

## Supporting Information

### **Rational Design of Dimeric Lysine *N*-Alkylamides as Potent and Broad-Spectrum Antibacterial Agents**

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Yanfen Wu,<sup>†</sup> Jianfeng Cai,<sup>‡,\*</sup> and Xin-Shan Ye<sup>†,\*</sup>

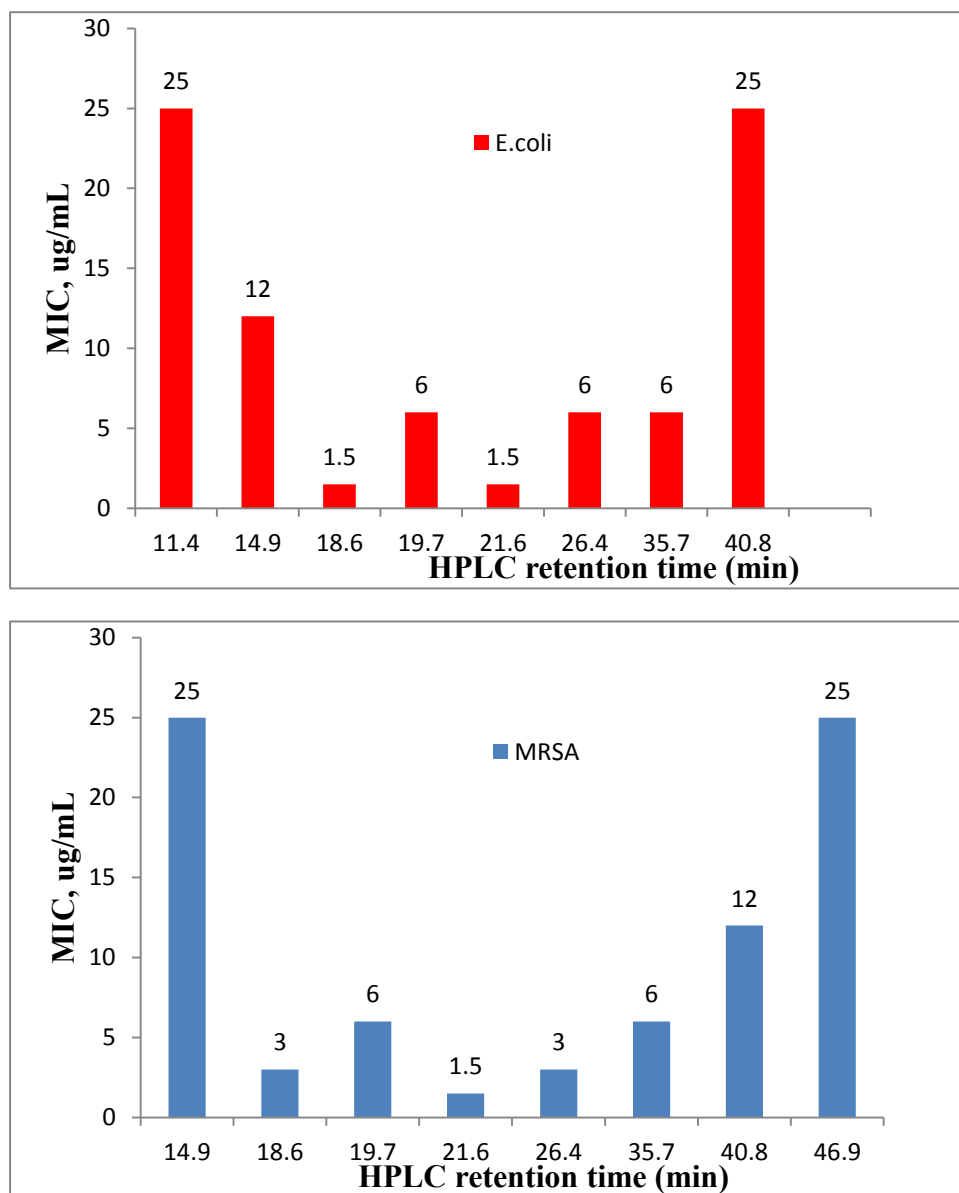
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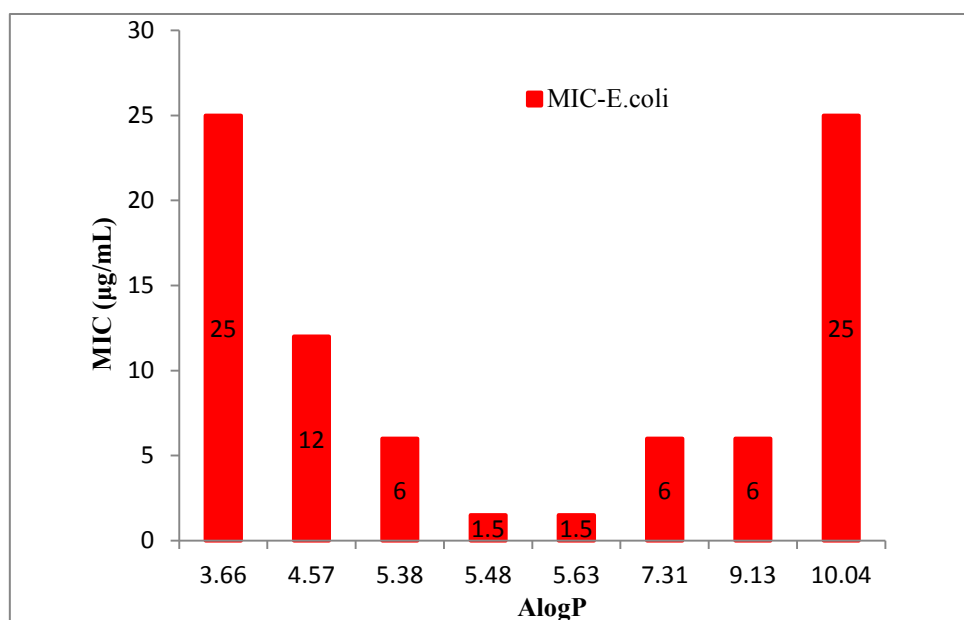
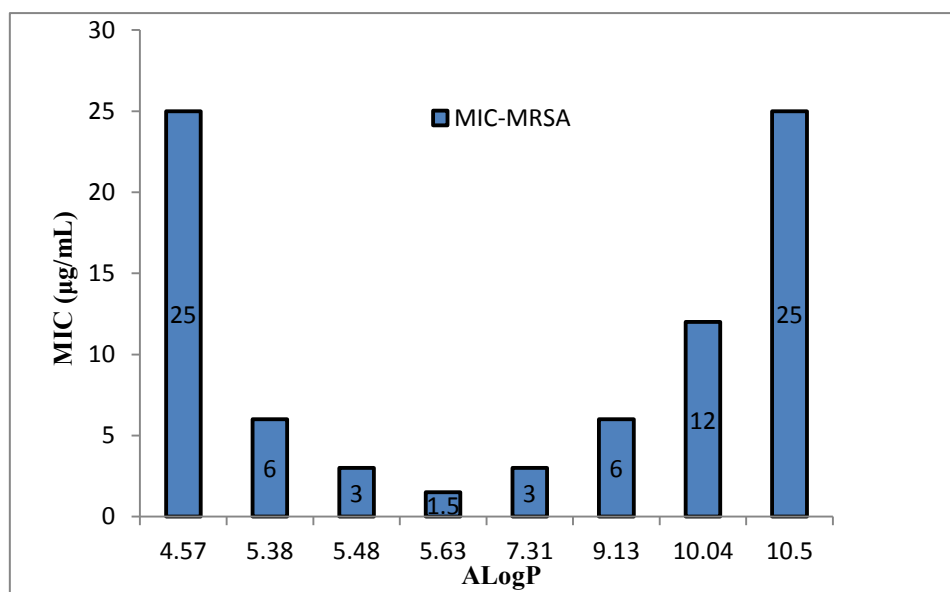
#### **Content:**

1. Correlation of antibacterial activity (MIC) against MRSA and *E. coli* vers AlogP of compounds **3a-3i**
2. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compounds **1, 2, 3a-3i**
3. HPLC analysis of compounds **3a-3i**

1. Correlation of antibacterial activity (MIC) against MRSA and *E. coli* vers AlogP of compounds **3a-3i**



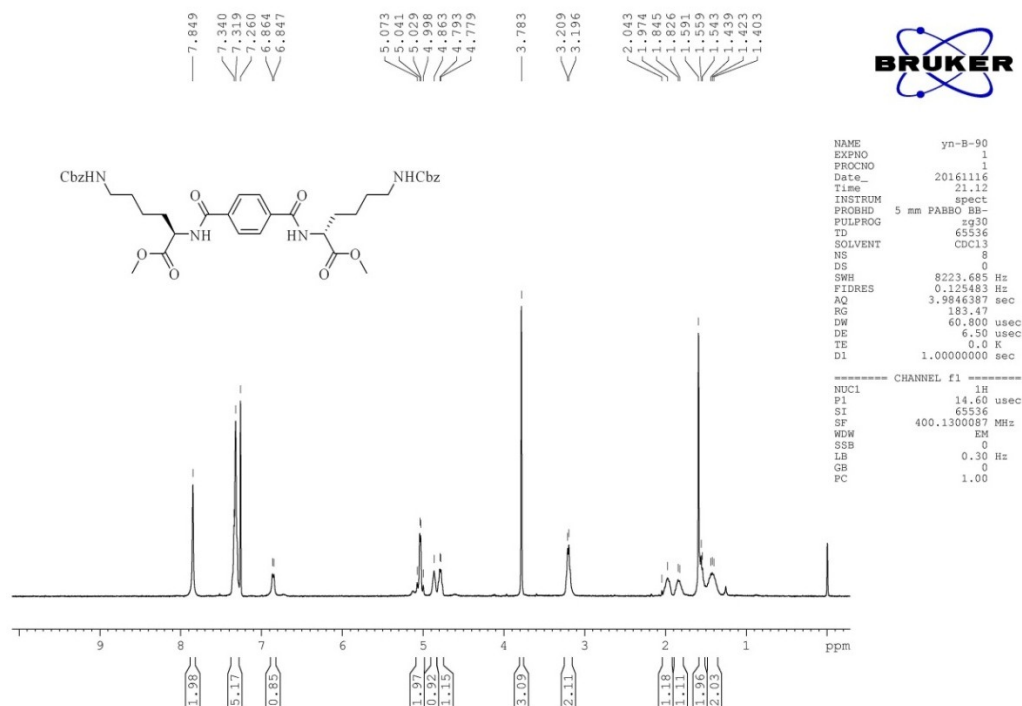
**Figure S1.** Correlation of antibacterial activity (MIC) against MRSA and *E. coli* with HPLC retention time of compounds **3a-3i**



