

## Supporting Information

### A new diterpenoid from *Salvia santolinifolia* Boiss.

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#### Abstract

Phytochemical study of the *Salvia santolinifolia* root extract resulted in the isolation of one  
new quinone diterpenoid, aegyptinone E (**1**) as well as two known ones, aegyptinone A (**2**)  
and aegyptinone D (**3**). All the isolated compounds were reported for the first time from *S.*  
*santolinifolia*. Spectroscopic analyses including 1D and 2D NMR and HRESIMS were used  
to determine the chemical structures. Aegyptinone A (**2**) showed moderate antibacterial  
activity against *Staphylococcus aureus*, *Staphylococcus epidermis*, and *Bacillus subtilis* with  
MIC of 25 µg/mL.

**Keywords:** Quinone diterpenoids, *Salvia*, antibacterial activity, Lamiaceae

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### List of Supporting Information

**Figure S1.**  $^1\text{H}$  NMR Spectrum (600 MHz,  $\text{CDCl}_3$ ) of compound **1**.

**Figure S2.**  $^{13}\text{C}$  NMR Spectrum (150 MHz,  $\text{CDCl}_3$ ) of compound **1**.

**Figure S3.** HSQC Spectrum ( $\text{CDCl}_3$ ) of compound **1**.

**Figure S4.** HMBC Spectrum ( $\text{CDCl}_3$ ) of compound **1**.

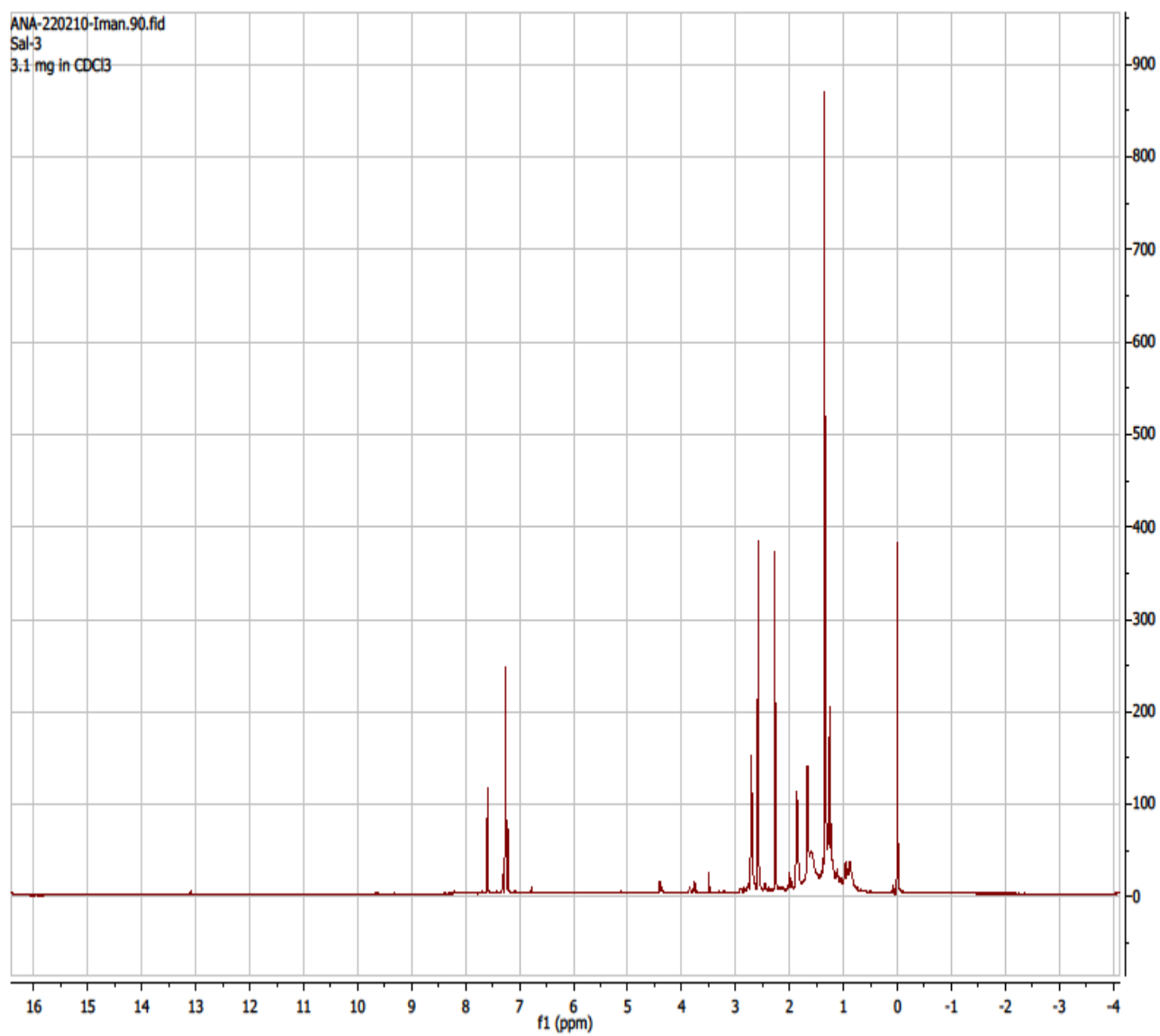
**Figure S5.** COSY Spectrum ( $\text{CDCl}_3$ ) of compound **1**.

