

## SUPPLEMENTARY INFORMATION

### Lipid structure influences the ability of glucose monocorynomycolate to signal through Mincle

Phillip L. van der Peet,<sup>a</sup> Masahiro Nagata,<sup>b</sup> Sayali Shah,<sup>a</sup> Jonathan M. White,<sup>a</sup> Sho Yamasaki,<sup>b</sup>  
Spencer J. Williams<sup>a,\*</sup>

<sup>a</sup> School of Chemistry and Bio21 Molecular Science and Biotechnology Institute, University of Melbourne, Parkville, Victoria, Australia 3010

<sup>b</sup> Division of Molecular Immunology, Medical Institute of Bioregulation, Kyushu University, Fukuoka 812-8582, Japan.

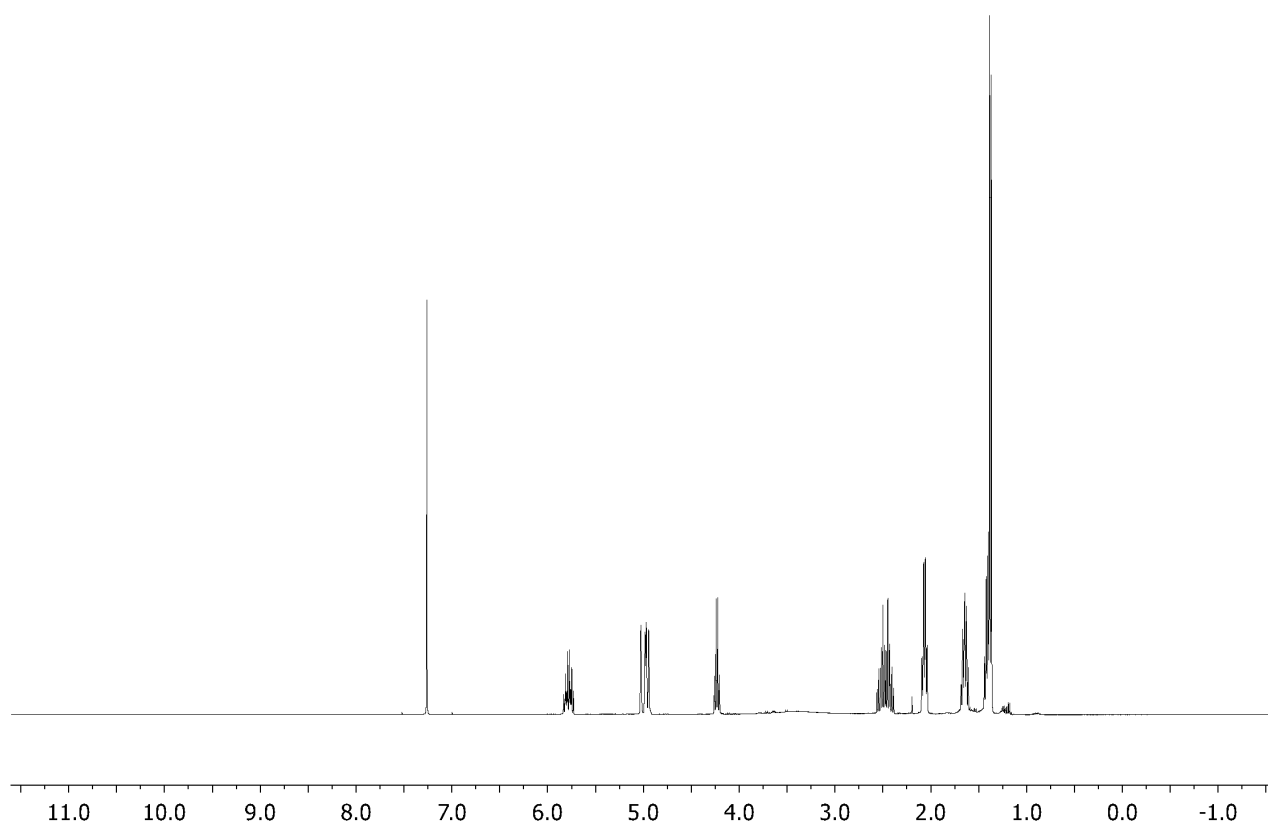
#### Table of Contents

|                                                                                                                                                                                     |    |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----|
| (S)-8-Hydroxy-7-oxo-non-1-ene (10) .....                                                                                                                                            | 3  |
| (S)-7-Oxonon-1-en-8-yl benzoate (11) .....                                                                                                                                          | 4  |
| <sup>1</sup> H NMR spectrum (CDCl <sub>3</sub> ) of crude (2S,4R,5R)-5-Hydroxy-3-oxo-4-(pent-4-enyl)eicosan-2-yl benzoate (12) plus diastereoisomer, before recrystallization ..... | 5  |
| (2S,4R,5R)-5-Hydroxy-3-oxo-4-(pent-4-enyl)eicosan-2-yl benzoate (12) .....                                                                                                          | 6  |
| (2S,4R/S,5R)-4-(Pent-4-en-1-yl)eicosane-2,3,5-triol (13).....                                                                                                                       | 7  |
| (2R,3R)-3-Hydroxy-2-(pent-4-en-1-yl)octadecanoic acid (15).....                                                                                                                     | 8  |
| (2R,3R)-3-Hydroxy-2-pentyloctadecanoic acid (16).....                                                                                                                               | 9  |
| 4-((5R,6R)-2,2-Dimethyl-4-oxo-6-pentadecyl-1,3-dioxan-5-yl)butanal (17).....                                                                                                        | 10 |
| 5-(Nonadecylthio)-1-phenyl-1H-tetrazole (18) .....                                                                                                                                  | 11 |
| 5-(Nonadecylsulfonyl)-1-phenyl-1H-tetrazole (20).....                                                                                                                               | 12 |
| 1-Phenyl-5-((8-phenyloctyl)thio)-1H-tetrazole (19) .....                                                                                                                            | 13 |
| 1-Phenyl-5-((8-phenyloctyl)sulfonyl)-1H-tetrazole (21).....                                                                                                                         | 14 |

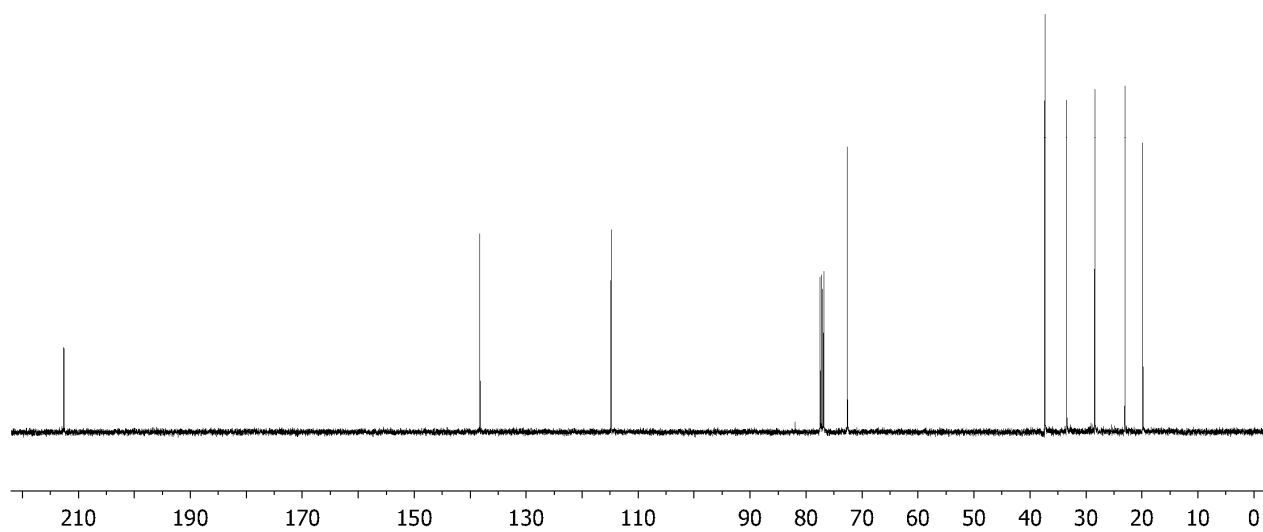
|                                                                                                                                                                       |           |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|
| <b>(2<i>R</i>,3<i>R</i>)-3-Hydroxy-2-(12-phenyldodec-4-en-1-yl)octadecanoic acid (23)</b> .....                                                                       | <b>15</b> |
| <b>(2<i>R</i>,3<i>R</i>)-3-Hydroxy-2-(12-phenyldodecyl)octadecanoic acid (25)</b> .....                                                                               | <b>16</b> |
| <b>(2<i>R</i>,3<i>R</i>)-3-Hydroxy-2-(tricosanyl)octadecanoic acid (24)</b> .....                                                                                     | <b>17</b> |
| <b>Benzyl 2,3,4-tri-<i>O</i>-benzyl-6-<i>O</i>-((2<i>R</i>,3<i>R</i>)-3-hydroxy-2-(pentyl)octadecanoyl)-<math>\beta</math>-D-glucopyranoside (28)</b> .....           | <b>18</b> |
| <b>6-<i>O</i>-((2<i>R</i>,3<i>R</i>)-3-Hydroxy-2-(pentyl)octadecanoyl)-D-glucopyranose (32)</b> .....                                                                 | <b>19</b> |
| <b>Benzyl 2,3,4-tri-<i>O</i>-benzyl-6-<i>O</i>-((2<i>R</i>,3<i>R</i>)-3-Hydroxy-2-(tricosanyl)octadecanoyl)-<math>\beta</math>-D-glucopyranoside (29)</b> .....       | <b>20</b> |
| <b>6-<i>O</i>-((2<i>R</i>,3<i>R</i>)-3-Hydroxy-2-(tricosanyl)octadecanoyl)-D-glucopyranose (33)</b> .....                                                             | <b>21</b> |
| <b>Benzyl 2,3,4-tri-<i>O</i>-benzyl-6-<i>O</i>-((2<i>R</i>,3<i>R</i>)-3-hydroxy-2-(12-phenyldodecyl)octadecanoyl)-<math>\beta</math>-D-glucopyranoside (30)</b> ..... | <b>22</b> |
| <b>6-<i>O</i>-((2<i>R</i>,3<i>R</i>)-3-Hydroxy-2-(12-phenyldodecyl)octadecanoyl)-D-glucopyranose (34)</b> .....                                                       | <b>23</b> |
| <b>6-<i>O</i>-(3'-Nonyl)dodecanoyl-D-glucose (35)</b> .....                                                                                                           | <b>24</b> |

