

# Supplementary Materials

## Chemical evidence for a missing intermediate in oxidative degradation of oak ellagitannin vescalagin

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Figure S1. <sup>1</sup>H NMR spectrum of **6** in acetone-*d*<sub>6</sub>.

Figure S2. <sup>13</sup>C NMR spectrum of **6** in acetone-*d*<sub>6</sub>.

Figure S3. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **6** in acetone-*d*<sub>6</sub>.

Figure S4. HSQC spectrum of **6** in acetone-*d*<sub>6</sub>.

Figure S5. HMBC spectrum of **6** in acetone-*d*<sub>6</sub>.

Figure S6. Roesy spectrum of **6** in acetone-*d*<sub>6</sub>.

Figure S7. HR-FAB-MS spectrum of **6**.

Figure S8. <sup>1</sup>H NMR spectrum of **7** in acetone-*d*<sub>6</sub>.

Figure S9. <sup>13</sup>C NMR spectrum of **7** in acetone-*d*<sub>6</sub>.

Figure S10. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **7** in acetone-*d*<sub>6</sub>.

Figure S11. HSQC spectrum of **7** in acetone-*d*<sub>6</sub>.

Figure S12. HMBC spectrum of **7** in acetone-*d*<sub>6</sub> (measured at 10Hz).

Figure S13. HMBC spectrum of **7** in acetone-*d*<sub>6</sub> (measured at 5Hz).

Figure S14. NOESY spectrum of **7**.

Figure S15. HR-FAB-MS spectrum of **7**.

Figure S16. <sup>1</sup>H NMR spectrum of **8** in acetone-*d*<sub>6</sub>.

Figure S17. <sup>13</sup>C NMR spectrum of **8** in acetone-*d*<sub>6</sub>.

Figure S18. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **8** in acetone-*d*<sub>6</sub>.

Figure S19. HSQC spectrum of **8** in acetone-*d*<sub>6</sub>.

Figure S20. HMBC spectrum of **8** in acetone-*d*<sub>6</sub>.

Figure S21. NOESY spectrum of **8**.

Figure S22. FAB-MS spectrum of **8**.

Figure S1.  $^1\text{H}$  NMR spectrum of **6** in acetone- $d_6$ .

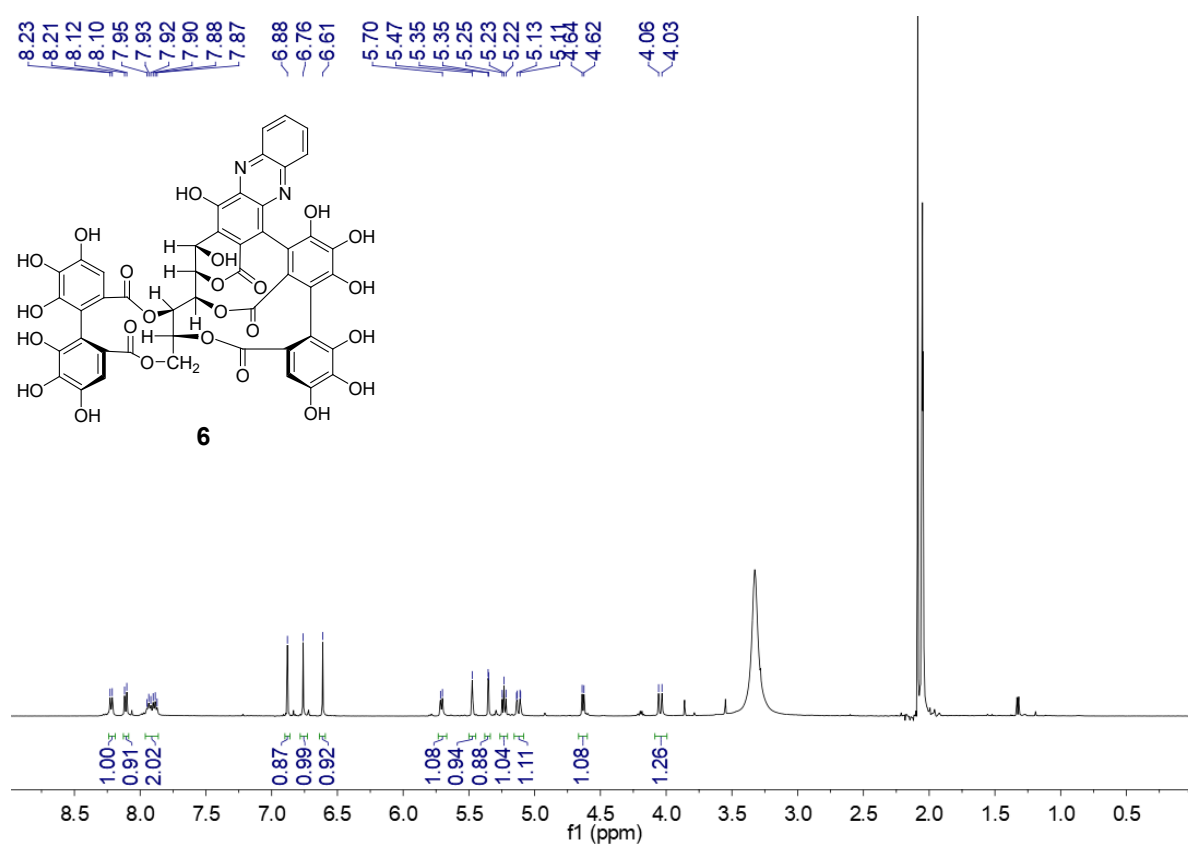


Figure S2.  $^{13}\text{C}$  NMR spectrum of **6** in acetone- $d_6$ .

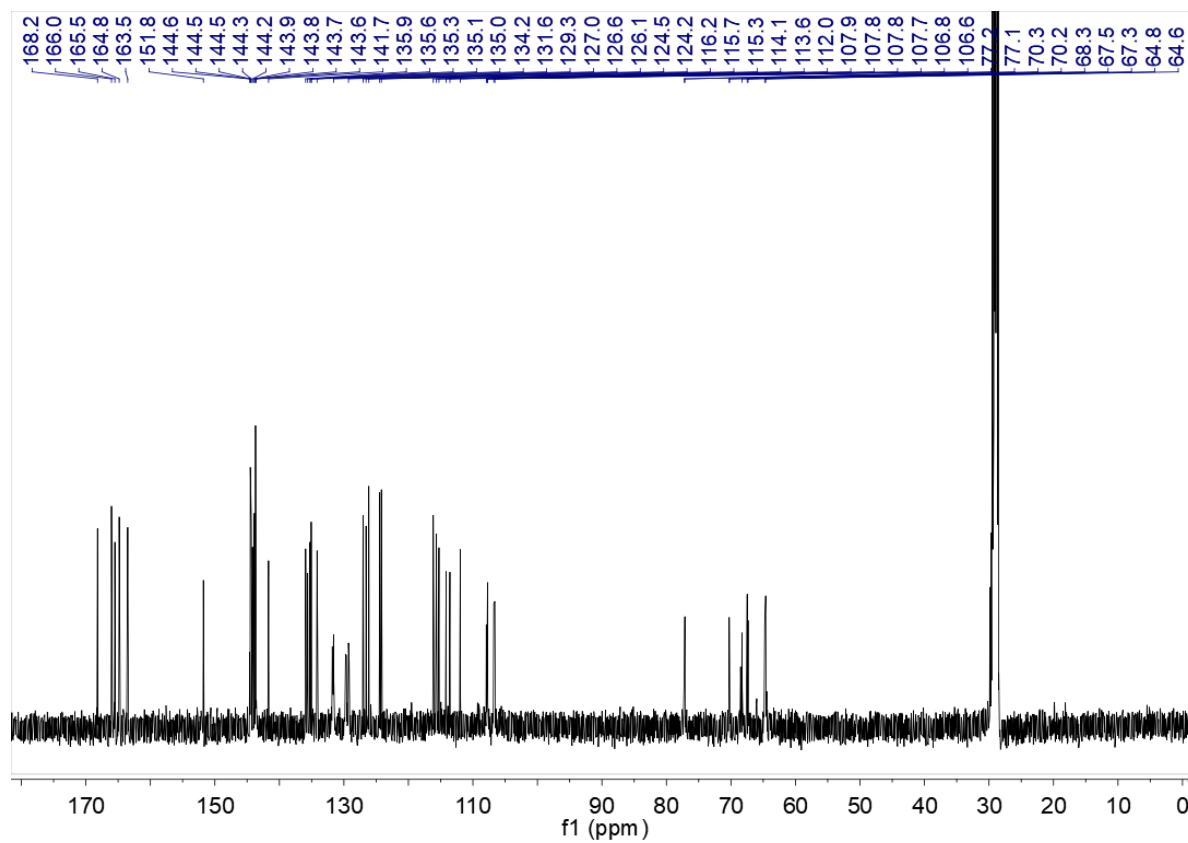




Figure S5. HMBC spectrum of **6** in acetone-*d*<sub>6</sub>.

