

## Supporting Information

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### A New Benzophenone Derivative from the Endophyte *Shiraia* sp. BYJB-1

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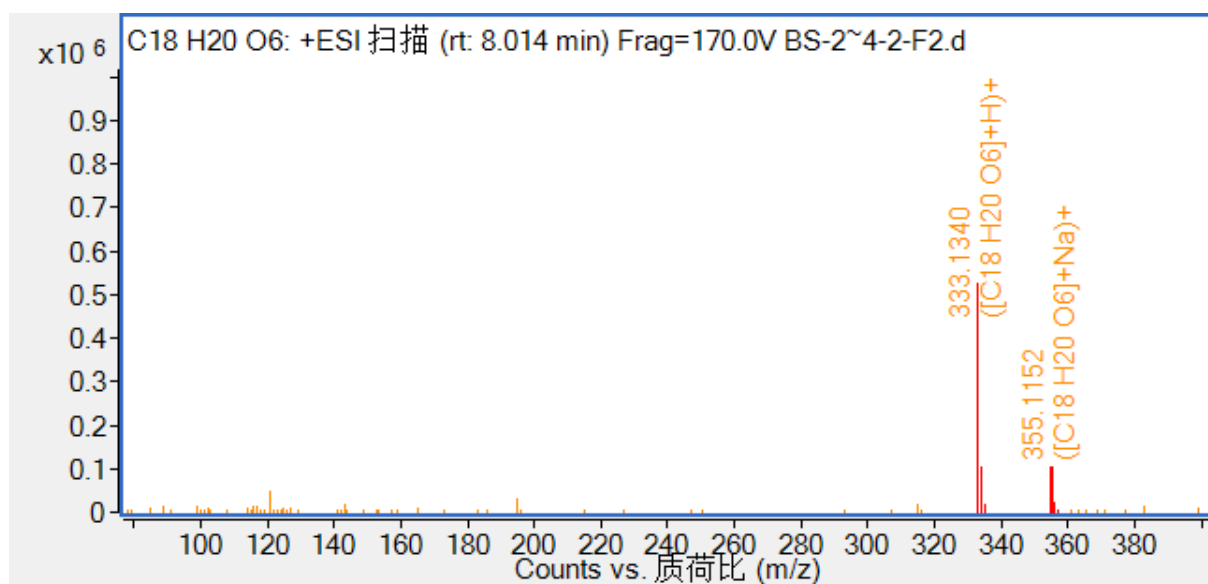
**Table S1:** Cytotoxicity activities of compounds **1-8**.

Compounds	IC50 <sup>c</sup> (μM)	
	SMMC7721	HepG2
<b>1</b>	N/A <sup>b</sup>	N/A
<b>2</b>	N/A	N/A
<b>3</b>	N/A	N/A
<b>4</b>	N/A	N/A
<b>5</b>	N/A	N/A
<b>6</b>	25.94 ± 2.07	50.48 ± 1.94
<b>7</b>	45.82 ± 1.32	N/A
<b>8</b>	N/A	N/A
Sorafenib <sup>a</sup>	2.19 ± 0.04	4.80 ± 0.08

