

Supporting Information

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Terpenes from the fresh stems of *Commiphora gileadensis* with antimicrobial activity

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| Table of Contents | Page |
|--|------|
| Characterization of diterpenes 1, 3-5. | 3 |
| Table S1: ¹ H NMR (500 MHz, CDCl ₃) spectrum of diterpenes 1, 3-5. | 3 |
| Table S2: ¹³ C NMR (125 MHz, CDCl ₃) spectrum of diterpenes 1, 3-5. | 4 |
| Figure S1: ¹ H NMR spectrum of 3. | 5 |
| Figure S2: ¹³ C NMR spectrum of 3. | 6 |
| Figure S3: DEPT135 spectrum of 3. | 7 |
| Figure S4: HSQC spectrum of 3. | 8 |
| Figure S5: HRESIMS spectrum of 3. | 9 |
| Figure S6: ¹ H NMR spectrum of 4. | 10 |
| Figure S7: ¹³ C NMR spectrum of 4. | 11 |
| Figure S8: DEPT135 spectrum of 4. | 12 |
| Figure S9: HSQC spectrum of 4. | 13 |
| Figure S10: HRESIMS spectrum of 4. | 14 |
| Figure S11: ¹ H NMR spectrum of 5. | 15 |
| Figure S12: ¹³ C NMR spectrum of 5. | 16 |
| Figure S13: DEPT135 spectrum of 5. | 17 |
| Figure S14: COSY spectrum of 5. | 18 |
| Figure S15: HSQC spectrum of 5. | 19 |
| Figure S16: HRESIMS spectrum of 5. | 20 |
| Figure S17: ¹ H NMR spectrum of 9. | 21 |

| | |
|---|----|
| Figure S18: ^{13}C NMR spectrum of 9 (Exp.). | 22 |
| Figure S19: ^{13}C NMR spectrum of 9 (Exp.). | 23 |
| Figure S20: DEPT135 spectrum of 9 . | 24 |
| Figure S21: COSY spectrum of 9 (Exp.). | 25 |
| Figure S22: COSY spectrum of 9 (Exp.). | 26 |
| Figure S23: HSQC spectrum of 9 . | 27 |
| Figure S24: HSQC spectrum of 9 (Exp.). | 28 |
| Figure S25: H2BC spectrum of 9 (Exp.). | 29 |
| Figure S26: H2BC spectrum of 9 (Exp.). | 30 |
| Figure S27: H2BC spectrum of 9 (Exp.). | 31 |
| Figure S28: H2BC spectrum of 9 (Exp.). | 32 |
| Figure S29: HMBC spectrum of 9 (Exp.). | 33 |
| Figure S30: HMBC spectrum of 9 (Exp.). | 34 |
| Figure S31: HMBC spectrum of 9 (Exp.). | 35 |
| Figure S32: HMBC spectrum of 9 (Exp.). | 36 |
| Figure S33: HRESIMS spectrum of 9 . | 37 |

(1*S*,3*E*,7*E*,11*R*)-(+)-*verticilla*-3,7,12(18)-*triene* (**1**): **C₂₀H₃₂**. Oily; $[\alpha]_D^{20} +152^\circ$ (*c* 0.63, CHCl₃). ¹H and ¹³C NMR: S1, S2. HRESIMS: *m/z* 269.2282 (*Cal.* 269.2269) [M⁺-3H], 268.2159 (*Cal.* 268.2191) [M⁺-4H] 267.2124 (*Cal.* 267.2113) [M⁺-5H].

(1*S*,14*S*)-*Ent*-13,14-*epoxyverticillol* (**3**): **C₂₀H₃₄O₂**. Colourless crystals; $[\alpha]_D^{20} -121^\circ$ (*c* 0.75, CHCl₃). ¹H and ¹³C NMR: Tables S1, S2. HRESIMS: *m/z* 289.2538 (*Cal.* 289.2531) [M⁺-OH].

(9*S*,10*S*)-*Ent*-9,10-*epoxyverticillol* (**4**): **C₂₀H₃₄O₂**. Colourless crystals; $[\alpha]_D^{20} -132^\circ$ (*c* 0.54, CHCl₃). ¹H and ¹³C NMR: S1, S2. HRESIMS: *m/z* 289.2541 (*Cal.* 289.2531) [M⁺-OH].

Ent-*Verticillol* (**5**): **C₂₀H₃₄O**. Amorphous solid; $[\alpha]_D^{20} +152^\circ$ (*c* 0.63, CHCl₃). ¹H and ¹³C NMR: Tables S1, S2. HRESIMS: *m/z* 273.2595 (M⁺-OH) (*Cal.* 273.2595), 271.2438 (M⁺-OH-2H) (*Cal.* 271.2426), 269.2280 (M⁺-OH-4H) (*Cal.* 269.2269).

Table S1 : ¹H NMR data of diterpenes **1, 3-5** (δ , *J* values in Hz).

| | 1 | 3 | 4 | 5 |
|-----------|-----------------------------------|----------------|--------------------------------|---------------------------|
| 2 | 1.40 m | 1.57 m | 1.47 m | 1.32 m |
| 3 | 1.60 m, 2.01 m | 1.68 m, 2.01 m | 1.67m, 2.00m | 1.50 m, 1.88 m |
| 4 | 2.24 m, 2.37 m | 1.72 m, 1.76 m | 1.67 m, 1.98 m | 1.59 m, 1.75 m |
| 6 | 2.83 bd (13.0) | 1.79 m | 2.26 m, 2.21 d (9.2) | 2.13 m |
| 7 | 1.24, 1.40 m | 1.35 m, 1.58 m | 1.55 m | 1.20 bd (13.4), 1.37 m |
| 8 | 1.76 td (13.0, 2.8), 1.93 m | 2.13 m, 2.24 m | 1.68 m, 2.01 m | 1.98 m, 2.13 m |
| 10 | 4.64 d (11.0) | 5.03 d (10.6) | 2.95 d (9.9) | 4.80 d (11.4) |
| 11 | 1.96 m, 2.37 m | 2.13 m, 2.32 m | 1.66m, 1.96 m | 1.98 m, 2.29 bq (11.8) |
| 12 | 1.99 m, 2.15 bd (11.2) | 1.24 m, 2.13 m | 1.97 bd (13.8), 2.15 bt (13.8) | 1.98 m, 2.13 m |
| 14 | 5.55 d (12.6) | 3.45 d (9.5) | 5.90 d (12.4) | 5.56 d (12.4) |
| 15 | 1.92 d (12.8), 2.66 td (2.9,12.8) | 1.82 m | 1.88m, 2.73 td (5.9, 14.0) | 1.75 m, 2.60 td (6, 13.8) |
| 16 | 0.79 s | 0.76 s | 0.96 s | 0.69 s |
| 17 | 0.67 s | 0.86 s | 0.80 | 0.62 s |
| 18 | 4.47 d (1.6), 4.74 d (1.6) | 1.30 s | 1.27 | 1.16 s |
| 19 | 1.49 s | 1.61 s | 1.26 | 1.44 s |
| 20 | 1.53 s | 1.26 | 1.62 | 1.41 s |

Table S2 : ^{13}C NMR data of diterpenes **1, 3-5**.

| | 1 | 3 | 4 | 5 |
|-----------|----------|----------|----------|----------|
| 1 | 37.68 | 36.85 | 37.36 | 37.10 |
| 2 | 44.78 | 42.88 | 43.83 | 43.32 |
| 3 | 30.26 | 28.27 | 28.12 | 28.77 |
| 4 | 36.09 | 41.08 | 41.35 | 41.24 |
| 5 | 149.61 | 75.46 | 75.49 | 75.79 |
| 6 | 42.60 | 46.15 | 45.21 | 44.76 |
| 7 | 19.45 | 21.74 | 21.10 | 20.76 |
| 8 | 37.70 | 40.44 | 39.72 | 41.06 |
| 9 | 133.90 | 133.89 | 62.24 | 133.23 |
| 10 | 128.37 | 129.63 | 66.37 | 129.88 |
| 11 | 26.40 | 24.39 | 26.28 | 26.03 |
| 12 | 41.29 | 40.50 | 38.72 | 41.16 |
| 13 | 132.90 | 63.60 | 133.14 | 132.90 |
| 14 | 127.37 | 64.32 | 127.97 | 127.67 |
| 15 | 33.52 | 34.90 | 33.56 | 34.08 |
| 16 | 27.33 | 28.93 | 29.44 | 27.92 |
| 17 | 24.46 | 25.62 | 24.78 | 26.57 |
| 18 | 105.27 | 24.50 | 24.88 | 24.04 |
| 19 | 15.60 | 16.46 | 16.58 | 15.92 |
| 20 | 15.00 | 15.84 | 15.20 | 15.21 |

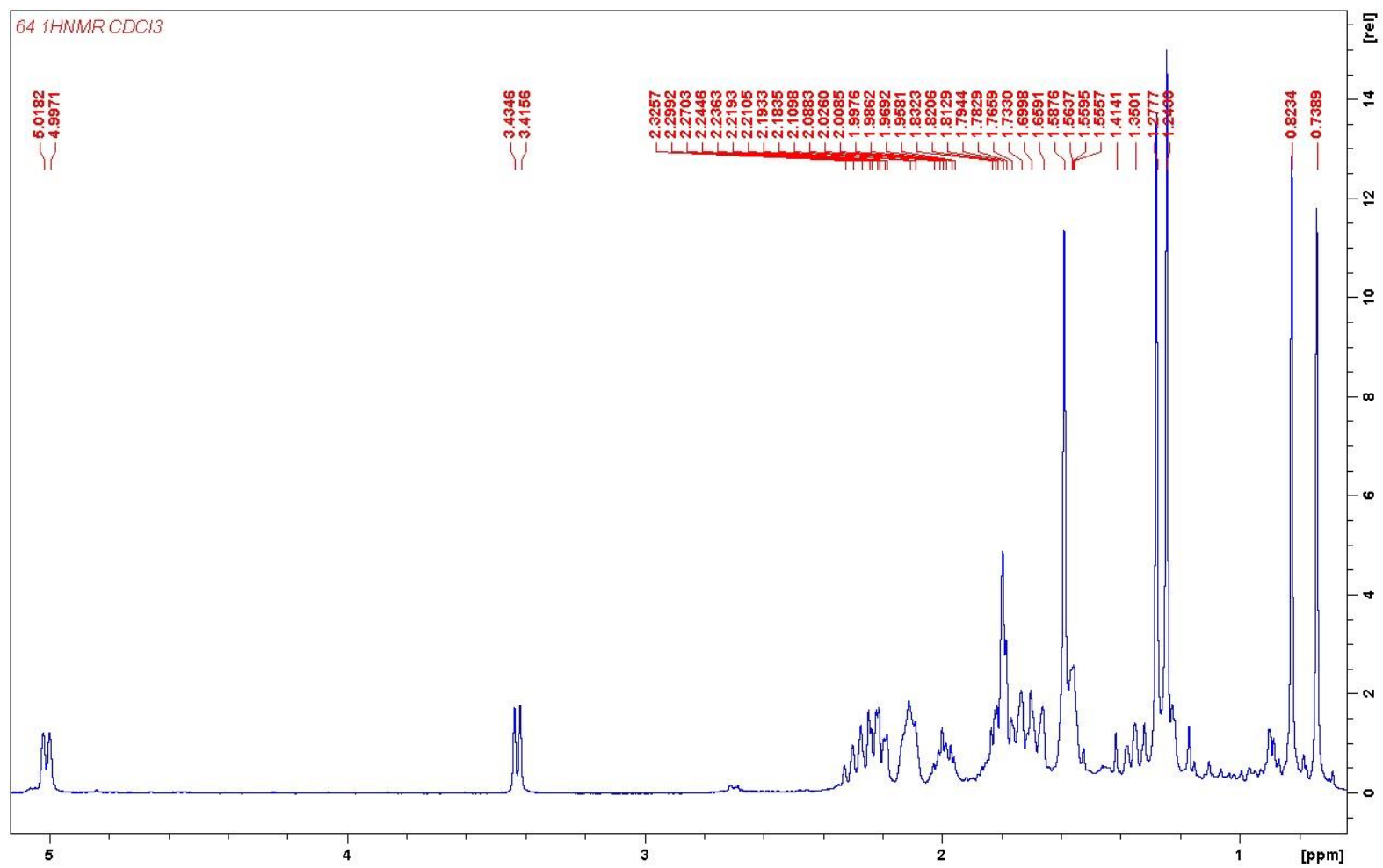


Figure S1: ¹H NMR spectrum of **3**.

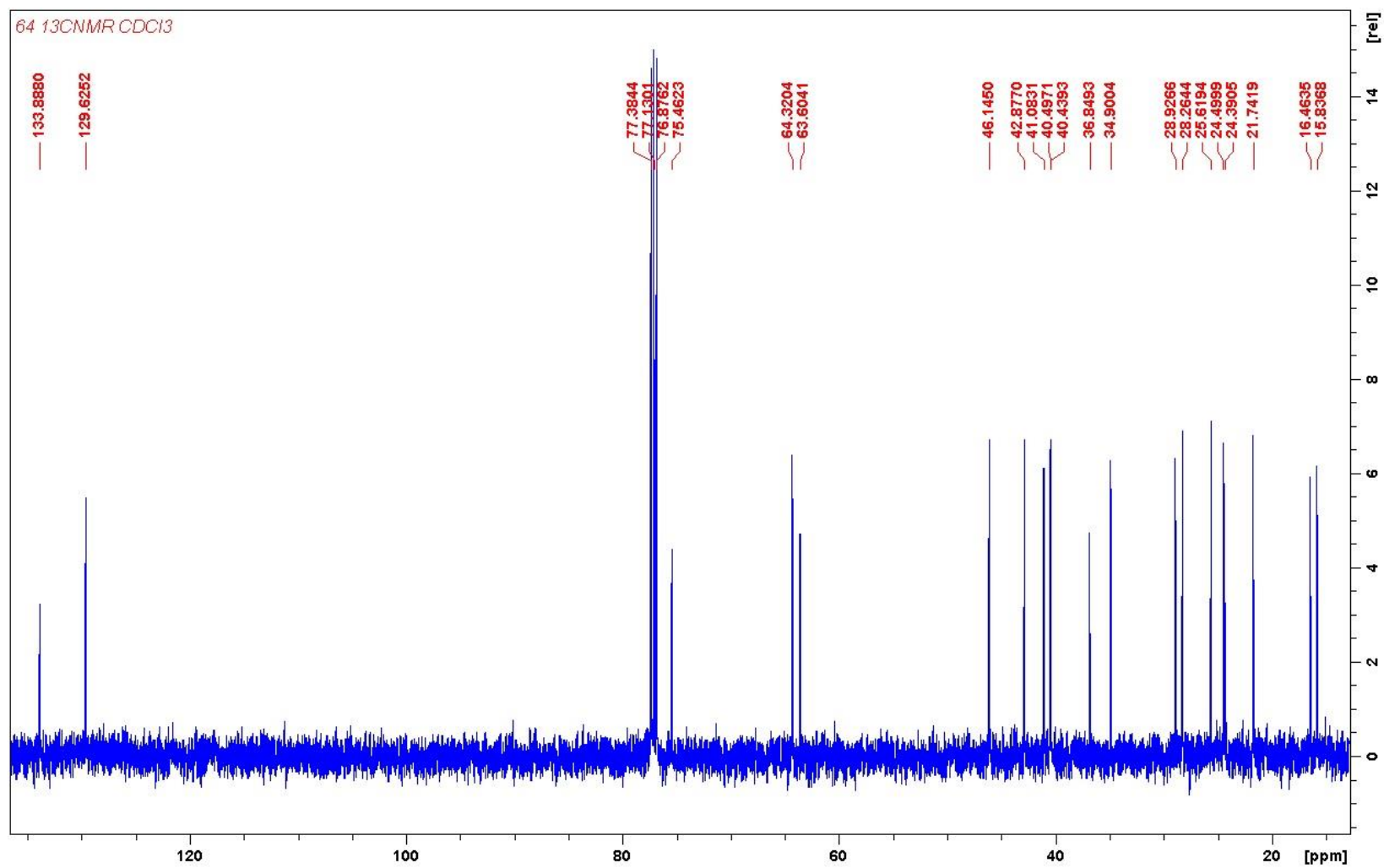


Figure S2: ¹³C NMR spectrum of **3**.

