



## Supporting Information

for

### **Synthesis and physicochemical evaluation of fluorinated lipopeptide precursors of ligands for microbubble targeting**

Masayori Hagimori, Estefanía E. Mendoza-Ortega and Marie Pierre Krafft

*Beilstein J. Org. Chem.* **2021**, *17*, 511–518. [doi:10.3762/bjoc.17.45](https://doi.org/10.3762/bjoc.17.45)

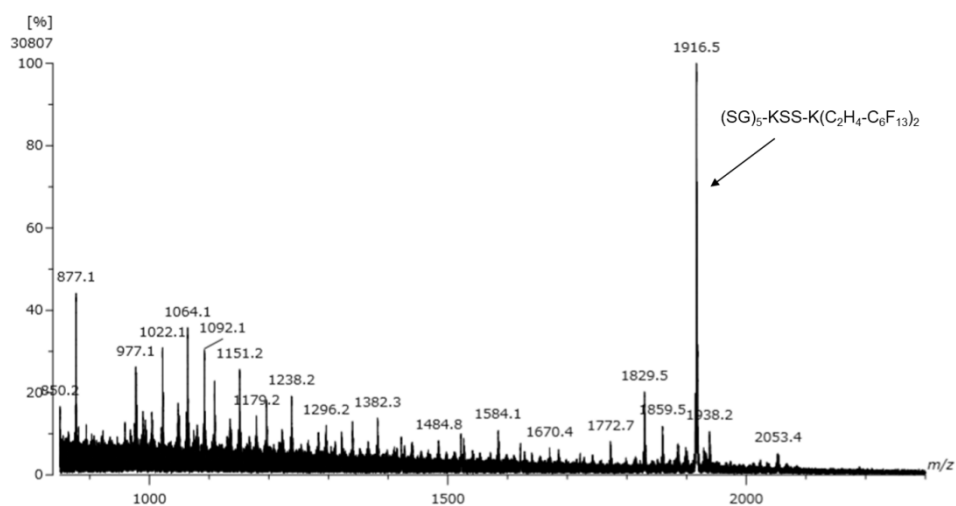
### **Mass spectrometry and FTIR data as well as RP-HPLC chromatograms of lipopeptides 1–4**

