

Supporting Information

Synthesis of ^{11}C -Labeled Thiamine and Fursultiamine for in Vivo Molecular Imaging of Vitamin B₁ and Its Prodrug Using Positron Emission Tomography

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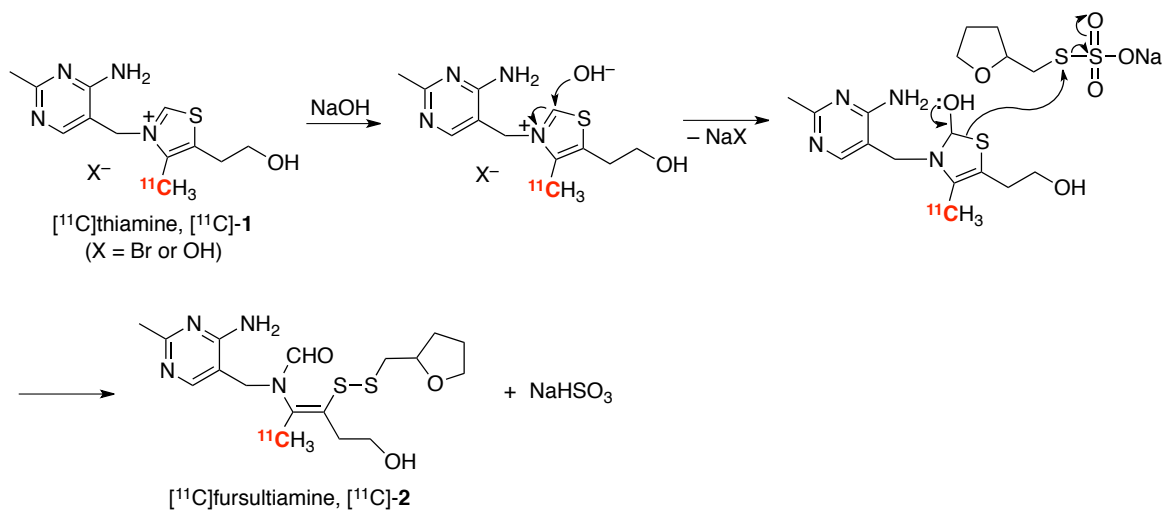
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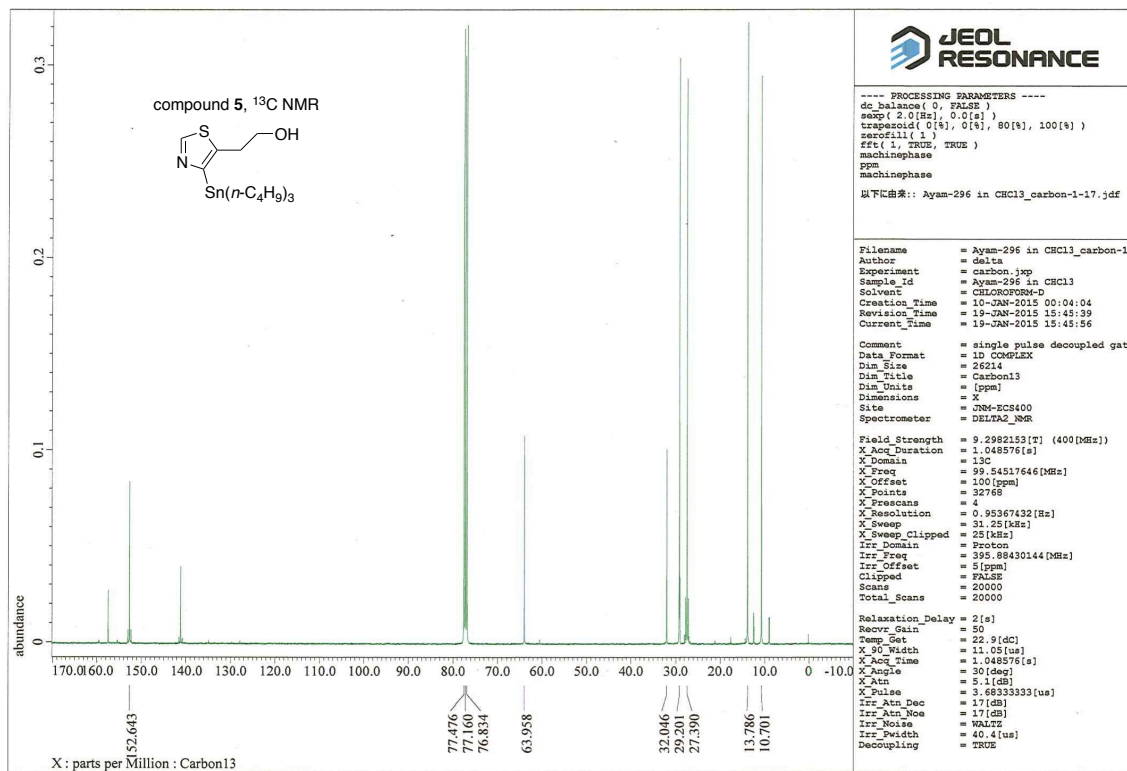
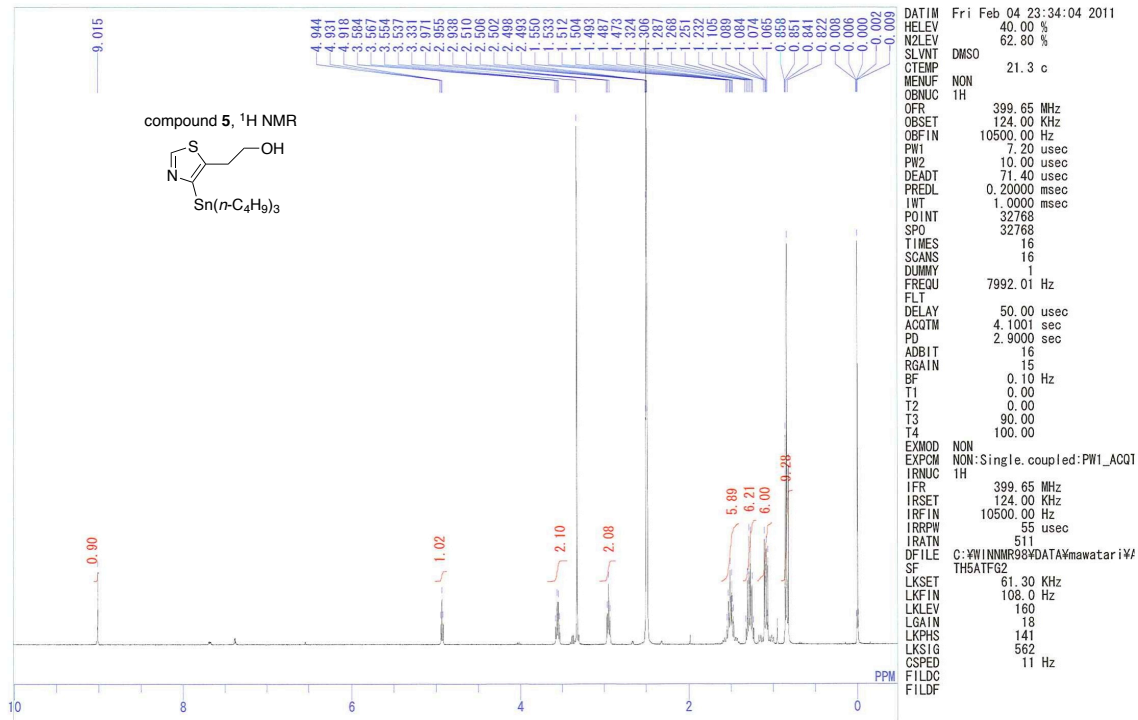
(1) Scheme S1. Possible reaction mechanism of production of [¹¹ C]fursultiamine ([¹¹ C]- 2) using [¹¹ C]thiamine ([¹¹ C]- 1) and <i>S</i> -tetrahydrofurfurylthiosulfuric acid, sodium salt (TFT-Na)	3
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(1) Scheme S1. Possible Reaction Mechanism of Production of [¹¹C]Fursultiamine ([¹¹C]-2) Using [¹¹C]Thiamine ([¹¹C]-1) and *S*-Tetrahydrofurfurylthiosulfuric Acid, Sodium Salt (TFT-Na)

