# Nidulaxanthone A, a Xanthone Dimer with Heptacyclic 6/6/6/6/6/6/6 Ring System from *Aspergillus* sp-F029

Fuqian Wang,[a,‡] Jie Jiang,[a,‡] Song Hu,[a,‡] Xincai Hao,[d,] You-sheng Cai,[c] Ying Ye,[b] Haoran Ma,[a] Weiguang Sun,[b] Lu Cheng,[a] Chuanqi Huang,[a] Hucheng Zhu,[b] Hong Zhang,[a] Geng Zhang,[a,*] Yonghui Zhang*[,b]

[a.] *Department of Pharmacy, Wuhan No.1 Hospital, Wuhan 430022, Hubei, People's Republic of China*

[b.] *Hubei Key Laboratory of Natural Medicinal Chemistry and Resource Evaluation, School of Pharmacy, Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430030, China.*

[c.] *Institute of TCM and Natural Products, School of Pharmaceutical Sciences, Wuhan University, 185 Donghu Road, Wuhan 430071, People's Republic of China*

[d.] *College of Pharmacy Hubei University of Medicine, Shiyan 442000, China*

*Corresponding author Tel.: (86) 27-83692892
E-mail: zhangyh@mails.tjmu.edu.cn; zhanggen888@126.com

# Contents of Supporting Information

**Table S1. $^{1}H$ (400 MHz), $^{13}C$ (100 MHz) and 2D NMR data (COSY, NOESY, HMBC) for compound 1 in $CDCl_3$, ($\delta$ in ppm, $J$ in Hz)**

| no | $\delta_H$[a] | $\delta_C$ | COSY | HMBC | NOESY |
|---|---|---|---|---|---|
| 1 | | 163.0 | | | |
| 1-OH | 12.05 s | | | 1 | |
| 2 | 6.38 s | 111.2 | | 1, 3, 6, 17 | |
| 3 | | 151.1 | | | |
| 4 | 6.31 s | 108.0 | | 2, 5, 6, 7, 17 | |
| 5 | | 158.4 | | | |
| 6 | | 104.8 | | | |
| 7 | | 181.3 | | | |
| 8 | | 129.3 | | | |
| 9 | | 82.8 | | | |
| 11 | 7.30 d (1.6) | 140.7 | 12 | 7, 8, 9, 13, 8’, 9’ | 11’ |
| 12 | 3.03 dd (10.0,1.6) | 39.4 | 11, 13 | 8, 9, 11, 13, 8’, 11’ | 13 |
| 13 | 3.41 m | 33.9 | 12, 13’, 14 | 11, 13’, 14’ | 12, 14 |
| 14 | 4.51 d (5.6) | 70.9 | 13 | 7, 8, 9, 12, 15 | 13 |
| 15 | | 168.5 | | | |
| 16 | 3.66 s | 53.4 | | 15 | |
| 17 | 2.30 s | 22.5 | | 2, 3, 4 | |
| 18 | | | | | |
| 1’ | | 162.5 | | | |
| 1’-OH | 11.60 s | | | 1’ | |
| 2’ | 6.50 s | 112.6 | | 1’, 4’, 6’, 17’ | |
| 3’ | | 150.6 | | | |
| 4’ | 6.43 s | 108.6 | | 2’, 5’, 6’, 7’ 17’ | |
| 5’ | | 156.8 | | | |
| 6’ | | 104.6 | | | |
| 7’ | | 196.4 | | | |
| 8’ | | 52.0 | | | |
| 9’ | | 84.2 | | | |
| 11’ | 6.63 d (8.4) | 125.9 | 12’ | 7’, 8’, 9’, 13’ | 11 |
| 12’ | 6.32 m | 133.0 | 11’, 13’ | 8’, 13’ | 14’ |
| 13’ | 3.26 m | 40.7 | 12’, 13, 14’ | 9’ | |
| 14’ | 3.99 d (3.2) | 70.4 | 13’ | 12’, 13, 15’ | 12’ |
| 15’ | | 170.3 | | | |
| 16’ | 3.64 s | 53.3 | | 15’ | |
| 17’ | 2.33 s | 22.6 | | 2’, 3’, 4’ | |

**Table S2. $^{1}$H (400 MHz), $^{13}$C (100 MHz) and 2D NMR data (COSY, NOESY, HMBC) for compound 2 in $CDCl_3$, ($\delta$ in ppm, $J$ in Hz)**

| no | $\delta_H$ [a] | $\delta_C$ | COSY | HMBC |
|---|---|---|---|---|
| 1 | | 163.0 | | |
| 1-OH | 12.08 s | | | 1, 2, 3, 6, 7 |
| 2 | 6.39 s | 111.8 | | 1, 4, 6, 17 |
| 3 | | 150.4 | | |
| 4 | 6.31 s | 108.7 | | 2, 5, 6, 7, 17 |
| 5 | | 157.7 | | |
| 6 | | 105.8 | | |
| 7 | | 185.0 | | |
| 8 | | 128.5 | | |
| 9 | | 81.5 | | |
| 11 | 7.20 t (3.2) | 138.5 | 12 | 7, 9, 12, 13 |
| 12 | 2.79 m | 28.4 | 11, 13 | 8, 11 |
| | 2.52 ddd (20.4,4.4,1.6) | | 11, 13 | 8, 11, 13, 14 |
| 13 | 3.77 m | 75.7 | 12, 14 | 9, 11, 14, 18 |
| 14 | 4.70 d (4.4) | 68.6 | 13 | 7, 8, 9, 12, 13, 14, 15 |
| 14-OH | 2.77 s | | | 7, 8, 9, 11, 13, 14, 15 |
| 15 | | 169.6 | | |
| 16 | 3.61 s | 53.3 | | 15 |
| 17 | 2.26 s | 22.6 | | 2, 3, 4 |
| 18 | 3.31 s | 57.9 | | 13 |

