

## SUPPLEMENTARY DATA

### Role of the thiosugar ring in the inhibitory activity of salacinol, a potent natural $\alpha$ -glucosidase inhibitor

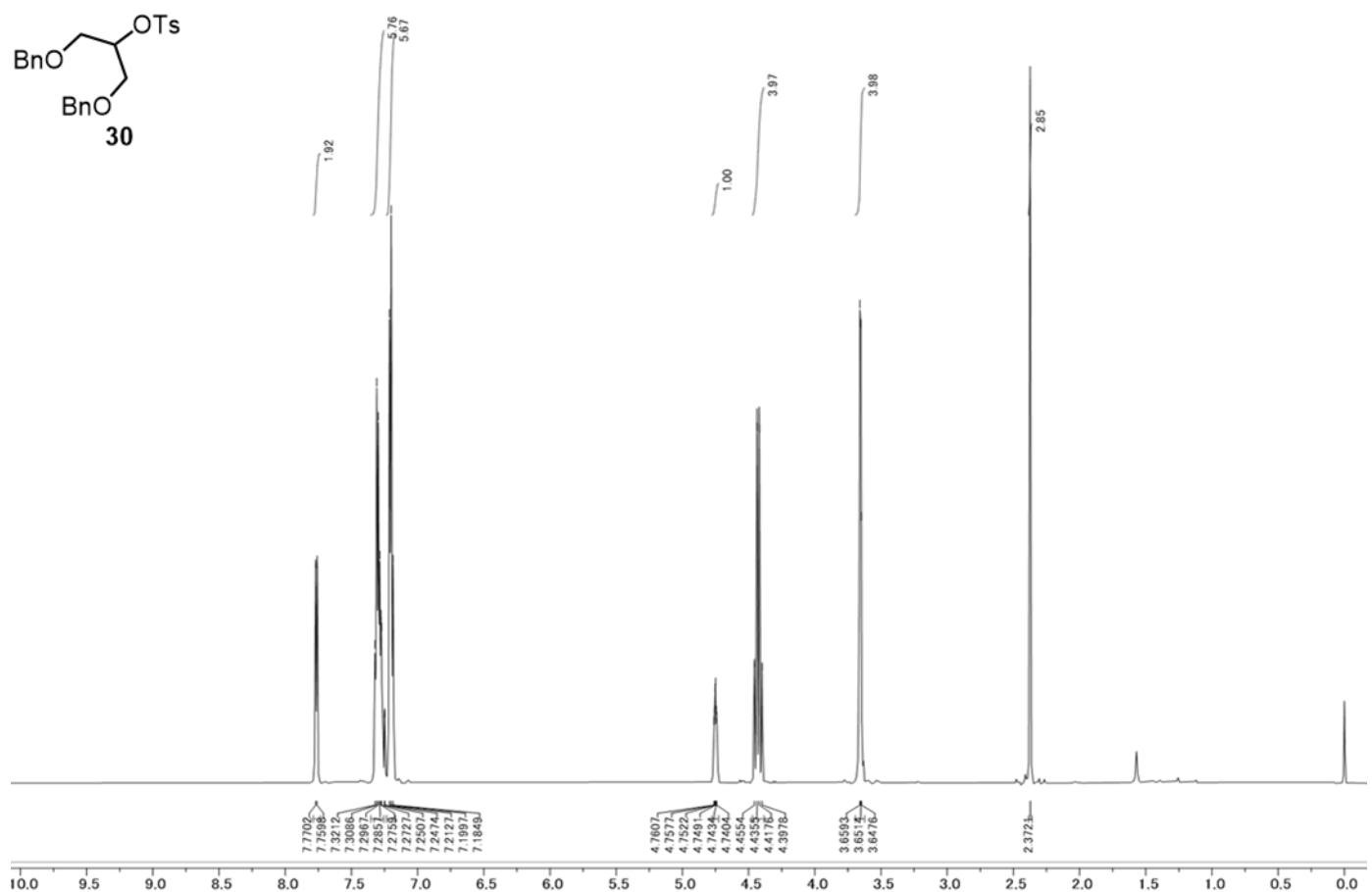
Katsuki Takashima,<sup>a</sup> Shinya Nakamura,<sup>a</sup> Fumihiro Ishikawa,<sup>a</sup> Maiko Nagayama,<sup>a</sup> Shinsuke Marumoto,<sup>c</sup> Weijia Xie,<sup>d</sup> Isao Nakanishi,<sup>a</sup> Osamu Muraoka,<sup>b</sup> Toshio Morikawa,<sup>b,\*</sup> and Genzoh Tanabe<sup>a,b,\*</sup>

<sup>a</sup>Faculty of Pharmay, <sup>b</sup>Pharmaceutical Research and Technology Institute, and <sup>c</sup>Joint Research Centere, Kindai University, 3-4-1 Kowakae, Higashi-osaka, Osaka 577-8502, Japan

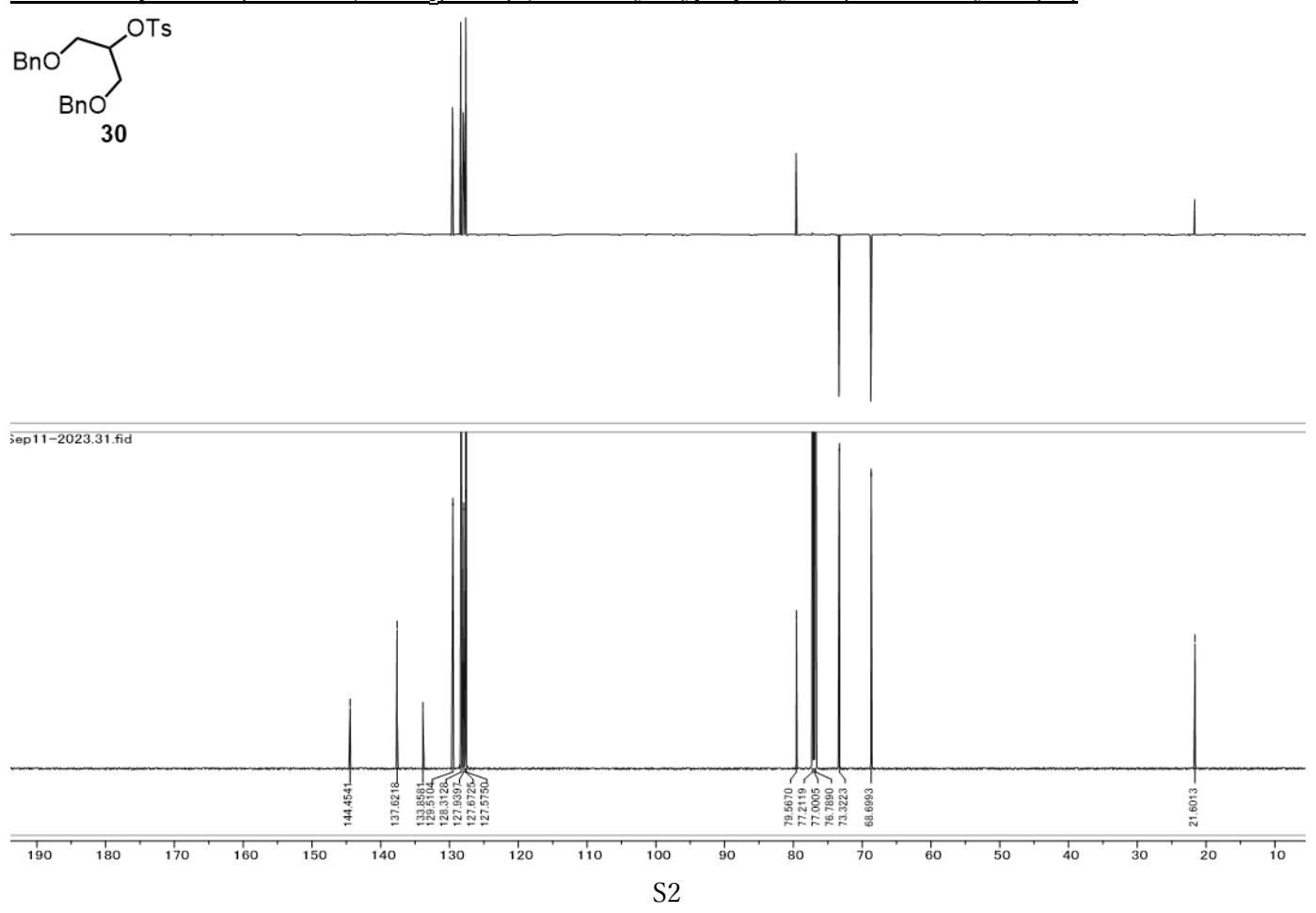
<sup>d</sup>State Key Laboratory of Natural Medicines, Department of Medicinal Chemistry, China Pharmaceutical University, Nanjing 2100009, P. R. China

<sup>1</sup>H and <sup>13</sup>C NMR spectroscopic data of synthetic compounds

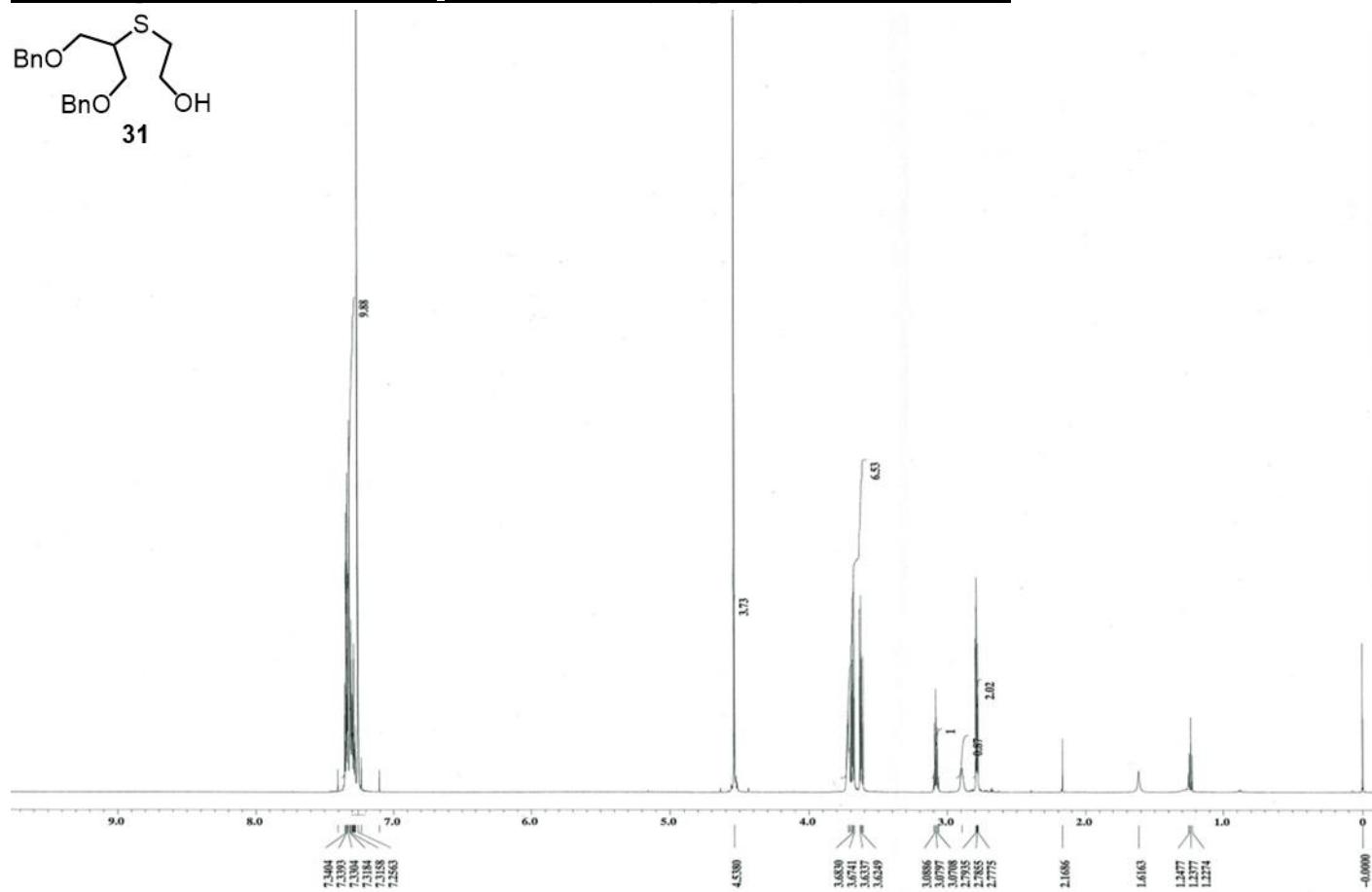
<sup>1</sup>H NMR spectrum (600 MHz, CDCl<sub>3</sub>) of 2-(1,3-Dibenoxyprop-2-ylthio)ethanol tosylate (30)



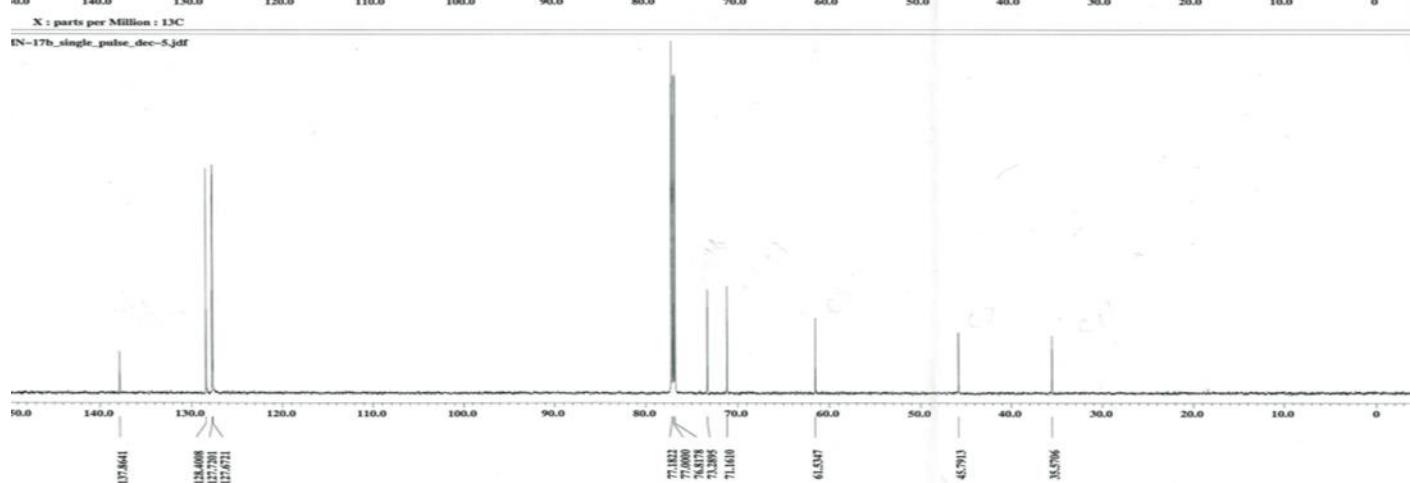
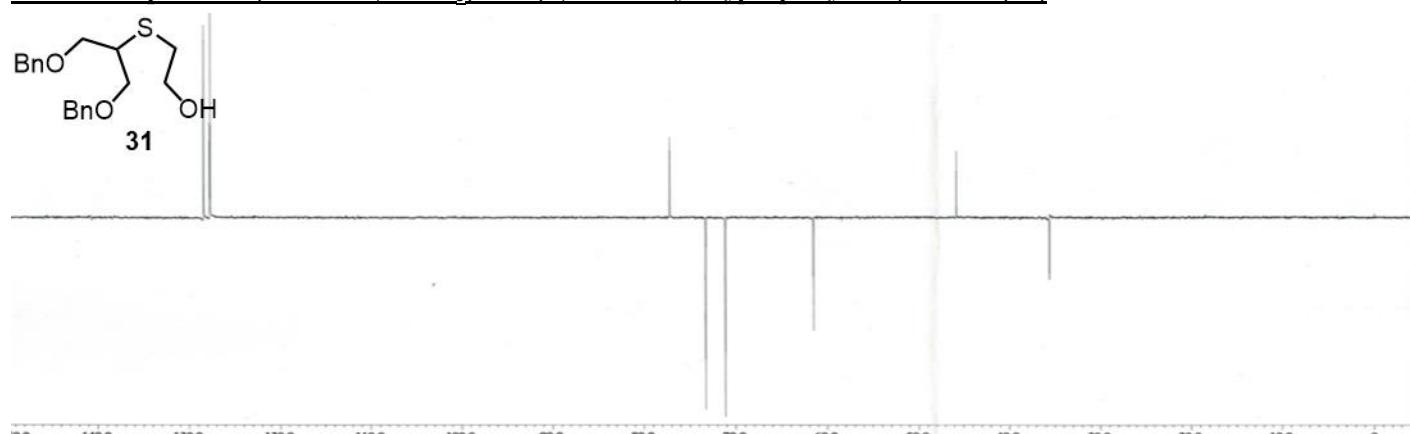
<sup>13</sup>C NMR spectrum (150 MHz, CDCl<sub>3</sub>) of 2-(1,3-Dibenoxyprop-2-ylthio)ethanol tosylate (30)