**Figure S6.** HRMS Spectrum of compound **1**.

**Table S1.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopic data of compound **1-3** (600 MHz in  $\text{CDCl}_3$ ,  $\delta$  in ppm,  $J$  in Hz).

**Table S2.** Antimicrobial properties of the isolated compounds.

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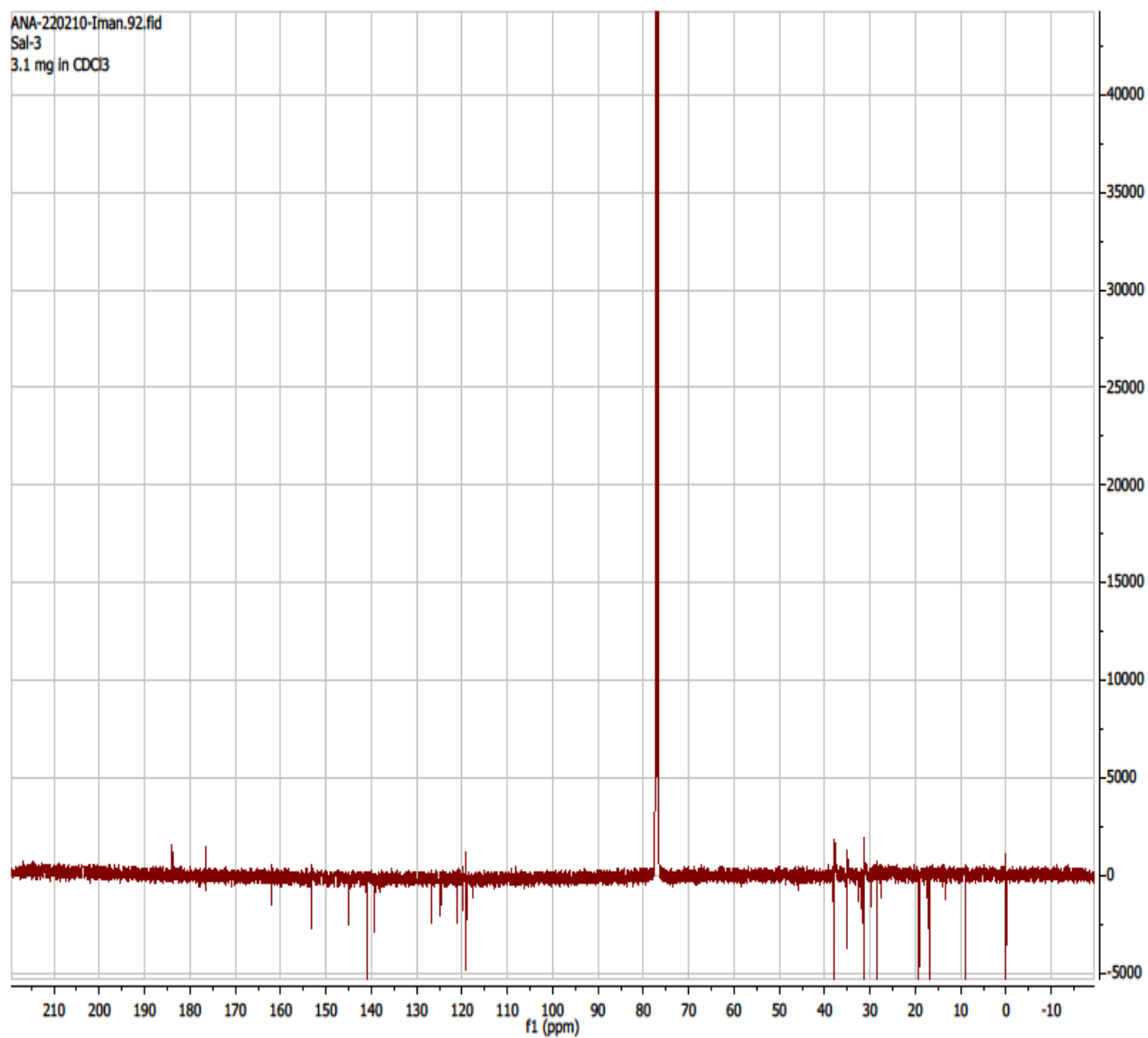
**Figure S1.** <sup>1</sup>H-NMR Spectrum (600 MHz, CDCl<sub>3</sub>) of compound **1**.

