

## *Supplementary Material*

# **Halogenase-Targeted Genome Mining Leads to the Discovery of ( $\pm$ ) Pestalachlorides A1a, A2a, and Their Atropisomers**

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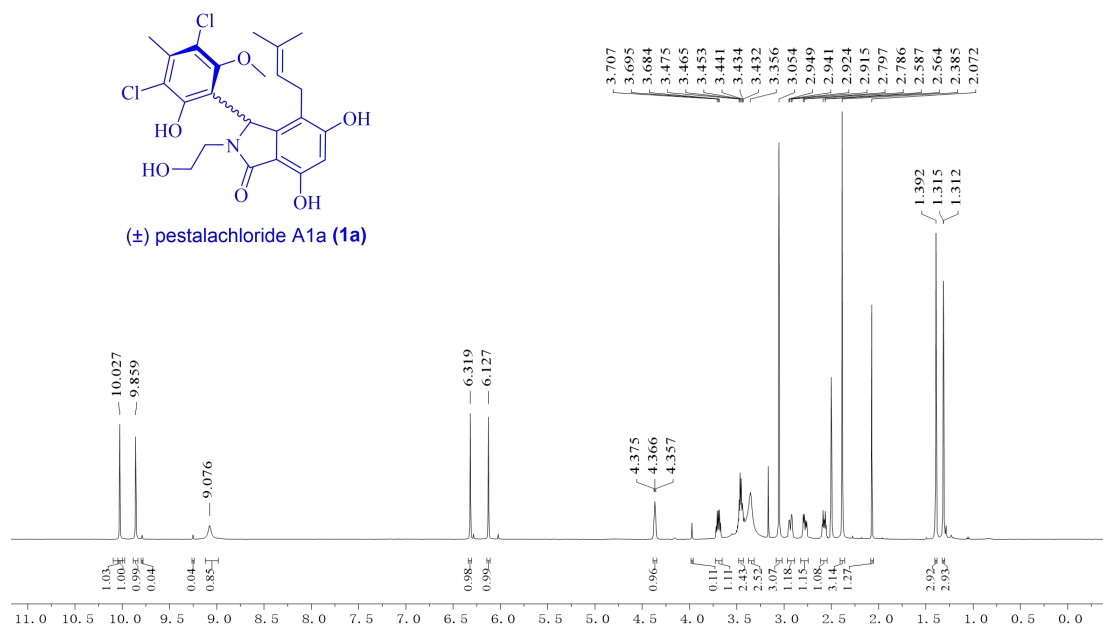
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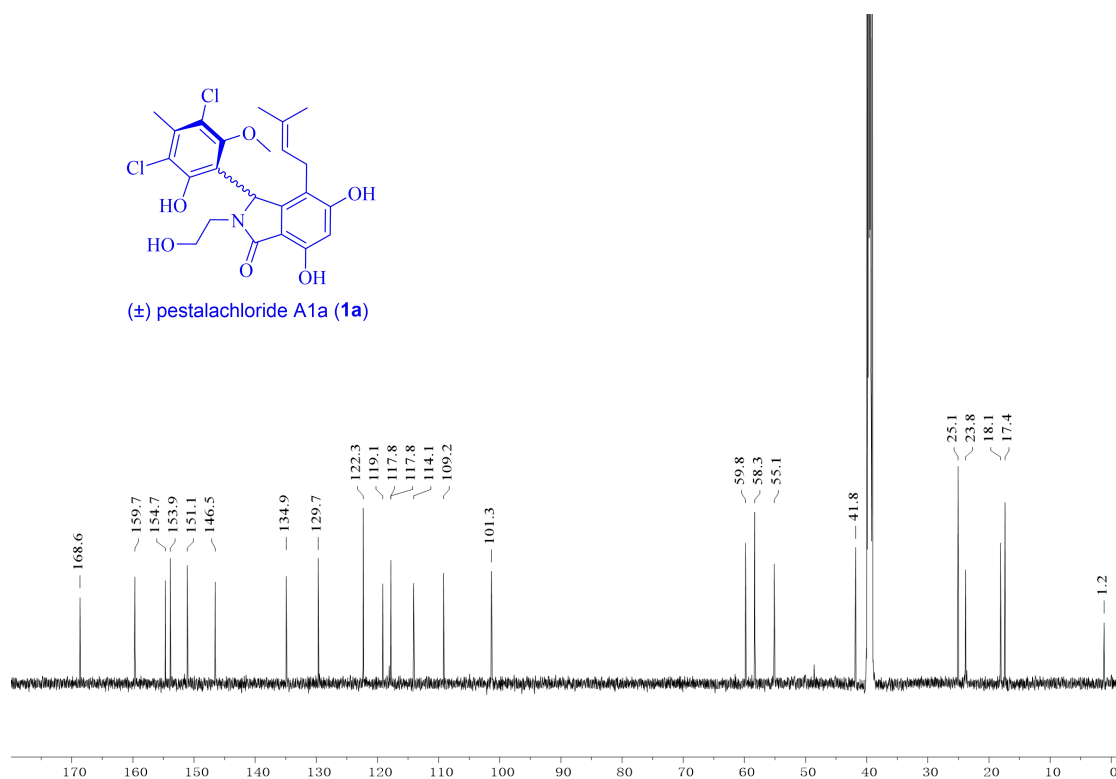
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**Figure S1.**  $^1\text{H}$  NMR for pestalachloride A1a (**1a**) in DMSO- $d_6$  (600 MHz)