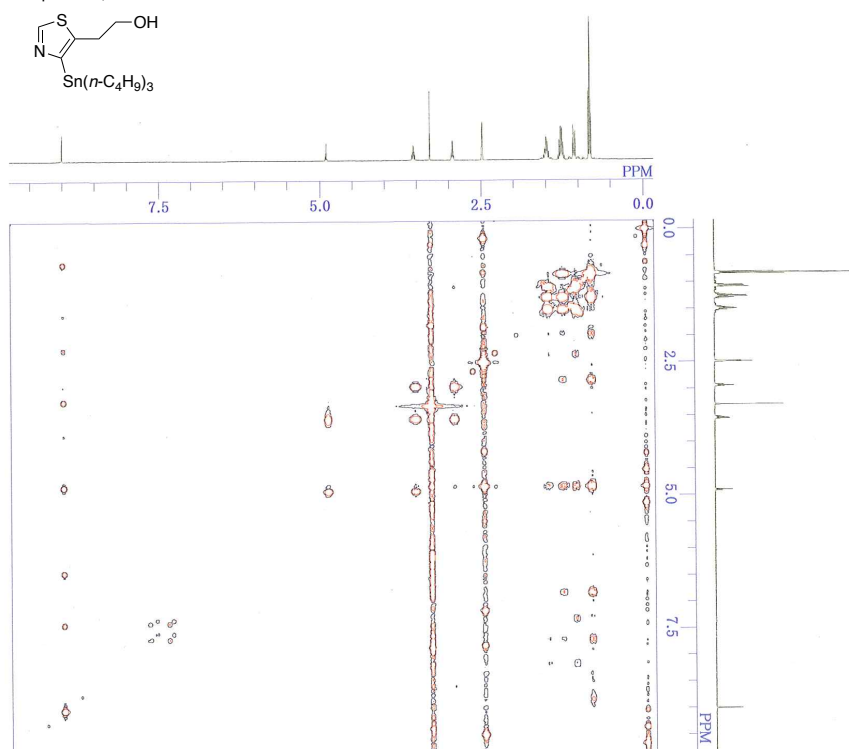


(2) ^1H , $^{13}\text{C}\{^1\text{H}\}$, and 2D NMR Spectra, and HRMS Analysis, of Compound 5

