

## Supplementary Information

### **Chroman-4-one and pyrano[4, 3-b]chromenone derivatives from the mangrove endophytic fungus *Diaporthe phaseolorum* SKS019**

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(Z. S.).

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Figure S41 HSQC spectrum (500 MHz, CDCl<sub>3</sub>) of (±)-diaporchromone A (**7**)

Figure S42 HMBC spectrum (500 MHz, CDCl<sub>3</sub>) of (±)-diaporchromone A (**7**)

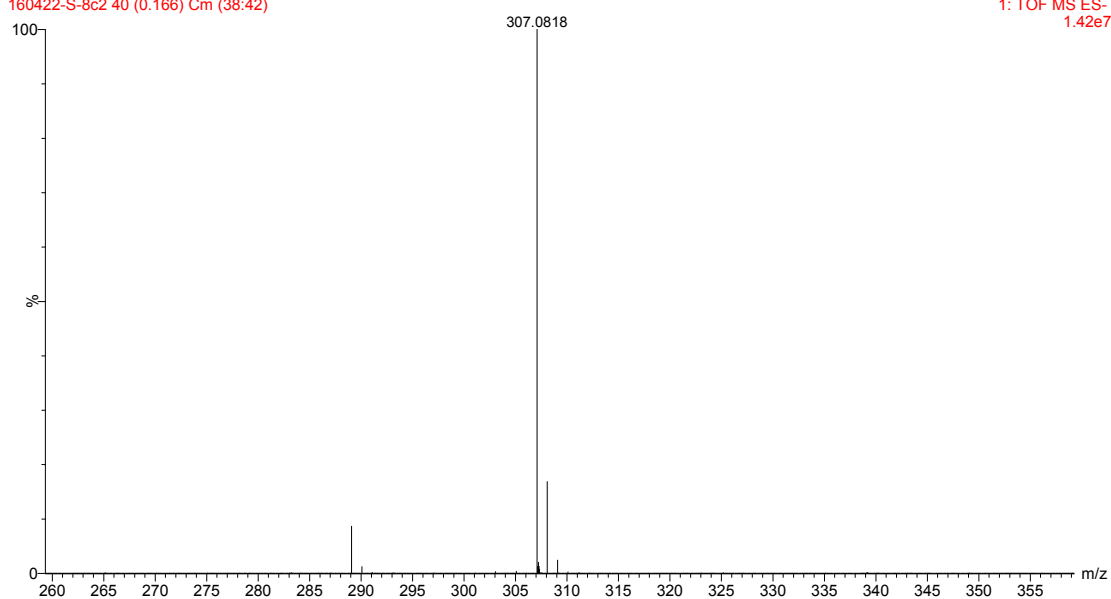
Figure S43 ECD Calculation section

Figure S1 HRESIMS of diaporchromanone A (1)

SYNAPT G2-Si#UGA489

160422-S-8c2.40 (0.166) Cm (38.42)

1: TOF MS ES-  
1.42e7



#### Elemental Composition Report

##### Single Mass Analysis

Tolerance = 4.0 PPM / DBE: min = -1.5, max = 50.0

Elements Used:

C: 0-50 H: 0-100 O: 0-50

Mass	Calc. Mass	mDa	PPM	DBE	Formula
307.0818	307.0818	0.0	0.0	8.5	C <sub>15</sub> H <sub>15</sub> O <sub>7</sub>

Figure S2 <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of diaporchromanone A (**1**)

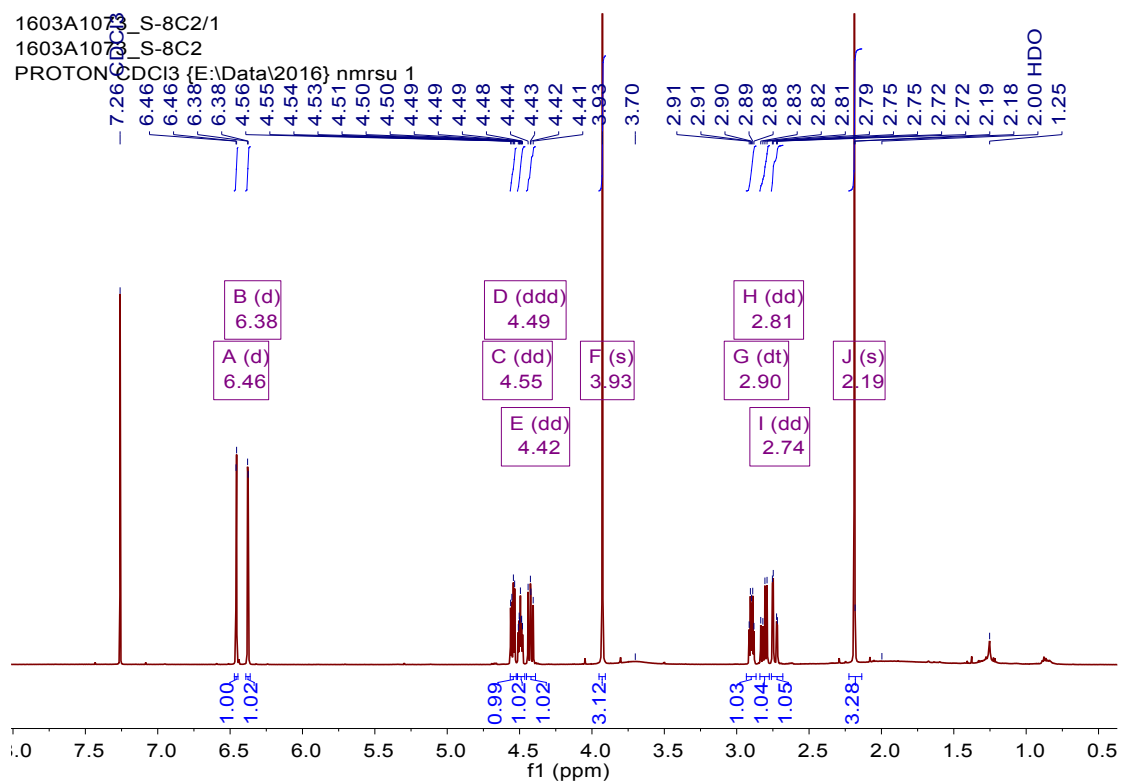


Figure S3 <sup>13</sup>C NMR spectrum (125 MHz, CDCl<sub>3</sub>) of diaporchromanone A (**1**)

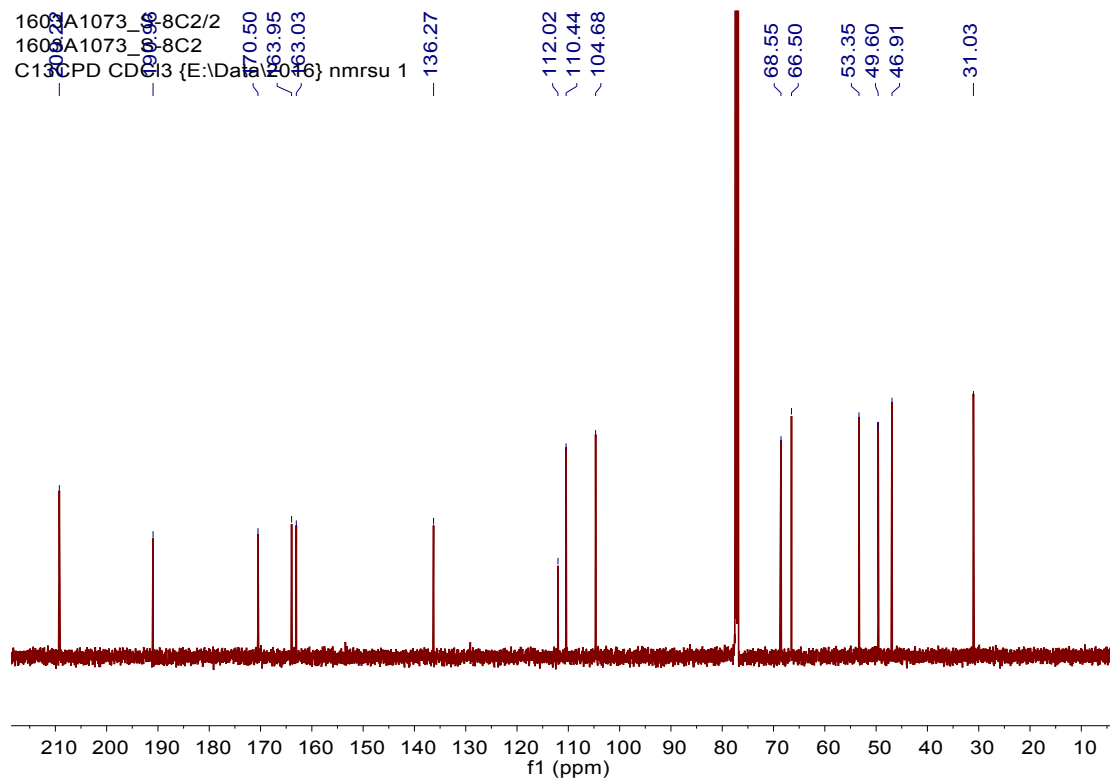


Figure S4 DEPT NMR spectrum (125 MHz, CDCl<sub>3</sub>) of diaporchromanone A (**1**)

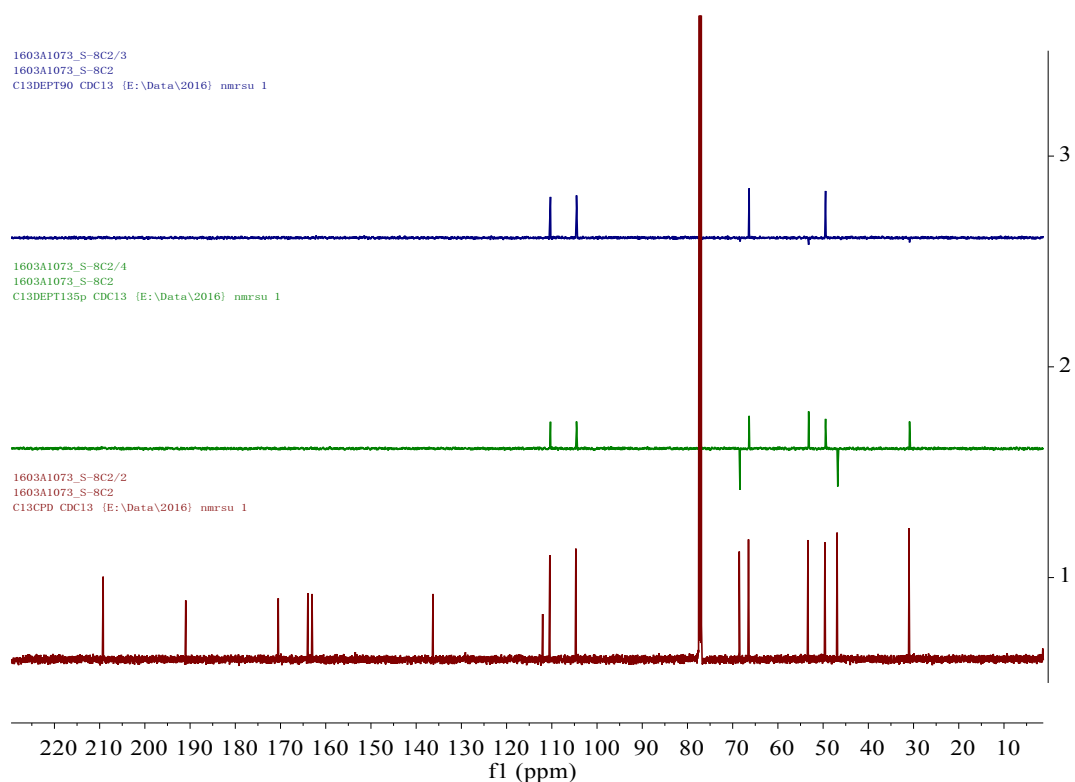


Figure S5 <sup>1</sup>H-<sup>1</sup>H COSY spectrum (500 MHz, CDCl<sub>3</sub>) of diaporchromanone A (**1**)

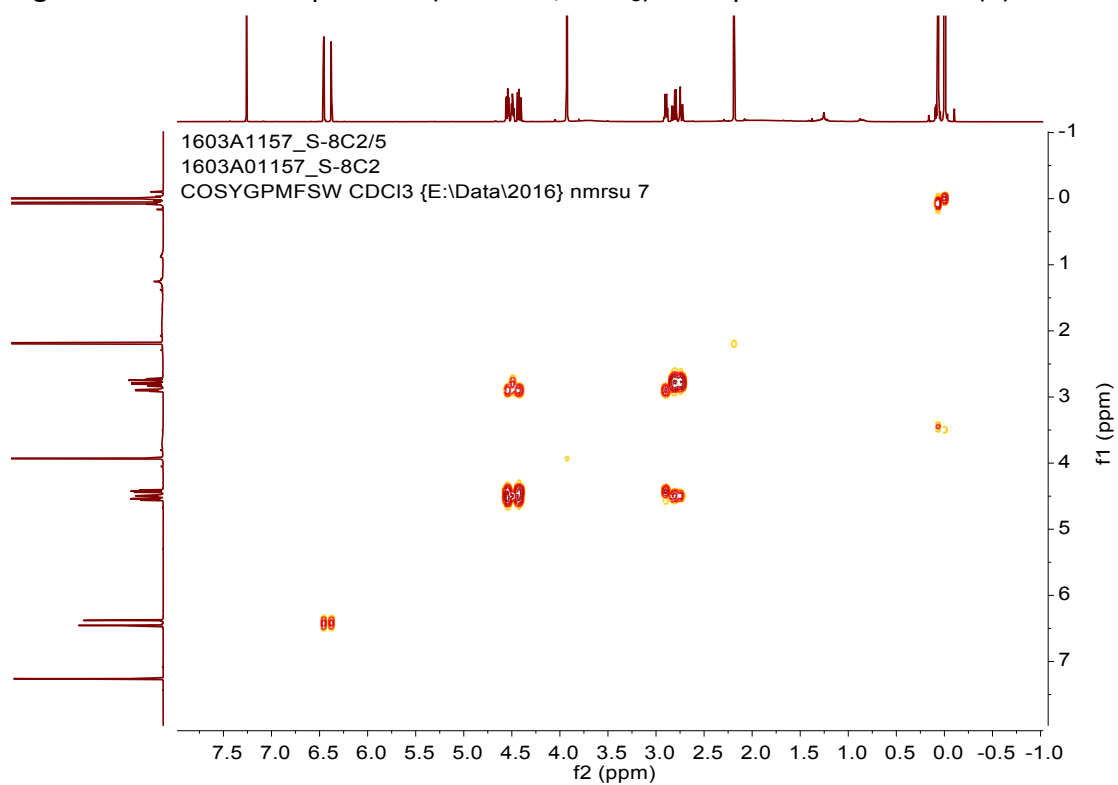


Figure S6 HSQC spectrum (500 MHz, CDCl<sub>3</sub>) of diaporchromanone A (**1**)