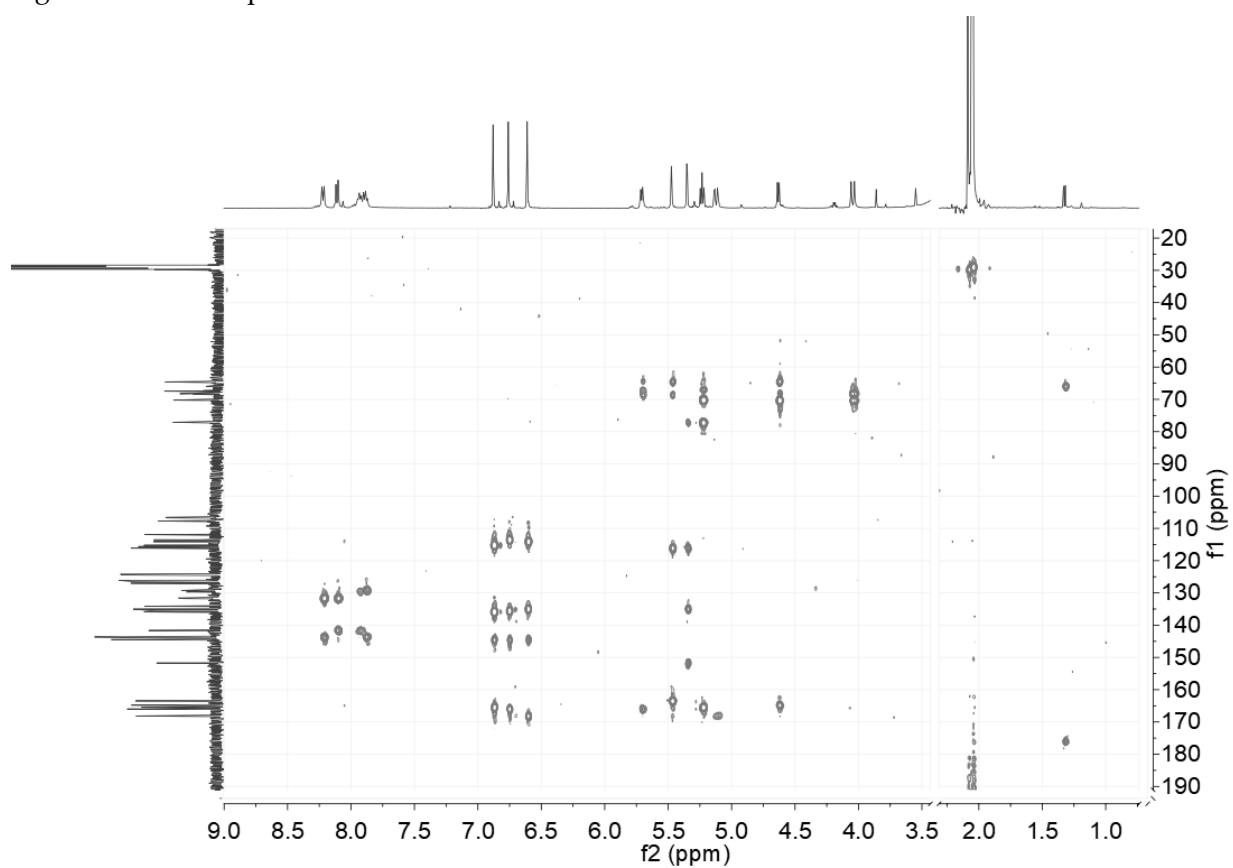


Figure S6. Roesy spectrum of **6** in acetone-*d*<sub>6</sub>.

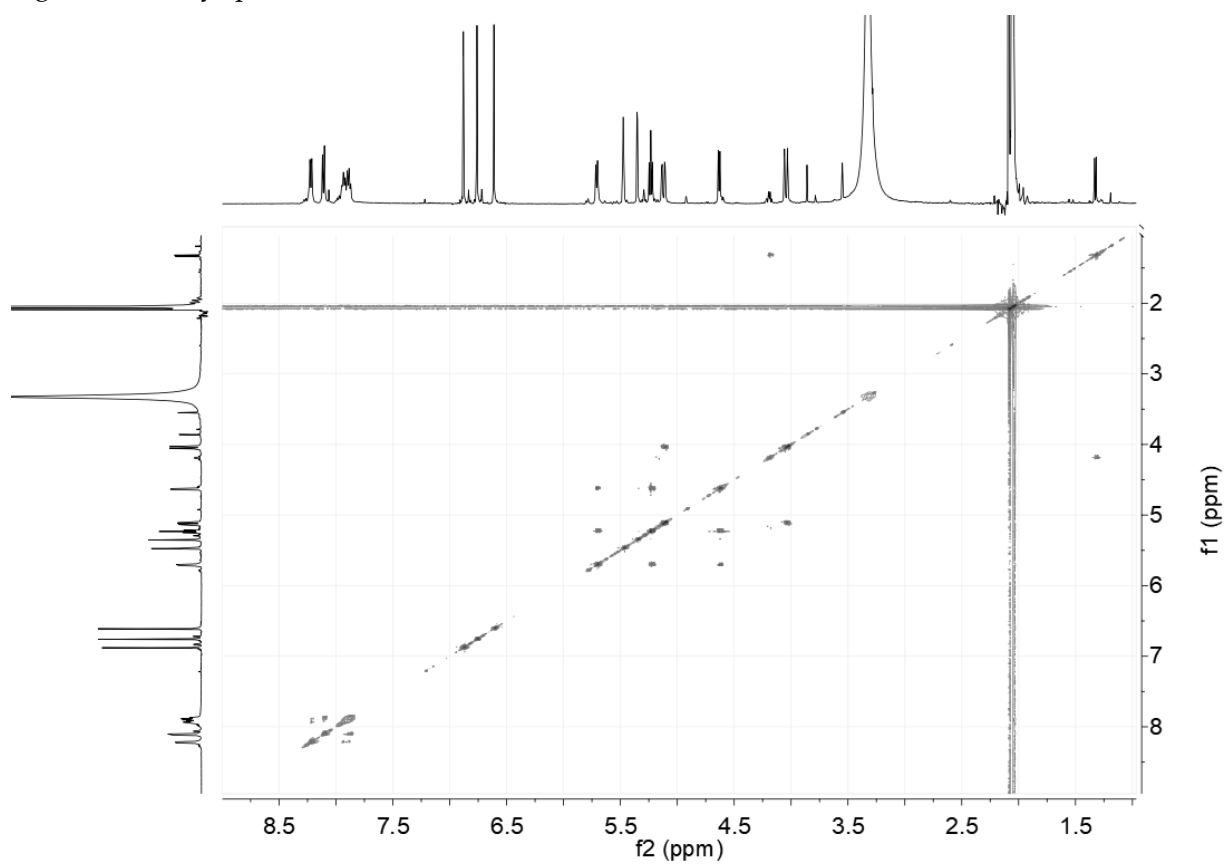
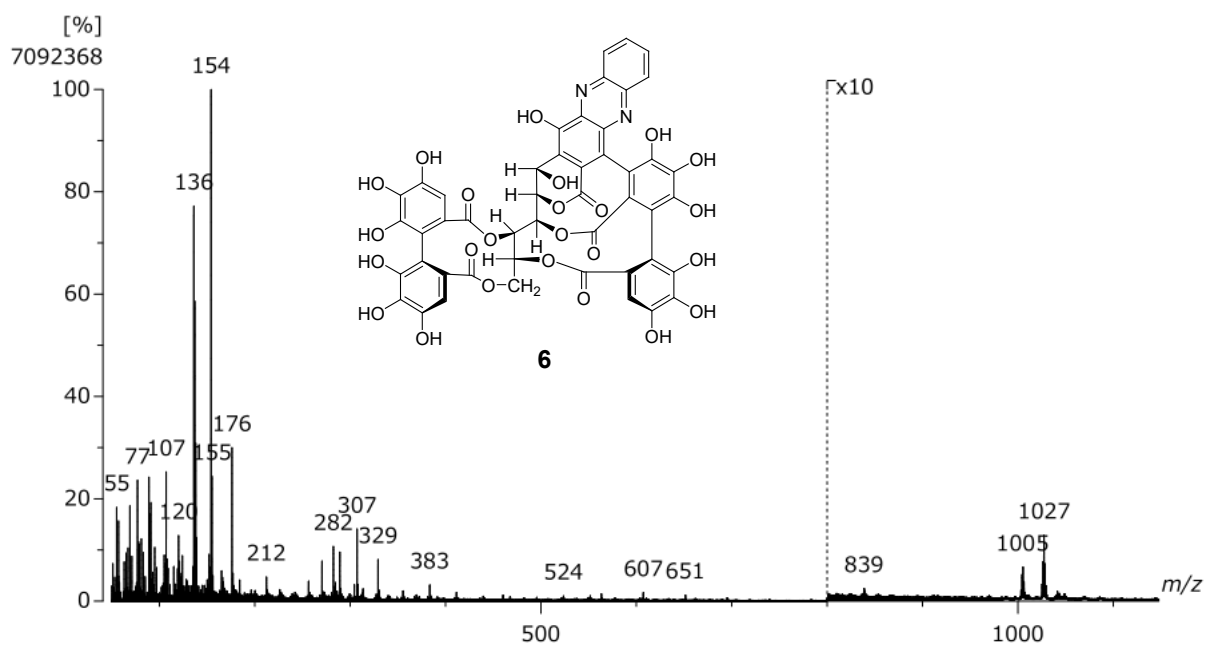