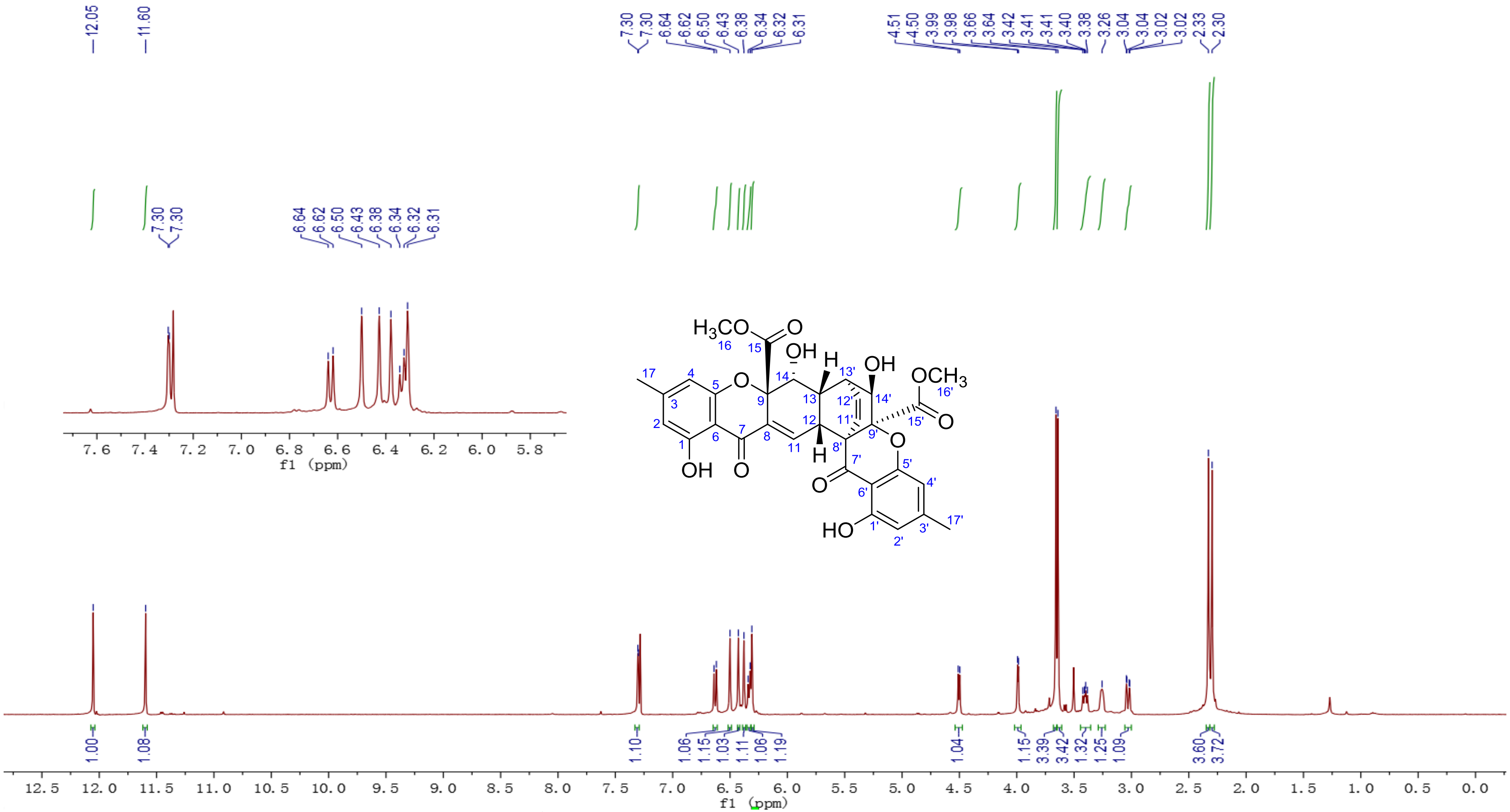

**Figure S1**. $^{1}$H NMR spectrum of nidulaxanthone A (**1**) in $CDCl_3$.

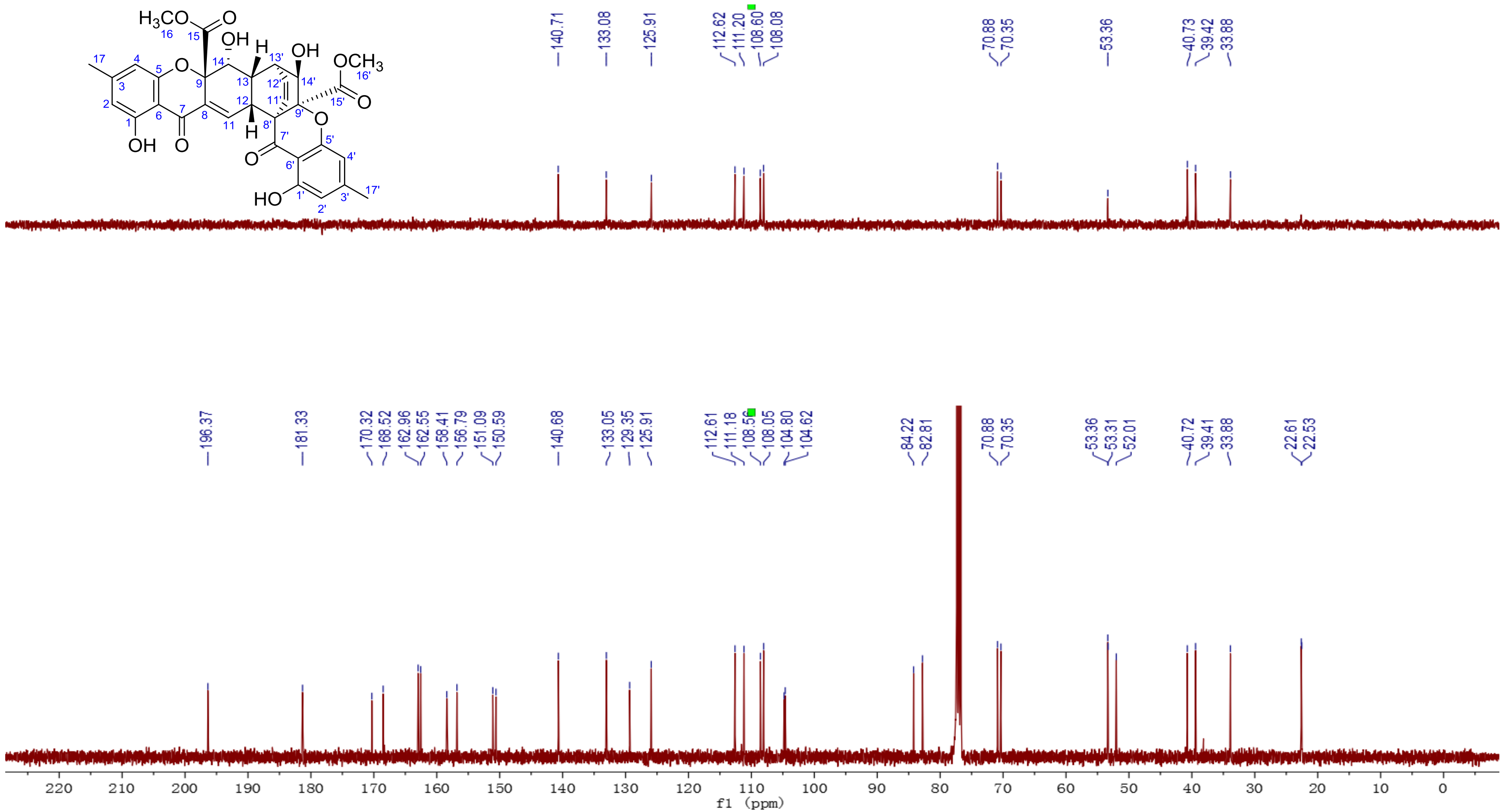


**Figure S2**. $^{13}$C NMR and DEPT spectra of nidulaxanthone A (**1**) in $CDCl_3$.

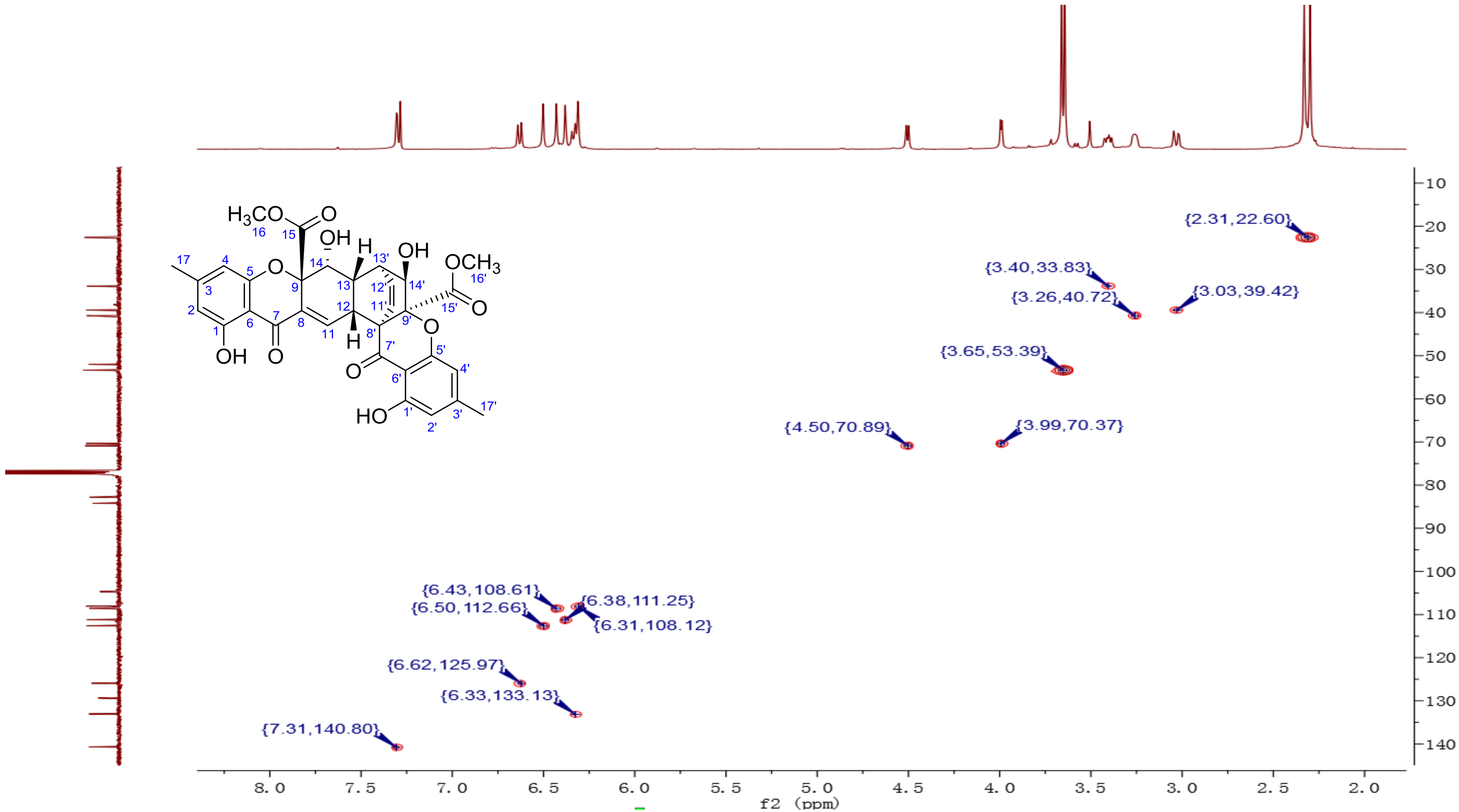


**Figure S3**. HSQC spectrum of nidulaxanthone A (**1**) in $CDCl_3$

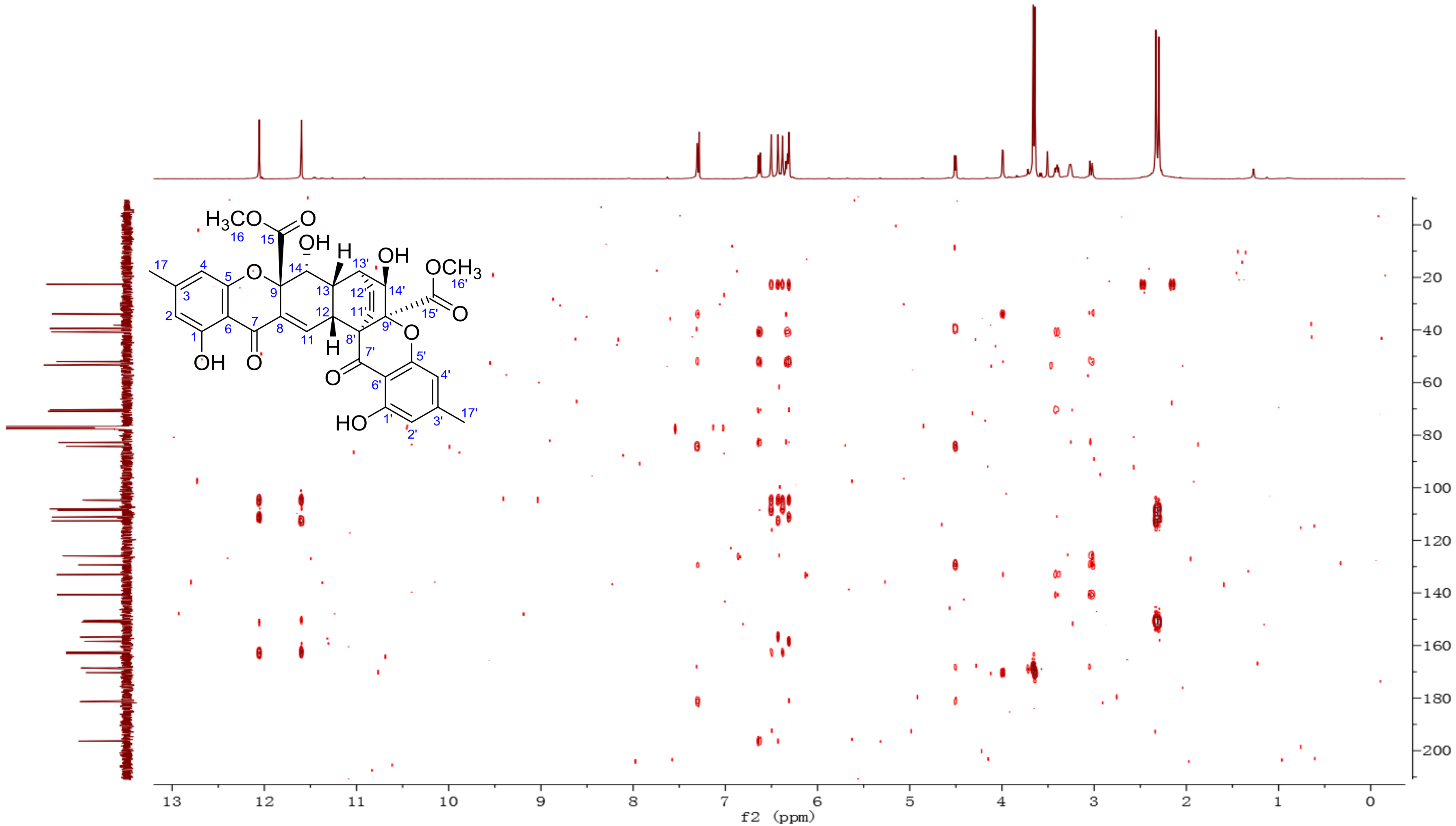


