Supporting Information

A Novel Cyclohexane Carboxylic Acid Derivative from Black Turtle Bean (*Phaseolus vulgaris* L.)

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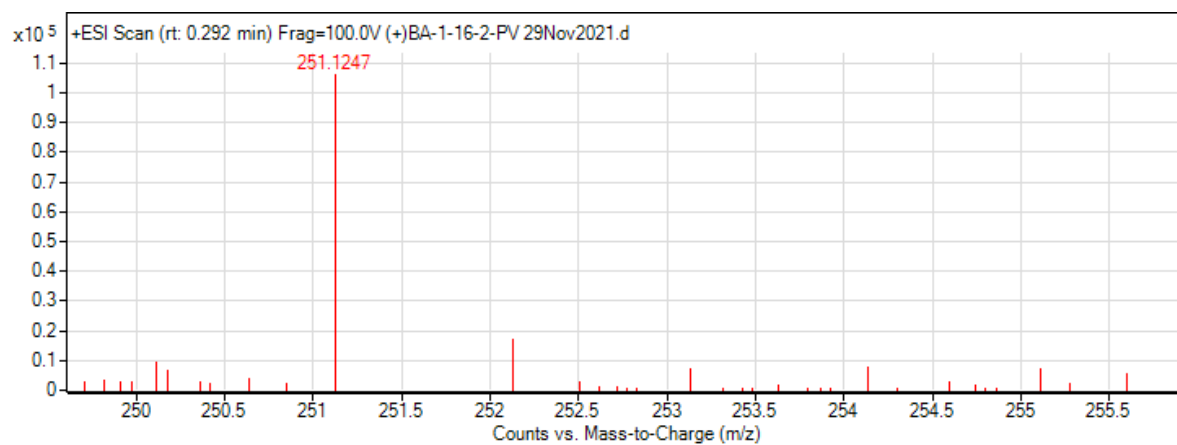