Figure S7. HR-FAB-MS spectrum of **6**



| Observed m/z | Int%   | Err [ppm / mmu] | U.S. Composition       |
|--------------|--------|-----------------|------------------------|
| 1027.0937    | 100.00 | +0.7 / +0.7     | 34.5 C47 H28 N2 O24 Na |

Figure S8. <sup>1</sup>H NMR spectrum of **7** in acetone-*d*<sub>6</sub>.

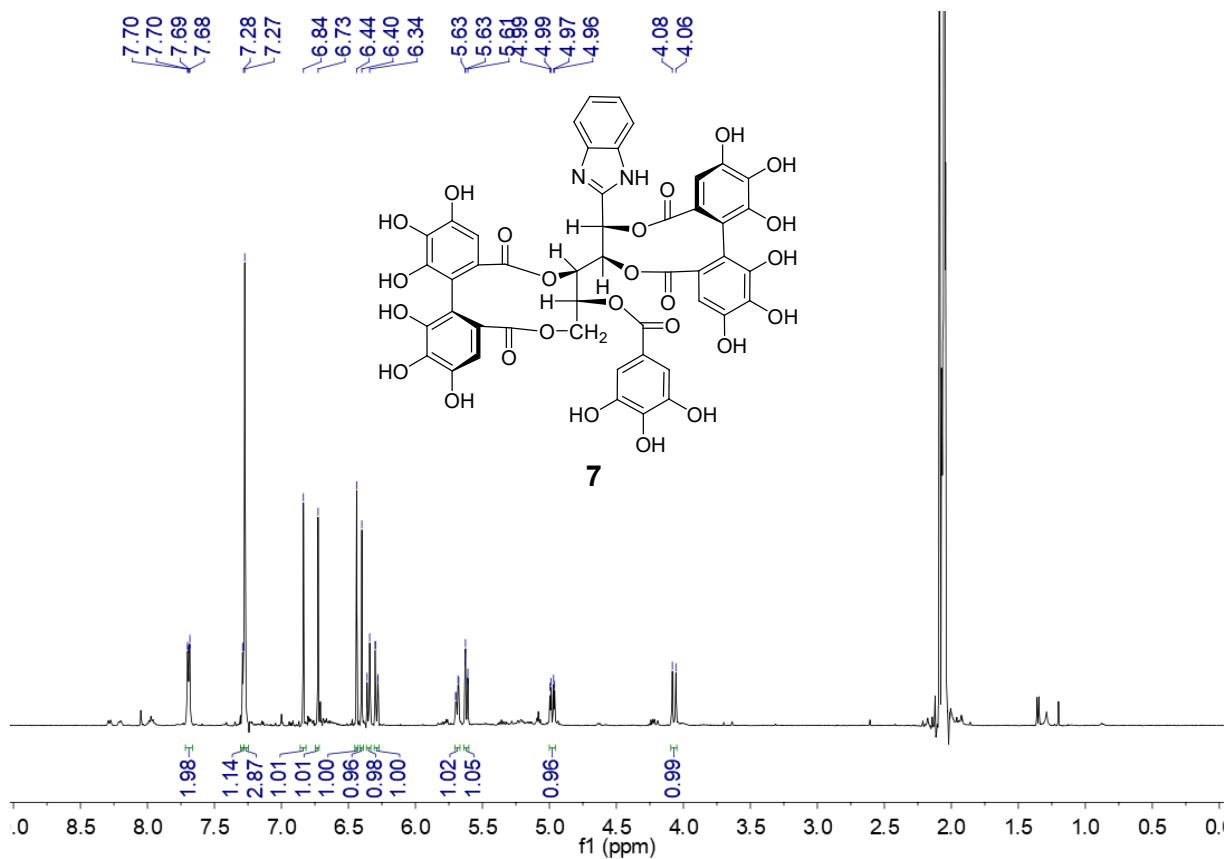


Figure S9.  $^{13}\text{C}$  NMR spectrum of **7** in acetone- $d_6$ .

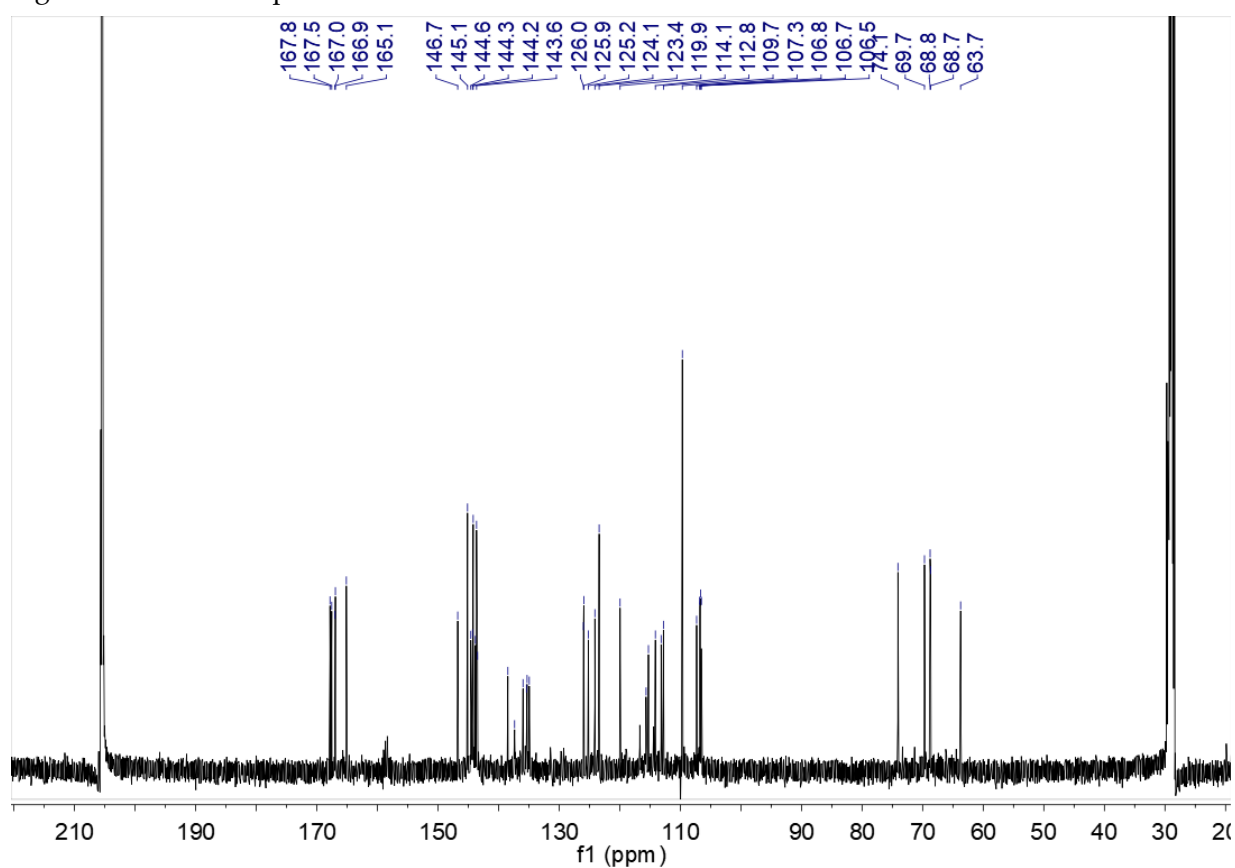


Figure S10.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **7** in acetone- $d_6$ .