**Figure S4**. HMBC spectrum of nidulaxanthone A (**1**) in $CDCl_3$.

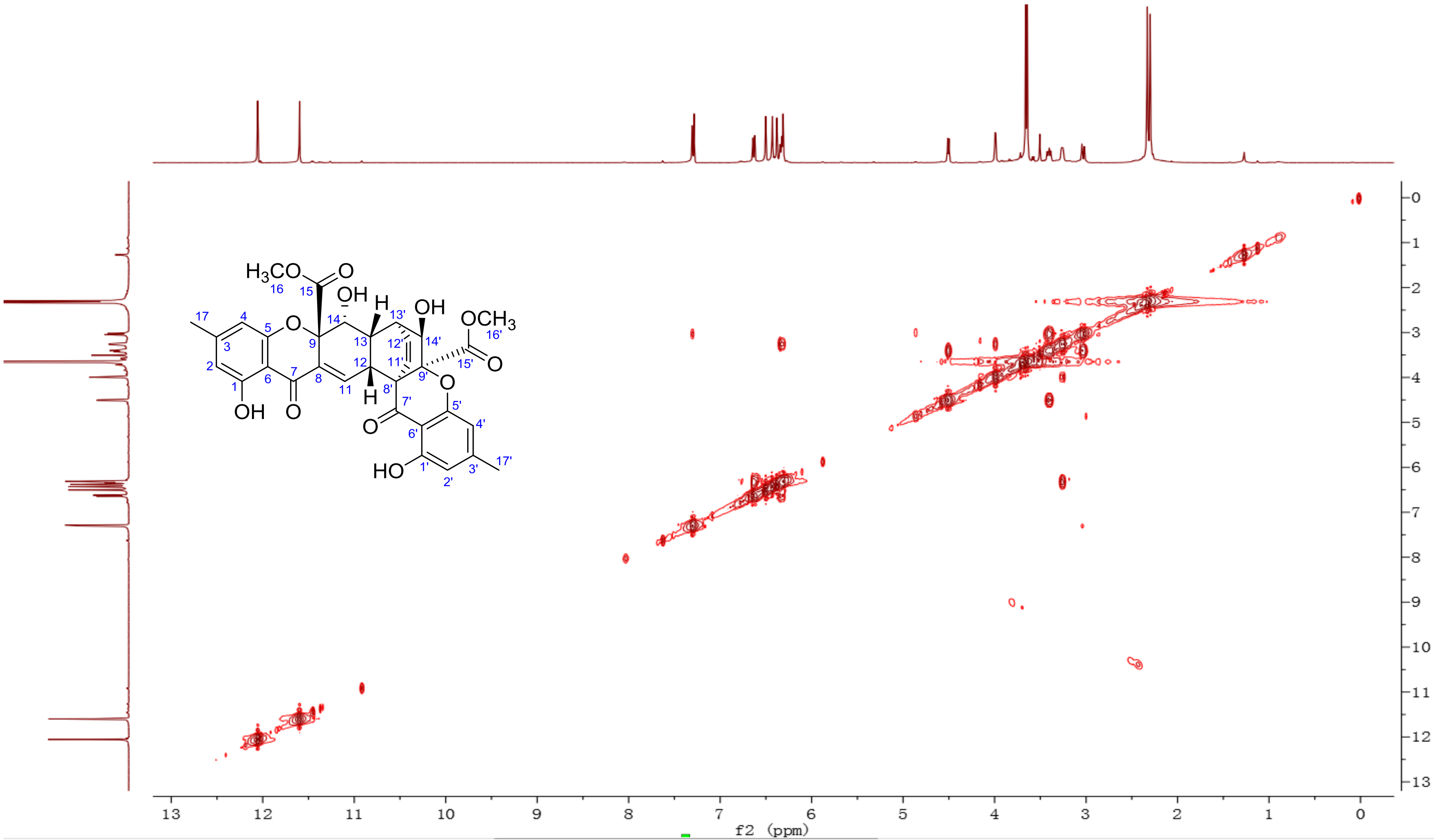

**Figure S5**. $^1H$–$^1H$ COSY spectrum of nidulaxanthone A (**1**) in $CDCl_3$.

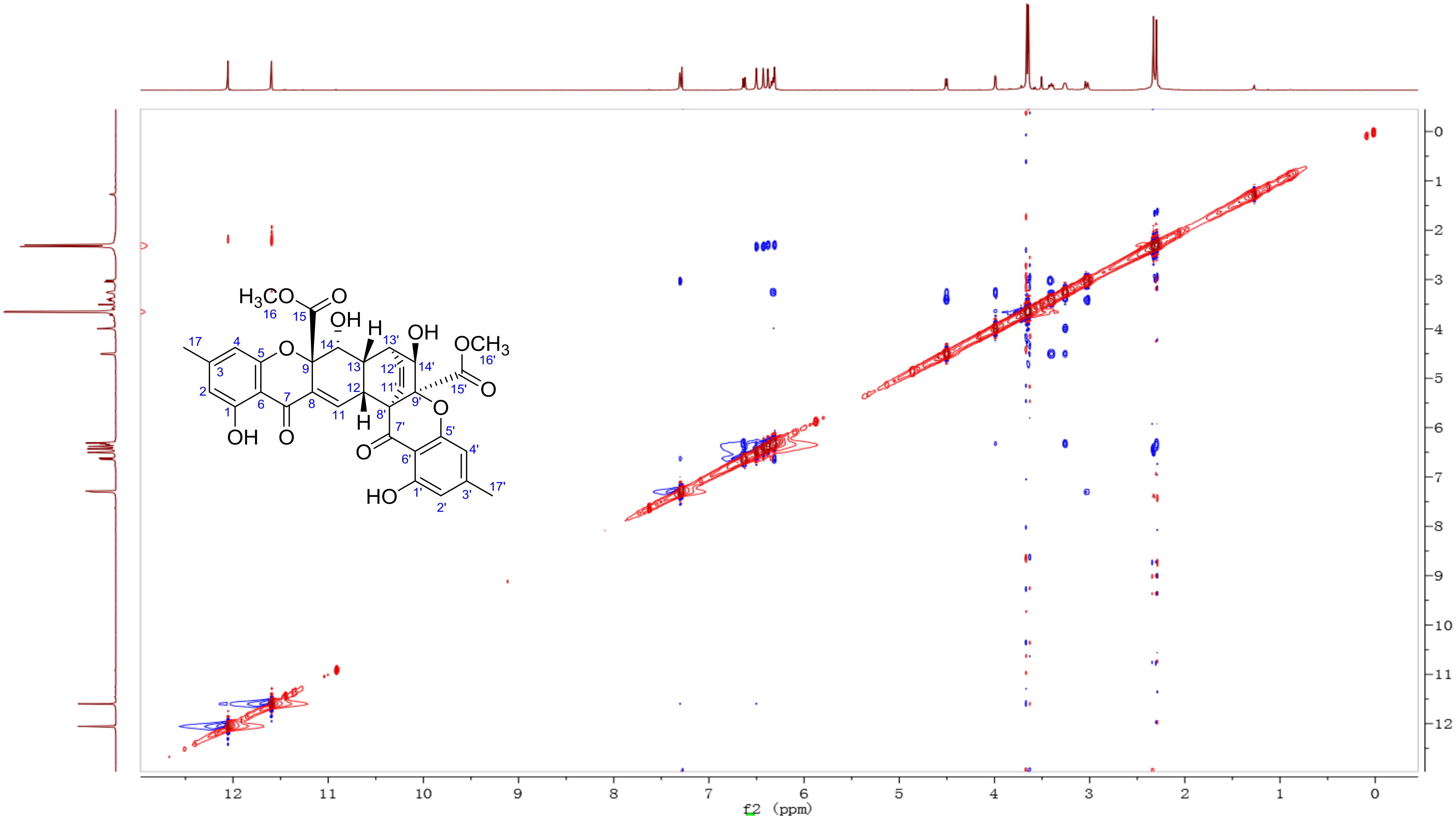


**Figure S6**. NOESY spectrum of spectrum of nidulaxanthone A (**1**) in $CDCl_3$.

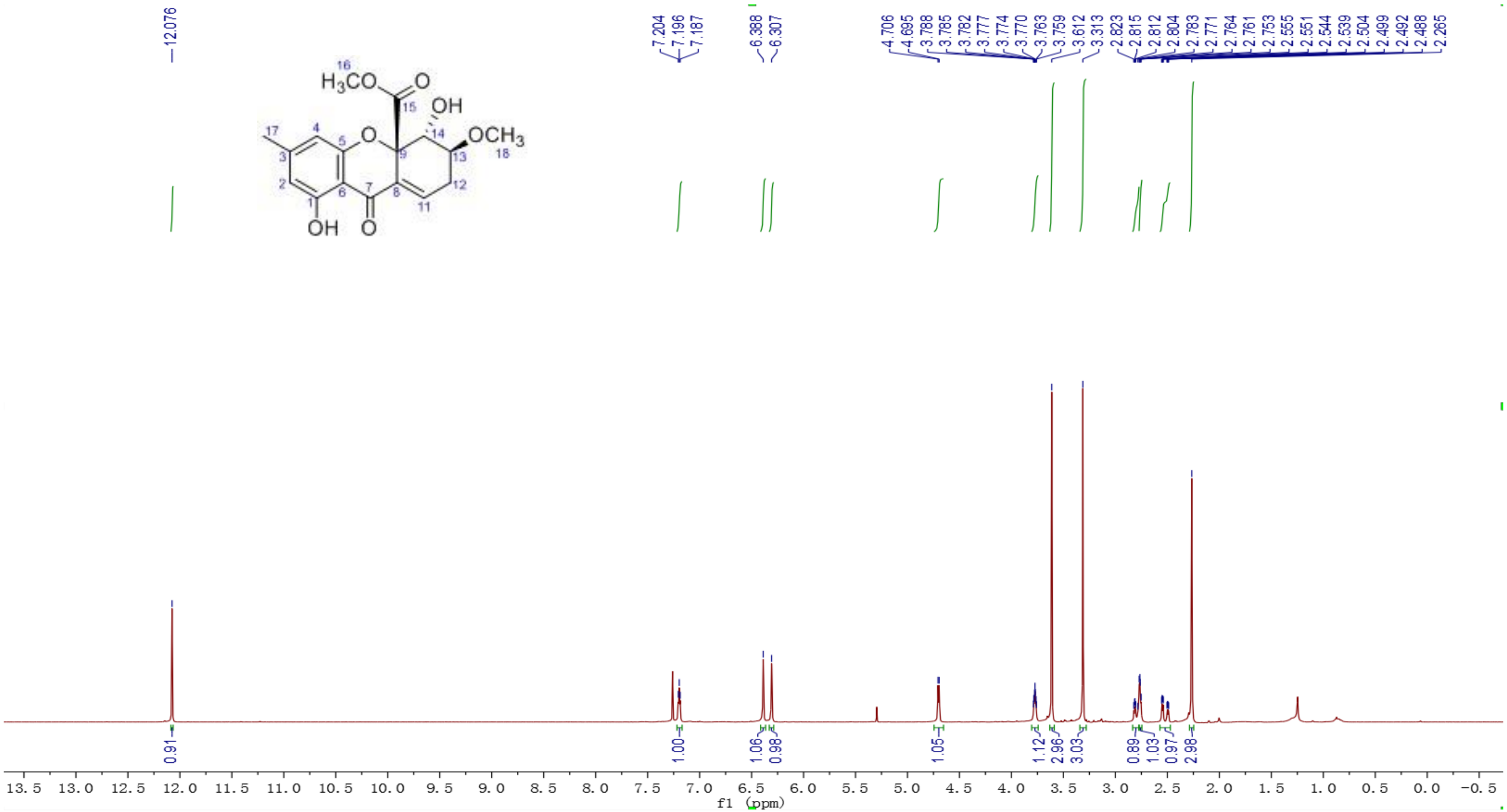

**Figure S7**. [1]H NMR spectrum of nidulalin D (**2**) in $CDCl_3$.

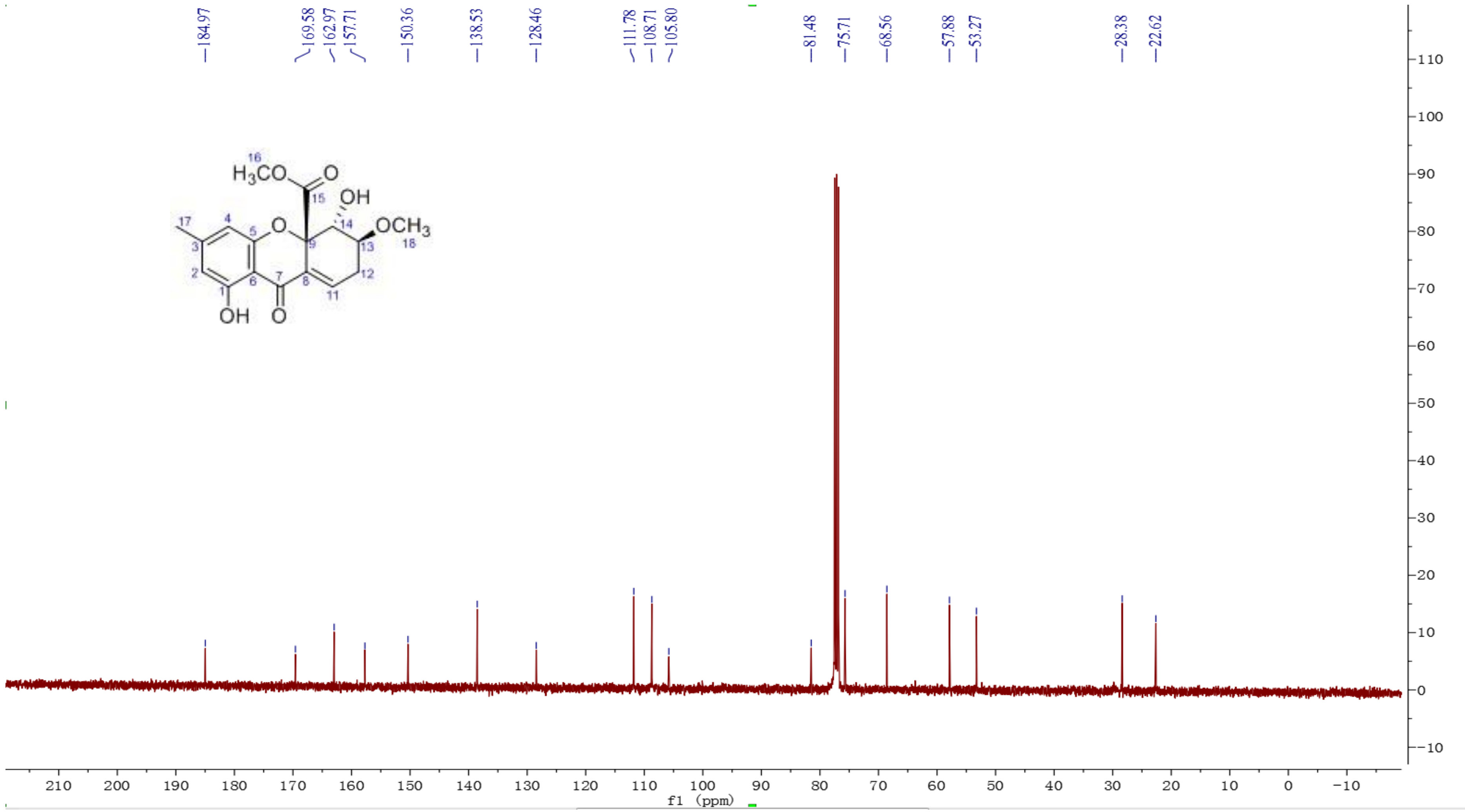