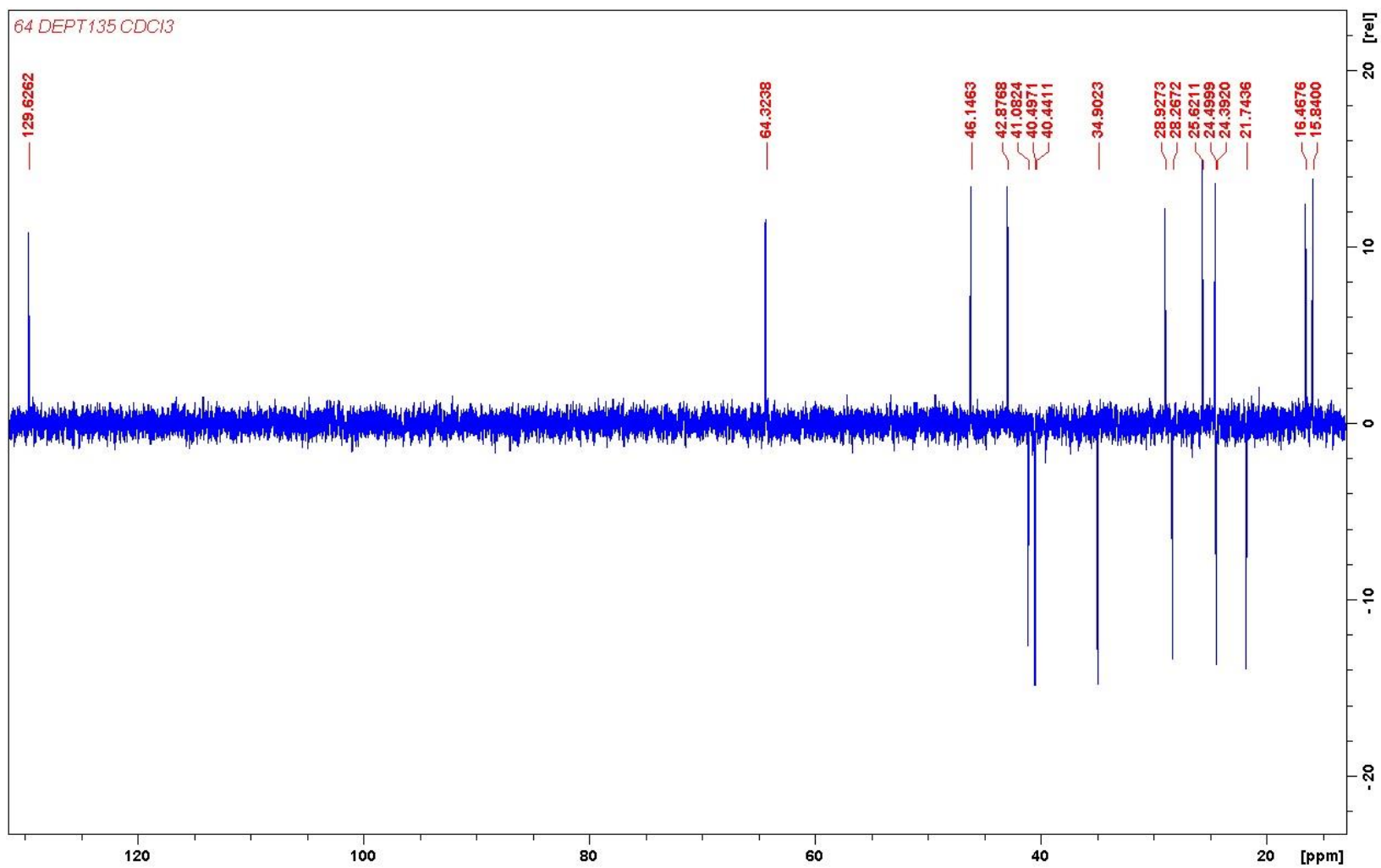


Figure S3: DEPT 135 spectrum of **3**.

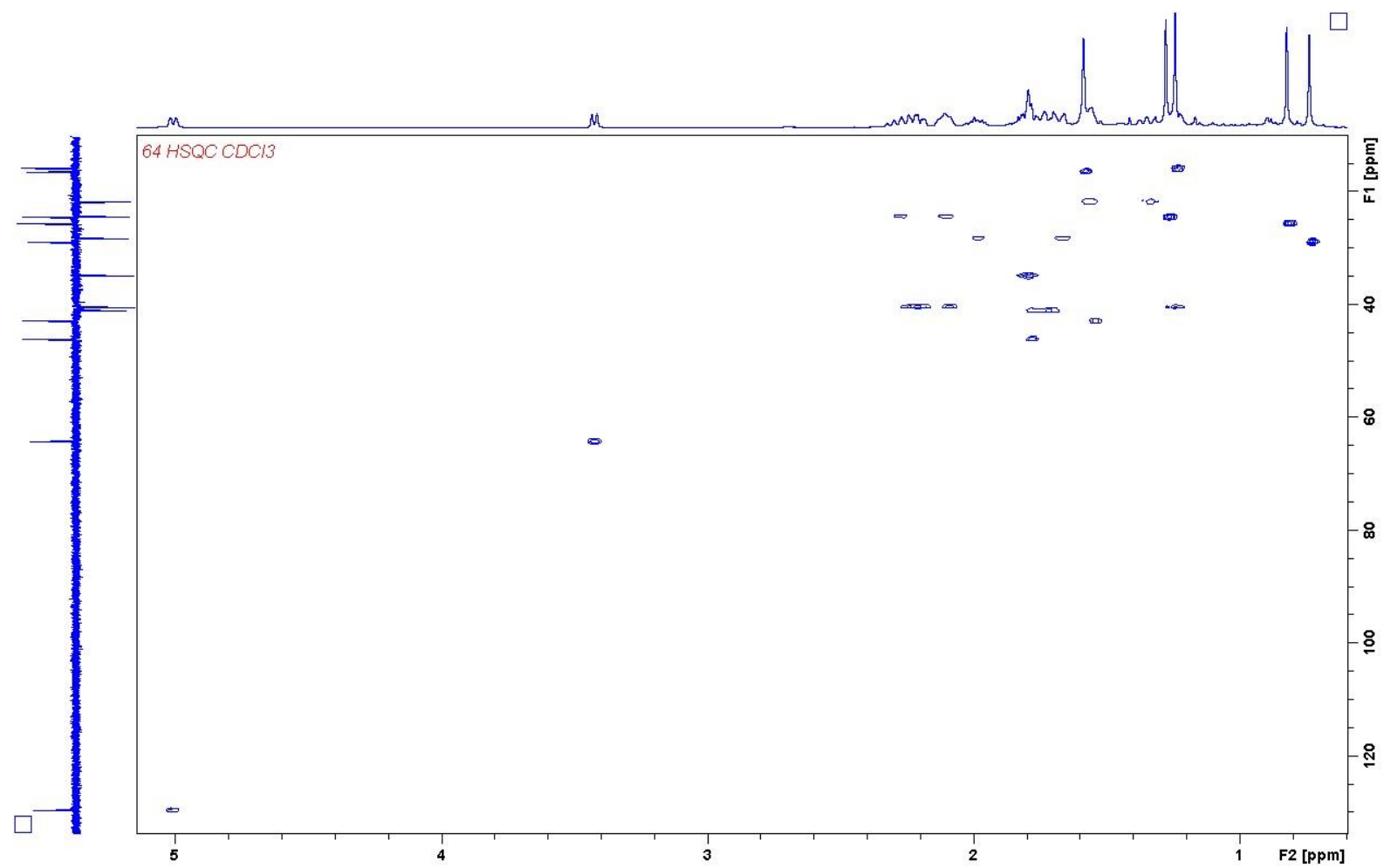


Figure S4: HSQC spectrum of **3**.

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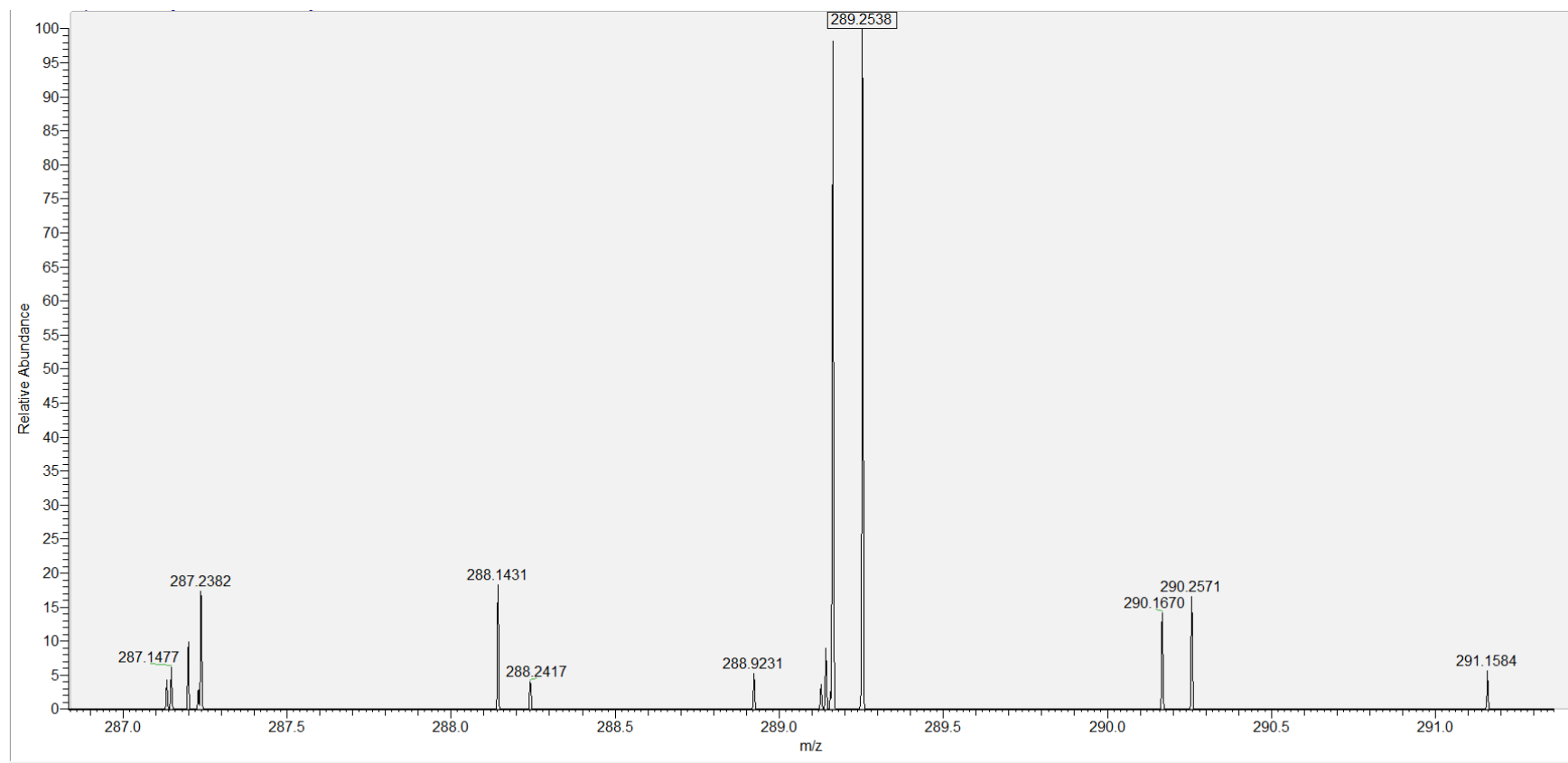


Figure S5: HRESIMS spectrum of 3.

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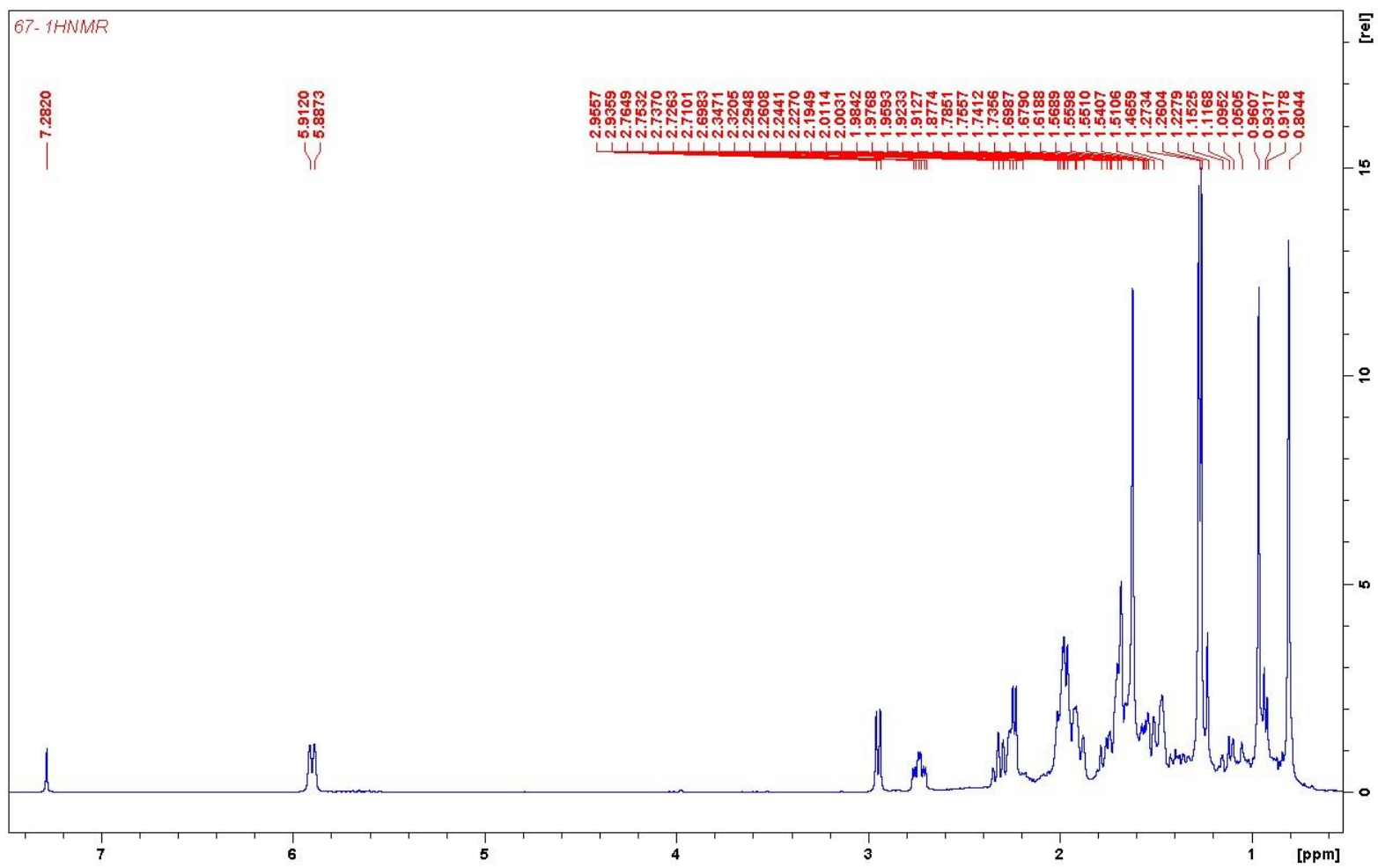


Figure S6: ¹H NMR spectrum of **4**.

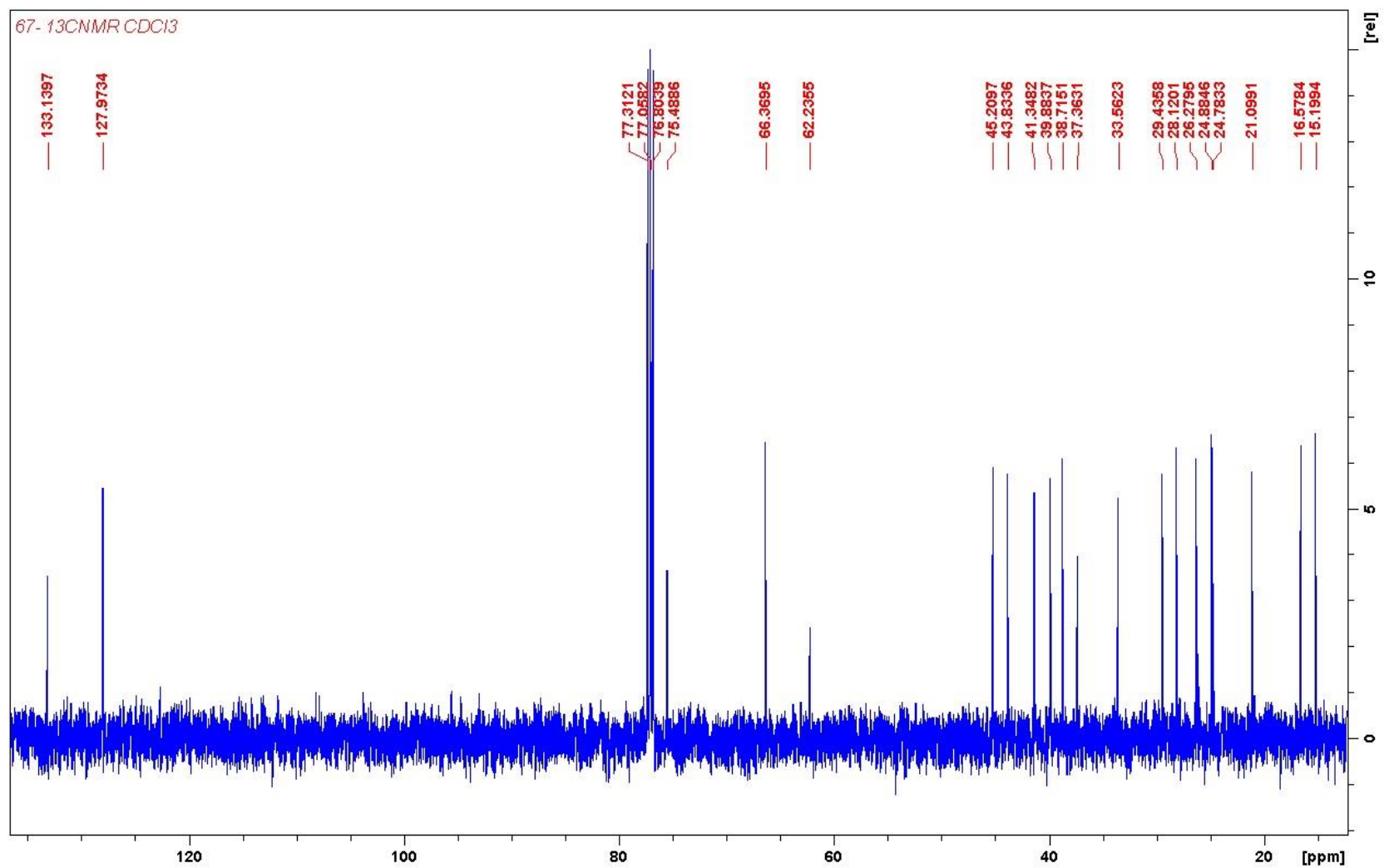


Figure S7: ¹³C NMR spectrum of **4**.

