SUPPLEMENTARY DATA

New natural furfural derivatives from the leaves and stems of *Pogostemon cablin*

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ABSTRACT

A new furfural derivative, pogoscafuran A (**1**), a new natural product, HMF levulinate (**2**), together with four known compounds (**3**–**6**) were isolated from an extract of the leaves and stems of *Pogostemon cablin* (Blanco) Benth. Their structures were elucidated on the basis of extensive spectroscopic analyses and single-crystal X-ray crystallography. Compound **1** was the first example of natural furfural derivative with a unique C5–C1′ linkage between a molecule of furfural and 3-methyl-2-cyclopentenone moiety. The plausible biogenetic pathway for the new compound **1** was proposed. All these isolated compounds were tested for their inhibitory effects on the nitric oxide (NO) production induced by lipopolysaccharide in RAW264.7 cells, and only compound **1** exhibited weak inhibitory activity.

Keywords: *Pogostemon cablin*; Labiatae; furfural derivatives; single-crystal X-ray crystallography

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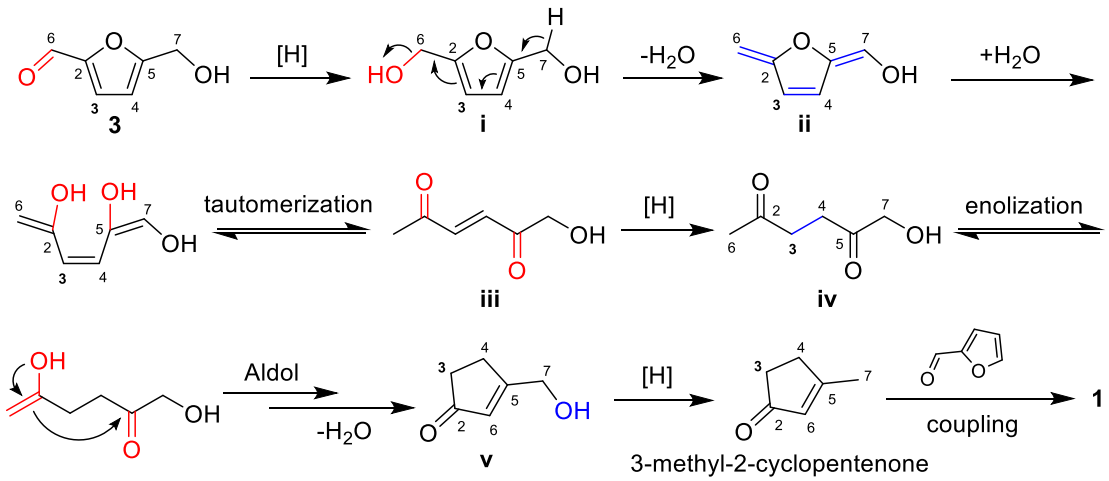

Scheme S1. Plausible biosynthetic pathway of compound **1**.

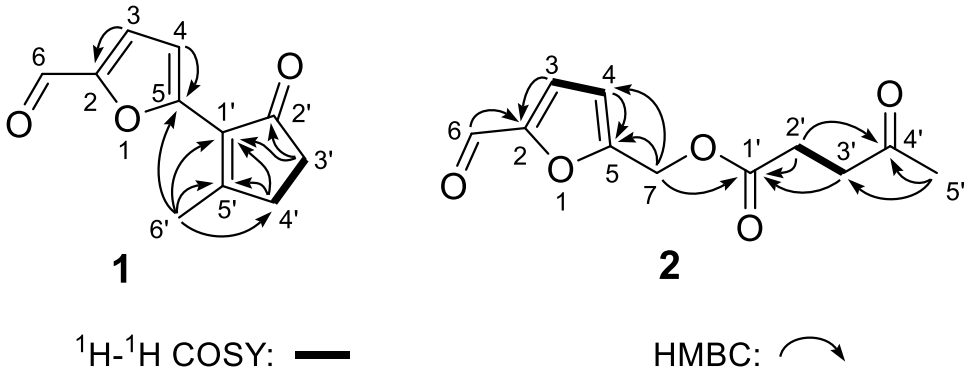

Figure S1. Key ^{1}H–^{1}H COSY and HMBC correlations of compounds **1** and **2**.

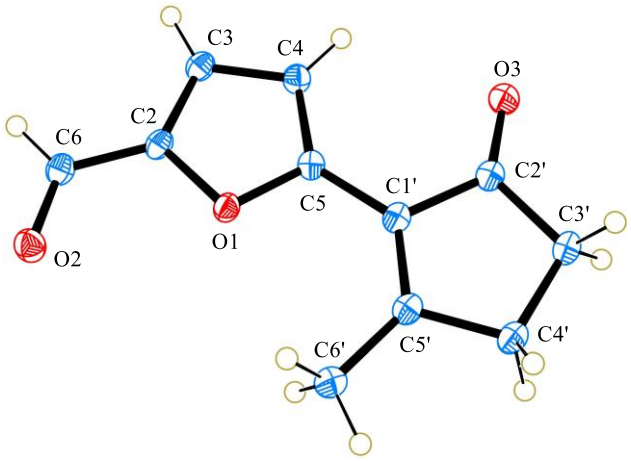

Figure S2. X-ray crystallographic structure of compound **1**.

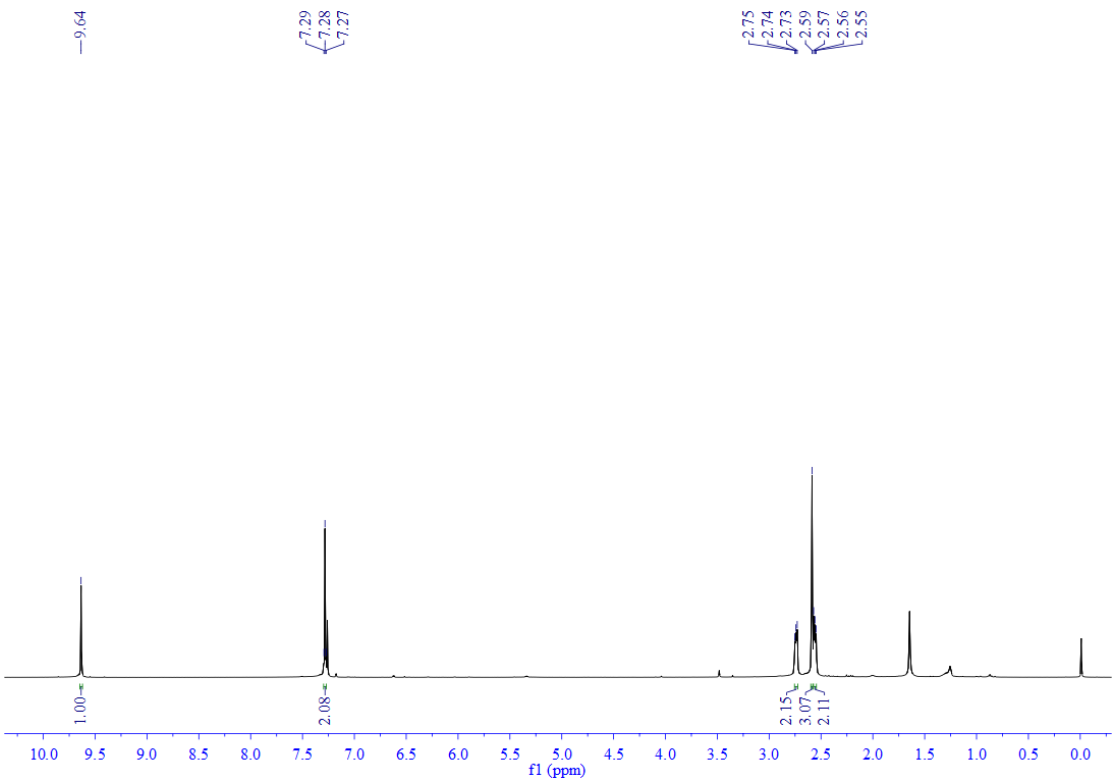

Figure S3. ^{1}H NMR (400 MHz) spectrum of compound **1** in $CDCl_3$.

