**SUPPLEMENTARY MATERIAL**

**Ricicomin A, a new alkaloid from the leaves of *Ricinus communis* Linn.**

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From the leaves of *Ricinus communis* Linn., one new alkaloid, named ricicomin A (**1**) together with three known ones, ricinine (**2**), *N*-demethylricinine (**3**) and 4-[2-formyl-5-(methoxymethyl)-1H-pyrrol-1-yl]butanoic acid (**4**) were justified by repeated chromatographic methods. Their structures were determined by comprehensive IR, HR-ESI-MS and NMR analyses. Compound **4** was identified for the first time from the genus *Ricinus*. DFT-NMR chemical shift calculations and subsequent DP4+ probability methods were applied to confirm the chemical structure of **1**. Compounds **1-3** did not display cytotoxic effect againstthree human cancer cell lines (MCF-7, HepG2 and HeLa)using SRB assay.

**Keywords:** *Ricinus communis*;Euphorbiaceae; alkaloid; ricicomin A.

**List of supporting information**

Table S1. NMR spectroscopic data for **1** recorded in DMSO-*d6* and acetone-*d*6.

Table S2.Cytotoxic activity of alkaloids **1-3** at the concentration of 100 μg/mL.

Table S3. Relative energy at B3LYP/6-311++G(2d,2p).

Figure S1. Key COSY, HMBC and NOESY correlations of 1.

Figure S2. 1H-NMR spectrum (500 MHz) of compound **1** in DMSO-*d6*.

Figure S3. 13C-NMR spectrum (125 MHz) of compound **1** in DMSO-*d6*.

Figure S4. COSY spectrum of compound **1** in DMSO-*d6*.

Figure S5. HSQC spectrum of compound **1** in DMSO-*d6*.

Figure S6. HMBC spectrum of compound **1** in DMSO-*d6*.

Figure S7. NOESY spectrum of compound **1** in DMSO-*d6*.

Figure S8. 1H-NMR spectrum (500 MHz) of compound **1** in acetone-*d*6.

Figure S9. 13C-NMR spectrum (125 MHz) of compound **1** in acetone-*d*6.

Figure S10. DEPT spectrum of compound **1** in acetone-*d*6.

Figure S11. HSQC spectrum of compound **1** in acetone-*d*6.

Figure S12. HMBC spectrum of compound **1** in acetone-*d*6.

Figure S13. HR-ESI-MS spectrum (negative) of compound **1**.

Figure S14. IR spectrum of compound **1**.

Figure S15. Optimized structures at B3LYP/6-311++G(2d,2p) level of theory.

Table S1. NMR spectroscopic data for **1** recorded in DMSO-*d6* and acetone-*d*6.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Pos. | *δ*C, type *a* | *δ*H,multi. *a* | *δ*C, type *b* | *δ*H, multi. *b* | NOESY *a* | HMBC *a* |
| 1 | 168.2, C |  | 170.0, C |  |  |  |
| 2 | 109.1, C |  | 109.3, C |  |  |  |
| 3 | 164.1, C |  | 165.6, C |  |  |  |
| 4 | 100.8, CH | 6.60, s | 101.3, CH | 6.60, s | 10 | 1, 2, 3, 5, 6, 8 |
| 5 | 164.1, C |  | 168.3, C |  |  |  |
| 6 | 90.2, C |  | 93.0, C |  |  |  |
| 7 | 134.0, CH | 8.20, s | 134.2, CH | 8.09, s | NH | 1, 3, 5, 8, 4 *d*, 6 *d* |
| 8 | 116.5, C |  | 116.7, C |  |  |  |
| 9 | 25.8, CH3 | 2.79, d (4.5) | 26.3, CH3 | 2.91, s |  | 1 |
| 10 | 56.5, CH3 | 3.89, s | 57.0, CH3 | 3.96, s | 4 | 3, 4*d* |
| NH |  | 9.05, br.s |  | 8.42, br.s | 7 |  |
| OH |  | *c* |  | *c* |  |  |

*a  Recorded in DMSO-d6*

*b  Recorded in acetone-d6*

*c Not observed*

*d Weak signal*

Table S2.Cytotoxic activity of alkaloids **1-3** at the concentration of 100 μg/mL.

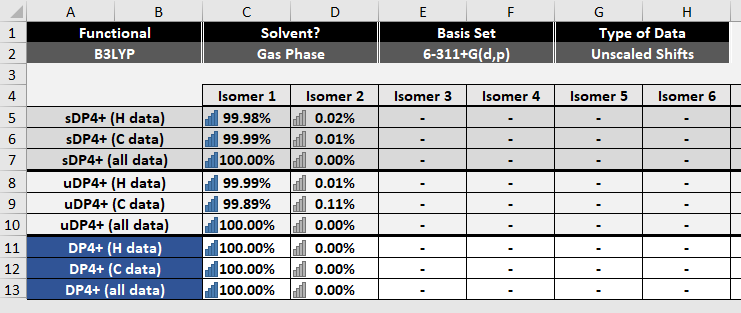
|  |  |  |
| --- | --- | --- |
| **Cell line** | **Fraction** | **Inhibition (%)** |
| HeLa | **1** | 2.67 ± 2.57 |
| Camptothecin\* | 65.08 ± 2.59 |
| HepG2 | **2** | 9.24 ± 1.39 |
| **3** | 5.03 ± 2.56 |
| Camptothecin# | 51.85 ± 0.32 |
| MCF-7 | **2** | 19.47 ± 1.76 |
| **3** | 12.29 ± 0.64 |
| Camptothecin$ | 51.85 ± 1.32 |
| *\*at the concentration of 1.00 (µg/mL)*  *#at the concentration of 0.07 (µg/mL)*  *$at the concentration of 0.01 (µg/mL)* | | |

Table S3. Relative energy at B3LYP/6-311++G(2d,2p).