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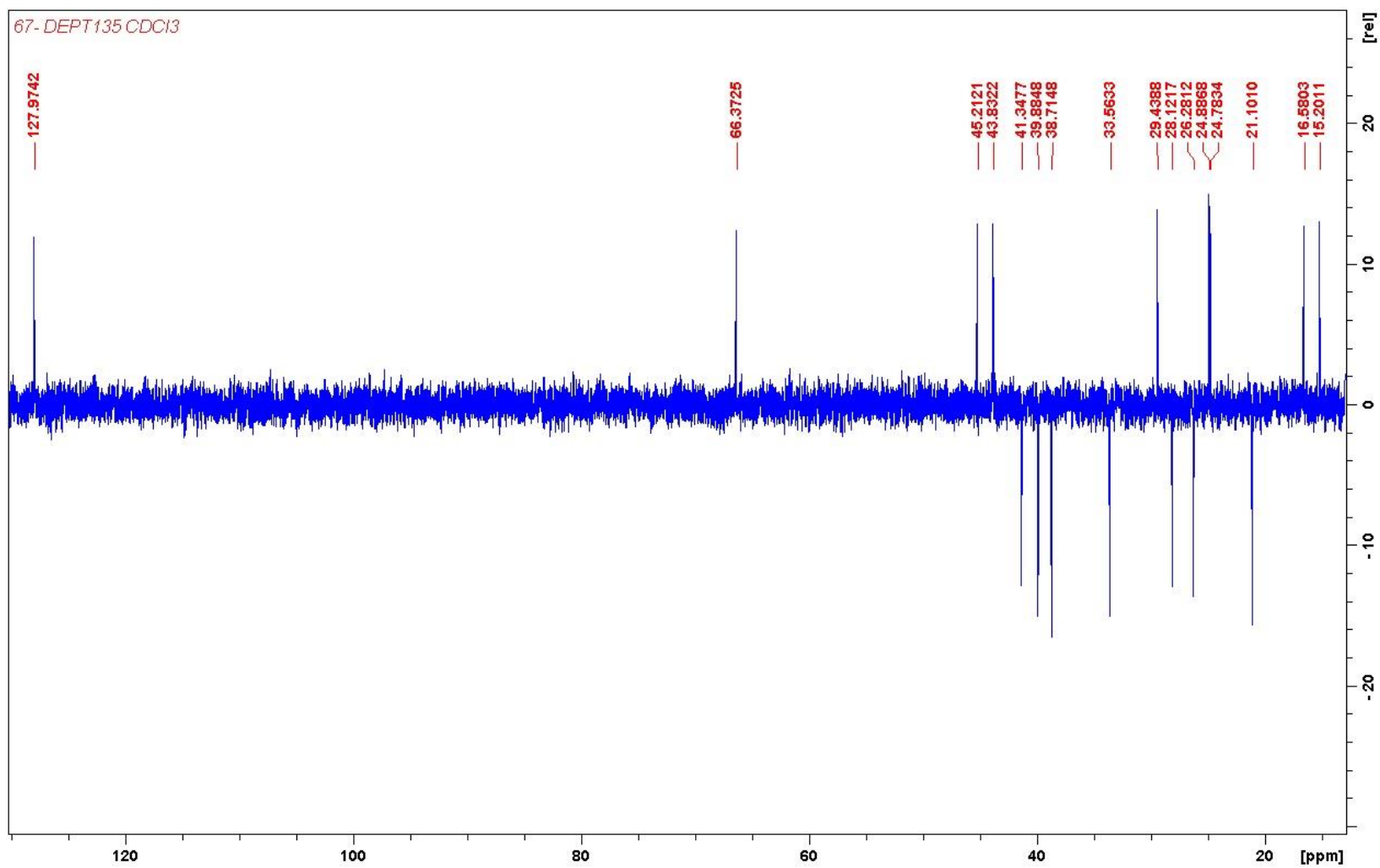


Figure S8: DEPT135 spectrum of **4**.

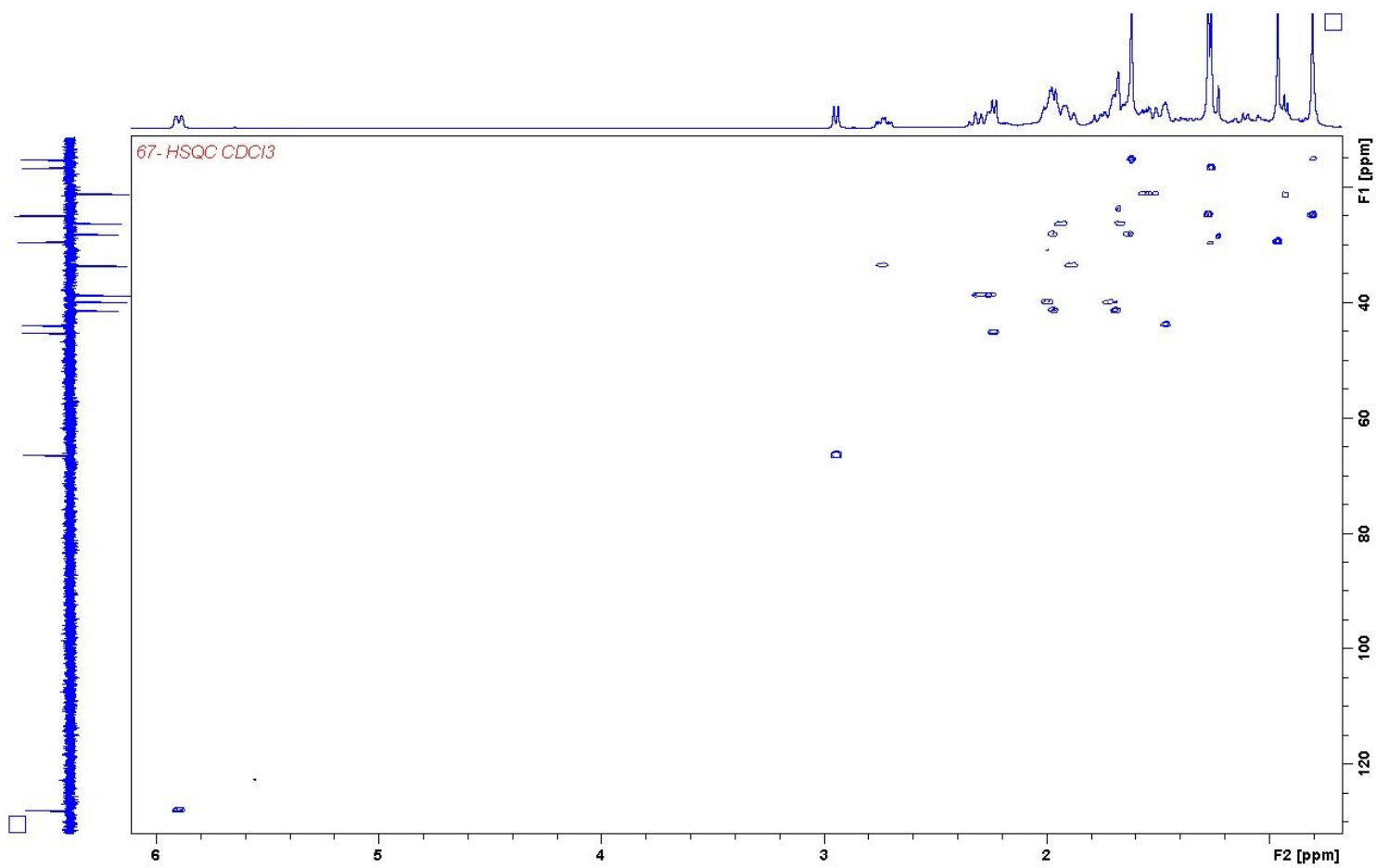


Figure S9: HSQC spectrum of **4**.

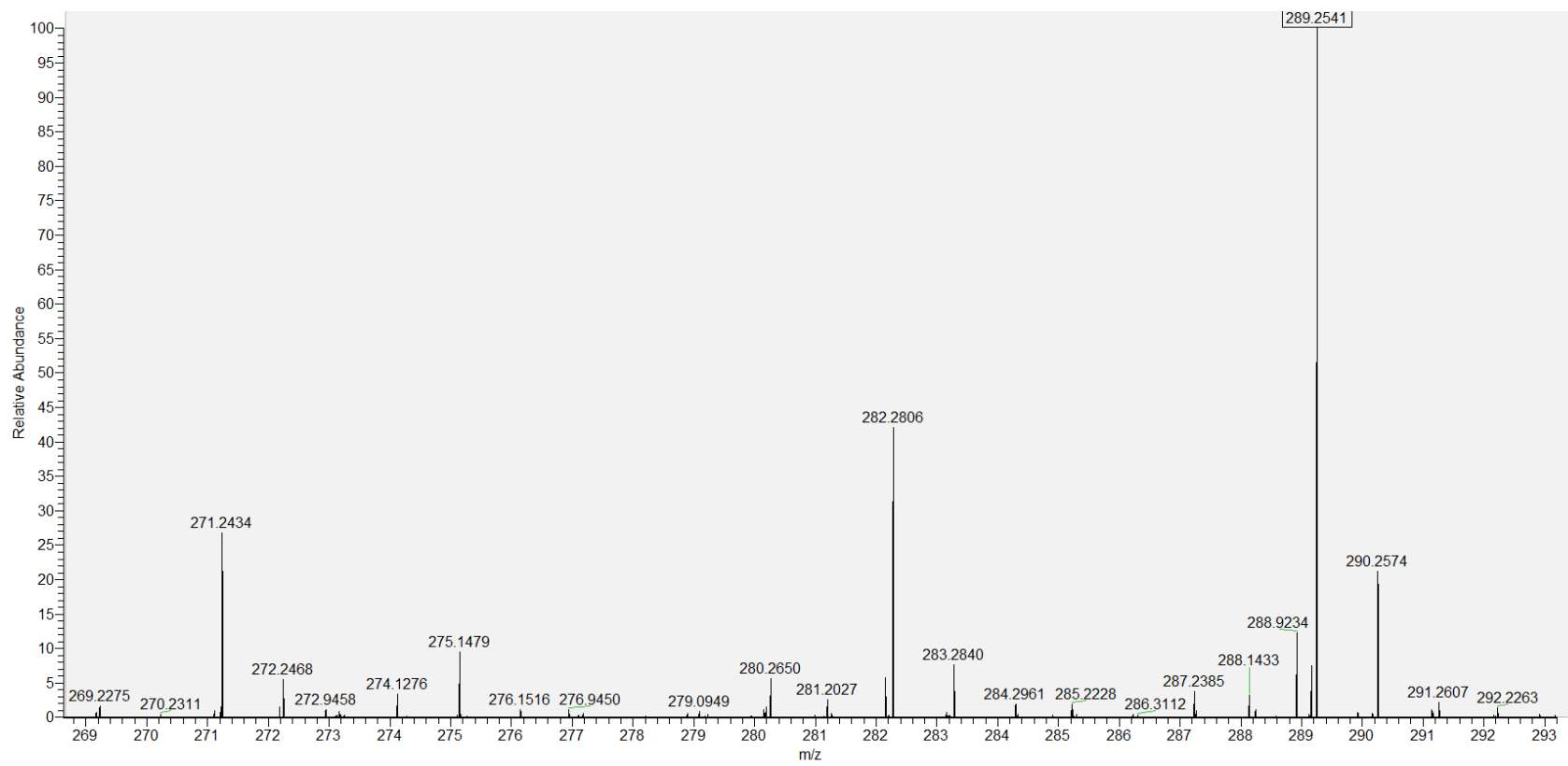


Figure S10: HRESIMS spectrum of 4.

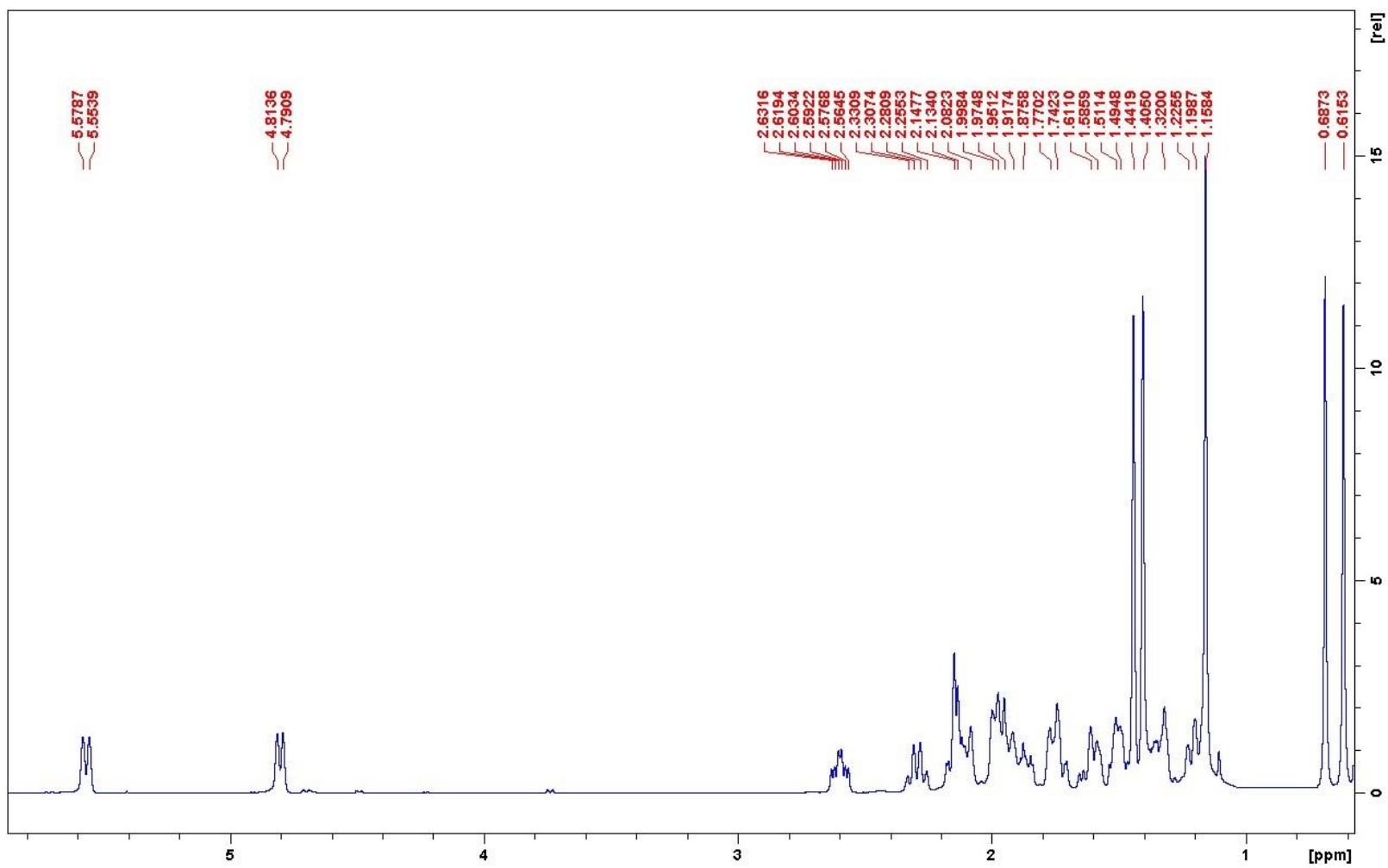


Figure S11: ^1H NMR spectrum of **5**.