Figure S1: HR-ESI-MS spectra of **1**
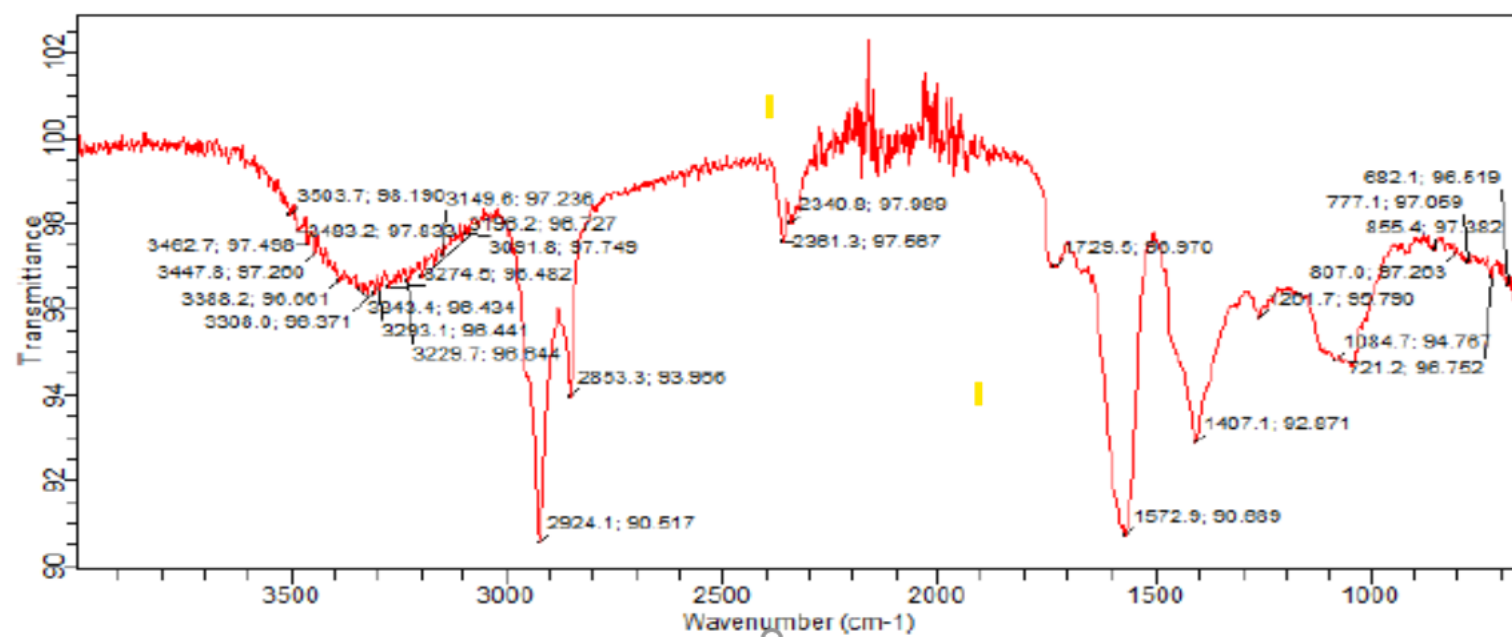
Figure S2: IR spectrum of **1**
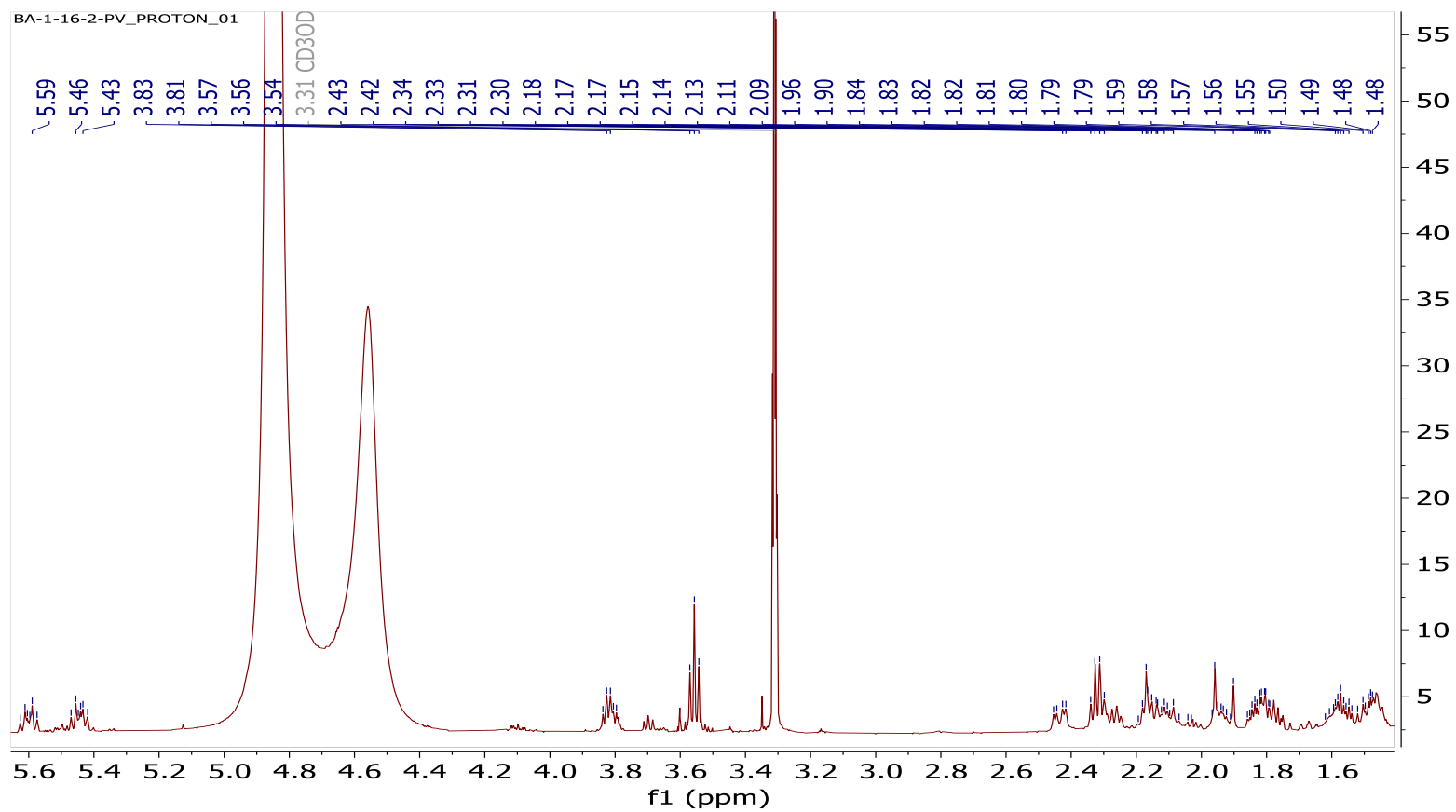
Figure S3: ^{1}H-NMR (500 MHz, CD$_3$OD) spectrum of **1**

