

# Supplementary Materials: Isoquercitrin Esters with Mono- or Dicarboxylic Acids: Enzymatic Preparation and Properties

Eva Vavříková, Fanny Langschwager, Lubica Jezova-Kalachova, Alena Křenková, Barbora Mikulová, Marek Kuzma, Vladimír Křen and Kateřina Valentová

| Content  | Page    |
|--|---------|
| Figure S1 Structures of compounds 2–11 .....                               | S3      |
| Table S1 <sup>13</sup> C NMR data of prepared compounds 2–8 .....          | S4      |
| Table S2 <sup>1</sup> H NMR data of prepared compounds 2 and 3 .....       | S6      |
| Table S3 <sup>1</sup> H NMR data of prepared compounds 4–8 .....           | S7      |
| Table S4 <sup>13</sup> C NMR data of prepared compounds 9–11 .....         | S9      |
| Table S5 <sup>1</sup> H NMR data of prepared compounds 9–11 .....          | S10     |
| Figure S2 <sup>13</sup> C NMR spectrum of compound 2 .....                 | S11     |
| Figure S3 <sup>1</sup> H NMR spectrum of compound 2 .....                  | S12     |
| Figure S4 HPLC chromatogram of compound 2 .....                            | S13     |
| Figure S5 <sup>13</sup> C NMR spectrum of compound 3 .....                 | S14     |
| Figure S6 <sup>1</sup> H NMR spectrum of compound 3 .....                  | S15     |
| Figure S7 HPLC chromatogram of compound 3 .....                            | S16     |
| Figure S8 <sup>13</sup> C NMR spectrum of compound 4 .....                 | S17     |
| Figure S9 <sup>1</sup> H NMR spectrum of compound 4 .....                  | S18     |
| Figure S10 HPLC chromatogram of compound 4 .....                           | S19     |
| Figure S11 <sup>13</sup> C NMR spectrum of compound 5 .....                | S20     |
| Figure S12 <sup>1</sup> H NMR spectrum of compound 5 .....                 | S21     |
| Figure S13 HPLC chromatogram of compound 5 .....                           | S22     |
| Figure S14 <sup>13</sup> C NMR spectrum of compound 6 .....                | S23     |
| Figure S15 <sup>1</sup> H NMR spectrum of compound 6 .....                 | S24     |
| Figure S16 HPLC chromatogram of compound 6 .....                           | S25     |
| Figure S17 <sup>13</sup> C NMR spectrum of compound 7 .....                | S26     |
| Figure S18 <sup>1</sup> H NMR spectrum of compound 7 .....                 | S27     |
| Figure S19 HPLC chromatogram of compound 7 .....                           | S28     |
| Figure S20 <sup>13</sup> C NMR spectrum of compound 8 .....                | S29     |
| Figure S21 <sup>1</sup> H NMR spectrum of compound 8 .....                 | S30     |
| Figure S22 HPLC chromatogram of compound 8 .....                           | S31     |
| Figure S23 <sup>13</sup> C NMR spectrum of compound 9 .....                | S32     |
| Figure S24 <sup>1</sup> H NMR spectrum of compound 9 .....                 | S33     |
| Figure S25–27 Details of <sup>1</sup> H NMR spectrum of compound 9 .....   | S34–S36 |
| Figure S28 HSQC NMR spectrum of compound 9 .....                           | S37     |
| Figure S29–31 Details of HSQC NMR spectrum of compound 9 .....             | S38–S40 |
| Figure S32 HMBC NMR spectrum of compound 9 .....                           | S41     |
| Figure S33–36 Details of HMBC NMR spectrum of compound 9 .....             | S42–S45 |
| Figure S37 COSY NMR spectrum of compound 9 .....                           | S46     |
| Figure S38–40 Details of COSY NMR spectrum of compound 9 .....             | S47–S49 |
| Figure S41 HPLC chromatogram of compound 9 .....                           | S50     |
| Figure S42 <sup>13</sup> C NMR spectrum of compound 10 .....               | S51     |
| Figure S43–45 Details of <sup>13</sup> C NMR spectrum of compound 10 ..... | S52–S54 |
| Figure S46 <sup>1</sup> H NMR spectrum of compound 10 .....                | S55     |
| Figure S47–49 Details of <sup>1</sup> H NMR spectrum of compound 10 .....  | S56–S58 |
| Figure S50 HSQC NMR spectrum of compound 10 .....                          | S59     |
| Figure S51–54 Details of HSQC NMR spectrum of compound 10 .....            | S60–S63 |

|   |         |
|---|---------|
| <b>Figure S55</b> HMBC NMR spectrum of compound <b>10</b> .....   | S64     |
| <b>Figure S56–62</b> Details of HMBC NMR spectrum of compound <b>10</b> .....   | S65–S71 |
| <b>Figure S63</b> COSY NMR spectrum of compound <b>10</b> .....   | S72     |
| <b>Figure S64–66</b> Details of COSY NMR spectrum of compound <b>10</b> .....   | S73–S75 |
| <b>Figure S67</b> HPLC chromatogram of compound <b>10</b> .....   | S76     |
| <b>Figure S68</b> <sup>1</sup> H NMR spectrum of compound <b>11</b> .....   | S77     |
| <b>Figure S69</b> <sup>1</sup> H NMR spectrum WET of compound <b>11</b> .....   | S78     |
| <b>Figure S70–72</b> Details of <sup>1</sup> H NMR spectrum WET of compound <b>11</b> .....   | S79–S81 |
| <b>Figure S73</b> HSQC NMR spectrum of compound <b>11</b> .....   | S82     |
| <b>Figure S74–76</b> Details of HSQC NMR spectrum of compound <b>11</b> .....   | S83–S85 |
| <b>Figure S77</b> HMBC NMR spectrum of compound <b>11</b> .....   | S86     |
| <b>Figure S78–82</b> Details of HMBC NMR spectrum of compound <b>11</b> .....   | S87–S91 |
| <b>Figure S83</b> COSY NMR spectrum of compound <b>11</b> .....   | S92     |
| <b>Figure S84–86</b> Details of COSY NMR spectrum of compound <b>11</b> .....   | S93–S95 |
| <b>Figure S87</b> HPLC chromatogram of compound <b>11</b> .....   | S96     |
| <b>Figure S88</b> HPLC chromatogram of the reaction mixture of isoquercitrin, succinic anhydride in the presence of Novozym 435®..... | S97     |
| <b>Figure S89</b> HPLC chromatogram of the reaction mixture of isoquercitrin, succinic anhydride in the absence of Novozym 435®.....  | S98     |
| <b>Figure S90</b> HPLC-MS (-) chromatogram of the monosuccinate of isoquercitrin .....  | S99     |
| <b>Figure S91</b> HPLC-MS (-) chromatogram of the disuccinate of isoquercitrin.....   | S100    |
| <b>Figure S92</b> HPLC-MS (-) chromatogram of the trisuccinate of isoquercitrin .....   | S101    |

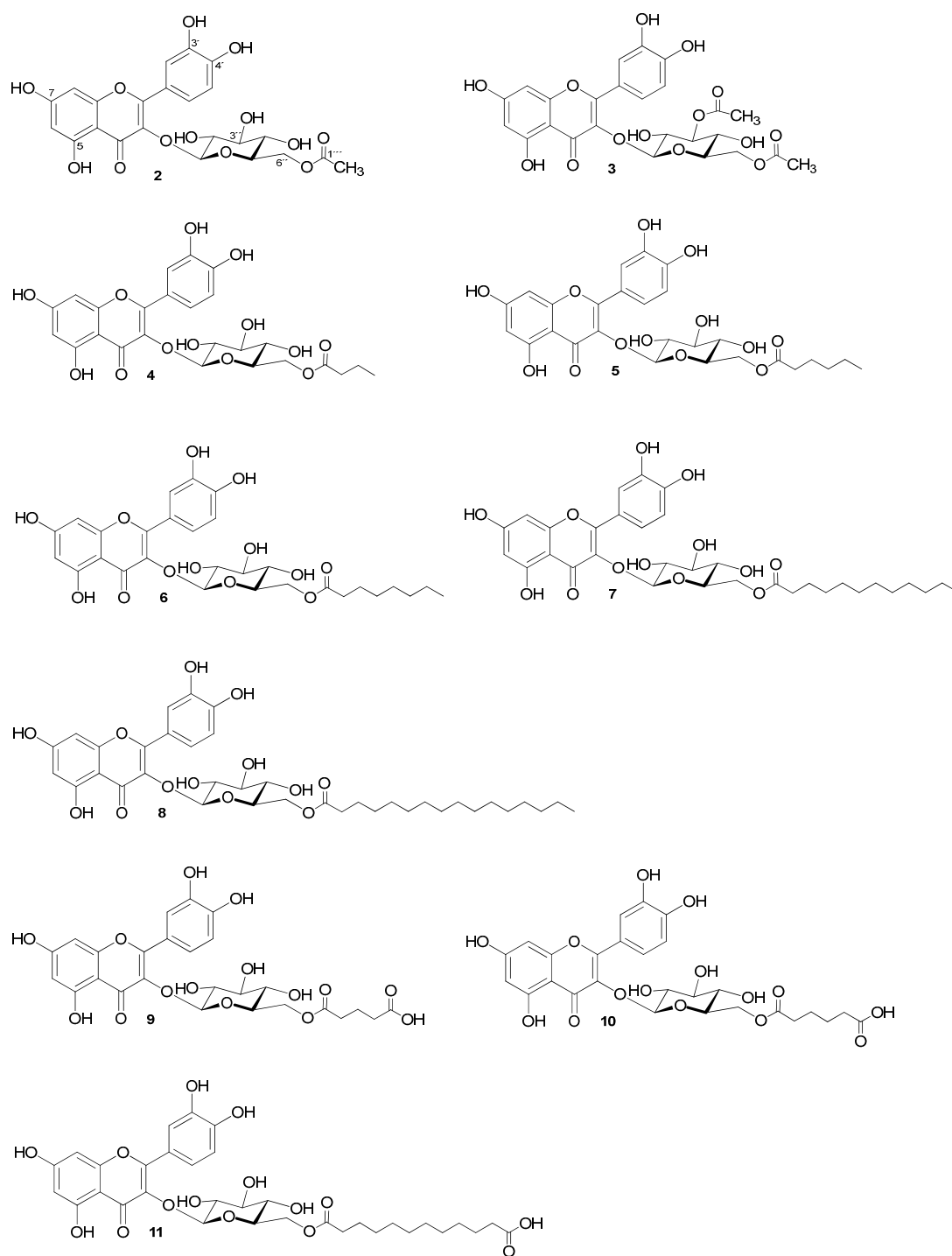


Figure S1. Structures of compounds 2–11.





Table S1. Cont.

| Comp.       | 2          |     | 3          |     | 4          |     | 5          |     | 6          |     | 7          |     | 8                   |     |
|-------------|------------|-----|------------|-----|------------|-----|------------|-----|------------|-----|------------|-----|---------------------|-----|
| Atom Number | $\delta C$ | m C | $\delta C$ | m C | $\delta C$ | m C | $\delta C$ | m C | $\delta C$ | m C | $\delta C$ | m C | $\delta C$          | m C |
| 1'''        | 169.88     | s   | -          | -   | 172.29     | s   | 172.42     | s   | 172.43     | s   | 172.44     | s   | 172.45              | s   |
| 2'''        | 20.12      | q   | -          | -   | 35.25      | t   | 33.19      | t   | 33.24      | t   | 33.24      | t   | 33.24               | t   |
| 3'''        | -          | -   | -          | -   | 17.81      | t   | 23.92      | t   | 24.24      | t   | 24.23      | t   | 24.24               | t   |
| 4'''        | -          | -   | -          | -   | 13.19      | q   | 30.51      | t   | 28.27      | t   | 28.31      | t   | 28.32               | t   |
| 5'''        | -          | -   | -          | -   | -          | -   | 21.61      | t   | 28.18      | t   | 28.52      | t   | 28.53               | t   |
| 6'''        | -          | -   | -          | -   | -          | -   | 13.75      | d   | 31.09      | t   | 28.73      | t   | 28.74               | t   |
| 7'''        | -          | -   | -          | -   | -          | -   | -          | -   | 22.03      | t   | 28.86      | t   | 28.87               | t   |
| 8'''        | -          | -   | -          | -   | -          | -   | -          | -   | 13.95      | q   | 29.00      | t   | 29.00               | t   |
| 9'''        | -          | -   | -          | -   | -          | -   | -          | -   | -          | -   | 29.02      | t   | 29.05               | t   |
| 10'''       | -          | -   | -          | -   | -          | -   | -          | -   | -          | -   | 31.33      | t   | 29.06               | t   |
| 11'''       | -          | -   | -          | -   | -          | -   | -          | -   | -          | -   | 22.12      | t   | -                   | -   |
| 12'''       | -          | -   | -          | -   | -          | -   | -          | -   | -          | -   | 13.98      | q   | 29.09 <sup>3C</sup> | t   |
| 13'''       | -          | -   | -          | -   | -          | -   | -          | -   | -          | -   | -          | -   | -                   | -   |
| 14'''       | -          | -   | -          | -   | -          | -   | -          | -   | -          | -   | -          | -   | 31.33               | t   |
| 15'''       | -          | -   | -          | -   | -          | -   | -          | -   | -          | -   | -          | -   | 22.12               | t   |
| 16'''       | -          | -   | -          | -   | -          | -   | -          | -   | -          | -   | -          | -   | 13.97               | q   |

<sup>3C</sup> ... three overlapped carbon signals.

**Table S2.** <sup>1</sup>H NMR data of prepared compounds **2** and **3** (DMSO-*d*<sub>6</sub>, 30 °C).

| Comp.         | <b>2</b>    |        |     |    | <b>3</b>  |        |     |     |               |
|---------------|-------------|--------|-----|----|-----------|--------|-----|-----|---------------|
|               | Atom Number | δ H    | n H | m  | J [Hz]    | δ H    | n H | m   | J [Hz]        |
| <b>2</b>      |             | -      | -   | -  | -         | -      | -   | -   | -             |
| <b>3</b>      |             | -      | -   | -  | -         | -      | -   | -   | -             |
| <b>4</b>      |             | -      | -   | -  | -         | -      | -   | -   | -             |
| <b>4a</b>     |             | -      | -   | -  | -         | -      | -   | -   | -             |
| <b>5</b>      |             | -      | -   | -  | -         | -      | -   | -   | -             |
| <b>6</b>      |             | 6.201  | 1   | d  | 2.1       | 6.210  | 1   | d   | 2.0           |
| <b>7</b>      |             | -      | -   | -  | -         | -      | -   | -   | -             |
| <b>8</b>      |             | 6.409  | 1   | d  | 2.1       | 6.414  | 1   | d   | 2.0           |
| <b>8a</b>     |             | -      | -   | -  | -         | -      | -   | -   | -             |
| <b>1'</b>     |             | -      | -   | -  | -         | -      | -   | -   | -             |
| <b>2'</b>     |             | -      | -   | -  | -         | -      | -   | -   | -             |
| <b>3'</b>     |             | 7.528  | 1   | d  | 2.2       | 7.543  | 1   | d   | 2.2           |
| <b>4'</b>     |             | -      | -   | -  | -         | -      | -   | -   | -             |
| <b>5'</b>     |             | 7.531  | 1   | dd | 9.0, 2.2  | 7.509  | 1   | dd  | 2.2, 8.4      |
| <b>6'</b>     |             | 6.832  | 1   | d  | 9.0       | 6.841  | 1   | d   | 8.4           |
| <b>1''</b>    |             | 5.372  | 1   | d  | 7.5       | 5.482  | 1   | d   | 7.7           |
| <b>2''</b>    |             | 3.27 H | 1   | m  | -         | 3.47 * | 1   | ddd | 7.7, 4.9, 9.3 |
| <b>3''</b>    |             | 3.25 H | 1   | m  | -         | 4.849  | 1   | dd  | 9.3, 9.3      |
| <b>4''</b>    |             | 3.147  | 1   | t  | 9.0       | 3.389  | 1   | ddd | 6.2, 9.3, 9.5 |
| <b>5''</b>    |             | 3.30 H | 1   | m  | -         | 3.46 * | 1   | ddd | 2.2, 5.6, 9.5 |
| <b>6''</b>    |             | 4.125  | 1   | dd | 11.8, 2.2 | 4.115  | 1   | dd  | 2.2, 11.9     |
|               |             | 3.941  | 1   | dd | 11.8, 6.1 | 3.983  | 1   | dd  | 5.6, 11.9     |
| <b>5-OH</b>   |             | 12.595 | 1   | s  | -         | 12.566 | 1   | s   | -             |
| <b>7-OH</b>   |             | n.a.   | -   | -  | -         | n.a.   | -   | -   | -             |
| <b>1'-OH</b>  |             | n.a.   | -   | -  | -         | n.a.   | -   | -   | -             |
| <b>2'-OH</b>  |             | n.a.   | -   | -  | -         | n.a.   | -   | -   | -             |
| <b>2''-OH</b> |             | n.a.   | -   | -  | -         | 5.649  | 1   | d   | 4.9           |
| <b>4''-OH</b> |             | n.a.   | -   | -  | -         | 5.400  | 1   | d   | 6.2           |
| <b>3''-CO</b> |             | -      | -   | -  | -         | -      | -   | -   | -             |
| <b>3''-Ac</b> |             | -      | -   | -  | -         | 2.056  | 3   | s   | -             |
| <b>6''-CO</b> |             | -      | -   | -  | -         | -      | -   | -   | -             |
| <b>6''-Ac</b> |             | 1.730  | 3   | s  | -         | 1.757  | 3   | s   | -             |

n.a.—not assigned due to lack of conclusive correlation from broadened OH signals; \*—HSQC readout.

Table S3. <sup>1</sup>H NMR data of prepared compounds 4–8 (DMSO-*d*<sub>6</sub>, 30 °C).

| Comp.                    | 4        |     |       |           | 5         |     |    |           | 6      |     |    |           | 7      |     |    |           | 8      |     |     |               |
|--------------------------|----------|-----|-------|-----------|-----------|-----|----|-----------|--------|-----|----|-----------|--------|-----|----|-----------|--------|-----|-----|---------------|
| Atom Number              | δ H      | n H | m     | J [Hz]    | δ H [ppm] | n H | m  | J [Hz]    | δ H    | n H | m  | J [Hz]    | δ H    | n H | m  | J [Hz]    | δ H    | n H | m   | J [Hz]        |
| 2                        | -        | -   | -     | -         | -         | -   | -  | -         | -      | -   | -  | -         | -      | -   | -  | -         | -      | -   | -   | -             |
| 3                        | -        | -   | -     | -         | -         | -   | -  | -         | -      | -   | -  | -         | -      | -   | -  | -         | -      | -   | -   | -             |
| 4                        | -        | -   | -     | -         | -         | -   | -  | -         | -      | -   | -  | -         | -      | -   | -  | -         | -      | -   | -   | -             |
| 4a                       | -        | -   | -     | -         | -         | -   | -  | -         | -      | -   | -  | -         | -      | -   | -  | -         | -      | -   | -   | -             |
| 5                        | -        | -   | -     | -         | -         | -   | -  | -         | -      | -   | -  | -         | -      | -   | -  | -         | -      | -   | -   | -             |
| 6                        | 6.216    | 1   | dd    | 2.0, 0.2  | 6.192     | 1   | d  | 2.0       | 6.189  | 1   | d  | 2.0       | 6.185  | 1   | d  | 2.0       | 6.183  | 1   | d   | 2.1           |
| 7                        | -        | -   | -     | -         | -         | -   | -  | -         | -      | -   | -  | -         | -      | -   | -  | -         | -      | -   | -   | -             |
| 8                        | 6.441    | 1   | dd    | 2.0, 0.9  | 6.839     | 1   | d  | 2.0       | 6.384  | 1   | d  | 2.0       | 6.379  | 1   | d  | 2.0       | 6.381  | 1   | d   | 2.1           |
| 8a                       | -        | -   | -     | -         | -         | -   | -  | -         | -      | -   | -  | -         | -      | -   | -  | -         | -      | -   | -   | -             |
| 1'                       | -        | -   | -     | -         | -         | -   | -  | -         | -      | -   | -  | -         | -      | -   | -  | -         | -      | -   | -   | -             |
| 2'                       | -        | -   | -     | -         | -         | -   | -  | -         | -      | -   | -  | -         | -      | -   | -  | -         | -      | -   | -   | -             |
| 3'                       | 7.542    | 1   | d     | 2.2       | 7.516     | 1   | d  | 2.2       | 7.515  | 1   | d  | 2.1       | 7.516  | 1   | d  | 2.2       | 7.520  | 1   | m   | -             |
| 4'                       | -        | -   | -     | -         | -         | -   | -  | -         | -      | -   | -  | -         | -      | -   | -  | -         | -      | -   | -   | -             |
| 5'                       | 7.521    | 1   | dd    | 8.3, 2.2  | 7.521     | 1   | dd | 2.2, 8.7  | 7.518  | 1   | dd | 2.1, 9.1  | 7.514  | 1   | dd | 2.2, 9.0  | 7.512  | 1   | dd  | 2.2, 8.2      |
| 6'                       | 6.845    | 1   | d     | 8.3       | 6.825     | 1   | d  | 8.7       | 6.824  | 1   | d  | 9.1       | 6.821  | 1   | d  | 9.0       | 6.822  | 1   | m   | -             |
| 1''                      | 5.436    | 1   | d     | 7.6       | 5.436     | 1   | d  | 7.4       | 5.434  | 1   | d  | 7.6       | 5.429  | 1   | d  | 7.6       | 5.428  | 1   | d   | 7.6           |
| 2''                      | 3.26 H   | 1   | m     | -         | 3.265     | 1   | m  | -         | 3.27 H | 1   | m  | -         | 3.26 H | 1   | m  | -         | 3.256  | 1   | m   | -             |
| 3''                      | 3.26 H   | 1   | m     | -         | 3.256     | 1   | m  | -         | 3.26 H | 1   | m  | -         | 3.25 H | 1   | m  | -         | 3.242  | 1   | m   | -             |
| 4''                      | 3.123    | 1   | br.t. | 7.5       | 3.126     | 1   | m  | -         | 3.126  | 1   | m  | -         | 3.12 H | 1   | m  | -         | 3.125  | 1   | dd  | 9.7, 8.5      |
| 5''                      | 3.29 H   | 1   | m     | -         | 3.298     | 1   | m  | -         | 3.30 H | 1   | m  | -         | 3.300  | 1   | m  | -         | 3.297  | 1   | ddd | 9.7, 7.1, 2.2 |
| 6''                      | 4.157    | 1   | dd    | 11.8, 2.2 | 4.155     | 1   | dd | 1.8, 11.8 | 4.155  | 1   | dd | 2.2, 11.7 | 4.152  | 1   | dd | 2.4, 11.7 | 4.149  | 1   | dd  | 11.7, 2.2     |
|                          | 3.940    | 1   | dd    | 11.8, 7.0 | 3.949     | 1   | dd | 7.0, 11.8 | 3.950  | 1   | dd | 7.1, 11.7 | 3.947  | 1   | dd | 7.1, 11.7 | 3.948  | 1   | dd  | 11.7, 7.1     |
| 5-OH                     | 12.612   | 1   | s     | -         | 12.612    | 1   | s  | -         | 12.610 | -   | -  | -         | 12.608 | 1   | s  | -         | 12.607 | 1   | s   | -             |
| 7-OH/<br>1'-OH/<br>2'-OH | 10.962 * | 1   | br.s. | -         | n.a.      | -   | -  | -         | n.a.   | -   | -  | -         | n.a.   | -   | -  | -         | 10.819 | 1   | s   | -             |
| 2''-OH                   | 9.725 *  | 1   | br.s. | -         | n.a.      | -   | -  | -         | n.a.   | -   | -  | -         | n.a.   | -   | -  | -         | 9.655  | 1   | s   | -             |
| 3''-OH                   | 9.249 *  | 1   | br.s. | -         | n.a.      | -   | -  | -         | n.a.   | -   | -  | -         | n.a.   | -   | -  | -         | 9.183  | 1   | s   | -             |
| 4''-OH                   | 5.173    | 1   | br.s. | -         | n.a.      | -   | -  | -         | n.a.   | -   | -  | -         | n.a.   | -   | -  | -         | 5.341  | 1   | s   | -             |
| 5''-OH                   | 5.377    | 1   | br.d  | 2.6       | n.a.      | -   | -  | -         | n.a.   | -   | -  | -         | n.a.   | -   | -  | -         | 5.147  | 1   | s   | -             |
| 6''-OH                   | 5.173    | 1   | br.s. | -         | n.a.      | -   | -  | -         | n.a.   | -   | -  | -         | n.a.   | -   | -  | -         | 5.147  | 1   | s   | -             |

Table S3. Cont.

| Comp.       | 4          |     |   |        | 5                |     |   |        | 6          |     |   |        | 7           |     |   |        | 8          |     |   |        |     |
|-------------|------------|-----|---|--------|------------------|-----|---|--------|------------|-----|---|--------|-------------|-----|---|--------|------------|-----|---|--------|-----|
| Atom Number | $\delta$ H | n H | m | J [Hz] | $\delta$ H [ppm] | n H | m | J [Hz] | $\delta$ H | n H | m | J [Hz] | $\delta$ H  | n H | m | J [Hz] | $\delta$ H | n H | m | J [Hz] |     |
| 1'''        | -          | -   | - | -      | -                | -   | - | -      | -          | -   | - | -      | -           | -   | - | -      | -          | -   | - | -      | -   |
| 2'''        | 1.961      | 2   | m | -      | 1.968            | 2   | m | -      | 1.971      | 2   | m | -      | 1.970       | 2   | m | -      | 1.969      | 2   | m | -      | -   |
| 3'''        | 1.246      | 2   | m | -      | 1.238 H          | 2   | m | -      | 1.24 H     | 2   | m | -      | 1.23 H      | 2   | m | -      | 1.233      | 2   | m | -      | -   |
| 4'''        | 0.649      | 3   | t | 7.4    | 1.030            | 2   | m | -      | 1.05 H     | 2   | m | -      | 1.04 H      | 2   | m | -      | 1.035      | 2   | m | -      | -   |
| 5'''        | -          | -   | - | -      | 1.118            | 2   | m | -      | 1.09 H     | 2   | m | -      | -           | -   | - | -      | 1.078      | 2   | m | -      | -   |
| 6'''        | -          | -   | - | -      | 0.778            | 3   | t | 7.0    | 1.12 H     | 2   | m | -      | -           | -   | - | -      | 1.236      | 2   | m | -      | -   |
| 7'''        | -          | -   | - | -      | -                | -   | - | -      | 1.21 H     | 2   | m | -      | 1.05–1.22 H | 10  | m | -      | 1.142      | 2   | m | -      | -   |
| 8'''        | -          | -   | - | -      | -                | -   | - | -      | 0.837      | 3   | t | 7.2    | -           | -   | - | -      | 1.191      | 2   | m | -      | -   |
| 9'''        | -          | -   | - | -      | -                | -   | - | -      | -          | -   | - | -      | -           | -   | - | -      | 1.210      | 2   | m | -      | -   |
| 10'''       | -          | -   | - | -      | -                | -   | - | -      | -          | -   | - | -      | 1.23 H      | 2   | m | -      | 1.233      | 2   | m | -      | -   |
| 11'''       | -          | -   | - | -      | -                | -   | - | -      | -          | -   | - | -      | 1.25 H      | 2   | m | -      | -          | -   | - | -      | -   |
| 12'''       | -          | -   | - | -      | -                | -   | - | -      | -          | -   | - | -      | 0.857       | 3   | t | 7.1    | 1.233      | 6   | m | -      | -   |
| 13'''       | -          | -   | - | -      | -                | -   | - | -      | -          | -   | - | -      | -           | -   | - | -      | -          | -   | - | -      | -   |
| 14'''       | -          | -   | - | -      | -                | -   | - | -      | -          | -   | - | -      | -           | -   | - | -      | 1.233      | 2   | m | -      | -   |
| 15'''       | -          | -   | - | -      | -                | -   | - | -      | -          | -   | - | -      | -           | -   | - | -      | 1.250      | 2   | m | -      | -   |
| 16'''       | -          | -   | - | -      | -                | -   | - | -      | -          | -   | - | -      | -           | -   | - | -      | 0.849      | 3   | t | -      | 7.1 |

n.a.—not assigned due to lack of conclusive correlation from broadened OH signals; <sup>3</sup>C ... three overlapped carbon signals; \*—HSQC readout.

Table S4. <sup>13</sup>C NMR data of prepared compounds 9–11.

| Comp.       | 9 <sup>a</sup> |     | 10 <sup>b</sup> |     | 11 <sup>c</sup>    |     |
|-------------|----------------|-----|-----------------|-----|--------------------|-----|
| Atom Number | δ C            | m C | δ C             | m C | δ C                | m C |
| 2           | 157.33         | s   | 158.47          | s   | 158.1 <sup>M</sup> | s   |
| 3           | 133.35         | s   | 135.65          | s   | 135.4 <sup>M</sup> | s   |
| 4           | 177.08         | s   | 179.18          | s   | 179.0 <sup>M</sup> | s   |
| 4a          | 103.53         | s   | 105.63          | s   | 105.2 <sup>M</sup> | s   |
| 5           | 159.53         | s   | 163.23          | S   | 163.1 <sup>M</sup> | s   |
| 6           | 99.22          | d   | 100.33          | d   | 100.6 <sup>H</sup> | d   |
| 7           | 164.68         | s   | 166.51          | s   | 167.6 <sup>M</sup> | s   |
| 8           | 94.62          | d   | 95.09           | d   | 95.2 <sup>H</sup>  | d   |
| 8a          | 156.11         | s   | 158.12          | s   | 158.2 <sup>M</sup> | s   |
| 9           | 147.40         | s   | 151.27          | s   | 151.4 <sup>M</sup> | s   |
| 10          | 143.22         | s   | 147.38          | s   | 147.4 <sup>M</sup> | s   |
| 11          | 116.42         | d   | 118.13          | d   | 118.0 <sup>H</sup> | d   |
| 12          | 121.38         | s   | 122.83          | s   | 122.6 <sup>M</sup> | s   |
| 13          | 122.26         | d   | 123.28          | d   | 123.1 <sup>H</sup> | d   |
| 14          | 114.99         | d   | 116.62          | d   | 116.6 <sup>H</sup> | d   |
| 1'          | 102.07         | d   | 104.77          | d   | 104.5 <sup>H</sup> | d   |
| 2'          | 73.56          | d   | 76.46           | d   | 76.3 <sup>H</sup>  | d   |
| 3'          | 75.34          | d   | 78.91           | d   | 78.9 <sup>H</sup>  | d   |
| 4'          | 69.24          | d   | 71.65           | d   | 71.8 <sup>H</sup>  | d   |
| 5'          | 73.18          | d   | 76.29           | d   | 76.2 <sup>H</sup>  | d   |
| 6'          | 62.66          | t   | 64.69           | t   | 64.7 <sup>H</sup>  | t   |
| 5-OH        | -              | -   | -               | -   | -                  | -   |
| 7-OH        | -              | -   | -               | -   | -                  | -   |
| 9-OH        | -              | -   | -               | -   | -                  | -   |
| 10-OH       | -              | -   | -               | -   | -                  | -   |
| 2'-OH       | -              | -   | -               | -   | -                  | -   |
| 3'-OH       | -              | -   | -               | -   | -                  | -   |
| 4'-OH       | -              | -   | -               | -   | -                  | -   |
| 1''         | 175.30         | s   | 173.77          | s   | 174.0 <sup>M</sup> | s   |
| 2''         | 32.96          | t   | 34.42           | t   | 34.7 <sup>H</sup>  | t   |
| 3''         | 20.85          | t   | 25.30           | t   | 25.5 <sup>H</sup>  | t   |
| 4''         | 36.37          | t   | 25.53           | t   | 29.6 <sup>H</sup>  | t   |
| 5''         | 182.31         | s   | 34.95           | t   | 29.7 <sup>H</sup>  | t   |
| 6''         |                |     | 176.29          | s   | 29.8 <sup>H</sup>  | t   |
| 7''         | -              | -   | -               | -   | 30.0 <sup>H</sup>  | t   |
| 8''         | -              | -   | -               | -   | 29.9 <sup>H</sup>  | t   |
| 9''         | -              | -   | -               | -   | 30.0 <sup>H</sup>  | t   |
| 10''        | -              | -   | -               | -   | 26.7 <sup>H</sup>  | t   |
| 11''        | -              | -   | -               | -   | 37.1 <sup>H</sup>  | t   |
| 12''        | -              | -   | -               | -   | 179.3 <sup>H</sup> | s   |
| 5''-OH      | -              | -   | -               | -   | -                  | -   |
| 6''-OH      | -              | -   | n.d.            | -   | -                  | -   |
| 12''-OH     | -              | -   | -               | -   | -                  | -   |

<sup>a</sup> D<sub>2</sub>O, 293.2 K, 150.94 MHz for <sup>13</sup>C; <sup>b</sup> pyridin, 293.2 K, 150.94 MHz for <sup>13</sup>C; <sup>c</sup> pyridin, 293.2 K, 150.94 MHz for <sup>13</sup>C; H—HSQC readout; M—HMBC readout; n.d.—not detected.

**Table S5.** <sup>1</sup>H NMR data of prepared compounds 9–11.

| Comp.       | 9 <sup>a</sup> |     |       |          | 10 <sup>b</sup> |     |       |               | 11 <sup>c</sup> |     |       |           |
|-------------|----------------|-----|-------|----------|-----------------|-----|-------|---------------|-----------------|-----|-------|-----------|
| Atom Number | δ H            | n H | m     | J [Hz]   | δ H [ppm]       | n H | m     | J [Hz]        | δ H             | n H | m     | J [Hz]    |
| 2           | -              | -   | -     | -        | -               | -   | -     | -             | -               | -   | -     | -         |
| 3           | -              | -   | -     | -        | -               | -   | -     | -             | -               | -   | -     | -         |
| 4           | -              | -   | -     | -        | -               | -   | -     | -             | -               | -   | -     | -         |
| 4a          | -              | -   | -     | -        | -               | -   | -     | -             | -               | -   | -     | -         |
| 5           | -              | -   | -     | -        | -               | -   | -     | -             | -               | -   | -     | -         |
| 6           | 5.874          | 1   | br.s. | -        | 6.731           | 1   | d     | 2.0           | 6.738           | 1   | br.s. | -         |
| 7           | -              | -   | -     | -        | -               | -   | -     | -             | -               | -   | -     | -         |
| 8           | 5.852          | 1   | br.s. | -        | 6.694           | 1   | d     | 2.0           | 6.787           | 1   | br.s. | -         |
| 8a          | -              | -   | -     | -        | -               | -   | -     | -             | -               | -   | -     | -         |
| 9           | -              | -   | -     | -        | -               | -   | -     | -             | -               | -   | -     | -         |
| 10          | -              | -   | -     | -        | -               | -   | -     | -             | -               | -   | -     | -         |
| 11          | 7.251          | 1   | br.s. | -        | 8.361           | 1   | d     | 2.1           | 8.361           | 1   | br.s. | -         |
| 12          | -              | -   | -     | -        | -               | -   | -     | -             | -               | -   | -     | -         |
| 13          | 7.032          | 1   | br.d  | 8.4      | 8.113           | 1   | dd    | 8.4, 2.1      | 8.144           | 1   | br.d. | 8.1       |
| 14          | 6.546          | 1   | d     | 8.4      | 7.313           | 1   | d     | 8.4           | 7.328           | 1   | br.d. | 8.1       |
| 1'          | 4.726          | 1   | d     | 7.8      | 6.157           | 1   | m     | -             | 6.206           | 1   | br.d. | 4.8       |
| 2'          | 3.420          | 1   | dd    | 7.8, 9.2 | 4.346           | 1   | m     | -             | 4.355           | 1   | m     | -         |
| 3'          | 3.344          | 1   | dd    | 9.2, 9.0 | 4.346           | 1   | m     | -             | 4.355           | 1   | m     | -         |
| 4'          | 3.283          | 1   | m     | -        | 4.059           | 1   | ddd   | 9.8, 6.0, 2.8 | 4.042           | 1   | m     | -         |
| 5'          | 3.283          | 1   | m     | -        | 4.128           | 1   | ddd   | 9.8, 6.1, 1.9 | 4.169           | 1   | m     | -         |
| 6'          | 3.952          | 2   | m     | -        | 4.841           | 1   | dd    | 11.6, 1.9     | 4.886           | 1   | br.d. | 11.6      |
|             |                |     |       |          | 4.685           | 1   | dd    | 11.6, 6.1     | 4.720           | 1   | dd    | 11.6, 5.8 |
| 5-OH        | n.d.           | -   | -     | -        | 13.205          | 1   | br.s. | -             | n.d.            | -   | -     | -         |
| 7-OH/       | n.d.           | -   | -     | -        | -               | -   | -     | -             | n.d.            | -   | -     | -         |
| 9-OH/       | n.d.           | -   | -     | -        | -               | -   | -     | -             | n.d.            | -   | -     | -         |
| 10-OH       | n.d.           | -   | -     | -        | -               | -   | -     | -             | n.d.            | -   | -     | -         |
| 2'-OH       | n.d.           | -   | -     | -        | -               | -   | -     | -             | n.d.            | -   | -     | -         |
| 3'-OH       | n.d.           | -   | -     | -        | -               | -   | -     | -             | n.d.            | -   | -     | -         |
| 4'-OH       | n.d.           | -   | -     | -        | -               | -   | -     | -             | n.d.            | -   | -     | -         |
| 1''         | -              | -   | -     | -        | -               | -   | -     | -             | n.d.            | -   | -     | -         |
| 2''         | 1.911          | 2   | m     | -        | 2.332           | 1   | m     | -             | -               | -   | -     | -         |
|             |                |     |       |          | 2.269           | 1   | m     | -             | -               | -   | -     | -         |
| 3''         | 1.441          | 2   | m     | -        | 1.672           | 2   | m     | -             | 2.269           | 2   | m     | -         |
| 4''         | 1.898          | 2   | m     | -        | 1.733           | 2   | m     | -             | 1.534           | 2   | m     | -         |
| 5''         | -              | -   | -     | -        | 2.424           | 2   | t     | 7.5           | 1.171           | 2   | m     | -         |
| 6''         | -              | -   | -     | -        | -               | -   | -     | -             | 1.124           | 2   | m     | -         |
| 7''         | -              | -   | -     | -        | -               | -   | -     | -             | 1.138           | 2   | m     | -         |
| 8''         | -              | -   | -     | -        | -               | -   | -     | -             | 1.211           | 2   | m     | -         |
| 9''         | -              | -   | -     | -        | -               | -   | -     | -             | 1.291           | 2   | m     | -         |
| 10''        | -              | -   | -     | -        | -               | -   | -     | -             | 1.473           | 2   | m     | -         |
| 11''        | -              | -   | -     | -        | -               | -   | -     | -             | 1.901           | 2   | m     | -         |
| 12''        | -              | -   | -     | -        | -               | -   | -     | -             | 2.634           | 2   | m     | -         |
| 5''-OH      | n.d.           | -   | -     | -        | n.d.            | -   | -     | -             | -               | -   | -     | -         |
| 6''-OH      | -              | -   | -     | -        | -               | -   | -     | -             | -               | -   | -     | -         |
| 12''-OH     | -              | -   | -     | -        | -               | -   | -     | -             | n.d.            | -   | -     | -         |

<sup>a</sup> D<sub>2</sub>O, 293.2 K, 600.23 MHz for <sup>1</sup>H; <sup>b</sup> pyridin, 293.2 K, 600.23 MHz for <sup>1</sup>H; <sup>c</sup> pyridin, 293.2 K, 600.23 MHz for <sup>1</sup>H; H—HSQC readout; M—HMBC readout; n.d.—not detected.

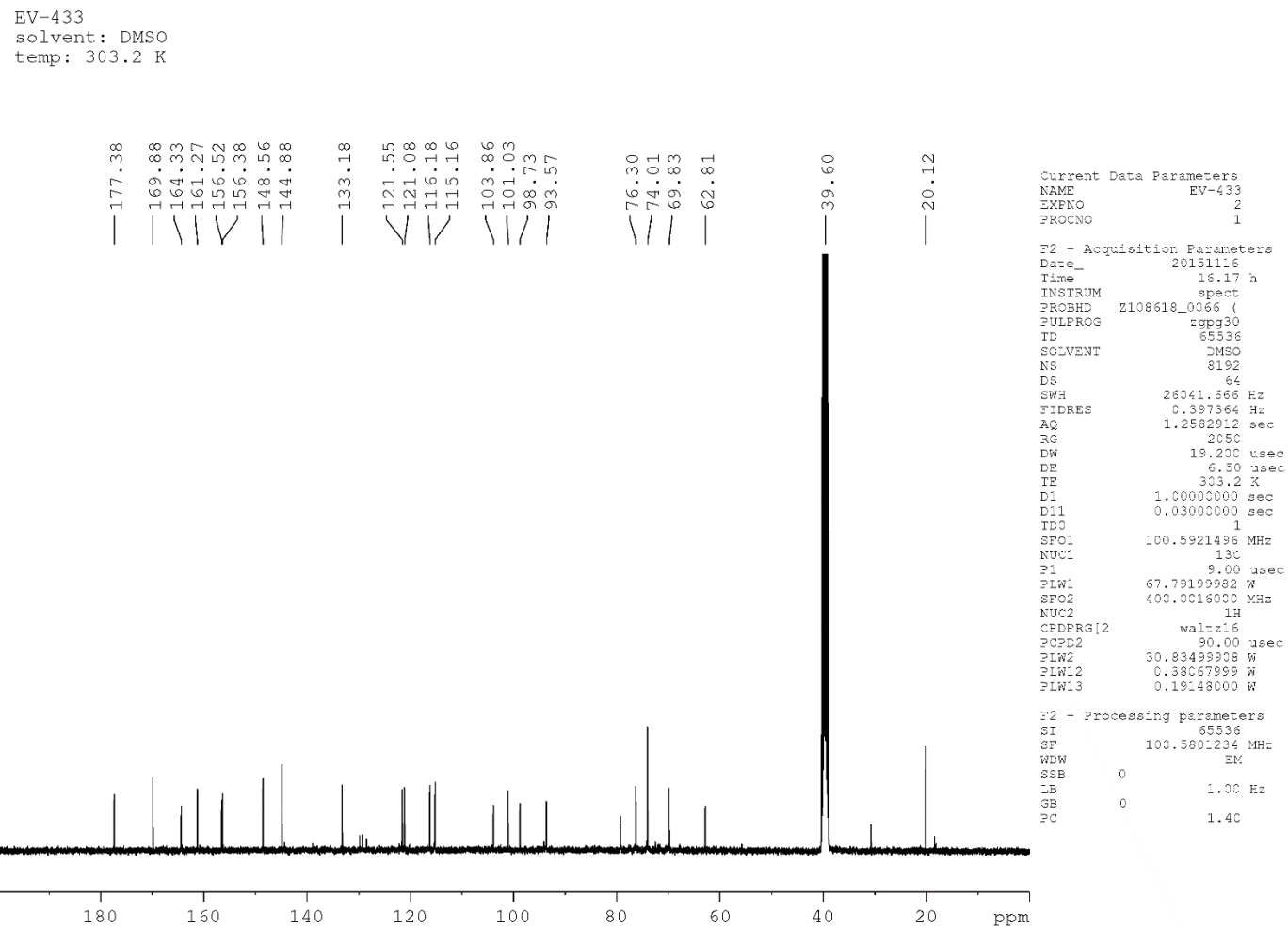


Figure S2. <sup>13</sup>C NMR spectrum of compound 2.

