Supporting information

Diastereoselectivity switch in the Pd(0)/InI-mediated reactions of β-lactams with aldehydes. An entry into nonracemic semi-protected (3*E*)-2,6-enediols.

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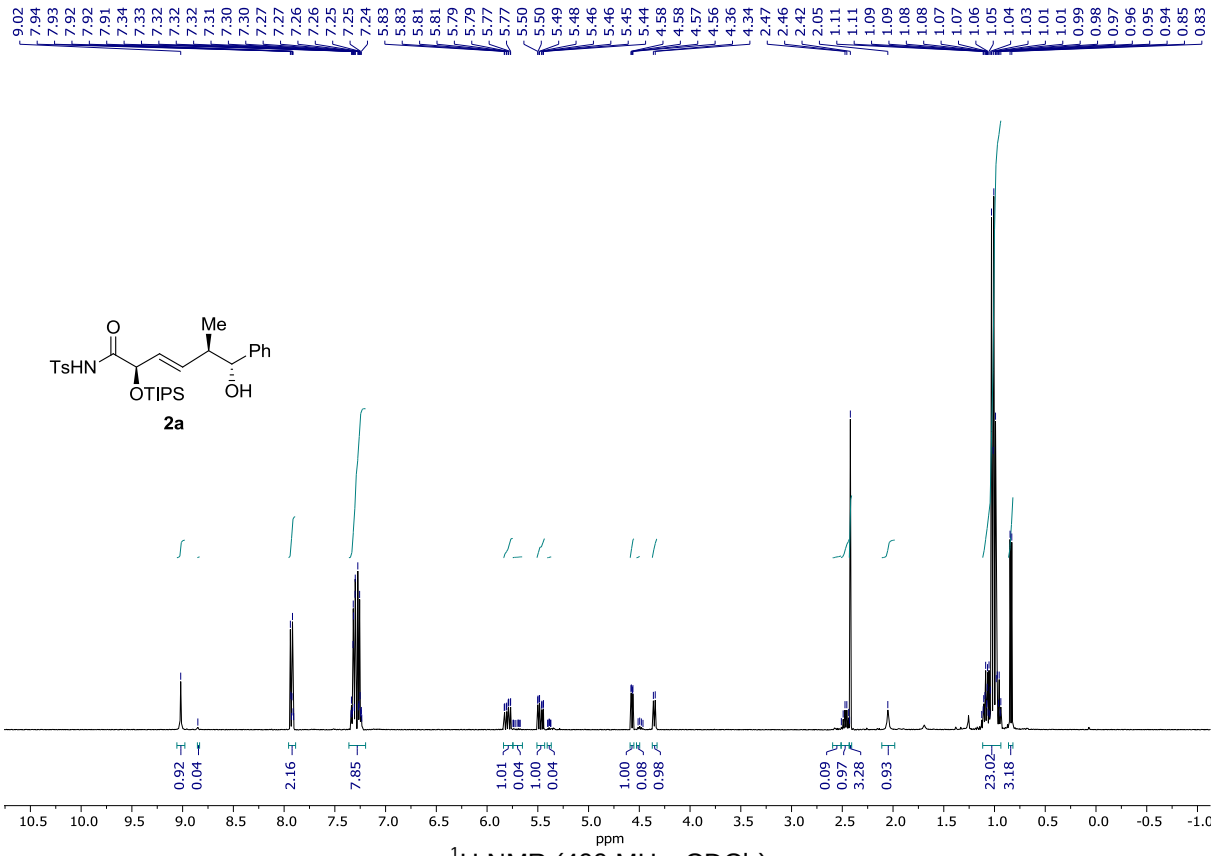
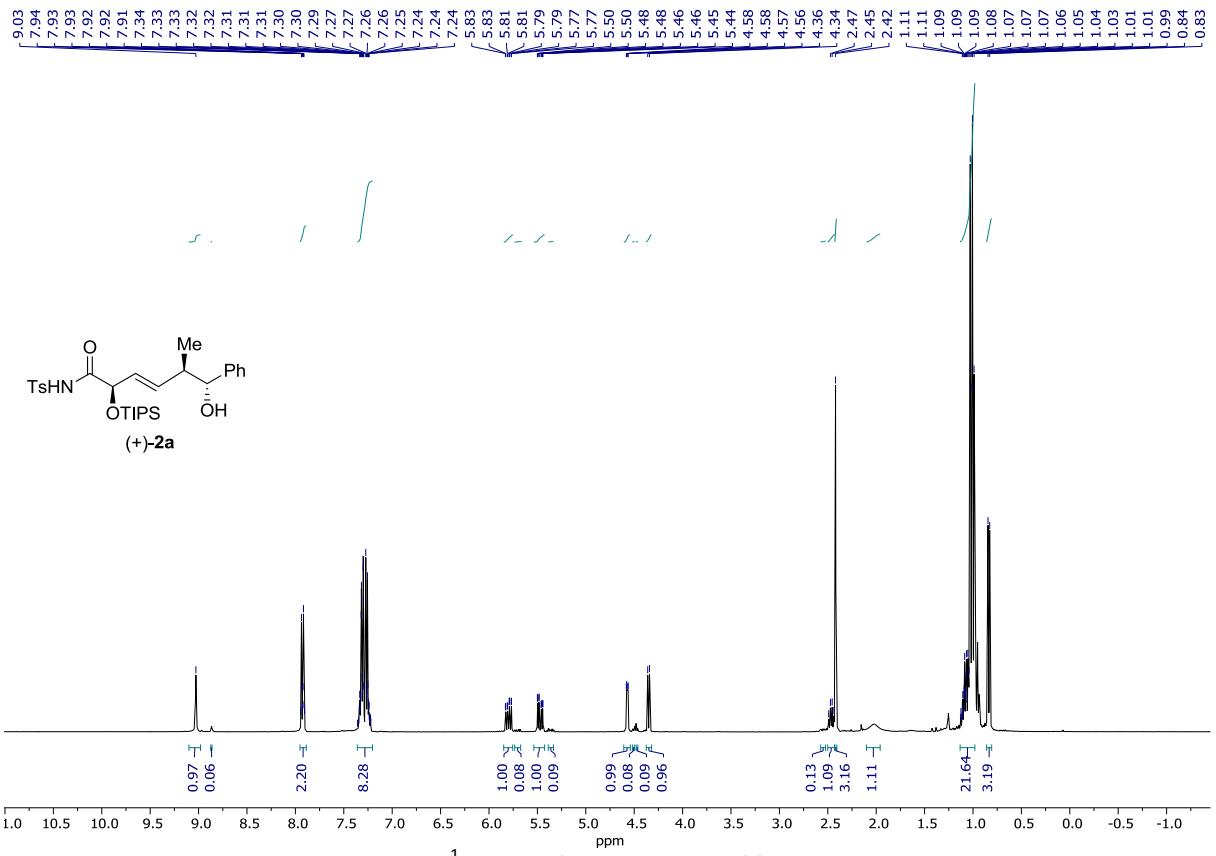
Contents

1. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra for all new and selected known compounds.



^{1}H NMR (400 MHz, $CDCl_3$)



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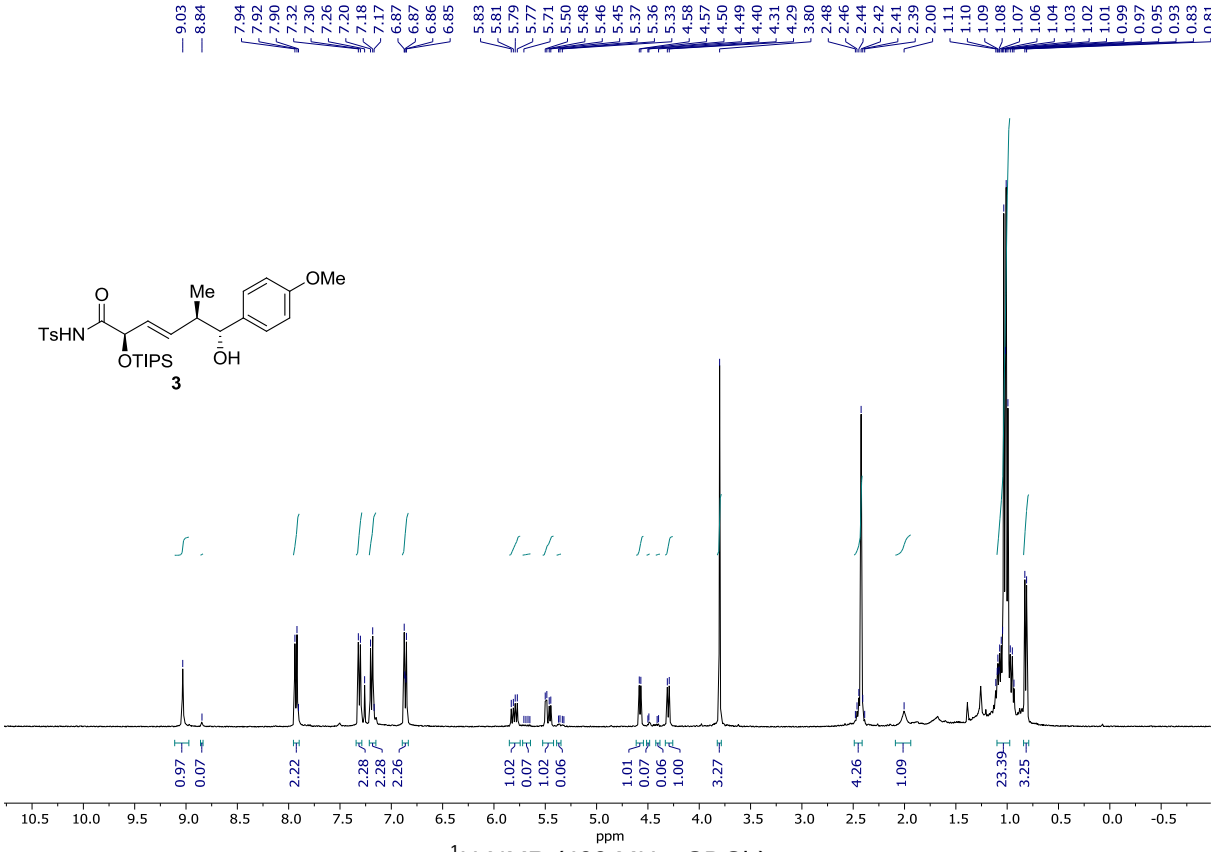

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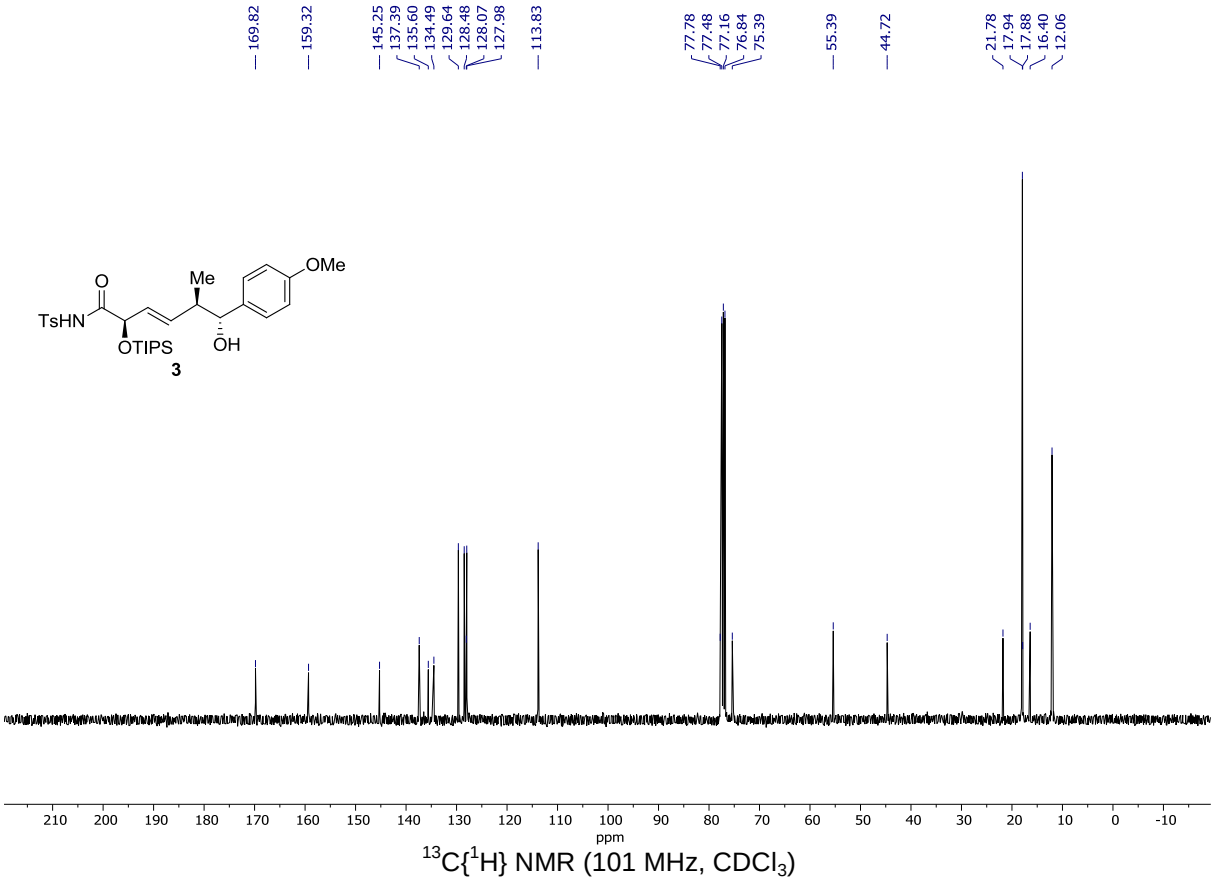
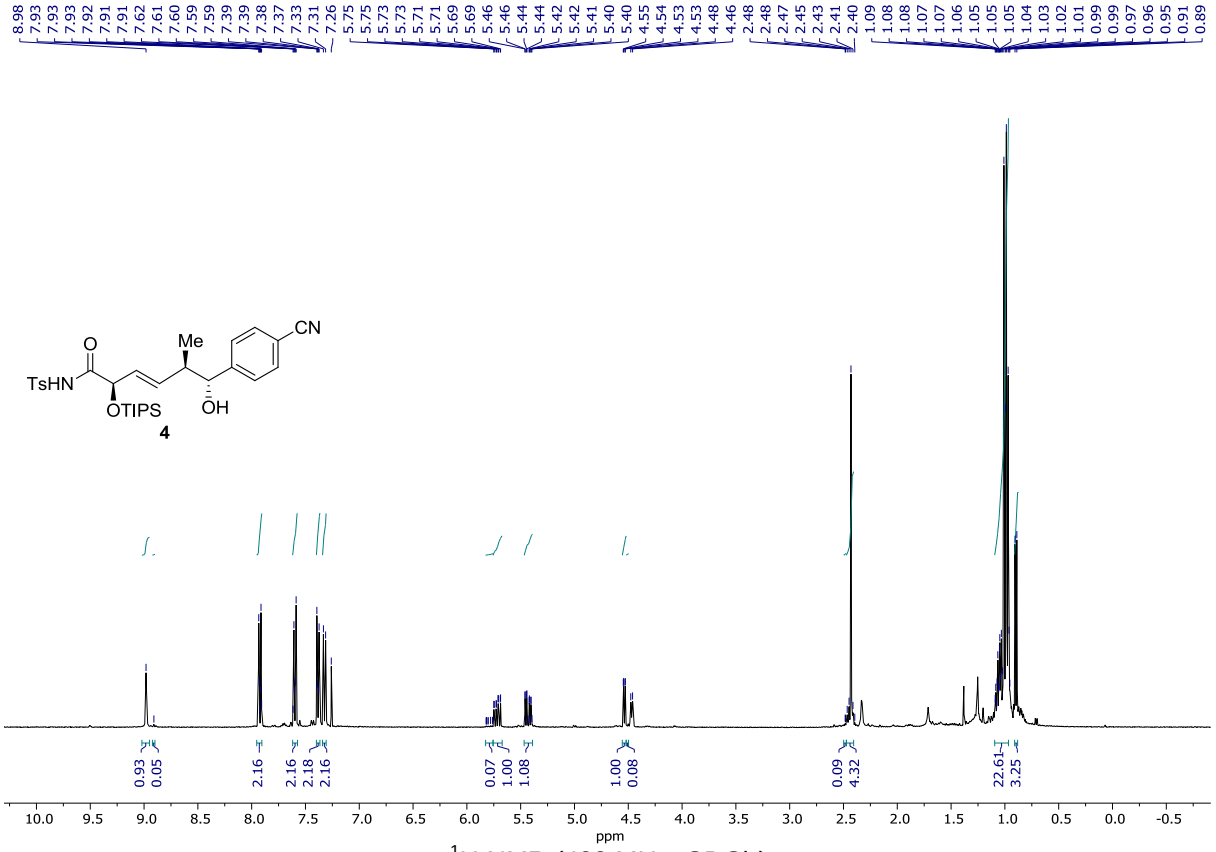


^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)