**Figure S2.**  $^{13}\text{C}$  NMR for pestalachloride A1a (**1a**) in DMSO- $d_6$  (150 MHz)

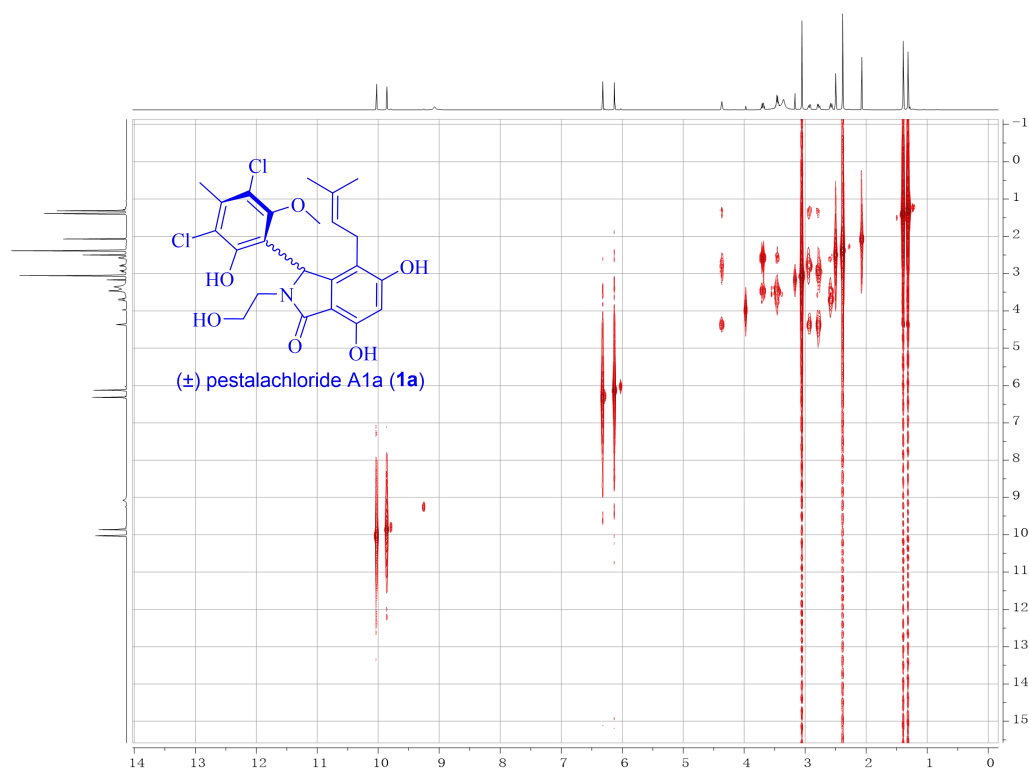