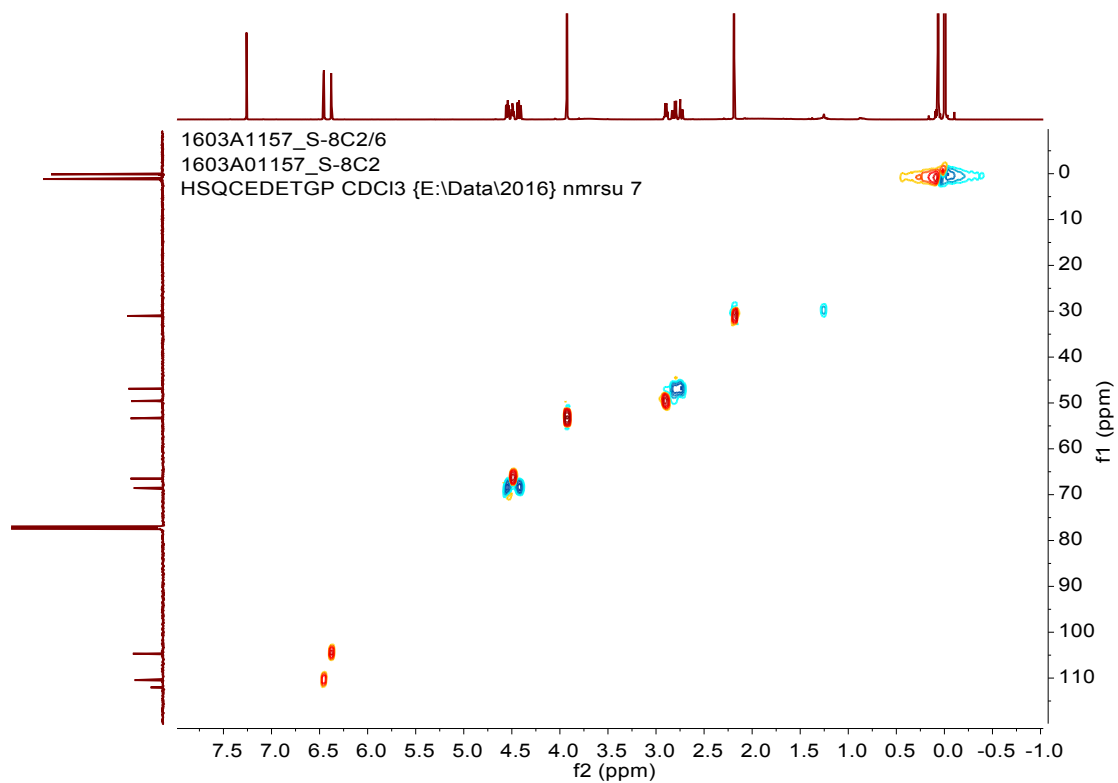


Figure S7 HMBC spectrum (500 MHz, CDCl<sub>3</sub>) of diaporchromanone A (**1**)

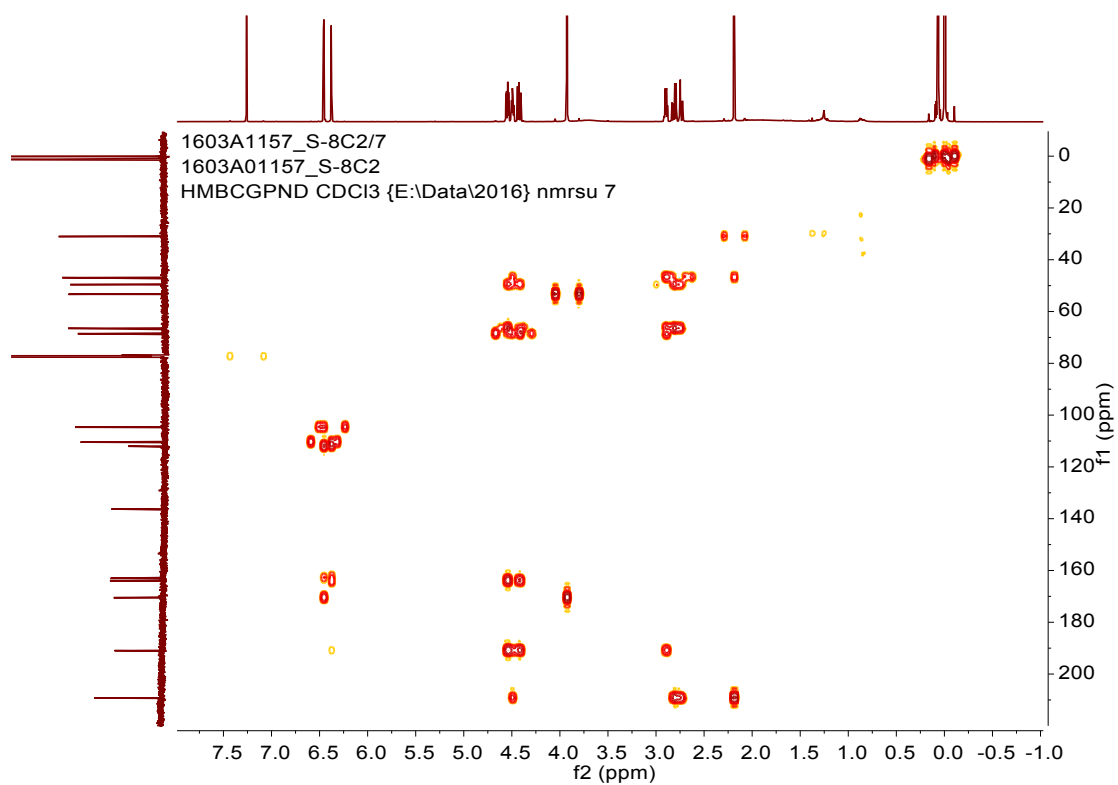
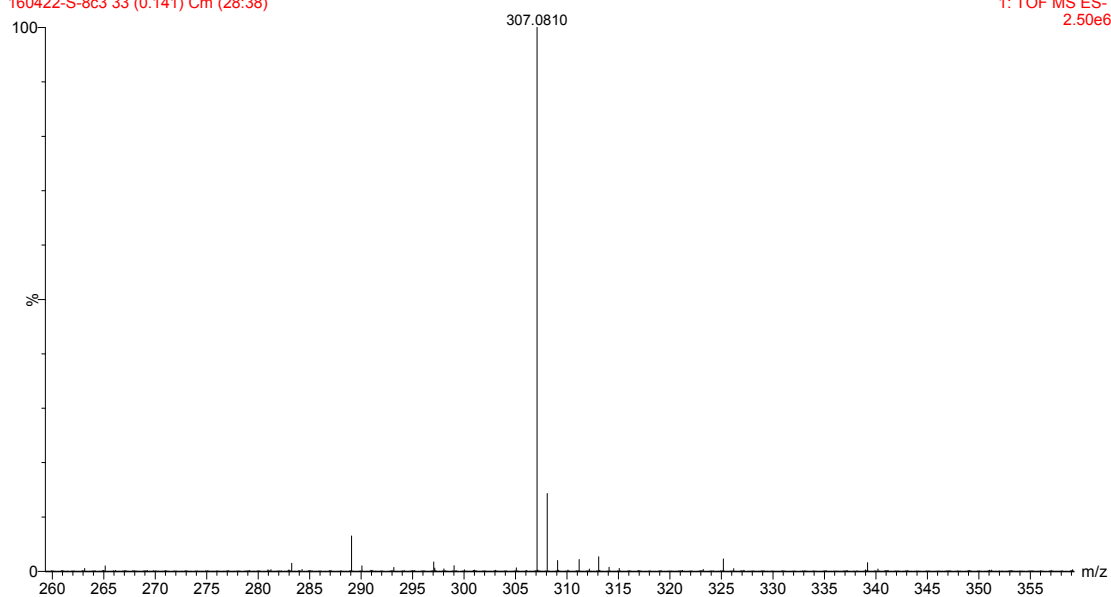


Figure S8 HRESIMS of diaporchromanone B (2)

SYNAPT G2-Si#UGA489

160422-S-8c3 33 (0.141) Cm (28:38)

1: TOF MS ES-  
2.50e6



### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 4.0 PPM / DBE: min = -1.5, max = 50.0

Elements Used:

C: 0-50 H: 0-100 O: 0-50

Mass	Calc. Mass	mDa	PPM	DBE	Formula
307.0810	307.0818	-0.8	-2.6	8.5	C <sub>15</sub> H <sub>15</sub> O <sub>7</sub>



Figure S9  $^1\text{H}$  NMR spectrum (500 MHz, acetone- $d_6$ ) of diaporchromanone B (**2**)

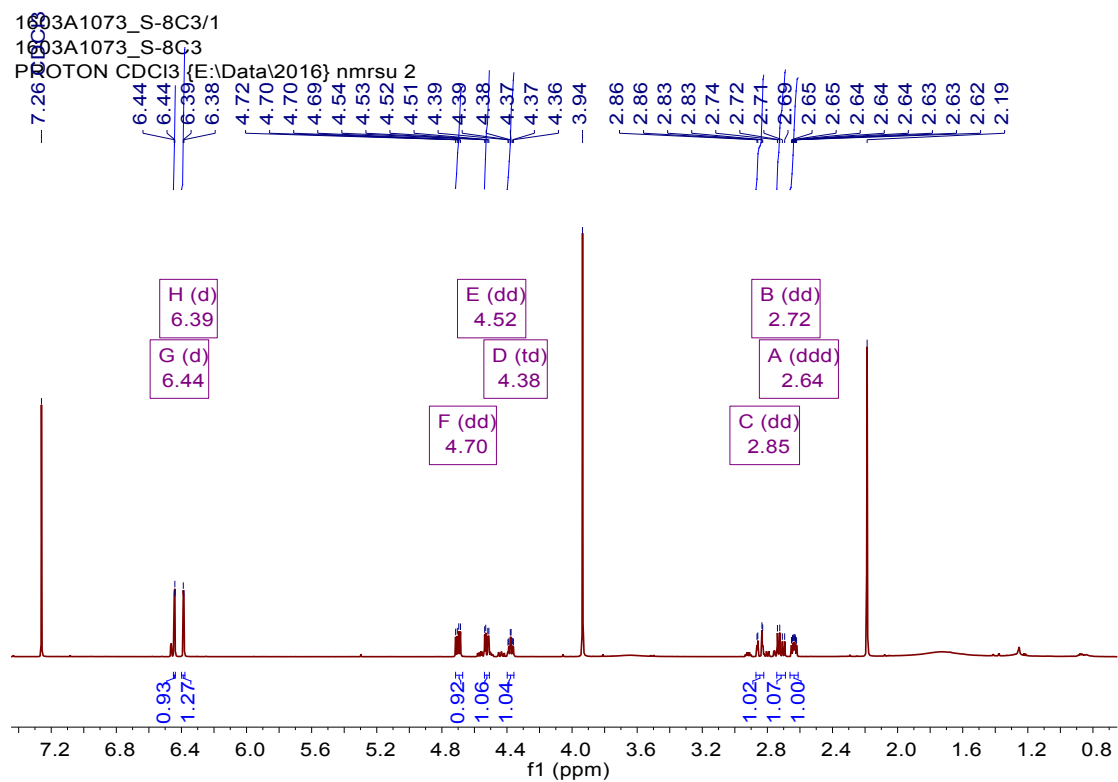


Figure S10  $^{13}\text{C}$  NMR spectrum (125 MHz, acetone- $d_6$ ) of diaporchromanone B (**2**)

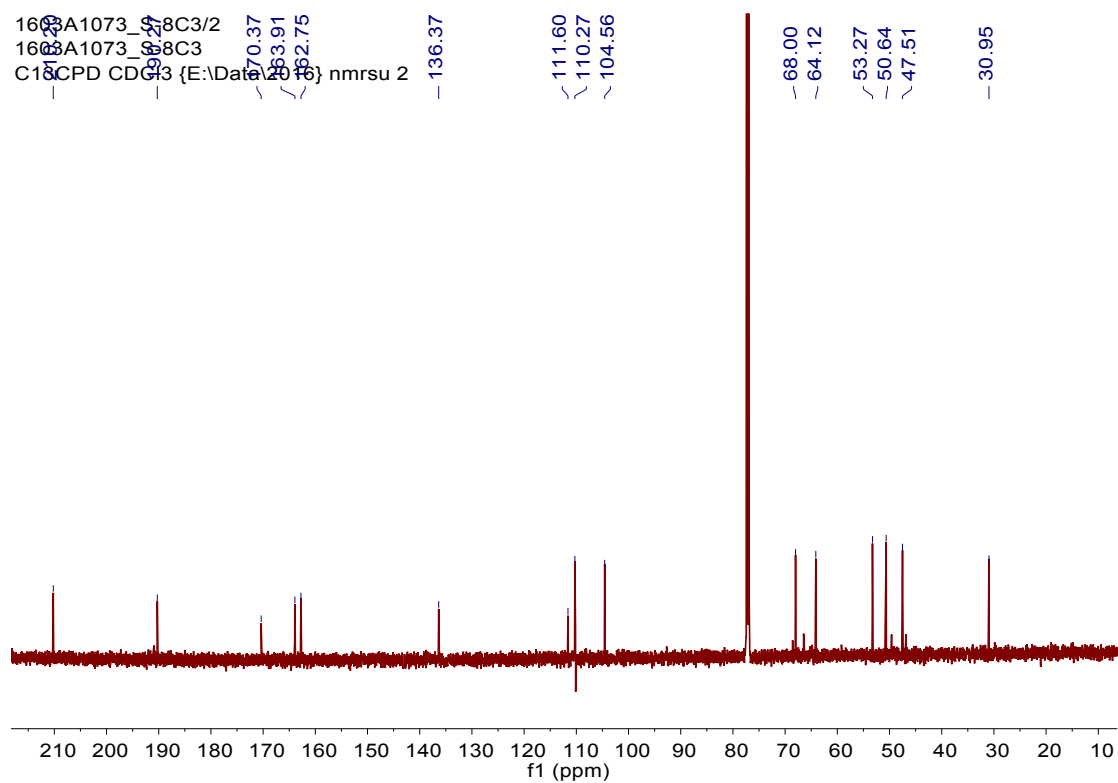


Figure S11  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (500 MHz,  $\text{CDCl}_3$ ) of diaporchromanone B (**2**)

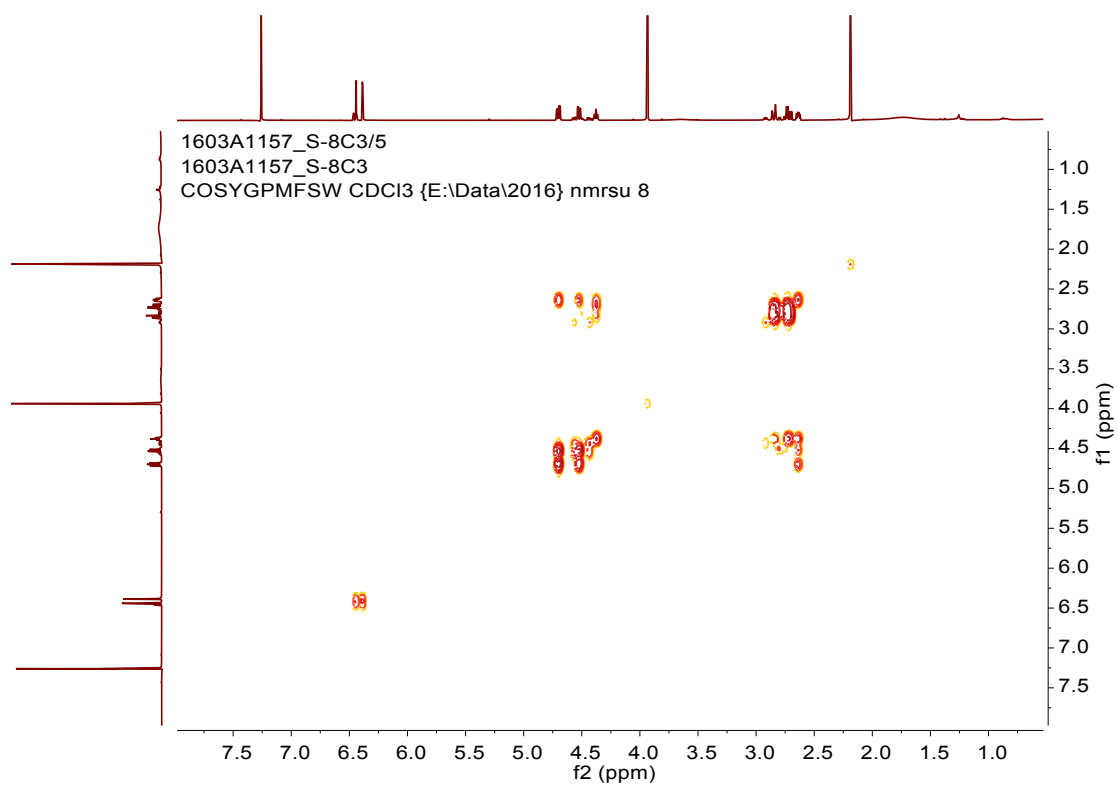


Figure S12 HSQC spectrum (500 MHz,  $\text{CDCl}_3$ ) of diaporchromanone B (**2**)