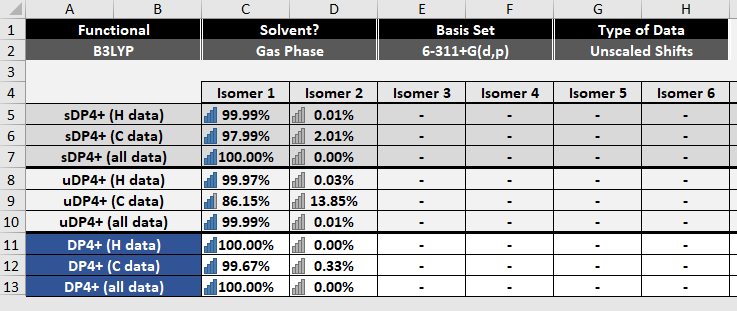
|  |  |  |  |
| --- | --- | --- | --- |
|  | **Relative Energy (with ZPE correction) (in kcal.mol-1)** | **Percentage according to Boltzmann analysis (%)** | **Note** |
| 1a\_1 | 12.3 | 0.003 |  |
| 1a\_2 | 6.2 | 99.997 | Isomer 1 in DP4+ |
| 1b\_1 | 0.0 | 99.999 | Isomer 2 in DP4+ |
| 1b\_2 | 5.7 | 0.001 |  |

**DP4+ results**

* **Type a (relative to the NMR data recorded in DMSO-d6)**



* **Type b (relative to the NMR data recorded in acetone-d6)**



**Cartesian coordinates at** B3LYP/6-311++G(2d,2p)

**1a\_1**

C -0.713412 -1.208219 -0.126693

C -1.915237 -0.507535 0.030178

C -1.886692 0.897568 0.066453

C -0.677107 1.572195 -0.054323

C 0.509347 0.856588 -0.193470

C 0.500965 -0.554662 -0.214785

H -0.734257 -2.286271 -0.189517

H -0.696265 2.649434 -0.043738

O -3.004631 1.644840 0.209532

H -3.784014 1.076694 0.272398

C -3.171793 -1.165215 0.148883

N -4.230427 -1.615222 0.256446

C 1.732610 -1.389812 -0.460696

O 1.773634 -2.150812 -1.417268

N 2.761243 -1.308521 0.424727

H 3.546946 -1.885894 0.168845

C 2.836915 -0.566068 1.669501

H 3.281131 -1.193651 2.441635

H 3.431400 0.342839 1.567520

H 1.838878 -0.289763 1.997703

O 1.717874 1.448113 -0.338024

C 1.787994 2.870563 -0.415310

H 1.208321 3.245390 -1.259849

H 1.438086 3.334343 0.508400

H 2.837497 3.103538 -0.563956

**1a\_2**

C 0.660720 -1.193135 0.000000

C 1.951482 -0.664378 0.000000

C 2.116180 0.731566 0.000001

C 0.998554 1.556119 0.000000

C -0.281657 1.009335 0.000000

C -0.473221 -0.394344 0.000000

H 0.509683 -2.262344 0.000000

H 1.162412 2.620611 0.000000

O 3.330075 1.323904 0.000000

H 4.029834 0.656807 0.000007

C 3.116901 -1.483465 -0.000001

N 4.116904 -2.061495 -0.000001

C -1.783854 -1.149331 0.000000

O -1.785790 -2.375435 0.000000

N -2.937689 -0.441839 0.000001

O -1.389293 1.800387 -0.000001

C -1.241006 3.221147 -0.000001

H -0.715349 3.559018 0.893343

H -0.715351 3.559018 -0.893345

H -2.250497 3.619937 0.000000

C -4.222877 -1.118528 0.000001

H -5.010066 -0.368459 0.000001

H -4.330786 -1.751411 -0.880503

H -4.330786 -1.751412 0.880504

H -2.890859 0.560807 0.000000

**1b\_1**

C 0.133684 1.035548 -0.000073

C 0.897927 -0.131049 -0.000050

C 0.204979 -1.370045 -0.000017

C -1.194332 -1.402728 0.000031

C -1.928003 -0.229050 0.000025

C -1.254655 1.019876 -0.000036

H 0.605445 2.007234 -0.000149

H -1.668132 -2.370612 0.000063

O 0.844368 -2.538141 -0.000029

H 1.818027 -2.321922 -0.000111

O -3.271065 -0.167337 0.000064

C -4.019654 -1.382526 0.000110

H -3.807612 -1.971712 -0.892981

H -3.807572 -1.971668 0.893221

H -5.061721 -1.080689 0.000126

C -1.986322 2.243544 -0.000066

N -2.546120 3.252347 -0.000089

C 2.379655 -0.147085 -0.000059

O 3.007085 -1.222772 -0.000187

N 3.057696 1.020417 0.000049

H 2.559065 1.889452 0.000443

C 4.513369 1.053051 0.000182

H 4.912133 0.553776 -0.881623

H 4.834305 2.091209 -0.000147

H 4.912037 0.554360 0.882373

**1b\_2**

C 0.297762 0.934978 -0.224675

C 1.028880 -0.249087 -0.118018

C 0.297102 -1.462591 0.004526

C -1.096977 -1.444794 0.113702

C -1.794931 -0.250823 0.041738

C -1.089058 0.963615 -0.152983

H 0.802238 1.870754 -0.396589

H -1.598566 -2.391945 0.225208

O 0.895926 -2.652156 0.019120

H 1.854196 -2.481550 -0.190333

O -3.132042 -0.142633 0.125556

C -3.913308 -1.322682 0.311265

H -3.789484 -2.009128 -0.527258

H -3.649379 -1.823311 1.243701

H -4.942926 -0.983833 0.356837

C -1.787186 2.201065 -0.273934

N -2.320666 3.219334 -0.372059

C 2.504391 -0.329906 -0.190150

O 3.054840 -1.413823 -0.465342

N 3.297860 0.750725 0.034797

C 3.016891 1.996970 0.737921

H 2.749536 2.807596 0.058610

H 2.218408 1.865144 1.463624

H 3.914230 2.293126 1.277098

H 4.270220 0.511145 -0.081092

**Calculated NMR data**

**Isotropic value based on GIAO calculations at B3LYP/6-311+G(d,p)**

|  |  |  |
| --- | --- | --- |
| **Position** | **Isomer 1** | **Isomer 2** |
| C7 | 39.0635 | 46.3733 |
| C6 | 87.7286 | 73.0310 |
| C5 | 13.4695 | 8.0452 |
| C4 | 84.2035 | 81.1347 |
| C3 | 14.8318 | 10.6055 |
| C2 | 63.1115 | 85.5206 |
| C8 | 64.5859 | 64.0833 |
| C1 | 16.8081 | 9.3343 |
| C10 | 127.0527 | 127.4358 |
| C9 | 155.8089 | 155.6801 |
| H7 | 23.0026 | 24.7996 |
| H4 | 25.6418 | 25.7663 |
| H10 | 28.2670  28.2670  27.8620 | 28.3901  28.3901  27.8212 |
|
|
| H9 | 29.6160  28.9005  28.9005 | 28.8895  29.5098  28.8907 |
| H(NH) | 24.9807 | 26.6495 |
| H(OH) | 26.3694 | 18.2529 |