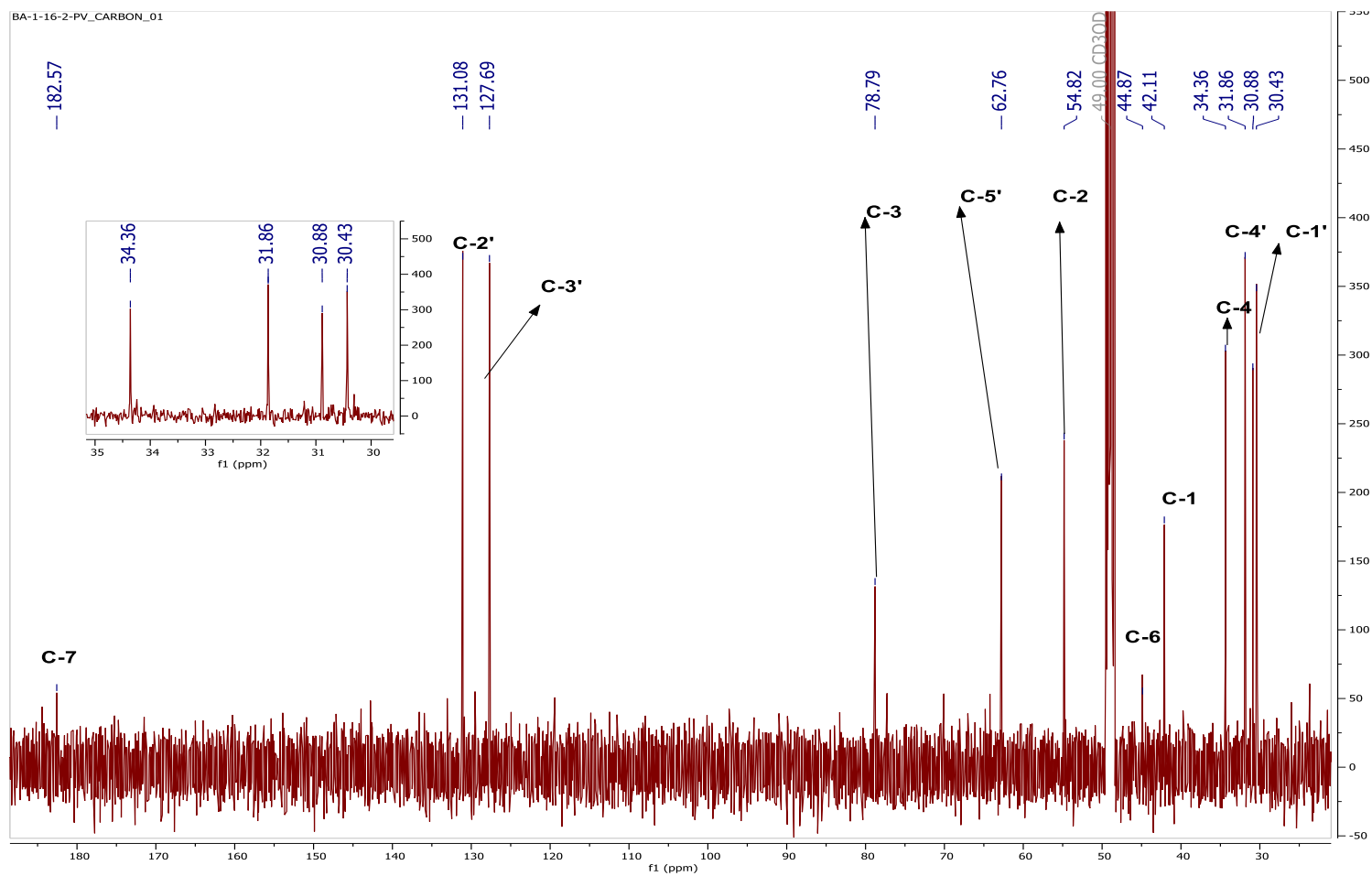**Figure S4:** ^{13}C-NMR (125 MHz, CD$_3$OD) spectrum of **1**
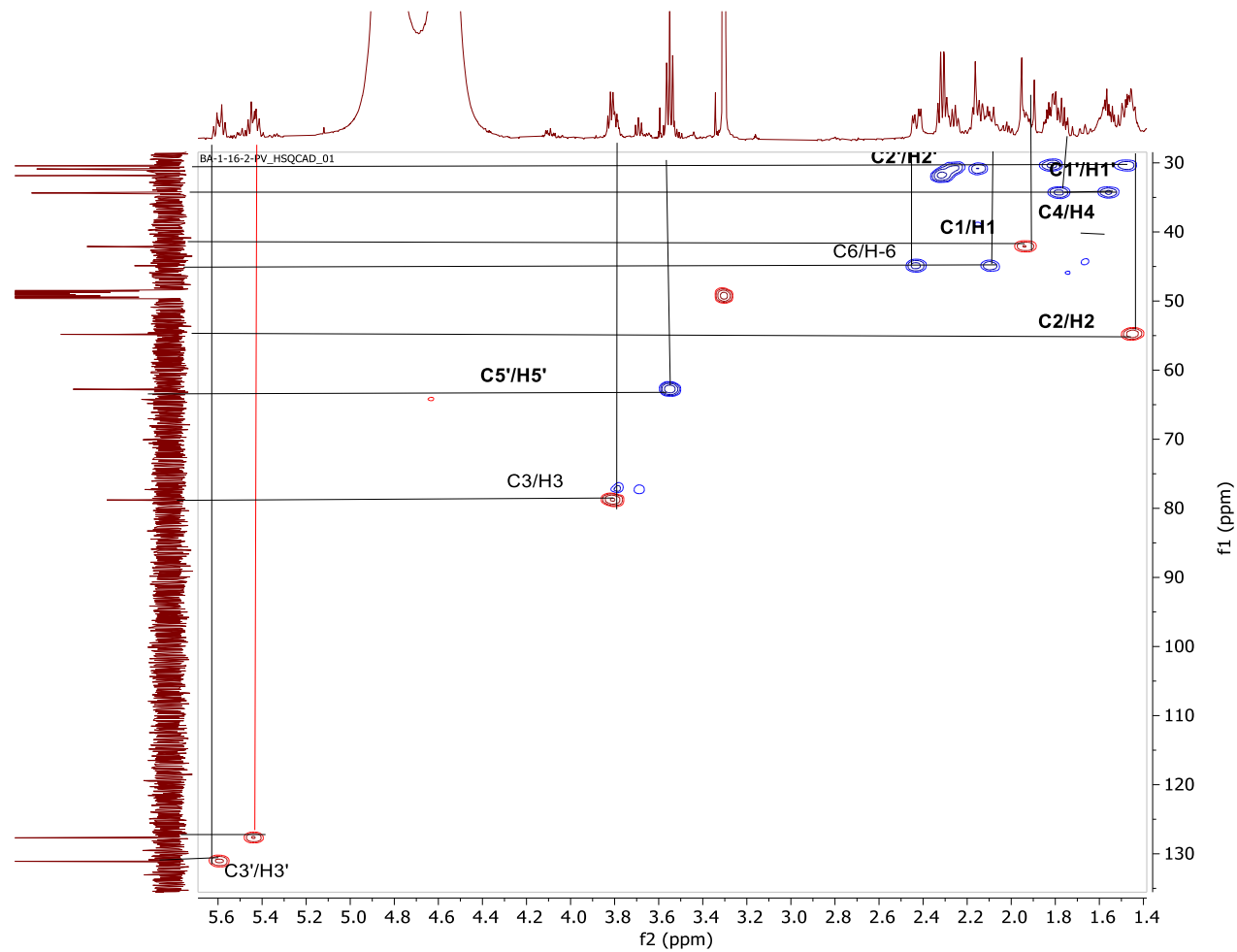
Figure S5: HSQC spectrum of **1,** (500 MHz, CD₃OD)