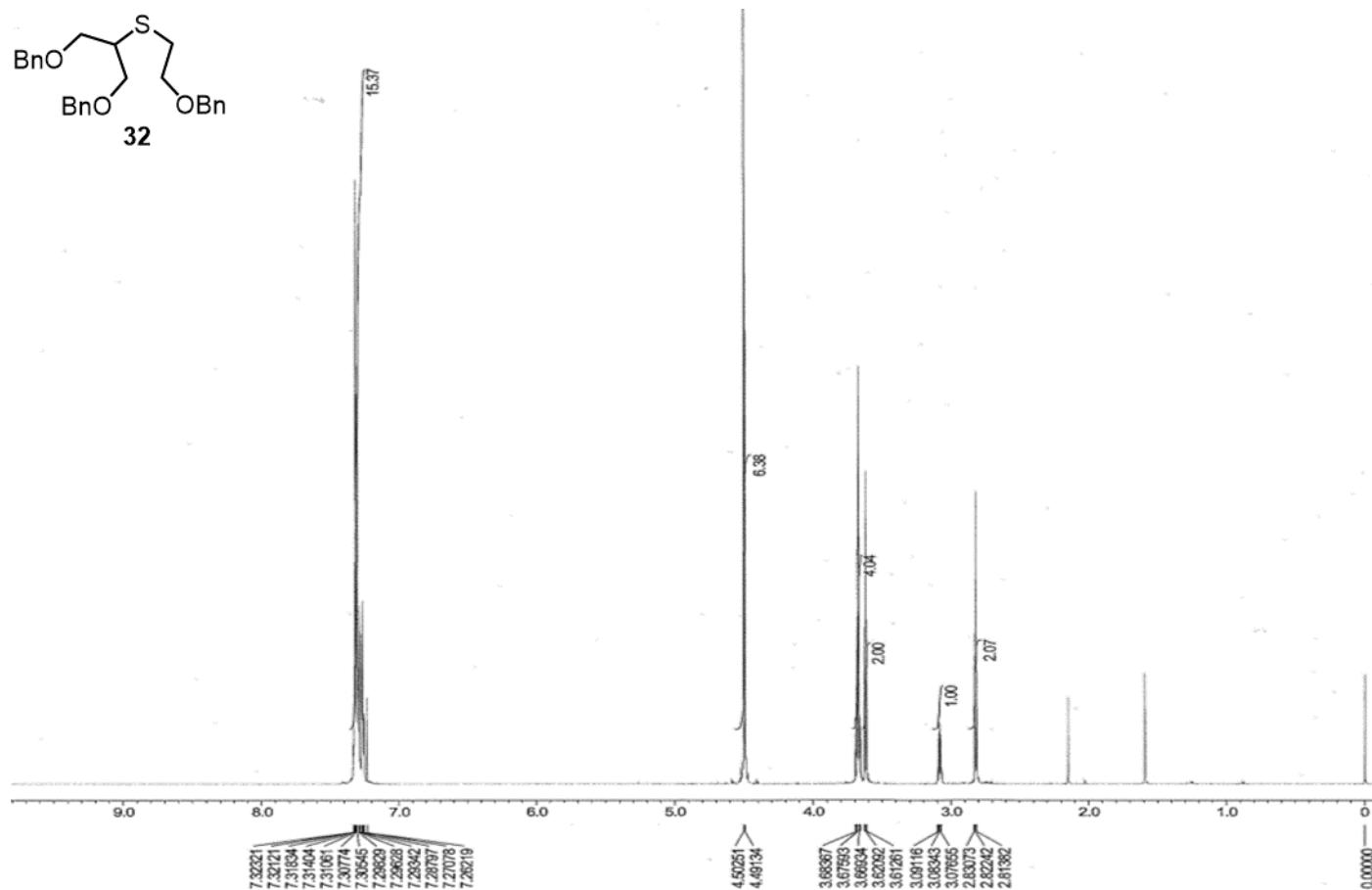
<sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of 2-(1,3-Dibenzoyloxyprop-2-ylthio)ethanol (31)



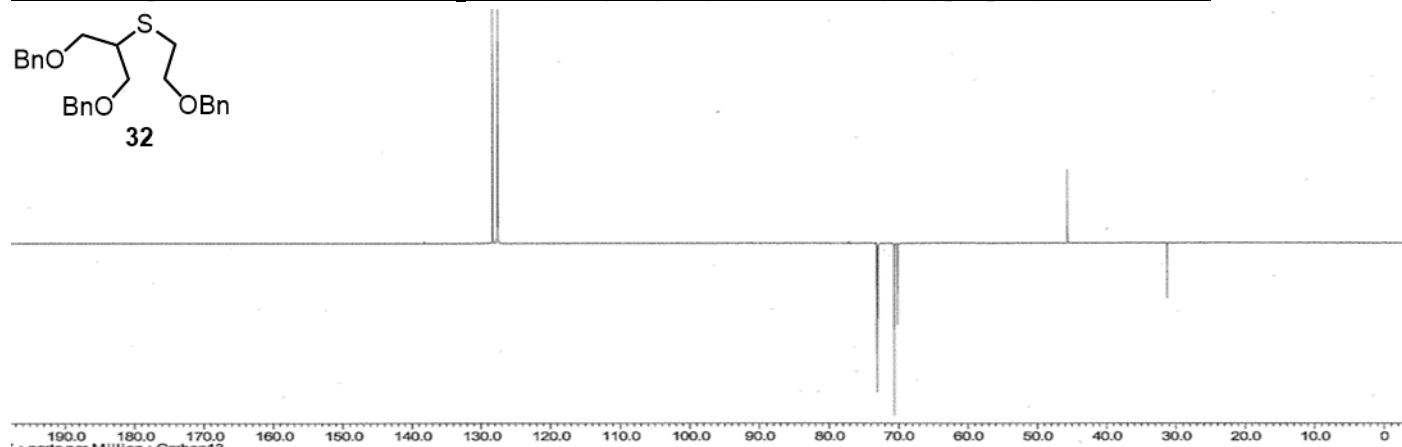
<sup>13</sup>C NMR spectrum (125 MHz, CDCl<sub>3</sub>) of 2-(1,3-Dibenzoyloxyprop-2-ylthio)ethanol (31)



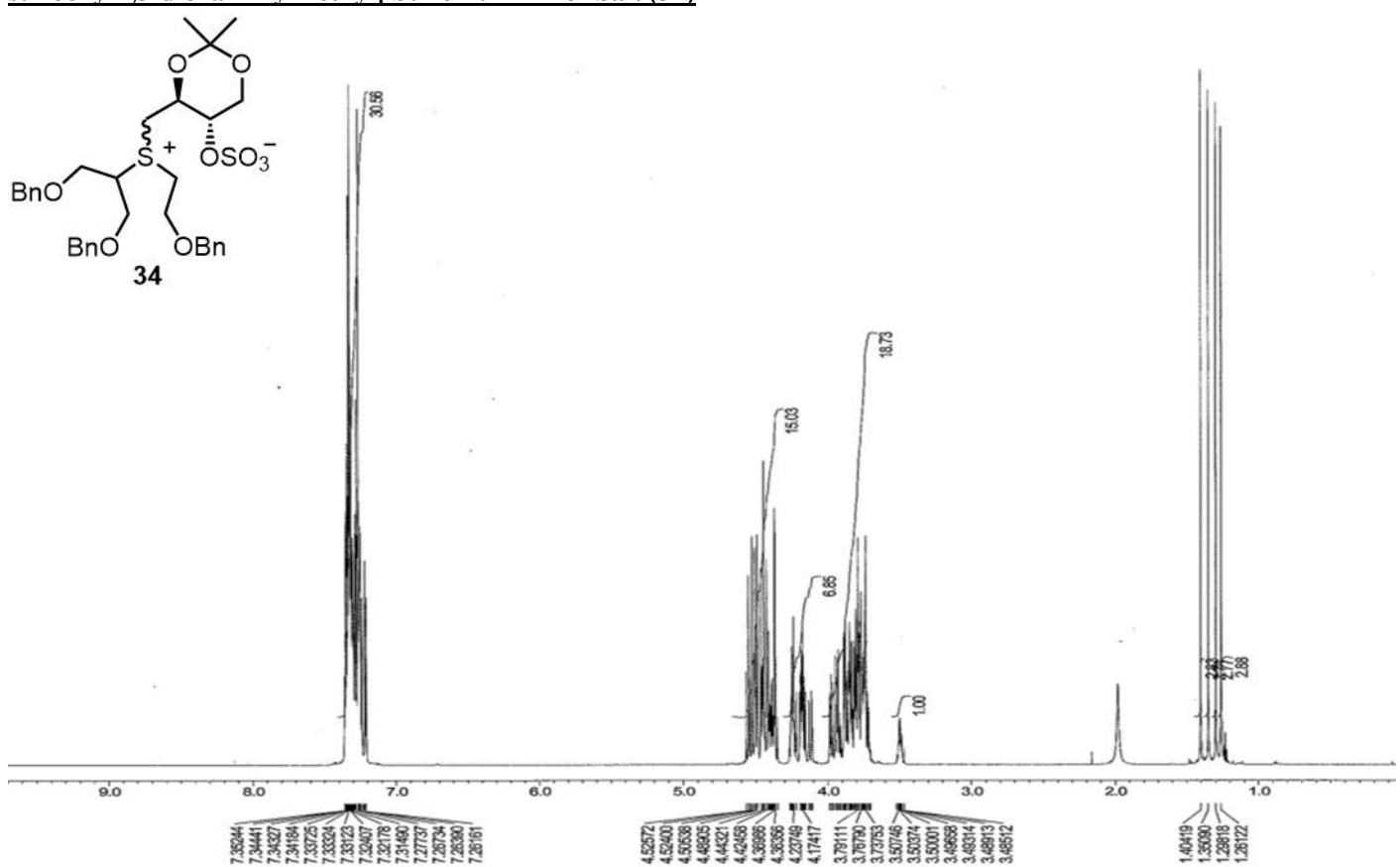
**<sup>1</sup>H NMR spectrum (800 MHz, CDCl<sub>3</sub>) of 2-(Benzylxoyethyl) (1,3-Dibenzylxoyprop-2-yl) Sulfide (32)**



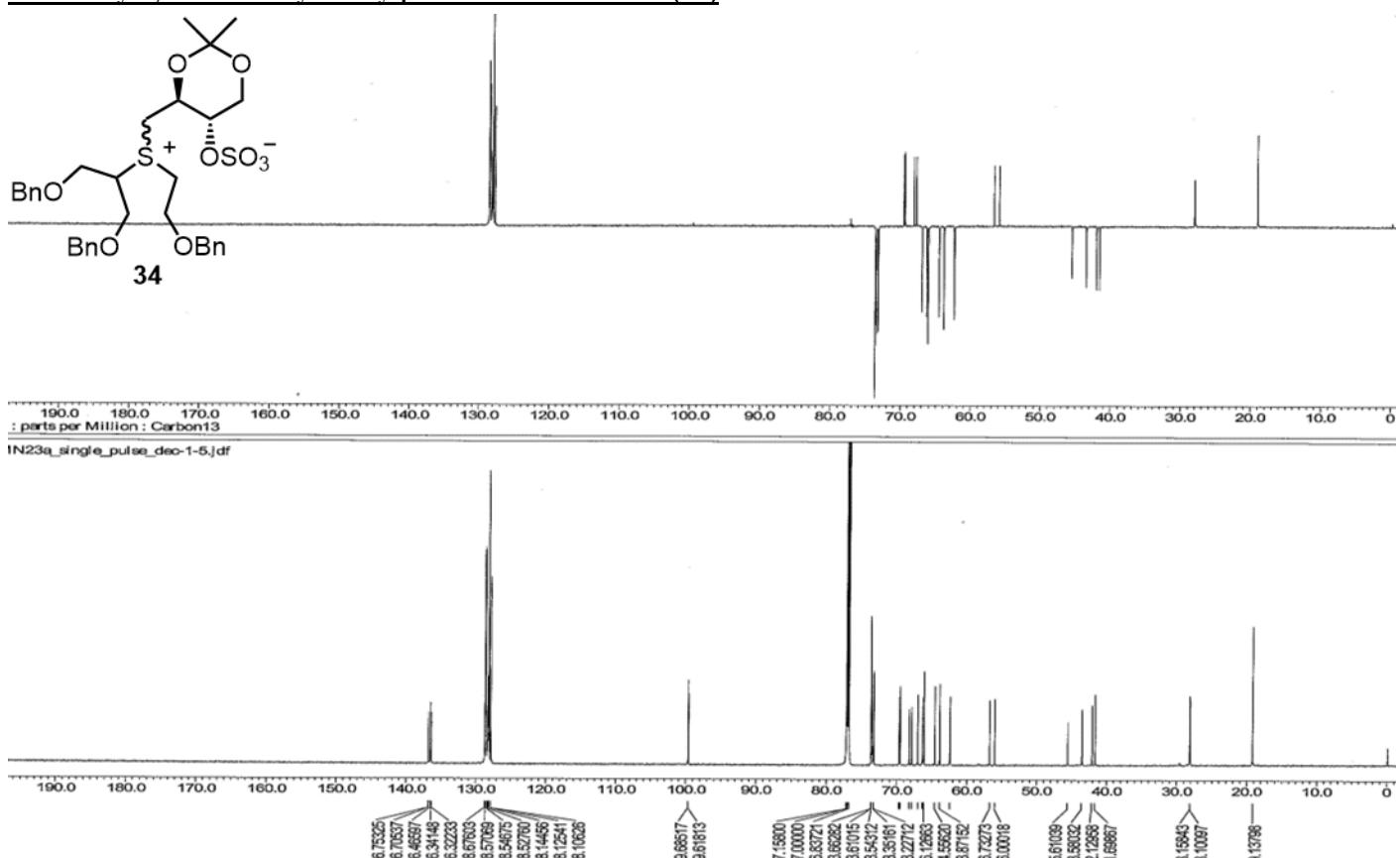
**<sup>13</sup>C NMR spectrum (200 MHz, CDCl<sub>3</sub>) of 2-(Benzylxoyethyl) (1,3-Dibenzylxoyprop-2-yl) Sulfide (32)**