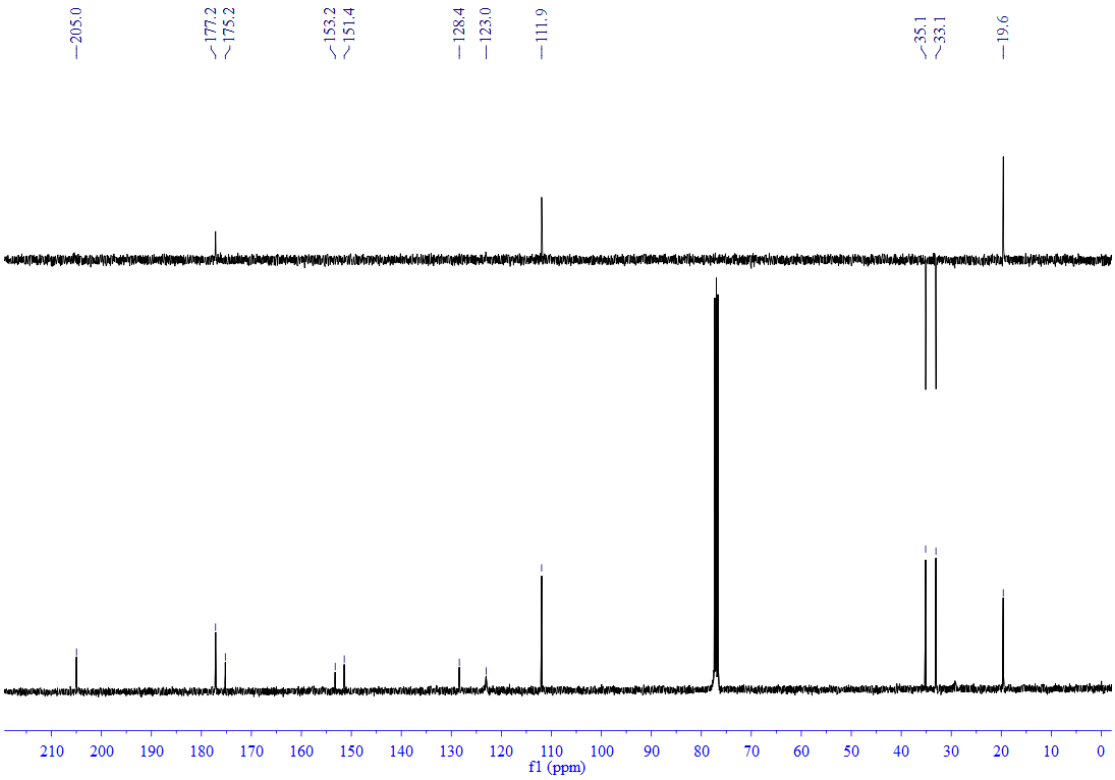

Figure S4. ^{13}C NMR and DEPT 135 (100 MHz) spectra of compound **1** in $CDCl_3$.

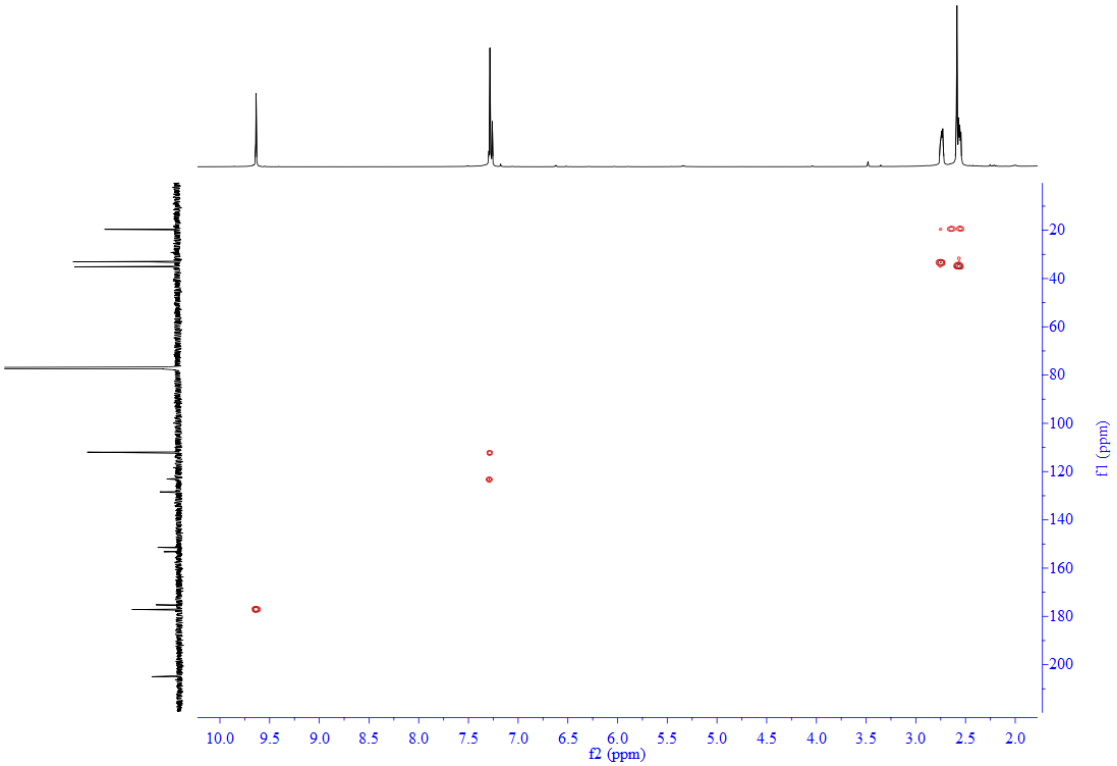

Figure S5. HSQC spectrum of compound **1** in $CDCl_3$.