Figure S3. gCOSY for pestalachloride A1a (1a) in DMSO- $d_6$

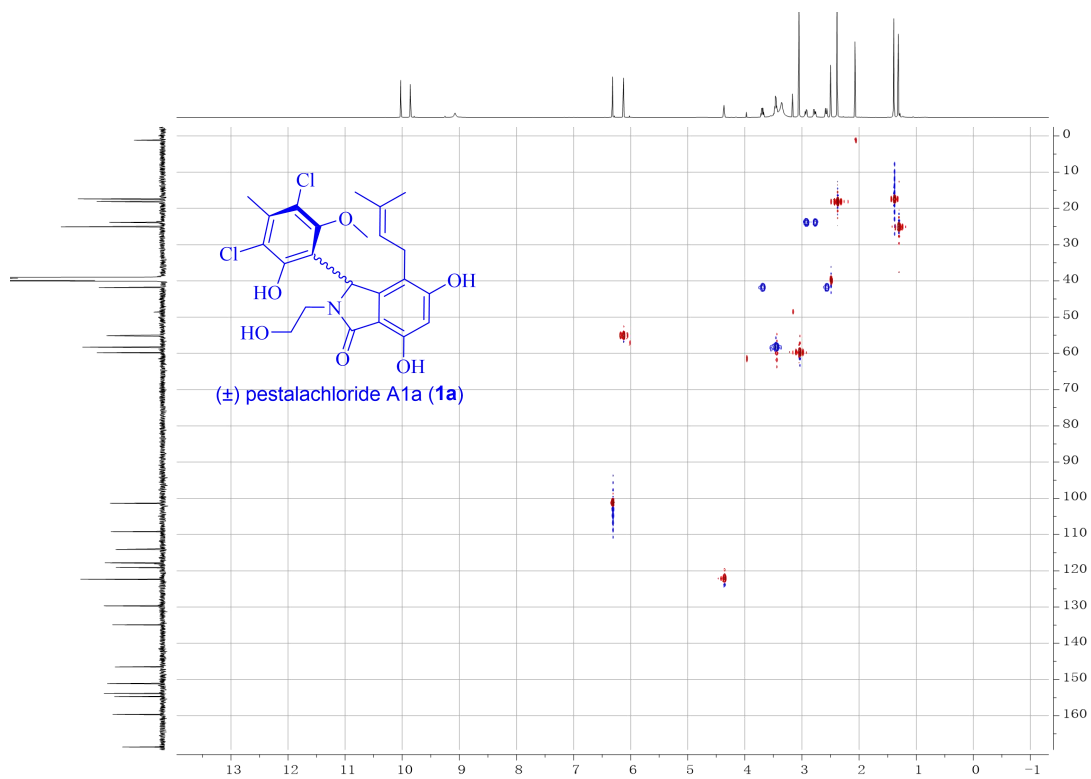
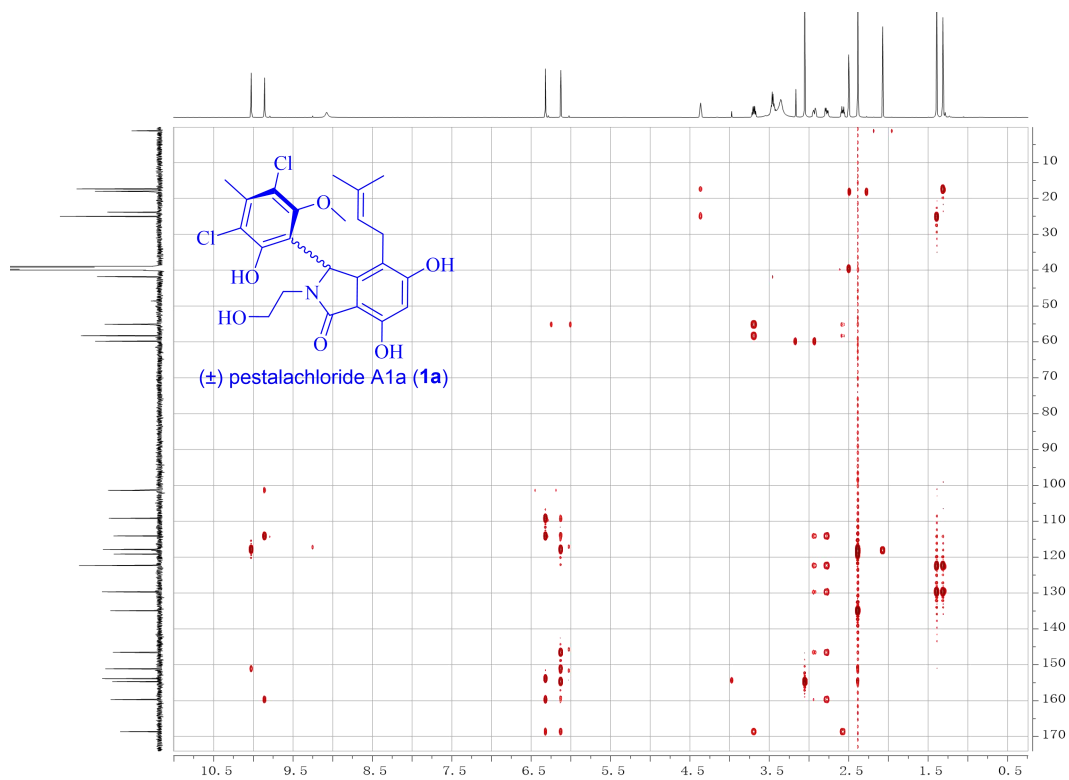
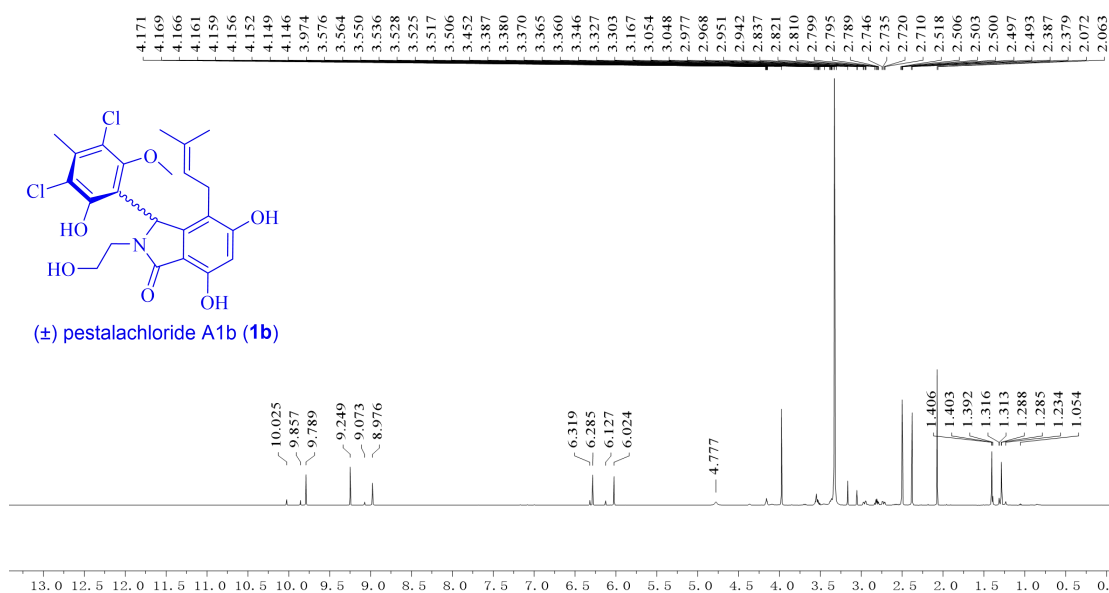