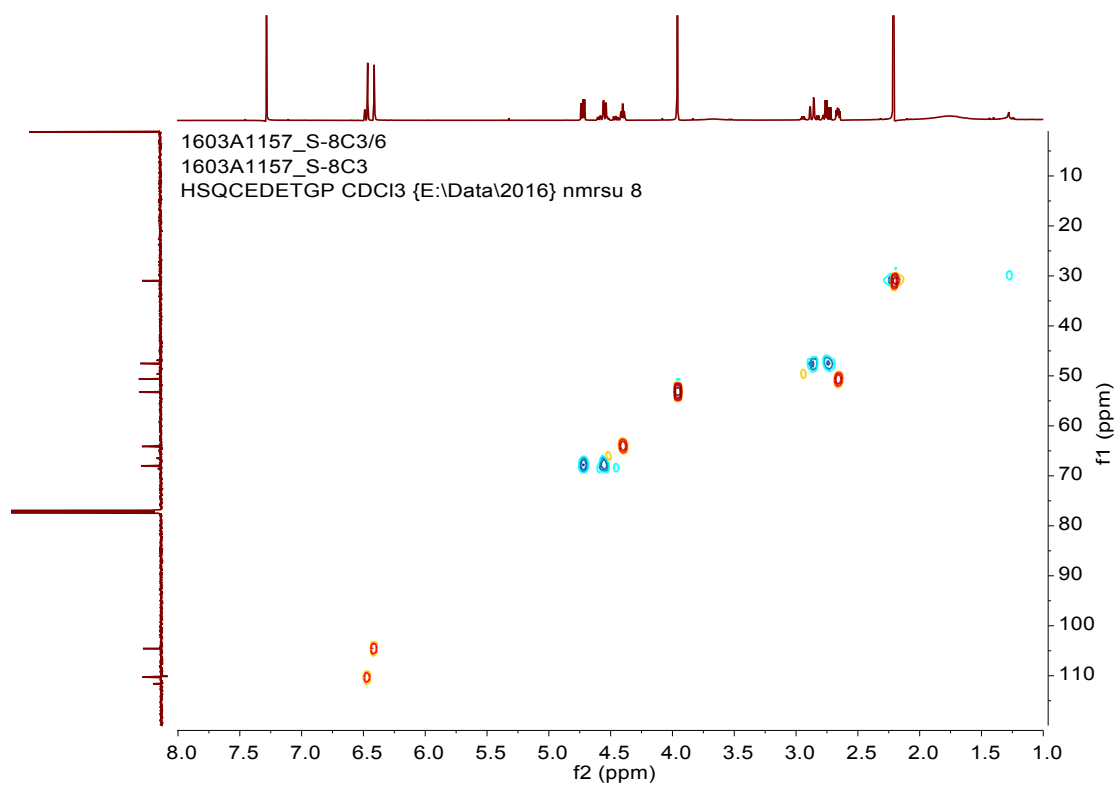


Figure S13 HMBC spectrum (500 MHz, CDCl<sub>3</sub>) of diaporchromanone B (**2**)

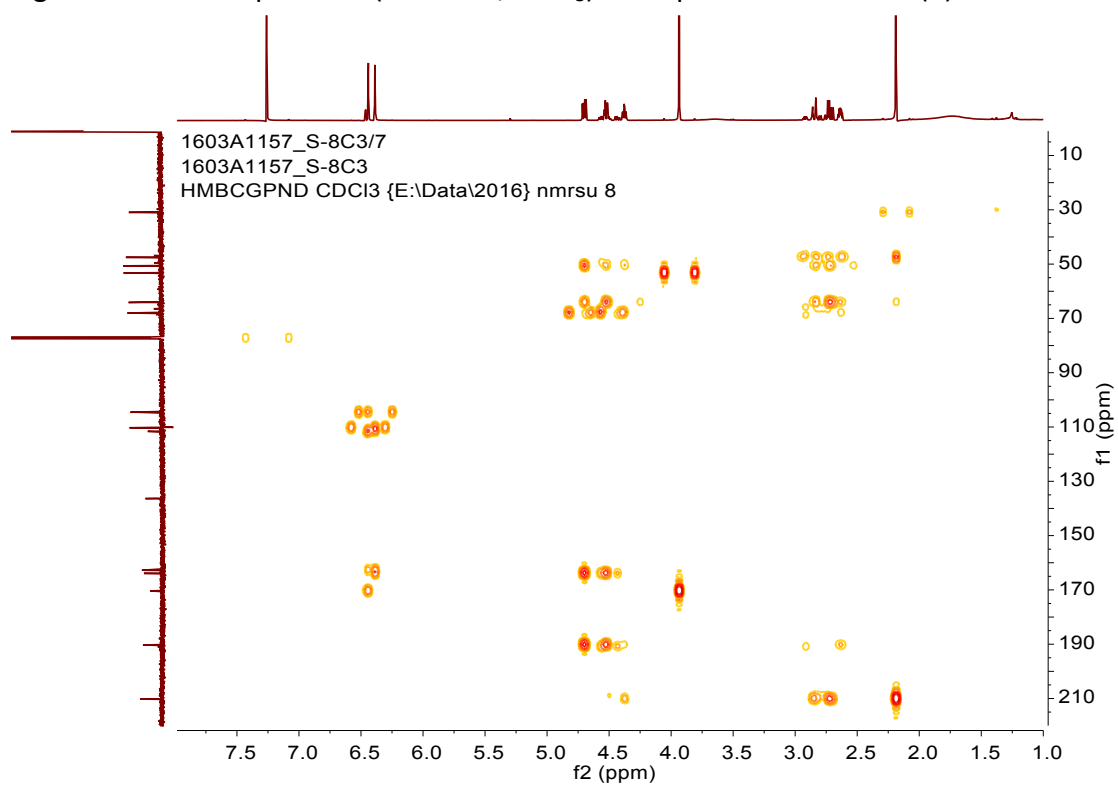
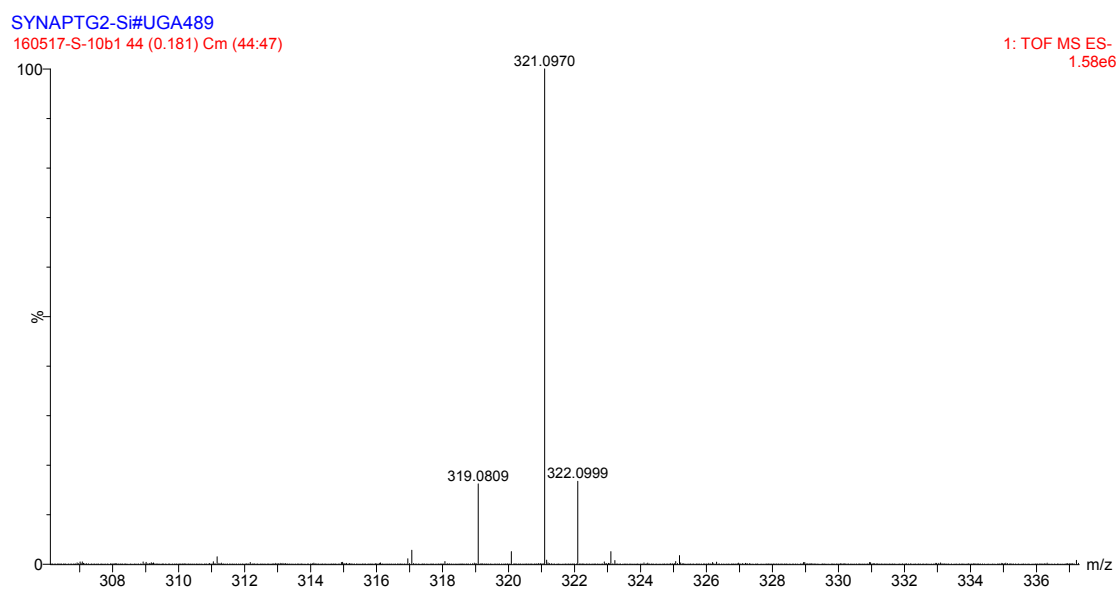


Figure S14 HRESIMS of diaporchromanone C (**3**)



### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Elements Used: C: 0-50 H: 0-100 O: 0-50

Mass	Calc. Mass	mDa	PPM	DBE	Formula
321.0970	321.0974	-0.4	-1.2	8.5	C <sub>16</sub> H <sub>17</sub> O <sub>7</sub>

Figure S15 <sup>1</sup>H NMR spectrum (500MHz, CDCl<sub>3</sub>) of diaporchromanone C (**3**)

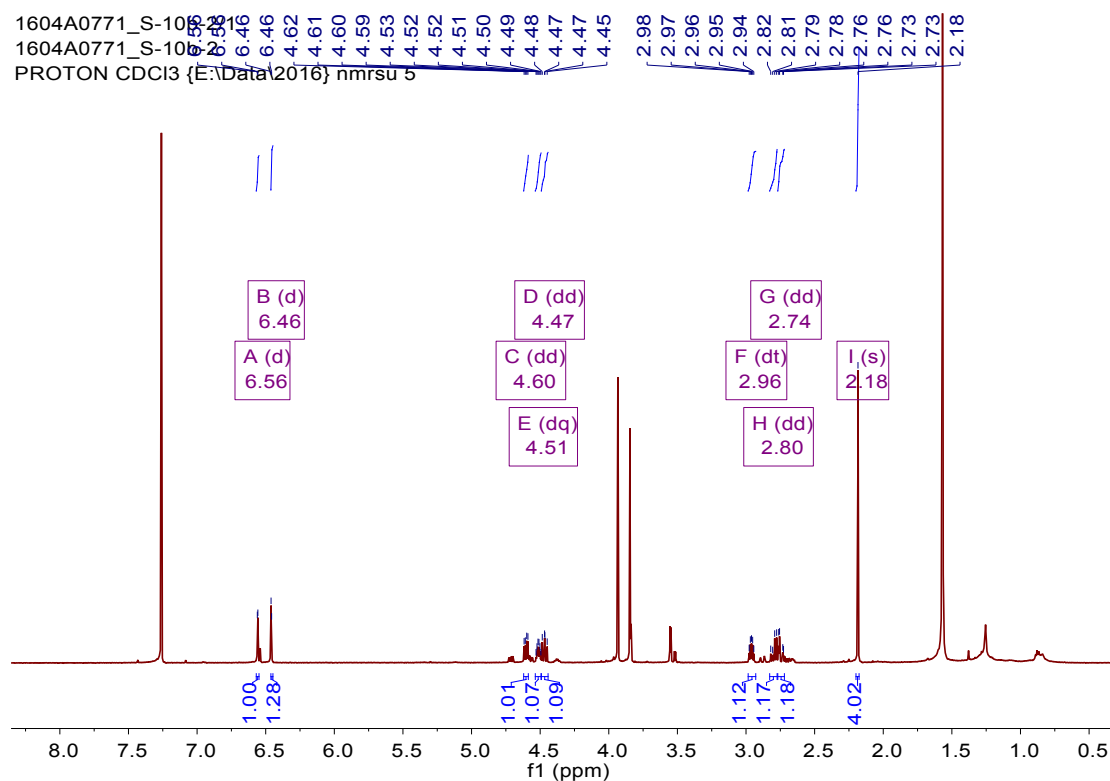


Figure S16 <sup>13</sup>C NMR spectrum (125 MHz, CDCl<sub>3</sub>) of diaporchromanone C (**3**)

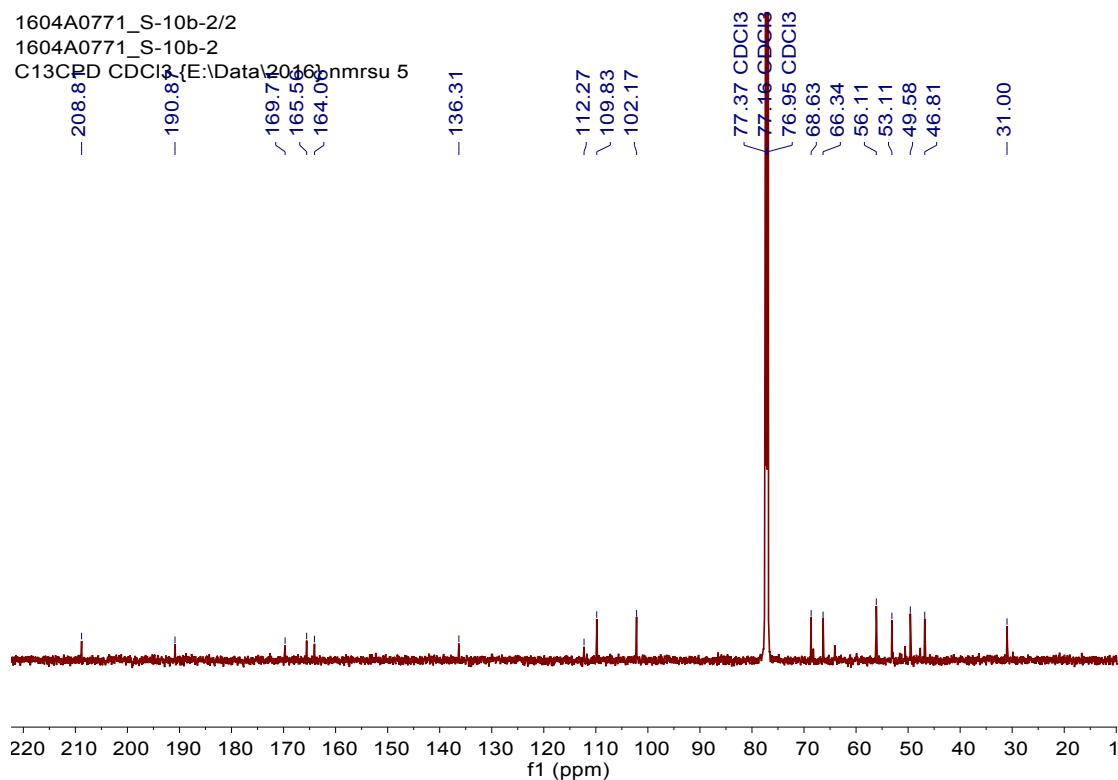


Figure S17  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (500 MHz,  $\text{CDCl}_3$ ) of diaporchromanone C (**3**)