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**Figure S2.** <sup>13</sup>C-NMR Spectrum (125 MHz, CDCl<sub>3</sub>) of compound **1**.

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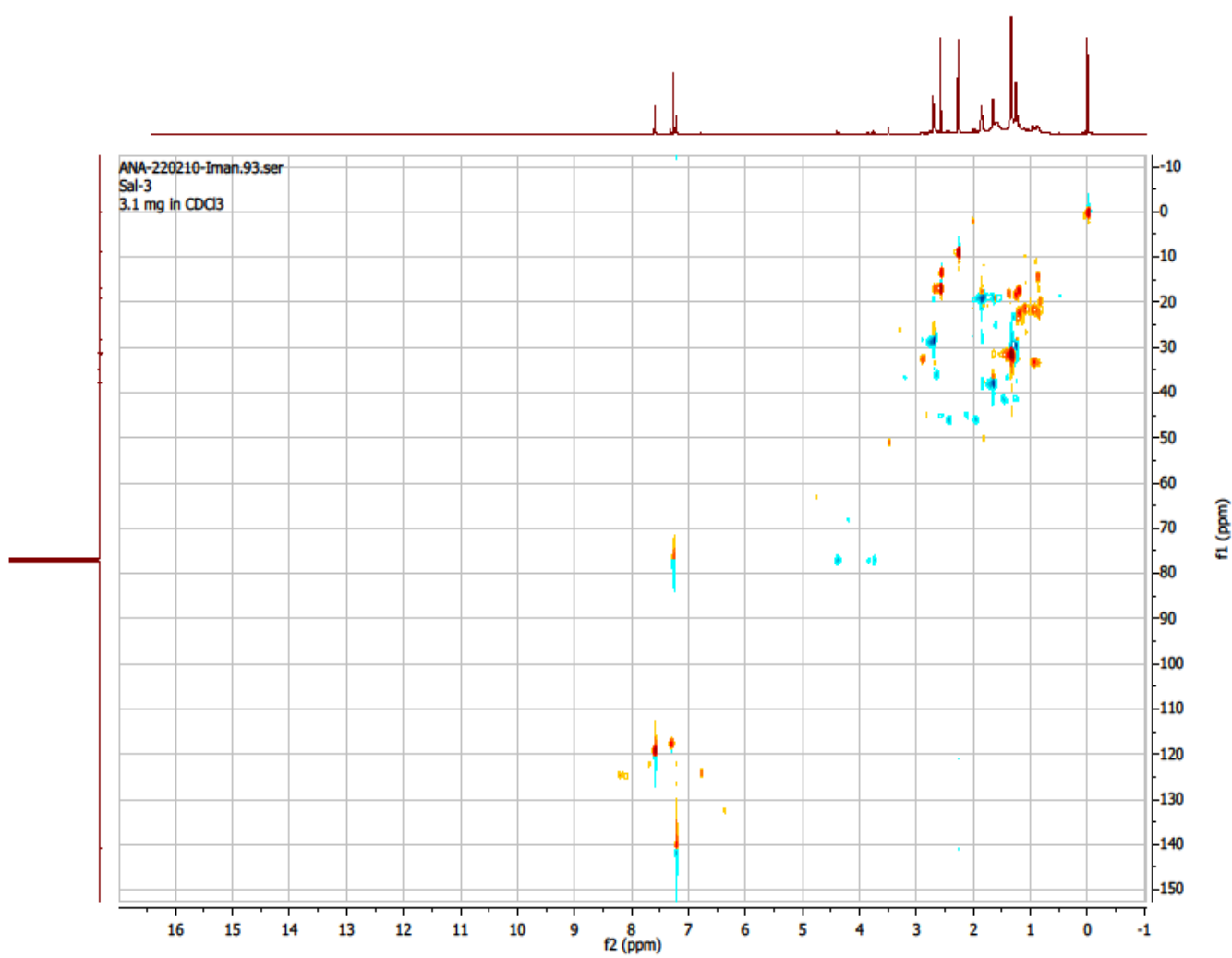