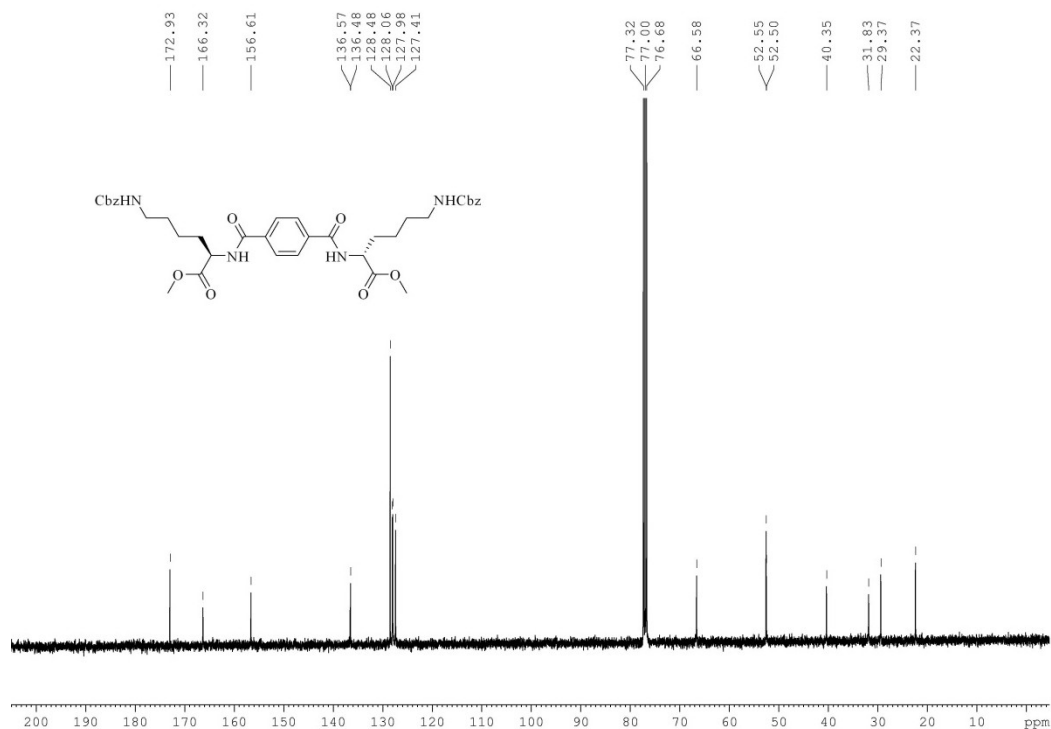
**Figure S2.** Correlation of antibacterial activity (MIC) against MRSA and *E. coli* with ALogP of compounds **3a-3i**

2.  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra of compounds **1**, **2**, **3a-3i**

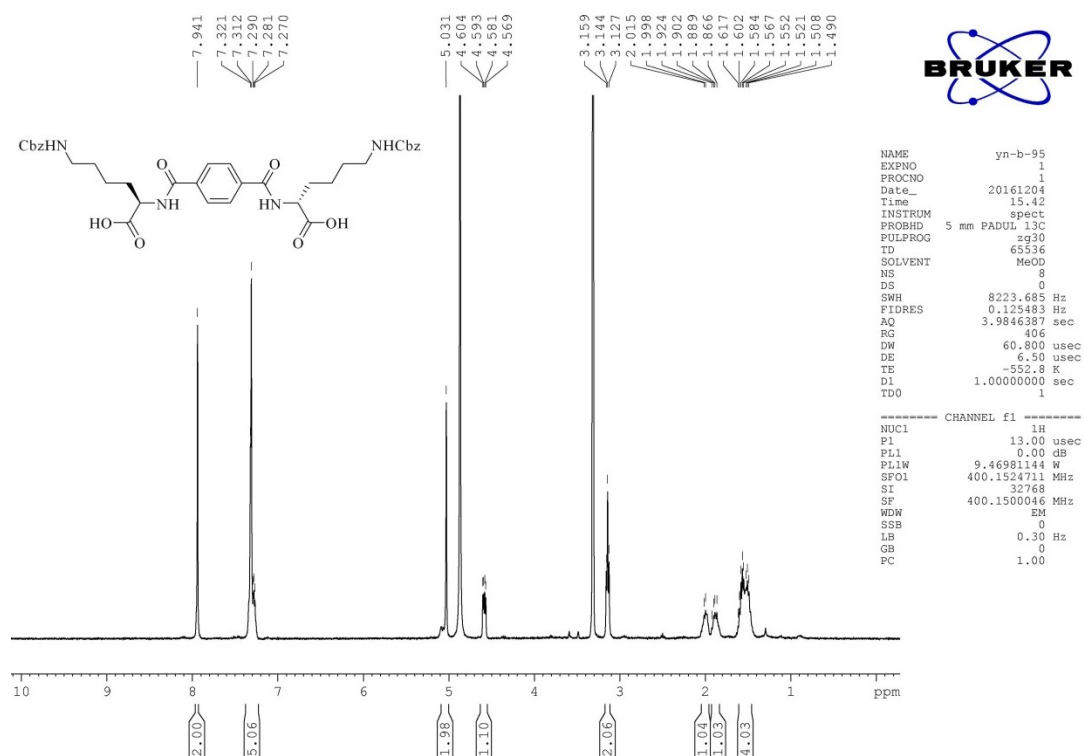
$^1\text{H}$  NMR (400MHz,  $\text{CDCl}_3$ ) spectrum of compound **1**



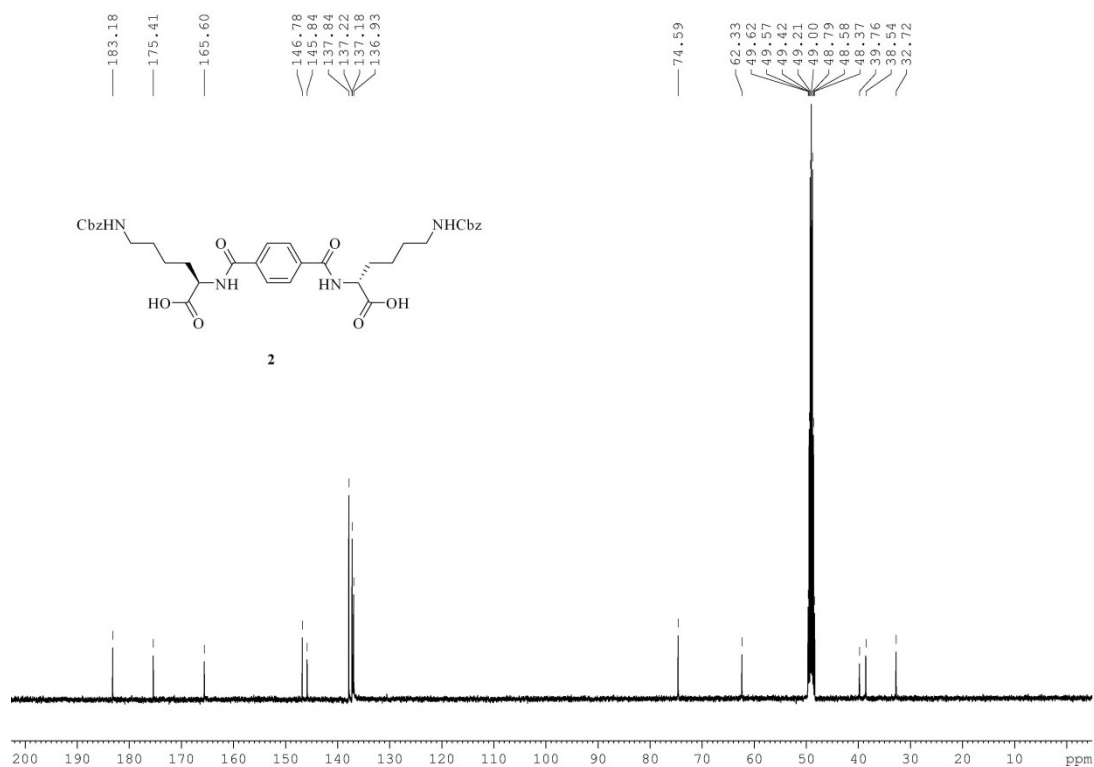
$^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ ) spectrum of compound **1**