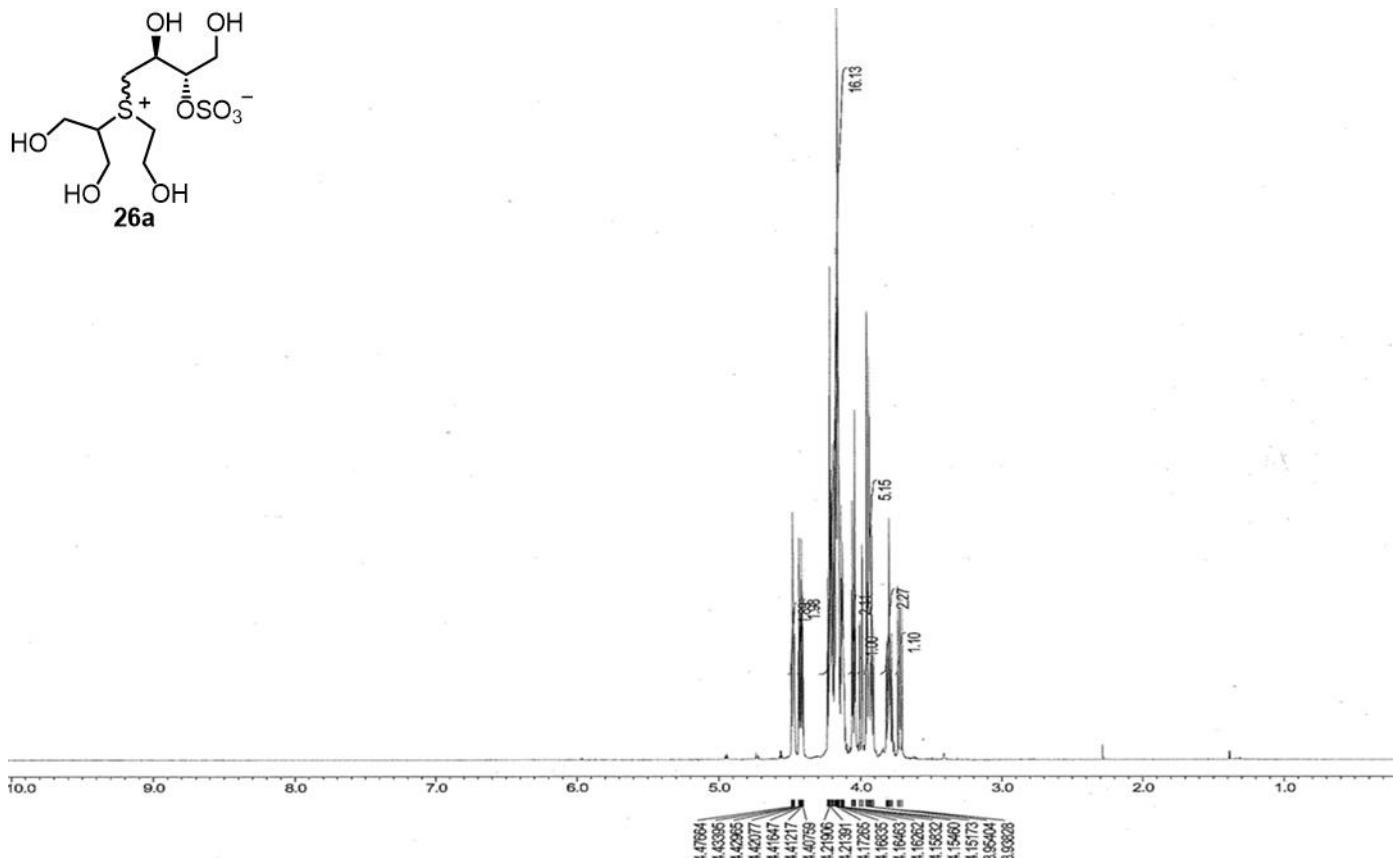
**<sup>1</sup>H NMR spectrum (800 MHz, CDCl<sub>3</sub>) of (2-Benzylxethyl) [1,3-Di(benzylx)propan-2-yl] [(4S,5S)-2,2-Dimethyl-5-sulfoxy-1,3-dioxan-4-ylmethyl] Sulfonium Inner Salt (34)**



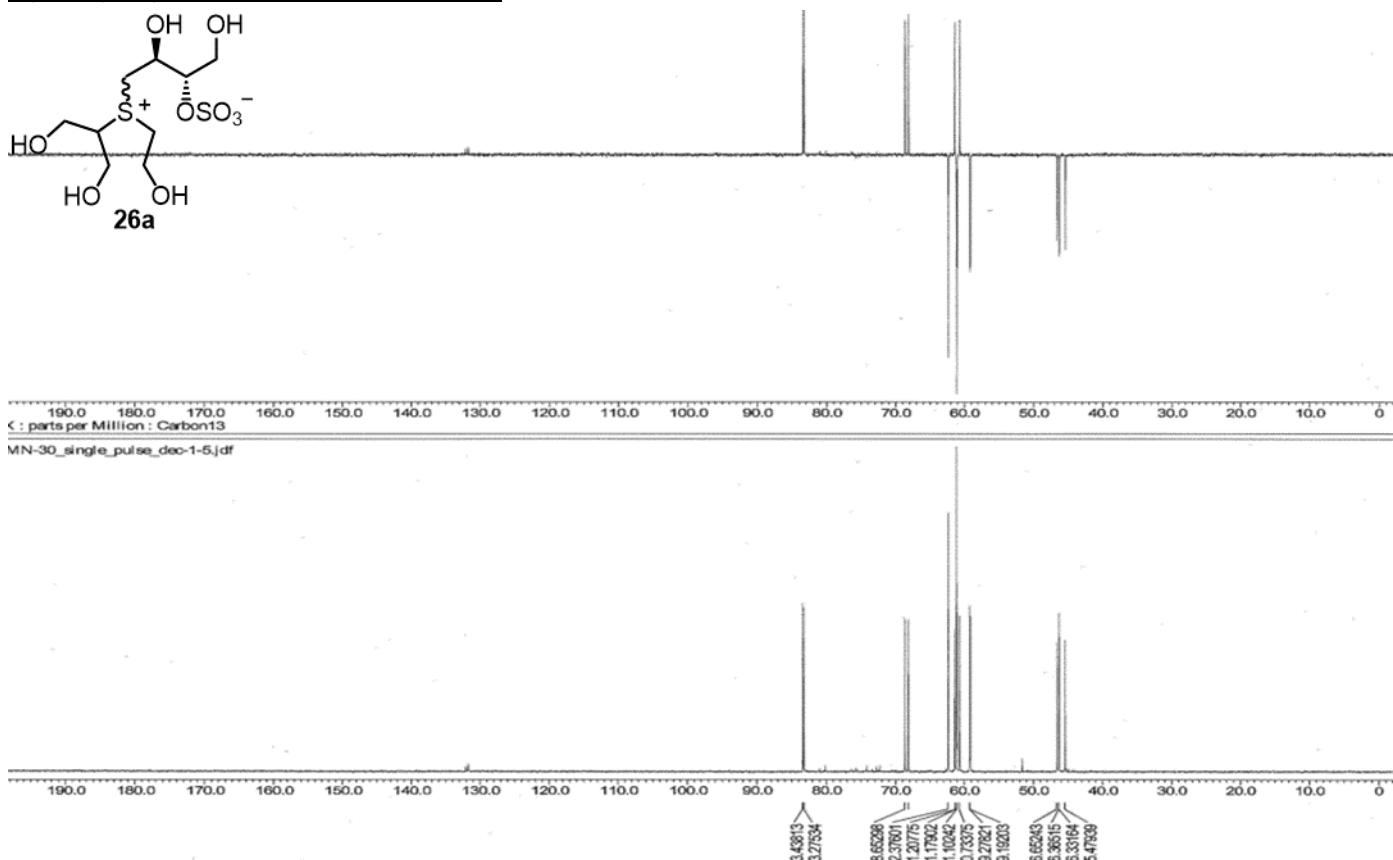
**<sup>13</sup>C NMR spectrum (200 MHz, CDCl<sub>3</sub>) of (2-Benzylxethyl) [1,3-Di(benzylx)propan-2-yl] [(4S,5S)-2,2-Dimethyl-5-sulfoxy-1,3-dioxan-4-ylmethyl] Sulfonium Inner Salt (34)**



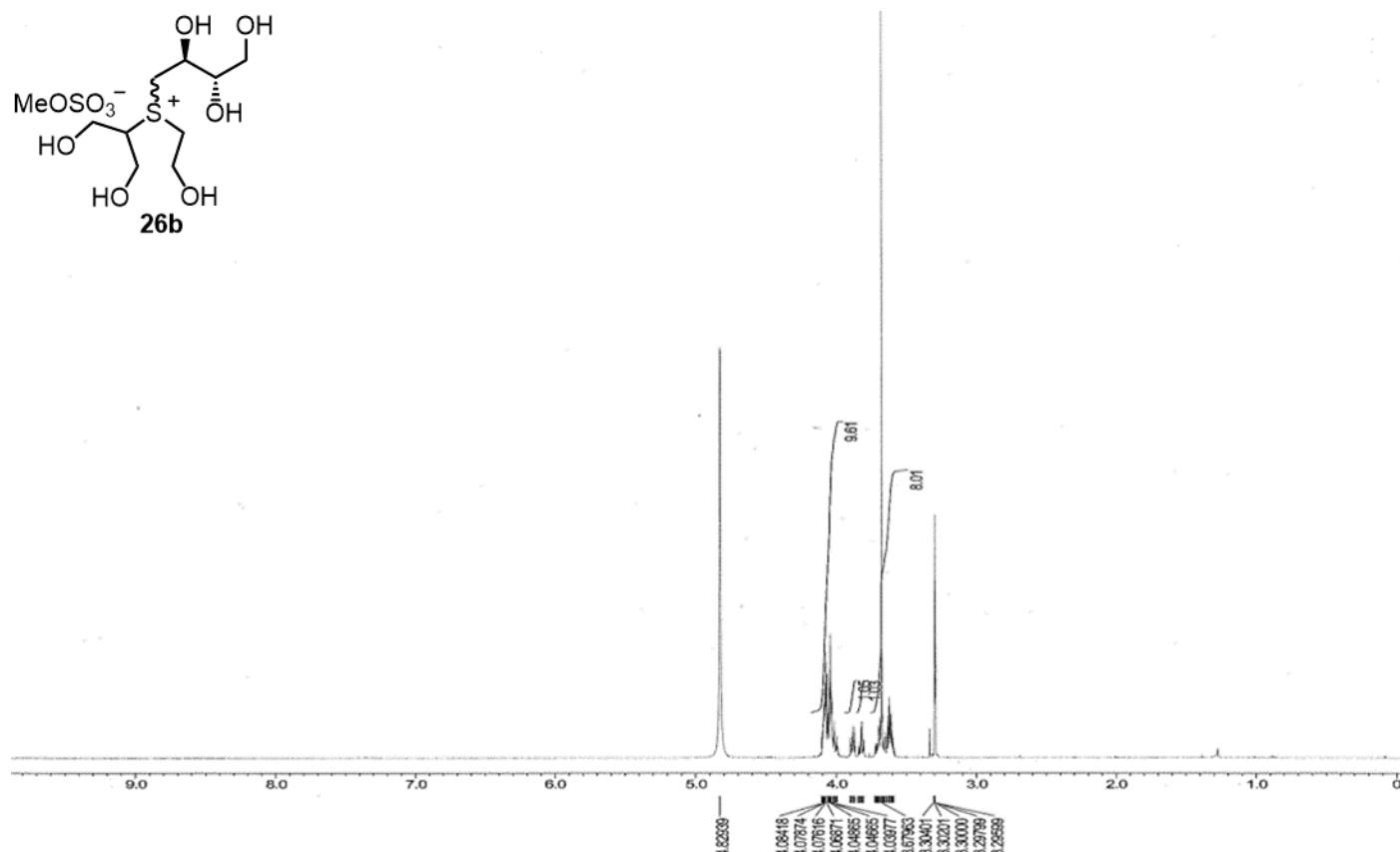
**<sup>1</sup>H NMR spectrum (800 MHz, D<sub>2</sub>O) of (1,3-Dihydroxypropan-2-yl) [(2S,3S)-2,4-Dihydroxy-3-sulfoxybutyl] (2-Hydroxyethyl) Sulfonium Inner Salt(26a)**



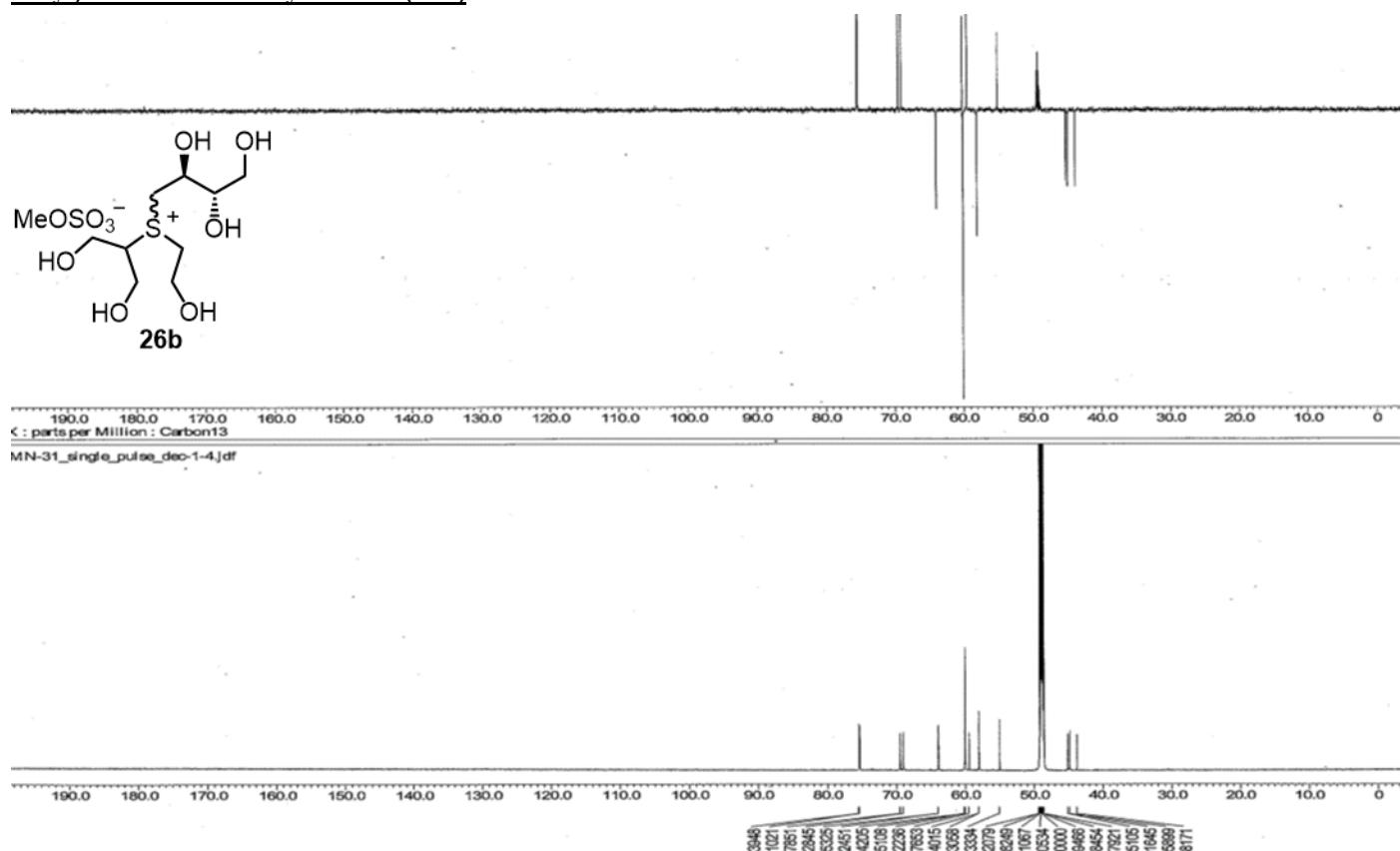
**<sup>13</sup>C NMR spectrum (200 MHz, D<sub>2</sub>O) of (1,3-Dihydroxypropan-2-yl) [(2S,3S)-2,4-Dihydroxy-3-sulfoxybutyl] (2-Hydroxyethyl) Sulfonium Inner Salt(26a)**