## Table of contents

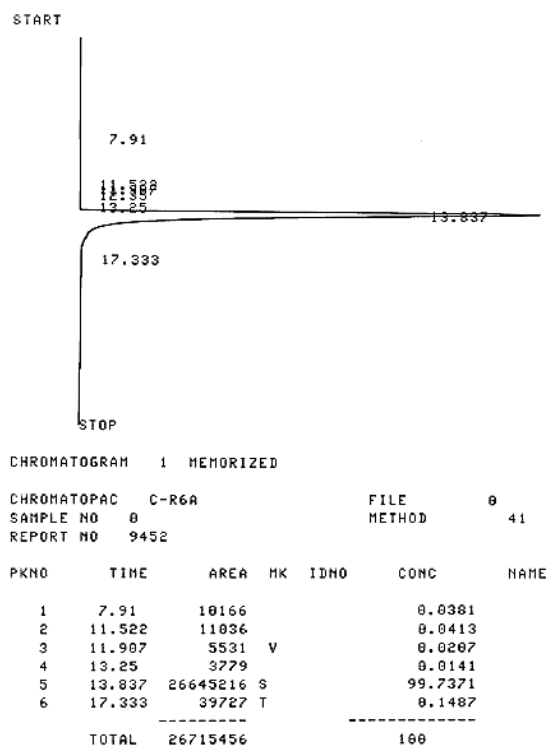
1. Instrumentation	S2
2. Figure S1: Mass spectrometry data of (SG) <sub>5</sub> -KSS-K(C <sub>2</sub> H <sub>4</sub> -C <sub>6</sub> F <sub>13</sub> ) <sub>2</sub> <b>1</b>	S2
3. Figure S2: RP-HPLC chromatogram of (SG) <sub>5</sub> -KSS-K(C <sub>2</sub> H <sub>4</sub> -C <sub>6</sub> F <sub>13</sub> ) <sub>2</sub> <b>1</b>	S3
4. Figure S3: FTIR spectrum of (SG) <sub>5</sub> -KSS-K(C <sub>2</sub> H <sub>4</sub> -C <sub>6</sub> F <sub>13</sub> ) <sub>2</sub> <b>1</b>	S3
5. Figure S4: Mass spectrometry data of (SG) <sub>5</sub> -KSS-K(C <sub>2</sub> H <sub>4</sub> -C <sub>7</sub> F <sub>15</sub> ) <sub>2</sub> <b>2</b>	S4
6. Figure S5: RP-HPLC chromatogram of (SG) <sub>5</sub> -KSS-K(C <sub>2</sub> H <sub>4</sub> -C <sub>7</sub> F <sub>15</sub> ) <sub>2</sub> <b>2</b>	S4
7. Figure S6: FTIR spectrum of (SG) <sub>5</sub> -KSS-K(C <sub>2</sub> H <sub>4</sub> -C <sub>7</sub> F <sub>15</sub> ) <sub>2</sub> <b>2</b>	S5
8. Figure S7: Mass spectrometry data of (SG) <sub>5</sub> -KSS-K(C <sub>2</sub> H <sub>4</sub> -C <sub>8</sub> F <sub>17</sub> ) <sub>2</sub> <b>3</b>	S5
9. Figure S8: RP-HPLC chromatogram of (SG) <sub>5</sub> -KSS-K(C <sub>2</sub> H <sub>4</sub> -C <sub>8</sub> F <sub>17</sub> ) <sub>2</sub> <b>3</b>	S6
10. Figure S9: FTIR spectrum of (SG) <sub>5</sub> -KSS-K(C <sub>2</sub> H <sub>4</sub> -C <sub>8</sub> F <sub>17</sub> ) <sub>2</sub> <b>3</b>	S6
11. Figure S10: Mass spectrometry data of (SG) <sub>5</sub> -KSS-K(C <sub>10</sub> H <sub>21</sub> ) <sub>2</sub> <b>4</b>	S7
12. Figure S11: RP-HPLC chromatogram of (SG) <sub>5</sub> -KSS-K(C <sub>10</sub> H <sub>21</sub> ) <sub>2</sub> <b>4</b>	S7
13. Figure S12: FTIR spectrum of (SG) <sub>5</sub> -KSS-K(C <sub>10</sub> H <sub>21</sub> ) <sub>2</sub> <b>4</b>	S8

### Instrumentation:

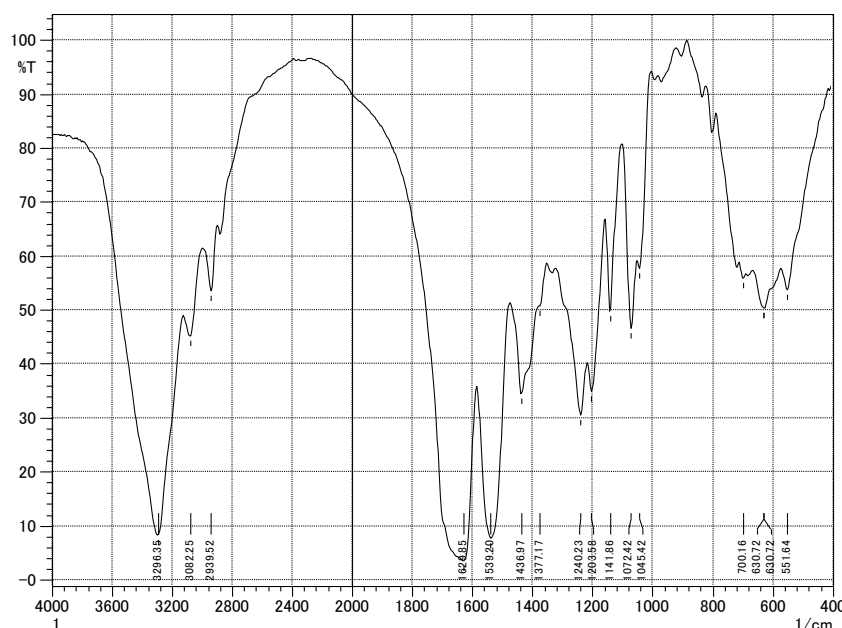
Mass spectra (MS) and HRMS were performed using a JMS-700 spectrometer (JEOL, Japan). RP-HPLC chromatograms were recorded on a Prominence system (Shimadzu, Japan). FTIR spectra were recorded on IRAffinity-1 (Shimadzu, Japan).