**(S)-8-Hydroxy-7-oxo-non-1-ene (10)**

**<sup>1</sup>H NMR**

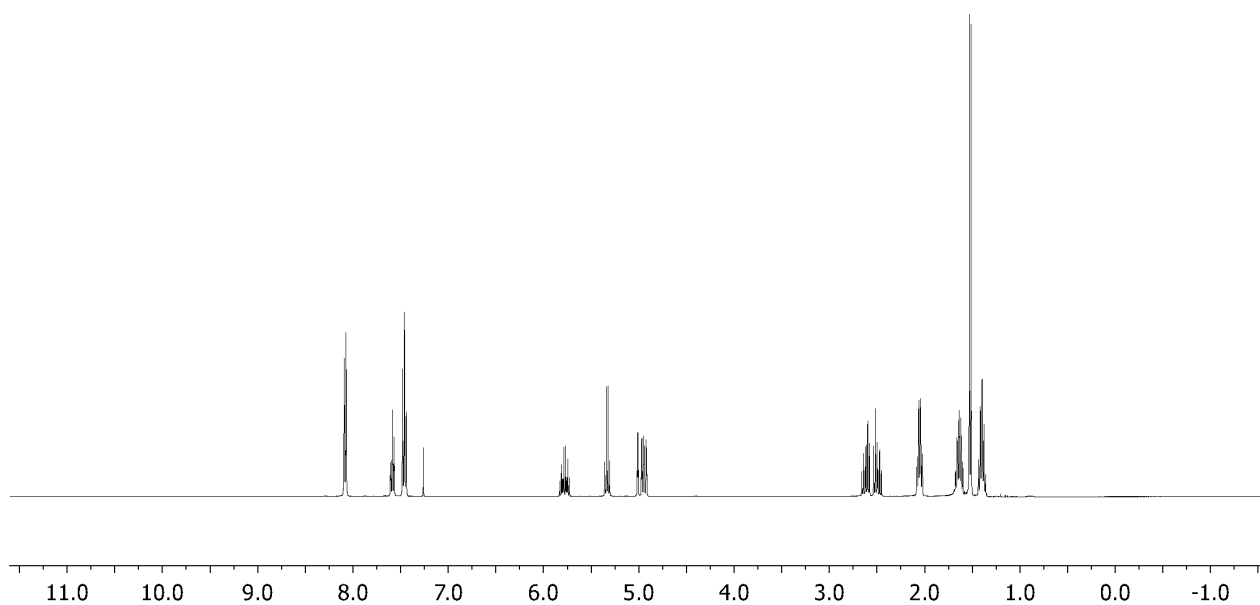


**<sup>13</sup>C NMR**

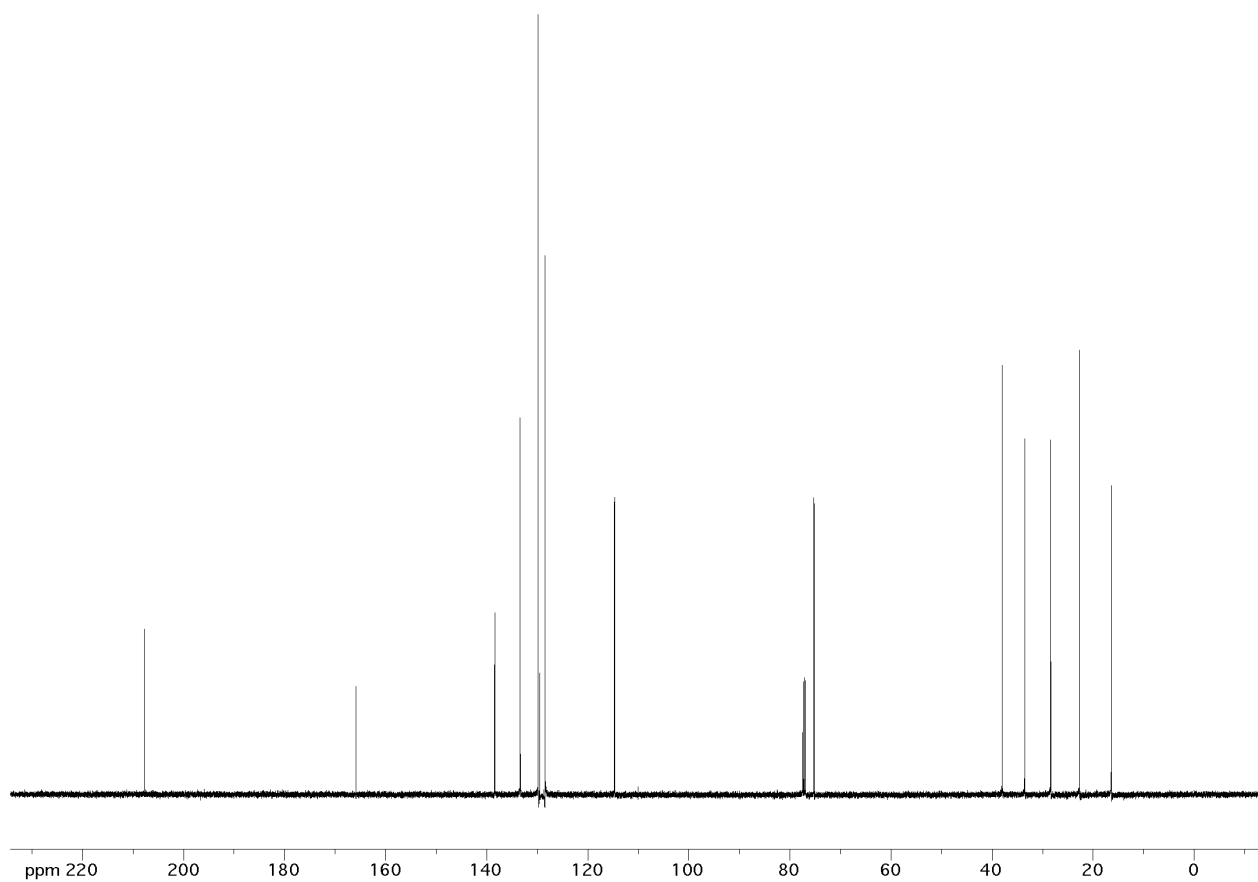


**(S)-7-Oxonon-1-en-8-yl benzoate (11)**

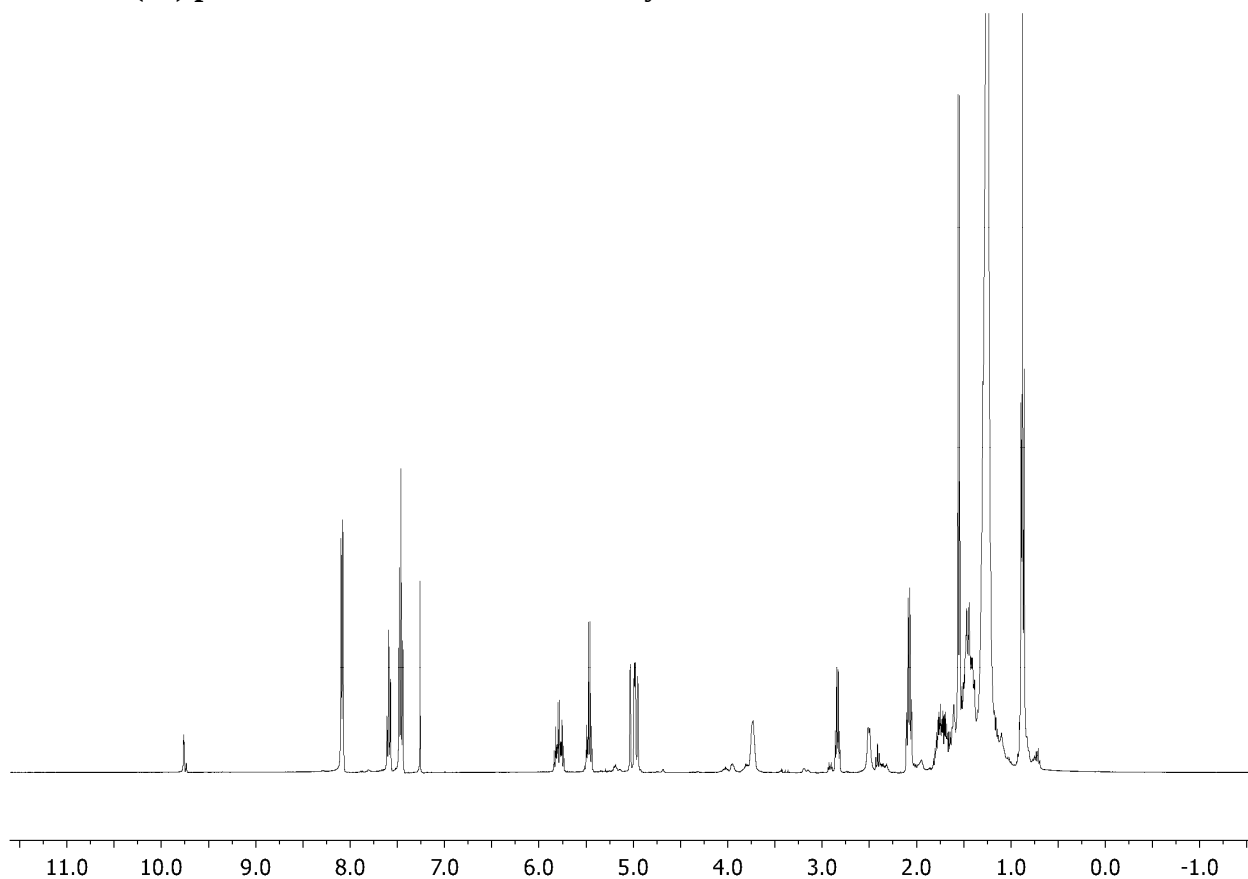
**<sup>1</sup>H NMR**



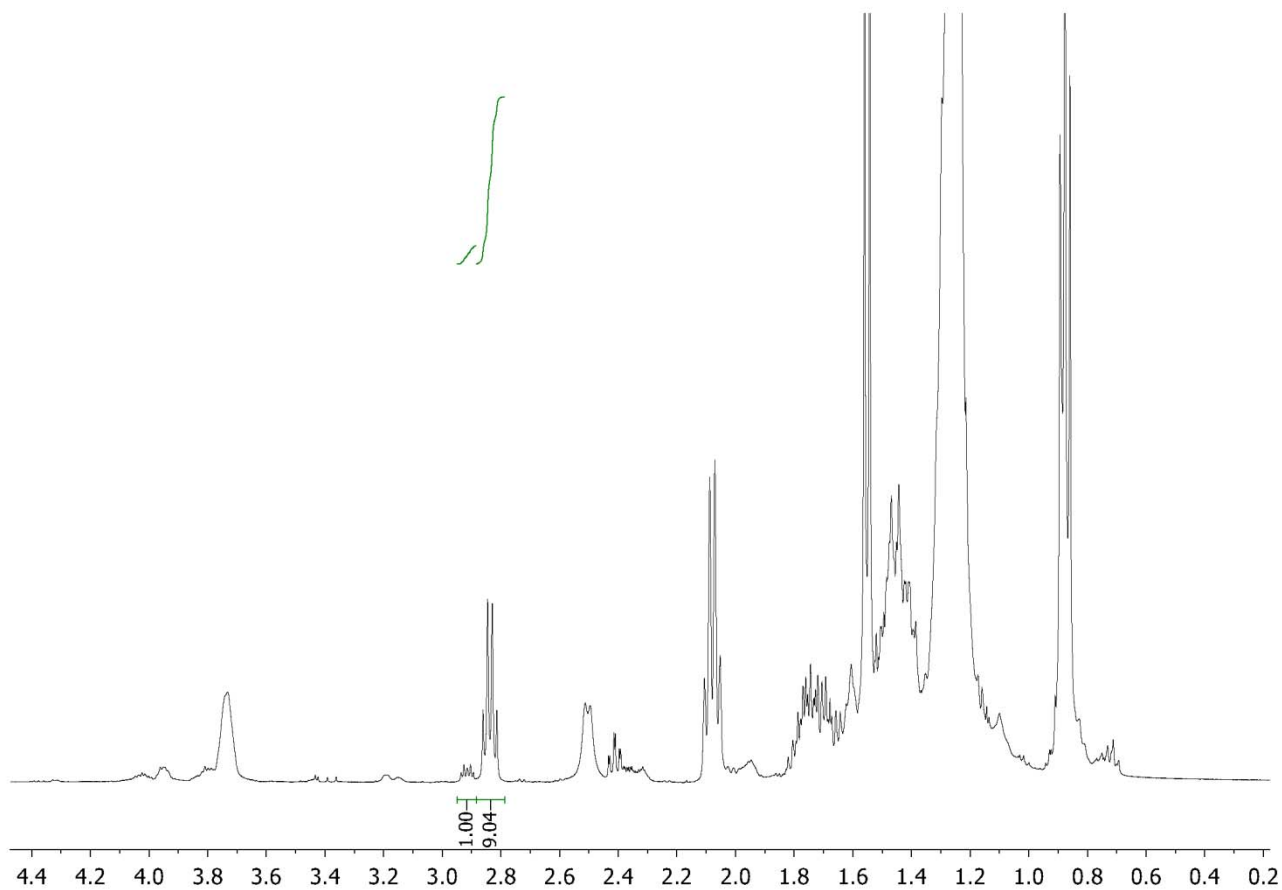
**<sup>13</sup>C NMR**



**$^1\text{H}$  NMR spectrum ( $\text{CDCl}_3$ ) of crude (2*S*,4*R*,5*R*)-5-Hydroxy-3-oxo-4-(pent-4-enyl)eicosan-2-yl benzoate (12) plus diastereoisomer, before recrystallization**