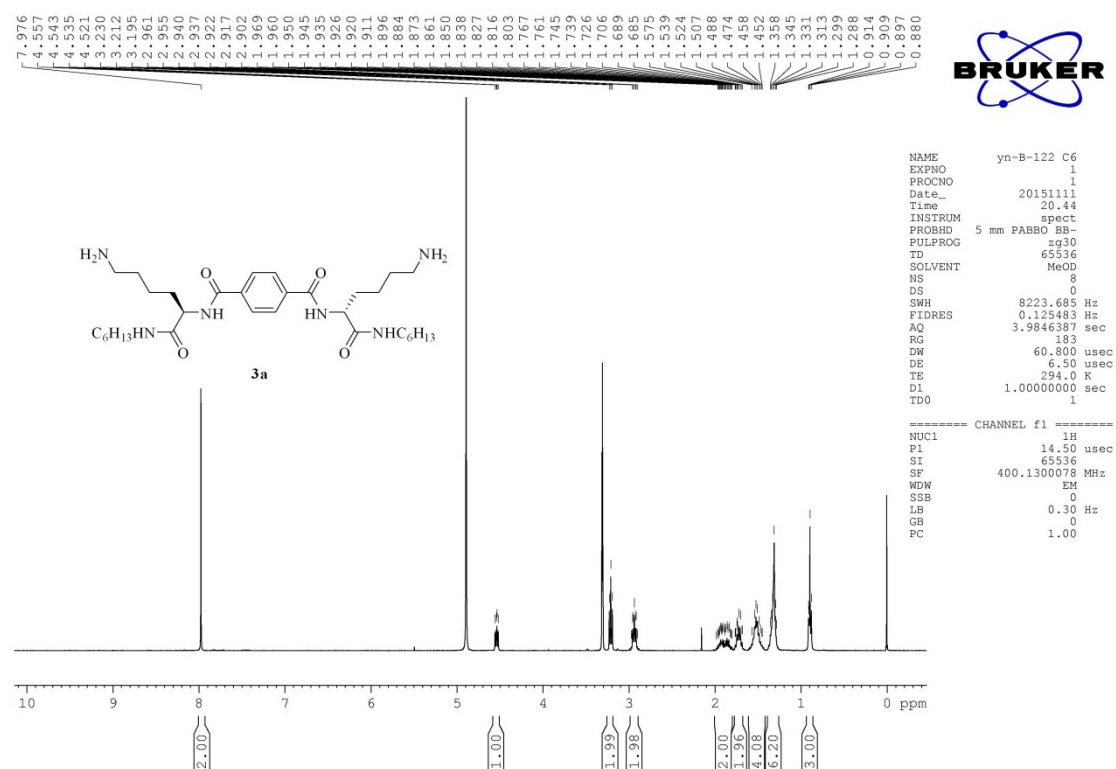
**<sup>1</sup>H NMR (400MHz, CD<sub>3</sub>OD) spectrum of compound 2**



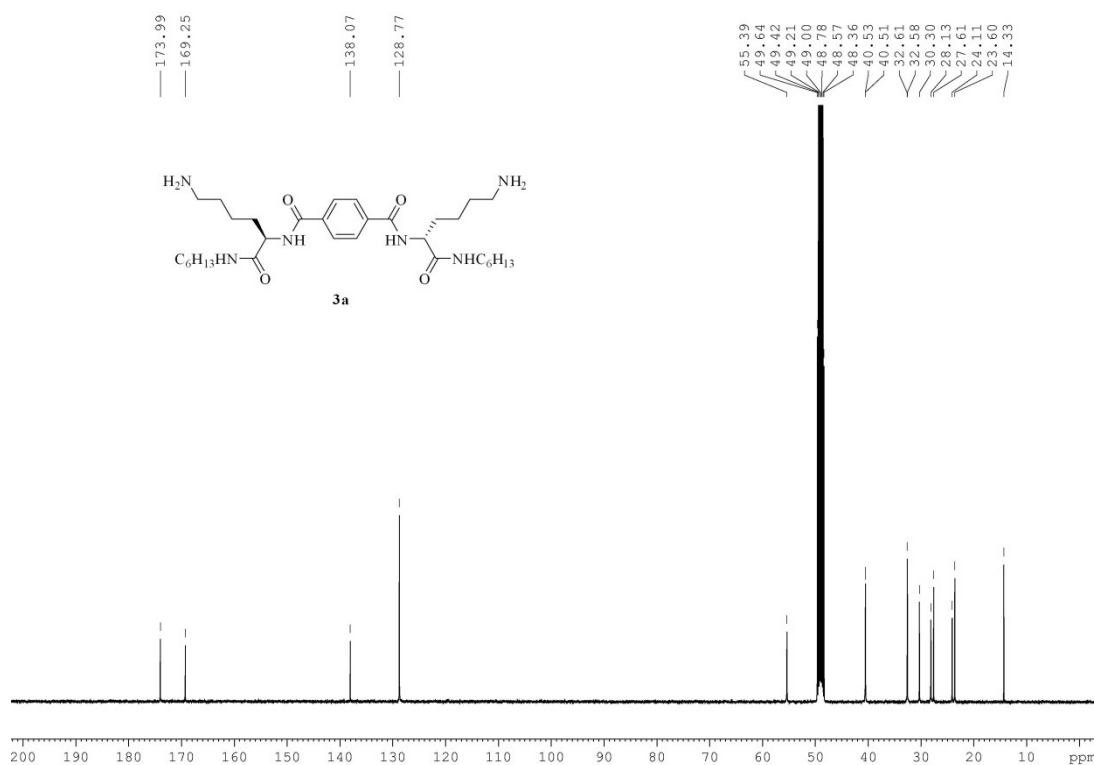
**<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD) spectrum of compound 2**



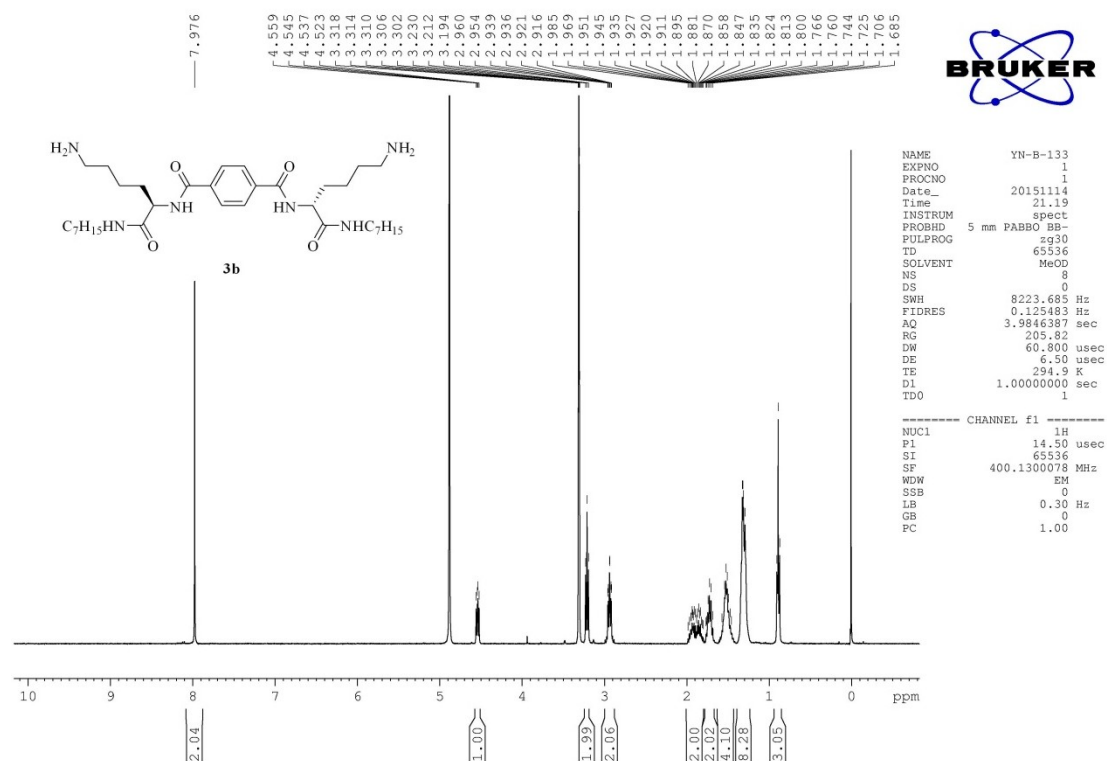
**$^1\text{H}$  NMR (400MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 3a**



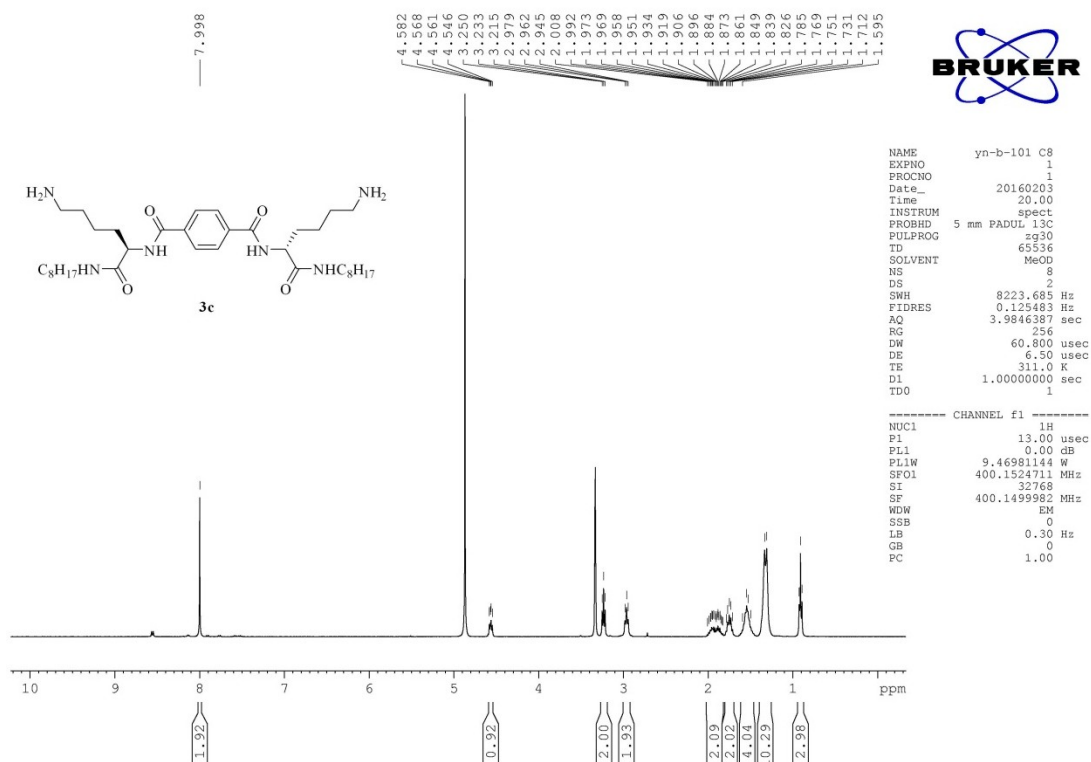
**$^{13}\text{C}$  NMR (101 MHz,  $\text{CD}_3\text{OD}$ ) spectrum of compound 3a**



