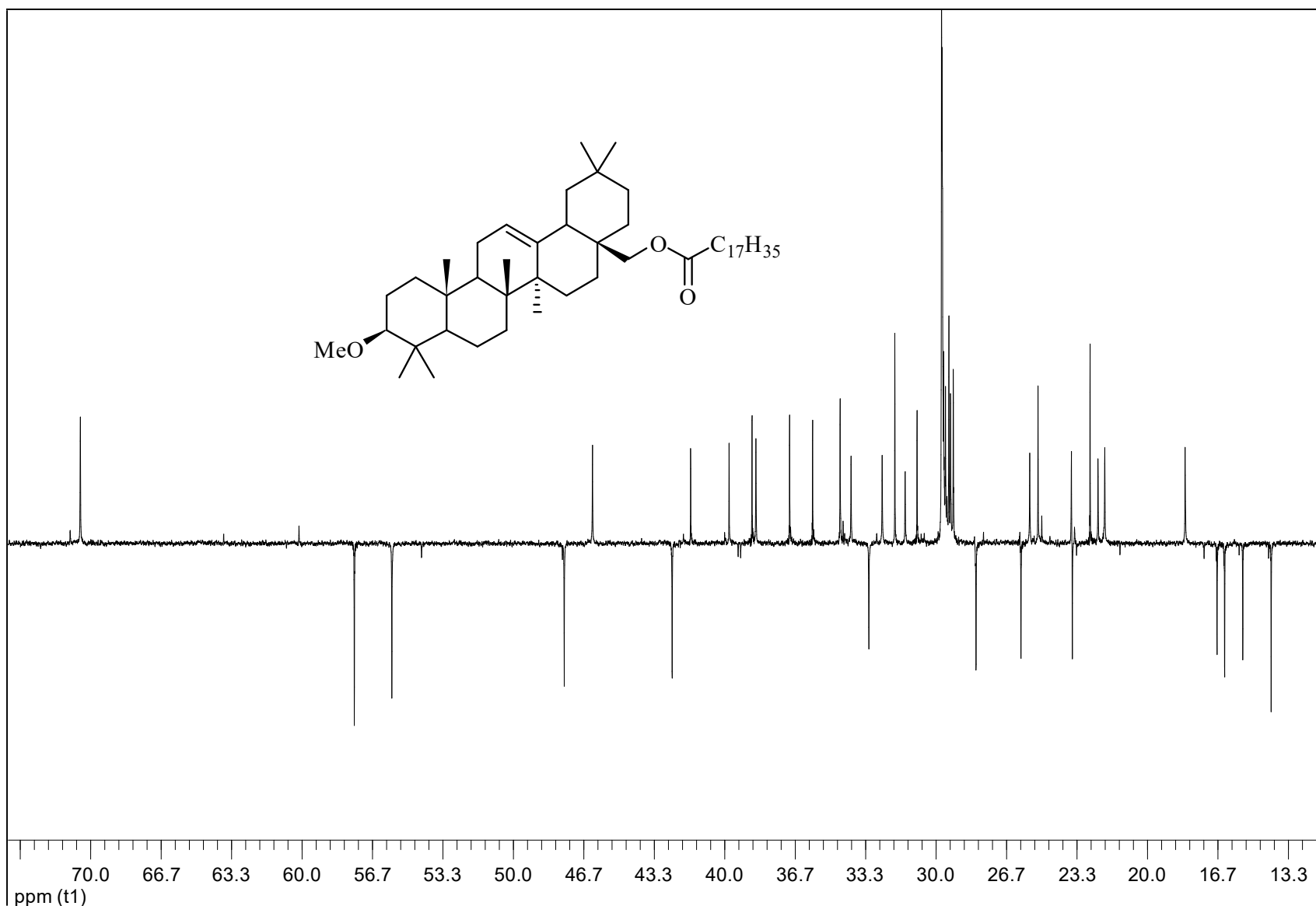


Figure 16: ¹³C-APT NMR Spectrum of Compound 5c (CDCl₃, 125 MHz)

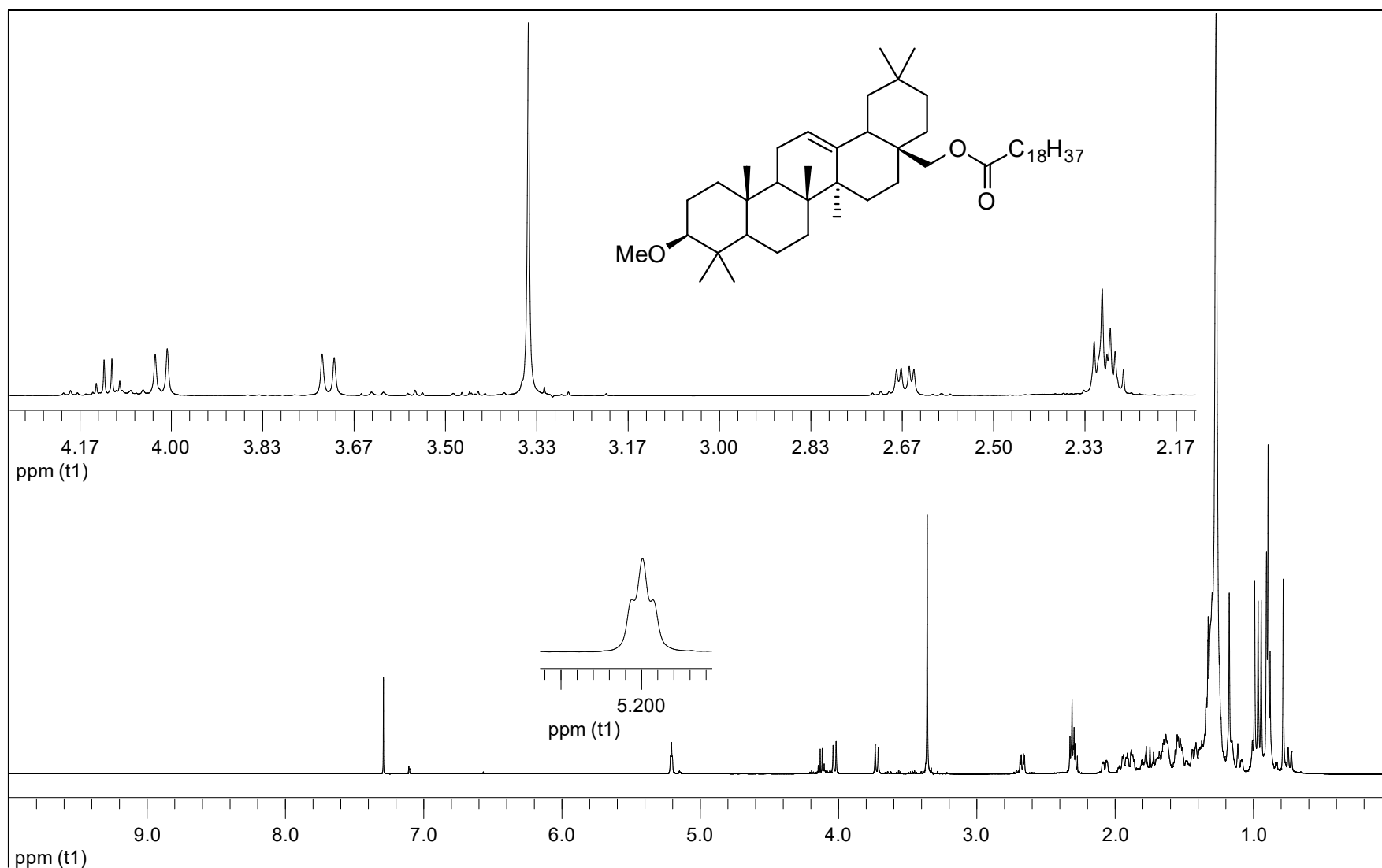


Figure 17: ¹H-NMR Spectrum of Compound **5d** (CDCl₃, 500 MHz)

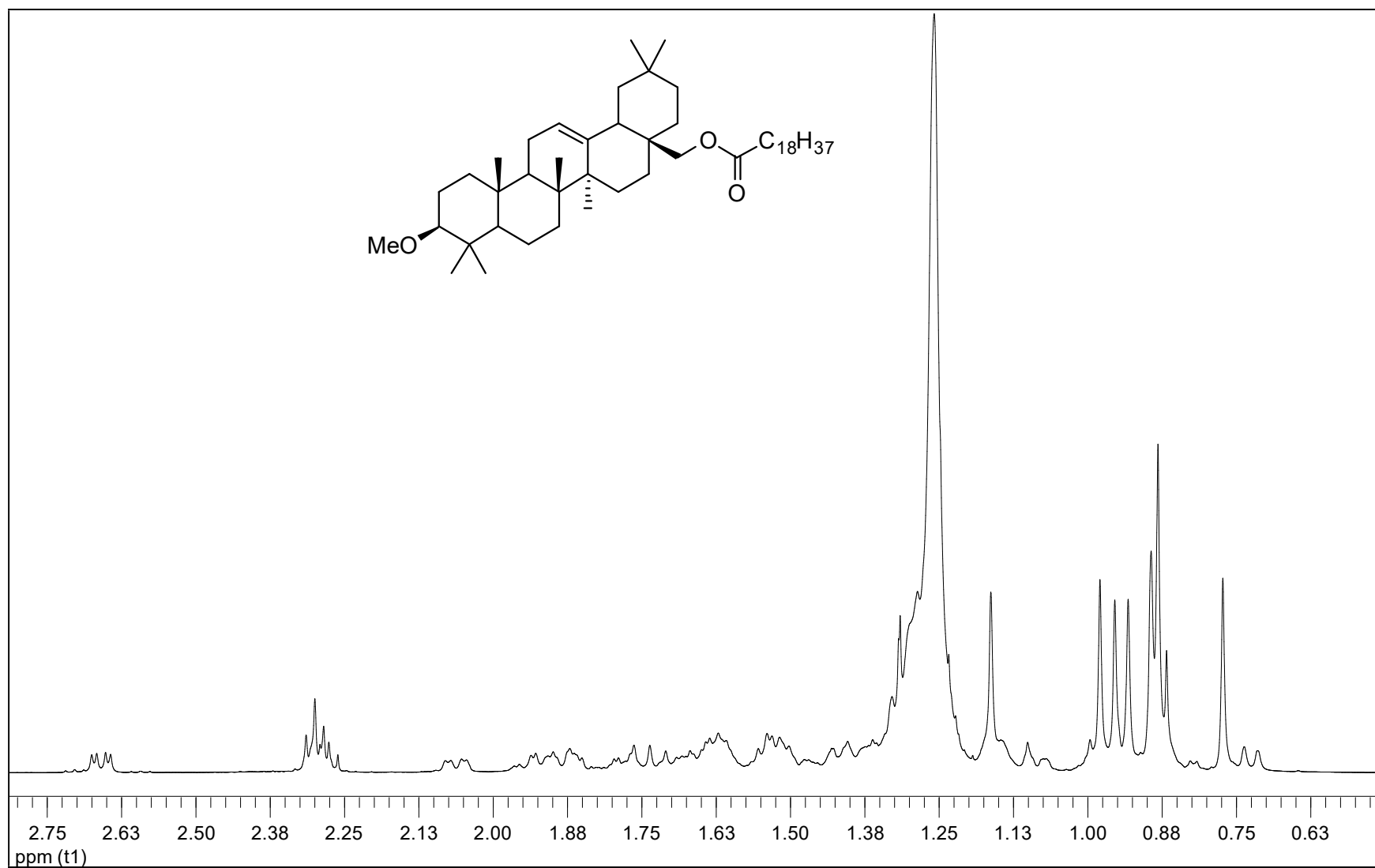


Figure 18: ¹H-NMR Spectrum of Compound **5d** (Extended) (CDCl₃, 500 MHz)

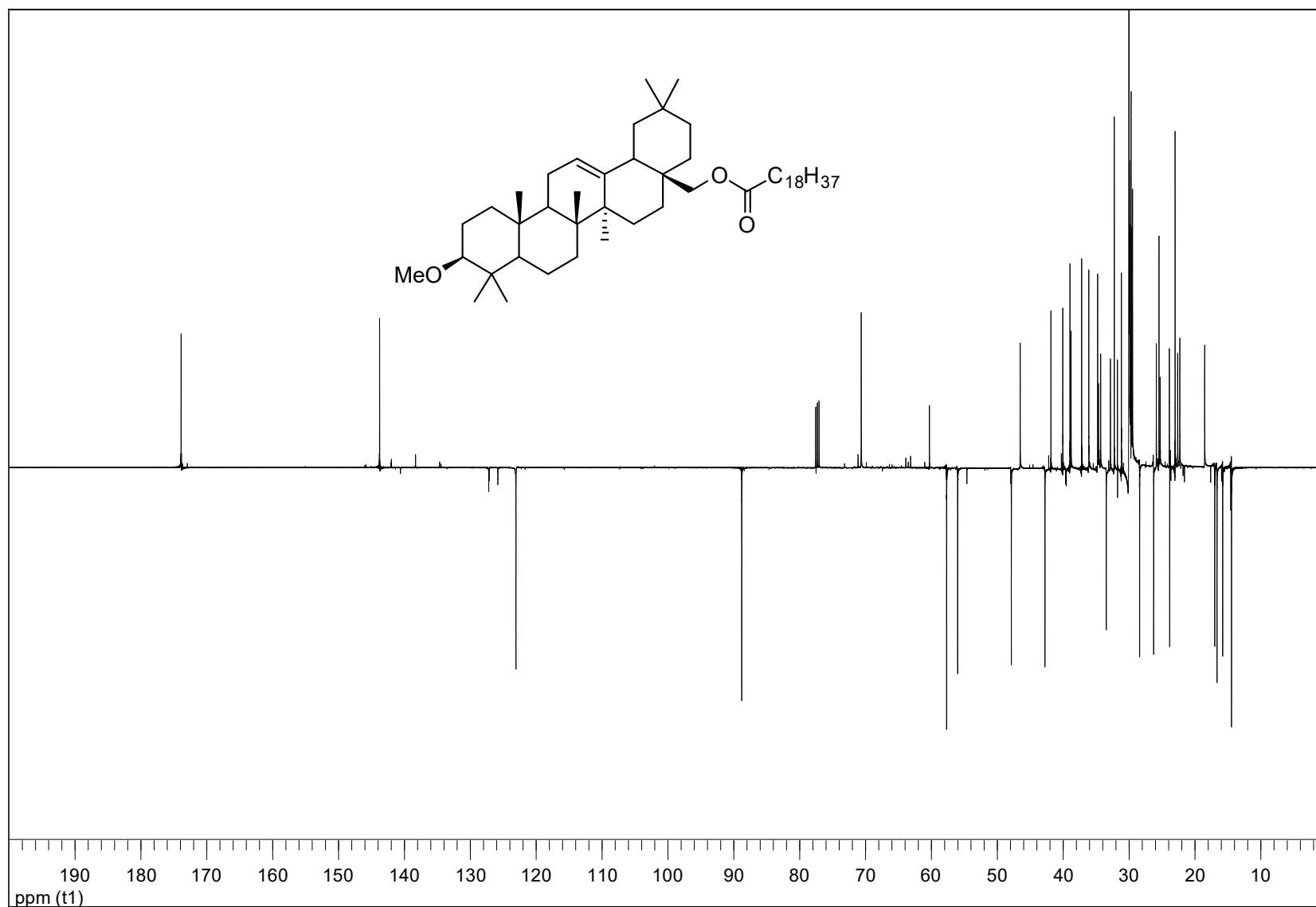


Figure 19: ^{13}C -APT NMR Spectrum of Compound **5d** (CDCl₃, 125 MHz)

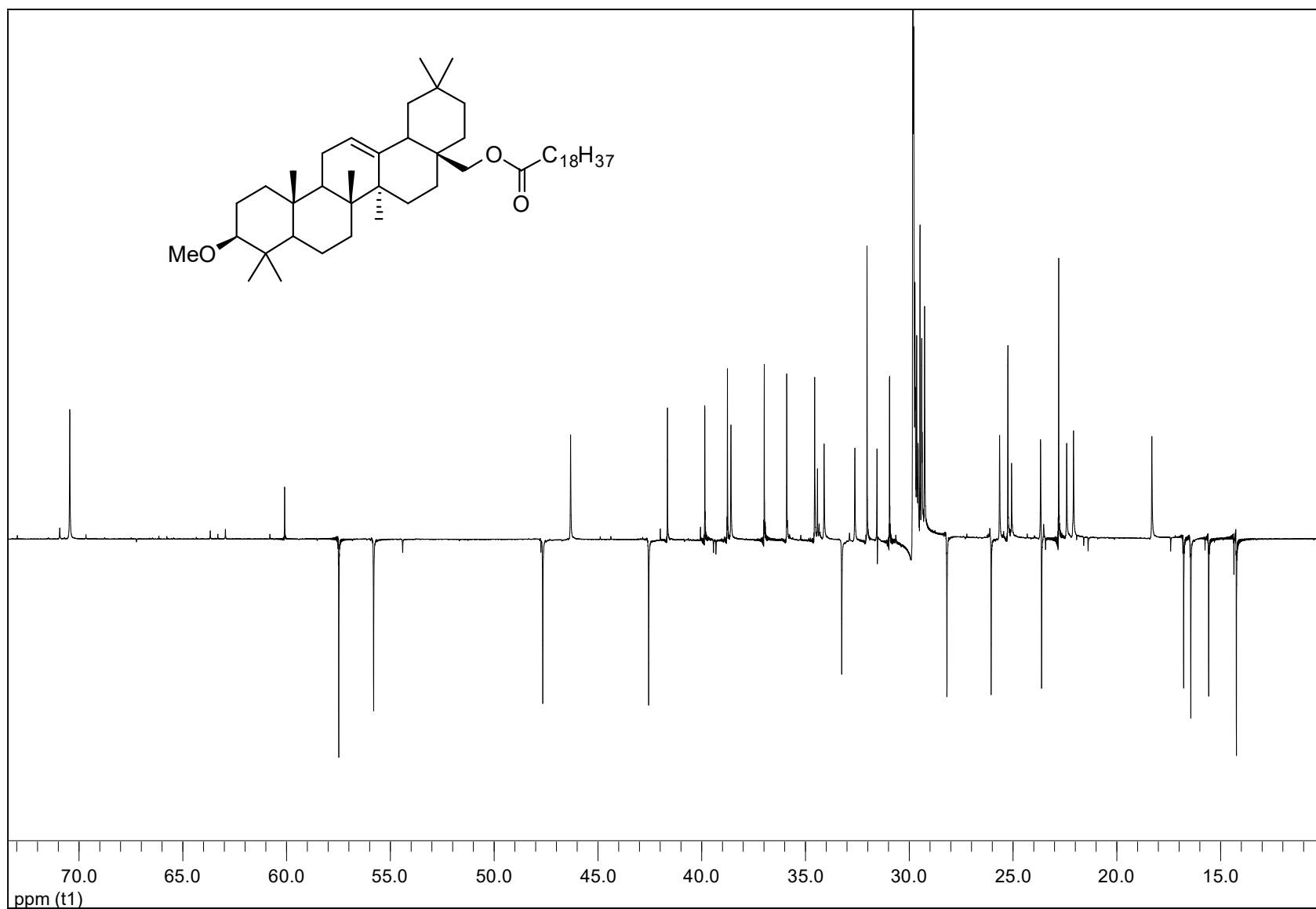


Figure 20: ^{13}C -APT NMR Spectrum of Compound **5d** (Extended) (CDCl_3 , 125 MHz)

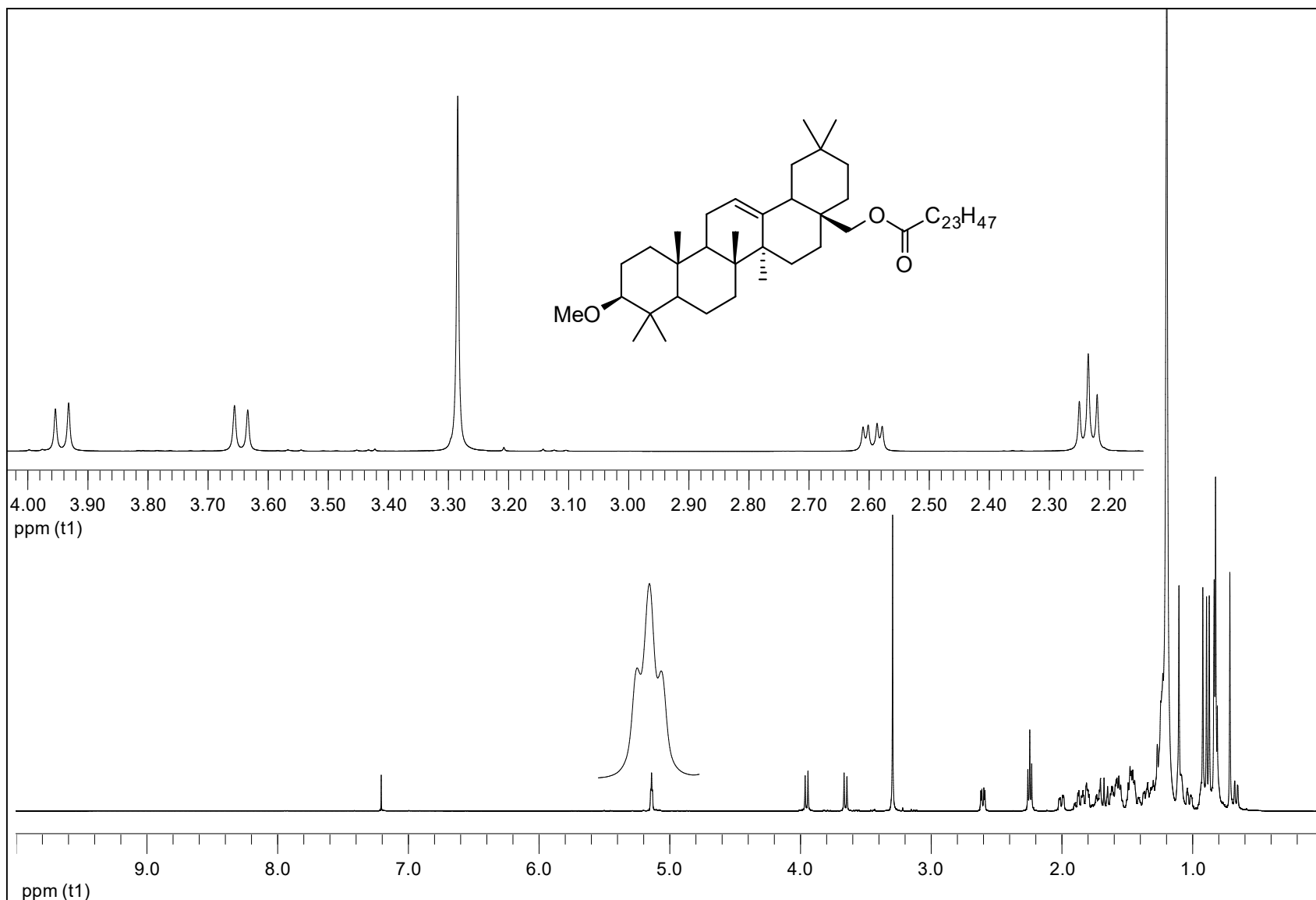


Figure 21: ¹H-NMR Spectrum of Compound 5e (CDCl₃, 500 MHz)

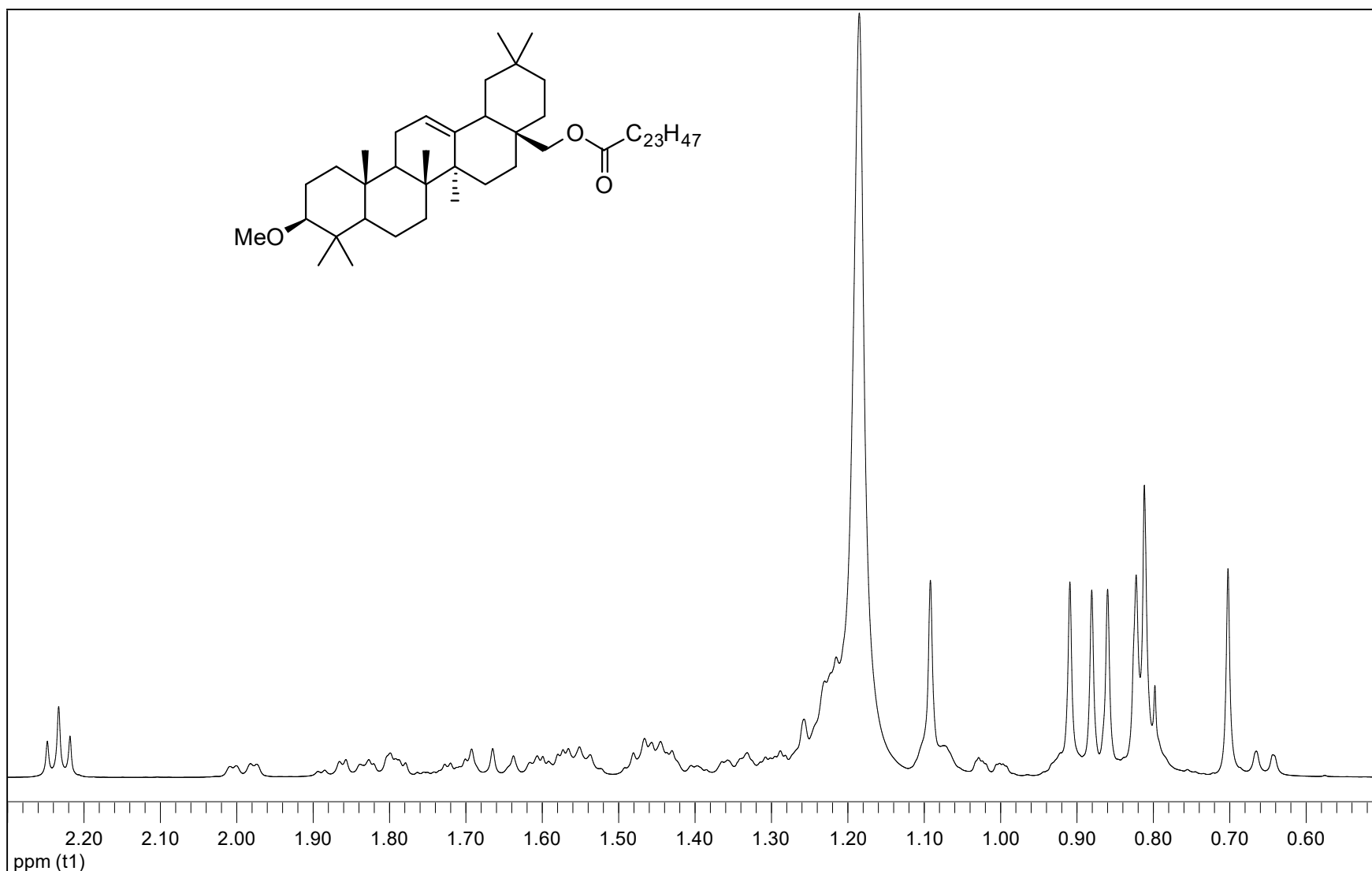


Figure 22: $^1\text{H-NMR}$ Spectrum of Compound **5e** (Extended) (CDCl_3 , 500 MHz)