**Figure S8**. $^{13}C$ NMR spectrum of nidulalin D (**2**) in $CDCl_3$.

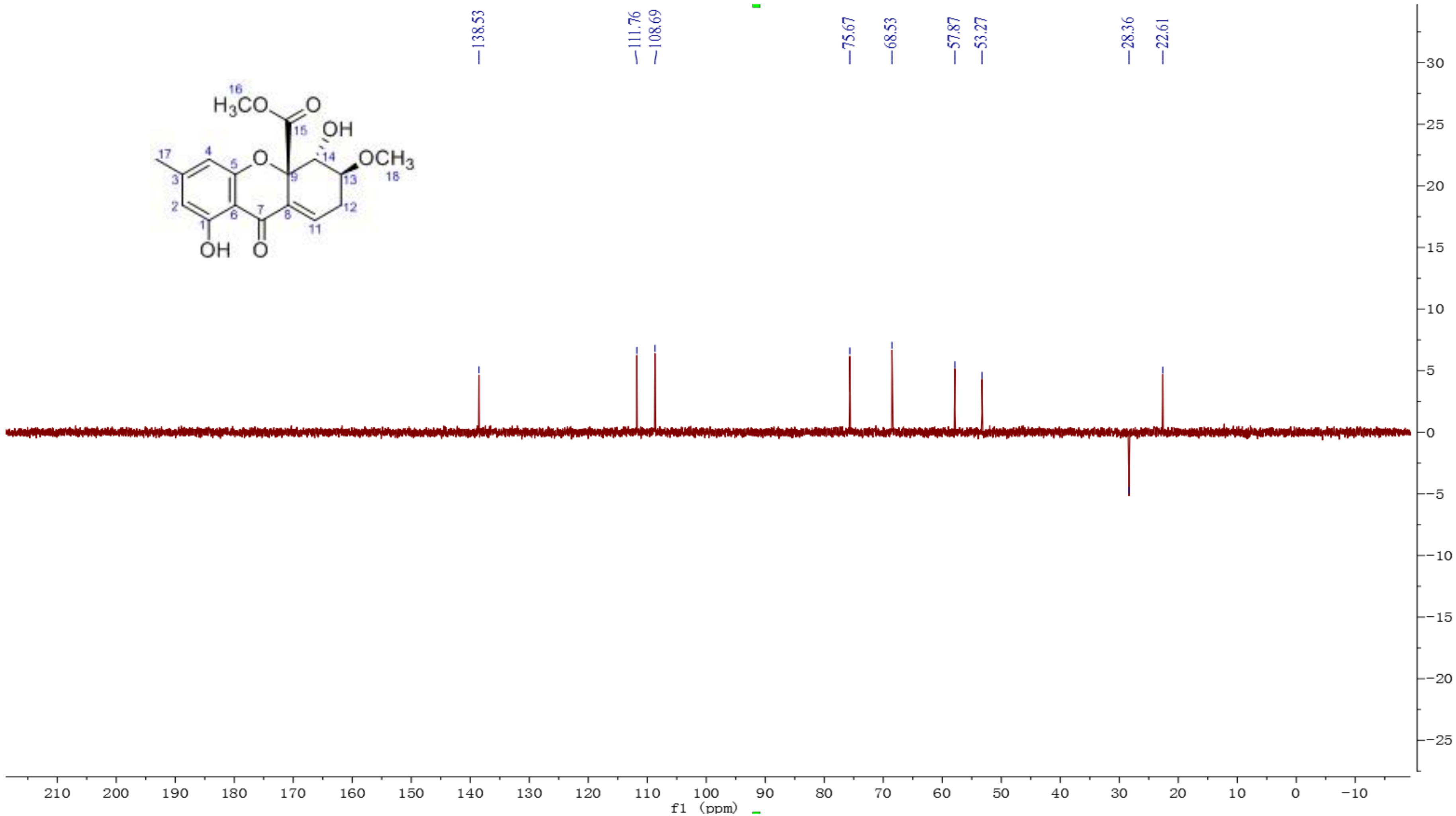


**Figure S9**. DEPT NMR spectrum of nidulalin D (**2**) in $CDCl_3$.

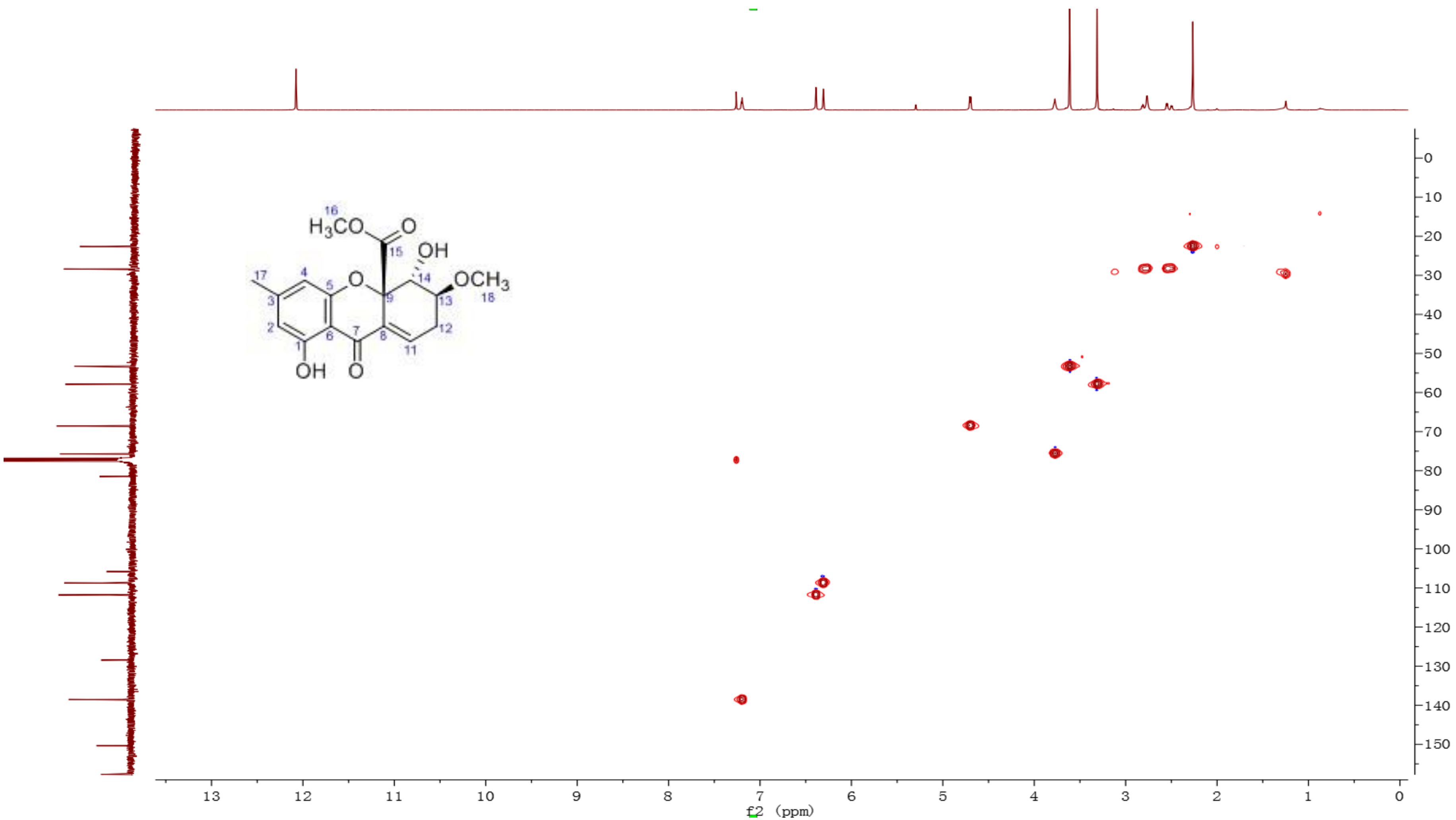


**Figure S10**. HSQC spectrum of nidulalin D (**2**) in $CDCl_3$.

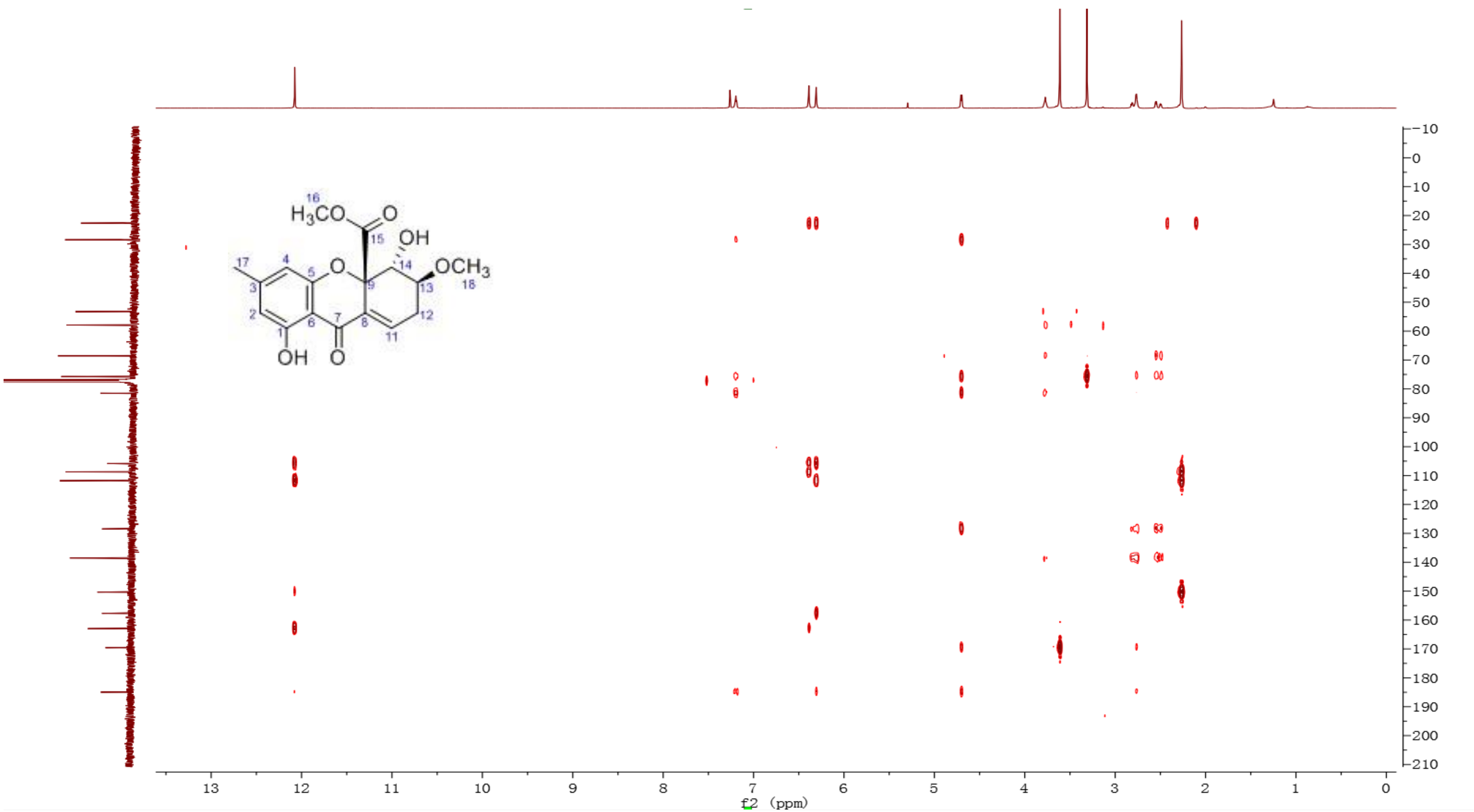


**Figure S11**. HMBC spectrum of nidulalin D (**2**) in $CDCl_3$.

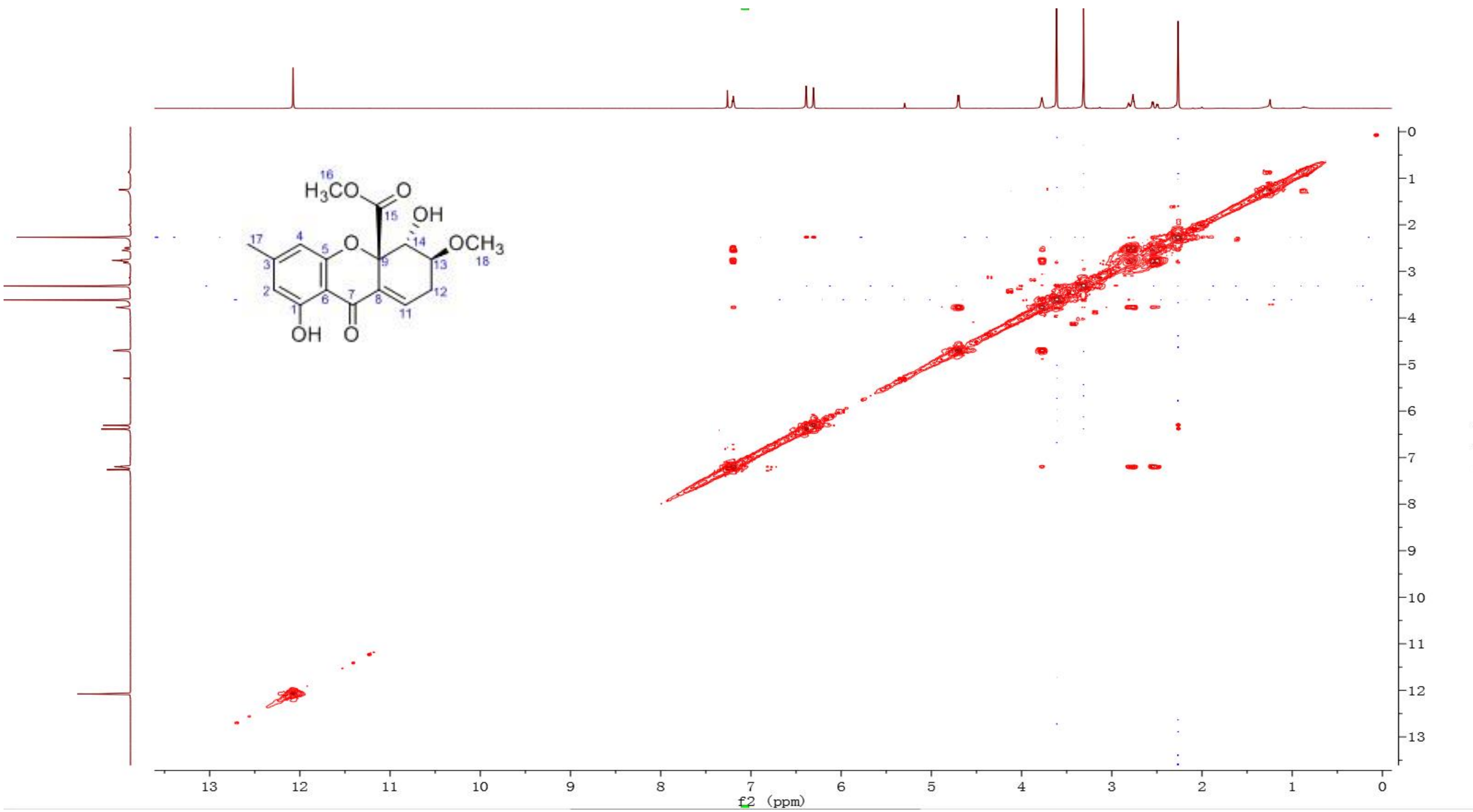