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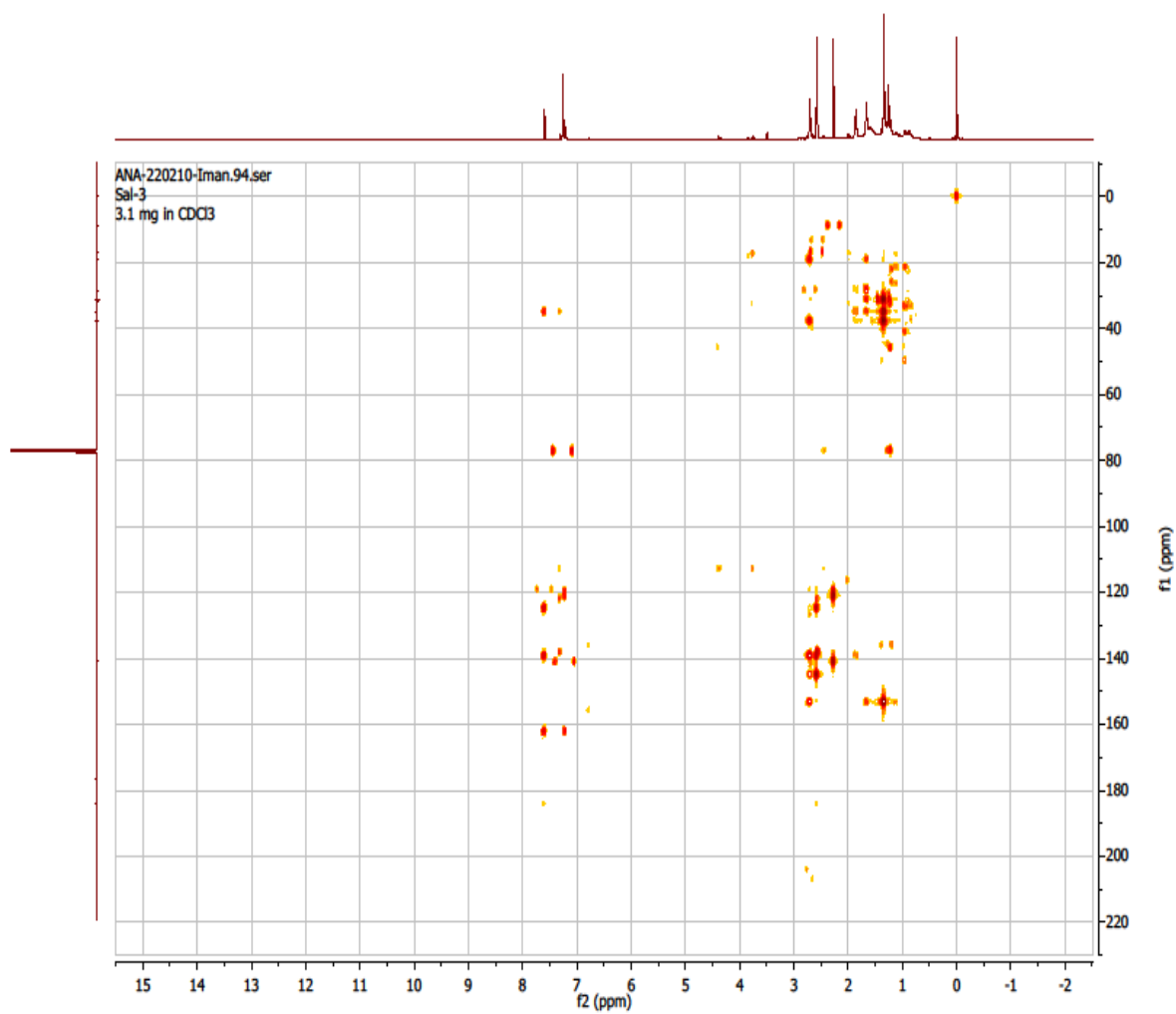
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**Figure S3.** HSQC Spectrum (CDCl<sub>3</sub>) of compound **1**.