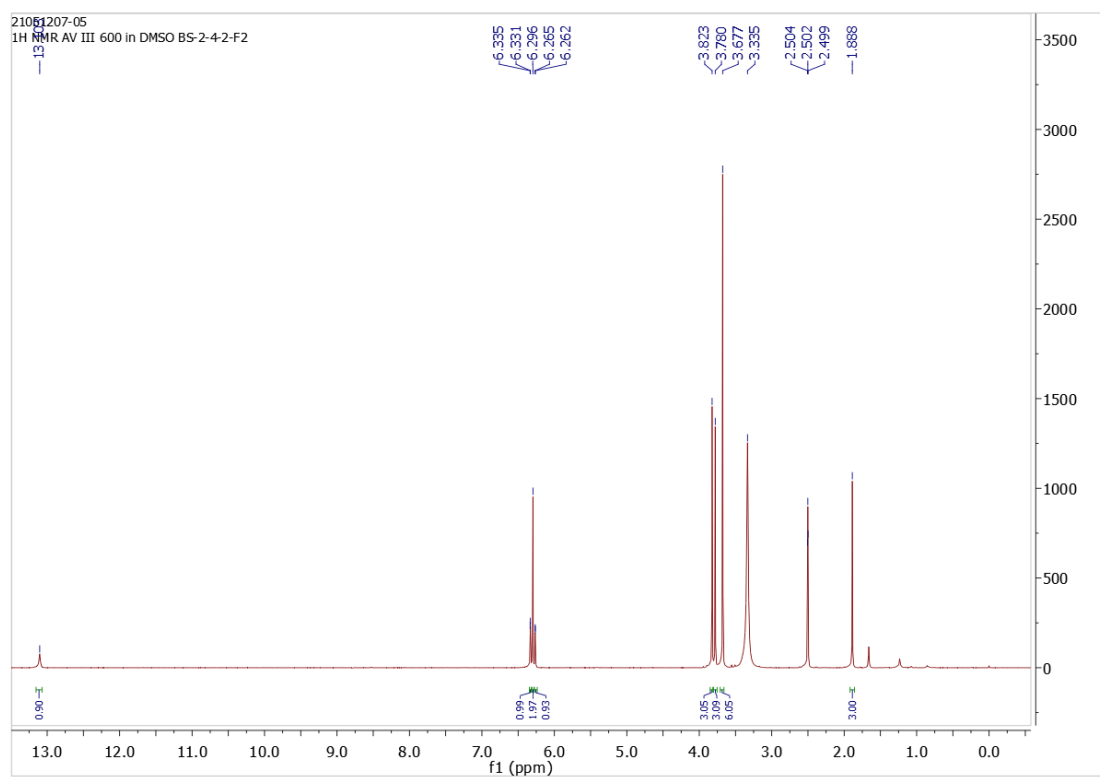
<sup>a</sup> positive control.<sup>b</sup> N/A: No active.<sup>c</sup> Results are the mean ± SD (*n* = 3).**Table S2 :** Antimicrobial activities of compounds **1-8**.

Compounds	MIC (μg/mL)	
	MRSA	<i>E. coil</i>
<b>1</b>	> 500	> 500
<b>2</b>	> 500	> 500
<b>3</b>	> 500	> 500
<b>4</b>	> 500	> 500
<b>5</b>	> 500	> 500
<b>6</b>	62.5	> 500
<b>7</b>	62.5	> 500
<b>8</b>	62.5	> 500
Vancomycin <sup>a</sup>	1.25	-
Kanamycin <sup>a</sup>	-	1.25

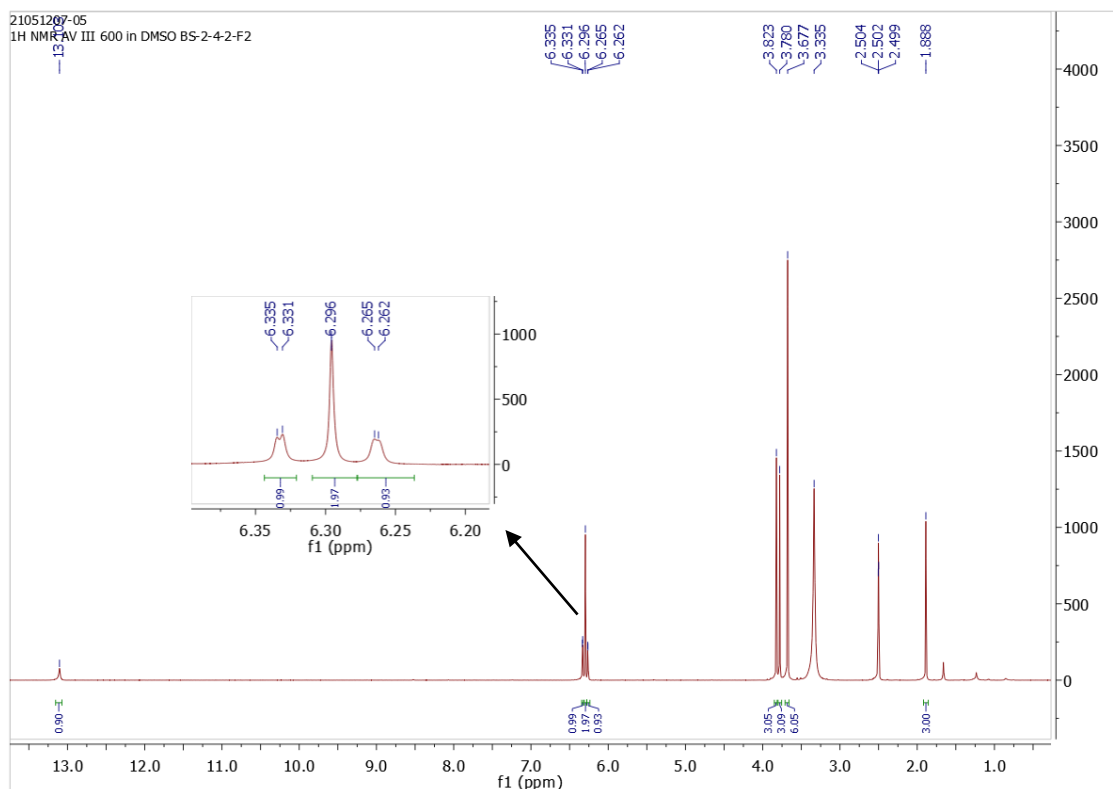
<sup>a</sup> positive control.