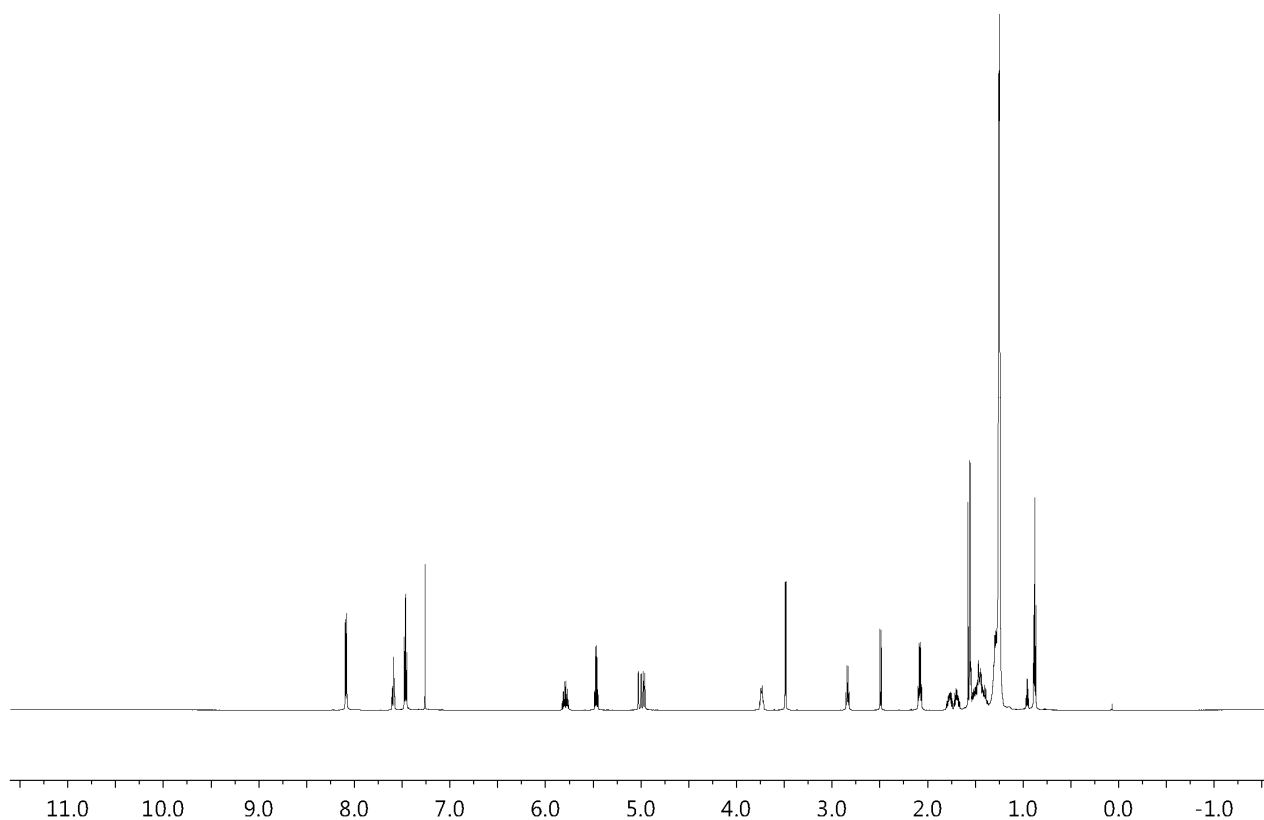


**Expansion**

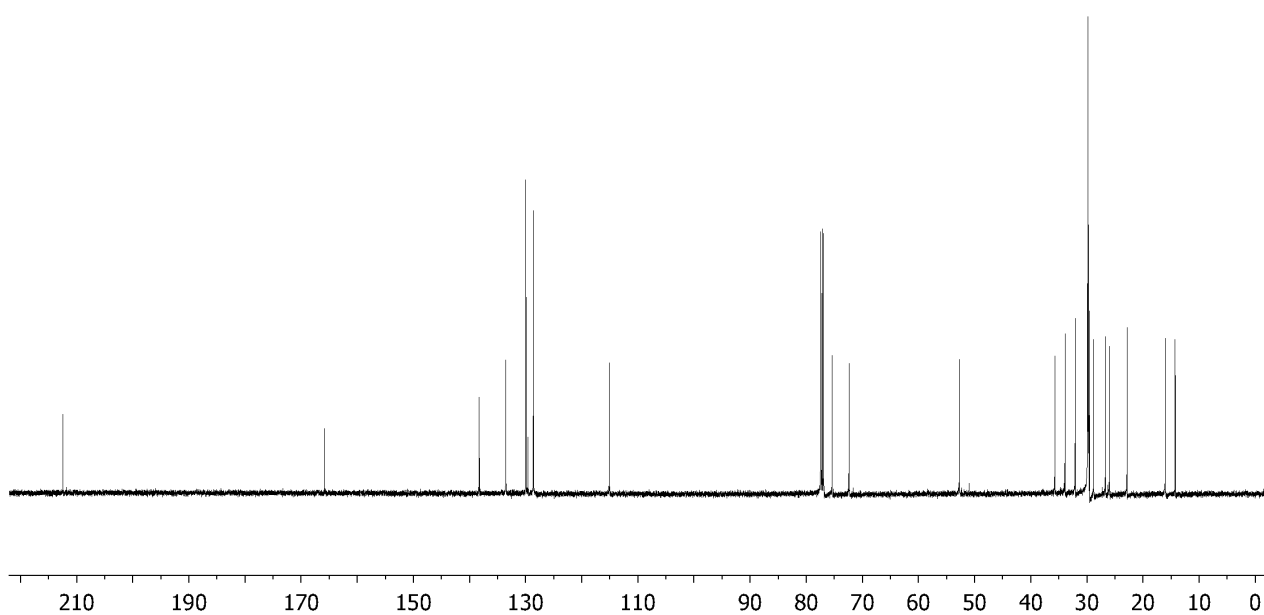


**(2*S*,4*R*,5*R*)-5-Hydroxy-3-oxo-4-(pent-4-enyl)eicosan-2-yl benzoate (12)**

**<sup>1</sup>H NMR**

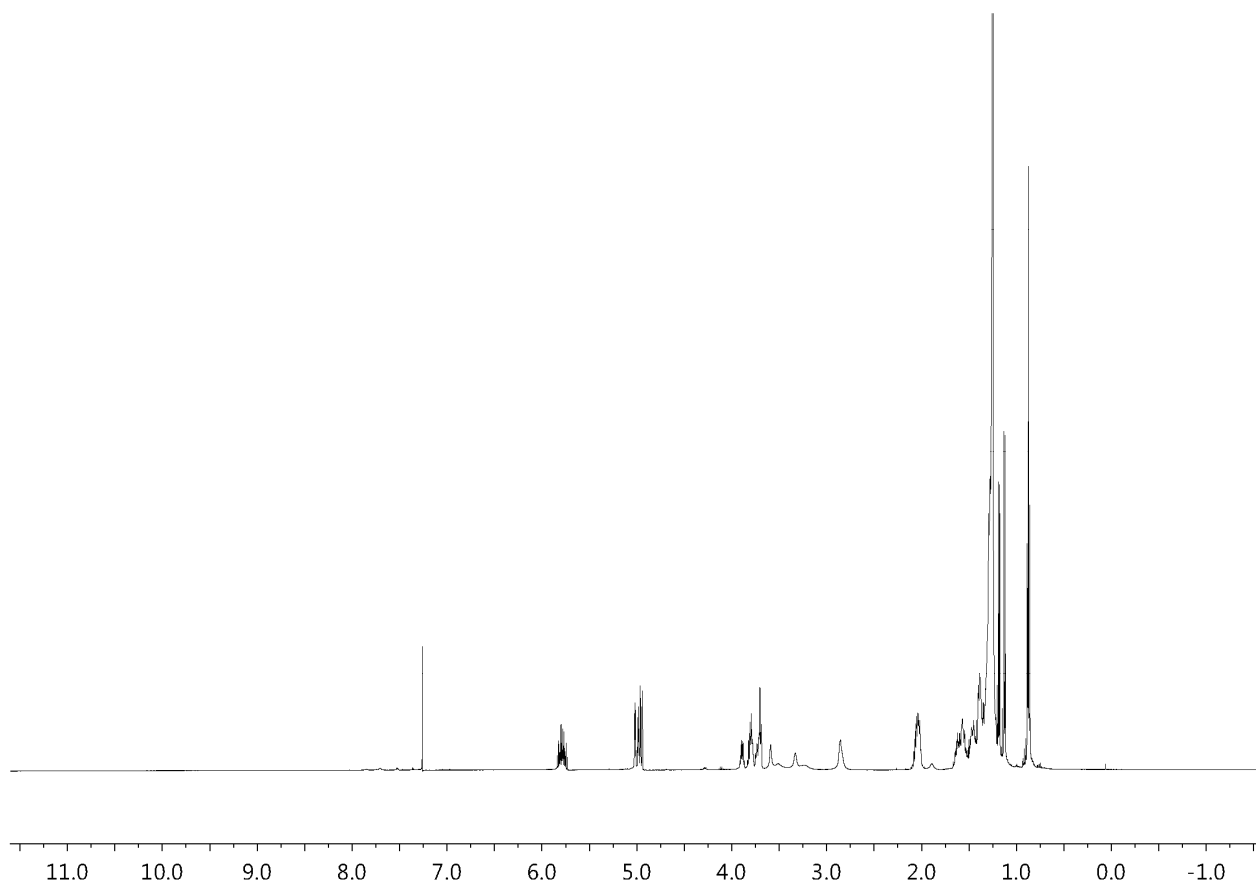


**<sup>13</sup>C NMR**

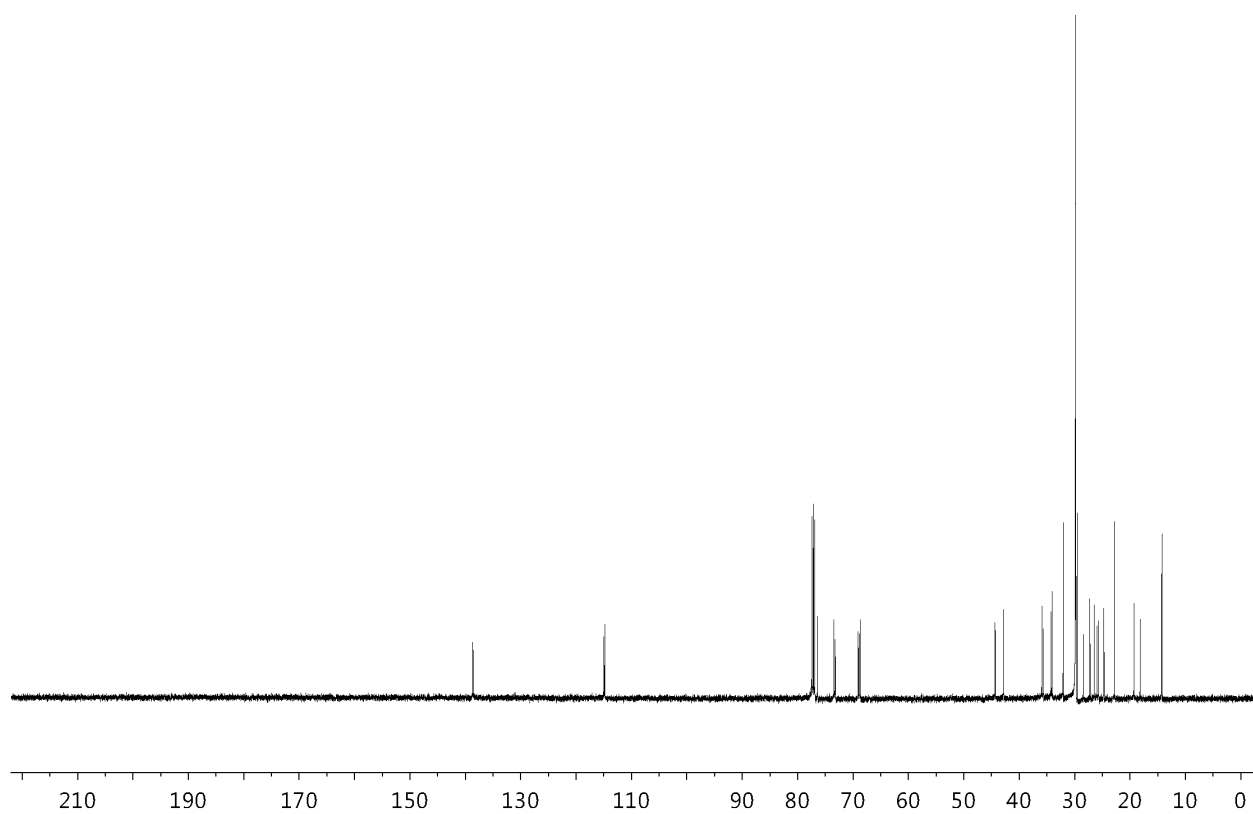


**(2S,4R/S,5R)-4-(Pent-4-en-1-yl)eicosane-2,3,5-triol (13)**

**<sup>1</sup>H NMR**

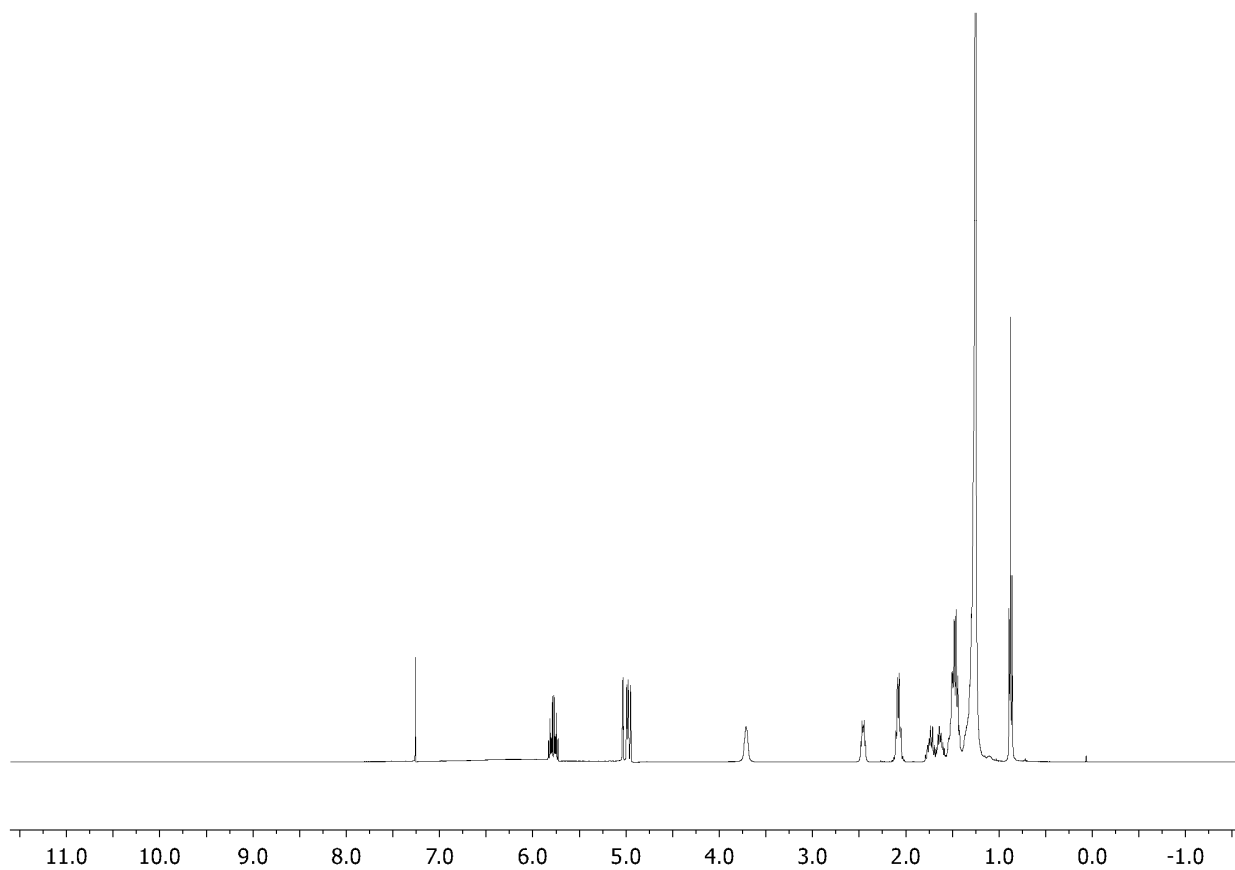


**<sup>13</sup>C NMR**

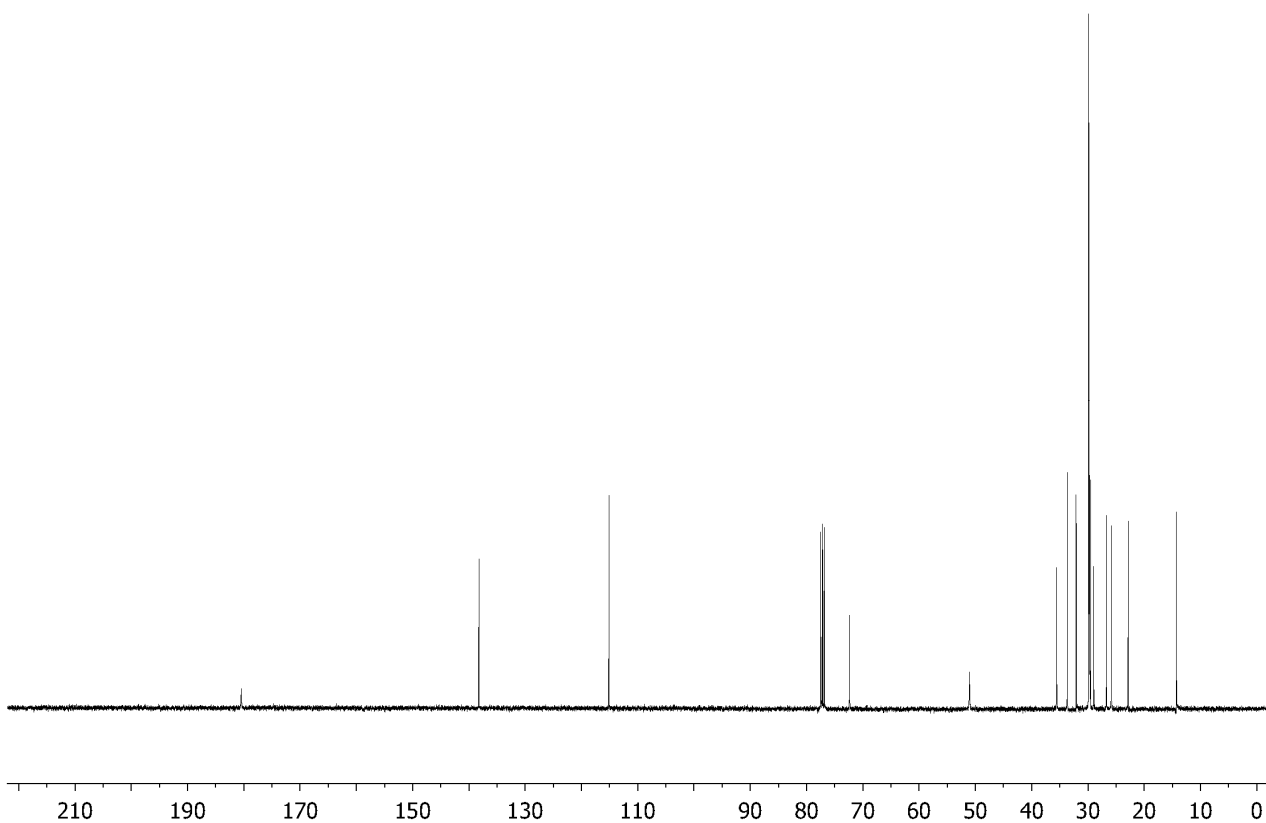


**(2*R*,3*R*)-3-Hydroxy-2-(pent-4-en-1-yl)octadecanoic acid (15)**

**<sup>1</sup>H NMR**

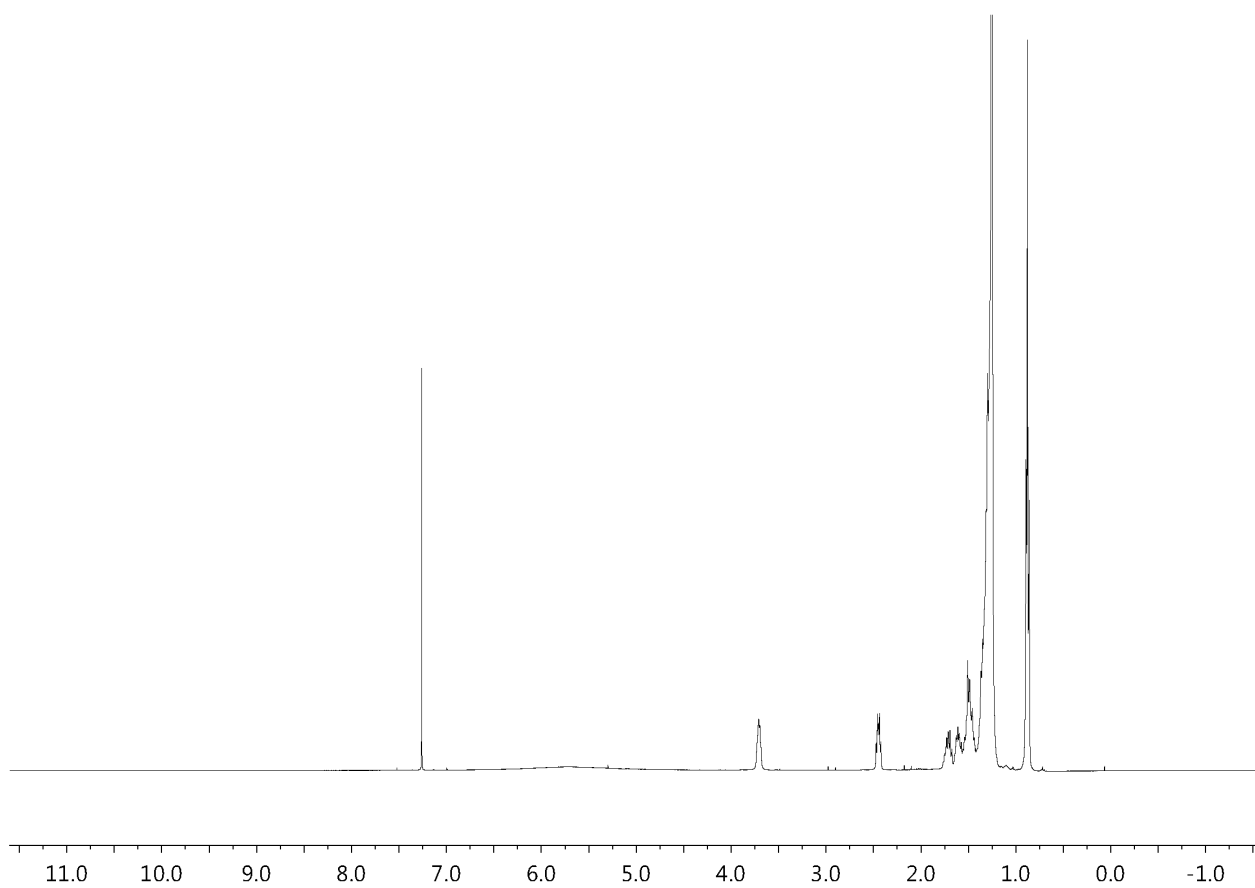