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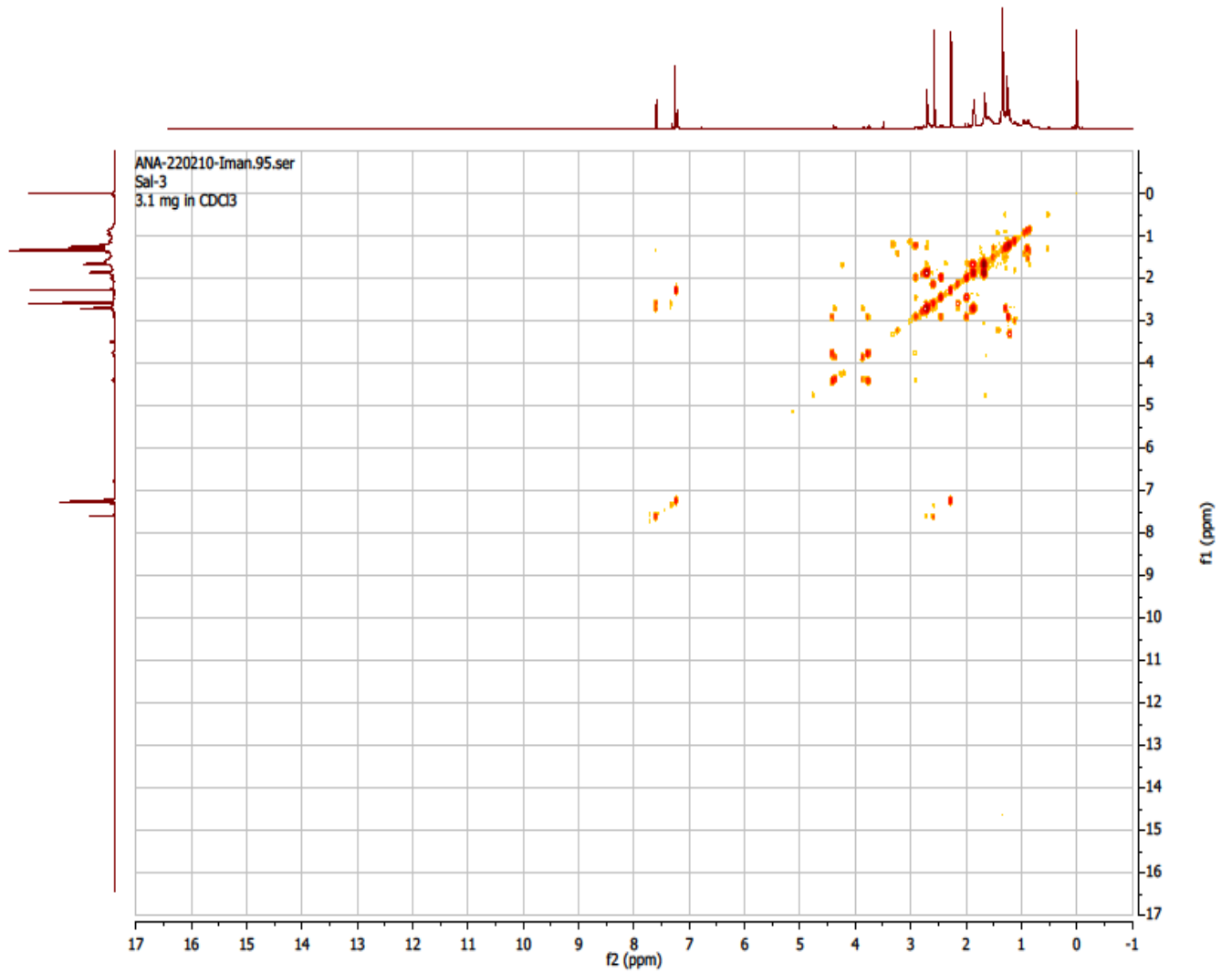
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**Figure S4.** HMBC Spectrum (CDCl<sub>3</sub>) of compound **1**.