Figure S1. Key COSY, HMBC and NOESY correlations of **1.**

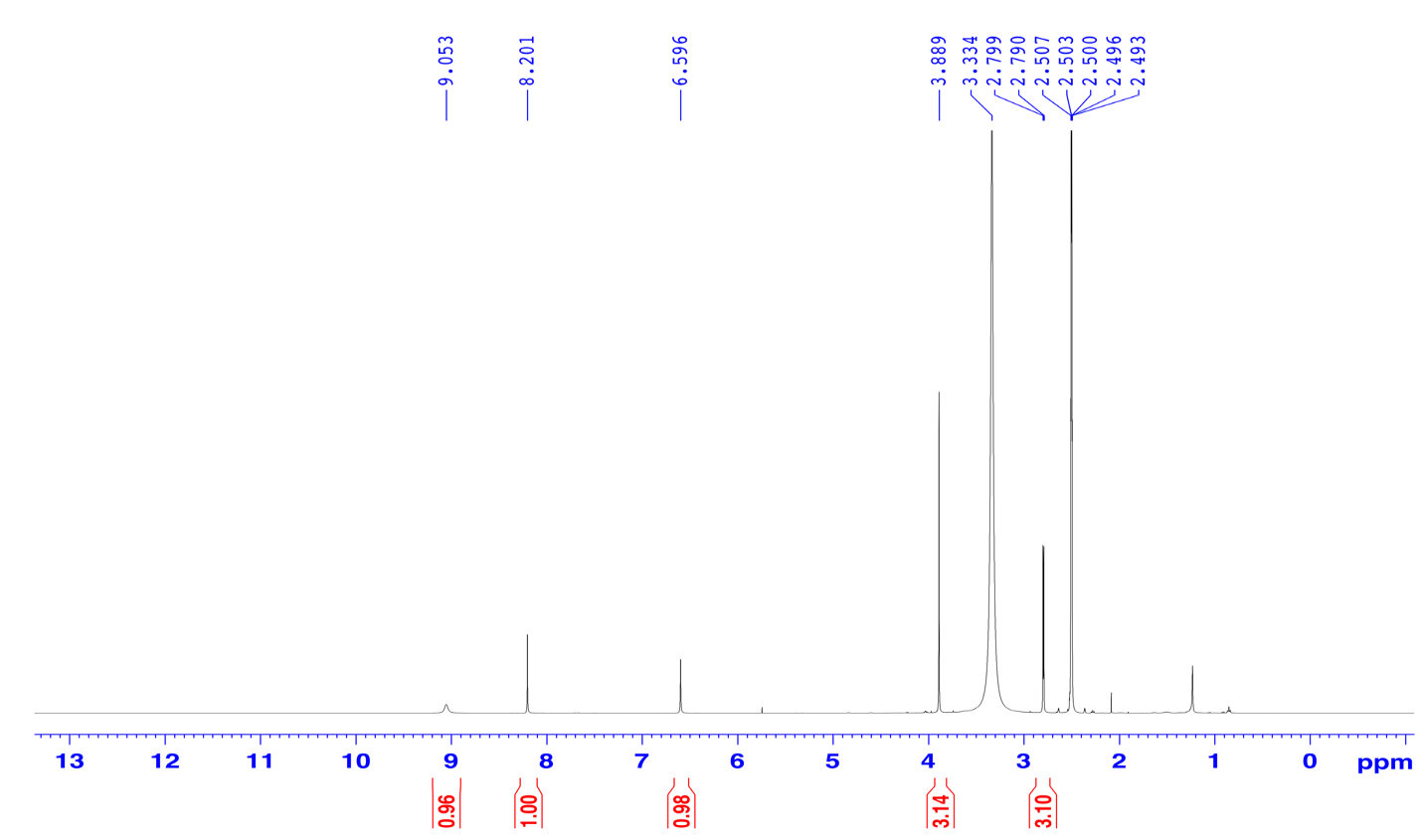


Figure S2. 1H-NMR spectrum (500 MHz) of compound **1** in DMSO-*d6*.

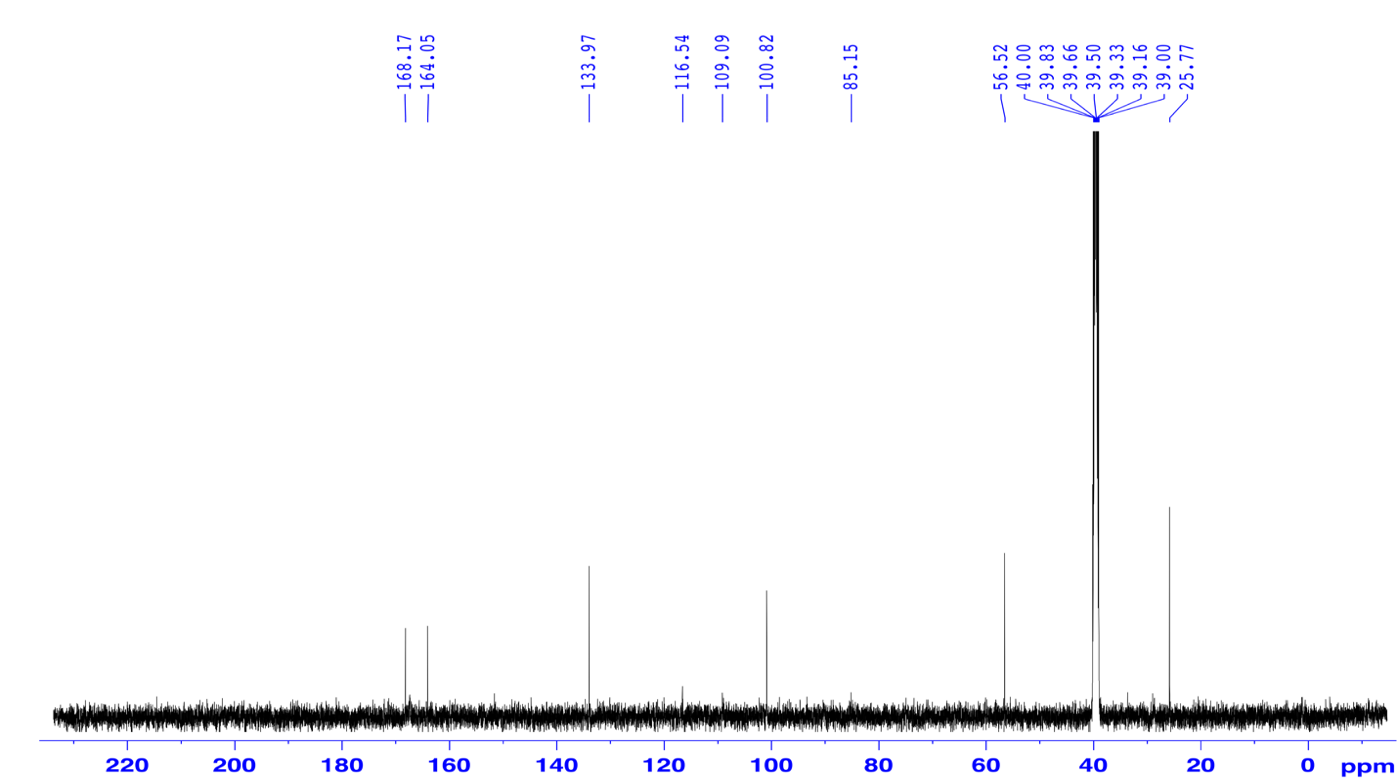


Figure S3. 13C-NMR spectrum (125 MHz) of compound **1** in DMSO-*d6*.