**<sup>13</sup>C NMR**

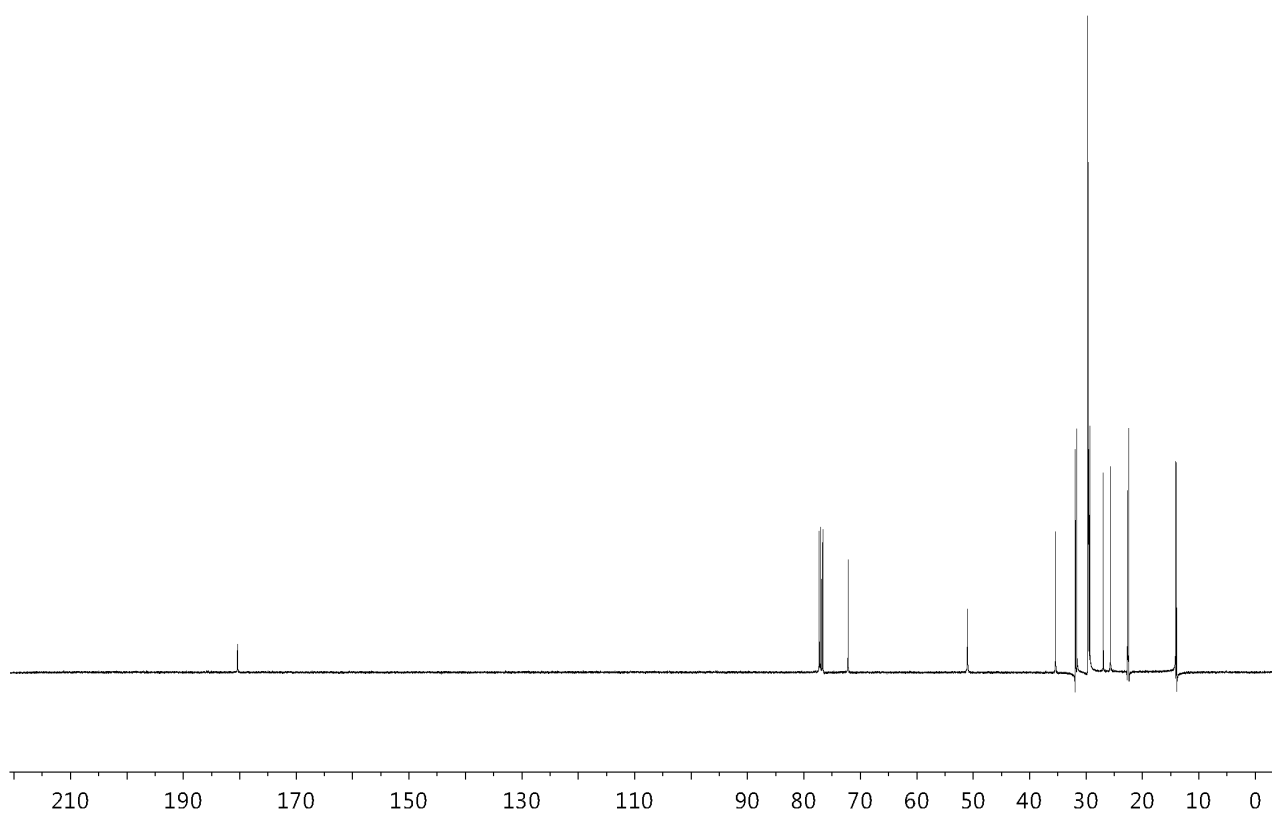


**(2*R*,3*R*)-3-Hydroxy-2-pentyloctadecanoic acid (16)**

**<sup>1</sup>H NMR**

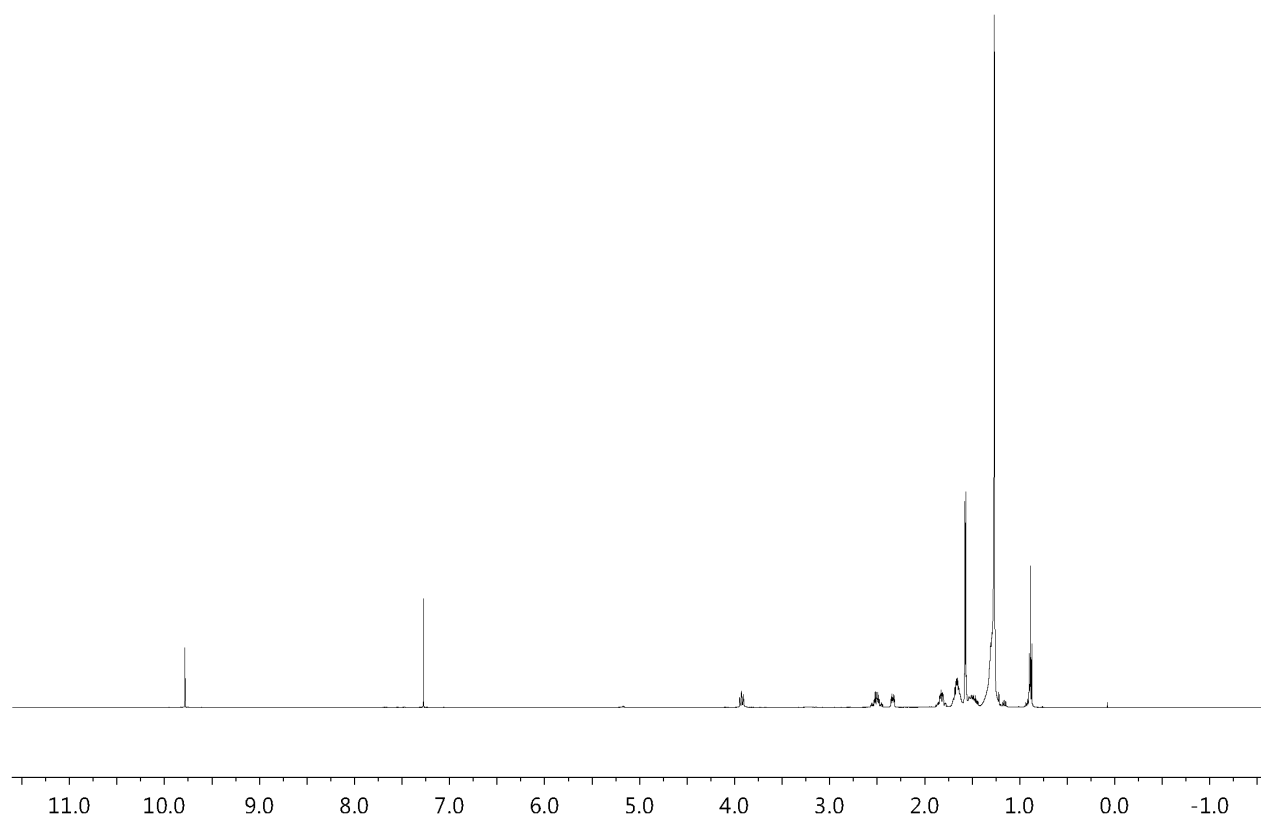


**<sup>13</sup>C NMR**

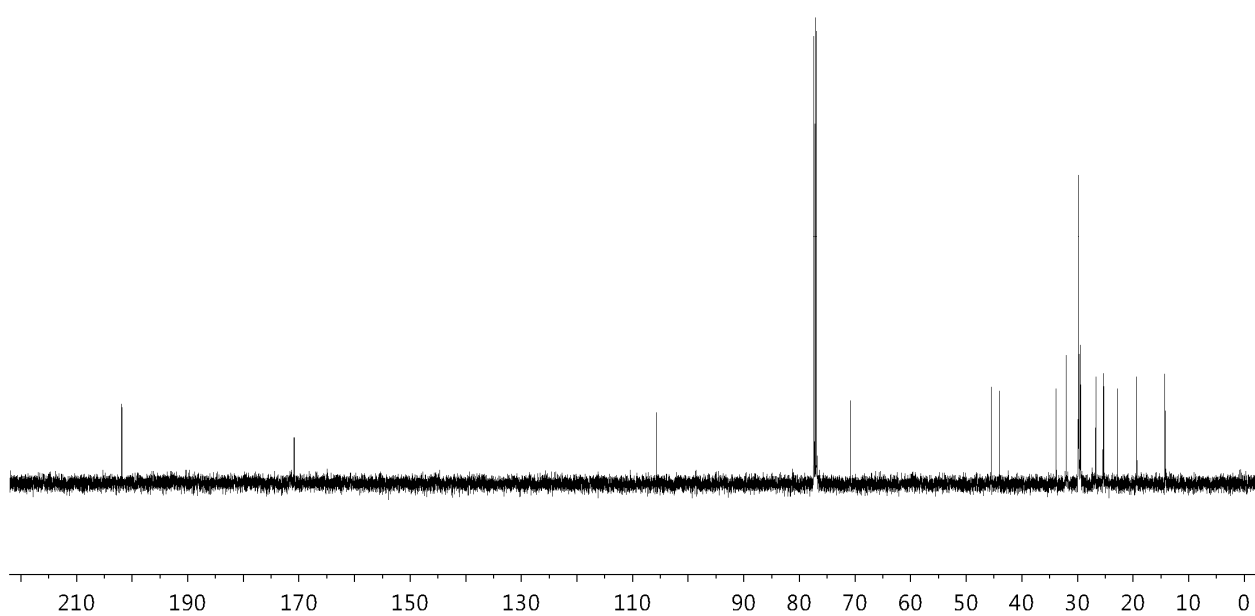


**4-((5*R*,6*R*)-2,2-Dimethyl-4-oxo-6-pentadecyl-1,3-dioxan-5-yl)butanal (17)**

**<sup>1</sup>H NMR**

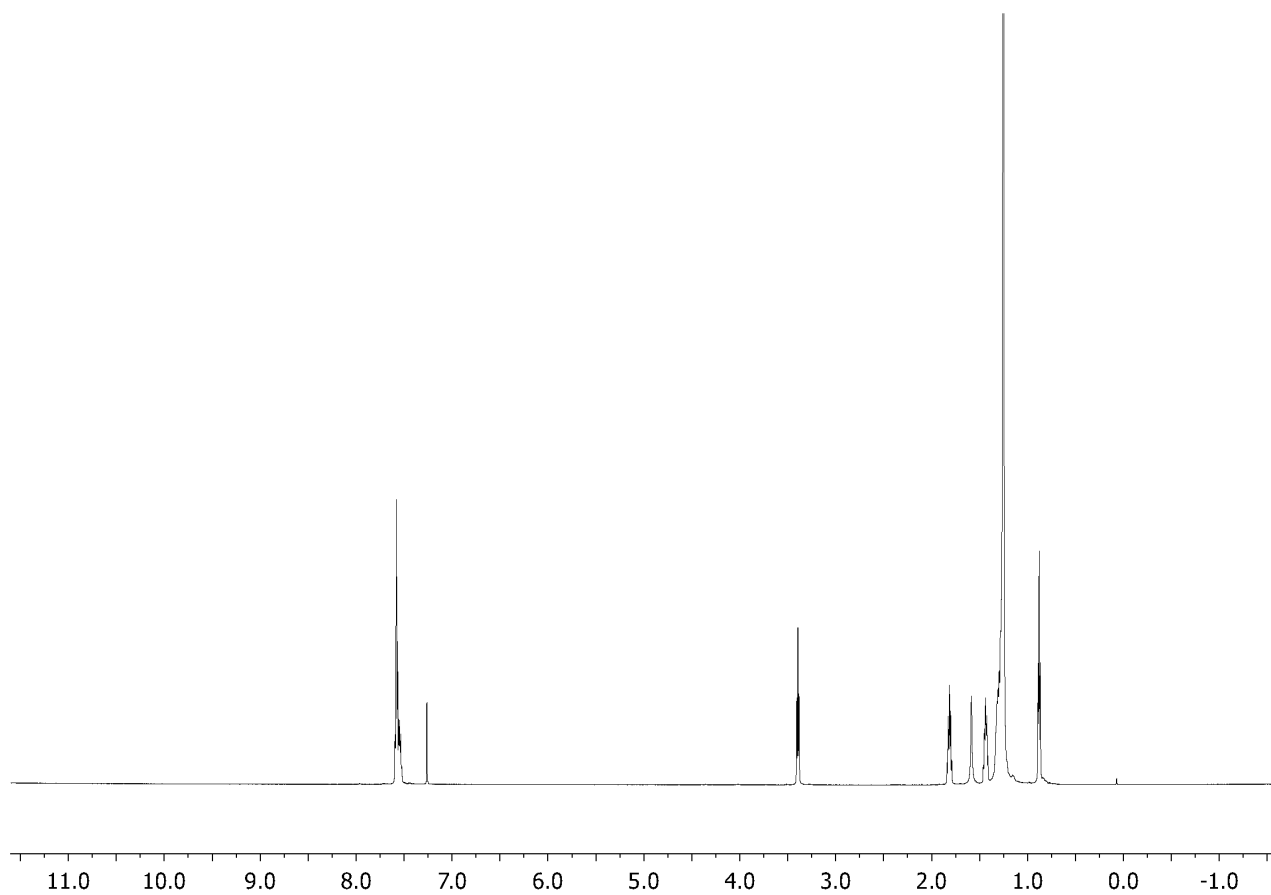


**<sup>13</sup>C NMR**

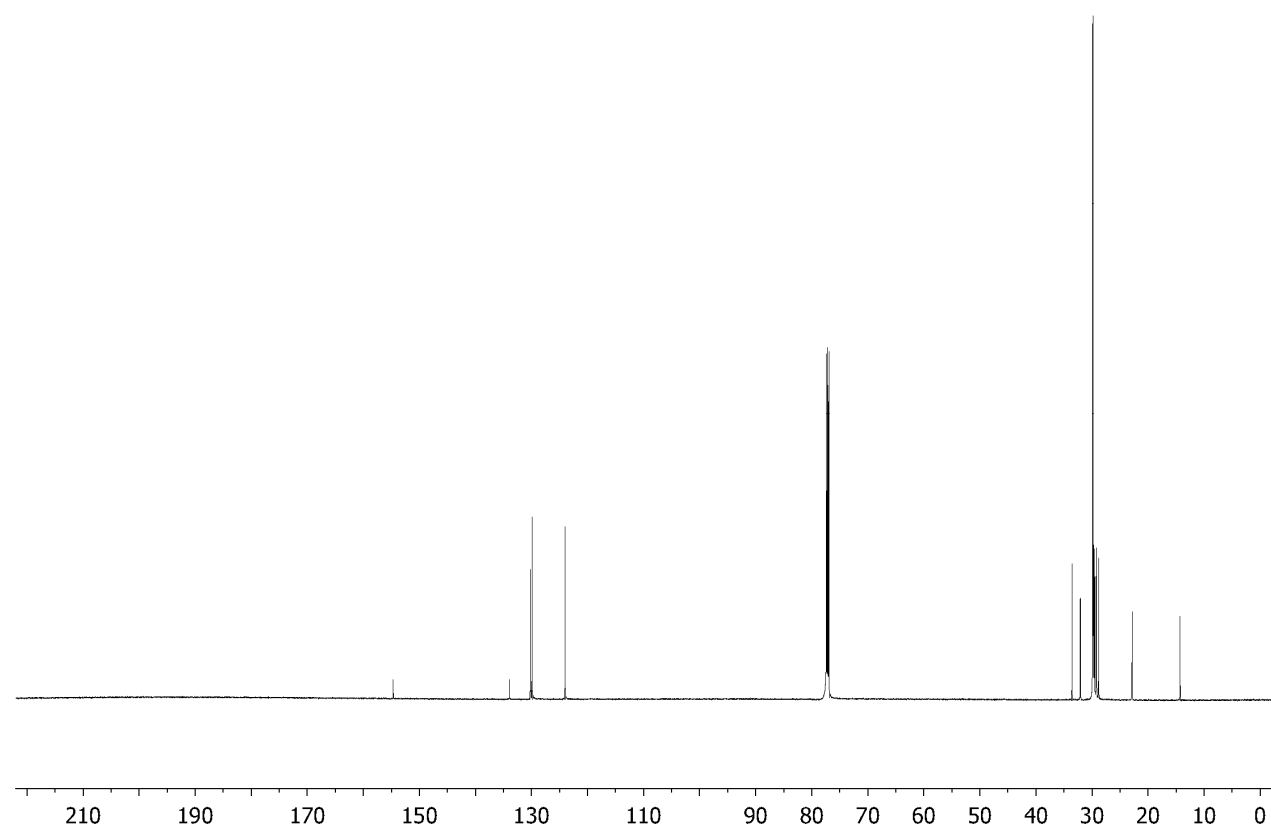


**5-(Nonadecylthio)-1-phenyl-1H-tetrazole (18)**

**<sup>1</sup>H NMR**

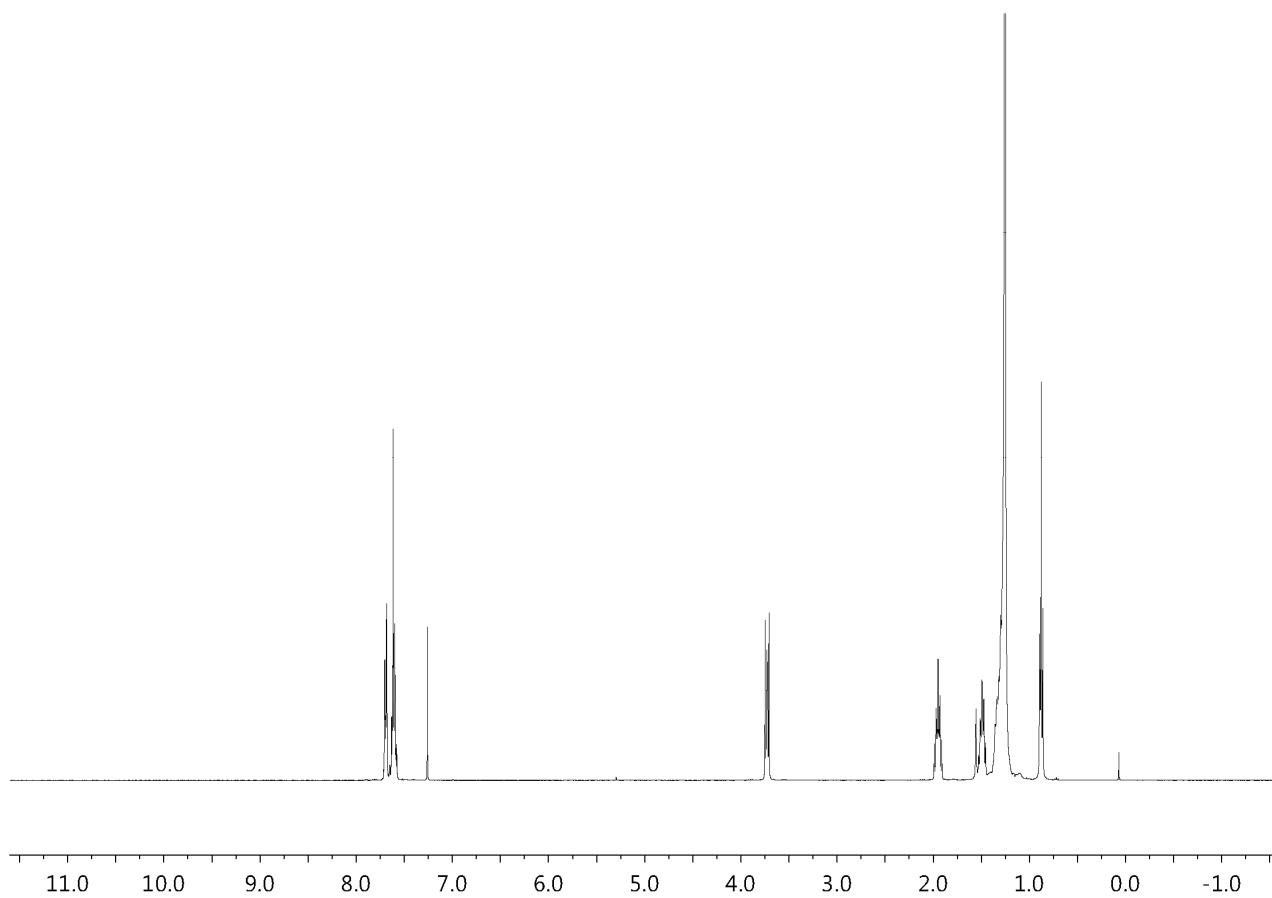