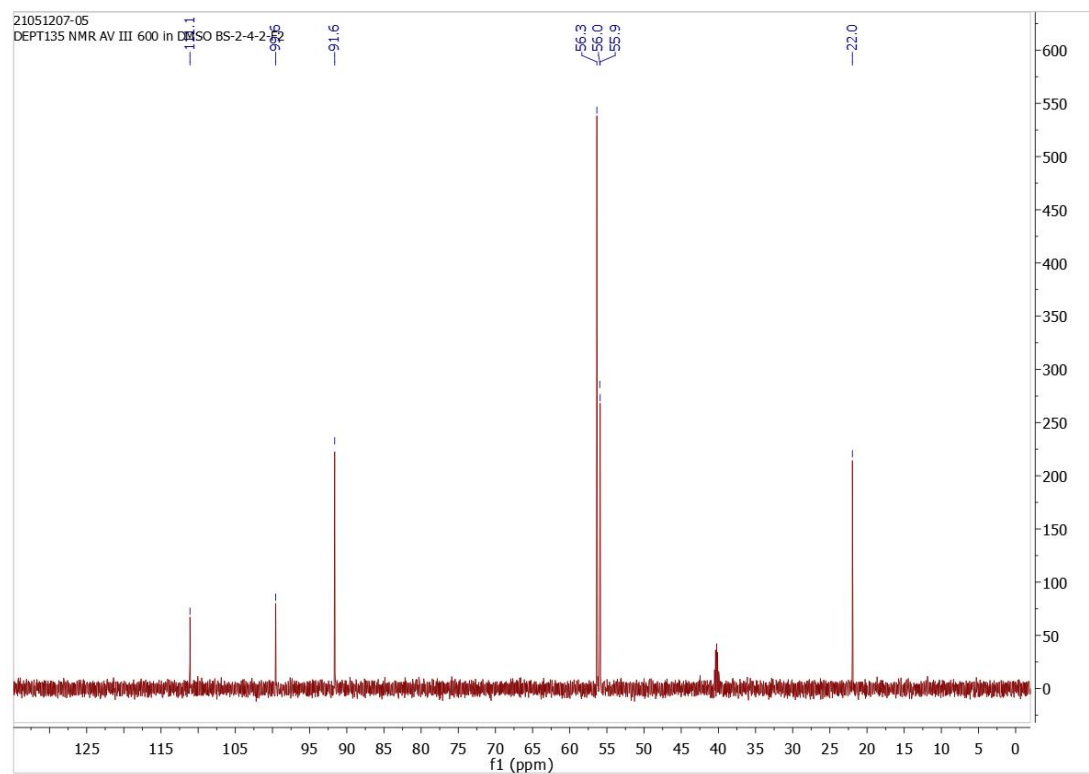
**Figure S1:** HR-ESI-MS spectrum of **1**