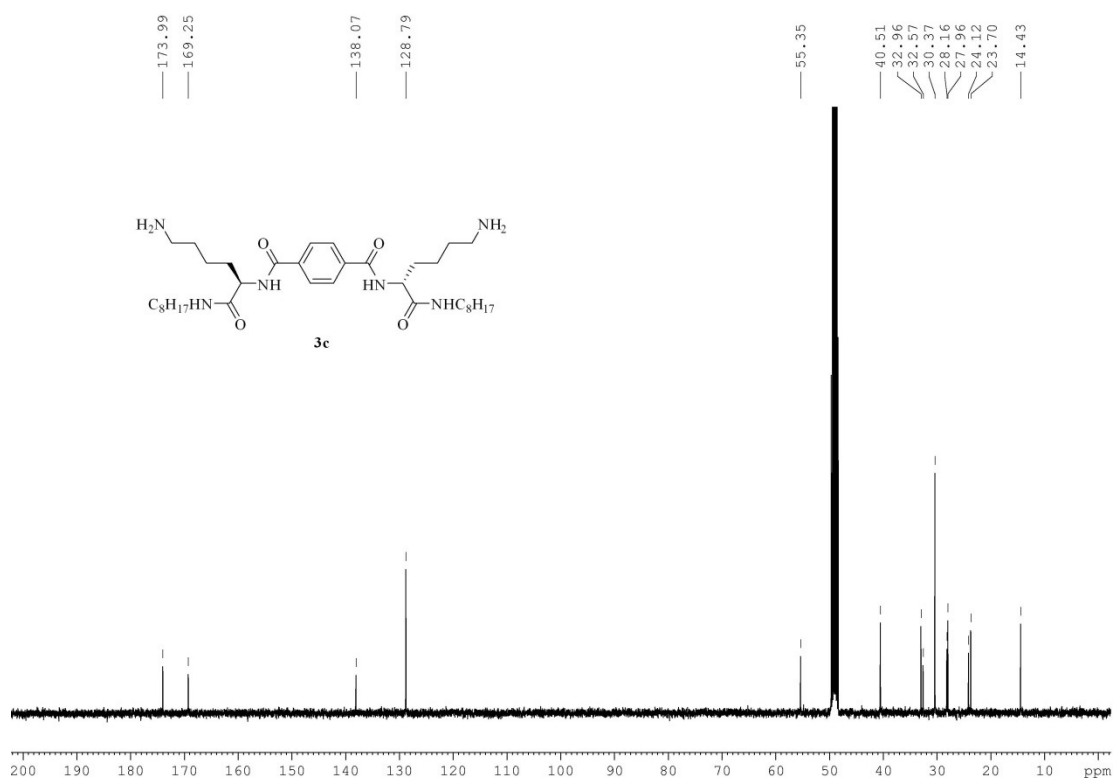
**<sup>1</sup>H NMR (400MHz, CD<sub>3</sub>OD) spectrum of compound 3b**