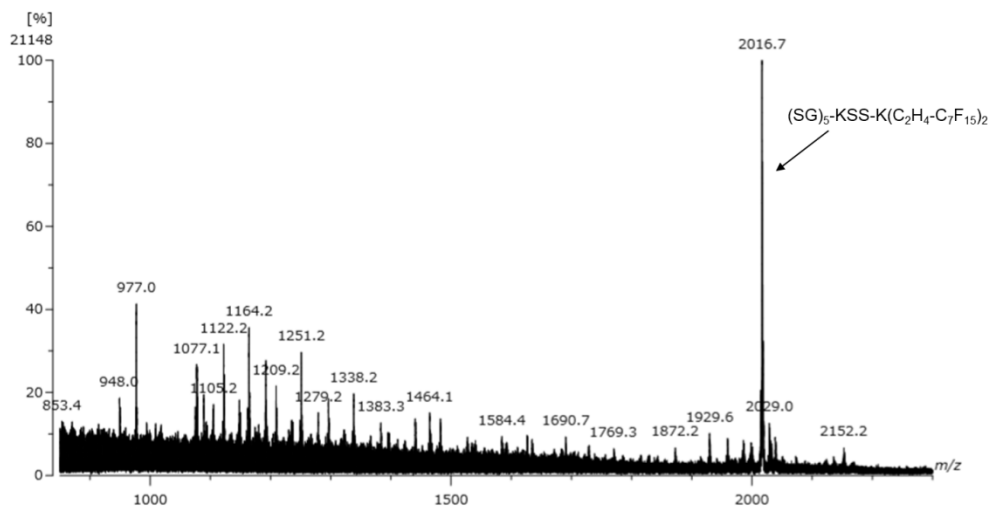
**Figure S1:** Mass spectrometry data of (SG)<sub>5</sub>-KSS-K(C<sub>2</sub>H<sub>4</sub>-C<sub>6</sub>F<sub>13</sub>)<sub>2</sub> **1**. Exact mass of the (SG)<sub>5</sub>-KSS-K(C<sub>2</sub>H<sub>4</sub>-C<sub>6</sub>F<sub>13</sub>)<sub>2</sub> [M + H]<sup>+</sup> was calculated 1916.5511 and found 1916.5509.



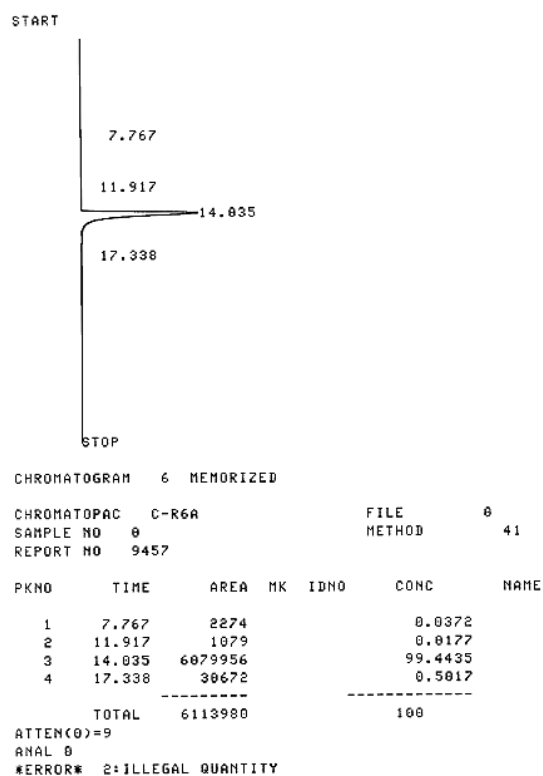
**Figure S2:** RP-HPLC chromatogram of  $(SG)_5\text{-KSS-K}(\text{C}_2\text{H}_4\text{-C}_6\text{F}_{13})_2$  **1**. HPLC conditions: the column was a COSMOSIL 5C18-AR-II 4.6 mm × 250 mm, flow rate was 0.5 mL/min, UV excitation at 220 nm, mobile phase systems were  $\text{CH}_3\text{CN}/\text{H}_2\text{O}$  80:20.