Figure S4. HSQC for pestalachloride A1a (1a) in DMSO- $d_6$

Figure S5. HMBC for pestalachloride A1a (**1a**) in DMSO-*d*<sub>6</sub>Figure S6. <sup>1</sup>H NMR for pestalachloride A1b (**1b**) in DMSO-*d*<sub>6</sub> (600 MHz)

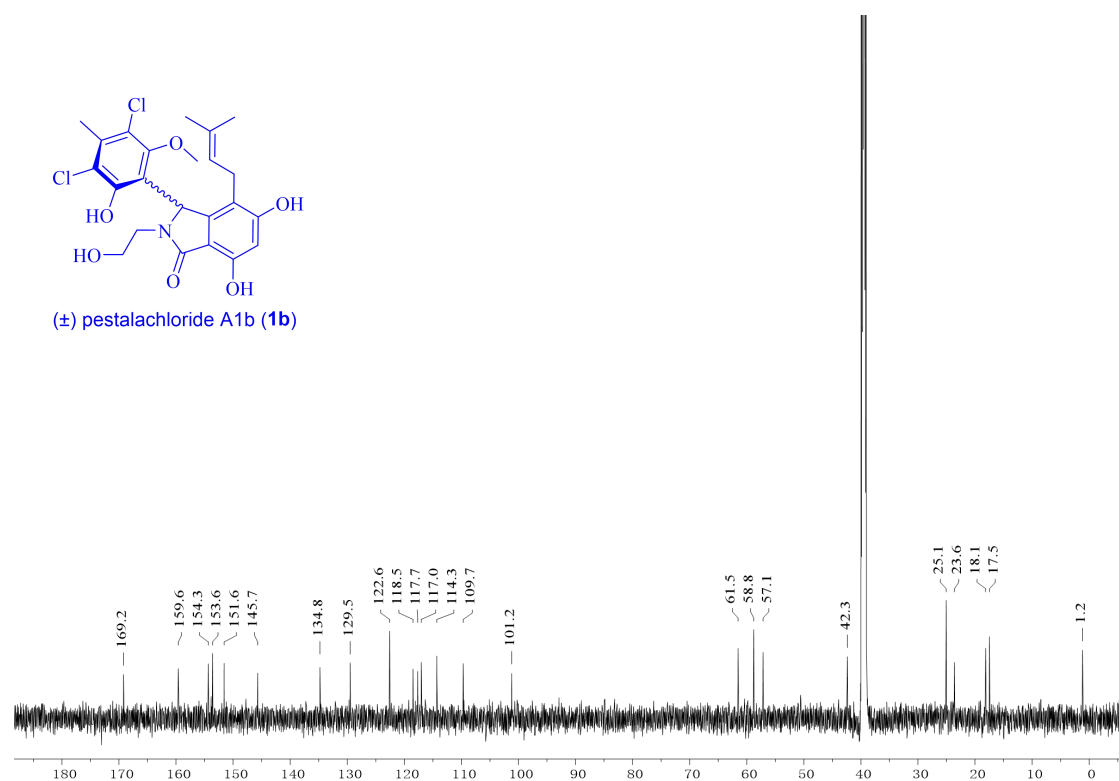


Figure S7.  $^{13}\text{C}$  NMR for pestalachloride A1b (1b) in  $\text{DMSO}-d_6$  (150 MHz)