EV-433  
solvent: DMSO  
temp: 303.2 K

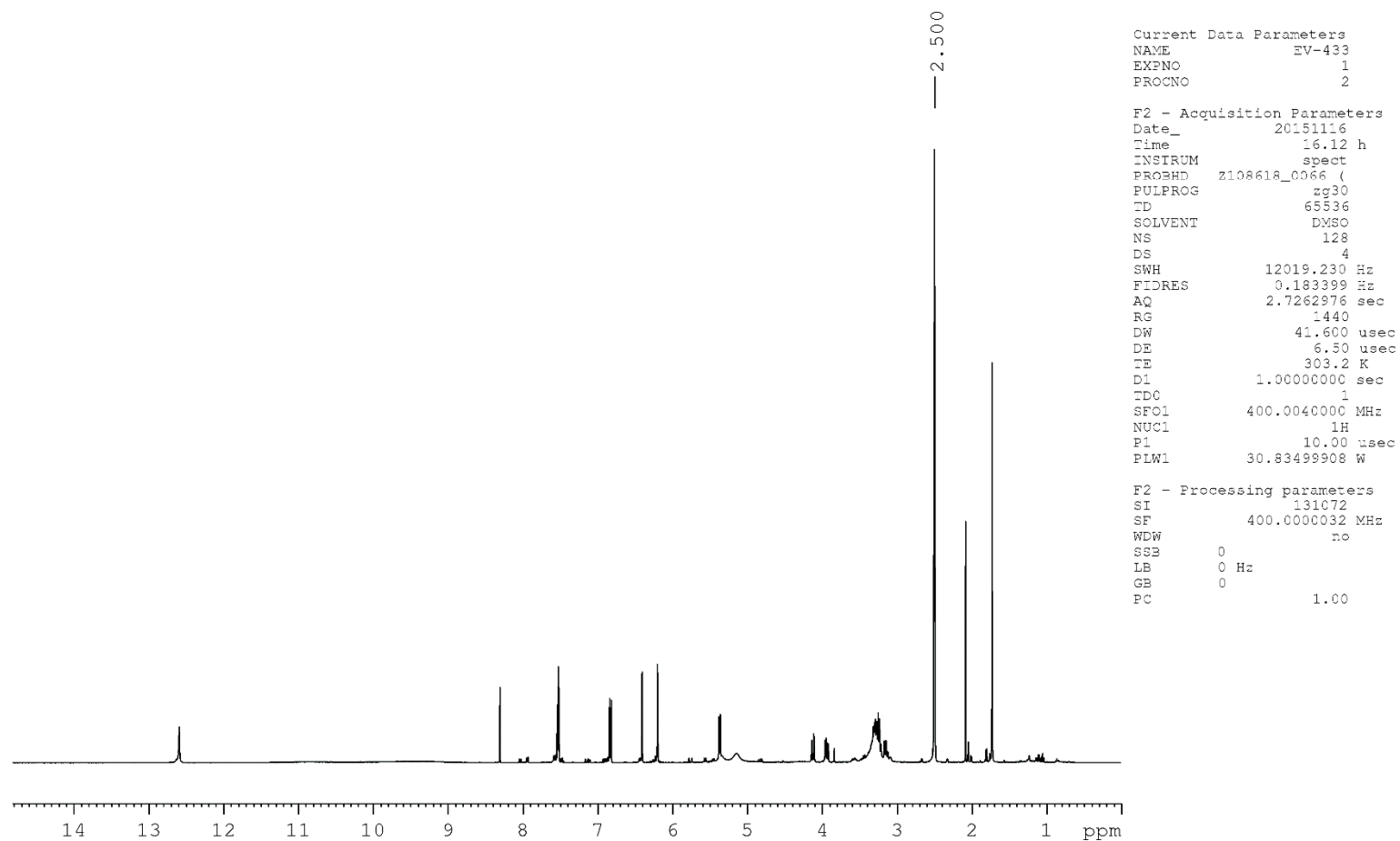


Figure S3. <sup>1</sup>H NMR spectrum of compound 2.



mAU

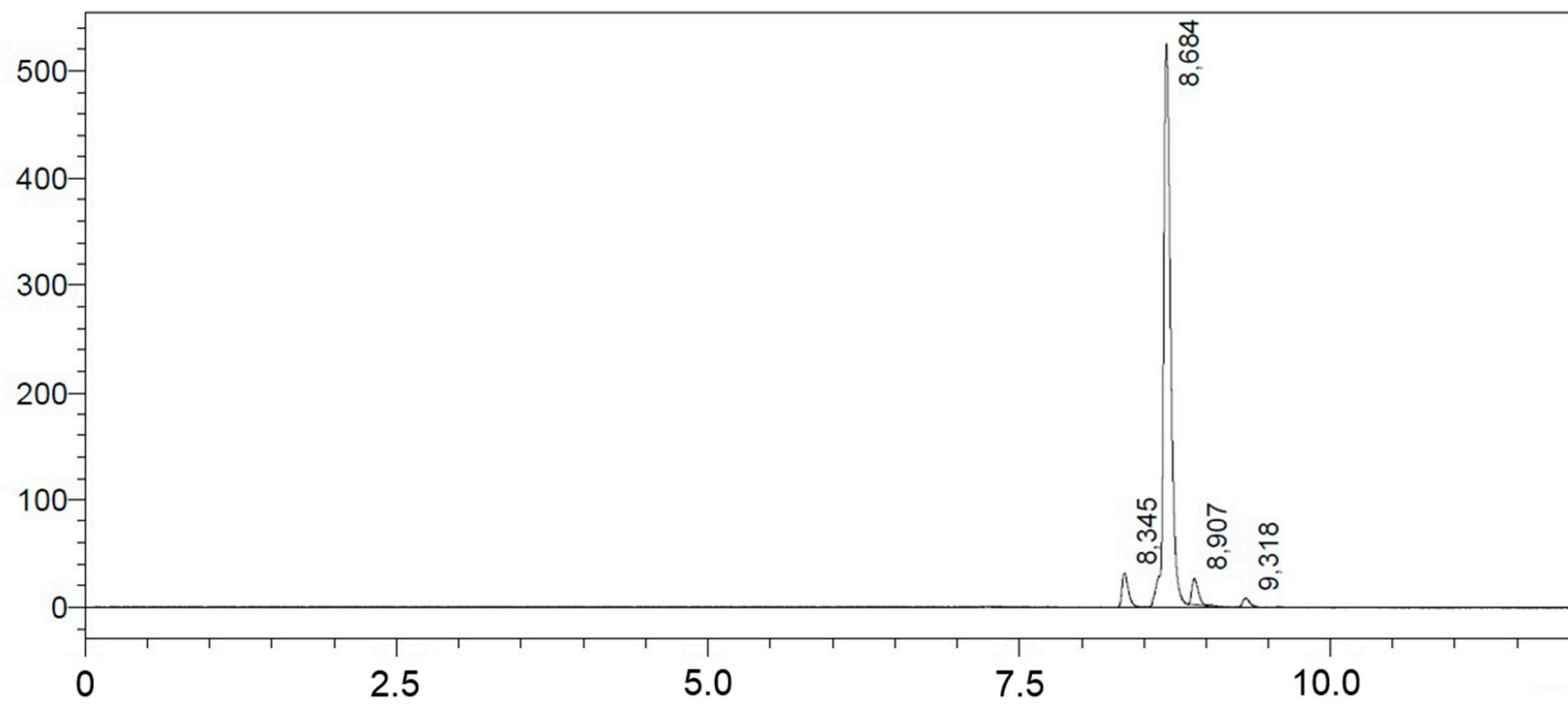


Figure S4. HPLC chromatogram of compound 2.

FL-002  
 solvent: DMSO  
 temp: 303.2 K  
 date: 28 Oct 2013

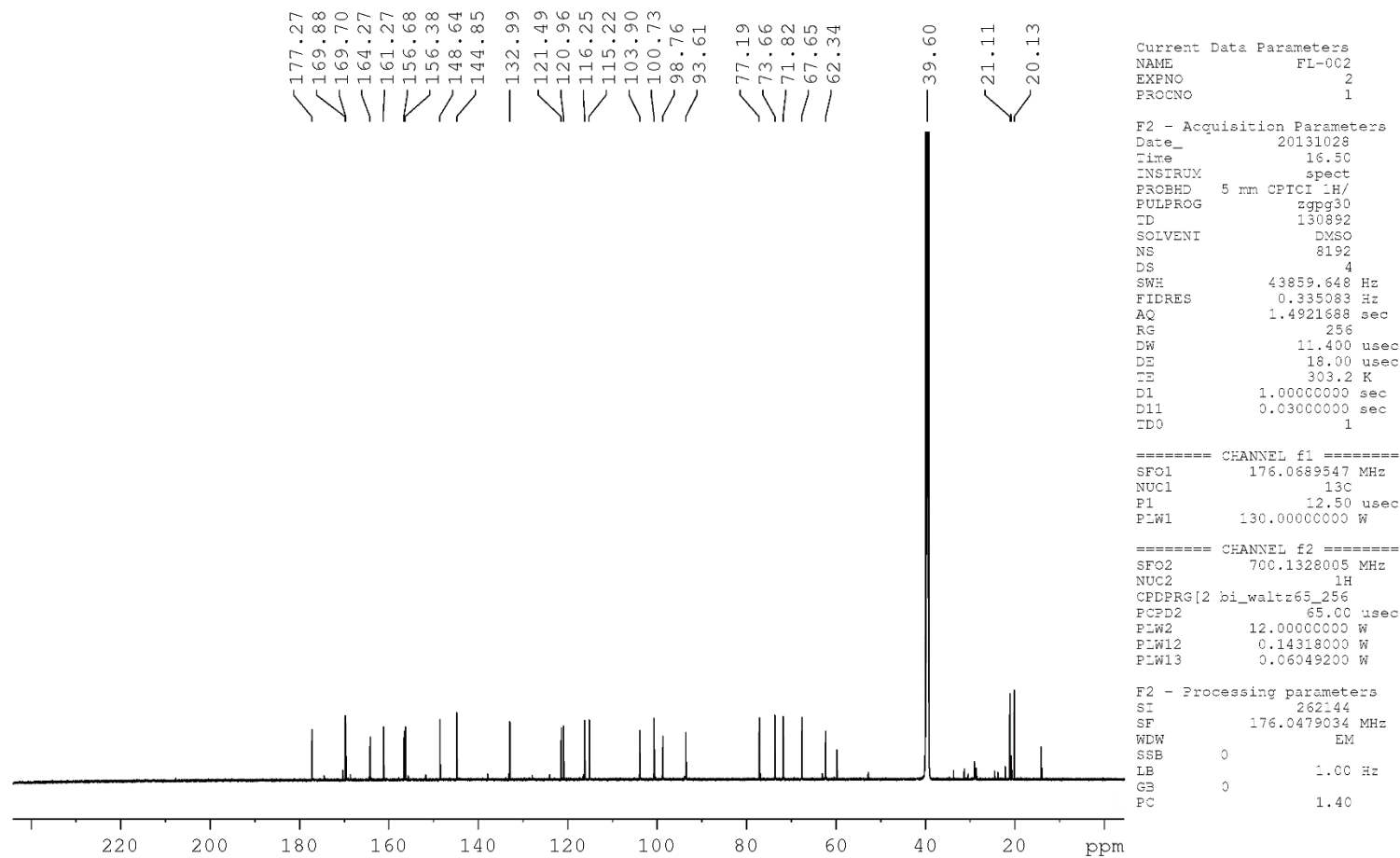


Figure S5. <sup>13</sup>C NMR spectrum of compound 3.

FL-002  
solvent: DMSO  
temp: 303.2 K  
date: 28 Oct 2013

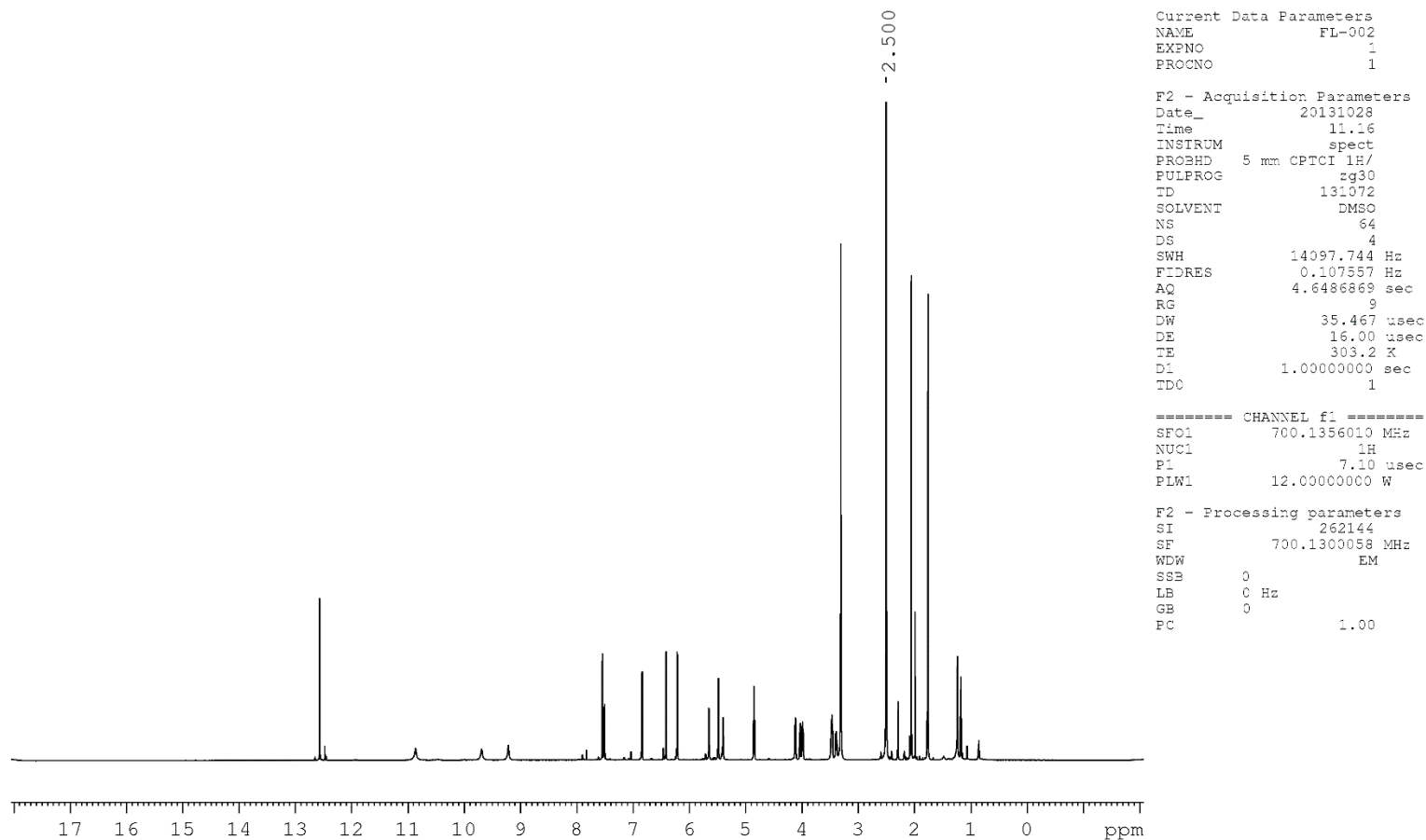


Figure S6. <sup>1</sup>H NMR spectrum of compound 3.

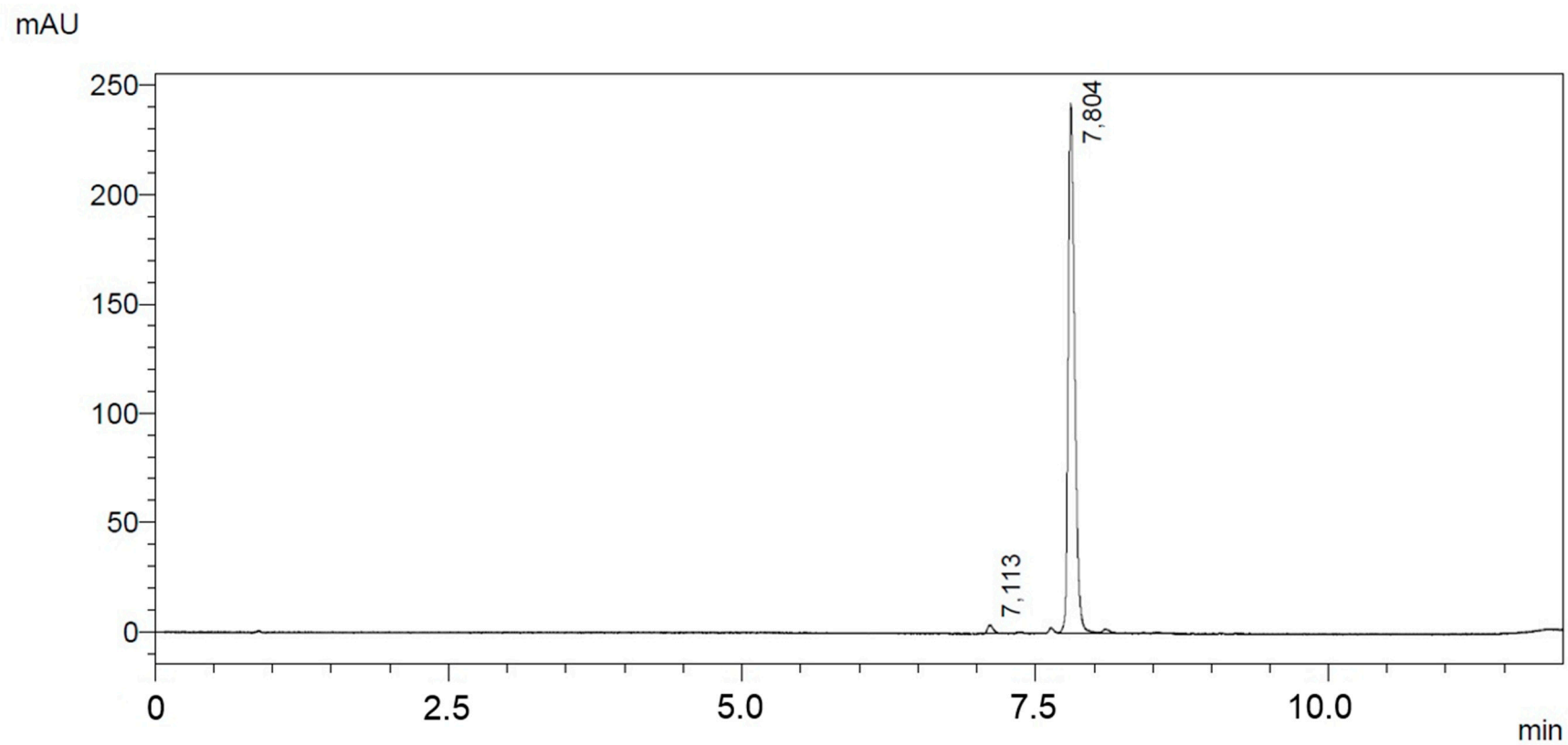


Figure S7. HPLC chromatogram of compound 3.

EV-415  
 solvent: DMSO  
 temp: 303.2 K

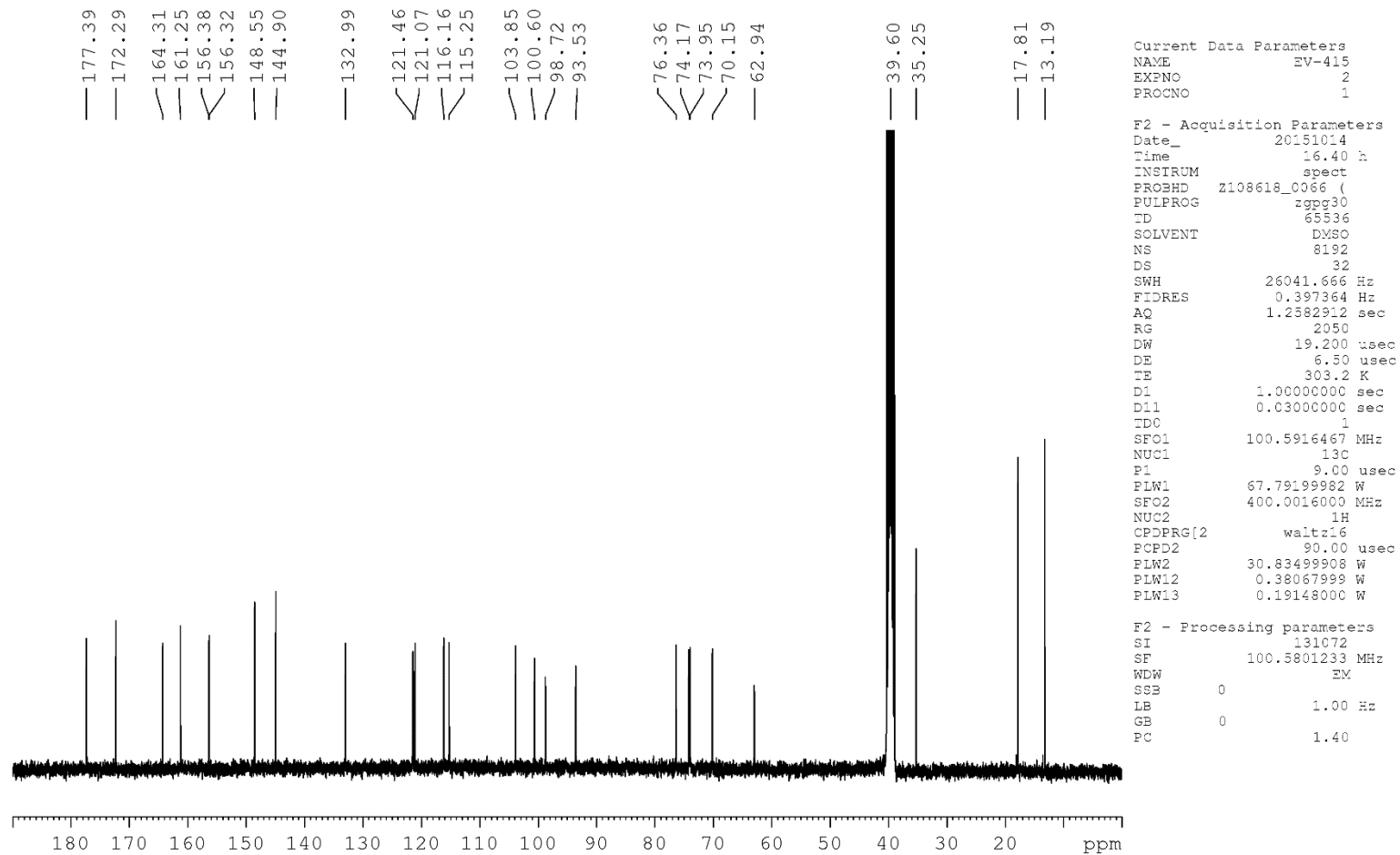


Figure S8.  $^{13}\text{C}$  NMR spectrum of compound 4.

EV-415  
solvent: DMSO  
temp: 303.2 K

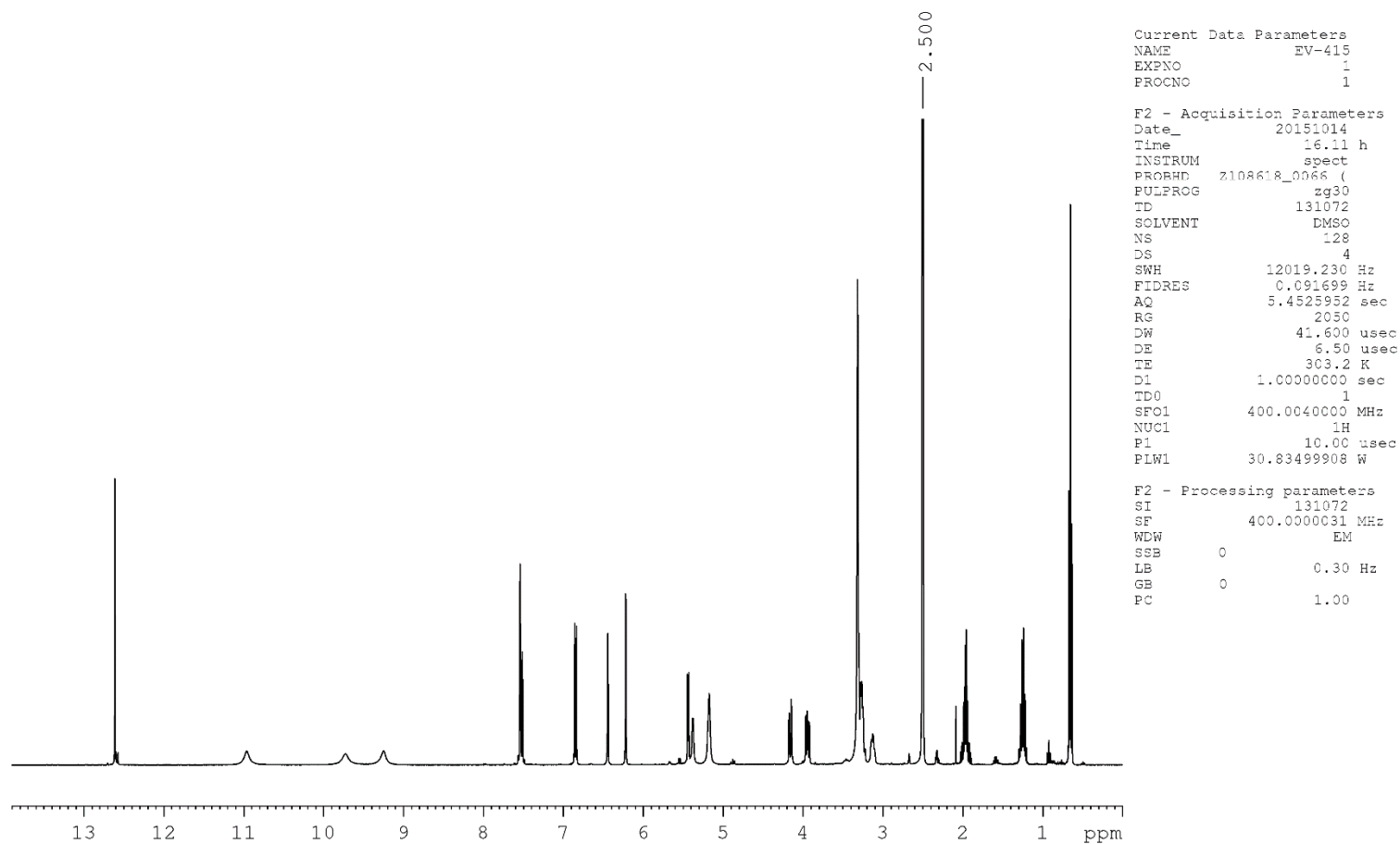


Figure S9. <sup>1</sup>H NMR spectrum of compound 4.

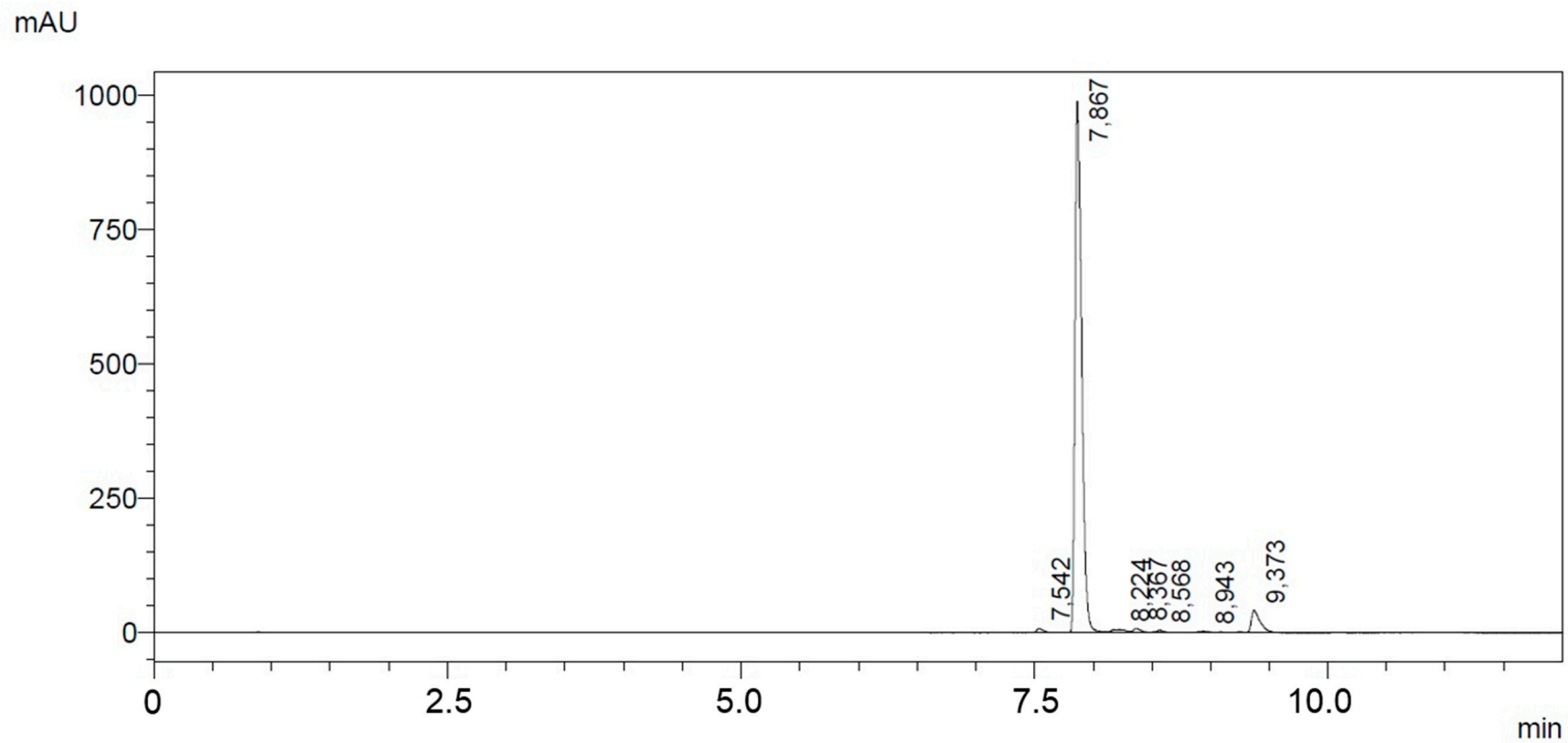
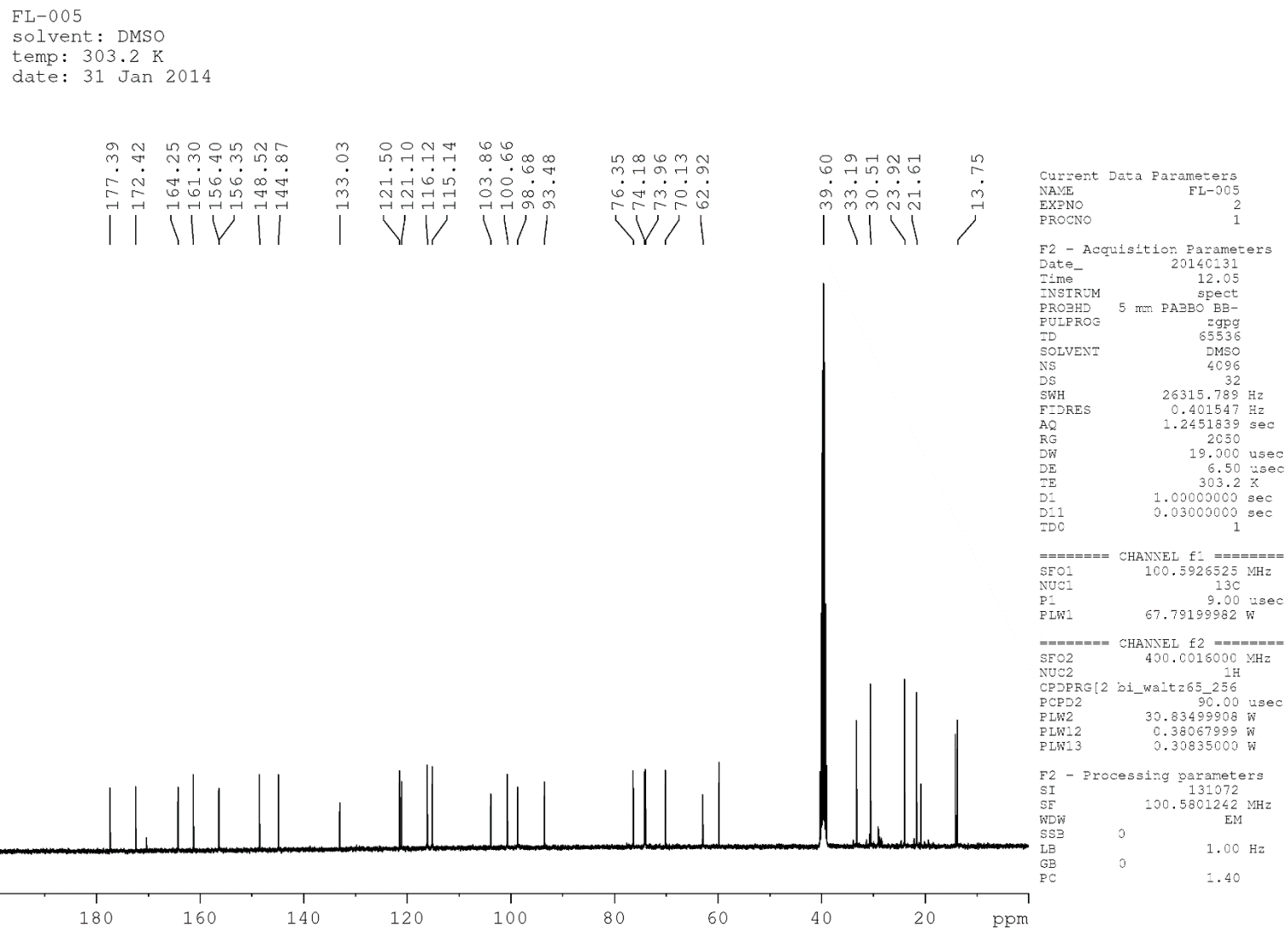


Figure S10. HPLC chromatogram of compound 4.

Figure S11.  $^{13}\text{C}$  NMR spectrum of compound 5.



FL-005  
 solvent: DMSO  
 temp: 303.2 K  
 date: 31 Jan 2014

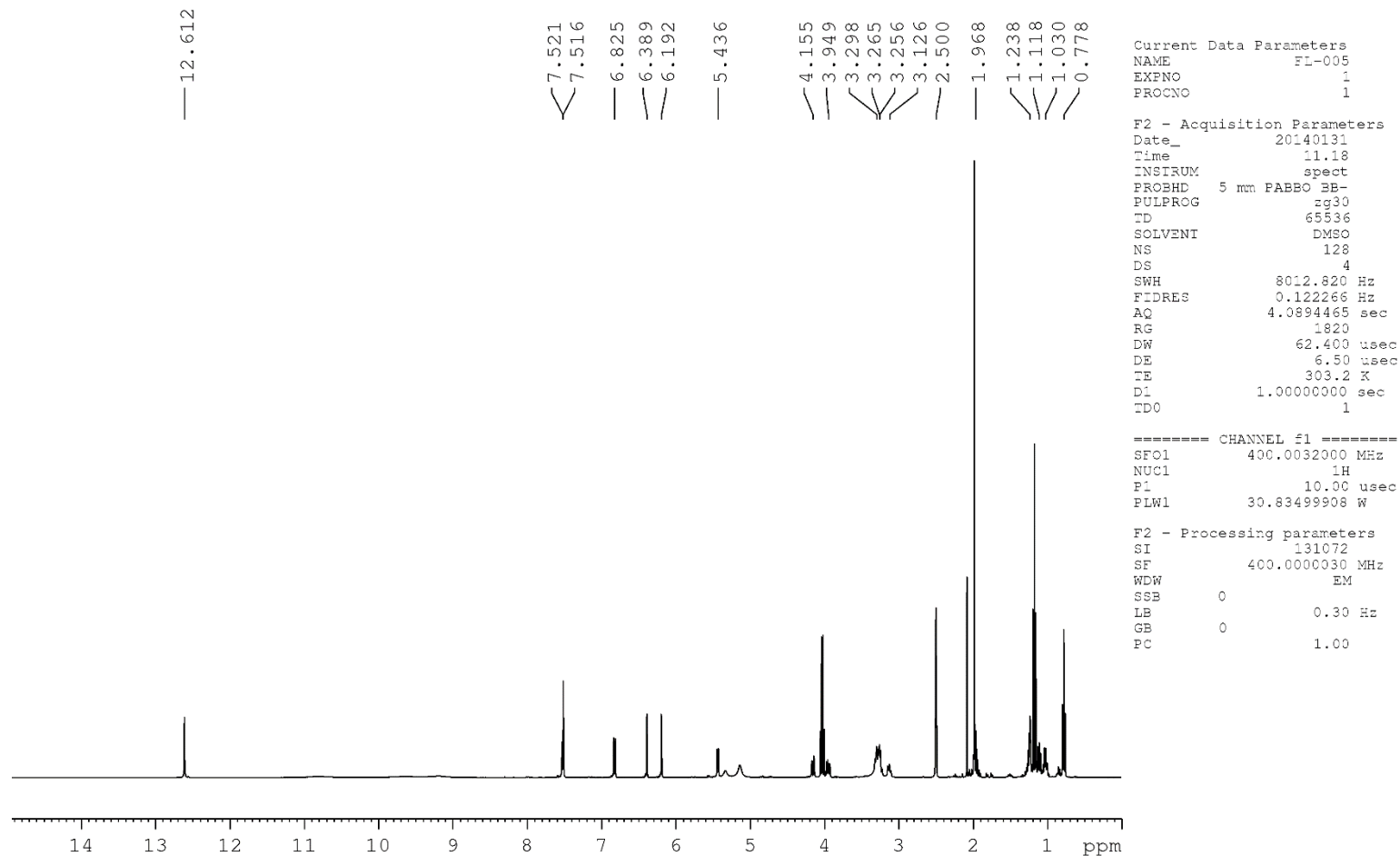


Figure S12. <sup>1</sup>H NMR spectrum of compound 5.

mAU

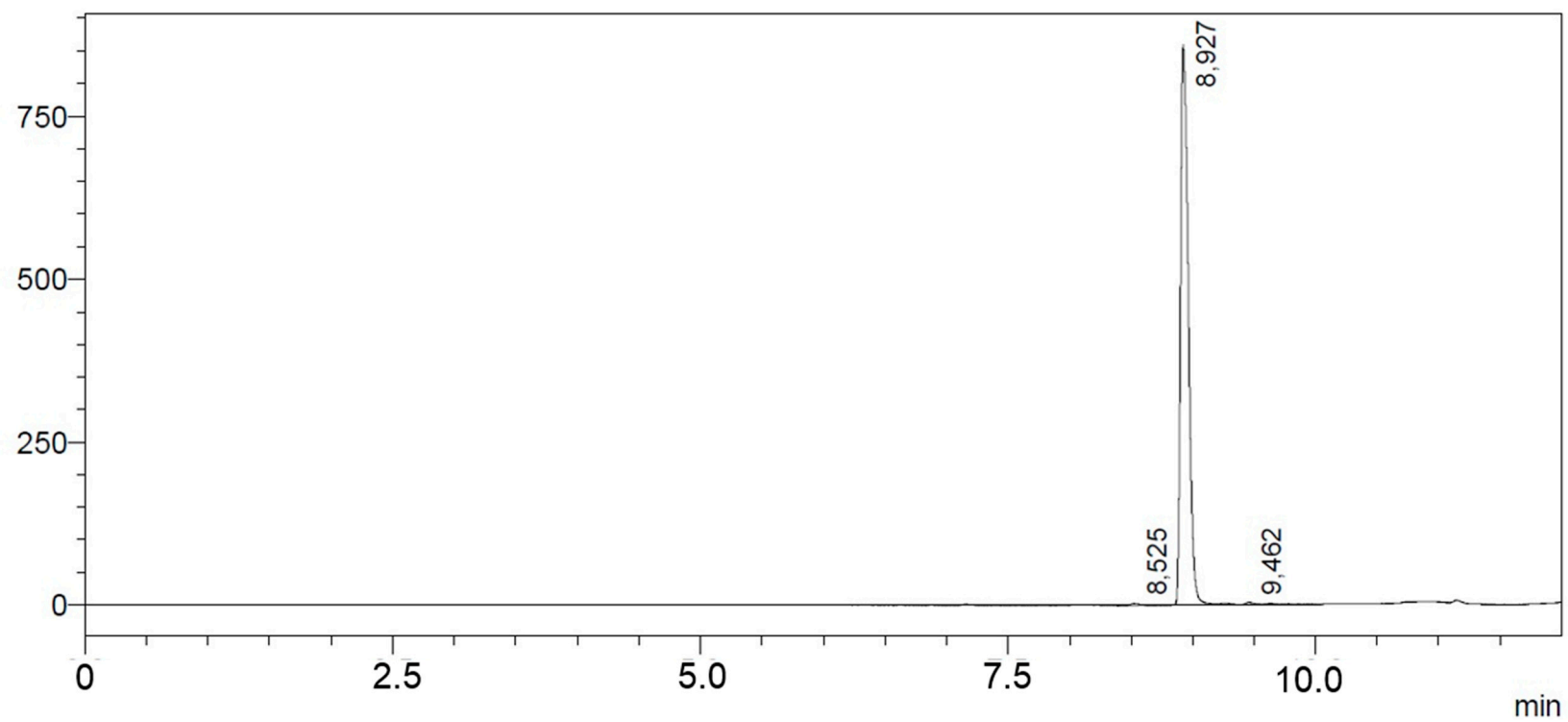


Figure S13. HPLC chromatogram of compound 5.

FL-004  
 solvent: DMSO  
 temp: 303.2 K  
 date: 22 Jan 2014

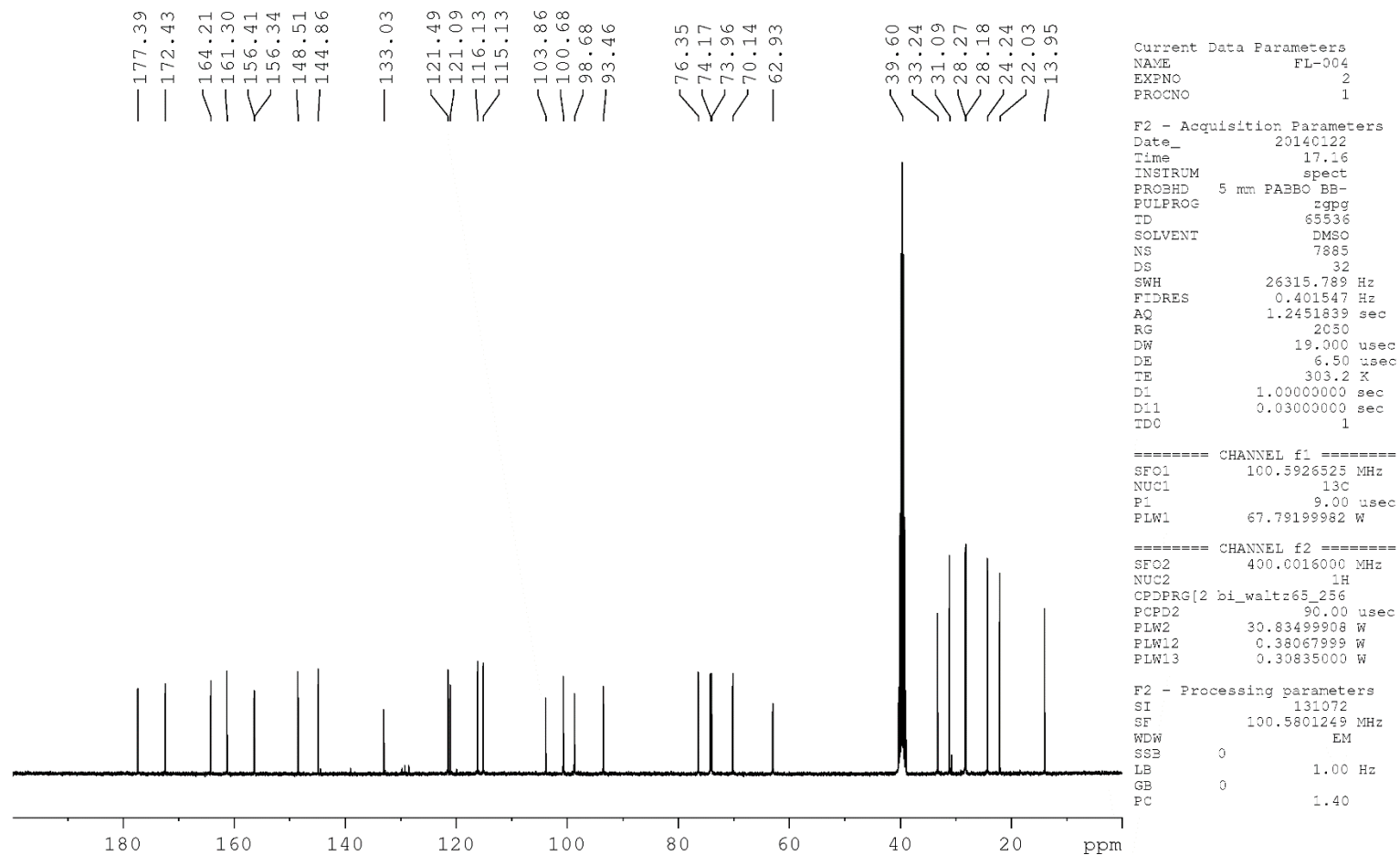


Figure S14. <sup>13</sup>C NMR spectrum of compound 6.

FL-004  
 solvent: DMSO  
 temp: 303.2 K  
 date: 22 Jan 2014

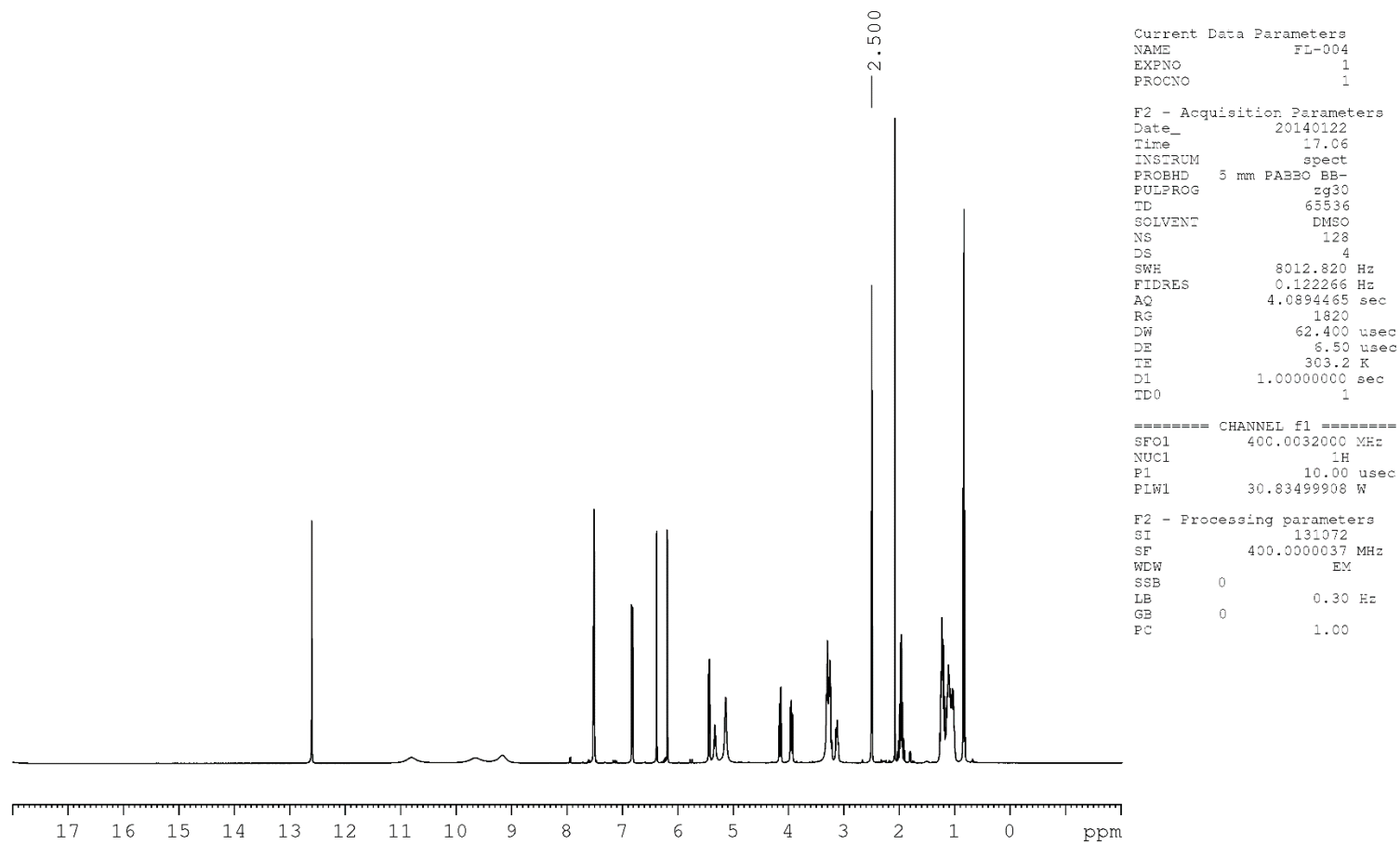


Figure S15. <sup>1</sup>H NMR spectrum of compound 6.