**<sup>13</sup>C NMR**

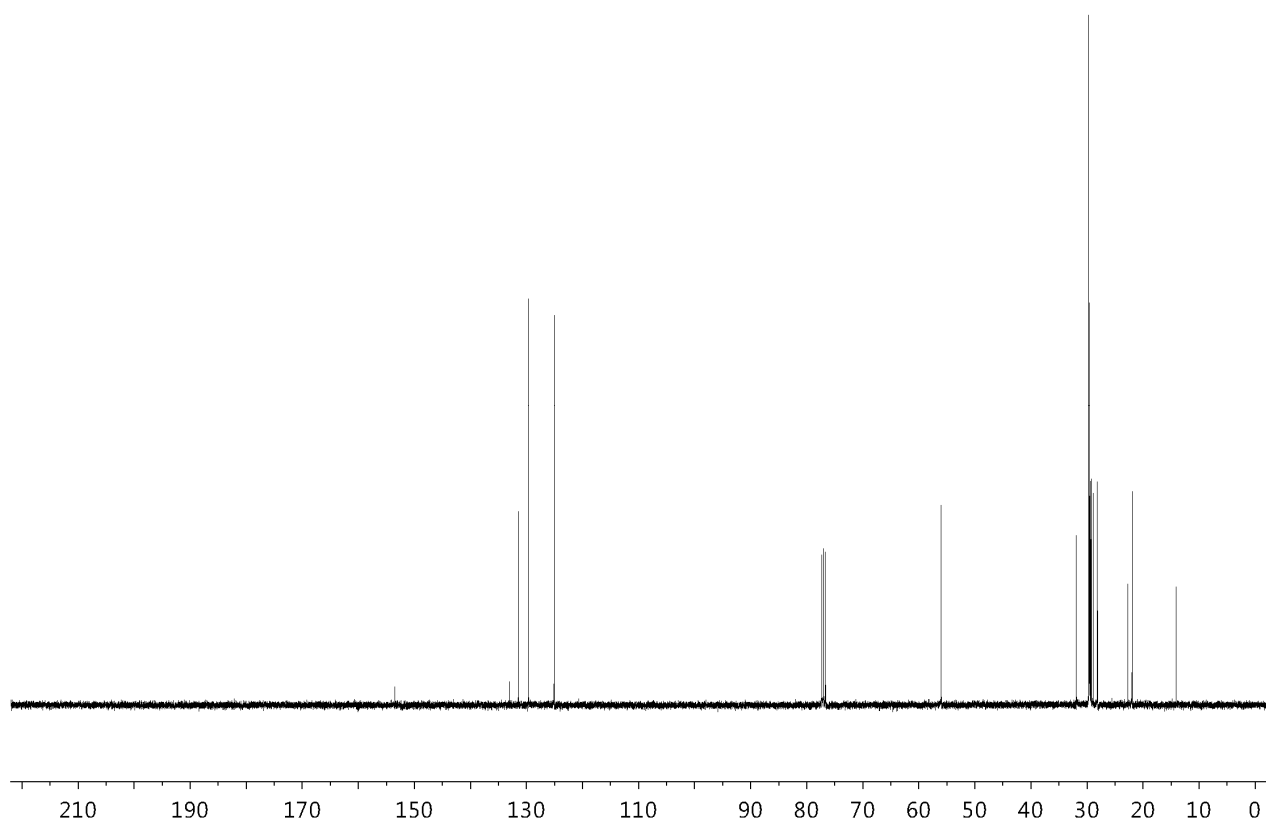


**5-(Nonadecylsulfonyl)-1-phenyl-1*H*-tetrazole (20)**

**<sup>1</sup>H NMR**

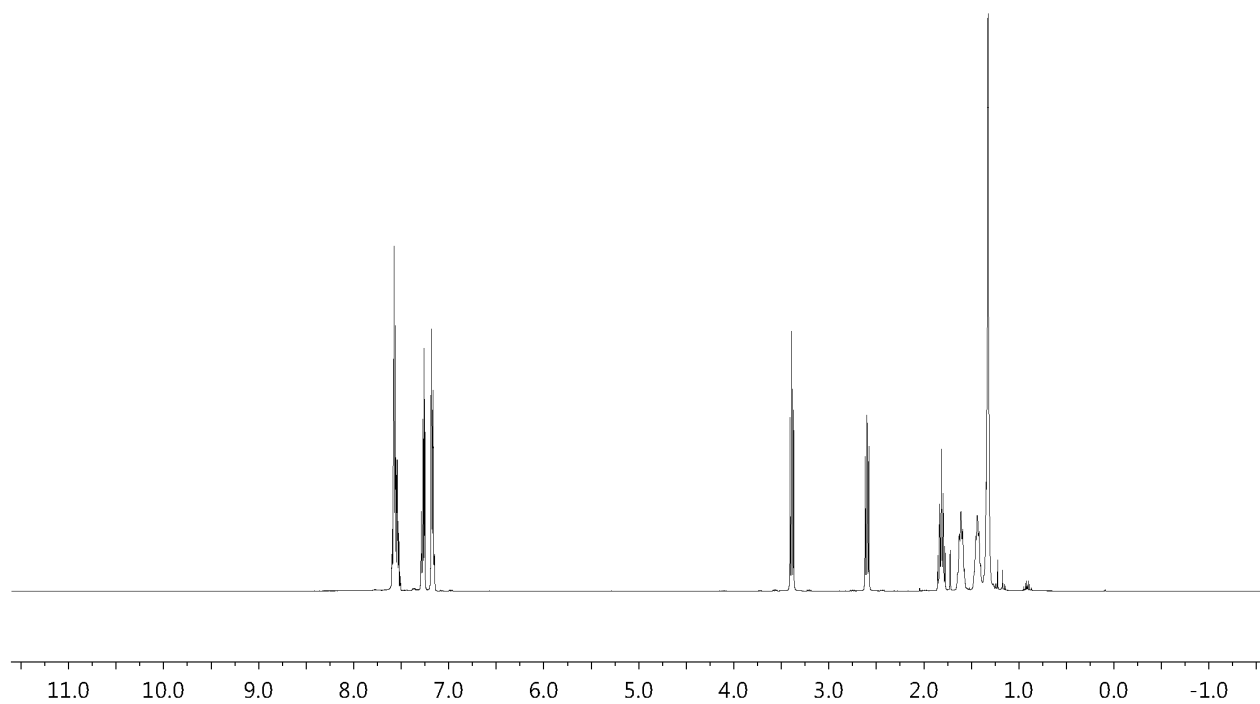


**<sup>13</sup>C NMR**

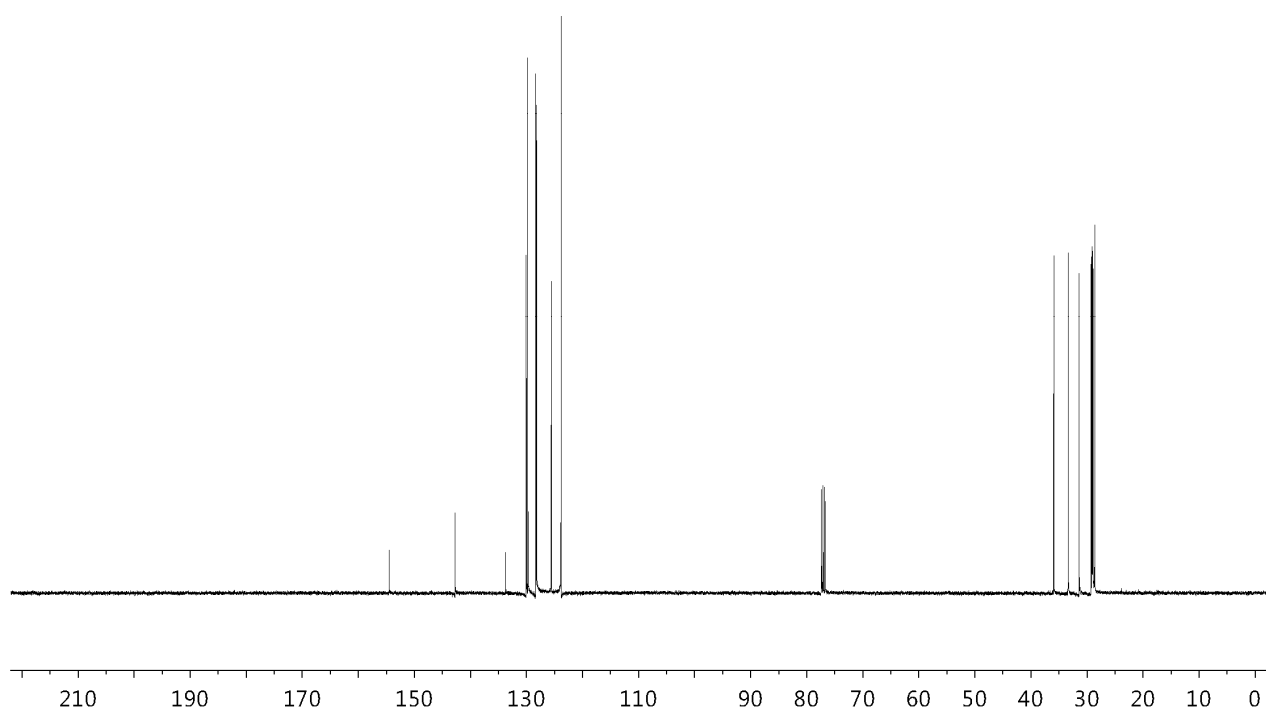


**1-Phenyl-5-((8-phenyloctyl)thio)-1*H*-tetrazole (19)**

**<sup>1</sup>H NMR**

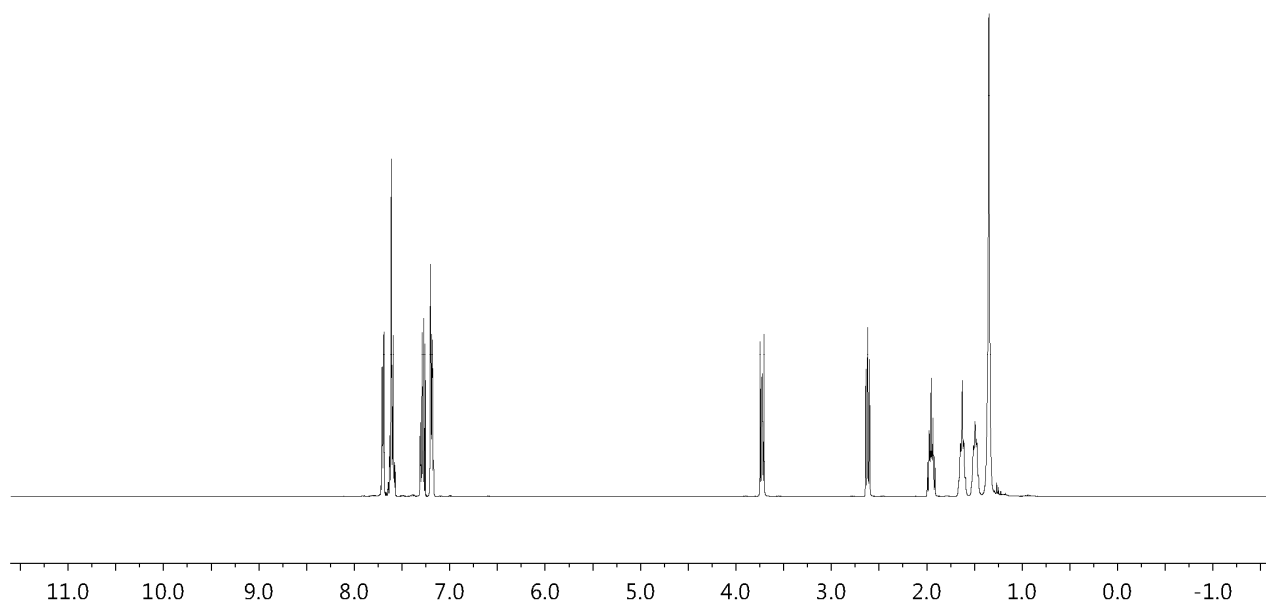


**<sup>13</sup>C NMR**

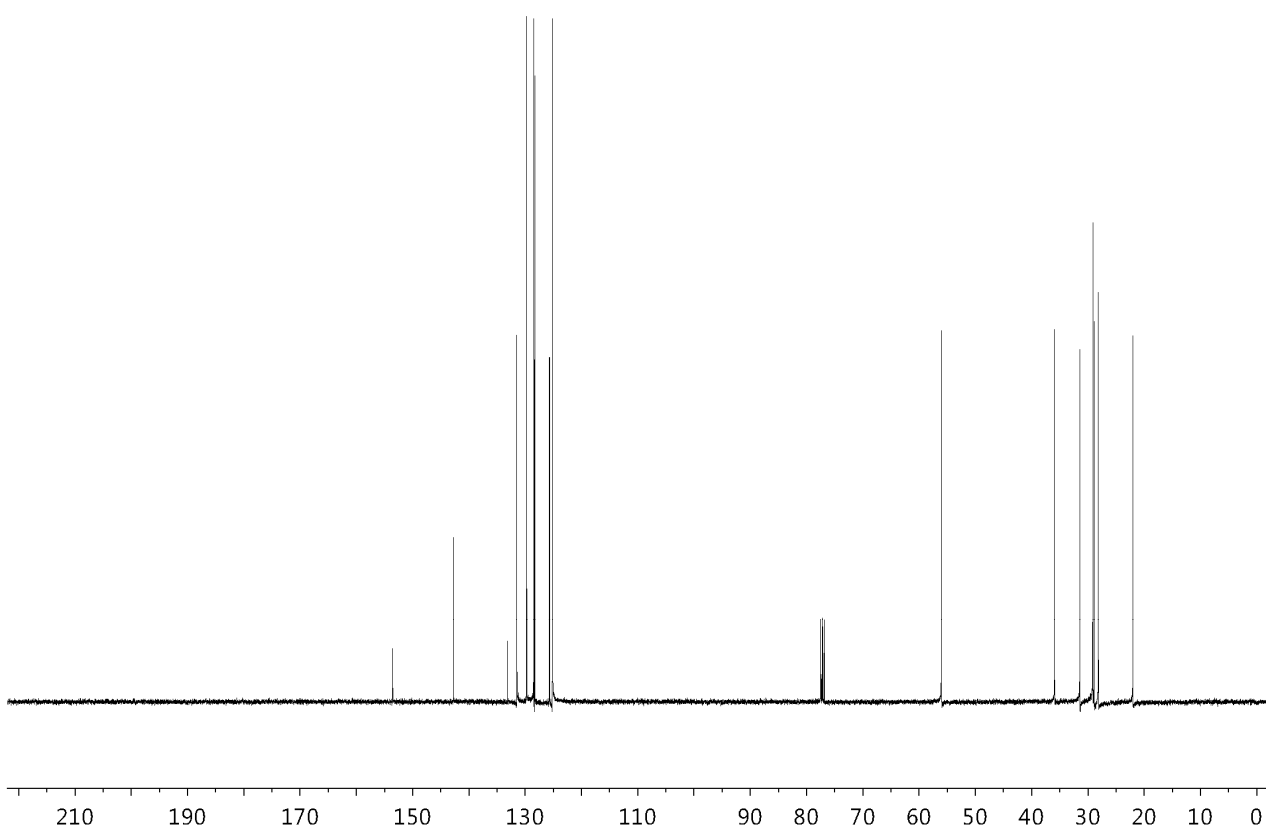


**1-Phenyl-5-((8-phenyloctyl)sulfonyl)-1*H*-tetrazole (21)**

**<sup>1</sup>H NMR**

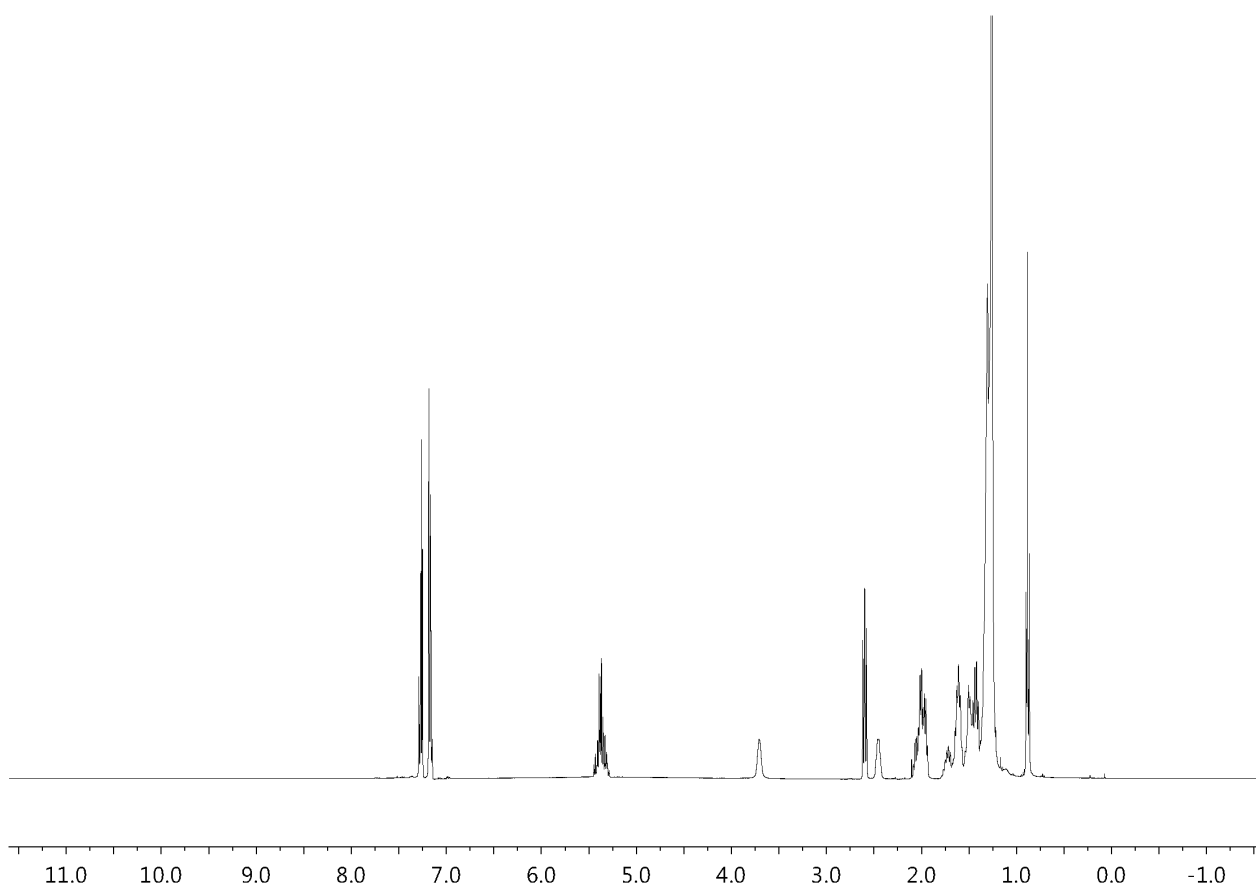


**<sup>13</sup>C NMR**

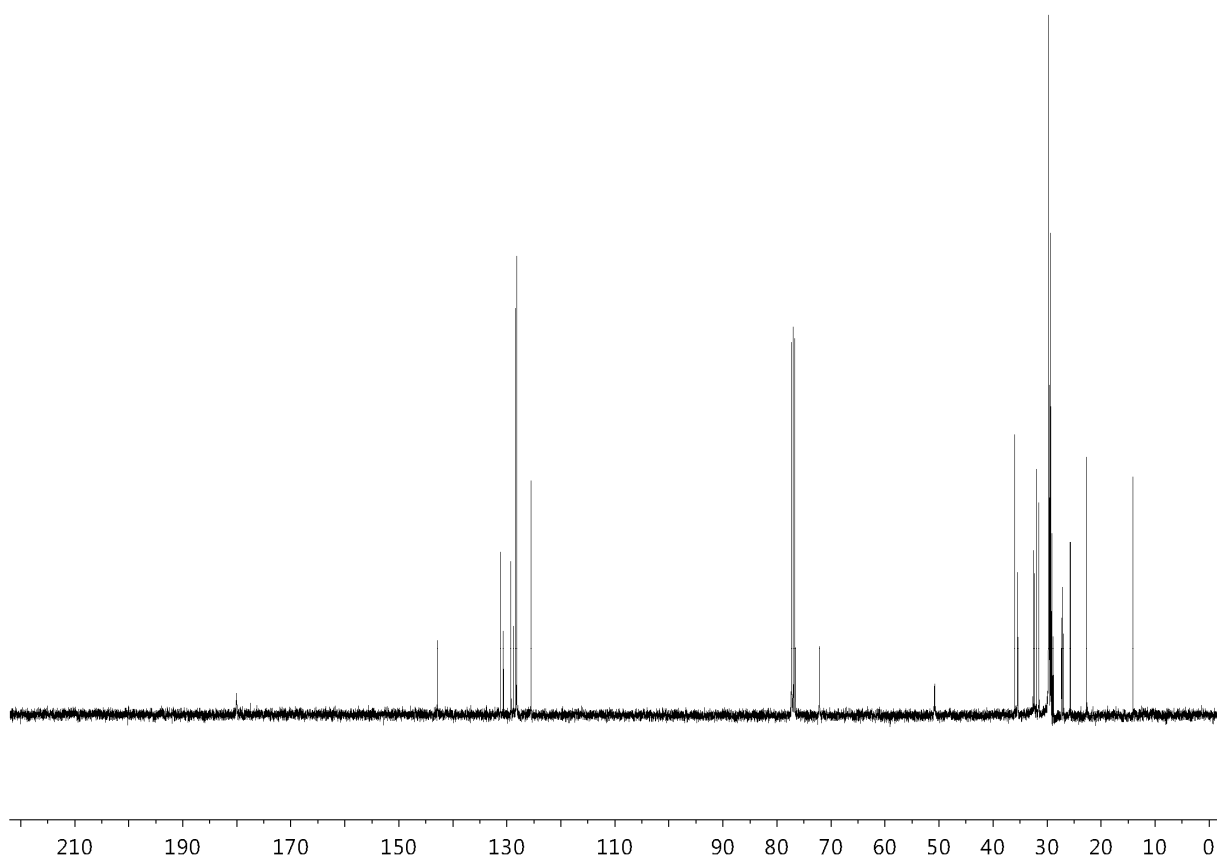