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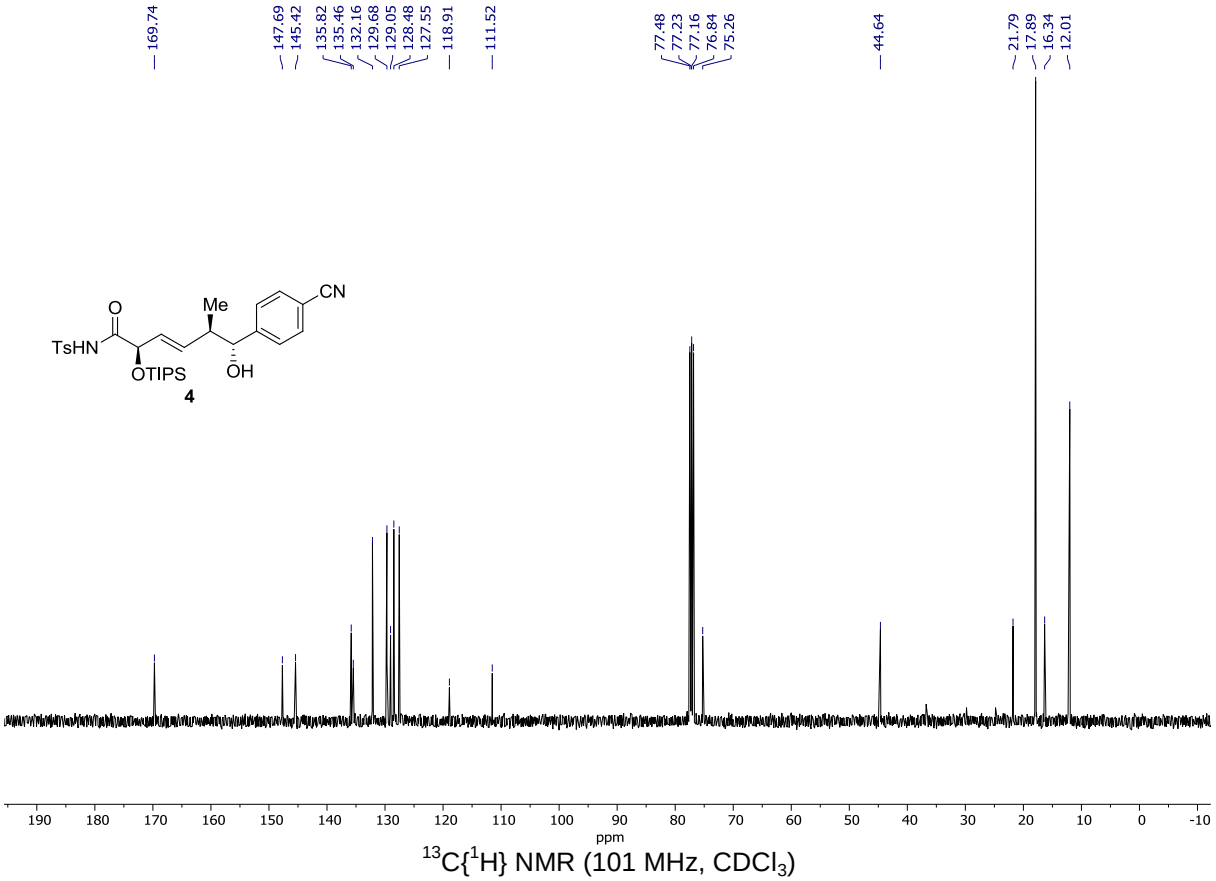

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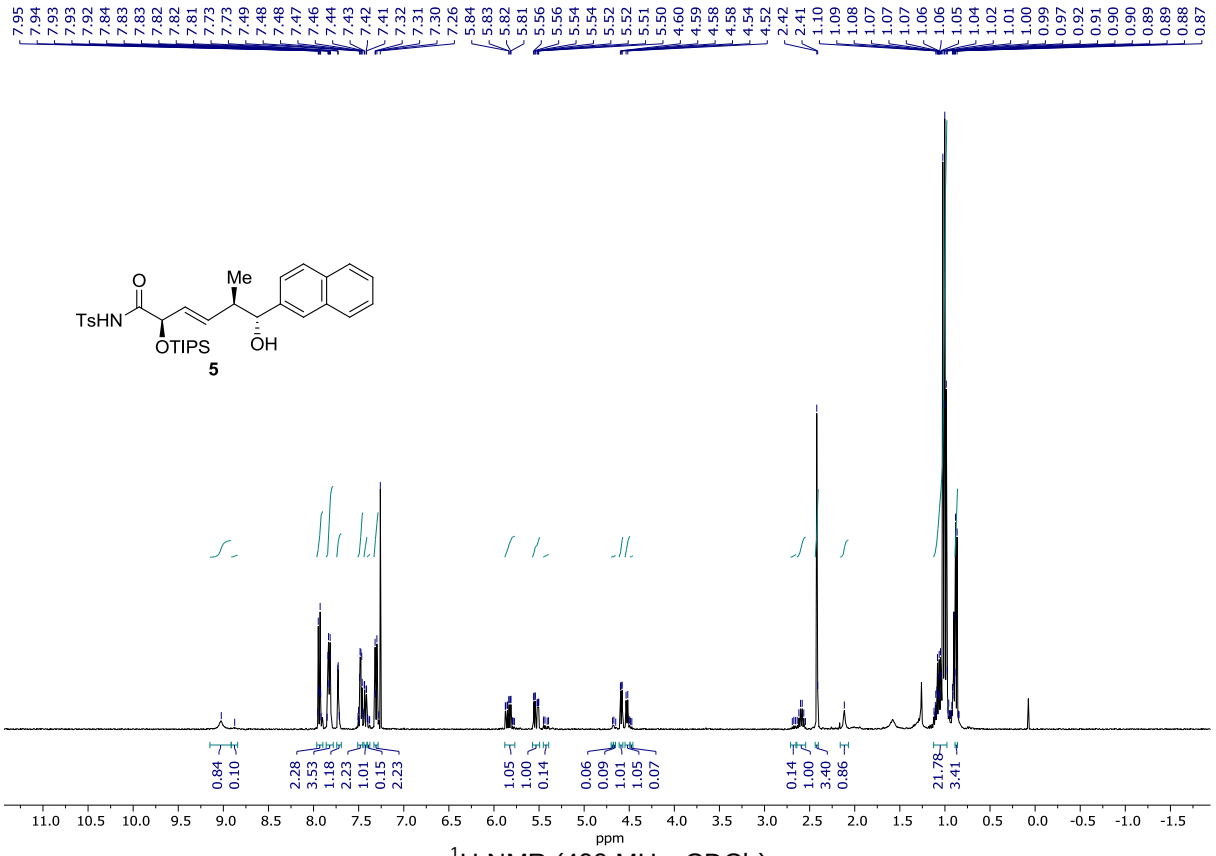

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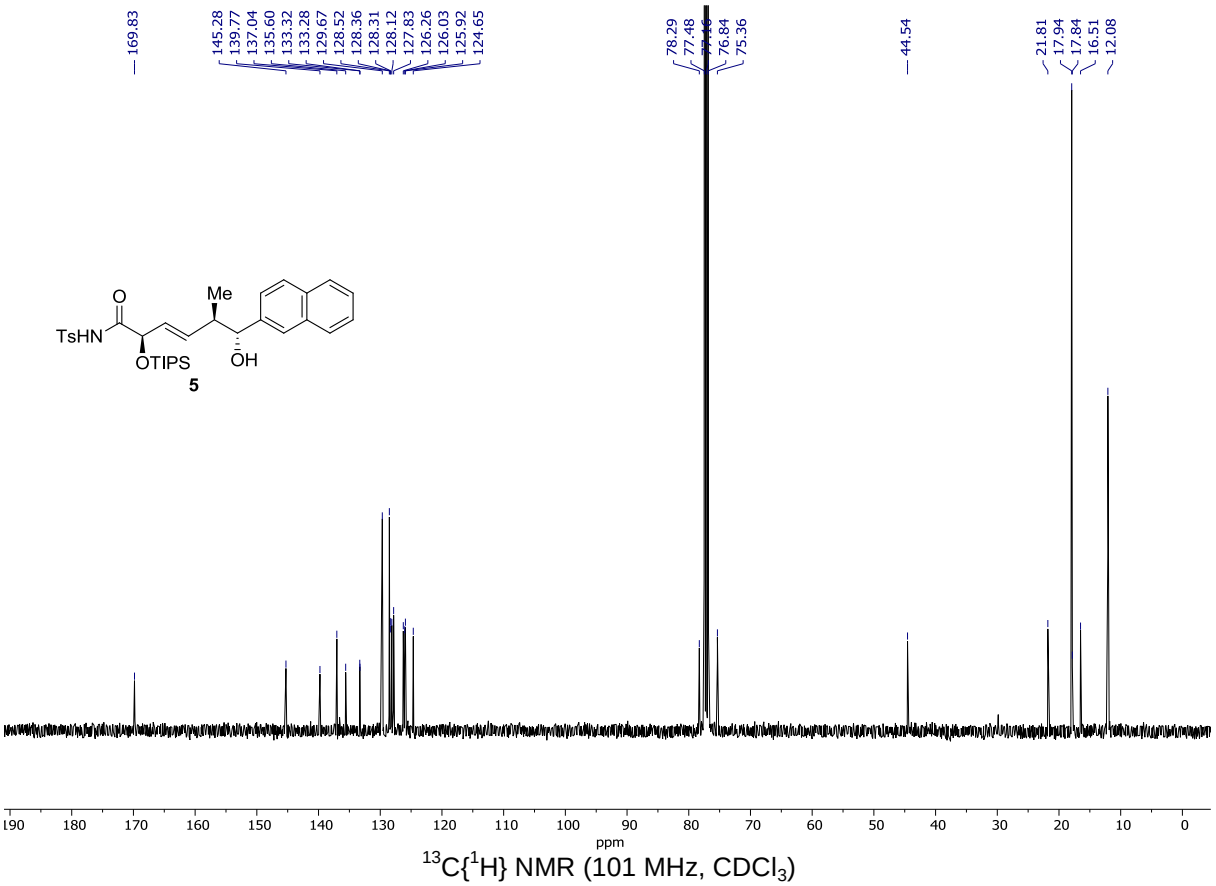

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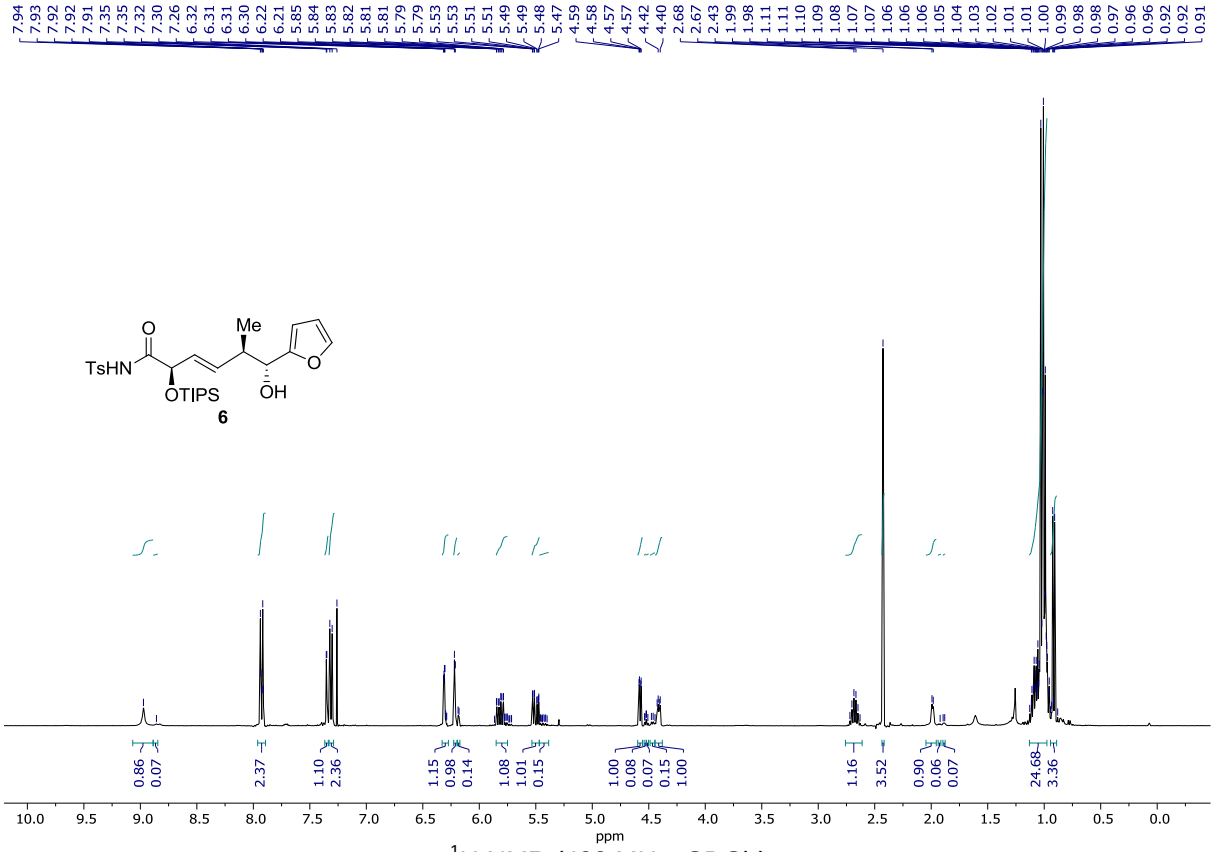

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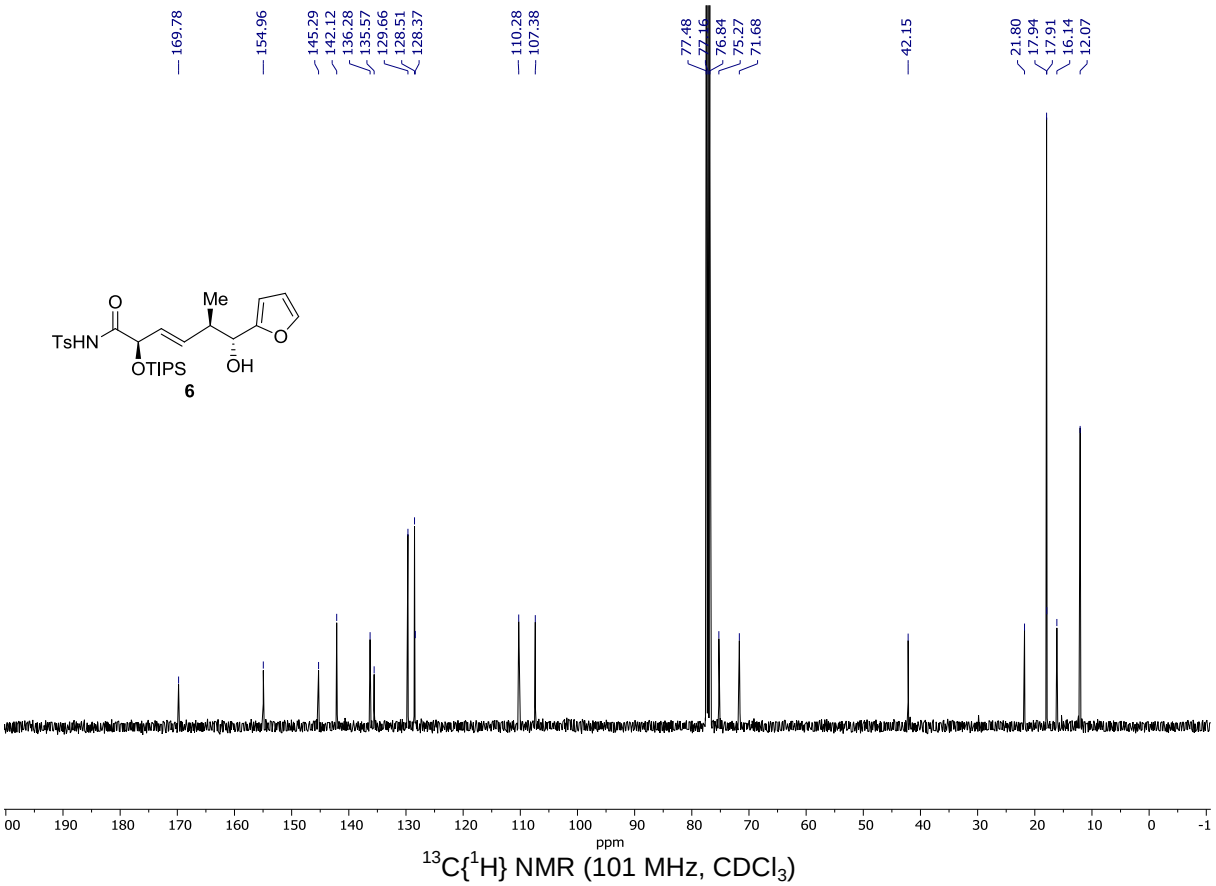