C:\VWINNMR98\DATA\mawatar\Yam-147-2 (DMSO).als



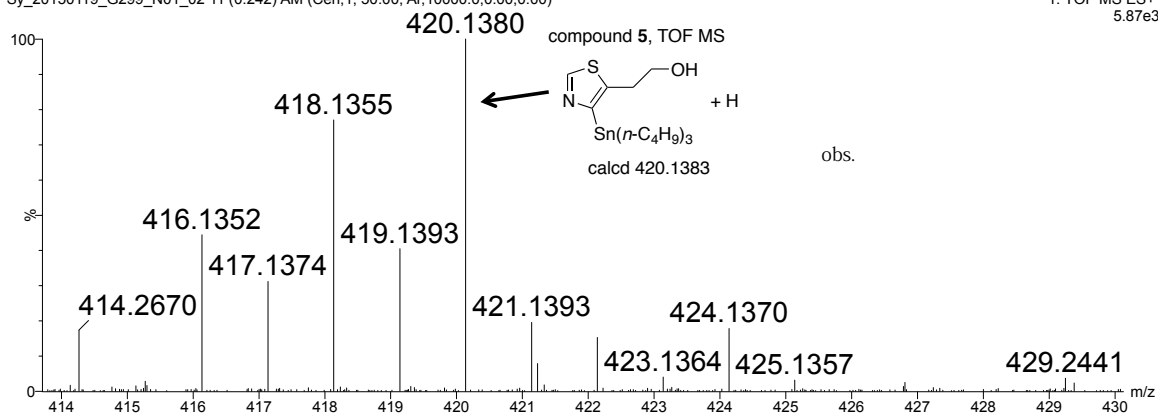
compound 5, ¹H-¹H COSY



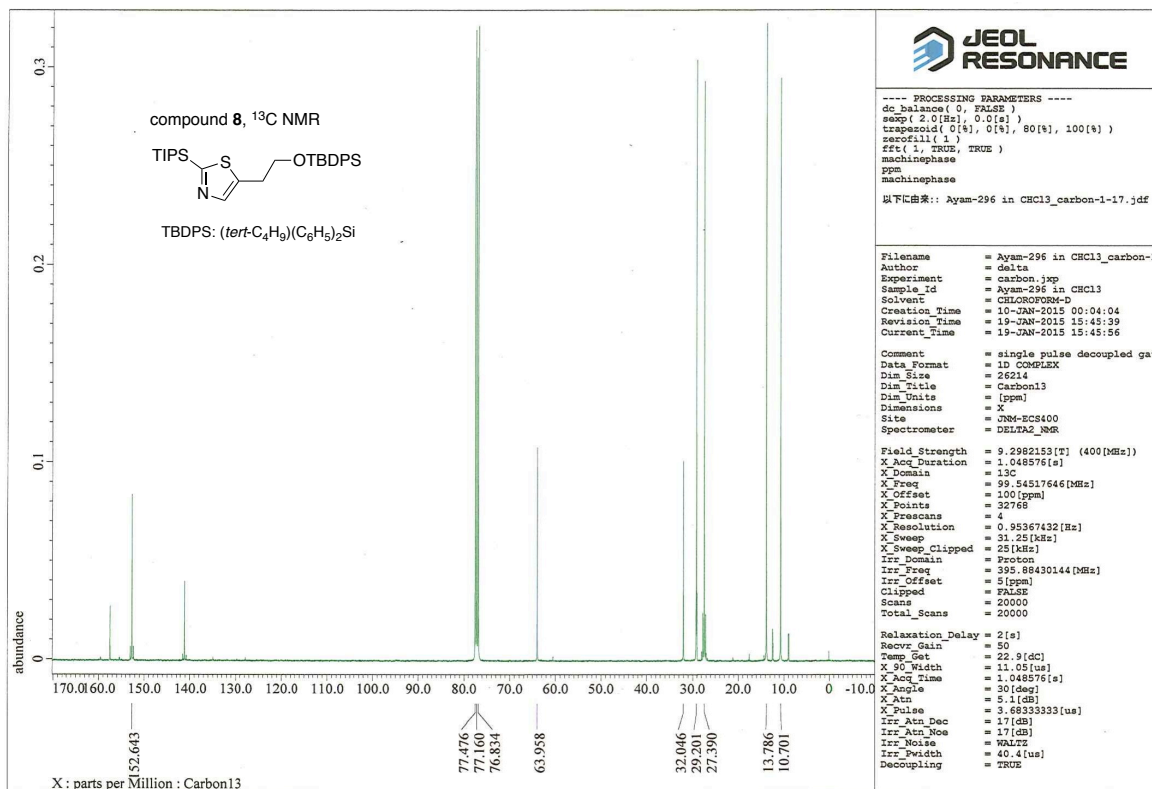
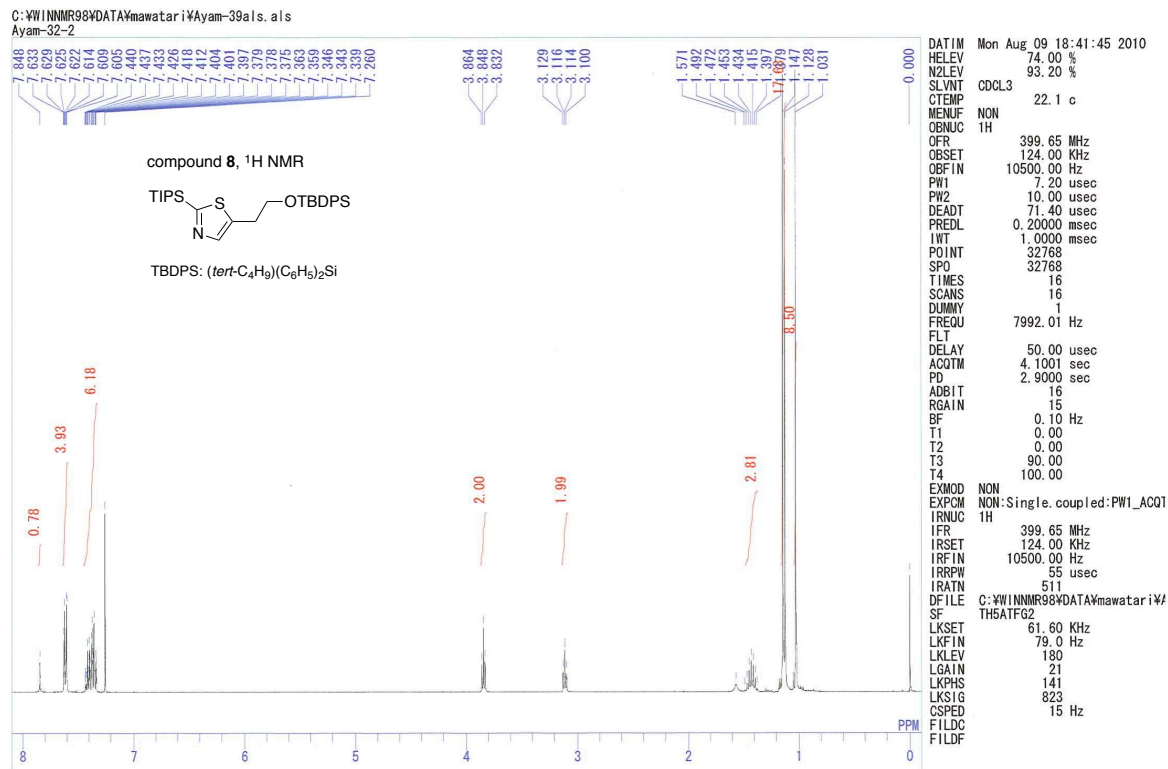
compound5-2D.als
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 134.40 KHz
 33.40 Hz
 512
 3988.04 Hz
 4096
 256
 3984.06 Hz
 4
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 1.5000 sec
 14.40 usec
 14.40 usec
 10.00 usec
 0.2510 msec
 0.2510 msec
 1.0000 msec
 1H
 23.8 c
 DMSO
 2.49 ppm
 2.49
 15
 511
 1