**Figure S12**. $^{1}H$–$^{1}H$ COSY spectrum of nidulalin D (**2**) in $CDCl_3$

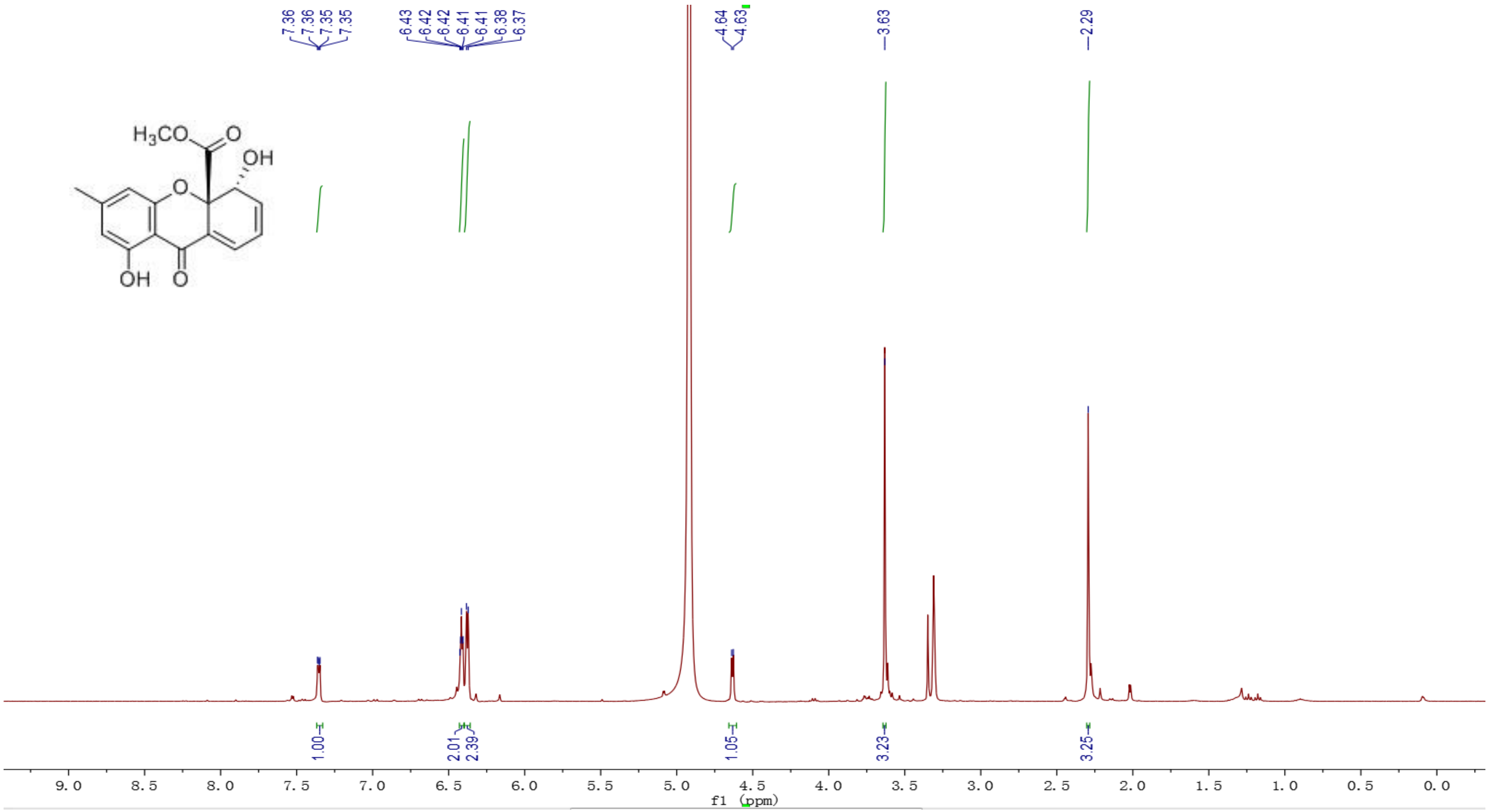


**Figure S13**. $^{1}$H NMR spectrum of nidulalin A (**3**) in $CD_3OD$.

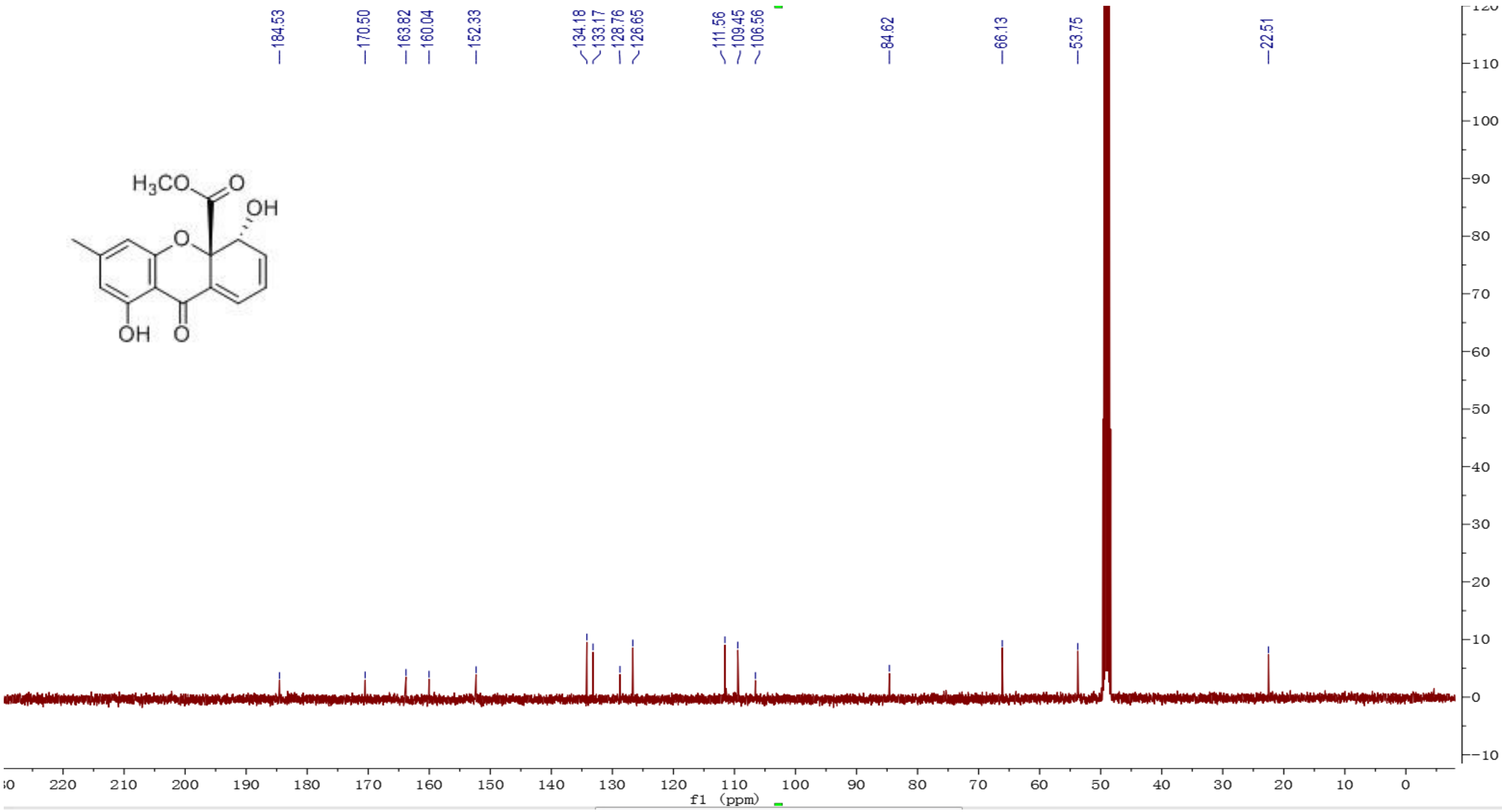


**Figure S14**. $^{13}$C NMR spectrum of nidulalin A (**3**) in $CD_3OD$.

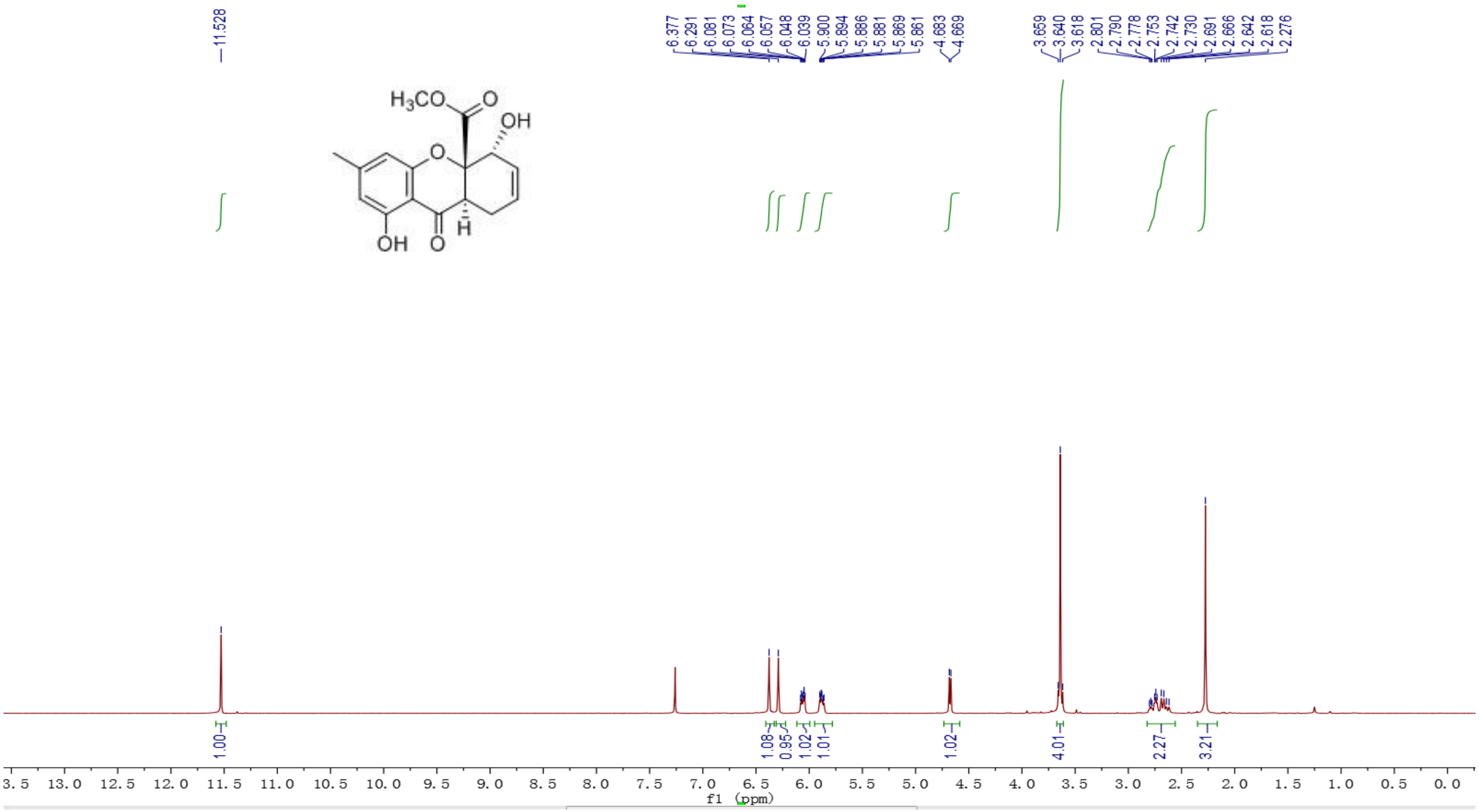