**<sup>1</sup>H NMR (400MHz, CD<sub>3</sub>OD) spectrum of compound 3c**

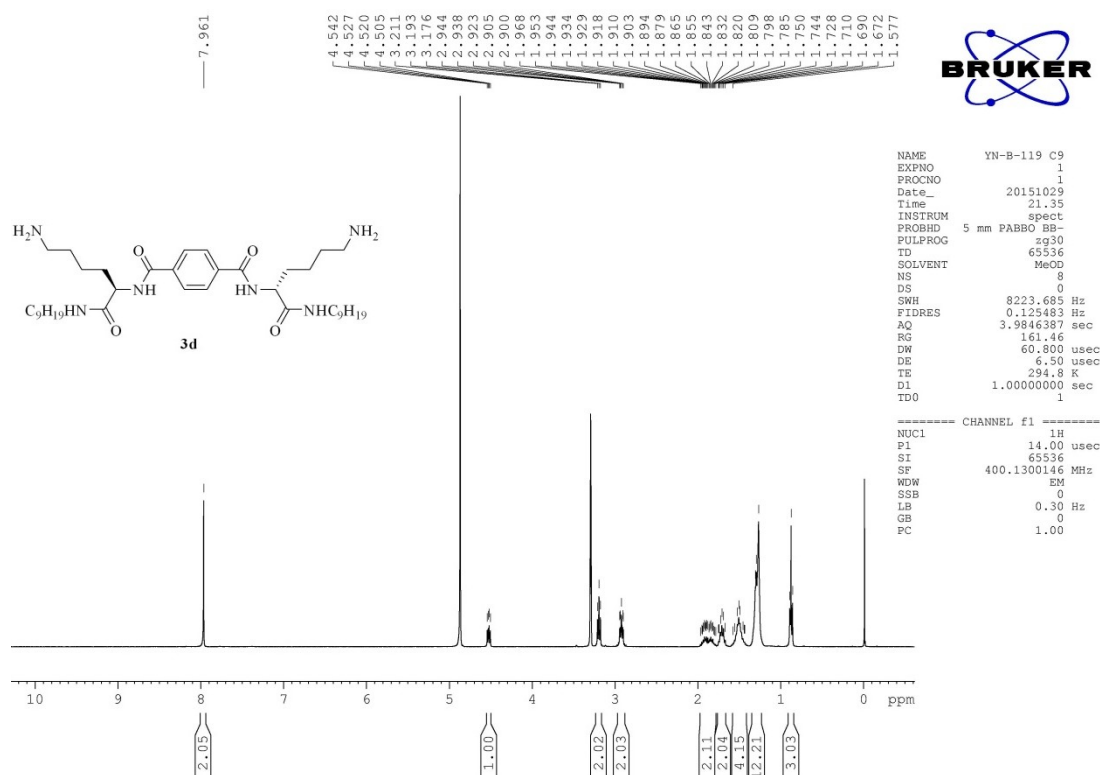


**<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD) spectrum of compound 3c**

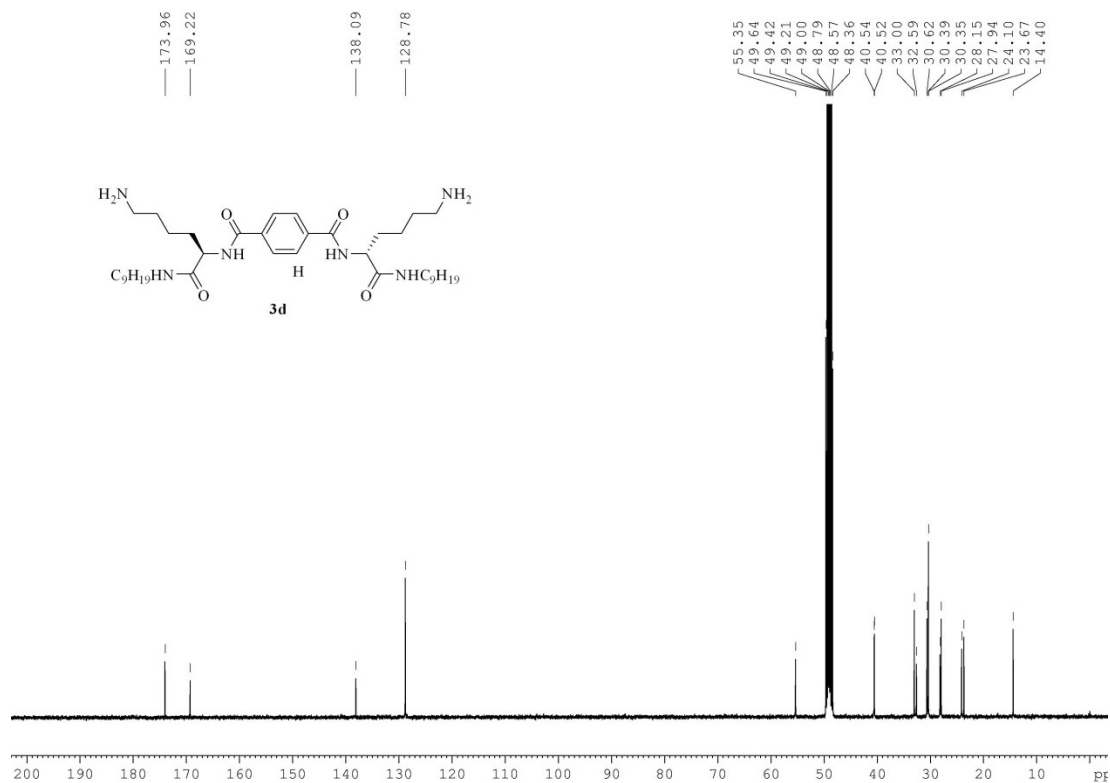




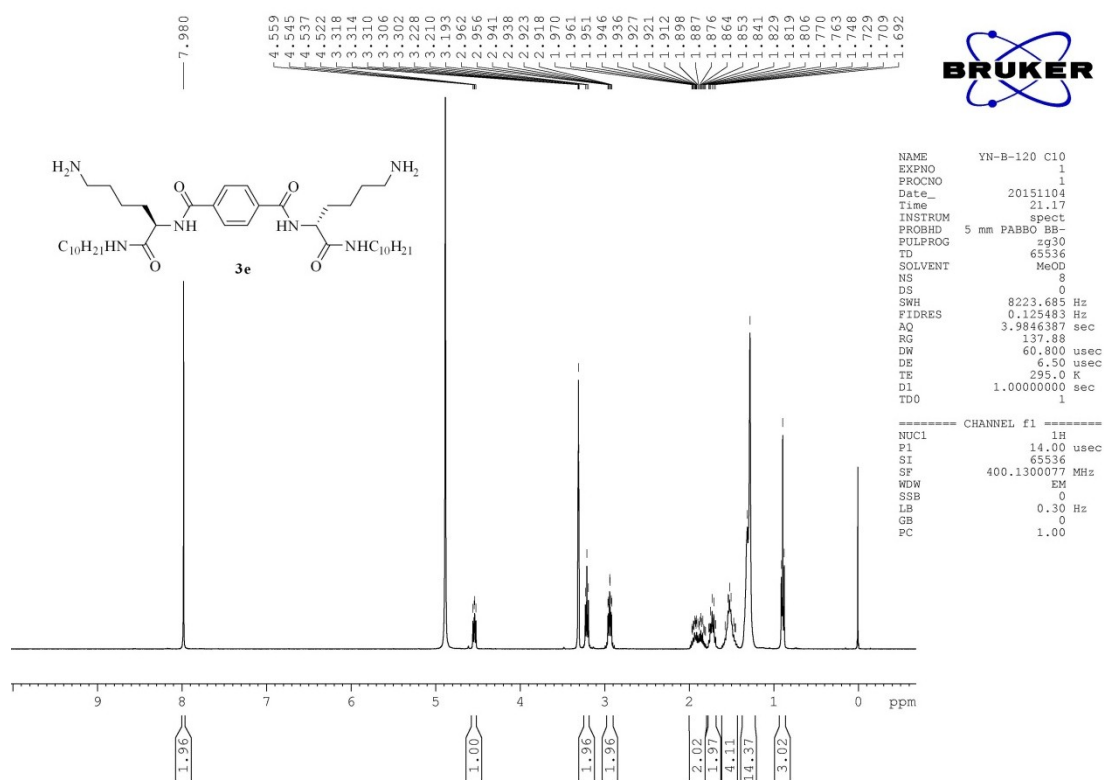
**<sup>1</sup>H NMR (400MHz, CD<sub>3</sub>OD) spectrum of compound 3d**



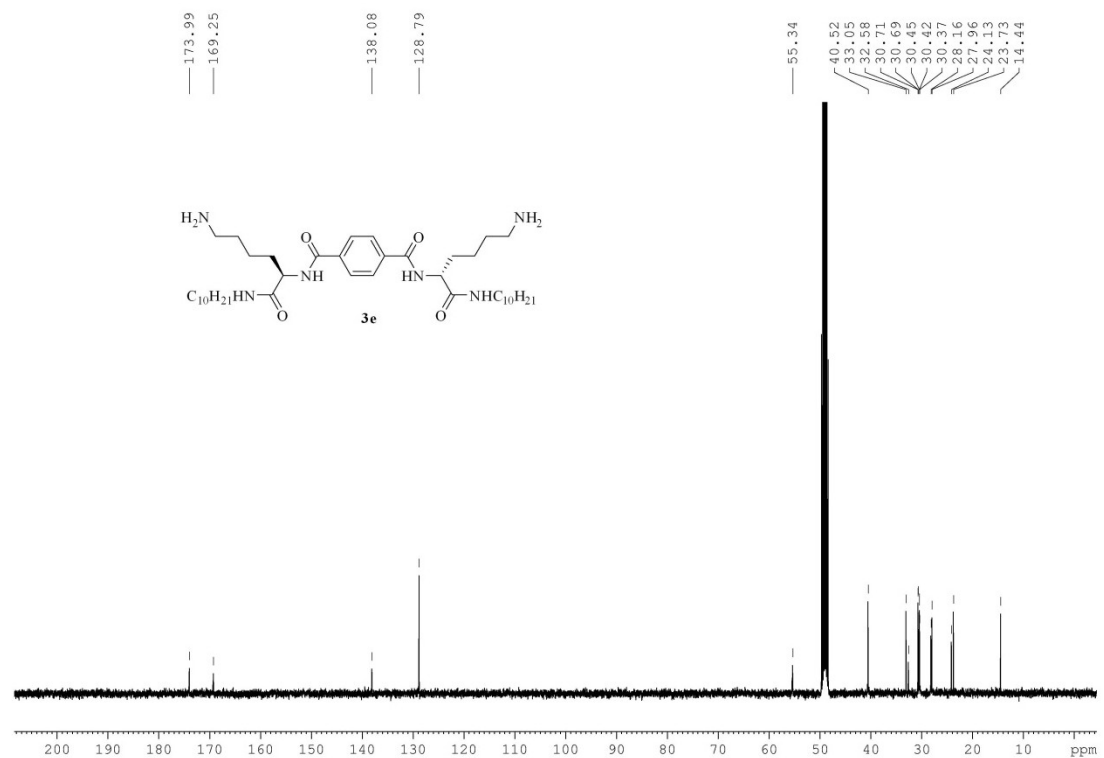
**<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD) spectrum of compound 3d**



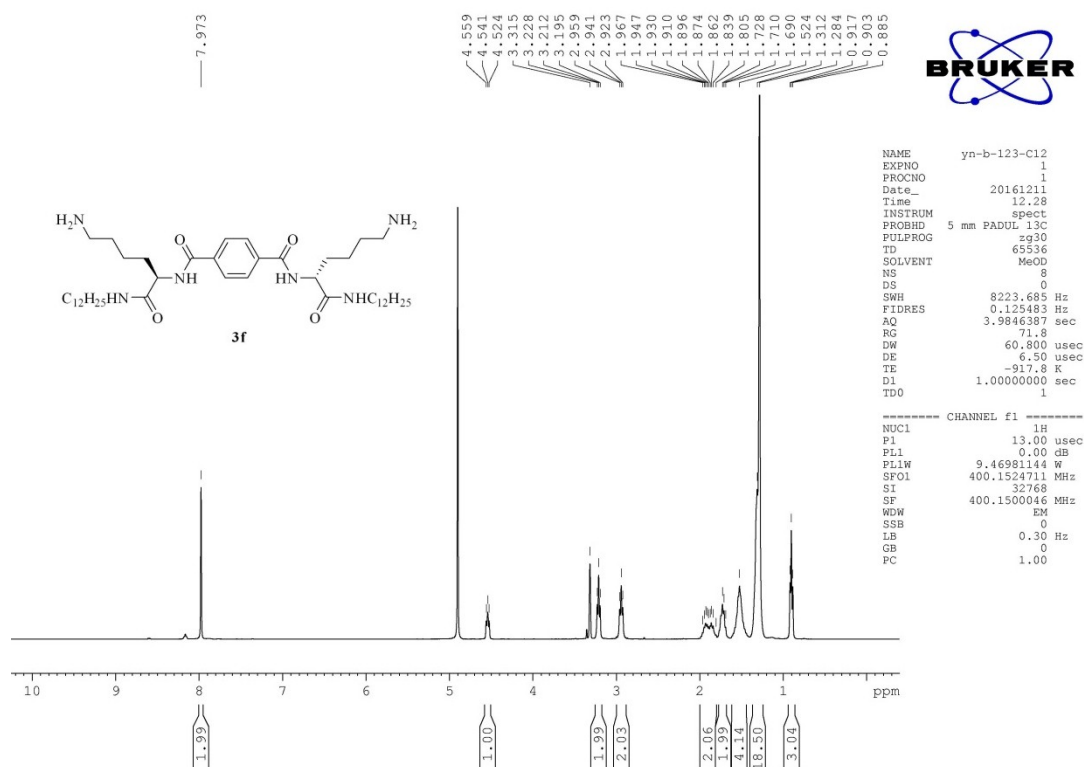
**<sup>1</sup>H NMR (400MHz, CD<sub>3</sub>OD) spectrum of compound 3e**



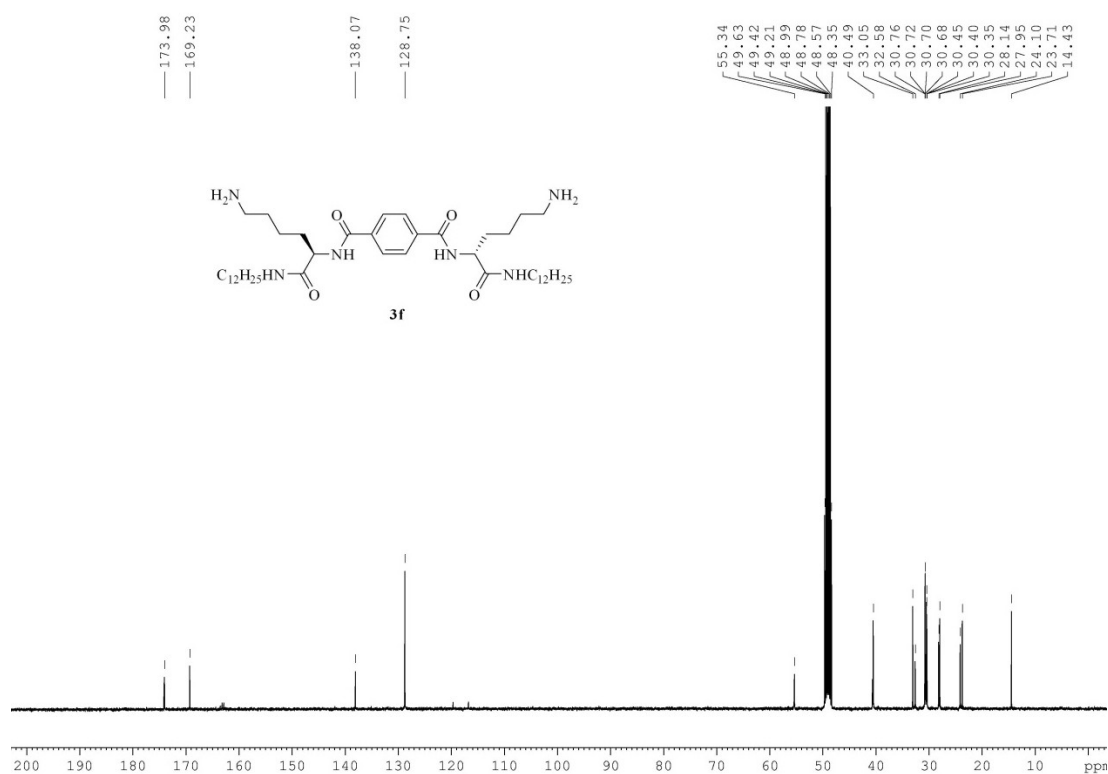
**<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD) spectrum of compound 3e**