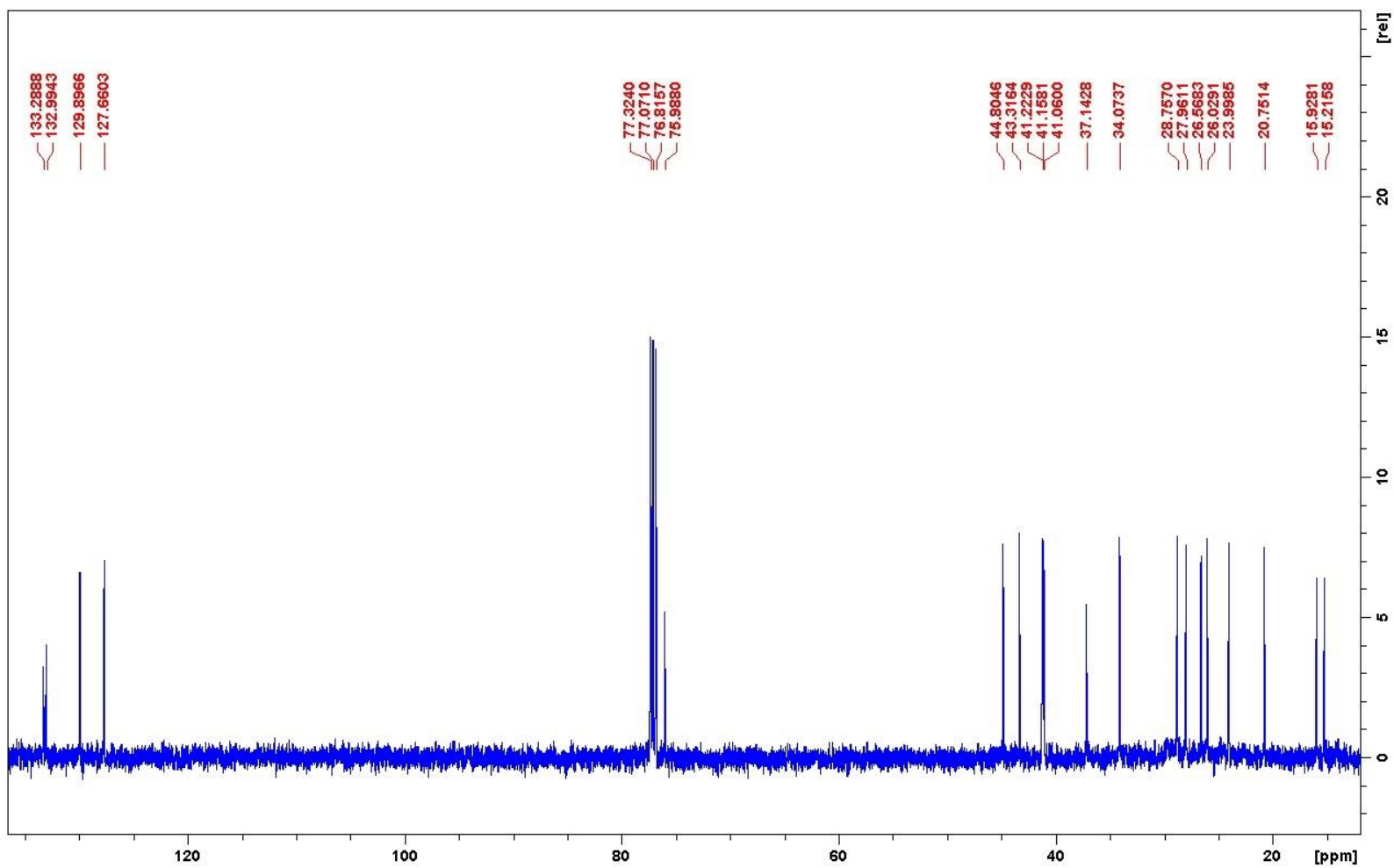


Figure S12: ^{13}C NMR spectrum of 5.

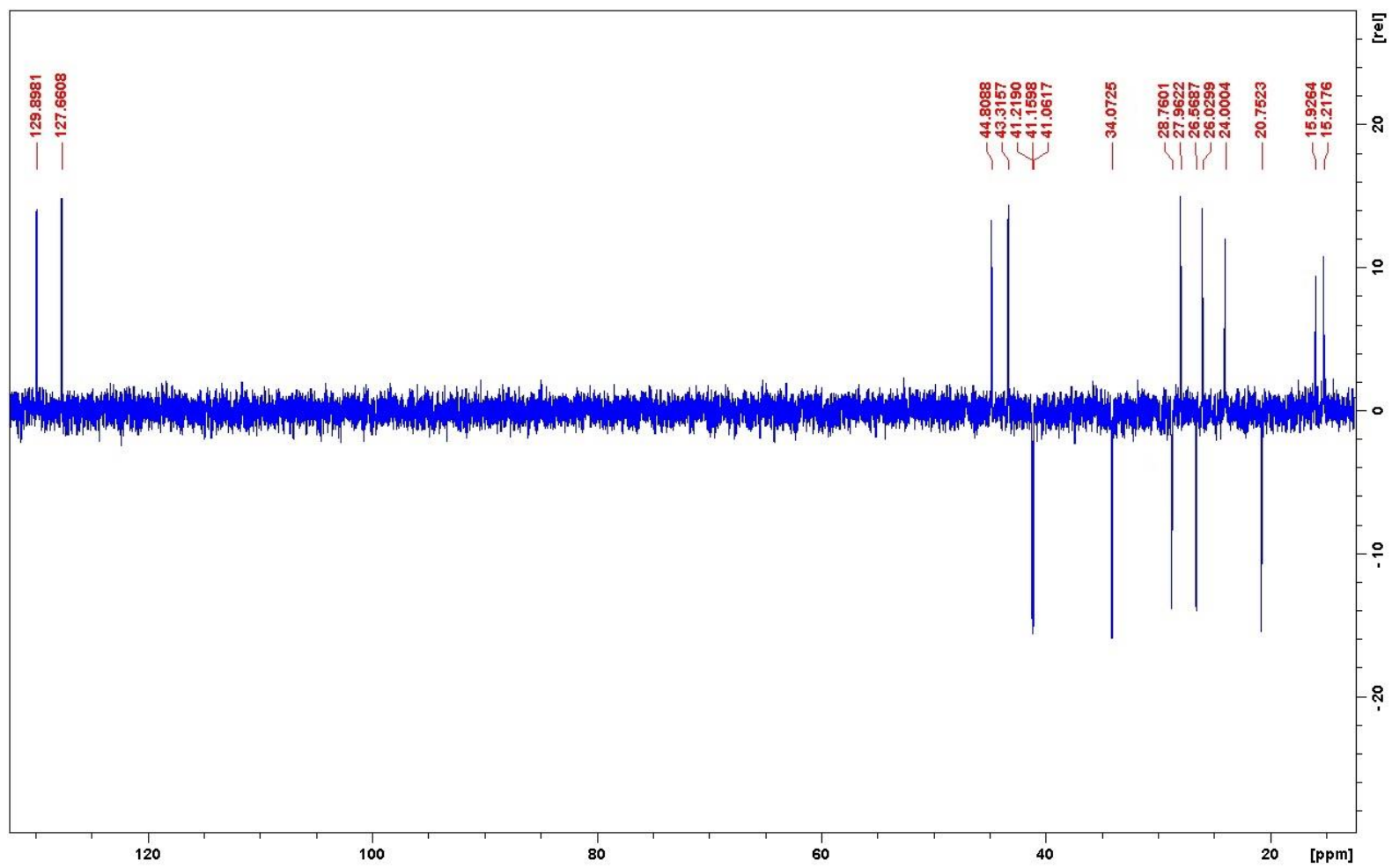


Figure S13: DEPT135 spectrum of **5**.

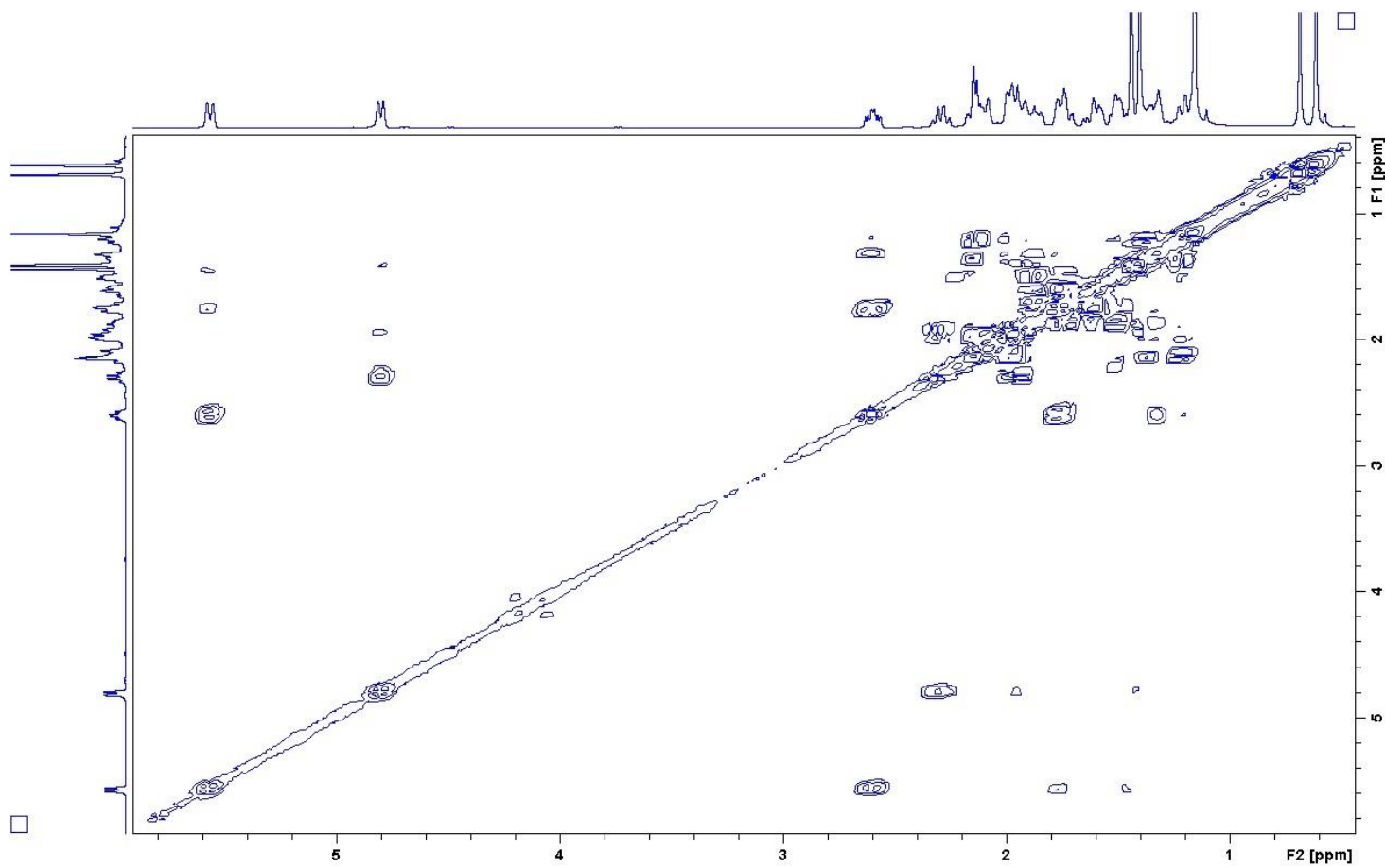


Figure S14: COSY spectrum of **5**.

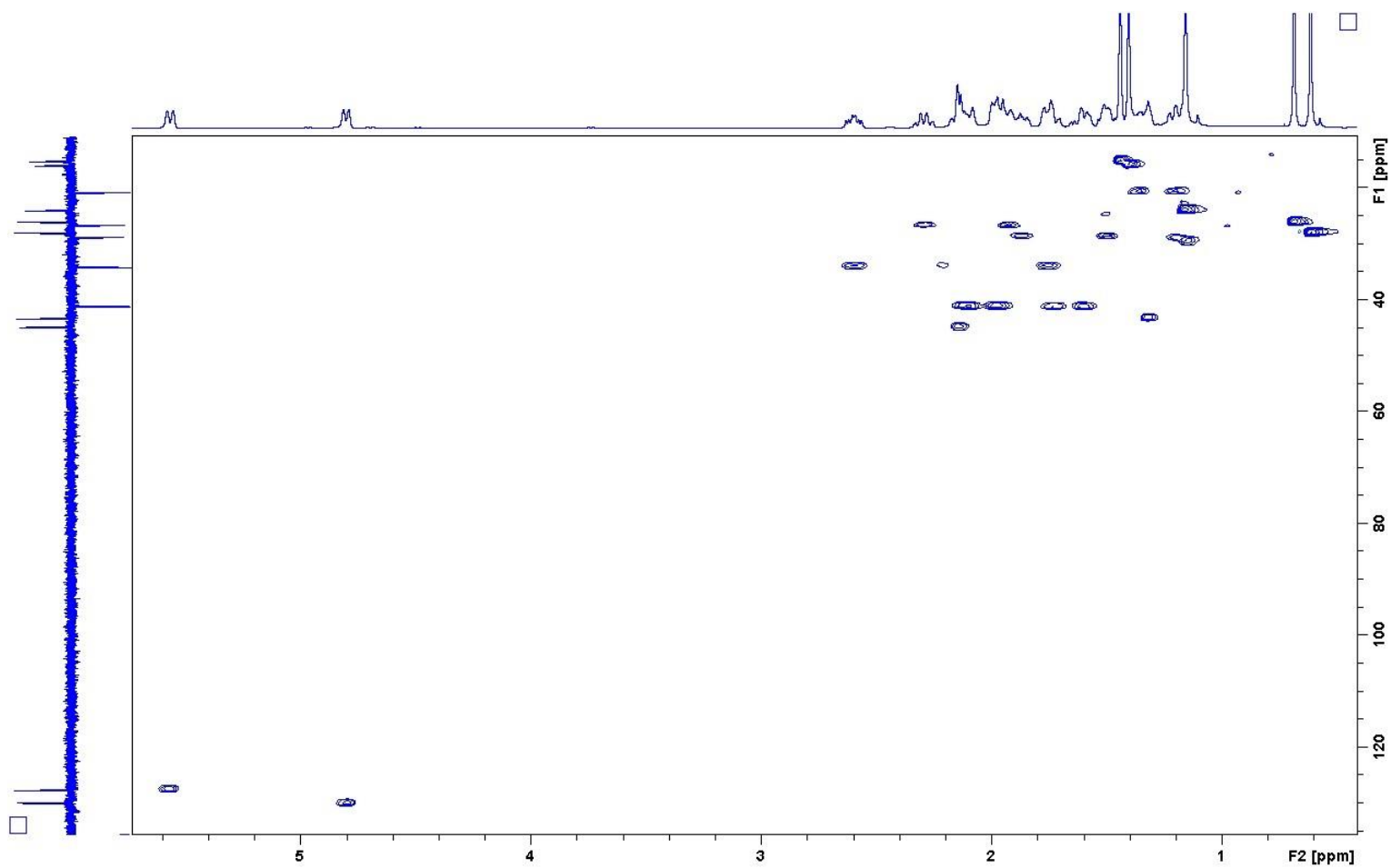


Figure S15: HSQC spectrum of **5**.