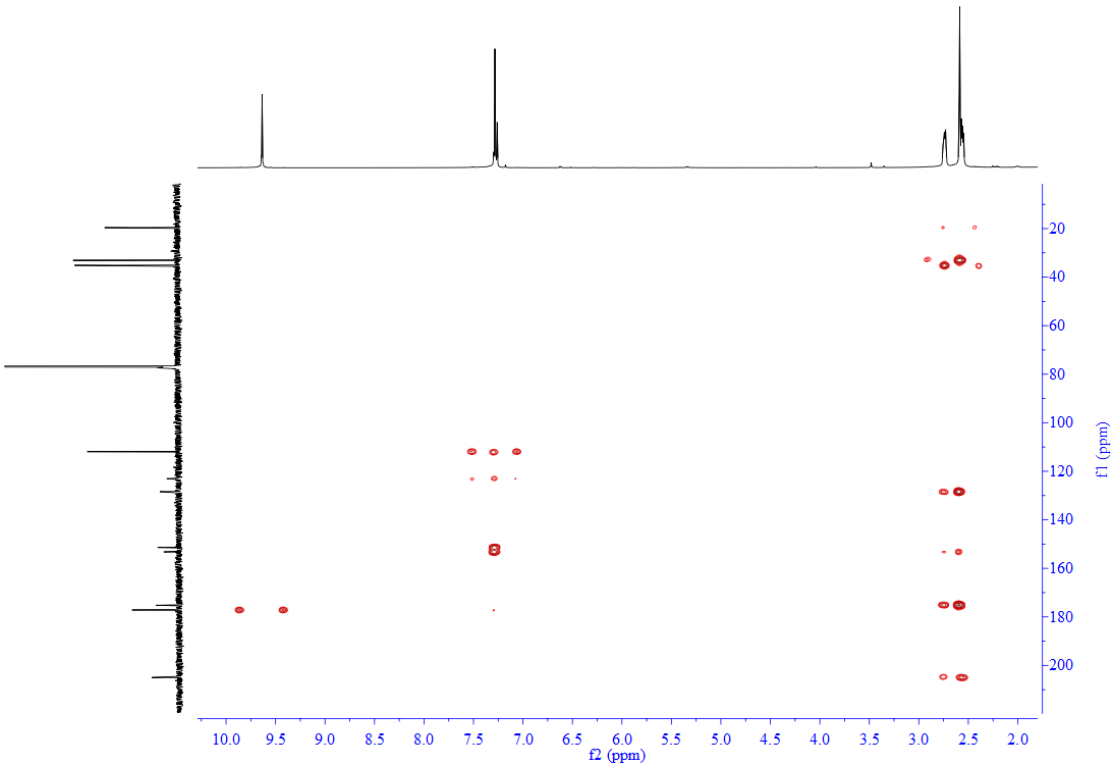

Figure S6. HMBC spectrum of compound **1** in $CDCl_3$.

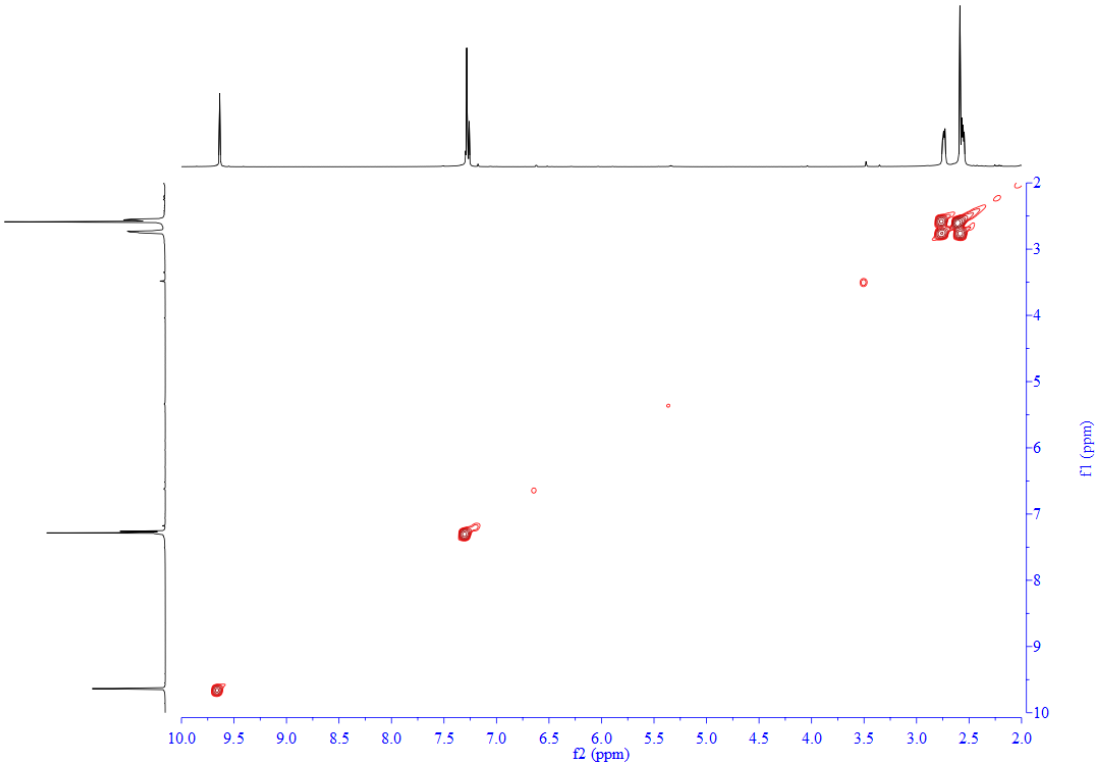

Figure S7. $^{1}H–^{1}H$ COSY spectrum of compound **1** in $CDCl_3$.

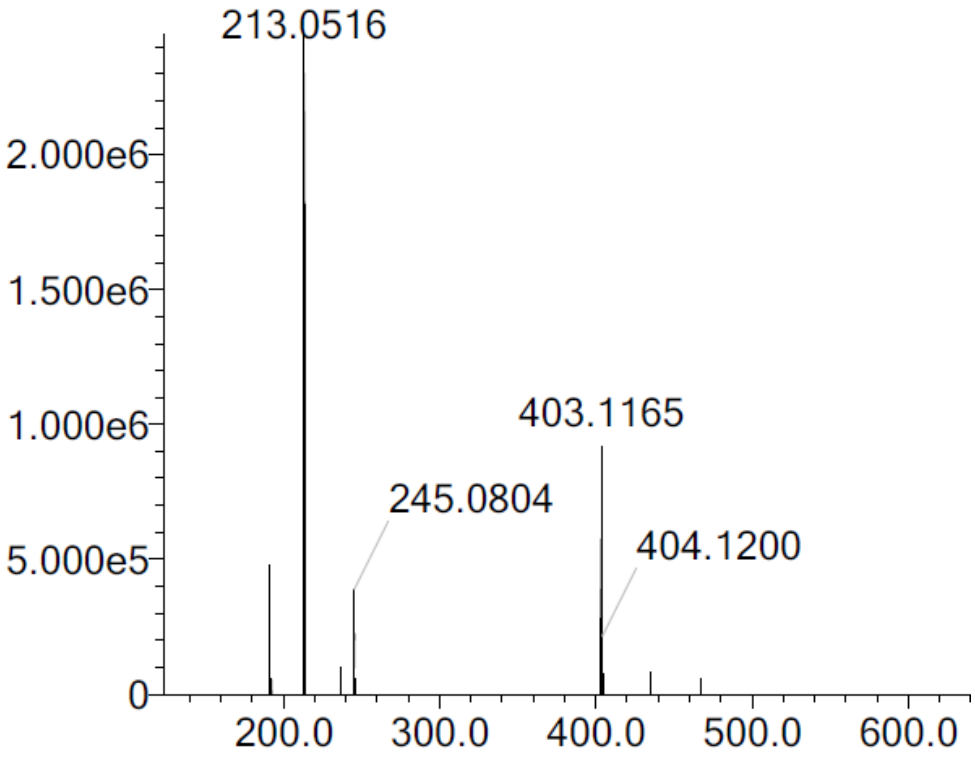

Figure S8. HRESIMS spectrum of compound **1**.