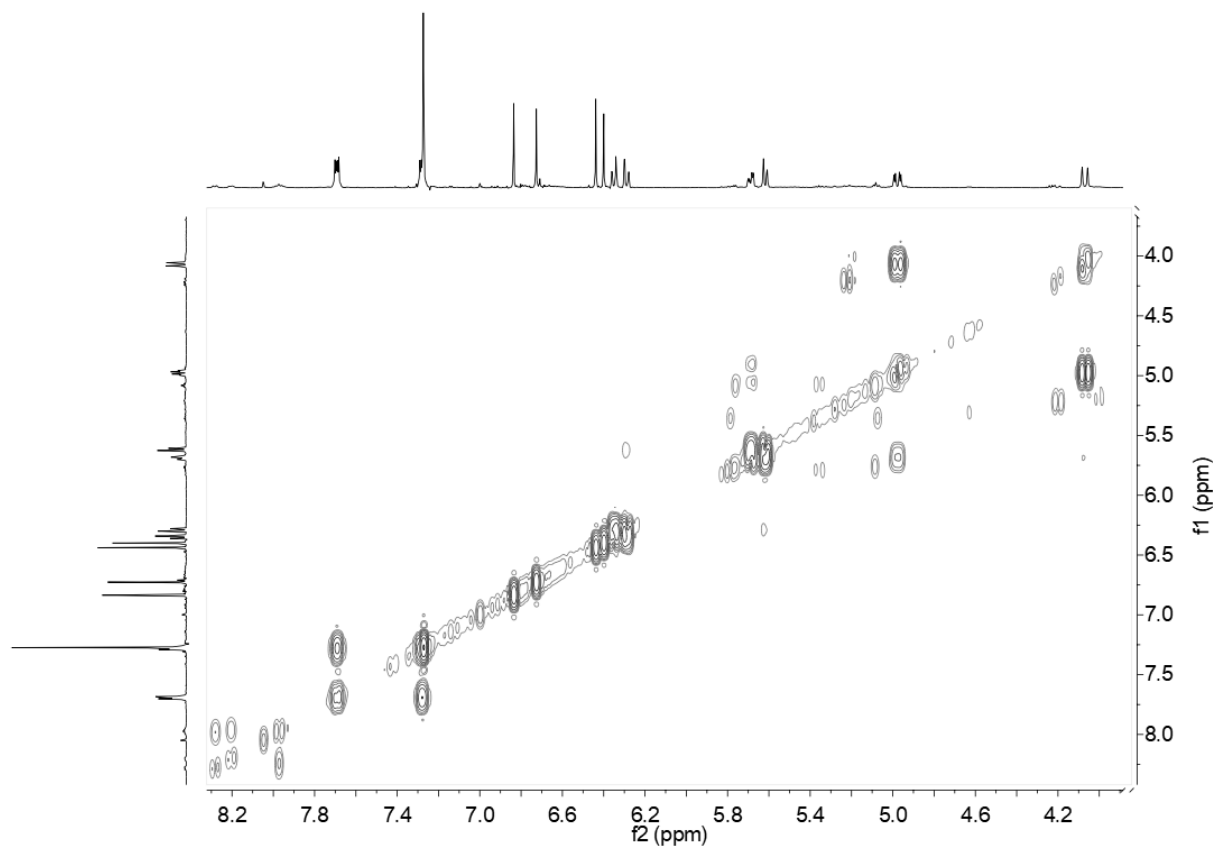


Figure S11. HSQC spectrum of **7** in acetone-*d*<sub>6</sub>.

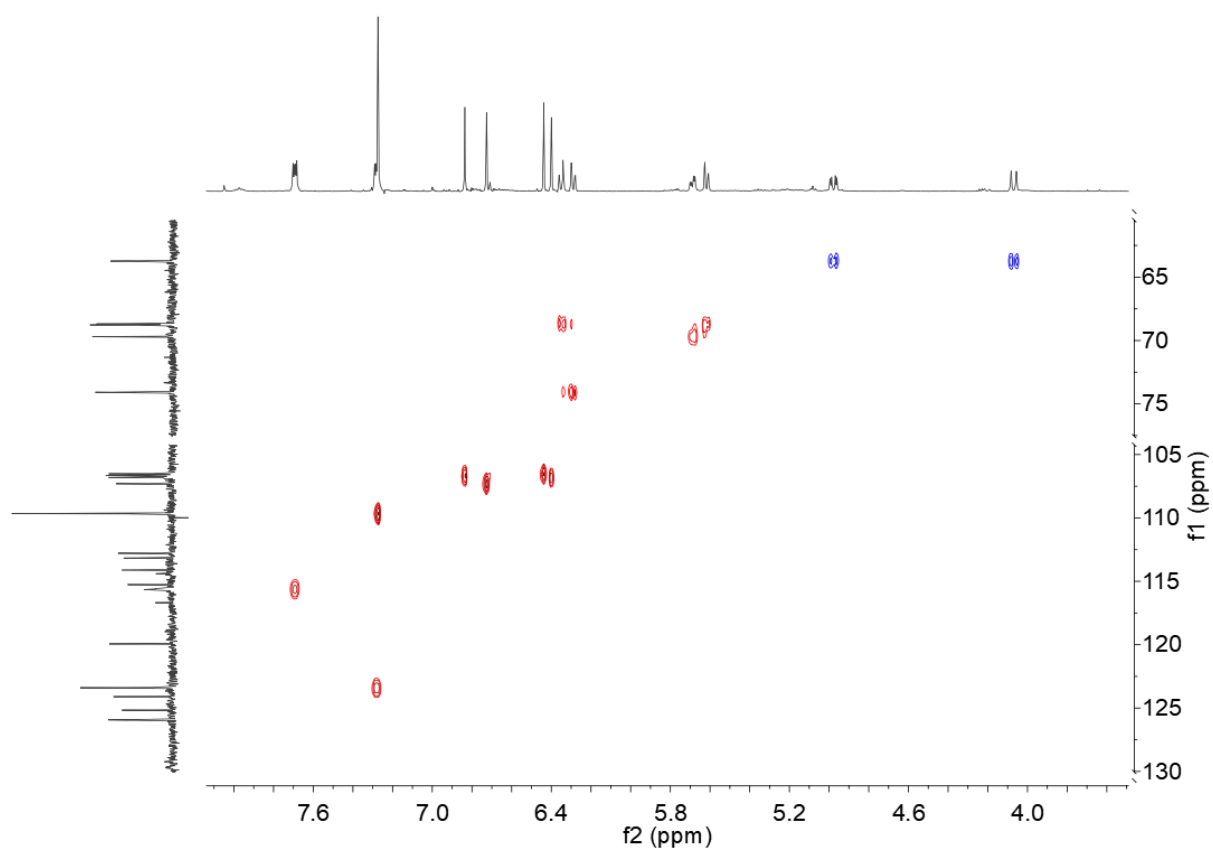


Figure S12. HMBC spectrum of **7** in acetone-*d*<sub>6</sub> (measured at 10Hz).