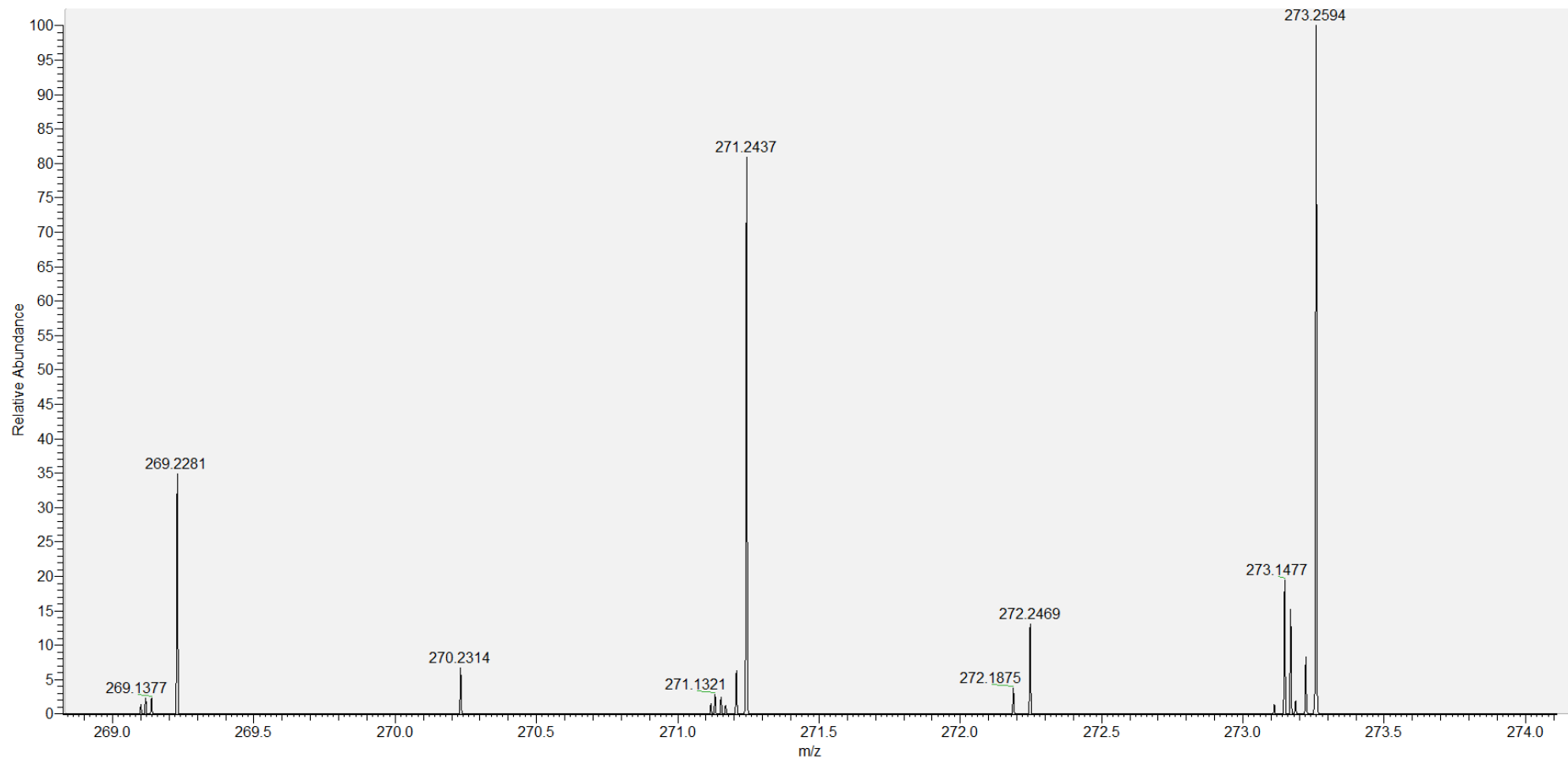


Figure S16: HRESIMS spectrum of **5**.

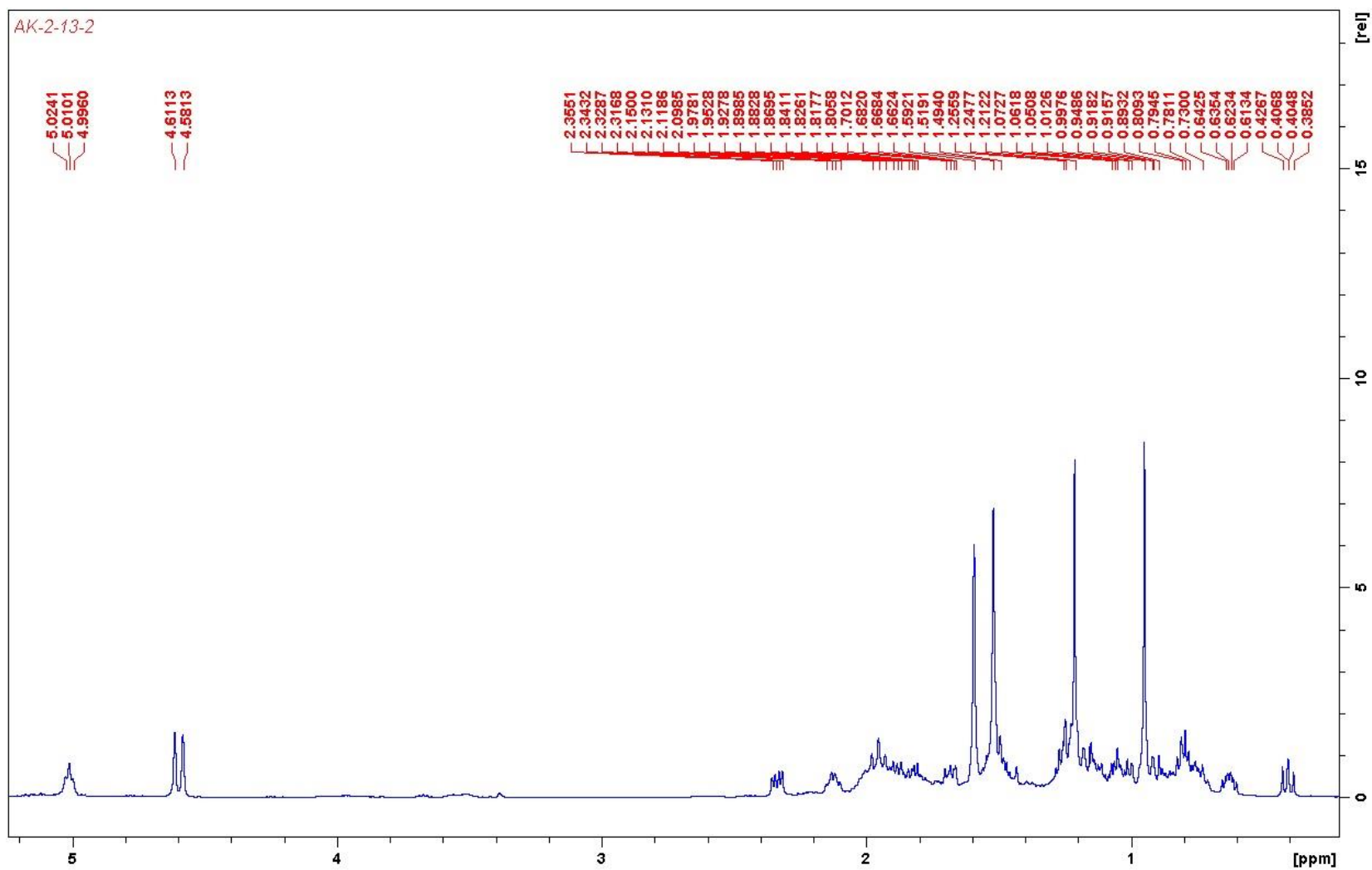


Figure S17: ^1H NMR spectrum of **9**.

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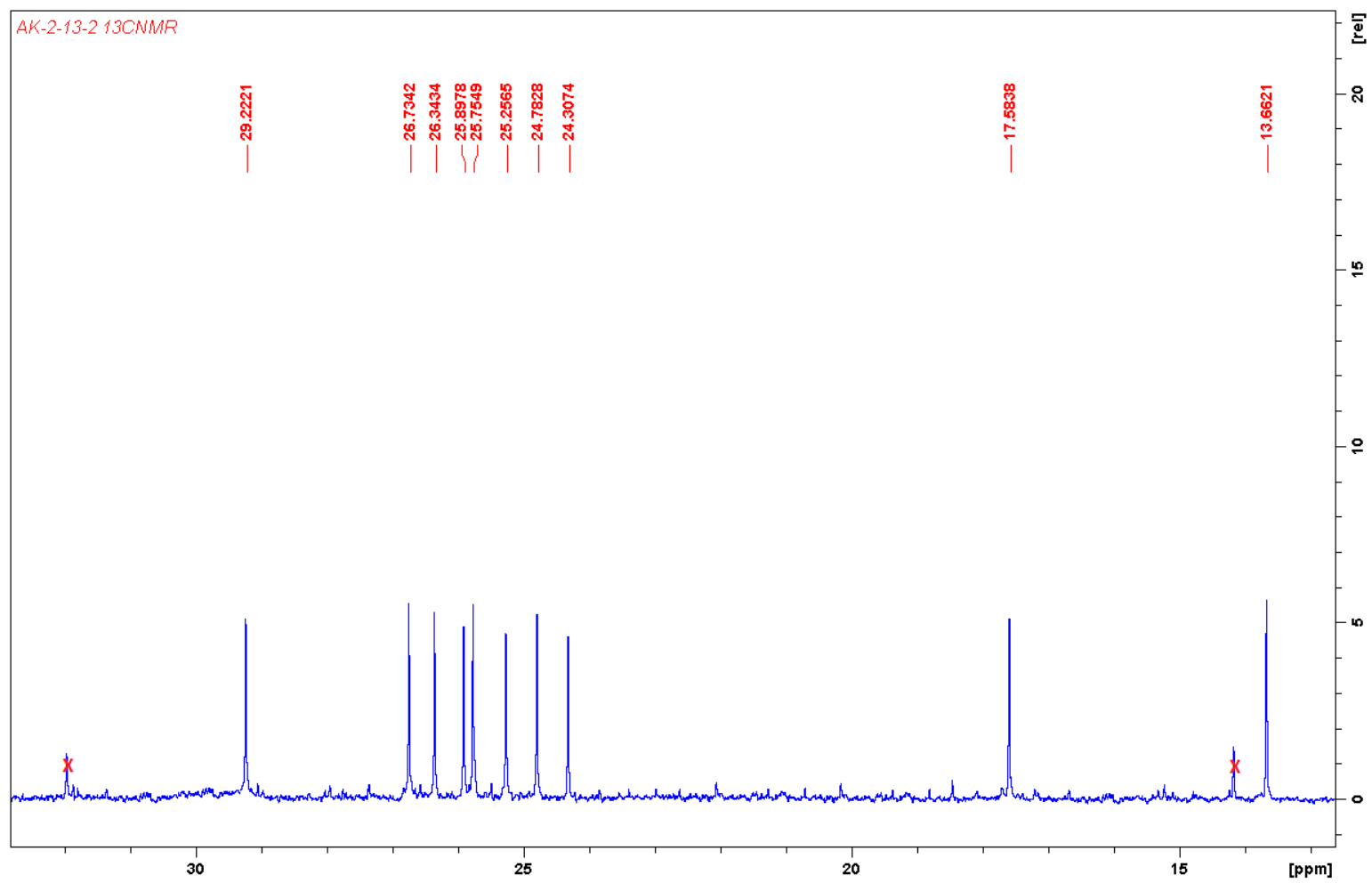


Figure S18: ¹³C NMR spectrum of **9** (Exp.).

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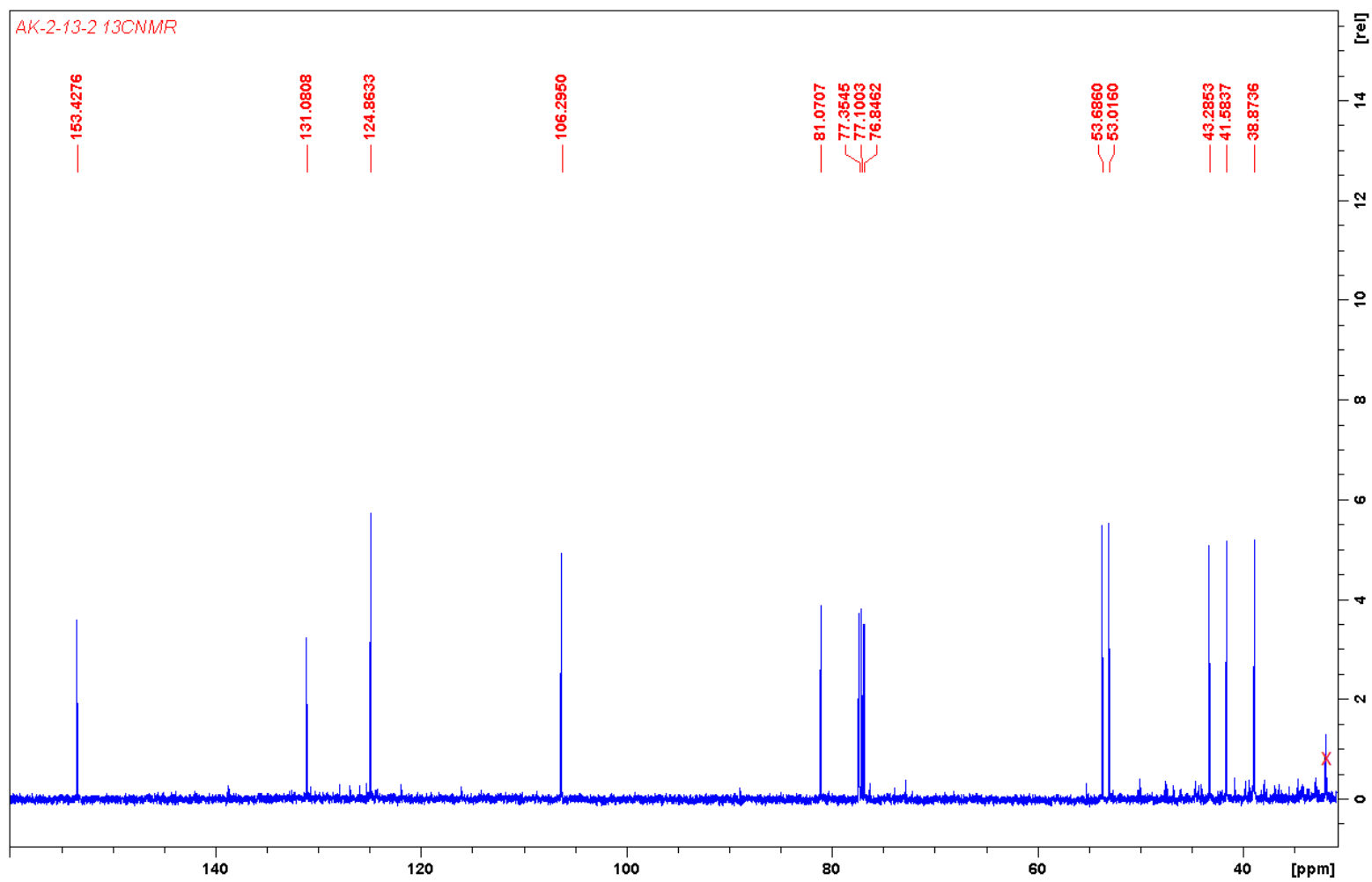


Figure S19: ¹³C NMR spectrum of **9** (Exp.).

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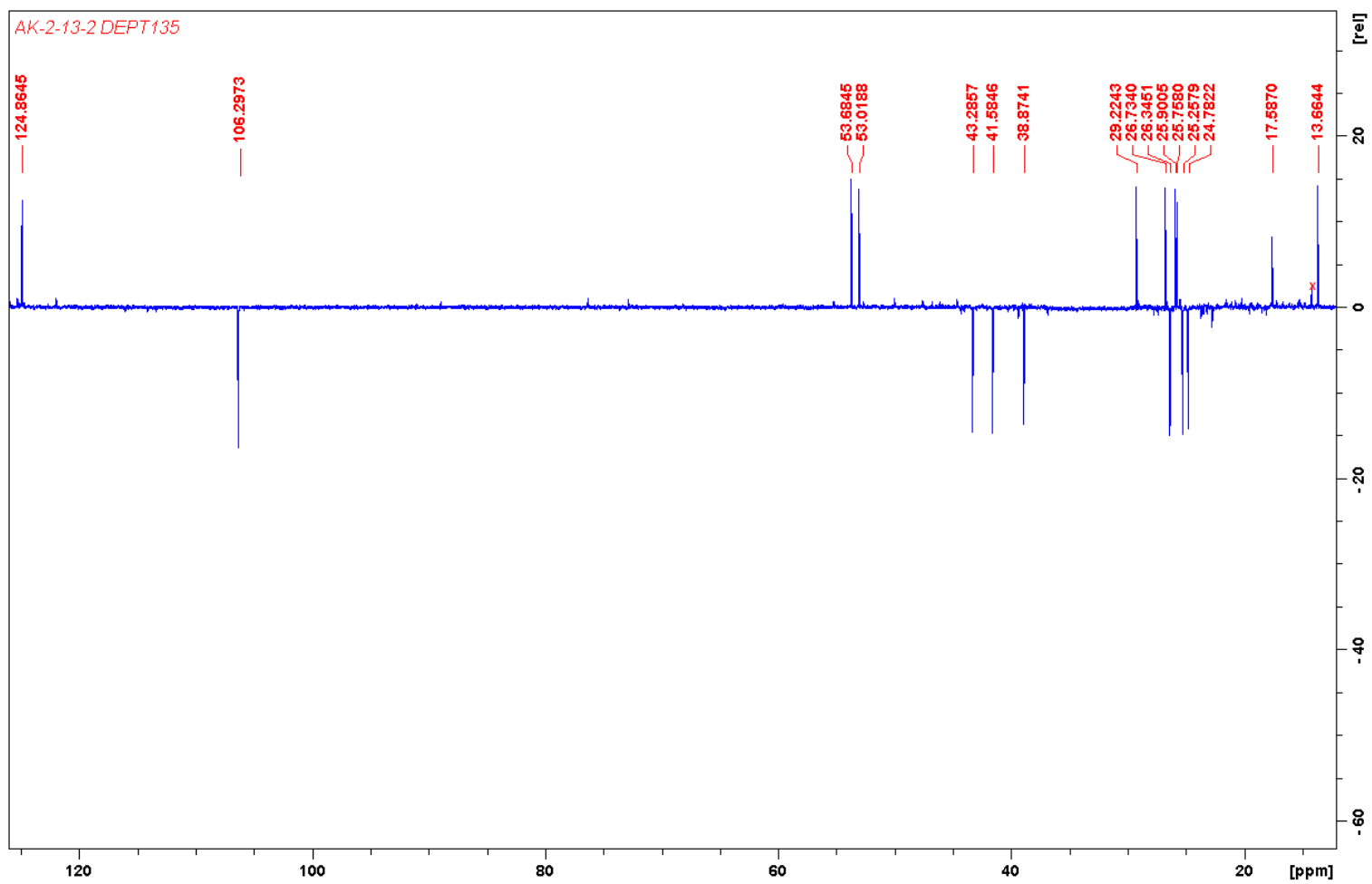


Figure S20: DEPT135 spectrum of **9**.