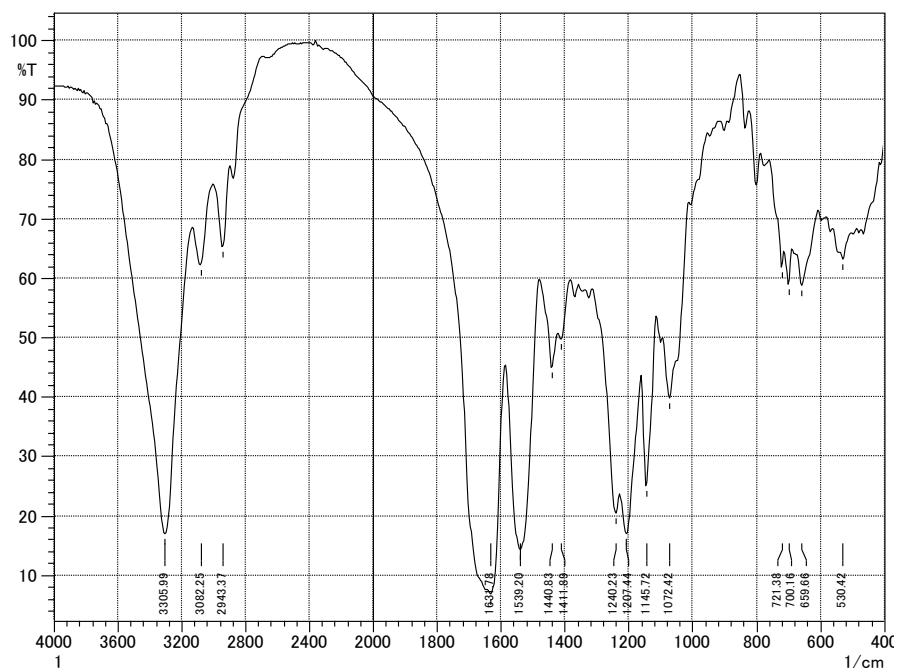
**Figure S3:** FTIR spectrum of  $(SG)_5\text{-KSS-K}(\text{C}_2\text{H}_4\text{-C}_6\text{F}_{13})_2$  **1**.



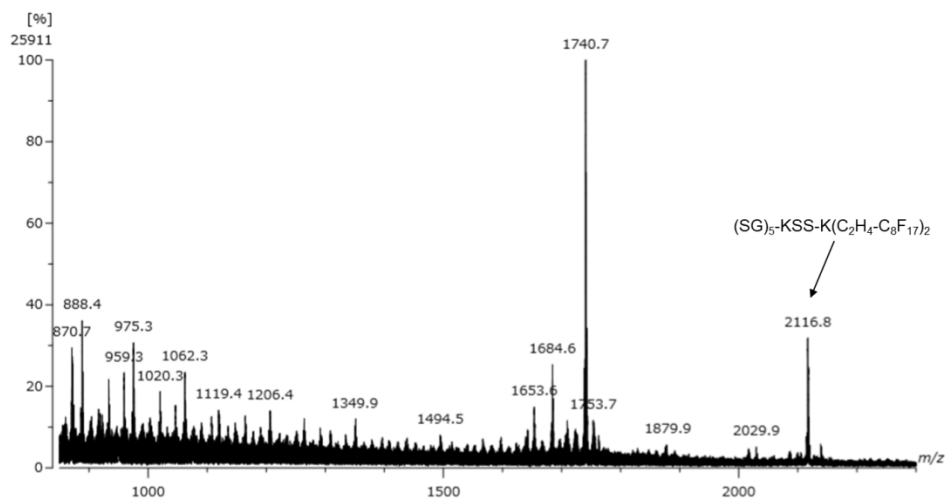
**Figure S4:** Mass spectrometry data of  $(SG)_5\text{-KSS-K}(C_2H_4\text{-}C_7F_{15})_2$  **2**. Exact mass of the  $(SG)_5\text{-KSS-K}(C_2H_4\text{-}C_7F_{15})_2 [M + H]^+$  was calculated 2016.5447 and found 2016.5448.