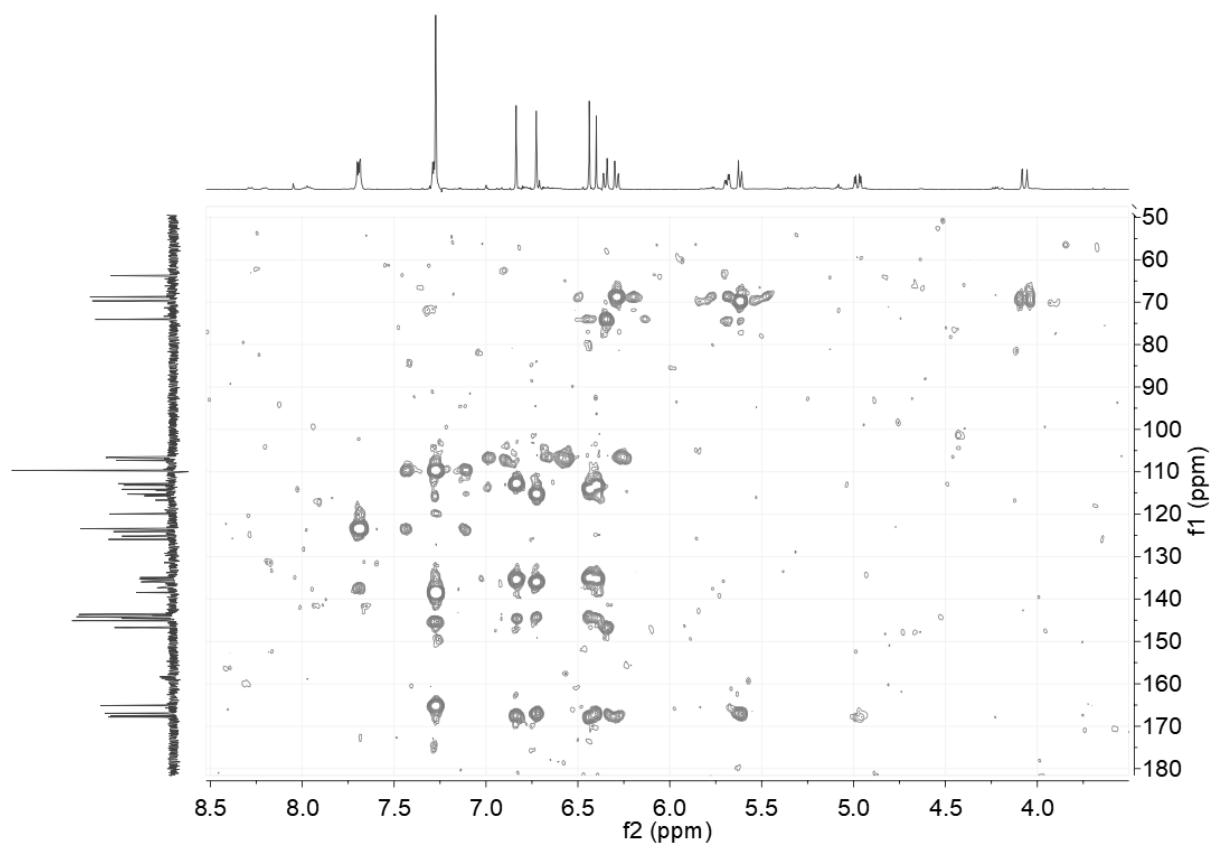


Figure S13. HMBC spectrum of **7** in acetone- $d_6$  (measured at 5Hz) .

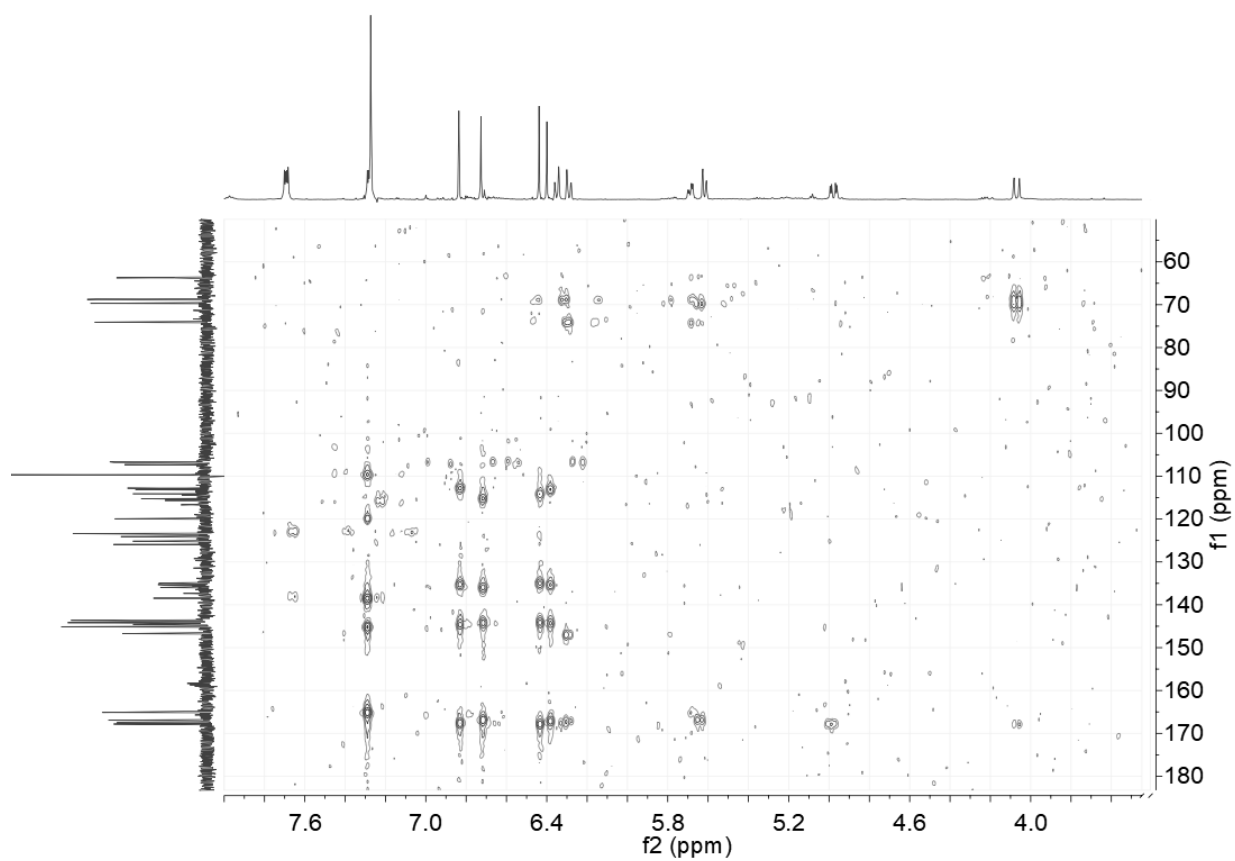


Figure S14. NOESY spectrum of **7** in acetone- $d_6$ .