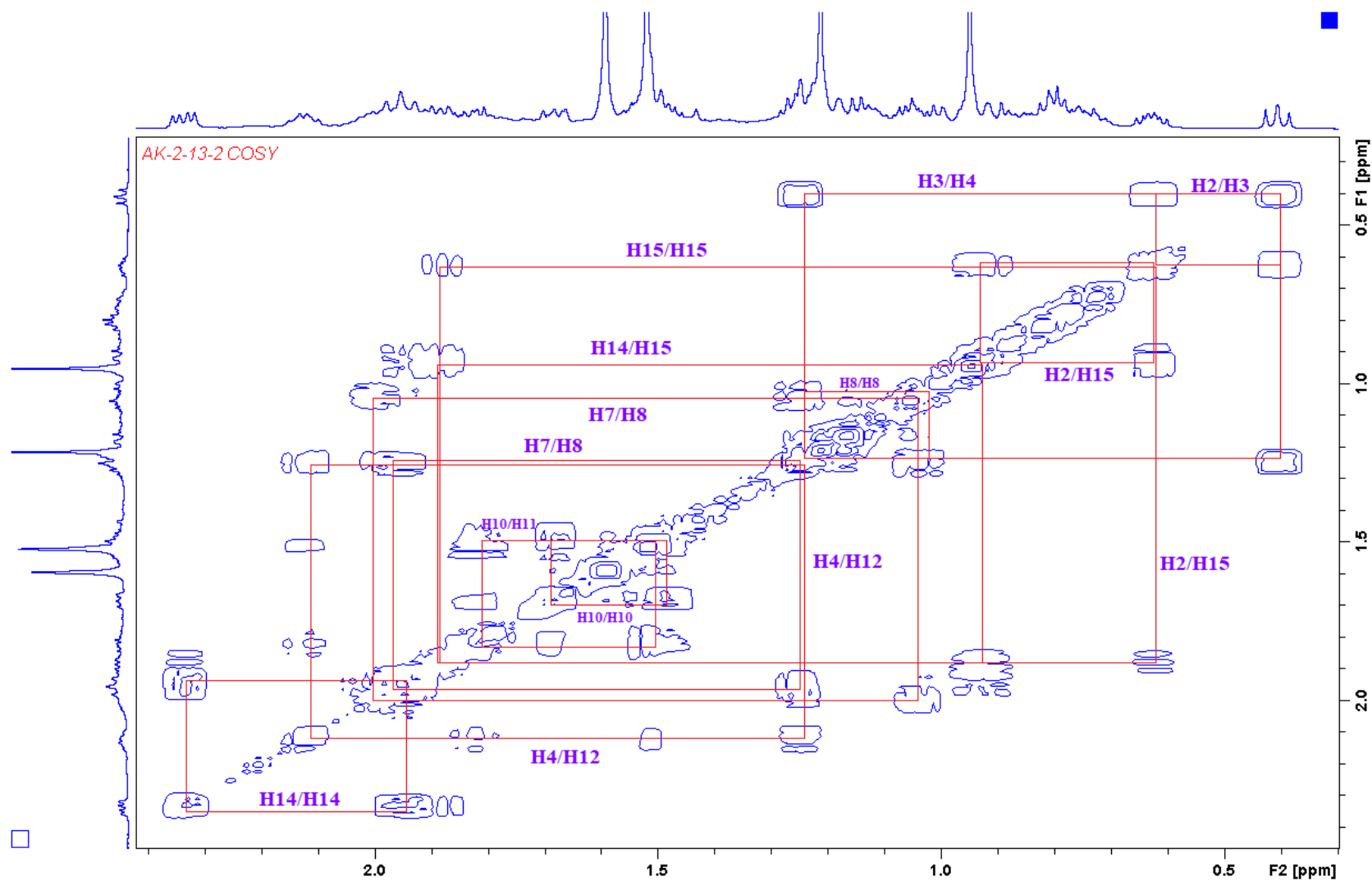


Figure S21: COSY spectrum of **9** (Exp.).

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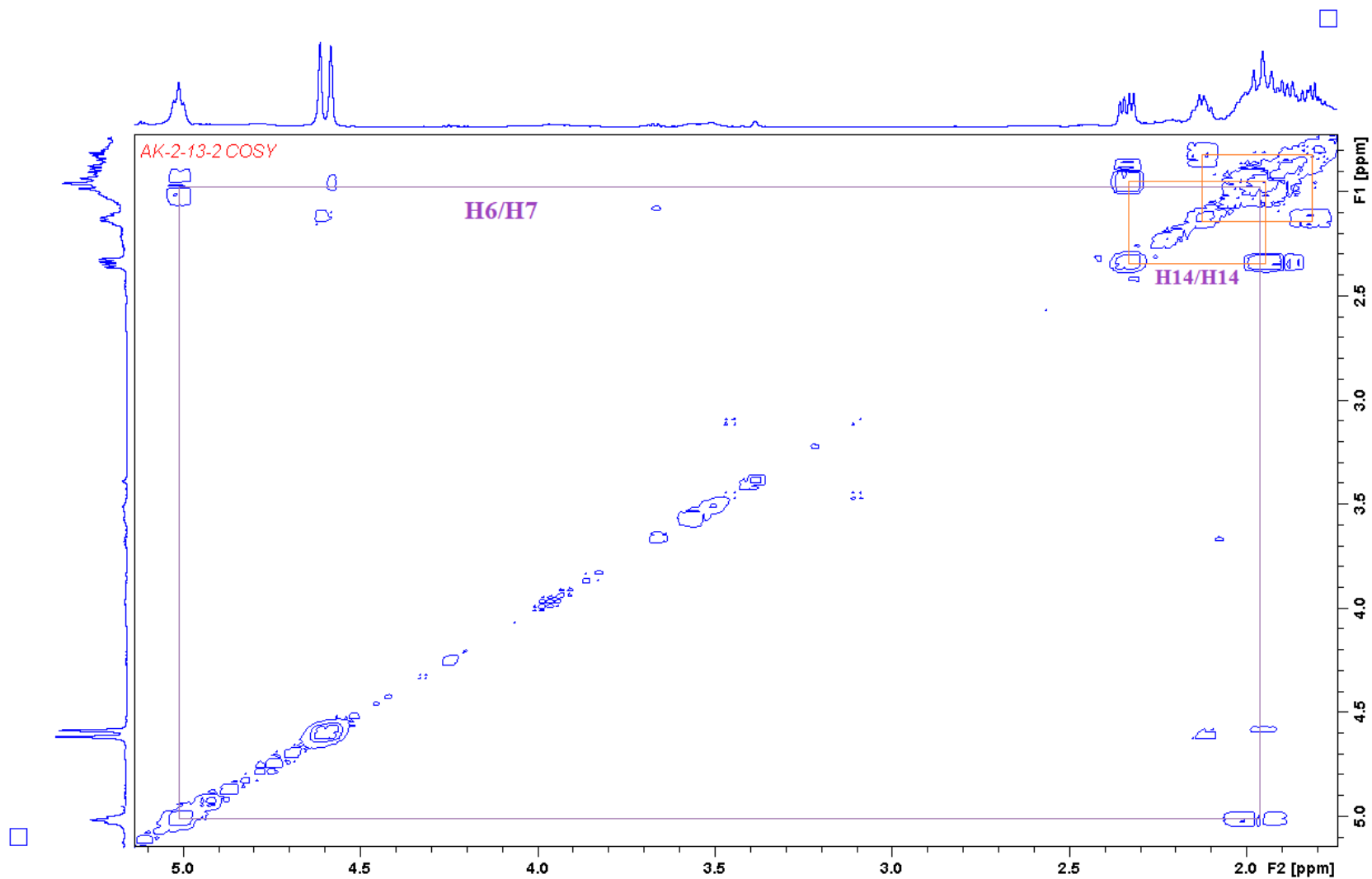


Figure S22: COSY spectrum of **9** (Exp.).

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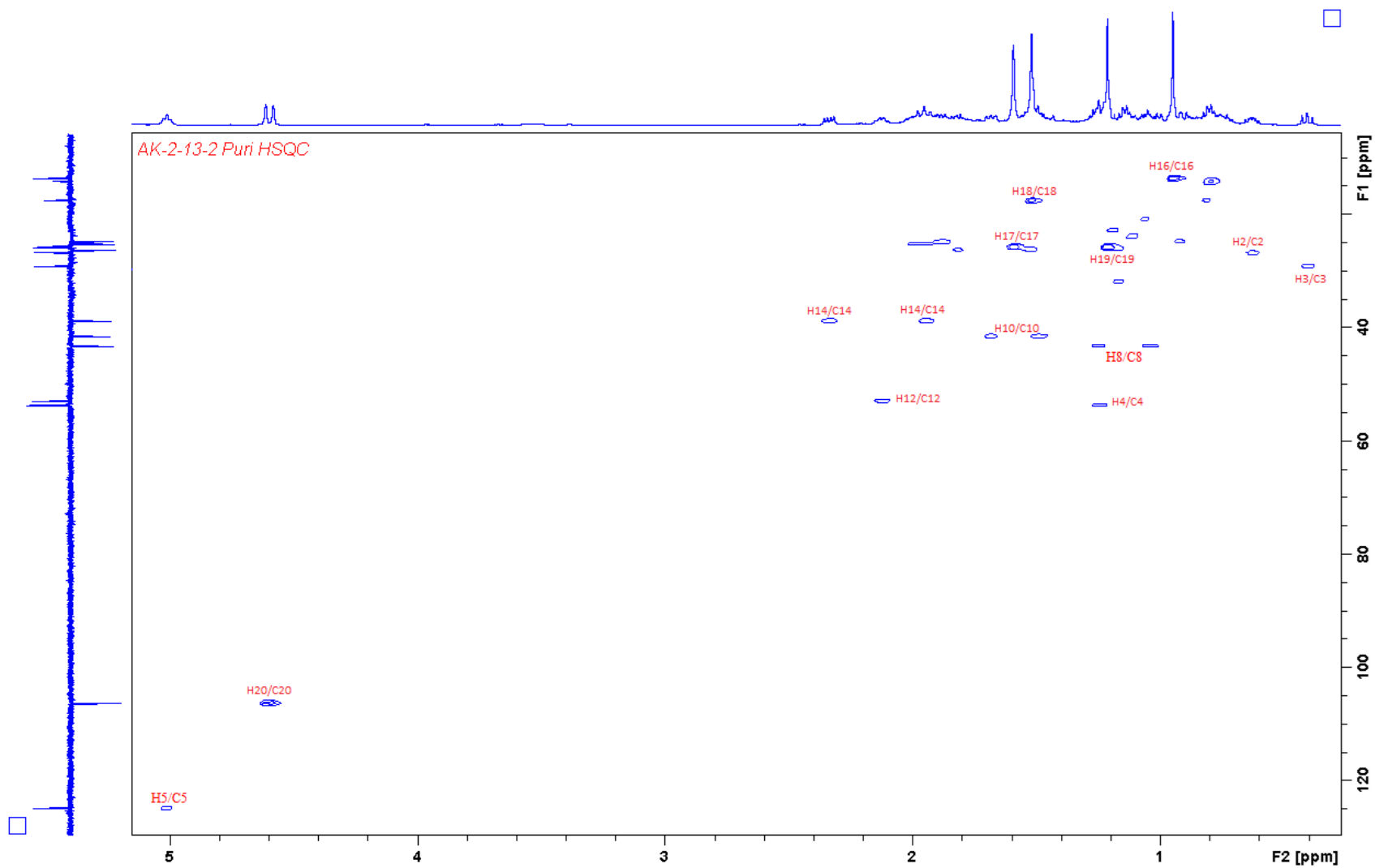


Figure S23: HSQC spectrum of **9**.

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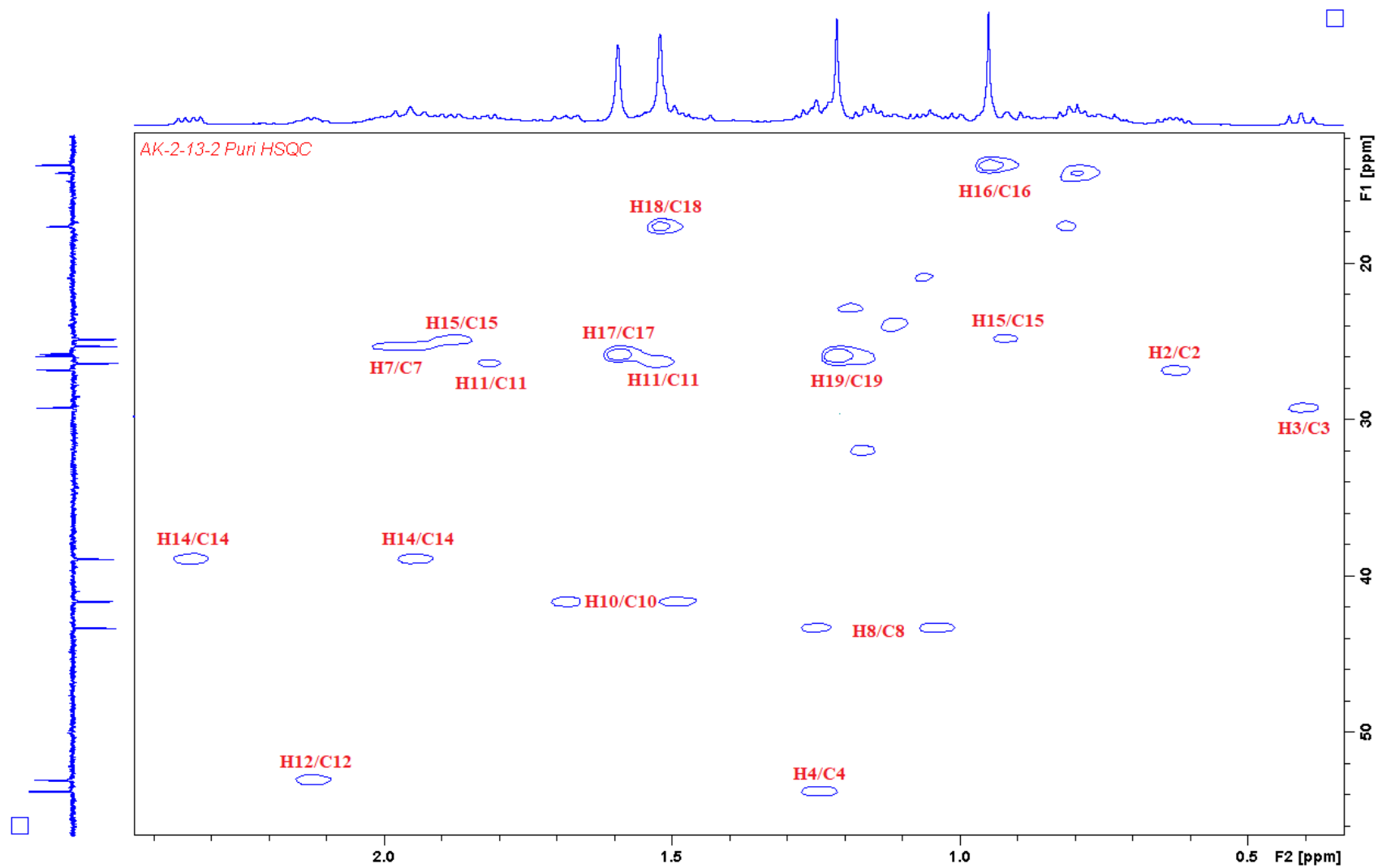


Figure S24: HSQC spectrum of **9** (Exp.).