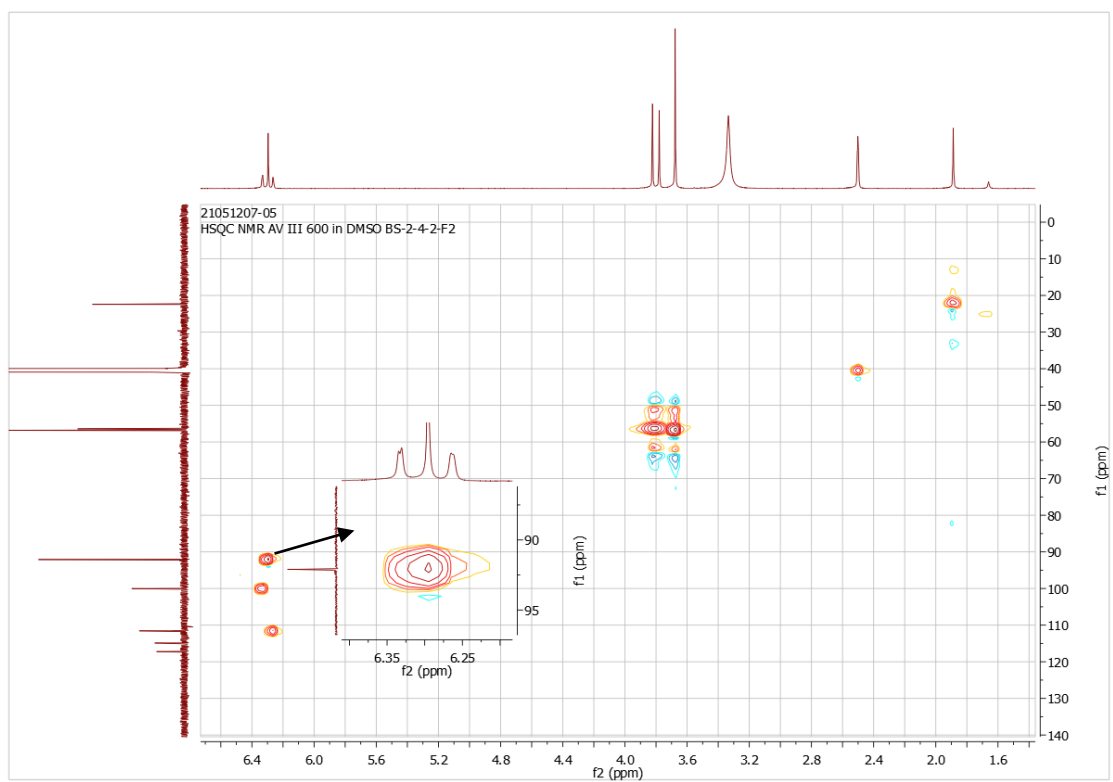
**Figure S2:**  $^1\text{H}$ -NMR (600 MHz,  $\text{DMSO}-d_6$ ) spectrum of **1**