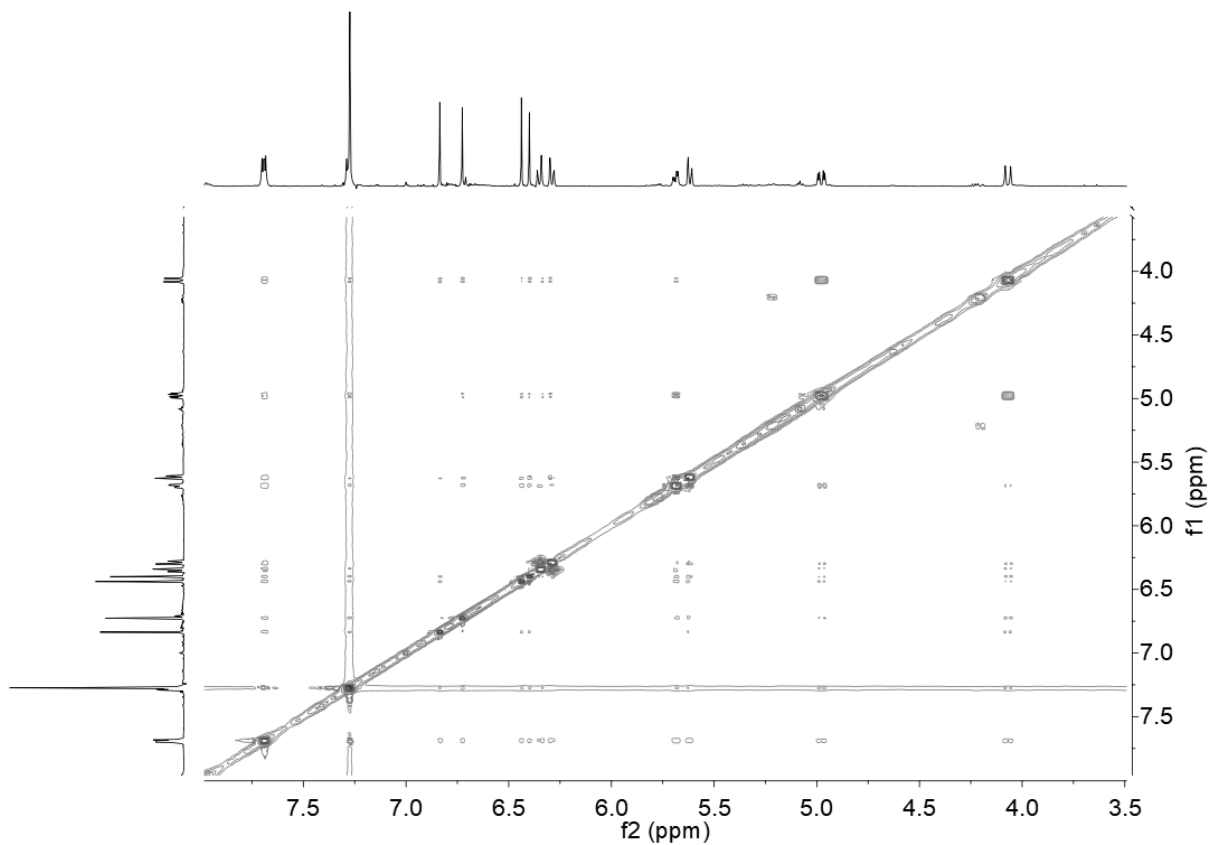




Figure S15. HR-FAB-MS spectrum of **7**.

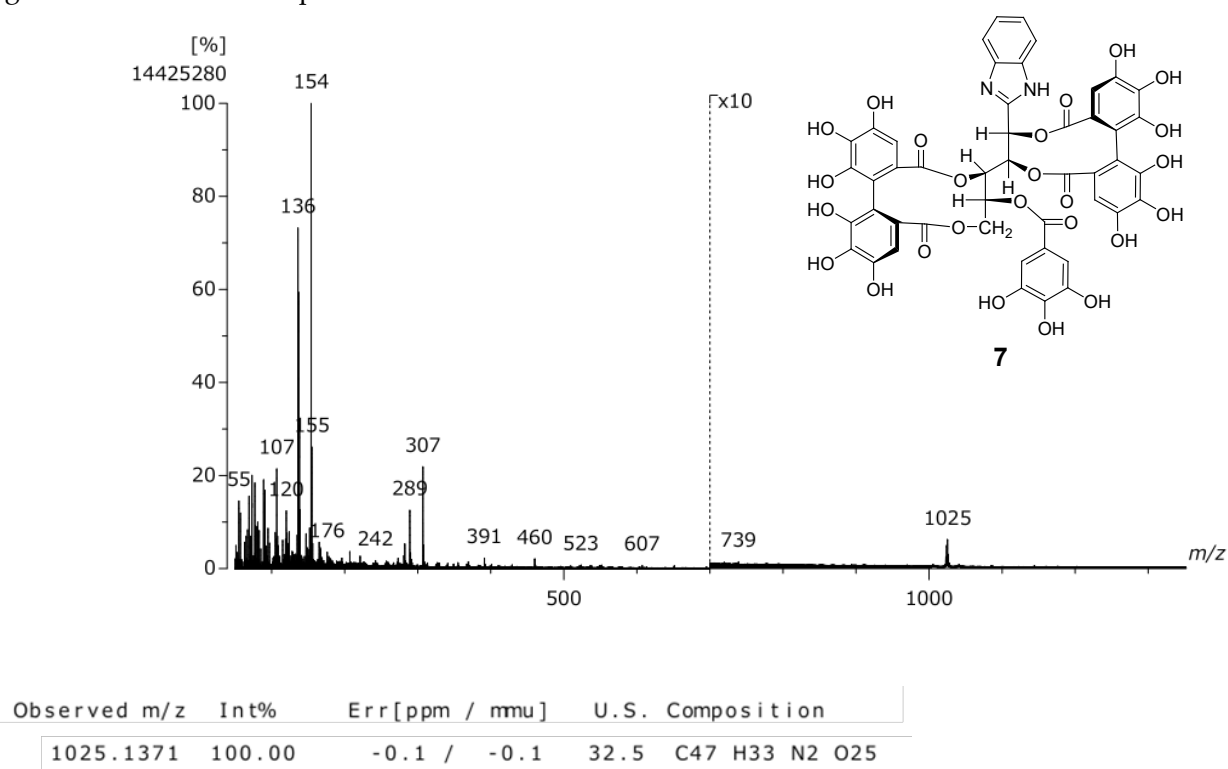


Figure S16.  $^1\text{H}$  NMR spectrum of **8** in acetone- $d_6$ .

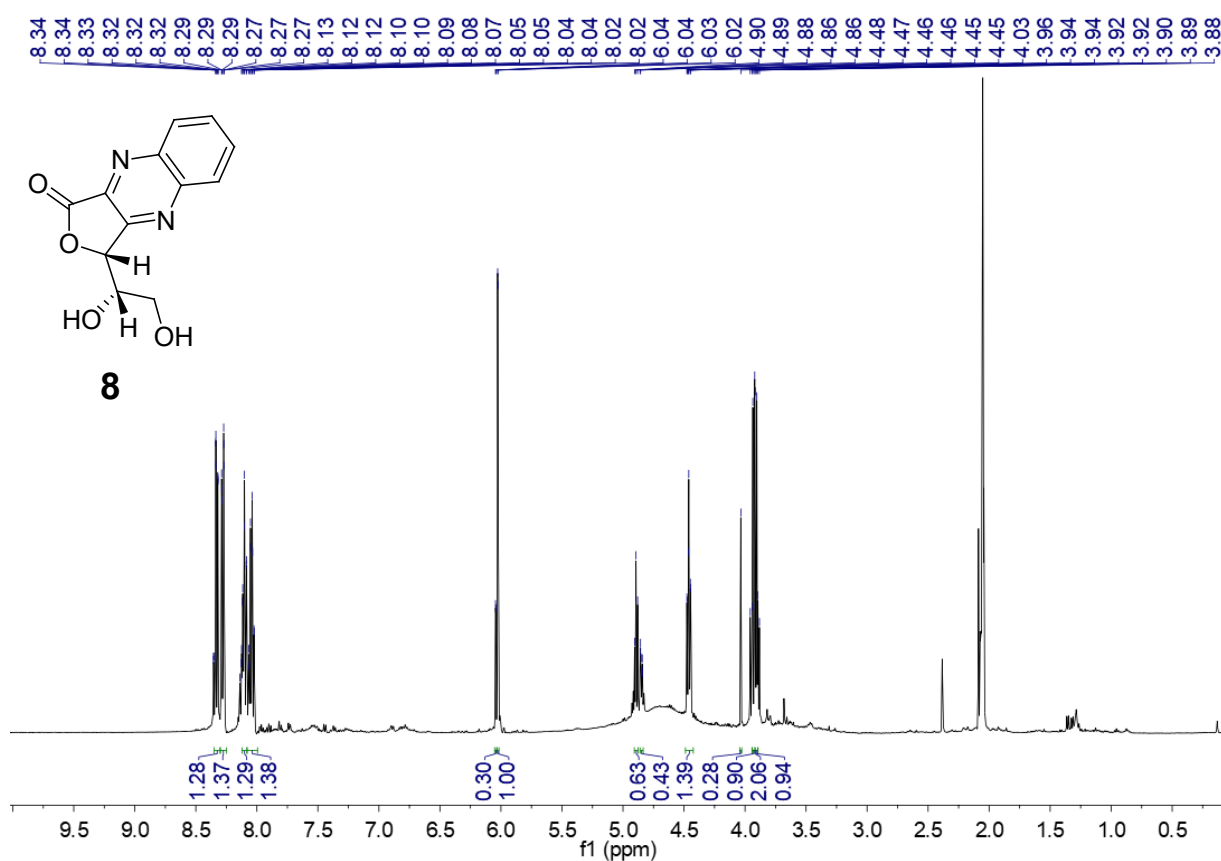


Figure S17.  $^{13}\text{C}$  NMR spectrum of **8** in acetone- $d_6$ .