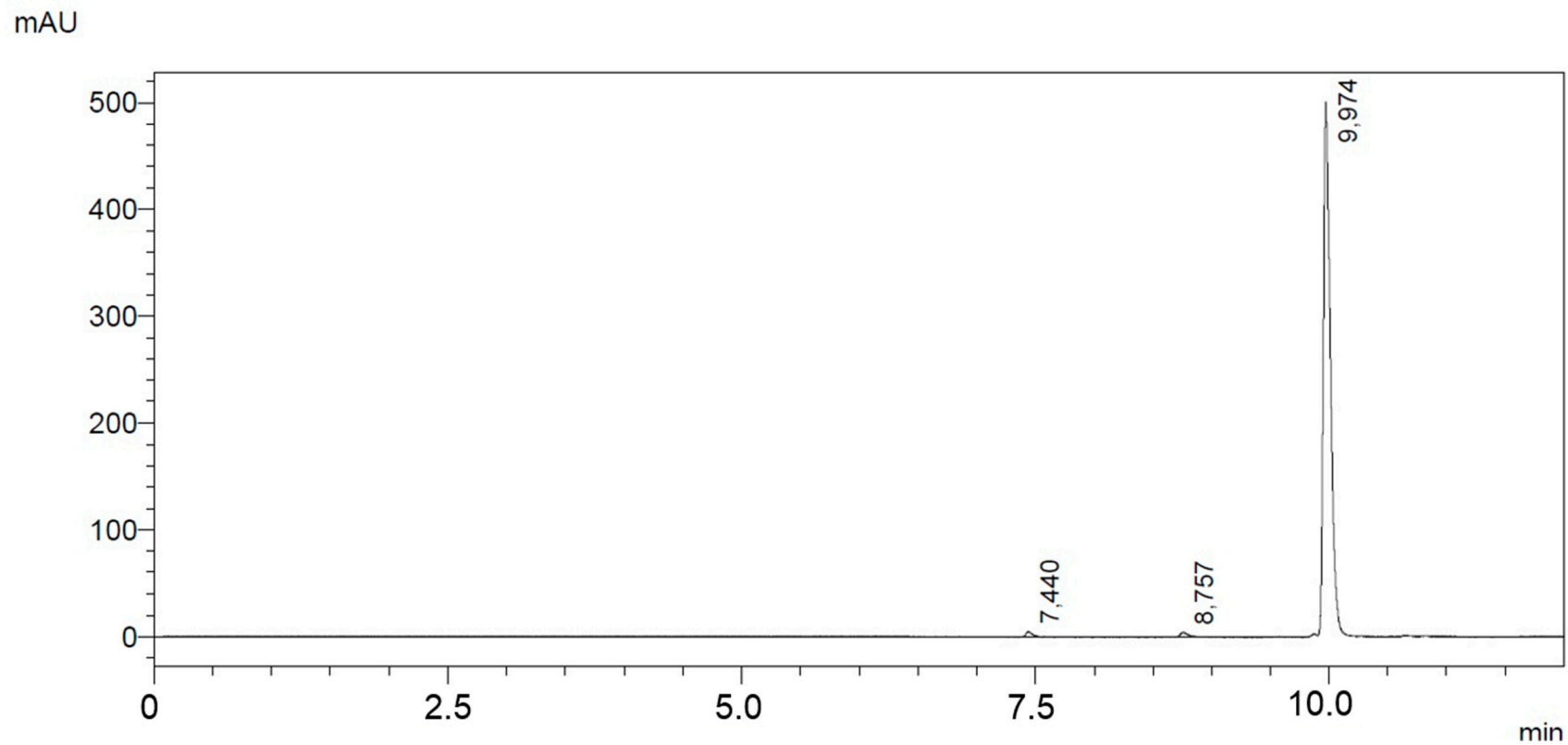


Figure S16. HPLC chromatogram of compound 6.

FL-006  
 solvent: DMSO  
 temp: 303.2 K  
 date: 24 Jan 2014

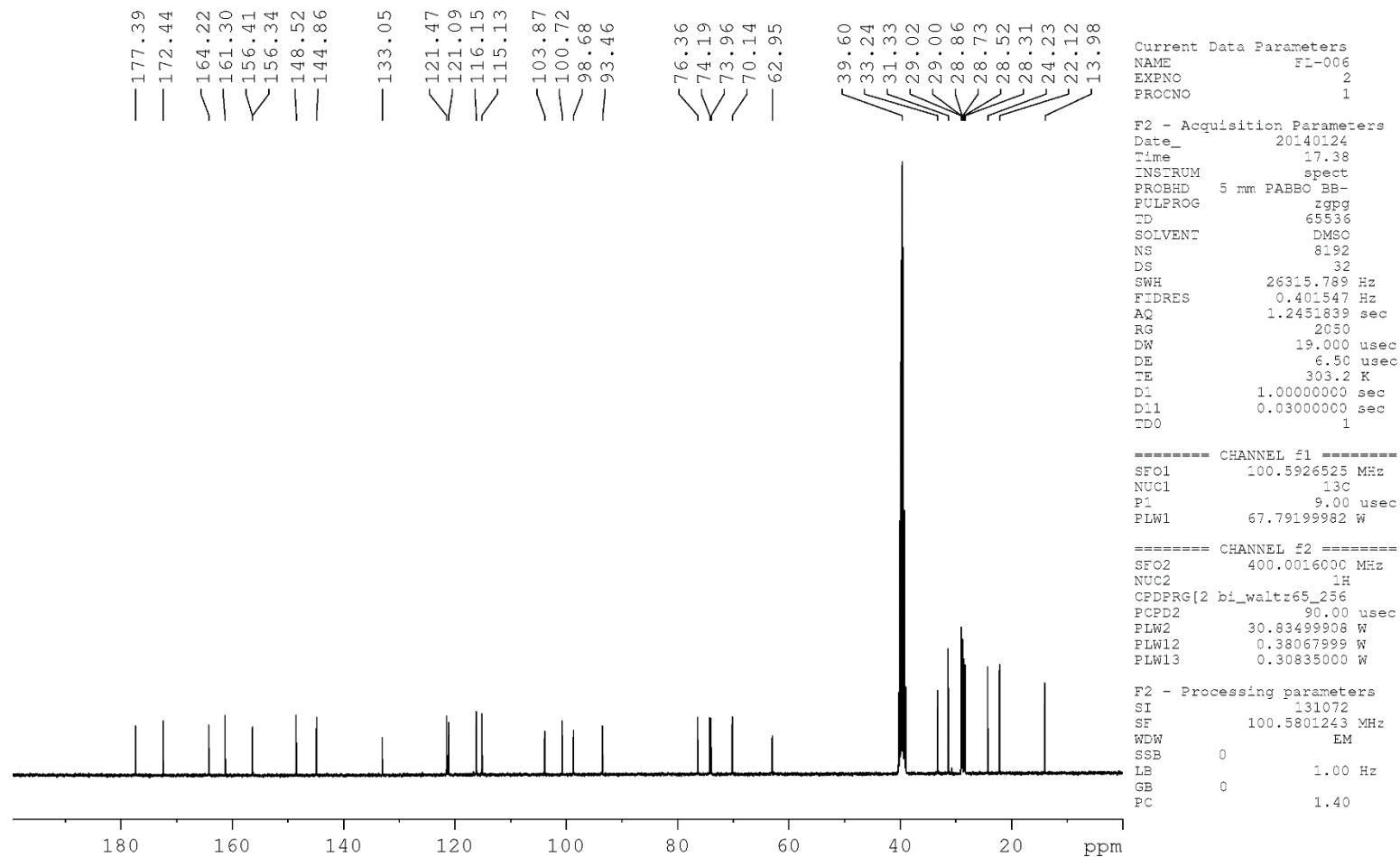


Figure S17. <sup>13</sup>C NMR spectrum of compound 7.

FL-006  
solvent: DMSO  
temp: 303.2 K  
date: 24 Jan 2014

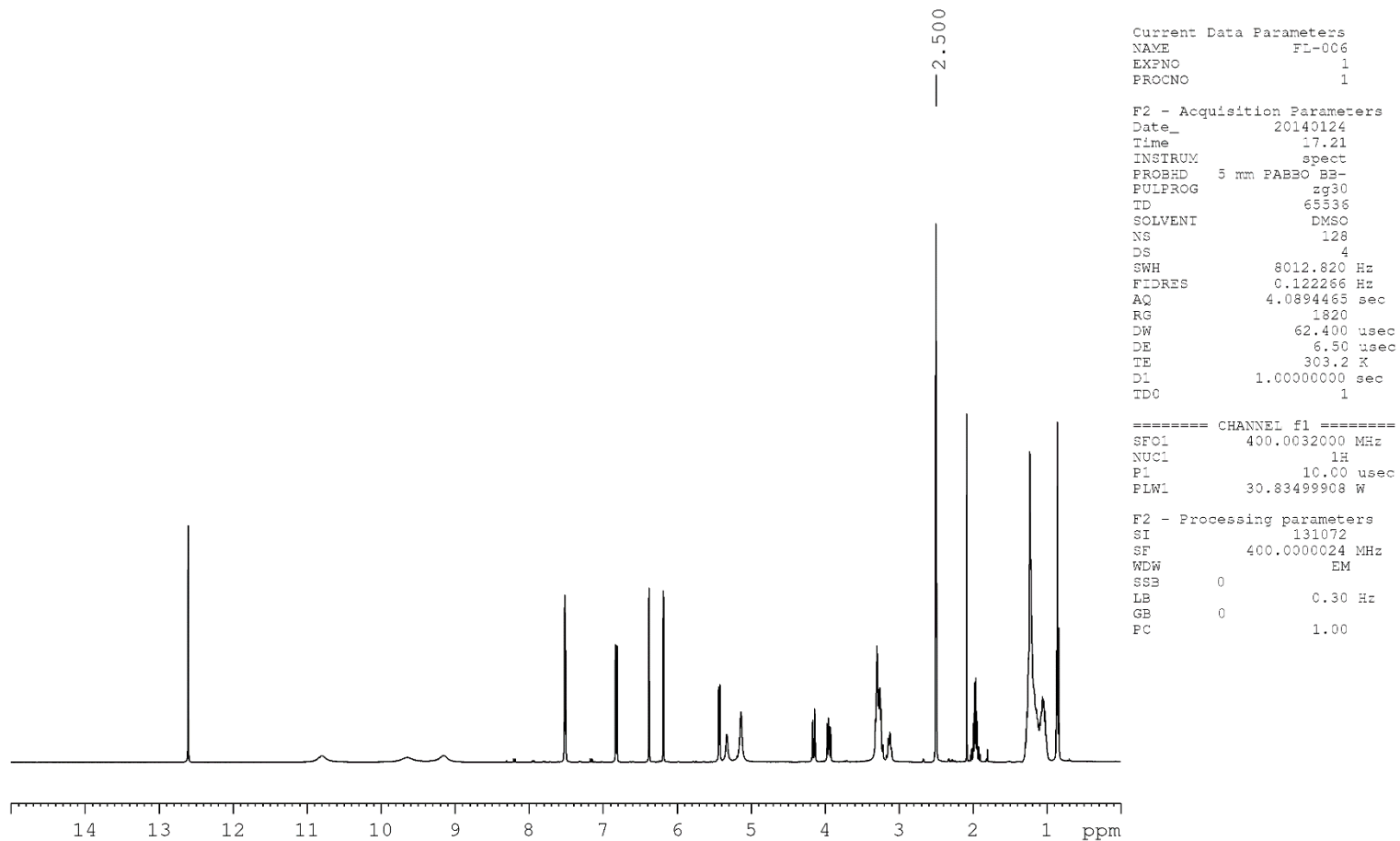


Figure S18. <sup>1</sup>H NMR spectrum of compound 7.

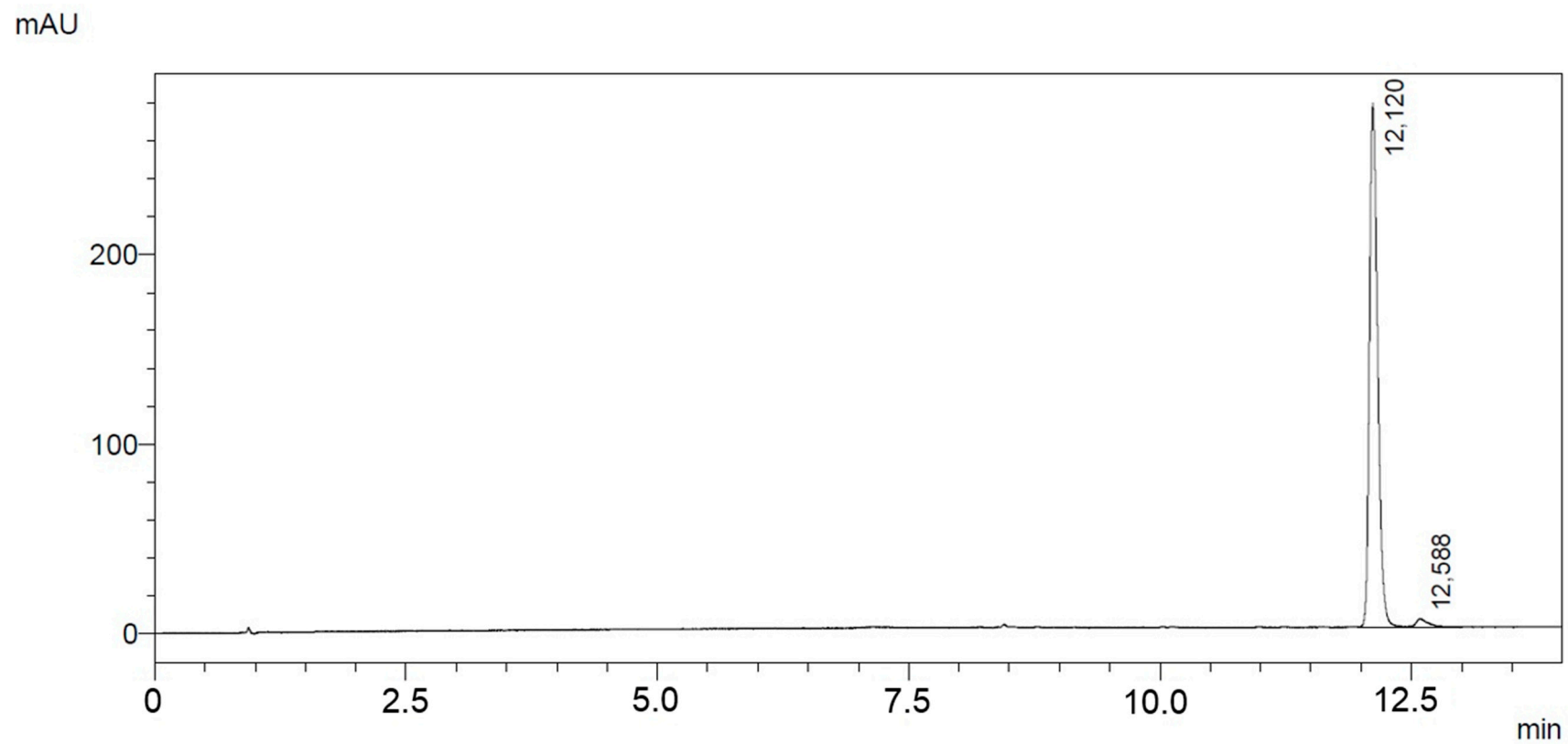


Figure S19. HPLC chromatogram of compound 7.



EV-428  
 solvent: DMSO  
 temp: 303.2 K

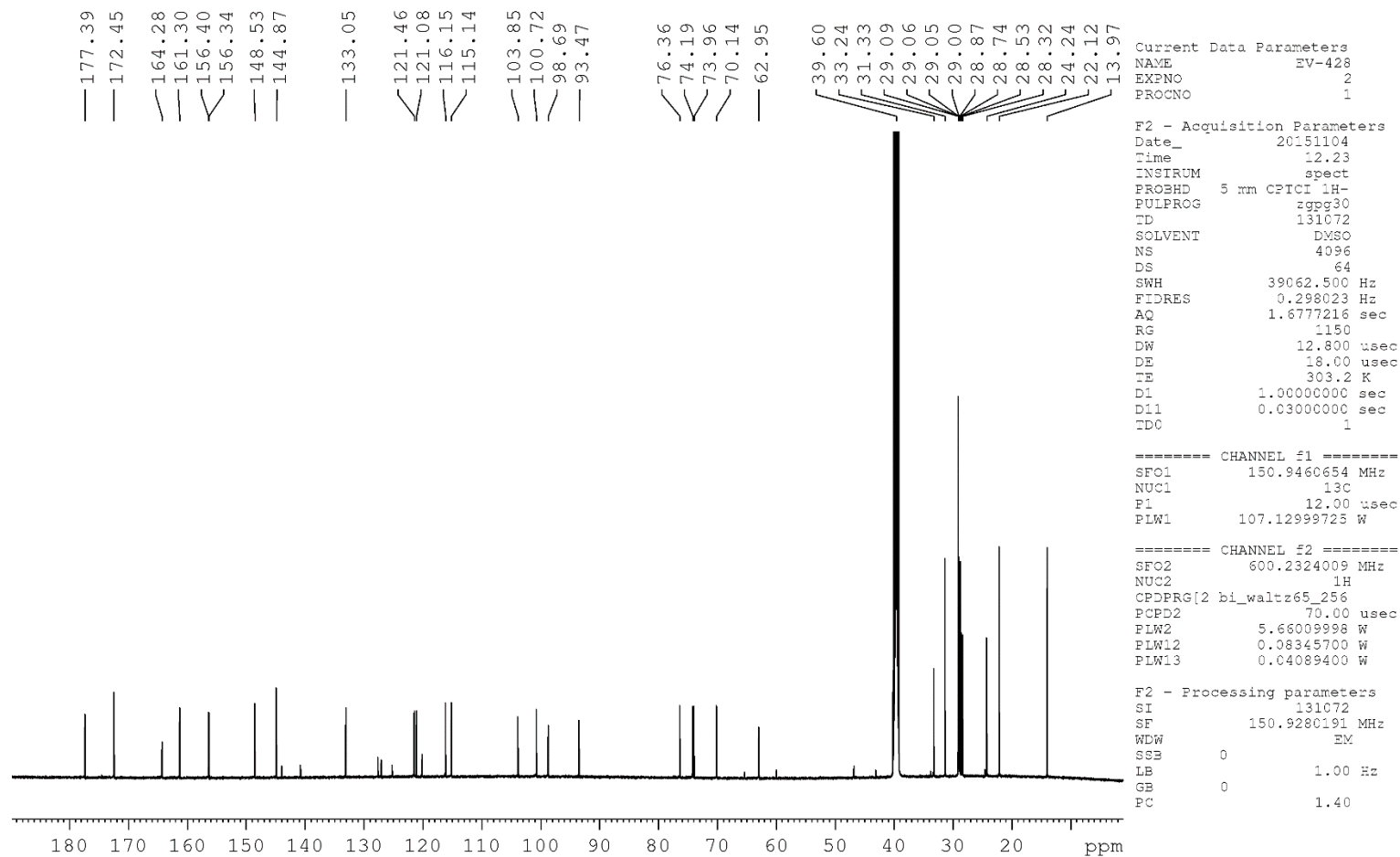


Figure S20. <sup>13</sup>C NMR spectrum of compound 8.

EV-428  
solvent: DMSO  
temp: 303.2 K

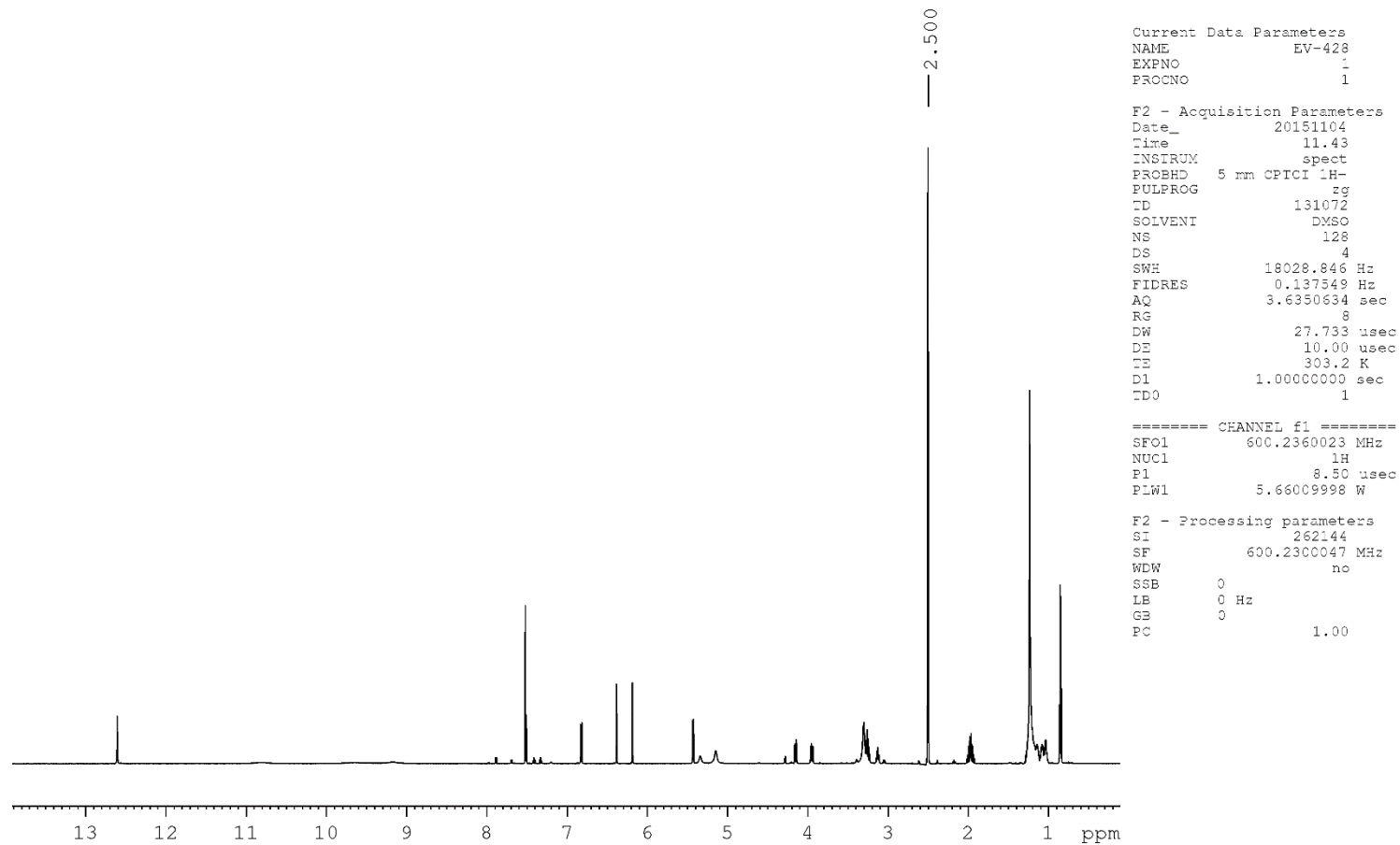


Figure S21. <sup>1</sup>H NMR spectrum of compound 8.

mAU

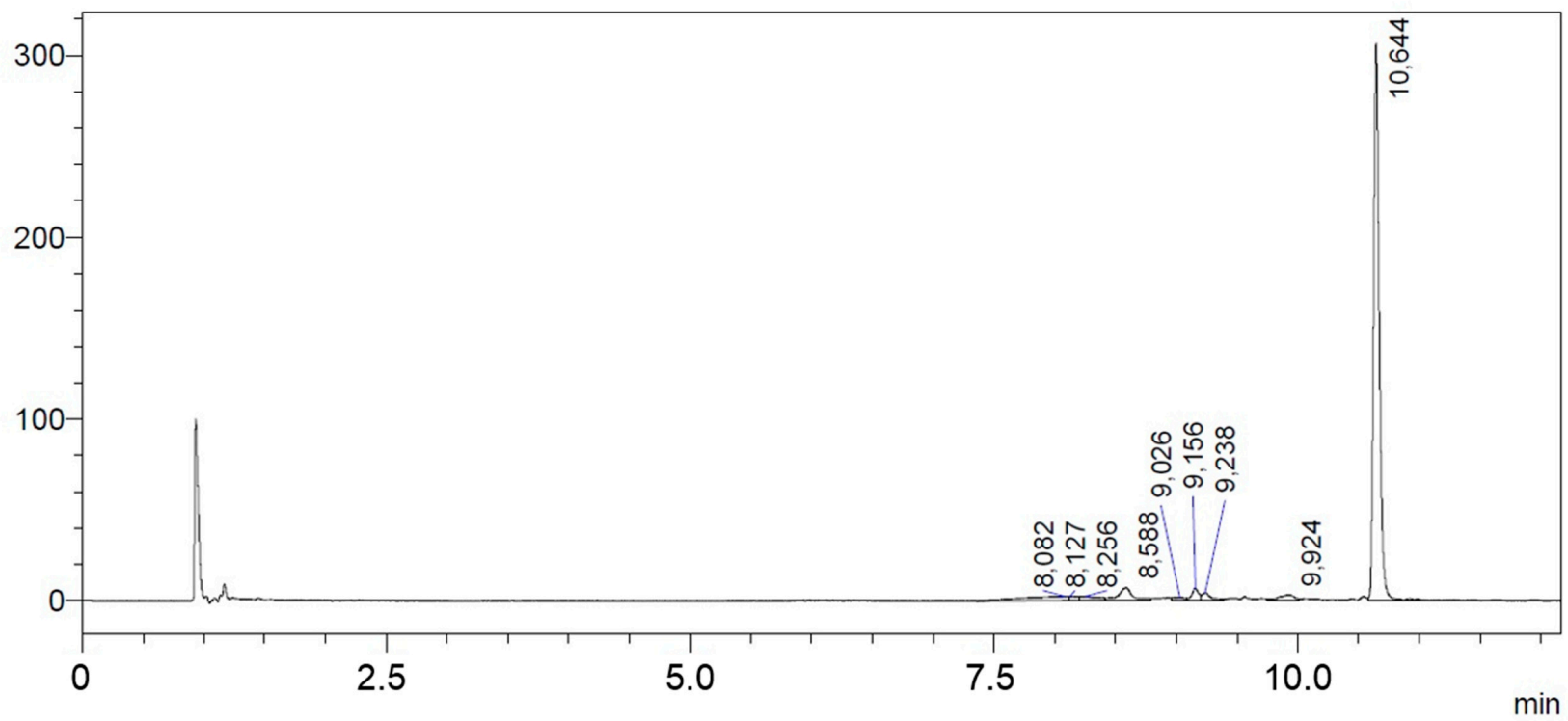
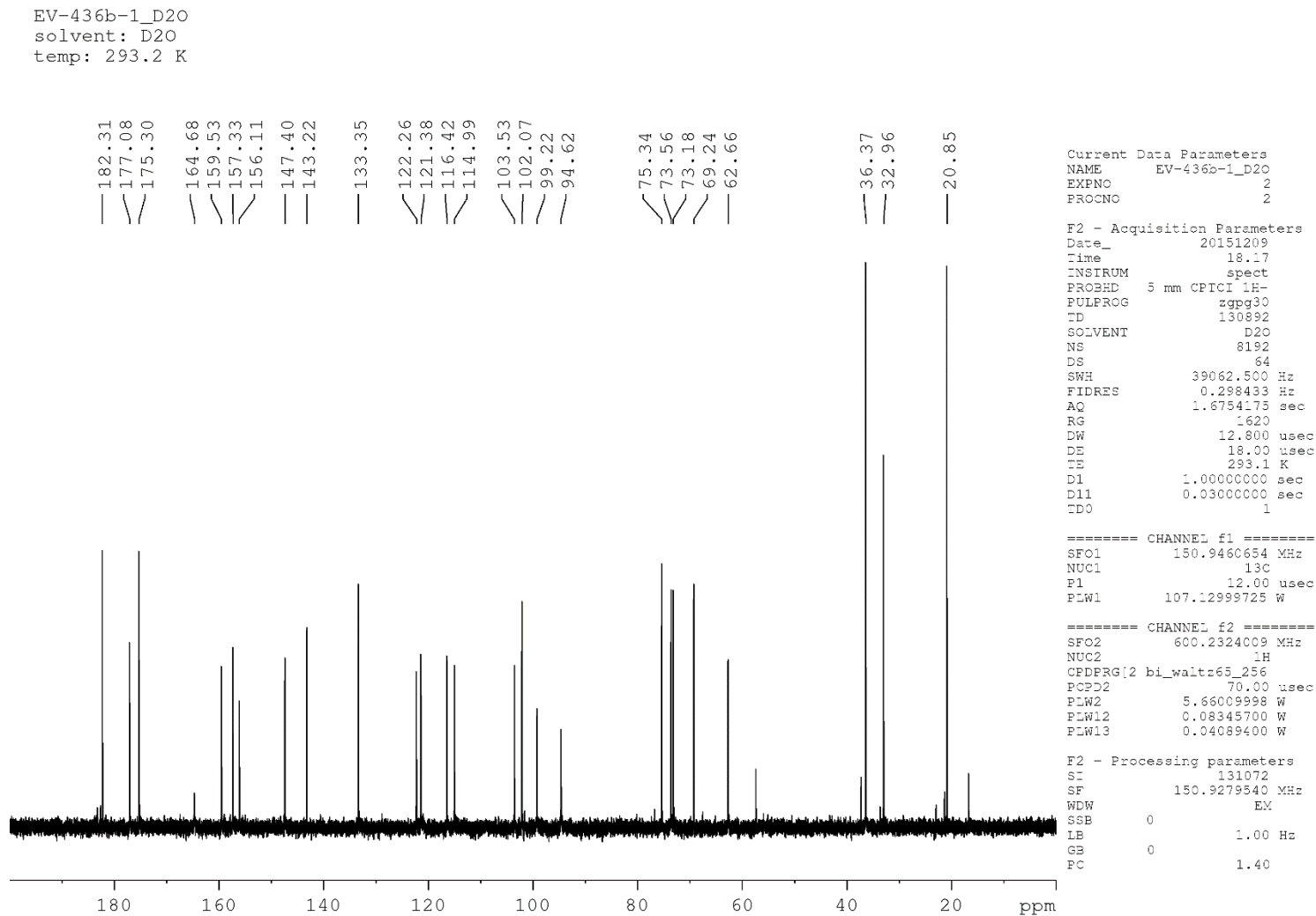


Figure S22. HPLC chromatogram of compound 8.

Figure S23. <sup>13</sup>C NMR spectrum of compound 9.

EV-436b-1\_D2O  
 solvent: D2O  
 temp: 293.2 K

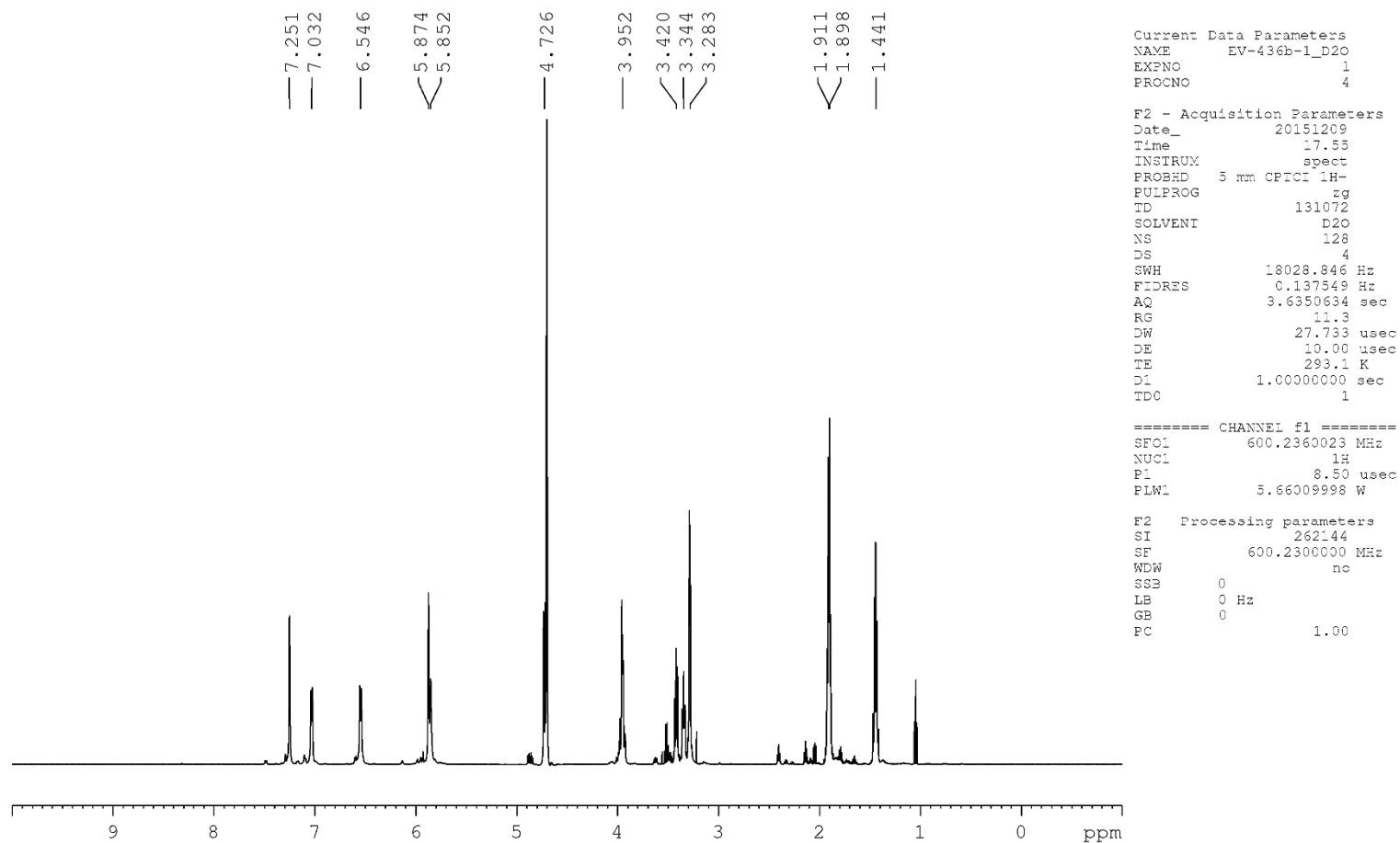


Figure S24. <sup>1</sup>H NMR spectrum of compound 9.

EV-436b-1\_D2O  
 solvent: D2O  
 temp: 293.2 K

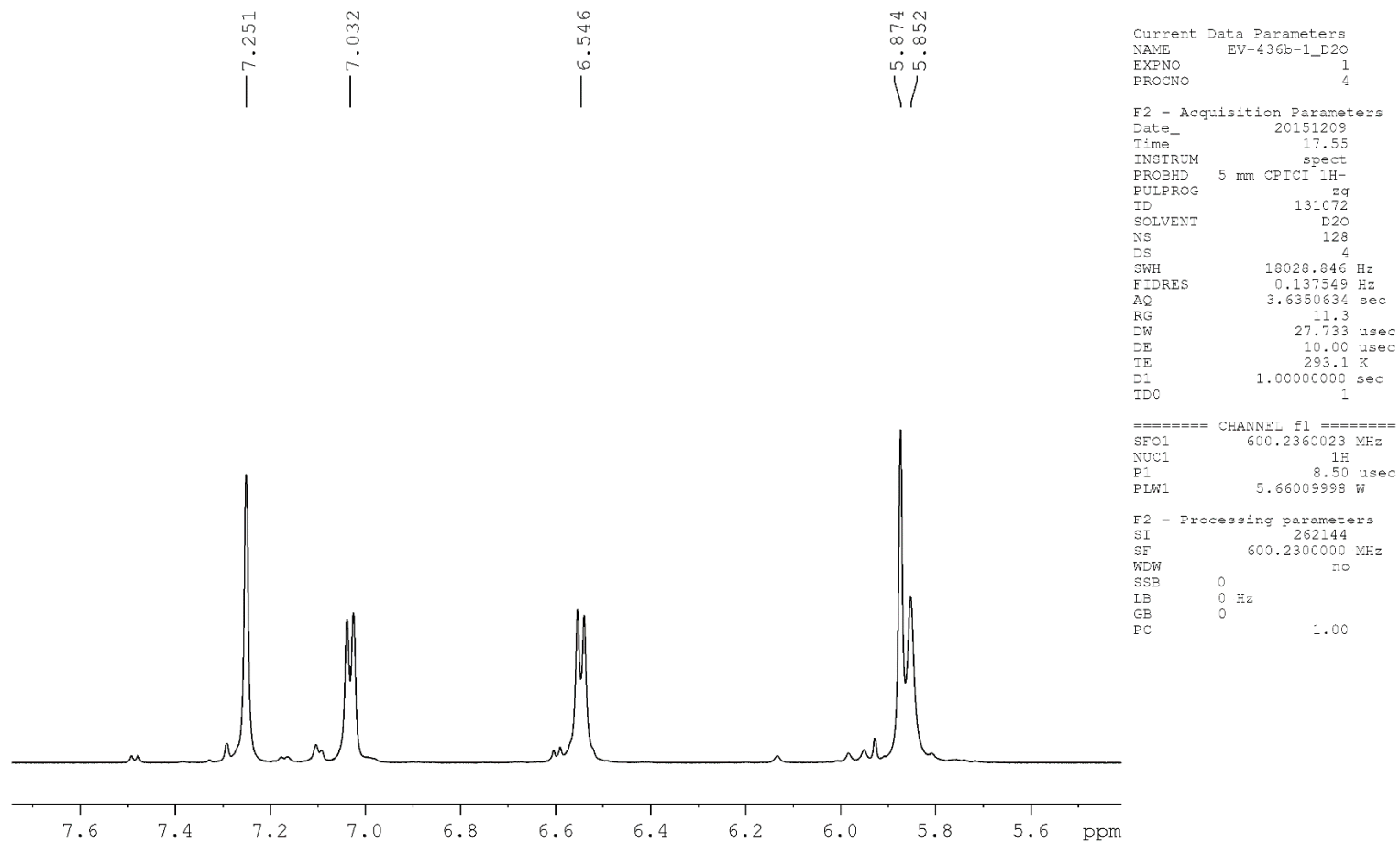


Figure S25. Detail (1/3) of <sup>1</sup>H NMR spectrum of compound 9.

EV-436b-1\_D2O  
 solvent: D2O  
 temp: 293.2 K

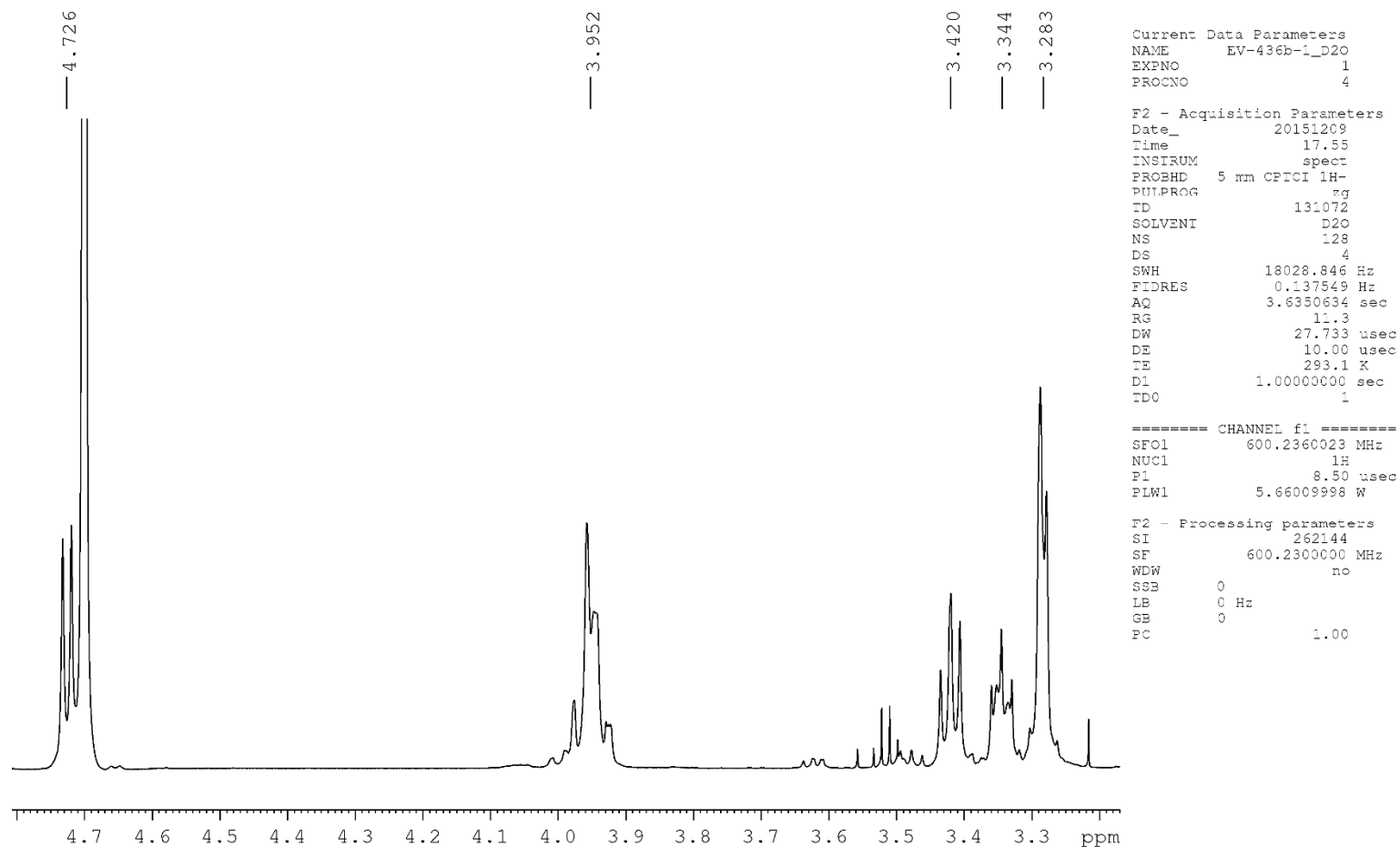


Figure S26. Detail (2/3) of <sup>1</sup>H NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D2O  
temp: 293.2 K

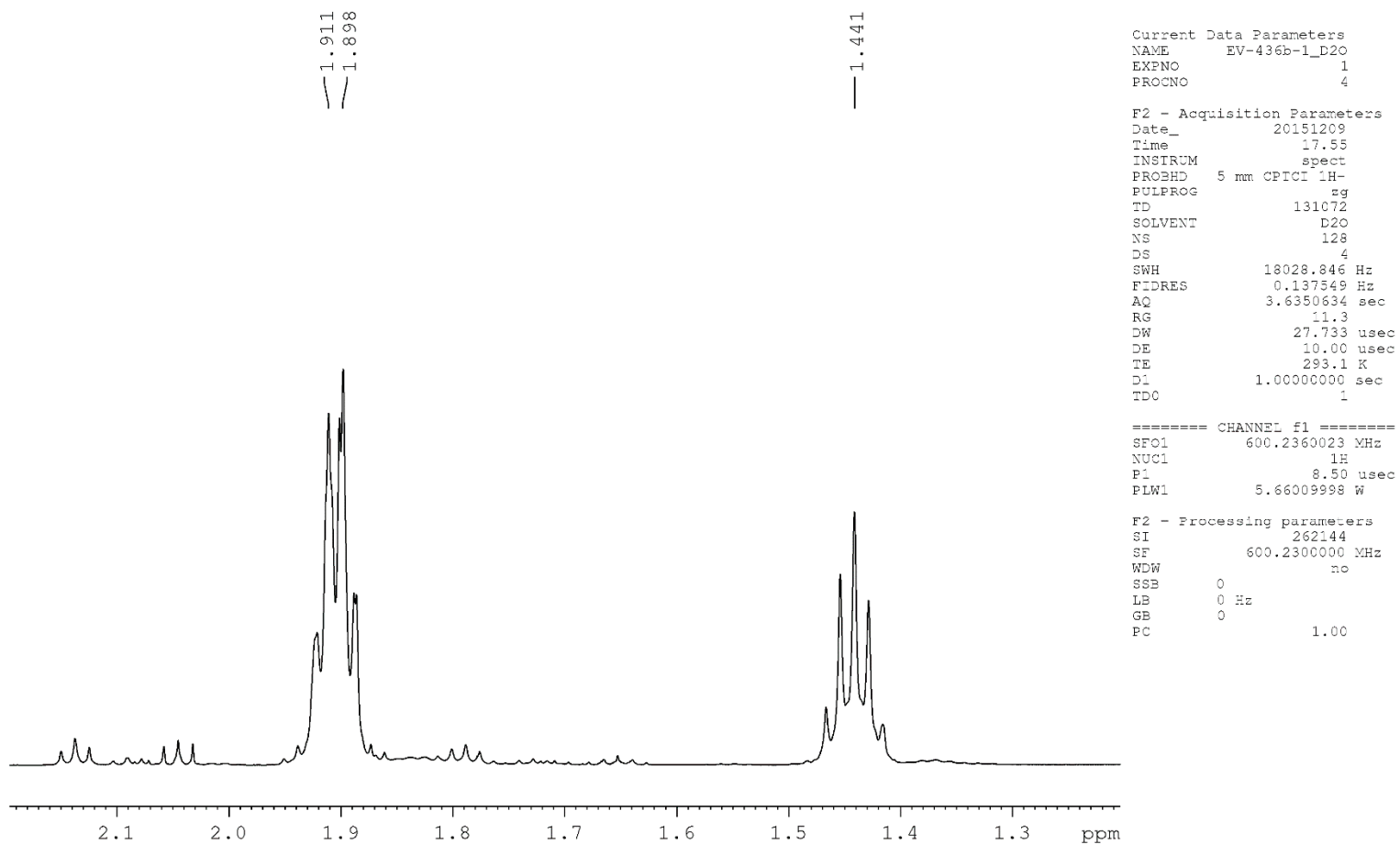


Figure S27. Detail (3/3) of <sup>1</sup>H NMR spectrum of compound 9.