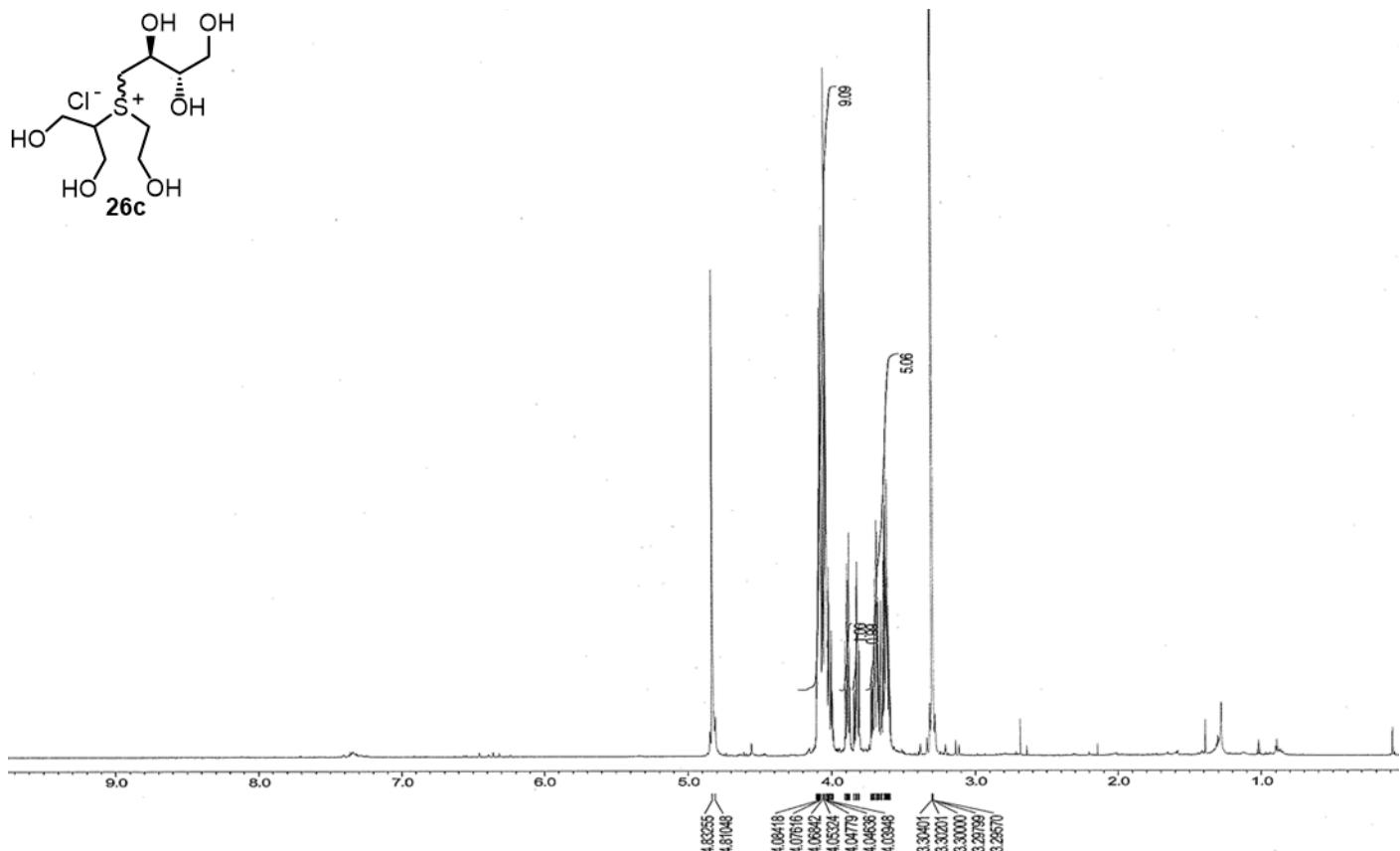
**<sup>1</sup>H NMR spectrum (800 MHz, CD<sub>3</sub>OD) of (1,3-Dihydroxypropan-2-yl) (2-Hydroxyethyl) [(2S,3S)-2,3,4-Trihydroxybutyl] Sulfonium Methyl Sulfate (26b)**



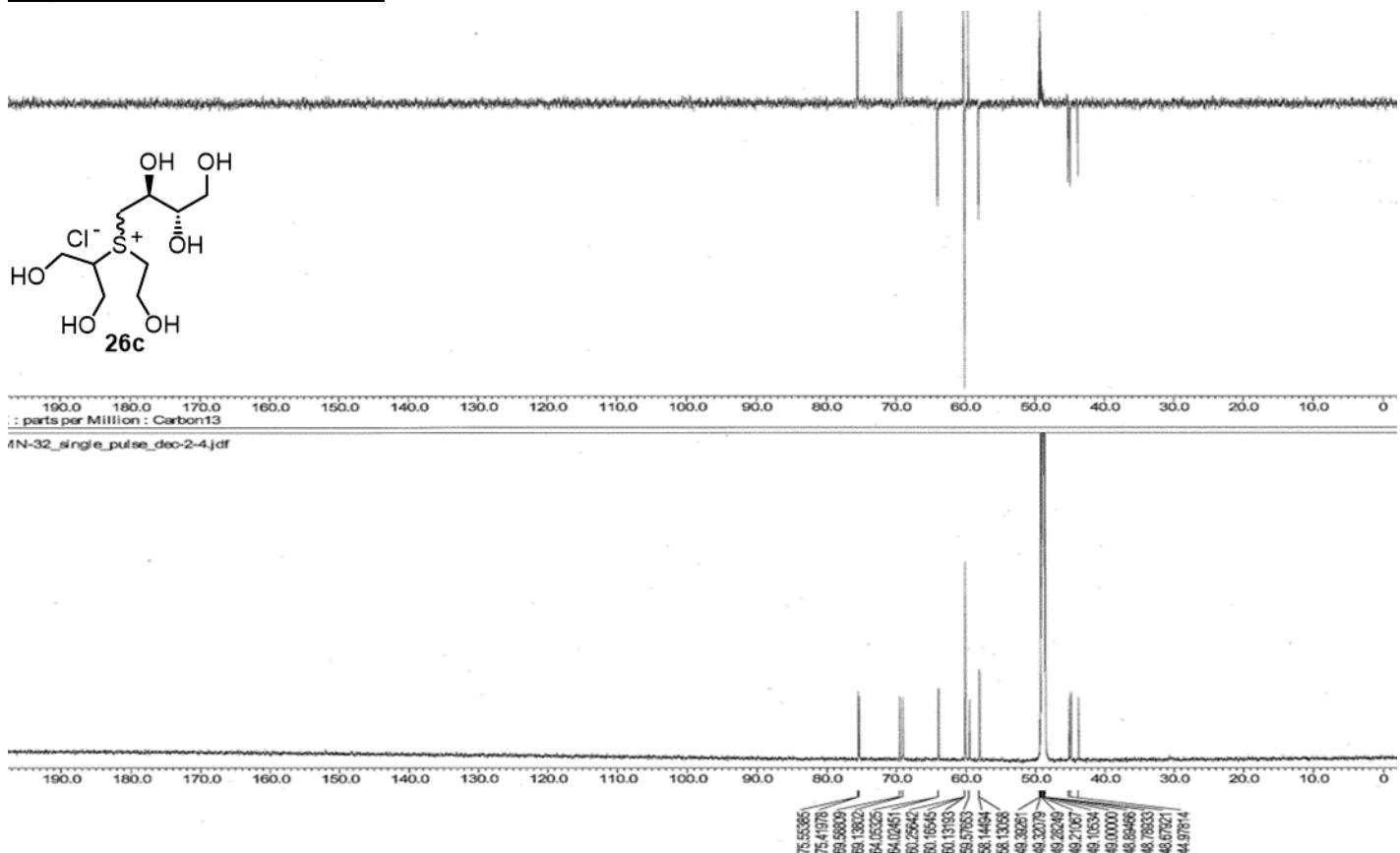
**<sup>13</sup>C NMR spectrum (200 MHz, CD<sub>3</sub>OD) of (1,3-Dihydroxypropan-2-yl) (2-Hydroxyethyl) [(2S,3S)-2,3,4-Trihydroxybutyl] Sulfonium Methyl Sulfate (26b)**



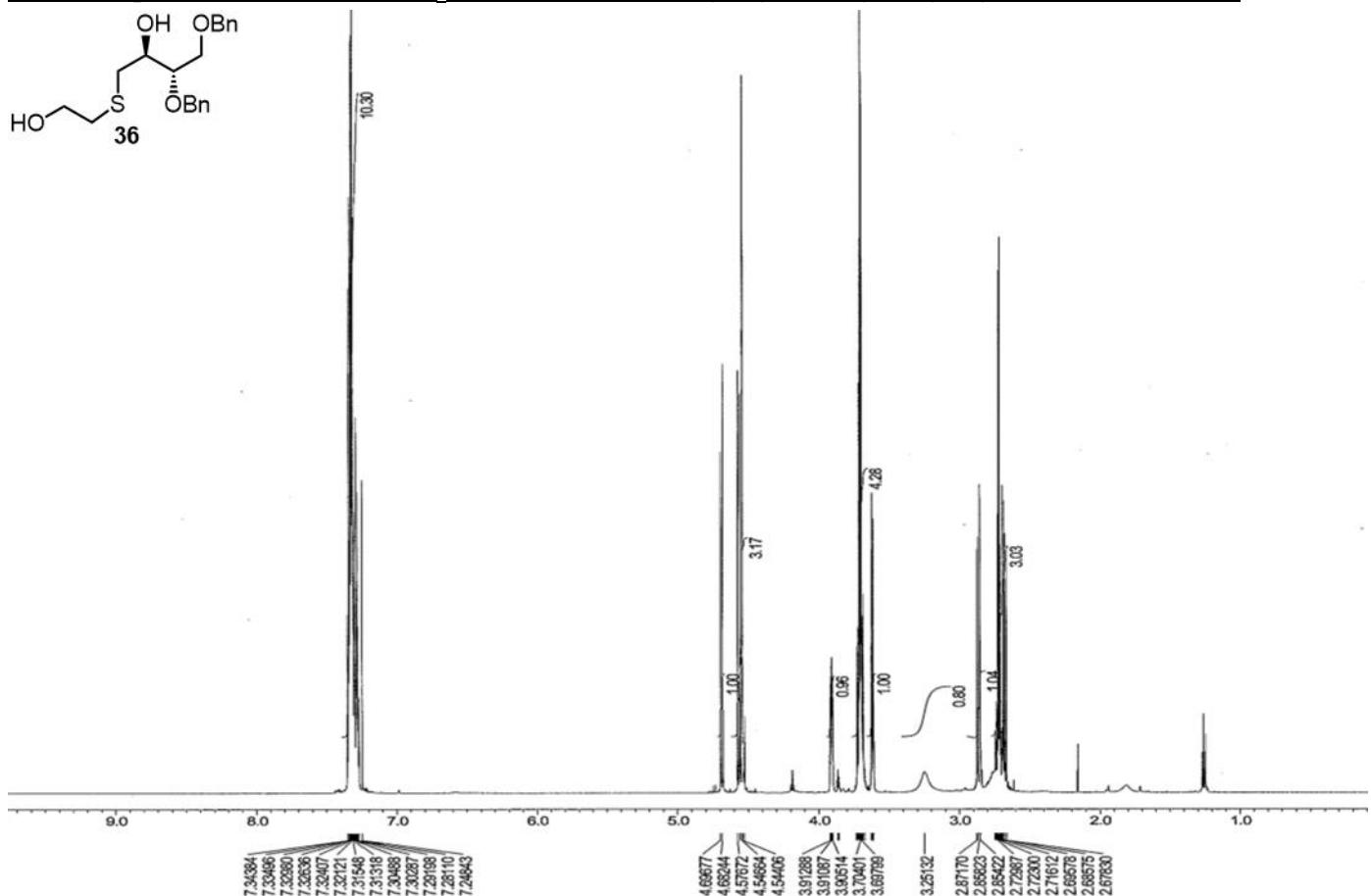
**<sup>1</sup>H NMR spectrum (800 MHz, CD<sub>3</sub>OD) of (1,3-Dihydroxypropan-2-yl) (2-Hydroxyethyl) [(2S,3S)-2,3,4-trihydroxybutyl] Sulfonium Chloride (26c)**



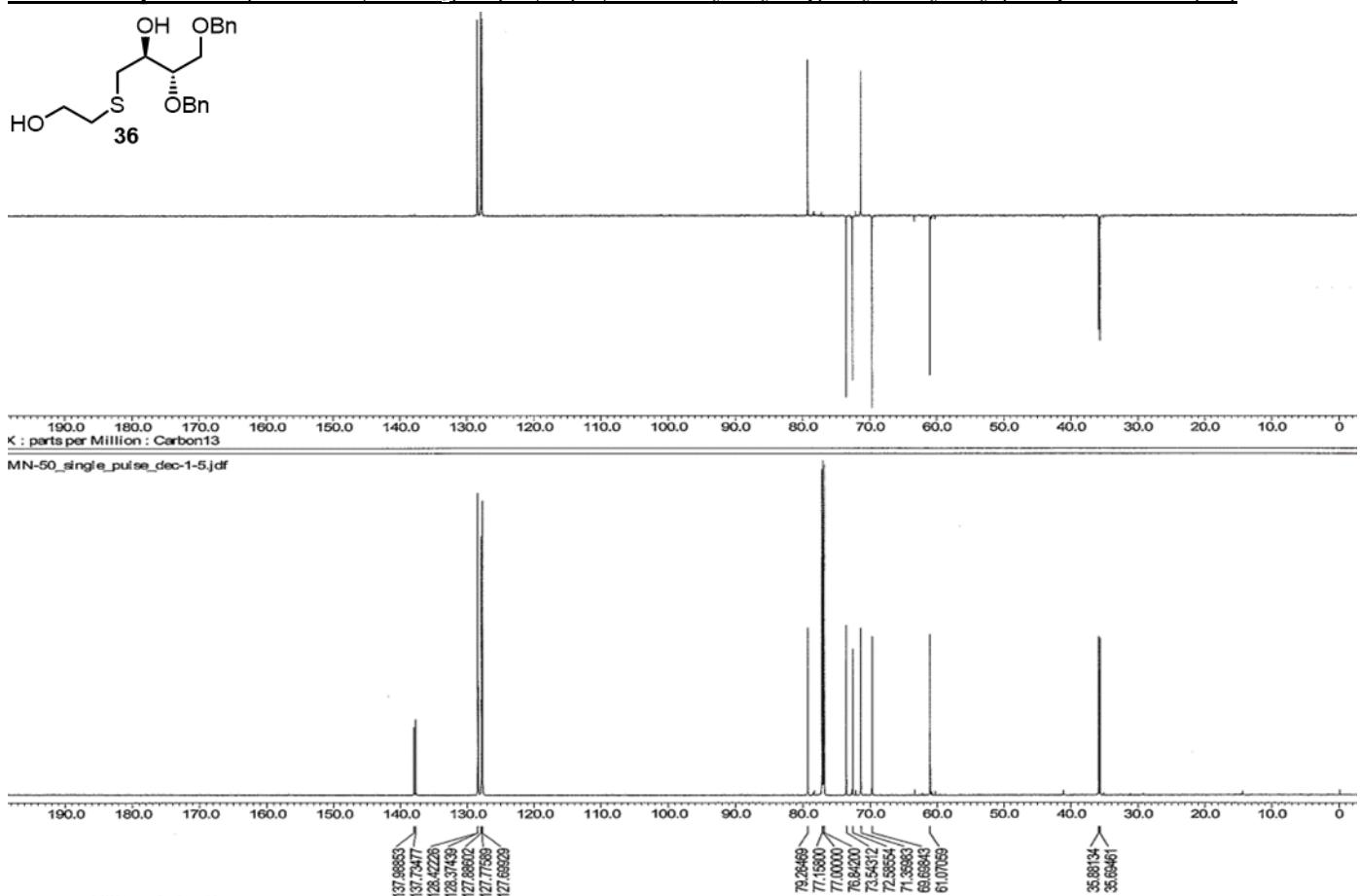
**<sup>13</sup>C NMR spectrum (200 MHz, CD<sub>3</sub>OD) of (1,3-Dihydroxypropan-2-yl) (2-Hydroxyethyl) [(2S,3S)-2,3,4-trihydroxybutyl] Sulfonium Chloride (26c)**