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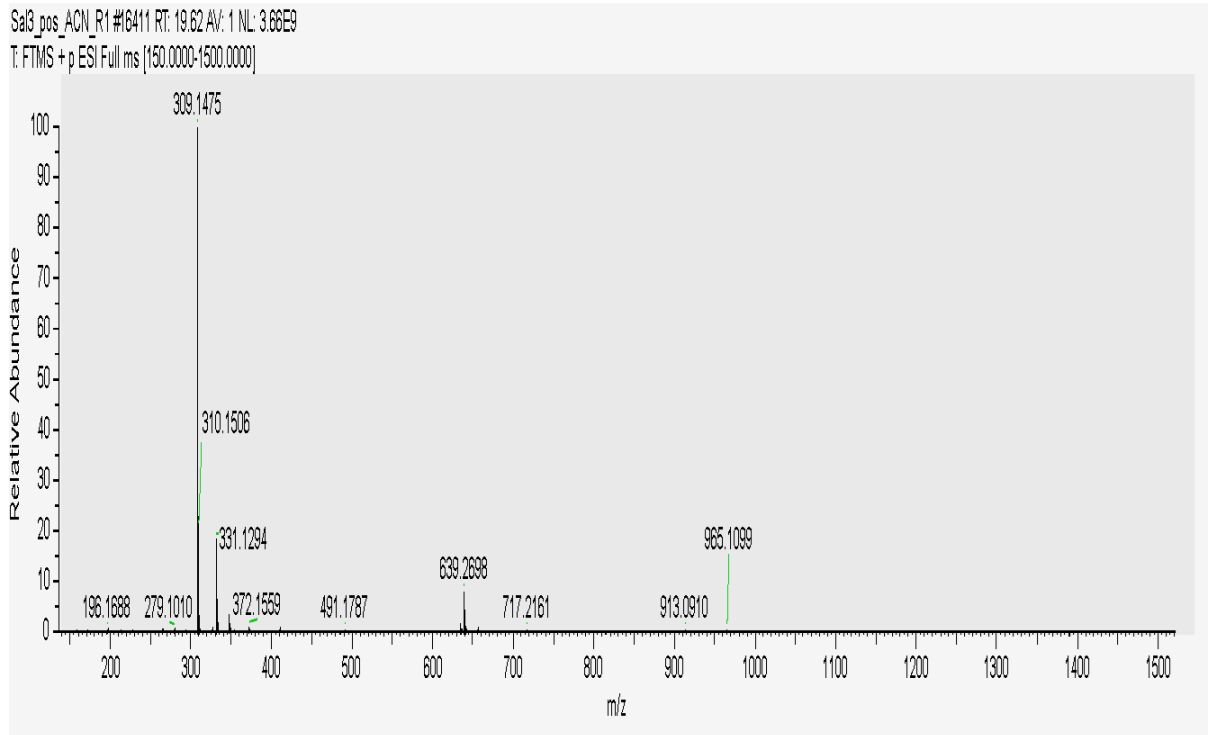
**Figure S5.** COSY Spectrum (CDCl<sub>3</sub>) of compound **1**.

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111 **Figure S6.** HRMS Spectrum of compound **1**.