EV-436b-1\_D2O  
 solvent: D2O  
 temp: 293.2 K

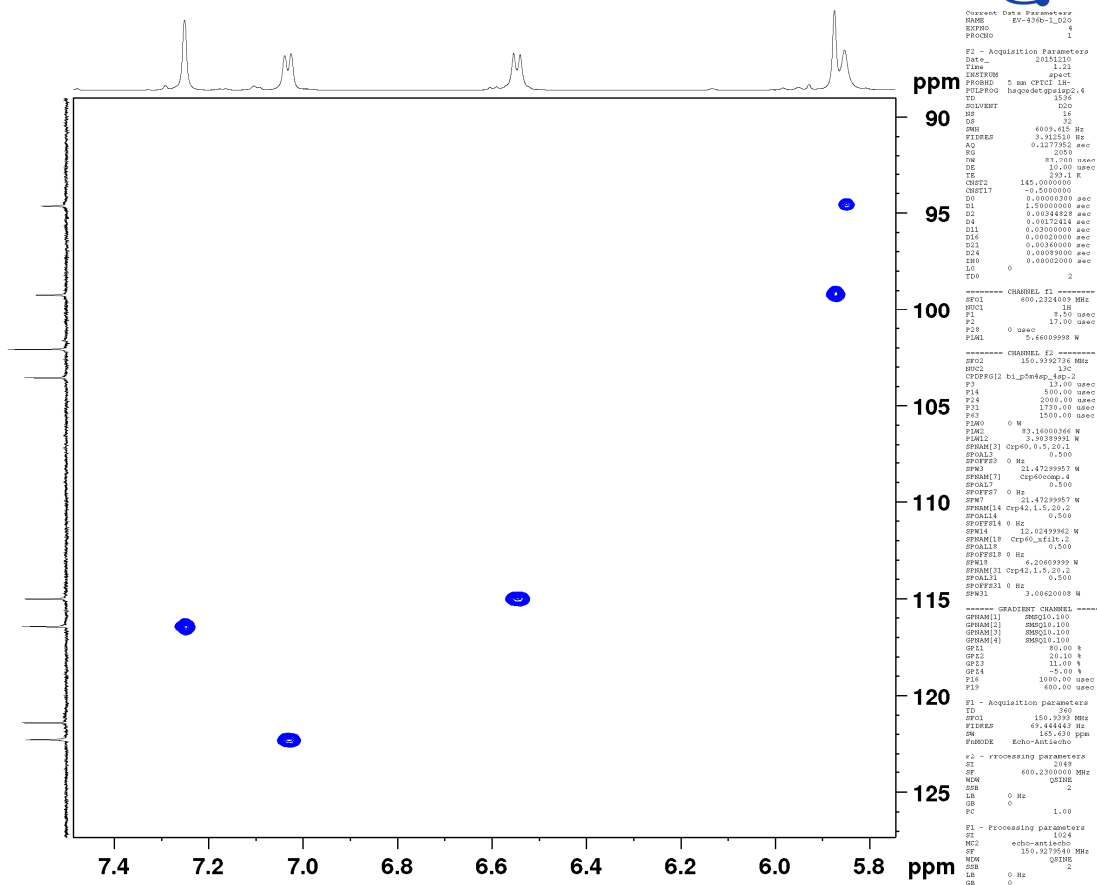


Figure S29. Detail (1/3) of HSQC NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D2O  
temp: 293.2 K

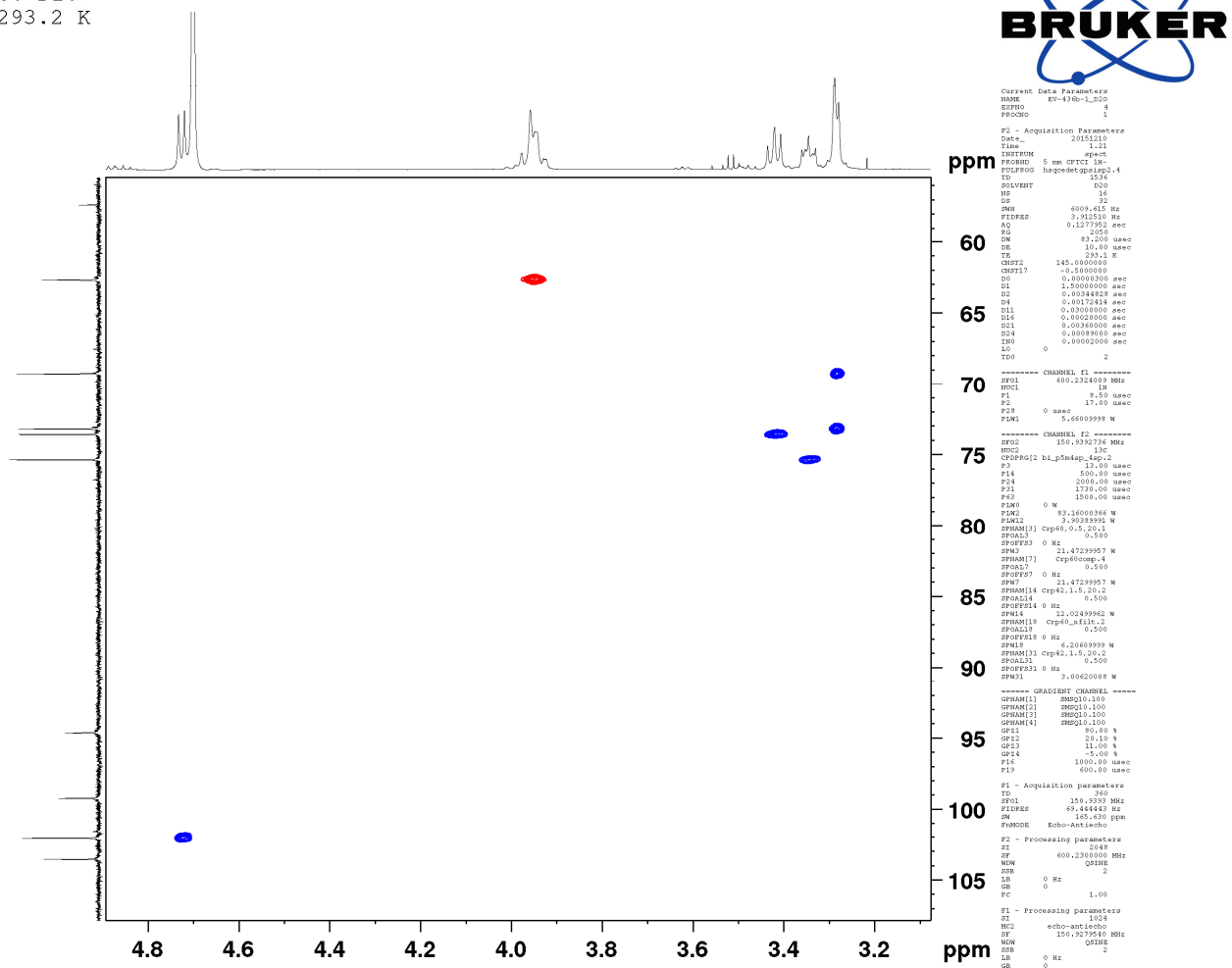


Figure S30. Detail (2/3) of HSQC NMR spectrum of compound 9.

EV-436b-1\_D2O  
 solvent: D2O  
 temp: 293.2 K

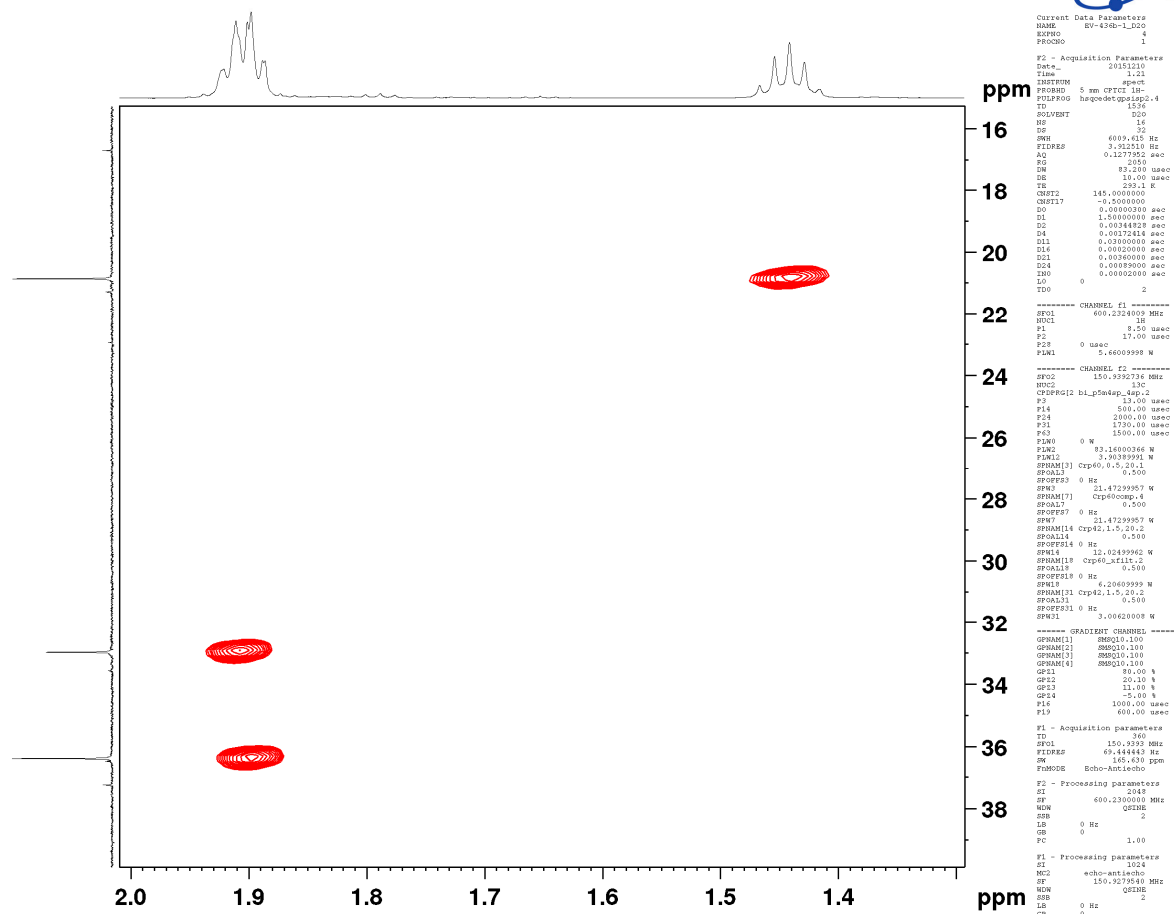


Figure S31. Detail (3/3) of HSQC NMR spectrum of compound 9.

EV-436b-1\_D2O  
 solvent: D2O  
 temp: 293.2 K

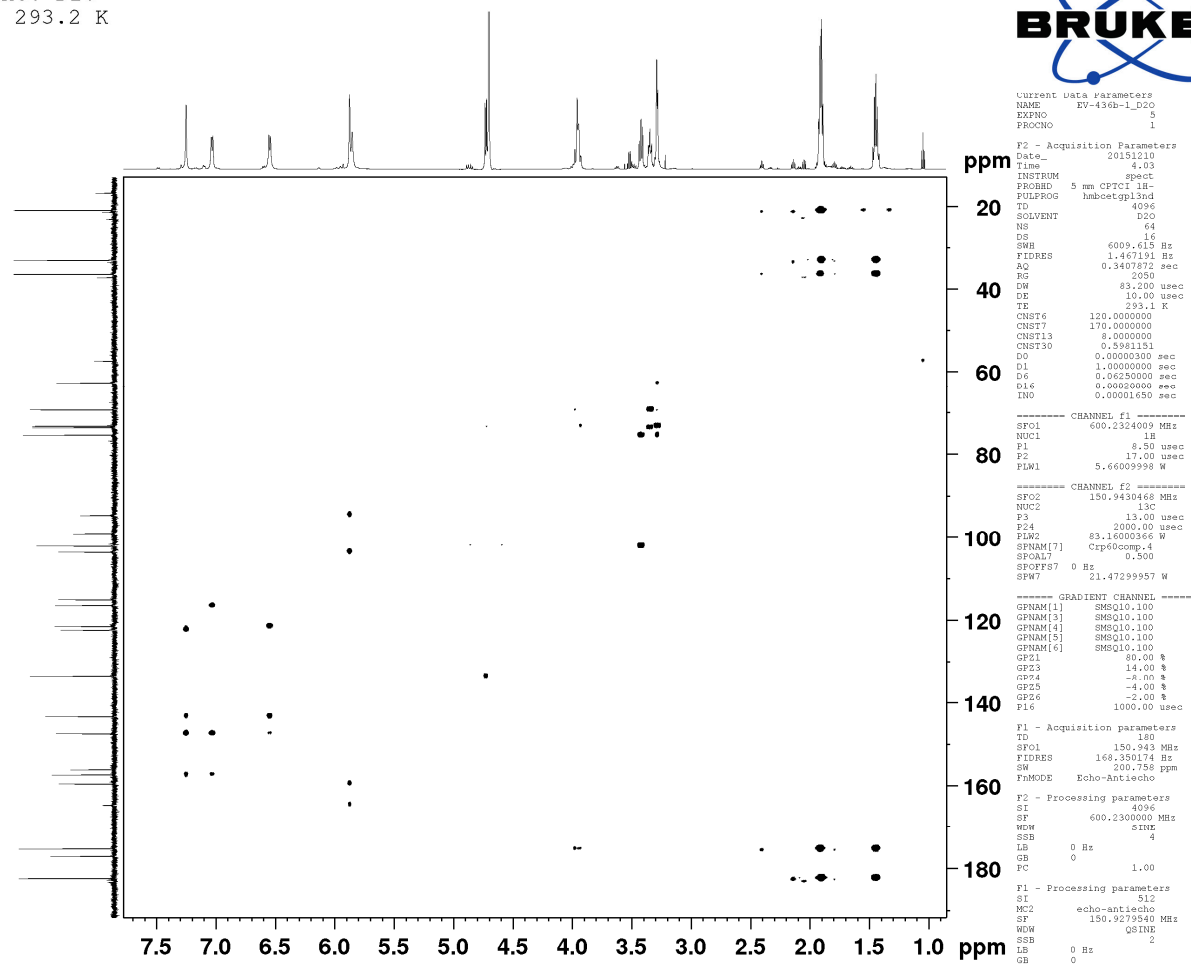


Figure S32. HMBC NMR spectrum of compound 9.

EV-436b-1\_D2O  
 solvent: D2O  
 temp: 293.2 K

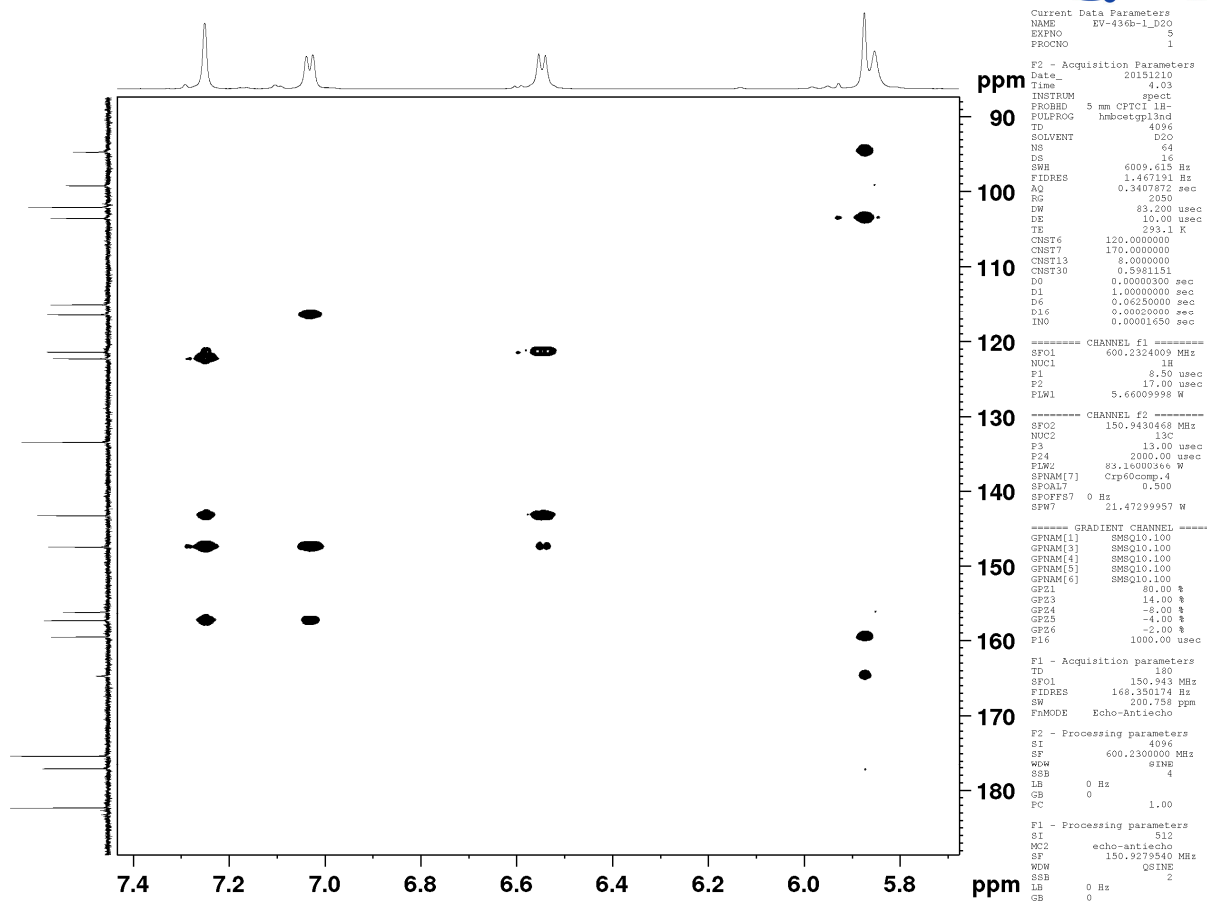


Figure S33. Detail (1/4) of HMBC NMR spectrum of compound 9.

EV-436b-1\_D2O  
 solvent: D2O  
 temp: 293.2 K

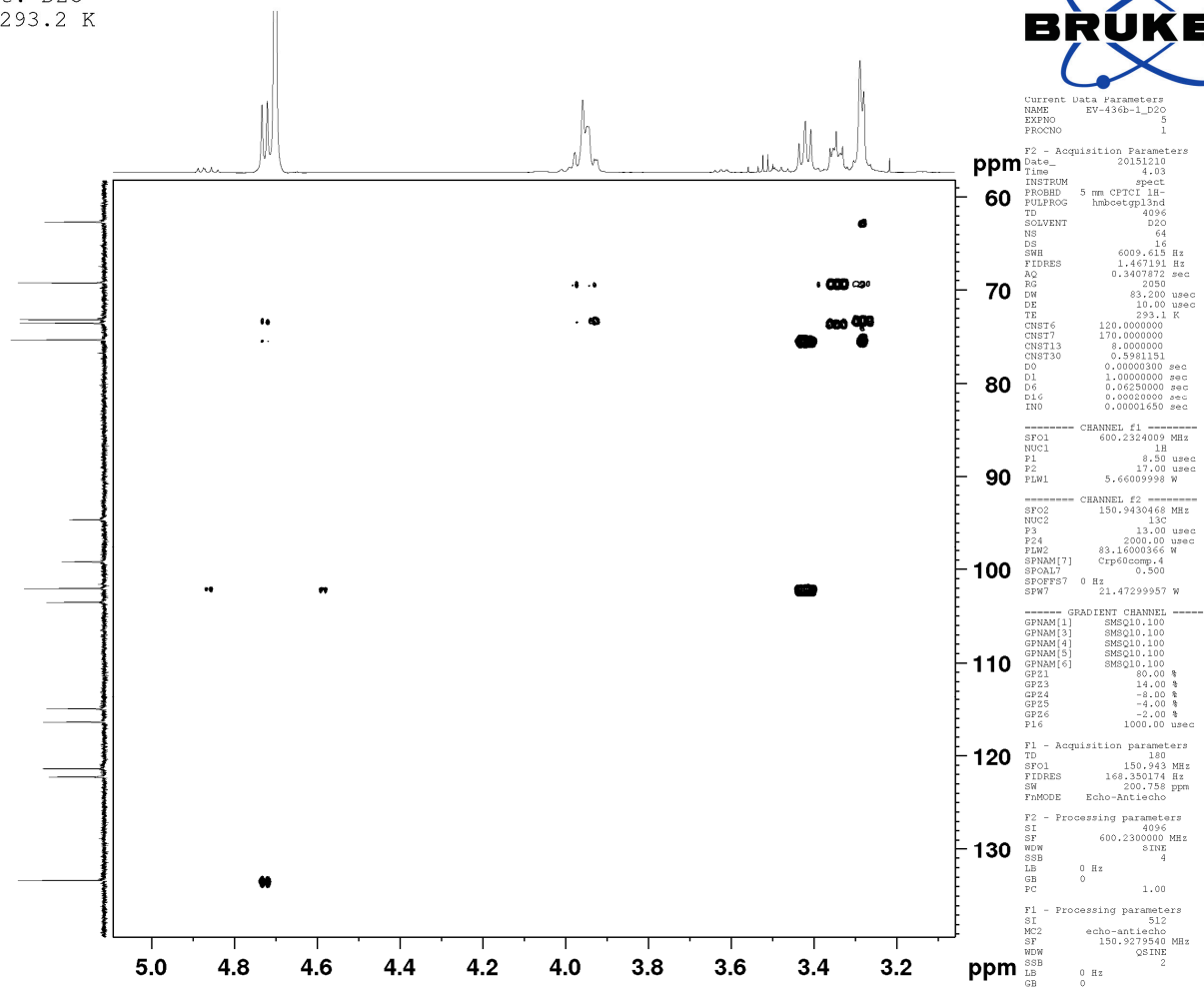


Figure S34. Detail (2/4) of HMBC NMR spectrum of compound 9.

EV-436b-1\_D2O  
 solvent: D2O  
 temp: 293.2 K

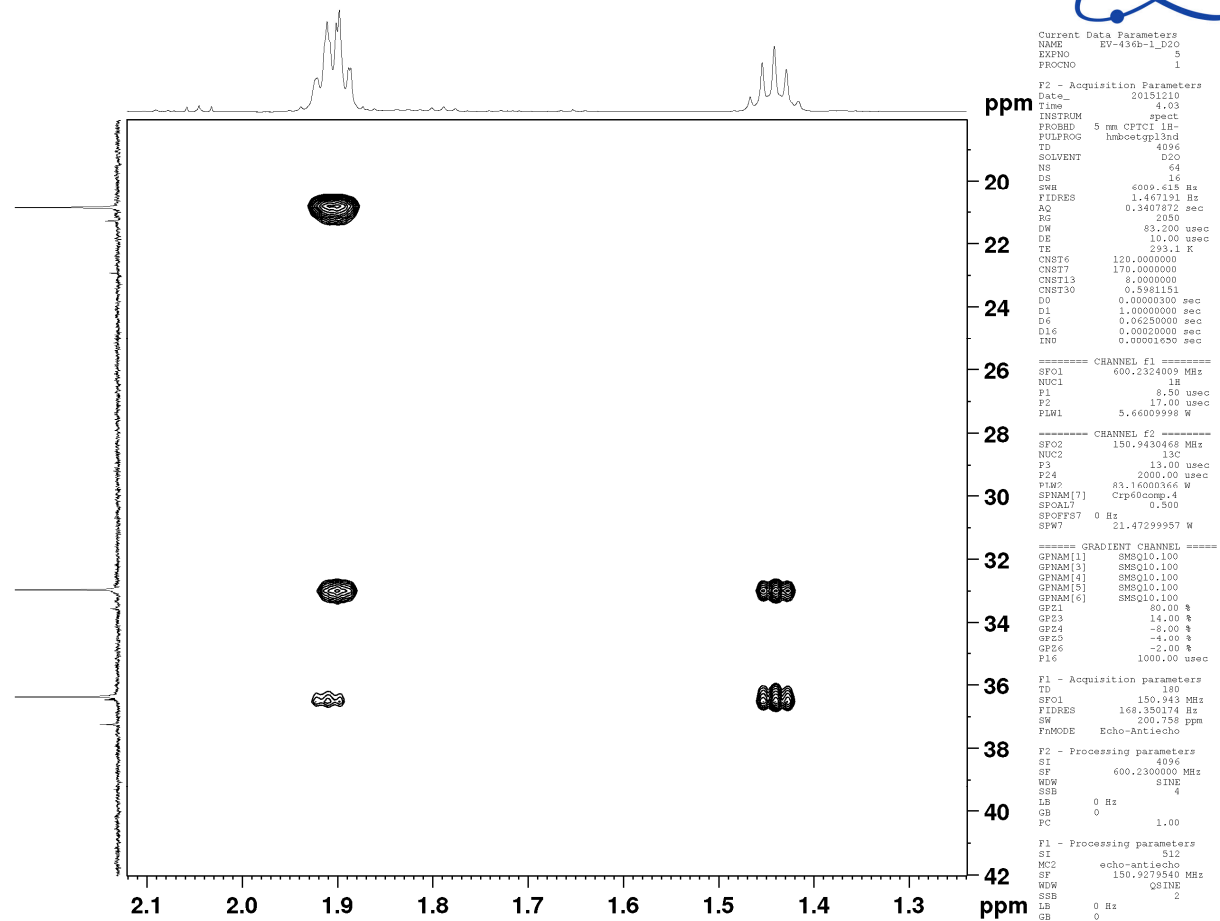


Figure S35. Detail (3/4) of HMBC NMR spectrum of compound 9.



EV-436b-1\_D2O  
 solvent: D2O  
 temp: 293.2 K

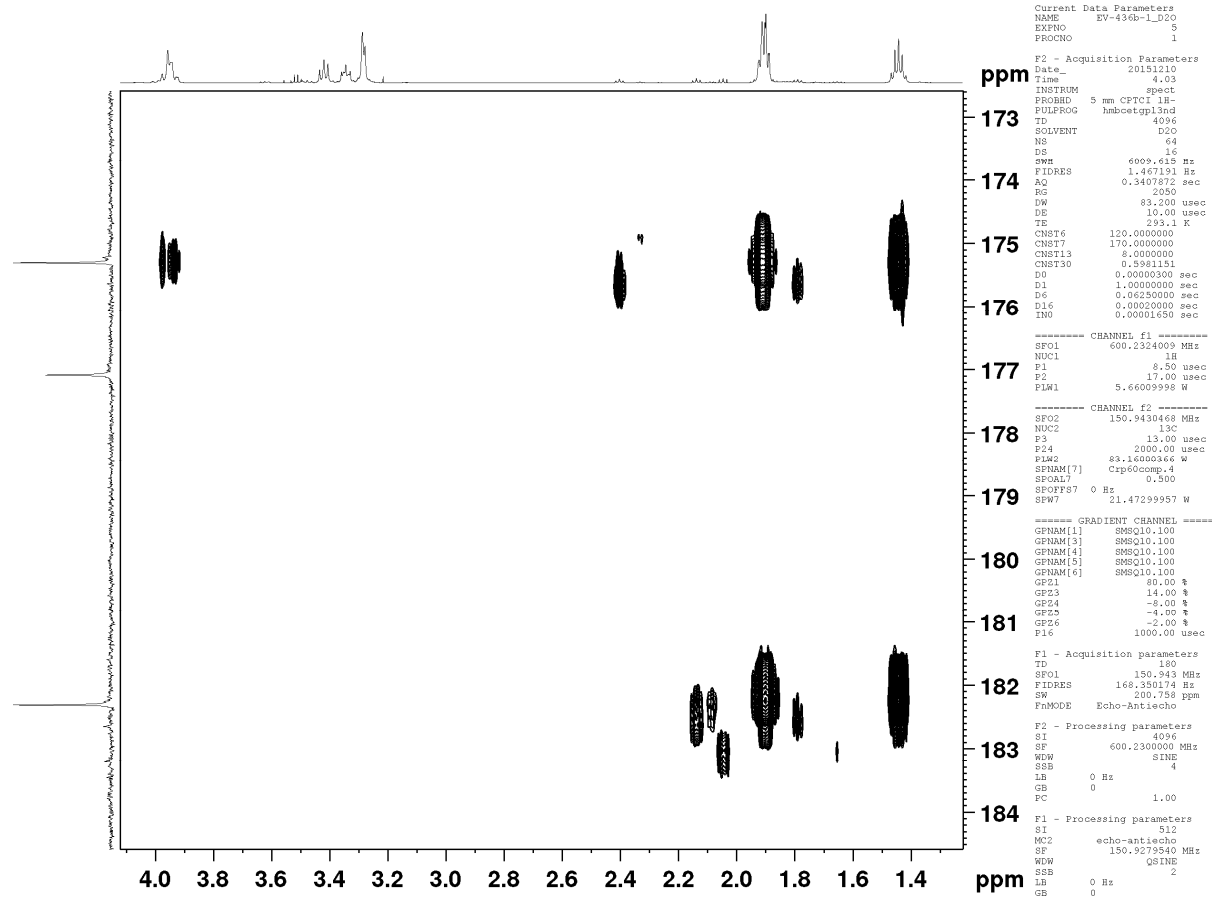


Figure S36. Detail (4/4) of HMBC NMR spectrum of compound 9.

EV-436b-1\_D2O  
 solvent: D2O  
 temp: 293.2 K

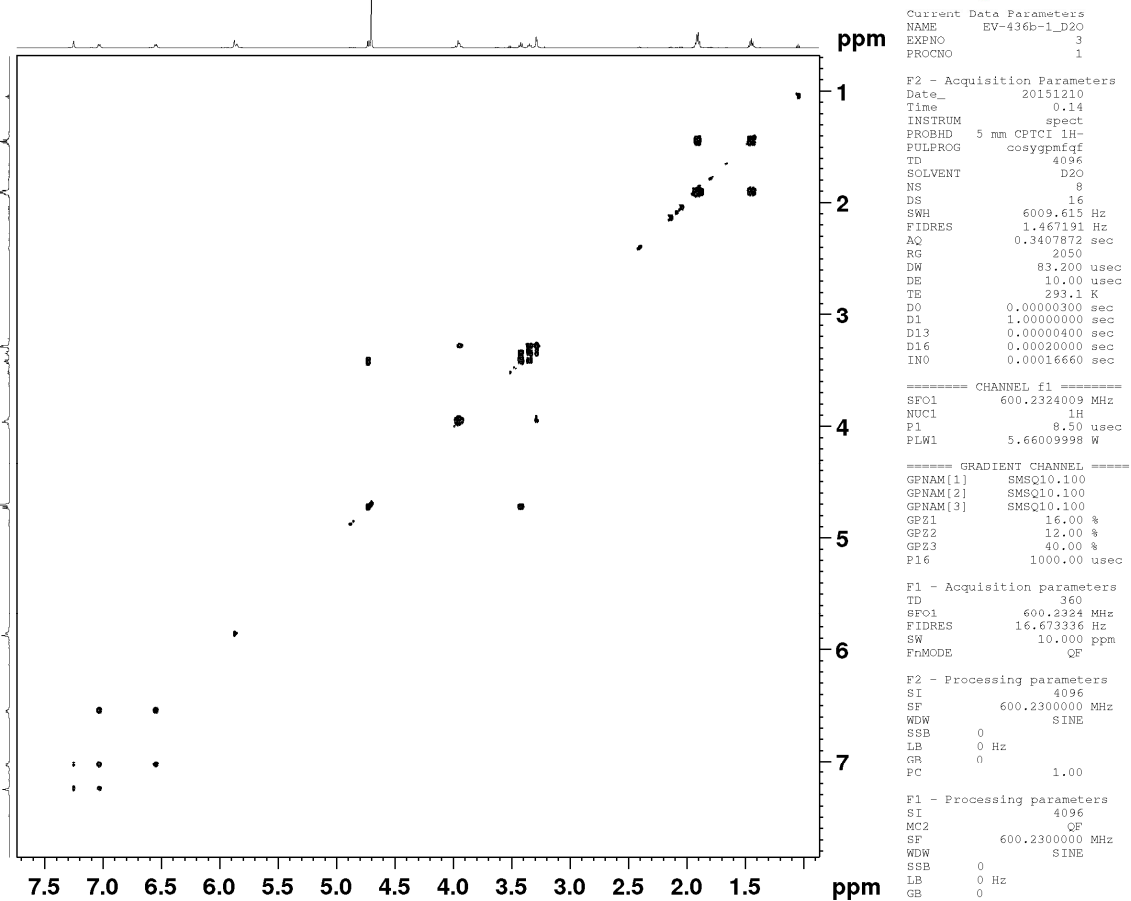


Figure S37. COSY NMR spectrum of compound 9.

EV-436b-1\_D2O  
 solvent: D2O  
 temp: 293.2 K

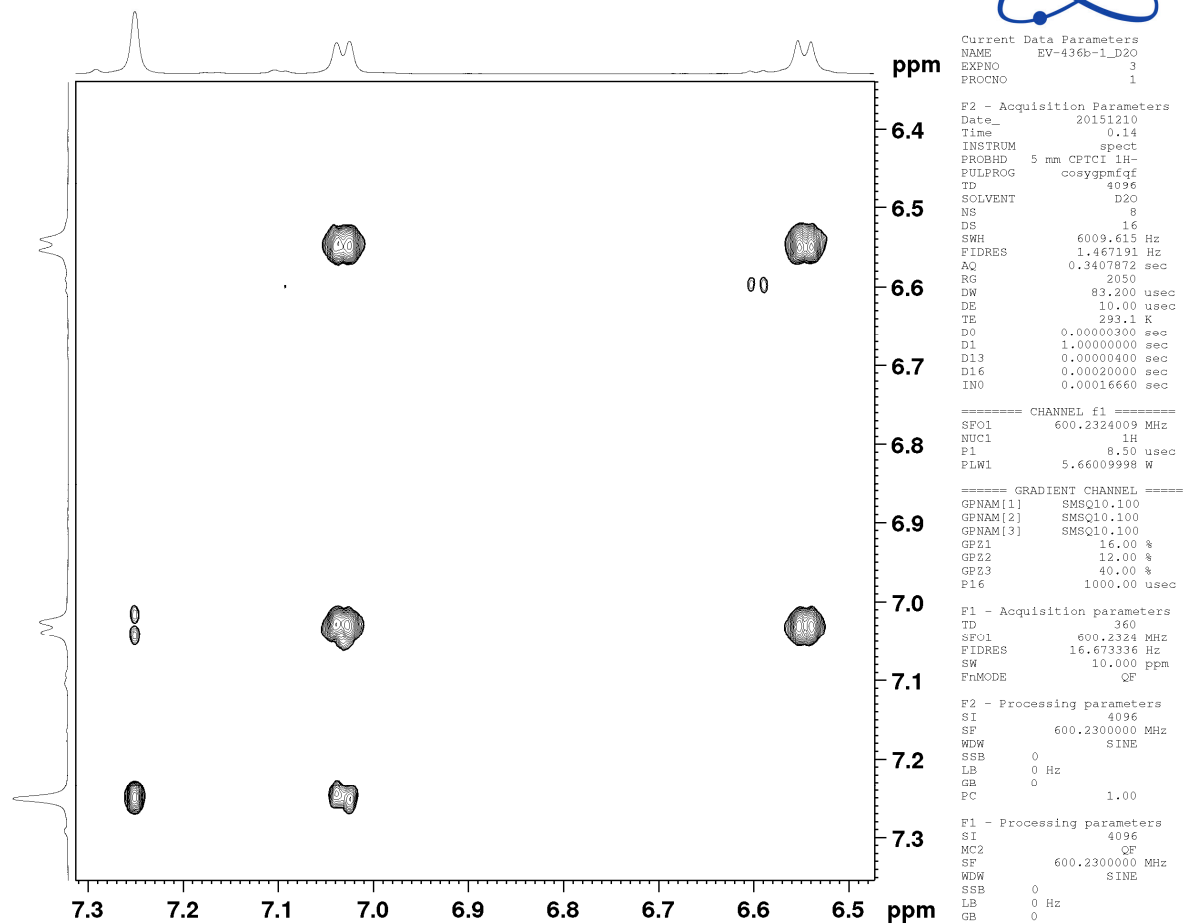


Figure S38. Detail (1/3) of COSY NMR spectrum of compound 9.

EV-436b-1\_D2O  
 solvent: D2O  
 temp: 293.2 K

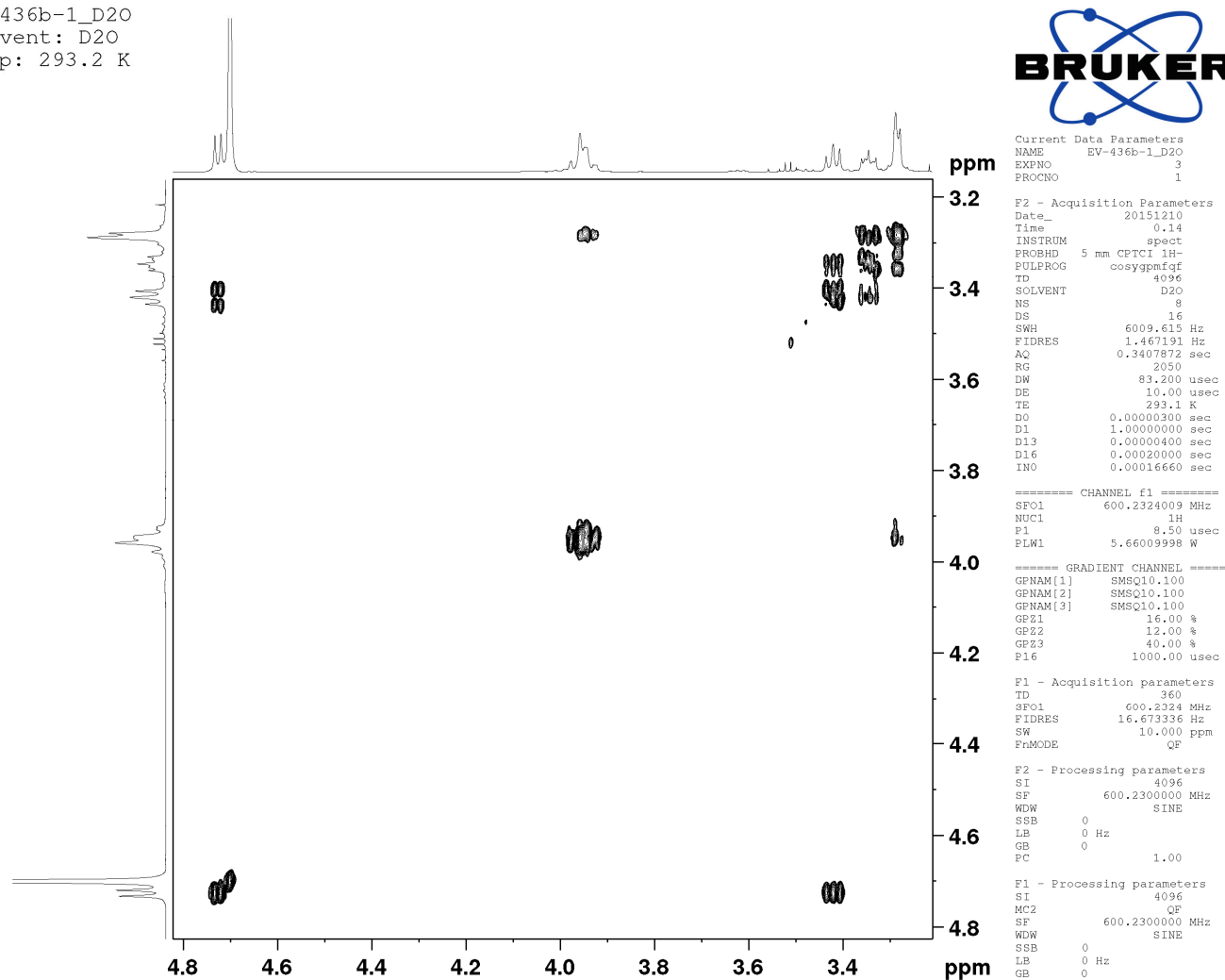


Figure S39. Detail (2/3) of COSY NMR spectrum of compound 9.

EV-436b-1\_D2O  
 solvent: D2O  
 temp: 293.2 K

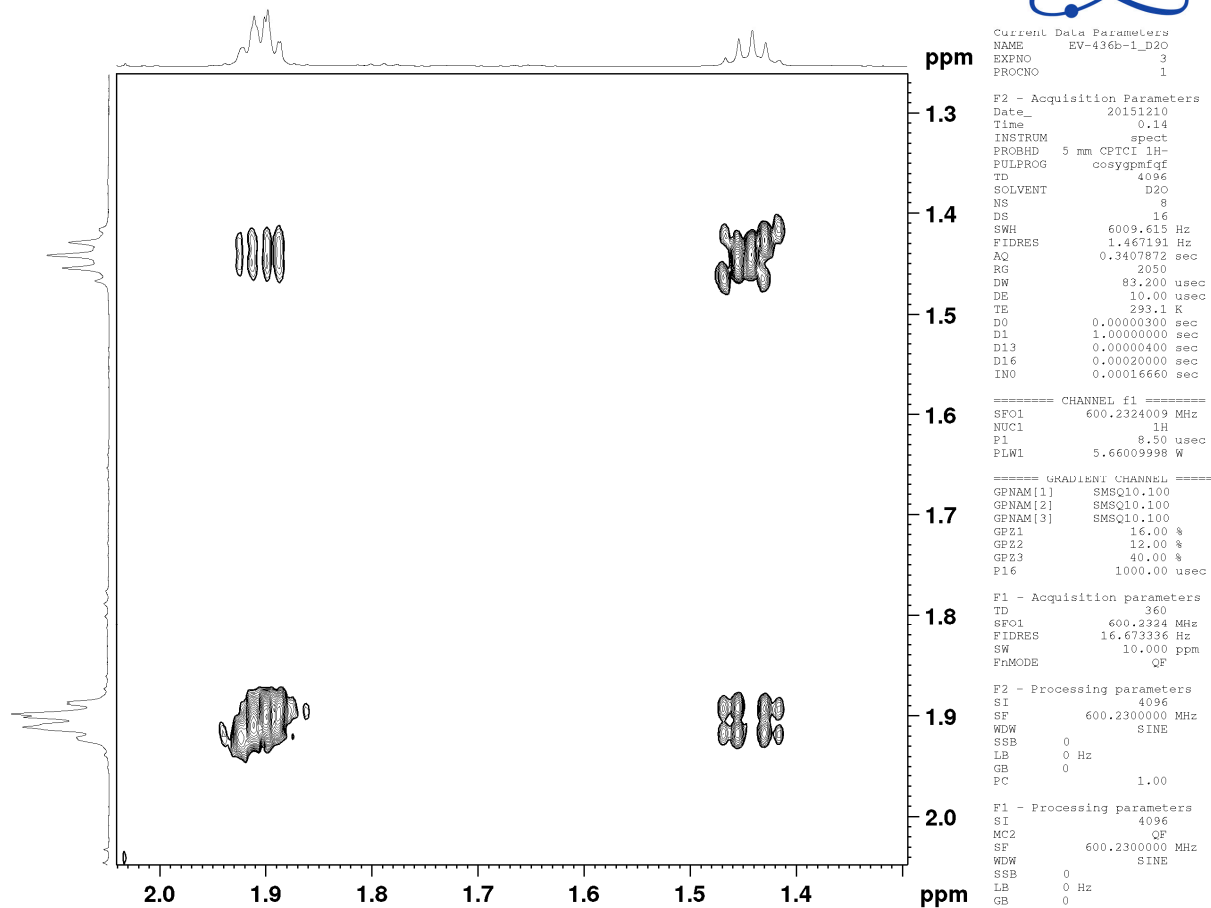


Figure S40. Detail (3/3) of COSY NMR spectrum of compound 9.

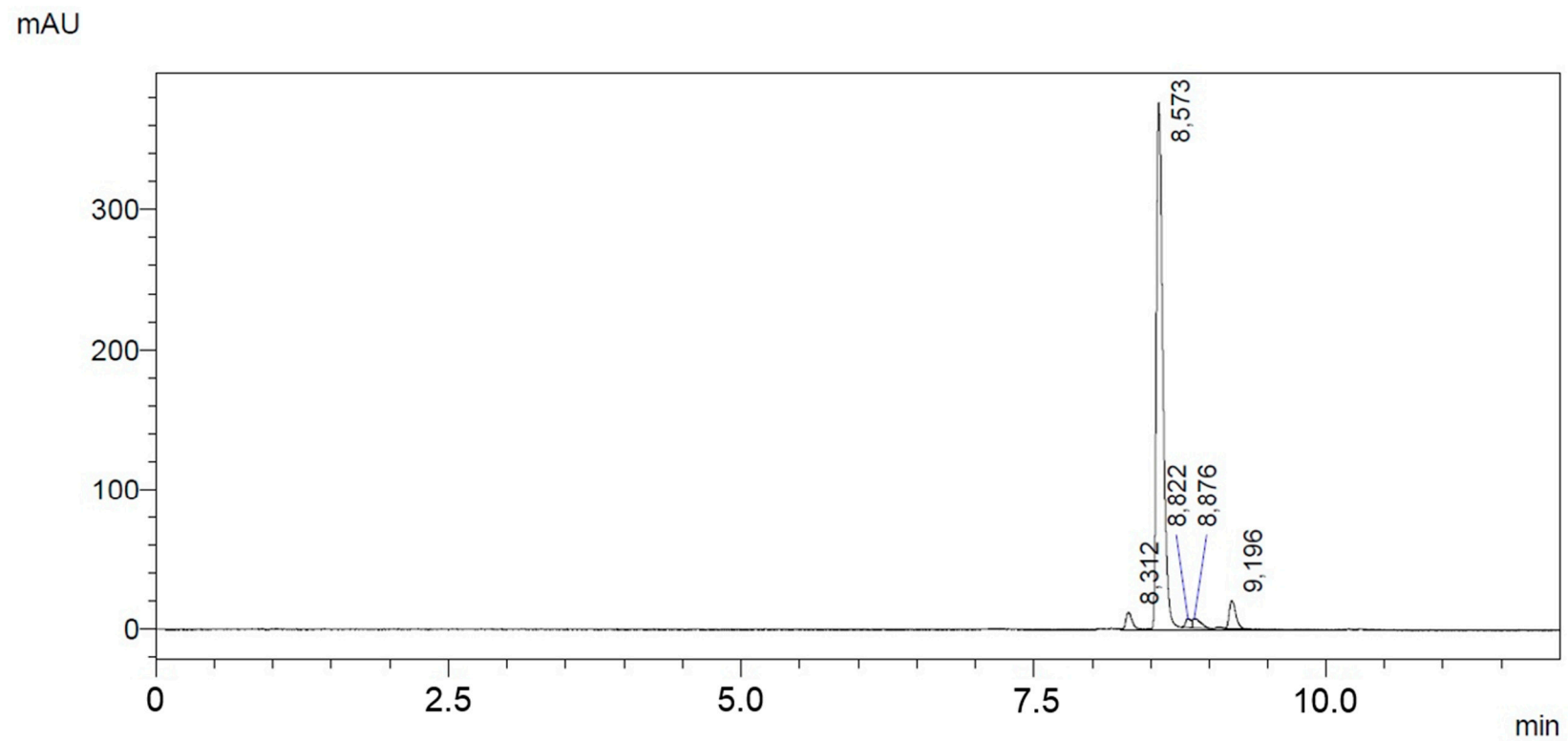
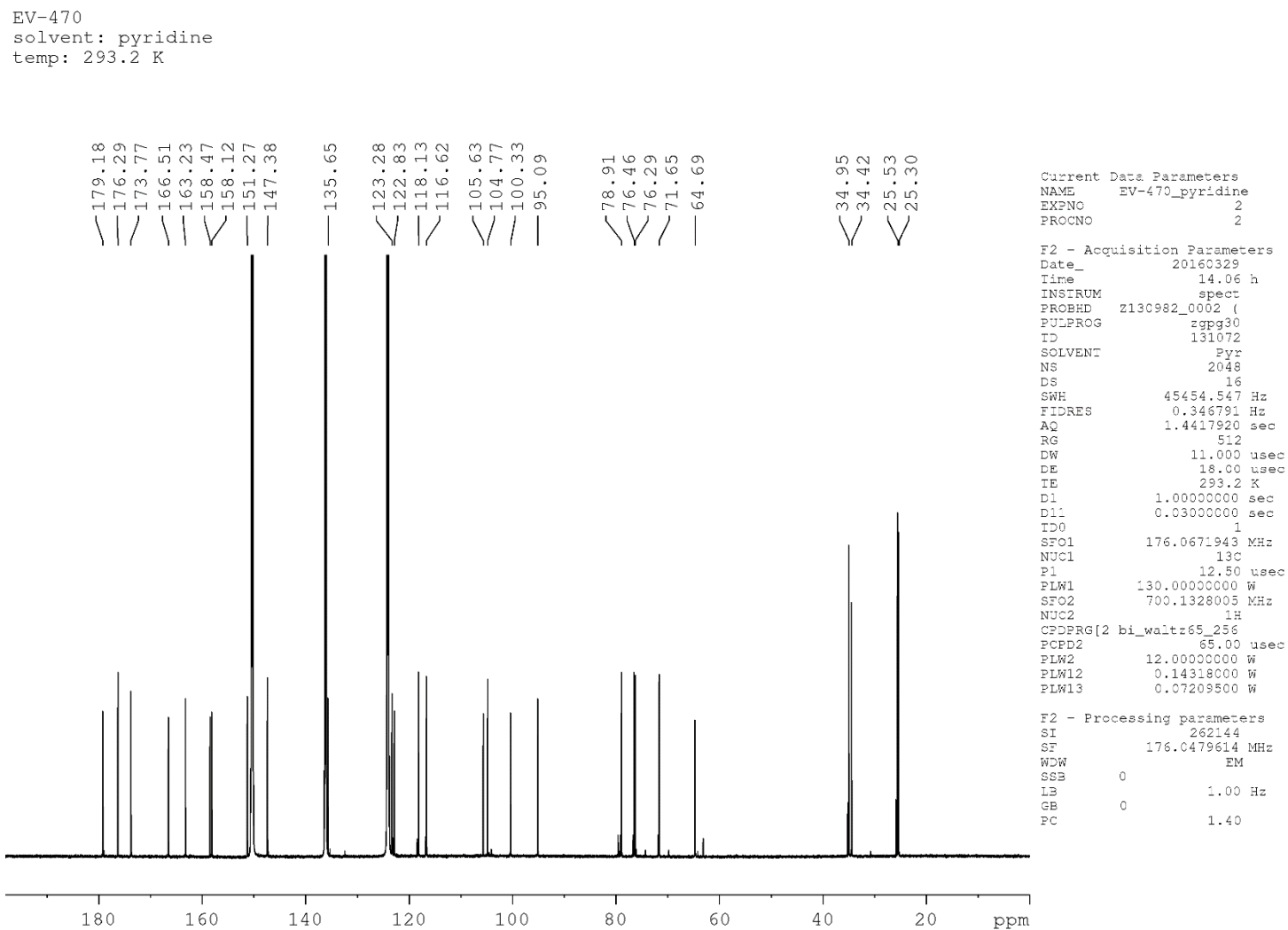


Figure S41. HPLC chromatogram of compound 9.