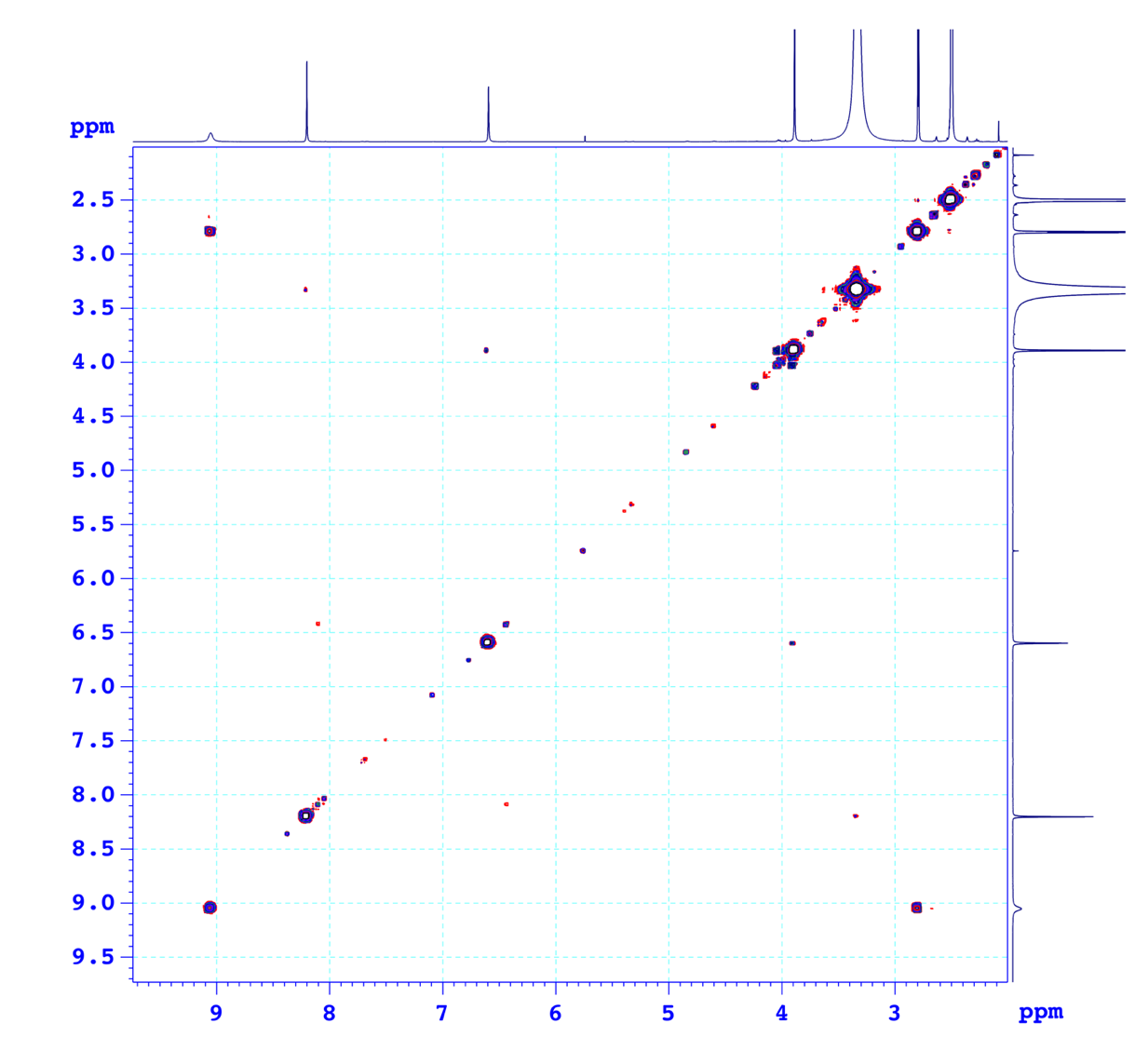


Figure S4. COSY spectrum of compound **1** in DMSO-*d6*.