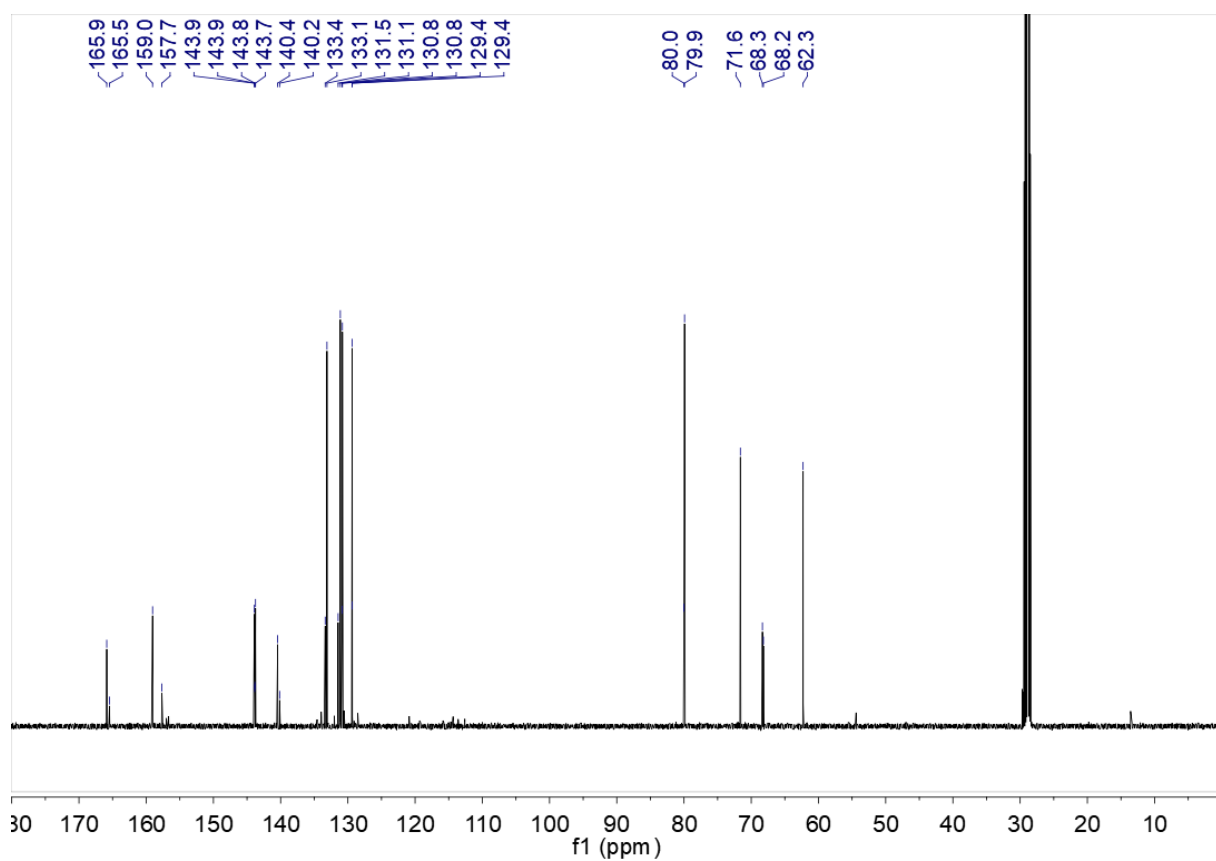


Figure S18.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **8** in acetone- $d_6$ .

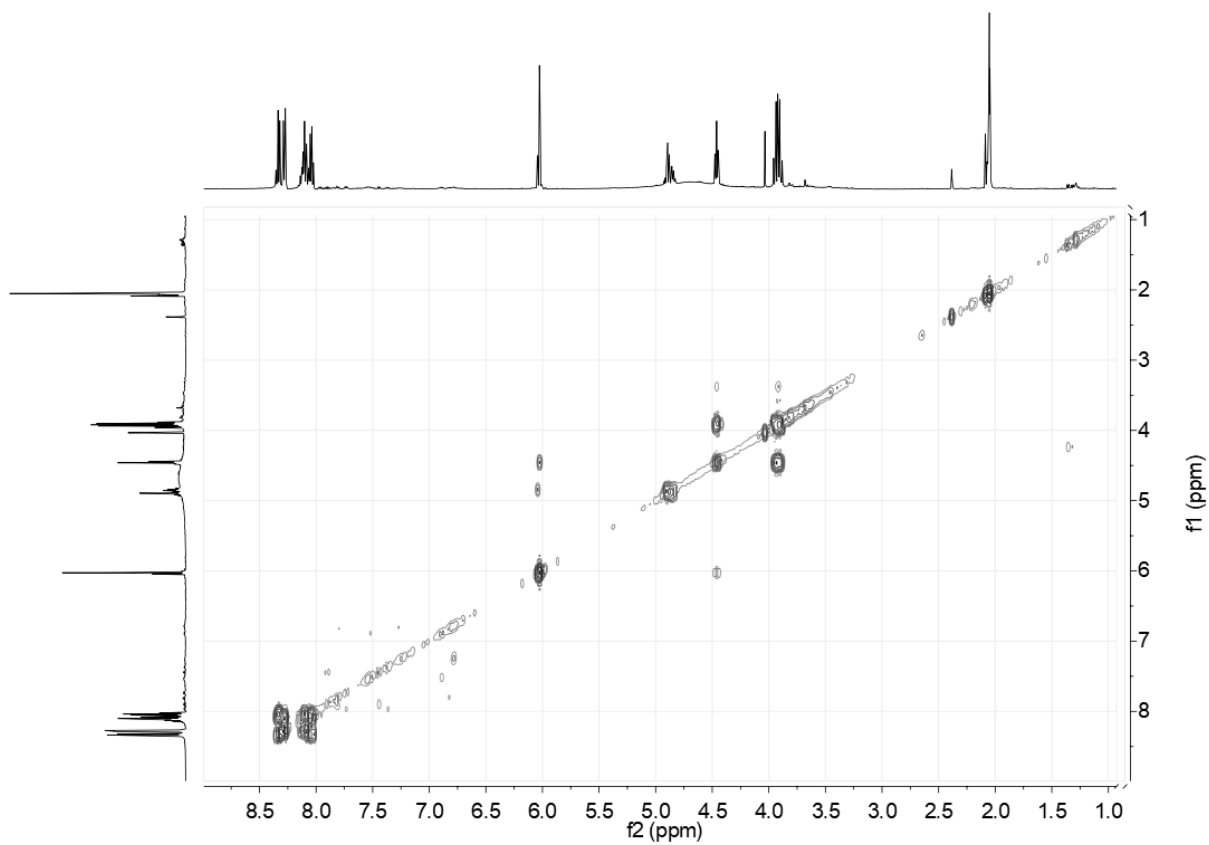


Figure S19. HSQC spectrum of **8** in acetone- $d_6$ .