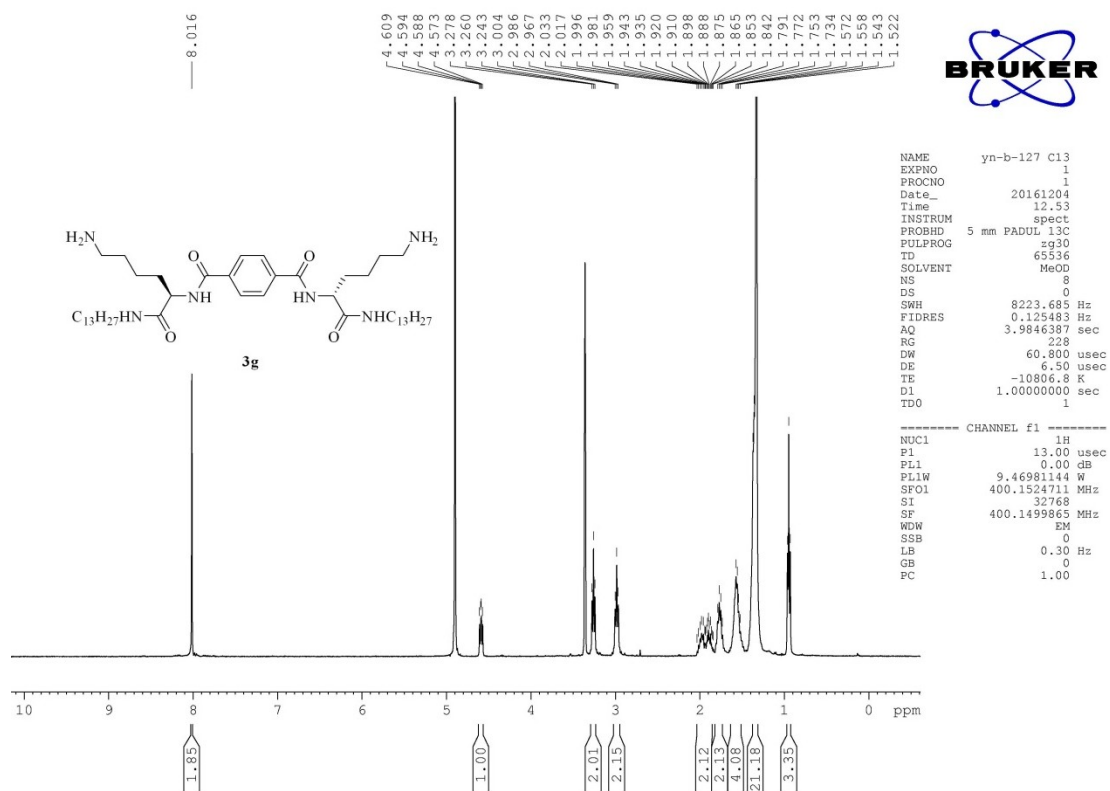
**<sup>1</sup>H NMR (400MHz, CD<sub>3</sub>OD) spectrum of compound 3f**



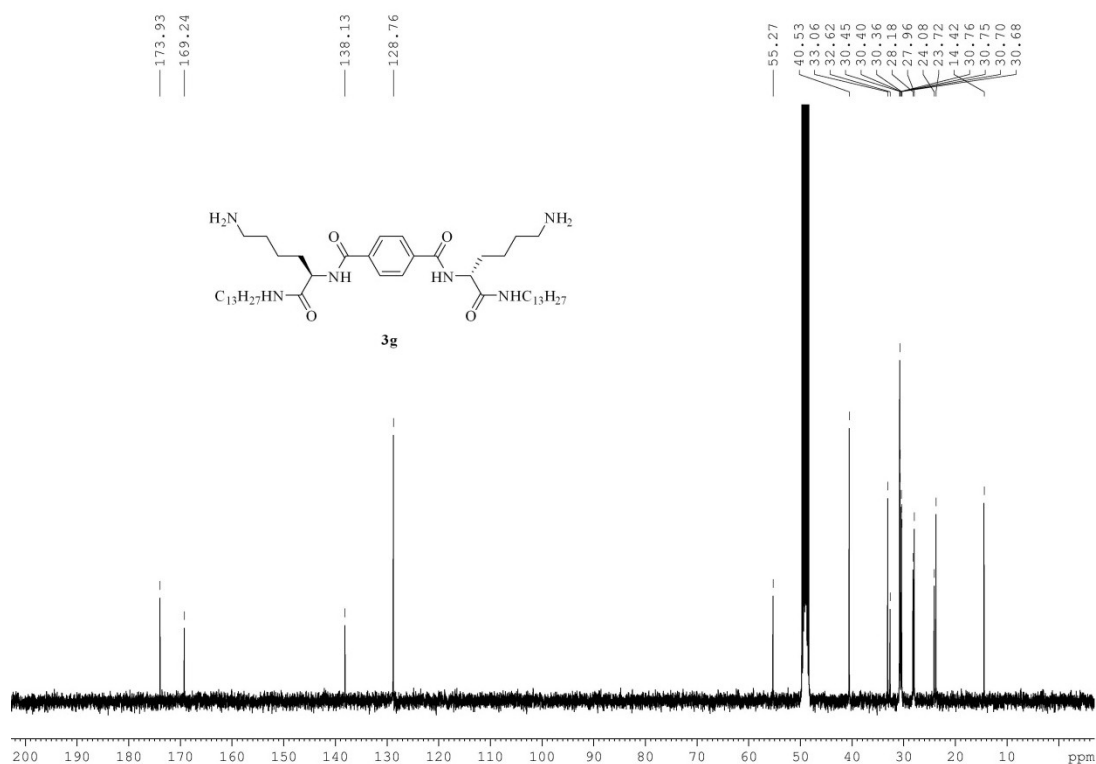
**<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD) spectrum of compound 3f**



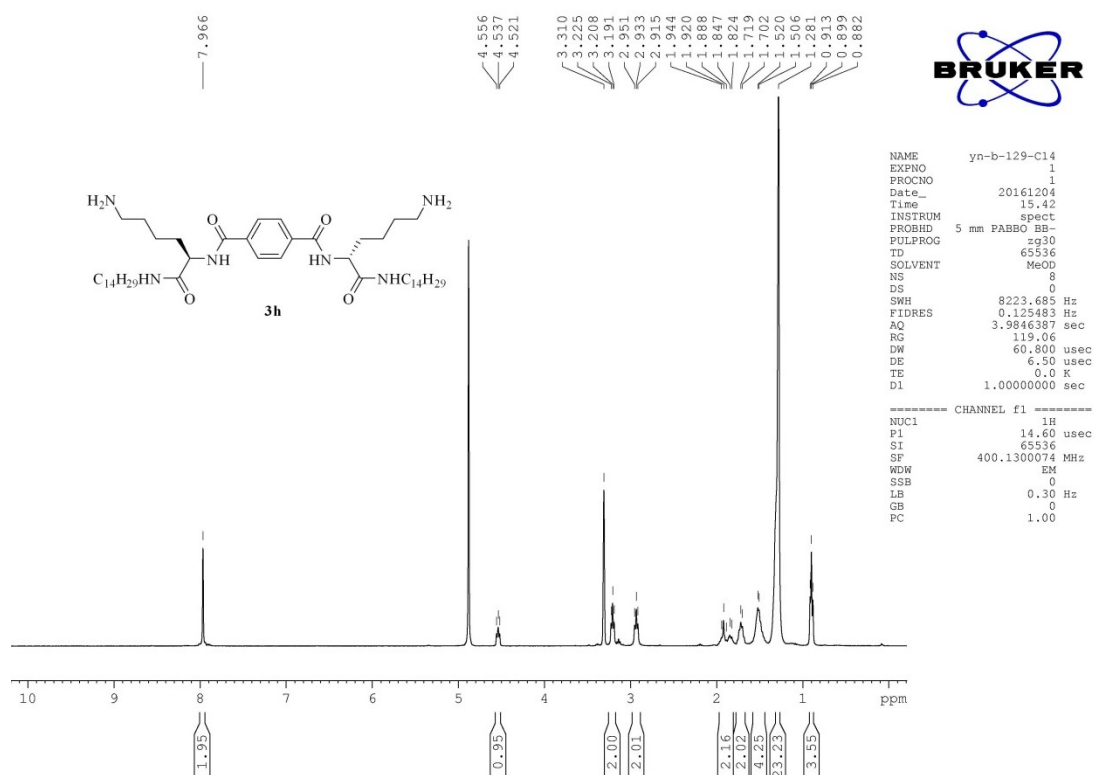
**<sup>1</sup>H NMR (400MHz, CD<sub>3</sub>OD) spectrum of compound 3g**