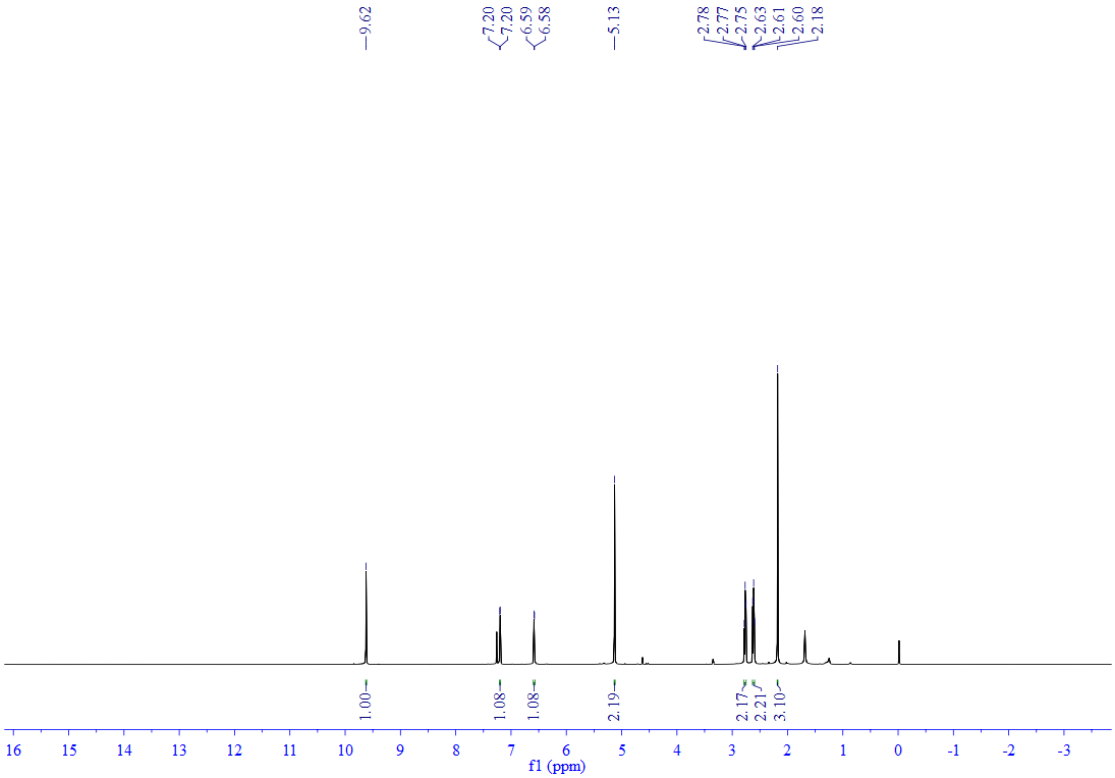

Figure S9. ^{1}H NMR (400 MHz) spectrum of compound **2** in $CDCl_3$.

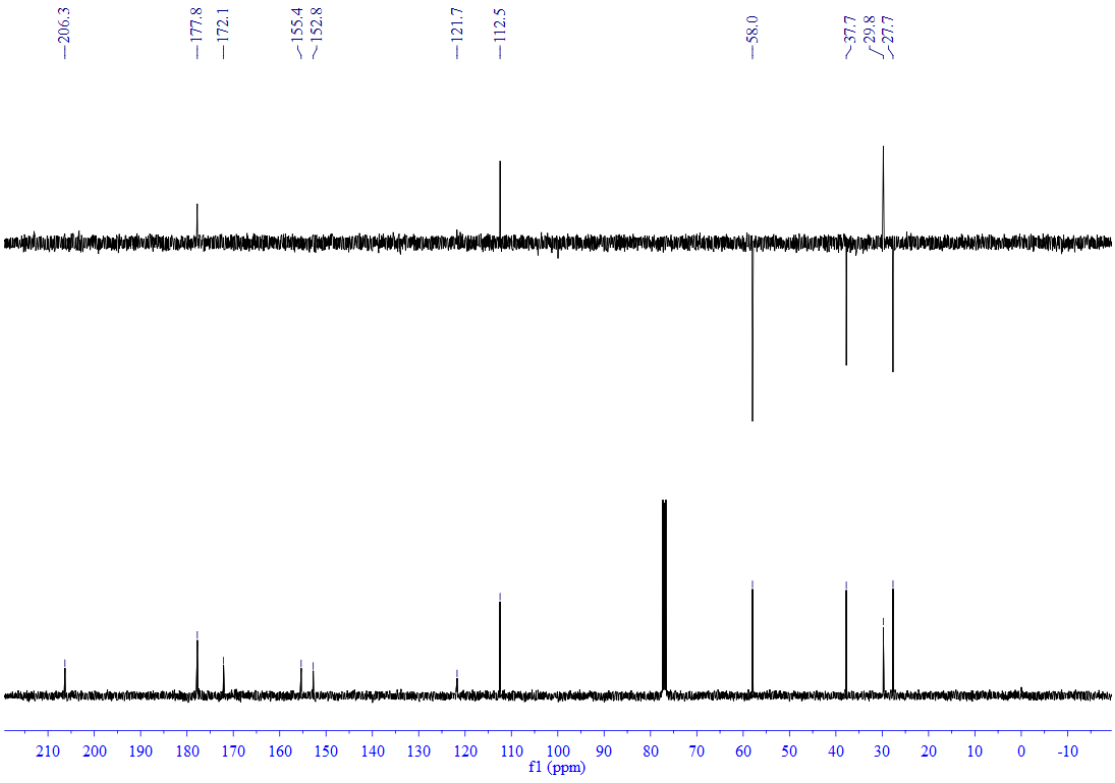

Figure S10. ^{13}C NMR and DEPT 135 (100 MHz) spectra of compound **2** in $CDCl_3$.

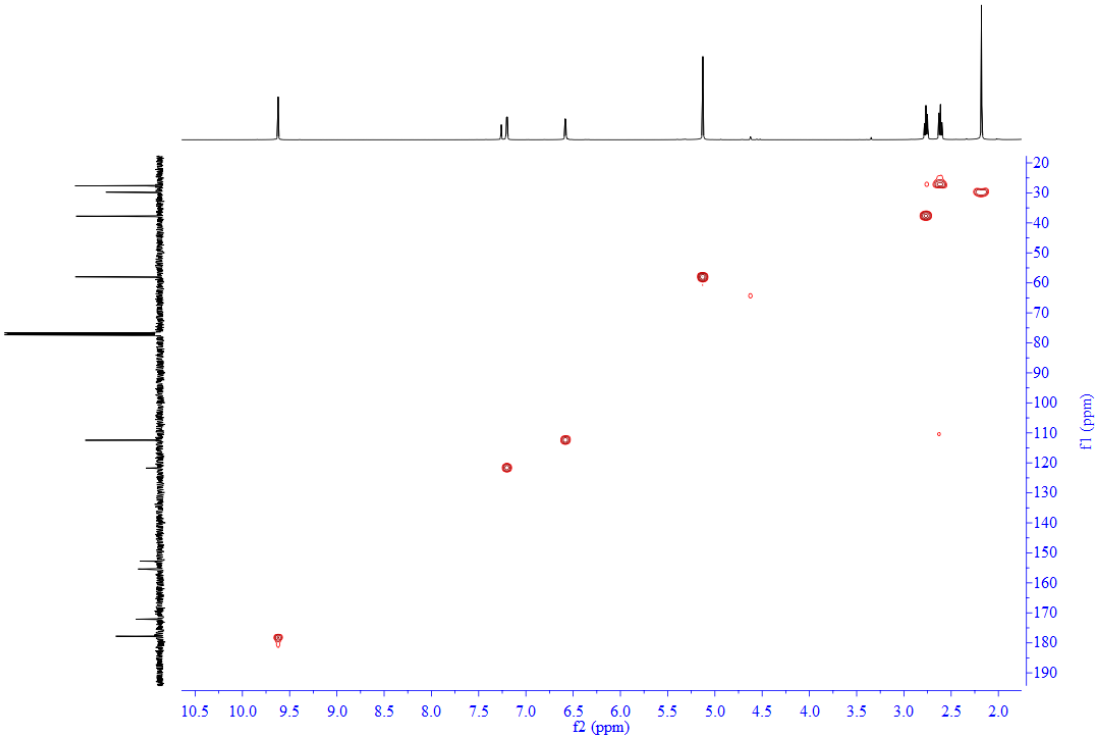

Figure S11. HSQC spectrum of compound **2** in $CDCl_3$.