Figure S42. <sup>13</sup>C NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K

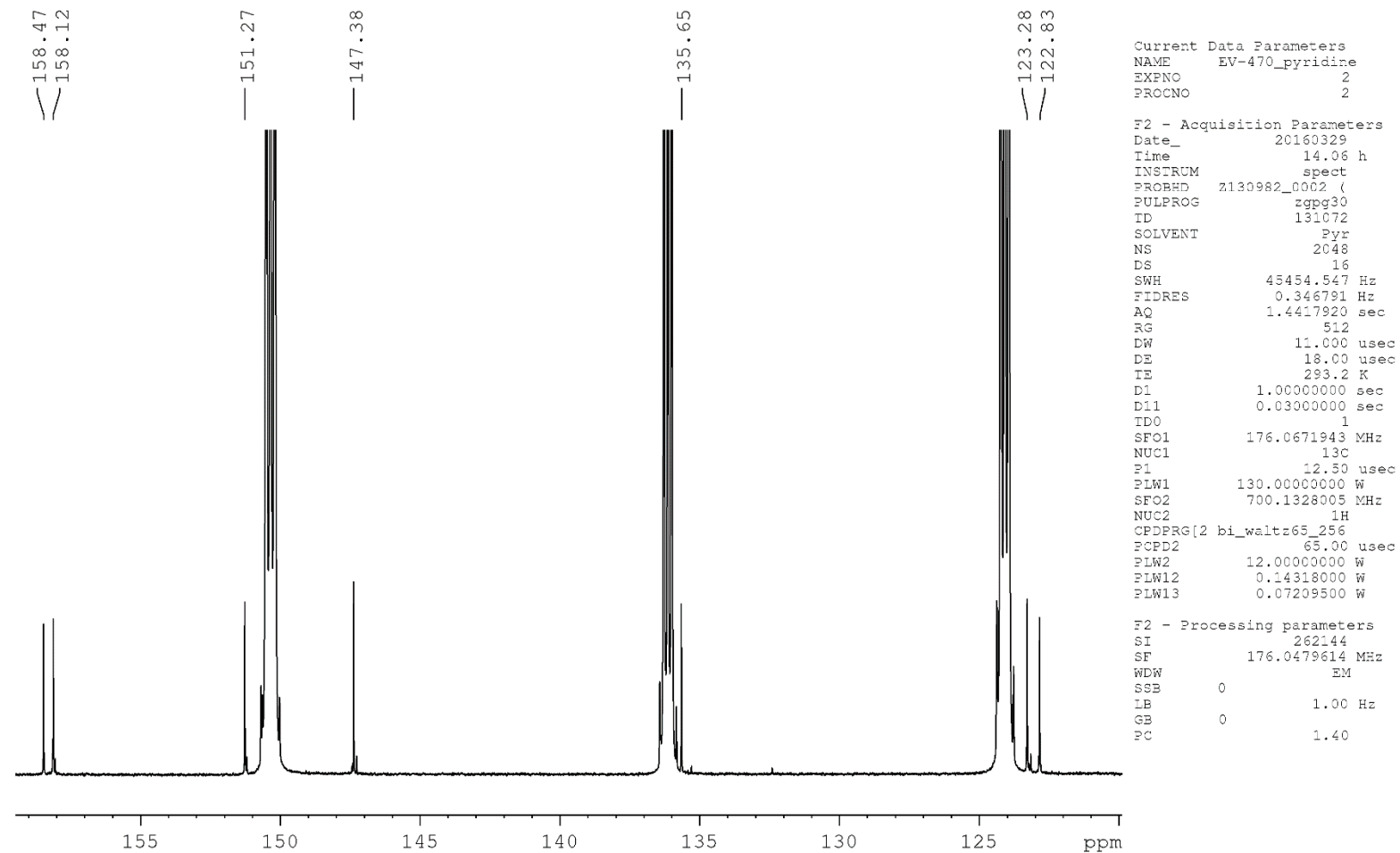


Figure S43. Detail (1/3) of  $^{13}\text{C}$  NMR spectrum of compound 10.



EV-470  
solvent: pyridine  
temp: 293.2 K

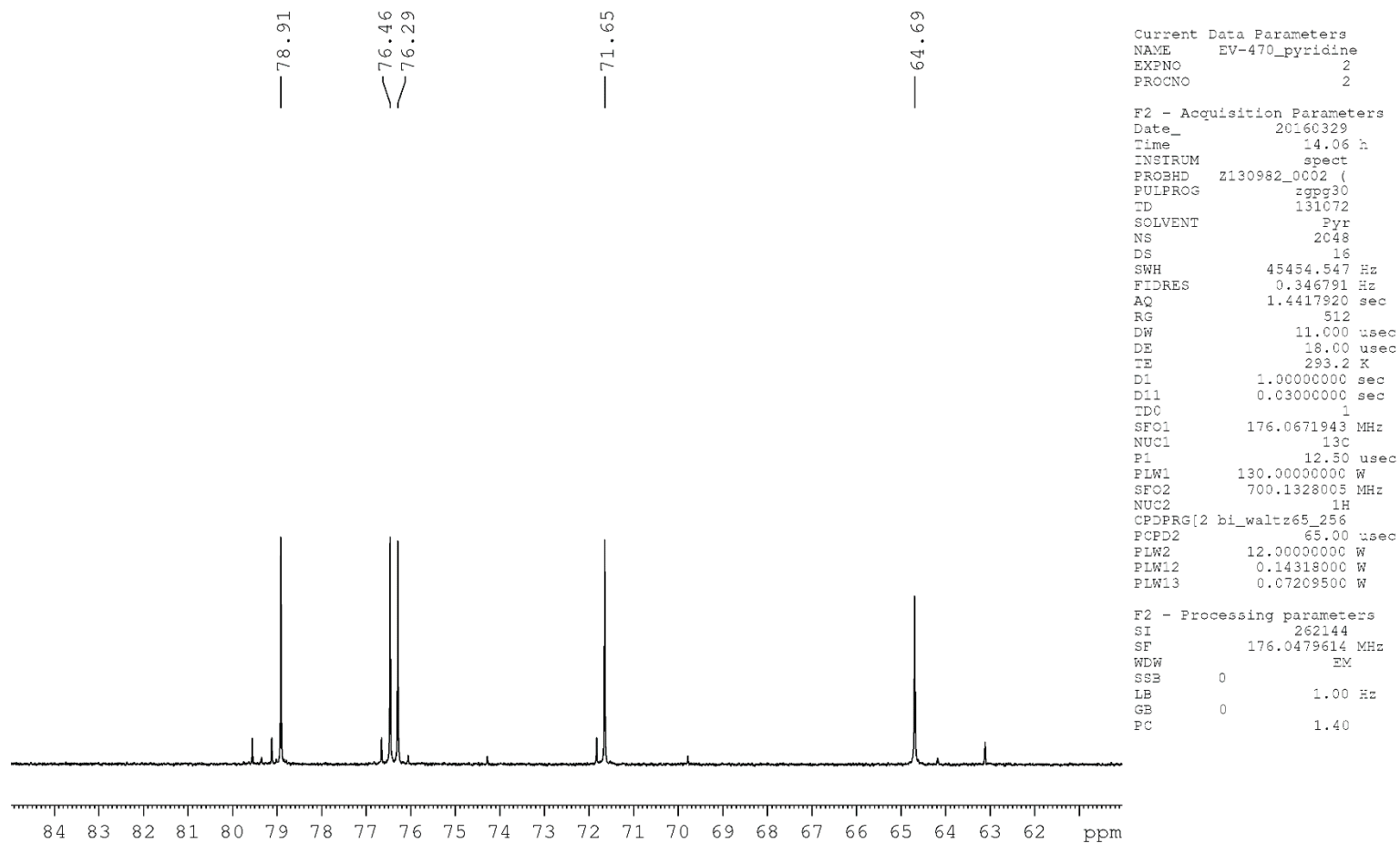


Figure S44. Detail (2/3) of  $^{13}\text{C}$  NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K

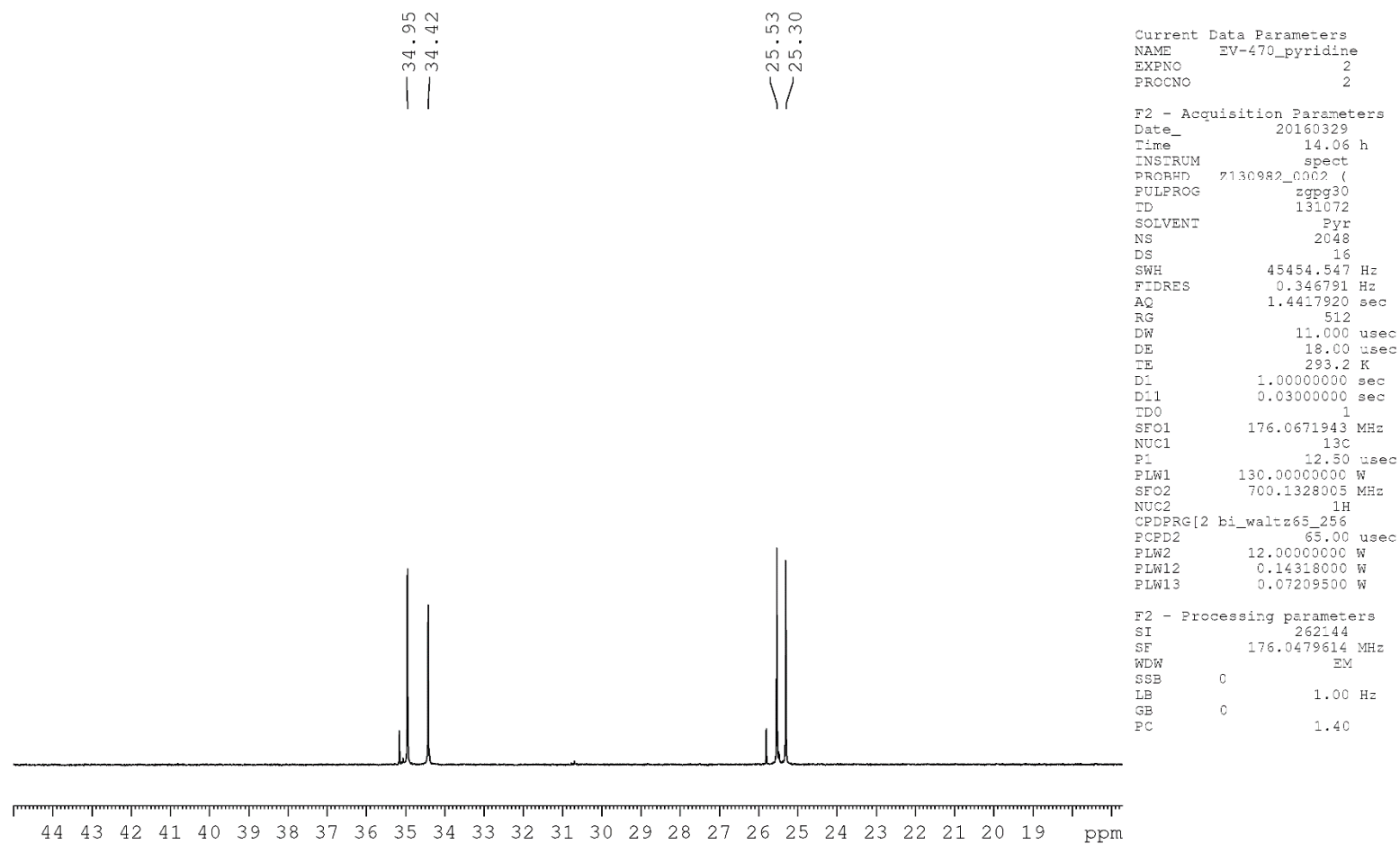


Figure S45. Detail (3/3) of <sup>13</sup>C NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K

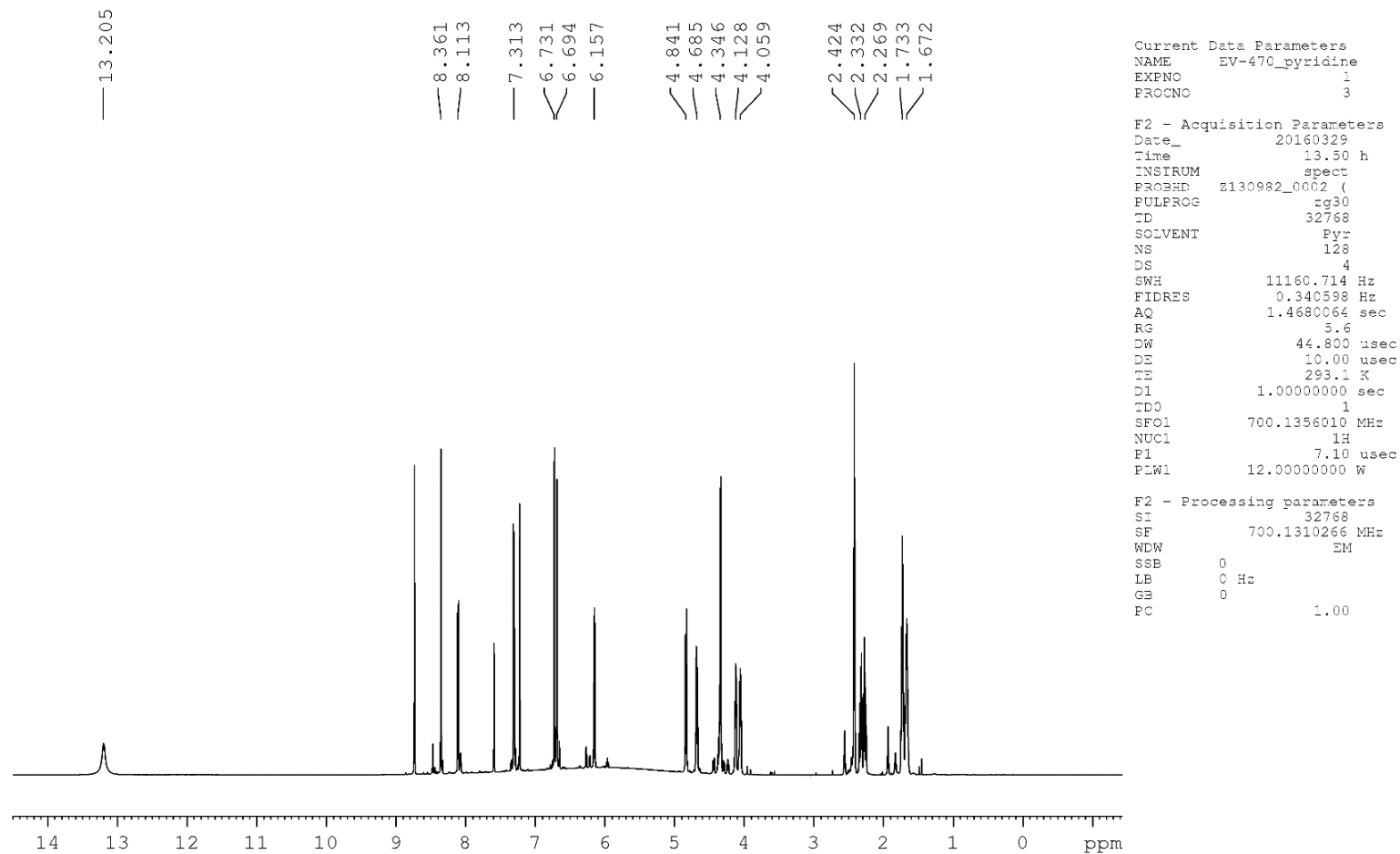


Figure S46. <sup>1</sup>H NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K

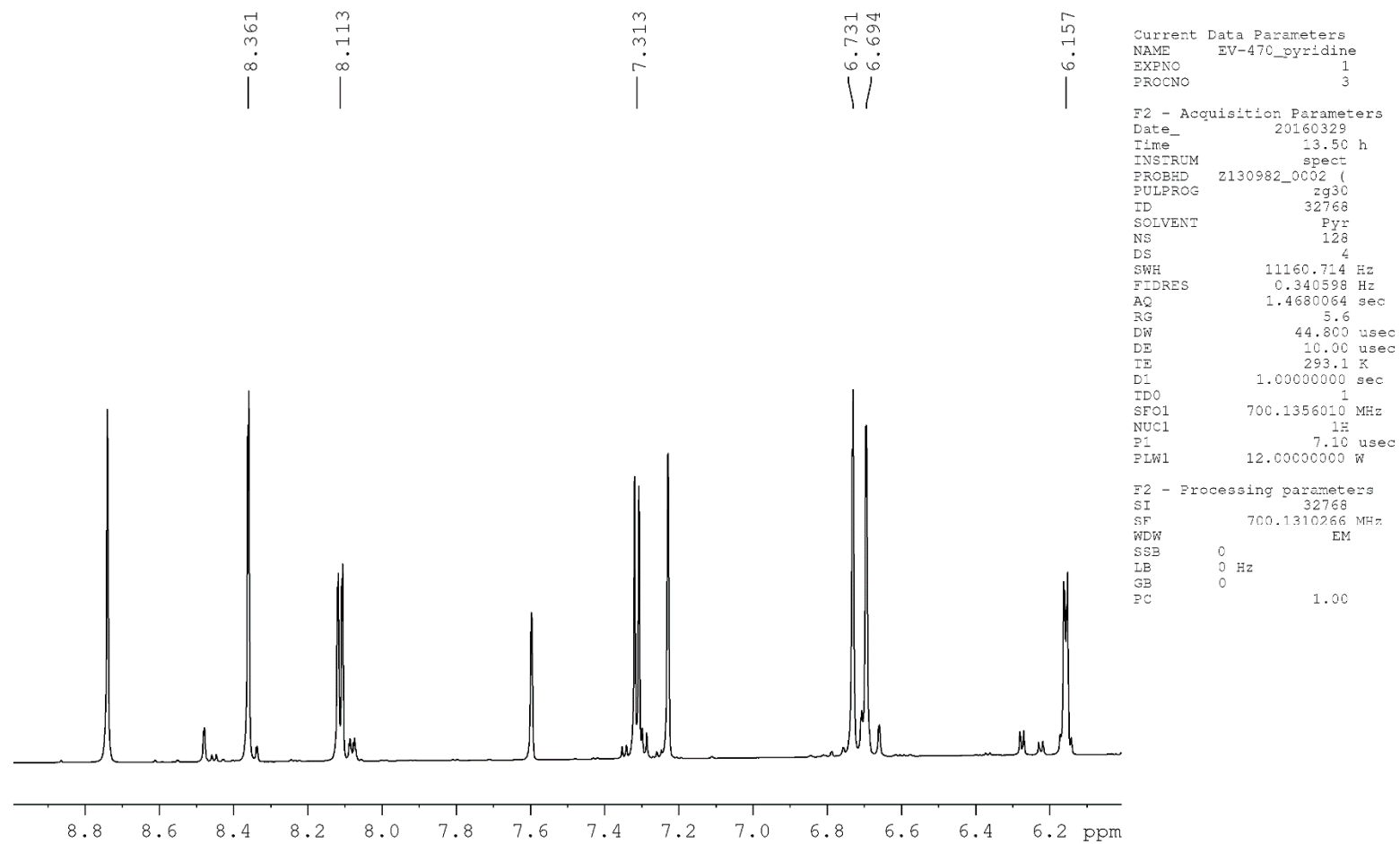


Figure S47. Detail (1/3) of  $^1\text{H}$  NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K

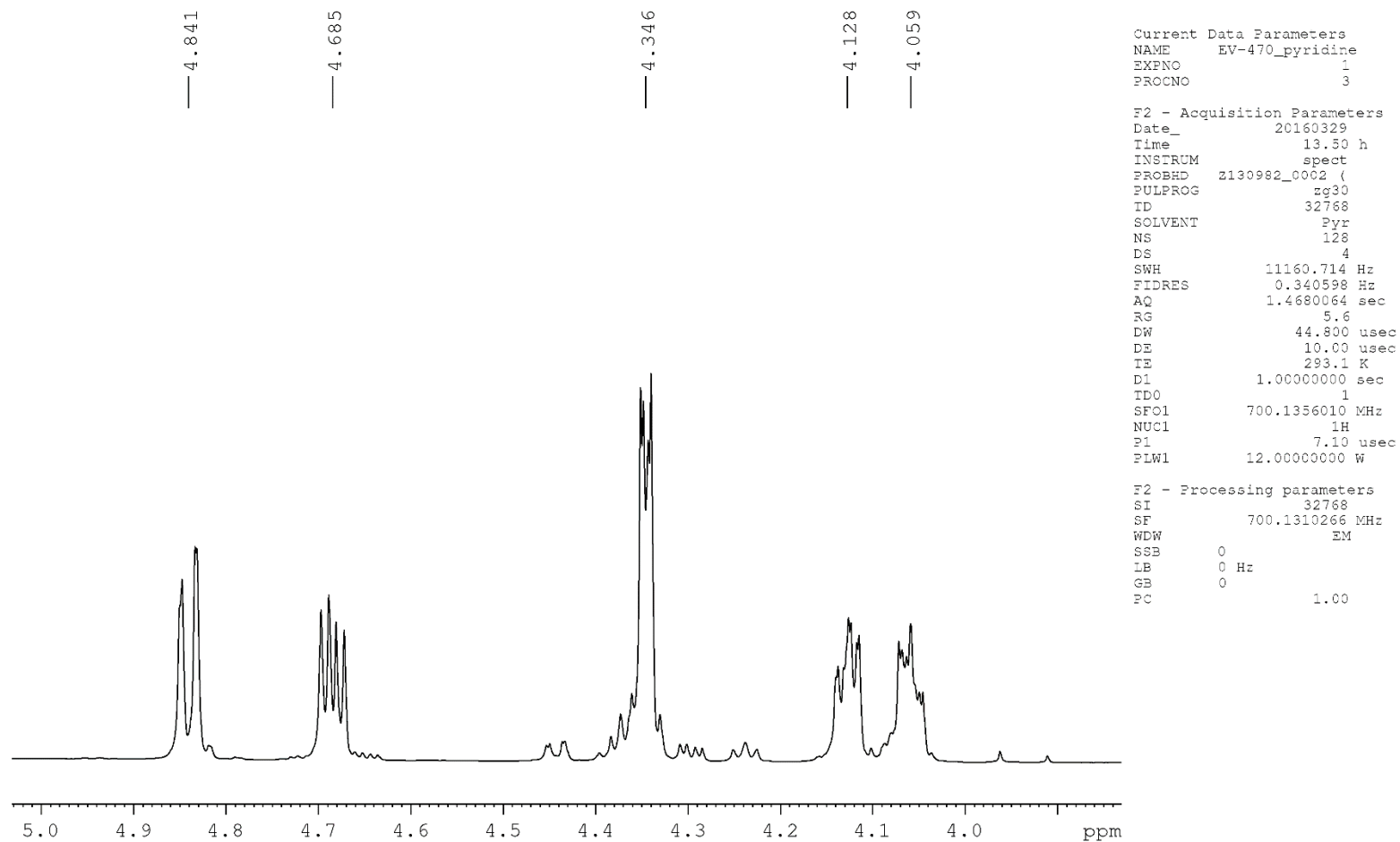


Figure S48. Detail (2/3) of <sup>1</sup>H NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K

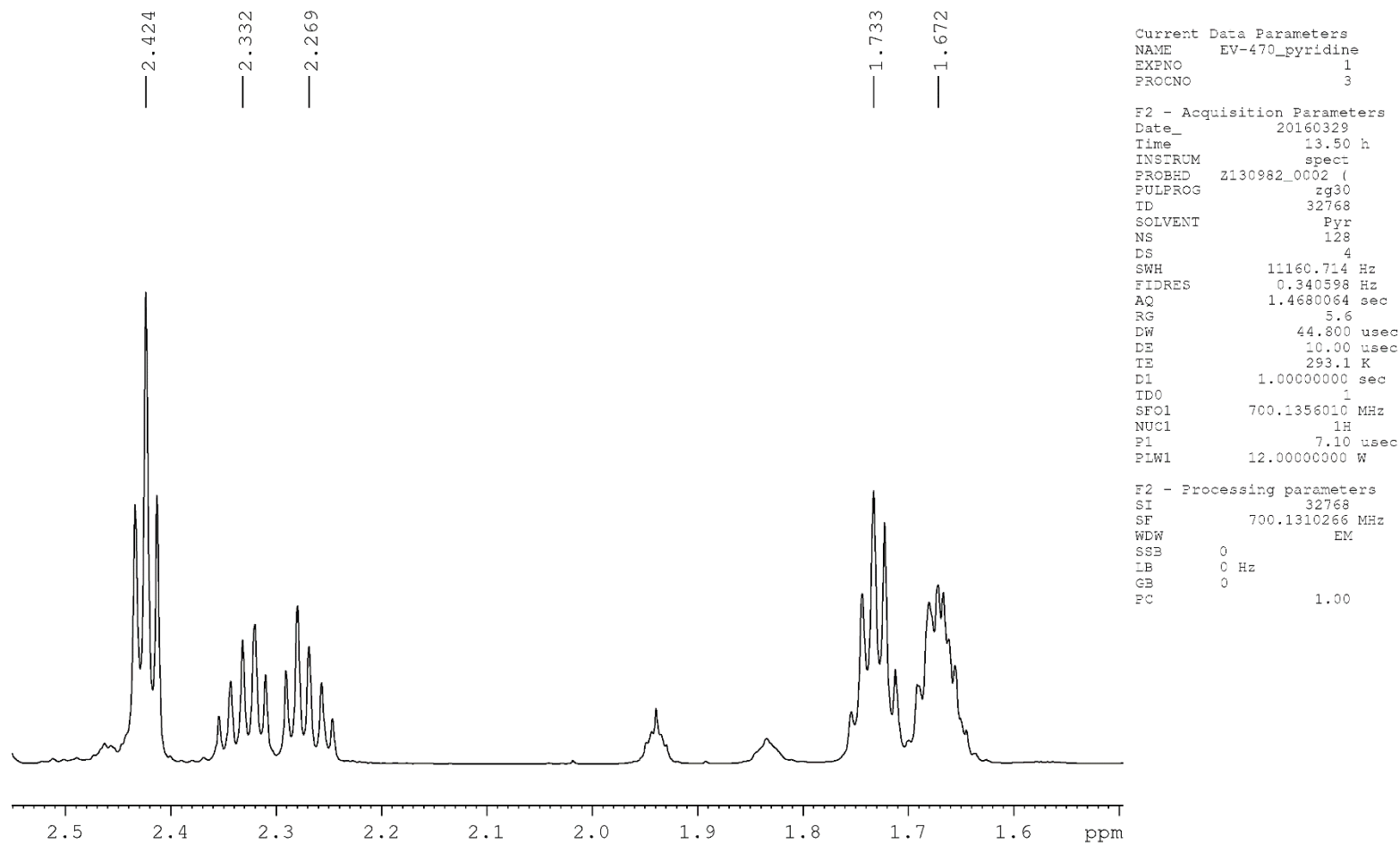


Figure S49. Detail (3/3) of <sup>1</sup>H NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K



Current Data Parameters  
 NAME EV-470\_pyridine  
 EXPNO 4  
 PROCNO 1

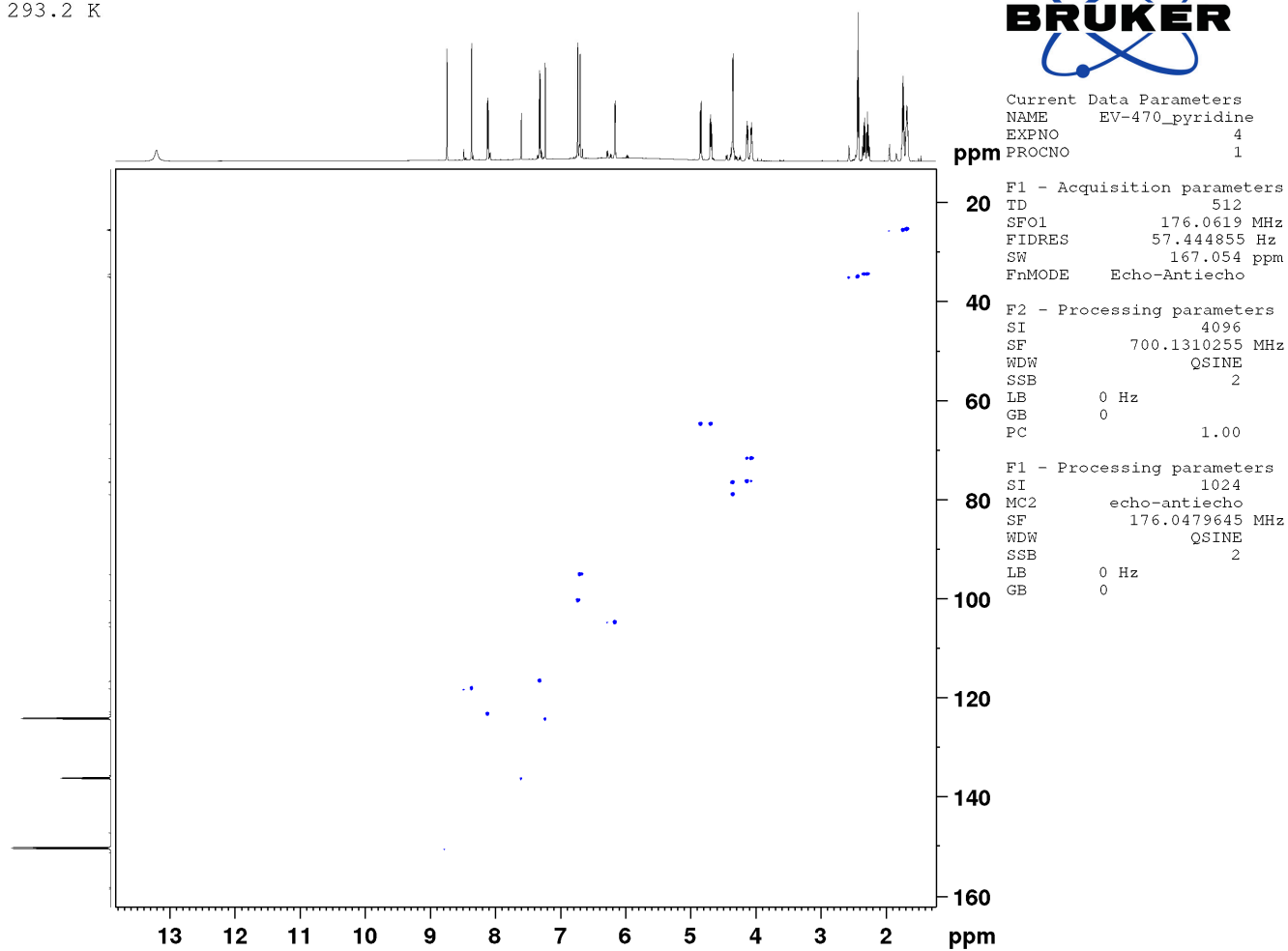


Figure S50. HSQC NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K

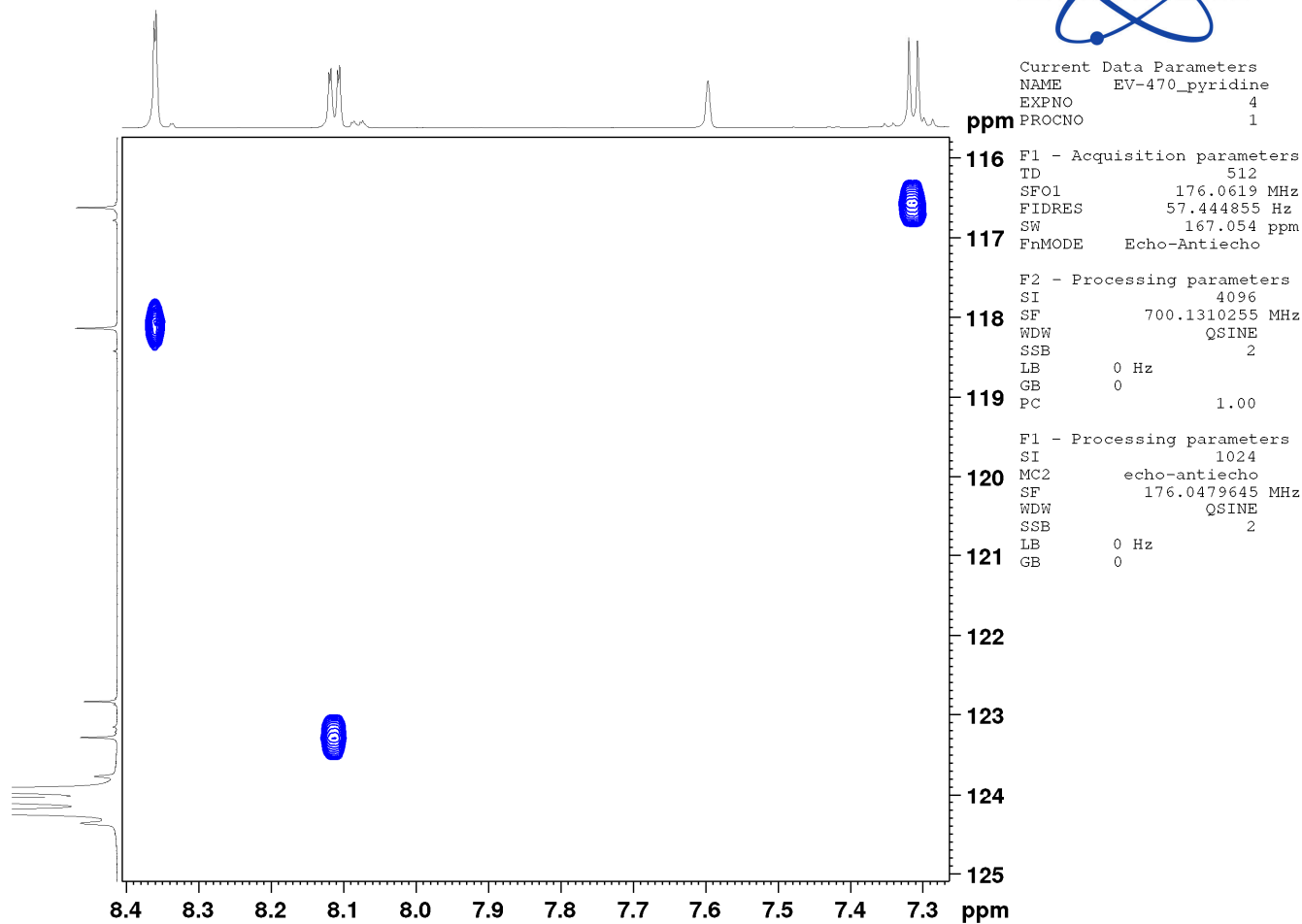


Figure S51. Detail (1/4) of HSQC NMR spectrum of compound 10.



EV-470  
 solvent: pyridine  
 temp: 293.2 K

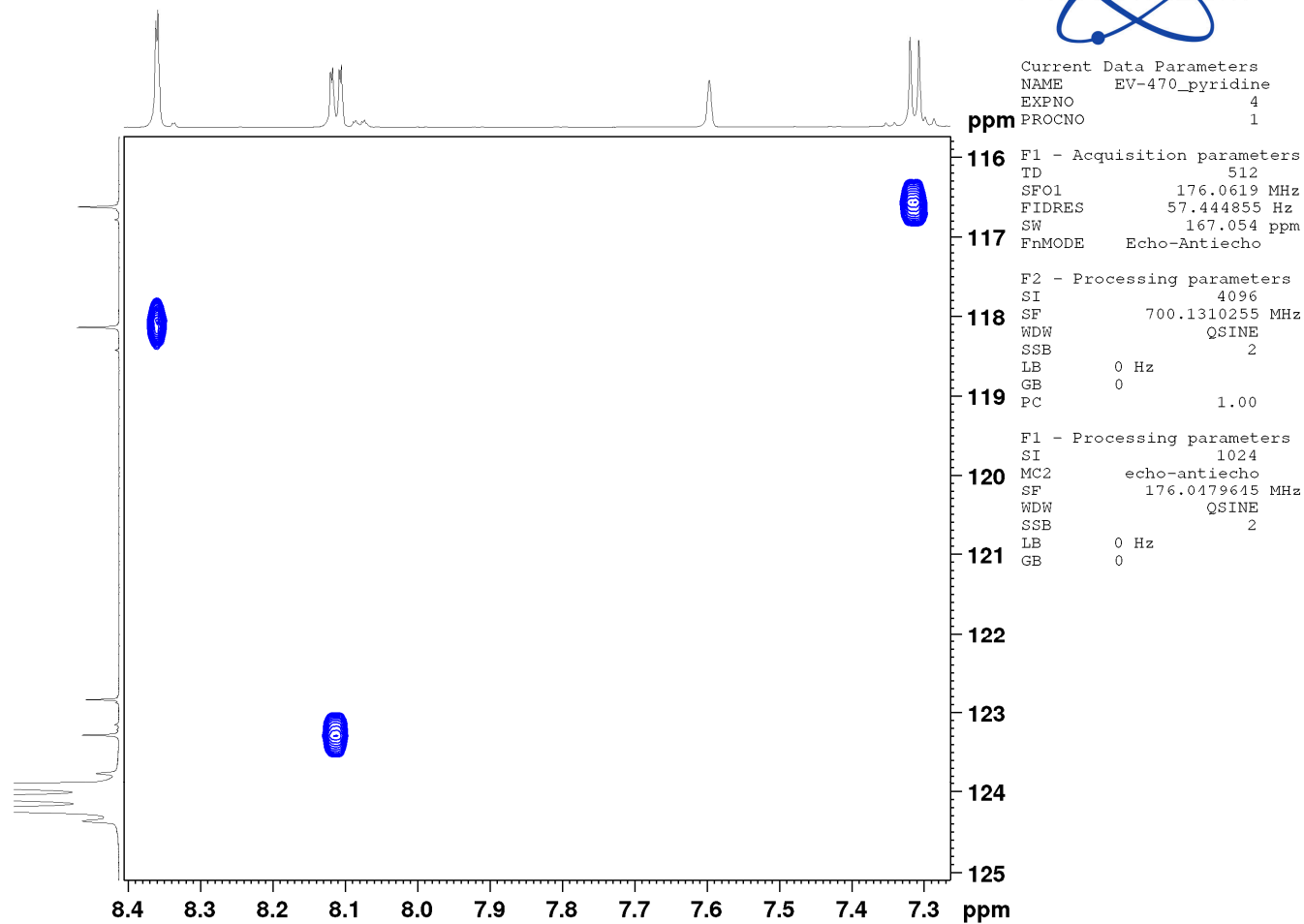


Figure S52. Detail (2/4) of HSQC NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K



Current Data Parameters  
 NAME EV-470\_pyridine  
 EXPNO 4  
 PROCNO 1

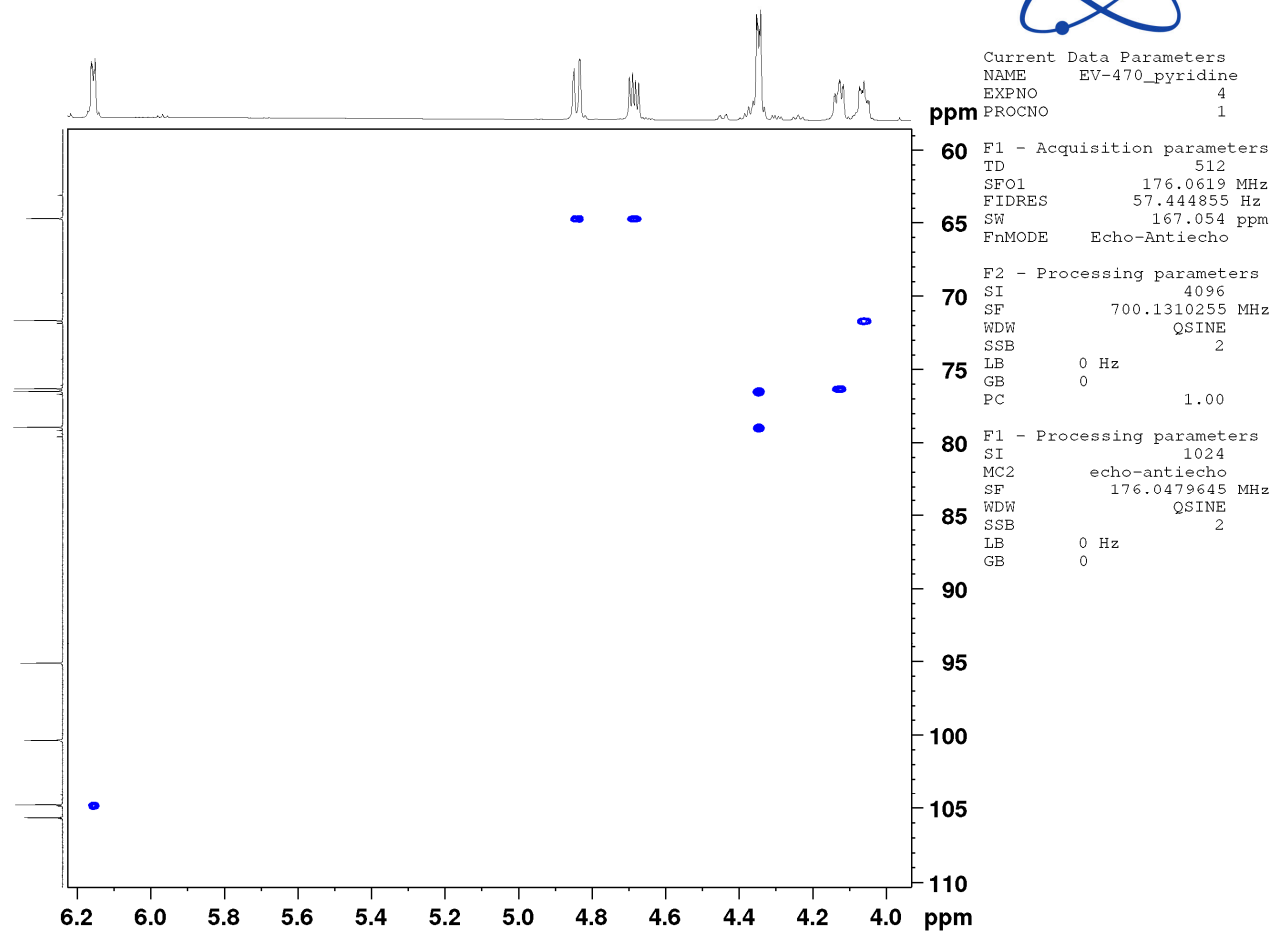


Figure S53. Detail (3/4) of HSQC NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K



Current Data Parameters  
 NAME EV-470\_pyridine  
 EXPNO 4  
 PROCNO 1

F1 - Acquisition parameters  
 TD 512  
 SFO1 176.0619 MHz  
 FIDRES 57.444855 Hz  
 SW 167.054 ppm  
 FhMODE Echo-Antiecho

F2 - Processing parameters  
 SI 4096  
 SF 700.1310255 MHz  
 WDW QSINE  
 SSB 2  
 LB 0 Hz  
 GB 0  
 PC 1.00

F1 - Processing parameters  
 SI 1024  
 MC2 echo-antiecho  
 SF 176.0479645 MHz  
 WDW QSINE  
 SSB 2  
 LB 0 Hz  
 GB 0

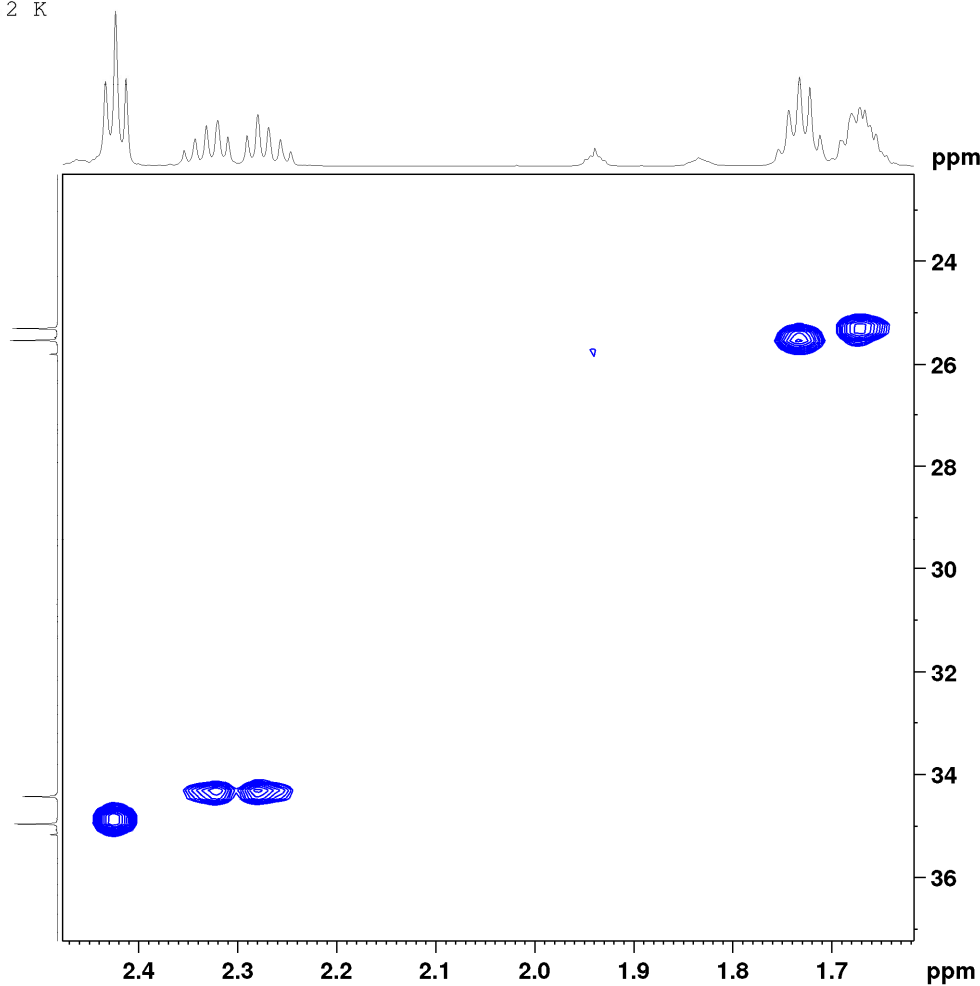


Figure S54. Detail (4/4) of HSQC NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K