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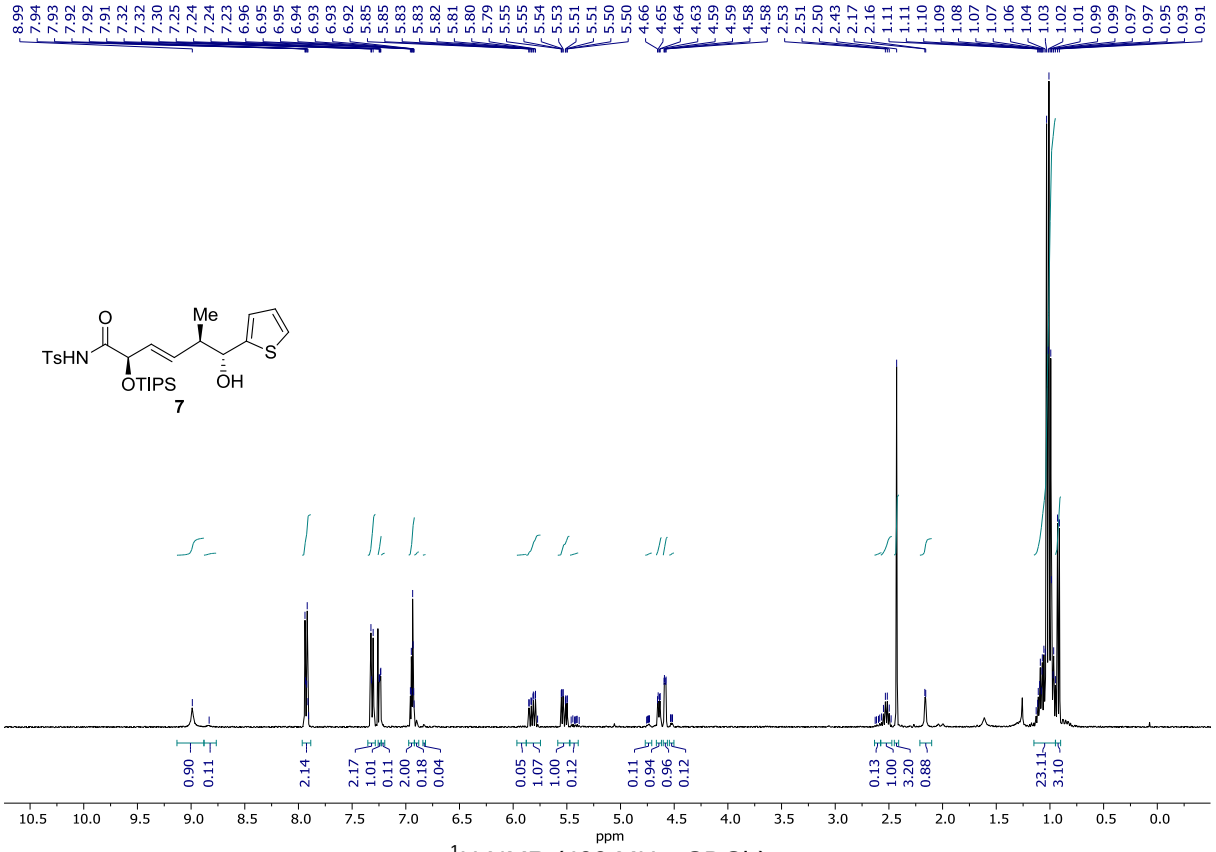

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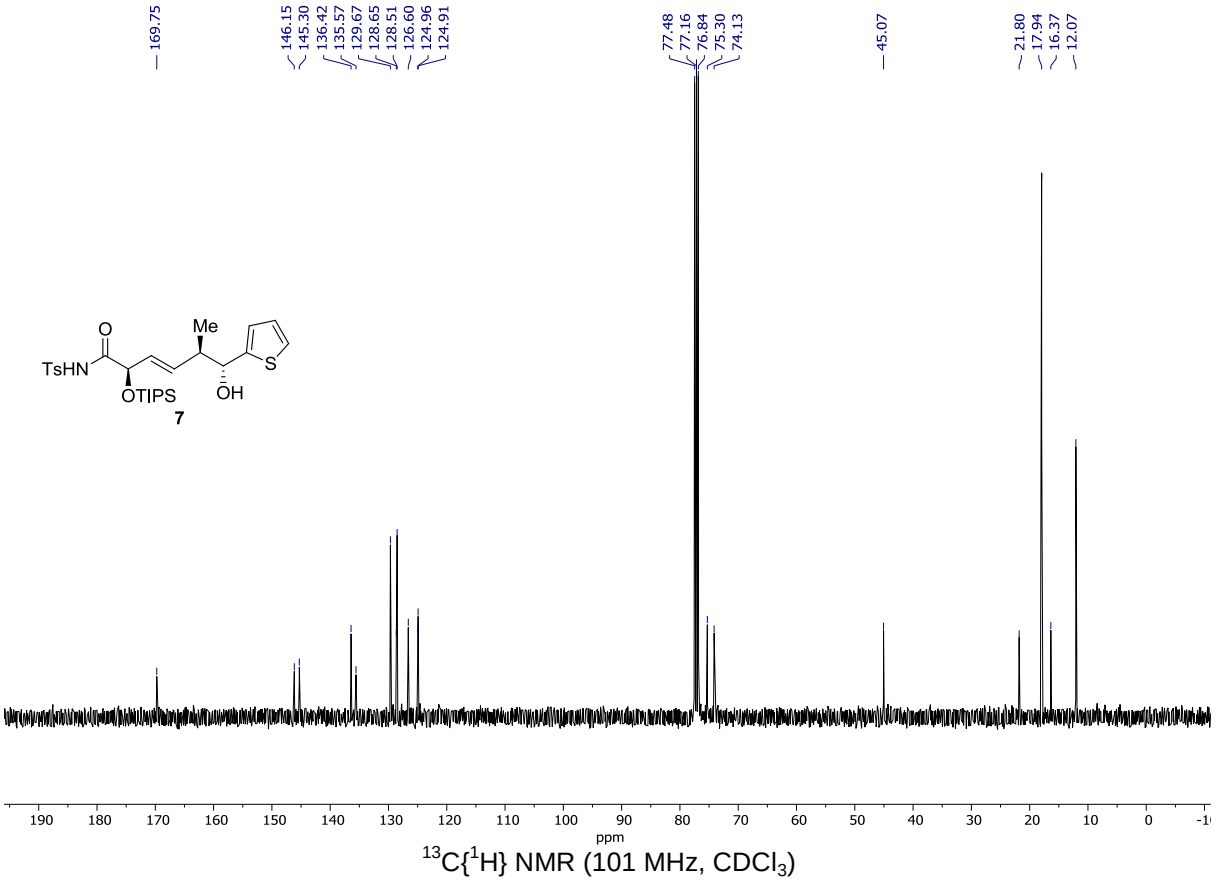

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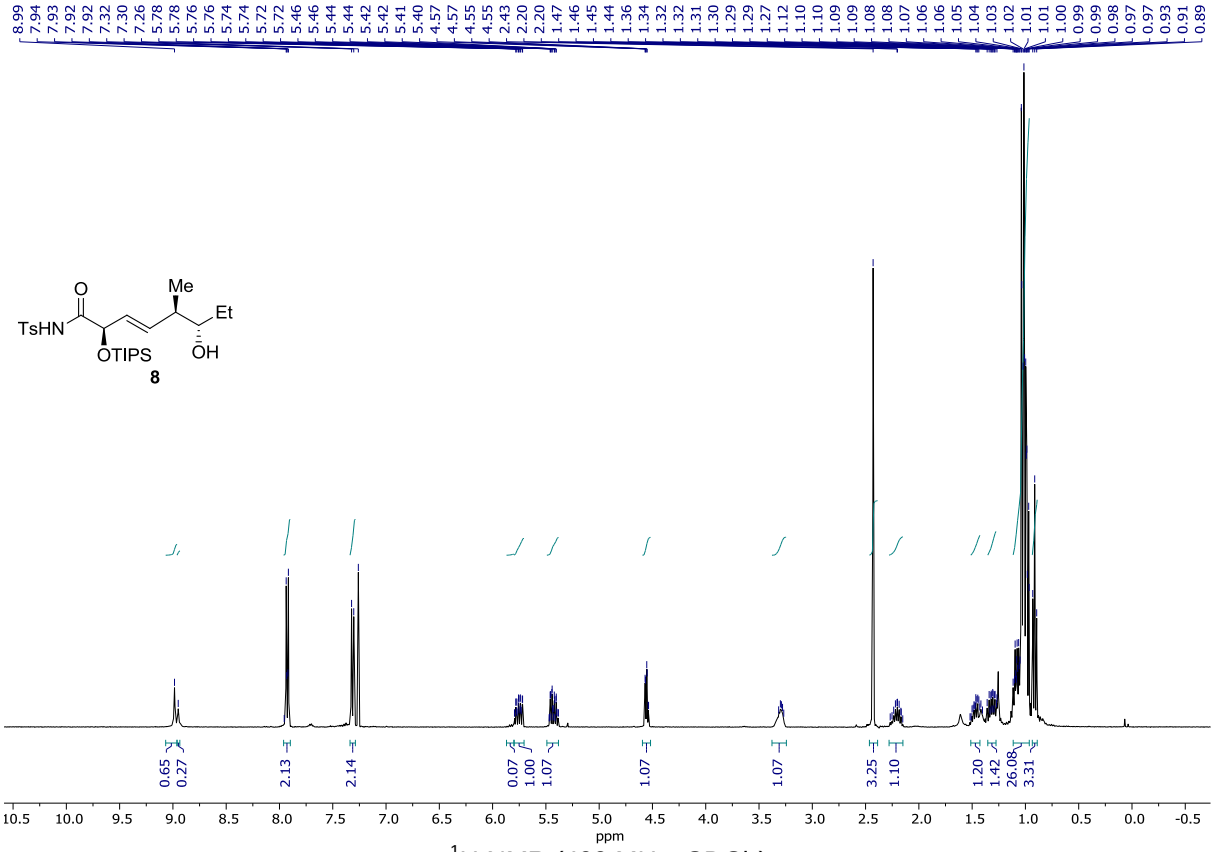

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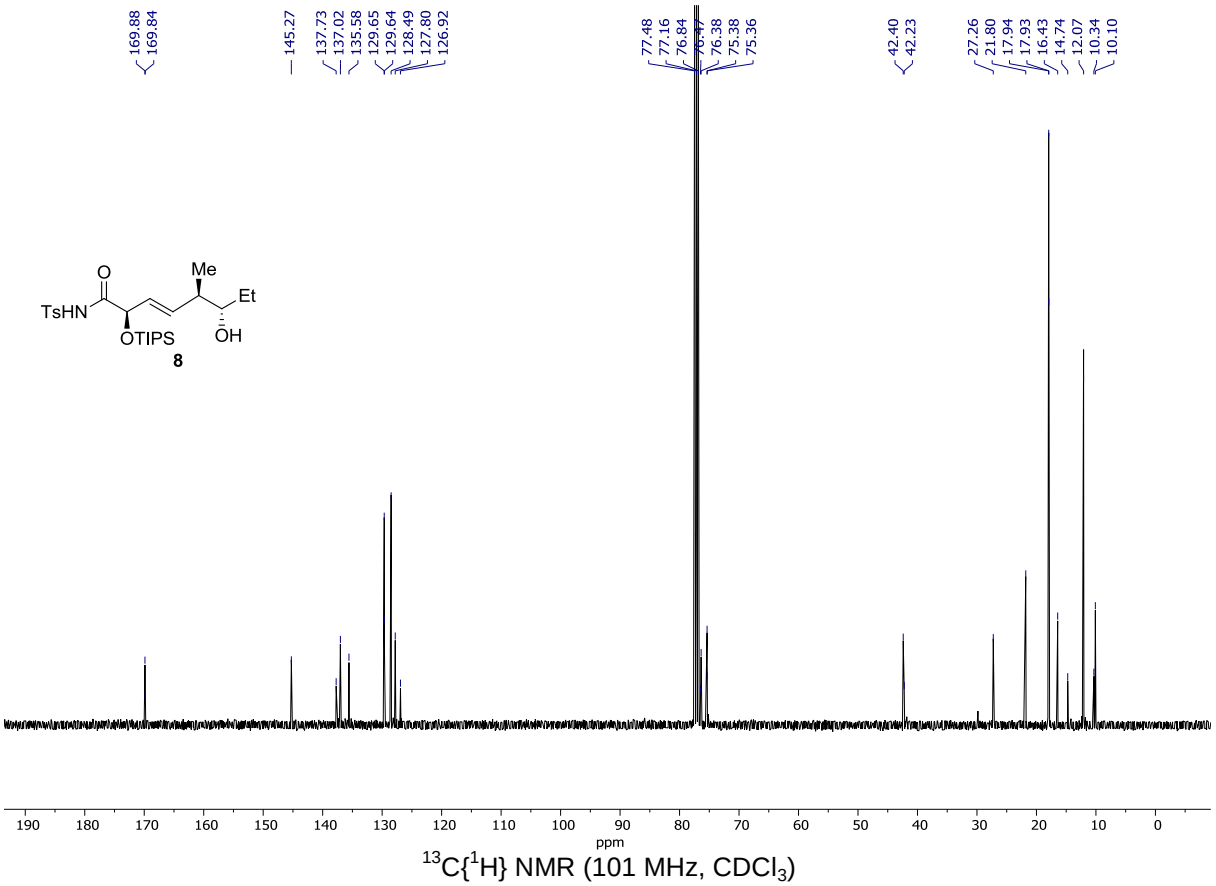

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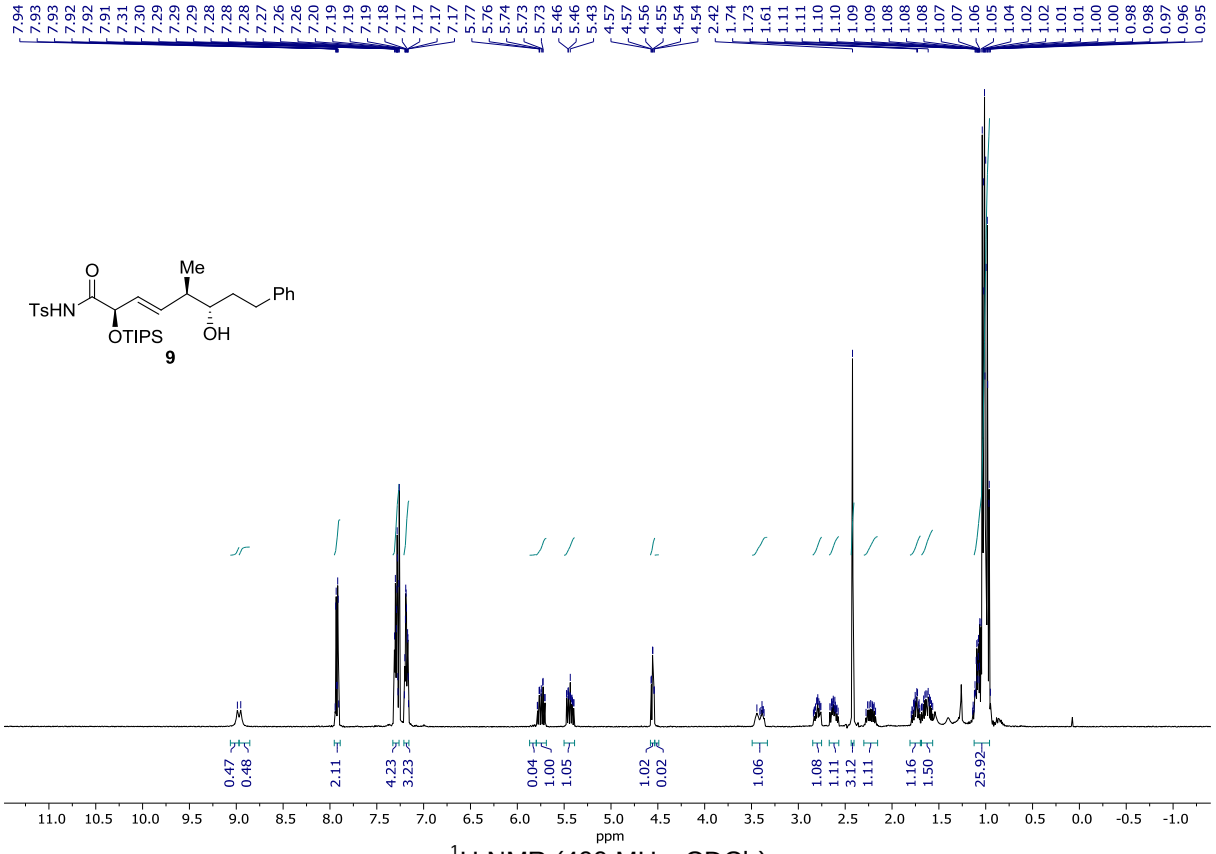