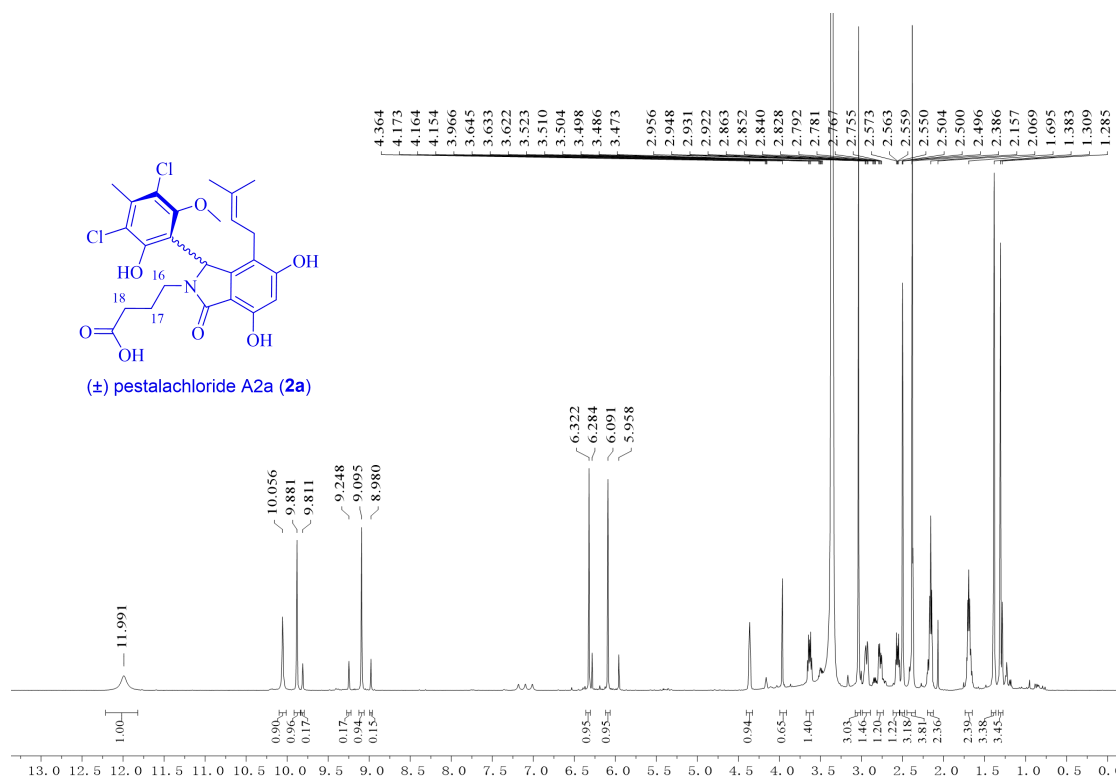


Figure S8.  $^1\text{H}$  NMR for pestalachloride A2a (2a) in  $\text{DMSO}-d_6$  (600 MHz)

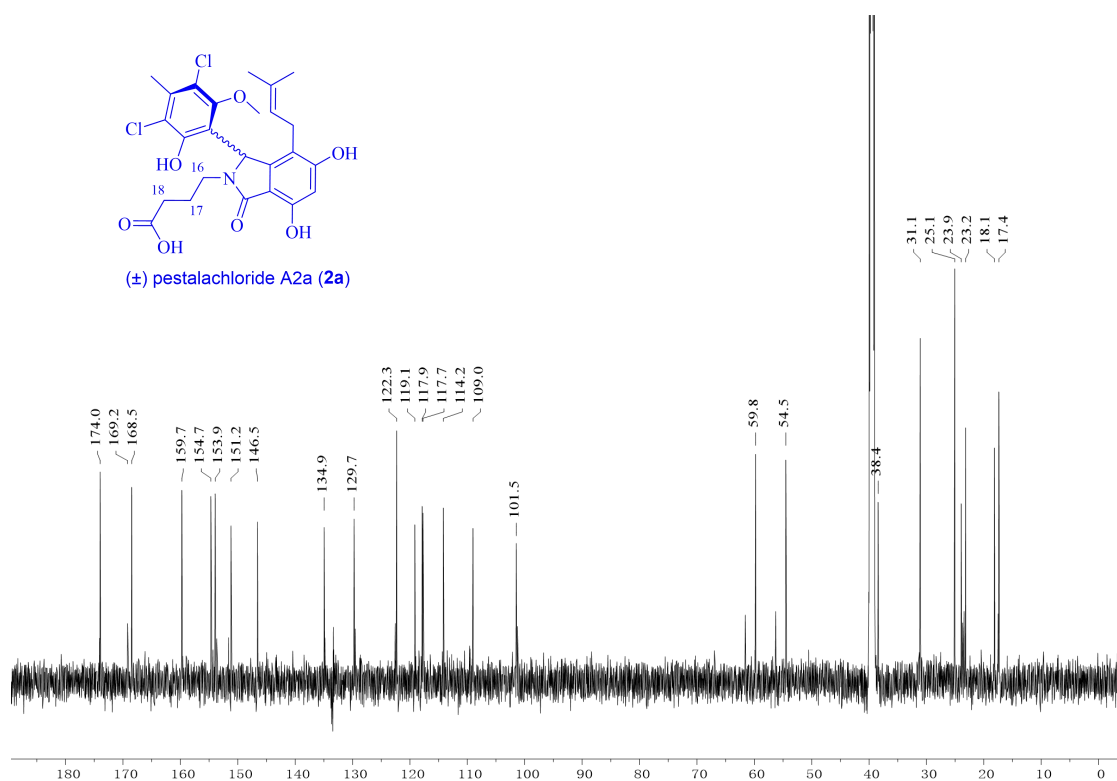


Figure S9.  $^{13}\text{C}$  NMR for pestalachloride A2a (**2a**) in  $\text{DMSO}-d_6$  (150 MHz)