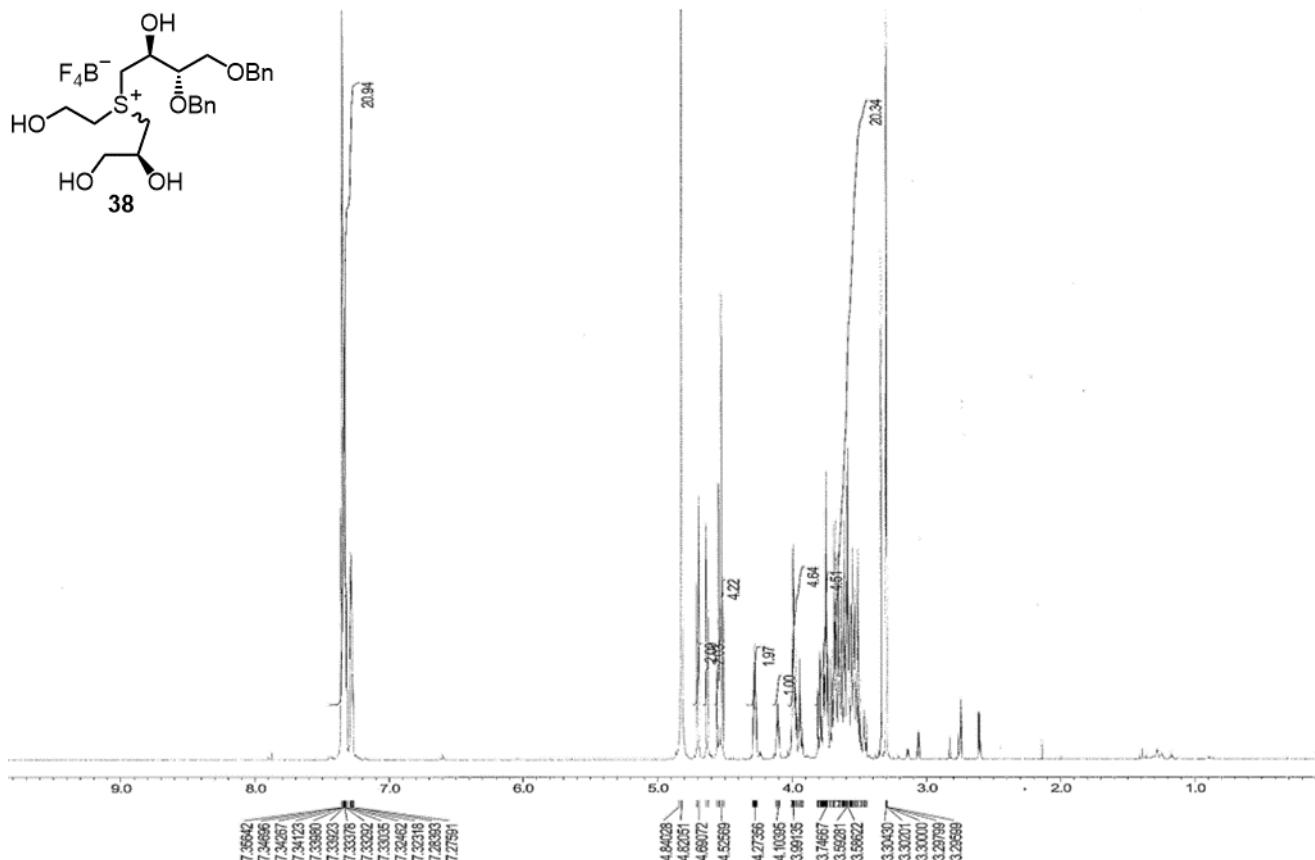
**<sup>1</sup>H NMR spectrum (800 MHz, CDCl<sub>3</sub>) of (2S,3S)-3,4-Dibenzyloxy-1-[(2-hydroxyethyl)thio]butan-2-ol (36)**



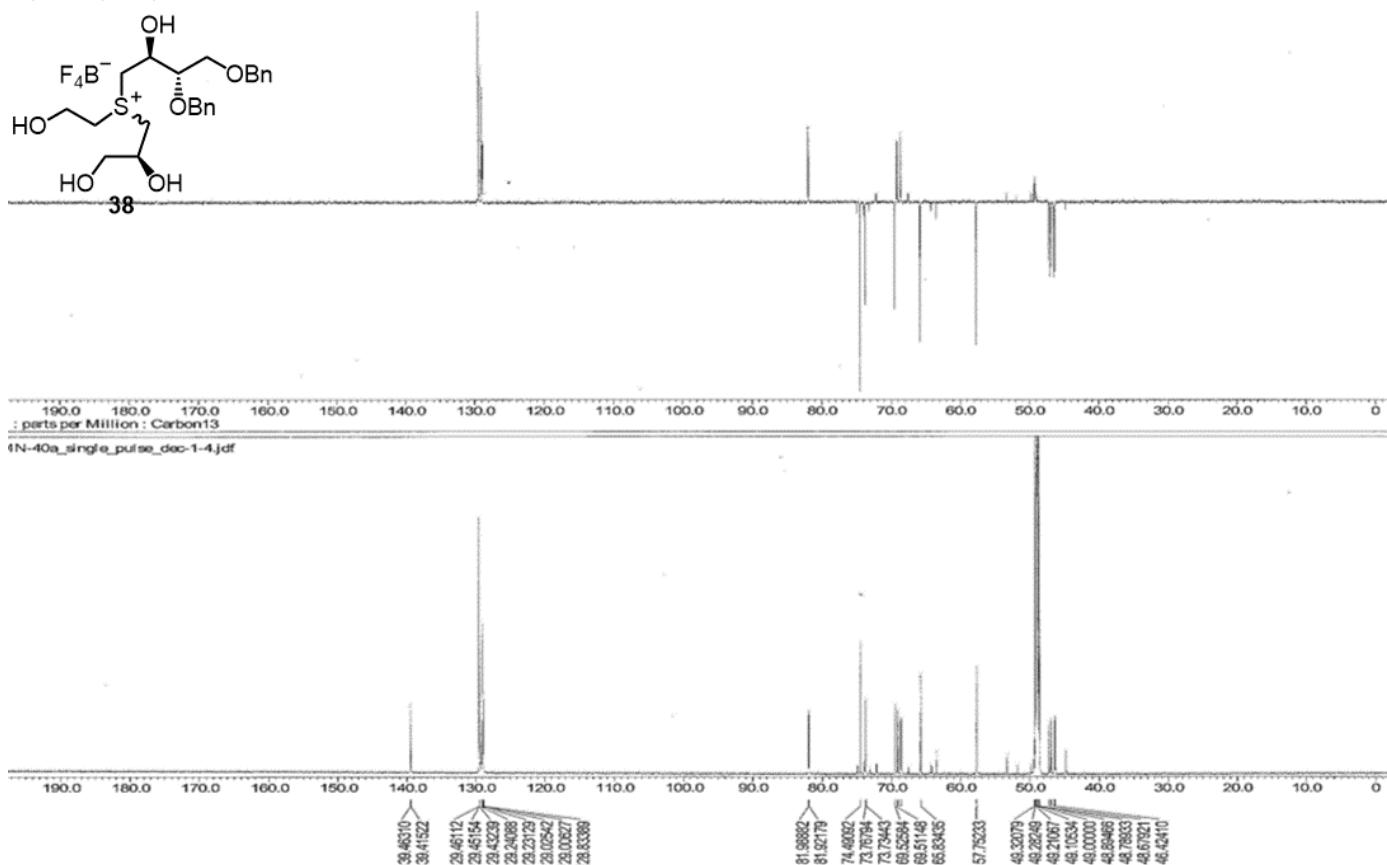
**<sup>13</sup>C NMR spectrum (200 MHz, CDCl<sub>3</sub>) of (2S,3S)-3,4-Dibenzyloxy-1-[(2-hydroxyethyl)thio]butan-2-ol (36)**



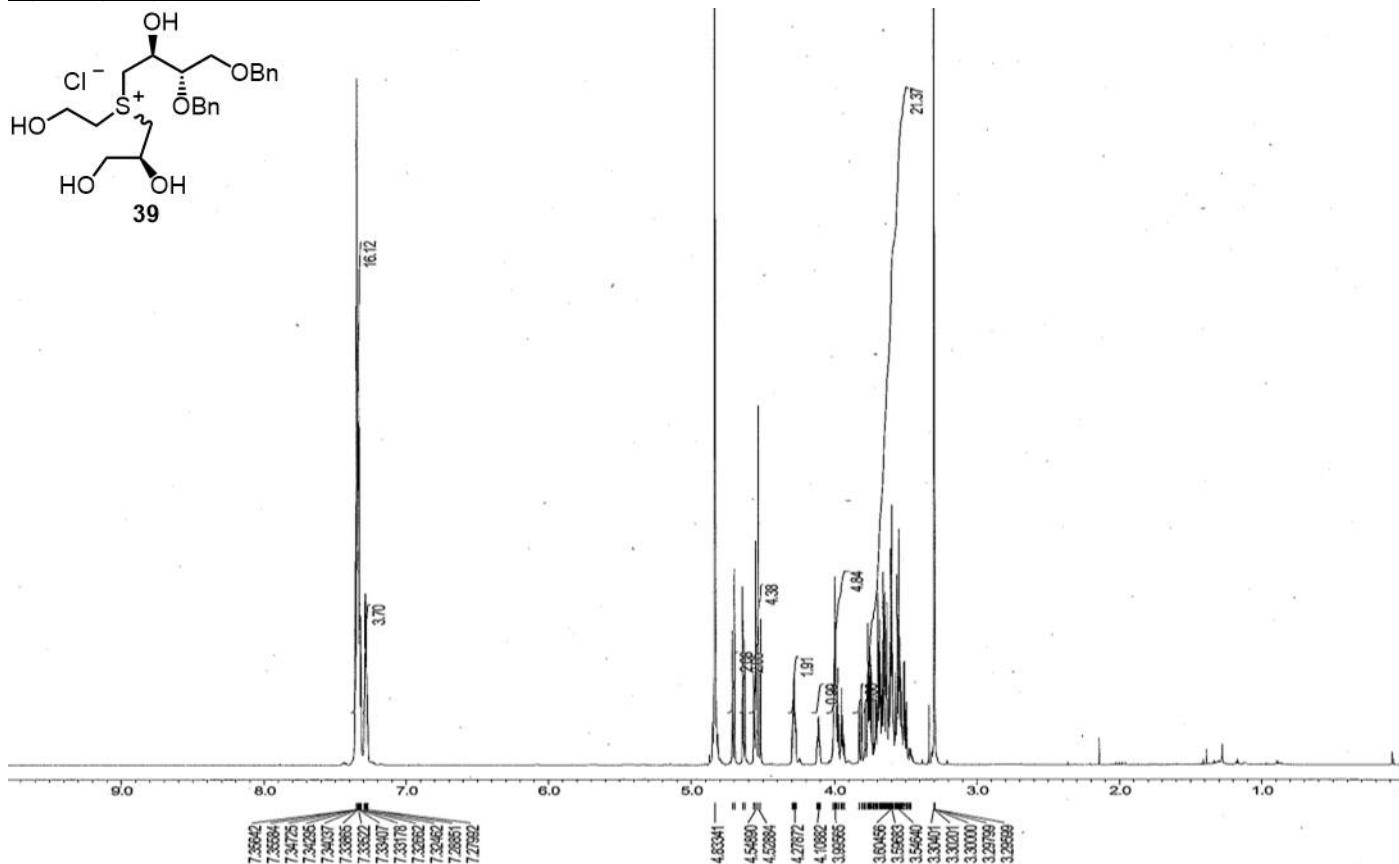
**<sup>1</sup>H NMR spectrum (800 MHz, CD<sub>3</sub>OD) of ((2*S*,3*S*)-3,4-Dibenzylxy-2-hydroxybutyl) [(*S*)-2,3-dihydroxy propyl] (2-Hydroxyethyl) Sulfonium Tetrafluoroborate (38)**



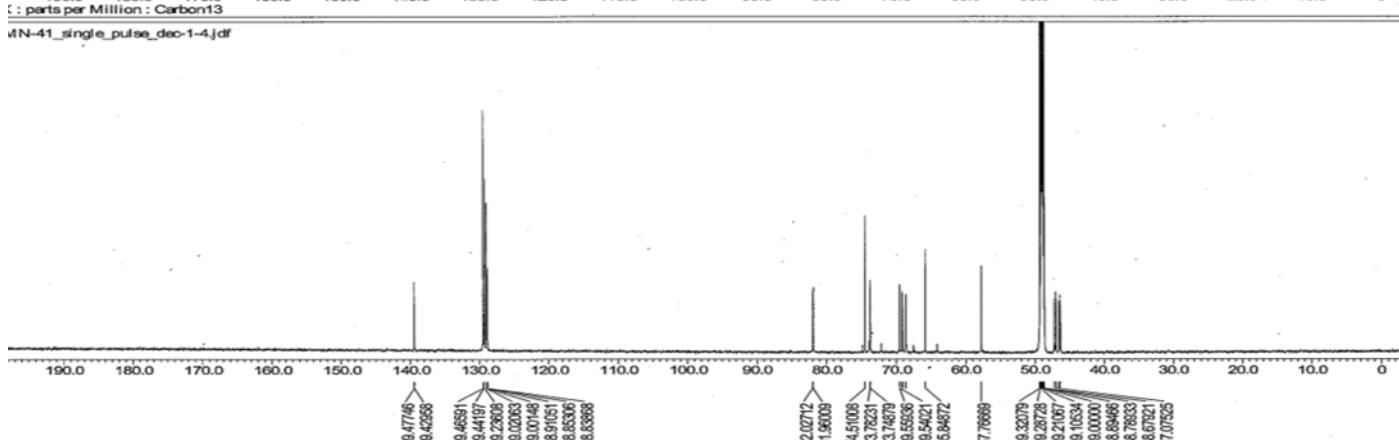
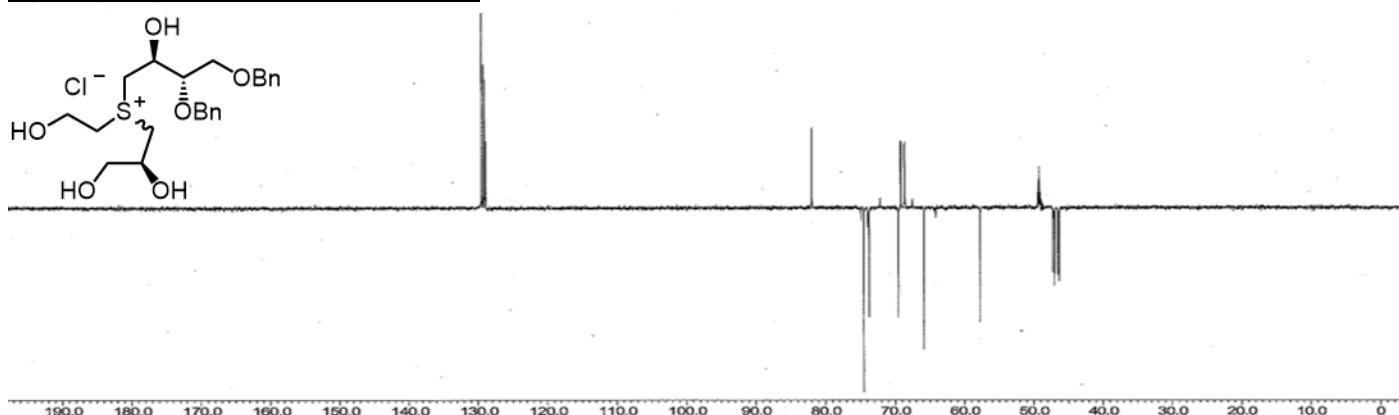
**<sup>13</sup>C NMR spectrum (200 MHz, CD<sub>3</sub>OD) of ((2*S*,3*S*)-3,4-Dibenzylxy-2-hydroxybutyl) [(*S*)-2,3-dihydroxy propyl] (2-Hydroxyethyl) Sulfonium Tetrafluoroborate (38)**



**<sup>1</sup>H NMR spectrum (800 MHz, CD<sub>3</sub>OD) of ((2S,3S)-3,4-Dibenzylxy-2-hydroxybutyl) [(S)-2,3-dihydroxy propyl] (2-Hydroxyethyl) Sulfonium Chloride (39)**