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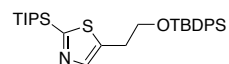
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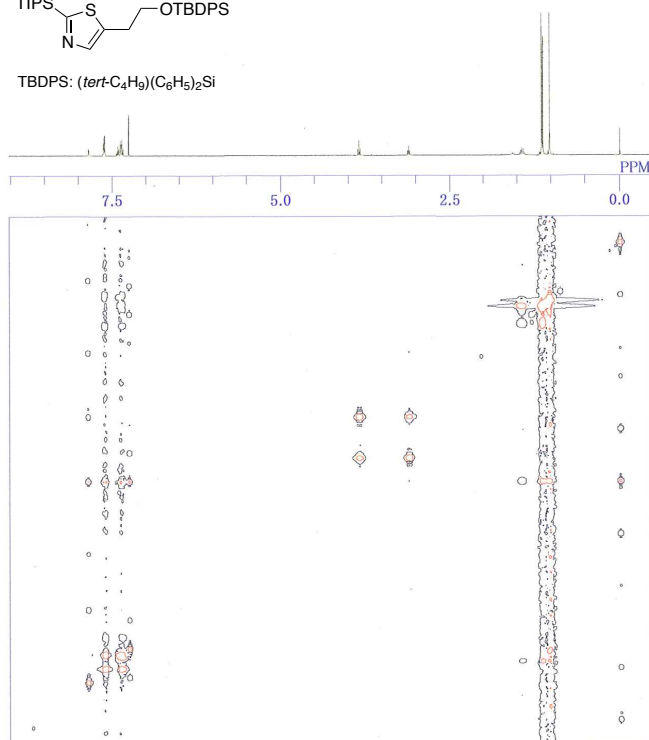
(3) ^1H , $^{13}\text{C}\{^1\text{H}\}$, and 2D NMR Spectra, and HRMS Analysis, of Compound 8