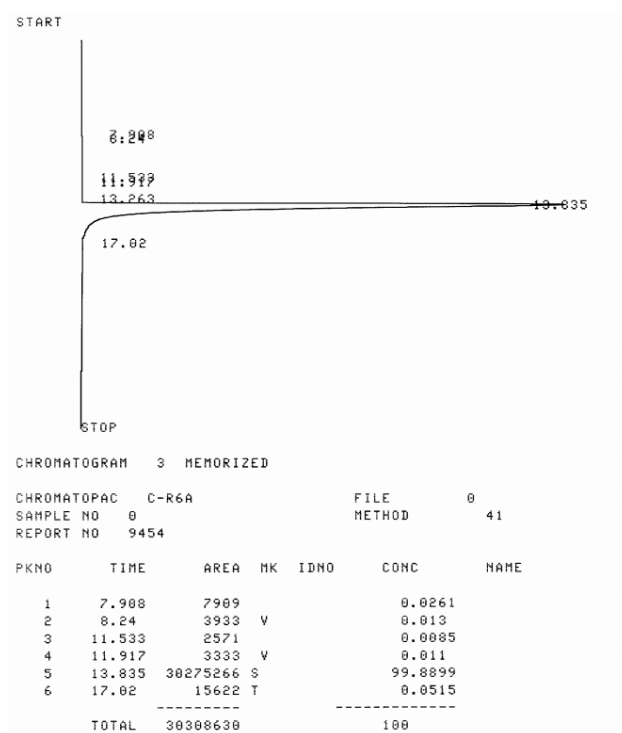
**Figure S5:** RP-HPLC chromatogram of  $(SG)_5\text{-KSS-K}(C_2H_4\text{-}C_7F_{15})_2$  **2**. HPLC conditions: the column was a COSMOSIL 5C18-AR-II 4.6 mm × 250 mm, flow rate was 0.5 mL/min, UV excitation at 220 nm, mobile phase systems were  $CH_3CN/H_2O$  80:20.



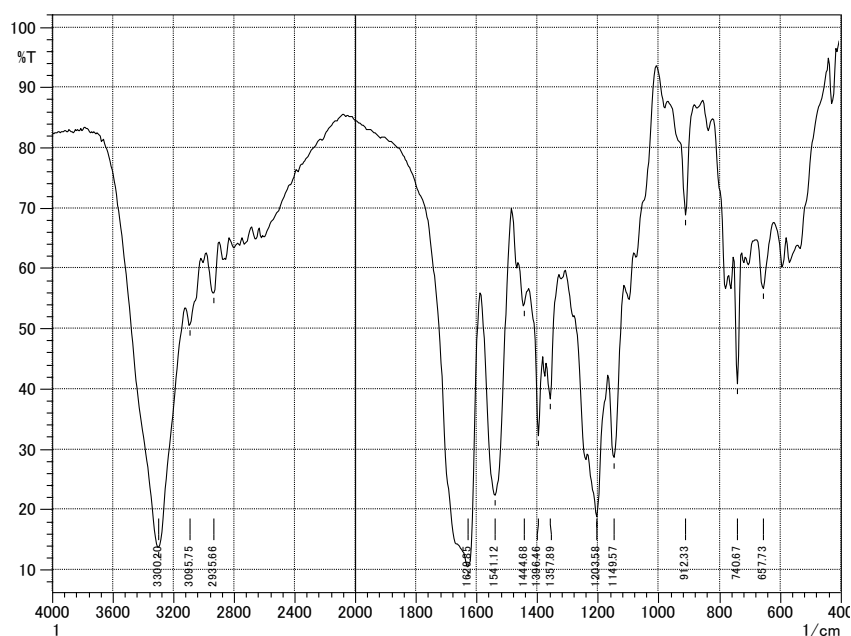
**Figure S6:** FTIR spectrum of  $(SG)_5\text{-KSS-K}(\text{C}_2\text{H}_4\text{-C}_7\text{F}_{15})_2$  **2**.