Figure S6: ^1H-^1H COSY spectrum of **1,** (500 MHz, CD$_3$OD)
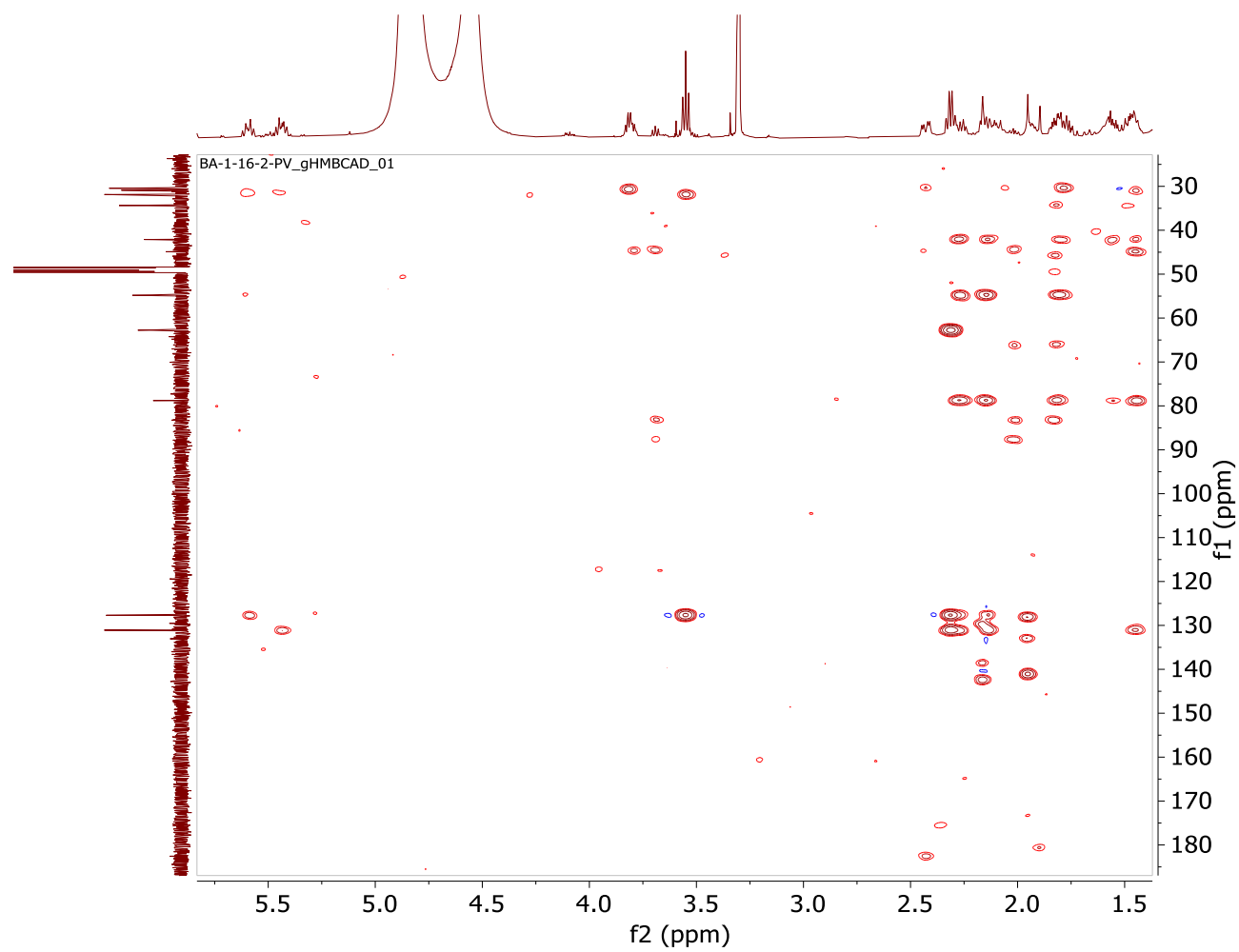
Figure S7: HMBC spectrum of **1,** (500 MHz, CD$_3$OD)