**(2*R*,3*R*)-3-Hydroxy-2-(12-phenyldodec-4-en-1-yl)octadecanoic acid (23)**

**<sup>1</sup>H NMR**

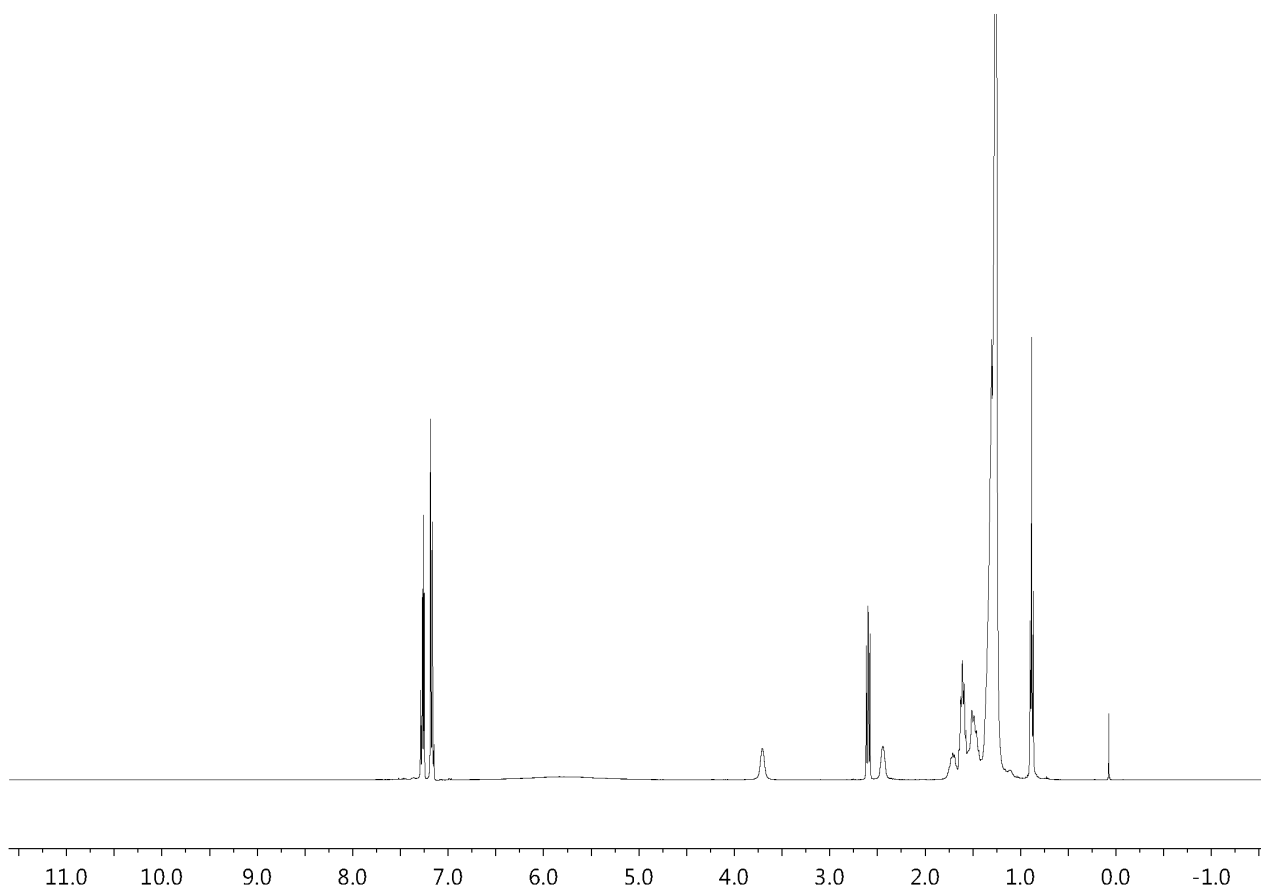


**<sup>13</sup>C NMR**

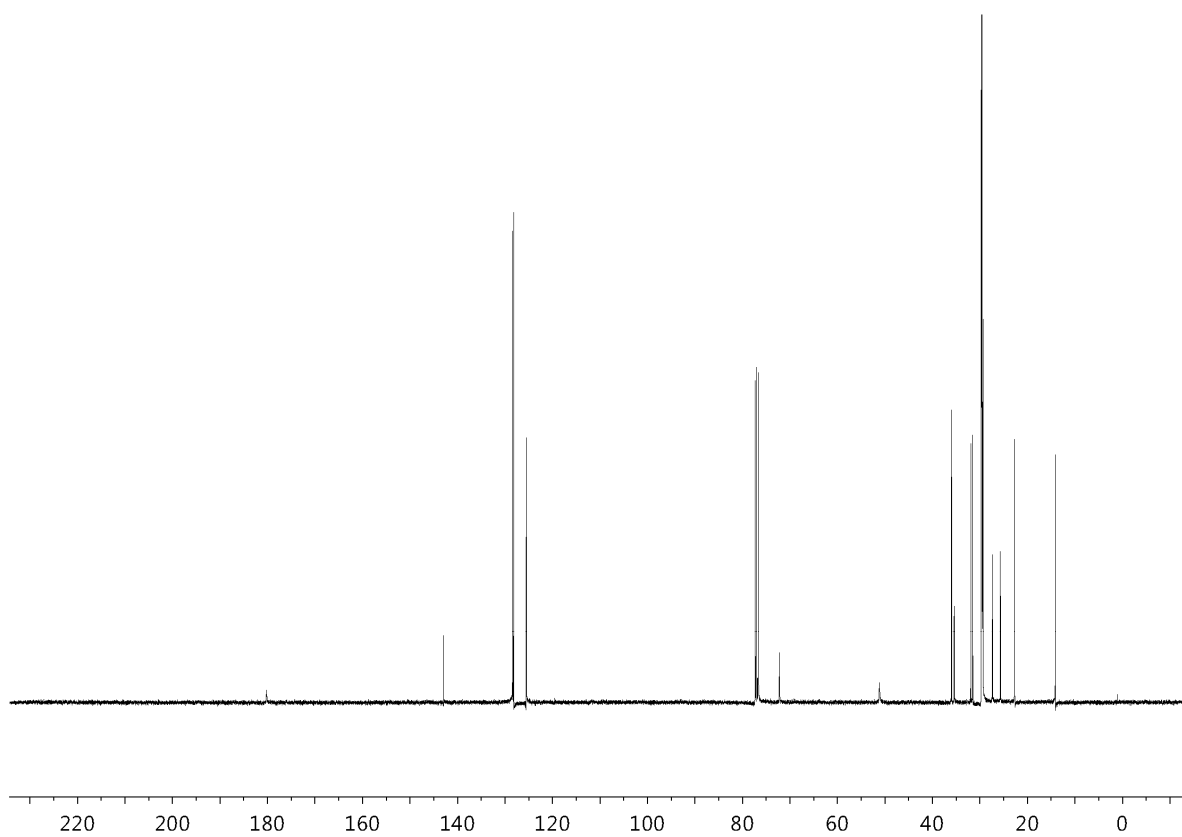


**(2*R*,3*R*)-3-Hydroxy-2-(12-phenyldodecyl)octadecanoic acid (25)**

**<sup>1</sup>H NMR**

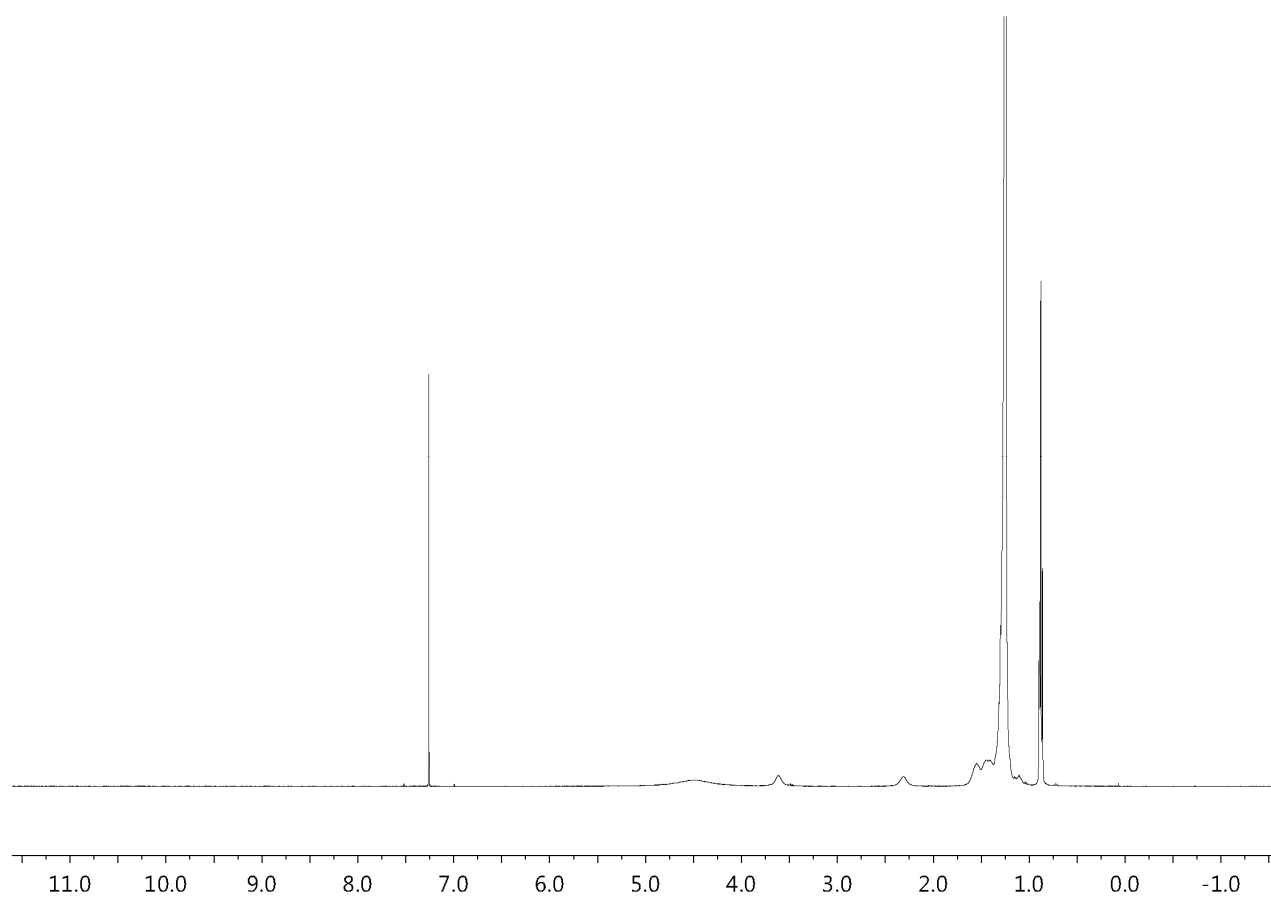


**<sup>13</sup>C NMR**

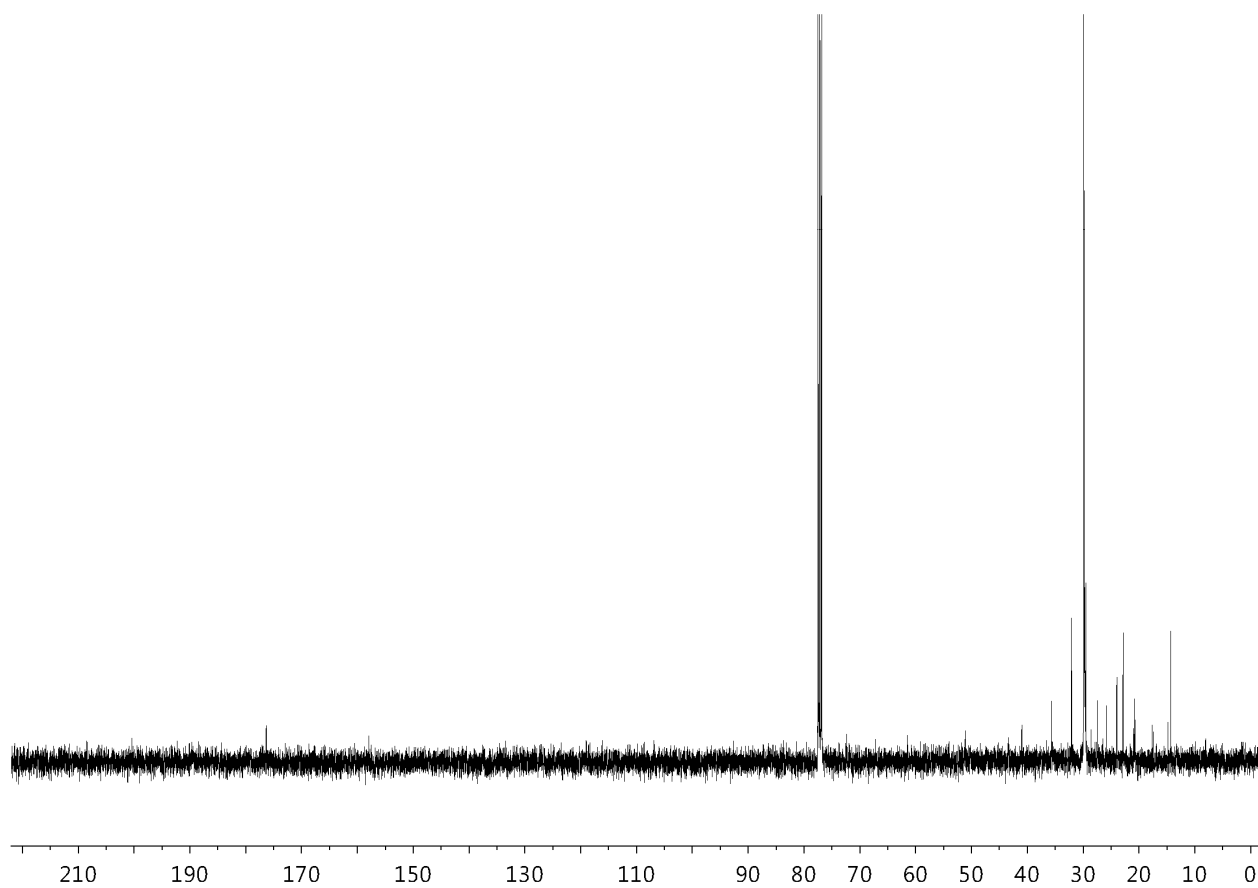


**(2*R*,3*R*)-3-Hydroxy-2-(tricosanyl)octadecanoic acid (24)**

**<sup>1</sup>H NMR**

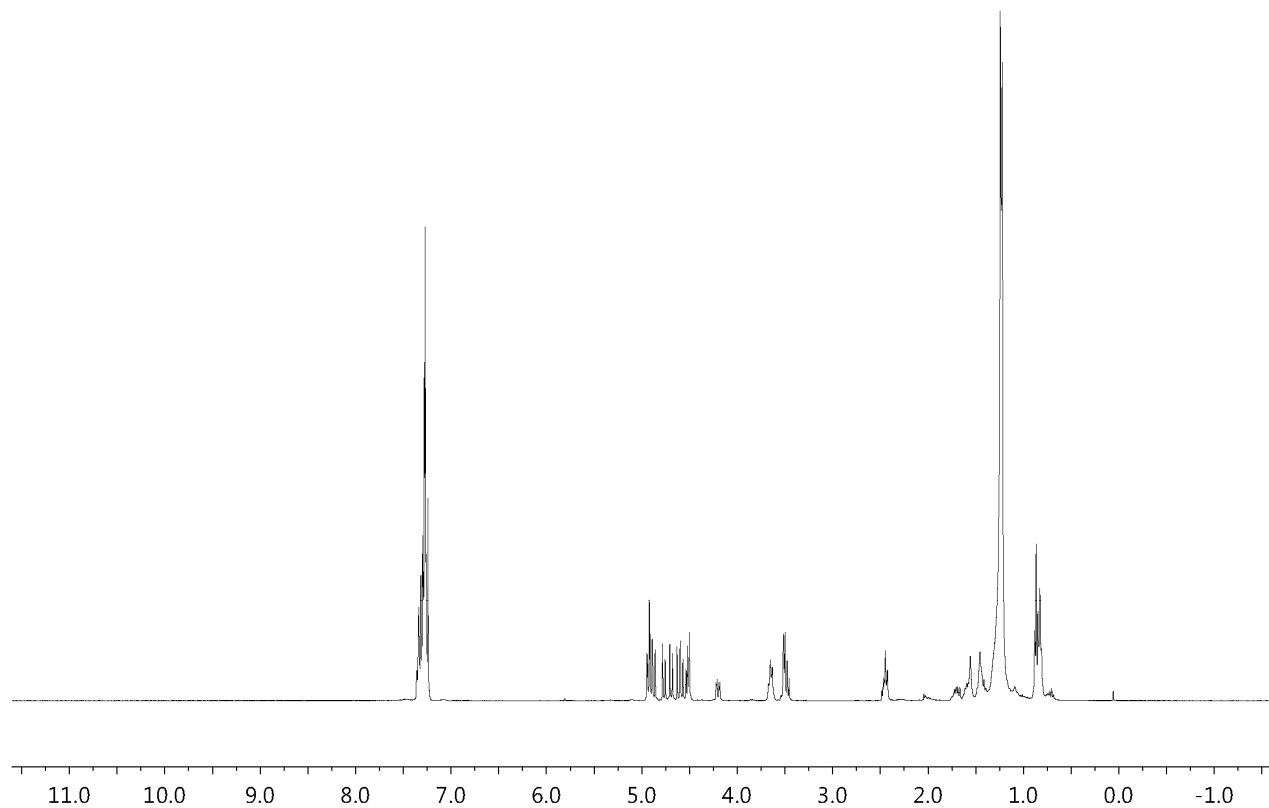


**<sup>13</sup>C NMR**

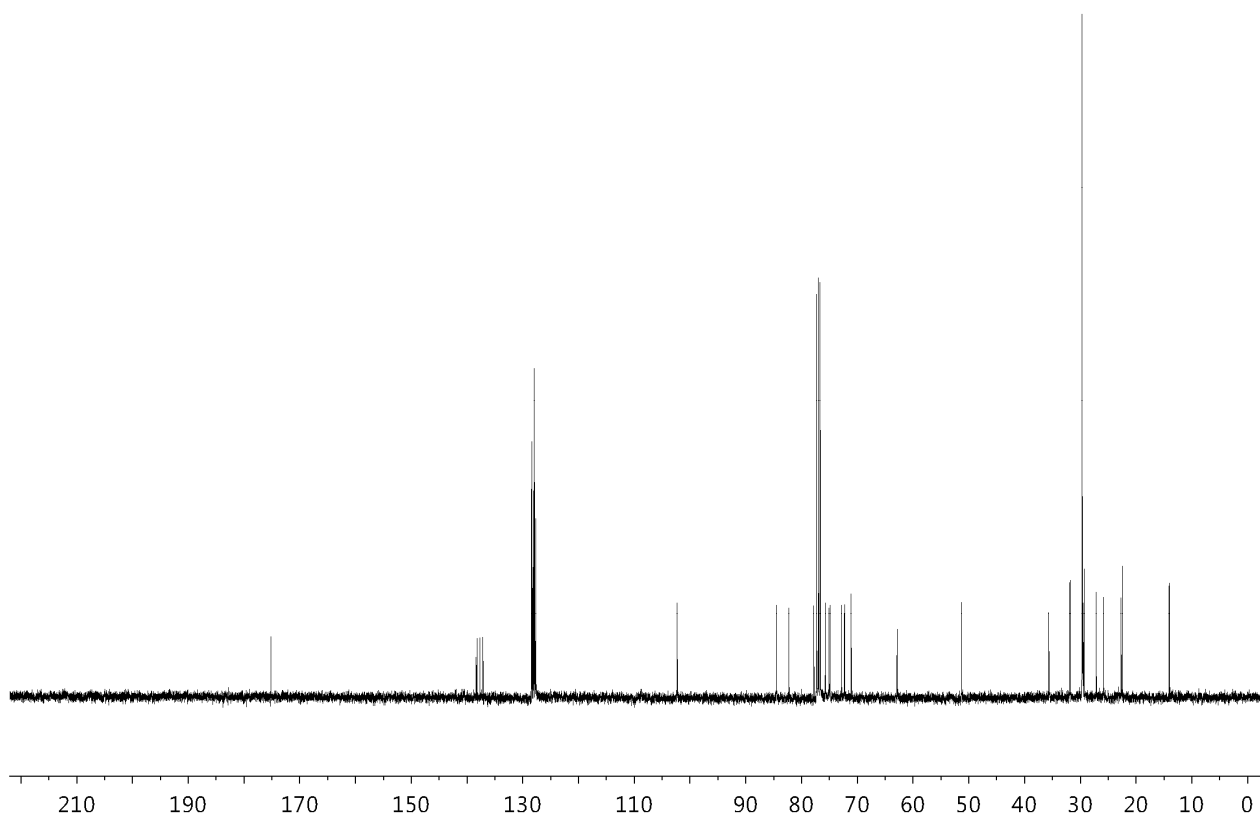