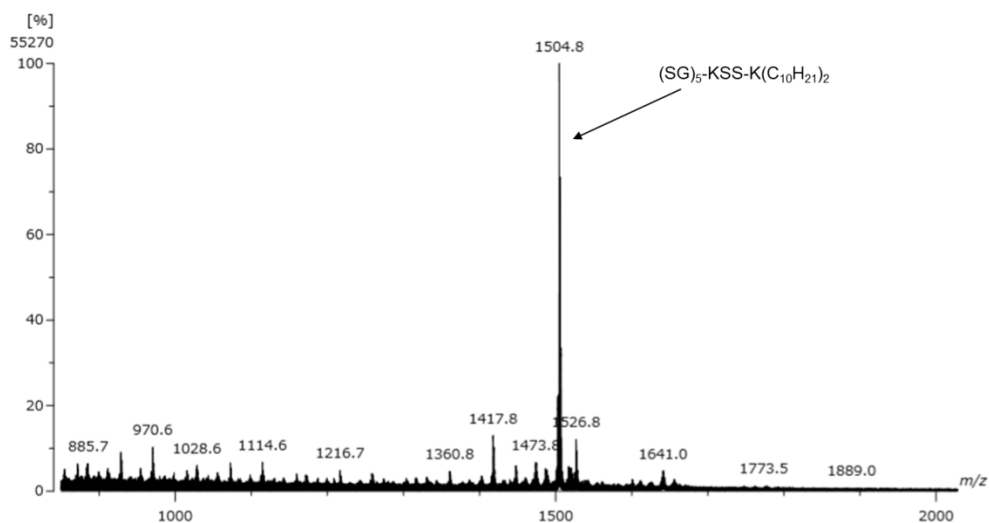
**Figure S7:** Mass spectrometry data of  $(SG)_5\text{-KSS-K}(\text{C}_2\text{H}_4\text{-C}_8\text{F}_{17})_2$  **3**. Exact mass of the  $(SG)_5\text{-KSS-K}(\text{C}_2\text{H}_4\text{-C}_8\text{F}_{17})_2$   $[\text{M} + \text{H}]^+$  was calculated 2116.5383 and found 2116.5381.