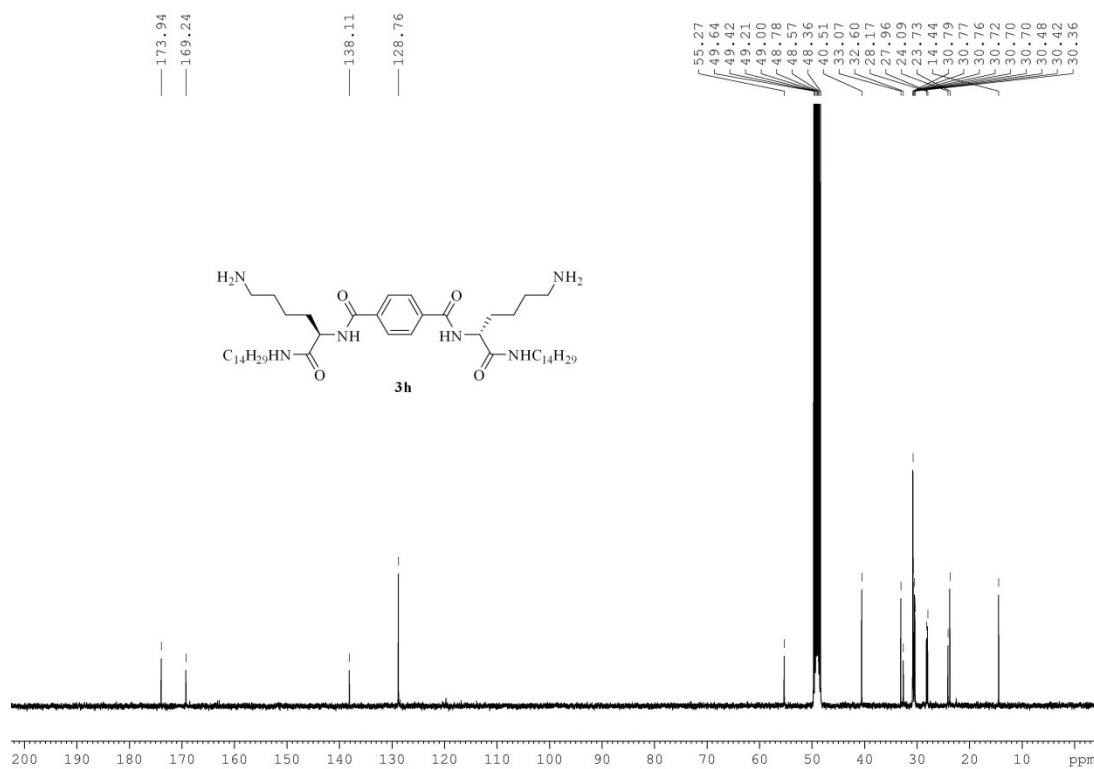
**<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD) spectrum of compound 3g**



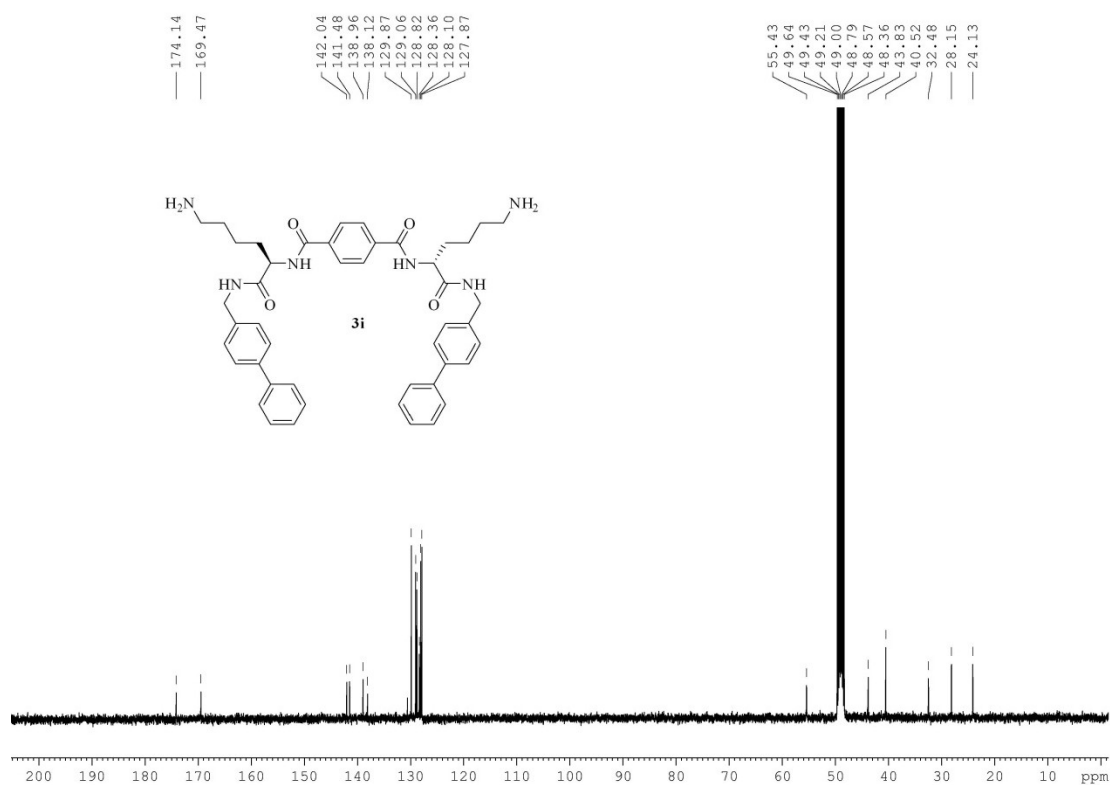
**<sup>1</sup>H NMR (400MHz, CD<sub>3</sub>OD) spectrum of compound 3h**



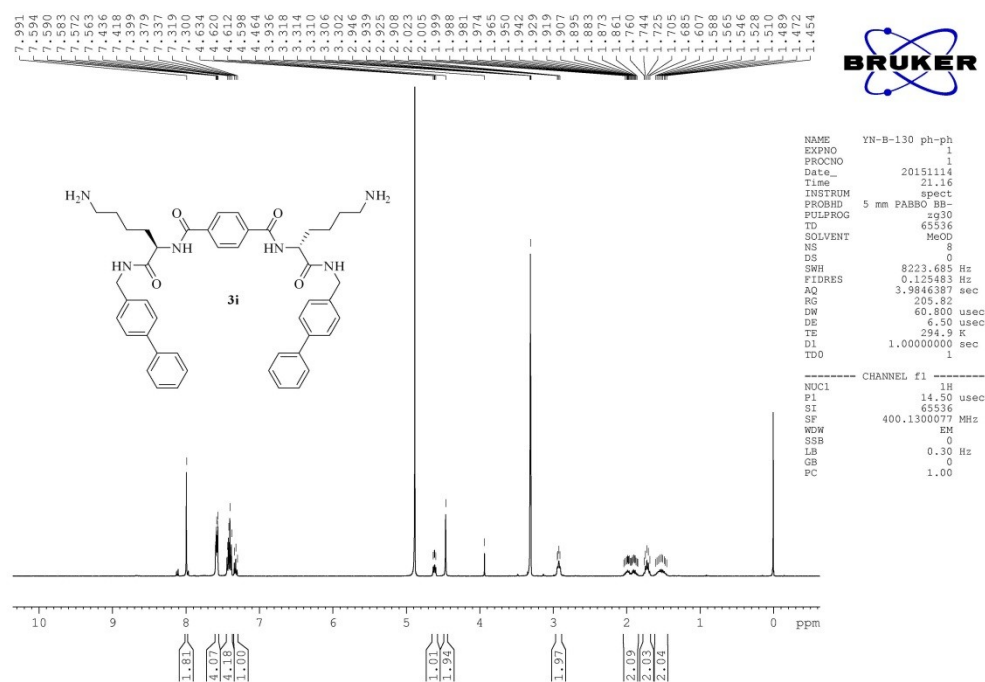
**<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD) spectrum of compound 3h**