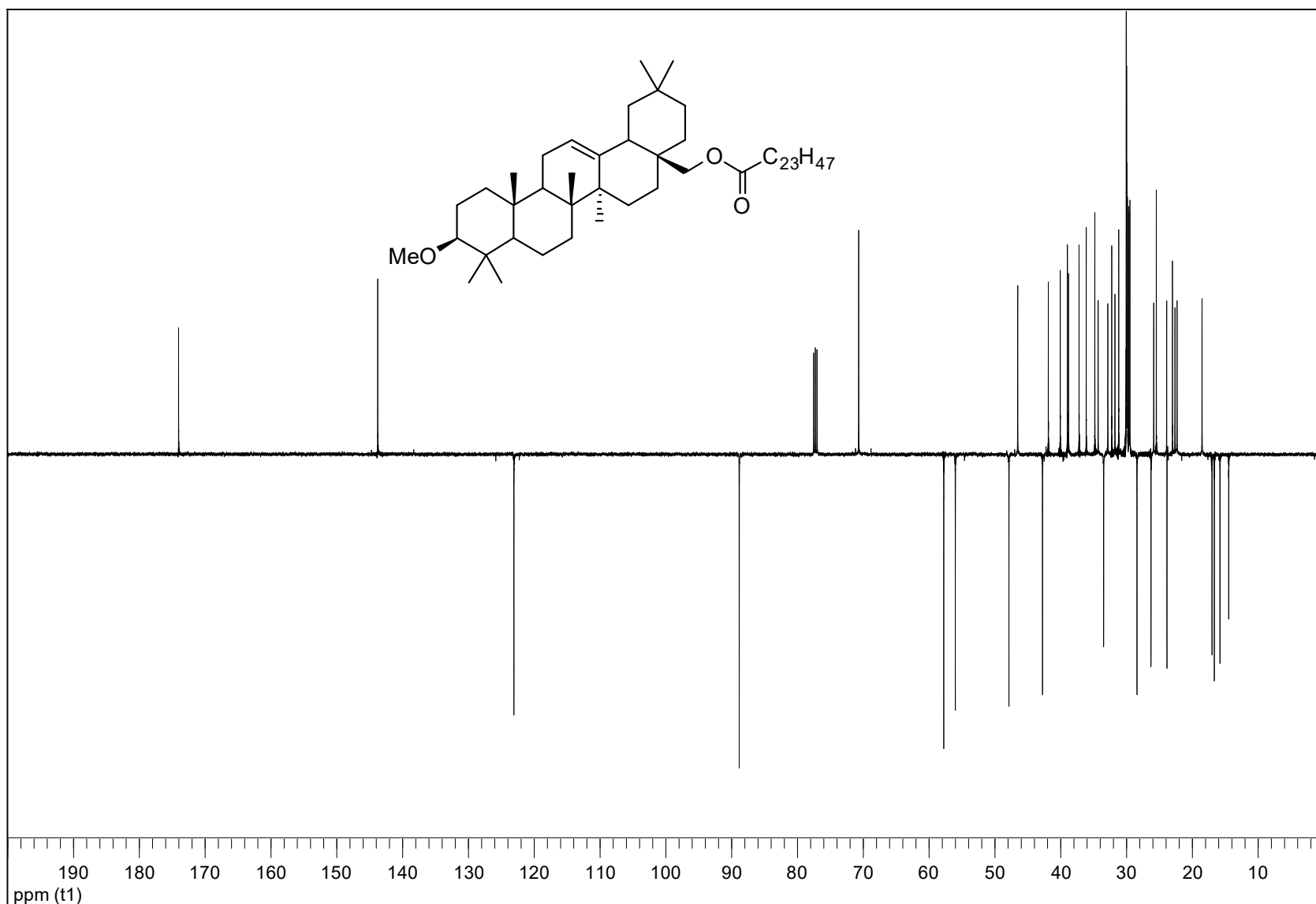


Figure 23: ^{13}C -APT NMR Spectrum of Compound 5e (CDCl₃, 125 MHz)

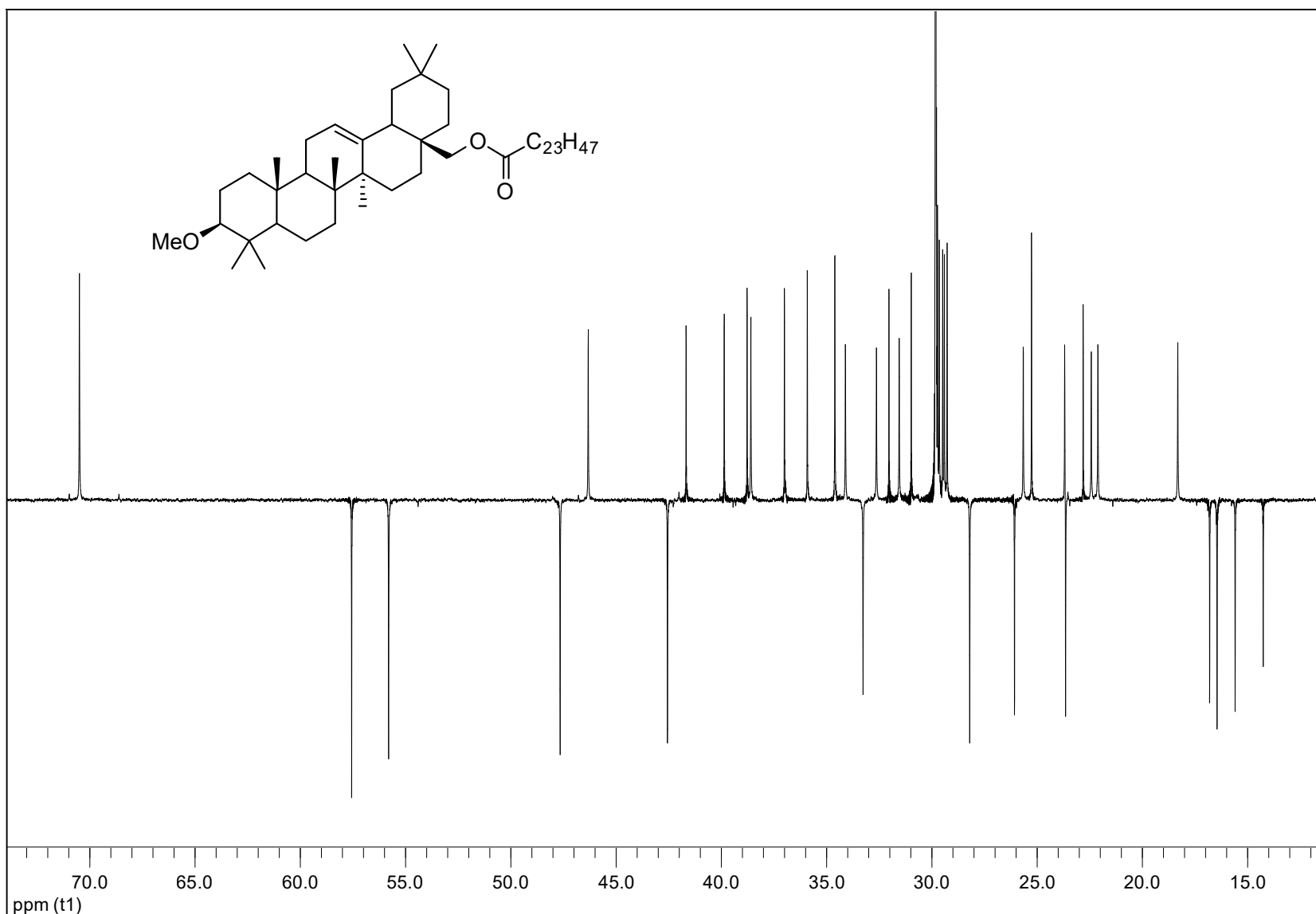


Figure 24: ^{13}C -APT NMR Spectrum of Compound **5e** (Extended) (CDCl_3 , 125 MHz)

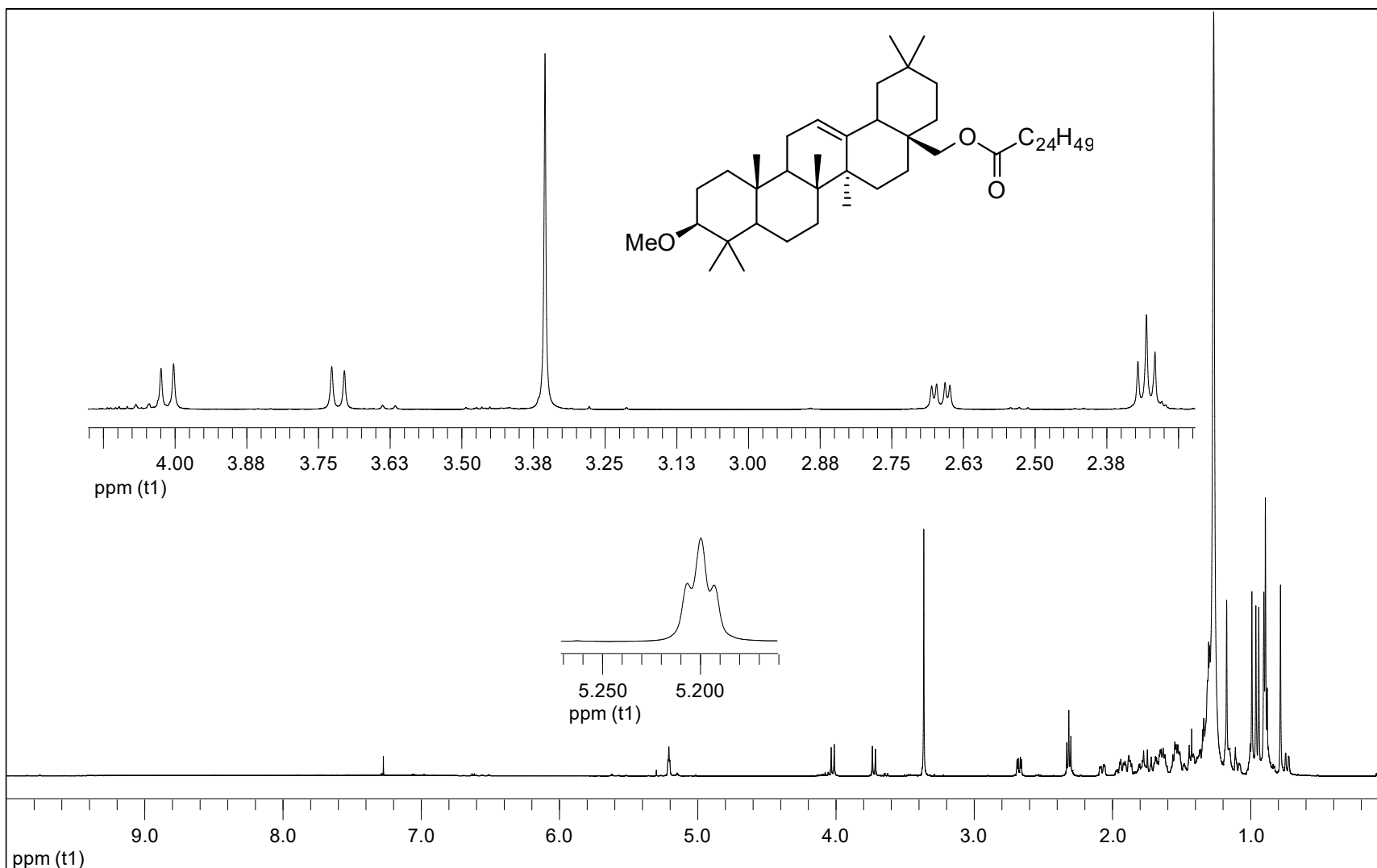


Figure 25: ¹H-NMR Spectrum of Compound **5f** (CDCl₃, 500 MHz)

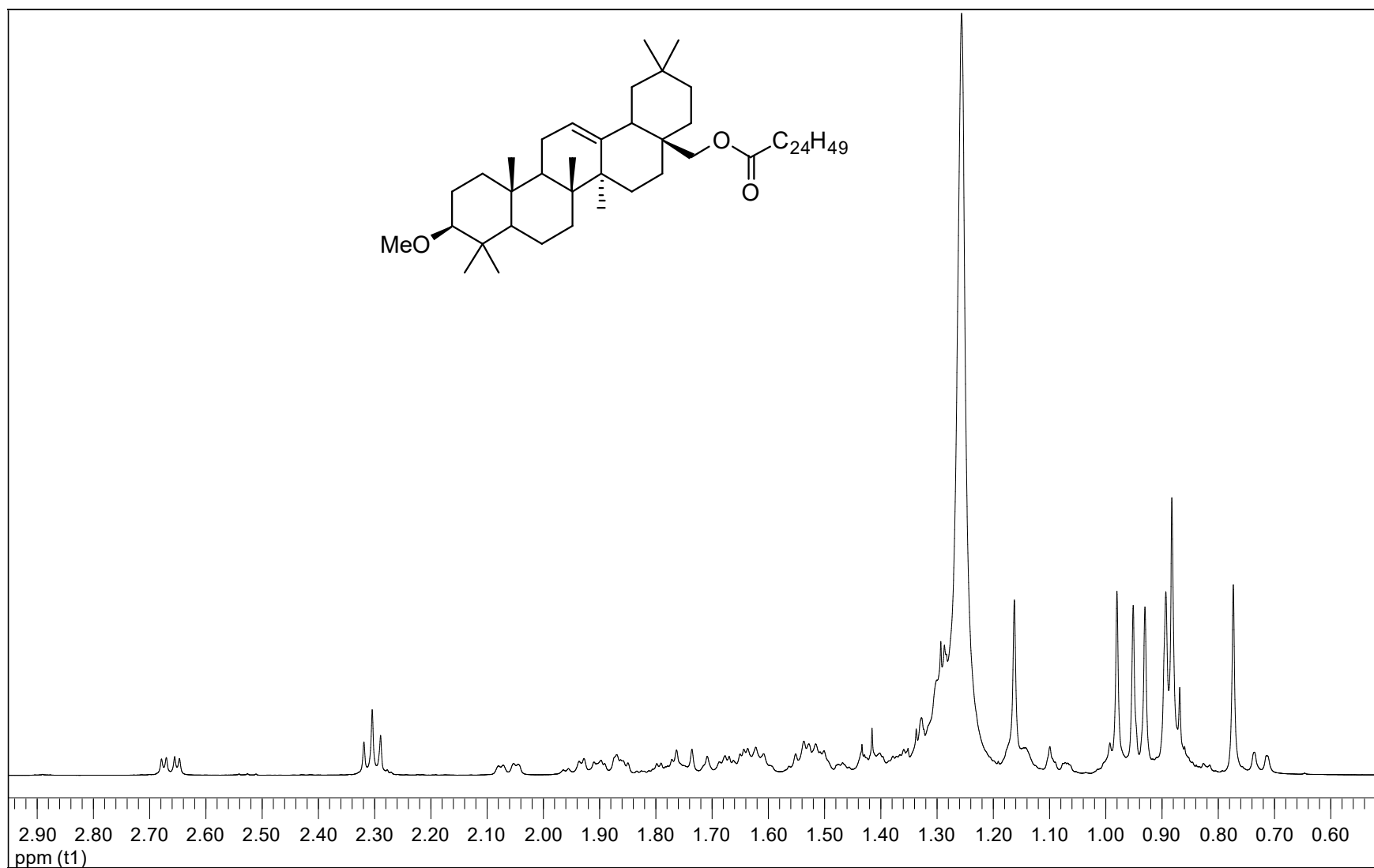


Figure 26: ¹H-NMR Spectrum of Compound 5e (Extended) (CDCl₃, 500 MHz)

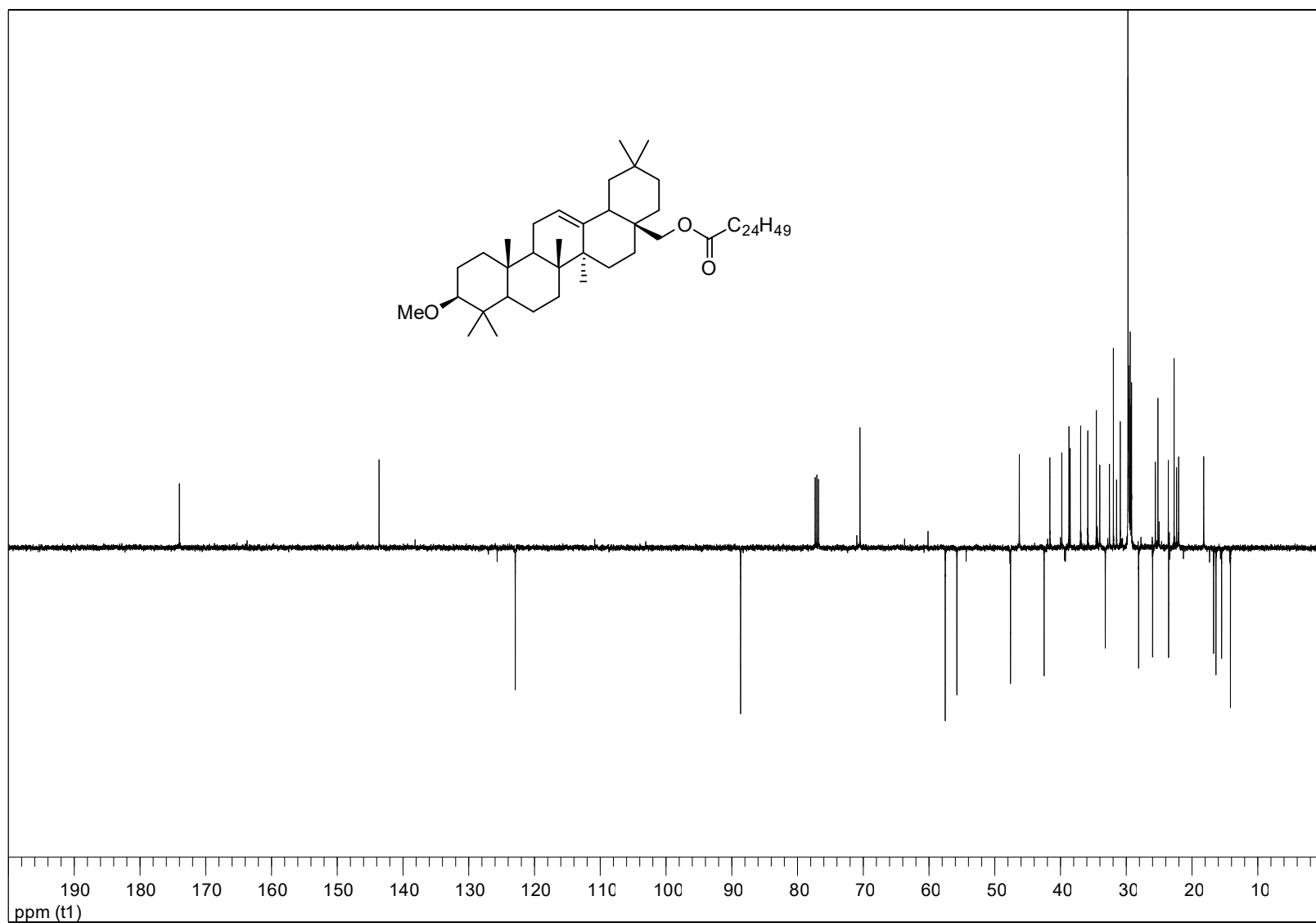


Figure 27: ¹³C-APT NMR Spectrum of Compound **5f** (CDCl₃, 125 MHz)

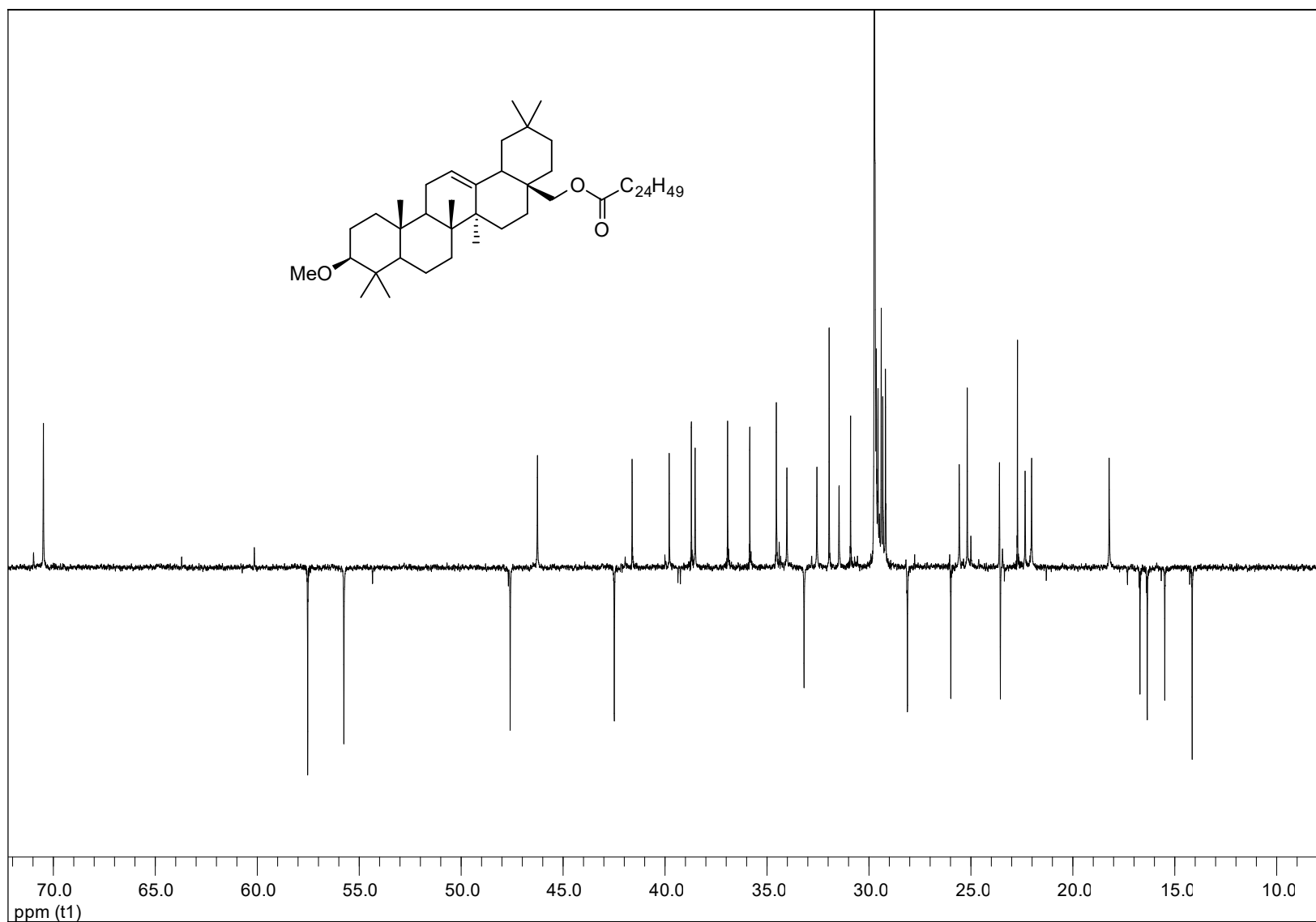


Figure 28: ¹³C-APT NMR Spectrum of Compound **5f** (Extended) (CDCl₃, 125 MHz)

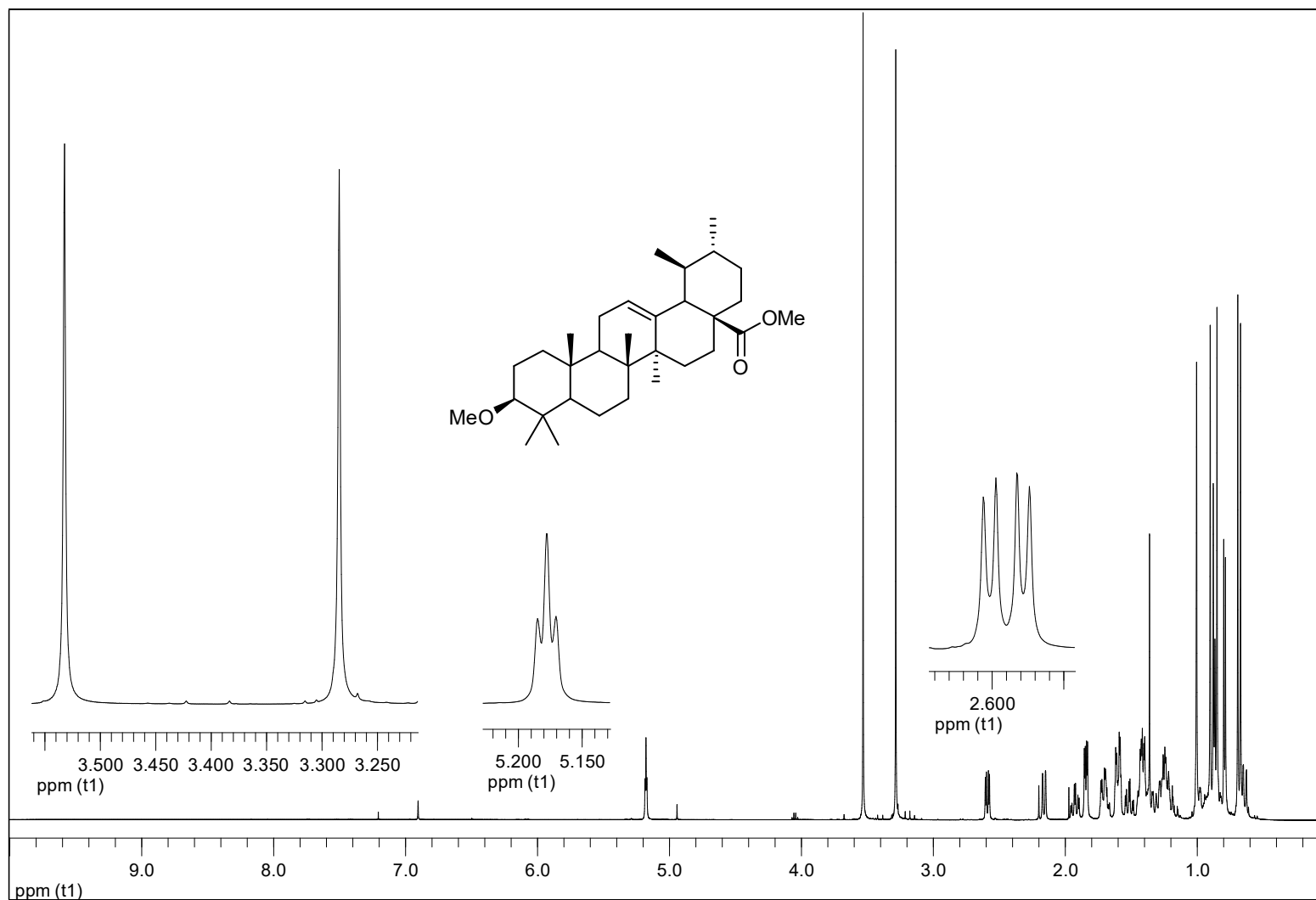


Figure 29: ¹H-NMR Spectrum of Compound 6 (CDCl₃, 500 MHz)

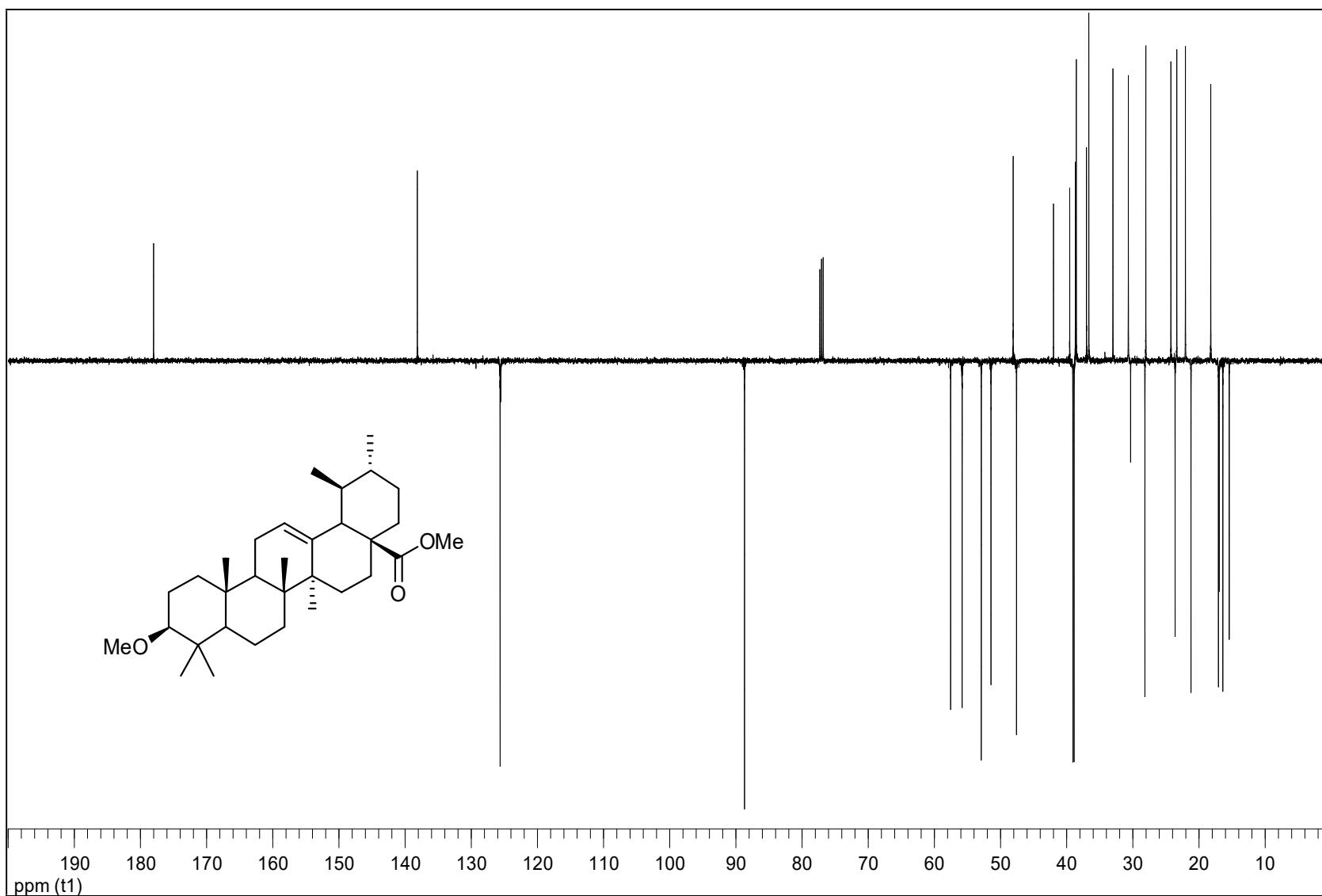


Figure 30: ^{13}C -APT NMR Spectrum of Compound 6 (125 MHz, CDCl_3)