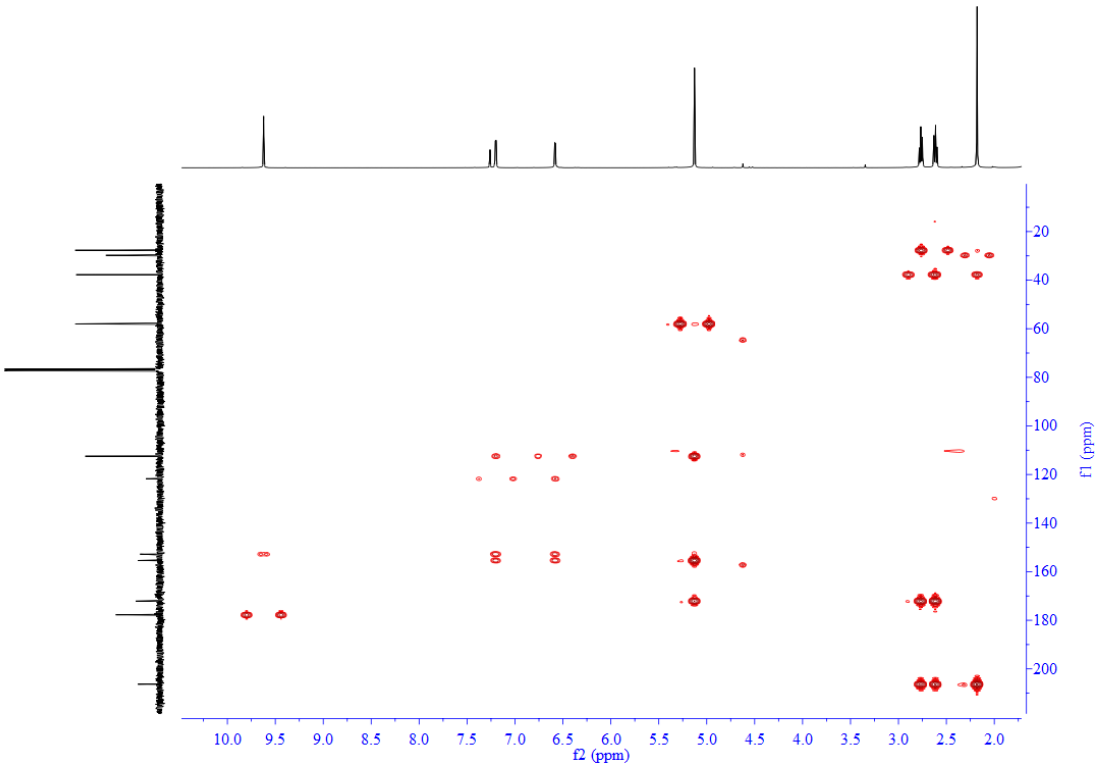

Figure S12. HMBC spectrum of compound **2** in $CDCl_3$.

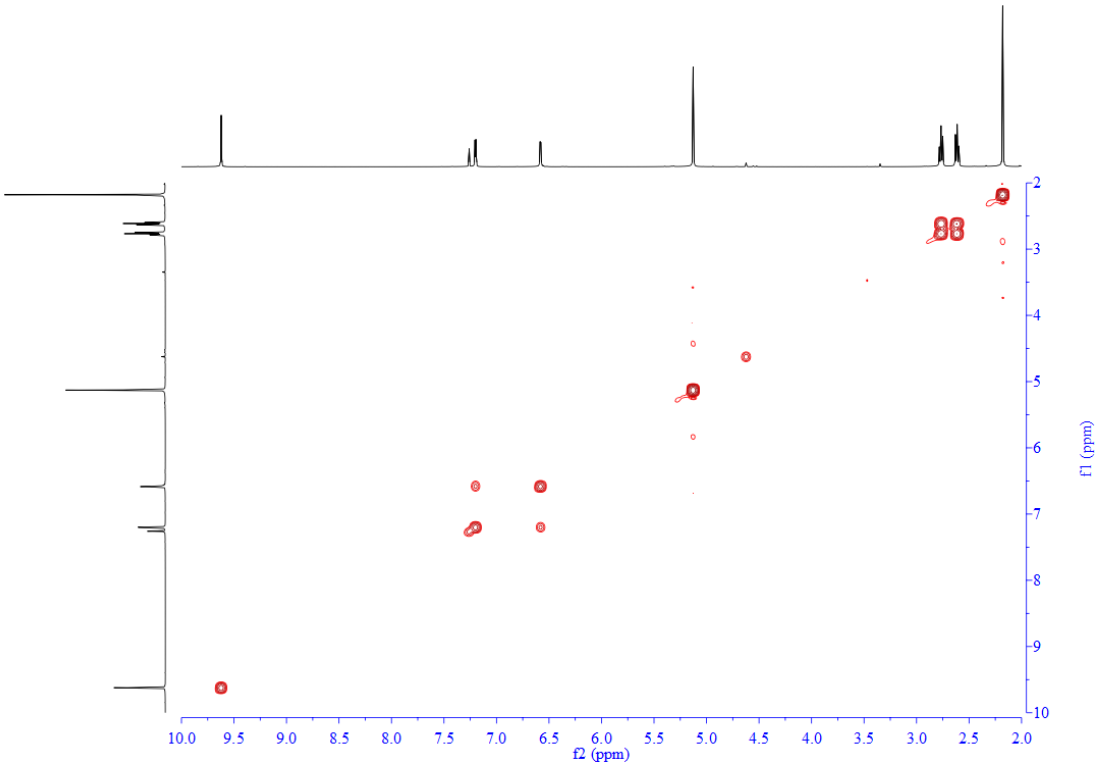

Figure S13. $^{1}H–^{1}H$ COSY spectrum of compound **2** in $CDCl_3$.

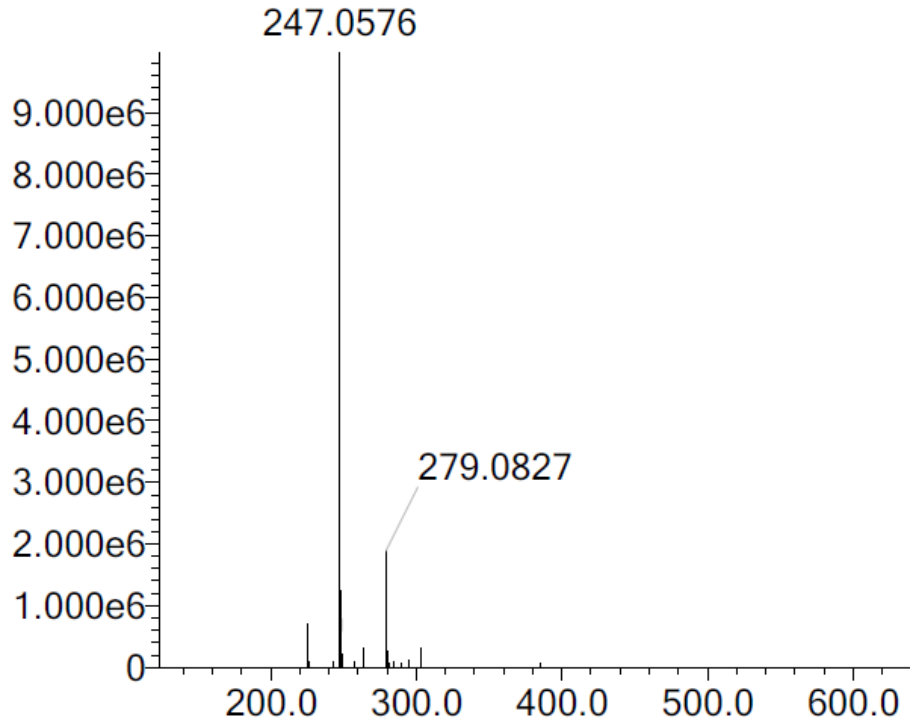

Figure S14. HRESIMS spectrum of compound **2**.