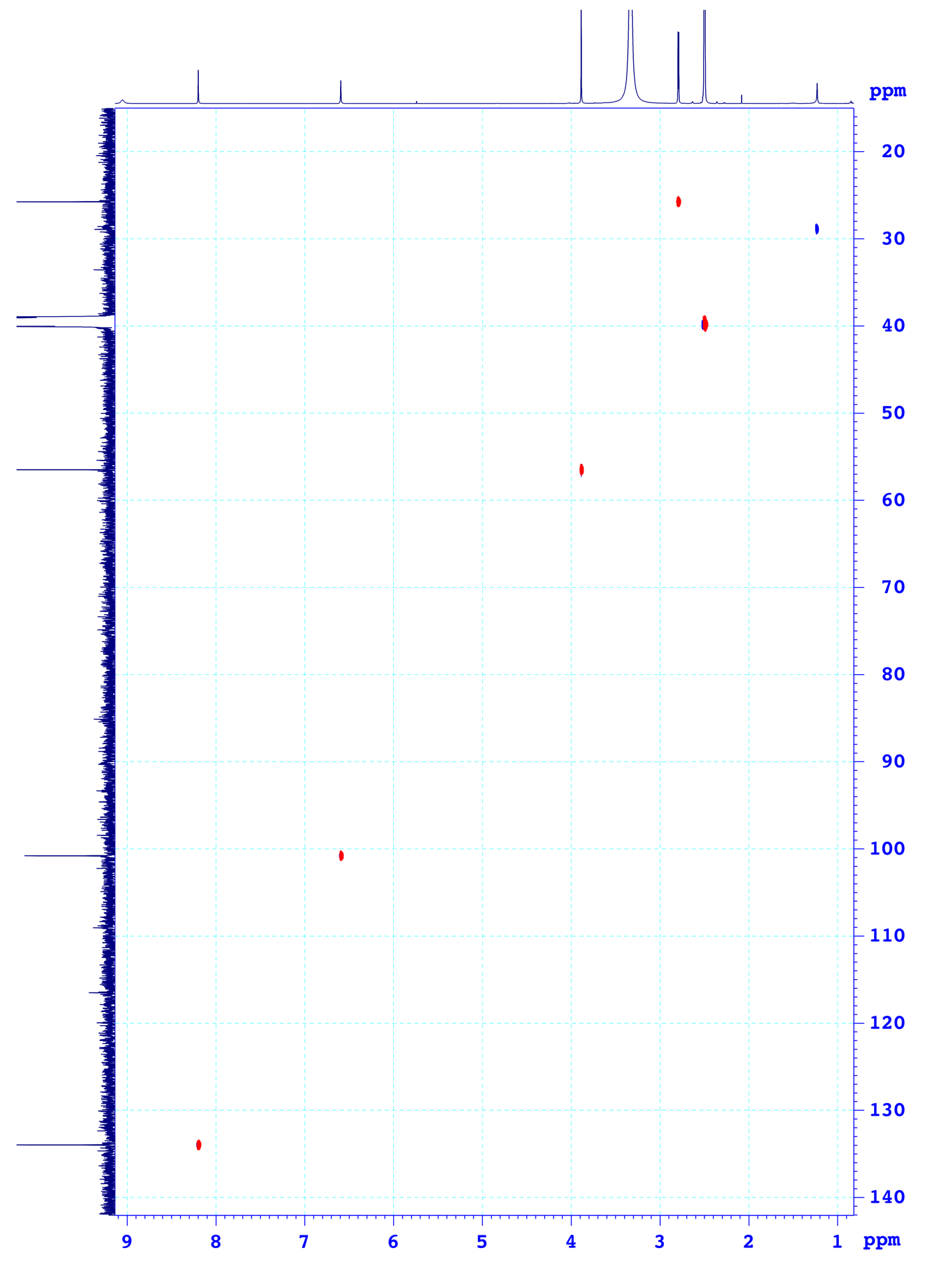


Figure S5. HSQC spectrum of compound **1** in DMSO-*d6*.

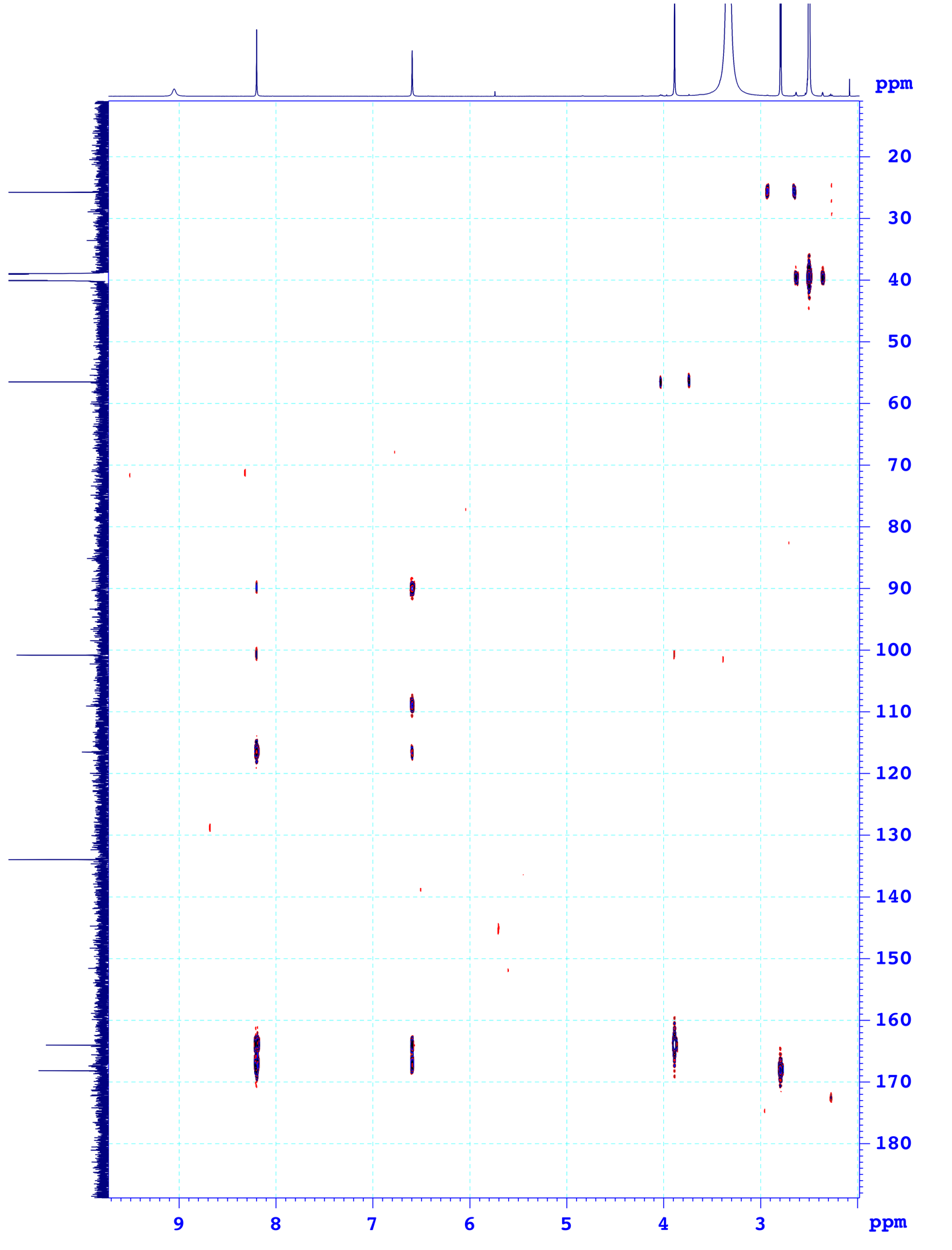


Figure S6. HMBC spectrum of compound **1** in DMSO-*d6*.