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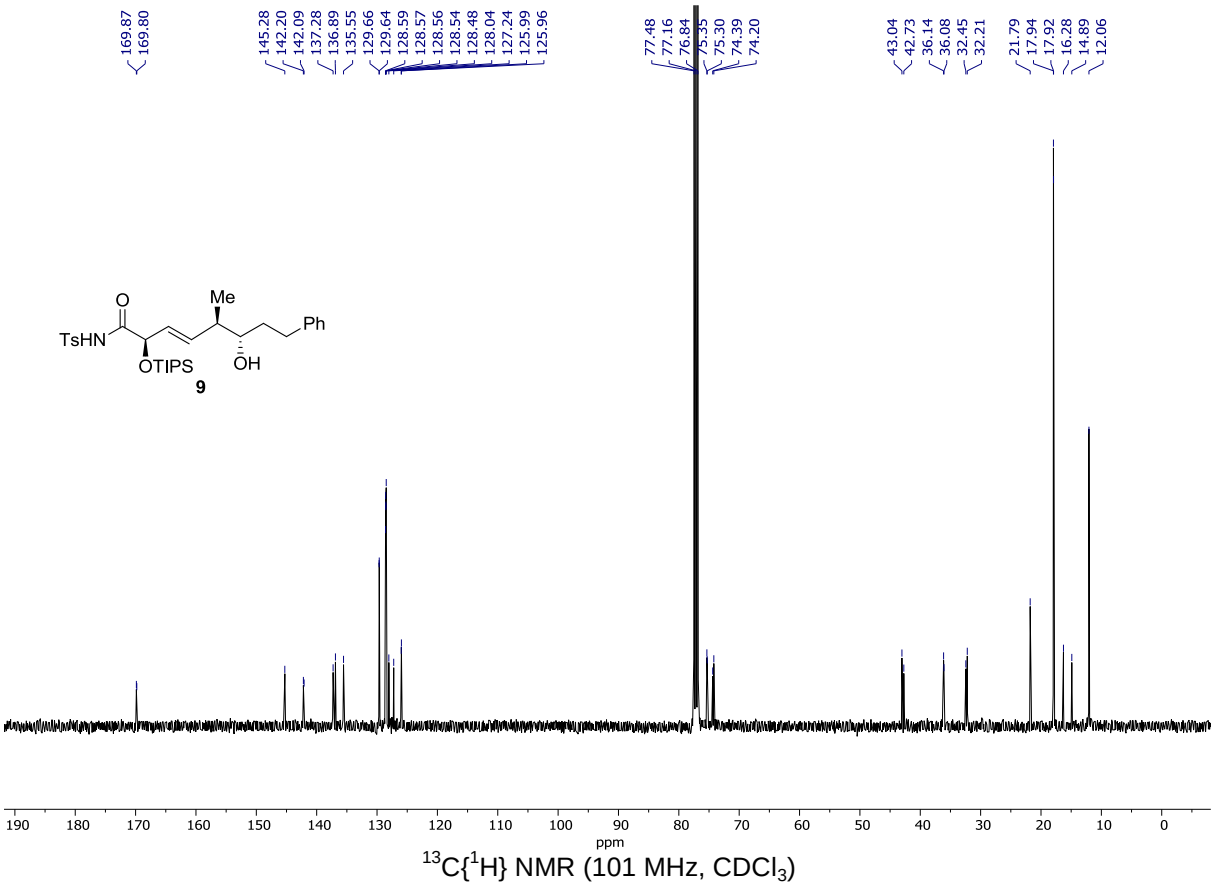

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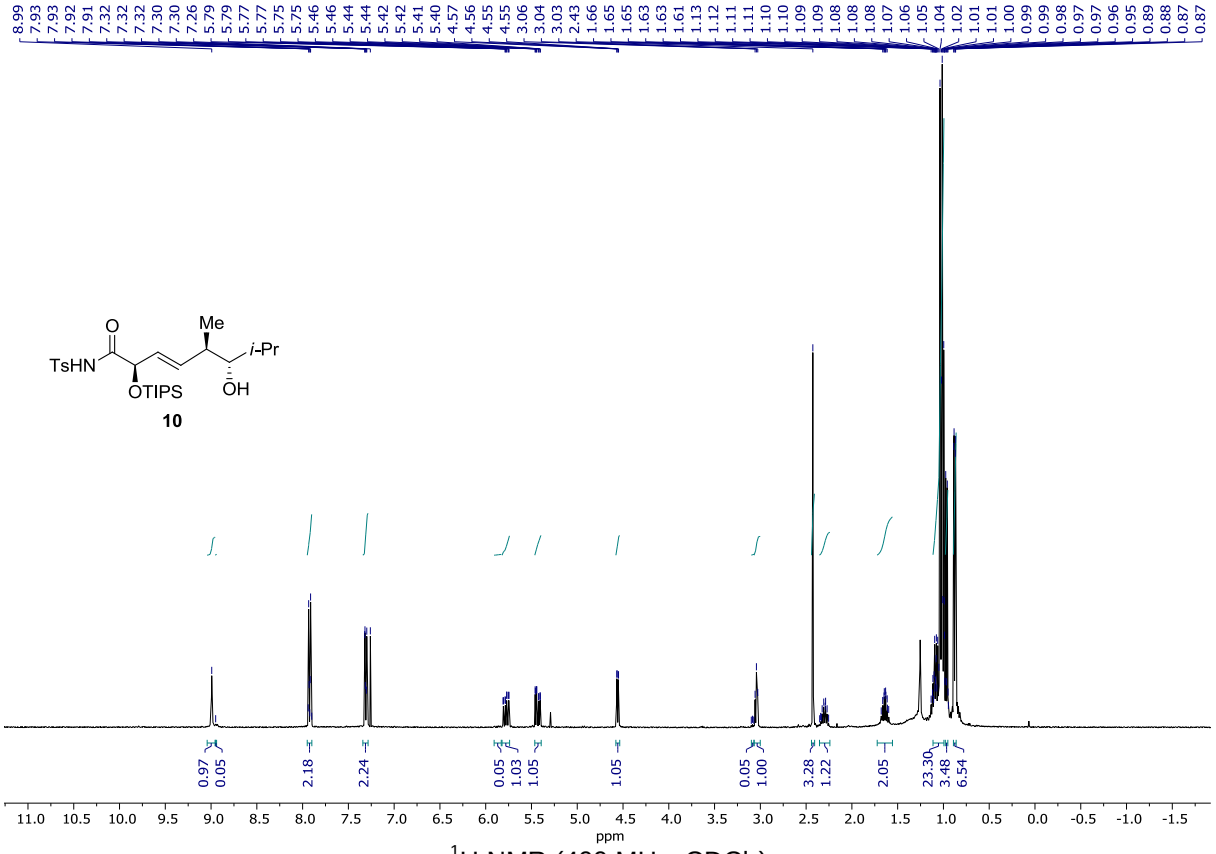

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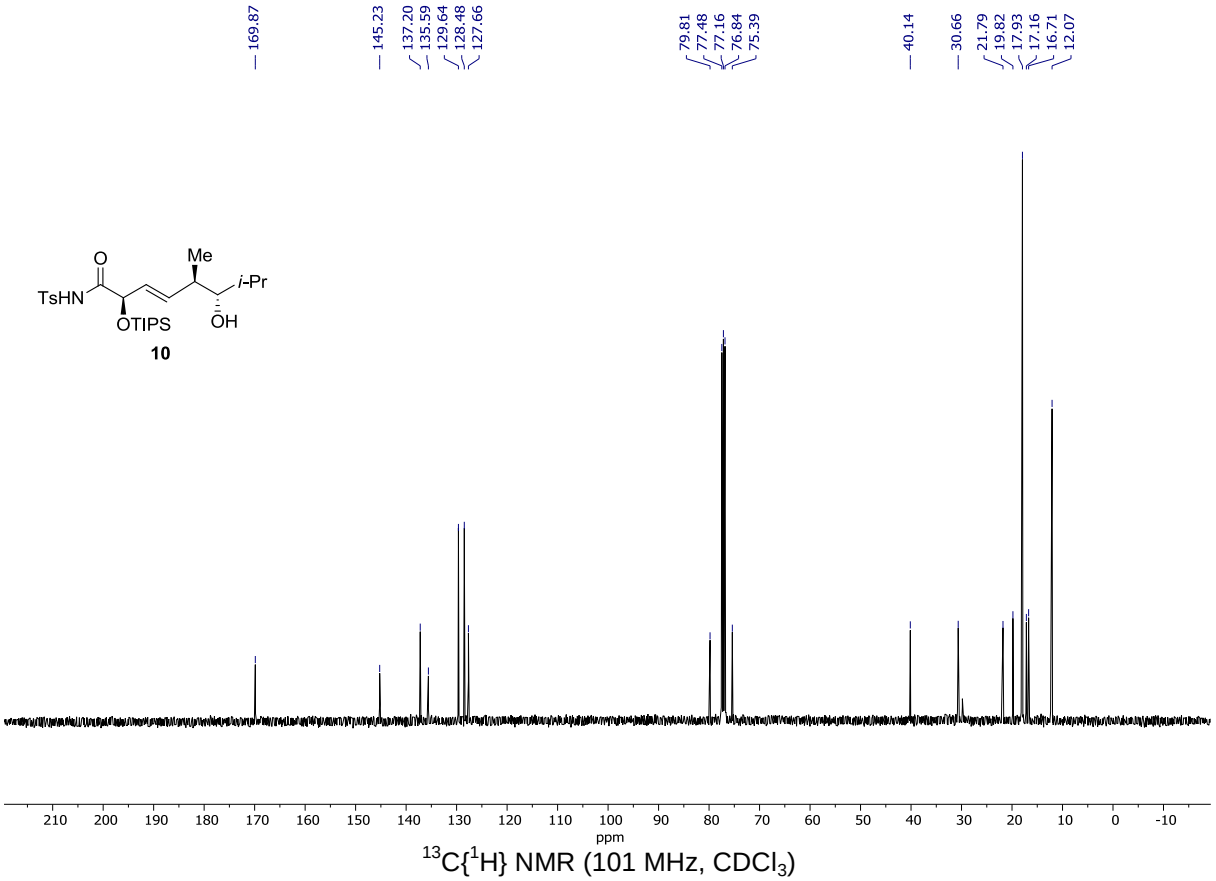

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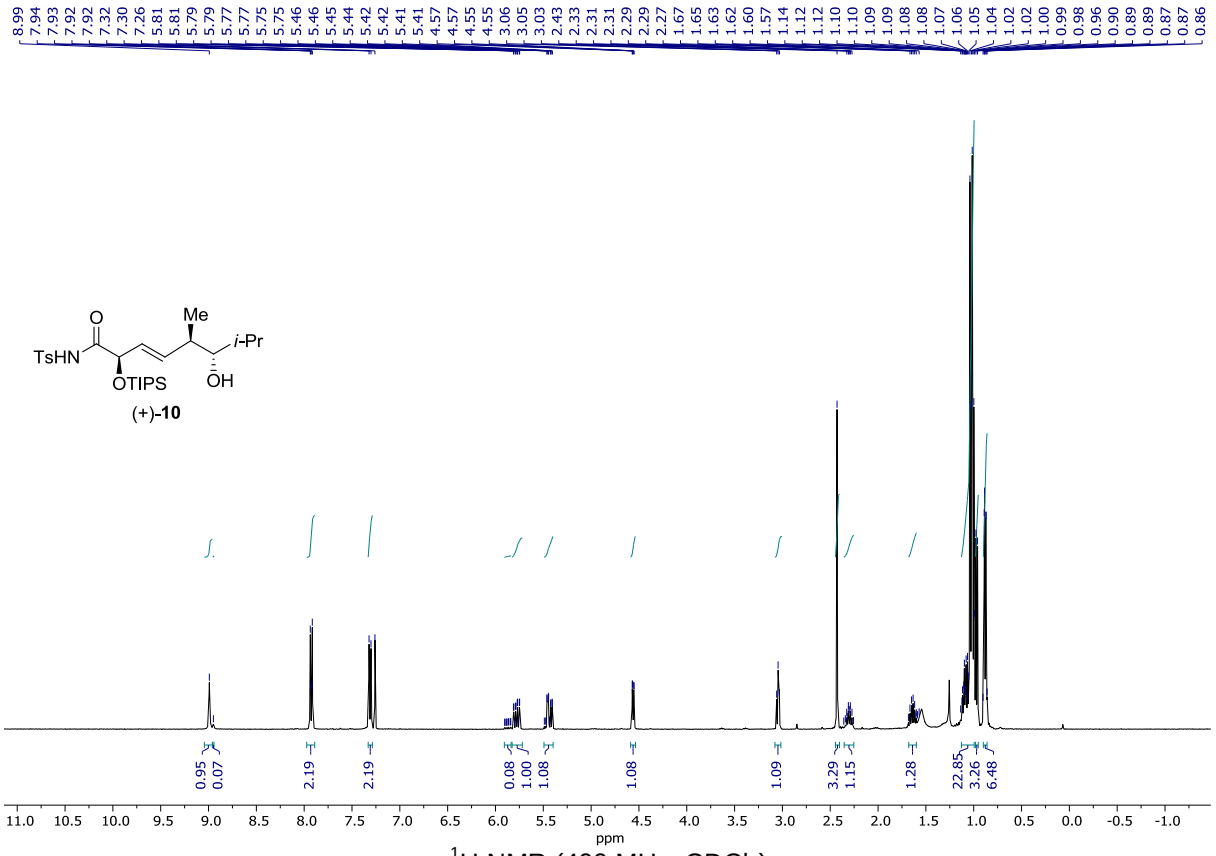

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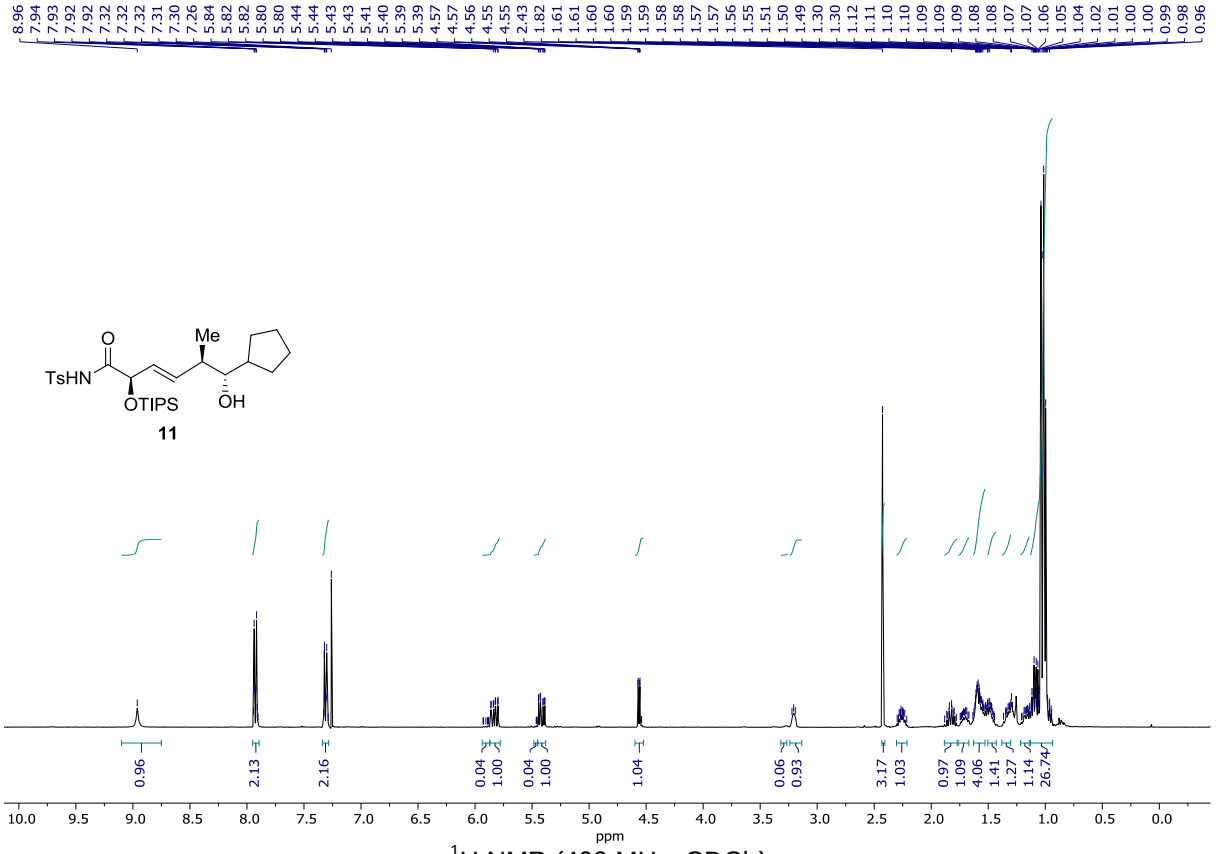