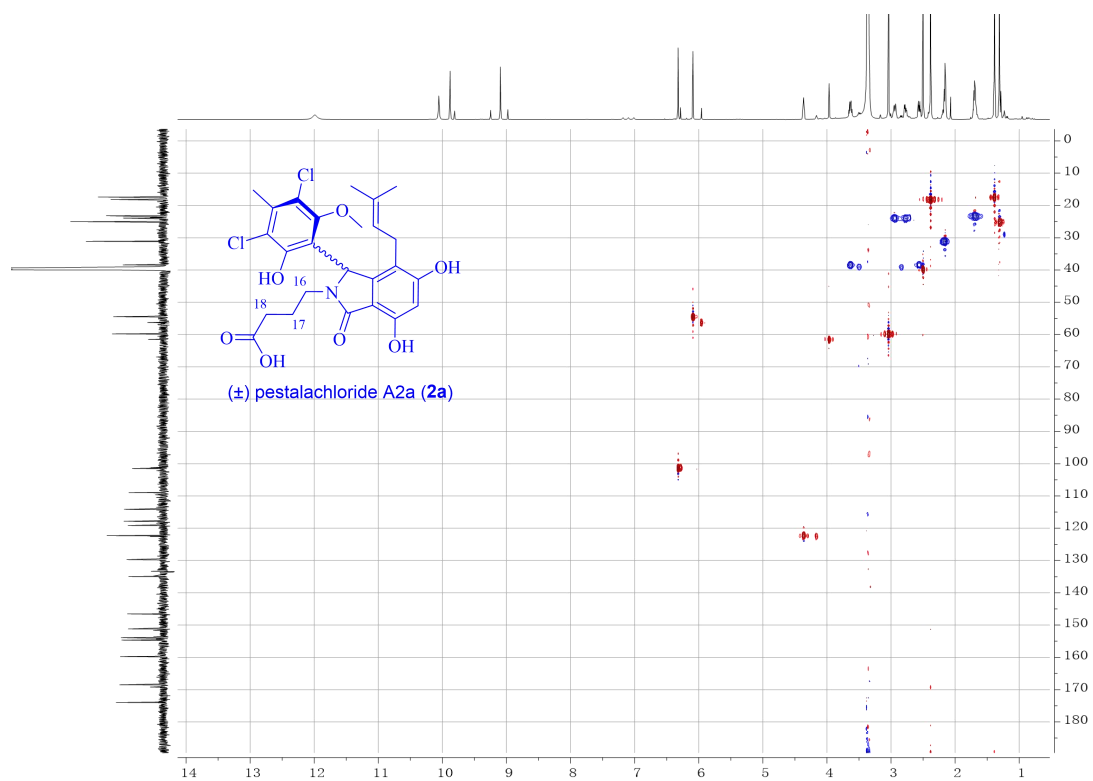


Figure S10. HSQC for pestalachloride A2a (**2a**) in  $\text{DMSO}-d_6$

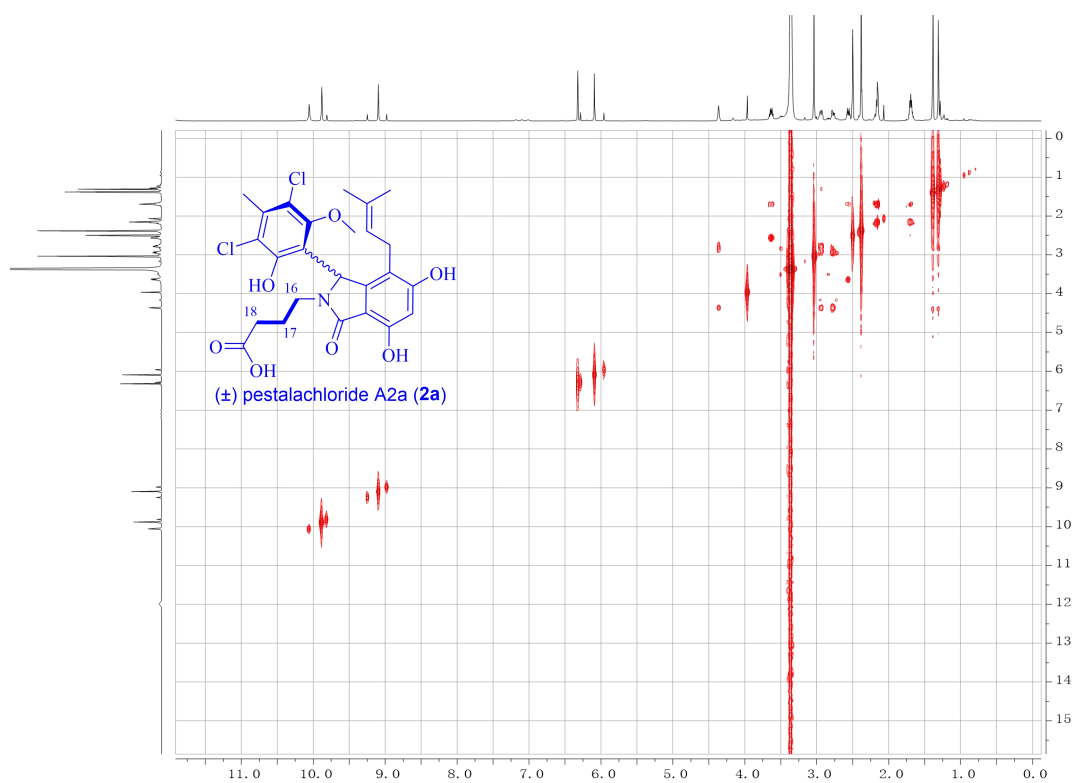


Figure S11. gCOSY for pestalachloride A2a (2a) in DMSO- $d_6$

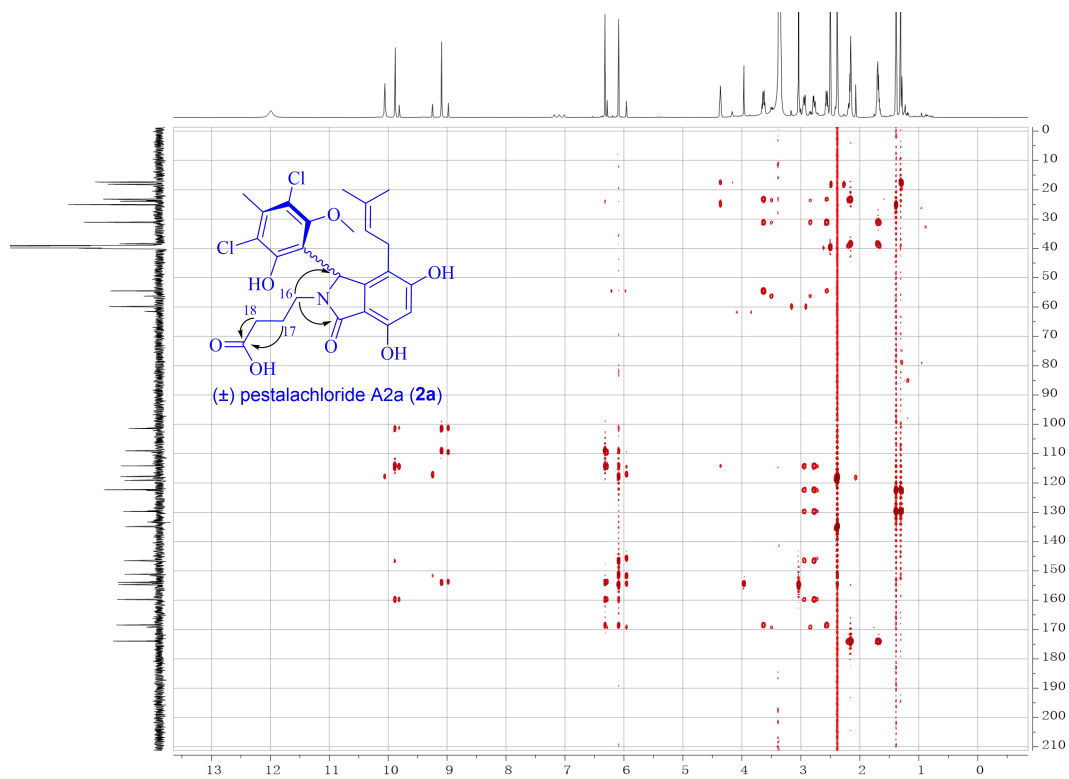