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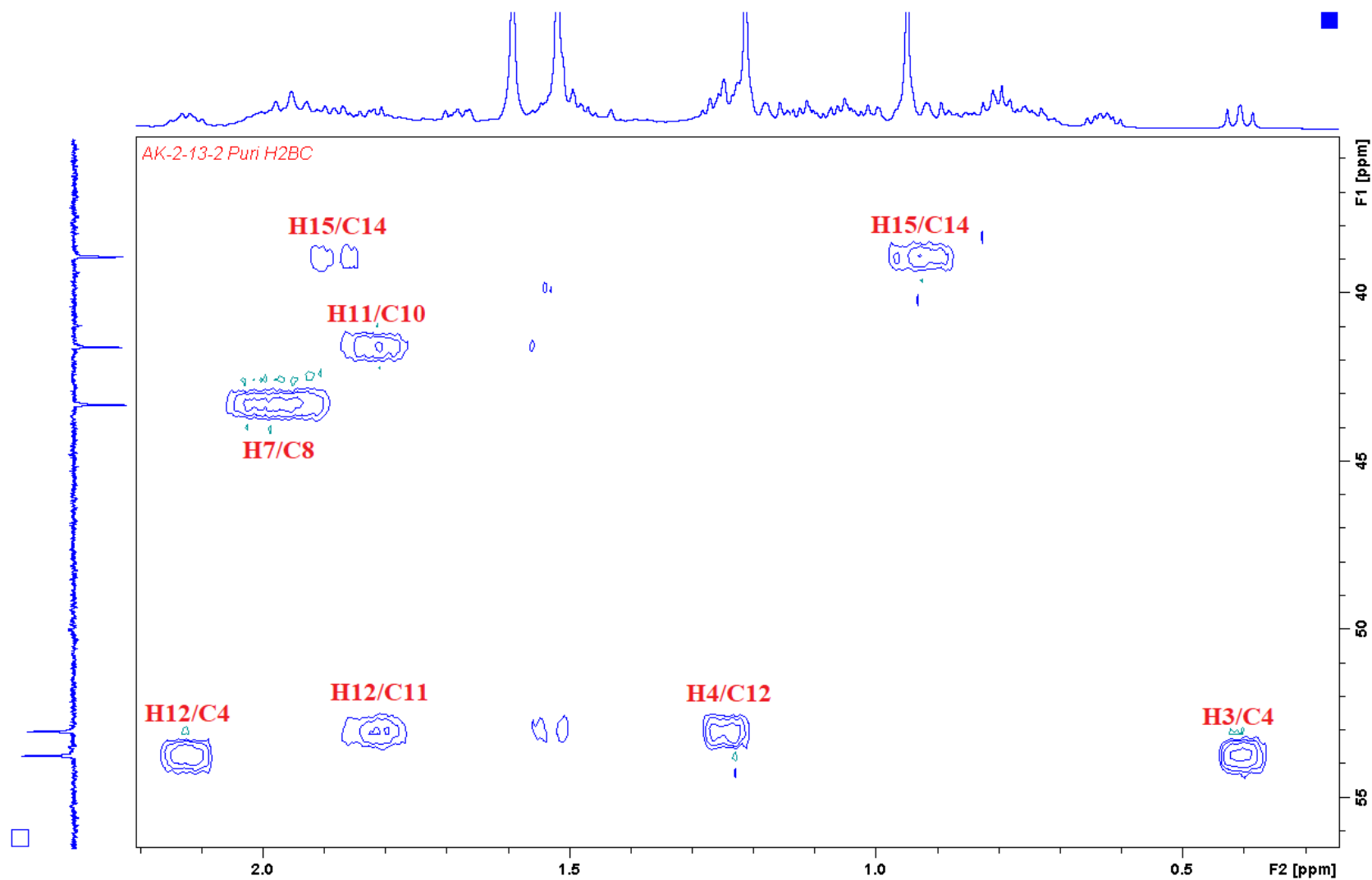


Figure S25: H2BC spectrum of **9** (Exp.).

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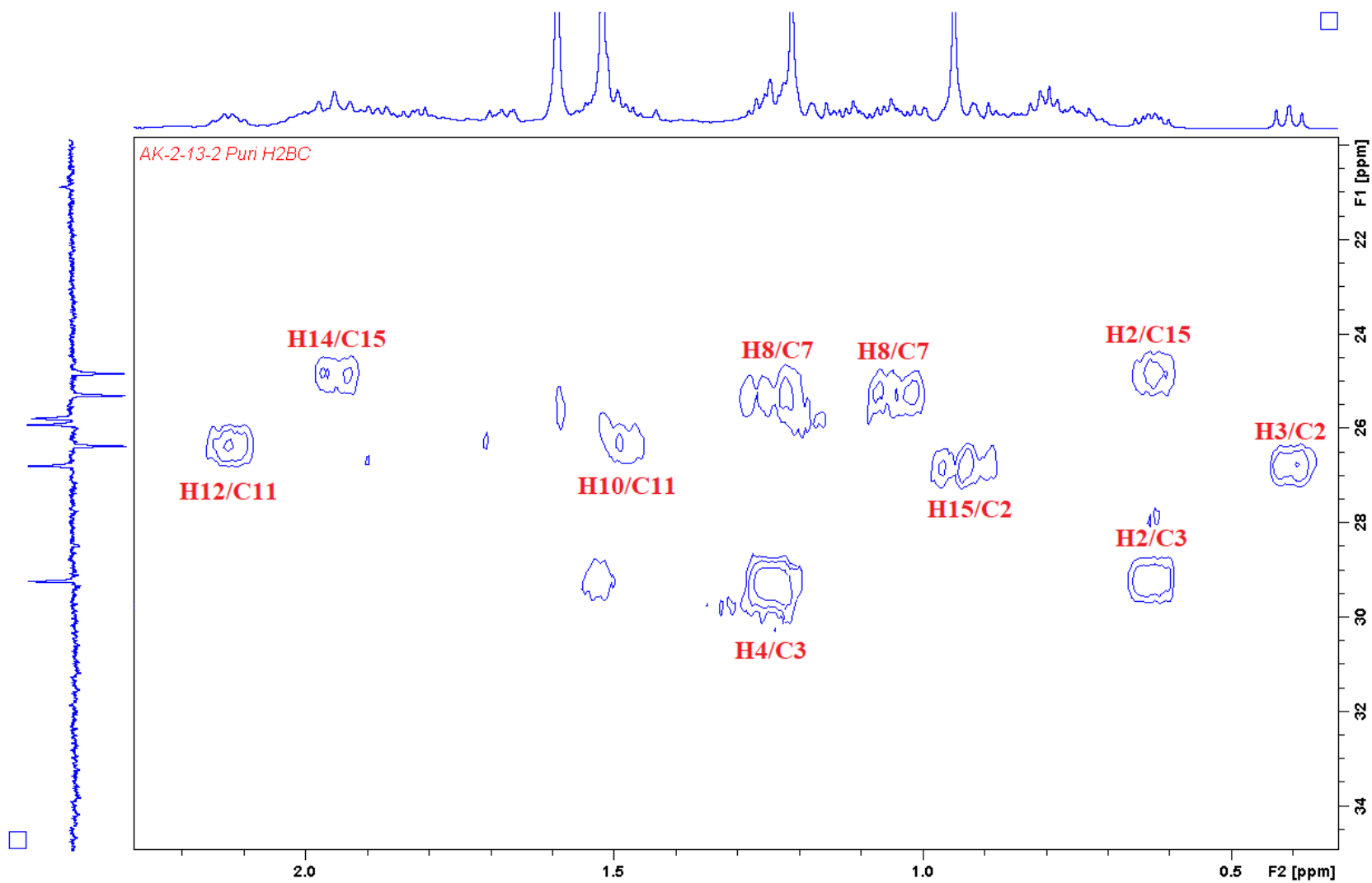


Figure S26: H2BC spectrum of **9** (Exp.).

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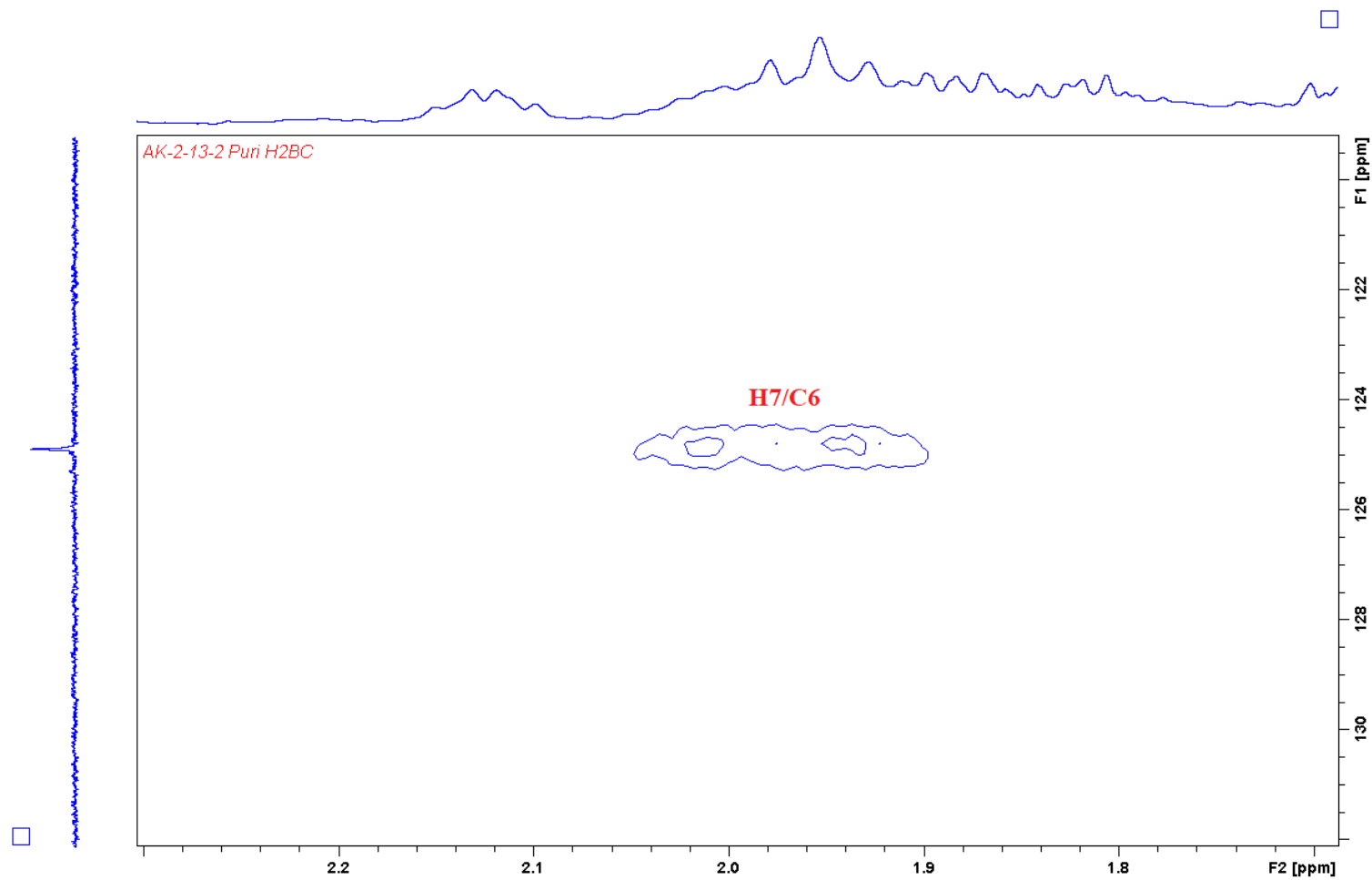


Figure S27: H2BC spectrum of **9** (Exp.).

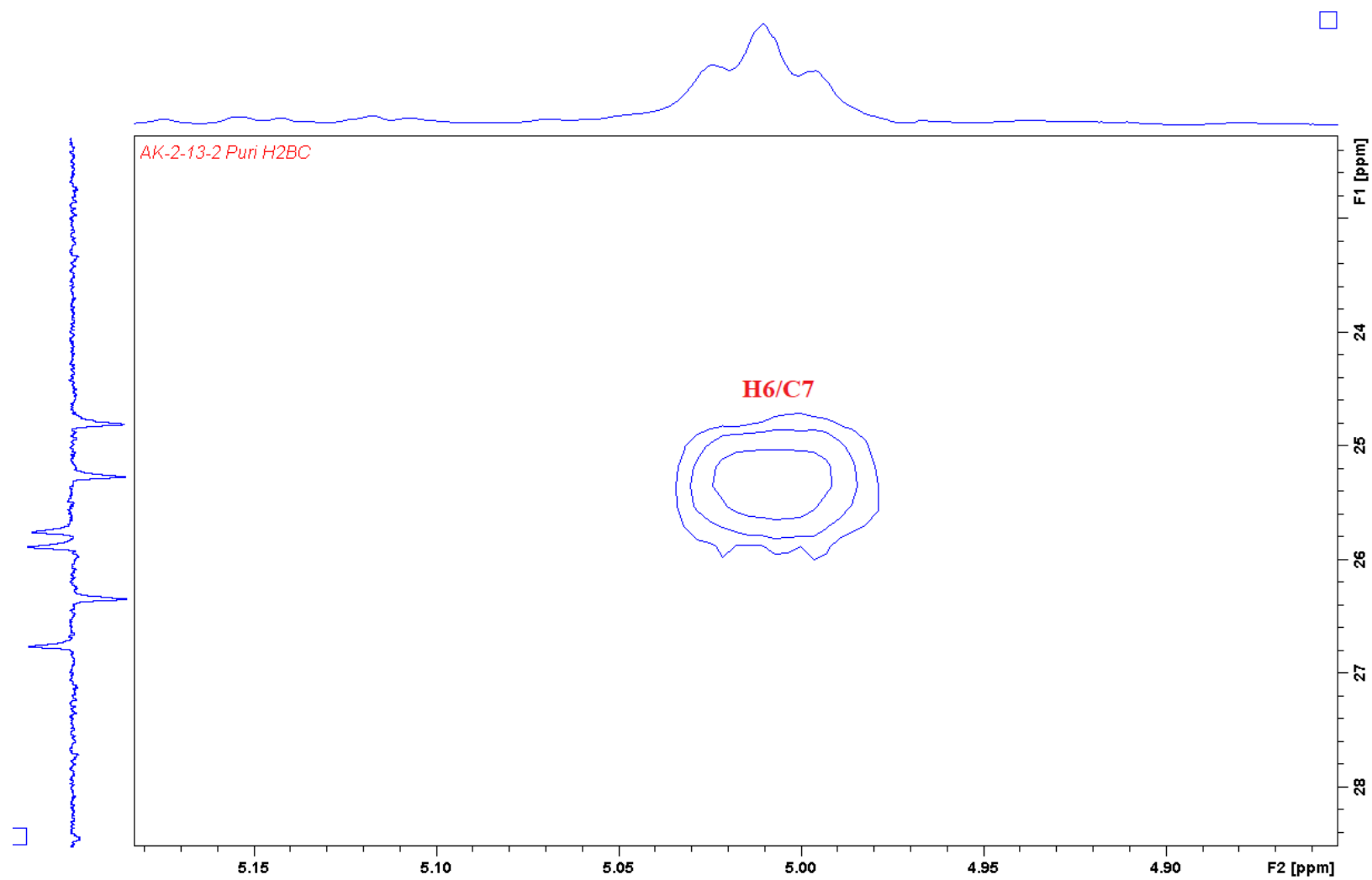


Figure S28: H2BC spectrum of **9** (Exp.).

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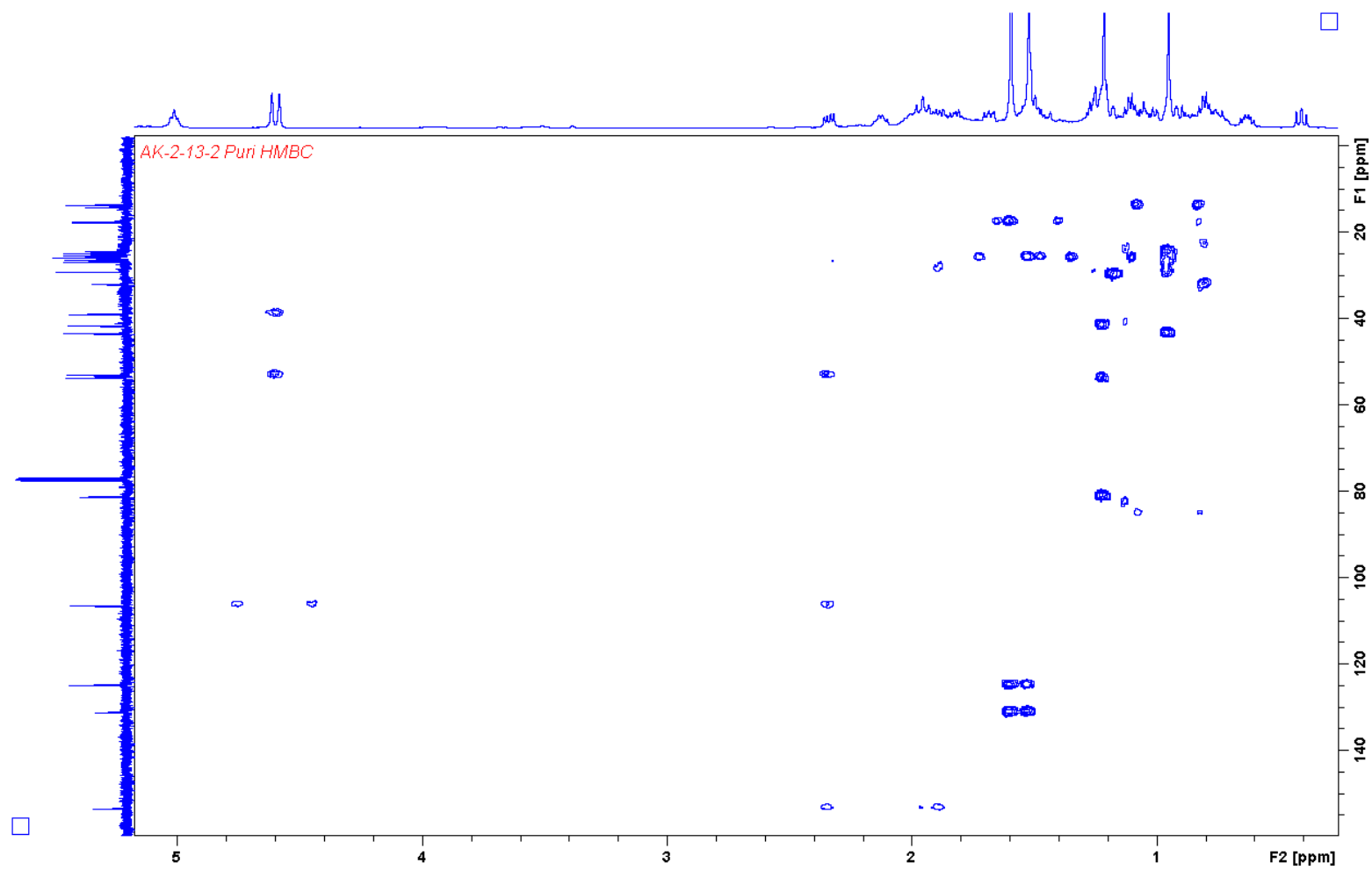


Figure S29: HMBC spectrum of **9** (Exp.).