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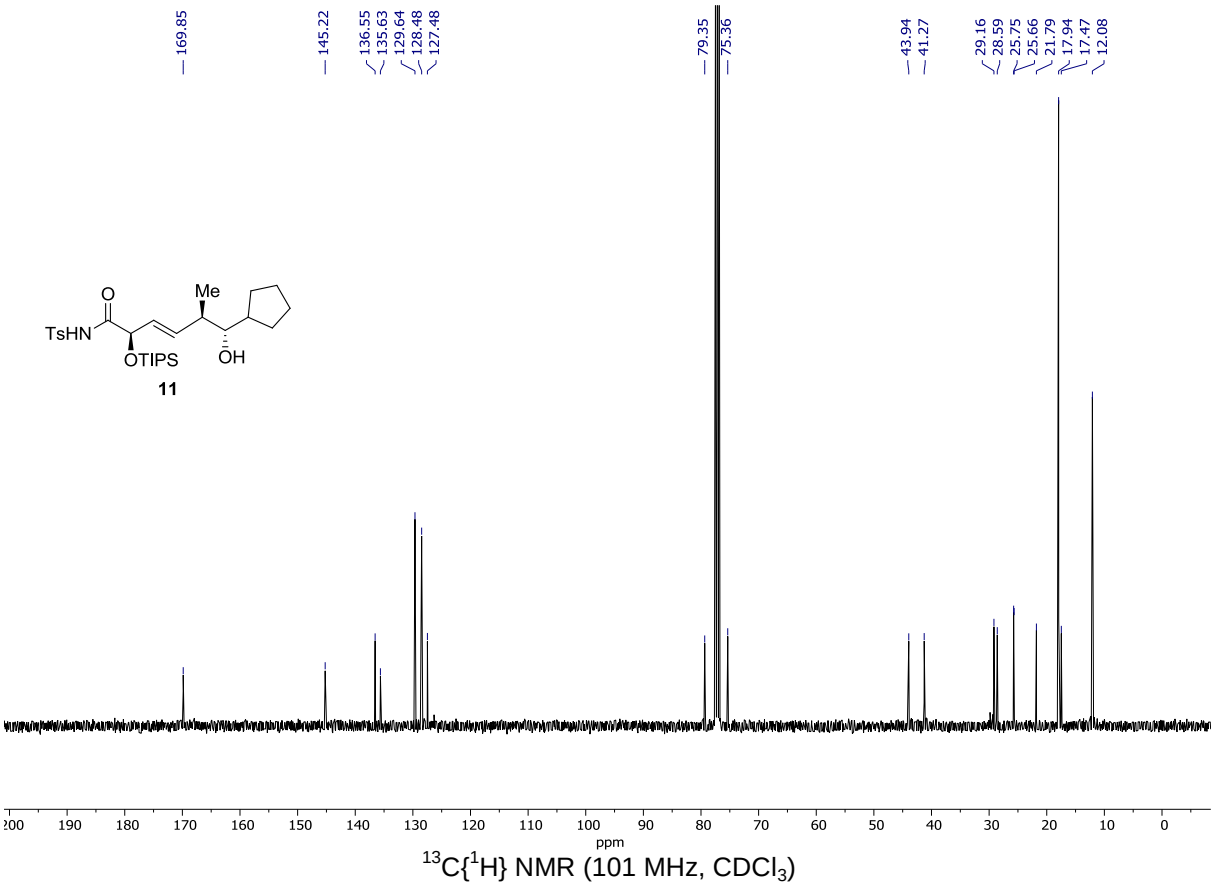

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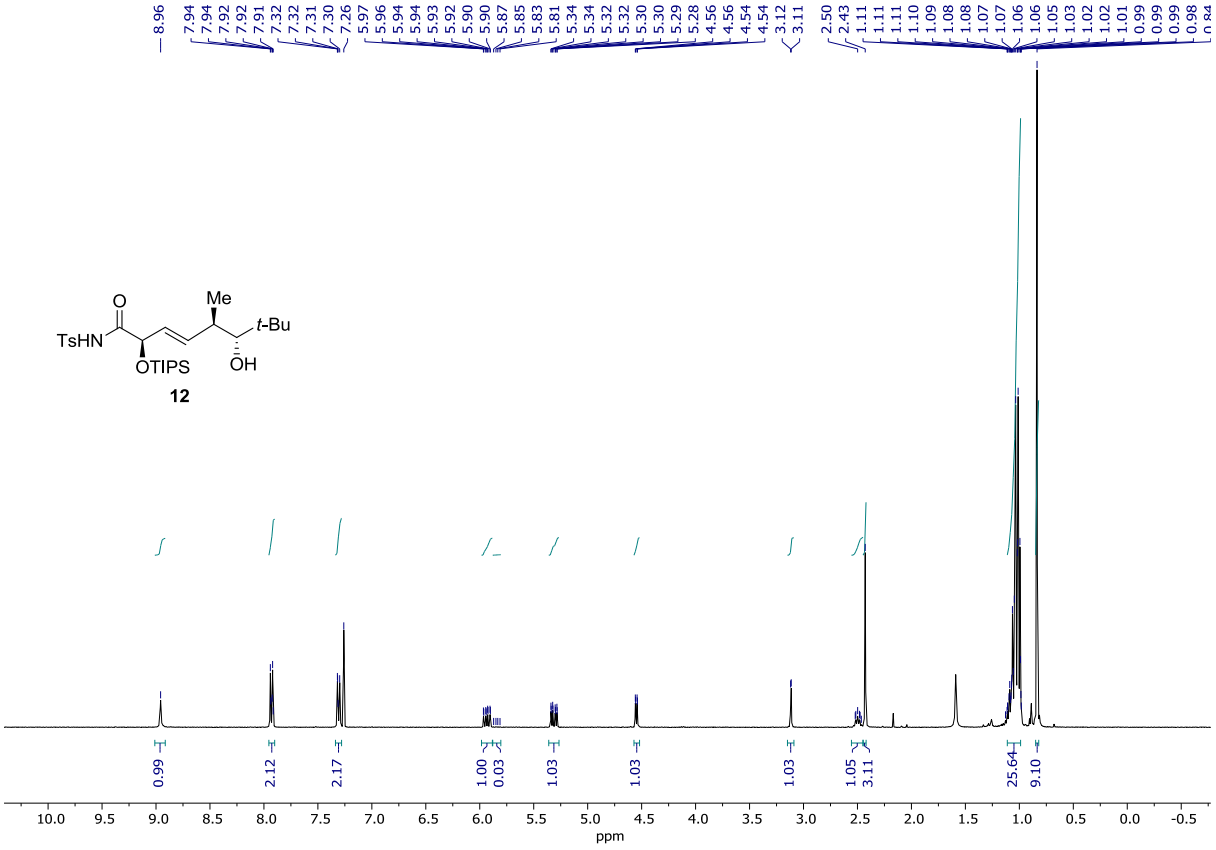

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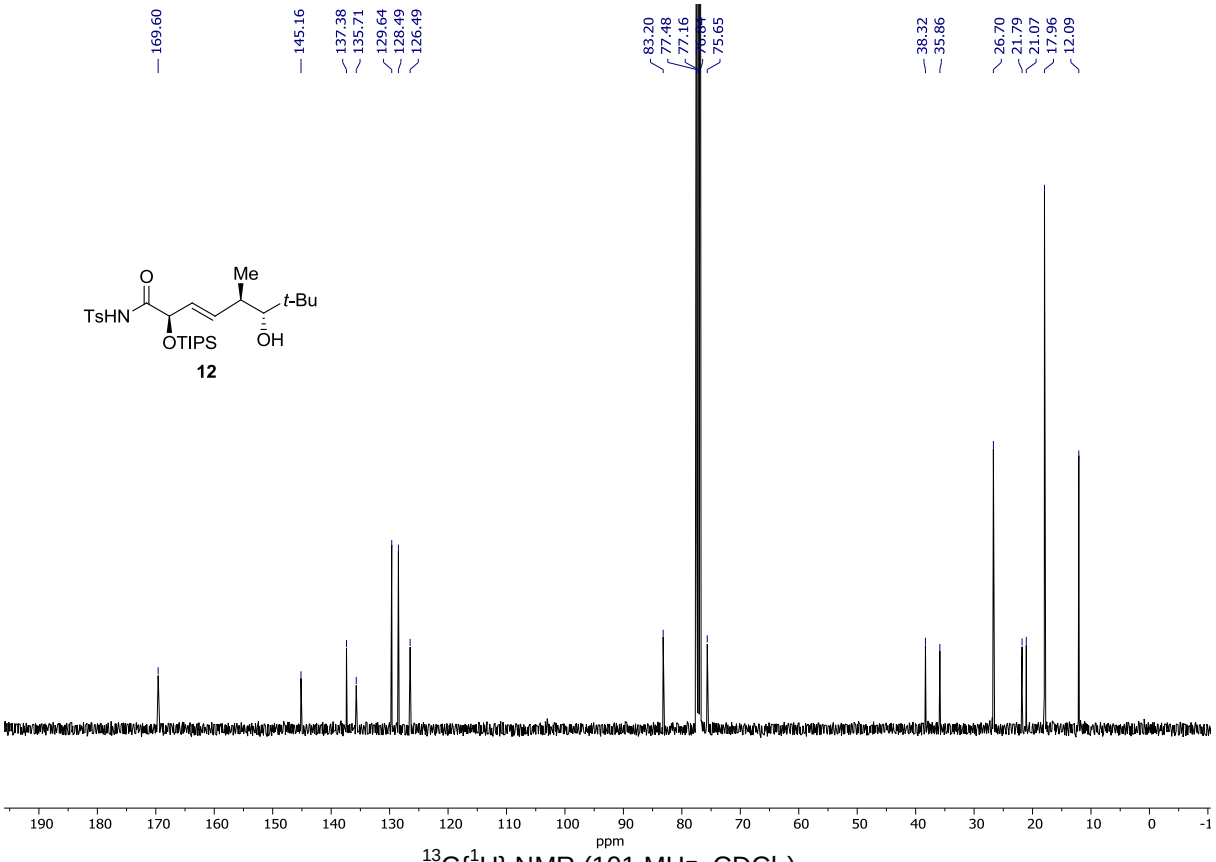

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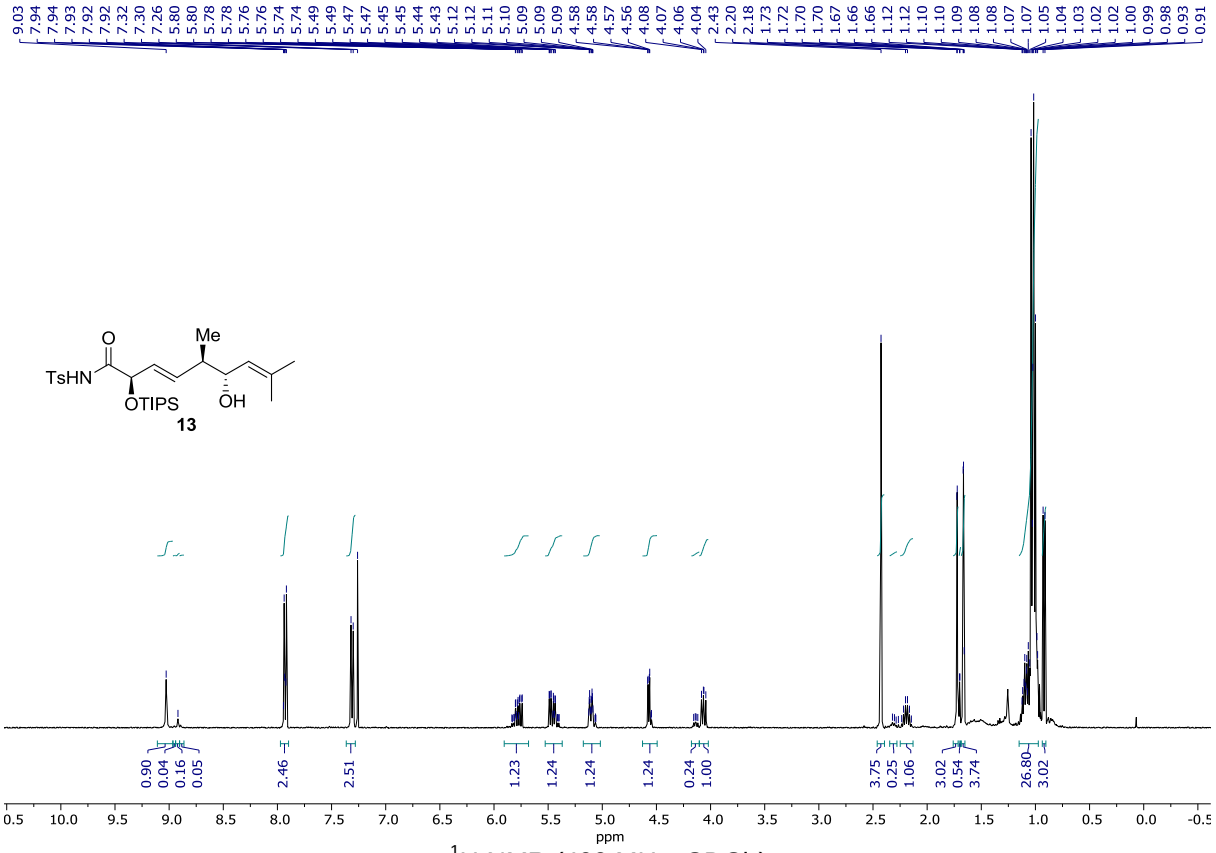

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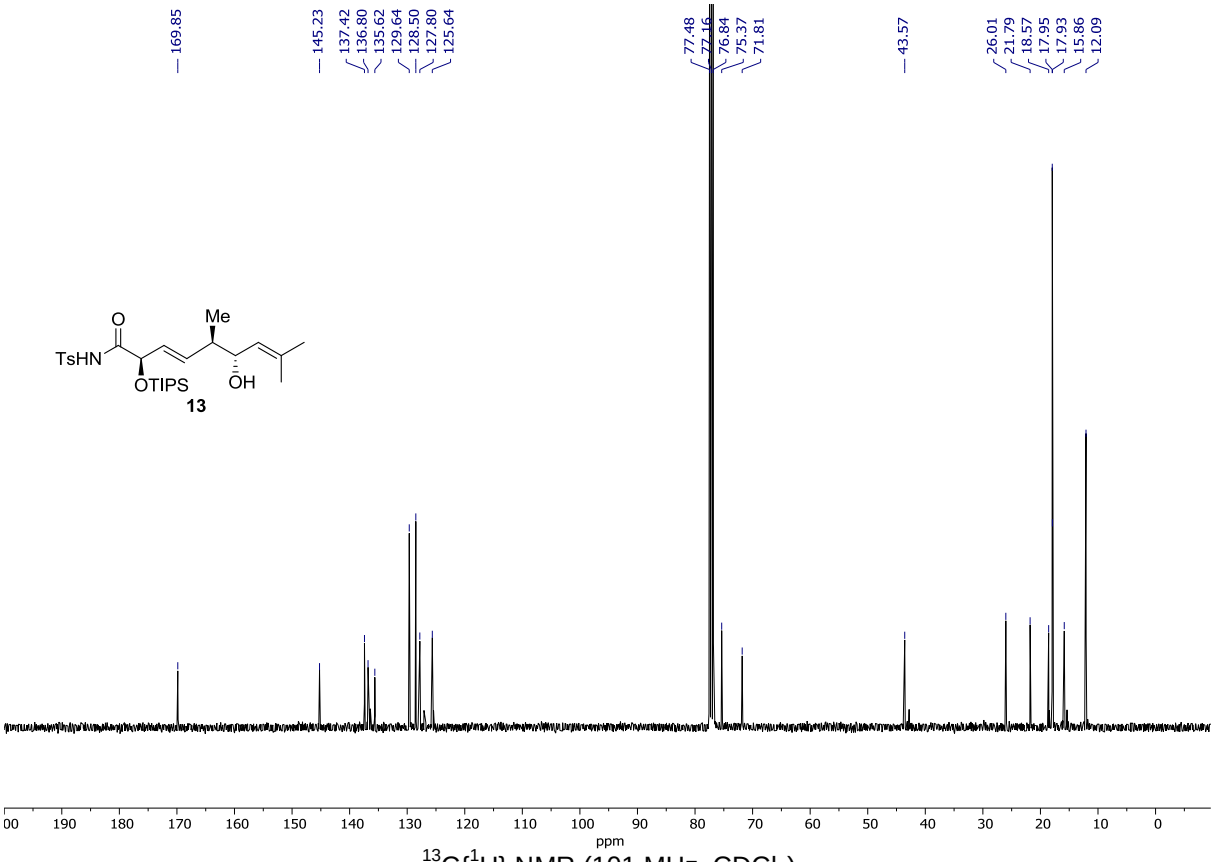

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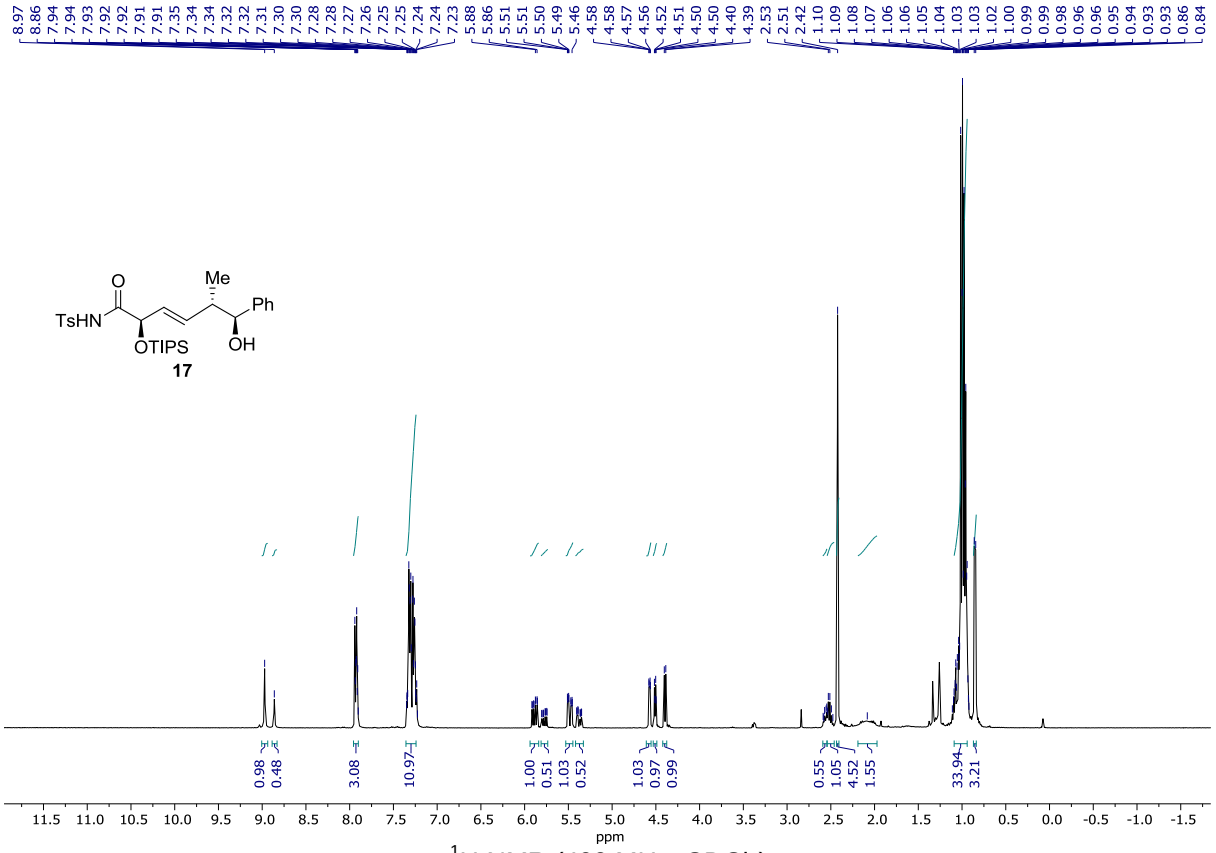