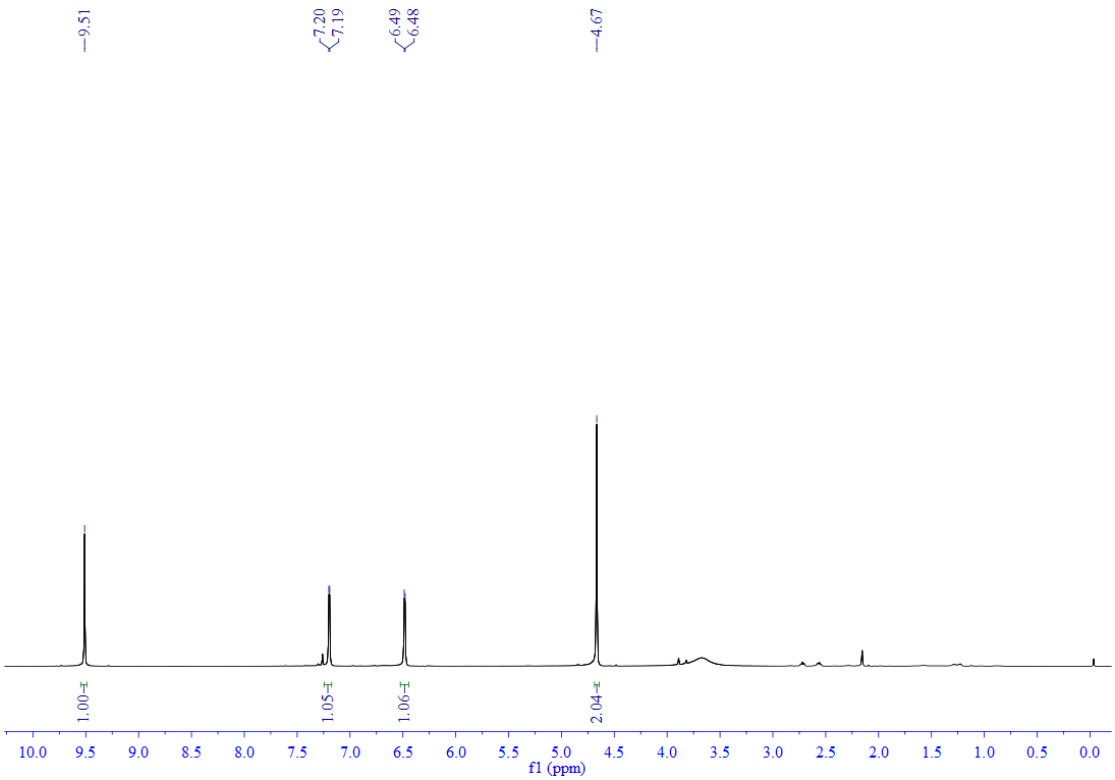

Figure S15. ^{1}H NMR (400 MHz) spectrum of compound **3** in $CDCl_3$.

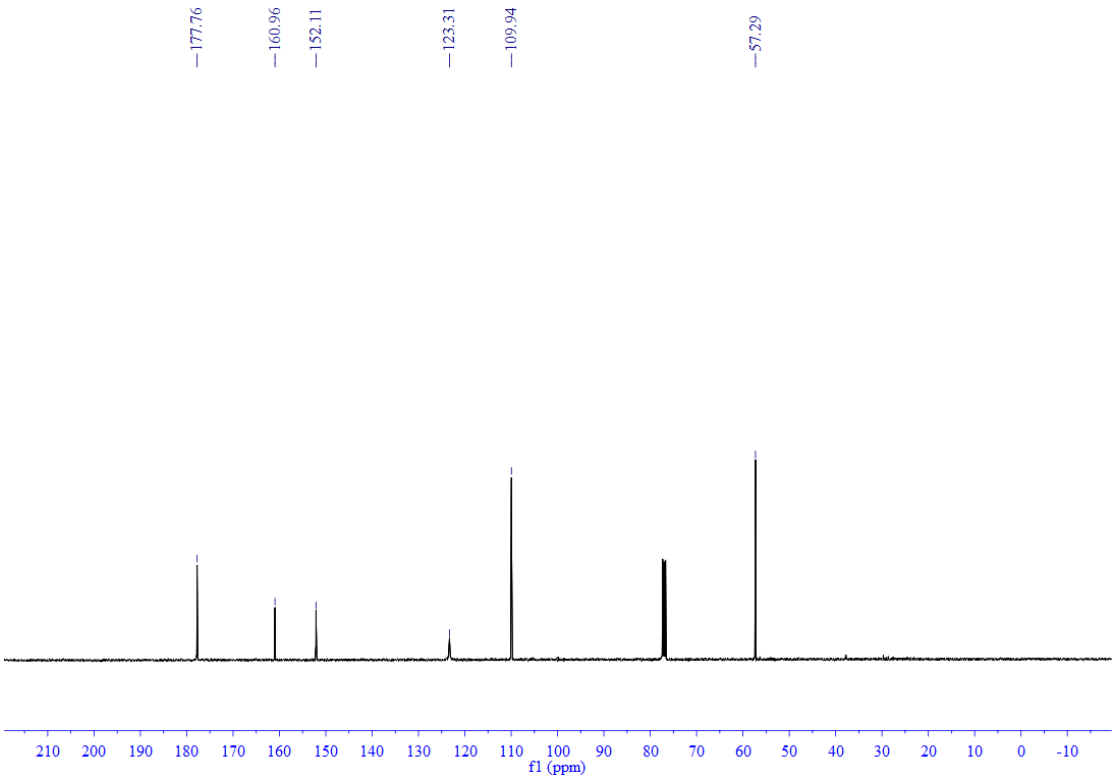

Figure S16. ^{13}C NMR (100 MHz) spectrum of compound **3** in $CDCl_3$.

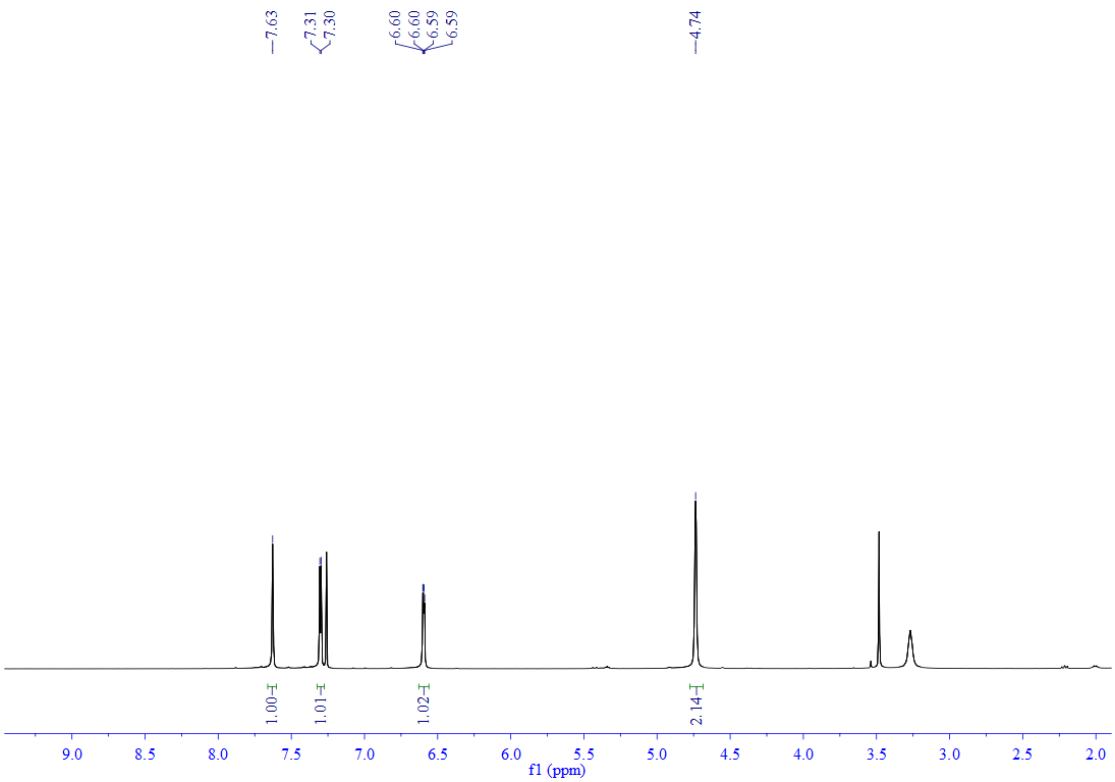

Figure S17. ^{1}H NMR (400 MHz) spectrum of compound **4** in $CDCl_3$.