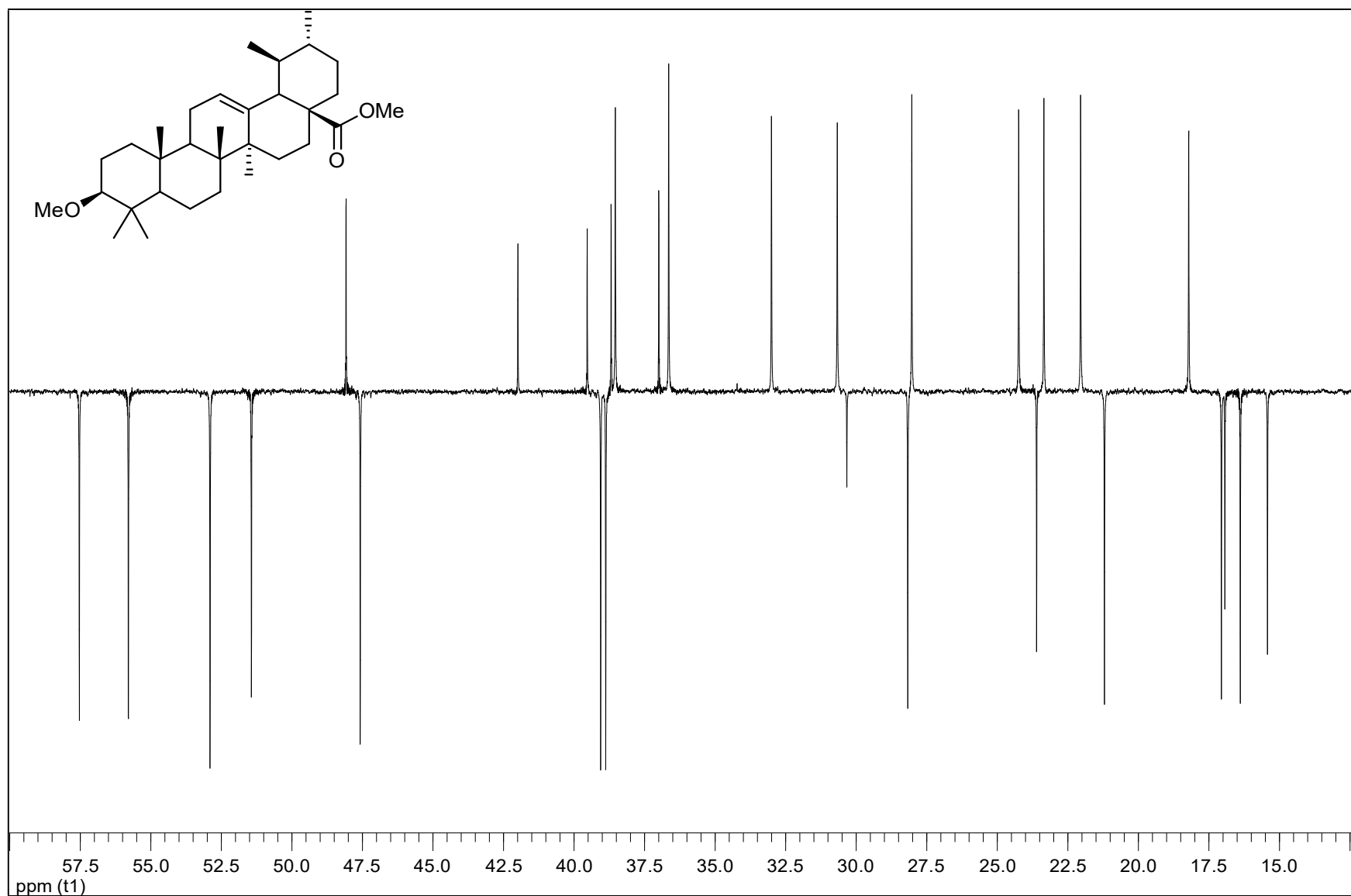


Figure 31: ¹³C-APT NMR Spectrum of Compound 6 (Extended) (125 MHz, CDCl₃)

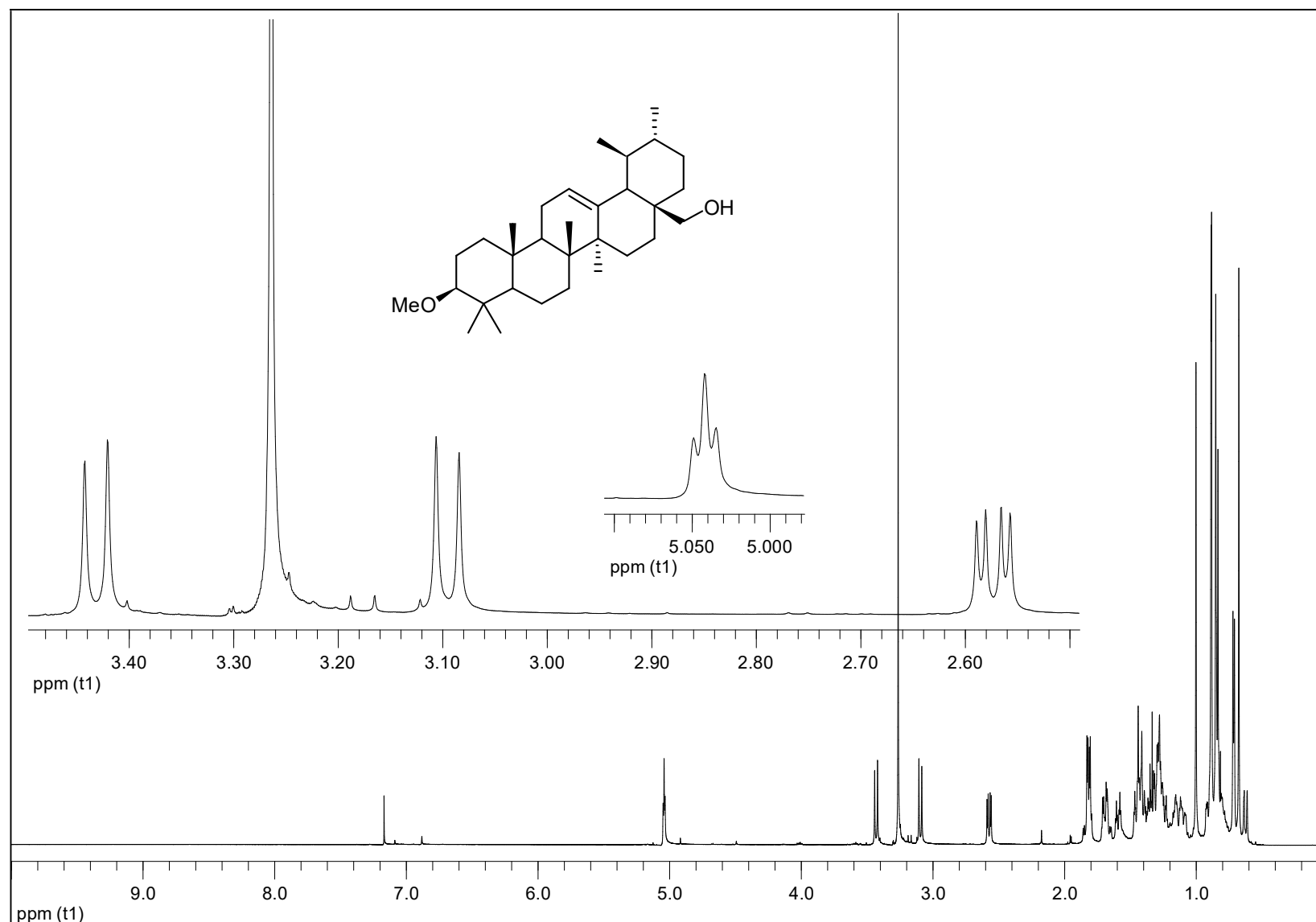


Figure 32: $^1\text{H-NMR}$ Spectrum of Compound 7 (CDCl_3 , 500 MHz)

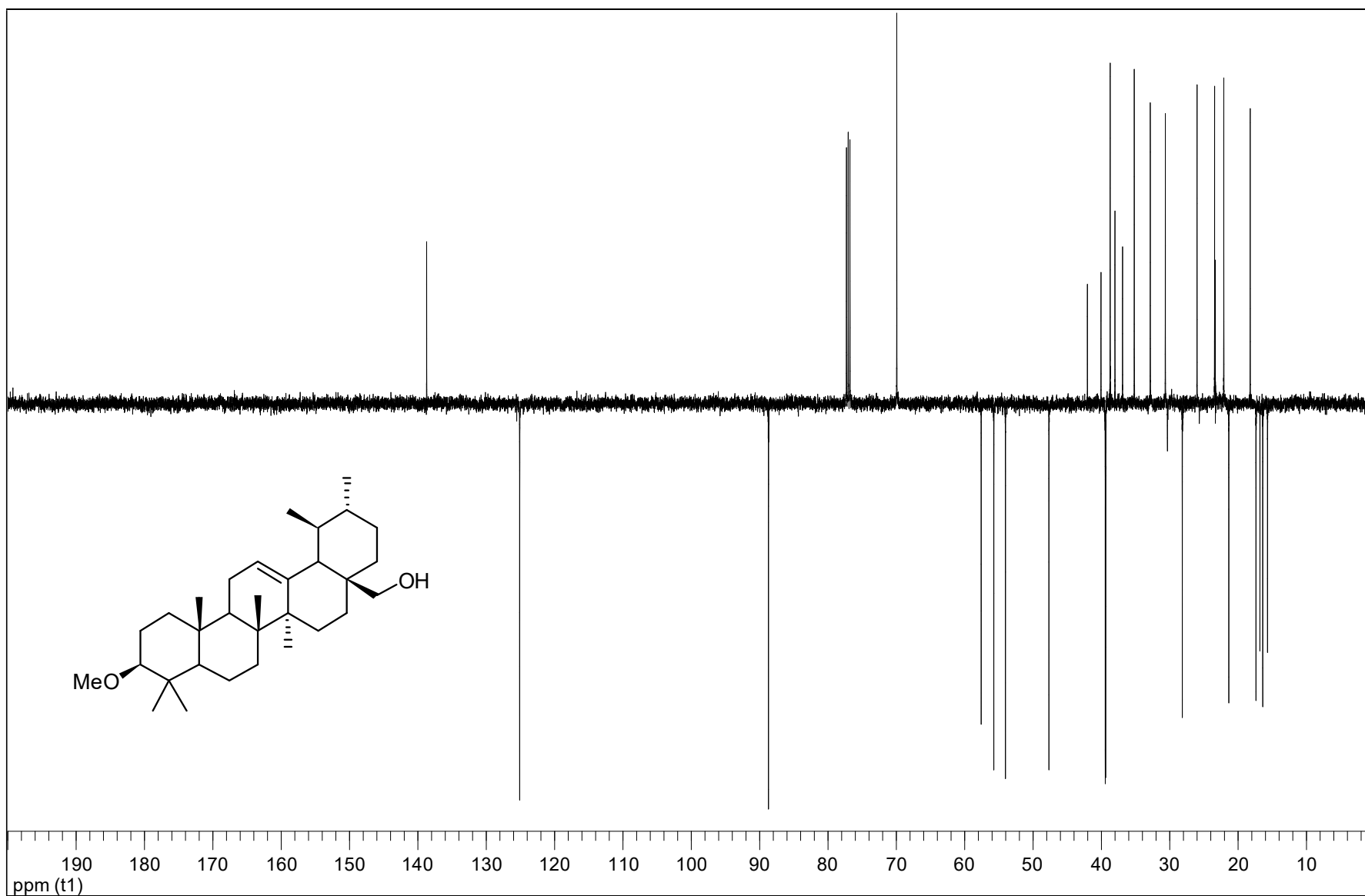


Figure 33: ^{13}C -APT NMR Spectrum of Compound 7 (CDCl_3 , 125 MHz)

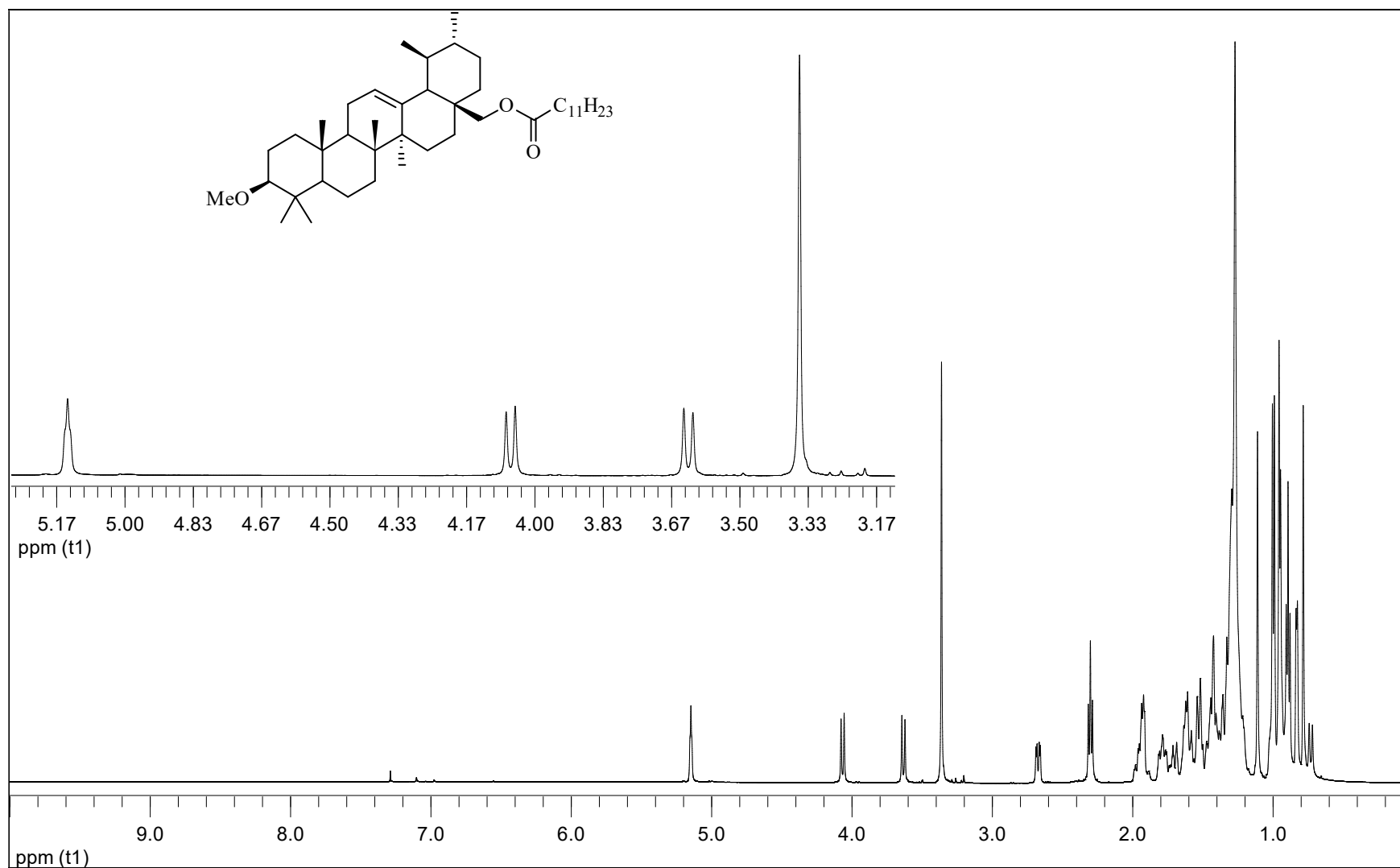


Figure 34: ¹H-NMR Spectrum of Compound **8a** (CDCl₃, 500 MHz)

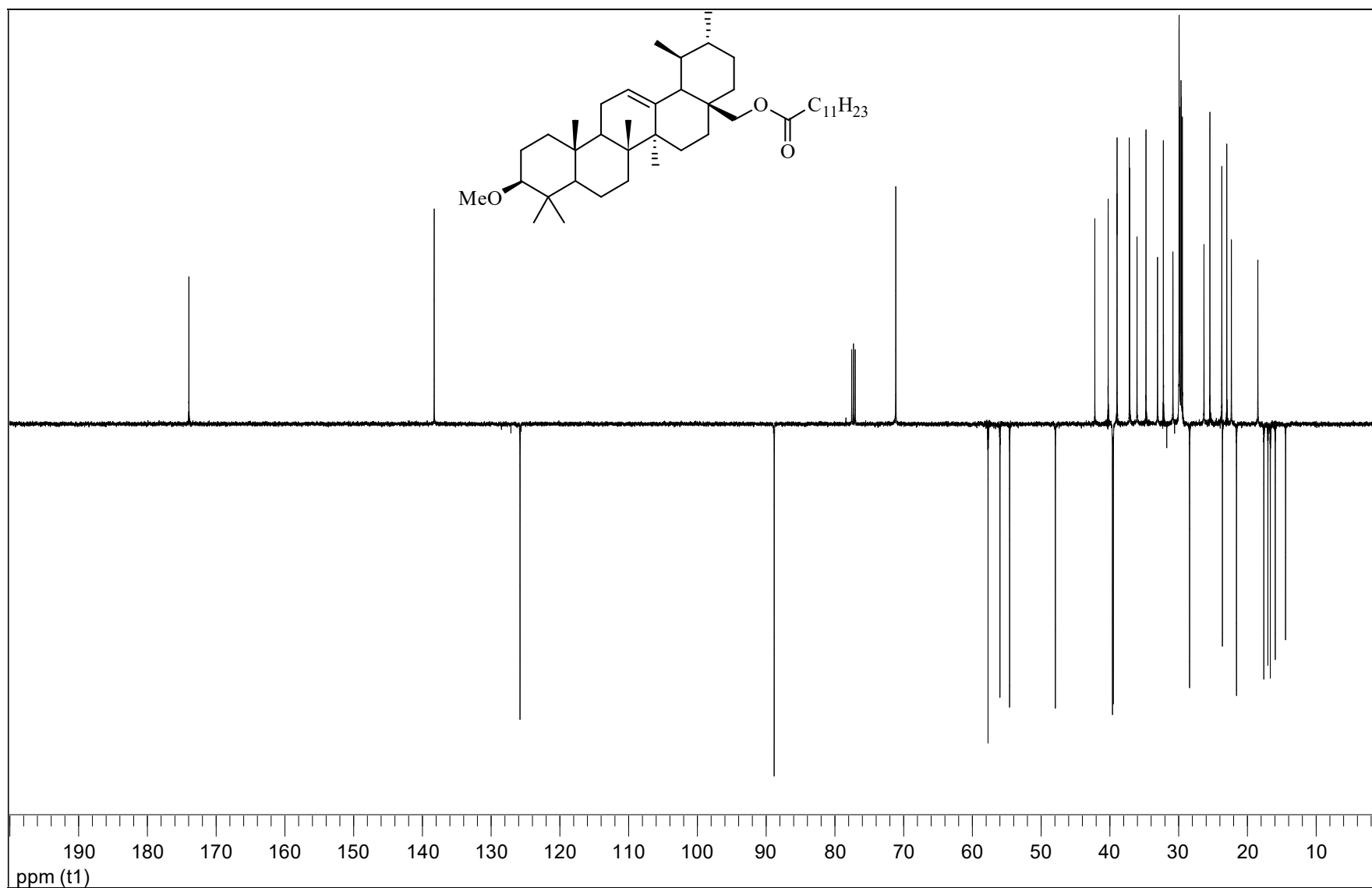


Figure 35: ¹³C APT NMR Spectrum of Compound **8a** (CDCl₃, 500 MHz)

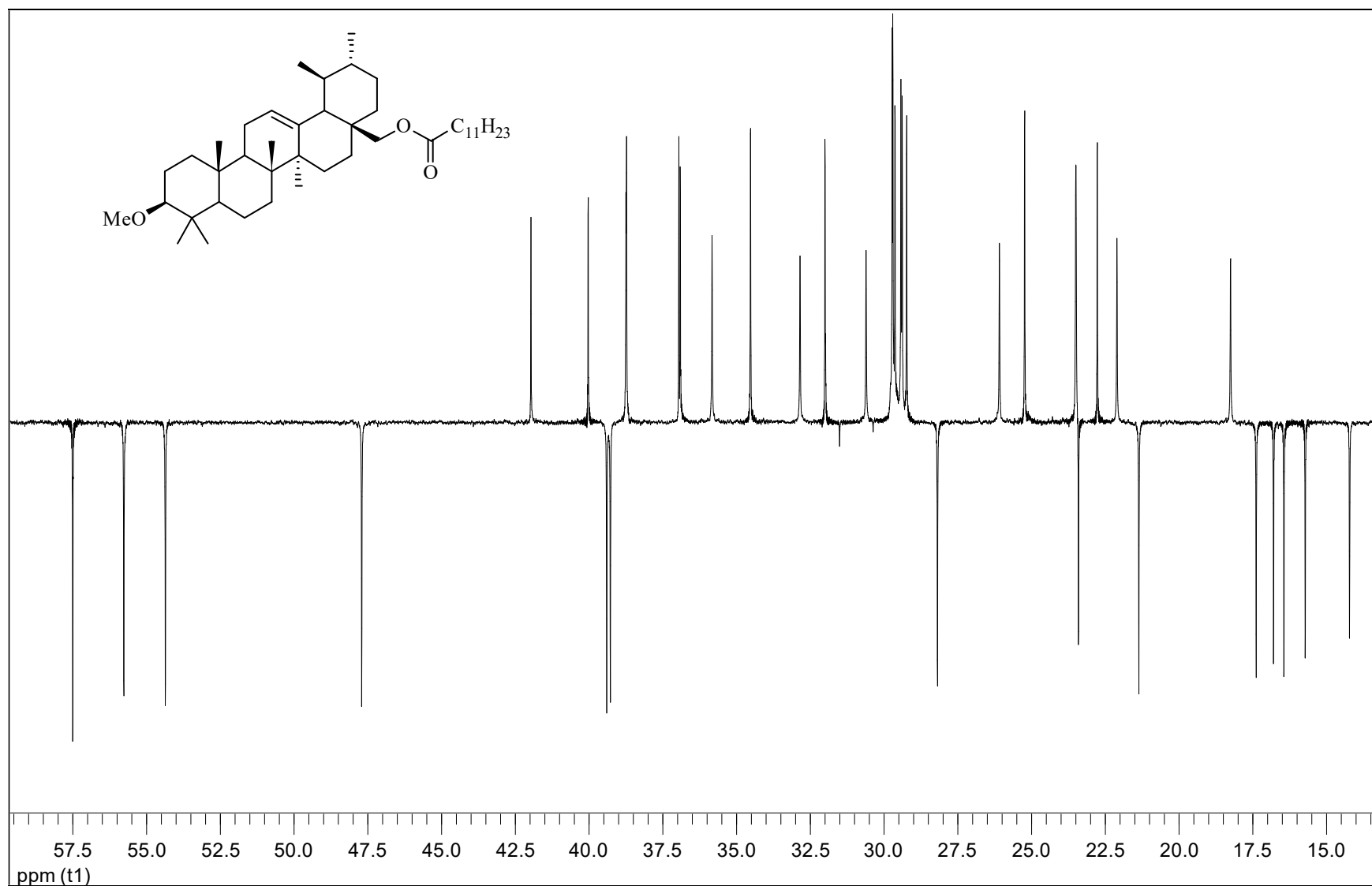


Figure 36: ^{13}C APT NMR Spectrum of Compound **8a** (Extended) (CDCl_3 , 500 MHz)

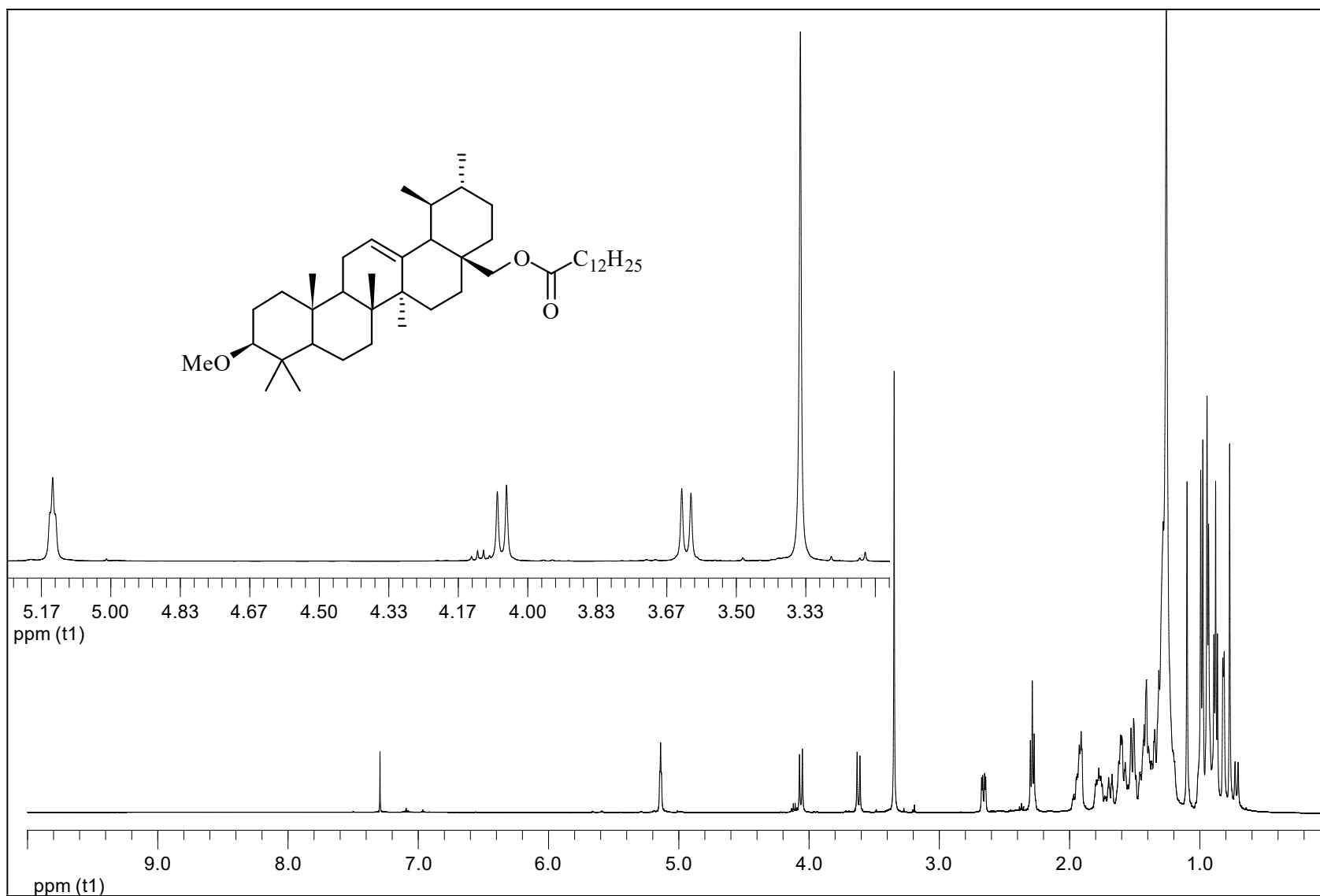


Figure 37: ¹H-NMR Spectrum of Compound **8b** (CDCl₃, 500 MHz)