**<sup>1</sup>H NMR (400MHz, CD<sub>3</sub>OD) spectrum of compound 3i**



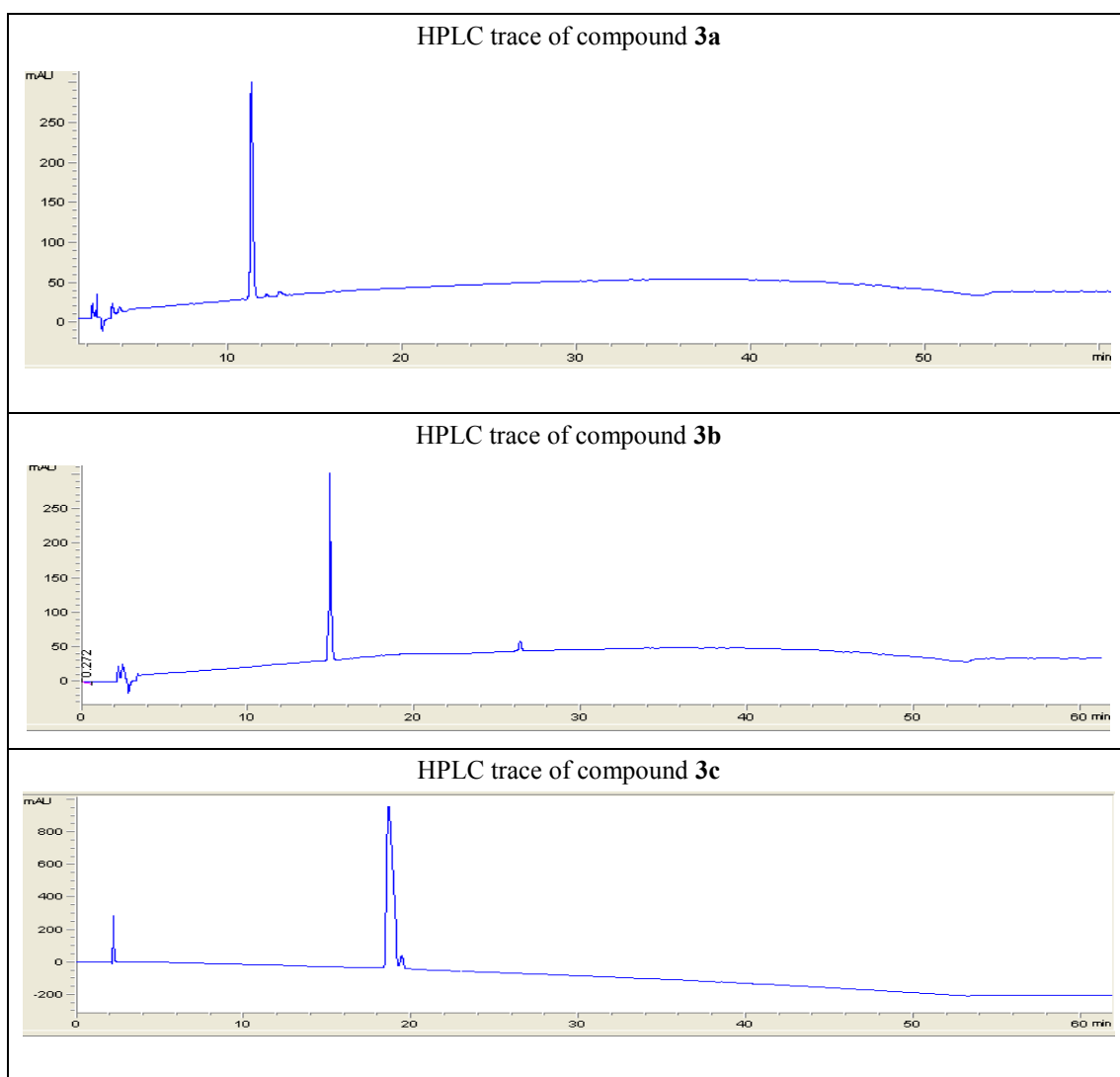
**<sup>13</sup>C NMR (101 MHz, CD<sub>3</sub>OD) spectrum of compound 3i**

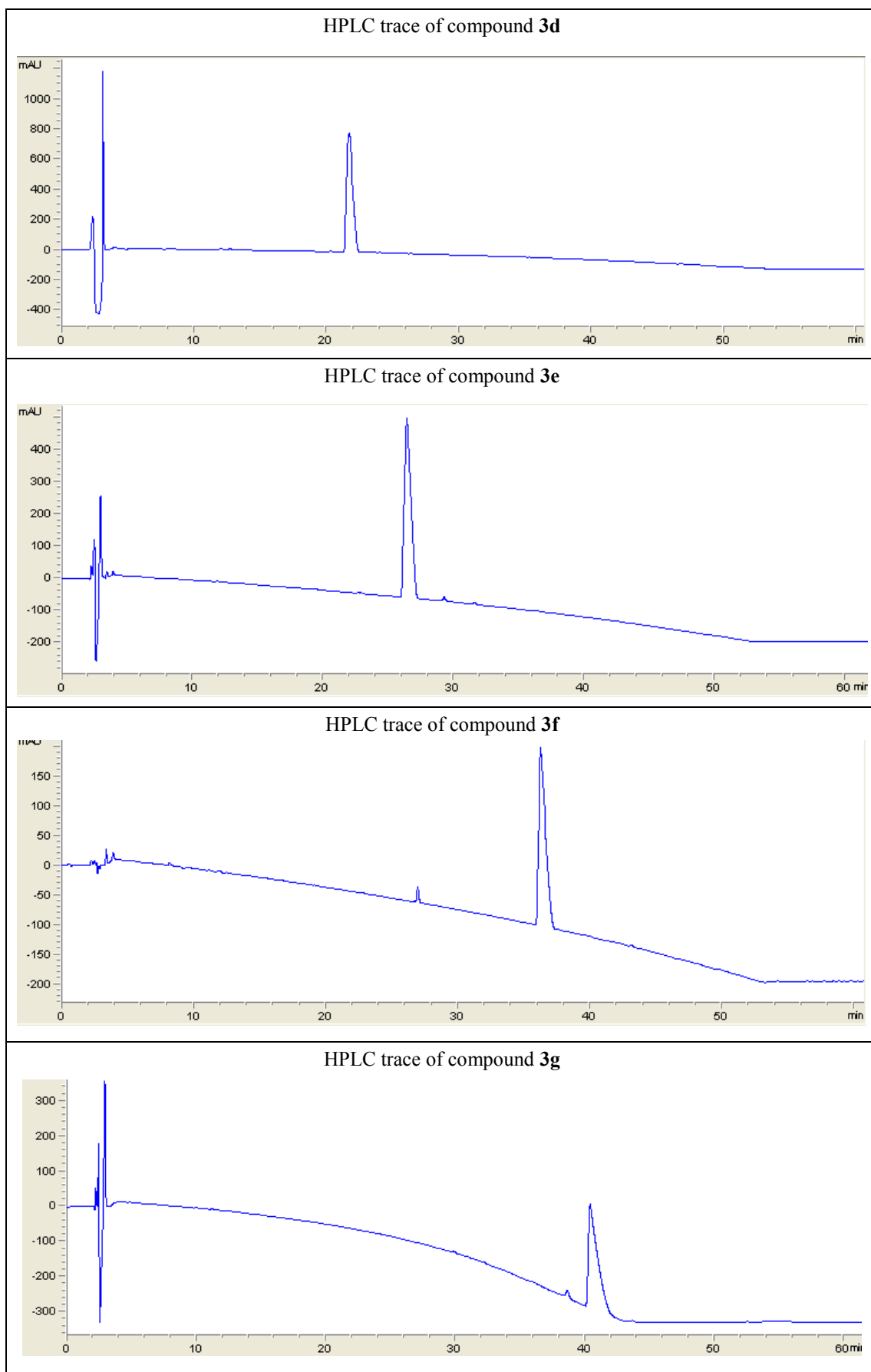


### 3. HPLC analysis of compounds **3a-3i**

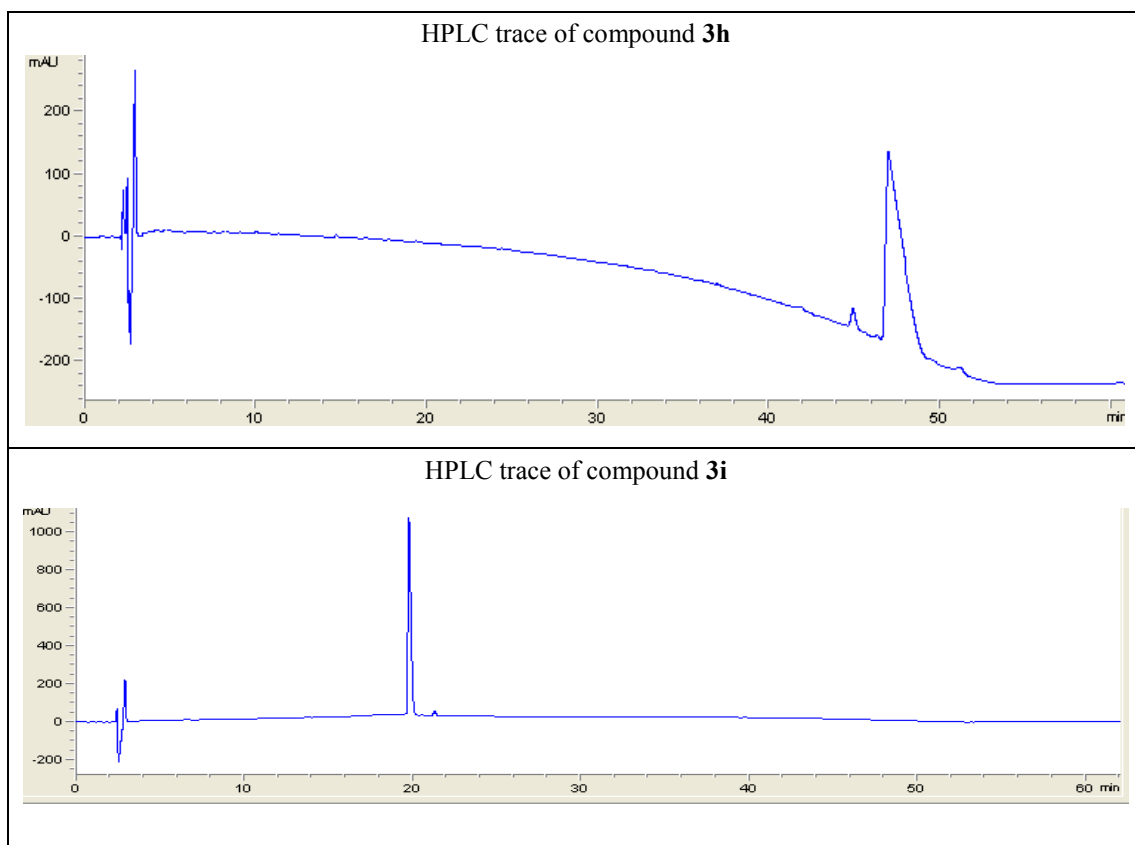
**Table S1.** HPLC purities and retention time of compounds **3a-3i**

compounds	<b>3a</b>	<b>3b</b>	<b>3c</b>	<b>3d</b>	<b>3e</b>	<b>3f</b>	<b>3g</b>	<b>3h</b>	<b>3i</b>
Retention time(min)	11.4	14.9	18.6	21.6	26.4	35.7	40.8	46.9	19.7
Purities (%)	96.4	96.3	97.3	99	>99	98.5	98.2	95.9	97.9









**Figure S3.** HPLC spectra of compound **3a-3i**