compound **8**, ^1H - ^1H COSY



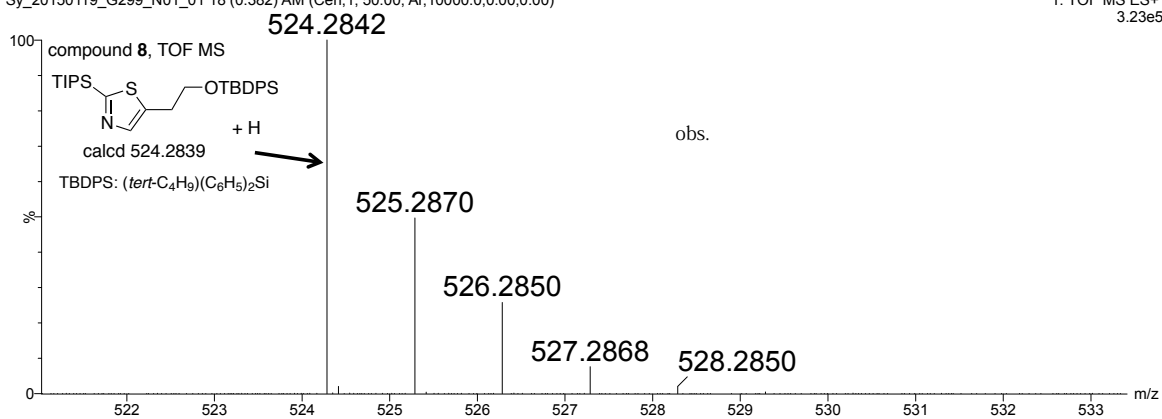
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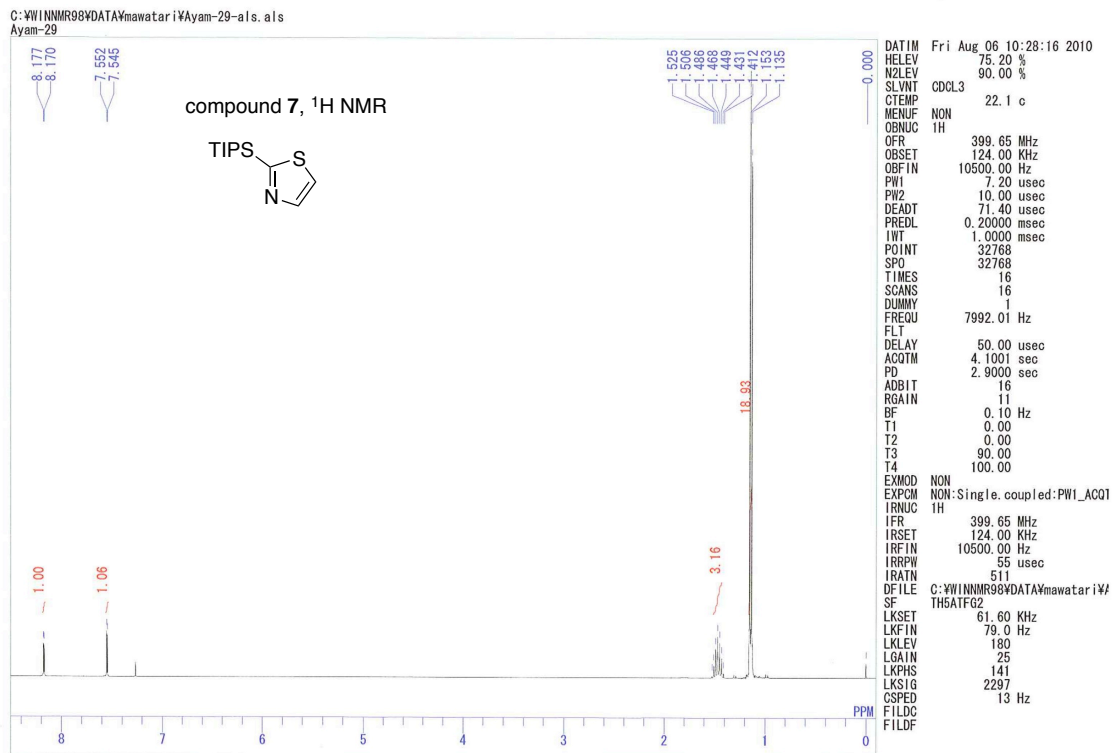
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 OBFIN 14.90 Hz
 POINT 512
 FREQU 3793.27 Hz
 CLPNT 1024
 TODAT 256
 CLFRQ 3787.88 Hz
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 PD 1.5000 sec
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 PW2 14.40 usec
 PW3 10.00 usec
 PI1 0.2640 msec
 PI2 0.2640 msec
 PI3 1.0000 msec
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 CTEMP 25.7 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 CLEXR 0.00
 RGAIN 15
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 LOOP1 1

Sy_20150119_G299_N01_01 18 (0.382) AM (Cen,1, 50.00, Ar,10000.0,0.00,0.00)

1: TOF MS ES+
3.23e5



(4) ^1H and 2D NMR Spectra of Compound 7



compound 7, ^1H - ^1H COSY