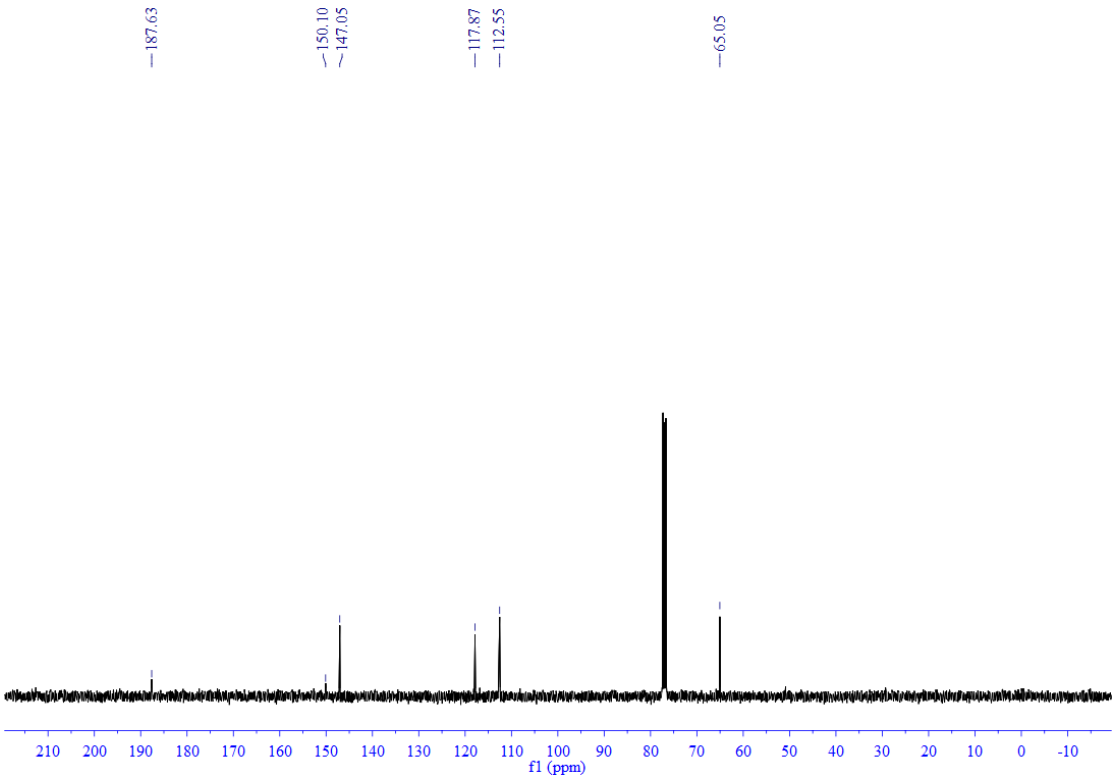

Figure S18. ^{13}C NMR (100 MHz) spectrum of compound **4** in $CDCl_3$.

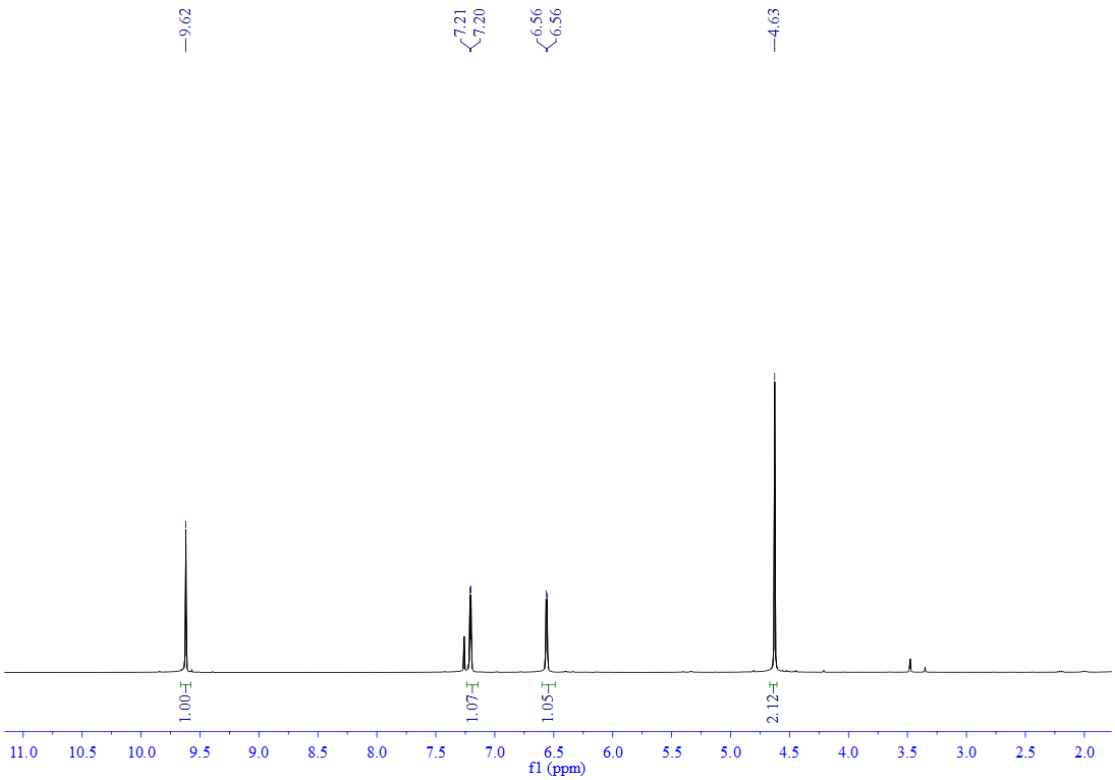

Figure S19. ^{1}H NMR (400 MHz) spectrum of compound **5** in $CDCl_3$.