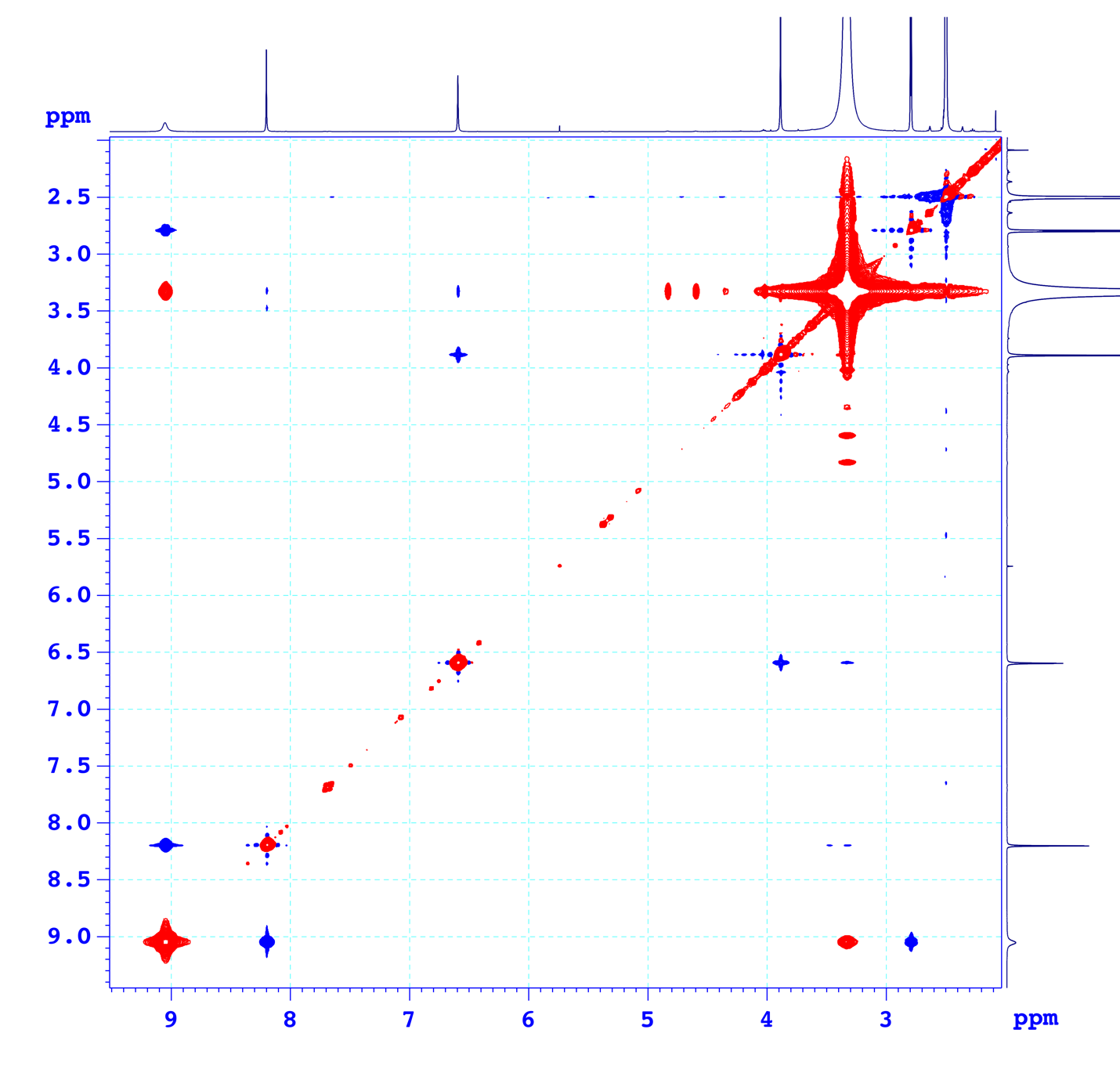


Figure S7. NOESY spectrum of compound **1** in DMSO-*d6*.

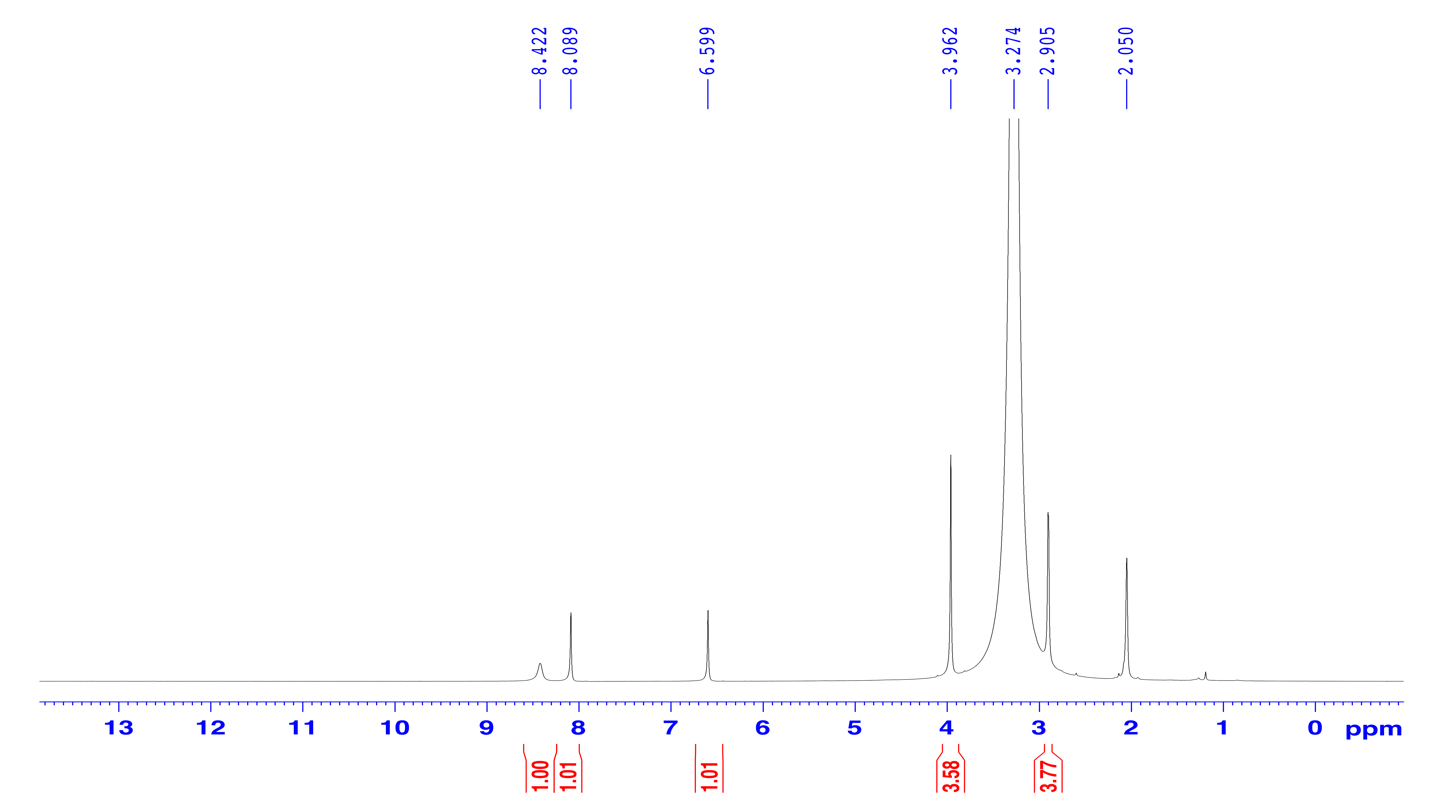


Figure S8. 1H-NMR spectrum (500 MHz) of compound **1** in acetone-*d*6.