BA-1-16-1-PV_PROTON_01
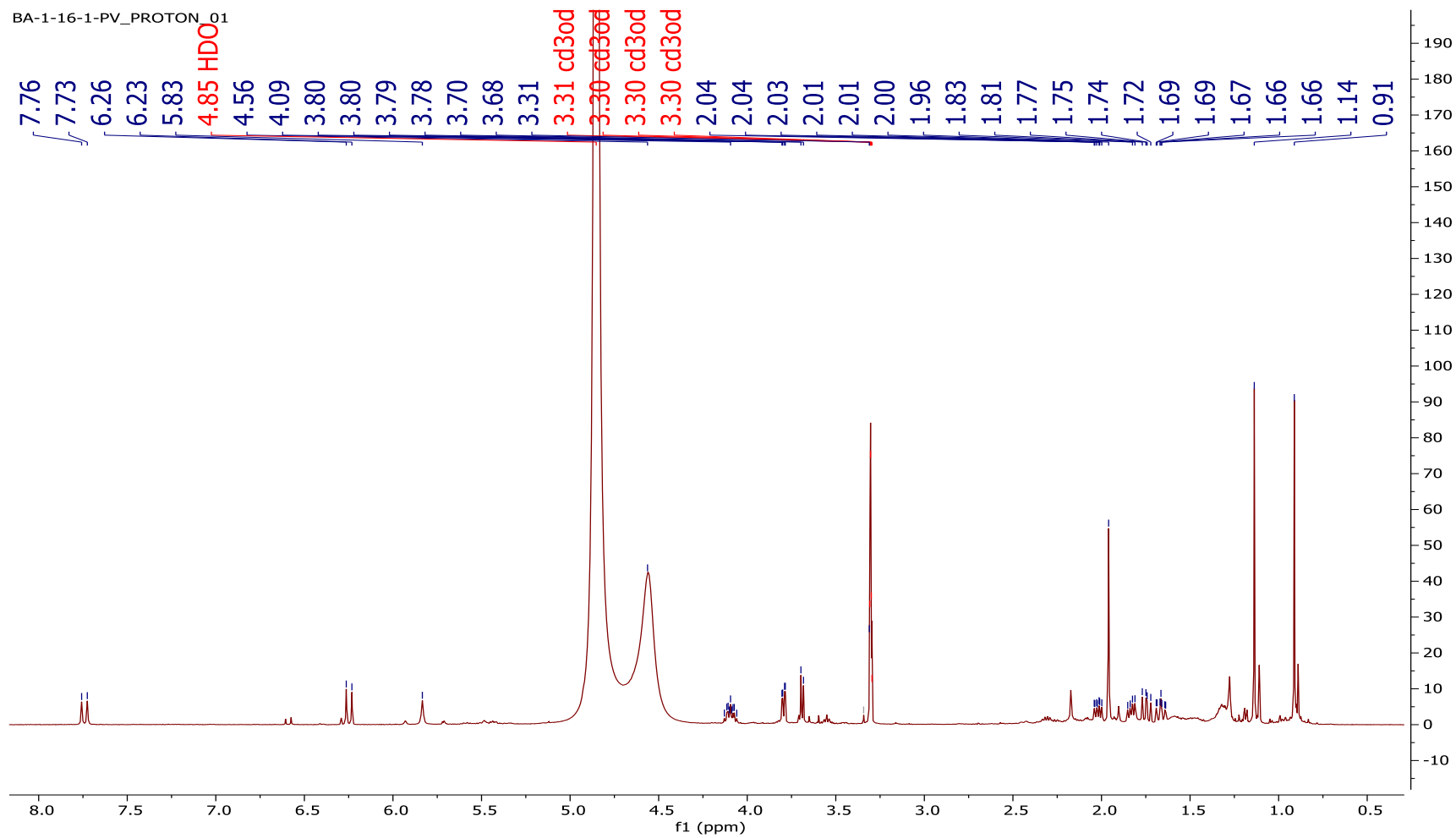
Figure S8: ^{1}H-NMR (500 MHz, CD$_3$OD) spectrum of **2**
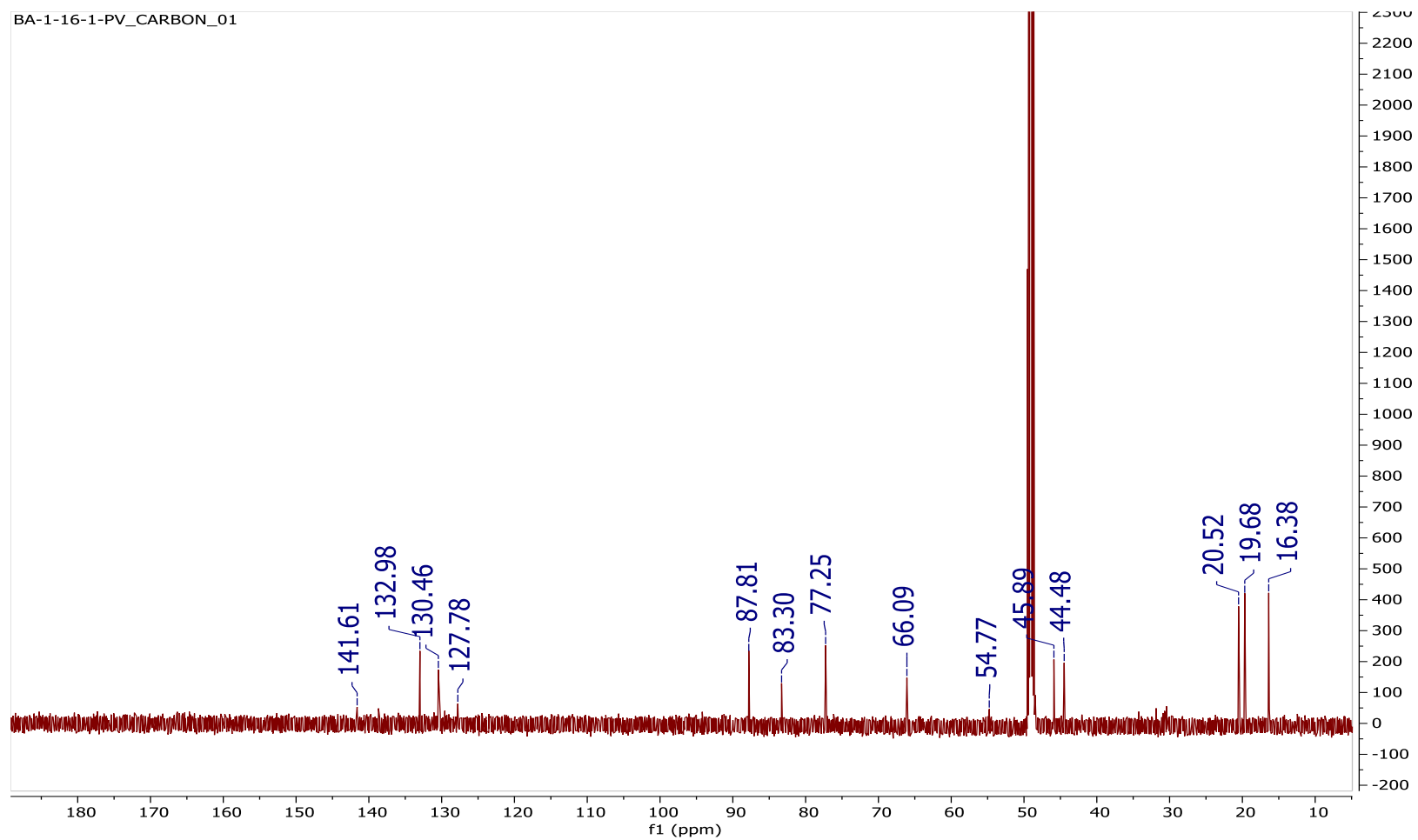
Figure **S9:** ^{13}C-NMR (125 MHz, CD$_3$OD) spectrum of **2**