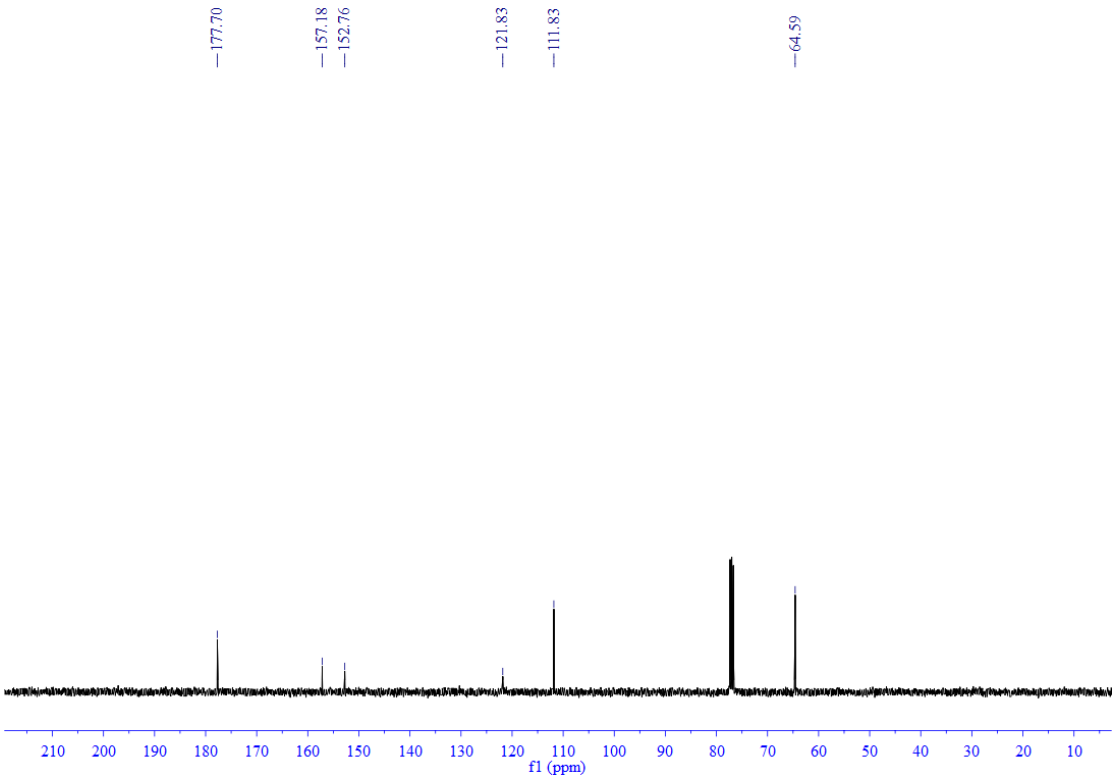

Figure S20. ^{13}C NMR (100 MHz) spectrum of compound **5** in $CDCl_3$.

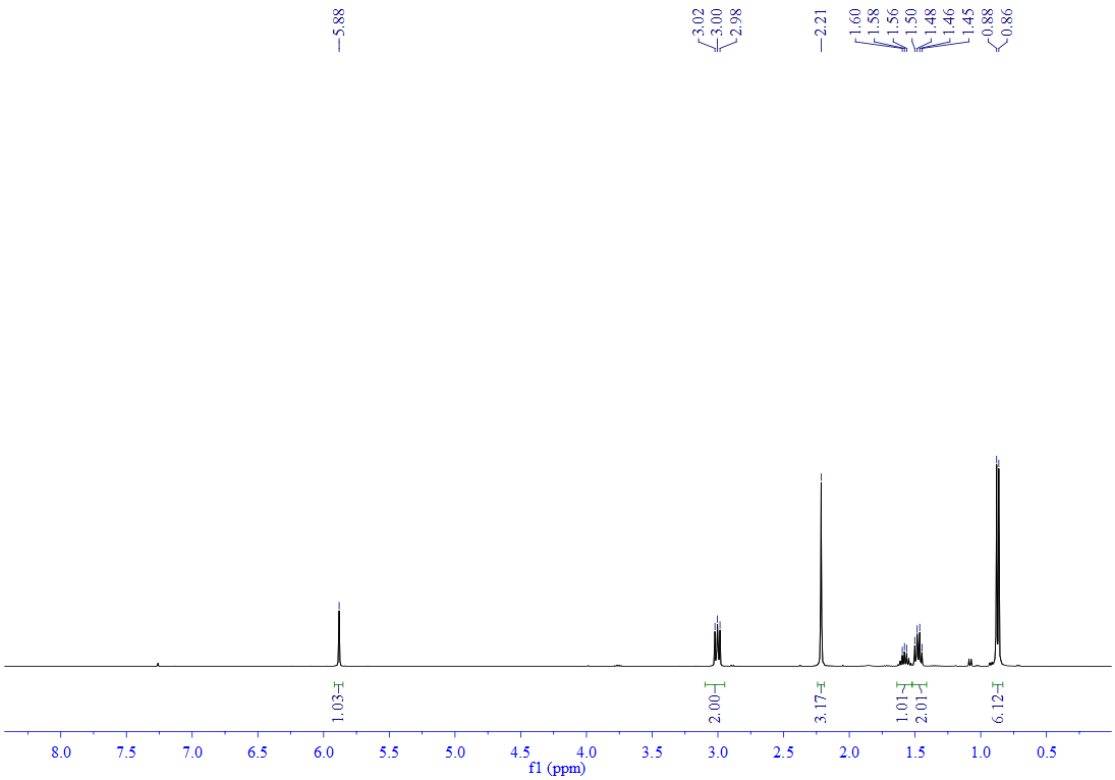

Figure S21. ^{1}H NMR (400 MHz) spectrum of compound **6** in $CDCl_3$.

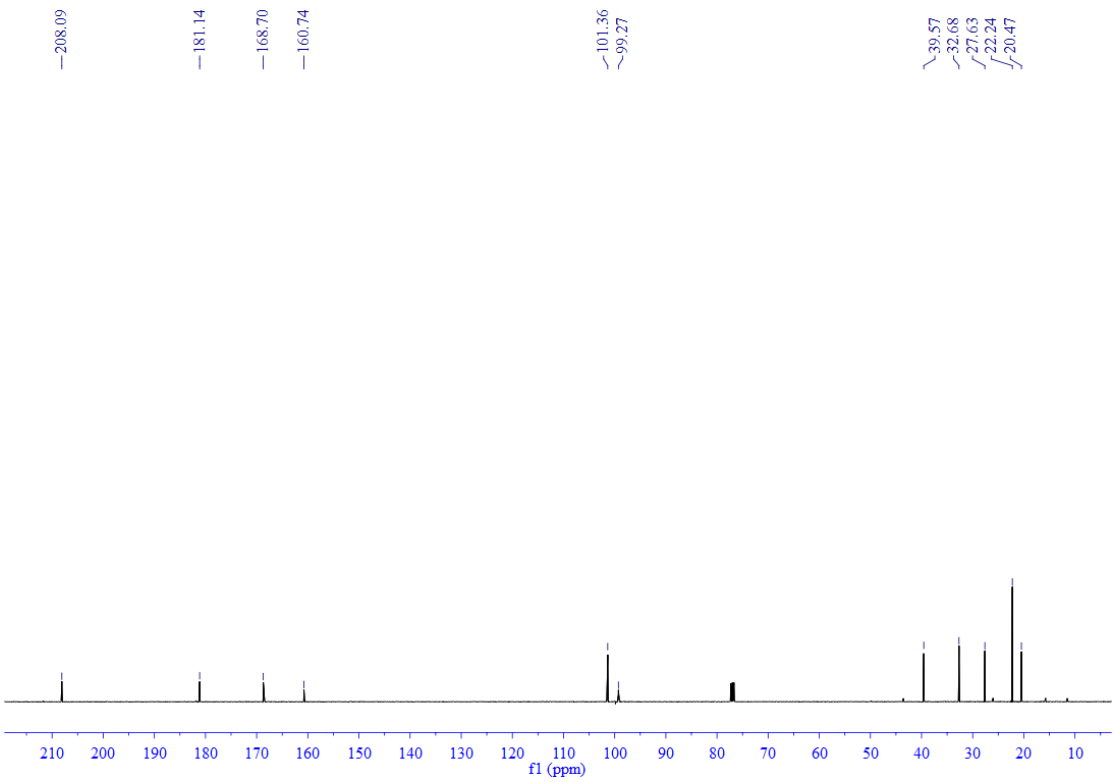

Figure S22. ^{13}C NMR (100 MHz) spectrum of compound **6** in $CDCl_3$.