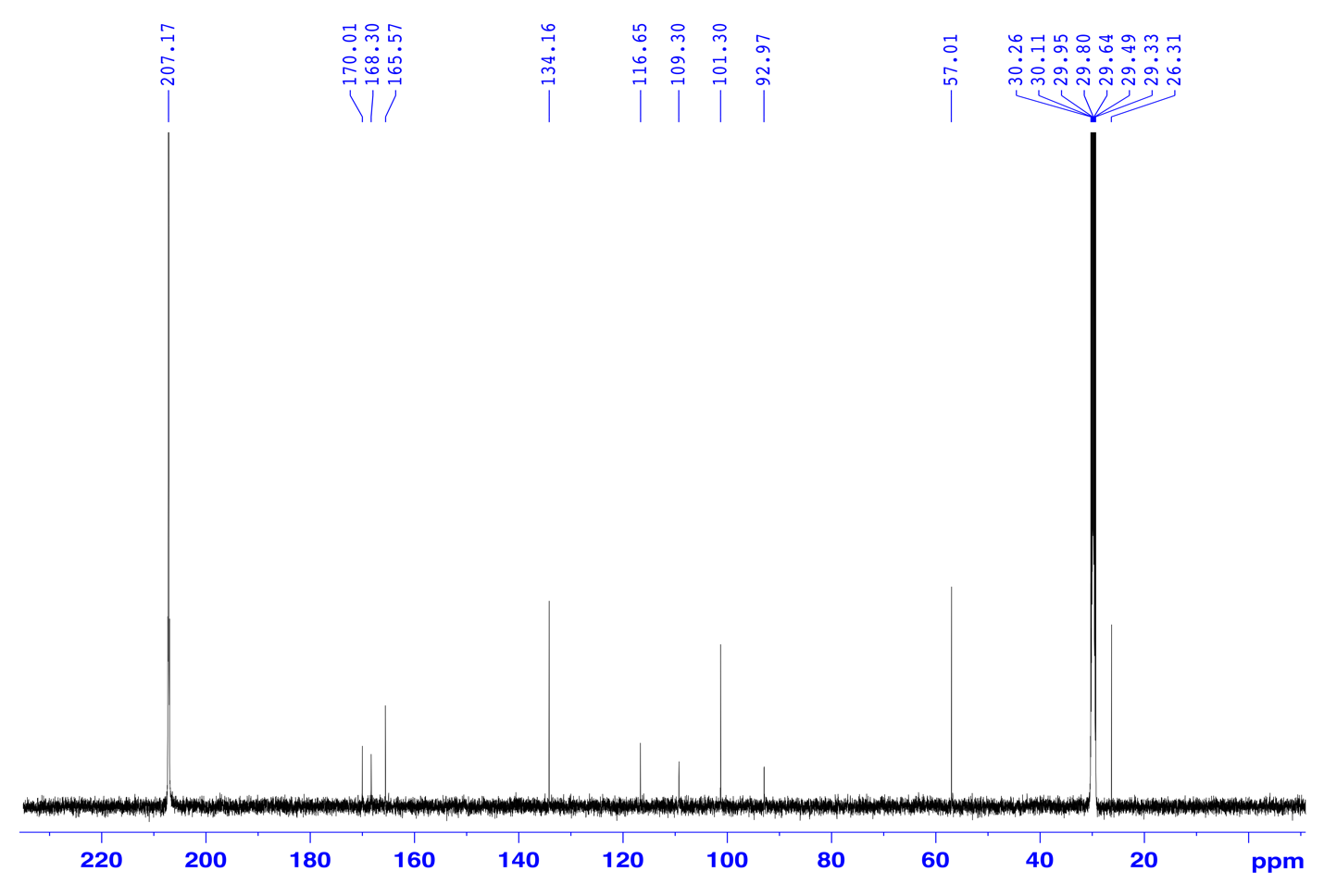


Figure S9. 13C-NMR spectrum (125 MHz) of compound **1** in acetone-*d*6.