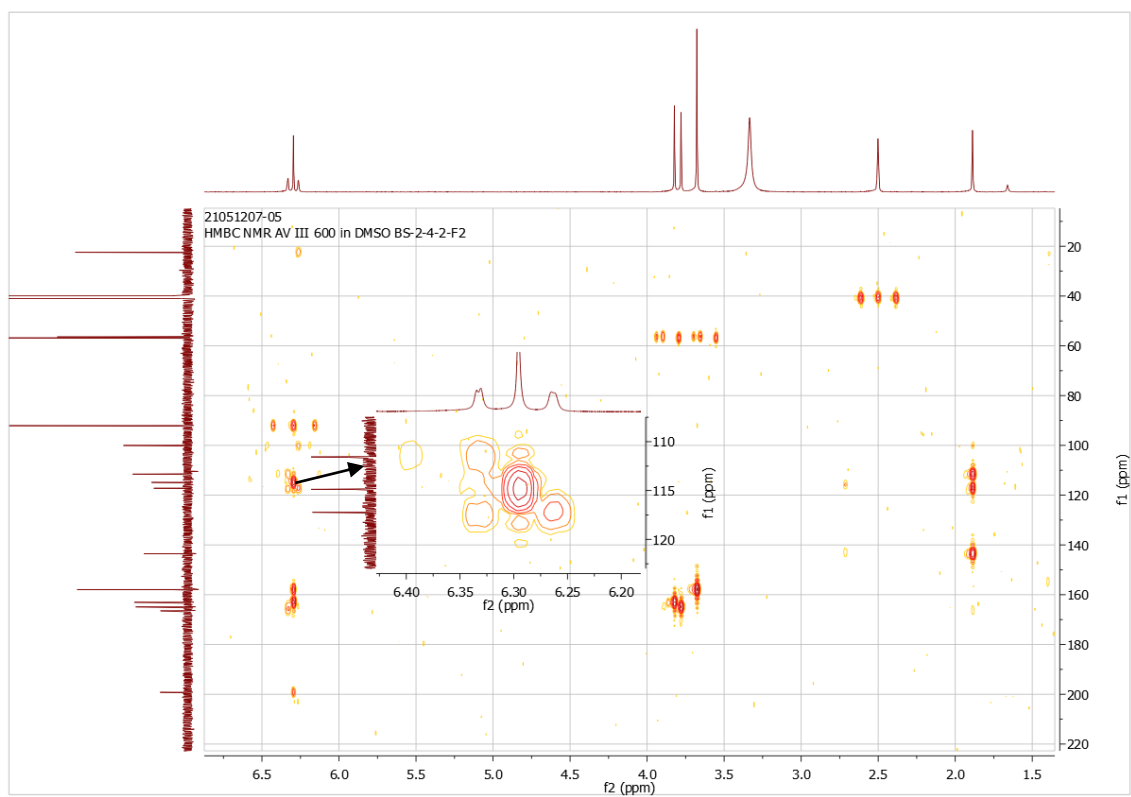
**Figure S3:**  $^1\text{H}$ -NMR (150 MHz,  $\text{DMSO}-d_6$ ) spectrum of **1**



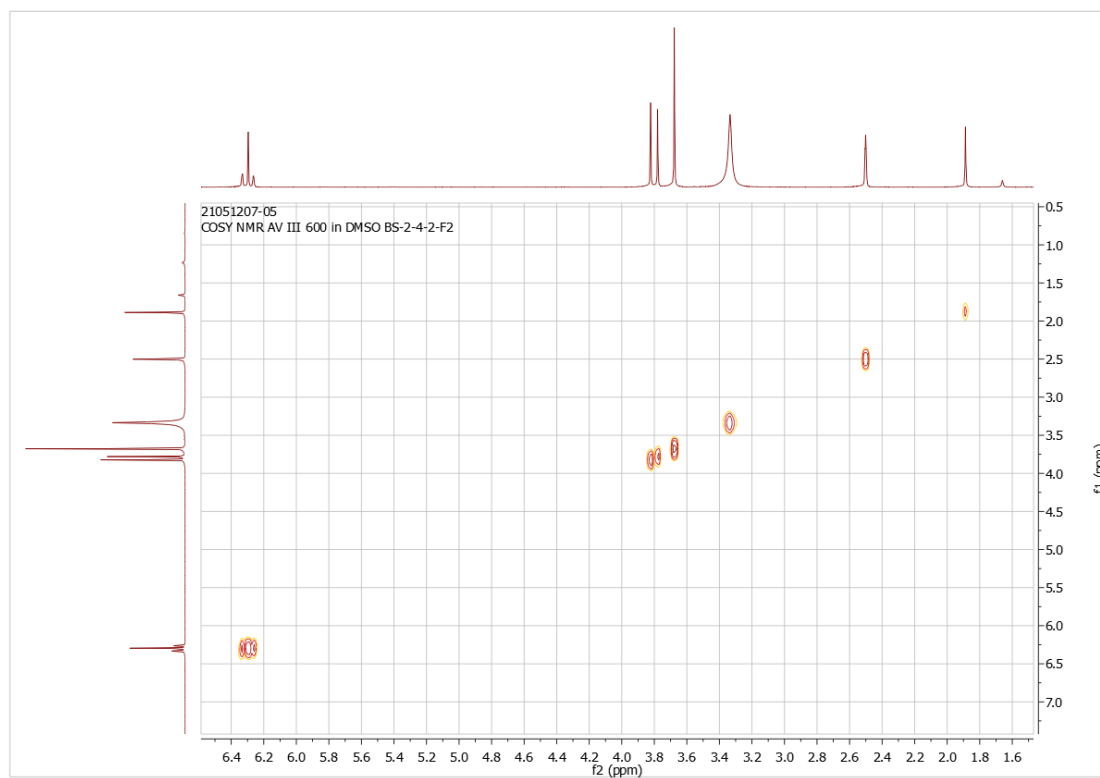
**Figure S4:** DEPT135 (150 MHz,  $\text{DMSO}-d_6$ ) spectrum of **1**