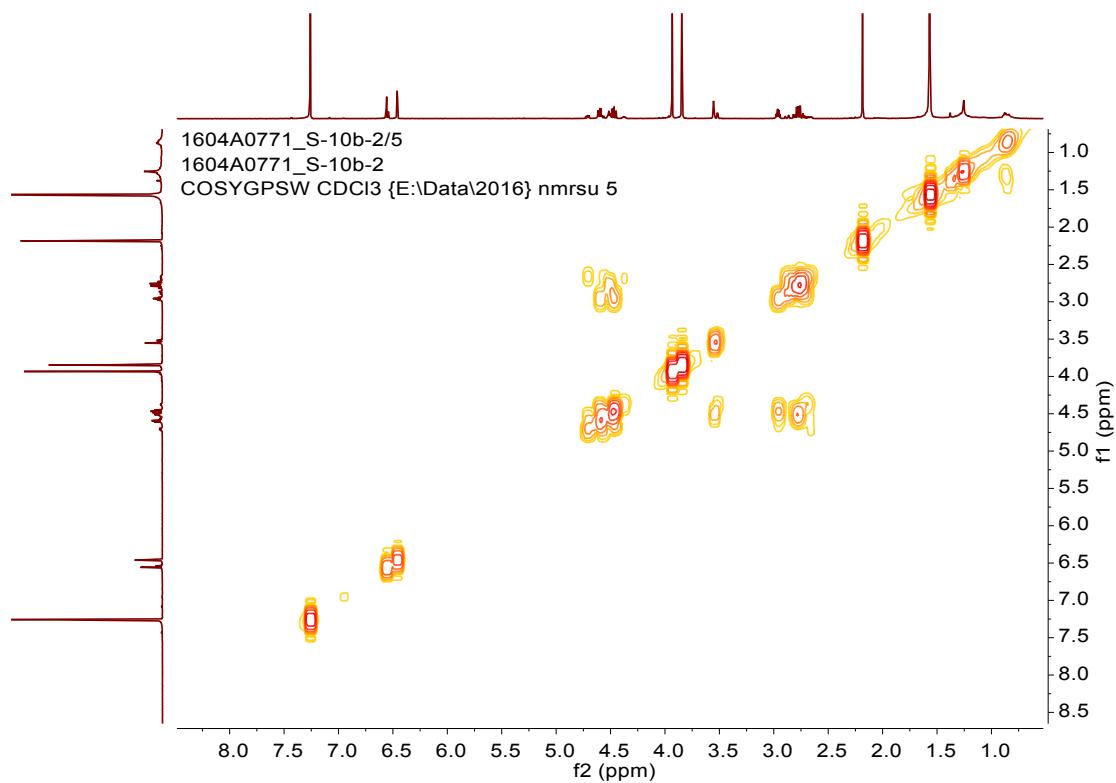


Figure S18 HSQC spectrum (500 MHz,  $\text{CDCl}_3$ ) of diaporchromanone C (**3**)

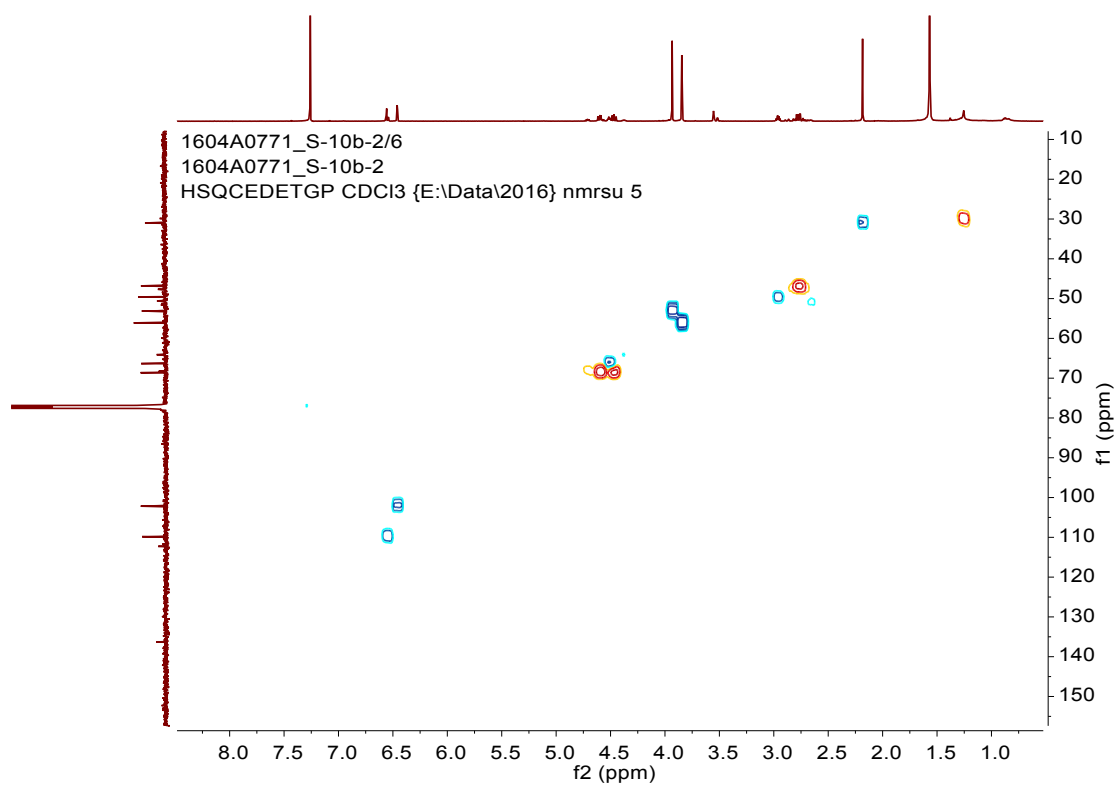


Figure S19 HMBC spectrum (500 MHz, CDCl<sub>3</sub>) of diaporchromanone C (**3**)

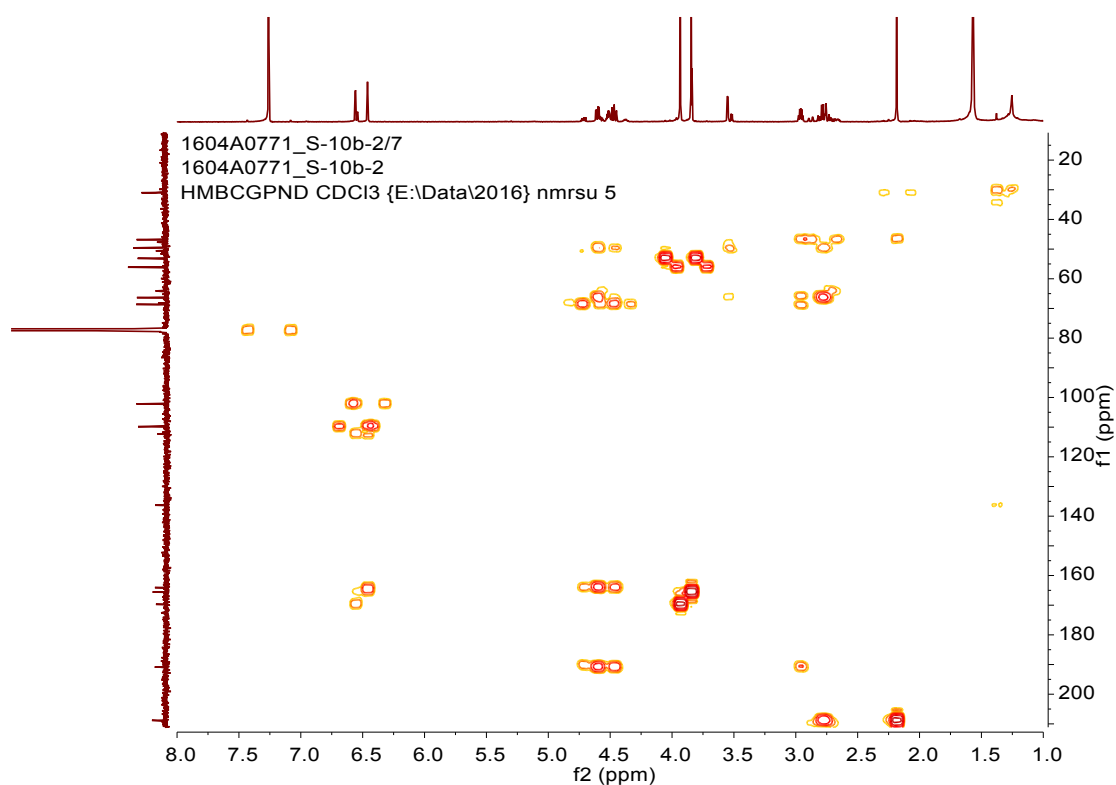
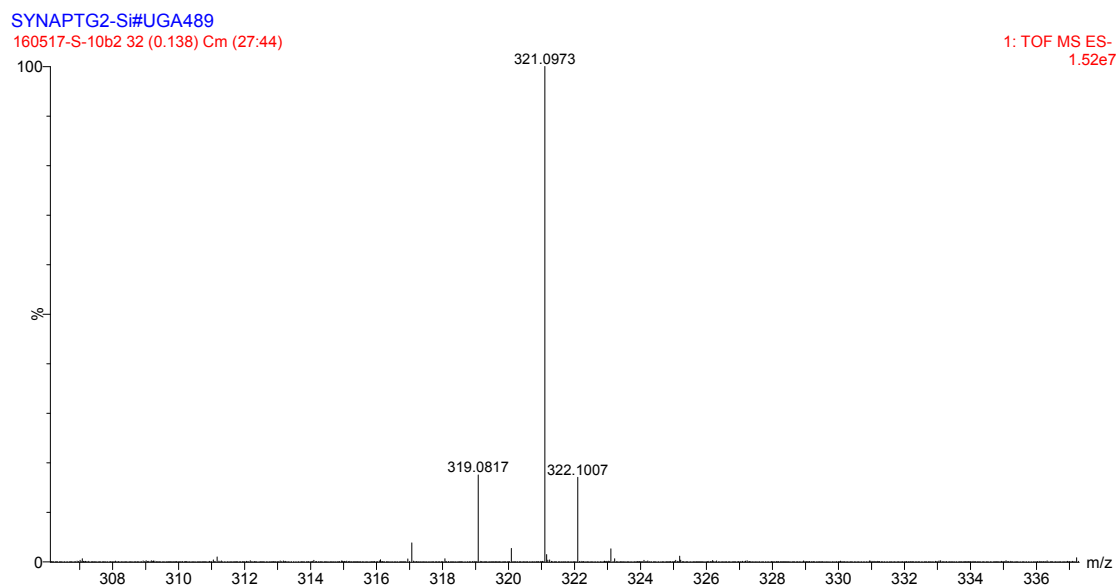


Figure S20 HRESIMS of diaporchromanone D (**4**)



### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Elements Used: C: 0-50 H: 0-100 O: 0-50

Mass	Calc. Mass	mDa	PPM	DBE	Formula
321.0973	321.0974	-0.1	-0.3	8.5	C <sub>16</sub> H <sub>17</sub> O <sub>7</sub>

Figure S21 <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of diaporchromanone D (**4**)

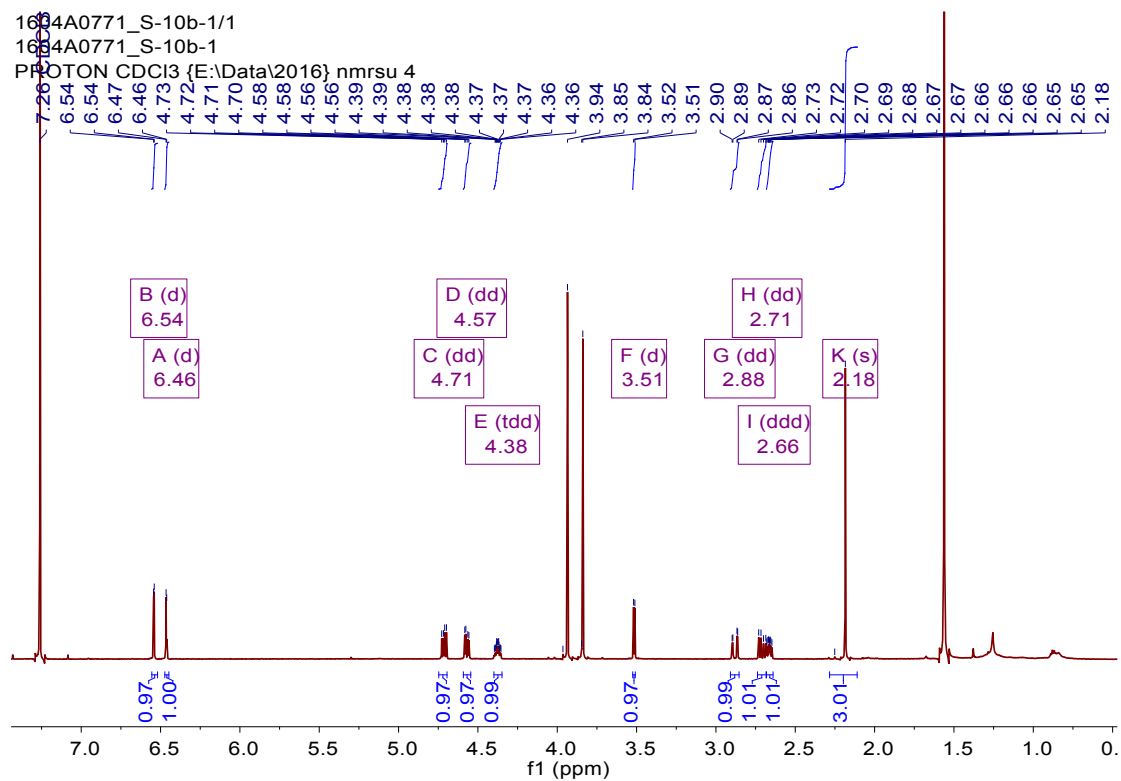


Figure S22 <sup>13</sup>C NMR spectrum (125 MHz, CDCl<sub>3</sub>) of diaporchromanone D (**4**)

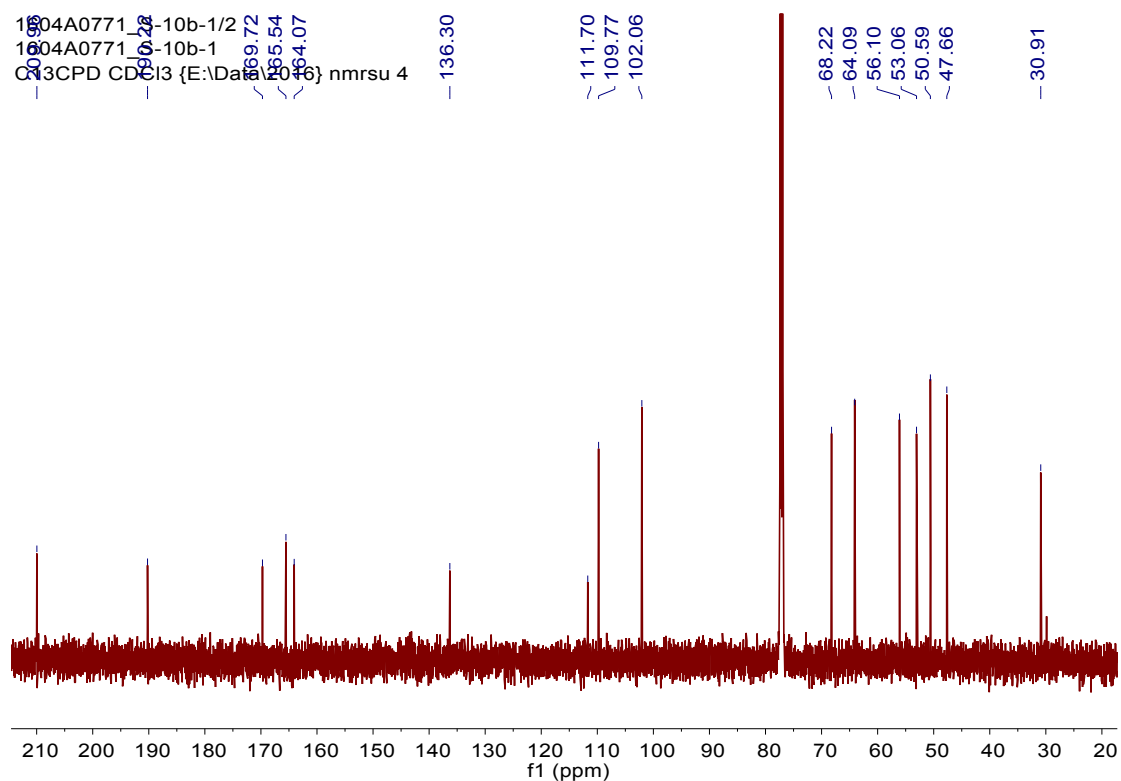


Figure S23  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (500 MHz,  $\text{CDCl}_3$ ) of diaporchromanone D (**4**)