**Benzyl**  
**glucopyranoside (28)**  
**<sup>1</sup>H NMR**

**2,3,4-tri-*O*-benzyl-6-*O*-((2*R*,3*R*)-3-hydroxy-2-(pentyl)octadecanoyl)-β-*D*-**

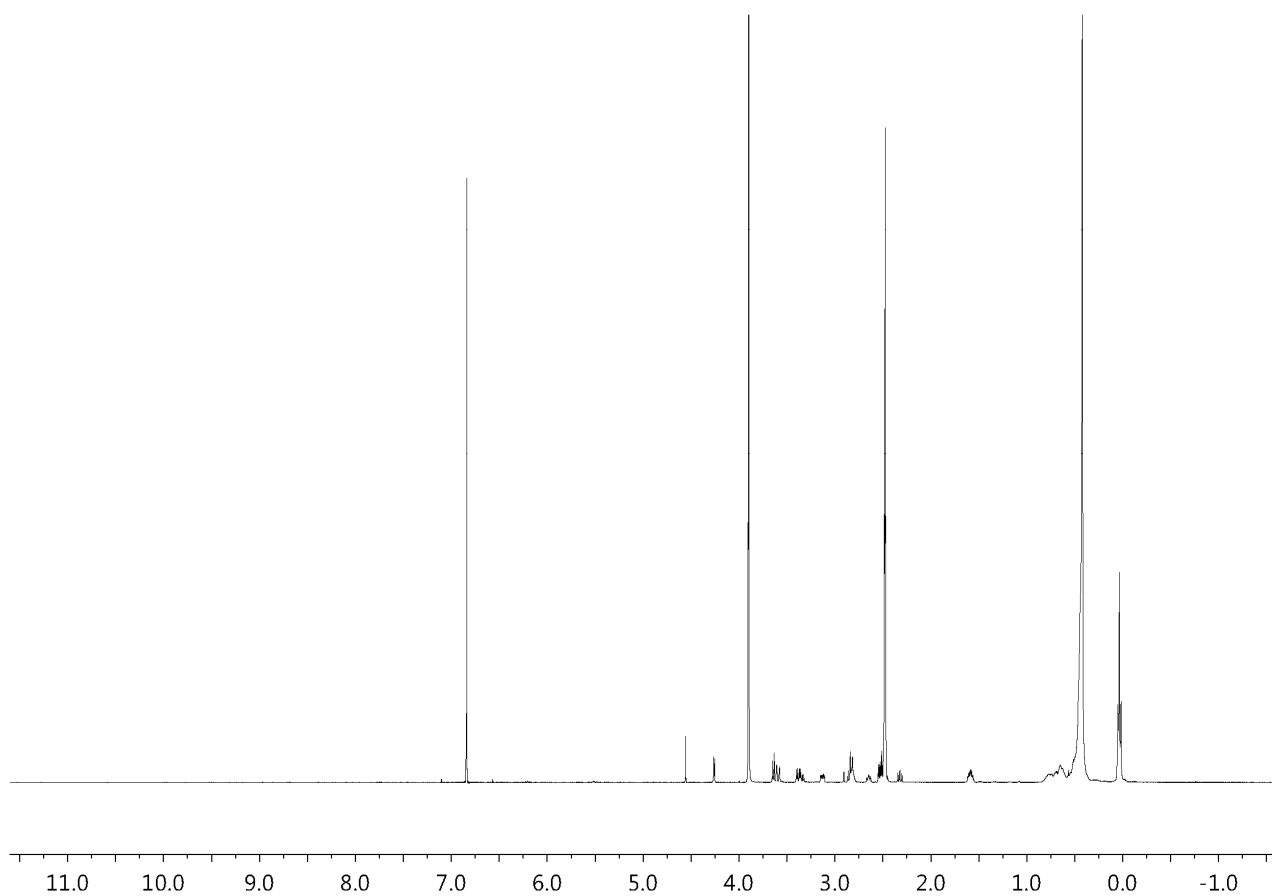


**<sup>13</sup>C NMR**

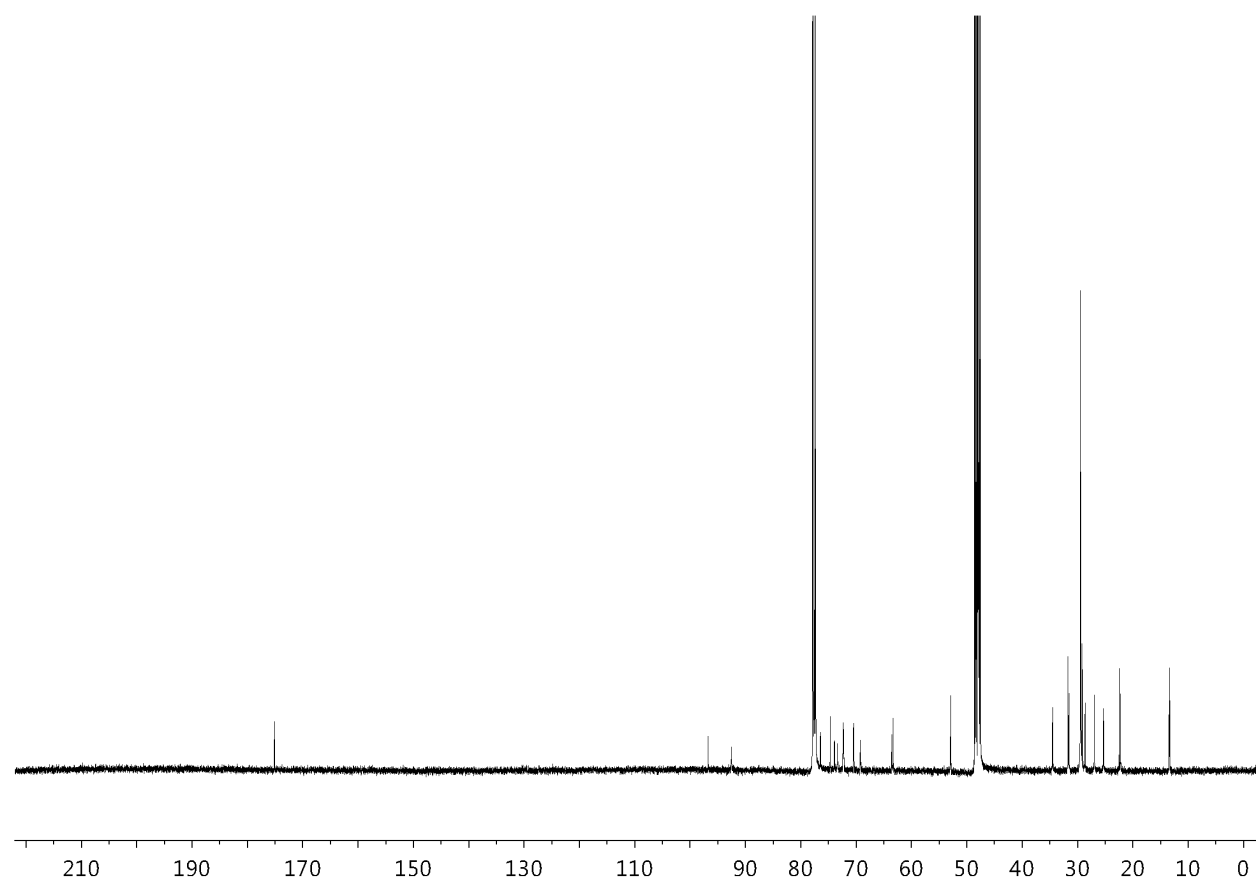


**6-O-((2*R*,3*R*)-3-Hydroxy-2-(pentyl)octadecanoyl)-D-glucopyranose (32)**

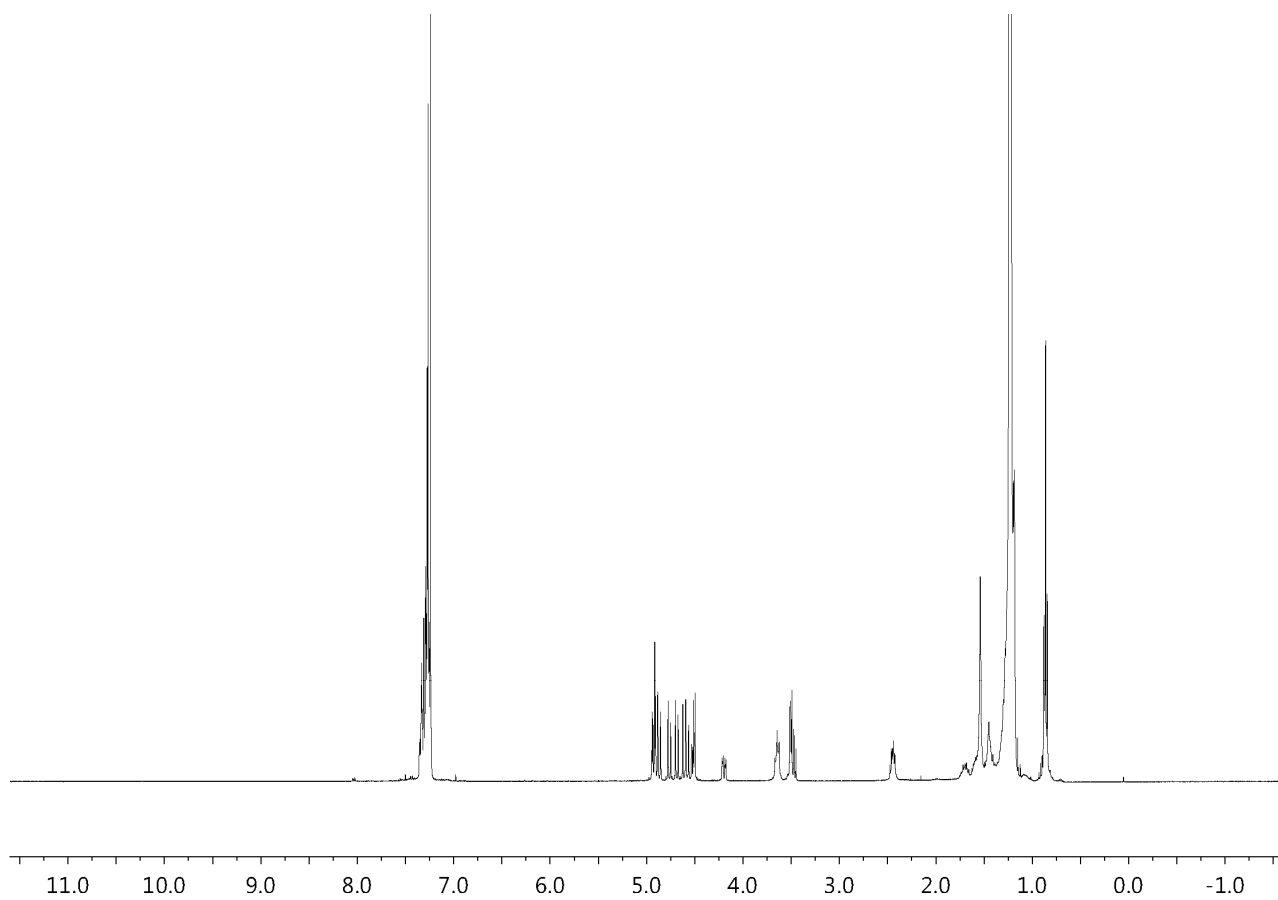
**<sup>1</sup>H NMR**



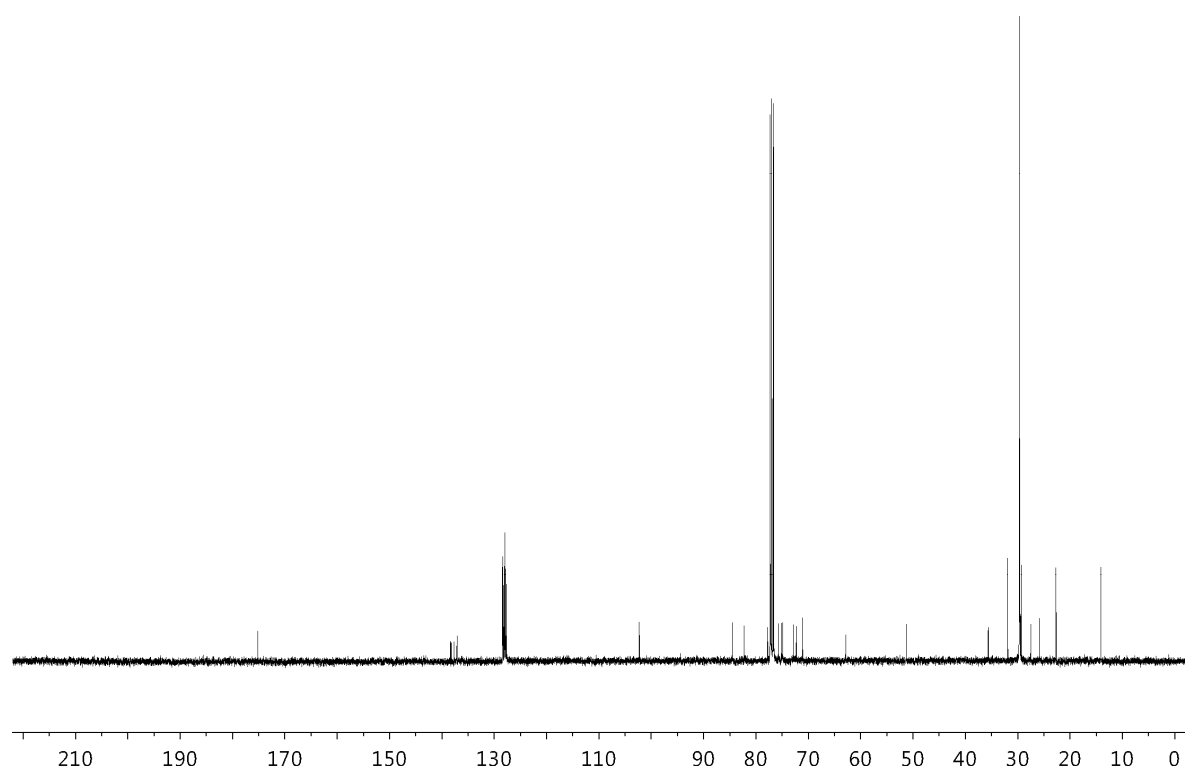
**<sup>13</sup>C NMR**



**Benzyl 2,3,4-tri-O-benzyl-6-O-((2*R*,3*R*)-3-Hydroxy-2-(tricosanyl)octadecanoyl)- $\beta$ -D-glucopyranoside (29)**  
 **$^1\text{H}$  NMR**