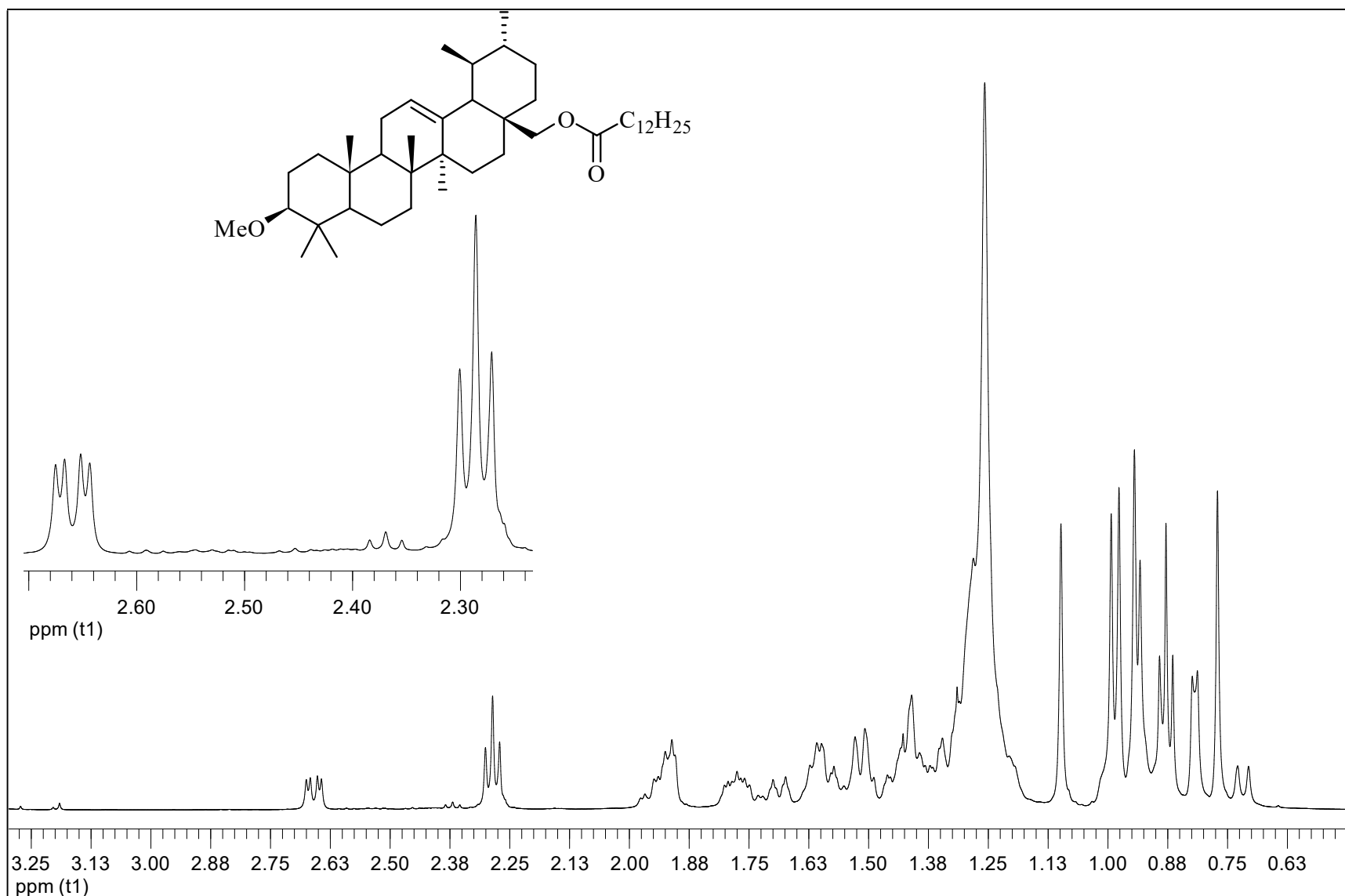


Figure 38: $^1\text{H-NMR}$ Spectrum of Compound **8b** (Extended) (CDCl_3 , 500 MHz)

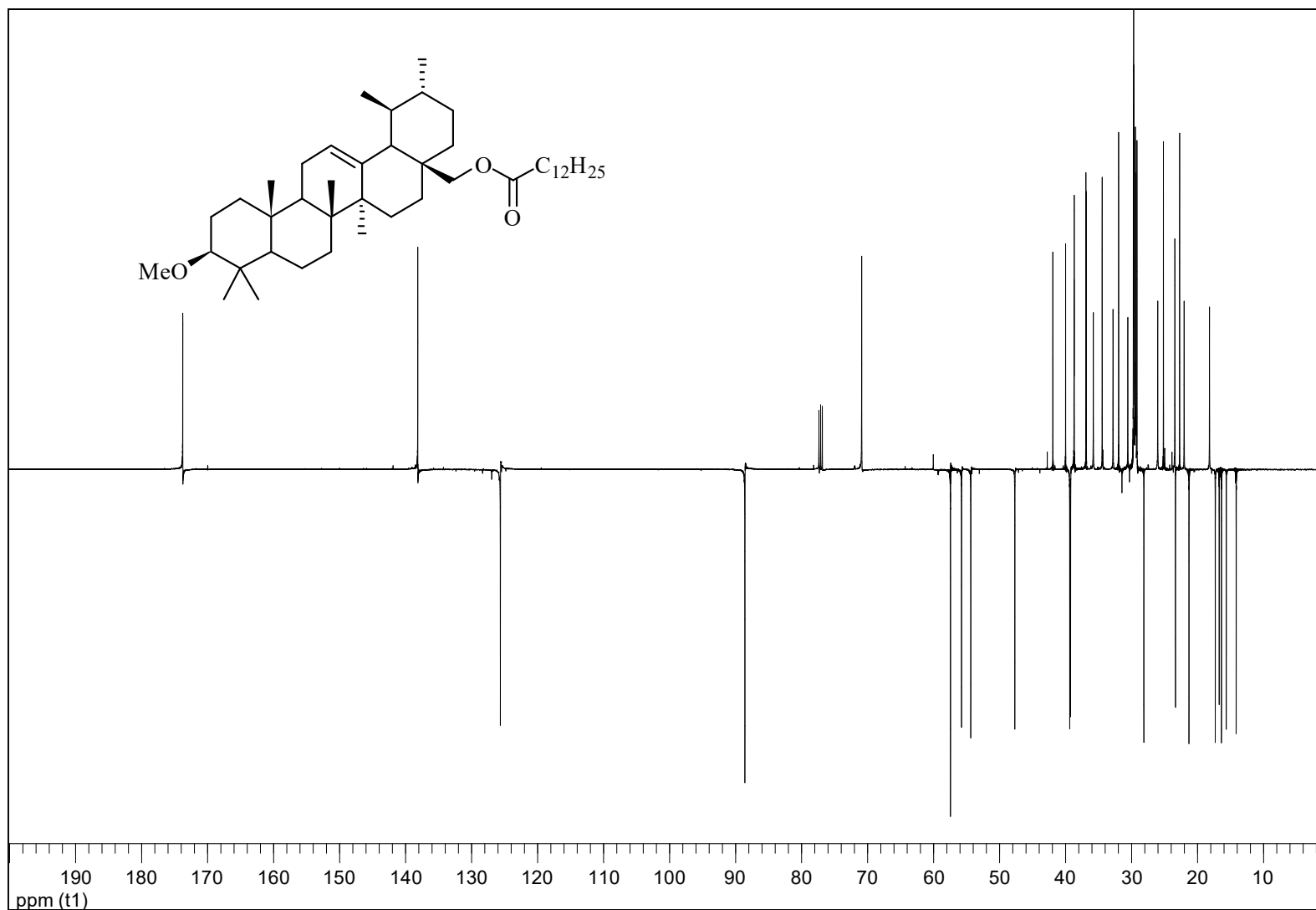


Figure 39: ^{13}C -APT NMR Spectrum of Compound **8b** (CDCl_3 , 125 MHz)

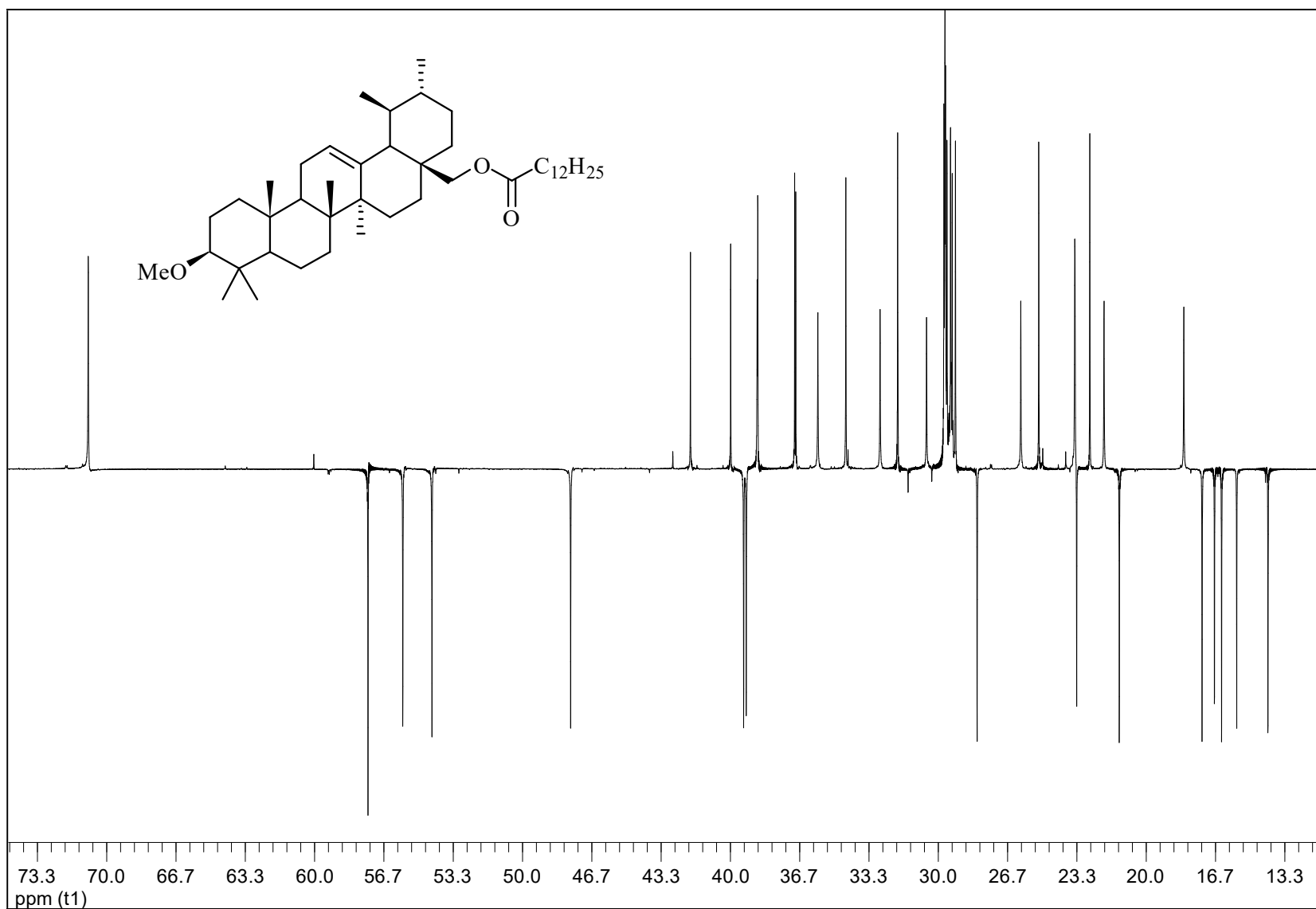


Figure 40: ^{13}C -APT NMR Spectrum of Compound **8b** (Extended) (CDCl_3 , 125 MHz)

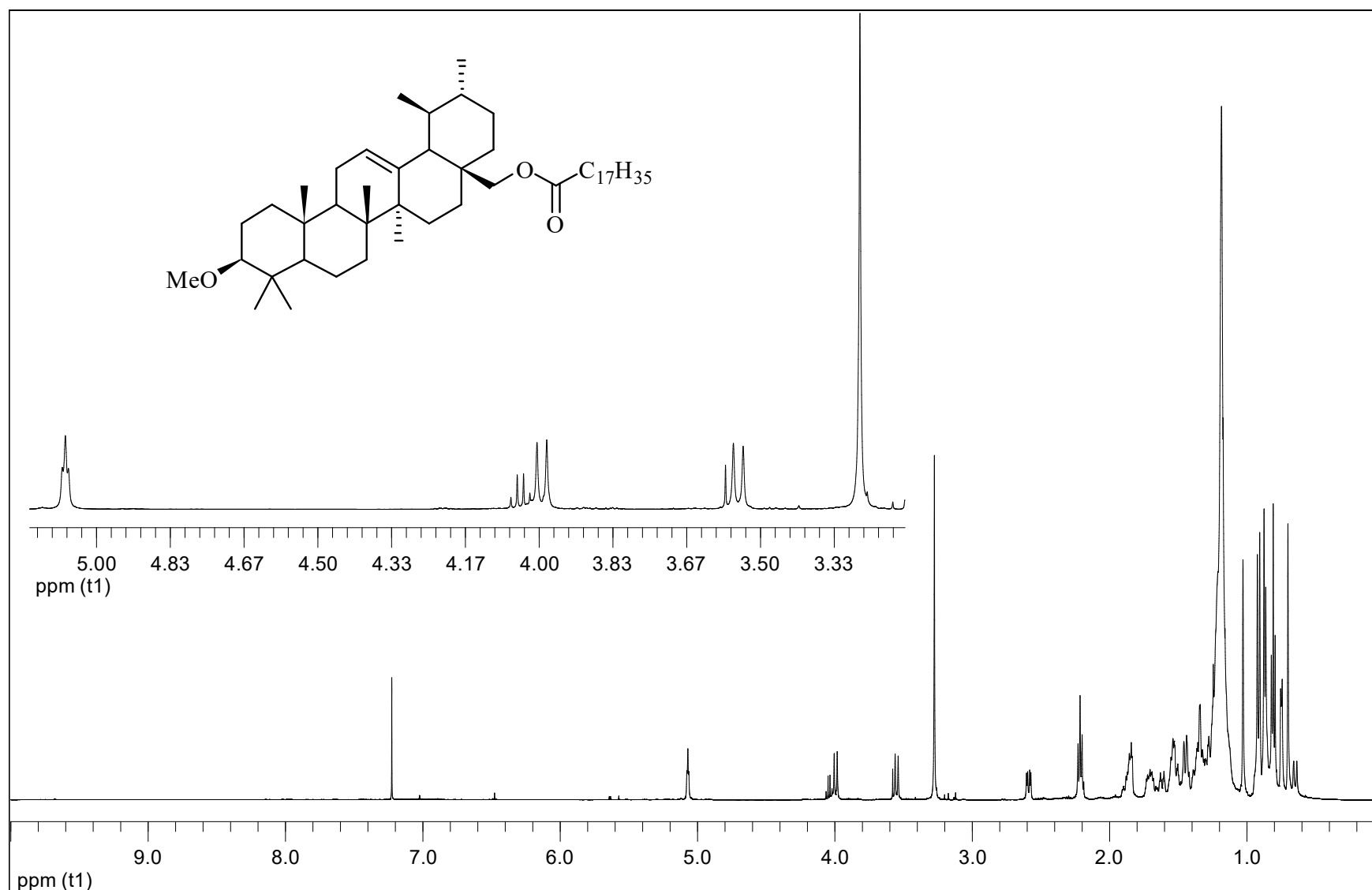


Figure 41: $^1\text{H-NMR}$ Spectrum of Compound **8c** (CDCl_3 , 500 MHz)

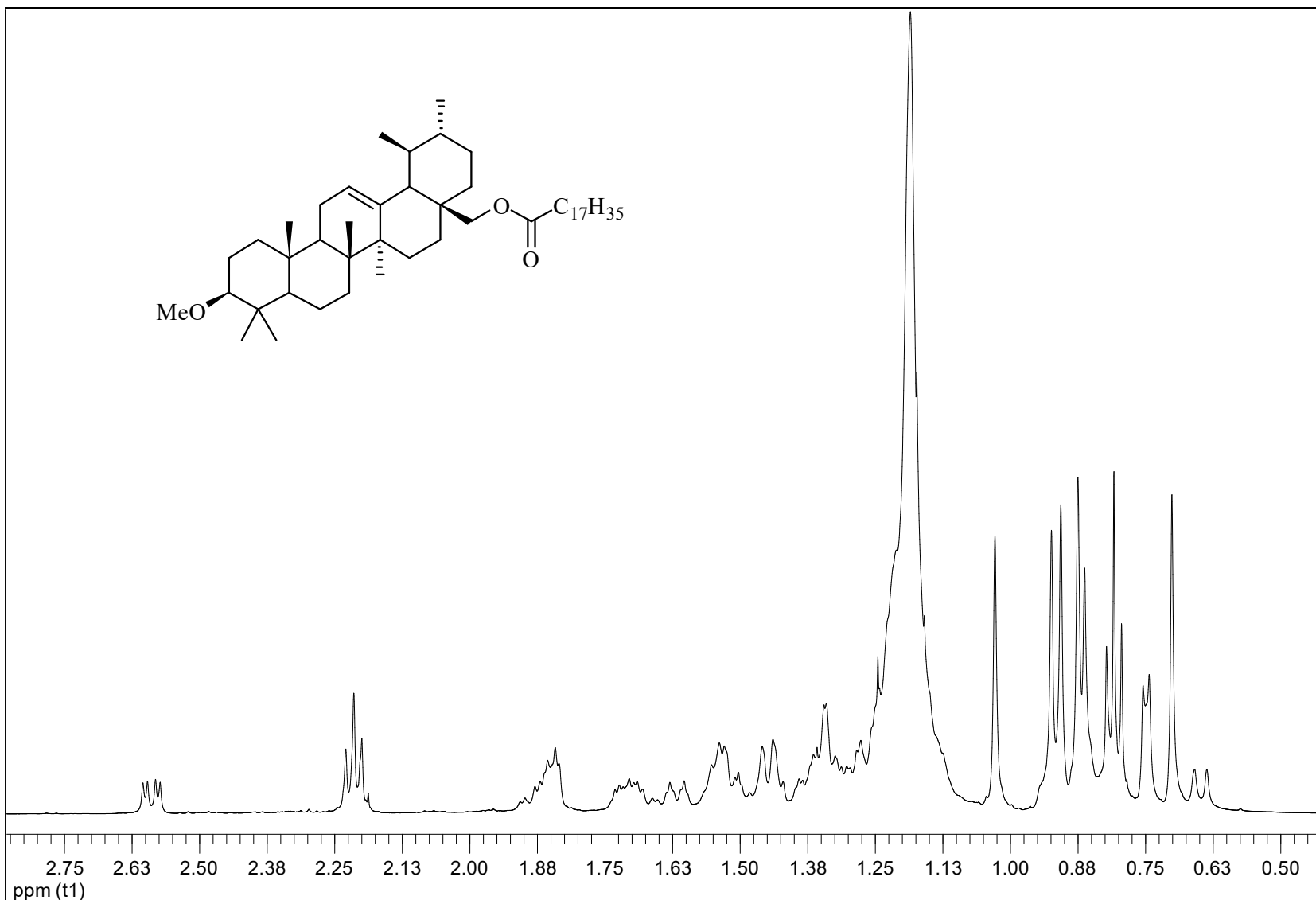


Figure 42: ¹H-NMR Spectrum of Compound **8c** (Extended) (CDCl₃, 500 MHz)

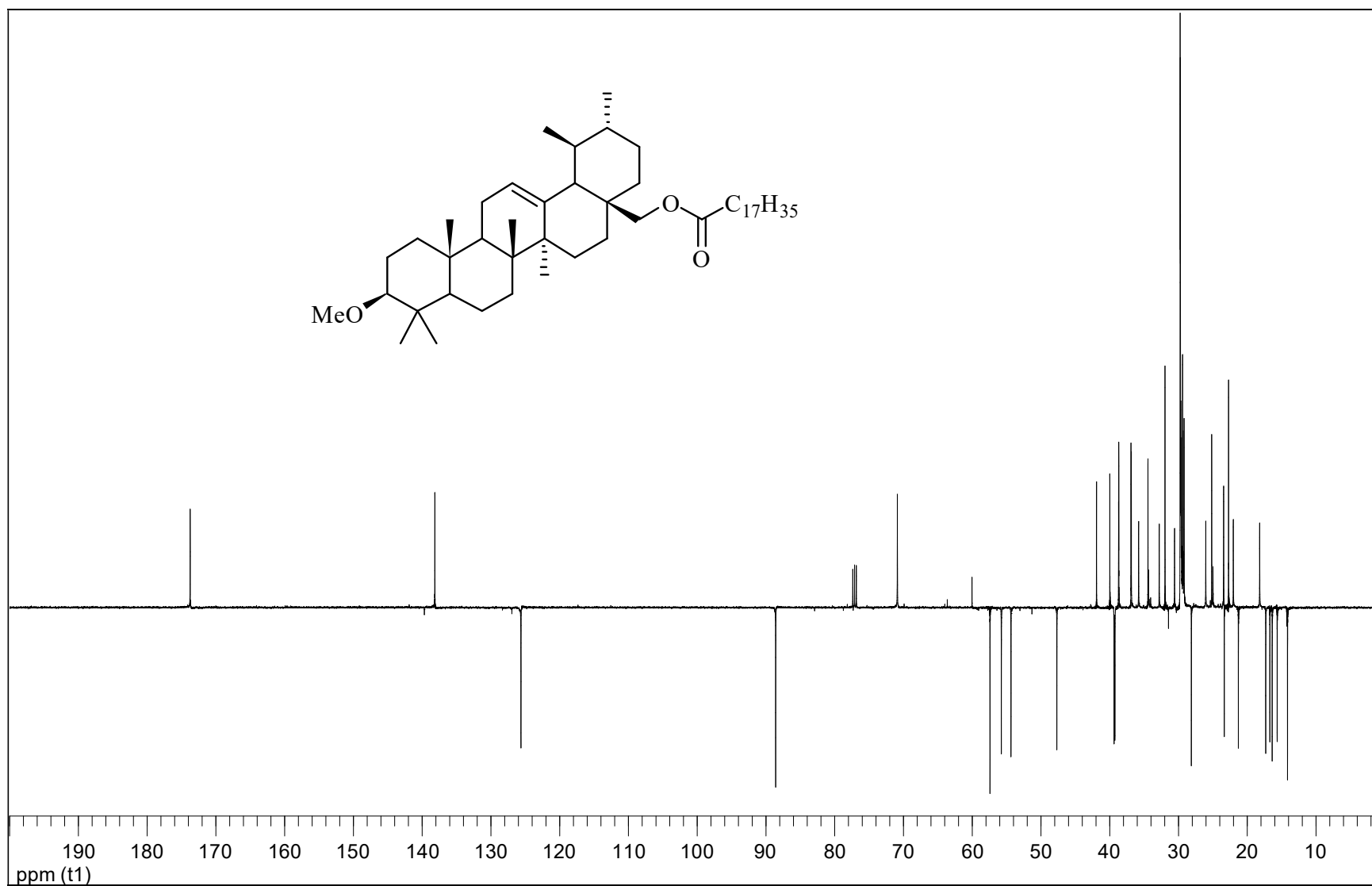


Figure 43: ¹³C-APT NMR Spectrum of Compound **8c** (CDCl₃, 125 MHz)

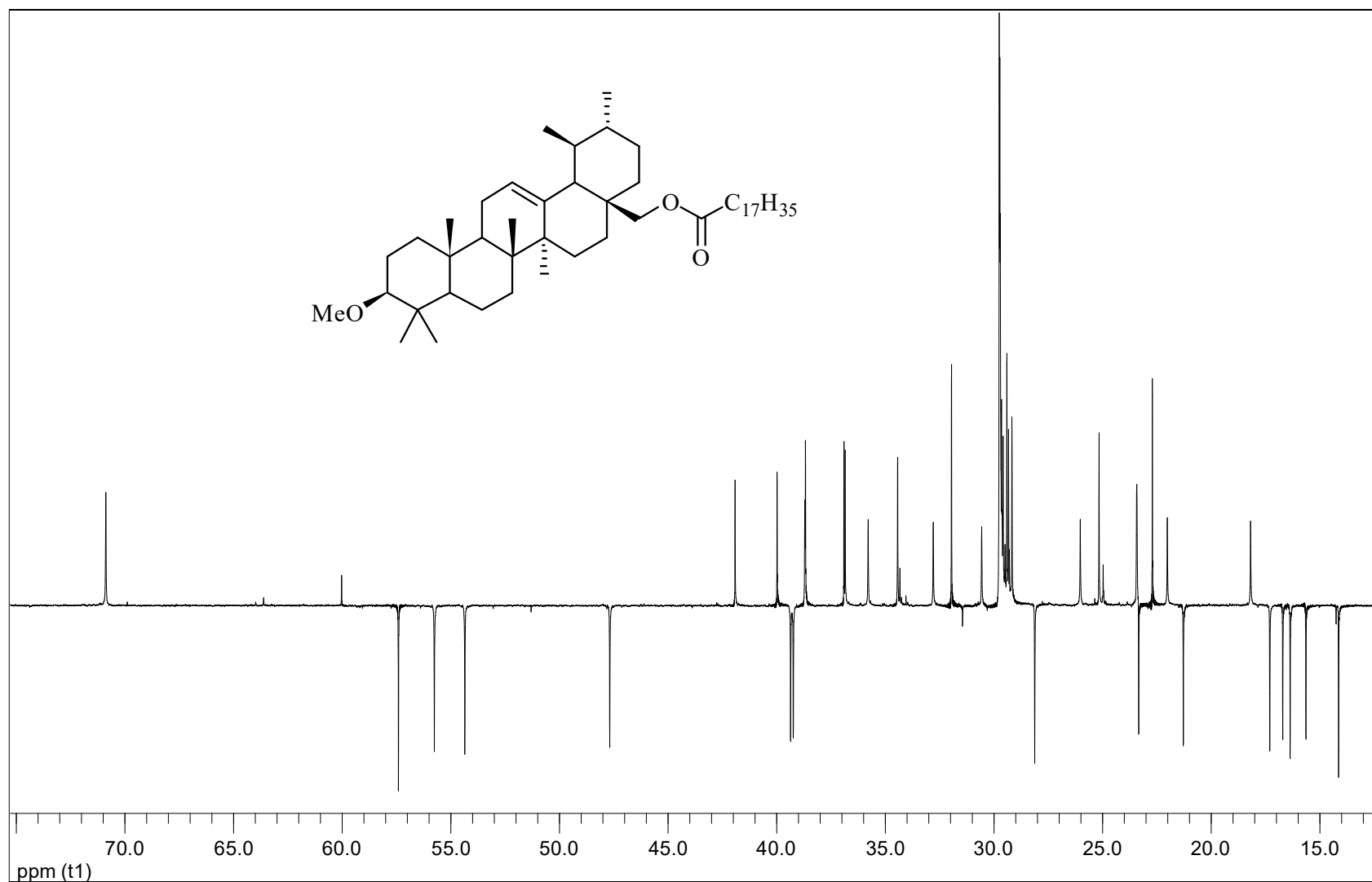


Figure 44: ¹³C-APT NMR Spectrum of Compound **8c** (Extended) (CDCl₃, 125 MHz)

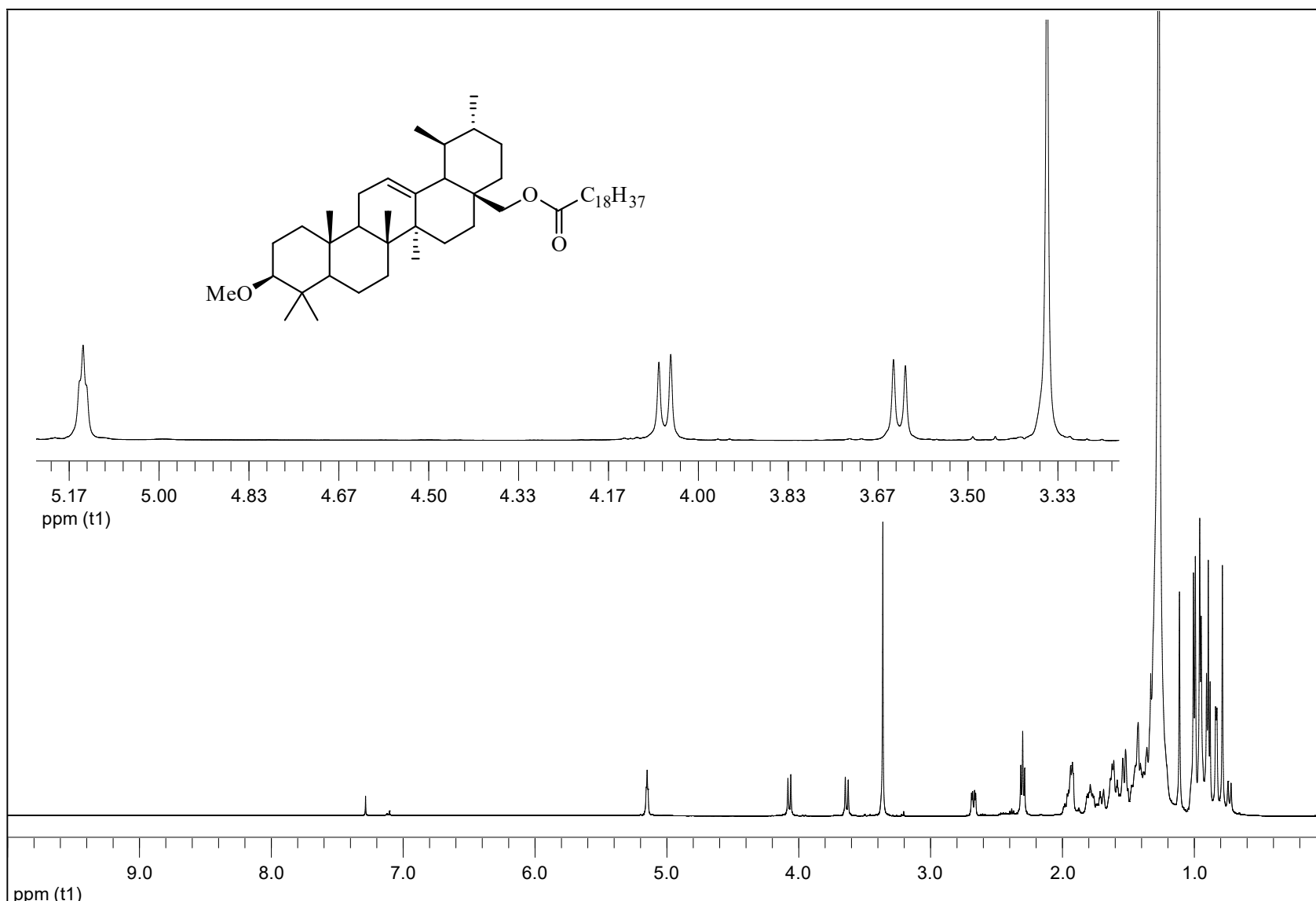


Figure 45: $^1\text{H-NMR}$ Spectrum of Compound **8d** (CDCl_3 , 500 MHz)