**Figure S15**. $^{1}$H NMR spectrum of (4*R*,4a*S*,9a*R*)-1,9a-dihydronidulalin A (**4**) in $CDCl_3$.

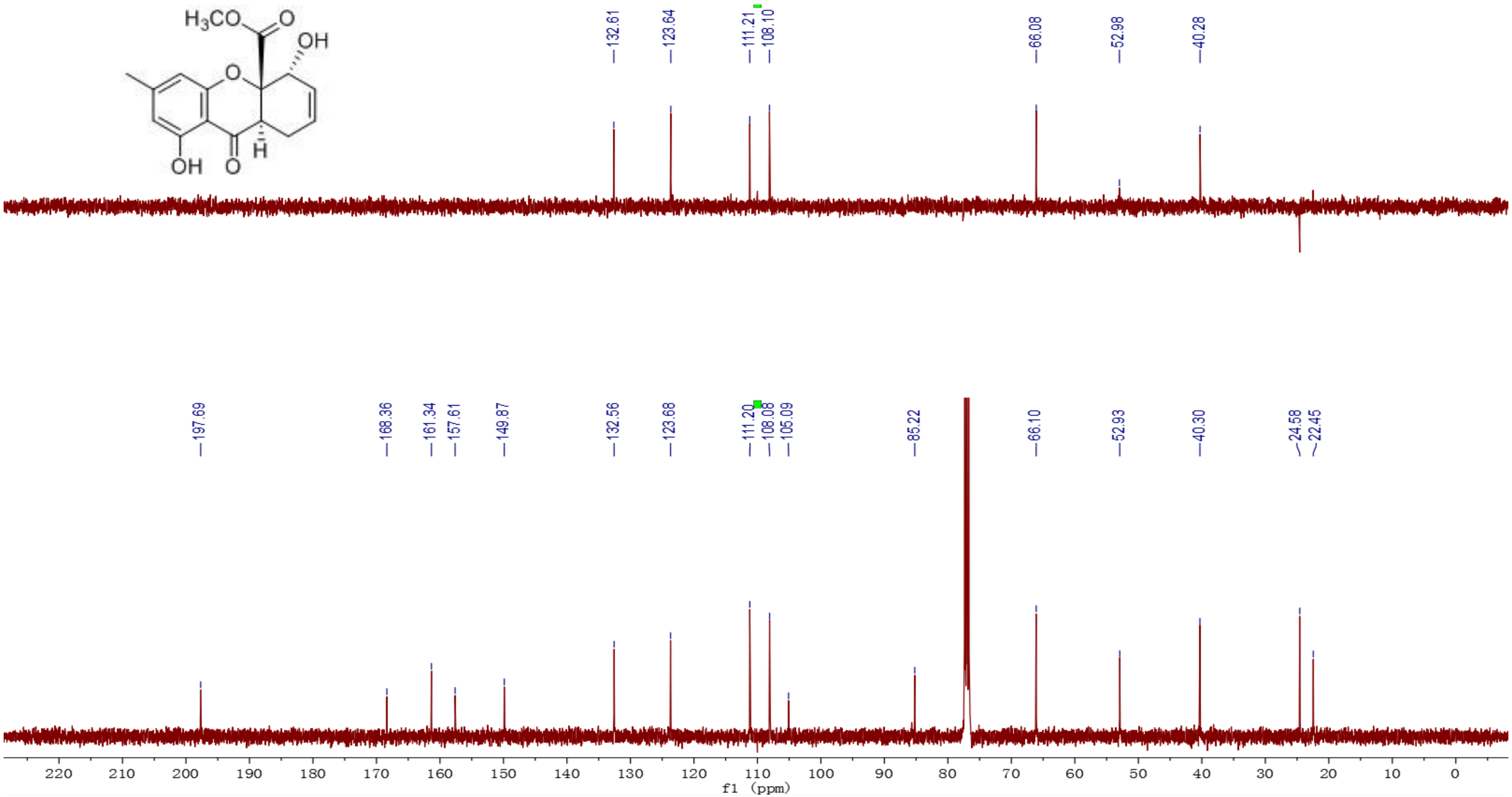


**Figure S16**. $^{13}$C NMR and DEPT spectra of (4*R*,4a*S*,9a*R*)-1,9a-dihydronidulalin A (**4**) in $CDCl_3$

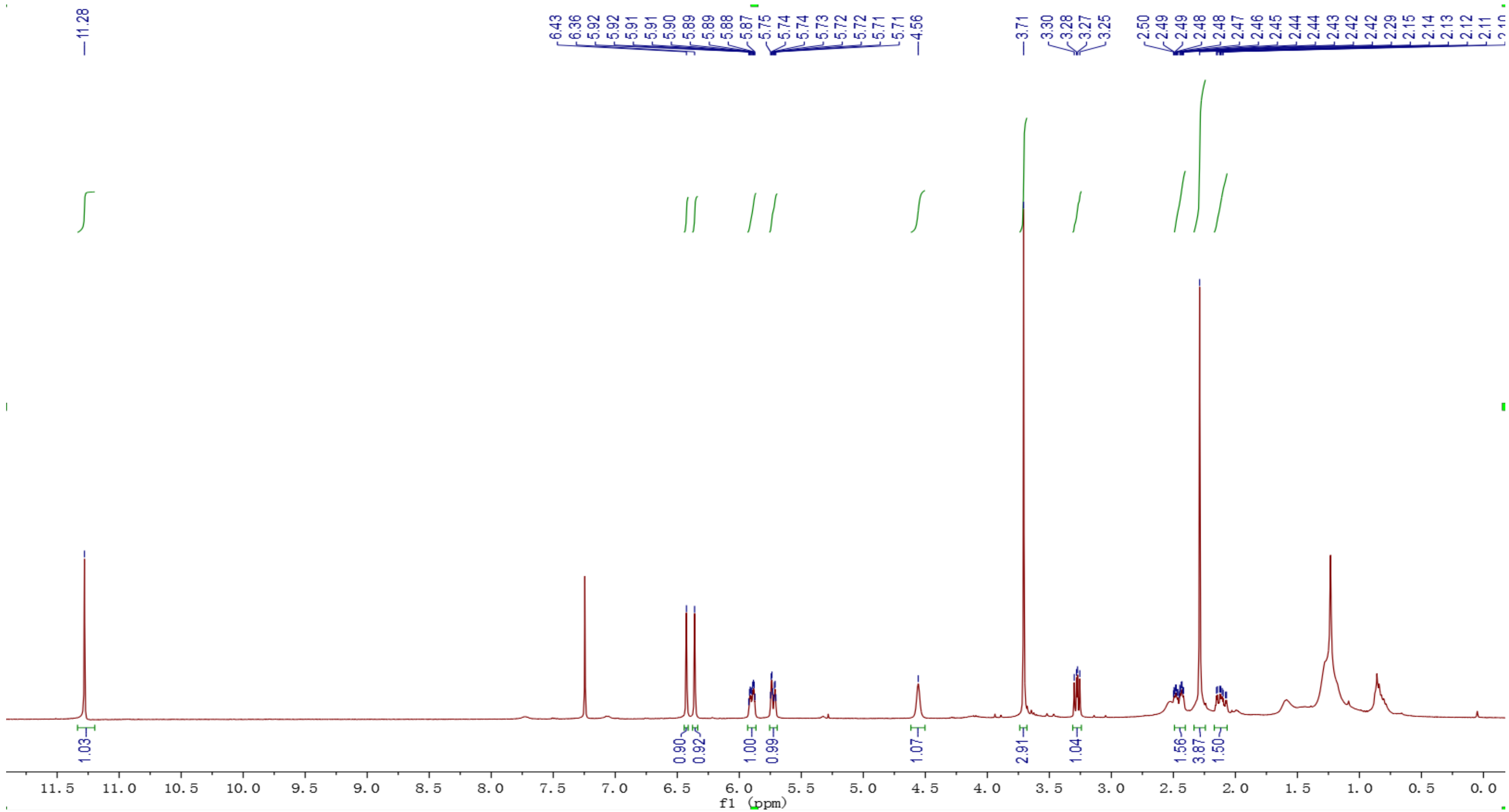


**Figure S17**. [1]H NMR spectrum of (4S,4aR,9aR)-4a-carbomethoxy-1,4,4a,9a-tetrahydro-4,8 dihydroxy-6-methylxanthone (**5**) in $CDCl_3$.