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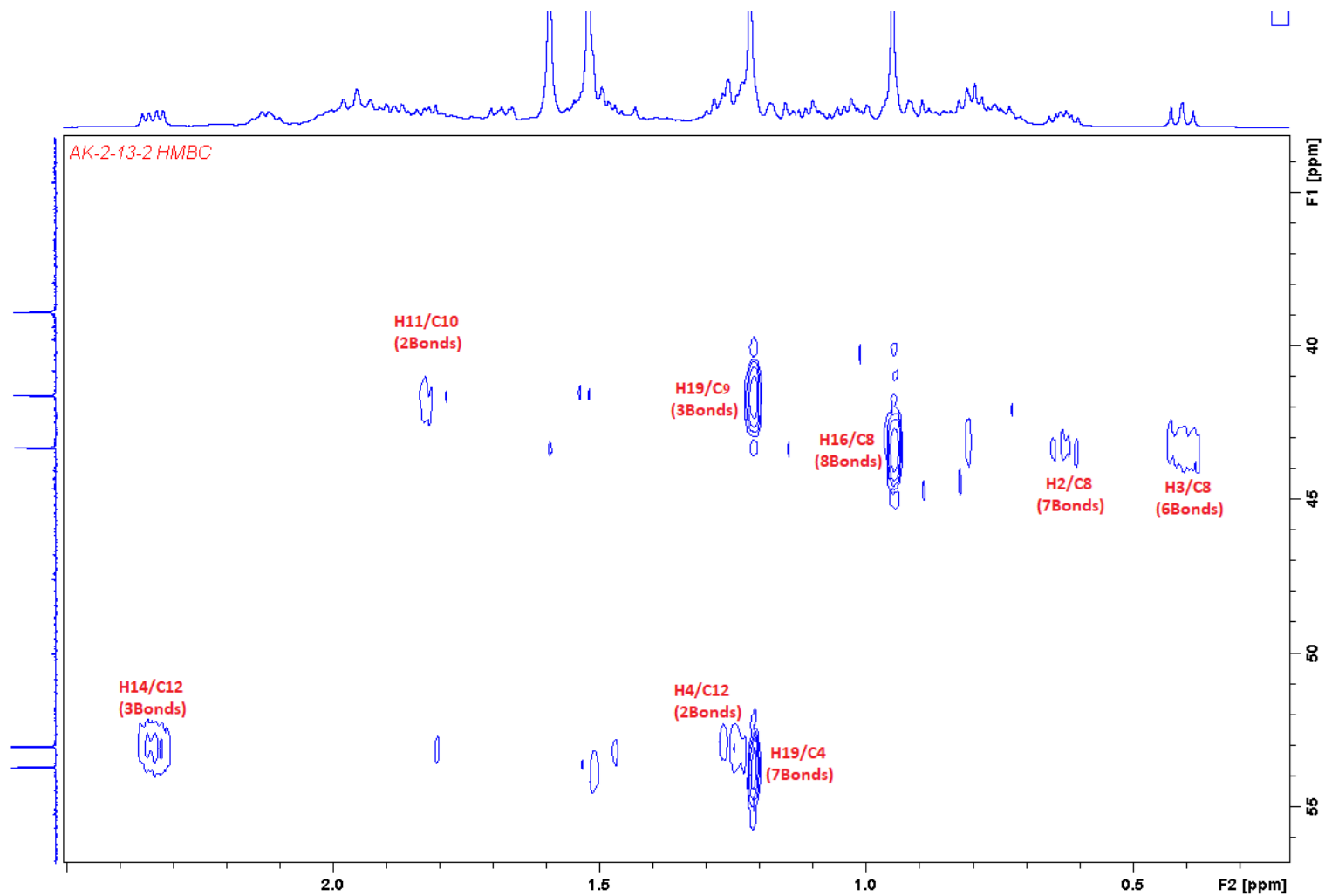


Figure S30: HMBC spectrum of **9** (Exp.).

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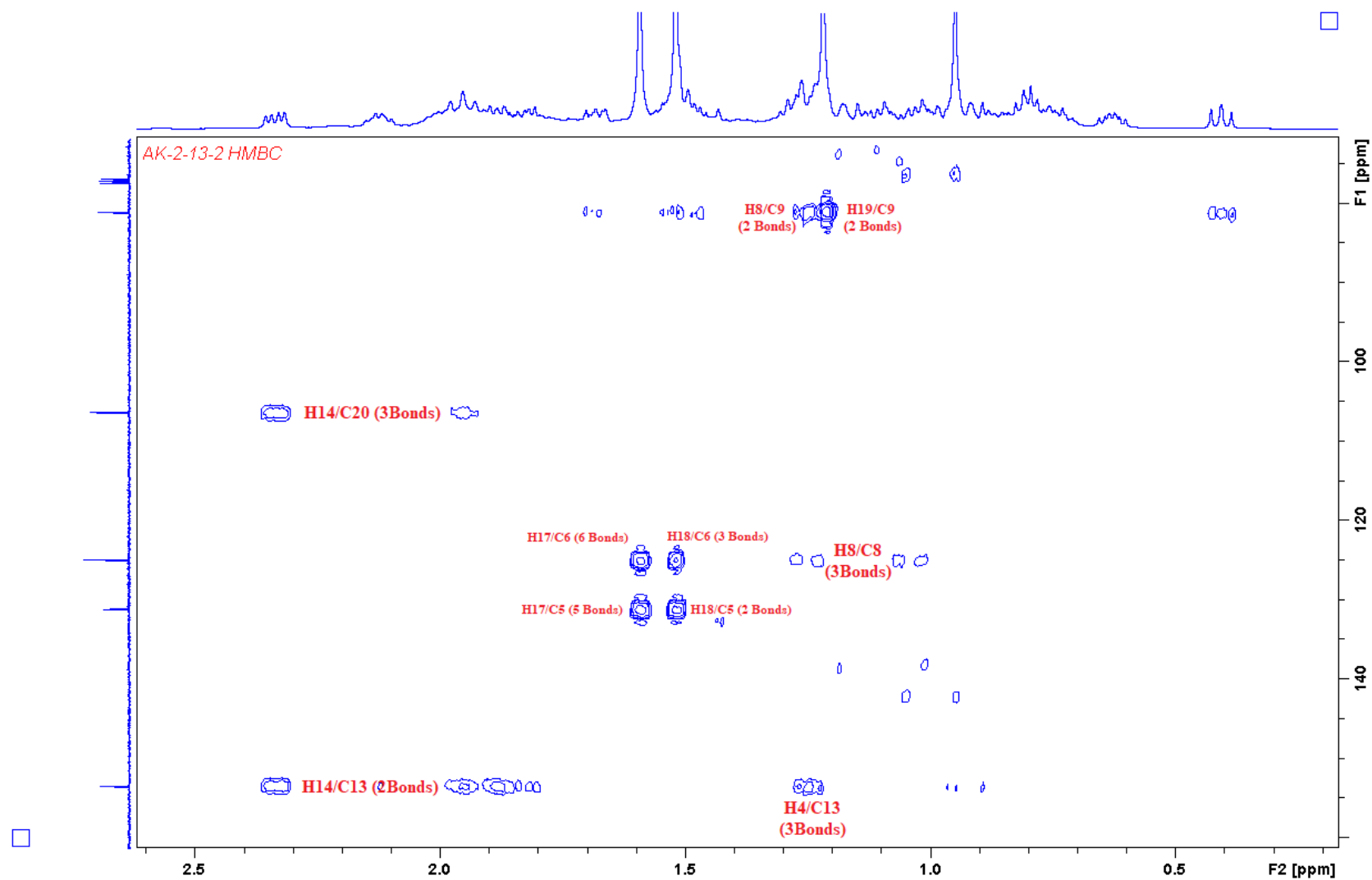


Figure S31: HMBC spectrum of **9** (Exp.).

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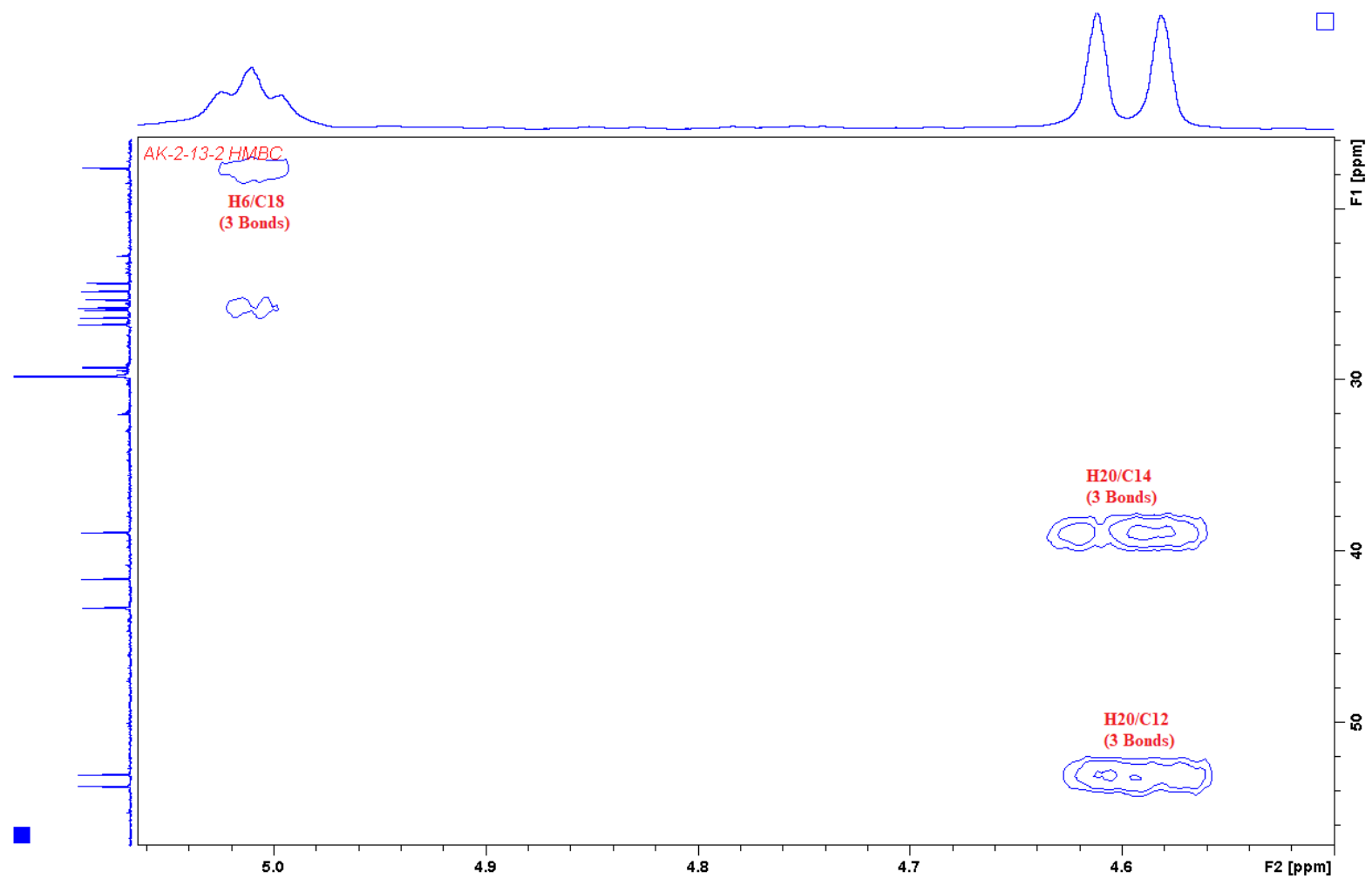


Figure S32: HMBC spectrum of **9** (Exp.).

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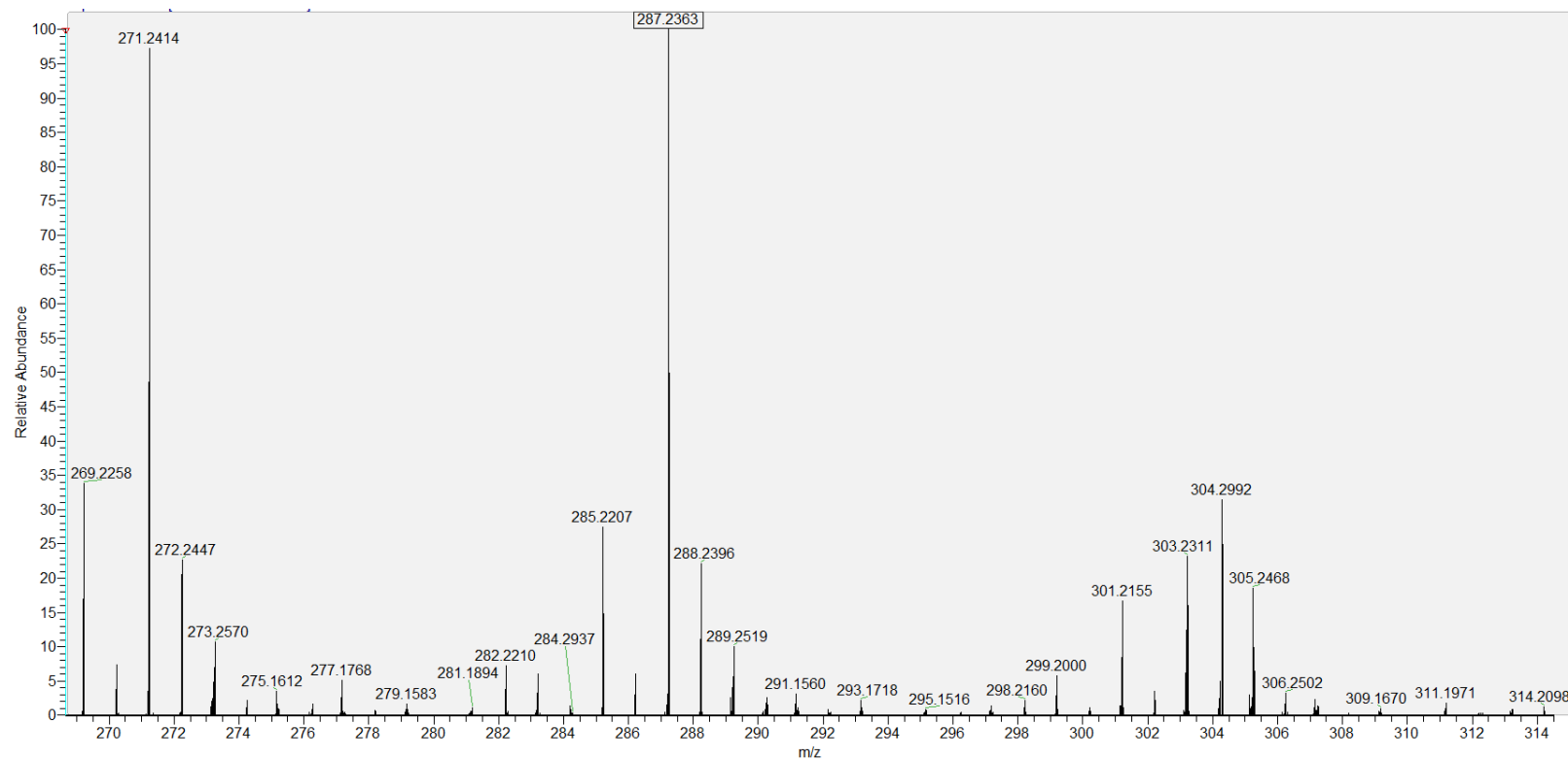


Figure S33: HRESIMS spectrum of **9**.