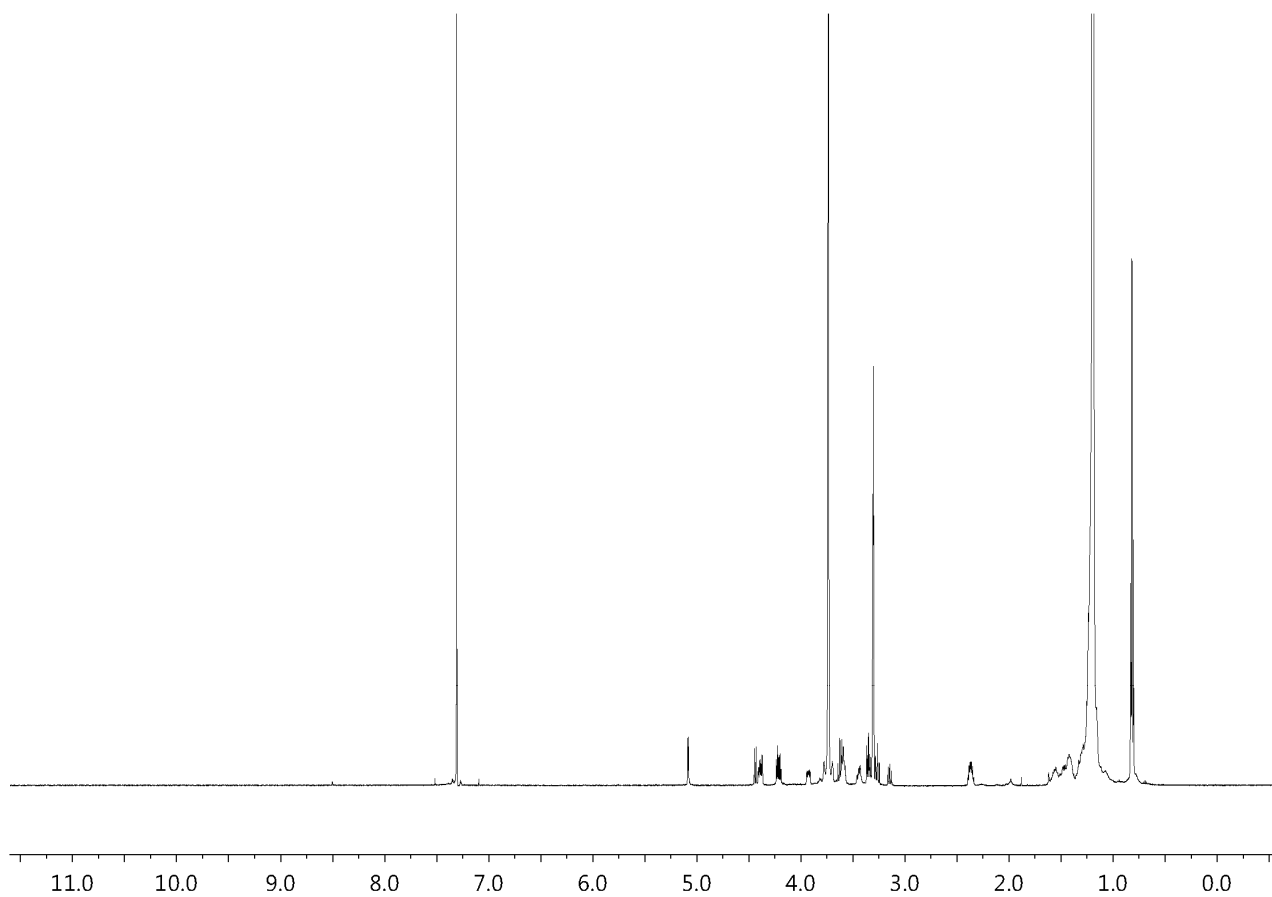


**$^{13}\text{C}$  NMR**

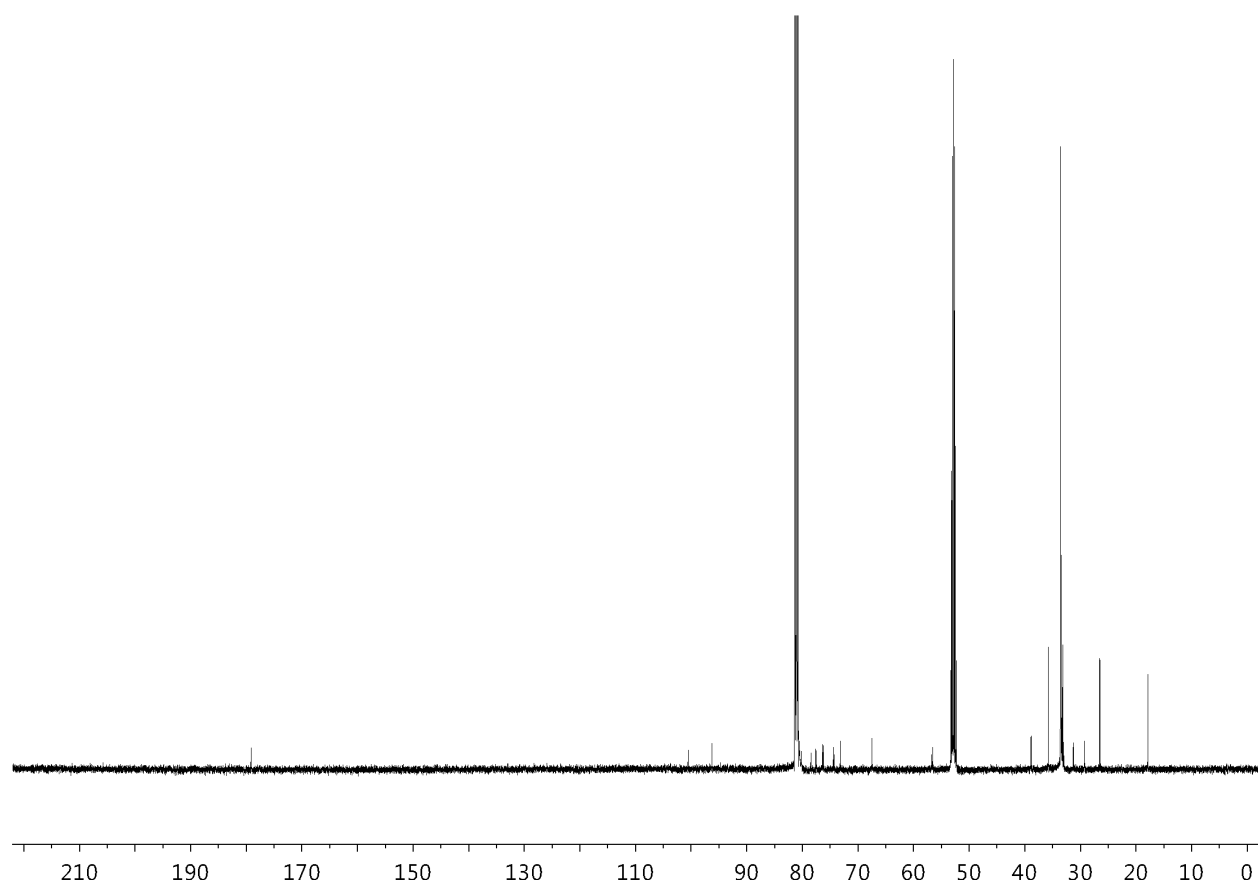


**6-O-((2*R*,3*R*)-3-Hydroxy-2-(tricosanyl)octadecanoyl)-D-glucopyranose (33)**

**<sup>1</sup>H NMR**

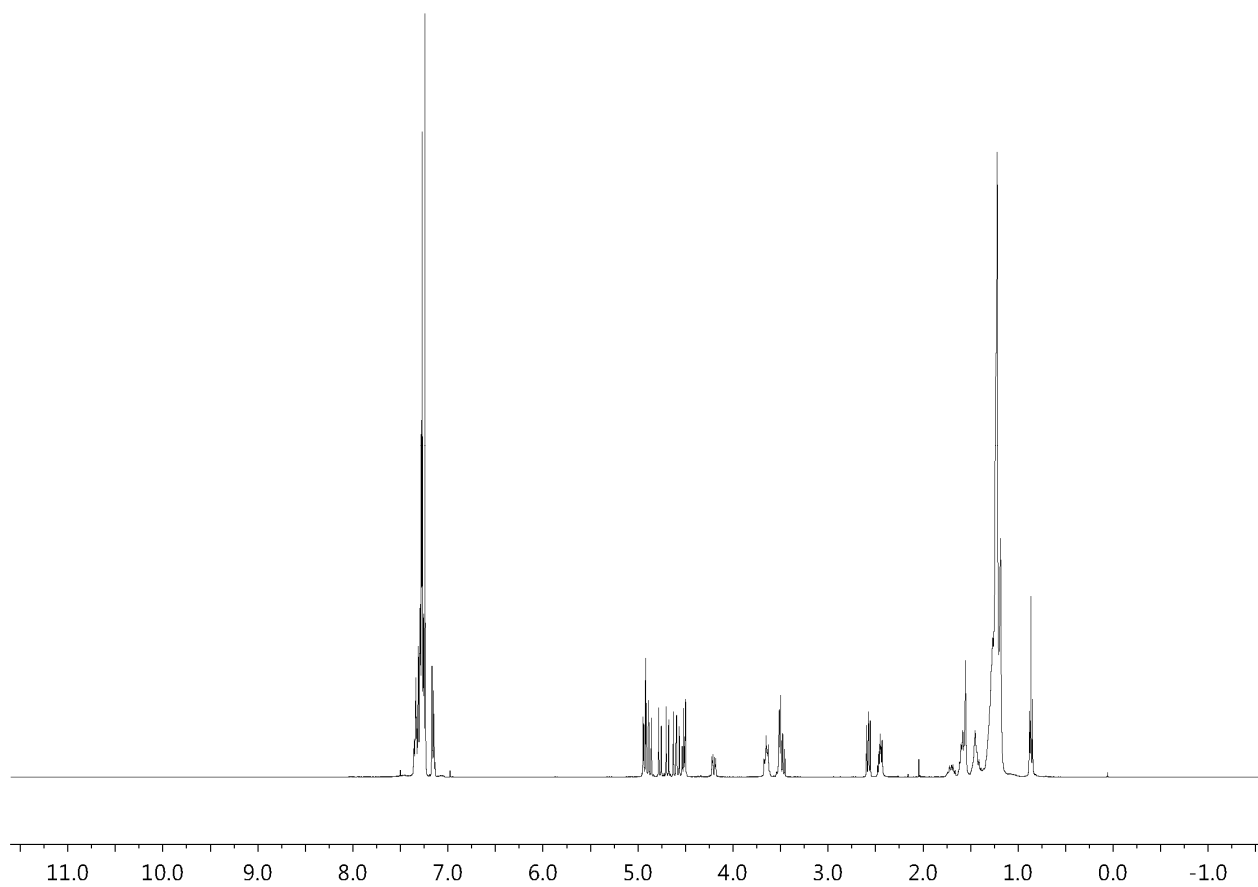


**<sup>13</sup>C NMR**

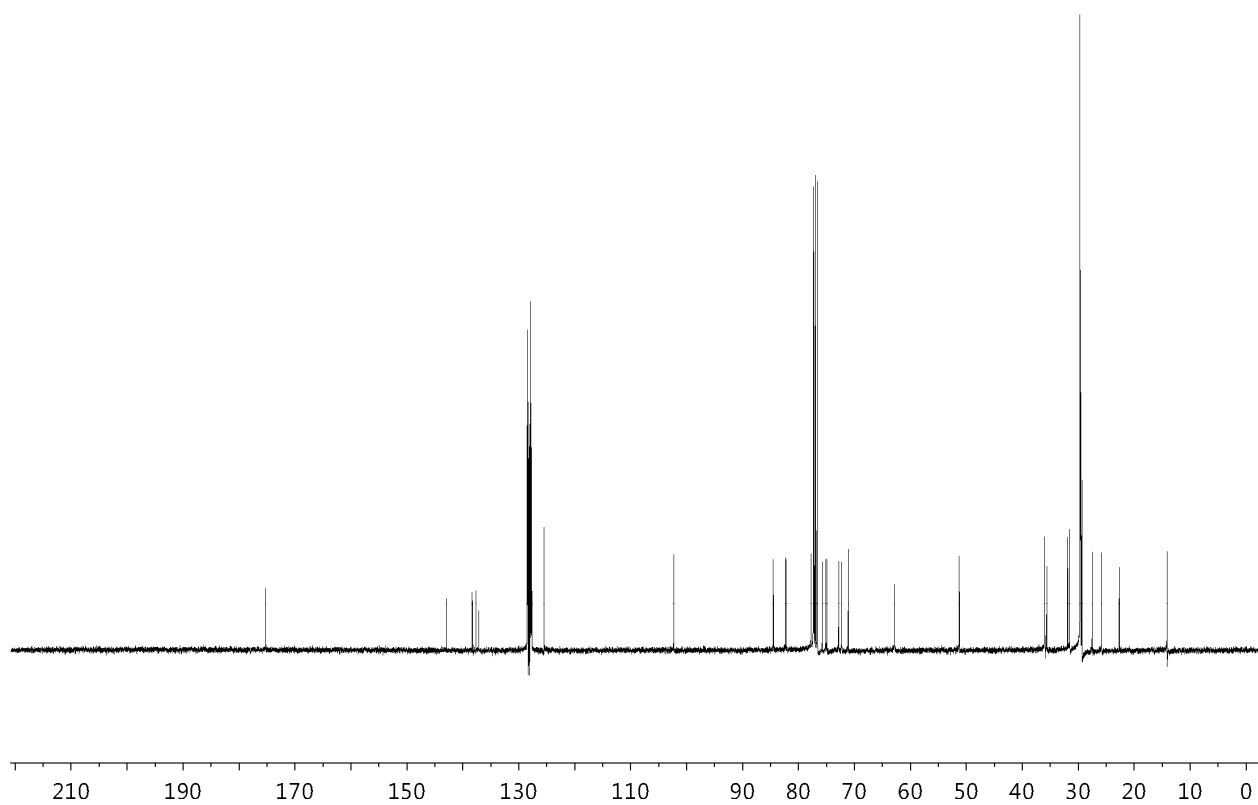


**Benzyl 2,3,4-tri-*O*-benzyl-6-*O*-((2*R*,3*R*)-3-hydroxy-2-(12-phenyldodecyl)octadecanoyl)- $\beta$ -D-glucopyranoside (30)**

**$^1\text{H}$  NMR**

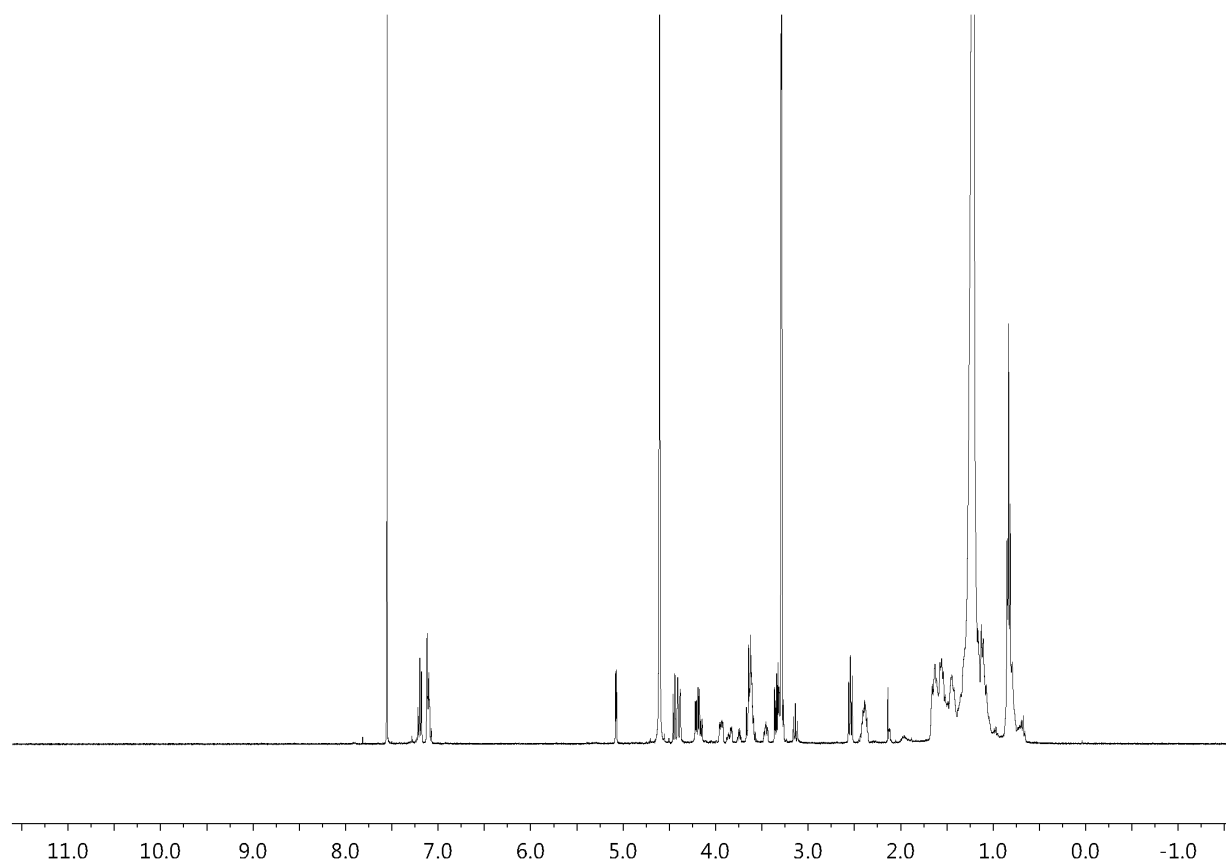


**$^{13}\text{C}$  NMR**

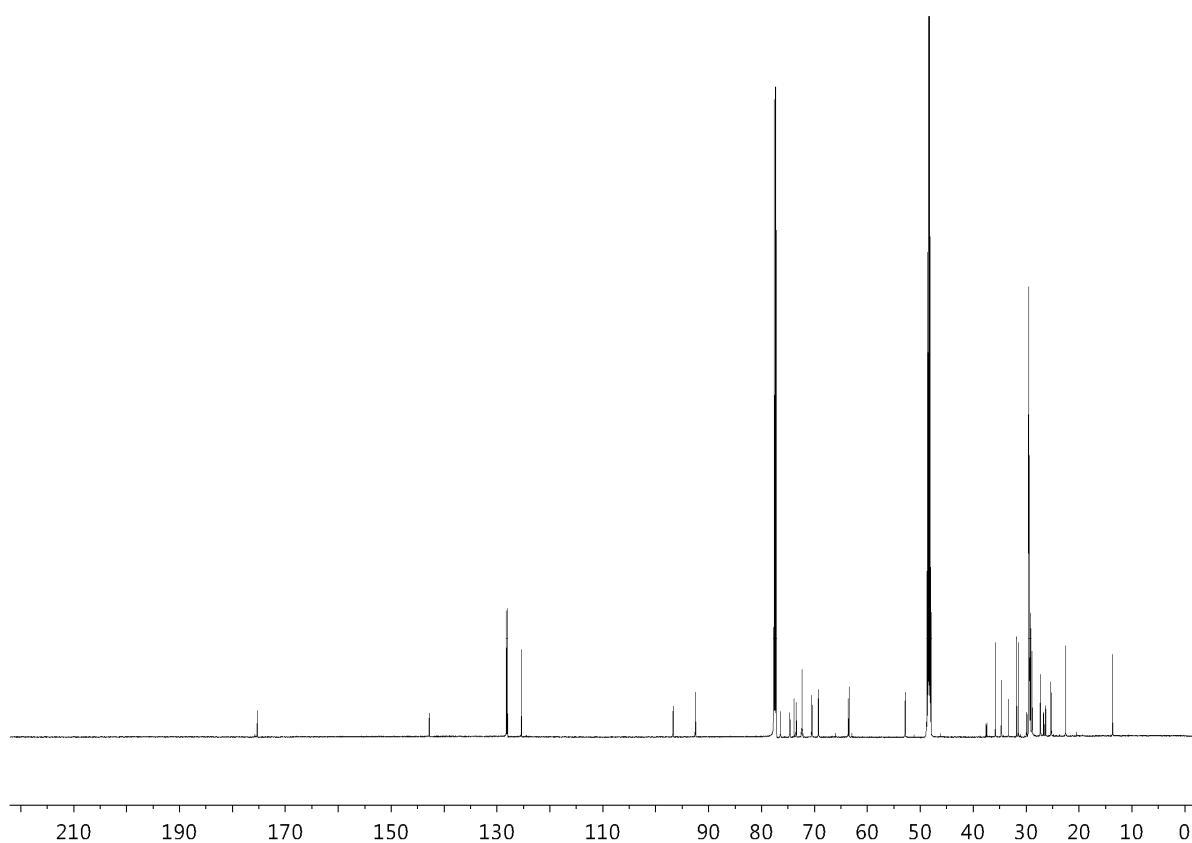


**6-O-((2*R*,3*R*)-3-Hydroxy-2-(12-phenyldodecyl)octadecanoyl)-D-glucopyranose (34)**

**<sup>1</sup>H NMR**

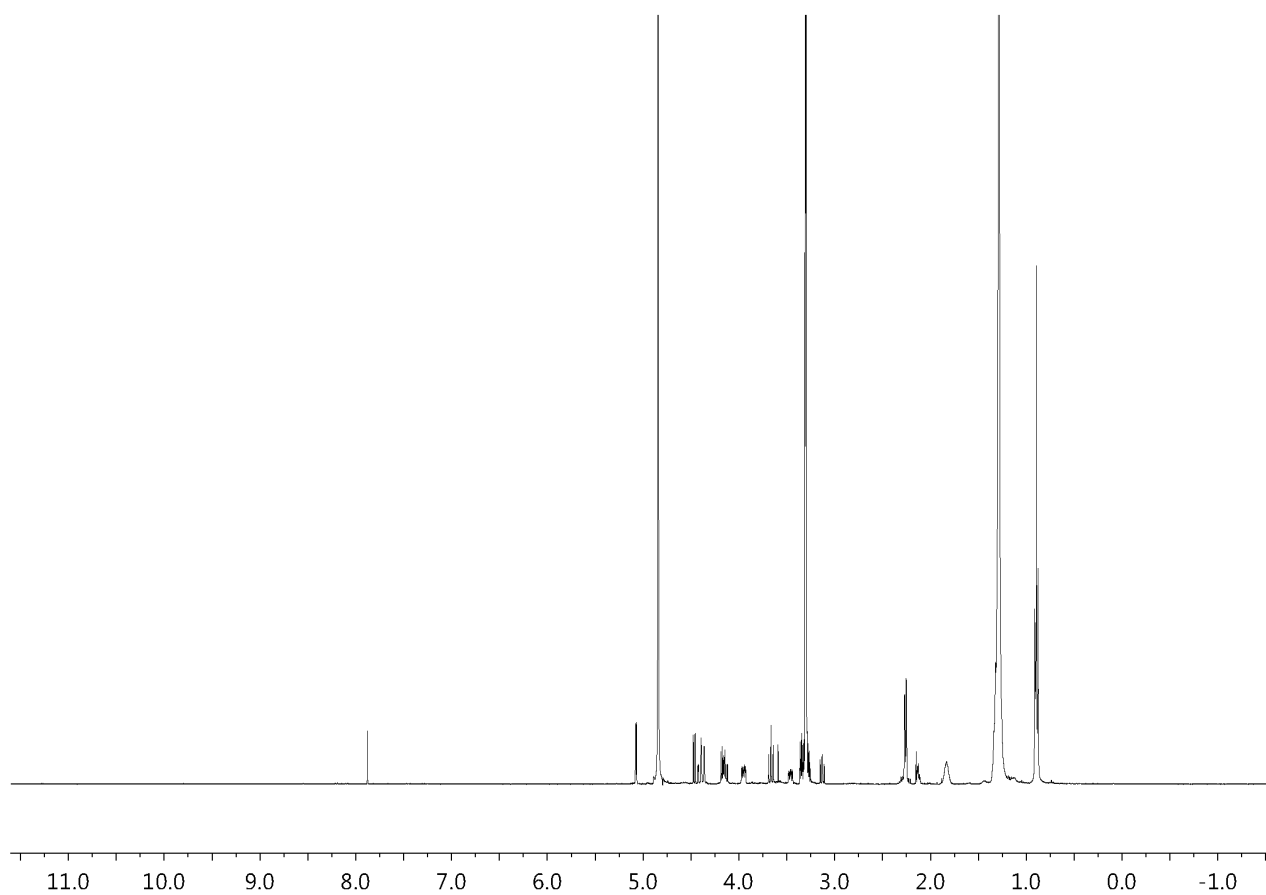


**<sup>13</sup>C NMR**



**6-O-(3'-Nonyl)dodecanoyl-D-glucose (35)**

**$^1\text{H}$  NMR**



**$^{13}\text{C}$  NMR**