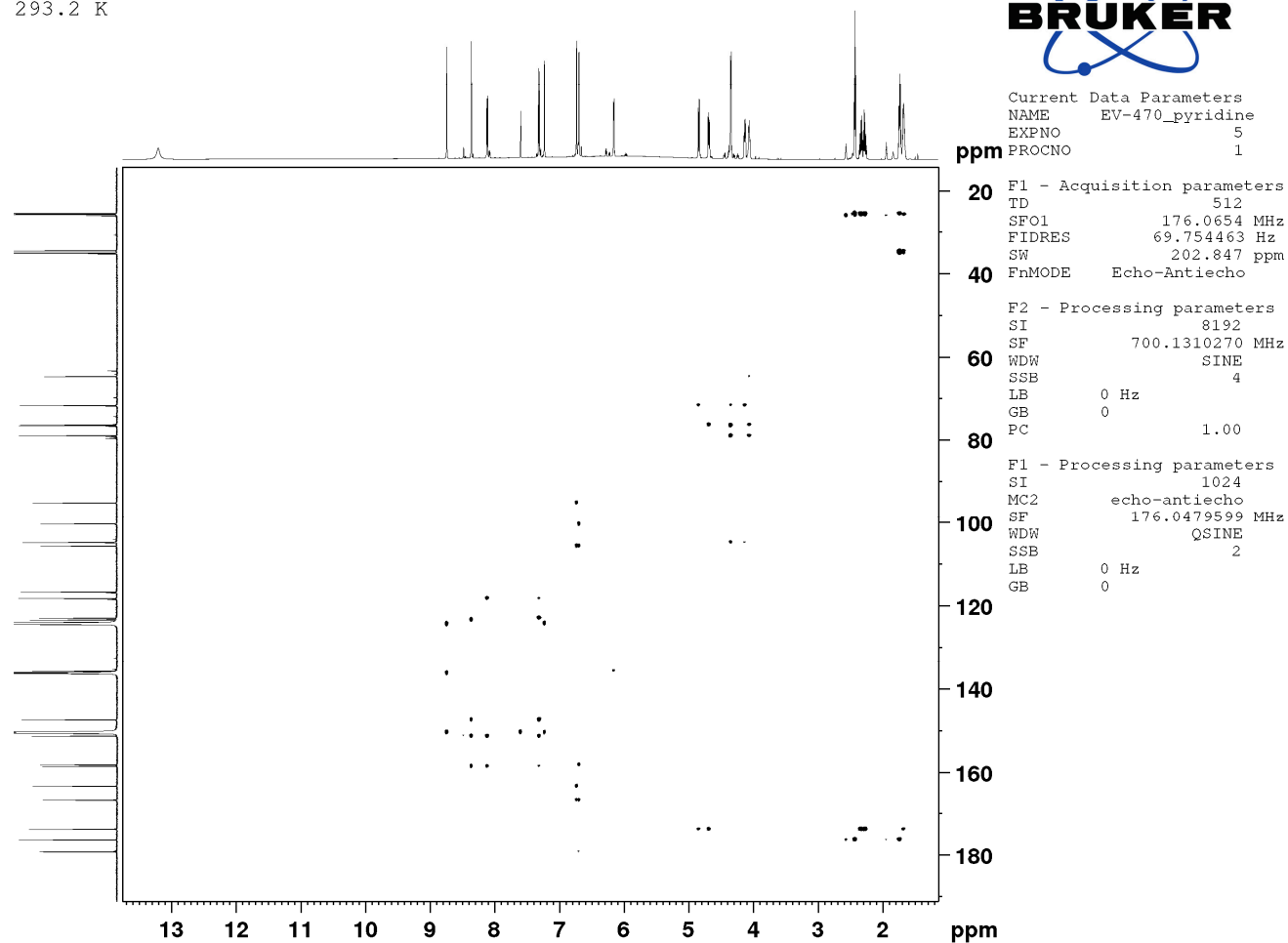


Figure S55. HMBC NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K

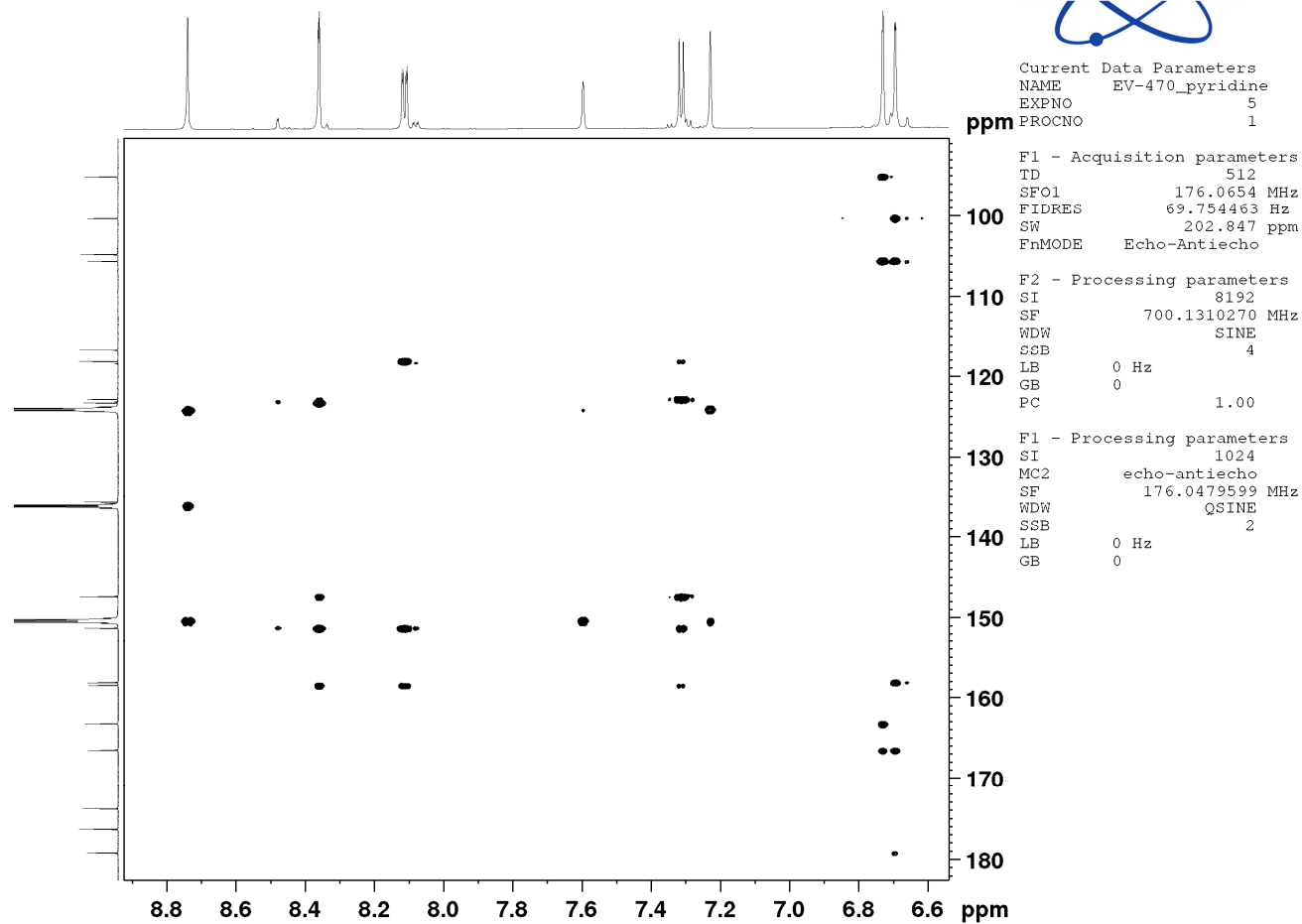


Figure S56. Detail (1/7) of HMBC NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K



Current Data Parameters  
 NAME EV-470\_pyridine  
 EXPNO 5  
 PROCNO 1

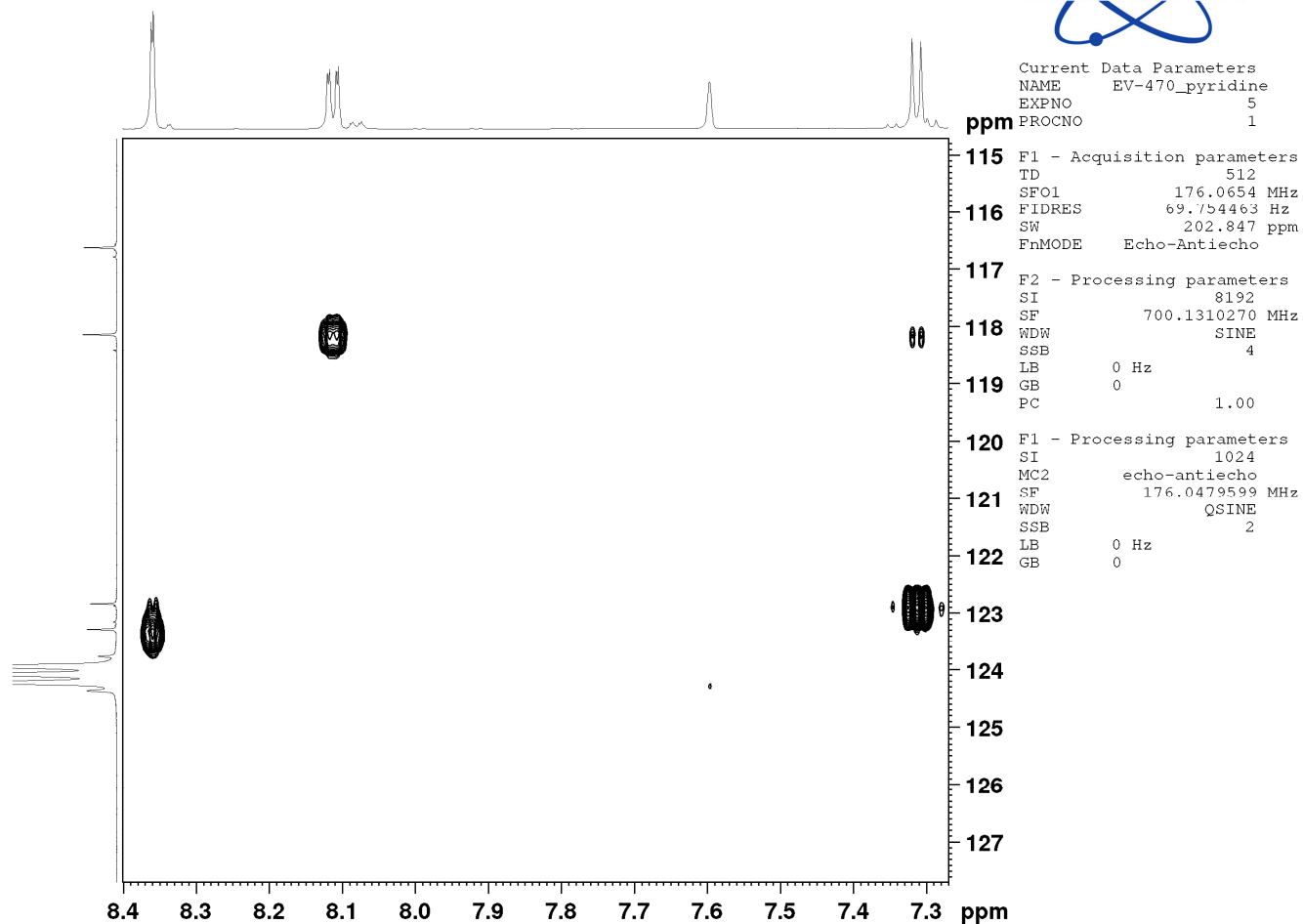


Figure S57. Detail (2/7) of HMBC NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K

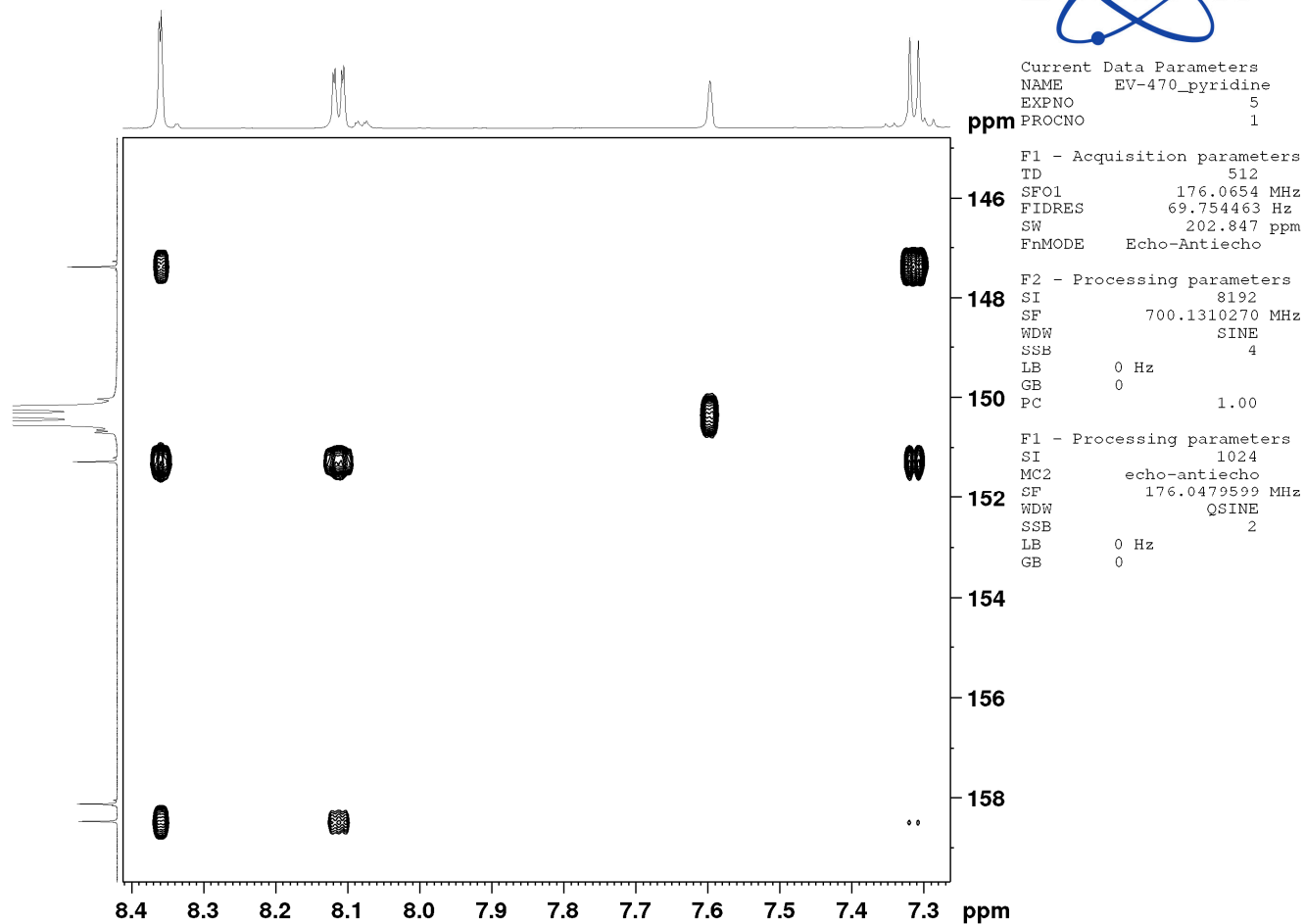


Figure S58. Detail (3/7) of HMBC NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K

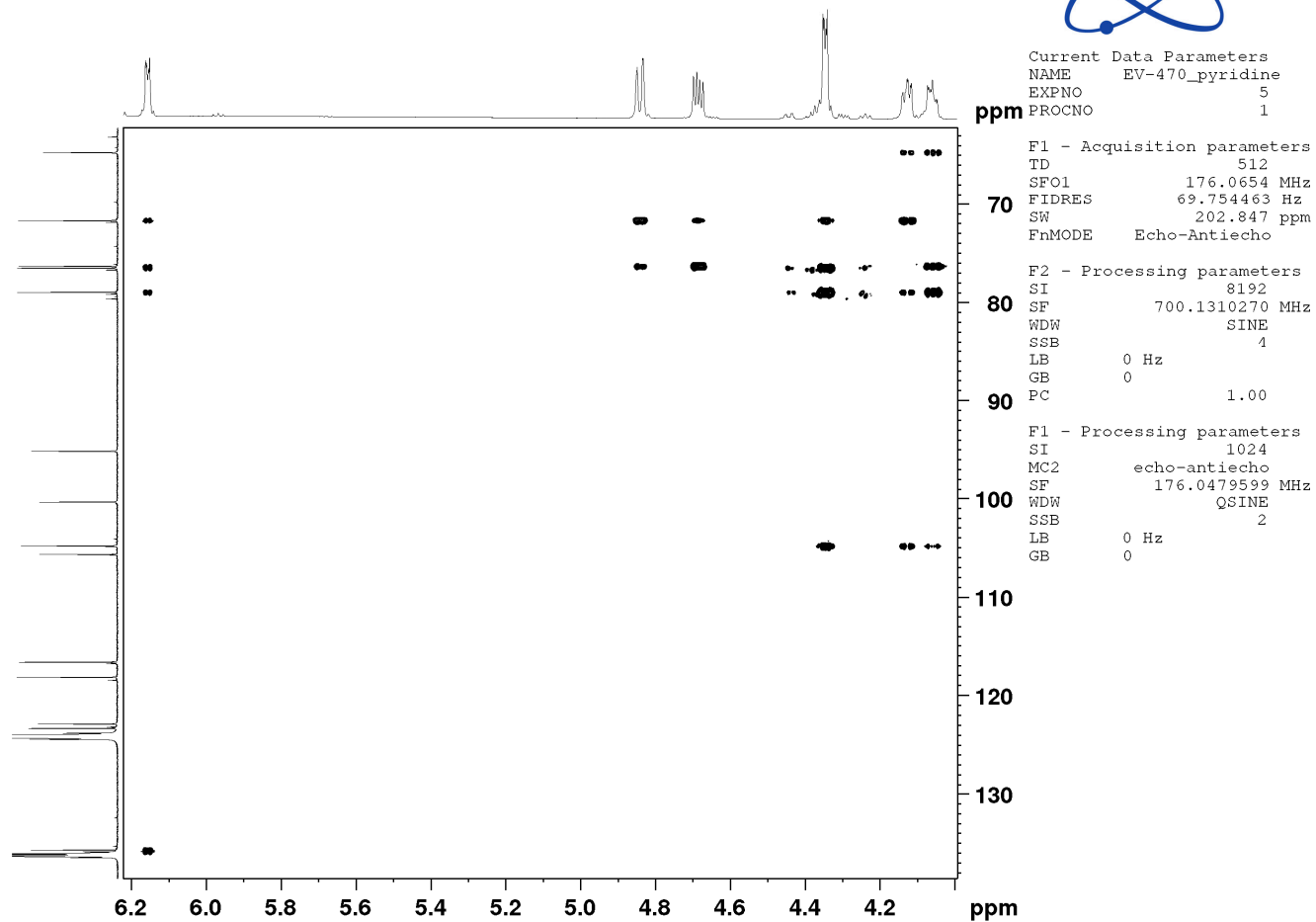


Figure S59. Detail (4/7) of HMBC NMR spectrum of compound 10.



EV-470  
 solvent: pyridine  
 temp: 293.2 K

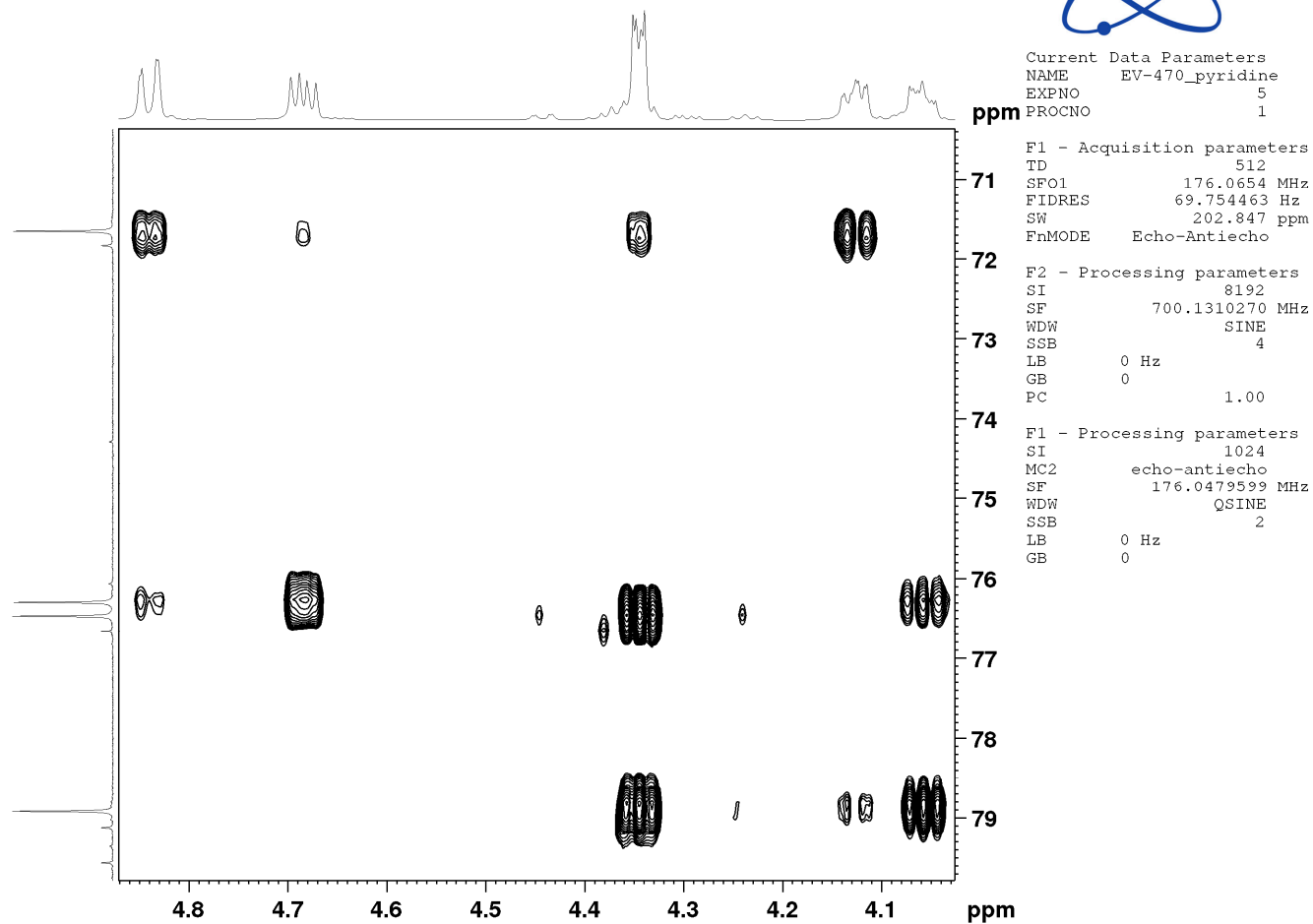


Figure S60. Detail (5/7) of HMBC NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K

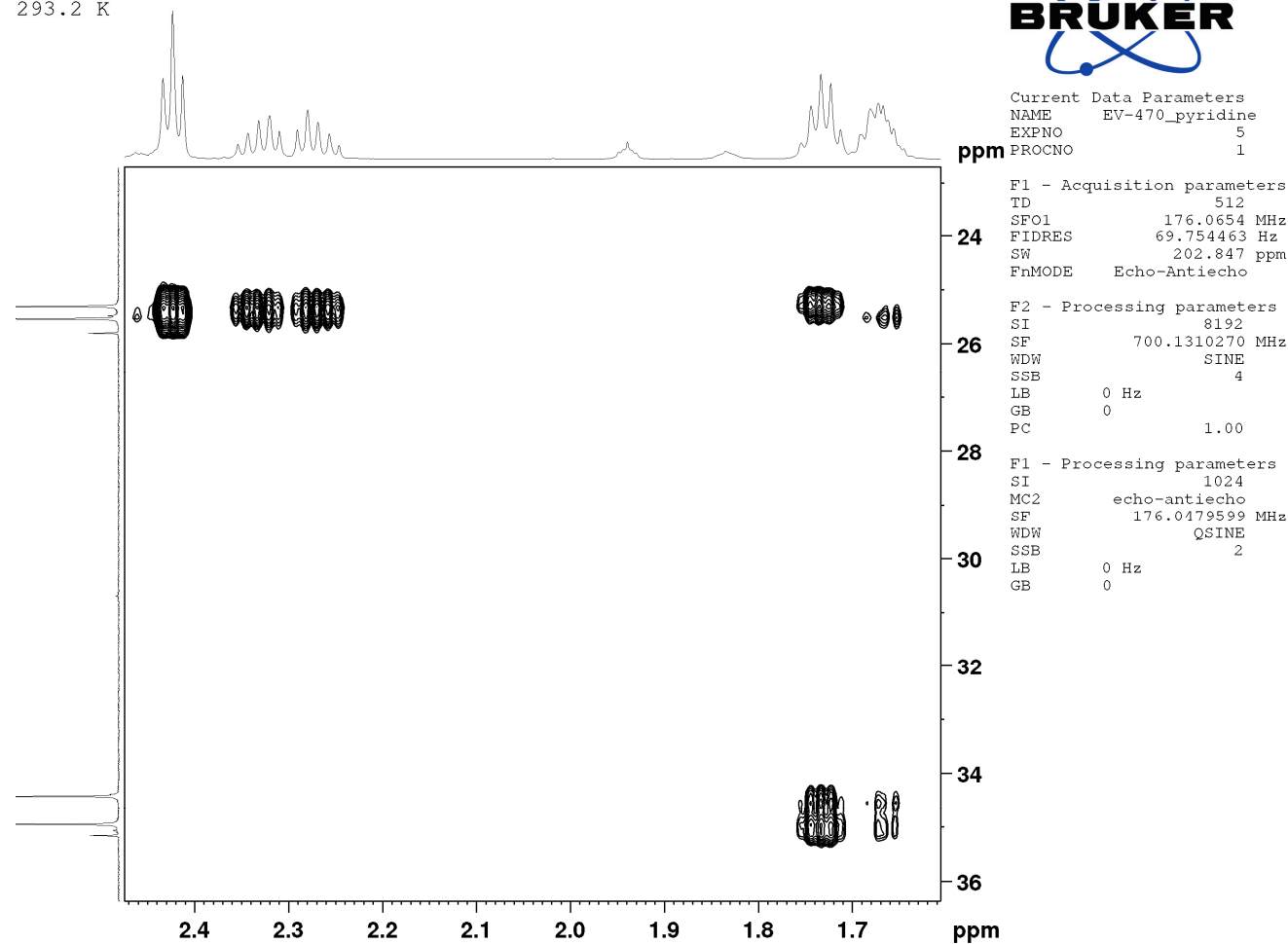


Figure S61. Detail (6/7) of HMBC NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K



Current Data Parameters  
 NAME EV-470\_pyridine  
 EXPNO 5  
 PROCNO 1

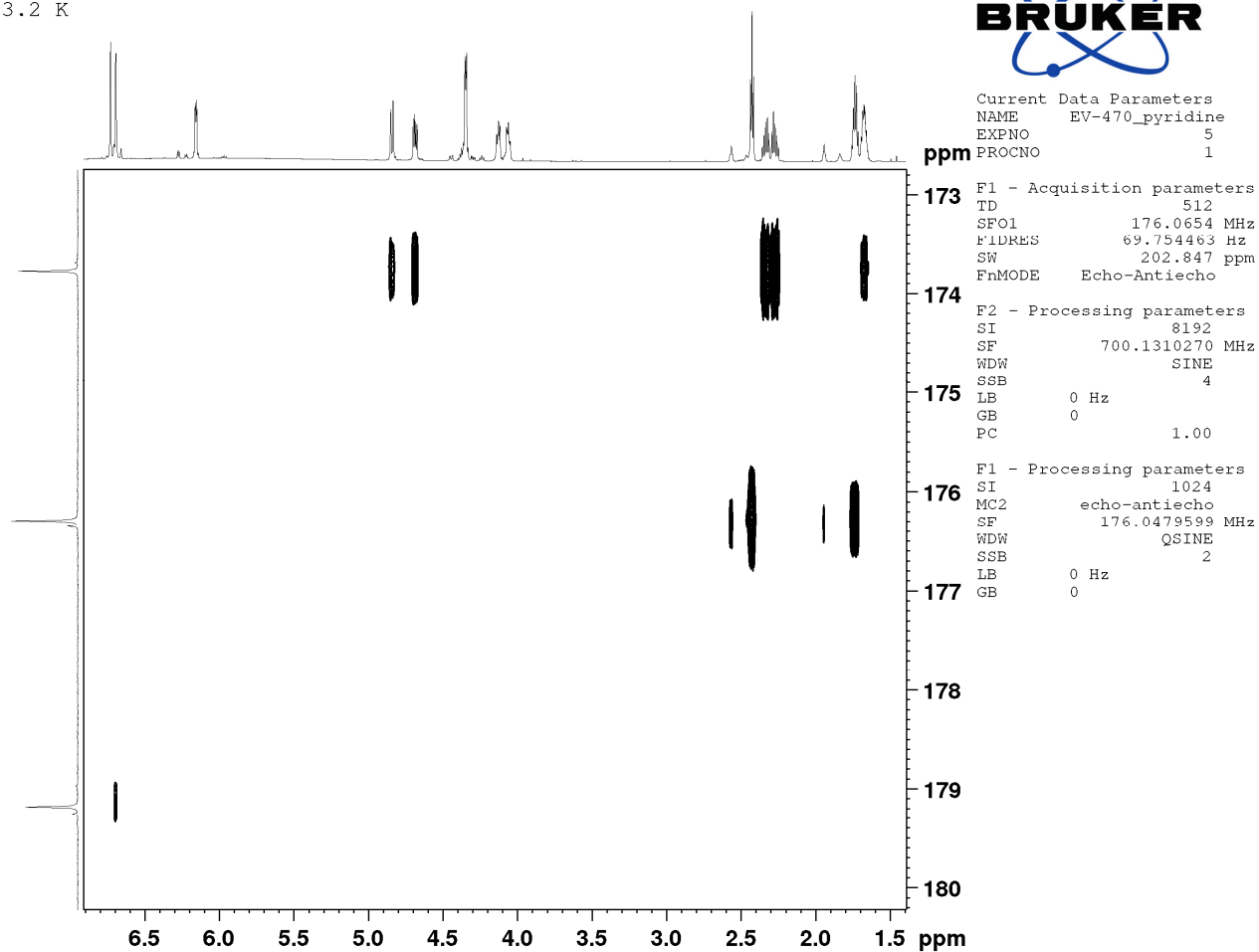


Figure S62. Detail (7/7) of HMBC NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K

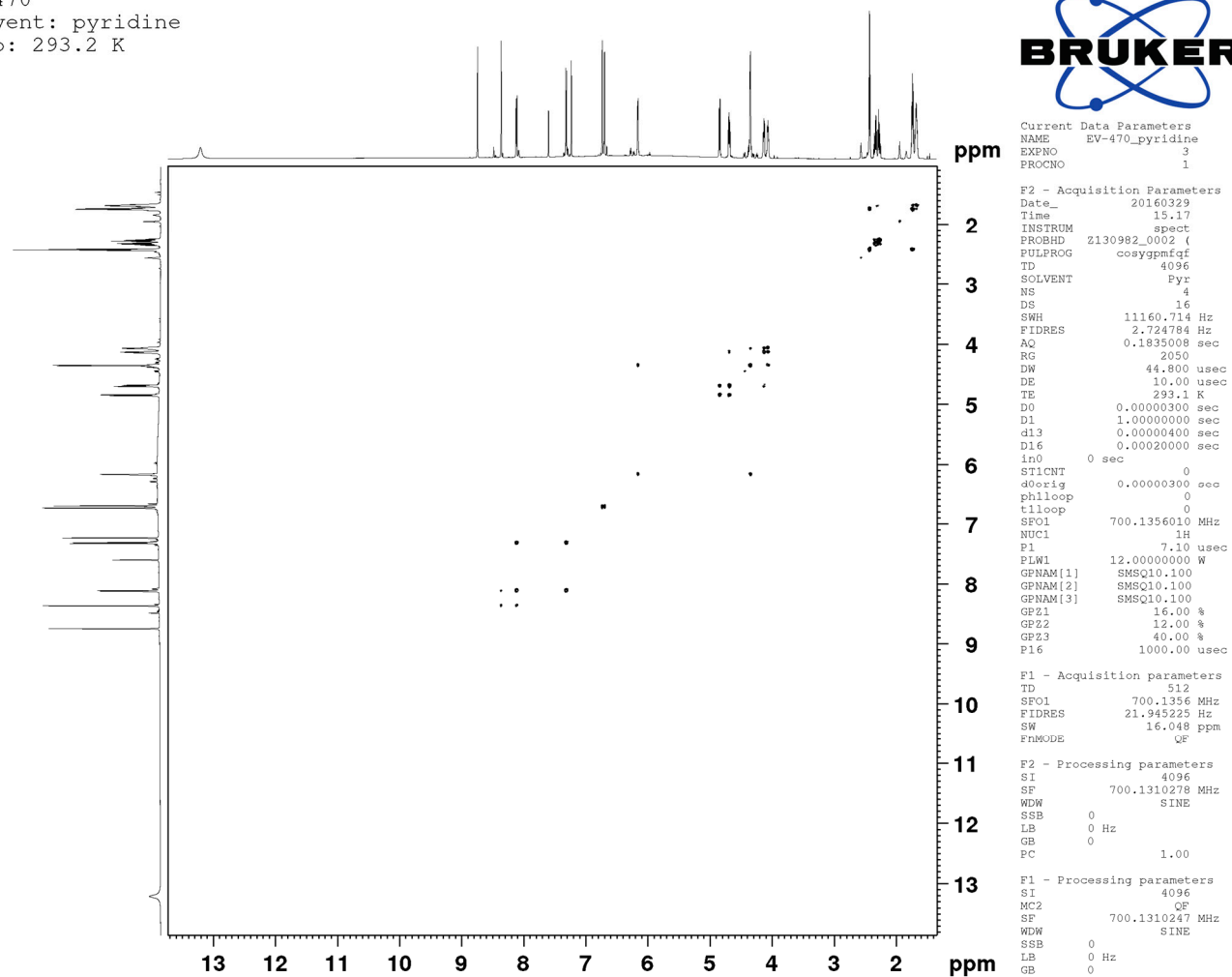


Figure S63. COSY NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K

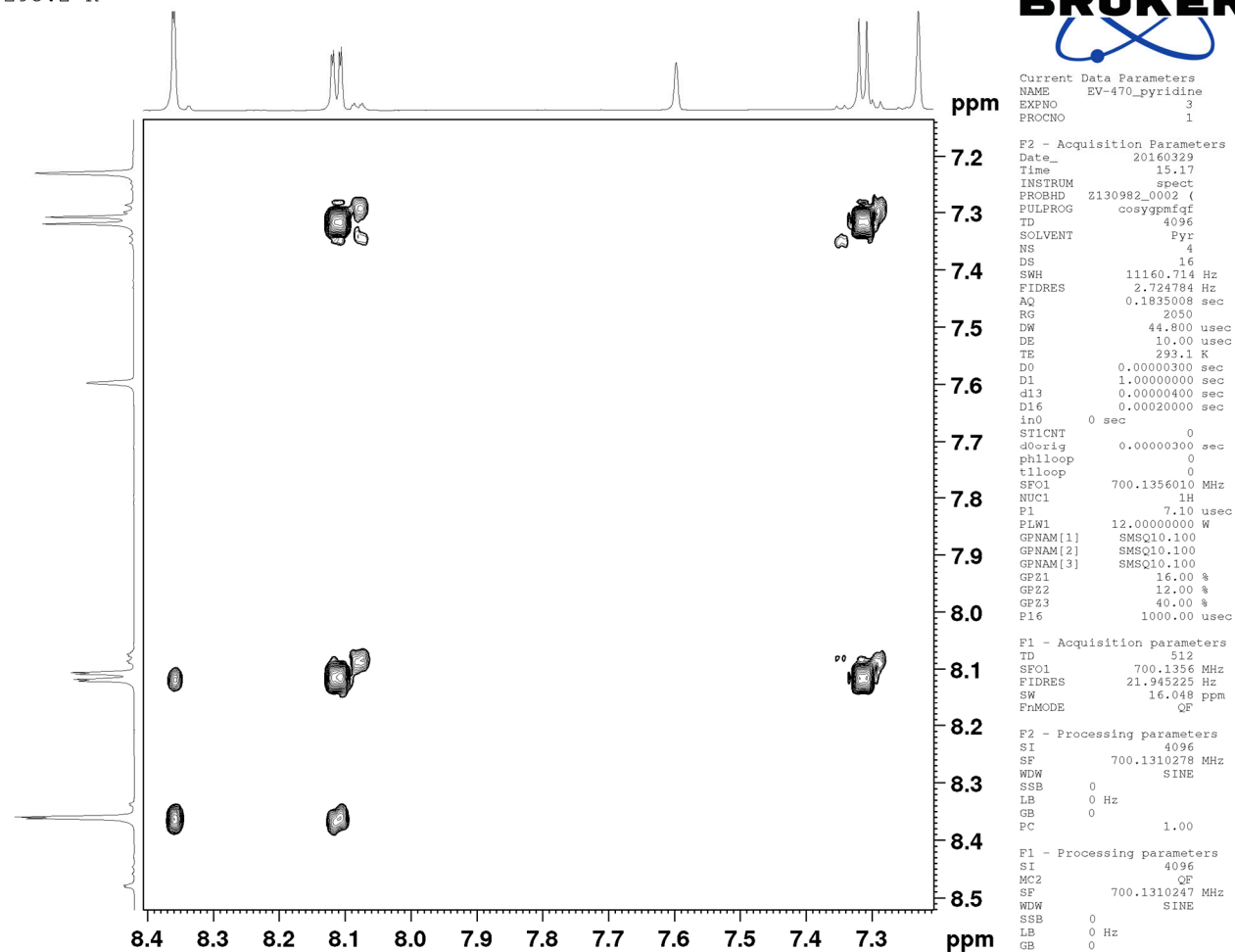


Figure S64. Detail (1/3) of COSY NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K

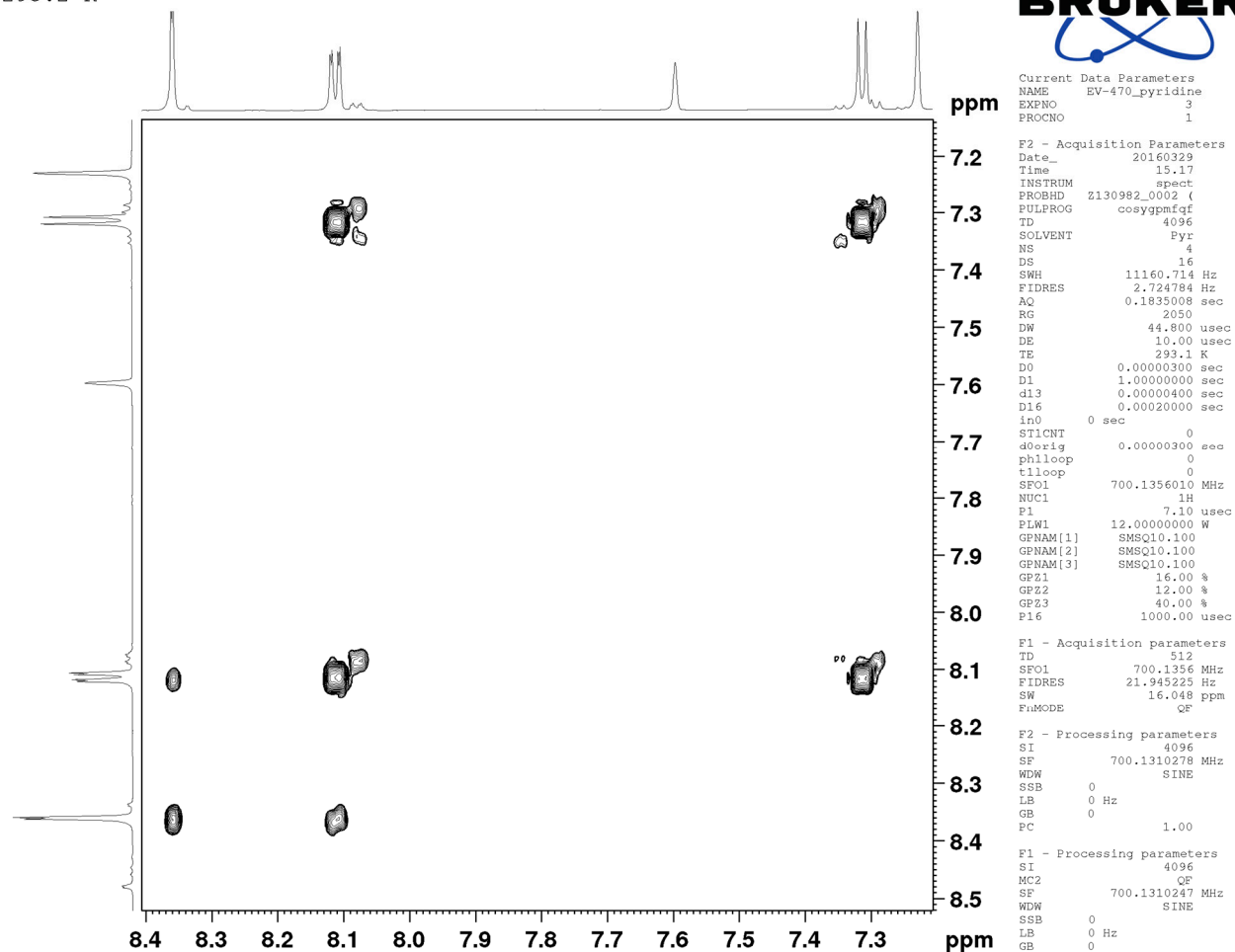


Figure S65. Detail (2/3) of COSY NMR spectrum of compound 10.