**Figure S5: HSQC spectrum of 1**



**Figure S6: HMBC spectrum of 1**



**Figure S7:**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1**

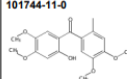
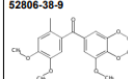
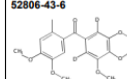
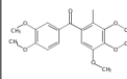
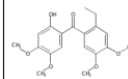
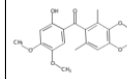
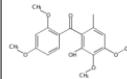
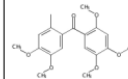
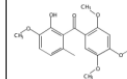
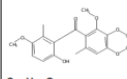
SciFinder®			Page 1
<p>Score: 99</p> <p>1.</p> <p><b>101744-11-0</b></p>  <p><b>C<sub>18</sub> H<sub>20</sub> O<sub>6</sub></b> Benzophenone, 2-hydroxy-4,4',5,5'-tetramethoxy-2'-methyl- (6CI)</p> <p><b>Key Physical Properties:</b> <b>Molecular Weight</b> 332.35 <b>Boiling Point (Predicted)</b> Value: 481.4±45.0 °C   Condition: Press: 760 Torr <b>Density (Predicted)</b> Value: 1.194±0.06 g/cm3   Condition: Temp: 20 °C Press: 760 Torr <b>pKa (Predicted)</b> Value: 7.58±0.48   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 1 References ~ 2 Commercial Sources</p>	<p>Score: 96</p> <p>2.</p> <p><b>52806-38-9</b></p>  <p><b>C<sub>19</sub> H<sub>22</sub> O<sub>6</sub></b> Methanone, (4,5-dimethoxy-2-methylphenyl)(3,4,5-trimethoxyphenyl)-</p> <p><b>Key Physical Properties:</b> <b>Molecular Weight</b> 346.37 <b>Boiling Point (Predicted)</b> Value: 485.5±45.0 °C   Condition: Press: 760 Torr <b>Density (Predicted)</b> Value: 1.139±0.06 g/cm3   Condition: Temp: 20 °C Press: 760 Torr</p> <p><b>Related Info:</b> ~ 1 References ~ 2 Commercial Sources</p>	<p>Score: 96</p> <p>3.</p> <p><b>52806-43-6</b></p>  <p><b>C<sub>19</sub> H<sub>20</sub> O<sub>2</sub> O<sub>6</sub></b> Methanone, (4,5-dimethoxy-2-methylphenyl)(3,4,5-trimethoxyphenyl)-2,6-d<sub>2</sub>- (9CI)</p> <p><b>Related Info:</b> ~ 1 References ~ 2 Commercial Sources</p>	
<p>Score: 96</p> <p>4.</p> <p><b>56890-08-5</b></p>  <p><b>C<sub>19</sub> H<sub>22</sub> O<sub>6</sub></b> Methanone, (3,4-dimethoxyphenyl)(3,4,5-trimethoxy-2-methylphenyl)-</p> <p><b>Key Physical Properties:</b> <b>Molecular Weight</b> 346.37 <b>Boiling Point (Predicted)</b> Value: 480.7±45.0 °C   Condition: Press: 760 Torr <b>Density (Predicted)</b> Value: 1.139±0.06 g/cm3   Condition: Temp: 20 °C Press: 760 Torr</p> <p><b>Related Info:</b> ~ 1 References ~ 5 Commercial Sources Spectra</p>	<p>Score: 96</p> <p>5.</p> <p><b>102162-90-3</b></p>  <p><b>C<sub>19</sub> H<sub>22</sub> O<sub>6</sub></b> Benzophenone, 2-ethyl-2'-hydroxy-4,4',5,5'-tetramethoxy- (6CI)</p> <p><b>Key Physical Properties:</b> <b>Molecular Weight</b> 346.37 <b>Boiling Point (Predicted)</b> Value: 537.3±50.0 °C   Condition: Press: 760 Torr <b>Density (Predicted)</b> Value: 1.174±0.06 g/cm3   Condition: Temp: 20 °C Press: 760 Torr <b>pKa (Predicted)</b> Value: 7.58±0.48   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 1 References ~ 2 Commercial Sources</p>	<p>Score: 96</p> <p>6.