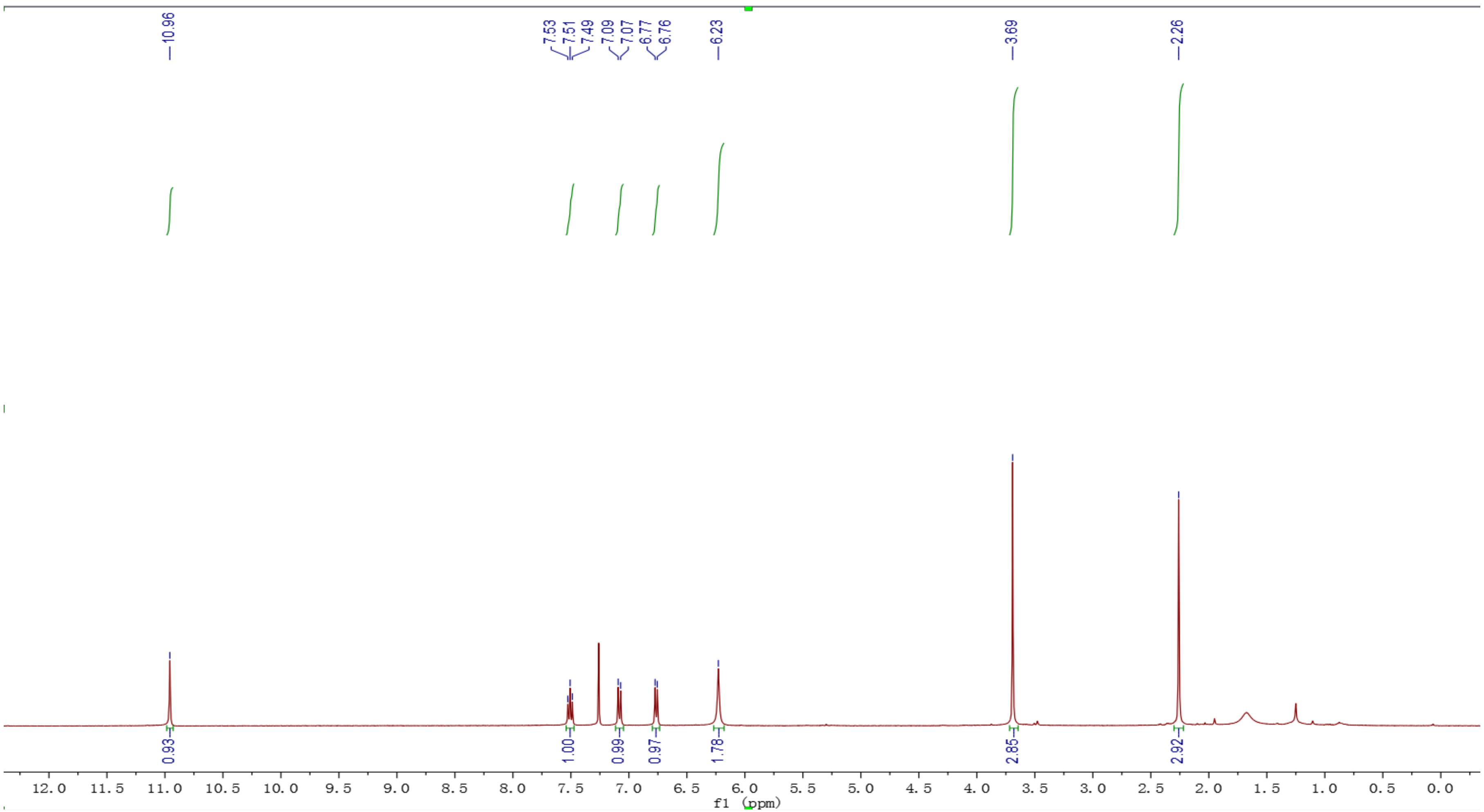


**Figure S18**. $^1H$ NMR spectrum of nidulalin B (**6**) in $CDCl_3$.

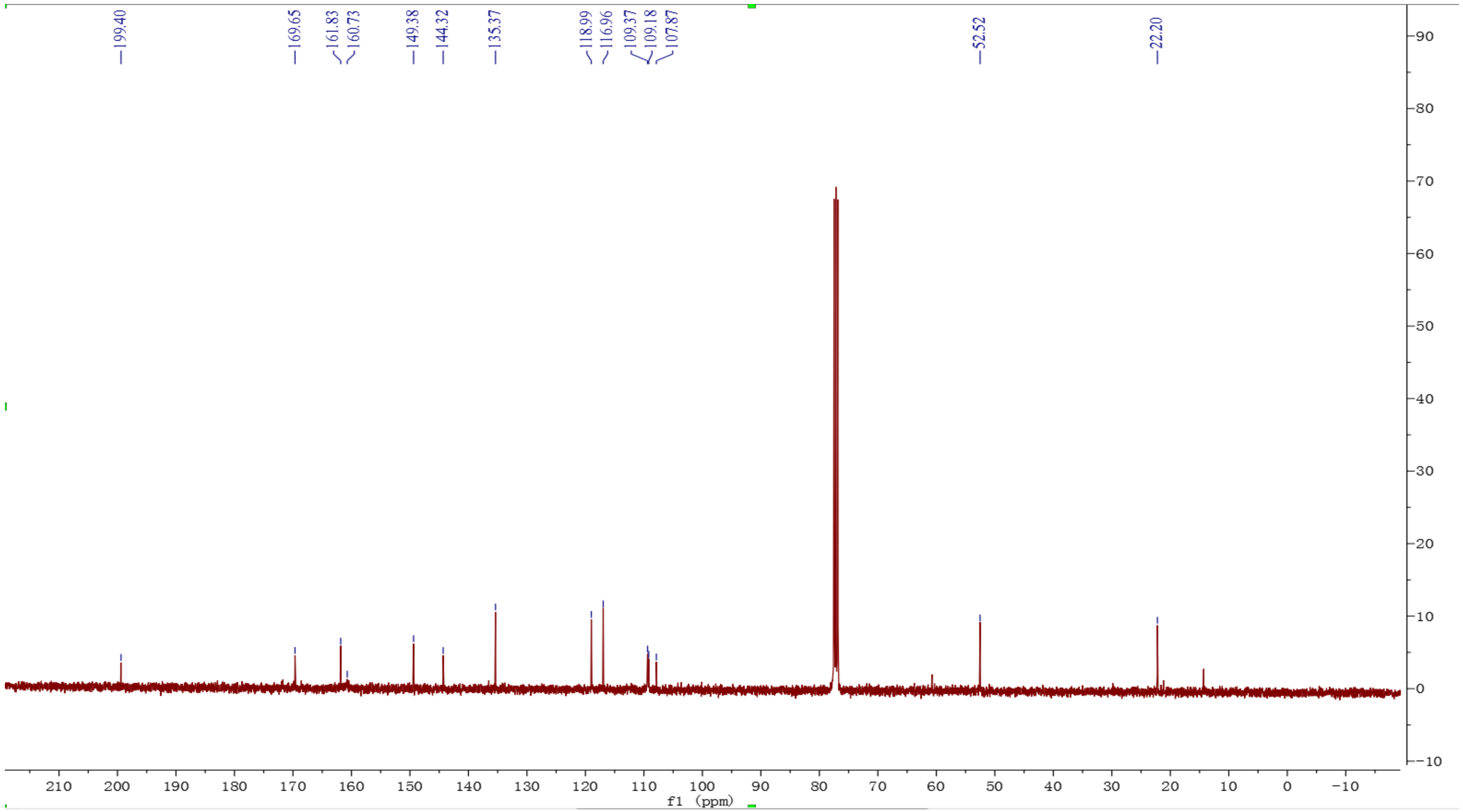


**Figure S19**. $^{13}C$ NMR spectrum of nidulalin B (**6**) in $CDCl_3$.

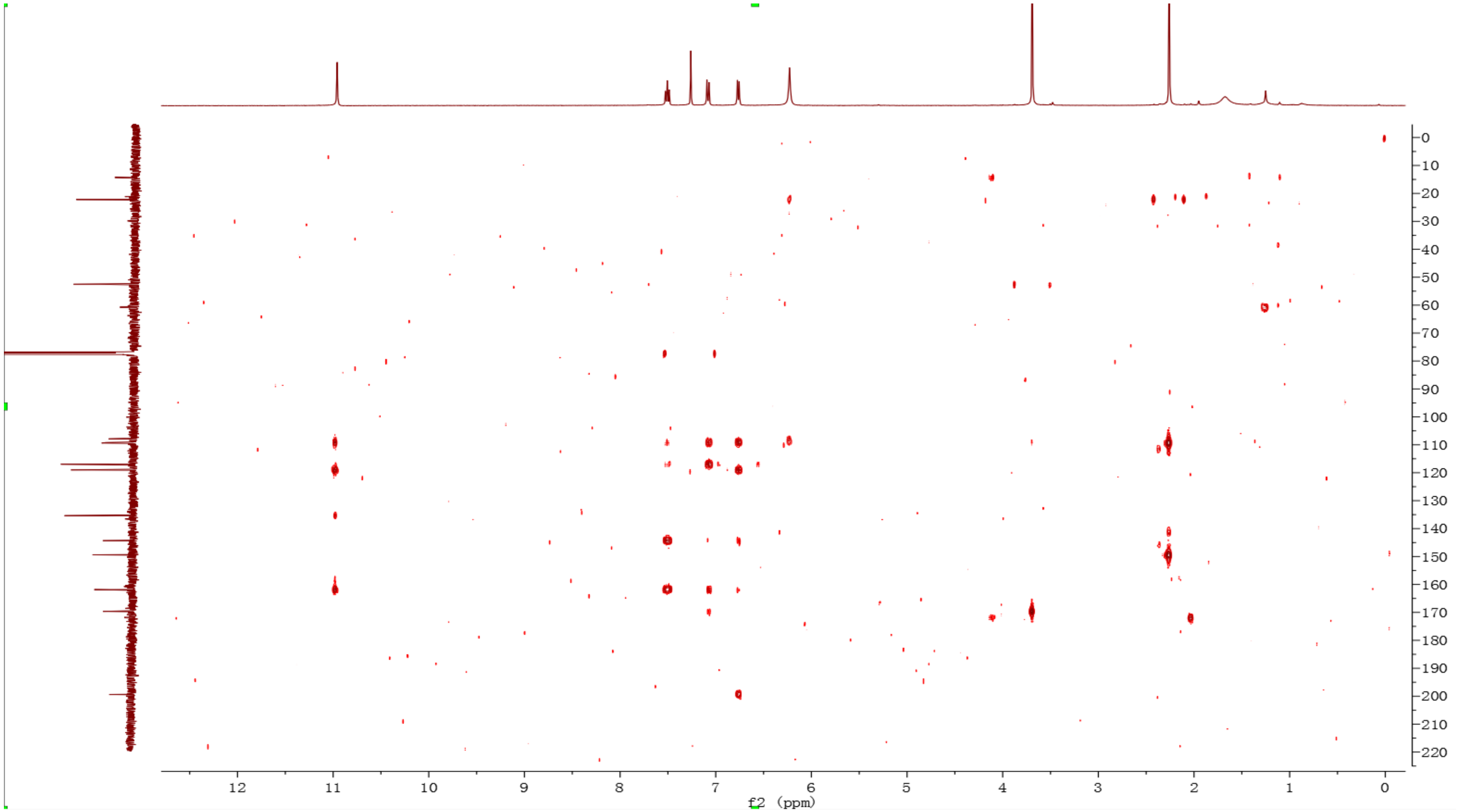


**Figure S20**. HMBC spectrum of nidulalin B (**6**) in $CDCl_3$..

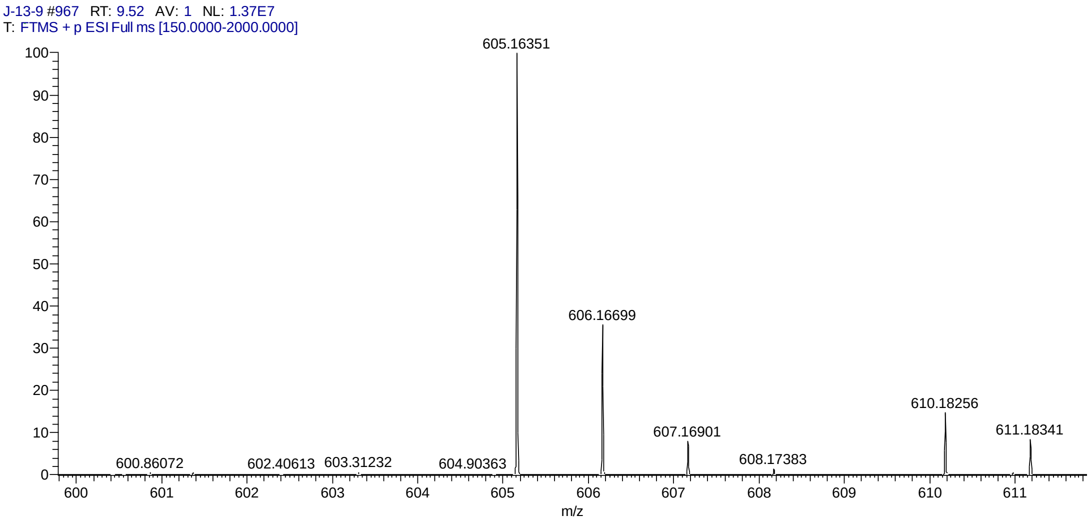


**Figure S21**. HRESIMS spectrum of nidulaxanthone A (**1**).

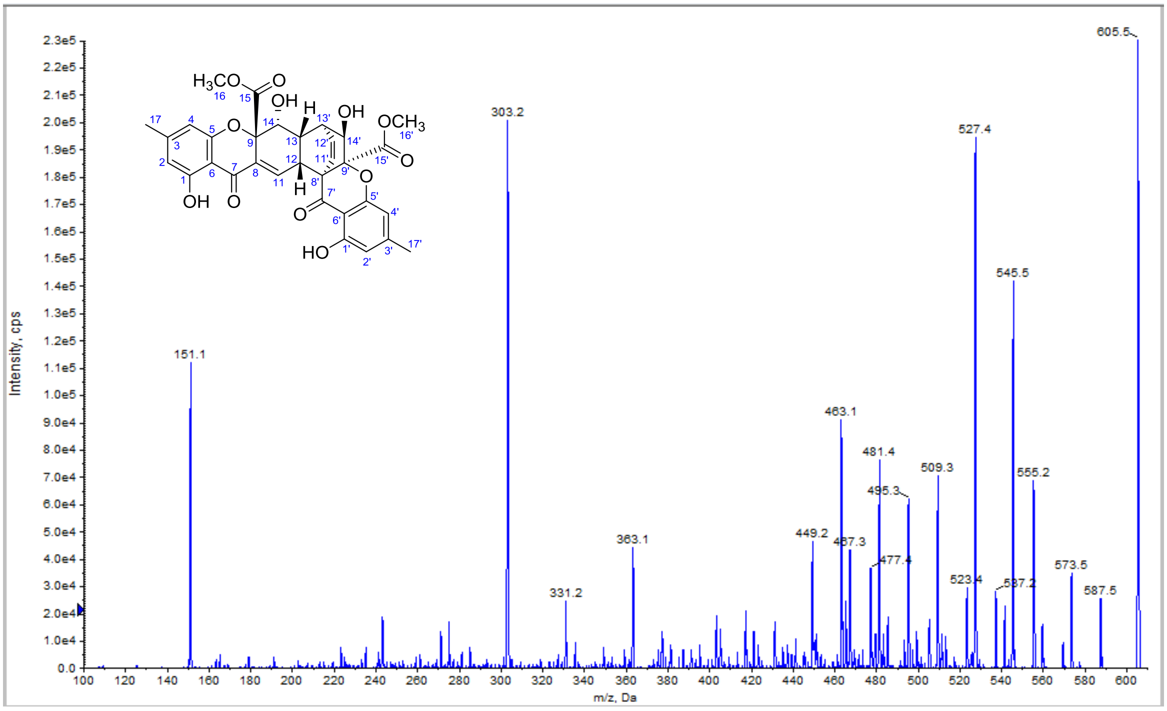


**Figure S22**. MS-MS spectrum of nidulaxanth one A (**1**). (de-hydroxy, de-methoxylation and de- acetylation fragments at m/z: 545, 573 and 587)