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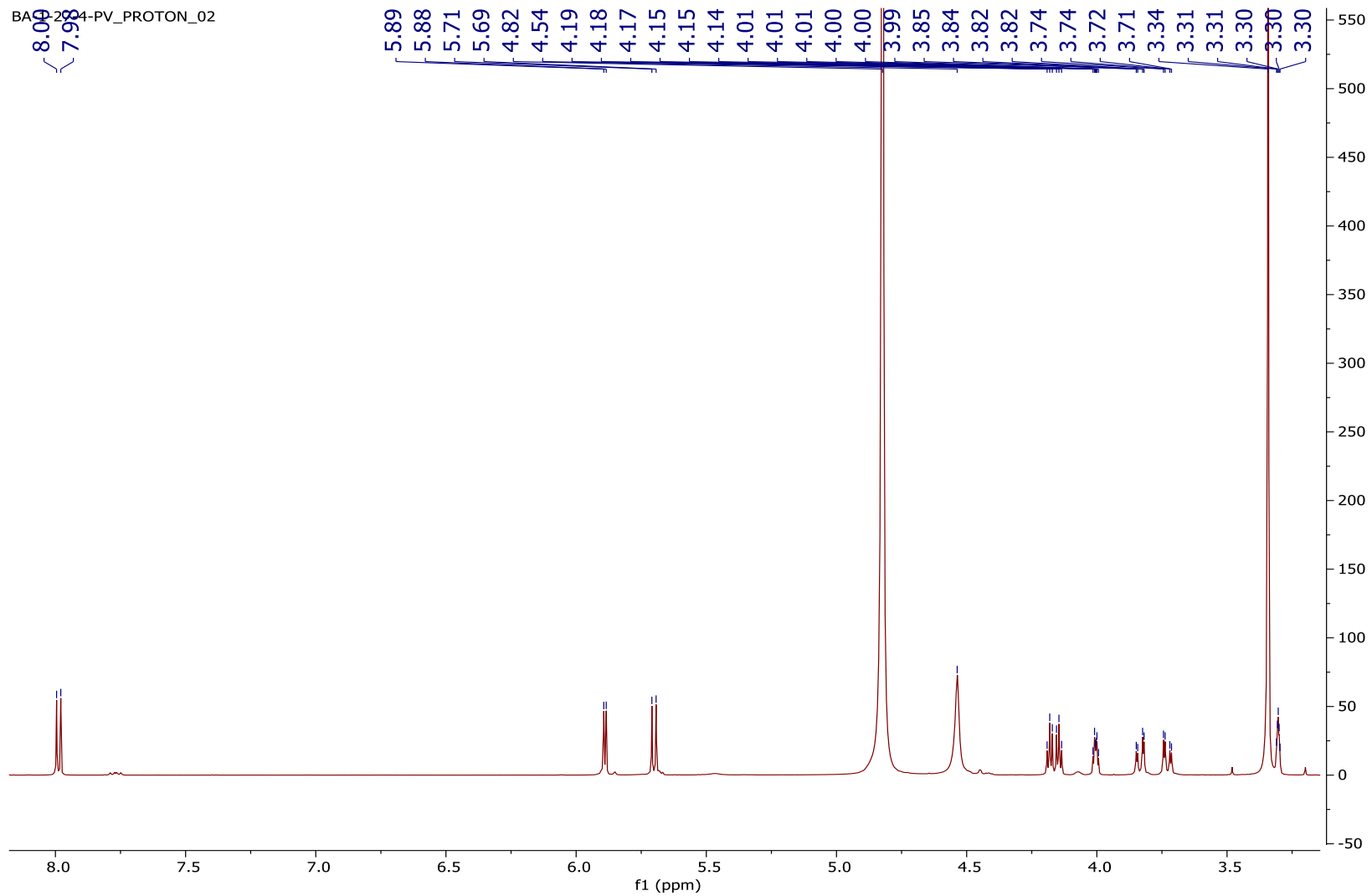
Figure S10: ^{1}H-NMR (500 MHz, CD$_3$OD) spectrum of **3**
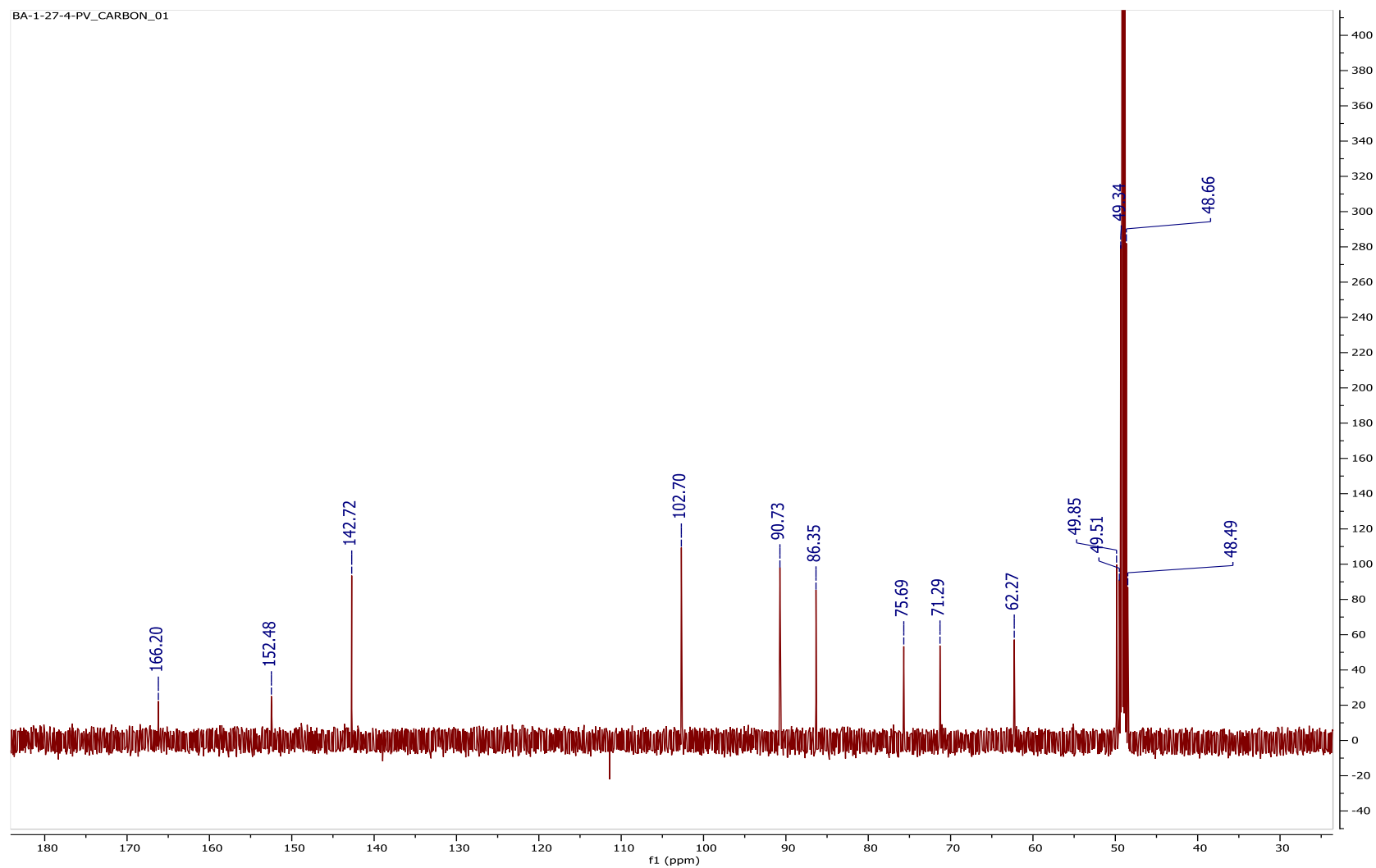
BA-1-27-4-PV_CARBON_01