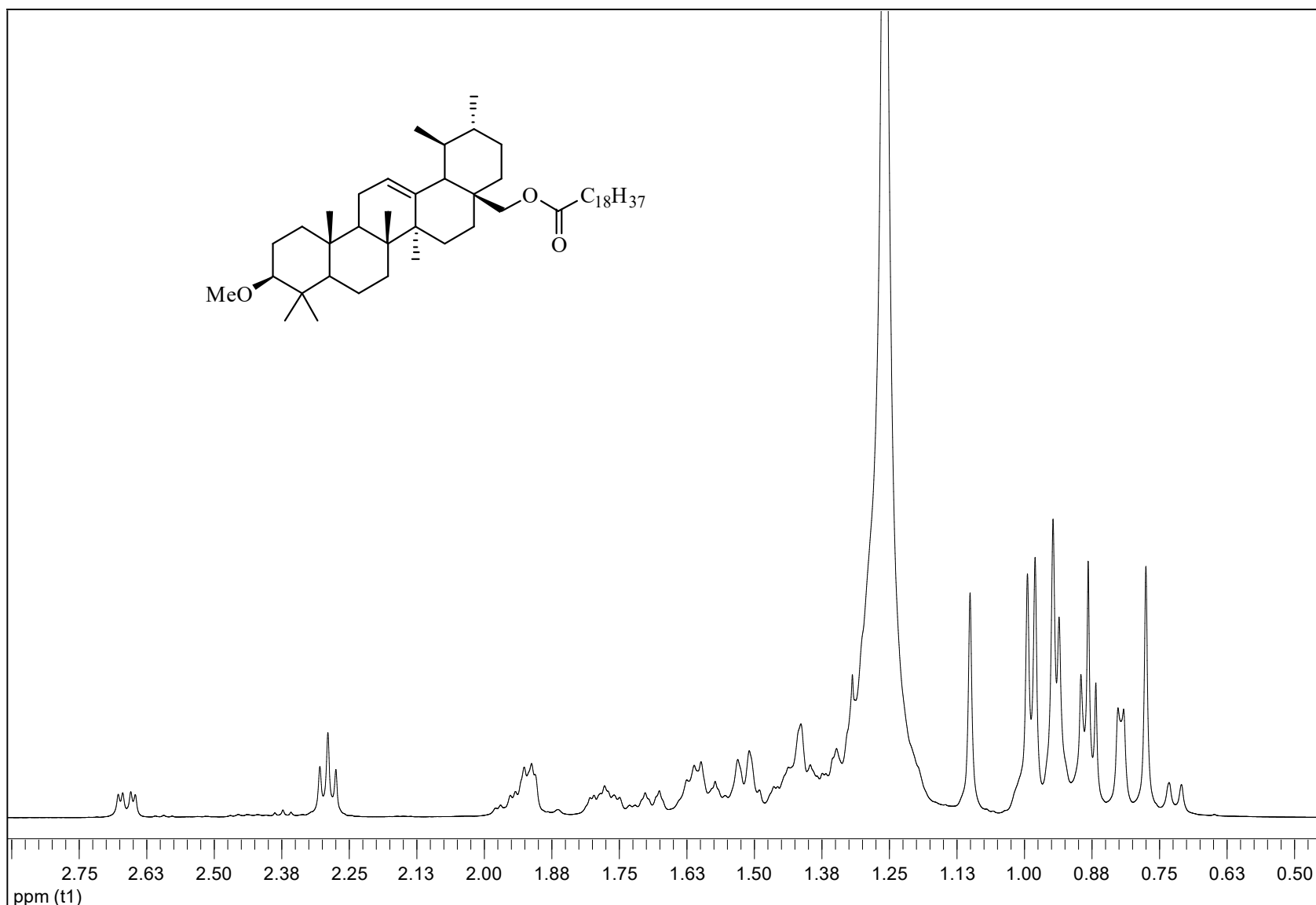


Figure 46: $^1\text{H-NMR}$ Spectrum of Compound **8d** (CDCl_3 , 500 MHz)

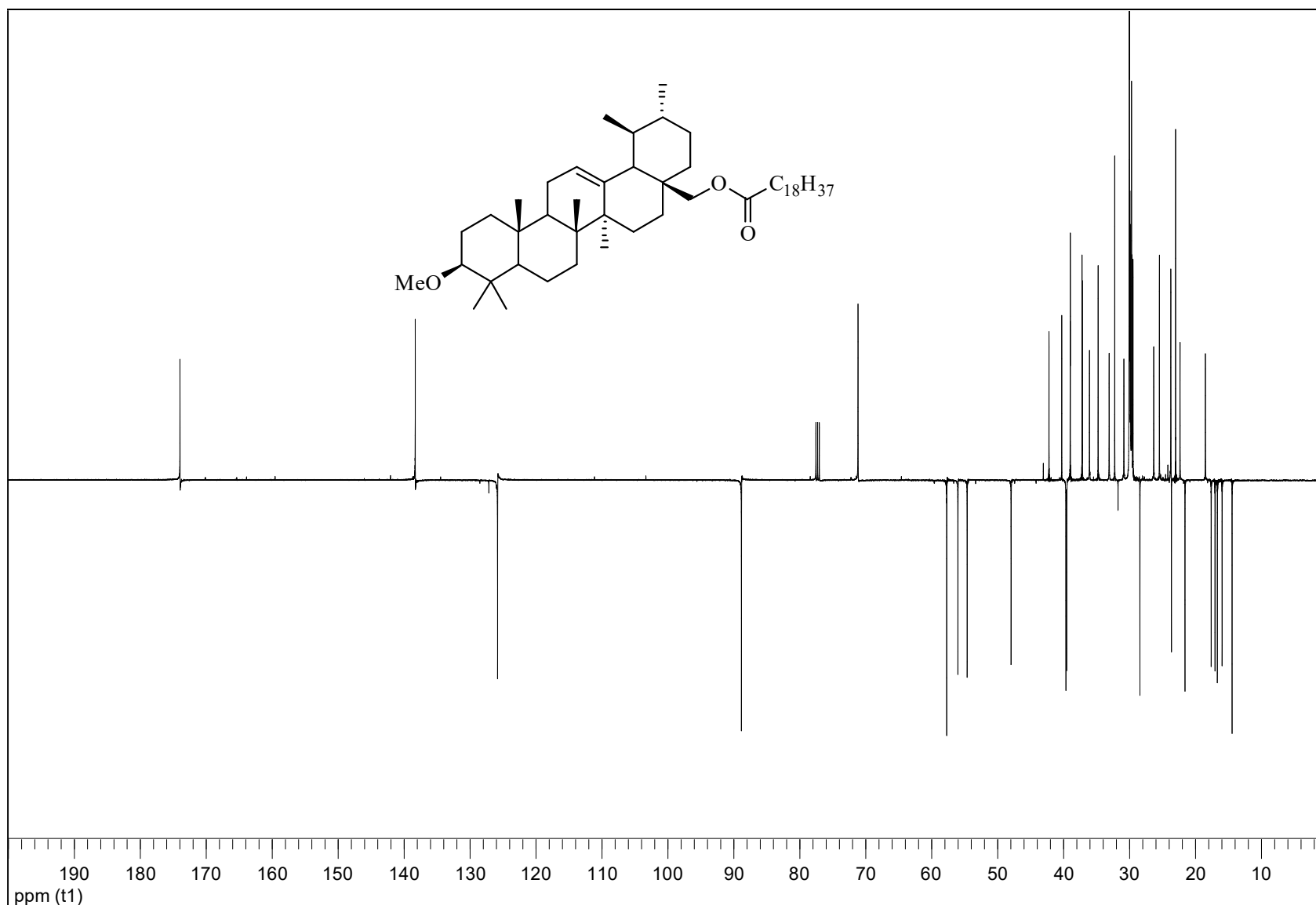


Figure 47: ¹³C-APT NMR Spectrum of Compound **8d** (CDCl₃, 125 MHz)

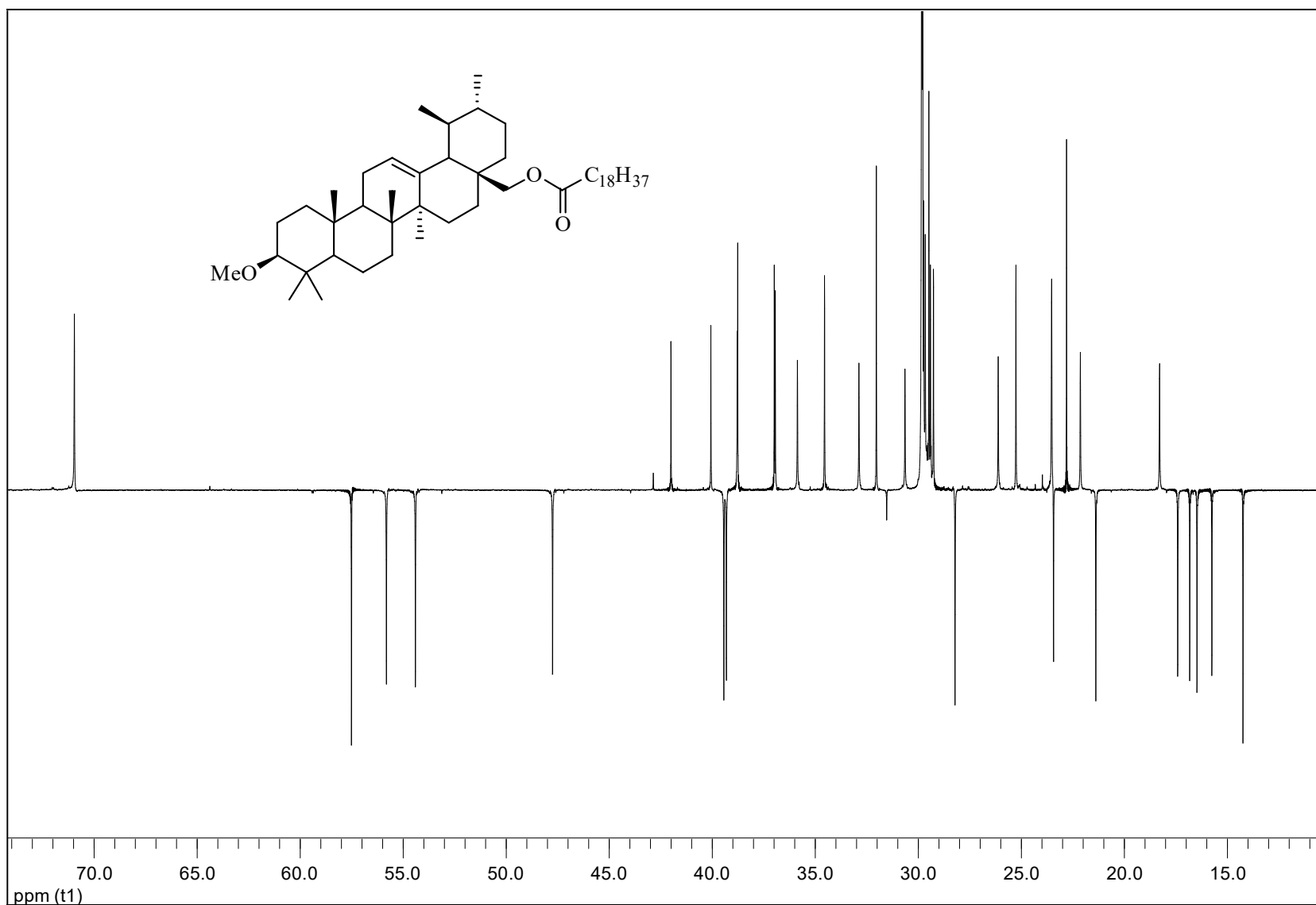


Figure 48: ^{13}C -APT NMR Spectrum of Compound **8d** (Extended) (CDCl₃, 125 MHz)

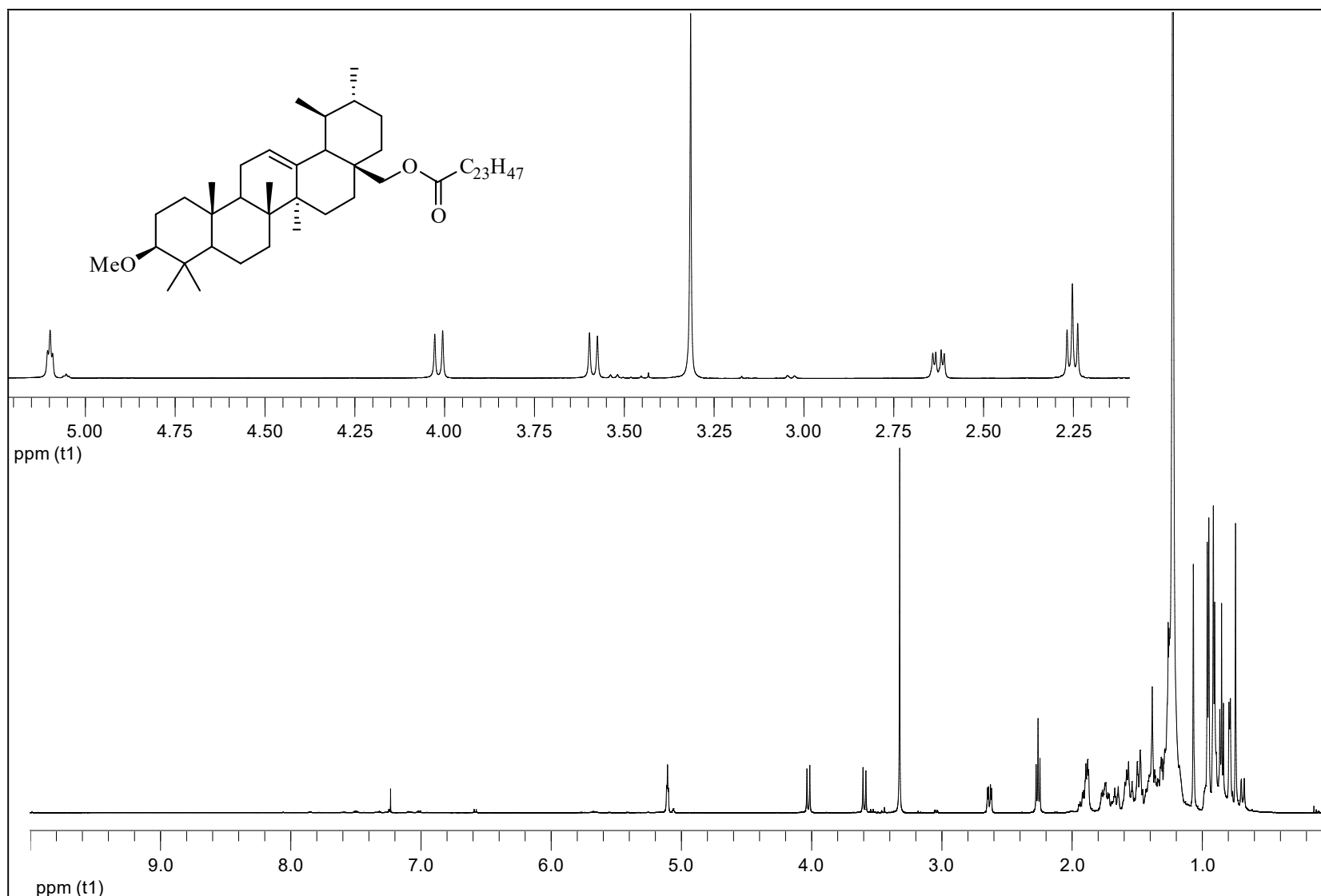


Figure 49: $^1\text{H-NMR}$ Spectrum of Compound **8e** (CDCl_3 , 500 MHz)

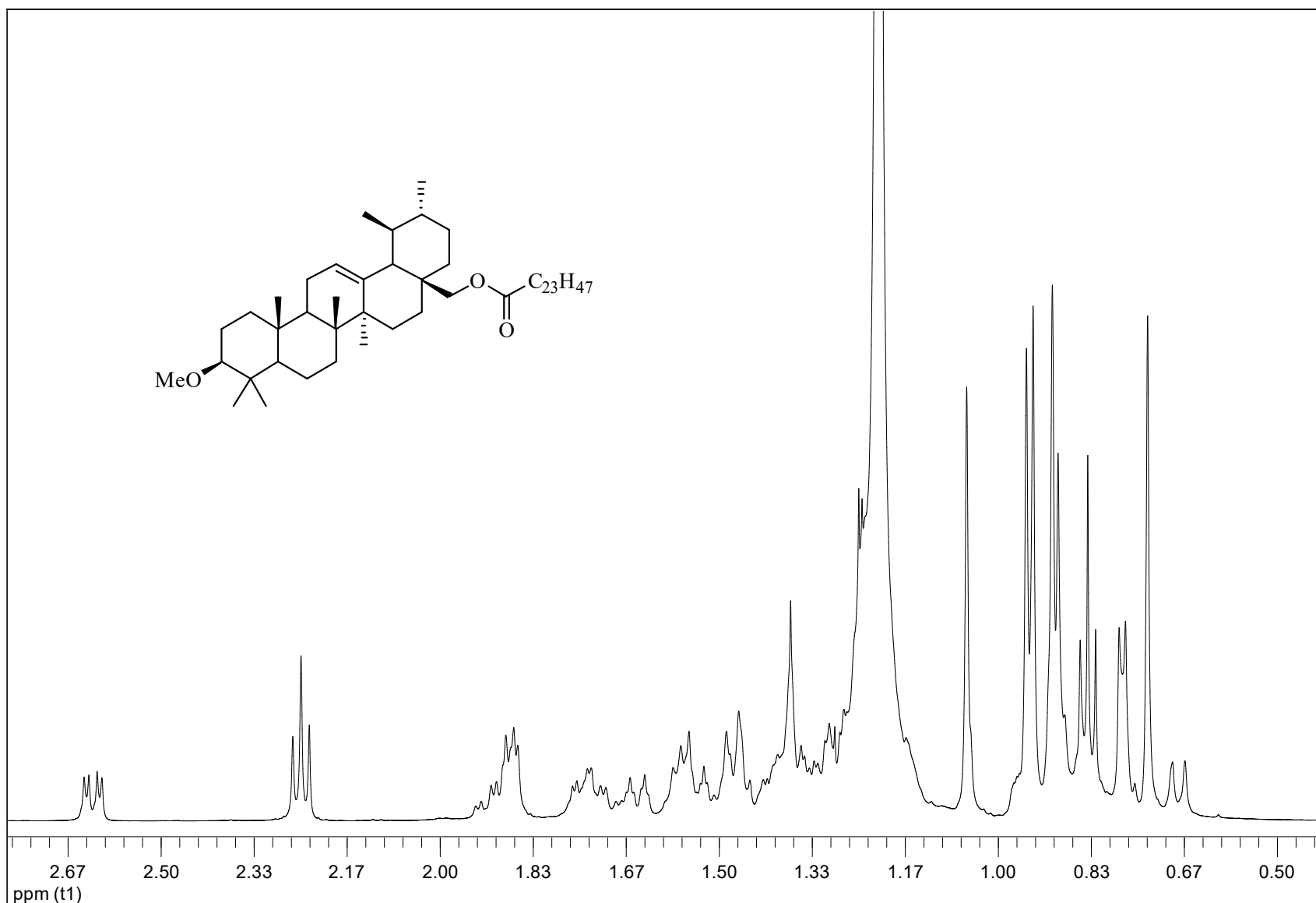


Figure 50: ¹H-NMR Spectrum of Compound **8e** (Extended) (CDCl₃, 500 MHz)

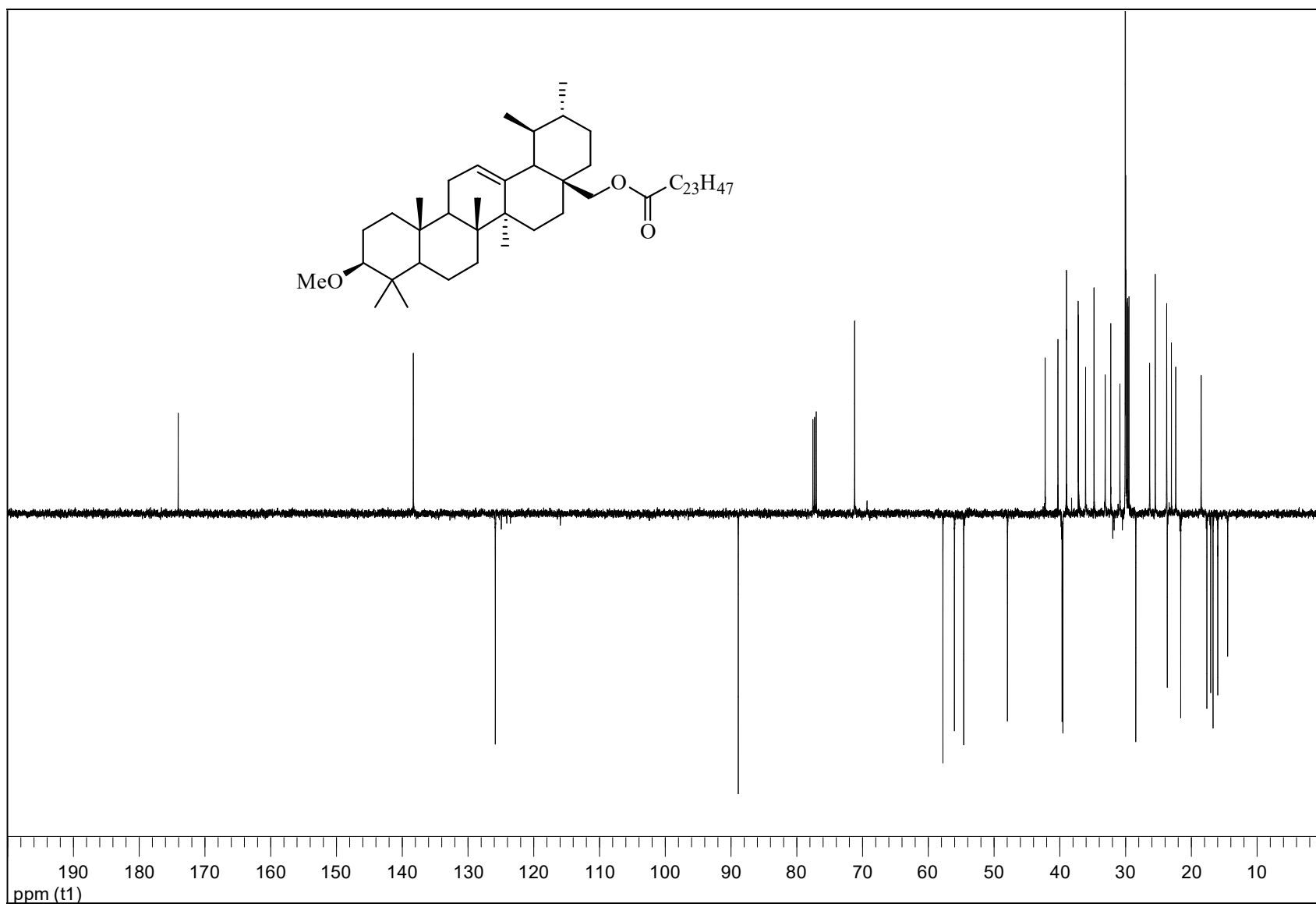


Figure 51: ^{13}C -APT NMR Spectrum of Compound **8e** (CDCl_3 , 125 MHz)

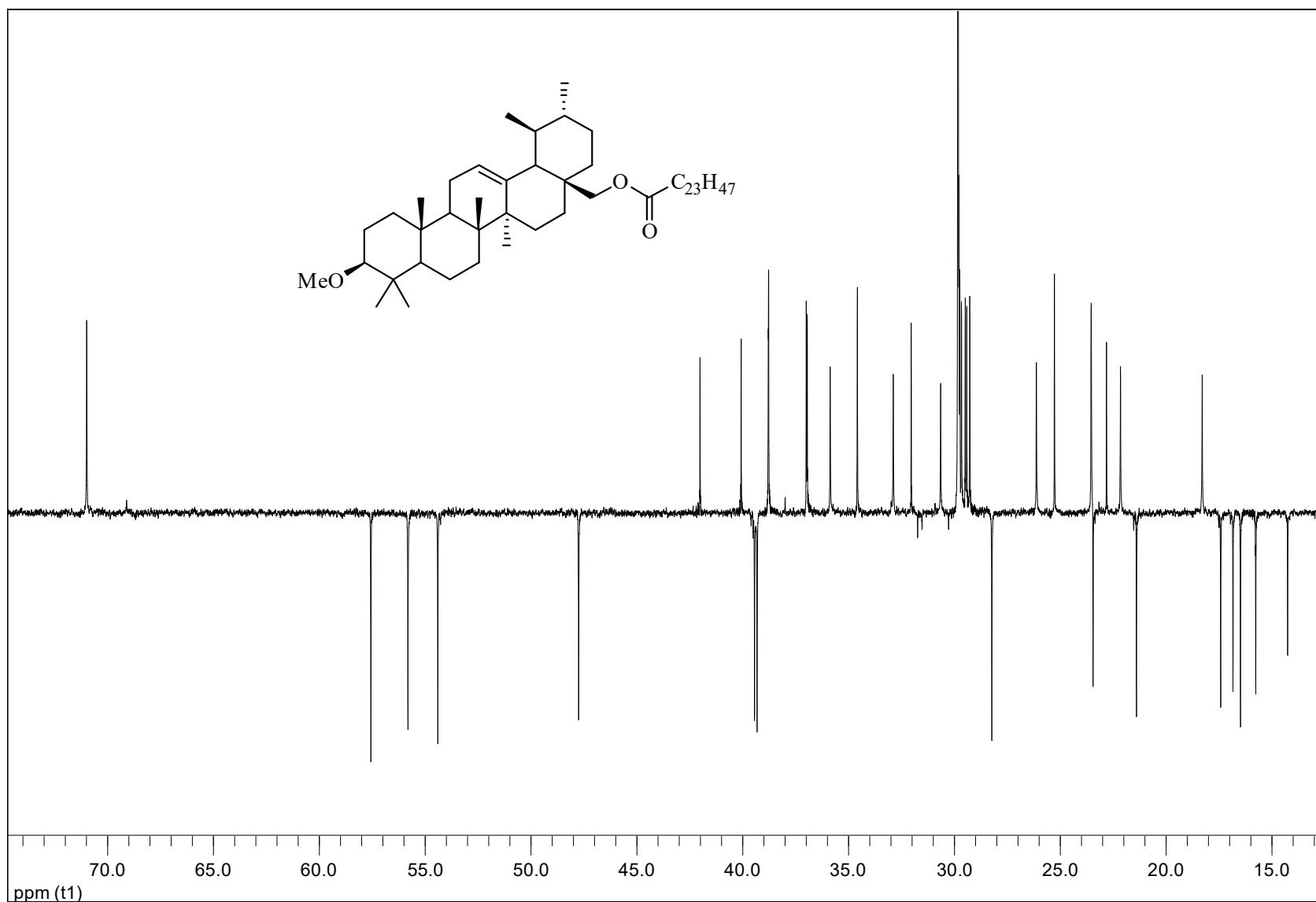


Figure 52: ^{13}C -APT NMR Spectrum of Compound **8e** (Extended) (CDCl_3 , 125 MHz)