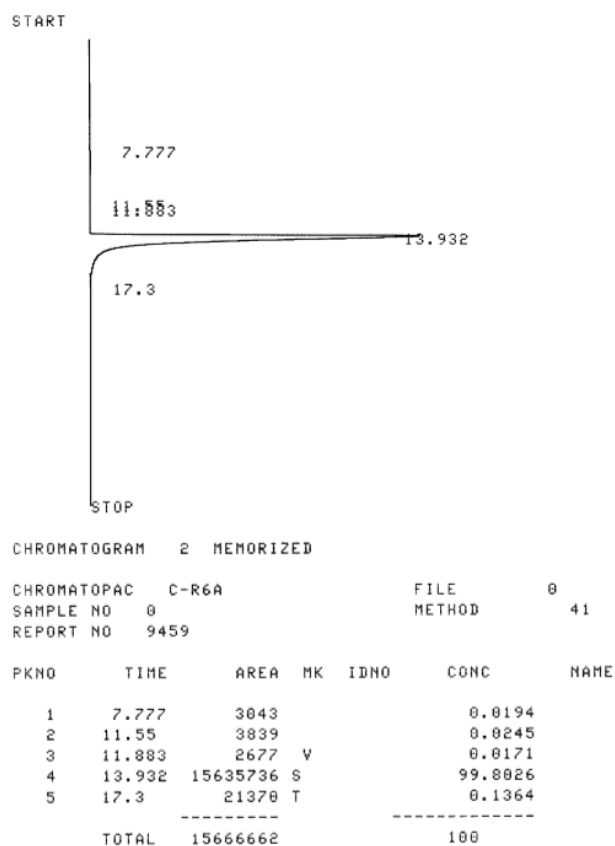
**Figure S8:** RP-HPLC chromatogram of  $(SG)_5\text{-KSS-K}(C_2H_4\text{-}C_8F_{17})_2$  **3**. HPLC conditions: the column was a COSMOSIL 5C18-AR-II 4.6 mm  $\times$  250 mm, flow rate was 0.5 mL/min, UV excitation at 220 nm, mobile phase systems were  $CH_3CN/H_2O$  80:20.



**Figure S9:** FTIR spectrum of  $(SG)_5\text{-KSS-K}(C_2H_4\text{-}C_8F_{17})_2$  **3**.

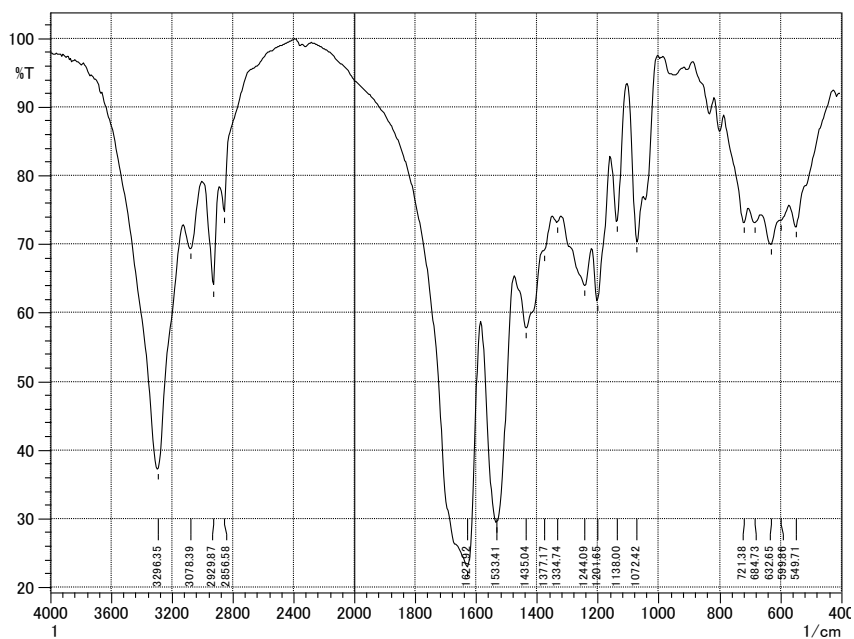


**Figure S10:** Mass spectrometry data of  $(SG)_5\text{-KSS-K}(C_{10}H_{21})_2$  **4**. Exact mass of the  $(SG)_5\text{-KSS-K}(C_{10}H_{21})_2 [M + H]^+$  was calculated 1504.8586 and found 1504.8585.



**Figure S11:** RP-HPLC chromatogram of  $(SG)_5\text{-KSS-K}(C_{10}H_{21})_2$  **4**. HPLC conditions: the column was a COSMOSIL 5C18-AR-II 4.6 mm × 250 mm, flow rate was 0.5 mL/min, UV excitation at 220 nm, mobile phase systems were  $CH_3CN/H_2O$  80:20.





**Figure S12:** FTIR spectrum of (SG)<sub>5</sub>-KSS-K(C<sub>10</sub>H<sub>21</sub>)<sub>2</sub> 4.