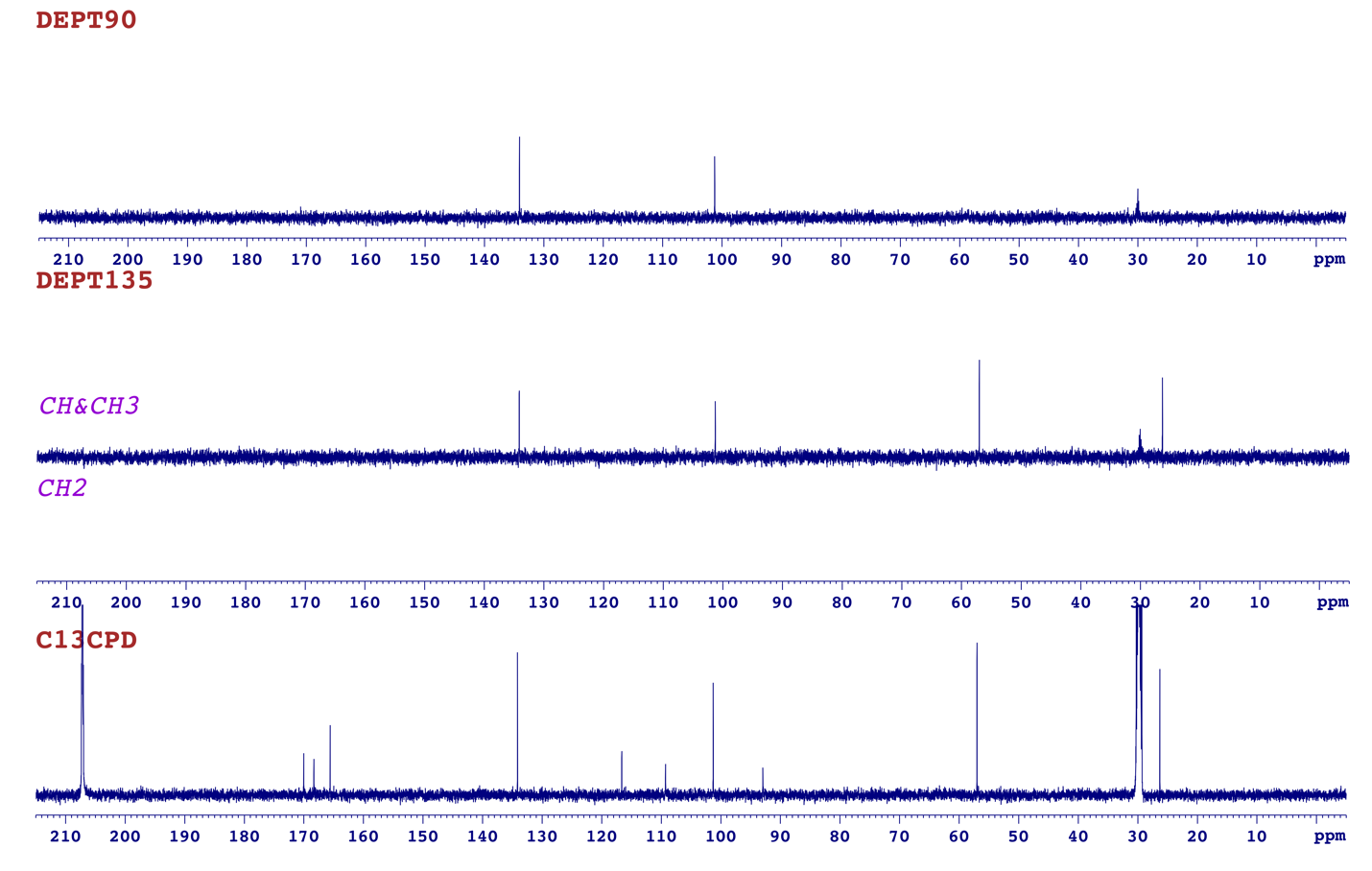


Figure S10. DEPT spectrum of compound **1** in acetone-*d*6.



Figure S11. HSQC spectrum of compound **1** in acetone-*d*6.

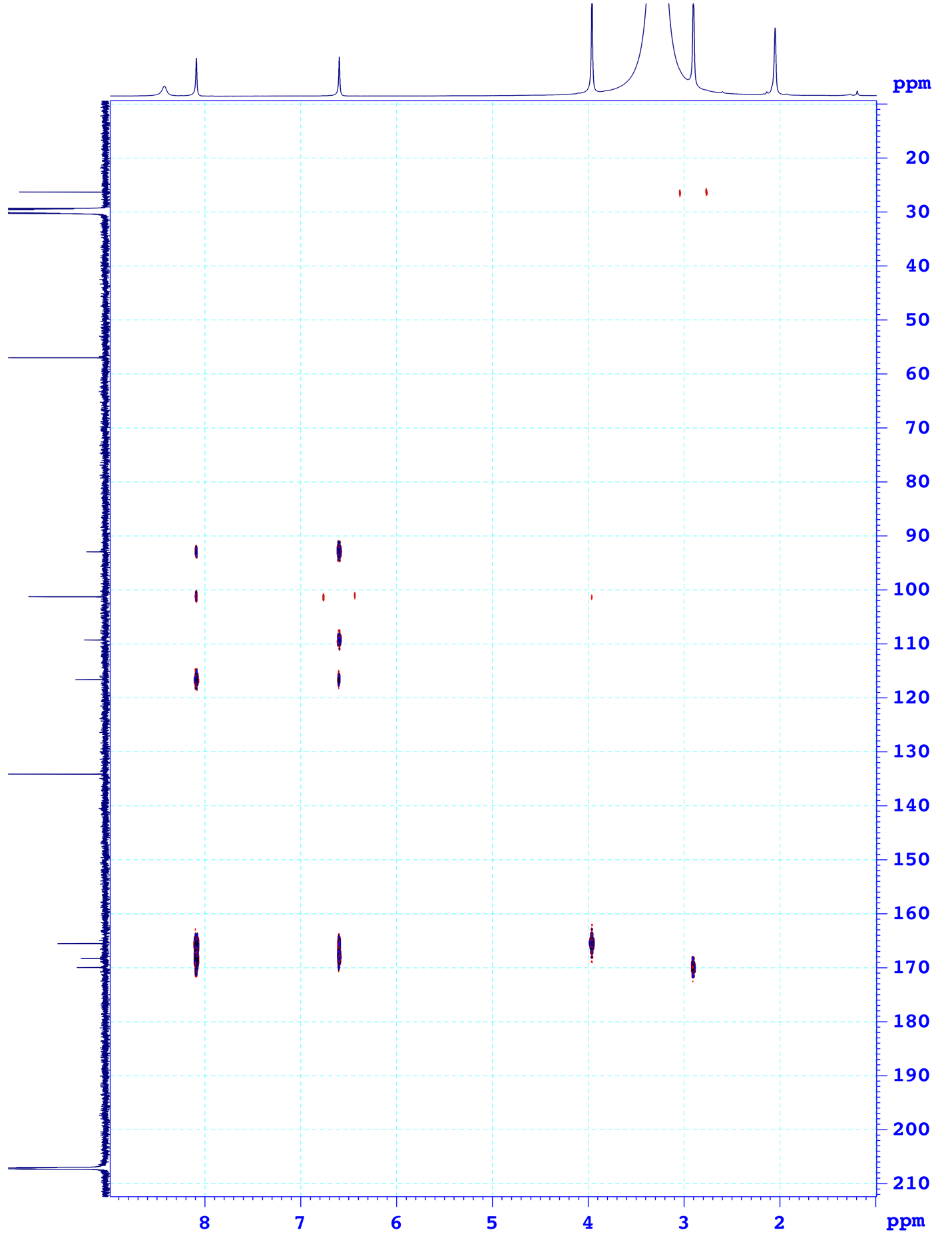


Figure S12. HMBC spectrum of compound **1** in acetone-*d*6.



Figure S13. HR-ESI-MS spectrum (negative) of compound **1**.



Figure S14. IR spectrum of compound **1**.

|  |  |
| --- | --- |
|  |  |
| 1a\_1 | 1a\_2 |
|  |  |
| 1b\_1 | 1b\_2 |

Figure S15. Optimized structures at B3LYP/6-311++G(2d,2p) level of theory.