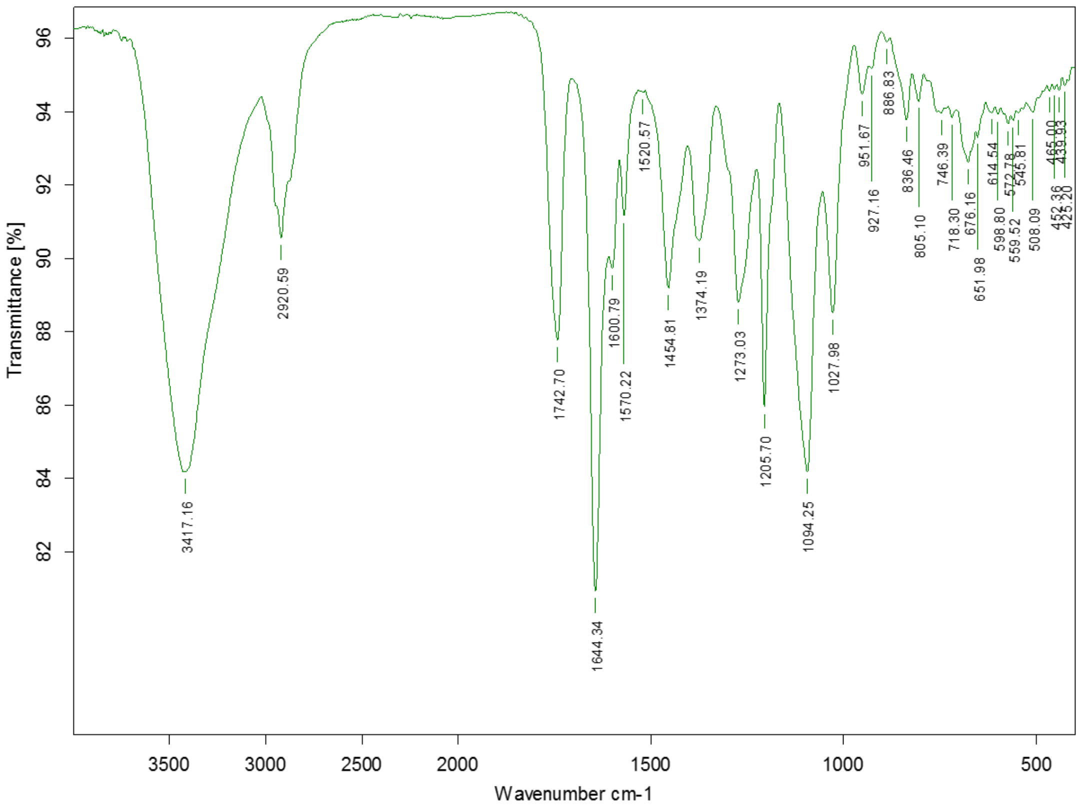


**Figure S23**. IR spectrum of nidulaxanthone A (**1**)

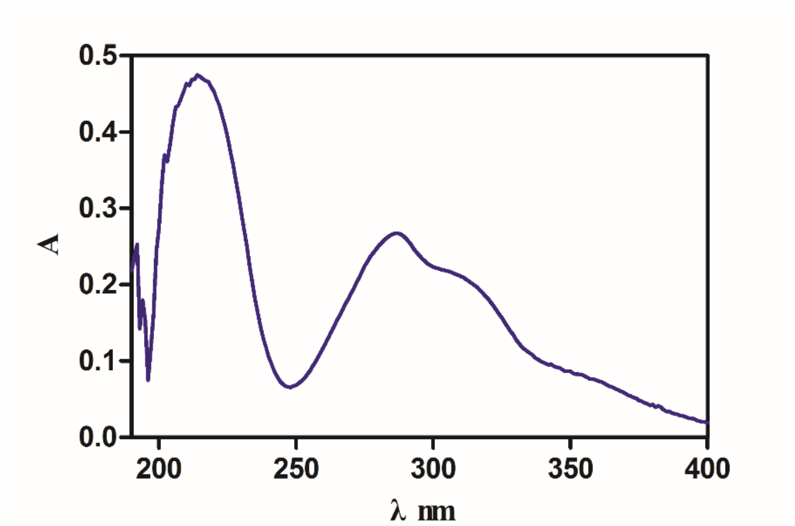


**Figure S24**. UV spectrum of nidulaxanthone A (**1**).

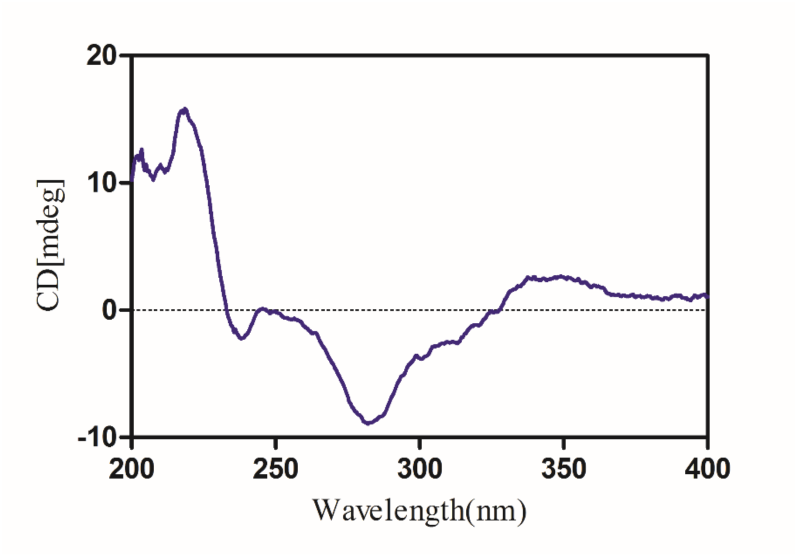


**Figure S25**. CD spectra of nidulaxanthone A (**1**)

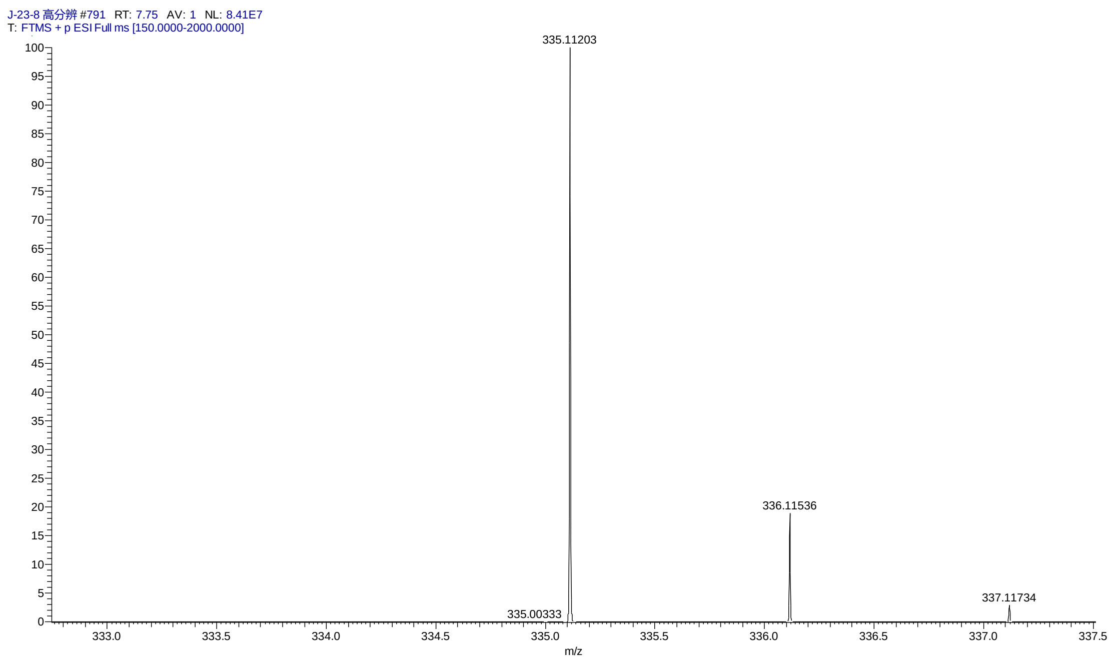


**Figure S26**. HRESIMS spectrum of nidulalin D (**2**).

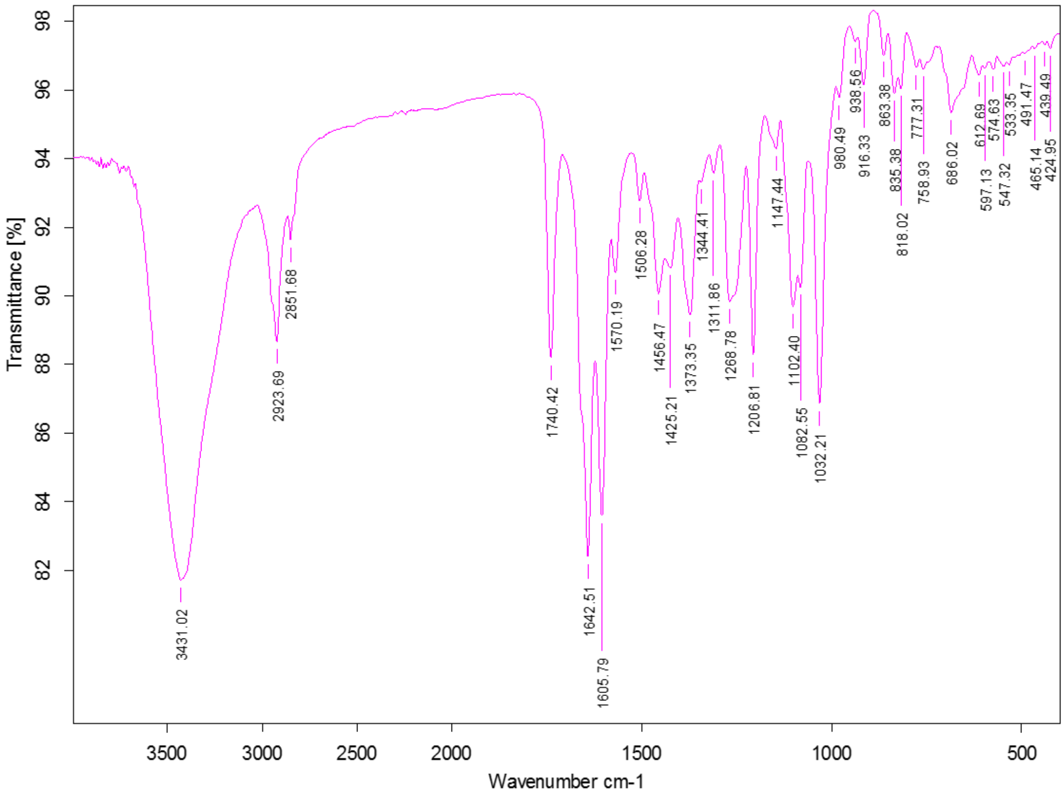


**Figure S27**. IR spectrum of nidulalin D (**2**).

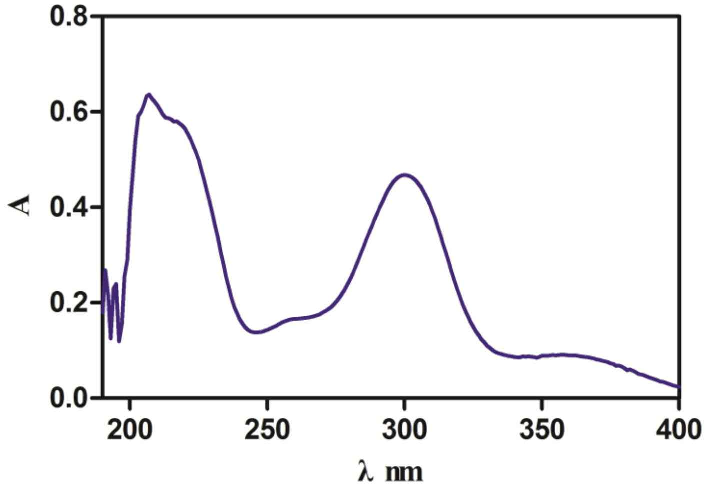


**Figure S28**. UV spectrum of nidulalin D (**2**).

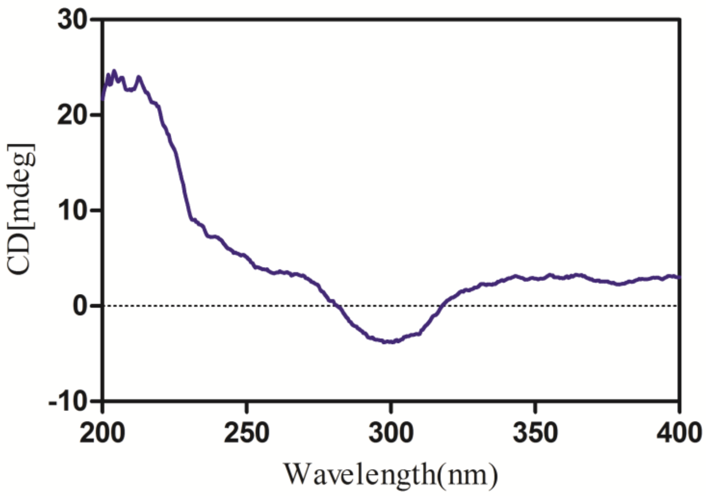


**Figure S29**. CD spectra of nidulalin D (**2**).

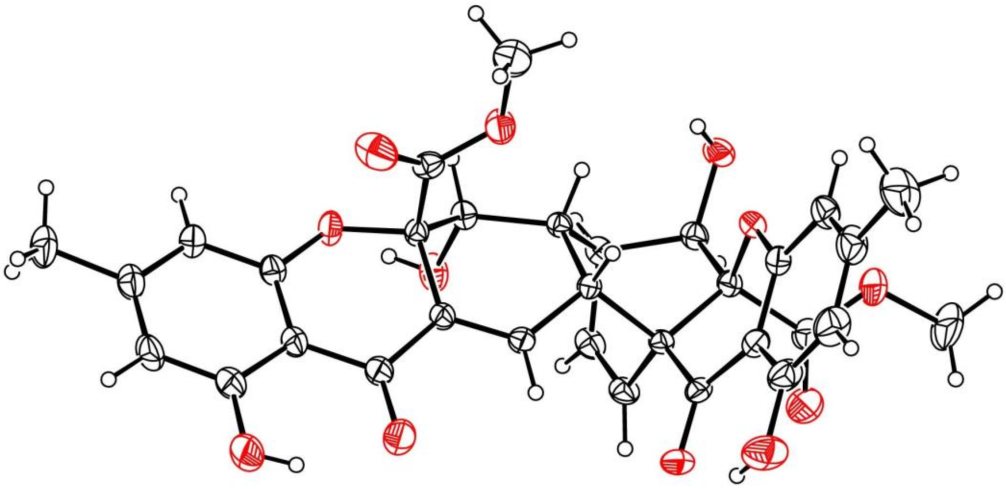

**Figure S22**. X-ray crystallographic structure of nidulaxanthone A (**1**).

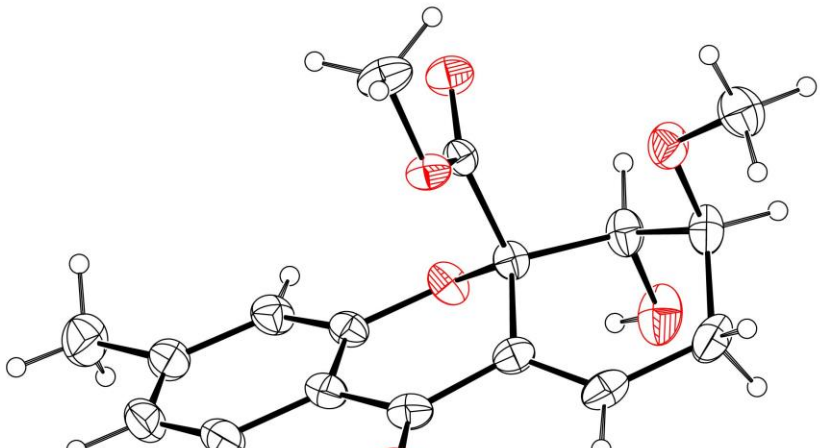

**Figure S23**. X-ray crystallographic structure of nidulalin D (**2**)