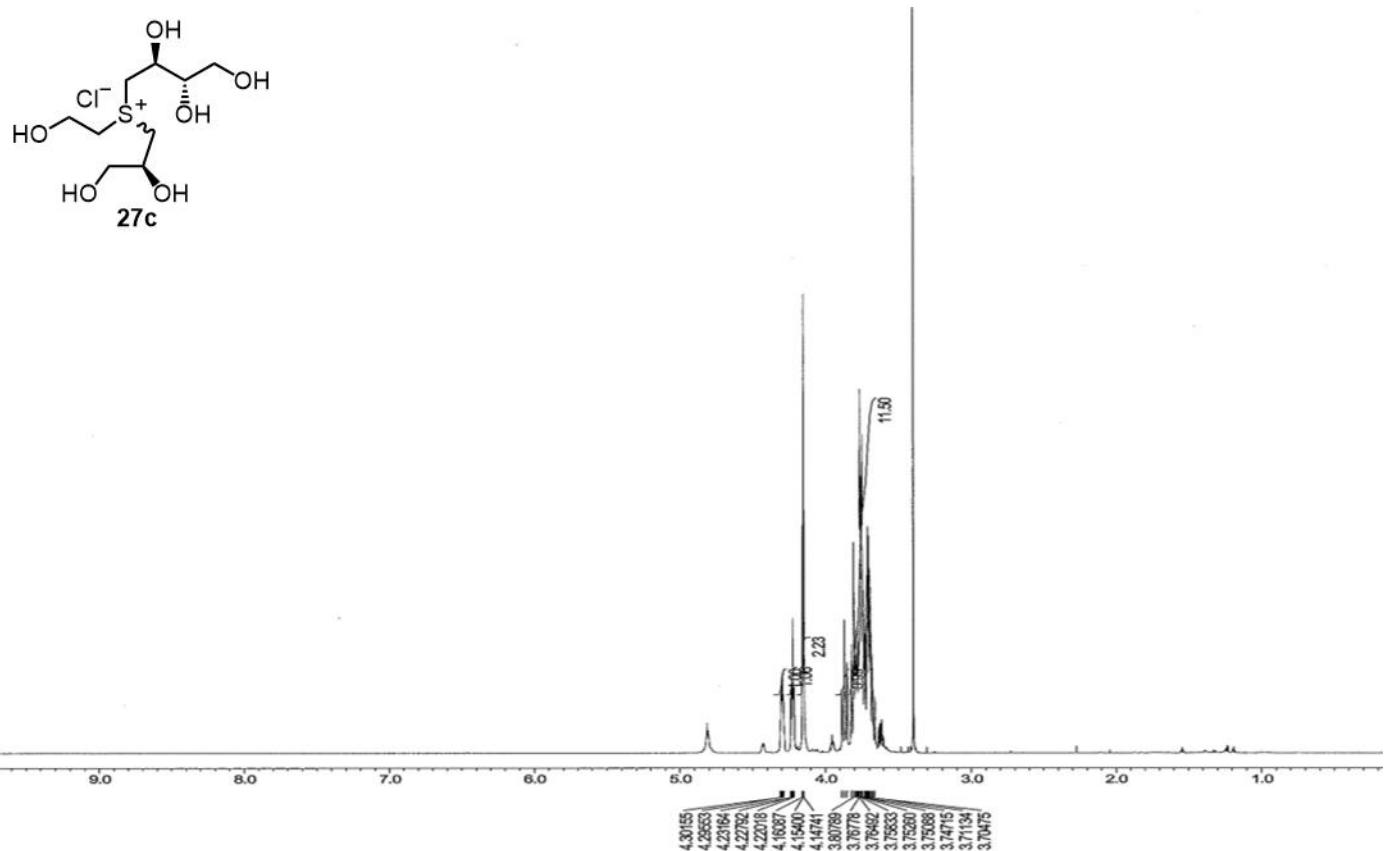


**<sup>13</sup>C NMR spectrum (200 MHz, CD<sub>3</sub>OD) of ((2S,3S)-3,4-Dibenzylxy-2-hydroxybutyl) [(S)-2,3-dihydroxy propyl] (2-Hydroxyethyl) Sulfonium Chloride (39)**



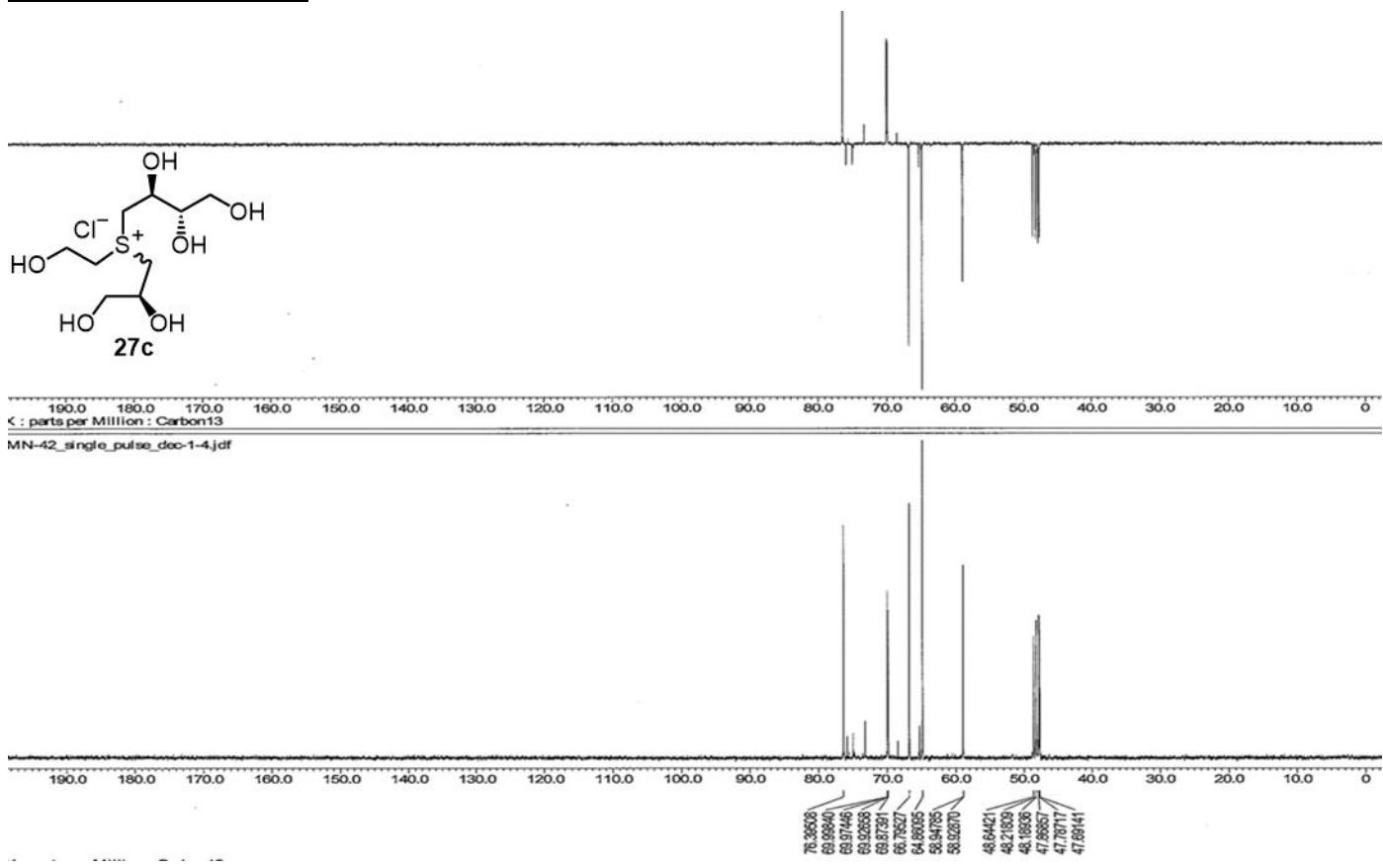
**<sup>1</sup>H NMR spectrum (800 MHz, D<sub>2</sub>O) of [(S)-2,3-Dihydroxypropyl] (2-Hydroxyethyl) ((2S,3S)-2,3,4-trihydroxybutyl)**

**Sulfonium Chloride (27c)**

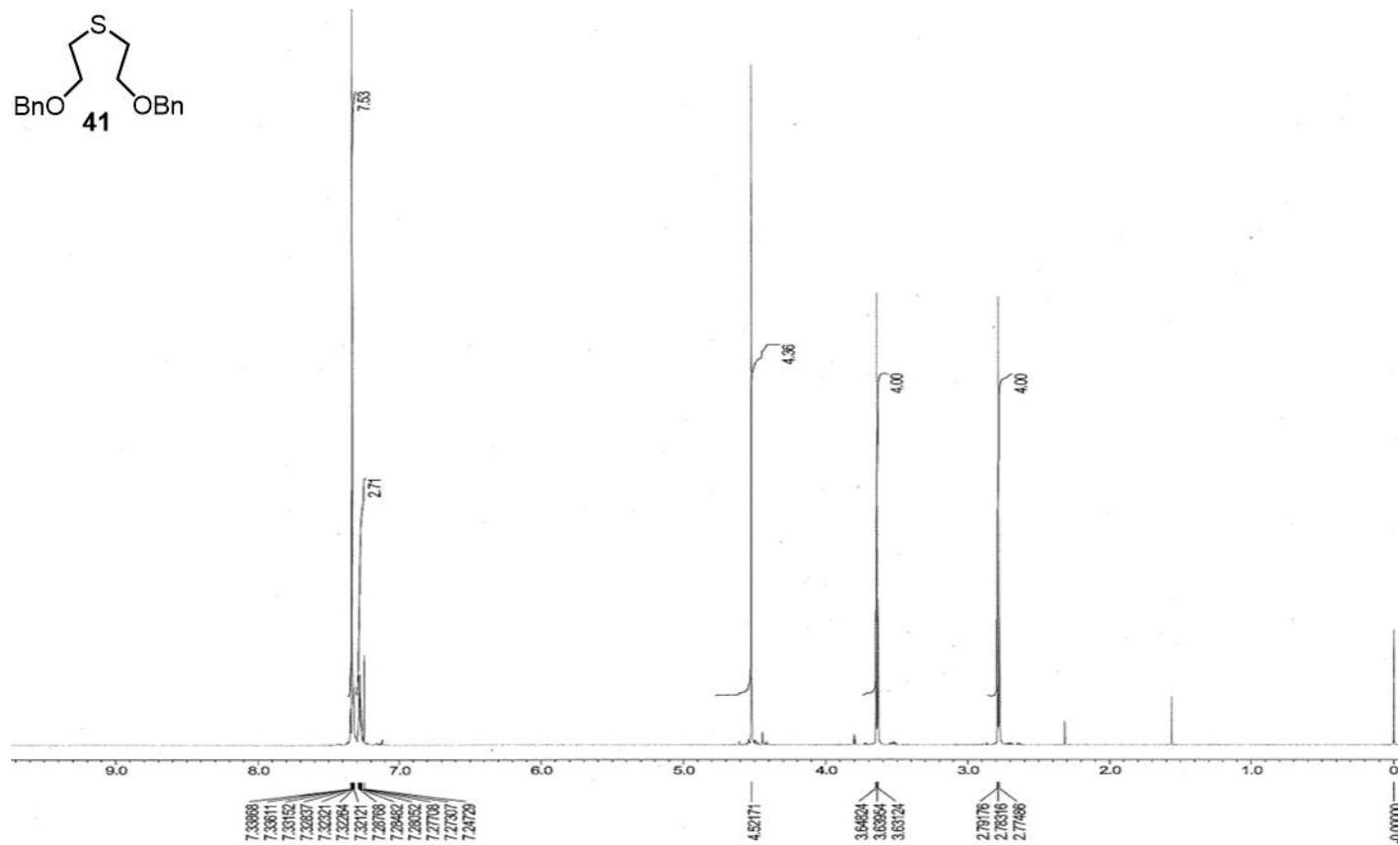


**<sup>13</sup>C NMR spectrum (200 MHz, D<sub>2</sub>O) of [(S)-2,3-Dihydroxypropyl] (2-Hydroxyethyl) ((2S,3S)-2,3,4-trihydroxybutyl)**

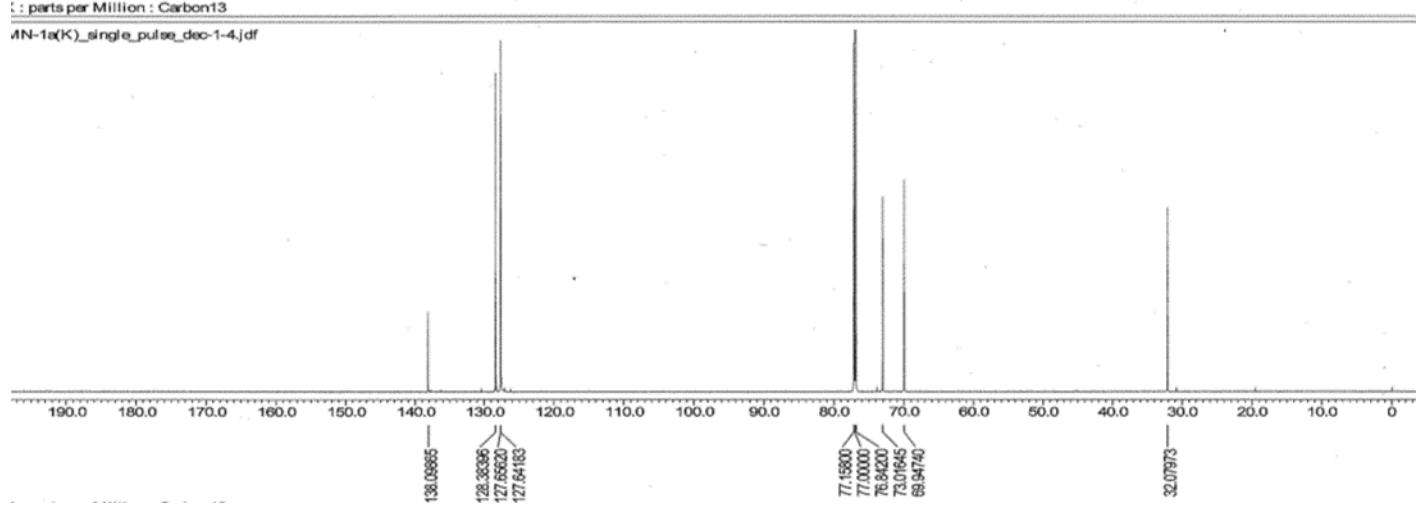
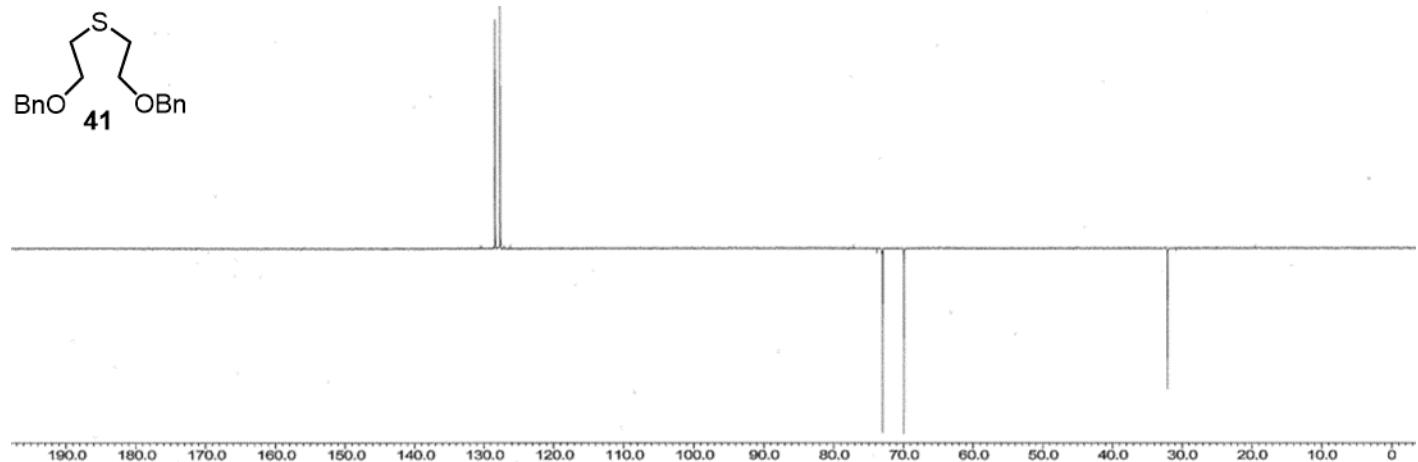
**Sulfonium Chloride (27c)**