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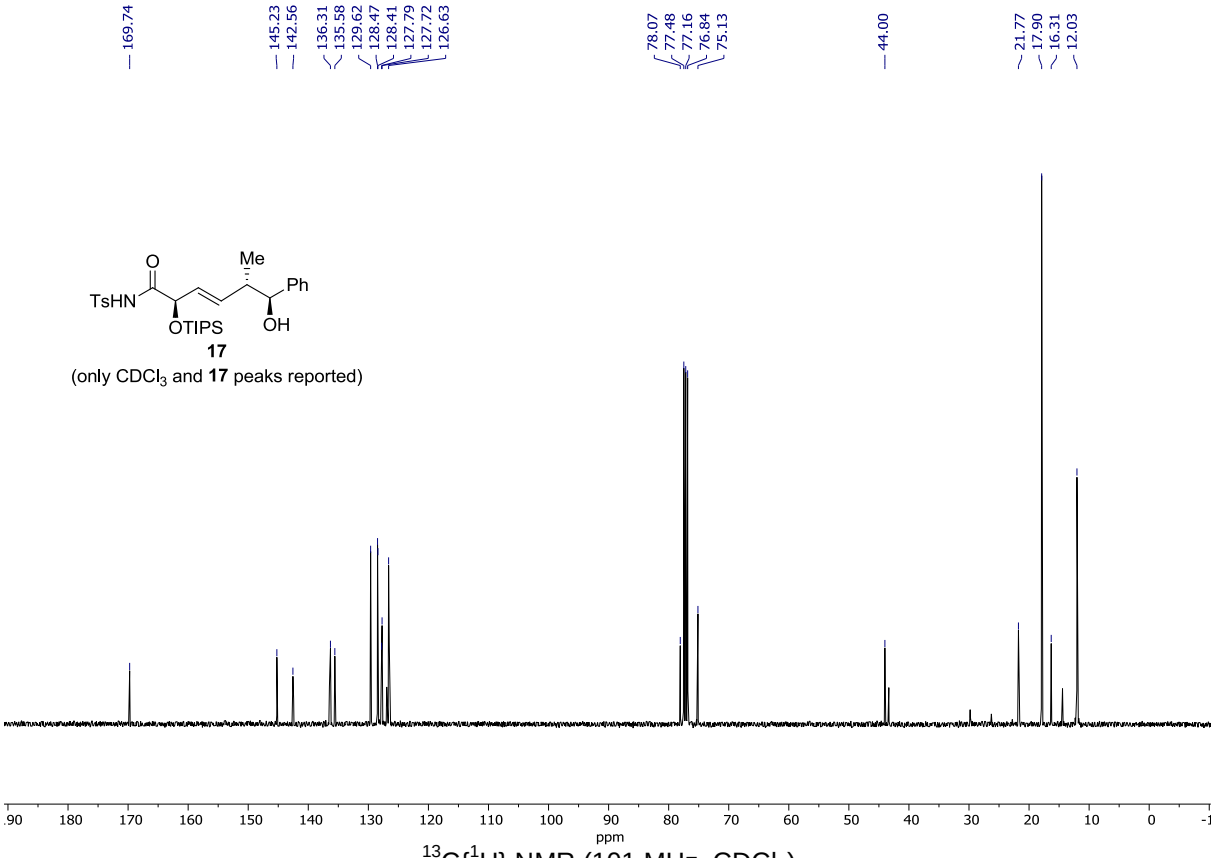
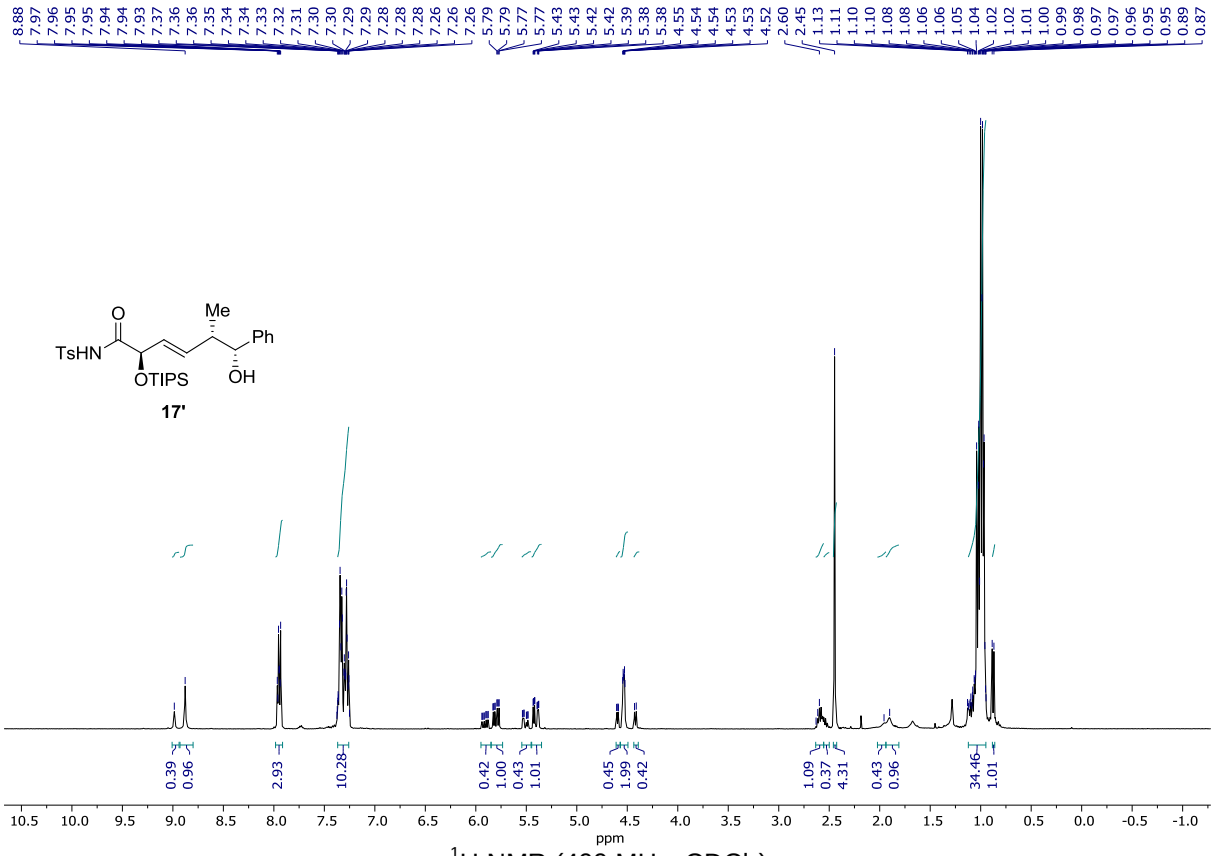
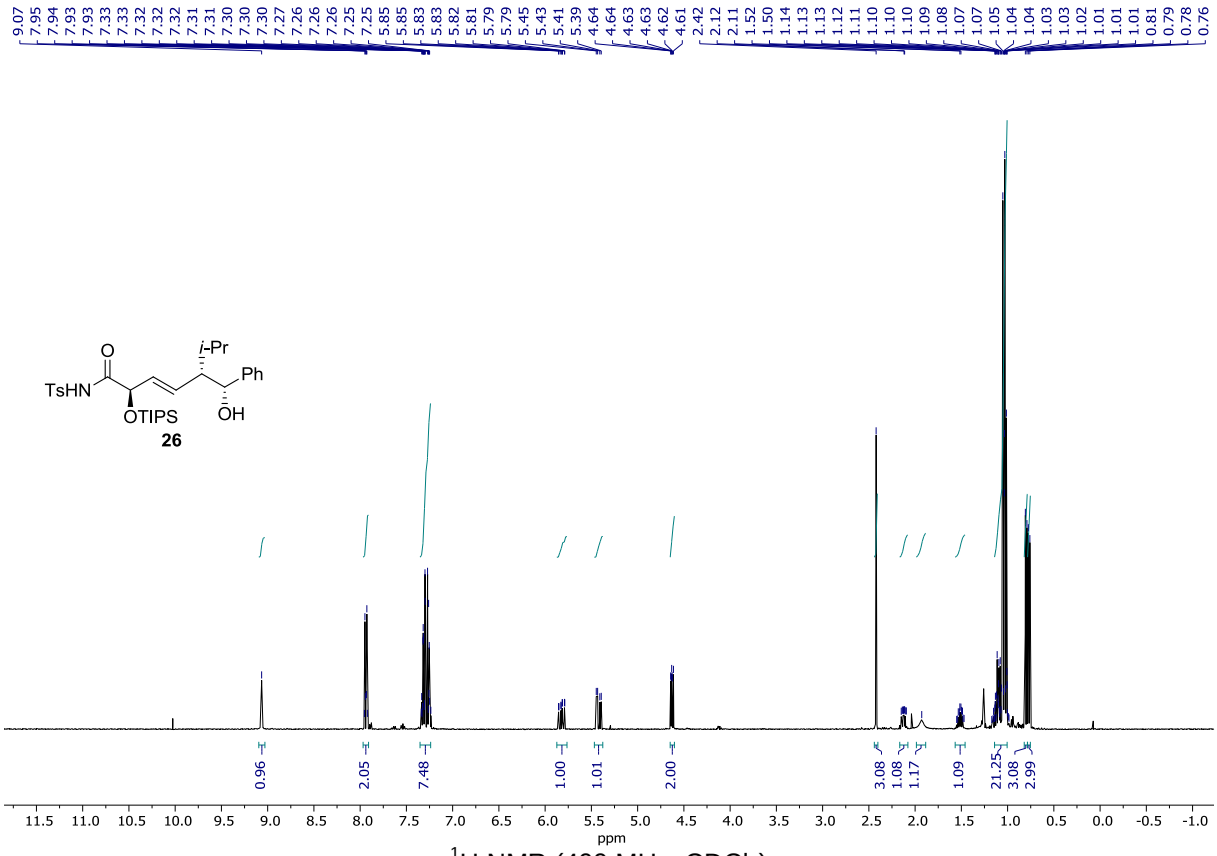


(only $CDCl_3$ and **17** peaks reported)

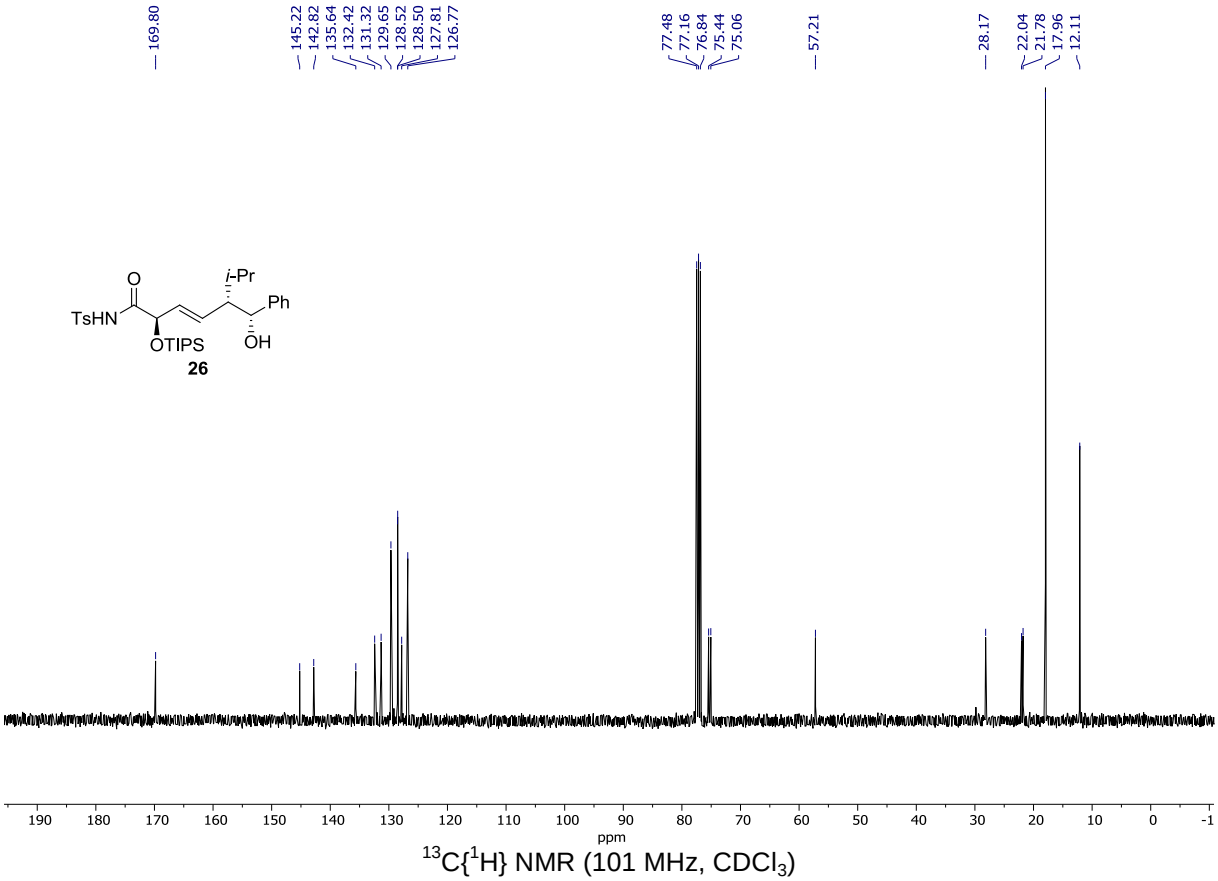
$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



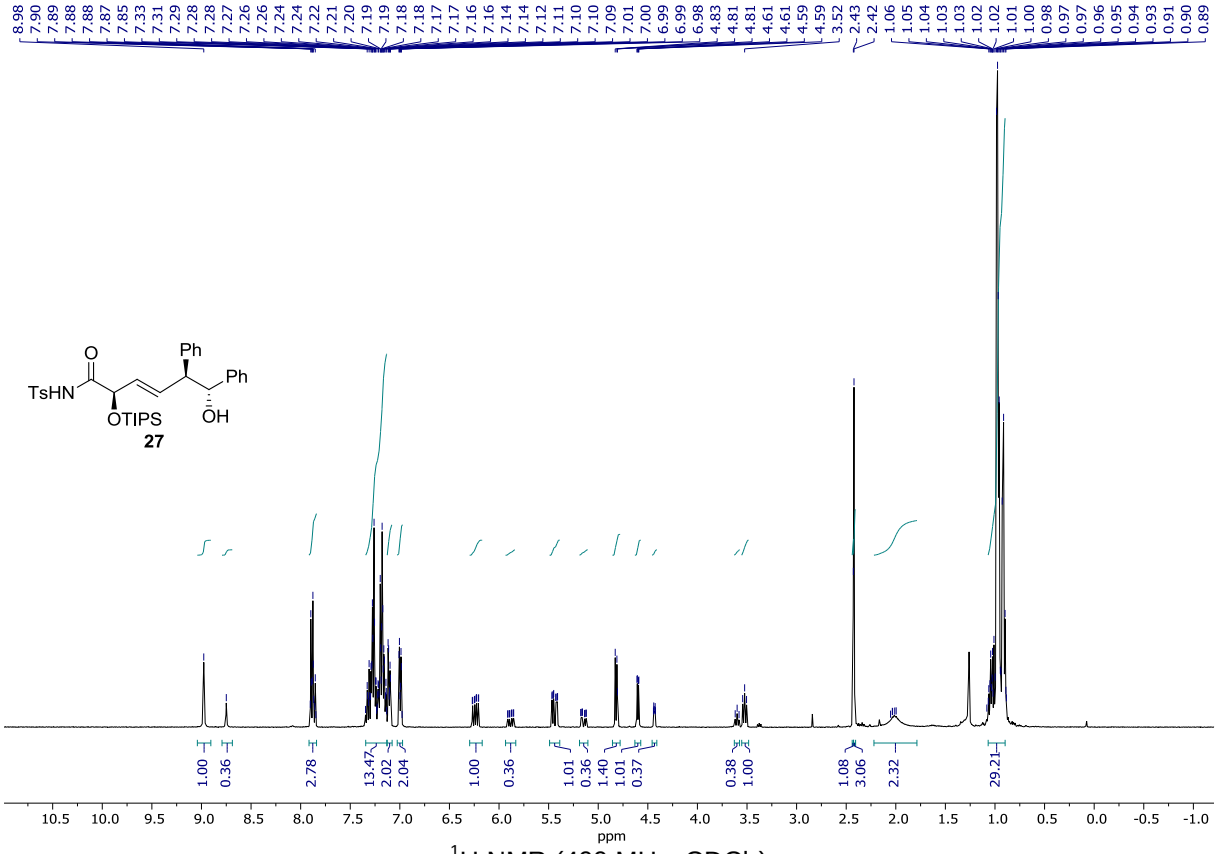
^{1}H NMR (400 MHz, $CDCl_3$)