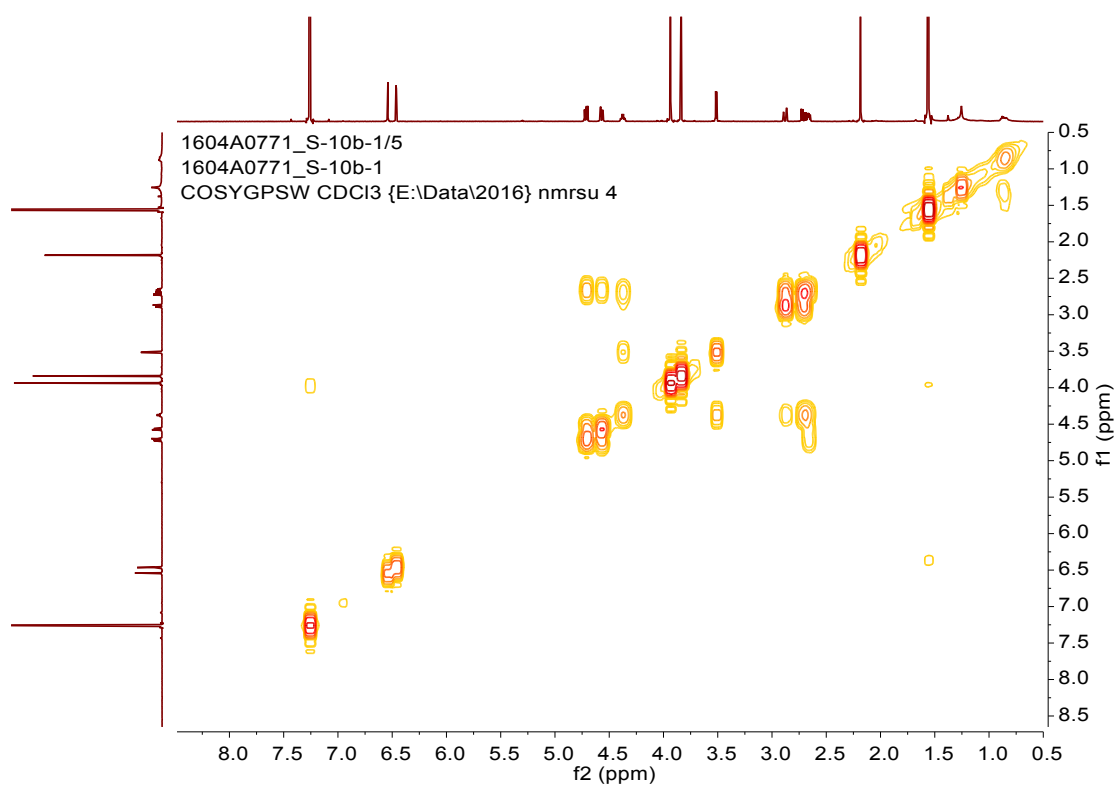


Figure S24 HSQC spectrum (500 MHz,  $\text{CDCl}_3$ ) of diaporchromanone D (**4**)

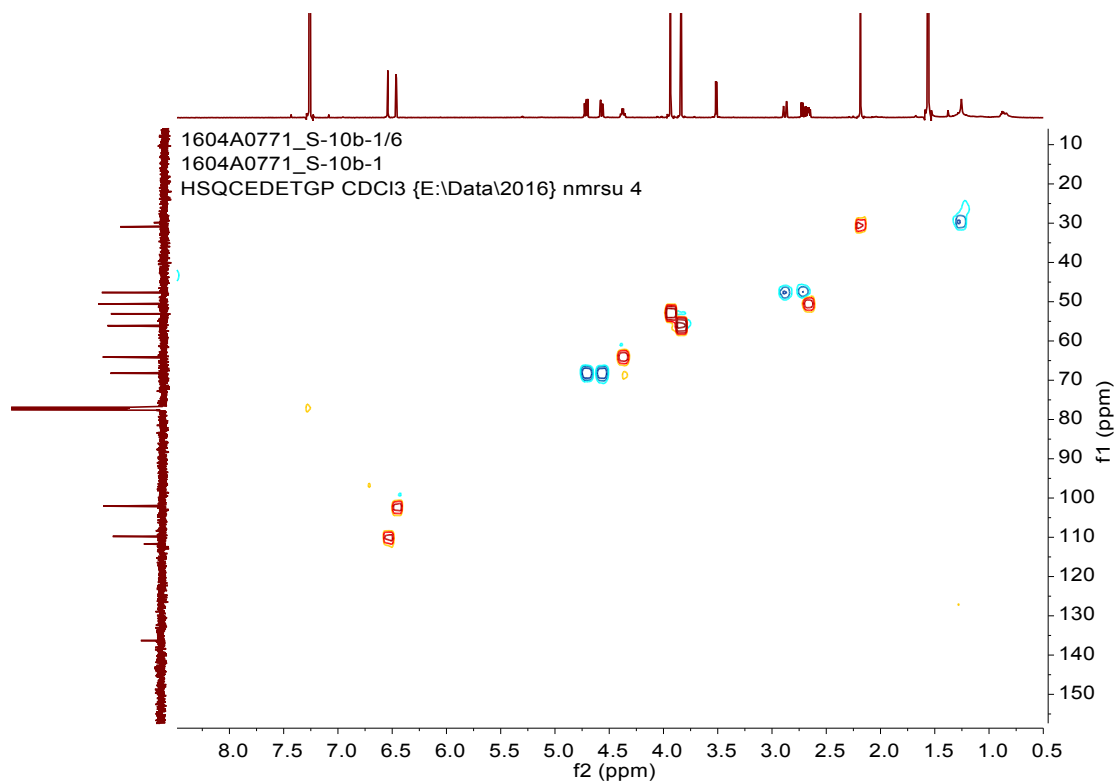




Figure S25 HMBC spectrum (500 MHz, CDCl<sub>3</sub>) of diaporchromanone D (**4**)

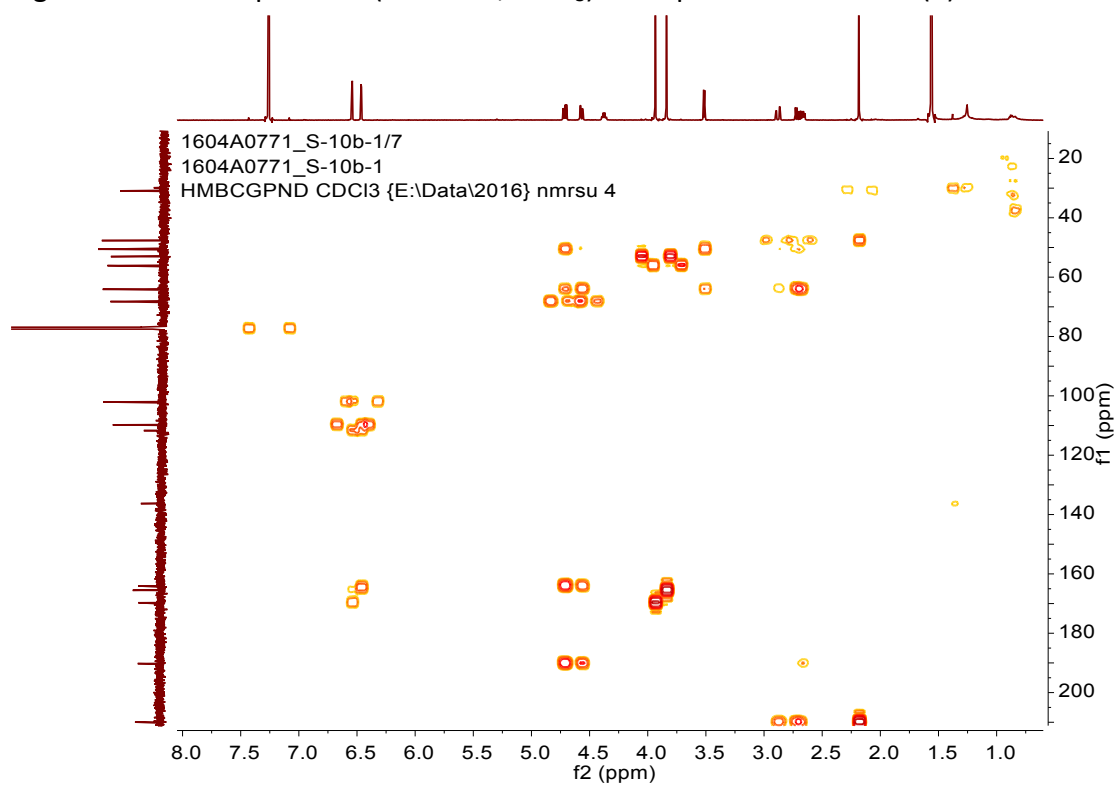
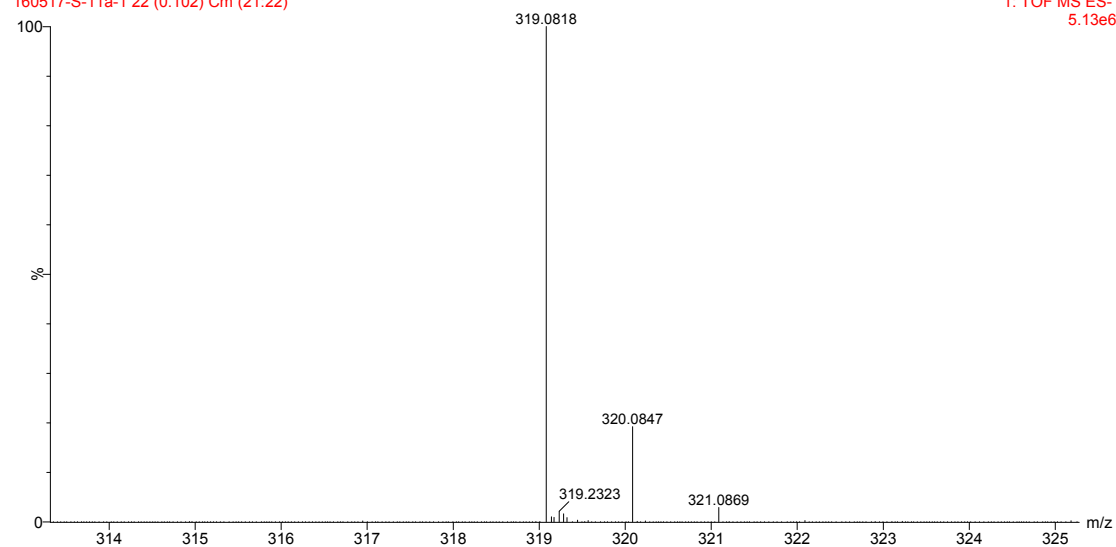


Figure S26 HRESIMS of (–) phomopsichin A (**5a**)

SYNAPT2-Si#UGA489

160517-S-11a-1 22 (0.102) Cm (21:22)

1: TOF MS ES-  
5.13e6



#### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0

Elements Used:		C: 0-50	H: 0-100	O: 0-50	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
319.0818	319.0818	0.0	0.0	9.5	C <sub>16</sub> H <sub>15</sub> O <sub>7</sub>

Figure S27 <sup>1</sup>H NMR spectrum (500 MHz, acetone-*d*<sub>6</sub>) of (–)-phomopsichin A (**5a**)

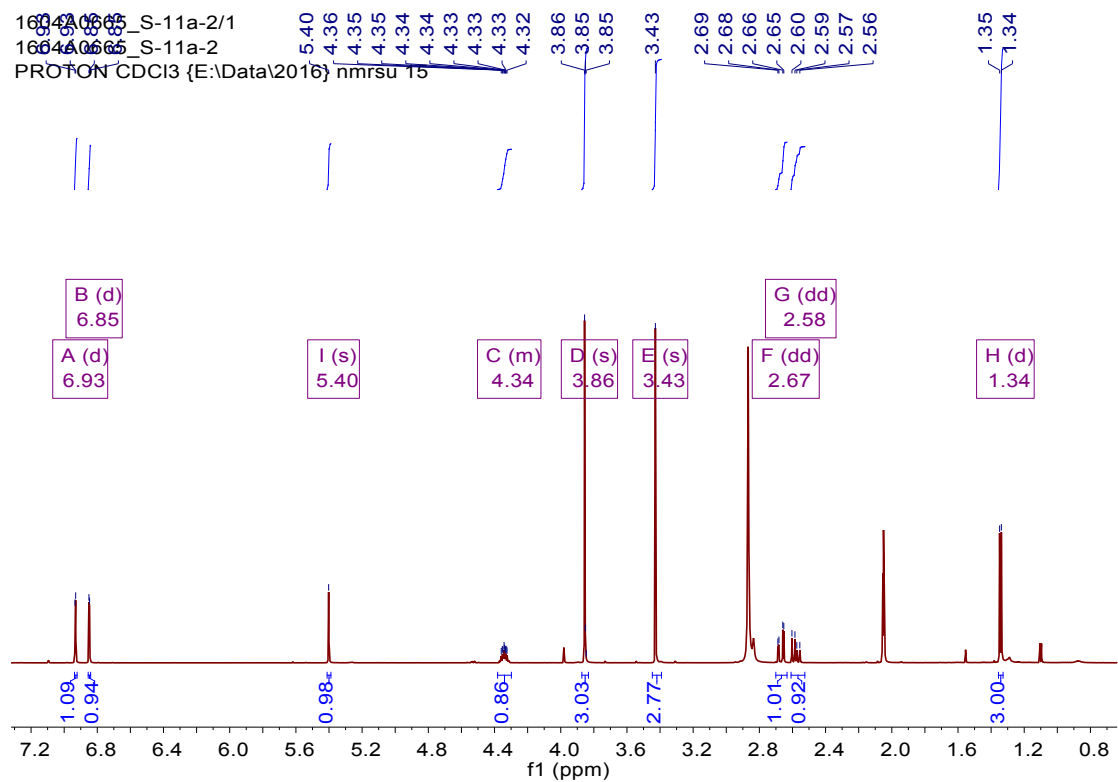


Figure S28 <sup>13</sup>C NMR spectrum (125 MHz, acetone-*d*<sub>6</sub>) of (–)-phomopsichin A (**5a**)