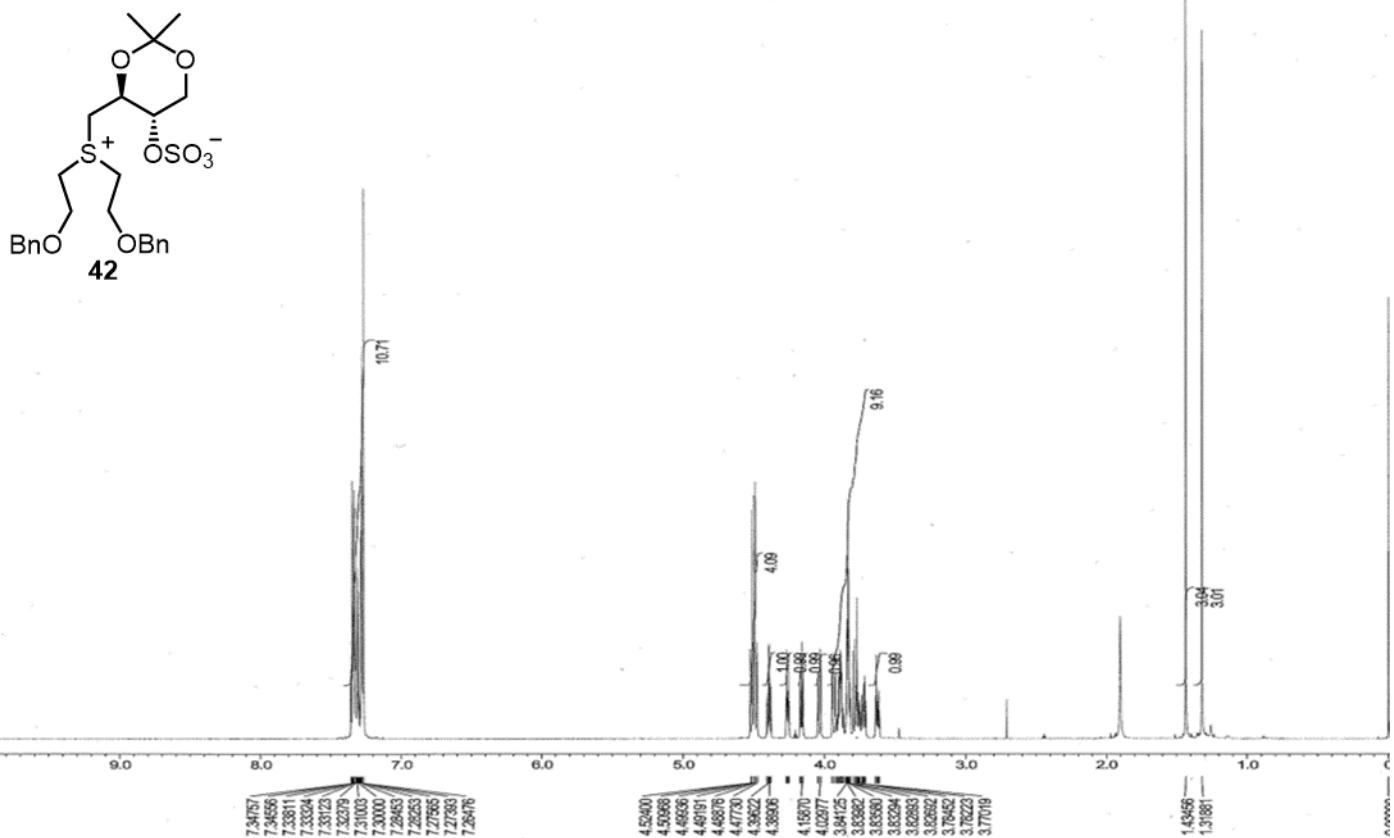
**<sup>1</sup>H NMR spectrum (800 MHz, CDCl<sub>3</sub>) of Di-O-benzyl-2,2'-thiodiethanol (41)**



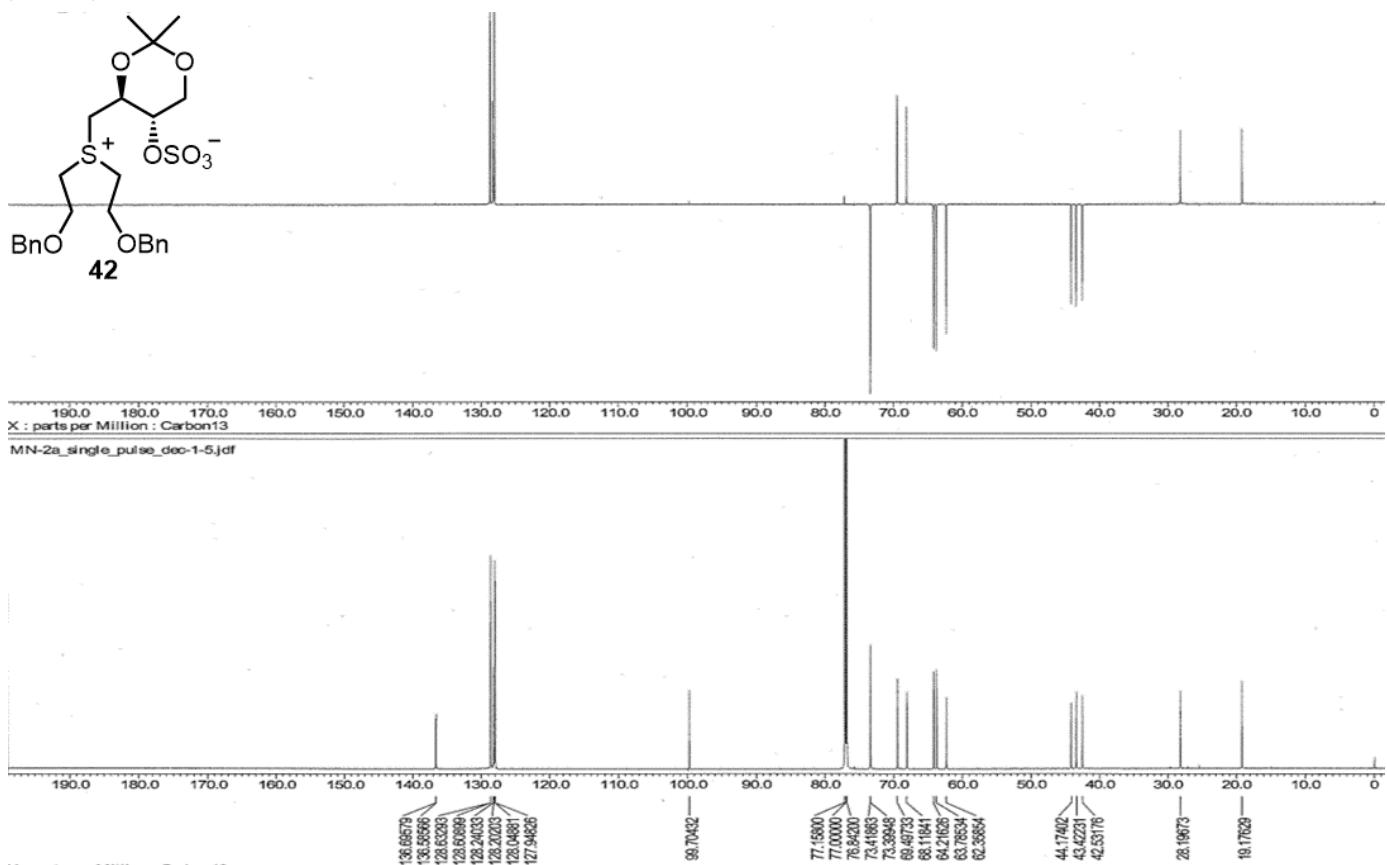
**<sup>13</sup>C NMR spectrum (200 MHz, CDCl<sub>3</sub>) of Di-O-benzyl-2,2'-thiodiethanol (41)**



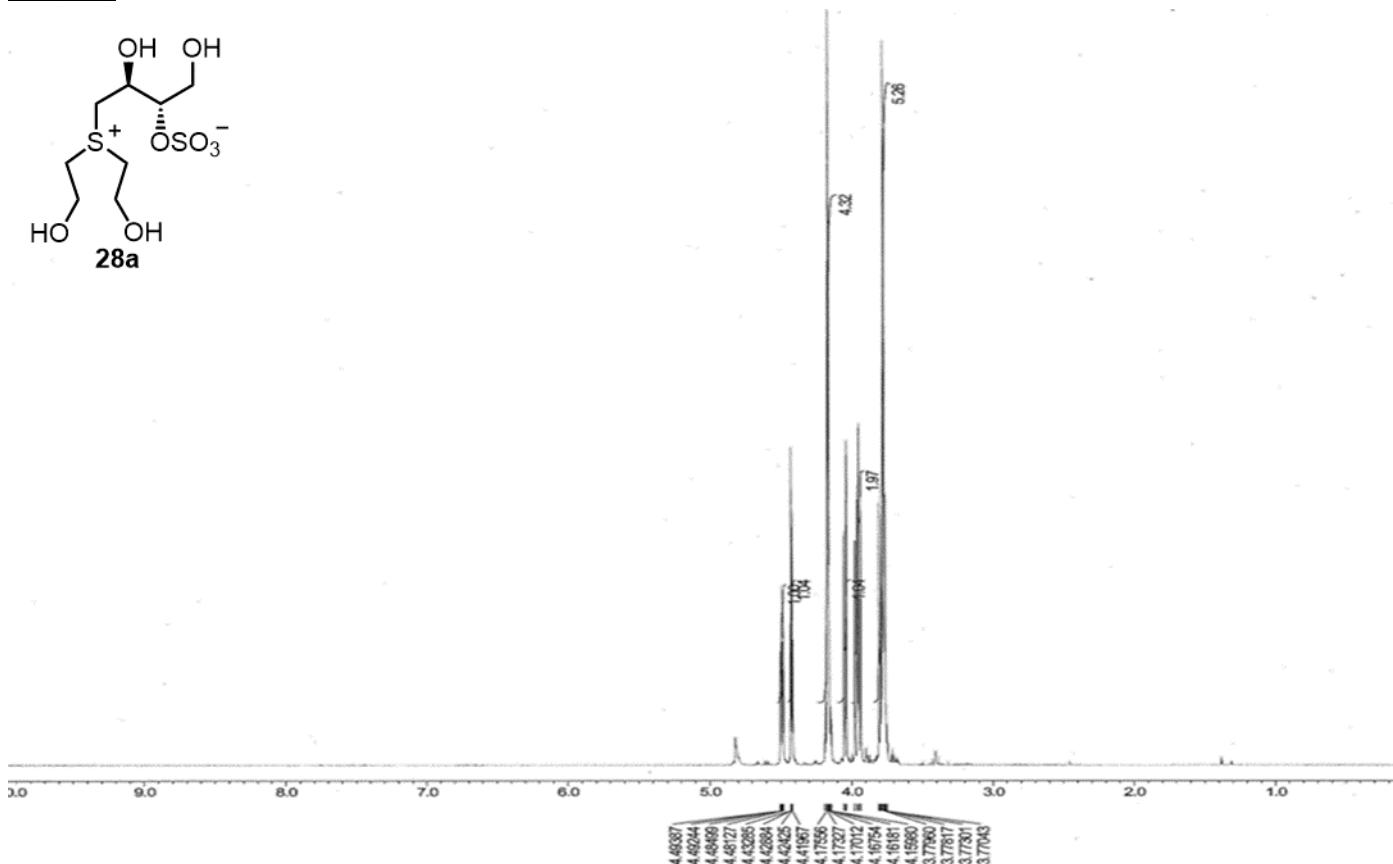
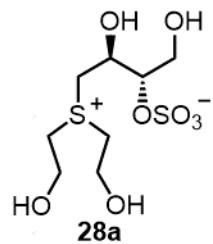
**<sup>1</sup>H NMR spectrum (800 MHz, CDCl<sub>3</sub>) of Di(2-benzyloxyethyl) [(4S,5S)-2,2-Dimethyl -5-sulfooxy-1,3-dioxan-4-ylmethyl] Sulfonium Inner Salt (42)**



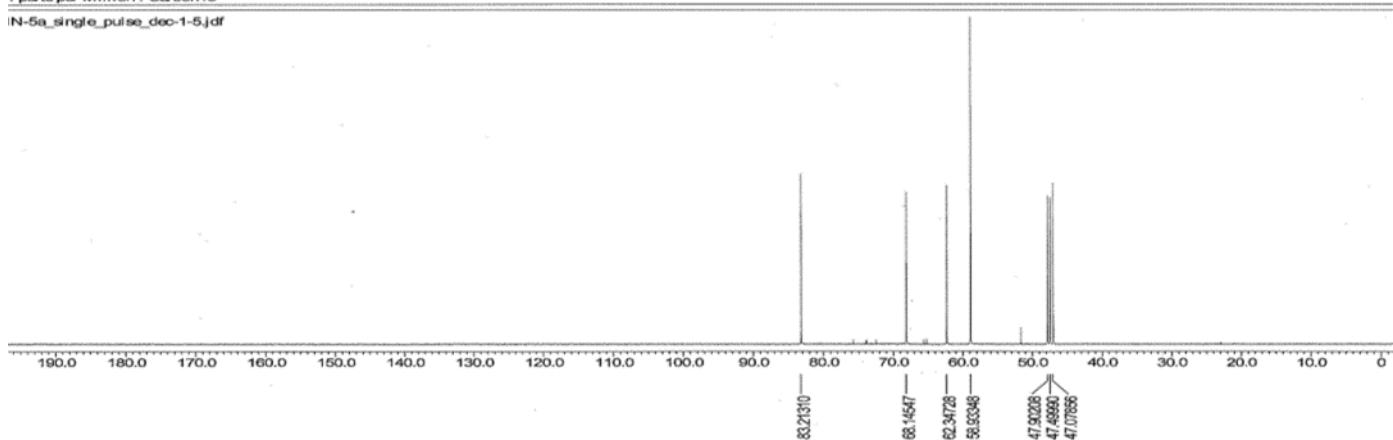
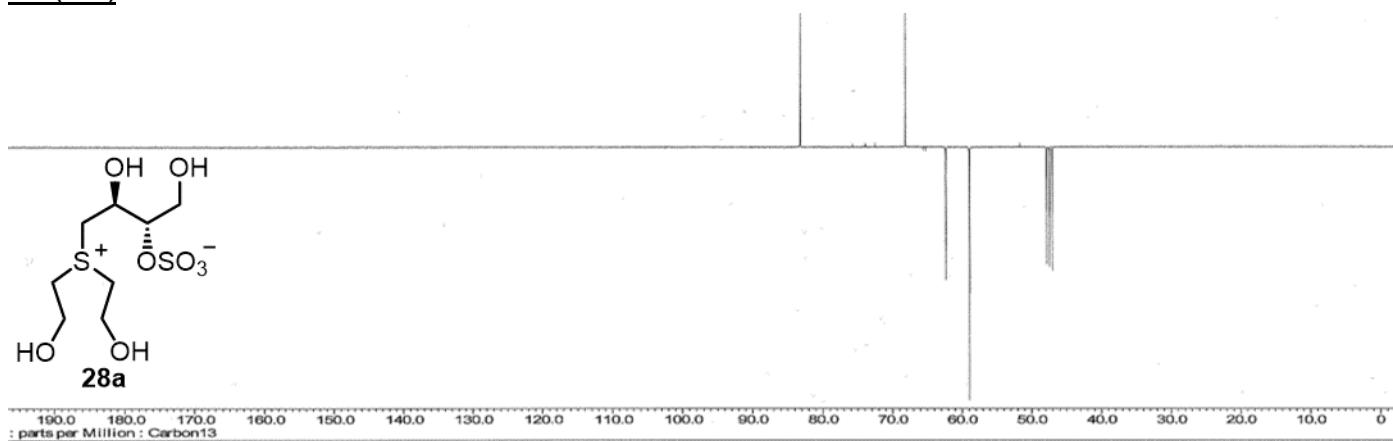
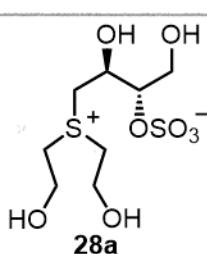
**<sup>13</sup>C NMR spectrum (200 MHz, CDCl<sub>3</sub>) of Di(2-benzyloxyethyl) [(4S,5S)-2,2-Dimethyl -5-sulfooxy-1,3-dioxan-4-ylmethyl] Sulfonium Inner Salt (42)**