</p> <p><b>102162-91-4</b></p>  <p><b>C<sub>19</sub> H<sub>22</sub> O<sub>6</sub></b> Benzophenone, 2'-hydroxy-3,4,4',5'-tetramethoxy-2,6-dimethyl- (6CI)</p> <p><b>Key Physical Properties:</b> <b>Molecular Weight</b> 346.37 <b>Boiling Point (Predicted)</b> Value: 471.2±45.0 °C   Condition: Press: 760 Torr <b>Density (Predicted)</b> Value: 1.175±0.06 g/cm3   Condition: Temp: 20 °C Press: 760 Torr <b>pKa (Predicted)</b> Value: 7.59±0.48   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 1 References ~ 2 Commercial Sources</p>	
SciFinder®			Page 2
<p>Score: 96</p> <p>7.</p> <p><b>2253623-31-1</b></p>  <p><b>C<sub>19</sub> H<sub>20</sub> O<sub>6</sub></b> INDEX NAME NOT YET ASSIGNED</p> <p><b>Key Physical Properties:</b> <b>Molecular Weight</b> 332.35 <b>Boiling Point (Predicted)</b> Value: 496.3±45.0 °C   Condition: Press: 760 Torr <b>Density (Predicted)</b> Value: 1.194±0.06 g/cm3   Condition: Temp: 20 °C Press: 760 Torr <b>pKa (Predicted)</b> Value: 7.21±0.45   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 3 References Reactions</p>	<p>Score: 95</p> <p>8.</p> <p><b>102162-92-5</b></p>  <p><b>C<sub>19</sub> H<sub>22</sub> O<sub>6</sub></b> Benzophenone, 2,4,4',5,5'-pentamethoxy-2'-methyl- (6CI)</p> <p><b>Key Physical Properties:</b> <b>Molecular Weight</b> 346.37 <b>Boiling Point (Predicted)</b> Value: 518.1±50.0 °C   Condition: Press: 760 Torr <b>Density (Predicted)</b> Value: 1.139±0.06 g/cm3   Condition: Temp: 20 °C Press: 760 Torr</p> <p><b>Related Info:</b> ~ 1 References ~ 2 Commercial Sources</p>	<p>Score: 95</p> <p>9.</p> <p><b>129103-92-0</b></p>  <p><b>C<sub>19</sub> H<sub>20</sub> O<sub>6</sub></b> Methanone, (2-hydroxy-3-methoxy-6-methylphenyl)(2,4,5-trimethoxyphenyl)-</p> <p><b>Key Physical Properties:</b> <b>Molecular Weight</b> 332.35 <b>Boiling Point (Predicted)</b> Value: 493.4±45.0 °C   Condition: Press: 760 Torr <b>Density (Predicted)</b> Value: 1.194±0.06 g/cm3   Condition: Temp: 20 °C Press: 760 Torr <b>pKa (Predicted)</b> Value: 7.49±0.40   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 2 References Reactions</p>	
<p>Score: 95</p> <p>10.</p> <p><b>1101903-04-1</b></p>  <p><b>C<sub>19</sub> H<sub>22</sub> O<sub>6</sub></b> Methanone, (6-hydroxy-3-methoxy-2-methylphenyl)(2,3,4-trimethoxy-6-methylphenyl)-</p> <p><b>Key Physical Properties:</b> <b>Molecular Weight</b> 346.37 <b>Boiling Point (Predicted)</b> Value: 486.6±45.0 °C   Condition: Press: 760 Torr <b>Density (Predicted)</b> Value: 1.175±0.06 g/cm3   Condition: Temp: 20 °C Press: 760 Torr <b>pKa (Predicted)</b> Value: 7.99±0.48   Condition: Most Acidic Temp: 25 °C</p> <p><b>Related Info:</b> ~ 1 References</p>			

Figure S8: Scifinder search reports