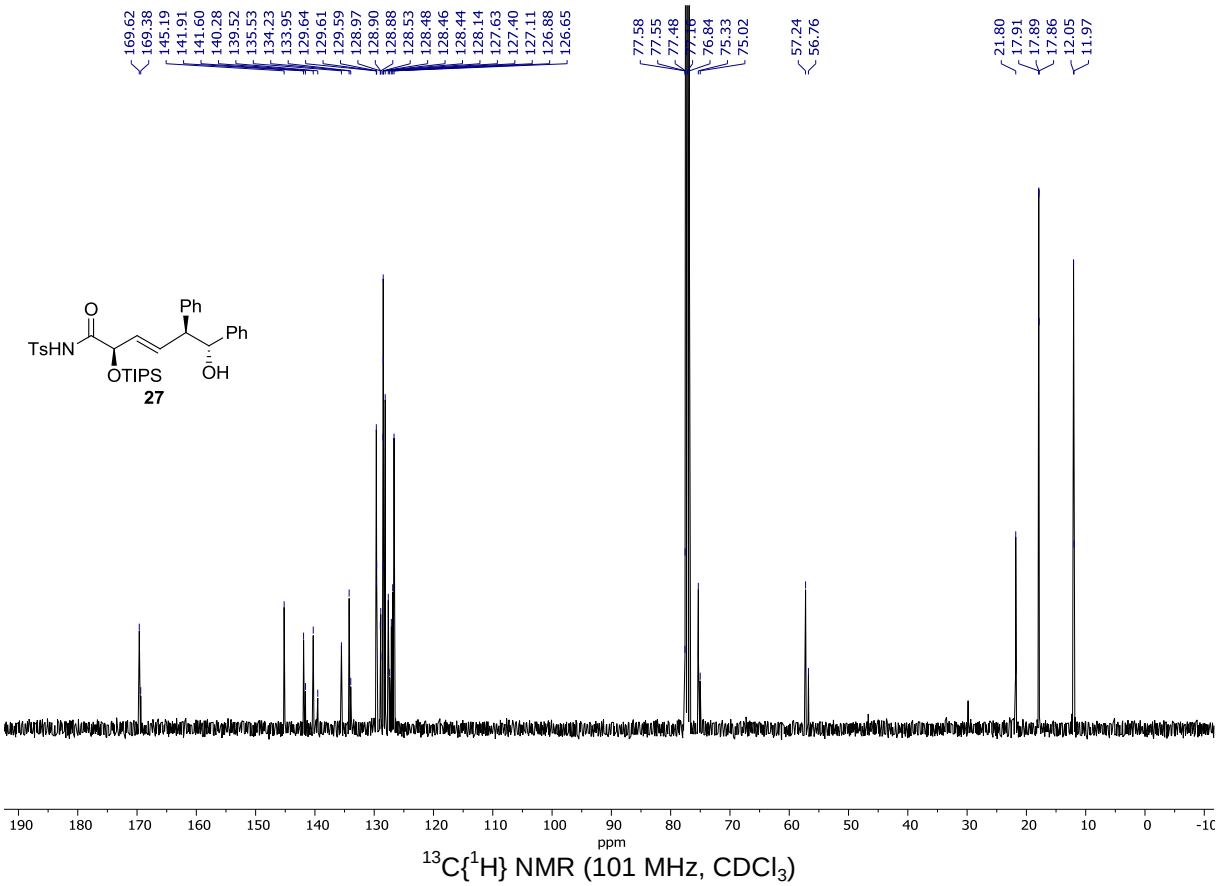
^{1}H NMR (400 MHz, $CDCl_3$)



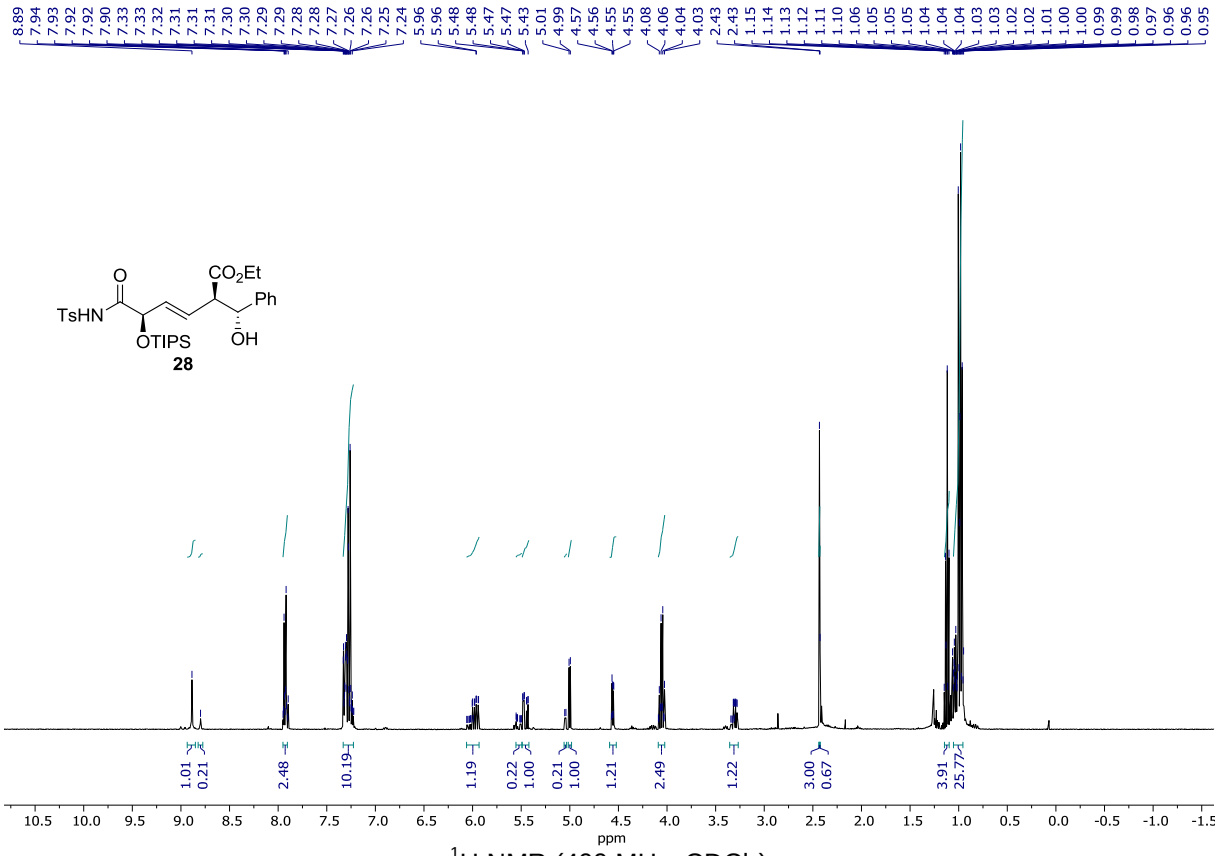
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



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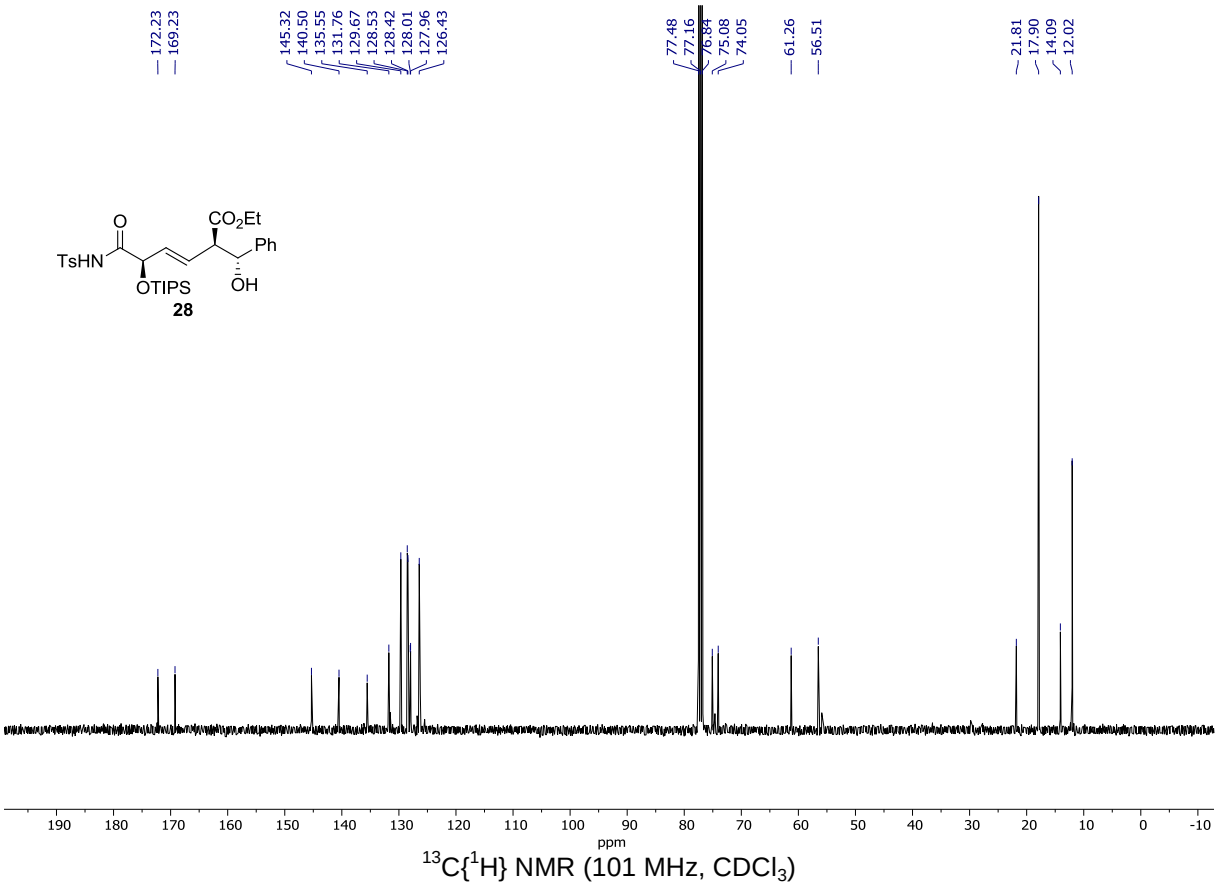
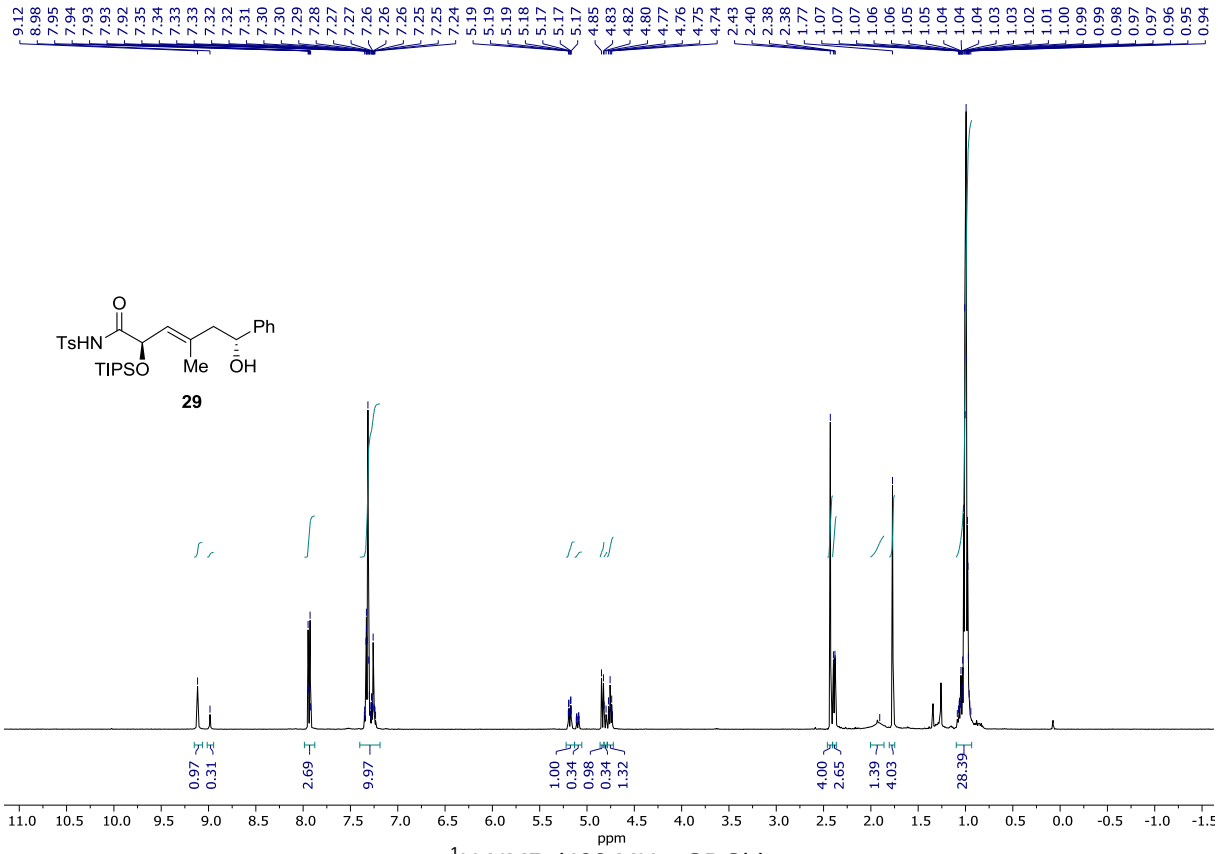


$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



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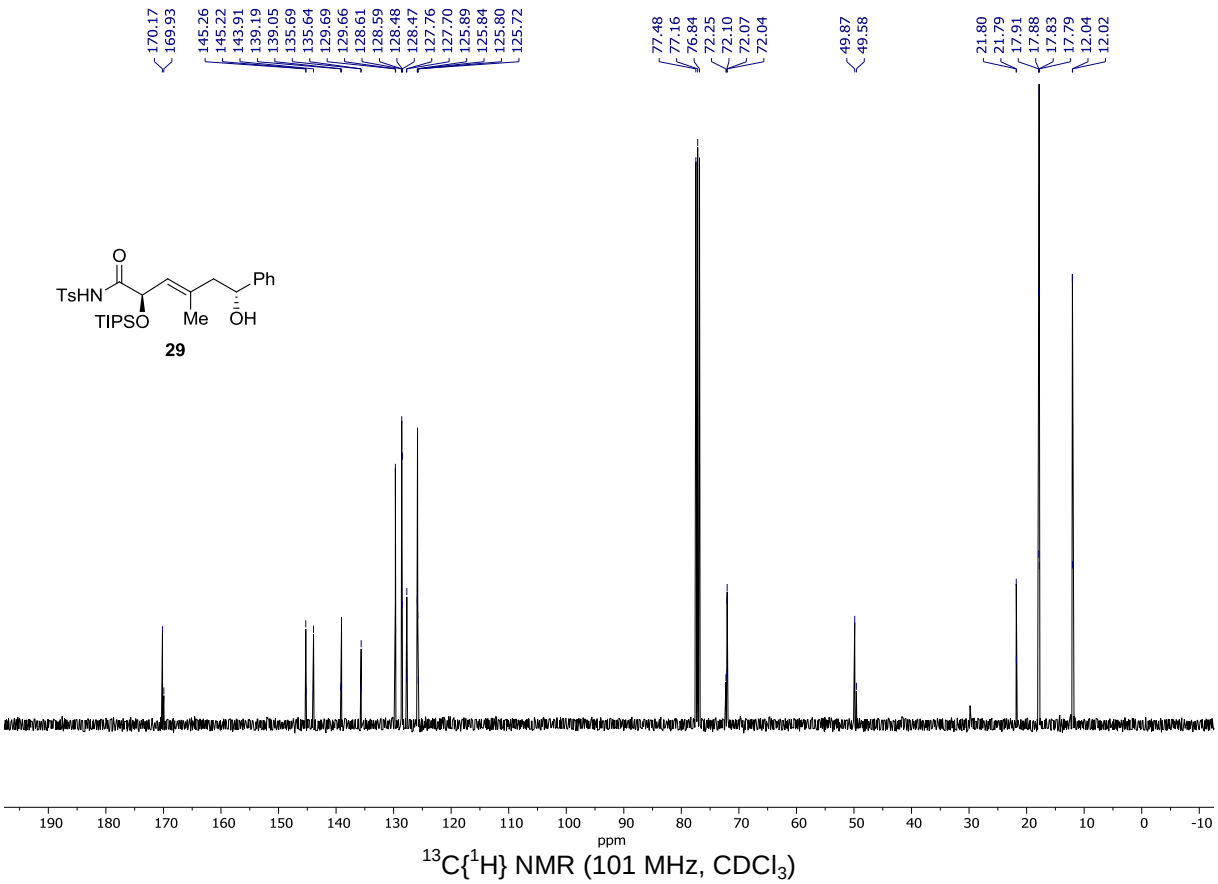