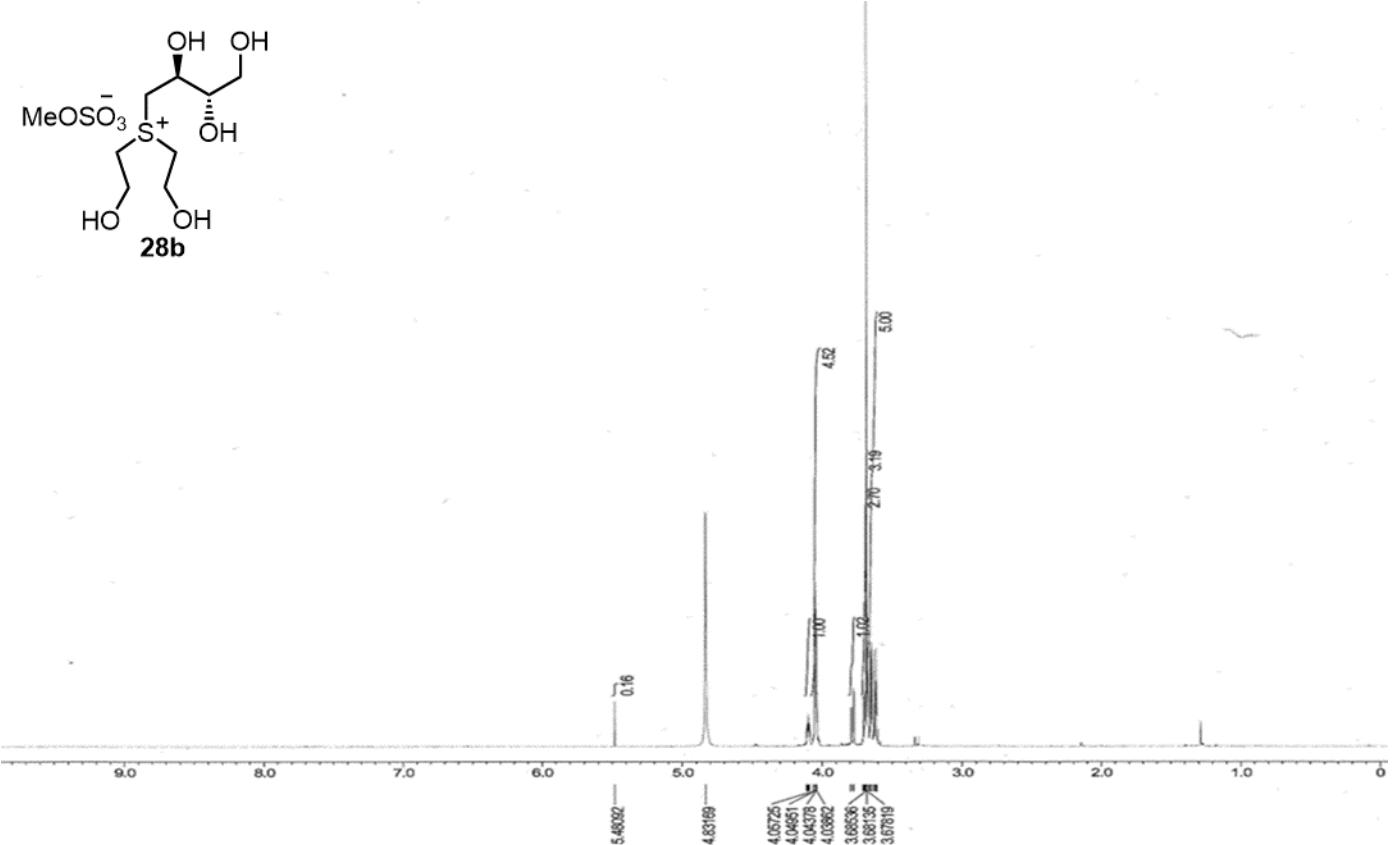
**<sup>1</sup>H NMR spectrum (800 MHz, D<sub>2</sub>O) of [(2S,3S)-2,4-Dihydroxy-3-sulfooxybutyl] Di(2-hydroxyethyl) Sulfonium Inner Salt(28a)**



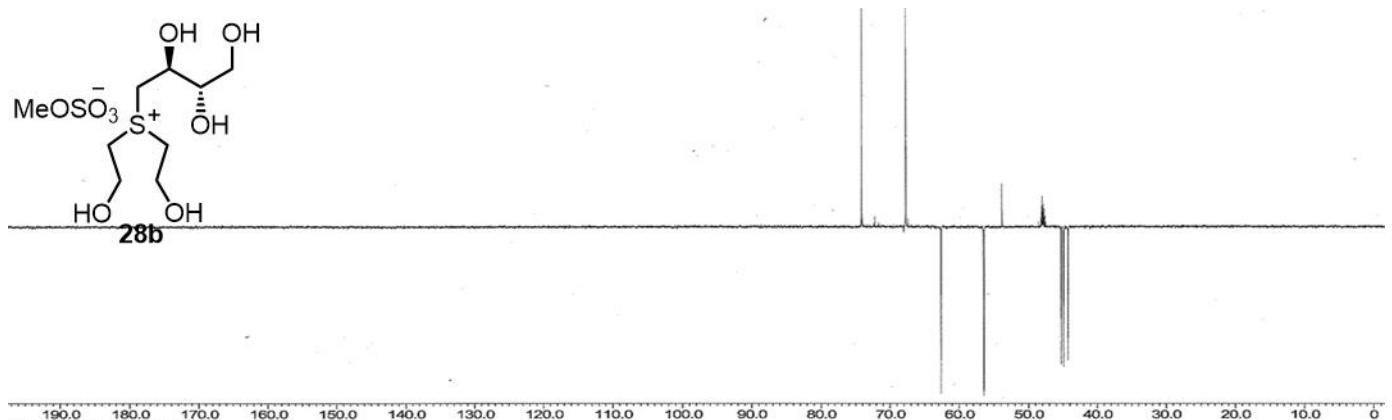
**<sup>13</sup>C NMR spectrum (200 MHz, D<sub>2</sub>O) of [(2S,3S)-2,4-Dihydroxy-3-sulfooxybutyl] Di(2-hydroxyethyl) Sulfonium Inner Salt(28a)**



**<sup>1</sup>H NMR spectrum (800 MHz, CD<sub>3</sub>OD) of Di(2-hydroxyethyl) [(2S,3S)-2,3,4-Trihydroxybutyl] Sulfoni m Methyl Sulfate (28b)**

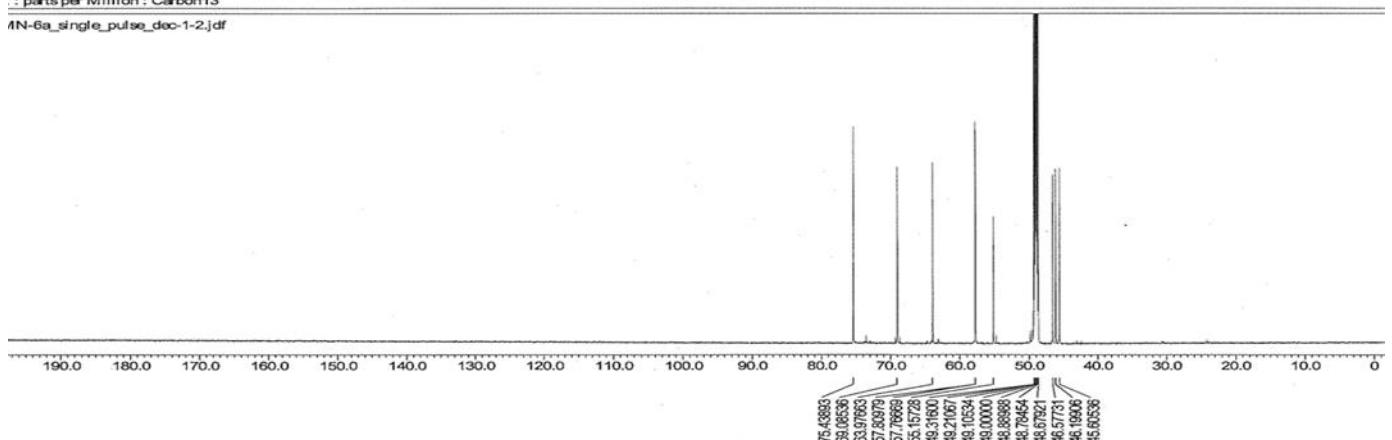


**<sup>13</sup>C NMR spectrum (200 MHz, CD<sub>3</sub>OD) of Di(2-hydroxyethyl) [(2S,3S)-2,3,4-Trihydroxybutyl] Sulfoni m Methyl Sulfate (28b)**

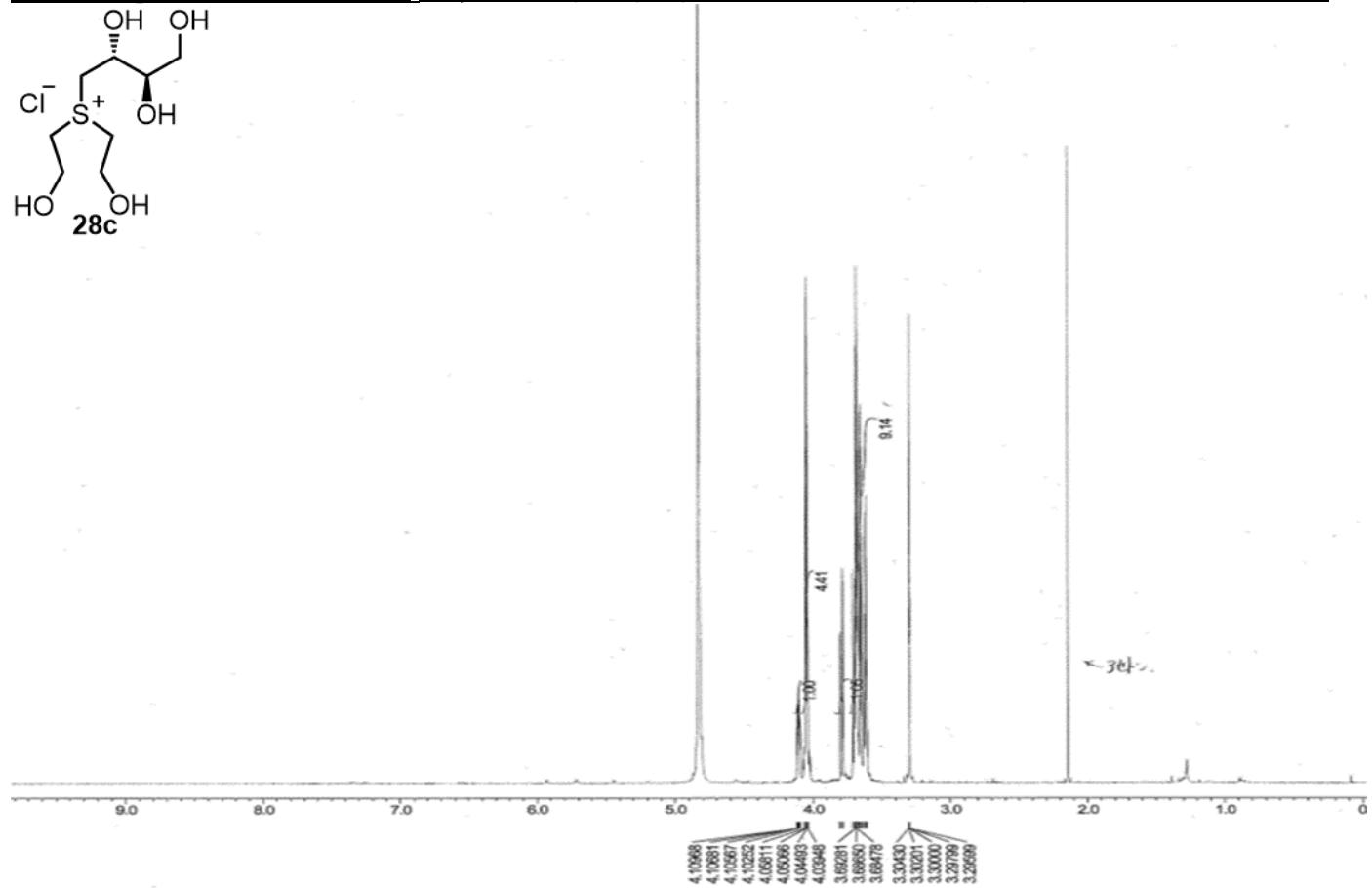


: parts per Million : Carbon13

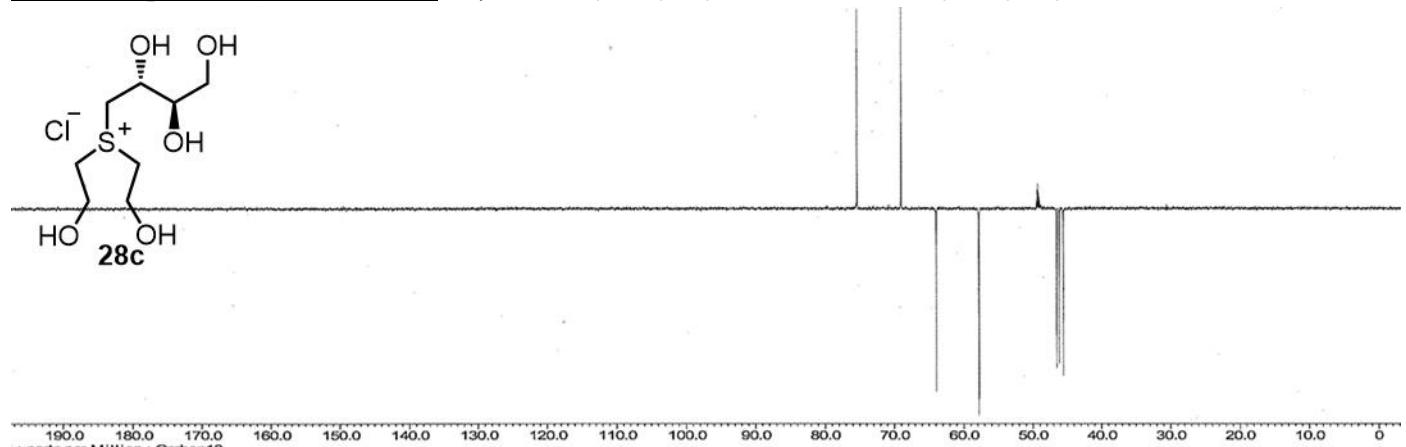
4N-6a\_single\_pulse\_dec-1-2.jdf



**<sup>1</sup>H NMR spectrum (800 MHz, CD<sub>3</sub>OD) of Di(2-hydroxyethyl) [(2S,3S)-2,3,4-Trihydroxybutyl] Sulfon ium Chloride (28c)**



**<sup>13</sup>C NMR spectrum (200 MHz, CD<sub>3</sub>OD) of Di(2-hydroxyethyl) [(2S,3S)-2,3,4-Trihydroxybutyl] Sulfon ium Chloride (28c)**



: parts per Million : Carbon13

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