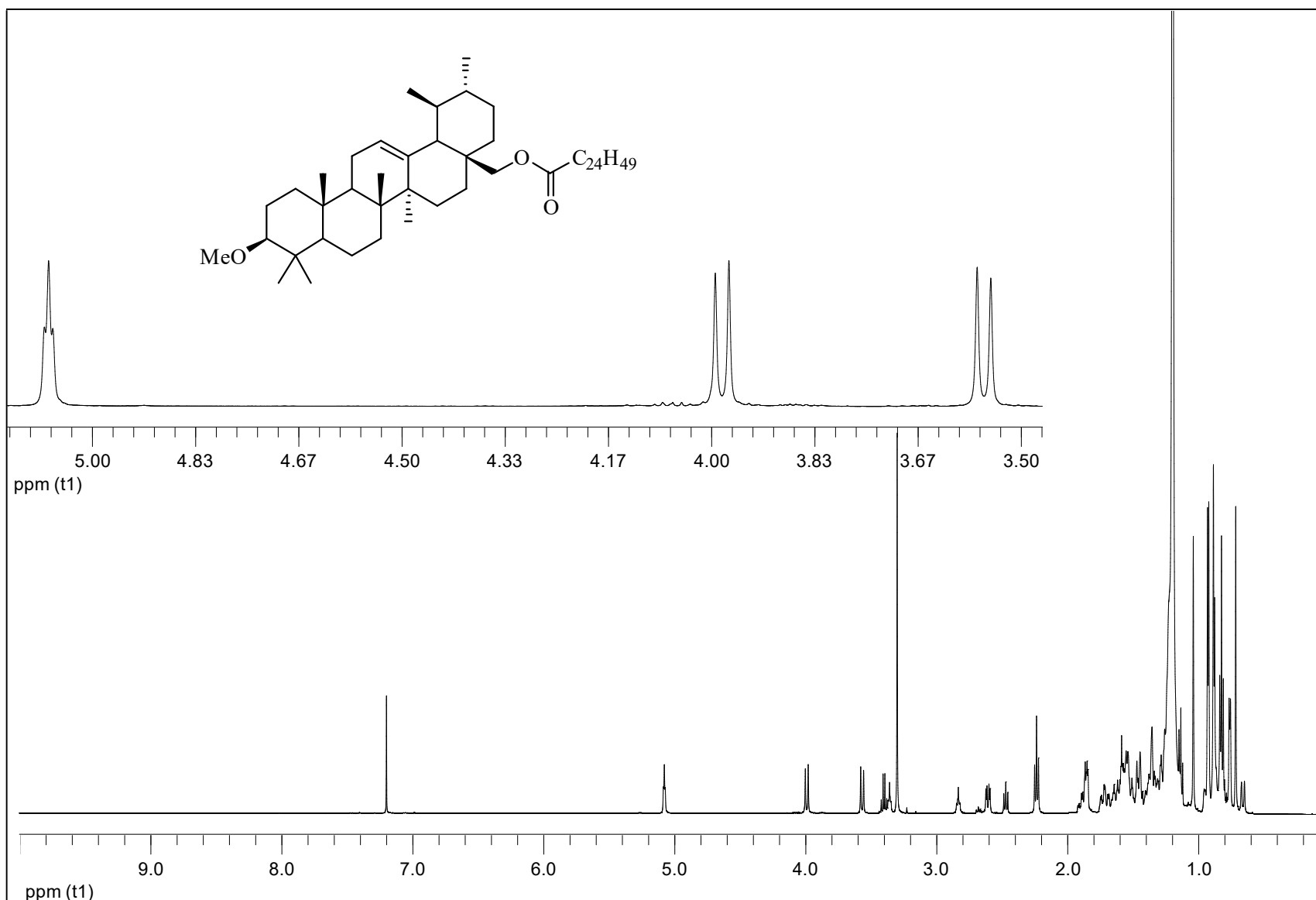


Figure 53: ¹H-NMR Spectrum of Compound **8f** (CDCl₃, 500 MHz)

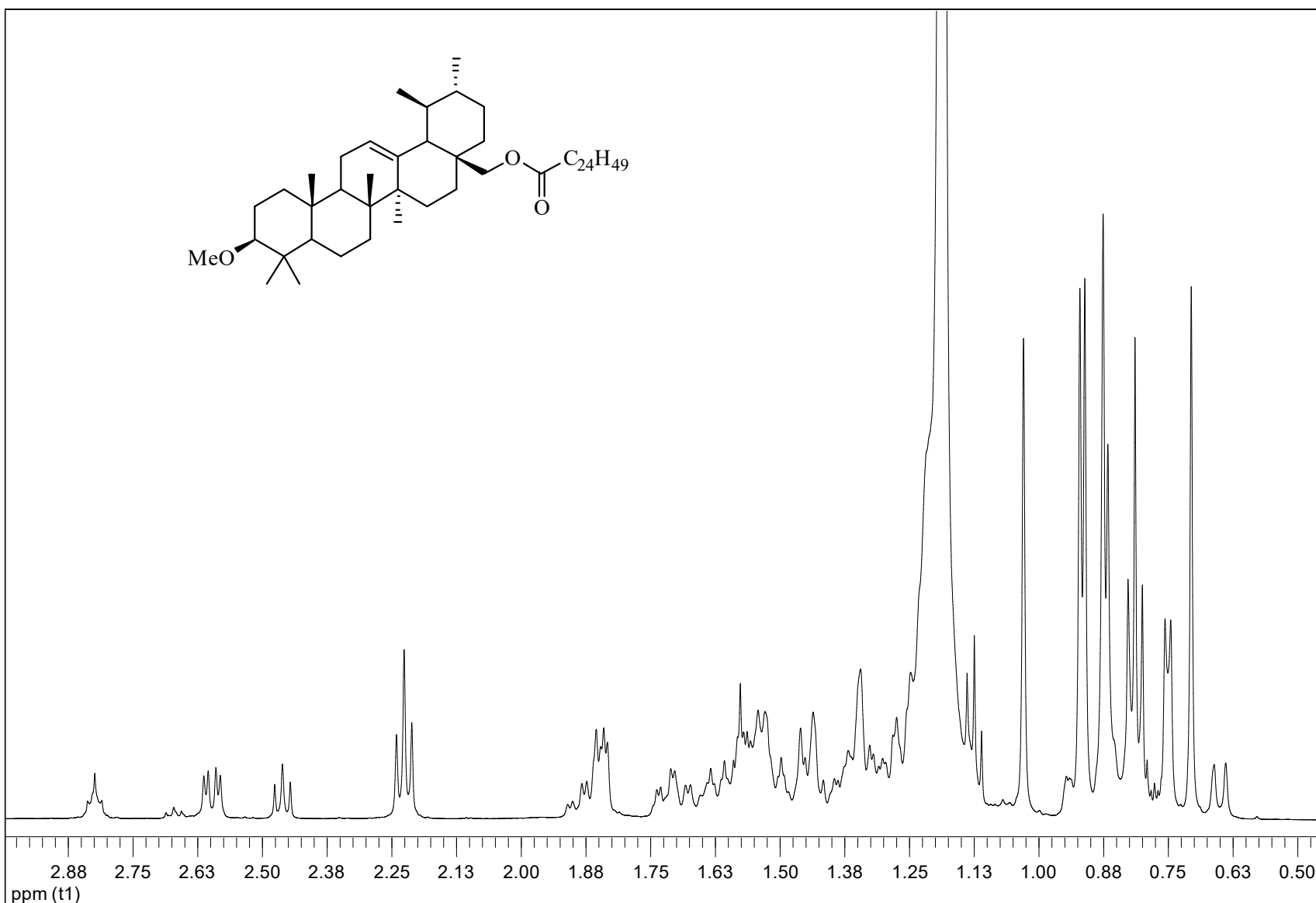


Figure 54: $^1\text{H-NMR}$ Spectrum of Compound **8f** (Extended) (CDCl_3 , 500 MHz)

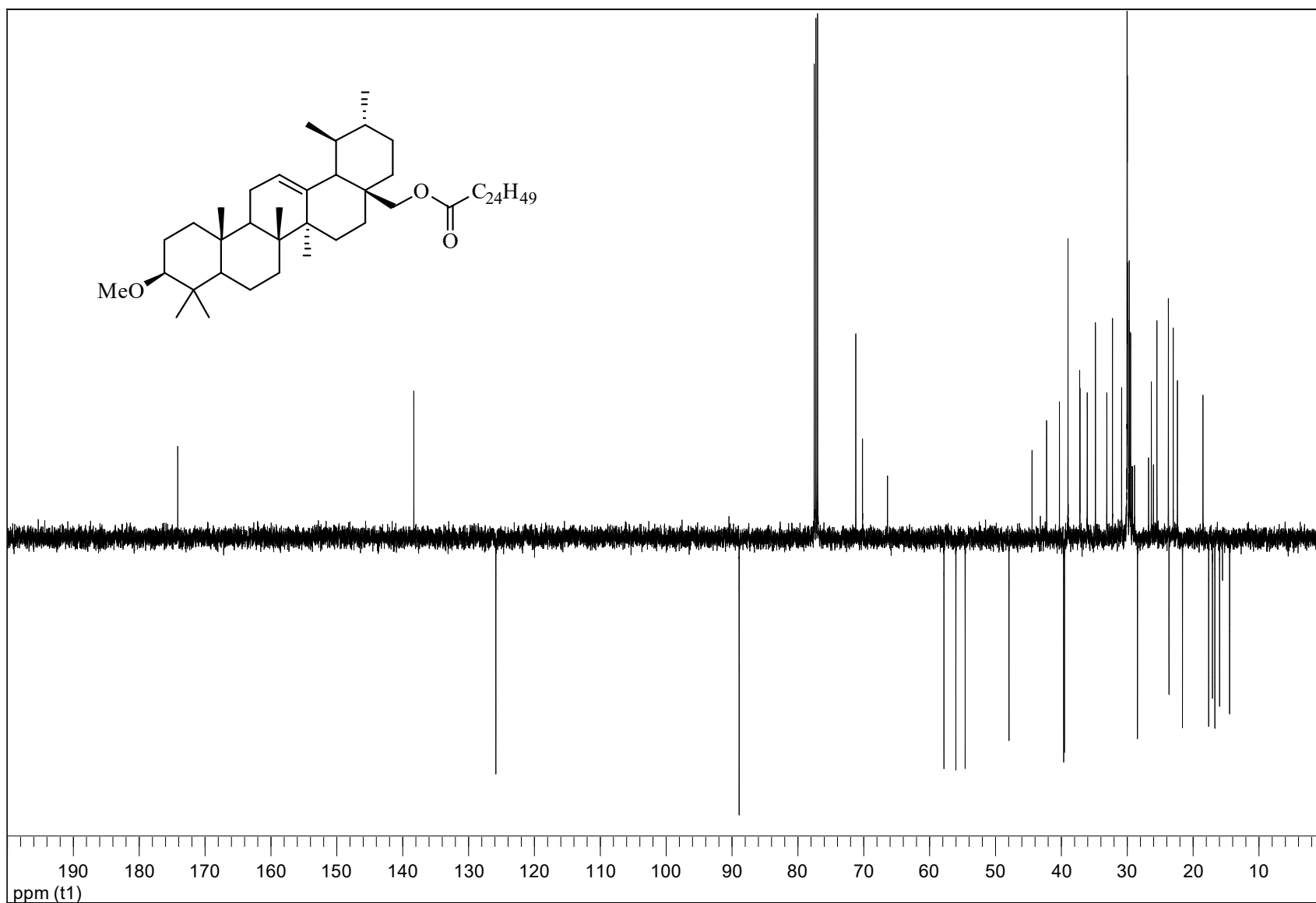


Figure 55: ^{13}C -APT NMR Spectrum of Compound **8f** (CDCl_3 , 125 MHz)

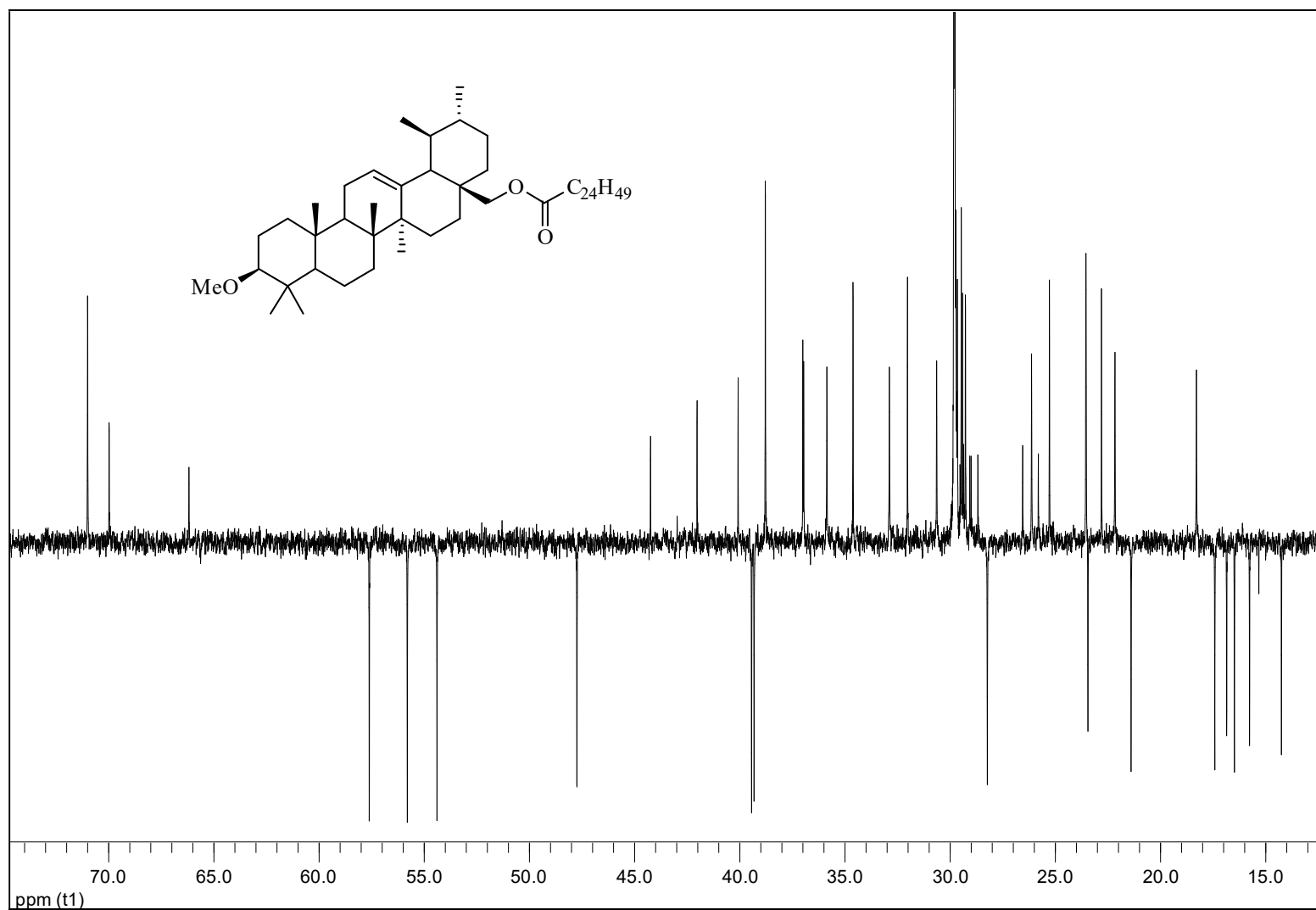


Figure 56: ¹³C-APT NMR Spectrum of Compound **8f** (Extended) (CDCl₃, 125 MHz)

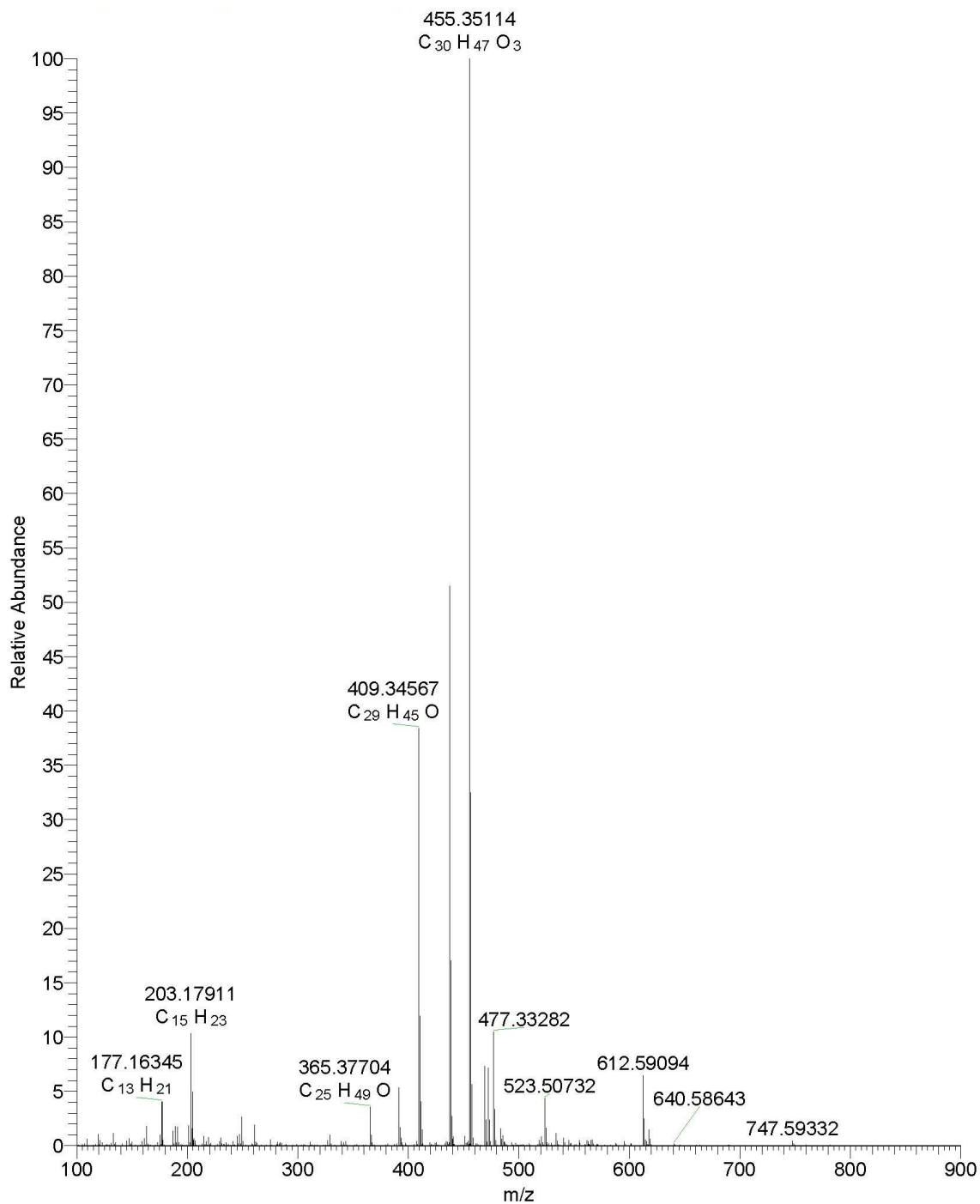


Figure 57: HRMS Spectrum of Compound **1** (oleanolic acid) (ESI MS M+1)

Molecular Formula: C₃₀H₄₆O₃; Exact Mass: 454.34470;

Calculated M+1: 455.35252; Experimental: M+1: 455.35114)

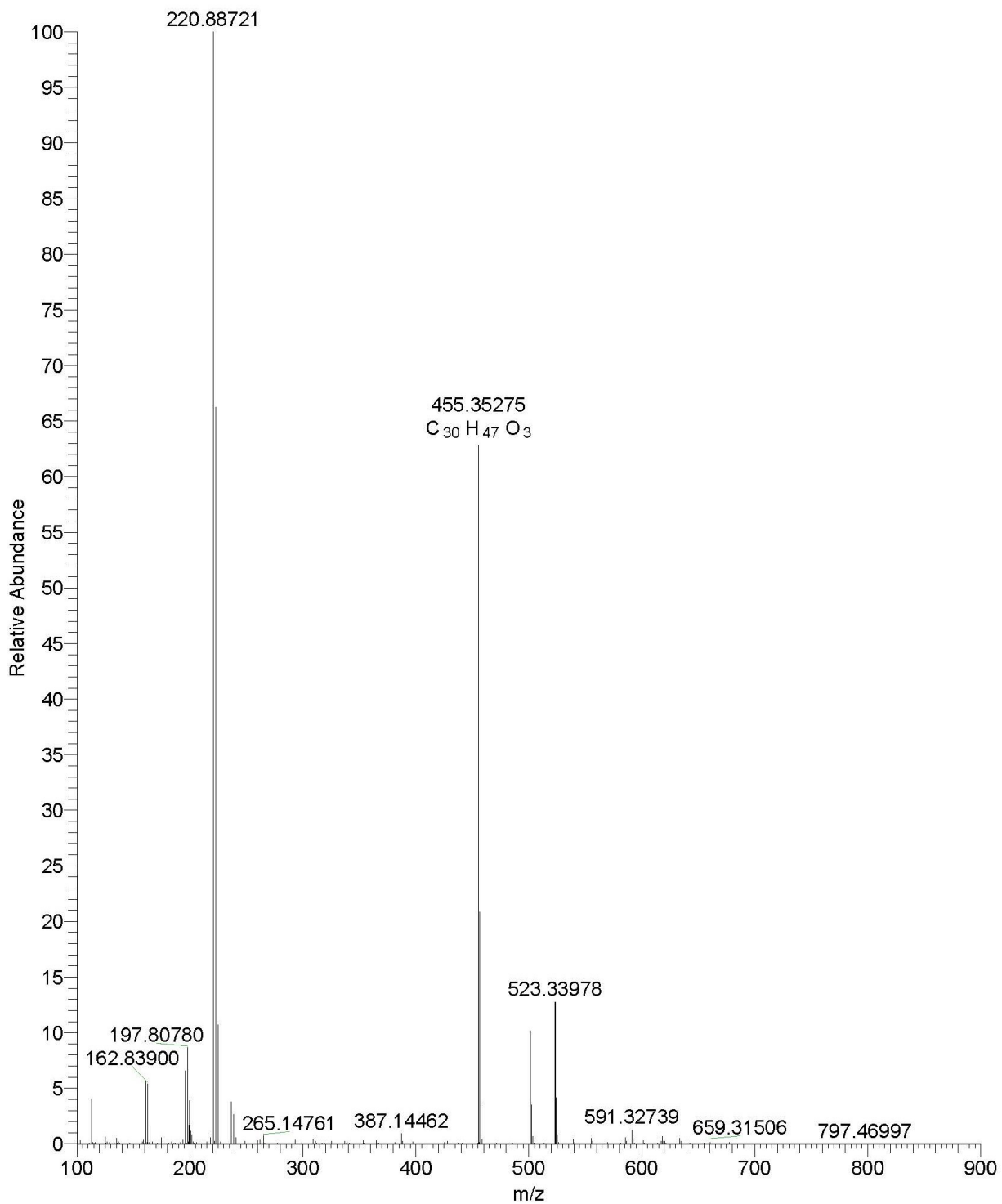


Figure 58: HRMS Spectrum of Compound 2 (ursolic acid) (ESI MS M+1)

Molecular Formula: C₃₀H₄₆O₃; Exact Mass: 454.34470;

Calculated M+1: 455.35252; Experimental: M+1: 455.35275

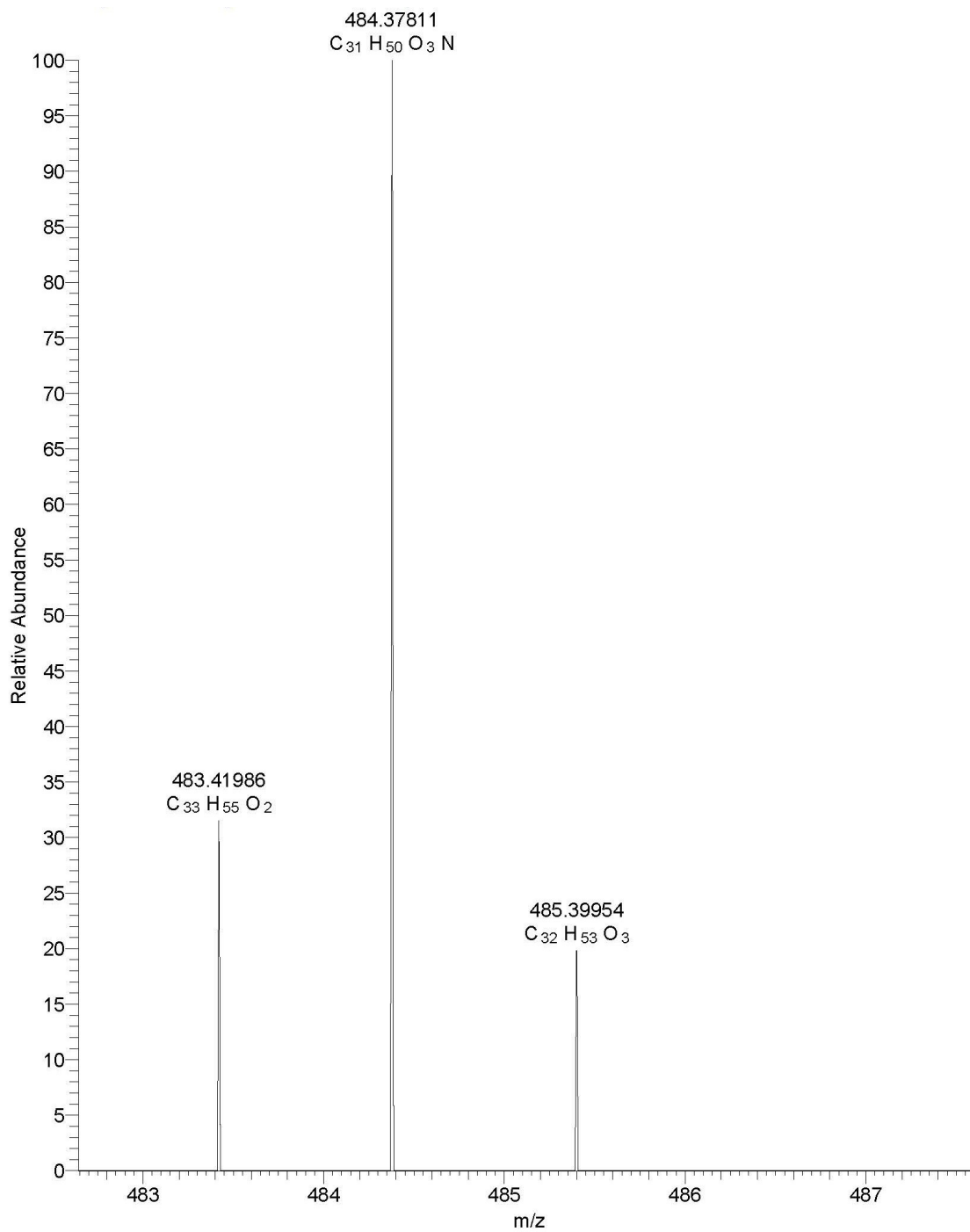


Figure 59: HRMS Spectrum of Compound **3** (ESI MS M+1)

Molecular Formula: C₃₂H₅₂O₃; Exact Mass: 484.39165;

Calculated M+1: 485.39947; Experimental: M+1: 485.39954

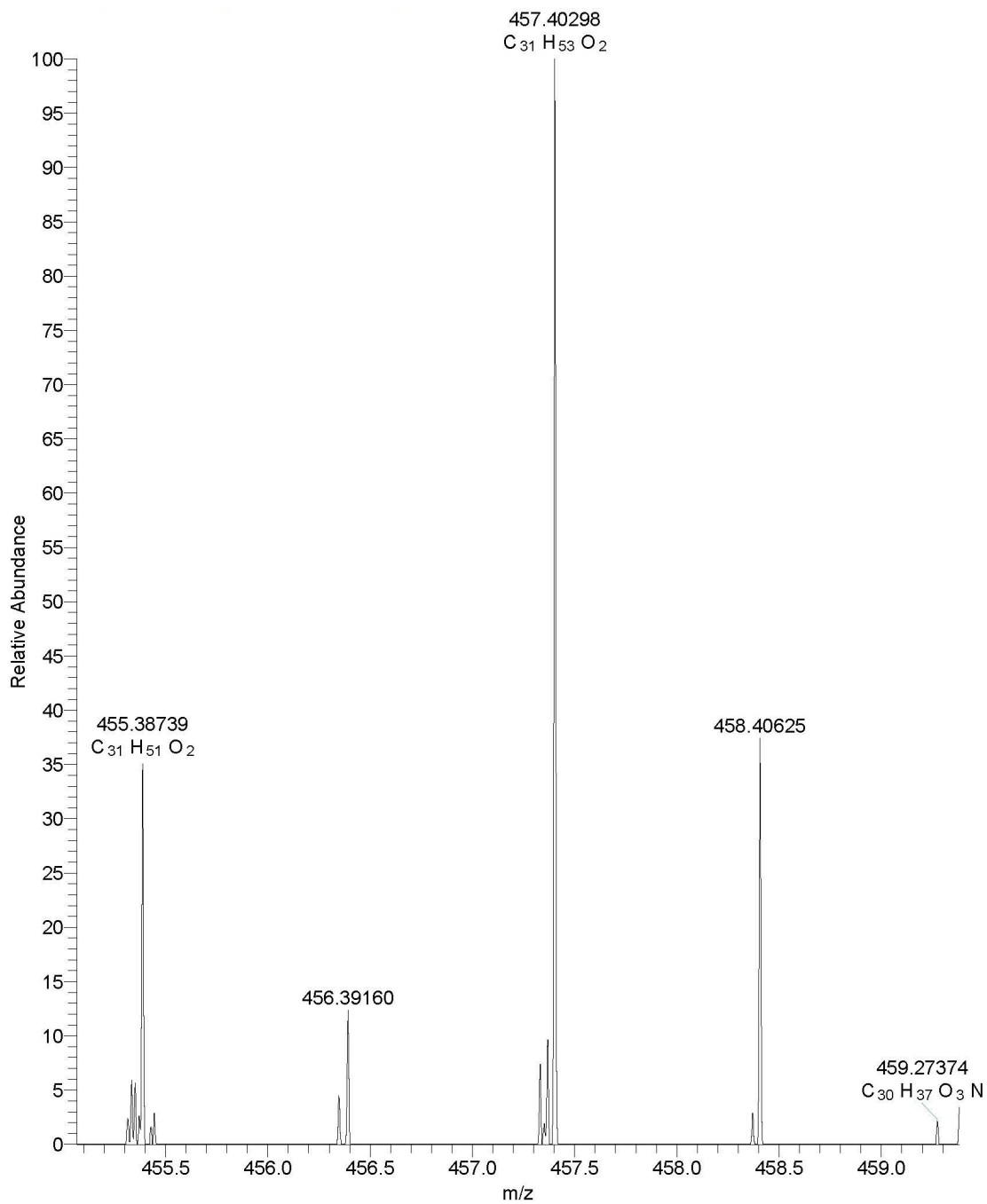


Figure 60: HRMS Spectrum of Compound **4** (ESI MS M+1)