Figure **S11**: ^{13}C-NMR (125 MHz, CD$_3$OD) spectrum of **3**
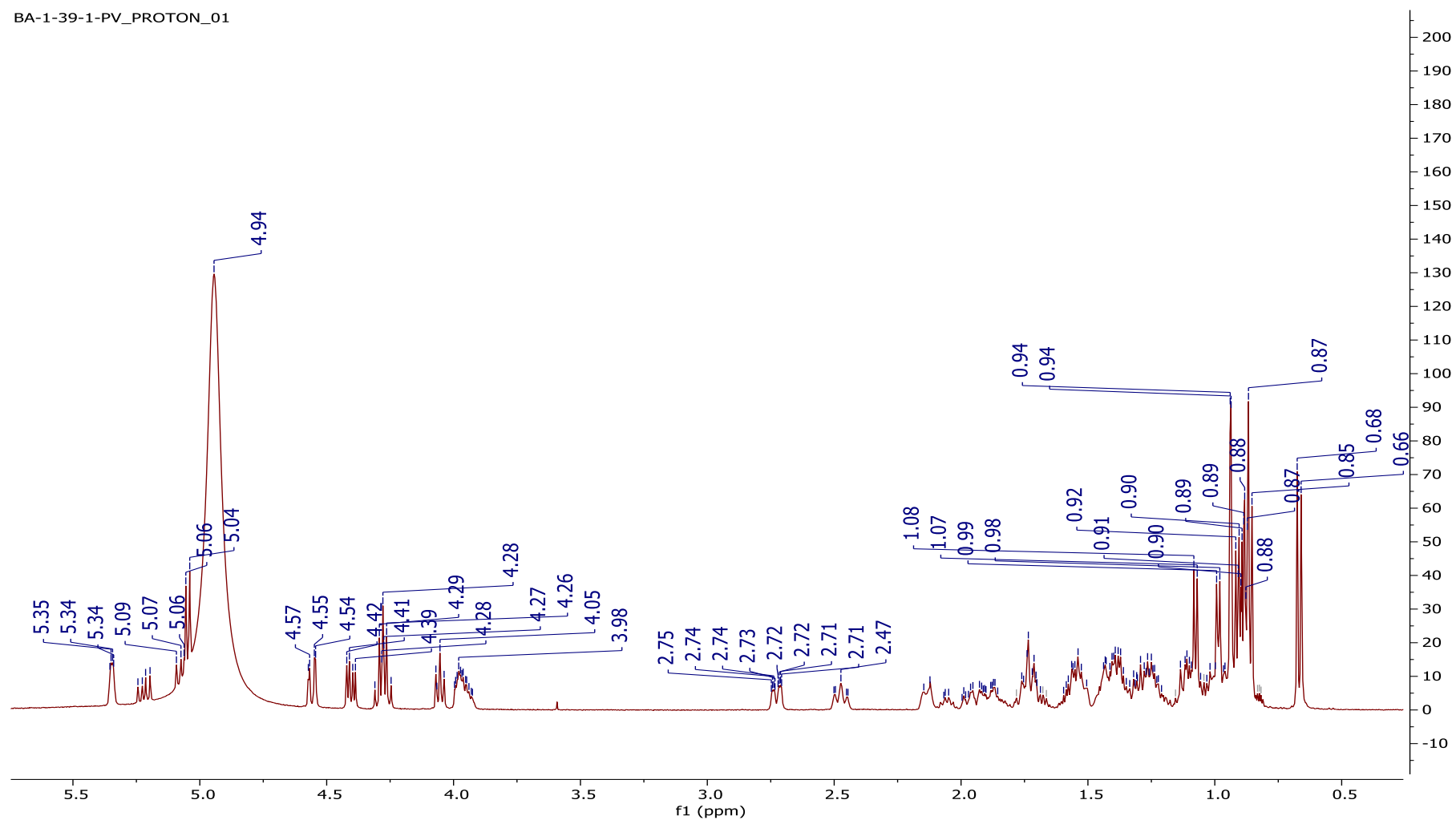
Figure S12: ^{1}H-NMR (500 MHz, C$_5$D$_5$N) spectrum of **4 and 5**
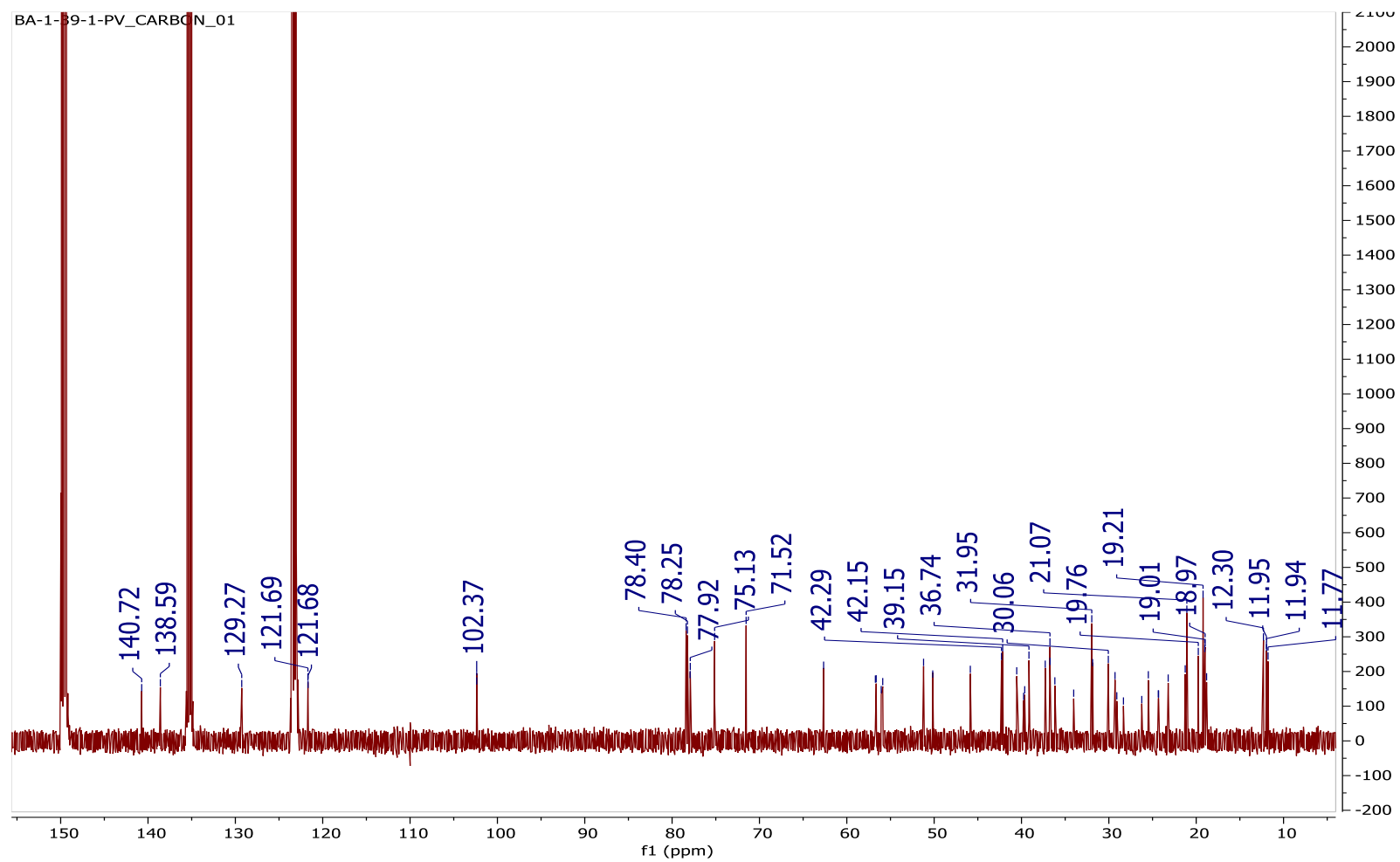
Figure **S11:** ^{13}C-NMR (125 MHz, C$_5$D$_5$N)) spectrum of **4** and **5**