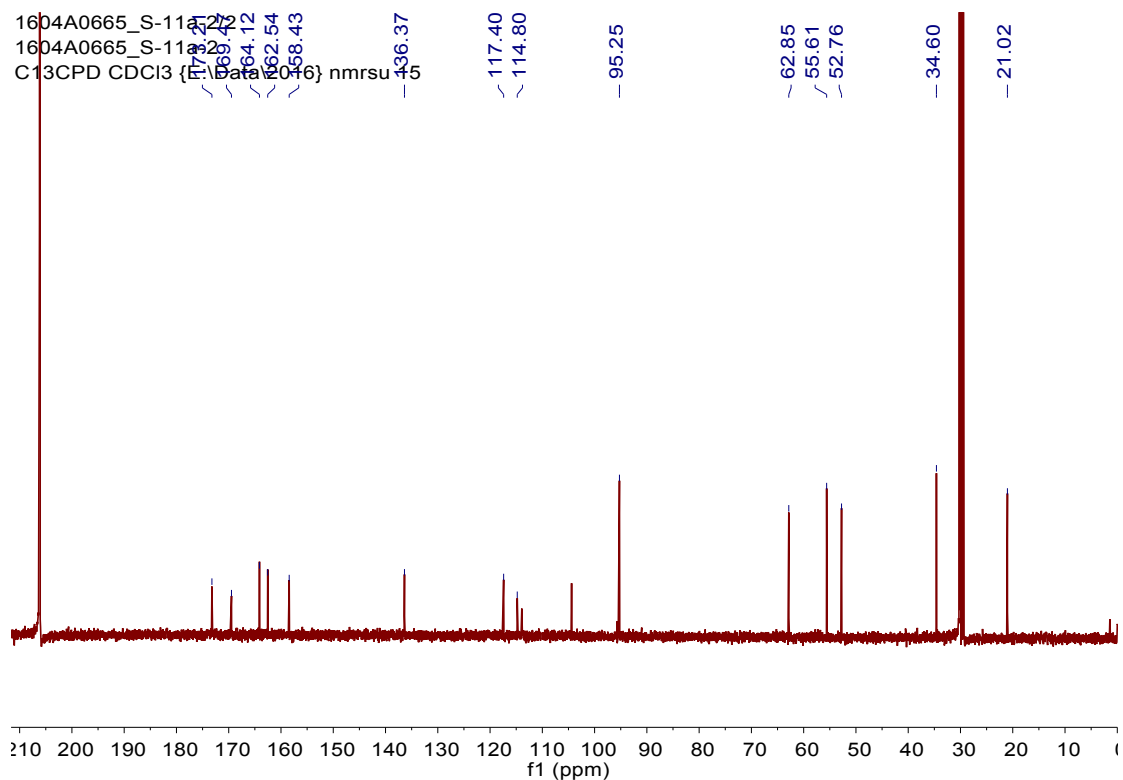


Figure S29  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (500 MHz, acetone- $d_6$ ) of (-)-phomopsichin A (**5a**)

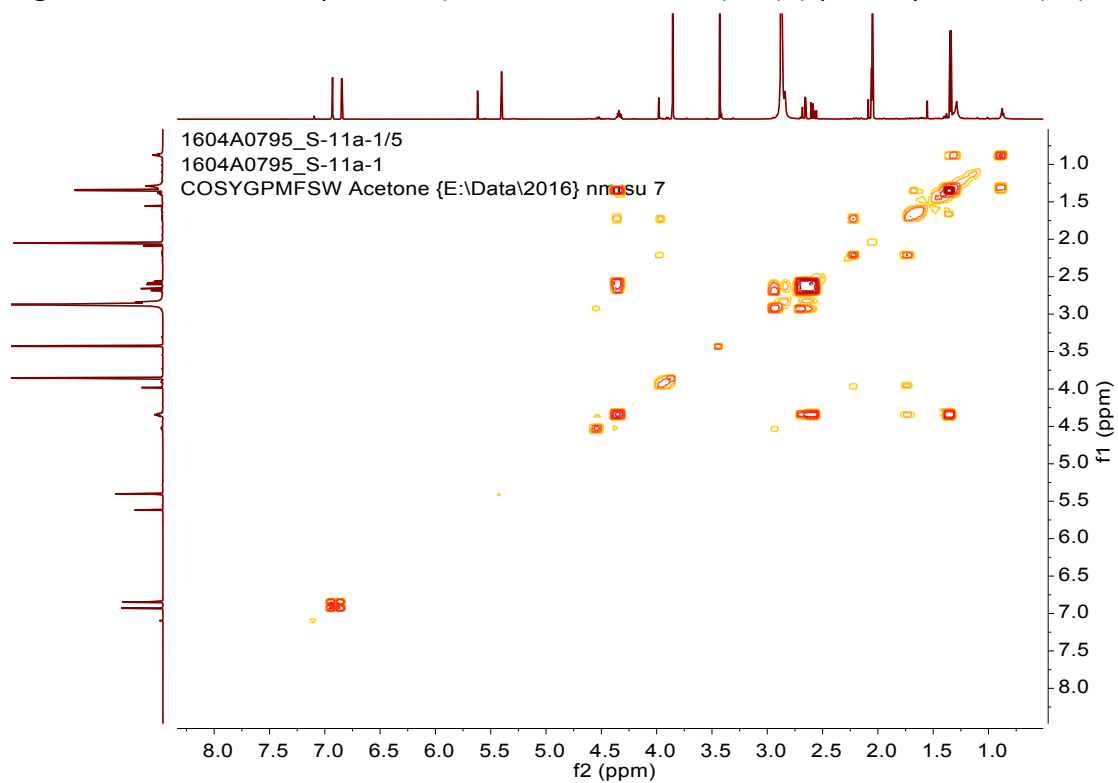


Figure S30 HSQC spectrum (500 MHz, acetone- $d_6$ ) of (-)-phomopsichin A (**5a**)

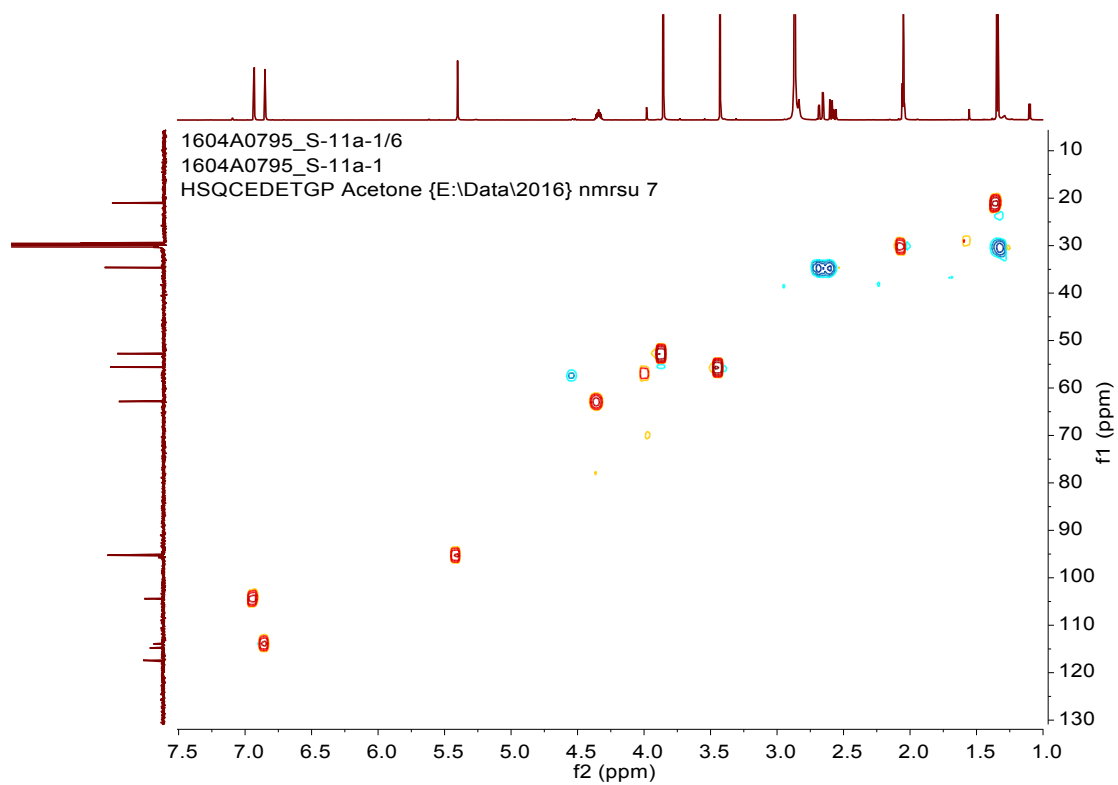


Figure S31 HMBC spectrum (500 MHz, acetone-*d*<sub>6</sub>) of (–)-phomopsichin A (5a)

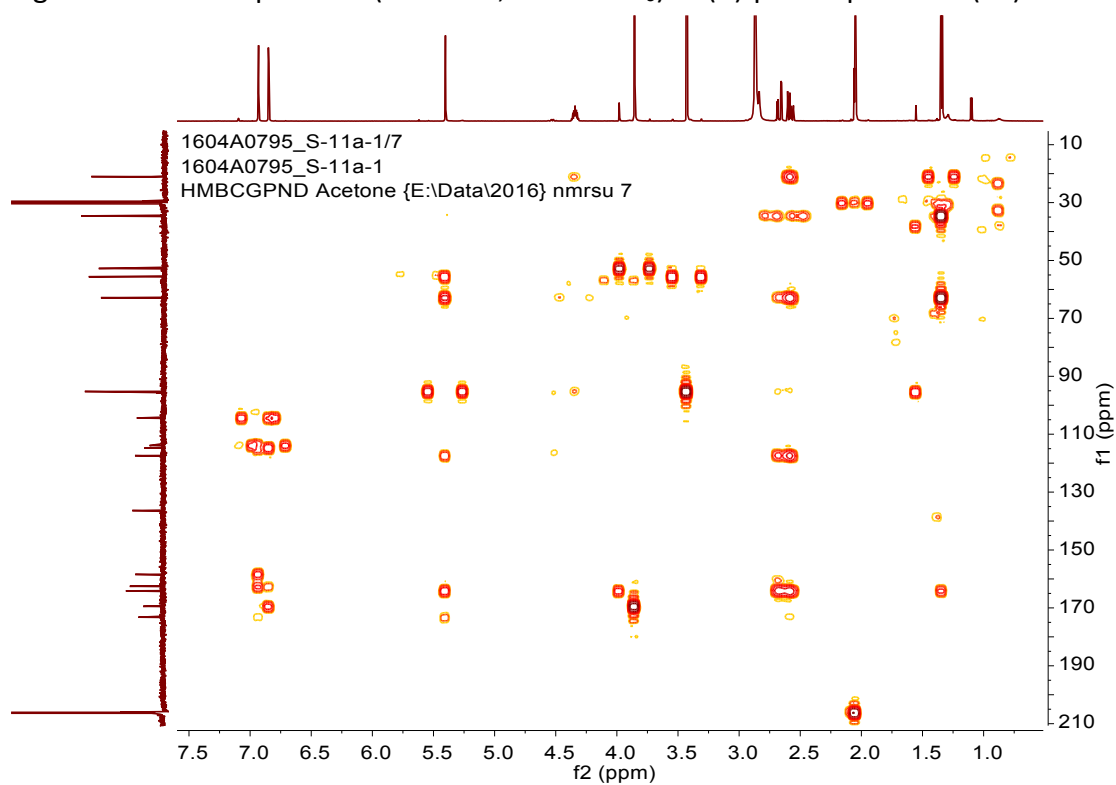
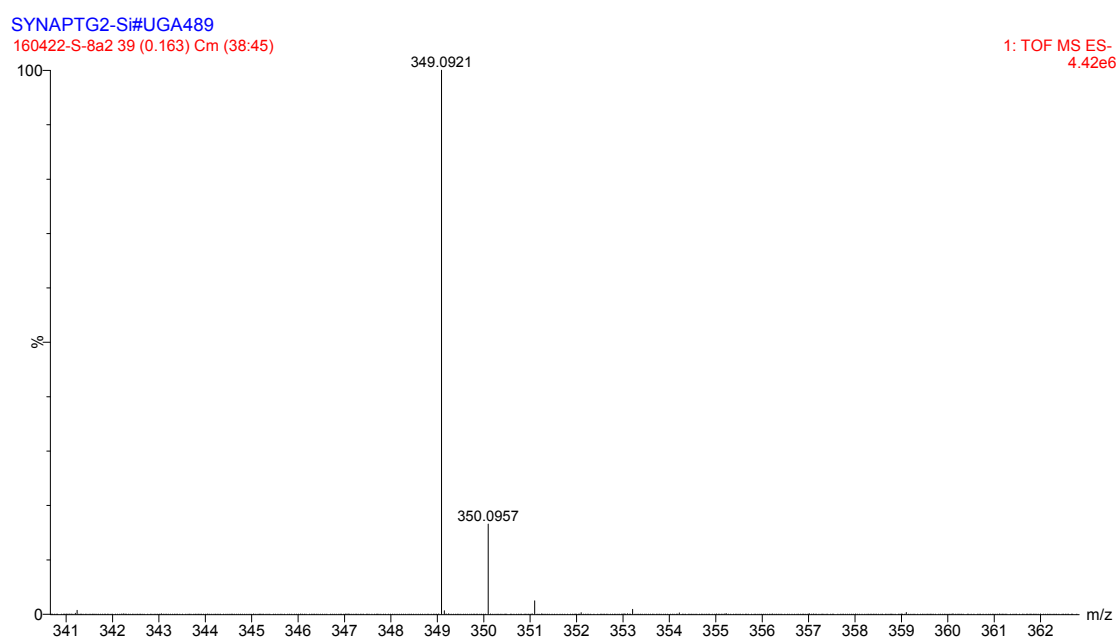


Figure S32 HRESIMS of (+)-phomopsichin B (6a)



### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 4.0 PPM DBE: min = -1.5, max = 50.0

C: 0-50 H: 0-100 O: 0-50

Mass	Calc. Mass	mDa	PPM	DBE	Formula
349.0921	349.0923	-0.2	-0.6	9.5	C <sub>17</sub> H <sub>17</sub> O <sub>8</sub>

Figure S33  $^1\text{H}$  NMR spectrum (500MHz,  $\text{CDCl}_3$ ) of (+)-phomopsichin B (**6a**)