EV-470  
 solvent: pyridine  
 temp: 293.2 K

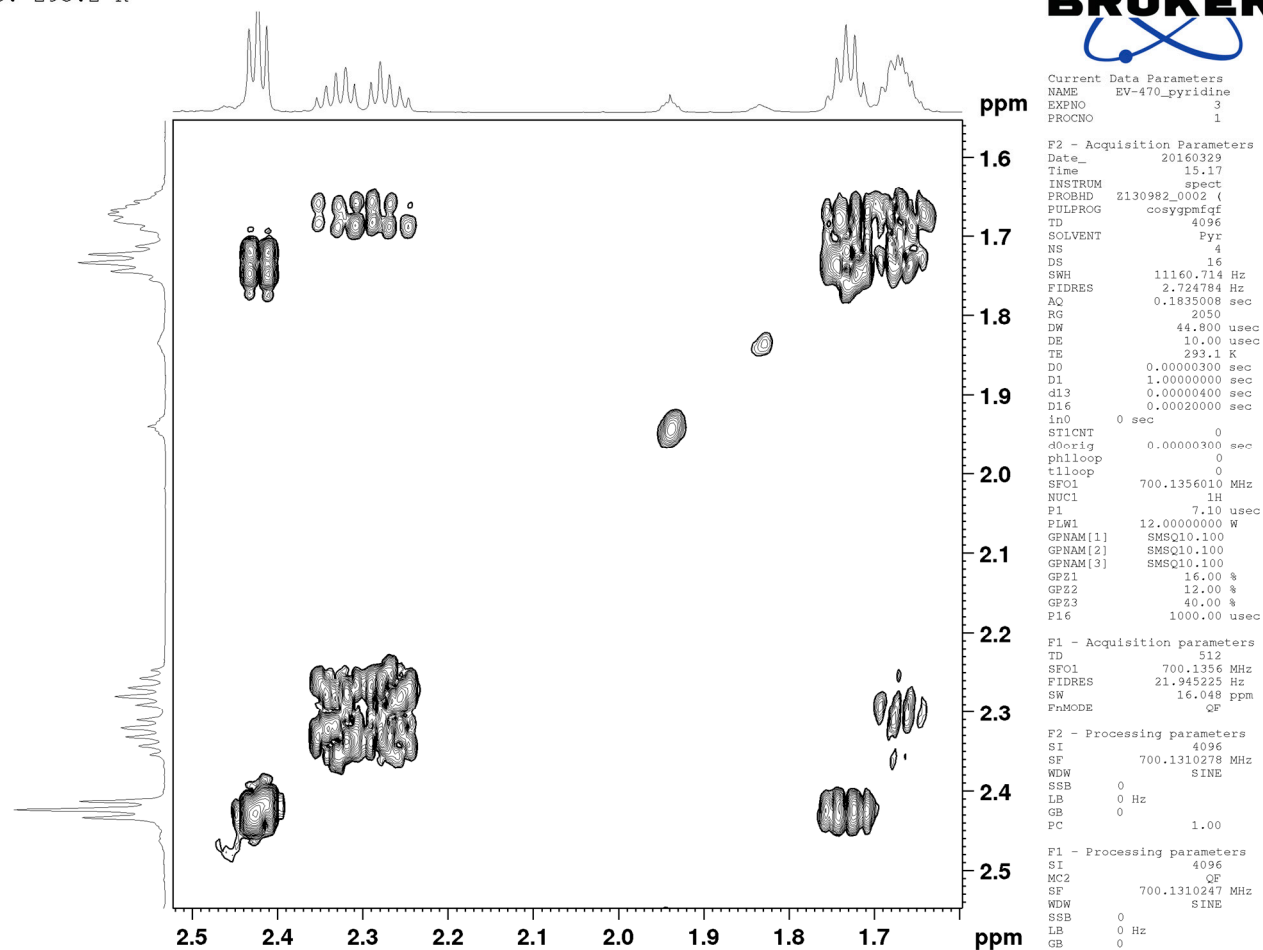


Figure S66. Detail (3/3) of COSY NMR spectrum of compound 10.

mAU

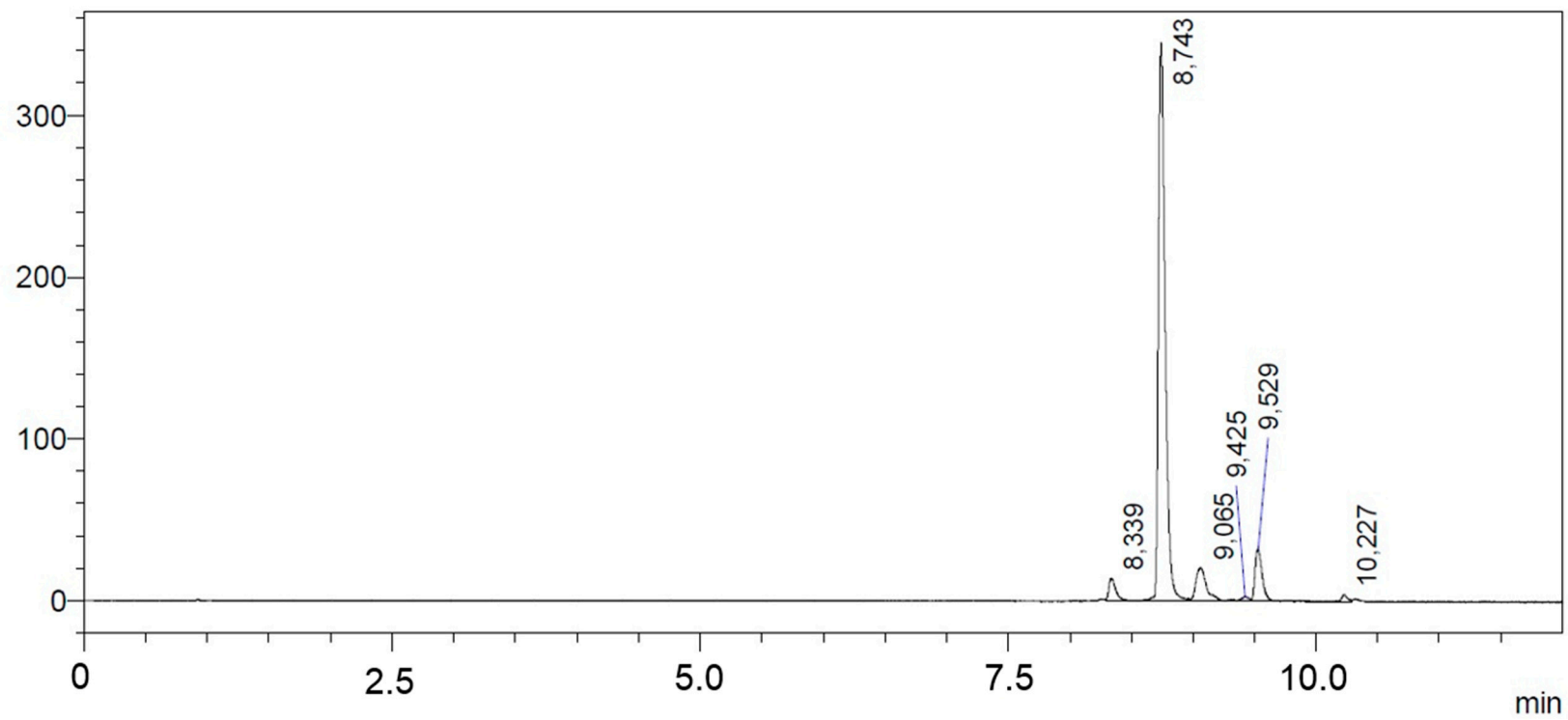
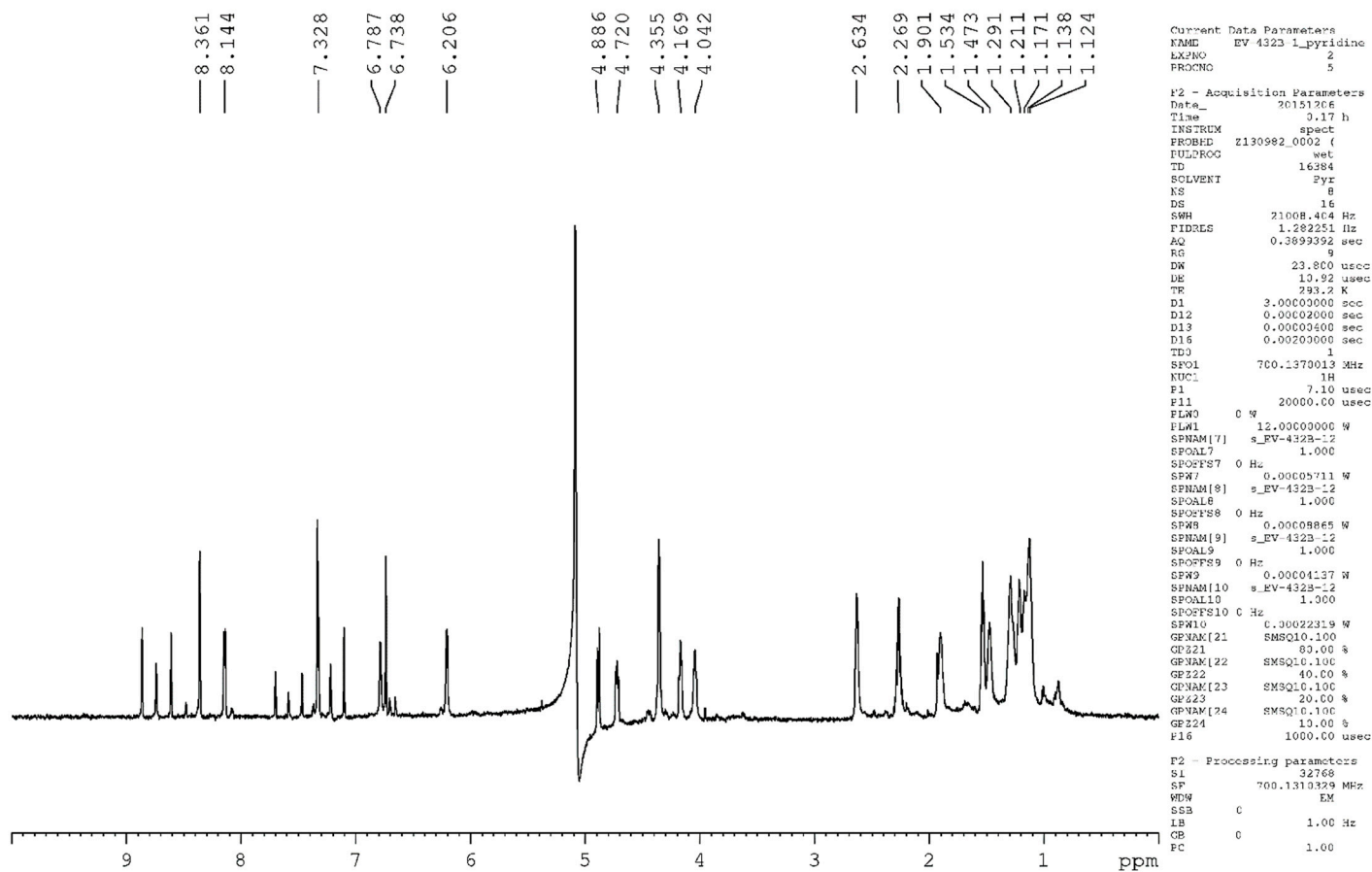


Figure S67. HPLC chromatogram of compound 10.



EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K  
 Summary : Main spectrum with NS 8 in 1.4min  
 Solvent(s) : 4 Off-resonance - residual signals of pyridine and water

Figure S68. <sup>1</sup>H NMR spectrum of compound 11.



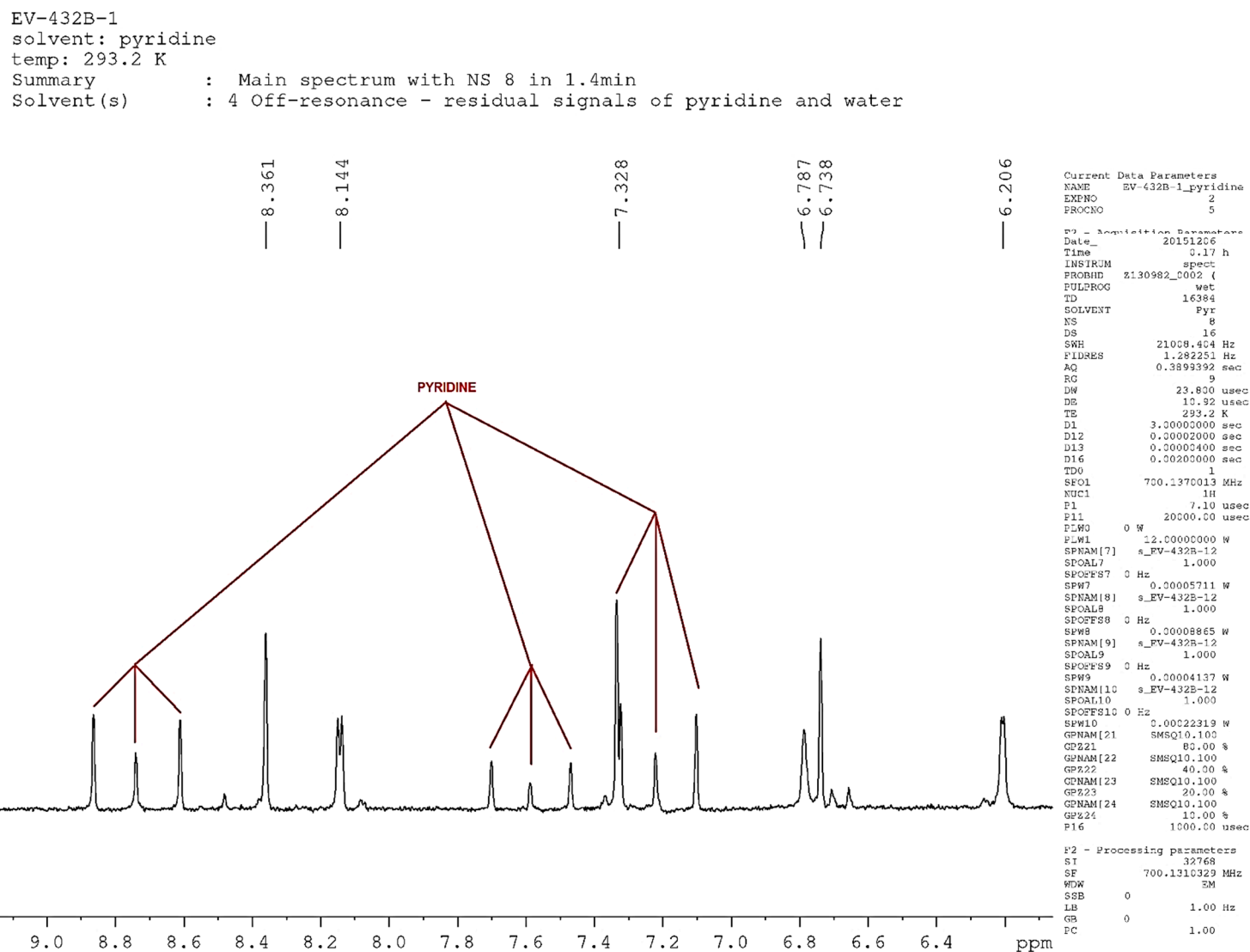
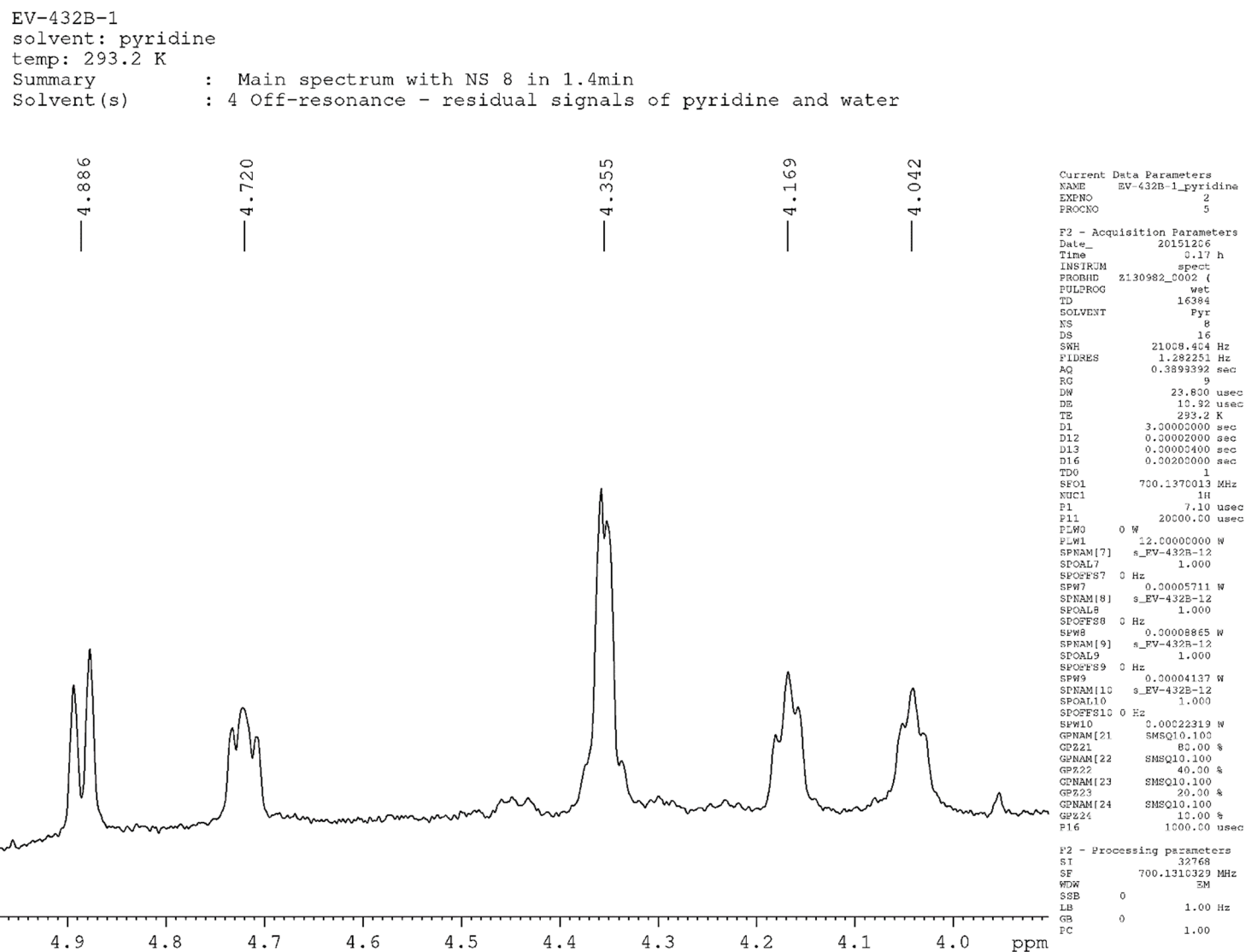
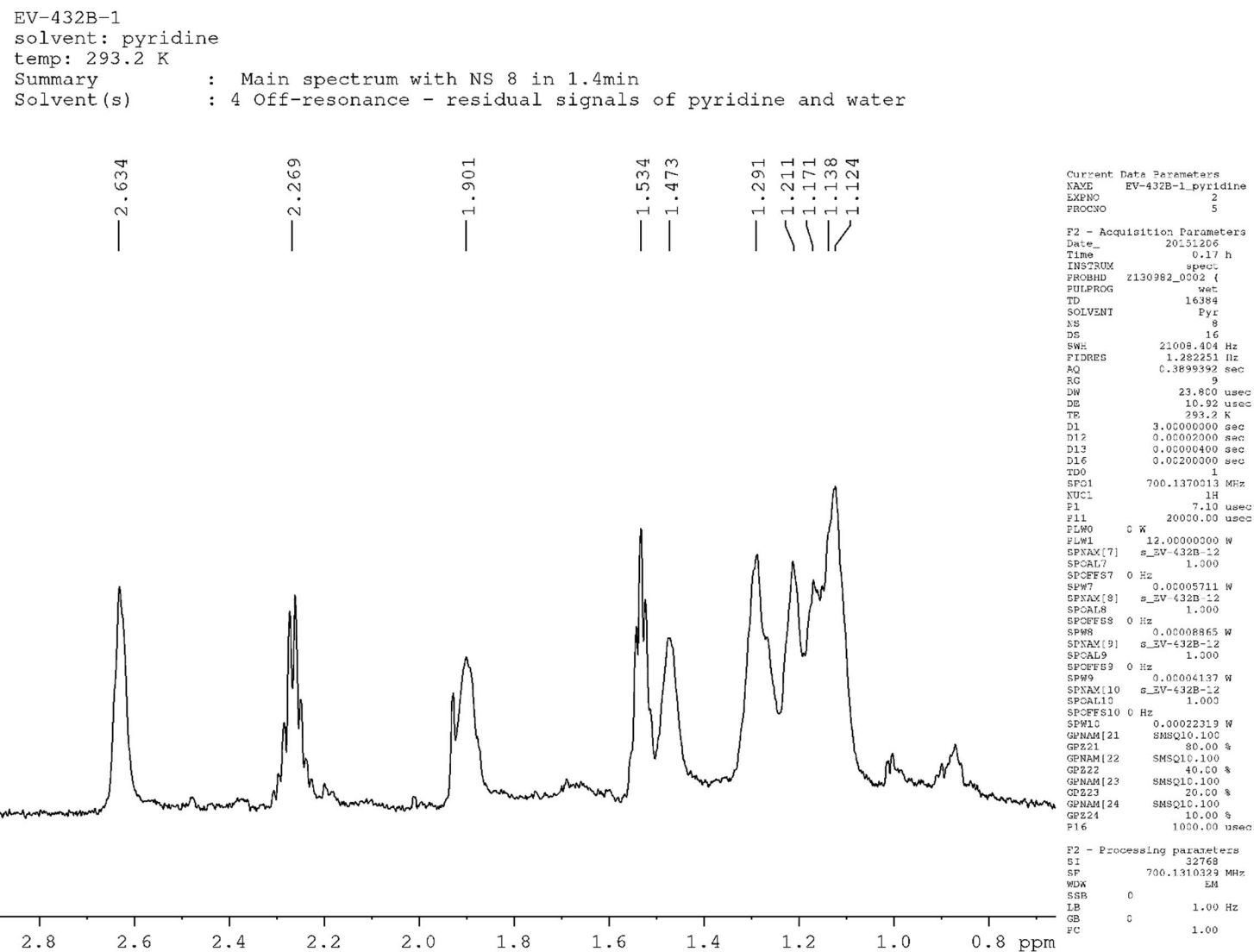


Figure S70. Detail (1/3) of <sup>1</sup>H NMR spectrum WET of compound 11.

Figure S71. Detail (2/3) of <sup>1</sup>H NMR spectrum WET of compound 11.

Figure S72. Detail (3/3) of <sup>1</sup>H NMR spectrum WET of compound 11.

EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K

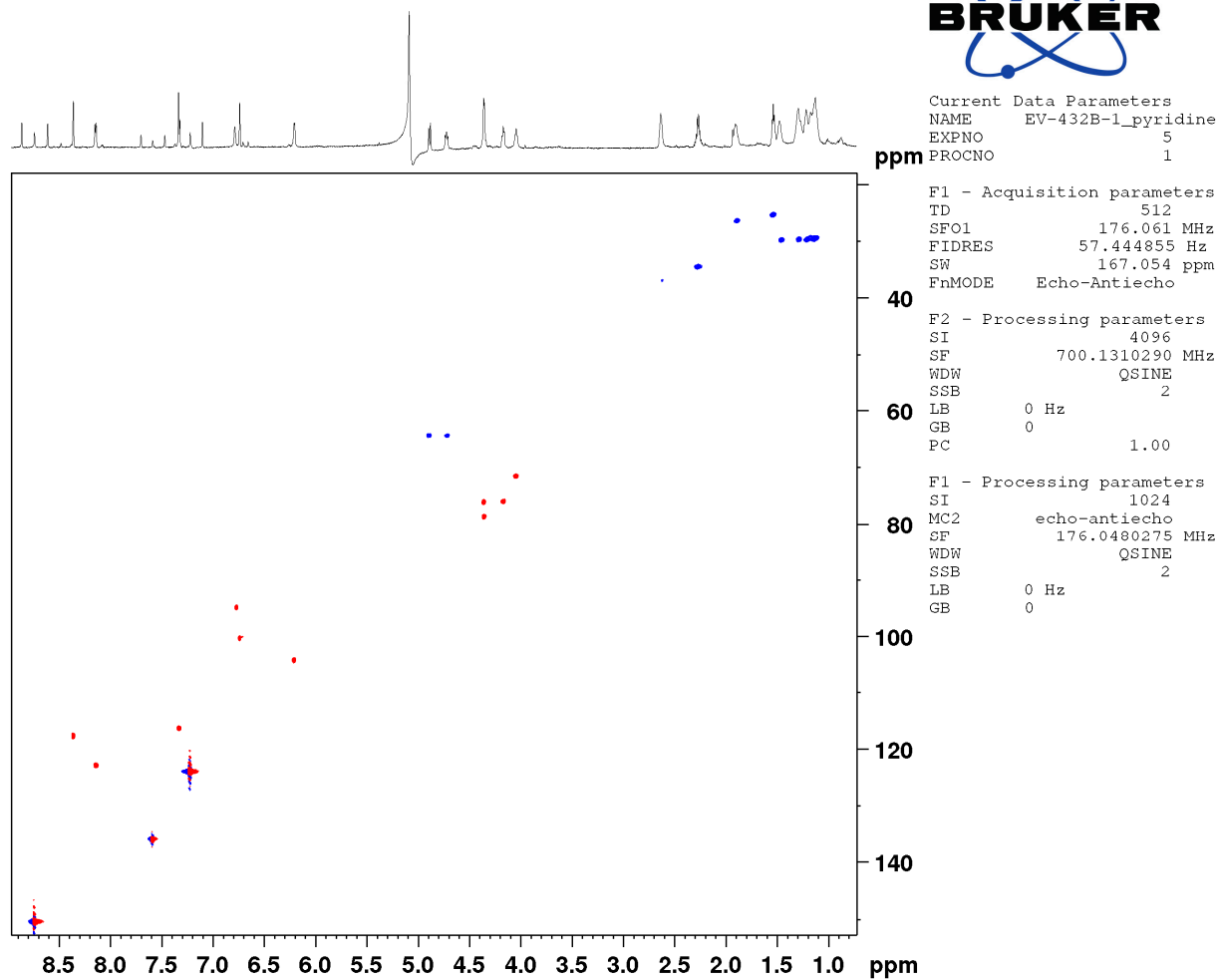


Figure S73. HSQC NMR spectrum of compound 11.

EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K

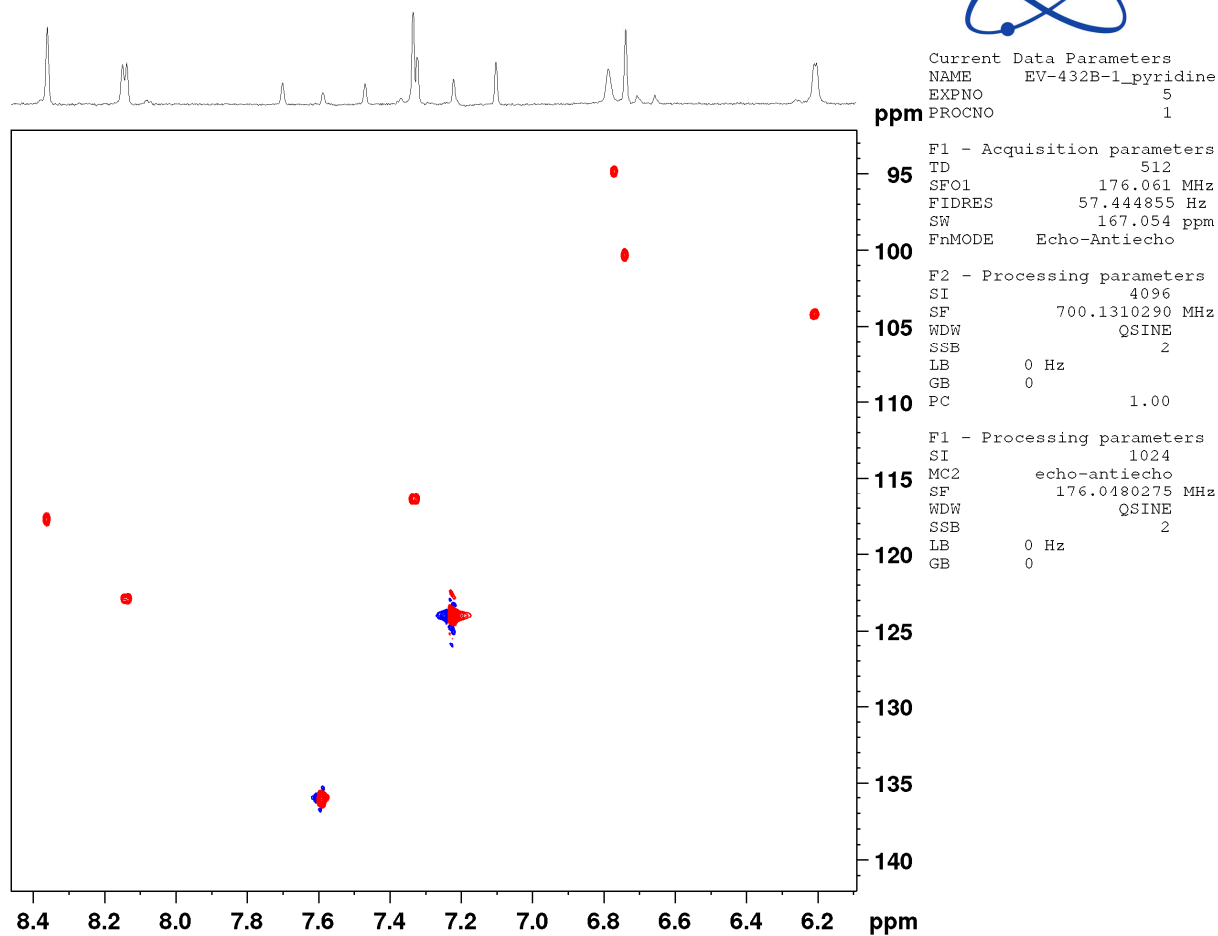


Figure S74. Detail (1/3) of HSQC NMR spectrum of compound 11.

EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K

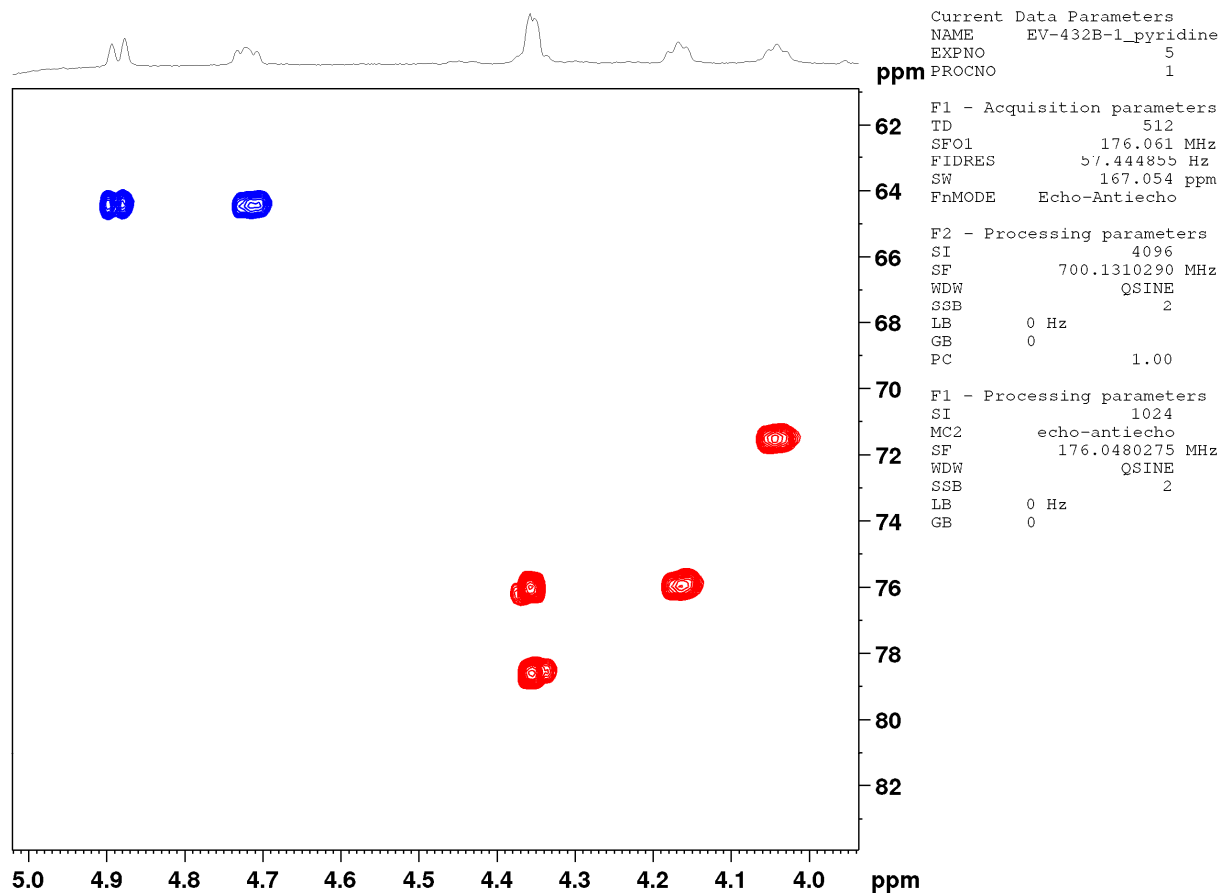


Figure S75. Detail (2/3) of HSQC NMR spectrum of compound 11.



EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K

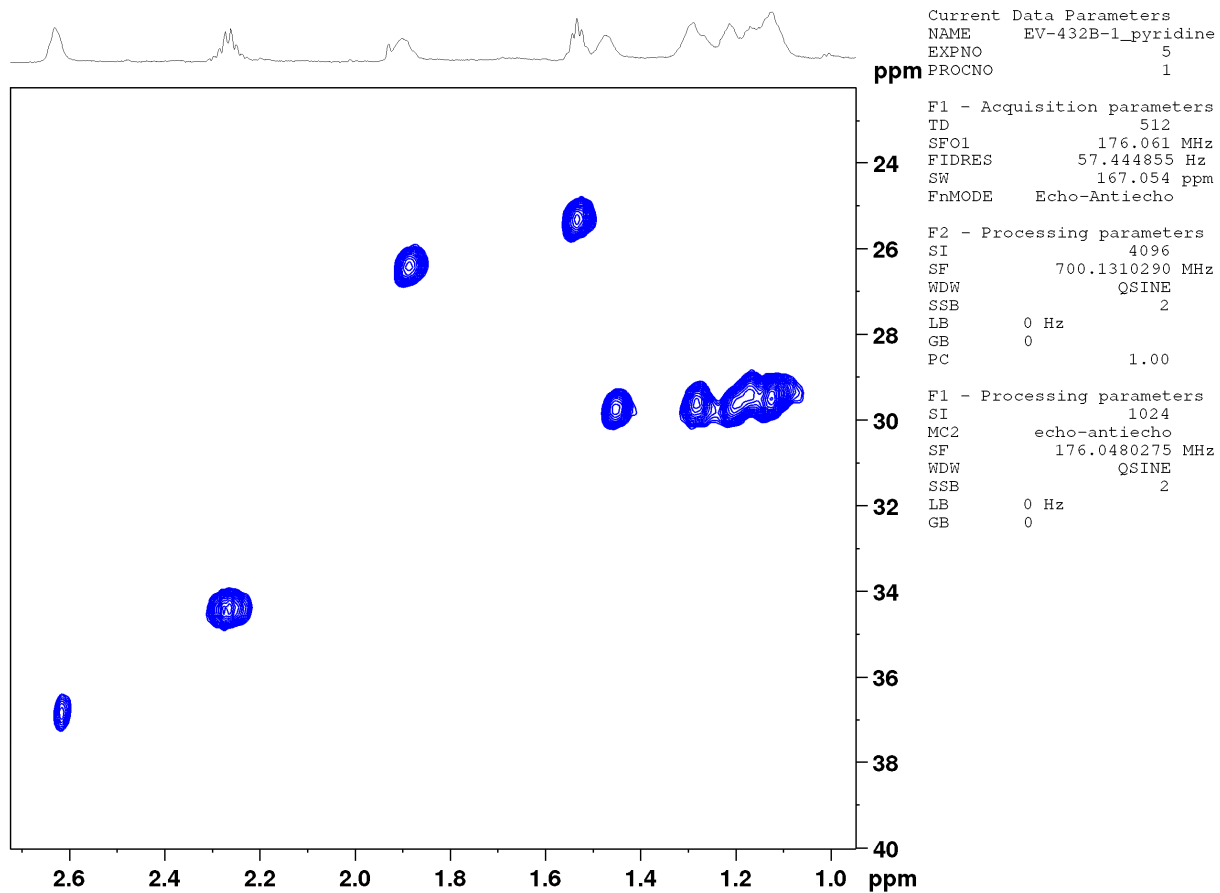


Figure S76. Detail (3/3) of HSQC NMR spectrum of compound 11.

EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K



Current Data Parameters  
 NAME EV-432B-1\_pyridine  
 EXPNO 6  
 PROCNO 1

F1 - Acquisition parameters  
 TD 512  
 SFO1 176.0654 MHz  
 FIDRES 75.120193 Hz  
 SW 218.450 ppm  
 FnmODE Echo-Antiecho

F2 - Processing parameters  
 SI 8192  
 SF 700.1310301 MHz  
 WDW SINE  
 SSB 4  
 LB 0 Hz  
 GB 0  
 PC 1.00

F1 - Processing parameters  
 SI 1024  
 MC2 echo-antiecho  
 SF 176.0479768 MHz  
 WDW QSINE  
 SSB 2  
 LB 0 Hz  
 GB 0

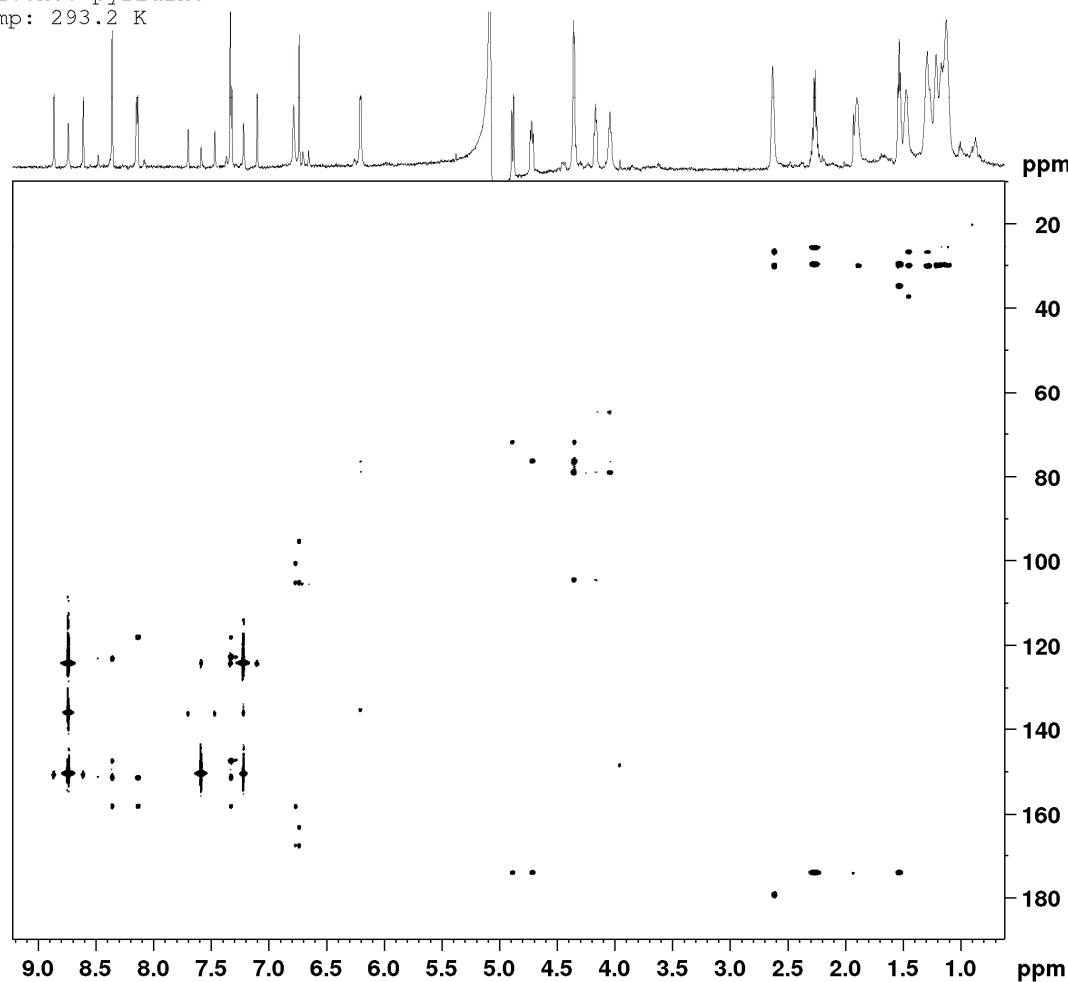
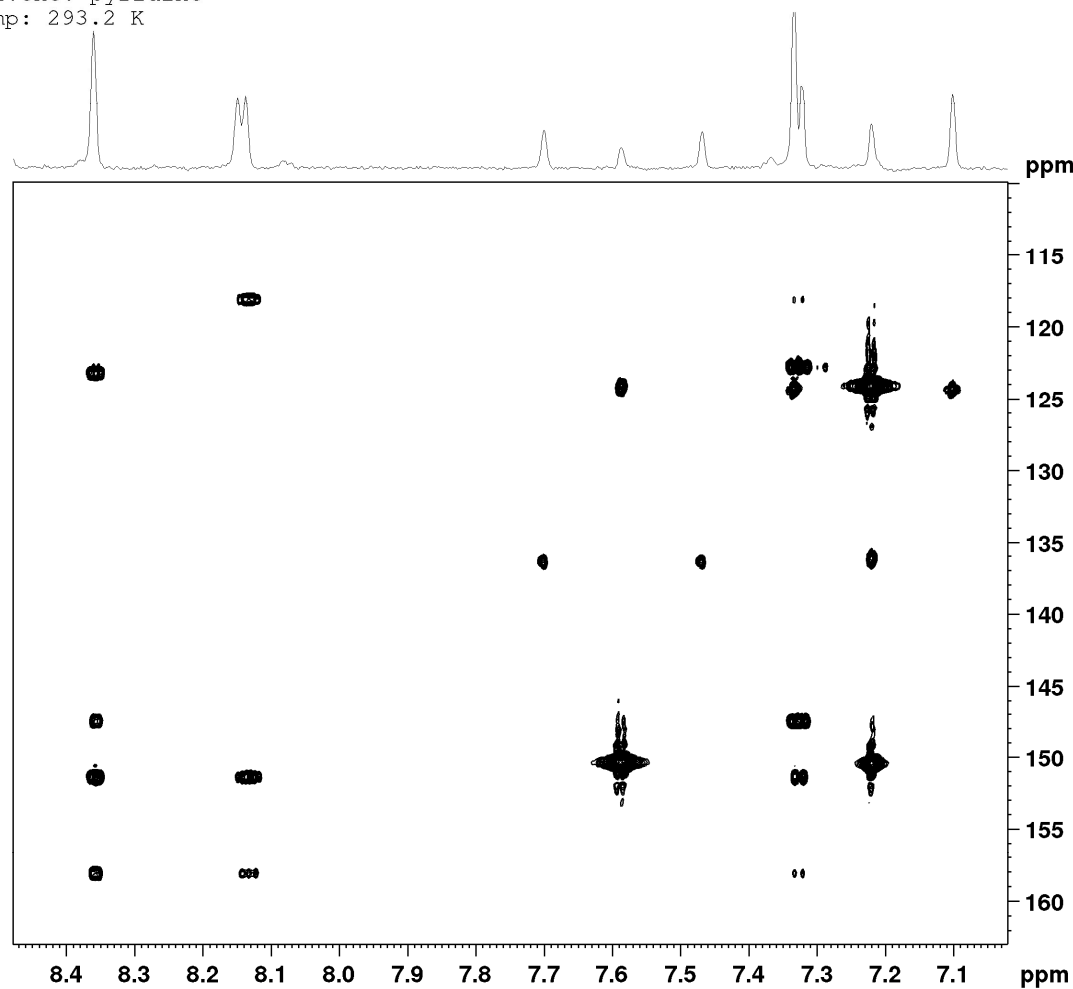


Figure S77. HMBC NMR spectrum of compound 11.

EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K



Current Data Parameters  
 NAME EV-432B-1\_pyridine  
 EXPNO 6  
 PROCNO 1



F1 - Acquisition parameters  
 TD 512  
 SFO1 176.0654 MHz  
 FIDRES 75.120193 Hz  
 SW 218.450 ppm  
 F1MODE Echo-Antiecho

F2 - Processing parameters  
 SI 8192  
 SF 700.1310301 MHz  
 WDW SINE  
 SSB 4  
 LB 0 Hz  
 GE 0  
 PC 1.00

F1 - Processing parameters  
 SI 1024  
 MC2 echo-antiecho  
 SF 176.0479768 MHz  
 WDW QSINE  
 SSB 2  
 LB 0 Hz  
 GE 0

Figure S78. Detail (1/5) of HMBC NMR spectrum of compound 11.

EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K



Current Data Parameters  
 NAME EV-432B-1\_pyridine  
 EXPNO 6  
 PROCNO 1

ppm  
 F1 - Acquisition parameters  
 TD 512  
 SFO1 176.0654 MHz  
 FIDRES 75.120193 Hz  
 SW 218.450 ppm  
 F2MODE Echo-Antiecho

F2 - Processing parameters  
 SI 8192  
 SF 700.1310301 MHz  
 WDW SINE  
 SSB 4  
 LB 0 Hz  
 GB 0  
 PC 1.00

F1 - Processing parameters  
 SI 1024  
 MC2 echo-antiecho  
 SF 176.0479768 MHz  
 WDW QSINE  
 SSB 2  
 LB 0 Hz  
 GB 0

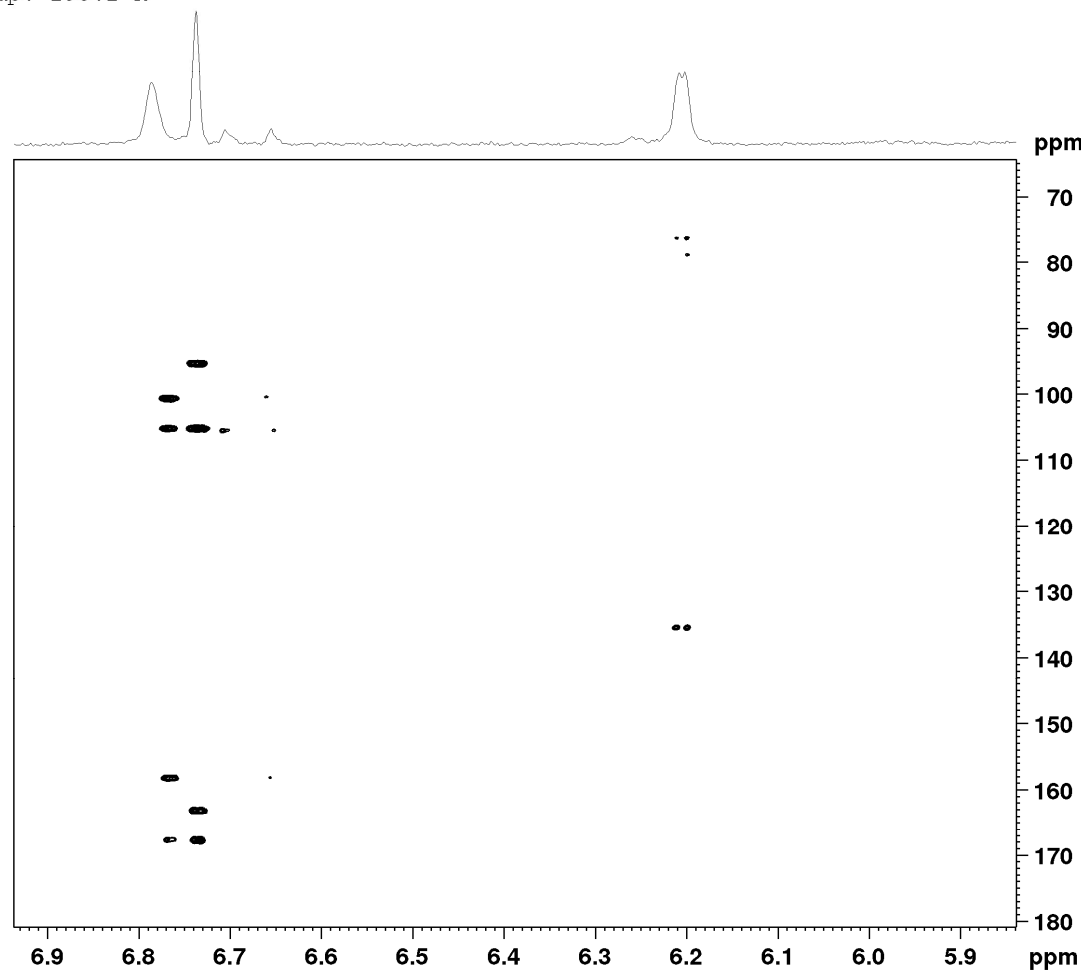


Figure S79. Detail (2/5) of HMBC NMR spectrum of compound 11.

EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K



Current Data Parameters  
 NAME EV-432B-1\_pyridine  
 EXPNO 6  
 PROCNO 1

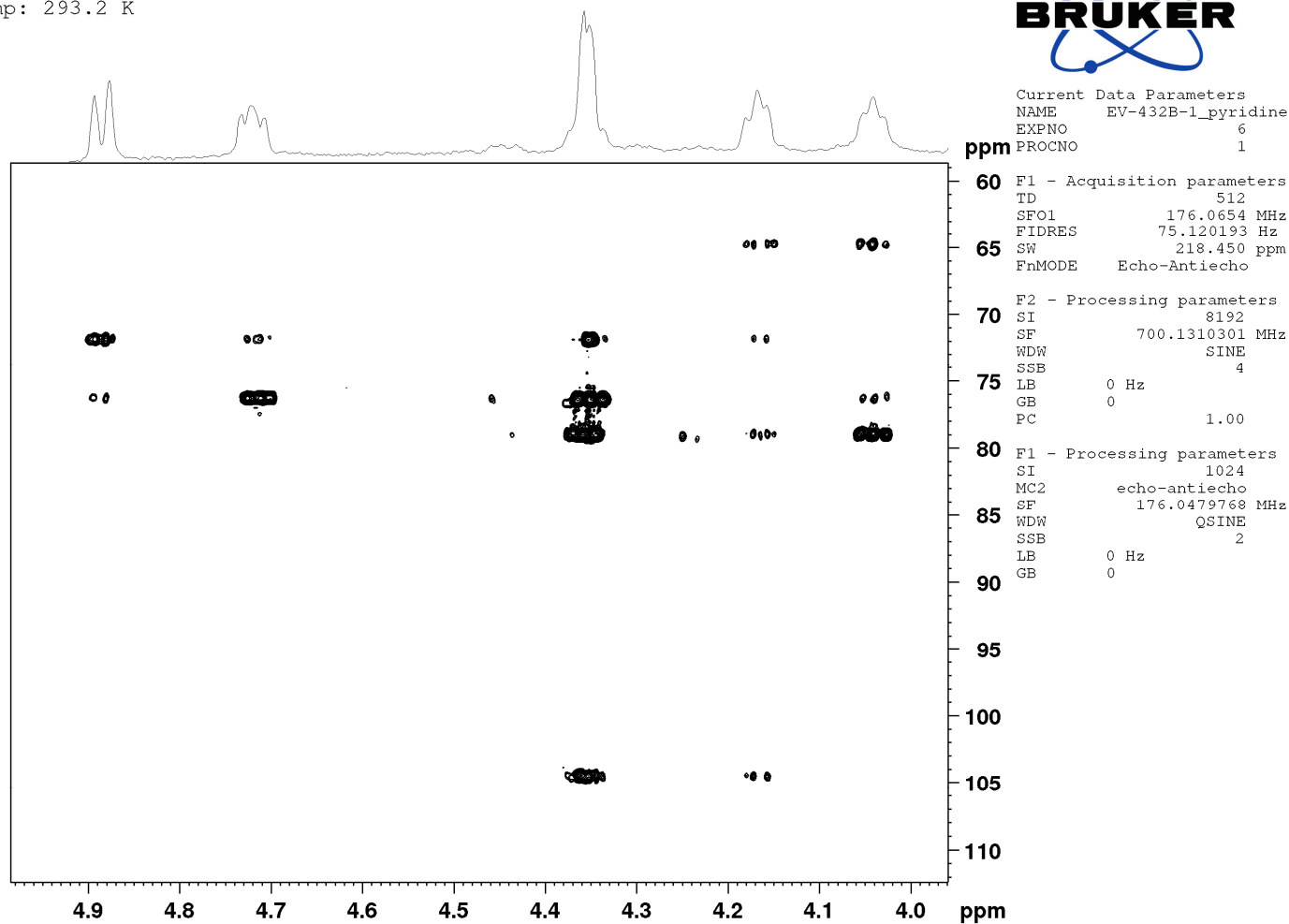


Figure S80. Detail (3/5) of HMBC NMR spectrum of compound 11.

EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K



Current Data Parameters  
 NAME EV-432B-1\_pyridine  
 EXPNO 6  
 PROCNO 1

F1 - Acquisition parameters  
 TD 512  
 SFO1 176.0654 MHz  
 FIDRES 75.120193 Hz  
 SW 218.450 ppm  
 FMODE Echo-Antiecho

F2 - Processing parameters  
 SI 8192  
 SF 700.1310301 MHz  
 WDW SINE  
 SSB 4  
 LB 0 Hz  
 GE 0  
 PC 1.00

F1 - Processing parameters  
 SI 1024  
 MC2 echo-antiecho  
 SF 176.0479768 MHz  
 WDW QSINE  
 SSB 2  
 LB 0 Hz  
 GB 0

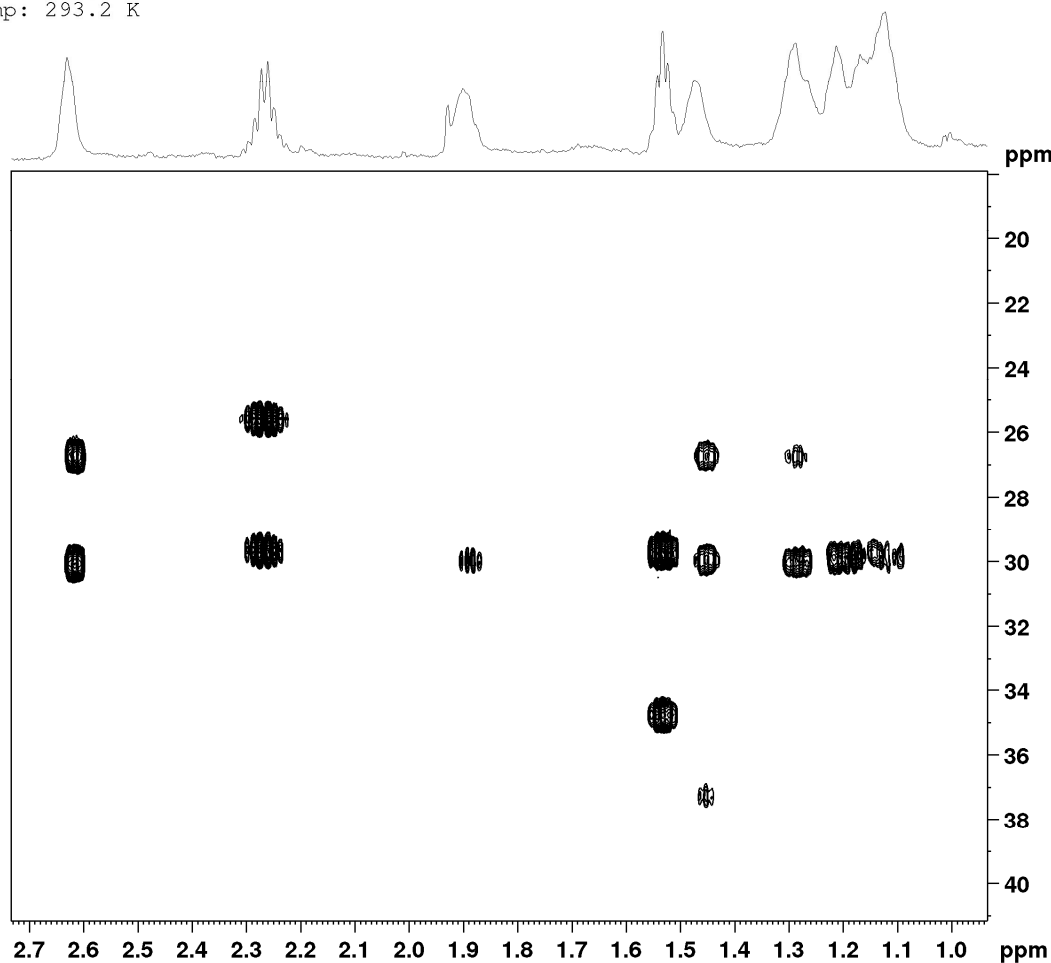


Figure S81. Detail (4/5) of HMBC NMR spectrum of compound 11.

EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K



Current Data Parameters  
 NAME EV-432B-1\_pyridine  
 EXPNO 6  
 PROCNO 1

ppm

F1 - Acquisition parameters  
 TD 512  
 SF01 176.0654 MHz  
 FIDRES 75.120193 Hz  
 SW 218.450 ppm  
 FnmODE Echo-Antiecho

172

173

F2 - Processing parameters  
 SI 8192  
 SF 700.1310301 MHz  
 WDW SINE  
 SSB 4  
 LB 0 Hz  
 GB 0  
 PC 1.00

174

175

F1 - Processing parameters  
 SI 1024  
 MC2 echo-antiecho  
 SF 176.0479768 MHz  
 WDW QSINE  
 SSB 2  
 LB 0 Hz  
 GB 0

176

177

178

179

180

181

182

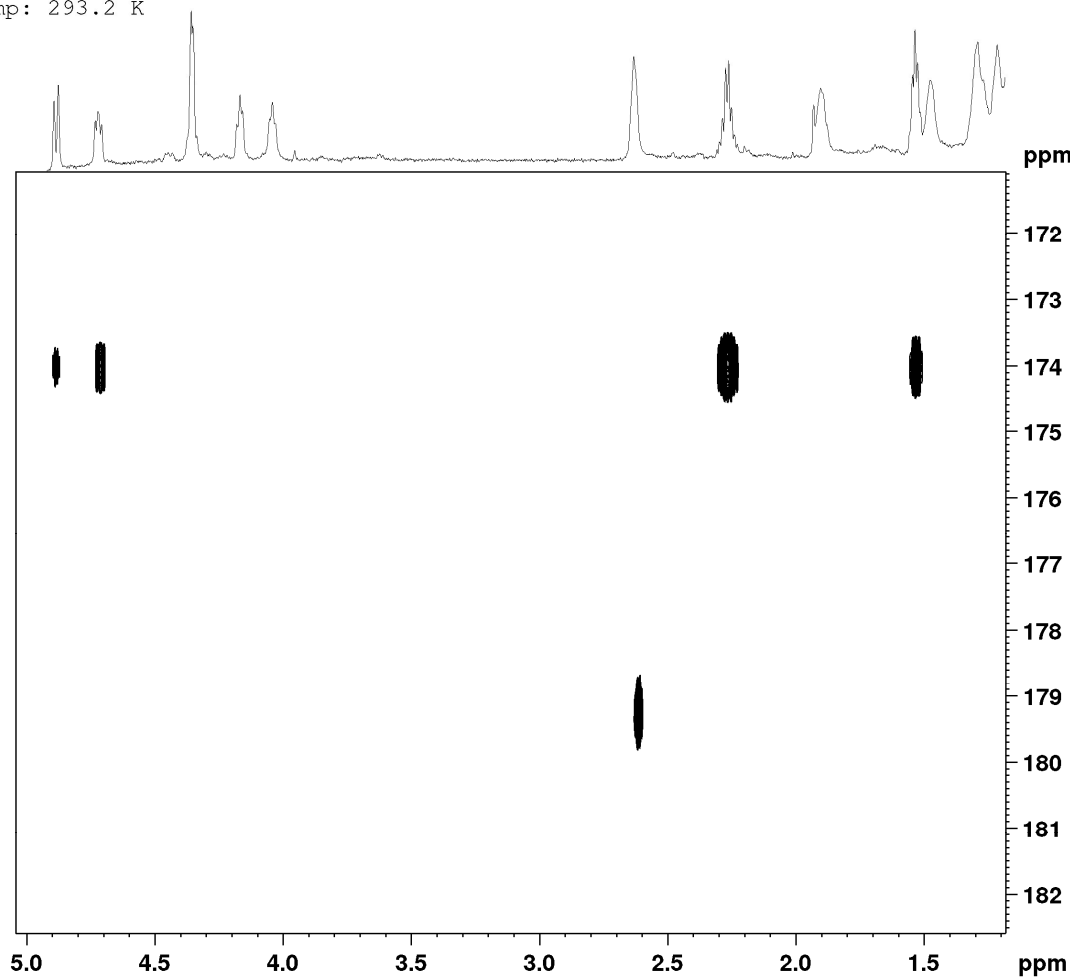


Figure S82. Detail (5/5) of HMBC NMR spectrum of compound 11.

EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K

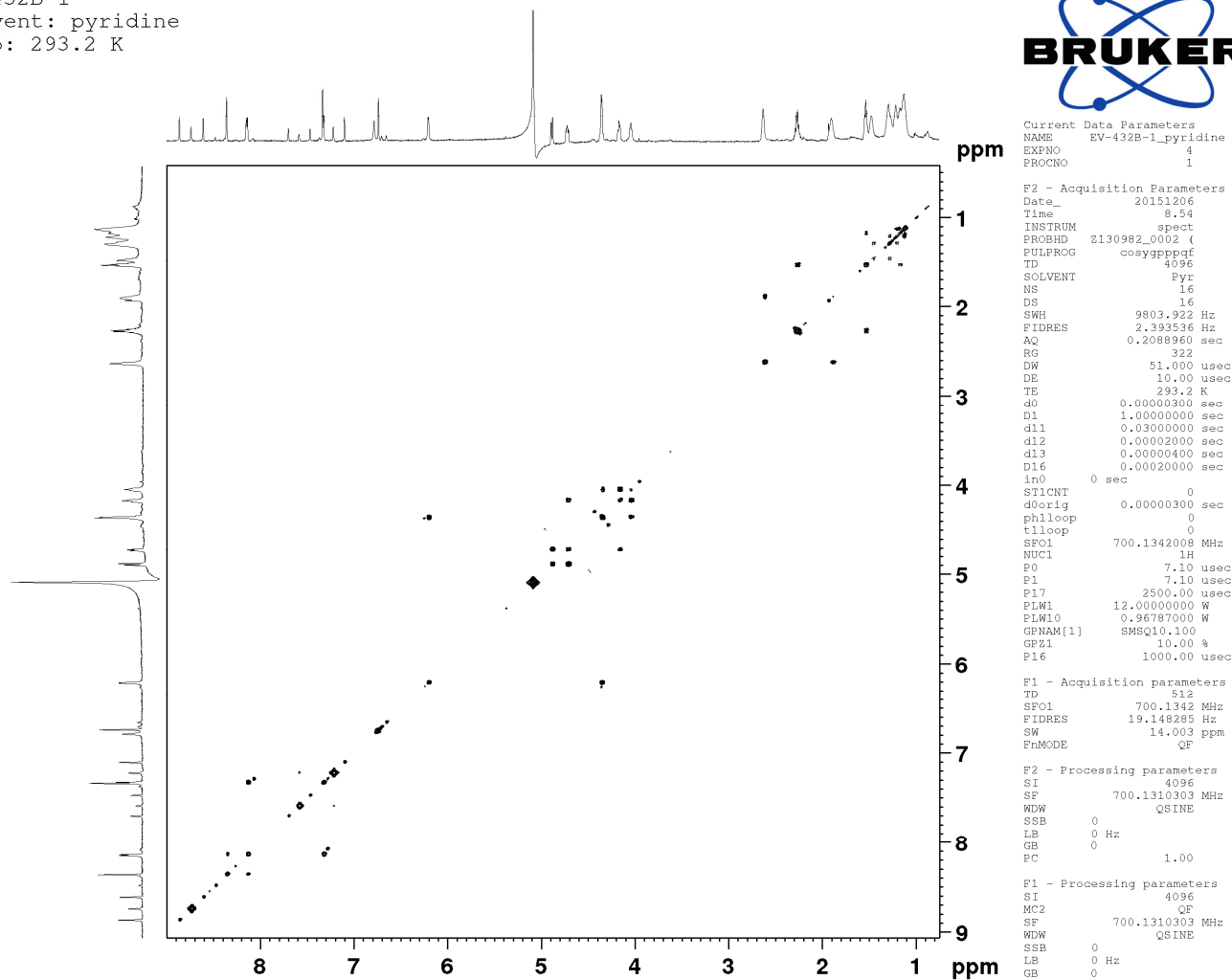


Figure S83. COSY NMR spectrum of compound 11.



EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K

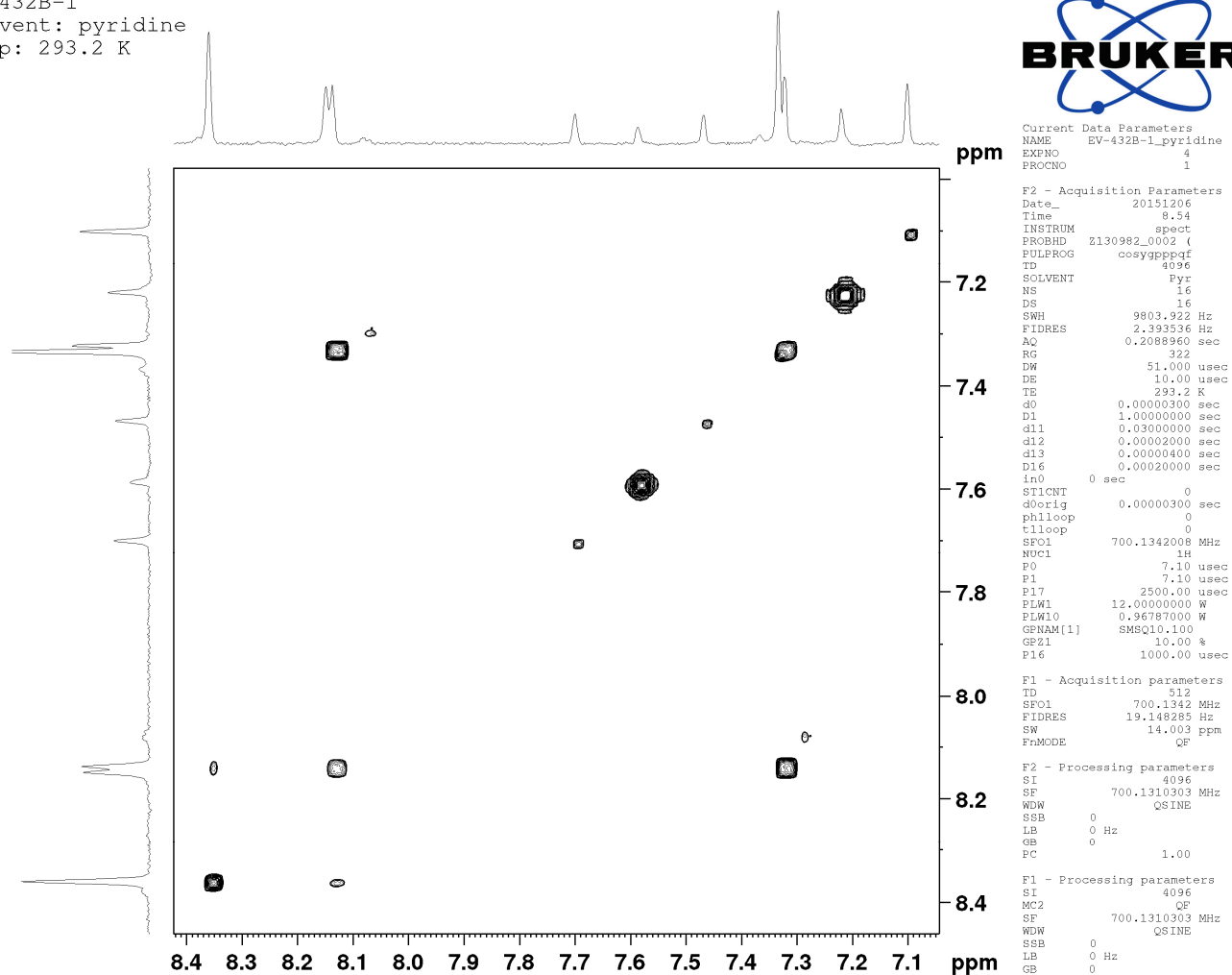


Figure S84. Detail (1/3) of COSY NMR spectrum of compound 11.

EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K

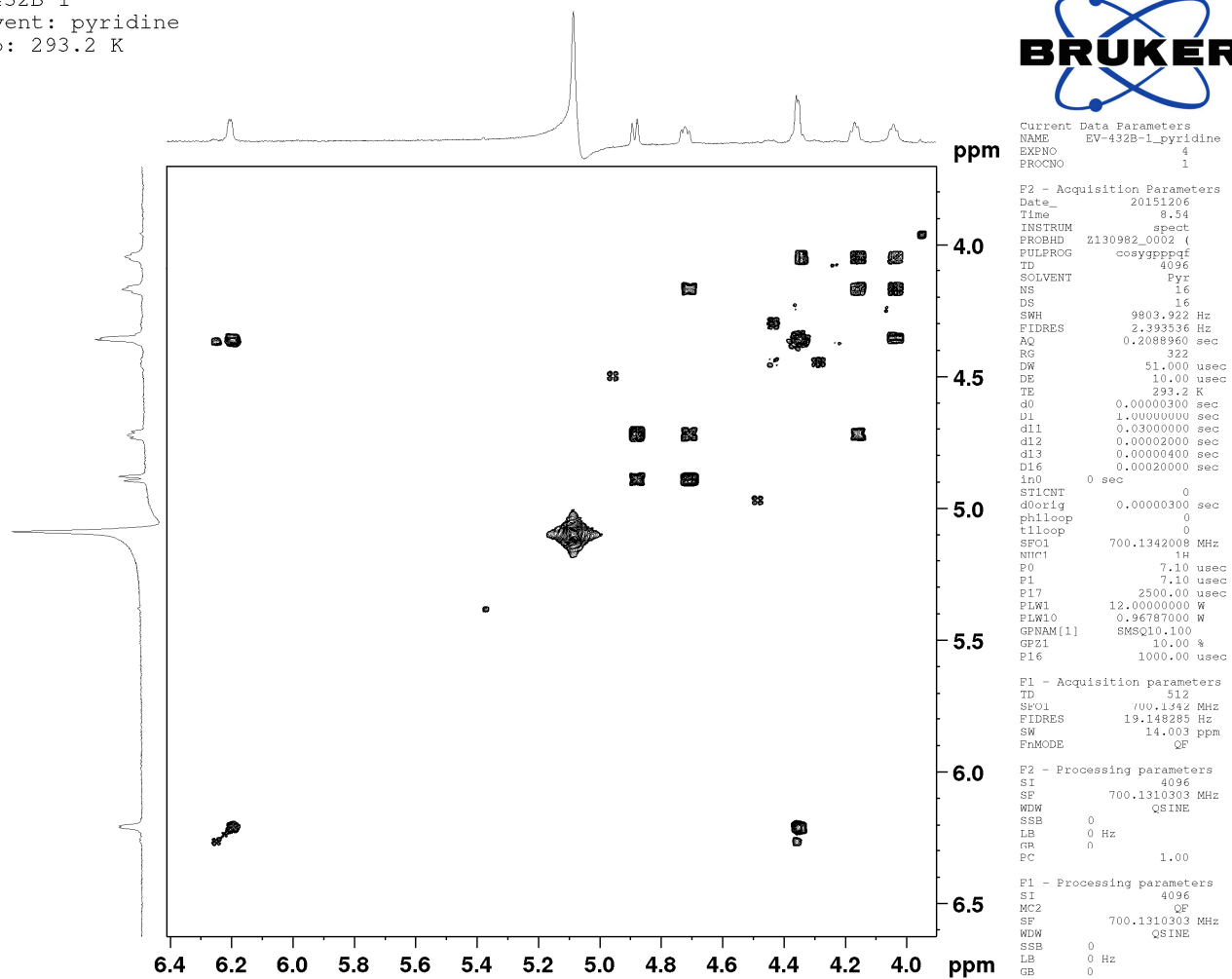


Figure S85. Detail (2/3) of COSY NMR spectrum of compound 11.

EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K

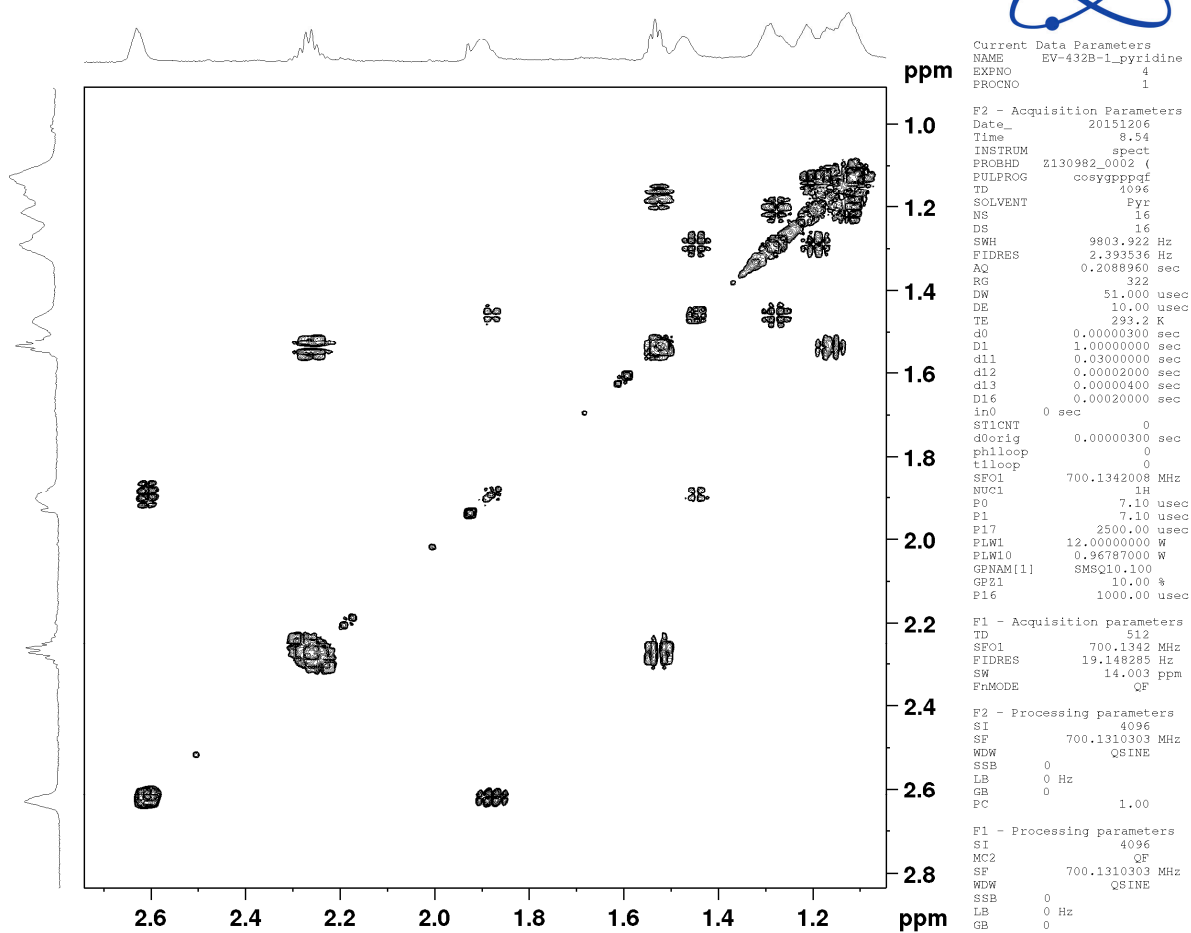


Figure S86. Detail (3/3) of COSY NMR spectrum of compound 11.

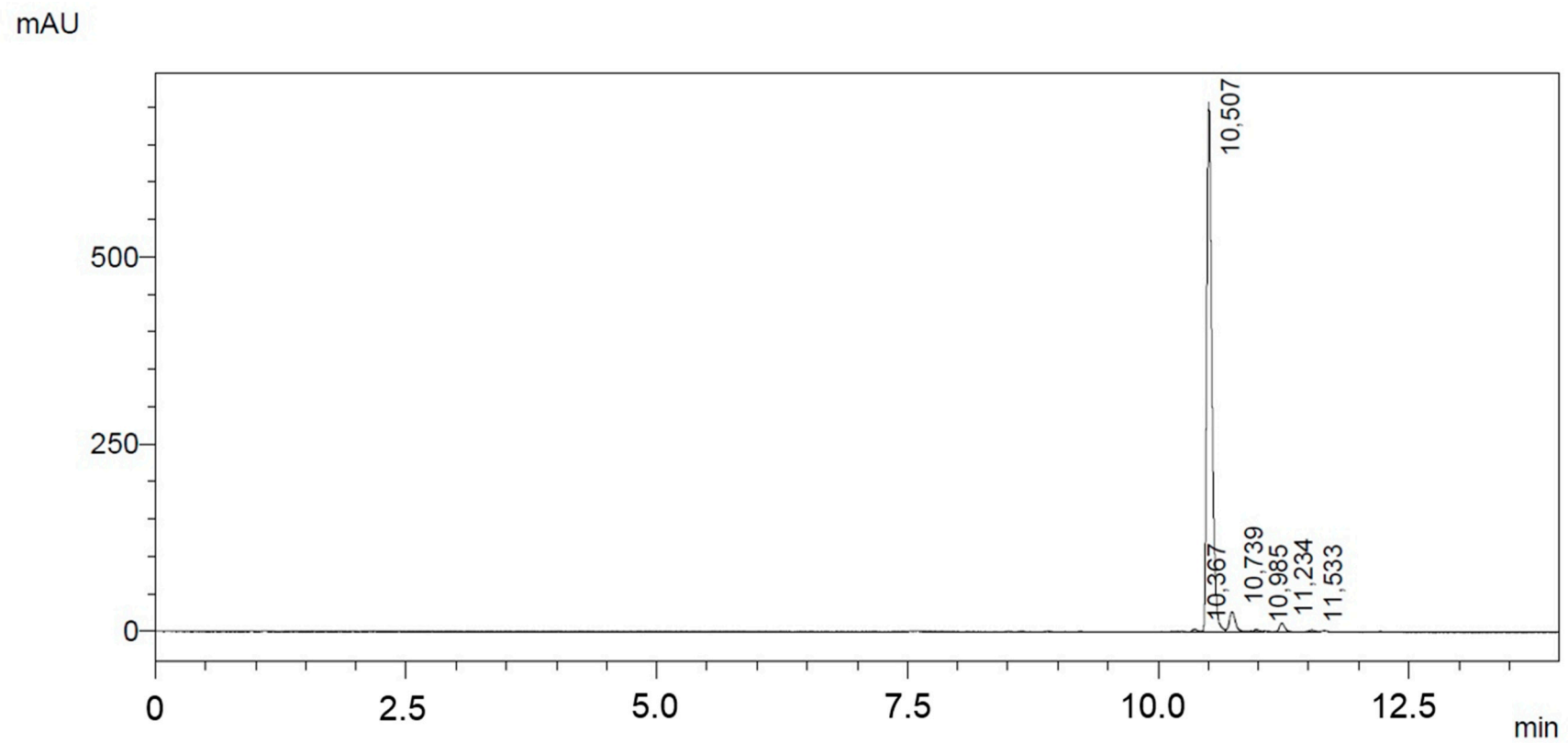
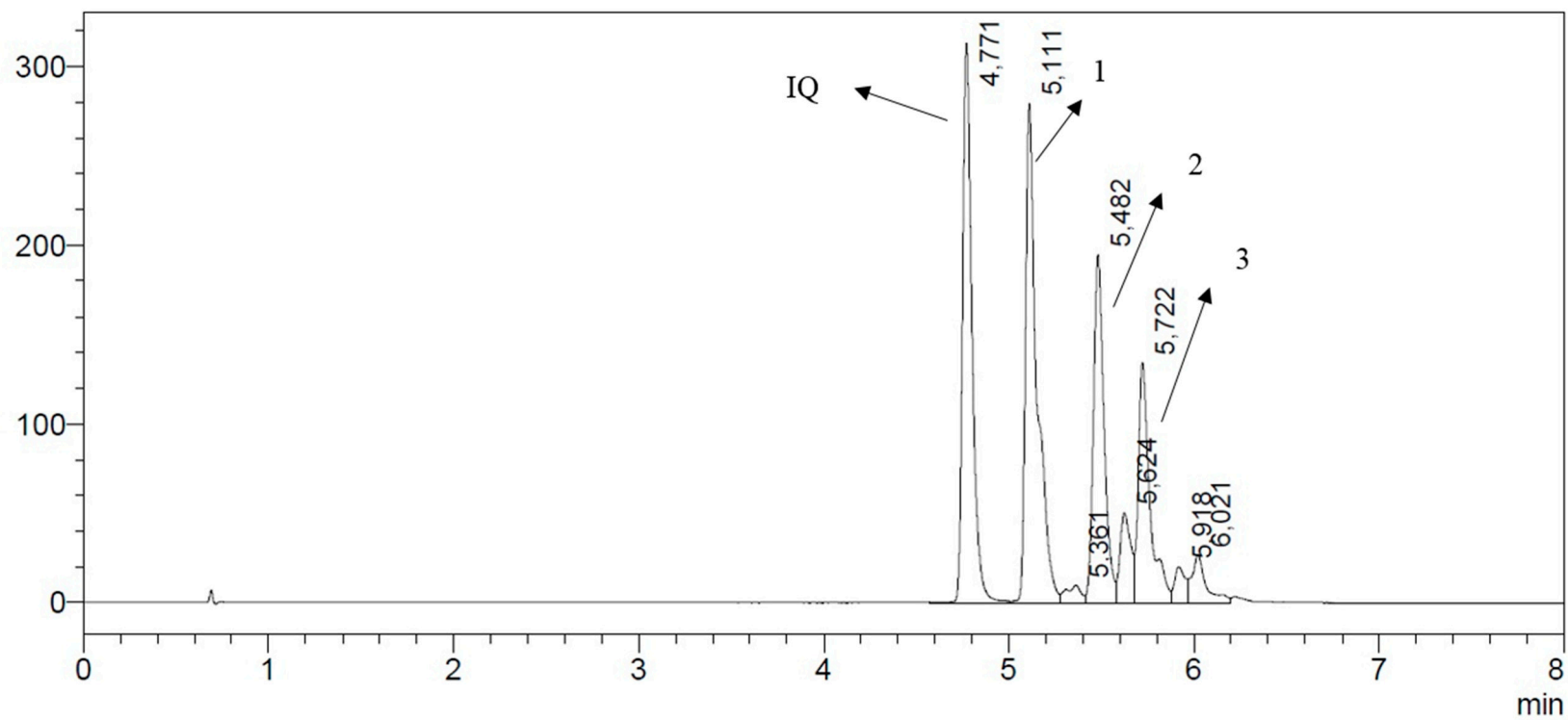
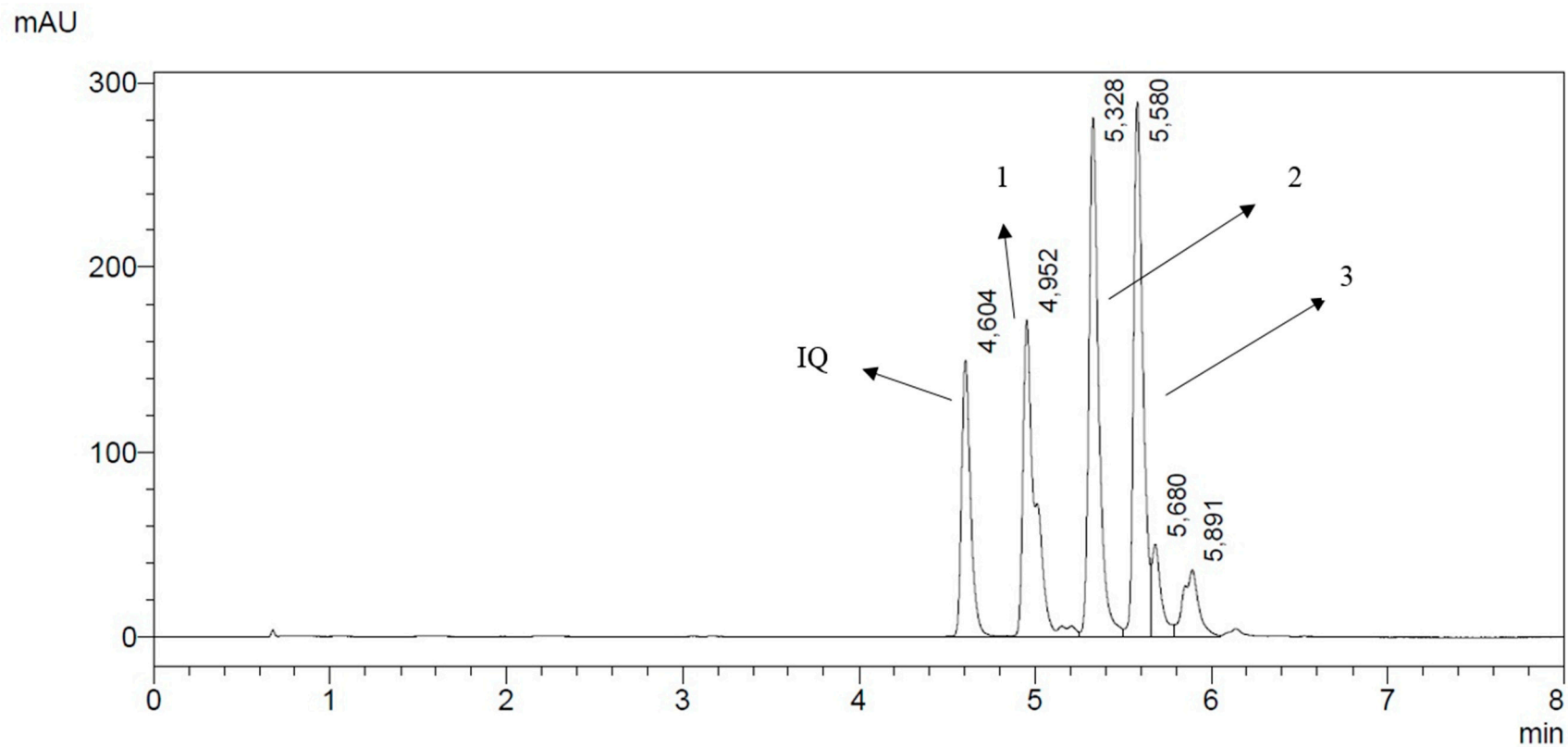


Figure S87. HPLC chromatogram of compound 11.

mAU



**Figure S88.** HPLC PDA chromatogram of the reaction mixture of isoquercitrin, succinic anhydride in the presence of Novozym 435®, acetone, 45 °C, 24 h. Peak 1: monosuccinate of isoquercitrin; Peak 2: disuccinate of isoquercitrin; Peak 3: trisuccinate of isoquercitrin.



**Figure S89.** HPLC PDA chromatogram of the reaction mixture of isoquercitrin, succinic anhydride in the absence of Novozym 435<sup>®</sup>, acetone, 45 °C, 24 h. Peak 1: monosuccinate of isoquercitrin; Peak 2: disuccinate of isoquercitrin; Peak 3: trisuccinate of isoquercitrin.

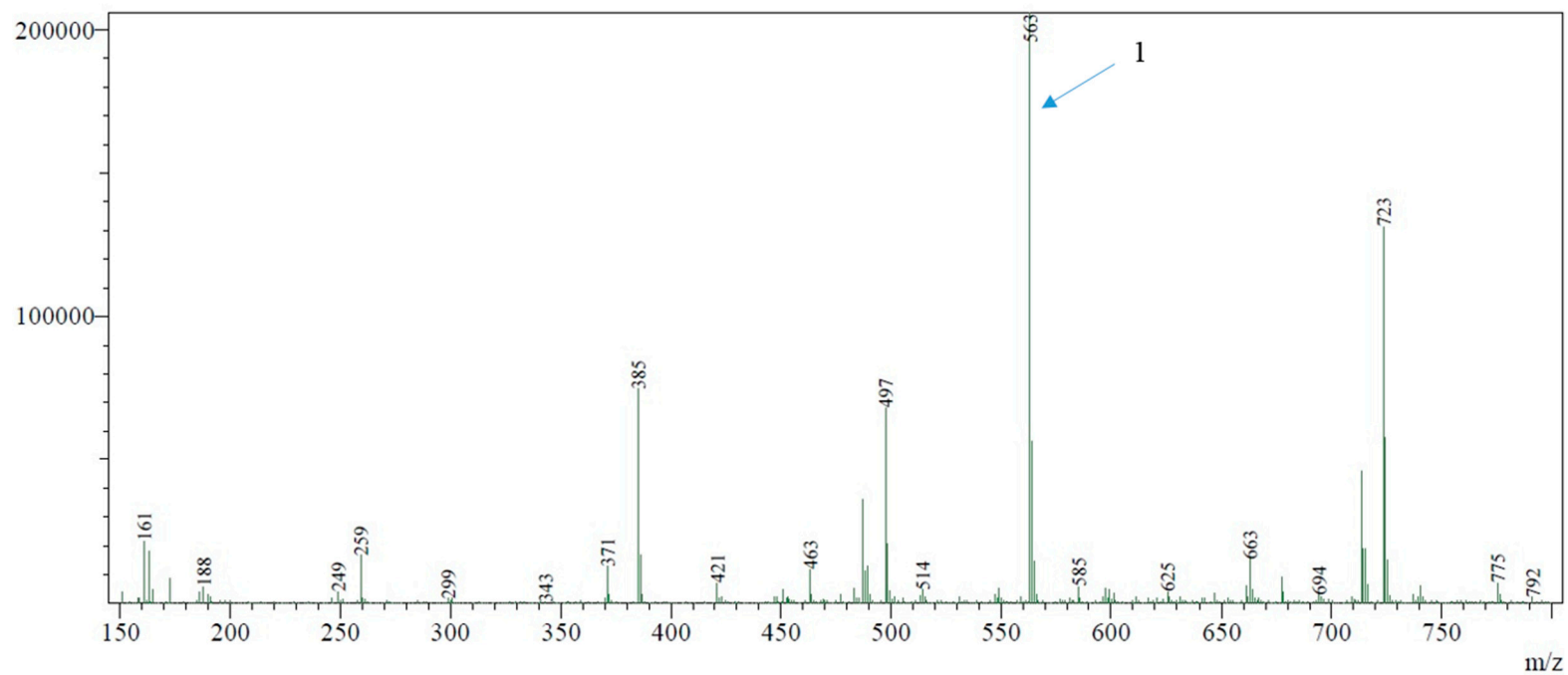


Figure S90. HPLC-MS (-) chromatogram of the monosuccinate of isoquercitrin (peak 1).

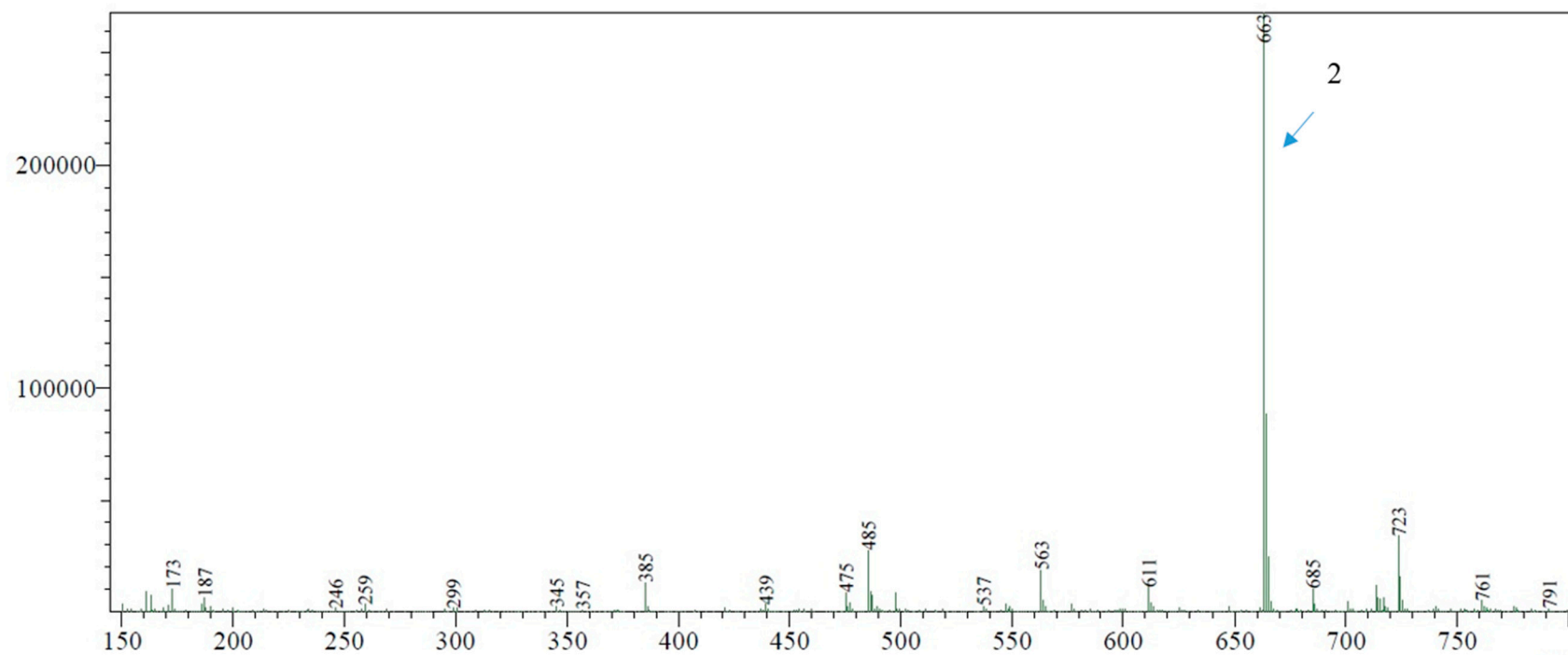


Figure S91. HPLC-MS (-) chromatogram of the disuccinate of isoquercitrin (peak 2).

m/z Figure



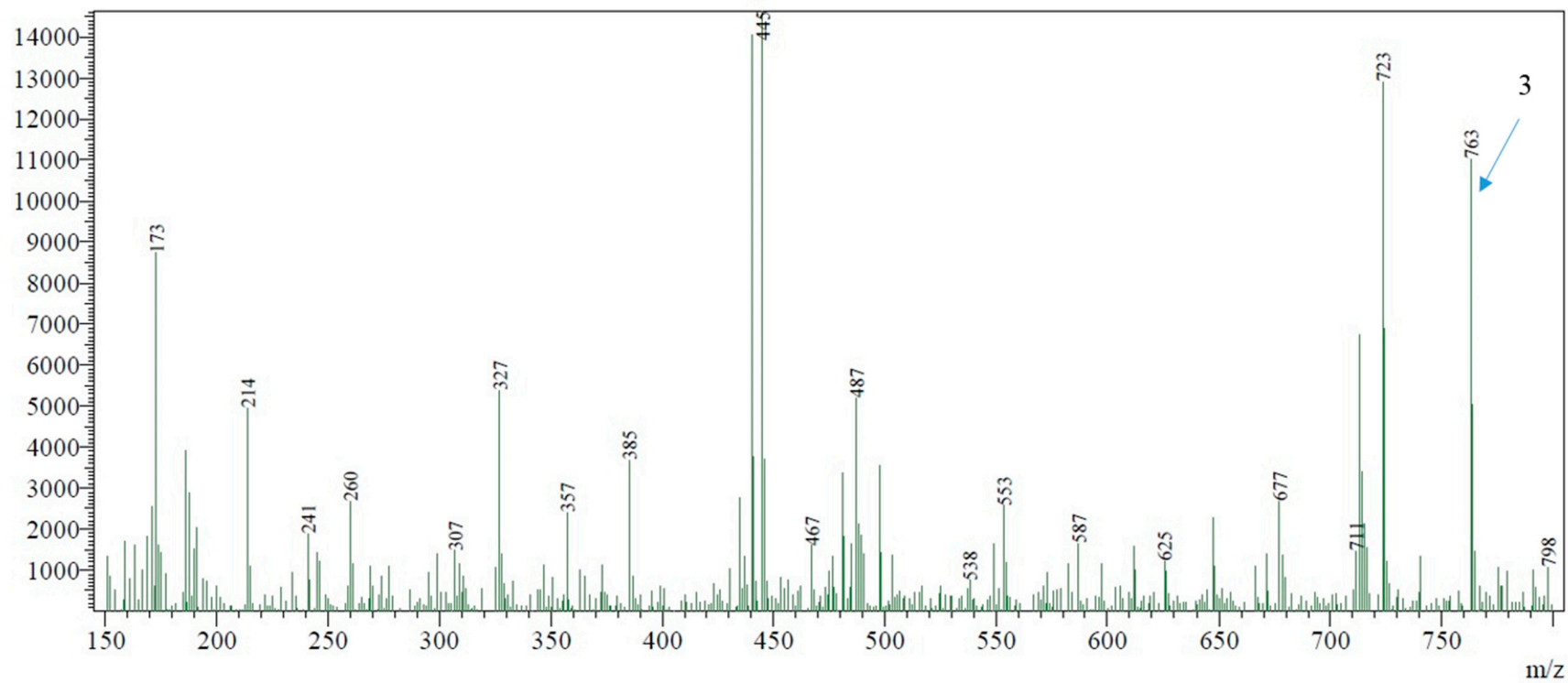


Figure S92. HPLC-MS (-) chromatogram of the trisuccinate of isoquercitrin (peak 3).