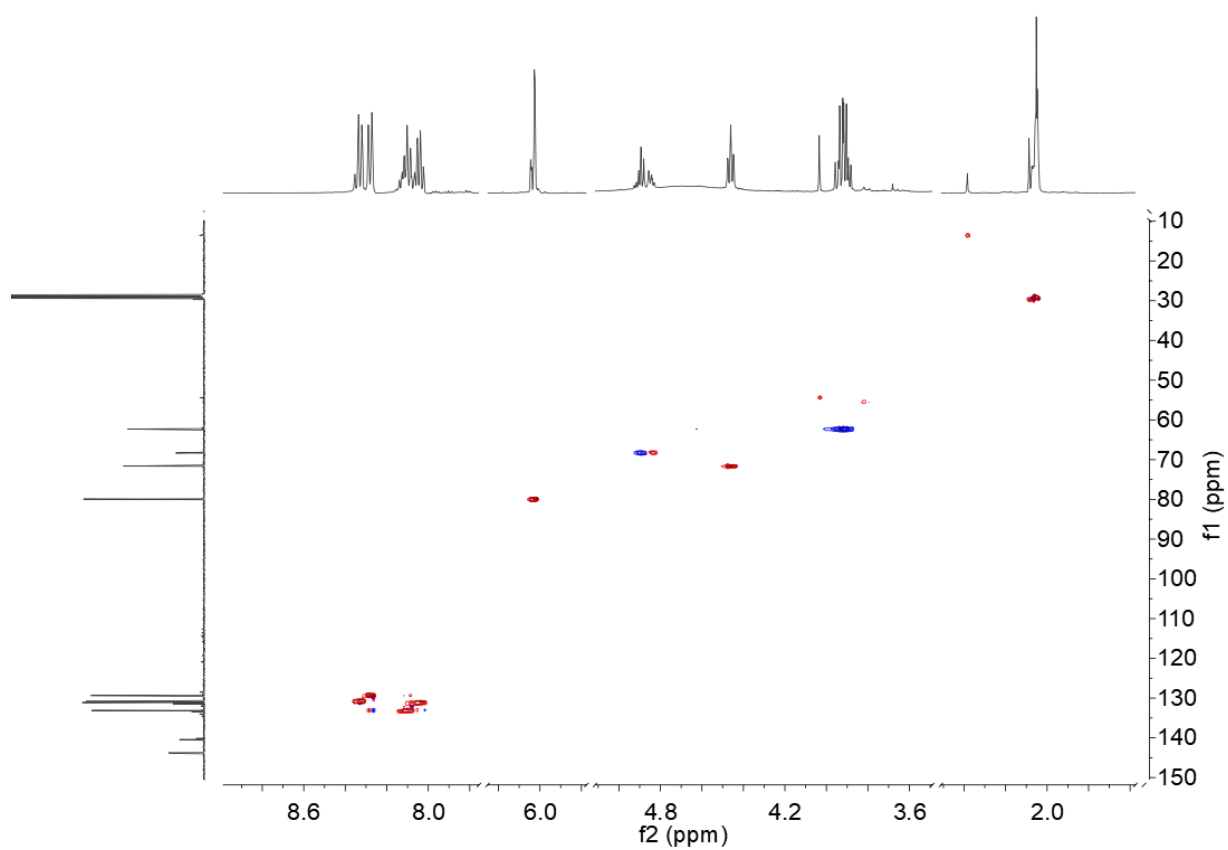


Figure S20. HMBC spectrum of **8** in acetone- $d_6$ .

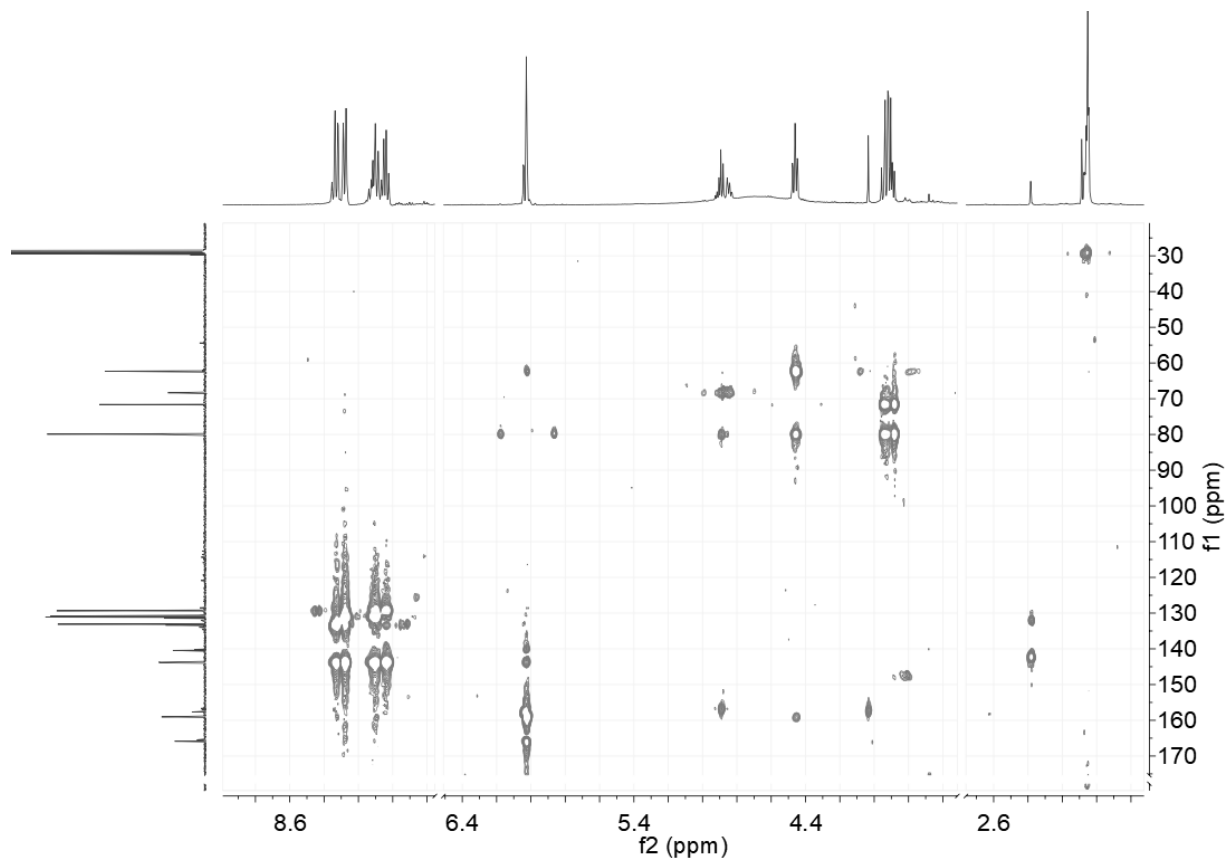


Figure S21. Roesy spectrum of 8 in acetone- $d_6$

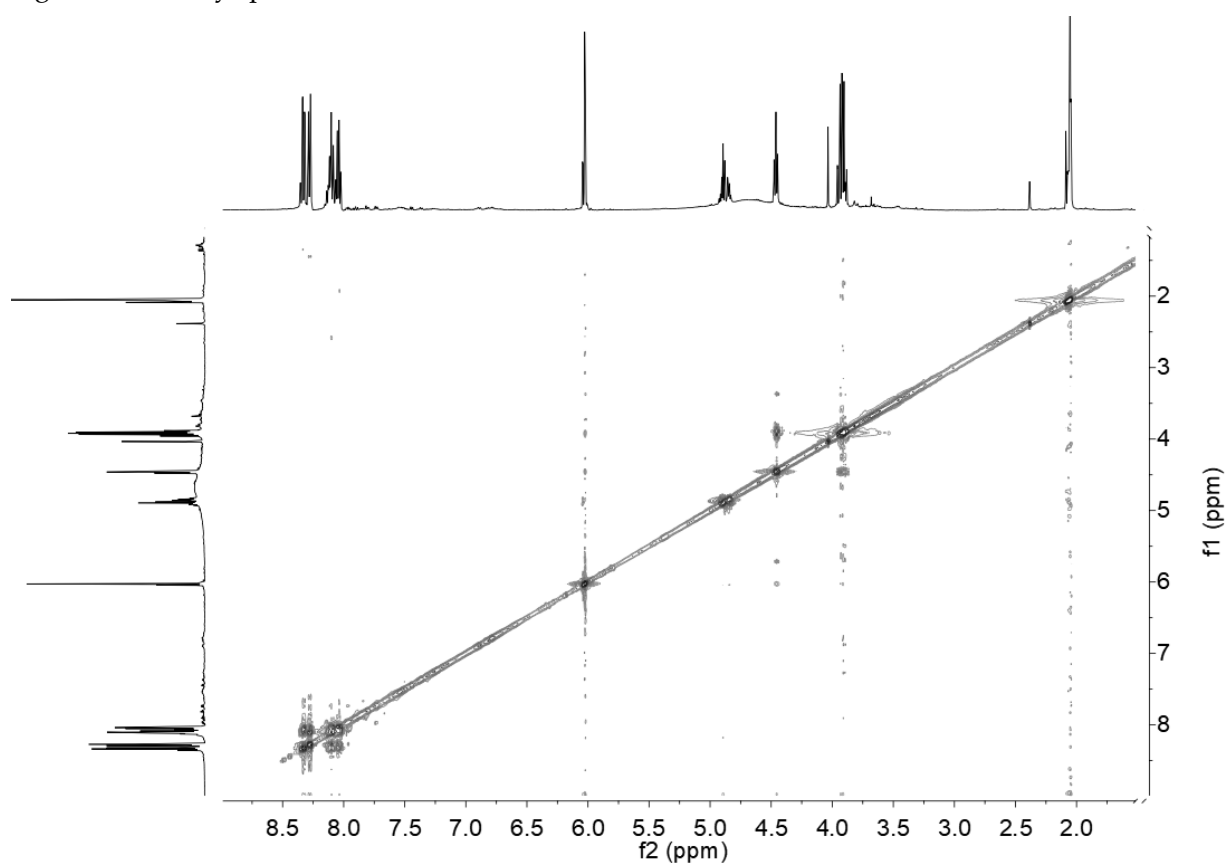


Figure S22. FAB-MS spectrum of 8