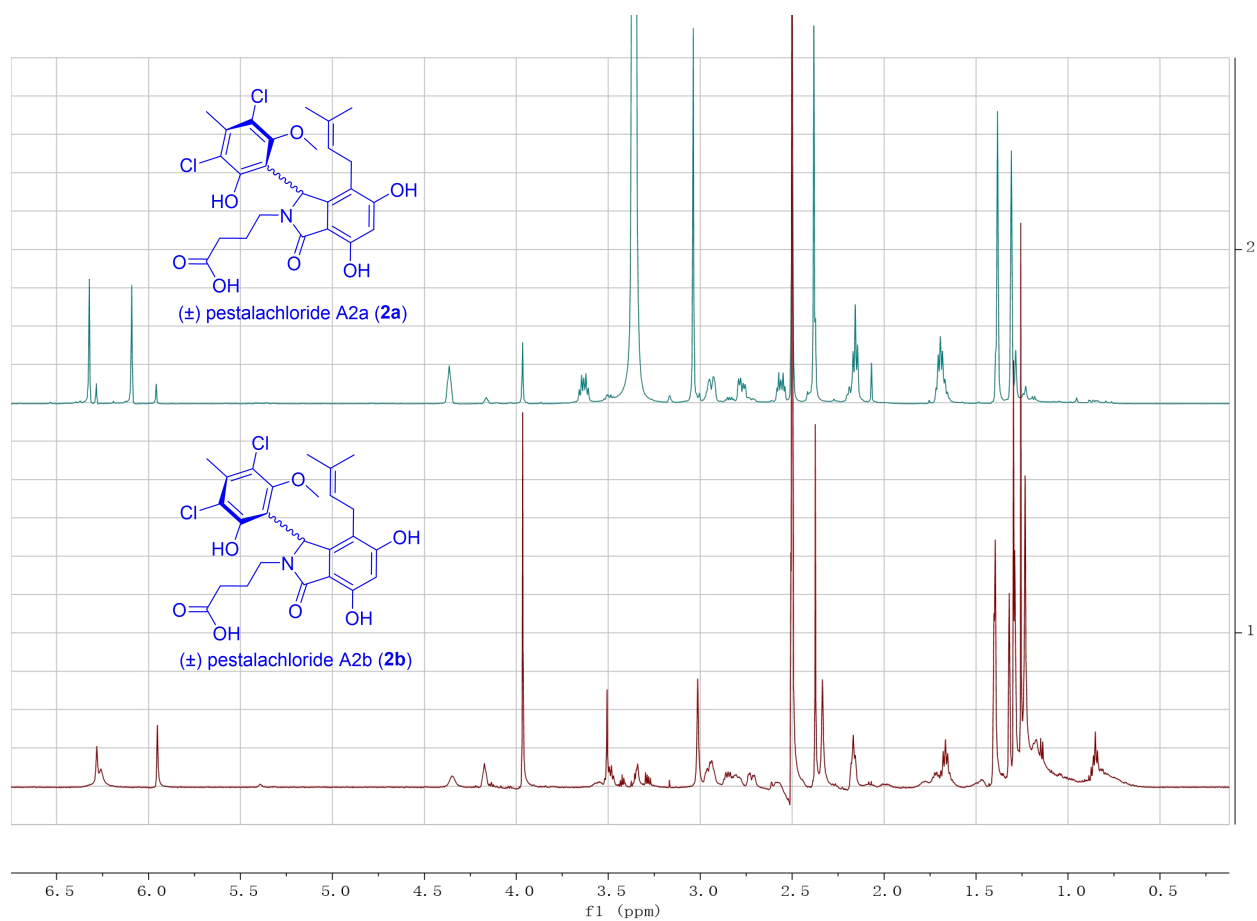
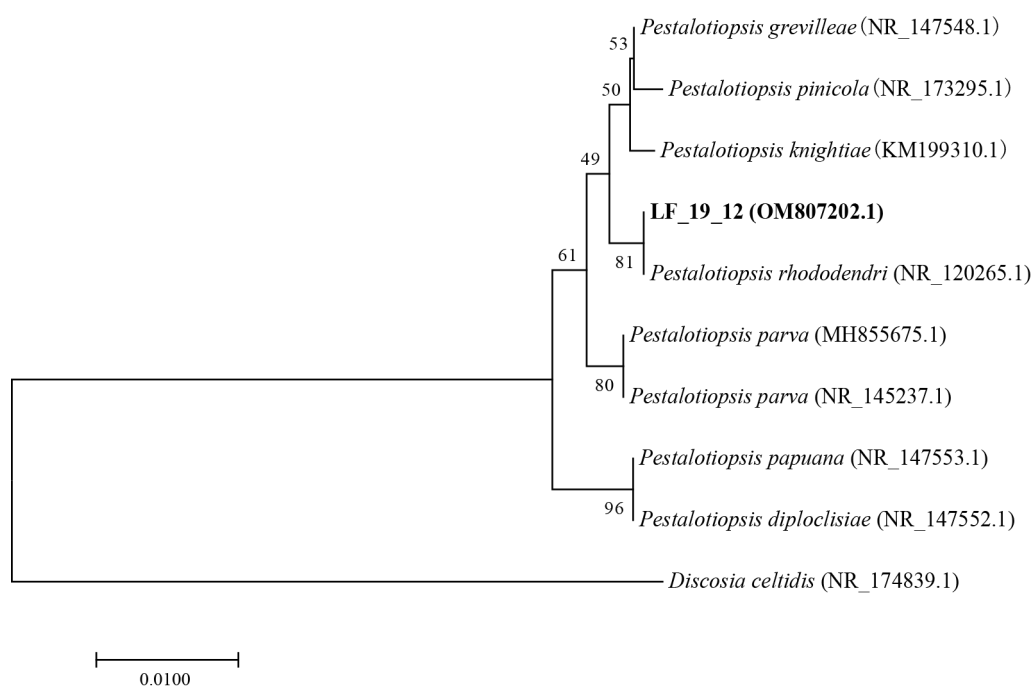


Figure S12. HMBC for pestalachloride A2a (2a) in DMSO- $d_6$



**Figure S13.**  $^1\text{H}$  NMR spectrum of pestalachloride A2b (**2b**) by comparison with that of pestalachloride A2a (**2a**) in  $\text{DMSO}-d_6$  (600 MHz)



**Figure S14.** Phylogenetic NJ tree based on ITS squences from LF-19-12 and related type strains . The ITS sequence of *Discosia celtidis* was used as an outgroup. The GenBank accessions are shown in parentheses.