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Table S1 : Published ^{1}H and ^{13}C NMR data of lasdiploic acid

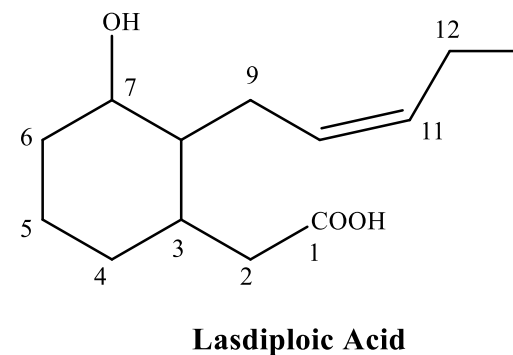| Position	δ_C	δ_H (J in Hz)
1	178.7	
2	35.3	2.47 (dd, 15.3, 9.4, 1H
		2.26 (dd, 15.5, 9.2, 1H)
3	36.6	2.69 (m, 1H)
4	28.3	2.15–1.91 (m, 1H)
		1.40–1.27 (m, 1H)
5	29.7	1.40–1.27 (m, 2H)
6	32.5	2.15–1.91 (m, 1H)
		1.62–1.56 (m, 1H)
7	77.6	4.04 (m, 1H)
8	50.5	2.15–1.91 (m, 1H)
9	25.3	2.15–1.91 (m, 2H)
10	127.0	5.38 (m, 1H)
11	133.3	5.48 (m, 1H)
12	20.7	2.15–1.91 (m, 2H)
13	14.2	0.98 (t, 7.5, 3H)

Lasdiploic Acid

Figure S14a: Structure and NMR data of lasdiploic acid which is the most similar to compound 1 according to Scifinder search.

S. Kumar, A.D. Pagar, F. Ahmad, V. Dwibedi, A. Wani, P.V. Bharatam, M. Chhibber, S. Saxena, and S. Pal I (2019). Xanthine oxidase inhibitors from an endophytic fungus Lasiodiplodia pseudotheobromae, *Bioorg. Chem.* **87,** 851–856.

Table S2 : Published ¹H and ¹³C NMR data of jasmonic acid

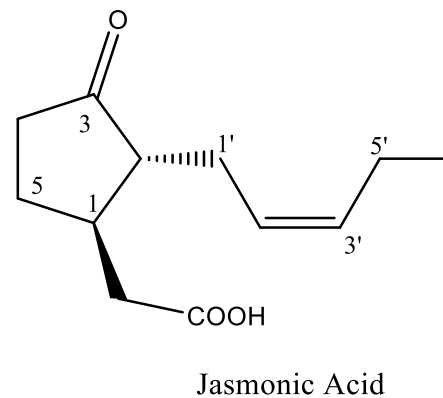| Position	δ_C	δ_H (J in Hz)
1	37.77	2.13 (m)
2	53.88	1.95 (m)
3	218.10	-
4	38.65	2.79, 2.37
5	27.15	2.33, 1.52
1	25.51	2.38
2	124.82	5.26 (dt, J=10.5, 5.5)
3	134.22	5.47 (dt, J=10.5, 5.5)
4	20.58	2.03, 1.64 (m)
5	14.05	0.97 (t, J=6.0)
CH₂	37.69	2.32
COOH	177.69	-

Jasmonic Acid

Figure S14b: Structure of -Jasmonic Acid which is 2nd most similar to compound 1 according to Scifinder search.

A.Husain, A. Ahmad and P.K. Agrawal (1993). (-)-Jasmonic acid, a phytotoxic substance from botryodiplodia theobromae: characterization by NMR spectroscopic methods, *J. Nat. Prod.* **56,** 2008–2011.