Molecular Formula: C₃₁H₅₂O₂; Exact Mass: 456.39673;

Calculated M+1: 457.40456; Experimental: M+1: 457.40298

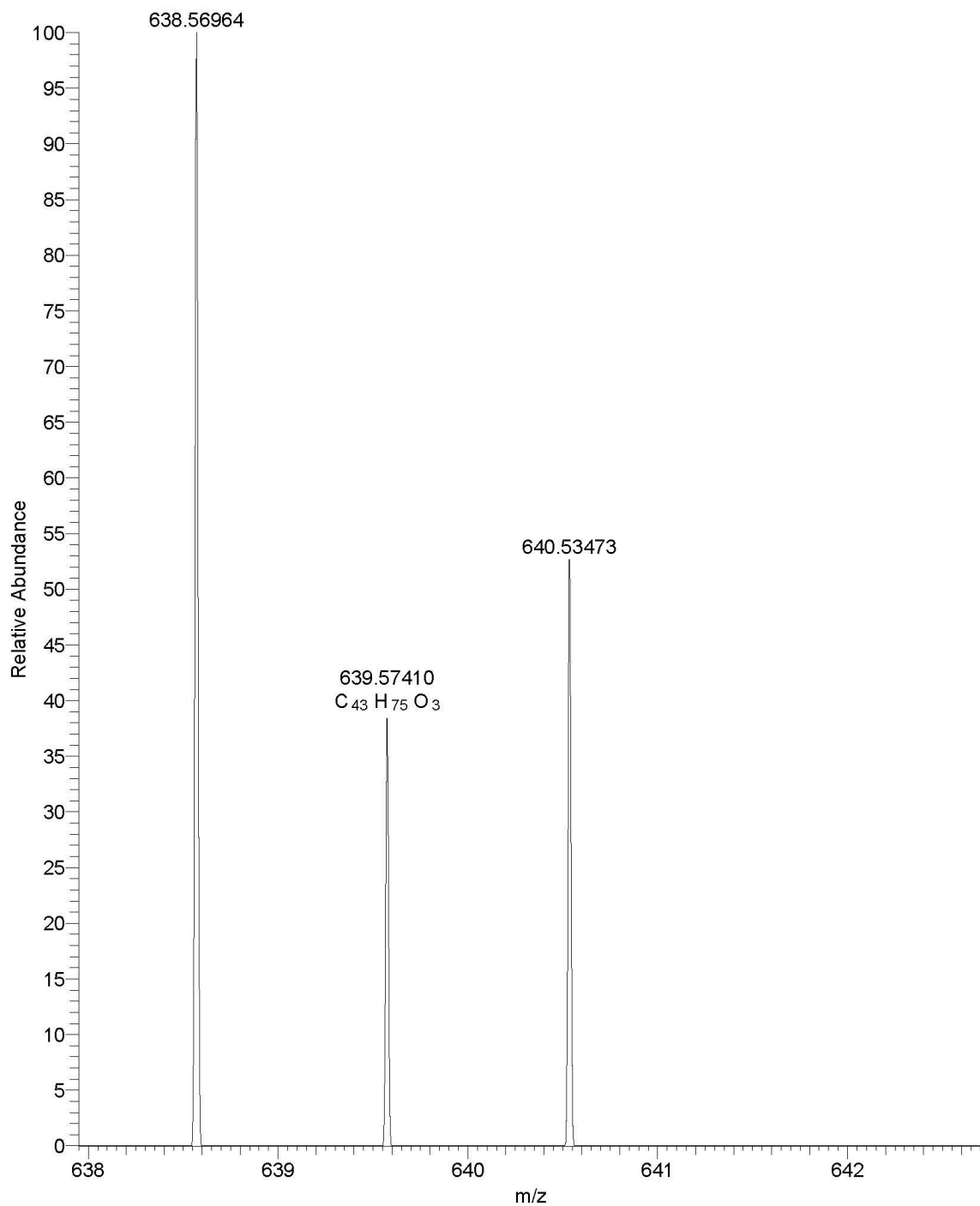


Figure 61: HRMS Spectrum of Compound **5a** (ESI MS M+1)

Molecular Formula: C₄₃H₇₄O₃; Exact Mass: 638.56380;

Calculated M+1: 639.57162; Experimental: M+1: 639.57410

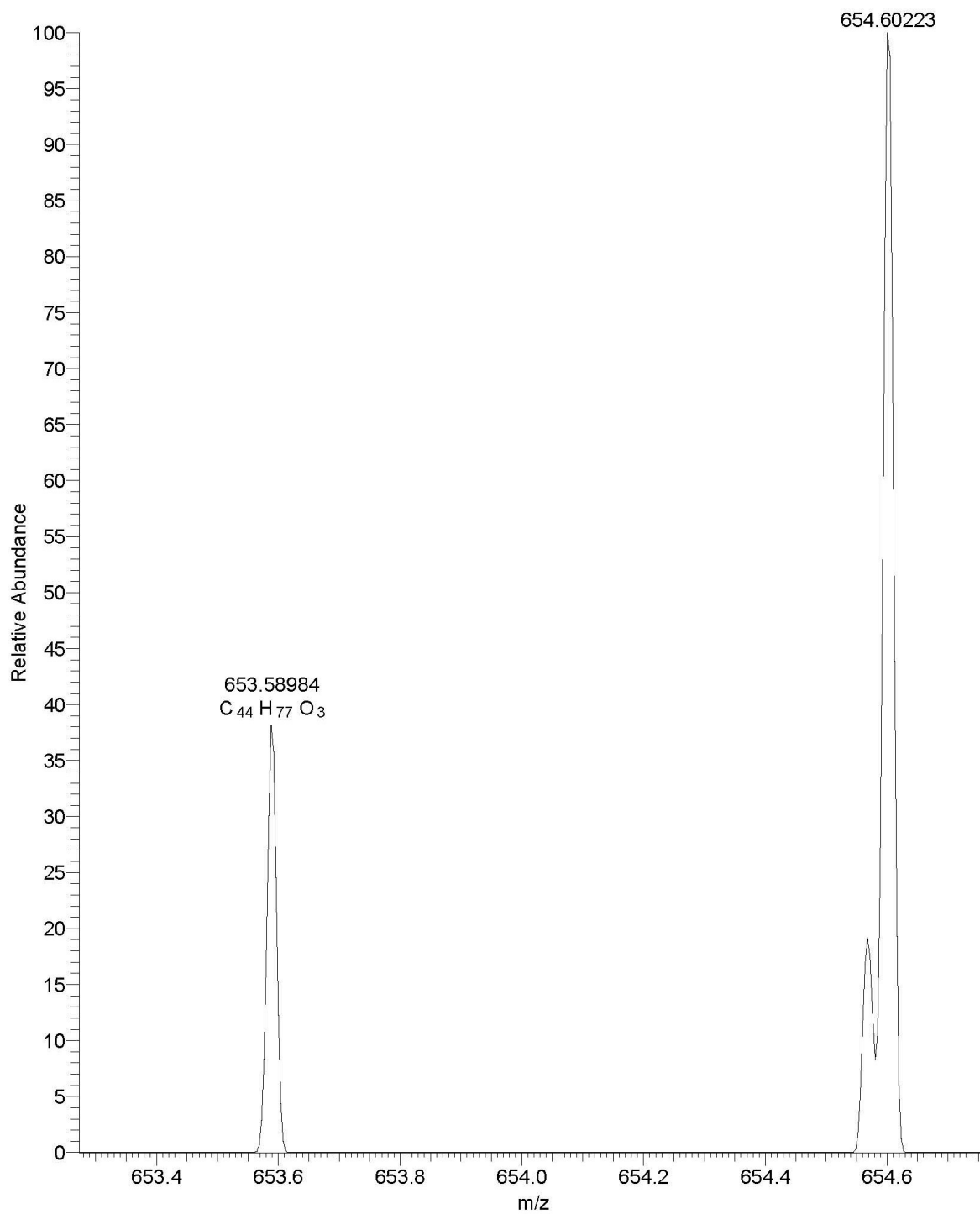


Figure 62: HRMS Spectrum of Compound **5b** (ESI MS M+1)

Molecular Formula: C₄₄H₇₆O₃; Exact Mass: 652.57945

Calculated M+1: 653.58727; Experimental: M+1: 653.58984

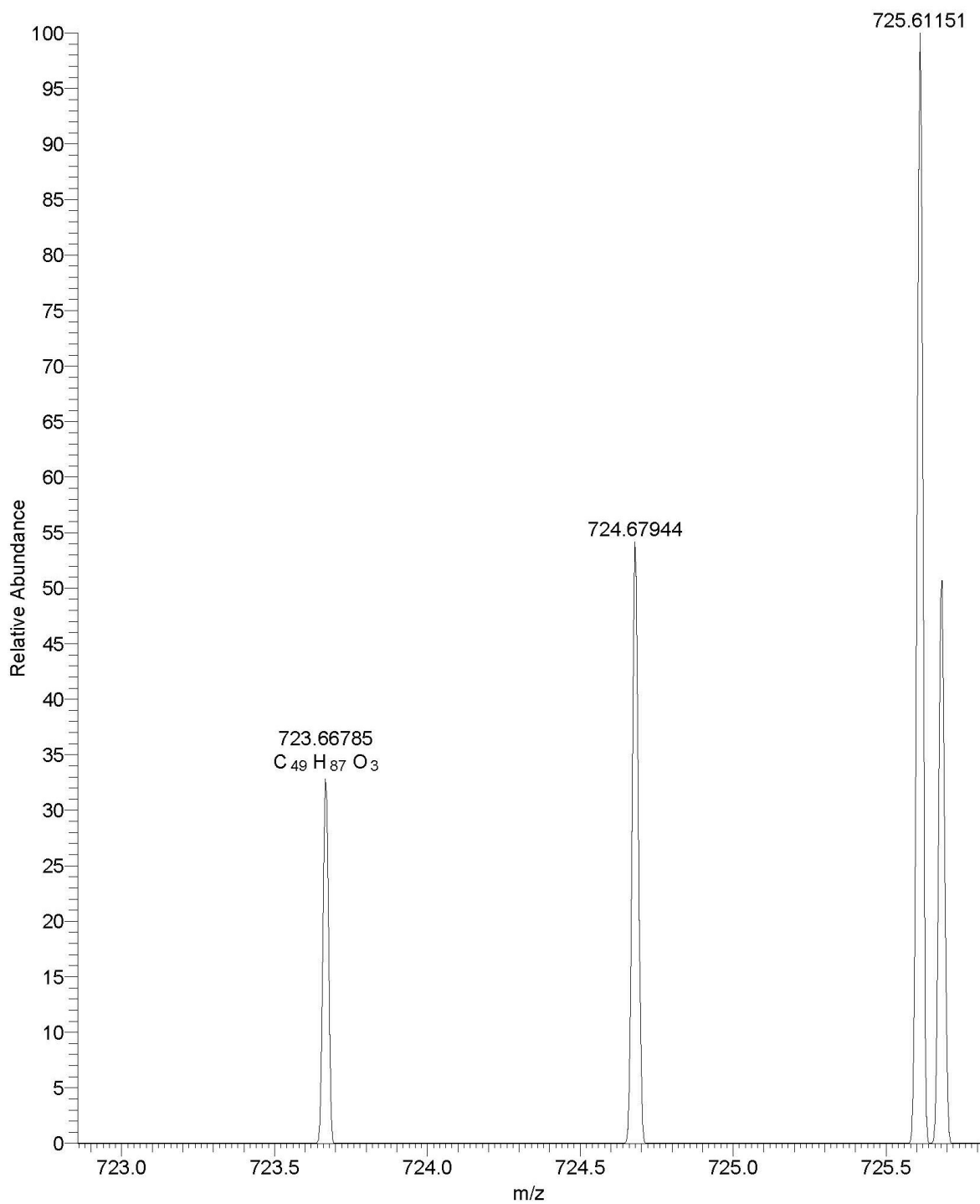


Figure 63: HRMS Spectrum of Compound **5c** (ESI MS M+1)

Molecular Formula: C₄₉H₈₆O₃; Exact Mass: 722.65770

Calculated M+1: 723.66552; Experimental: M+1: 723.66785

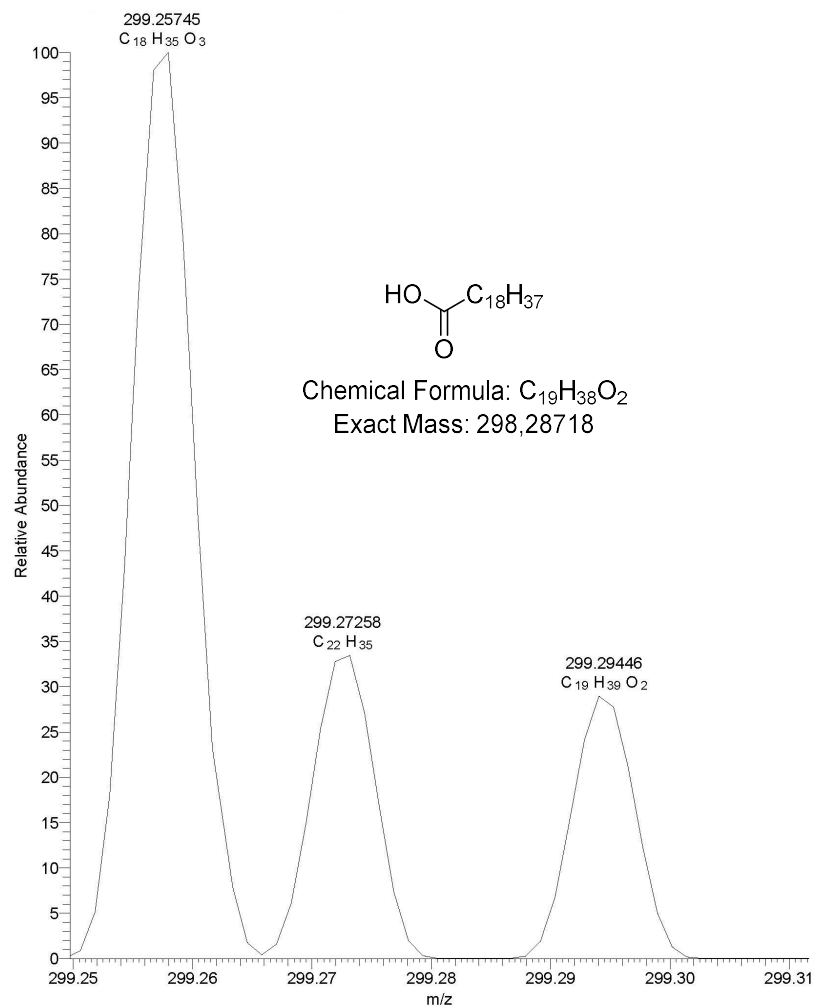
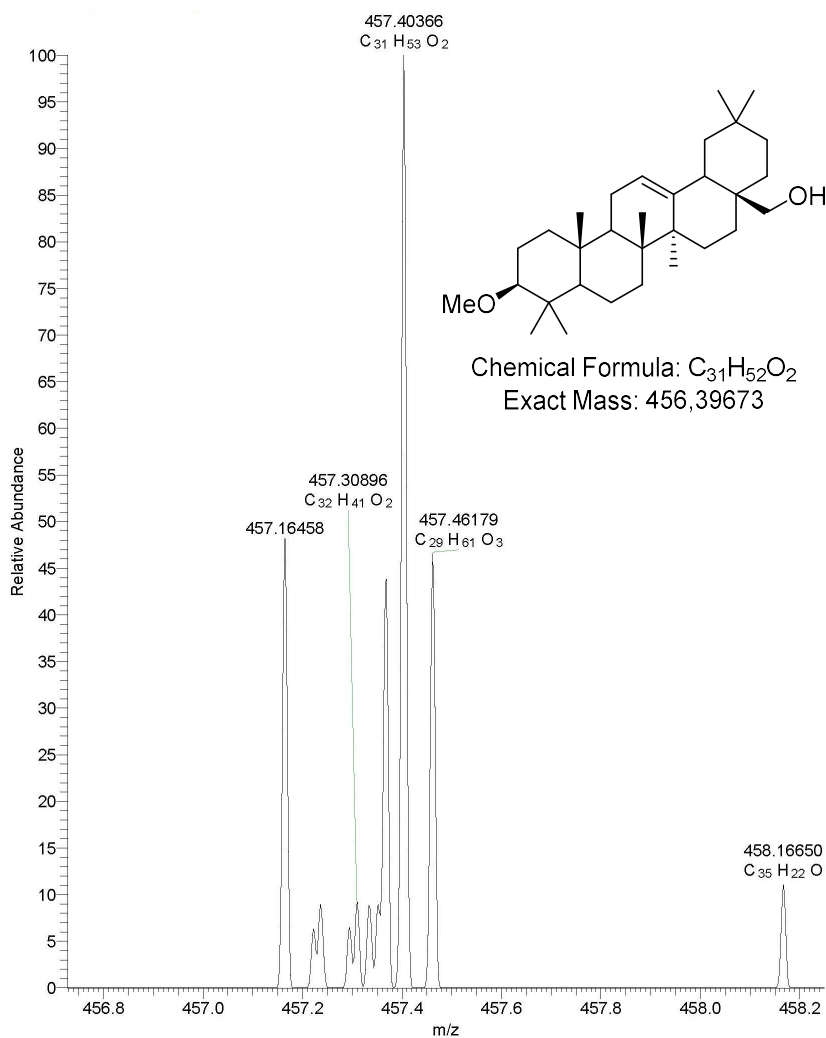


Figure 64: HRMS Spectrum of fragments of Compound **5d** (ESI MS M+1)
m/z: M+1: 457.40336, 299.25745

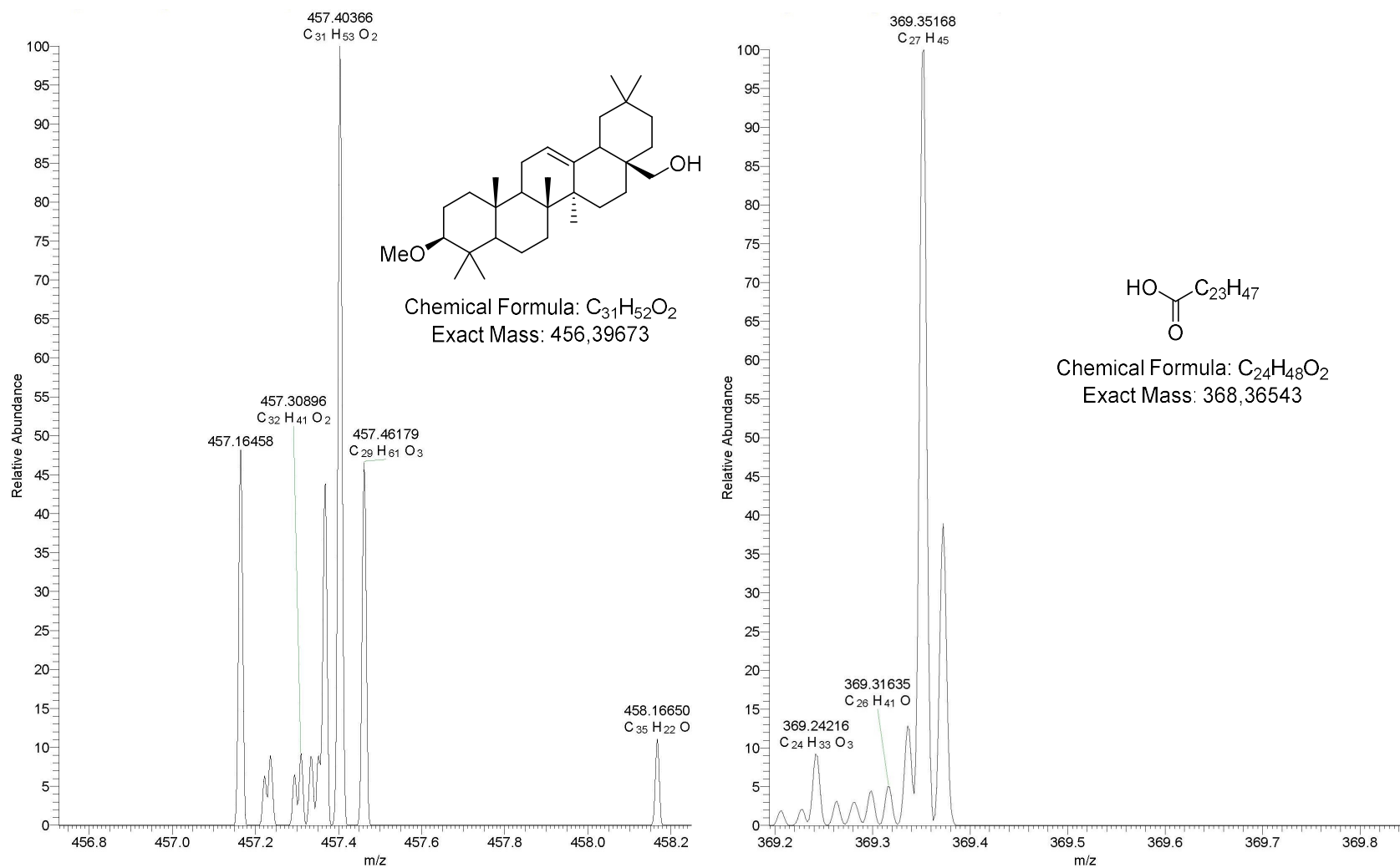


Figure 65: HRMS Spectrum of fragments of Compound **5e** (ESI MS M+1)
 m/z : M+1: 457.40336, 369.35168

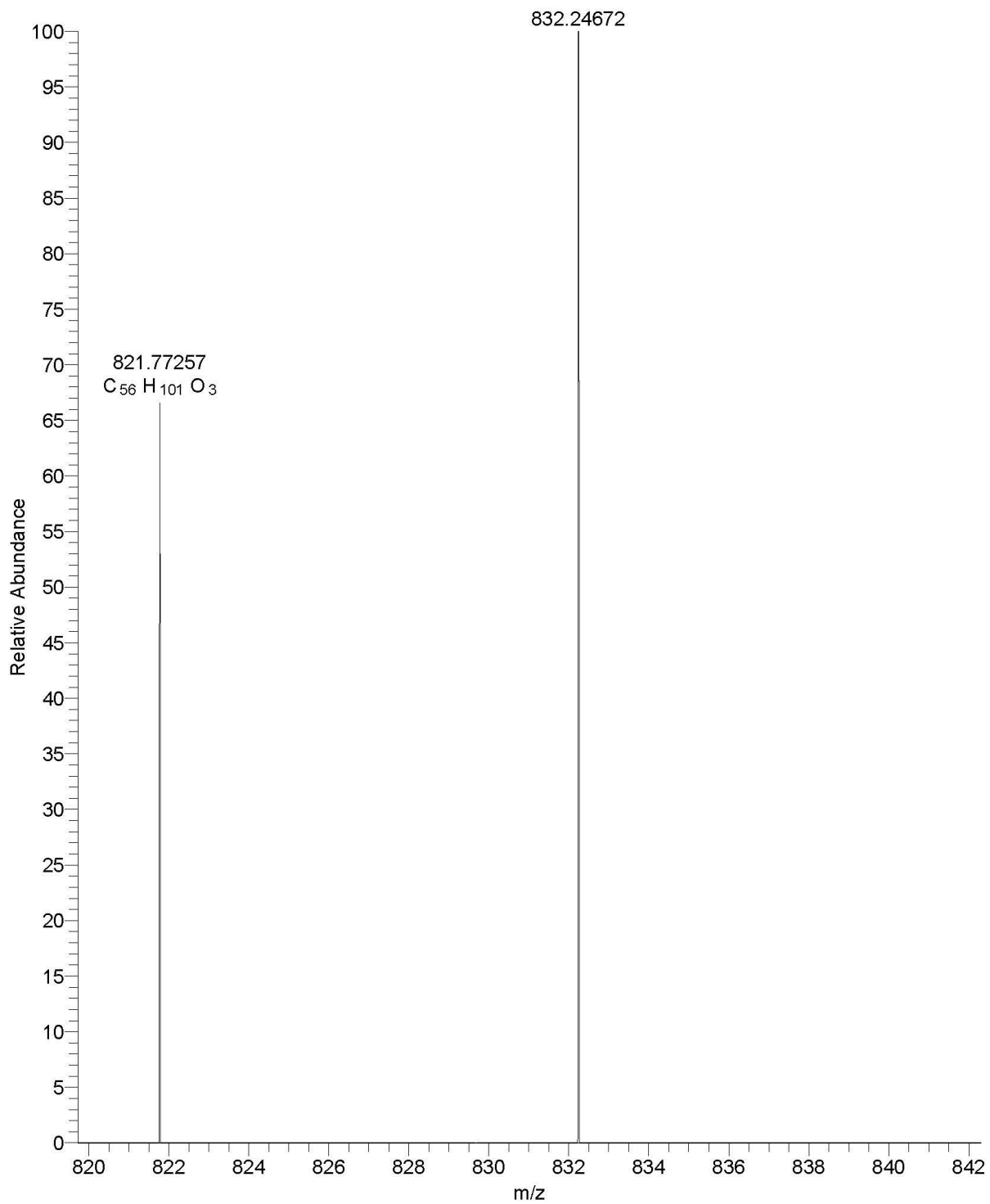


Figure 66: HRMS Spectrum of Compound **5f** (ESI MS M+1)

Molecular Formula: C₅₆H₁₀₀O₃; Exact Mass: 820.76725

Calculated M+1: 821.77507; Experimental: M+1: 821.77257

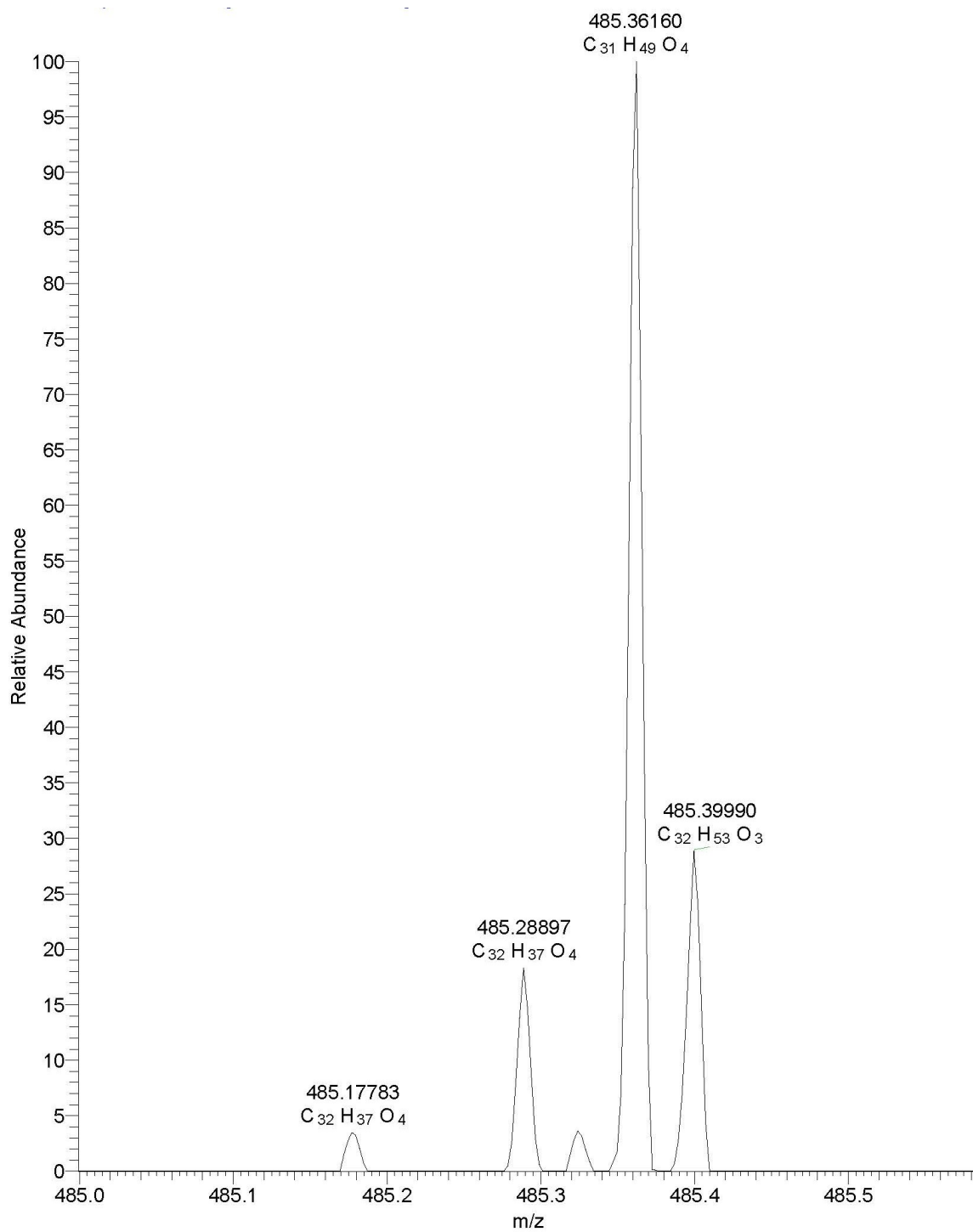


Figure 67: HRMS Spectrum of Compound **6** (ESI MS M+1)