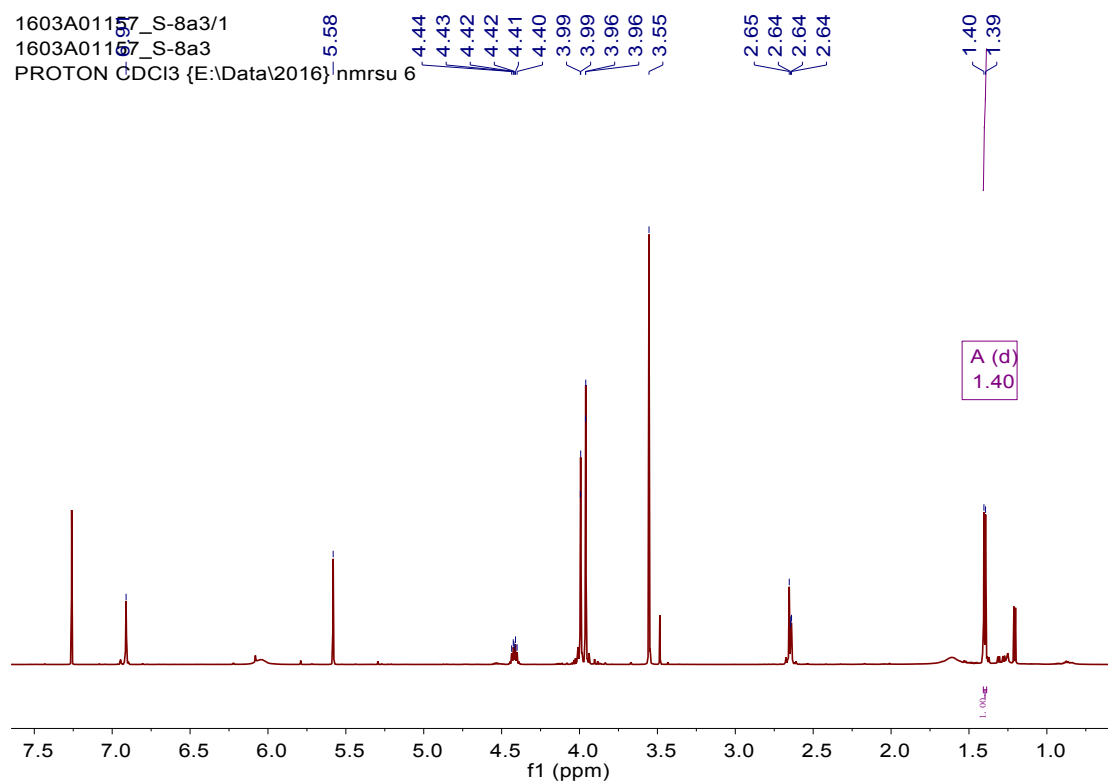


Figure S34  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ) of (+)-phomopsichin B (**6a**)

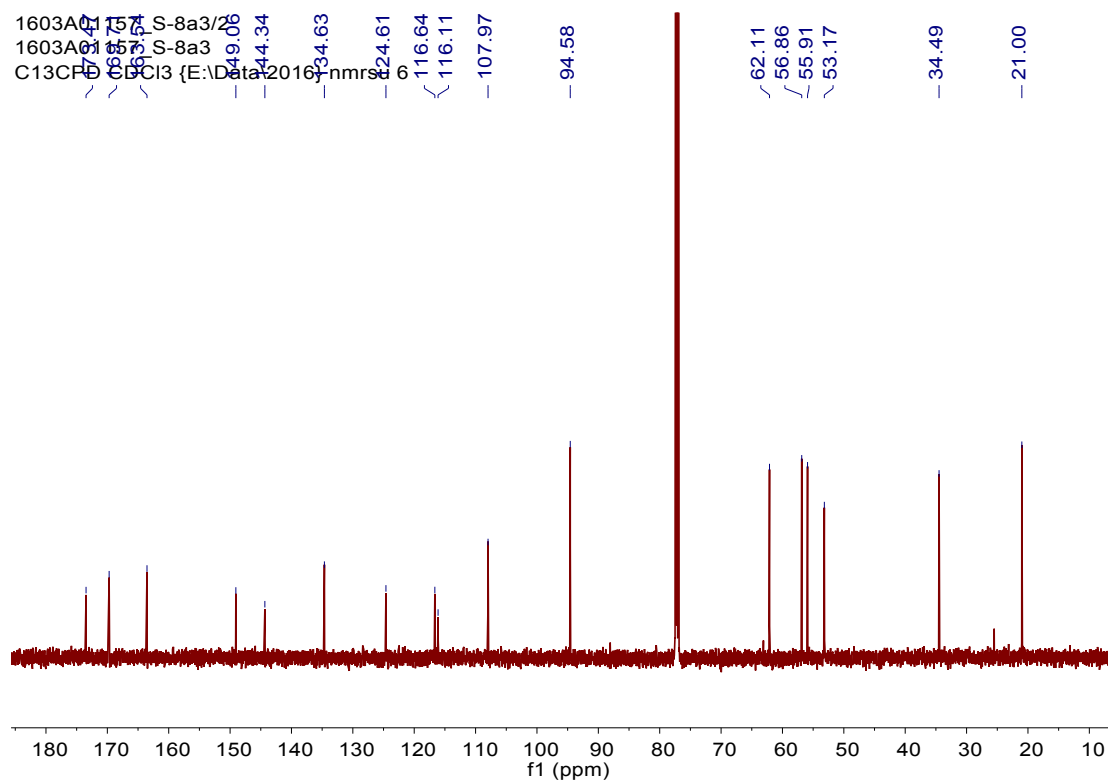


Figure S35  $^1\text{H}$ - $^1\text{H}$  COSY spectrum (500 MHz,  $\text{CDCl}_3$ ) of (+)-phomopsichin B (**6a**)

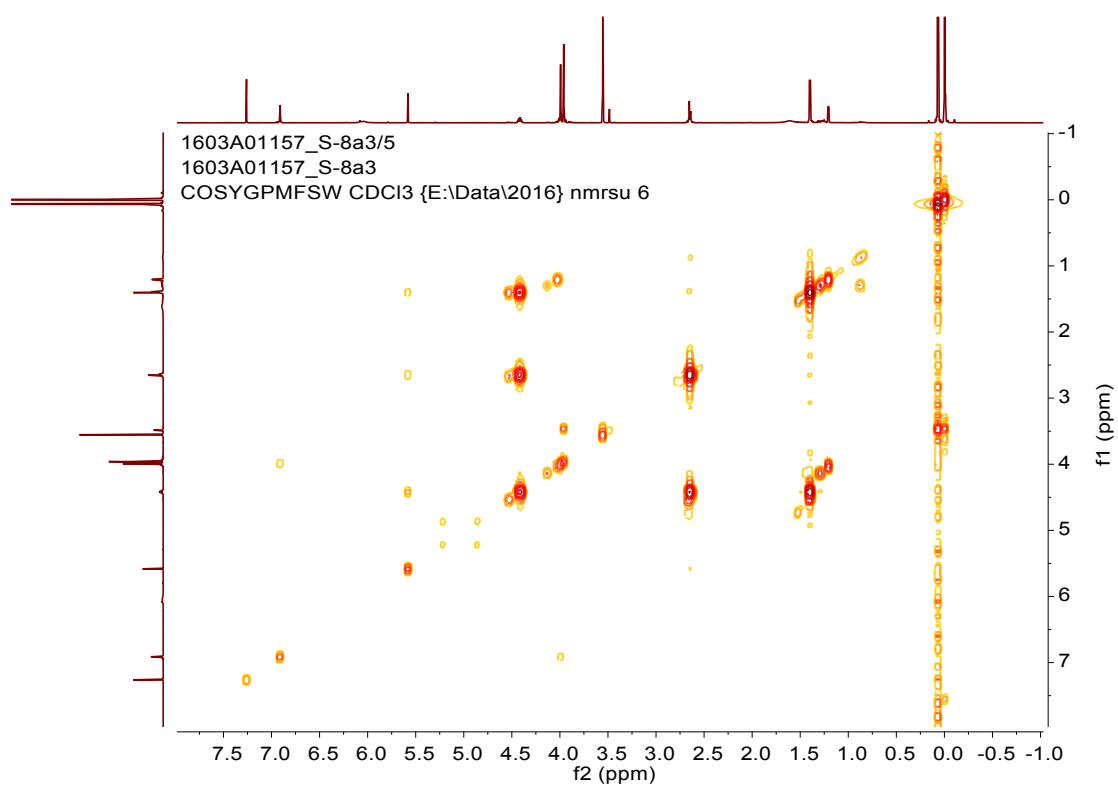


Figure S36 HSQC spectrum (500 MHz,  $\text{CDCl}_3$ ) of (+)-phomopsichin B (**6a**)

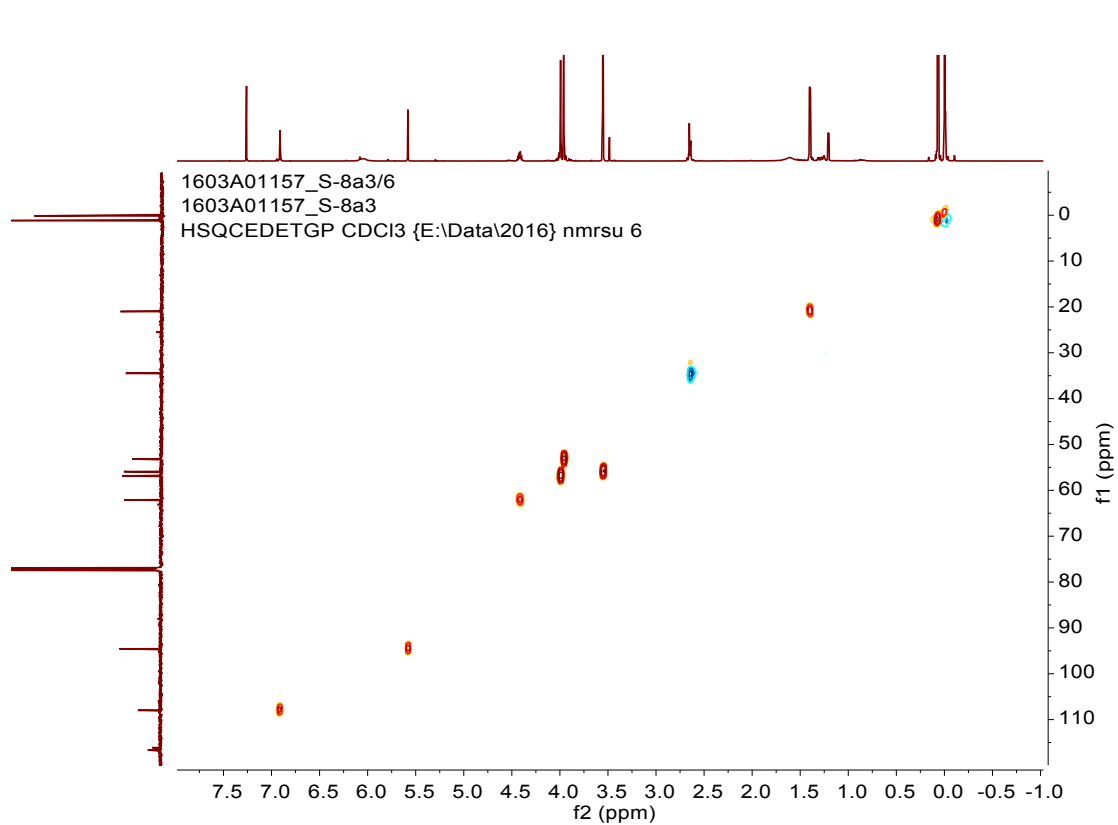


Figure S37 HMBC spectrum (500 MHz, CDCl<sub>3</sub>) of (+)-phomopsichin B (**6a**)

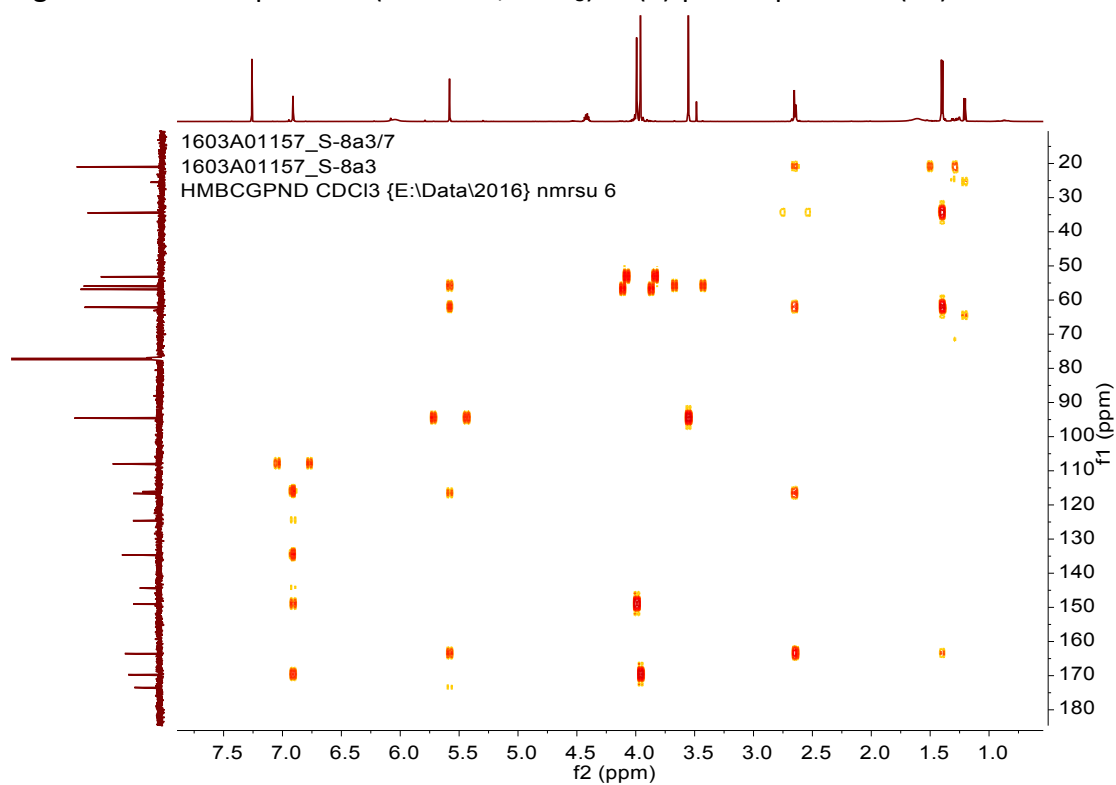
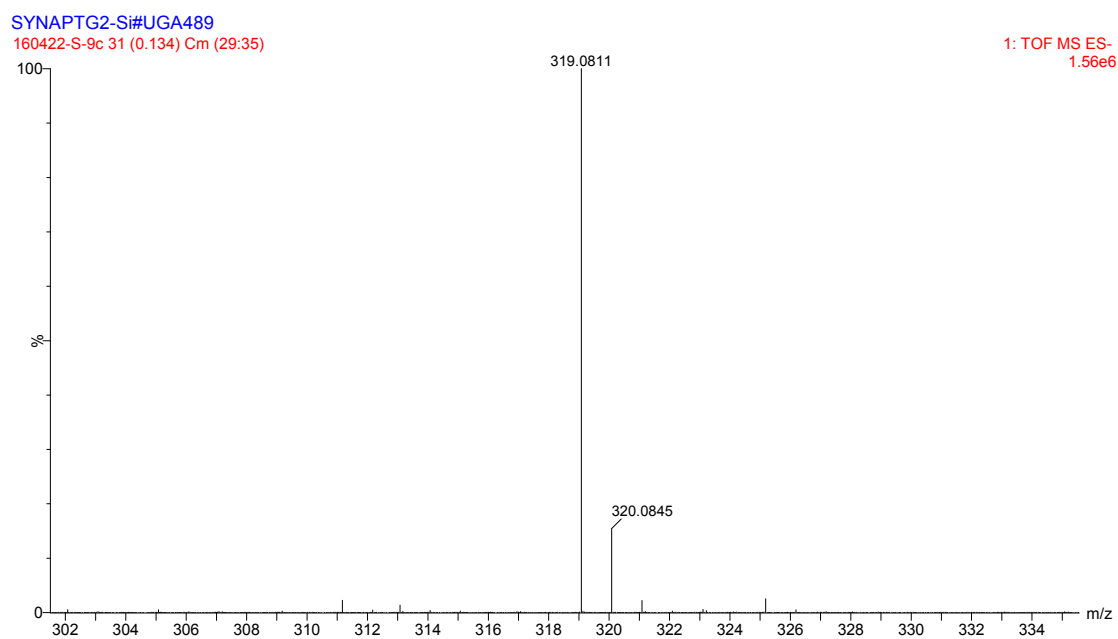