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124 **Table S1.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectroscopic data of compound **1-3** (600 MHz in  $\text{CDCl}_3$ ,  $\delta$  in  
 125 ppm,  $J$  in Hz).

Compound 1			Compound 2			Compound 3		
	$^1\text{H-NMR}$	$^{13}\text{C-NMR}$		$^1\text{H-NMR}$ ( $J$ , in Hz)	$^{13}\text{C-NMR}$		$^1\text{H-NMR}$	$^{13}\text{C-NMR}$
<b>1</b>	2.71 t (6.5)	28.2	<b>1</b>	2.61 t (6.4)	28.4	<b>1</b>	2.72 m	32.1
<b>2</b>	1.86 m	18.1	<b>2</b>	1.76 m	19.0	<b>2</b>	1.90 m	19.2
<b>3</b>	1.66 m	37.0	<b>3</b>	1.56 m	37.7	<b>3</b>	1.71 m	38.1
<b>4</b>	-	34.5	<b>4</b>	-	34.9	<b>4</b>	-	35.5
<b>5</b>	-	153.0	<b>5</b>	-	152.2	<b>5</b>	-	153.3
<b>6</b>	7.60 s	119.3	<b>6</b>	7.46 s	121.7	<b>6</b>	7.35 s	117.8
<b>7</b>	-	126.5	<b>7</b>	-	125.5	<b>7</b>	-	134.1
<b>8</b>	-	124.7	<b>8</b>	-	126.1	<b>8</b>	-	122.5
<b>9</b>	-	144.6	<b>9</b>	-	144.0	<b>9</b>	-	143.5
<b>10</b>	-	139.4	<b>10</b>	-	141.2	<b>10</b>	-	143.5
<b>11</b>	-	183.9	<b>11</b>	-	184.4	<b>11</b>	-	173.8
<b>12</b>	-	176.4	<b>12</b>	-	176.2	<b>12</b>	-	168.6
<b>13</b>	-	120.9	<b>13</b>	-	118.2	<b>13</b>	-	113.7
<b>14</b>	-	162.2	<b>14</b>	-	171.0	<b>14</b>	-	184.0
<b>15</b>	7.25 s	140.9	<b>15<math>\alpha</math></b>	4.28 dd (9.4, 6.0)	81.3	<b>15</b>	3.49 m	34.1
			<b>15<math>\beta</math></b>	4.82 t (9.4)				
<b>16</b>	-	119.6	<b>16</b>	3.51m	34.6	<b>16<math>\alpha</math></b>	4.42 dd (8.4, 5.0)	76.9
						<b>16<math>\beta</math></b>	3.2 t (8.4)	
<b>17</b>	2.27 s	8.6	<b>17</b>	1.25 d (6.8)	18.8	<b>17</b>	1.88 d (6.7)	19.0
<b>18</b>	1.35 s	31.4	<b>18</b>	1.23 s	30.9	<b>18</b>	1.36 s	31.1
<b>19</b>	1.35 s	31.3	<b>19</b>	1.23 s	30.9	<b>19</b>	1.36 s	31.1
<b>20</b>	2.57 s	16.7	<b>20</b>	2.49 s	16.6	<b>20</b>	2.60 s	13.3

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137 **Table S2.** Antimicrobial properties of the isolated compounds.

	<i>St. aur</i>		<i>St. epi</i>		<i>Ba. sub</i>		<i>Ps. aer</i>		<i>E. coli</i>	
	$\mu\text{g/mL}$									
n.o	MIC	MBC	MIC	MBC	MIC	MBC	MIC	MBC	MIC	MBC
<b>1</b>	n.a <sup>a</sup>	n.a	n.a	n.a	n.a	n.a	n.a	n.a	n.a	n.a
<b>2</b>	25	25	25	25	25	25	100	n.a	n.a	n.a
<b>3</b>	n.a <sup>a</sup>	n.a	n.a	n.a	n.a	n.a	n.a	n.a	n.a	n.a
<b>Cloxacillin</b>	-	-	-	-	0.39	0.39	-	-	-	-
<b>Tobramycin</b>	-	-	-	-	-	-	1.56	3.125	3.125	3.125

138 <sup>a</sup>not active (>100  $\mu\text{g/mL}$ )

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