Molecular Formula: C₃₂H₅₂O₃; Exact Mass: 484.39165;

Calculated M+1: 485.39947; Experimental: M+1: 485.39990

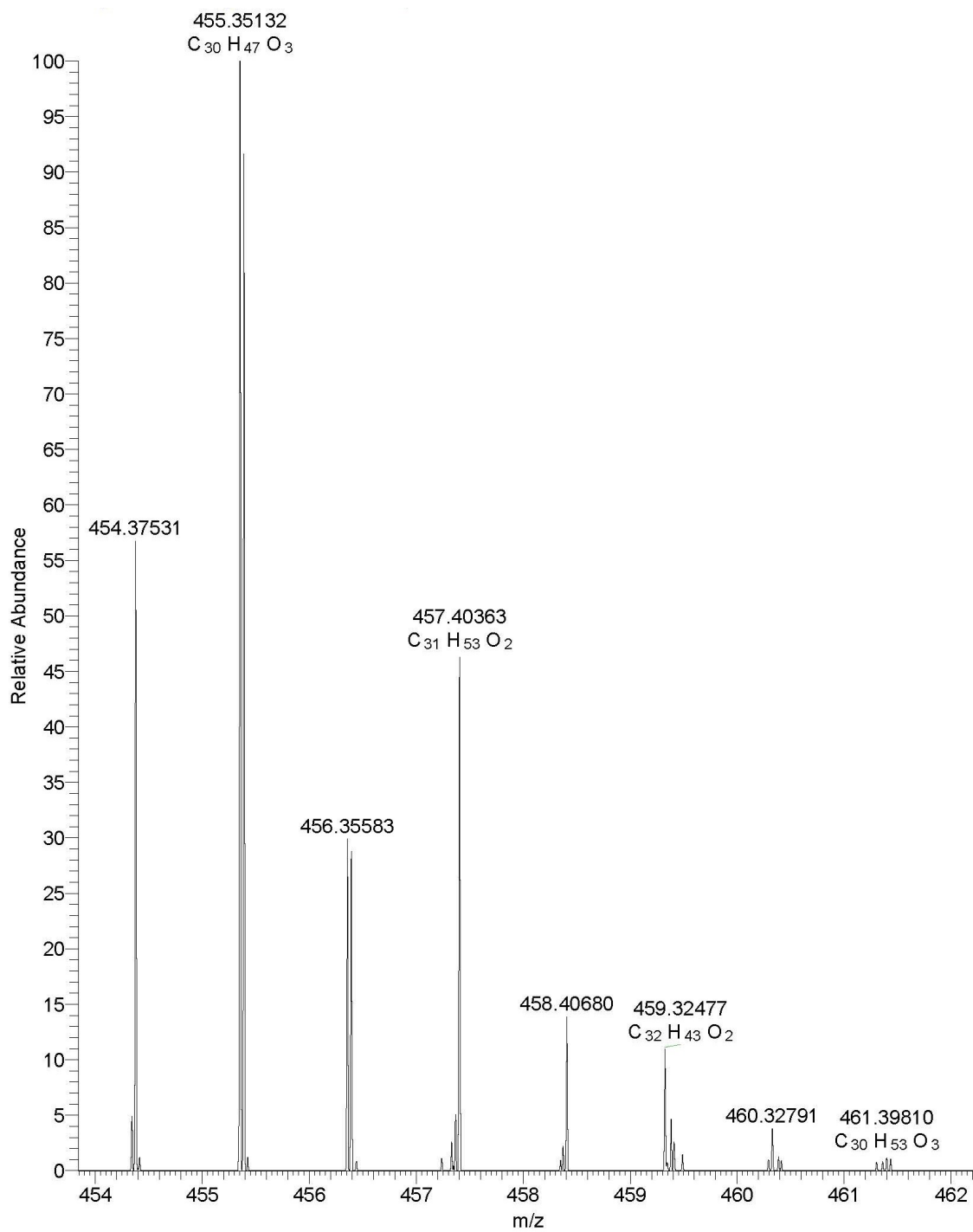


Figure 68: HRMS Spectrum of Compound 7 (ESI MS M+1)

Molecular Formula: C₃₁H₅₂O₂; Exact Mass: 456.39673;

Calculated M+1: 457.40456; Experimental: M+1: 457.40363

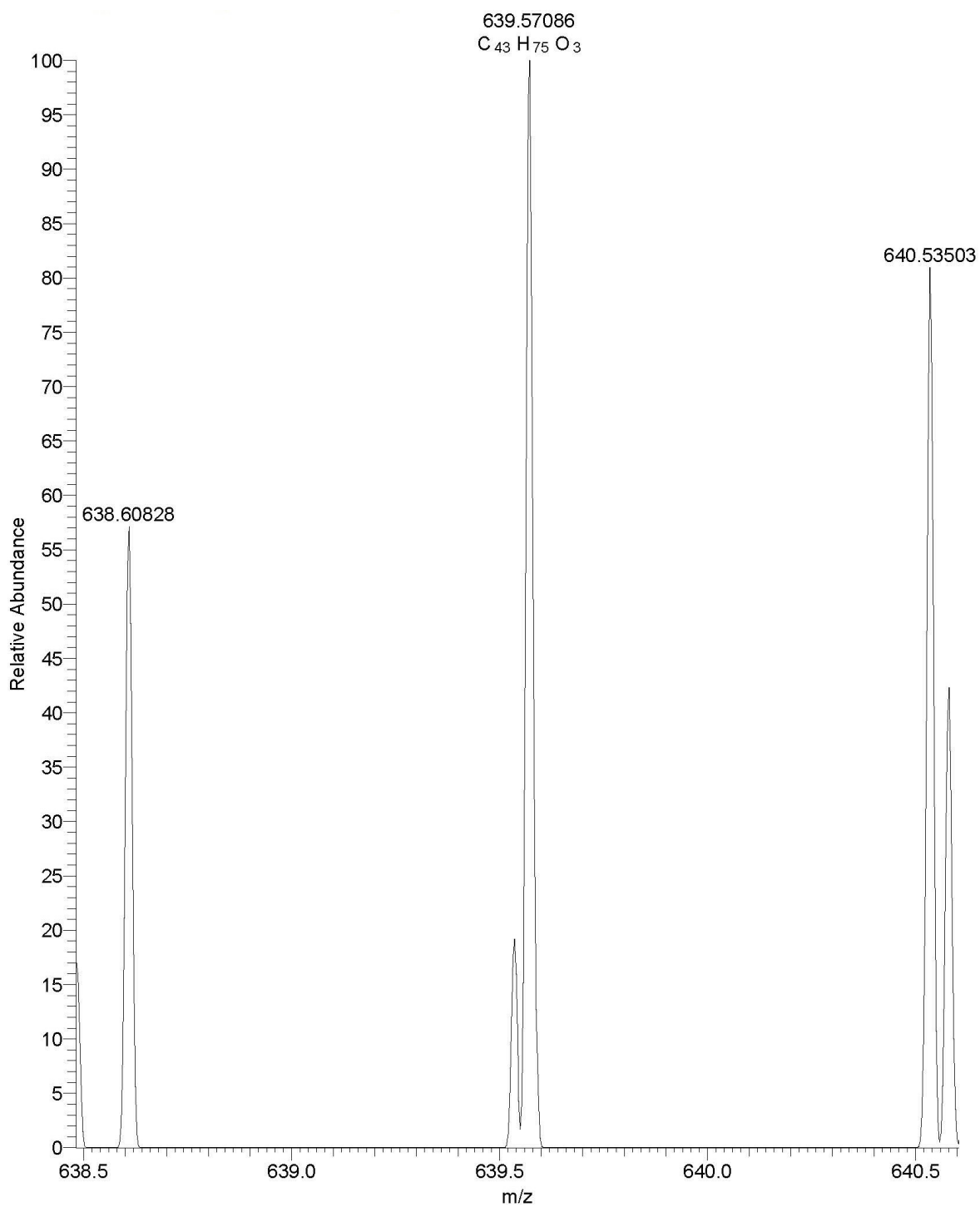


Figure 69: HRMS Spectrum of Compound **8a** (ESI MS M+1)

Molecular Formula: C₄₃H₇₄O₃; Exact Mass: 638.56380;

Calculated M+1: 639.57162; Experimental: M+1: 639.57086

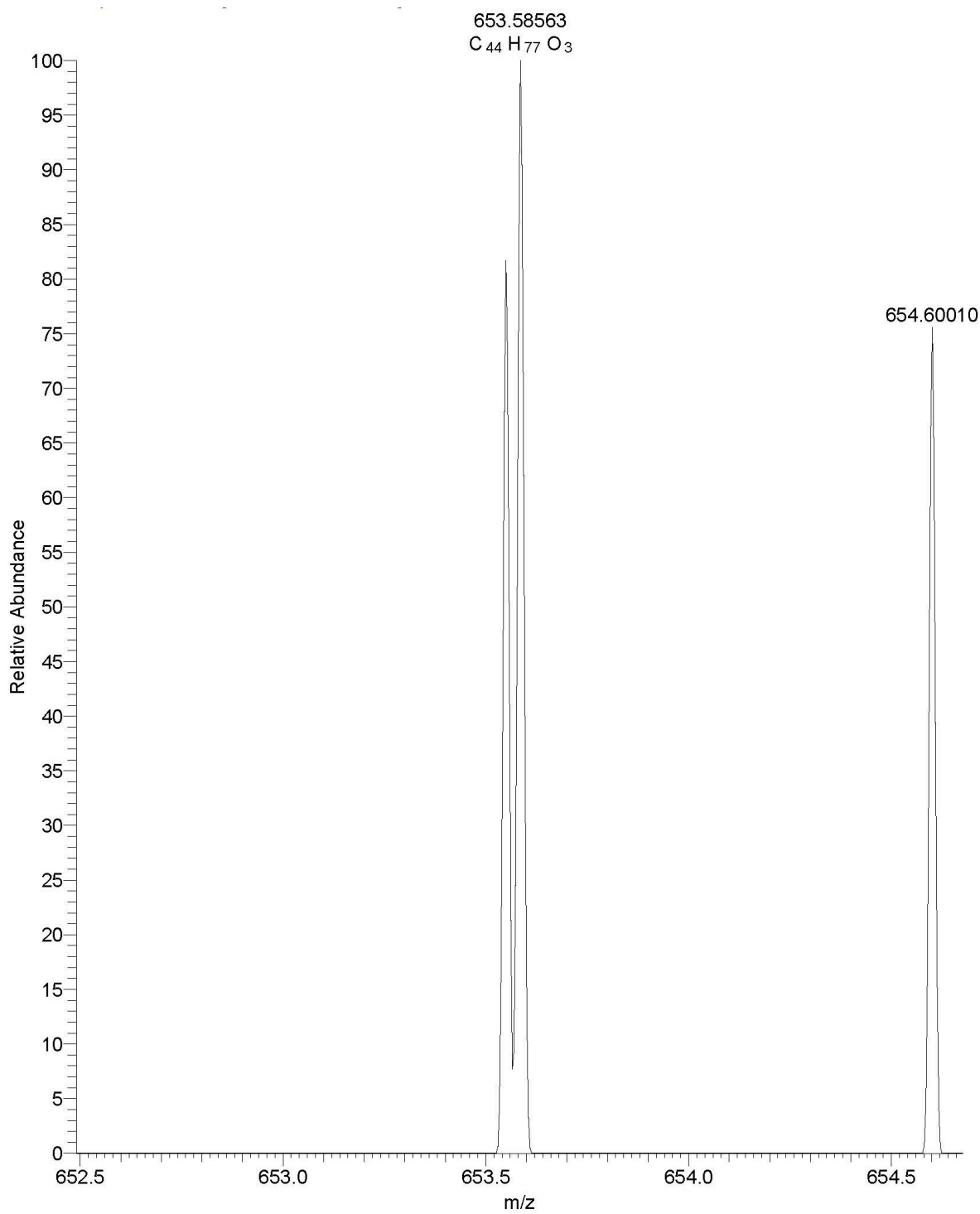


Figure 70: HRMS Spectrum of Compound **8b** (ESI MS M+1)

Molecular Formula: C₄₄H₇₆O₃; Exact Mass: 652.57945

Calculated M+1: 653.58727; Experimental: M+1: 653.58563

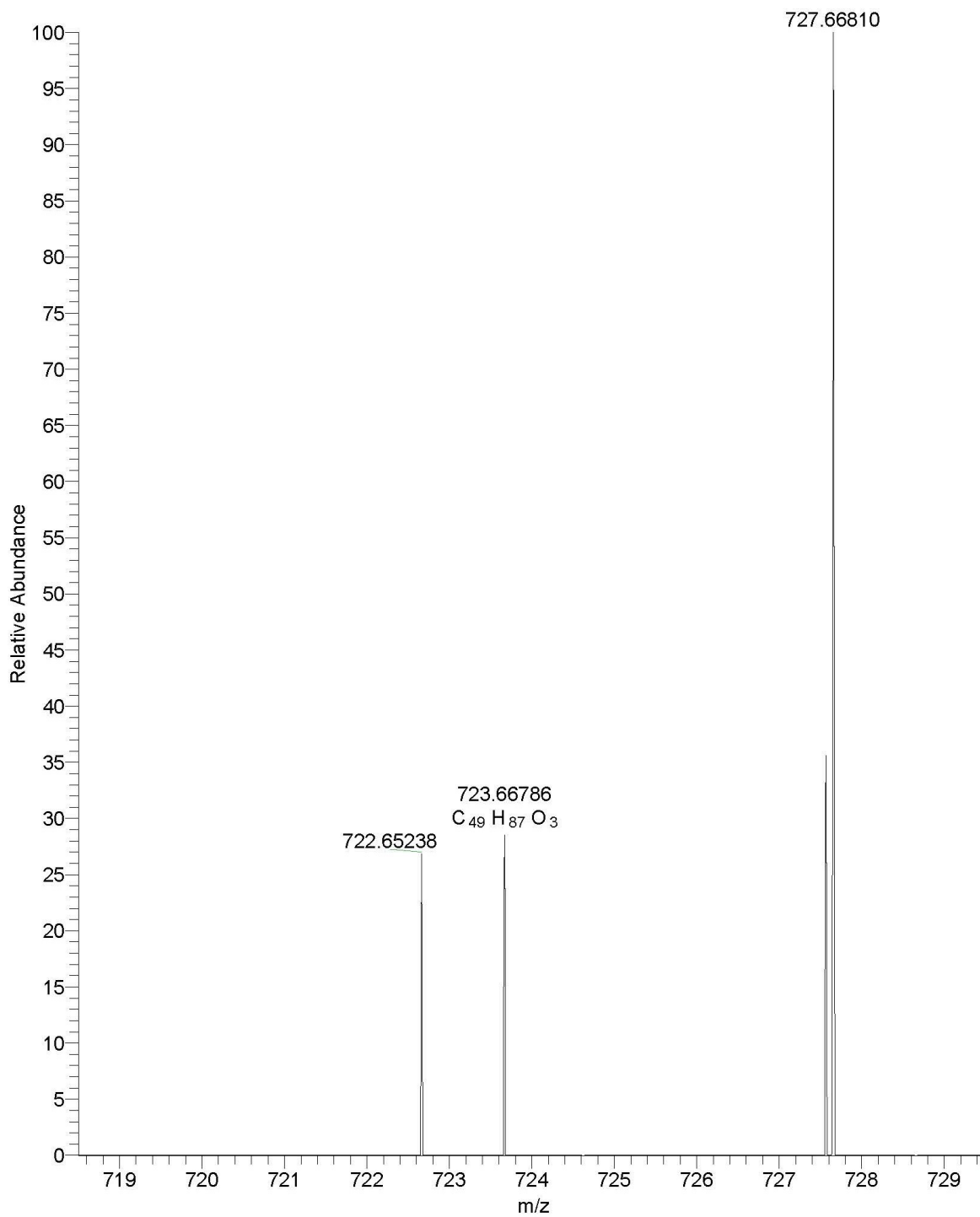


Figure 71: HRMS Spectrum of Compound **8c** (ESI MS M+1)

Molecular Formula: C₄₉H₈₆O₃; Exact Mass: 722.65770

Calculated M+1: 723.66552; Experimental: M+1: 723.66786

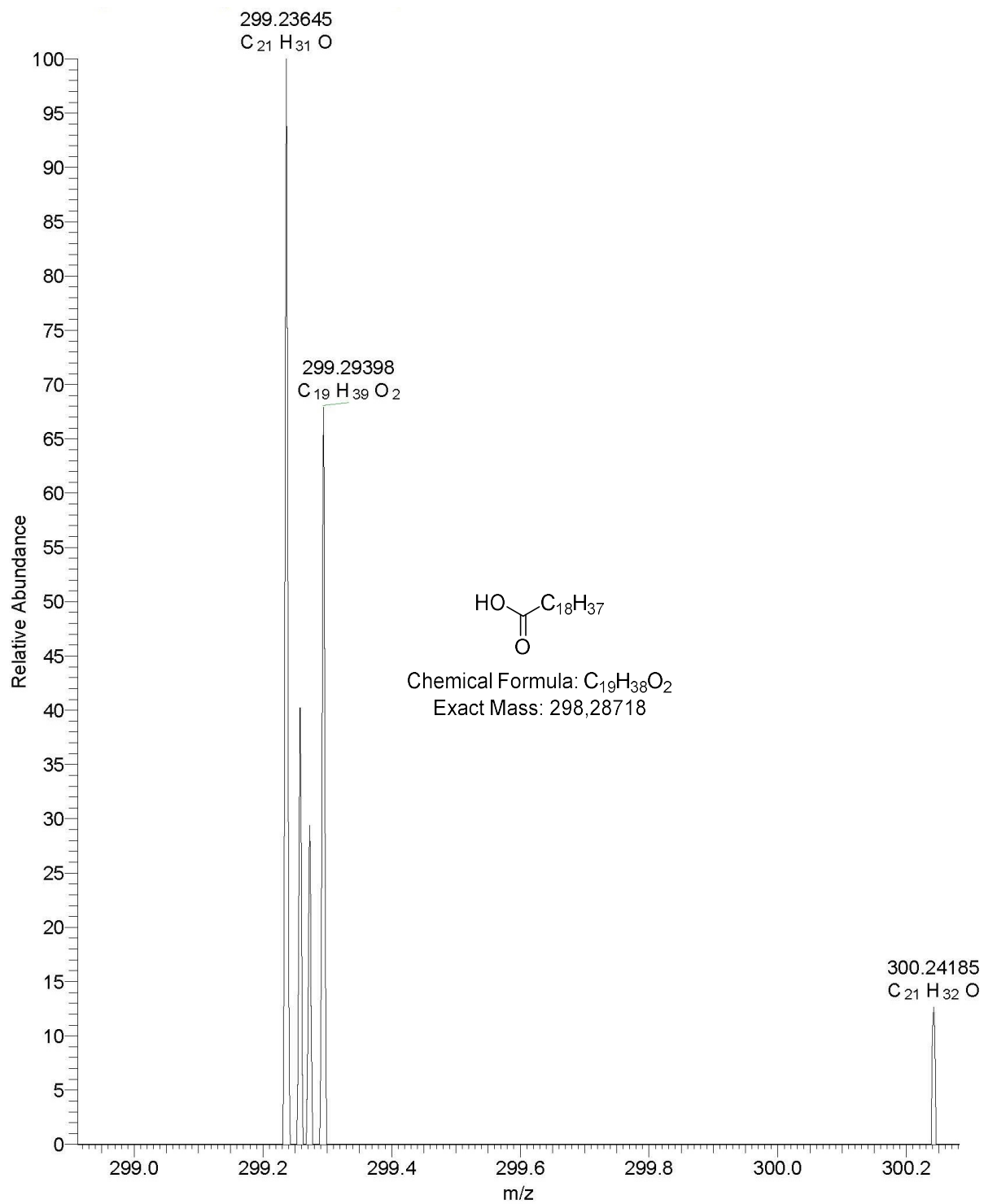


Figure 72: HRMS Spectrum of fatty acid fragments of Compound **8d** (ESI MS M+1)

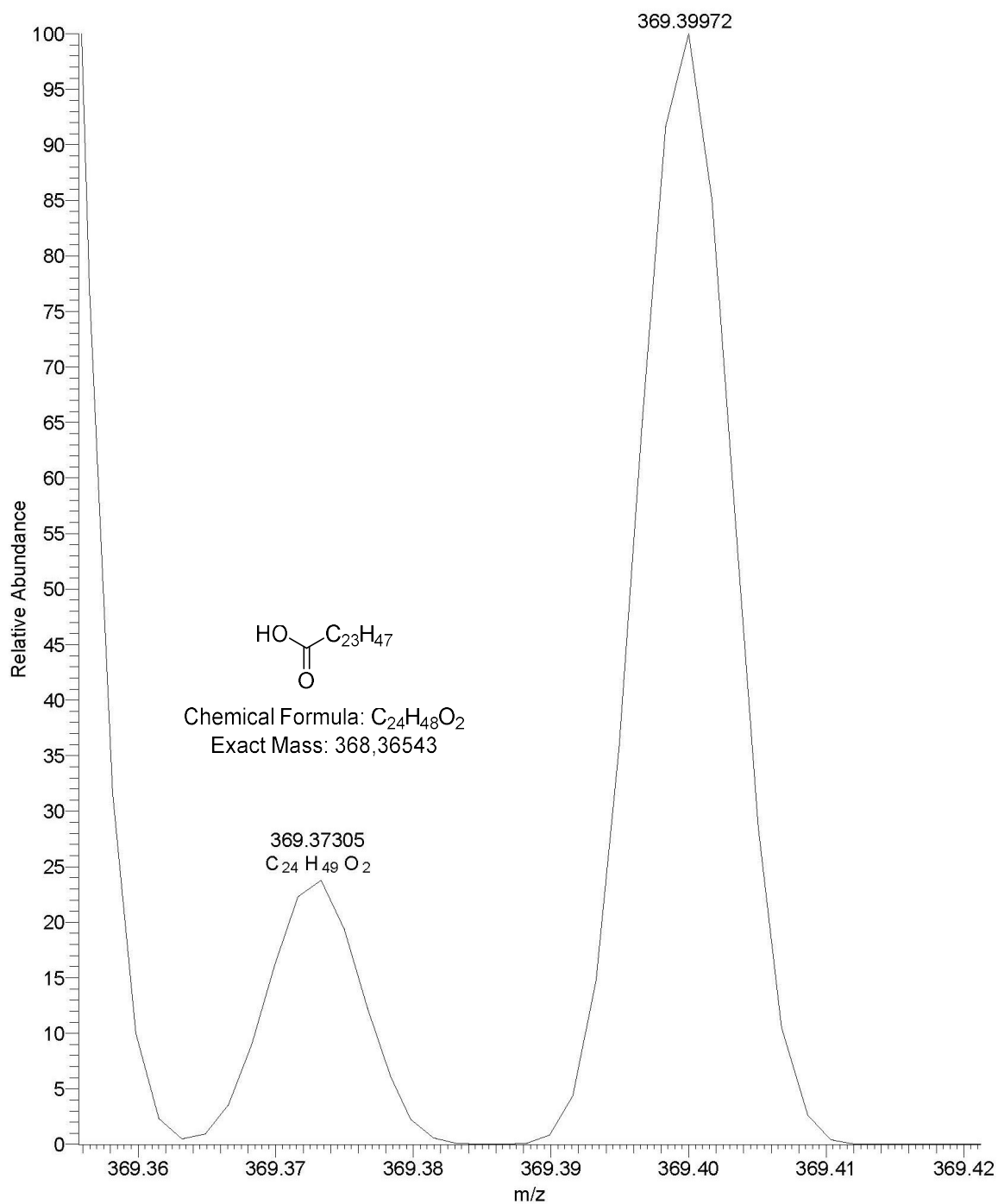


Figure 73: HRMS Spectrum of fatty acid fragments of Compound **8e** (ESI MS M+1)

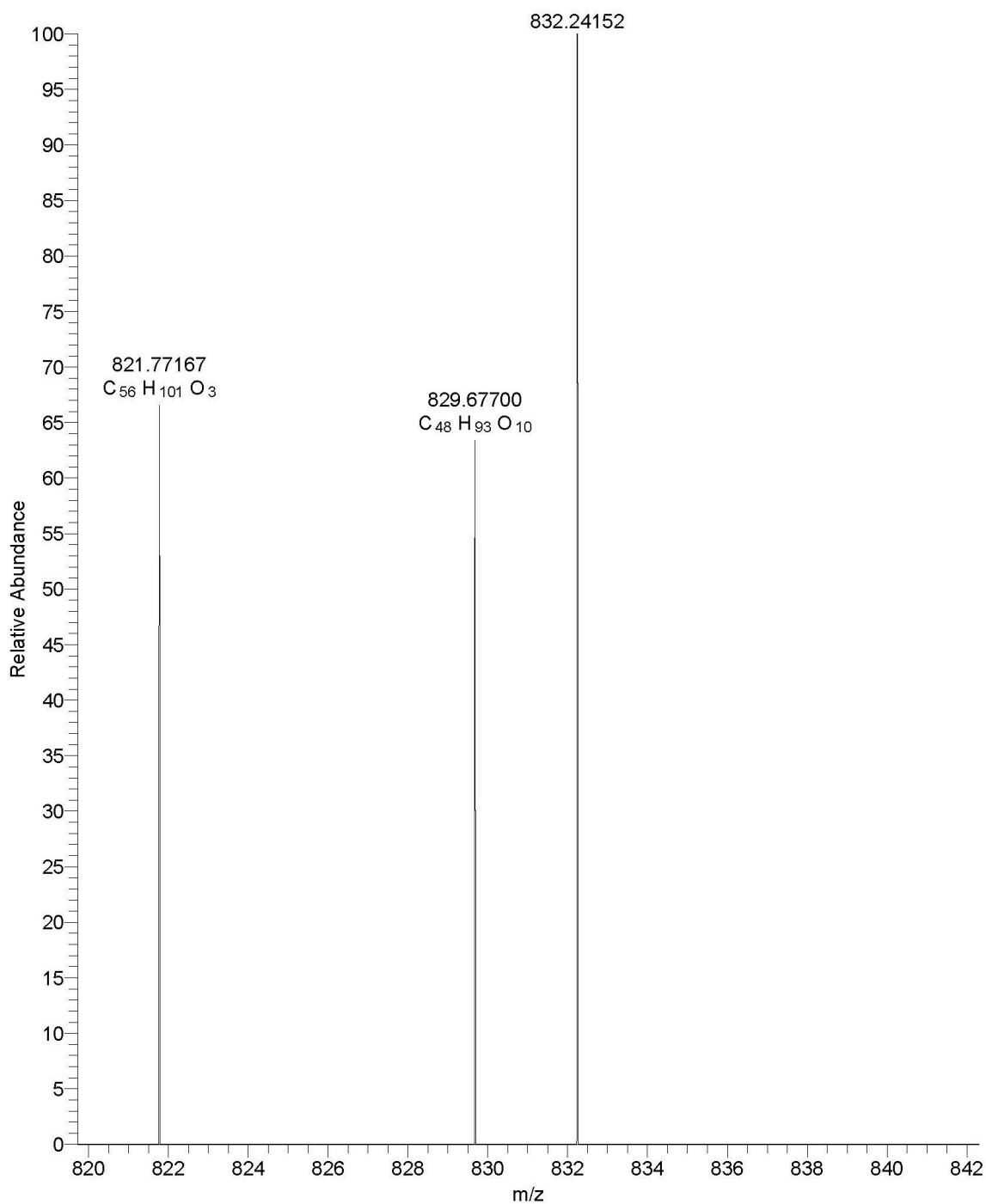


Figure 74: HRMS Spectrum of Compound **8f** (ESI MS M+1)

Molecular Formula: C₅₆H₁₀₀O₃; Exact Mass: 820.76725

Calculated M+1: 821.77507; Experimental: M+1: 821.77167