Figure S38 HRESIMS of (±)-diaporchromone A (**7**)



### Elemental Composition Report

#### Single Mass Analysis

Tolerance = 4.0 PPM / DBE: min = -1.5, max = 50.0

Monoisotopic Mass, Even Electron Ions

Elements Used:

C: 0-50 H: 0-100 O: 0-50

Mass	Calc. Mass	mDa	PPM	Formula
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319.0811 319.0818 -0.7 -2.2 C<sub>16</sub>H<sub>15</sub>O<sub>7</sub>

Figure S39 <sup>1</sup>H NMR spectrum (500MHz, CDCl<sub>3</sub>) of (±)-diaporchromone A (7)

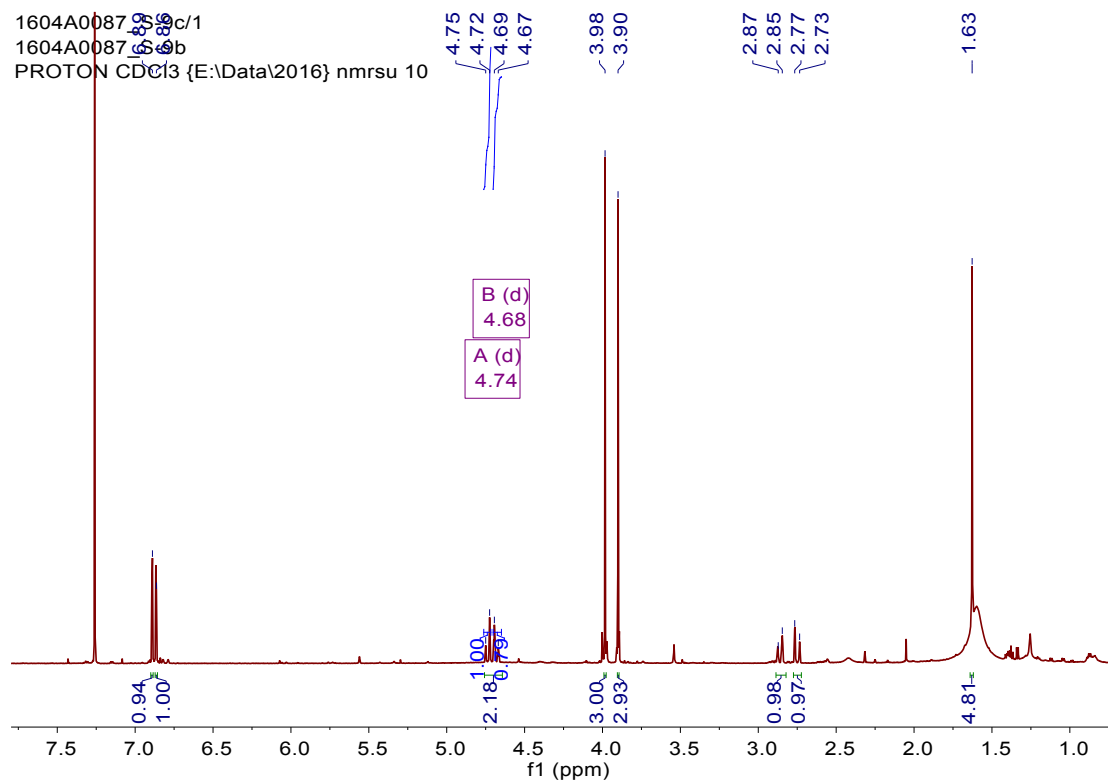


Figure S40 <sup>13</sup>C NMR spectrum (125 MHz, CDCl<sub>3</sub>) of (±)-diaporchromone A (7)

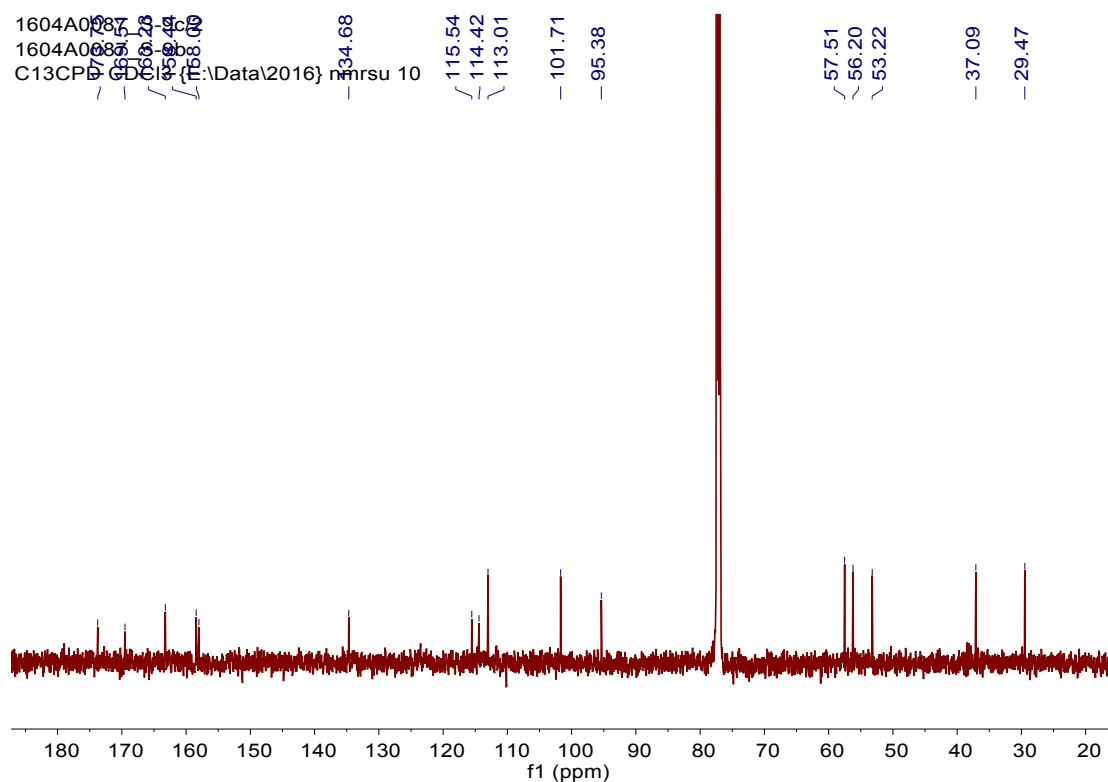




Figure S41 HSQC spectrum (500 MHz, CDCl<sub>3</sub>) of (±)-diaporchromone A (**7**)

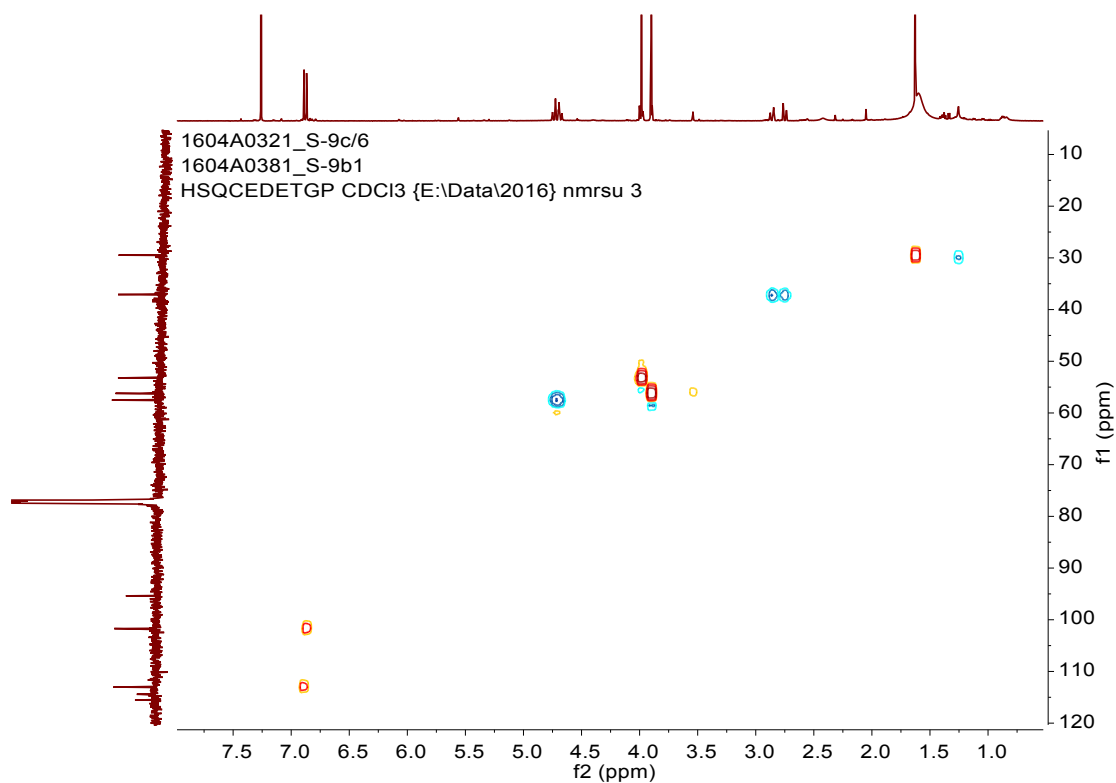
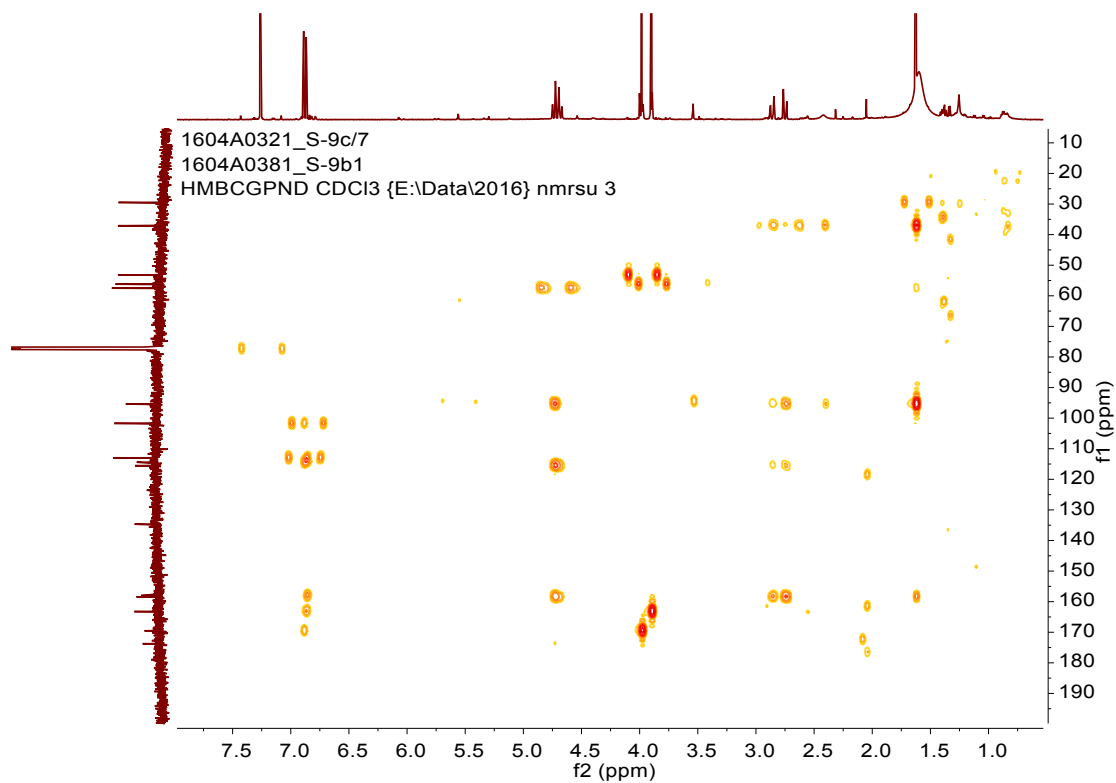


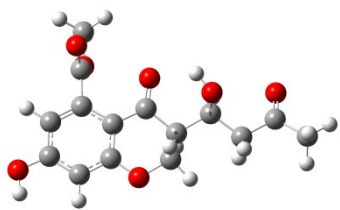
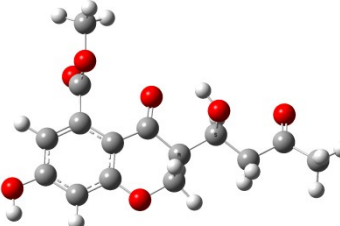
Figure S42 HSQC spectrum (500 MHz, CDCl<sub>3</sub>) of (±)-diaporchromone A (**7**)

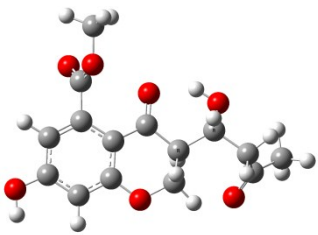
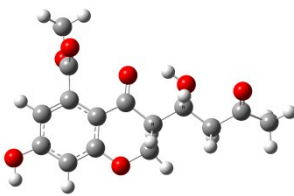
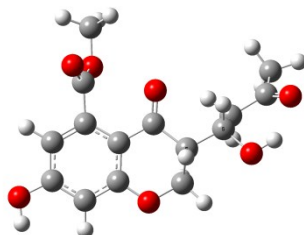
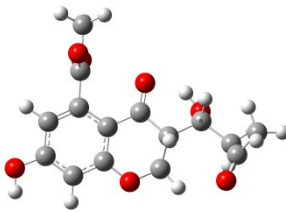
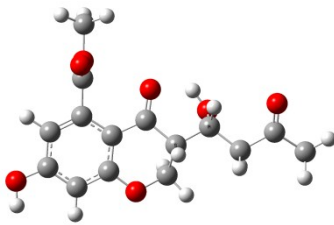


### Figure 43 ECD Calculation section

Conformational analysis was initially performed using Confab<sup>[1]</sup> at MMFF94 force field for one of the relative configurations for each compound. The conformers with Boltzmann-population of over 1% were chosen for ECD calculations. The energies and populations of all dominative conformers were provided in **Table 1**. The theoretical calculation was carried out using Gaussian 09<sup>[2]</sup>. First, the chosen conformer was optimized at B3LYP/6-311+g(2d,p) level, and conformers with low Boltzmann-populations were filtered. Then, the remaining conformers were further optimized at B3LYP/6-311+g(2d,p) in MeOH using the IEFPCM polarizable conductor calculation model. The theoretical calculation of ECD was conducted in MeOH using Time-dependent Density functional theory (TD-DFT) at the CAM-B3LYP/6-311+g(2d,p) level for compound **1**. Rotatory strengths for a total of 50 excited states were calculated. ECD spectra were generated using the program SpecDis 1.6 (University of Würzburg, Würzburg, Germany) and GraphPad Prism 5 (University of California San Diego, USA) from dipole-length rotational strengths by applying Gaussian band shapes with  $\sigma = 0.2$  eV<sup>[3]</sup>. All calculations were performed with the High-Performance Grid Computing Platform of Sun Yat-sen University.

**Table 1** The low energy conformers of the compound **1**.

Conformers	Low energy structure	$\Delta E$ (Kcal/mol)	Boltzmann Dist (%)
RS-1-a		0	63
RS-1-b		0.04	37

RR-1-a		0	81
RR-1-b		0.58	19
SR-1		0	100
SS-1-a		1.97	26.11
SS-1-b		0	73.9

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