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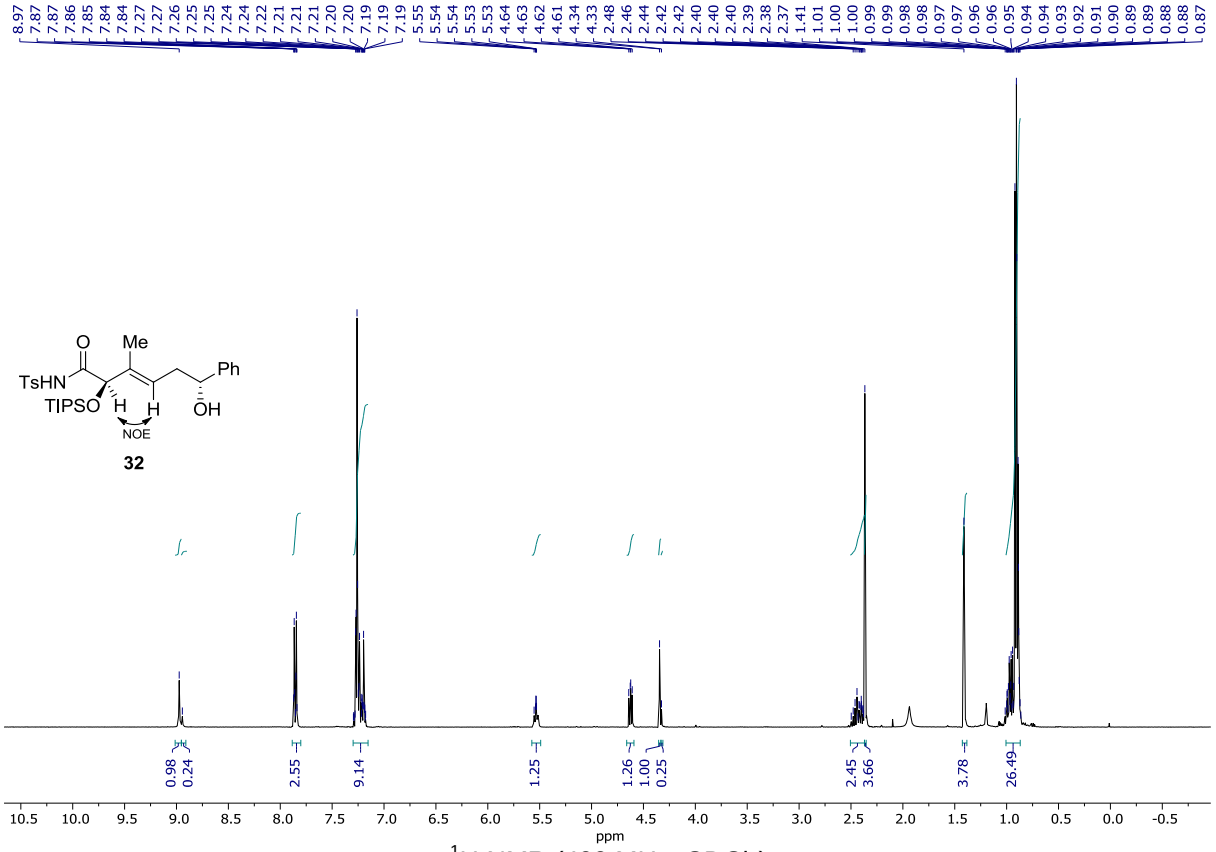
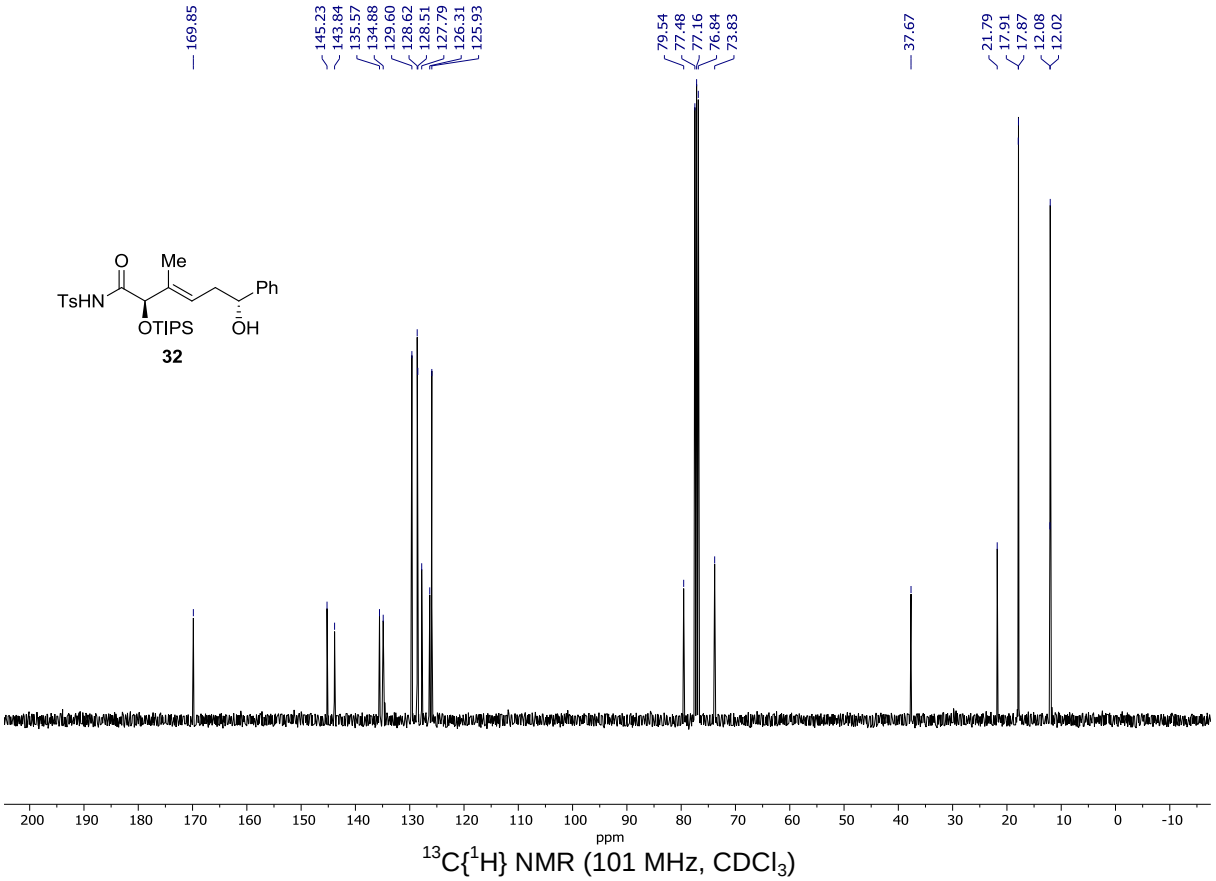
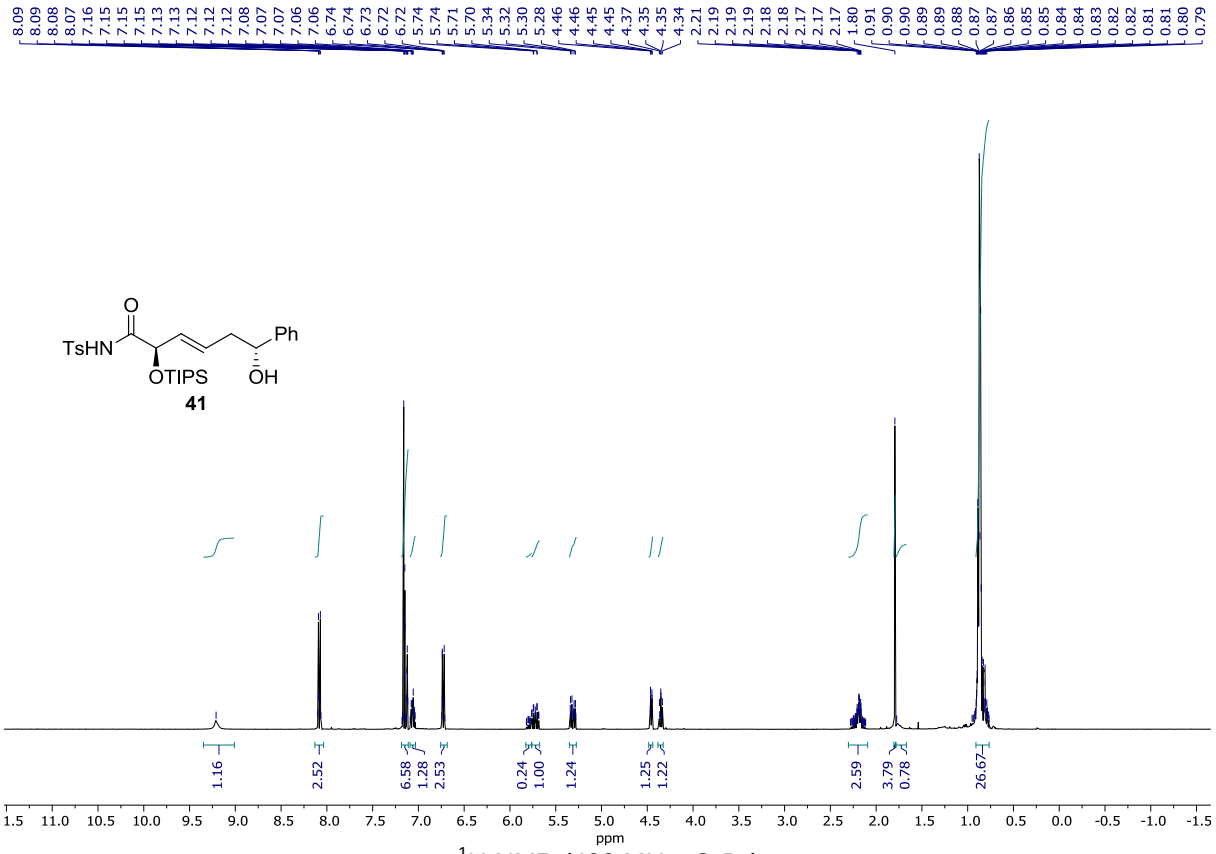


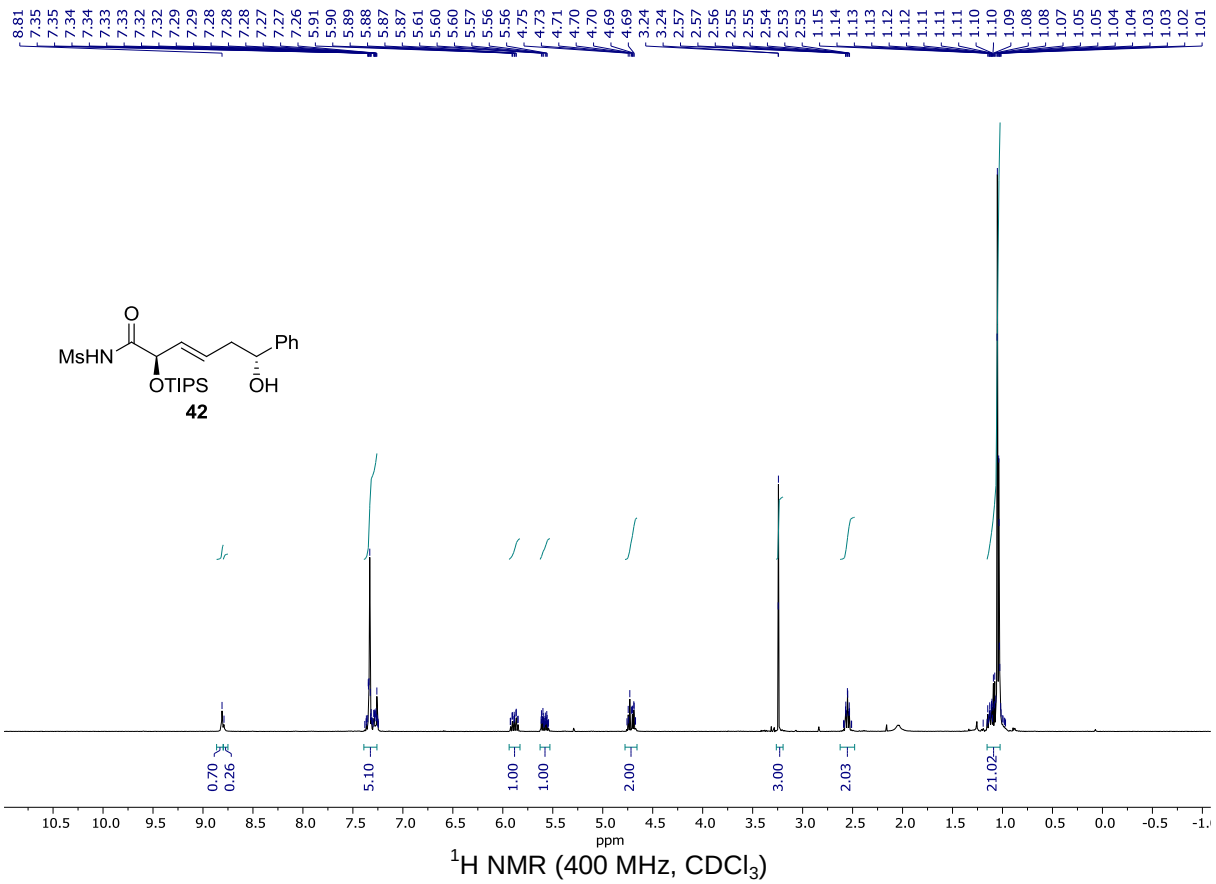
^{1}H NMR (400 MHz, $CDCl_3$)



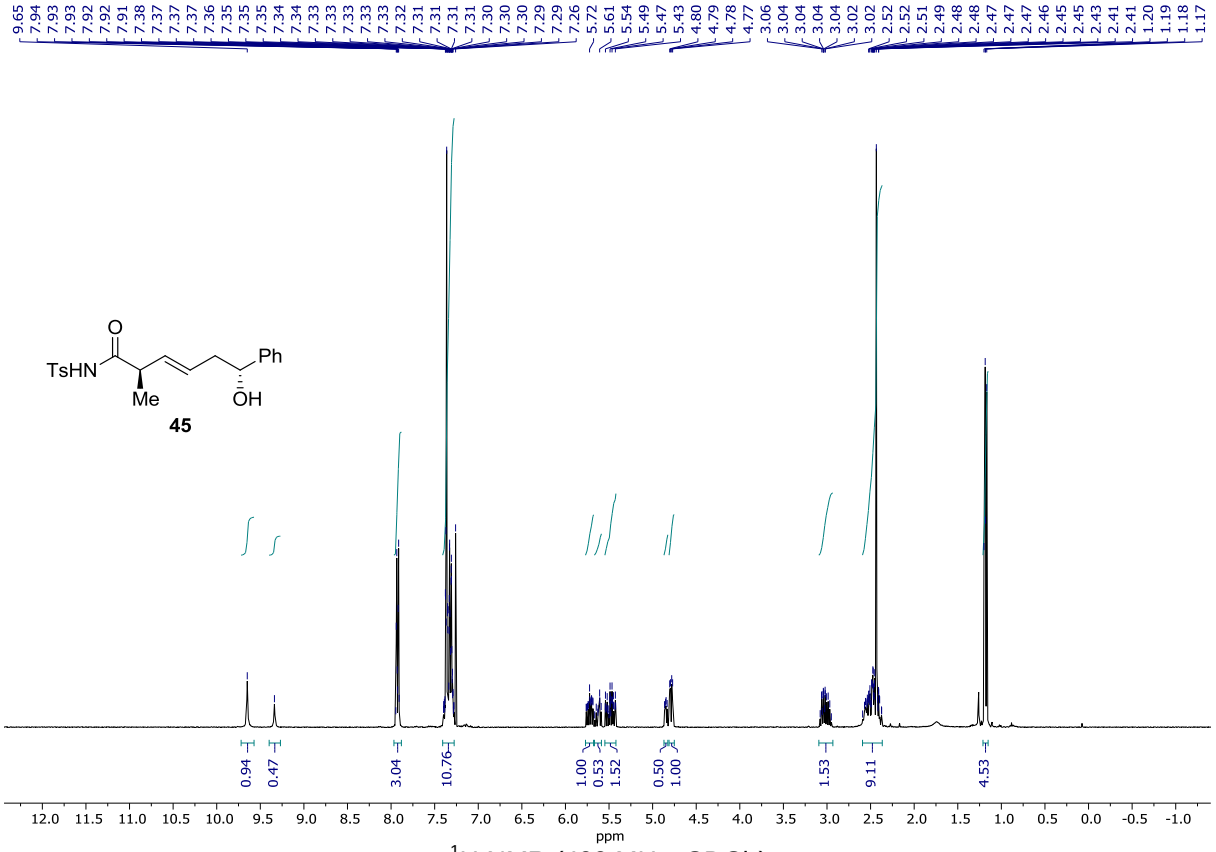
$^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$)



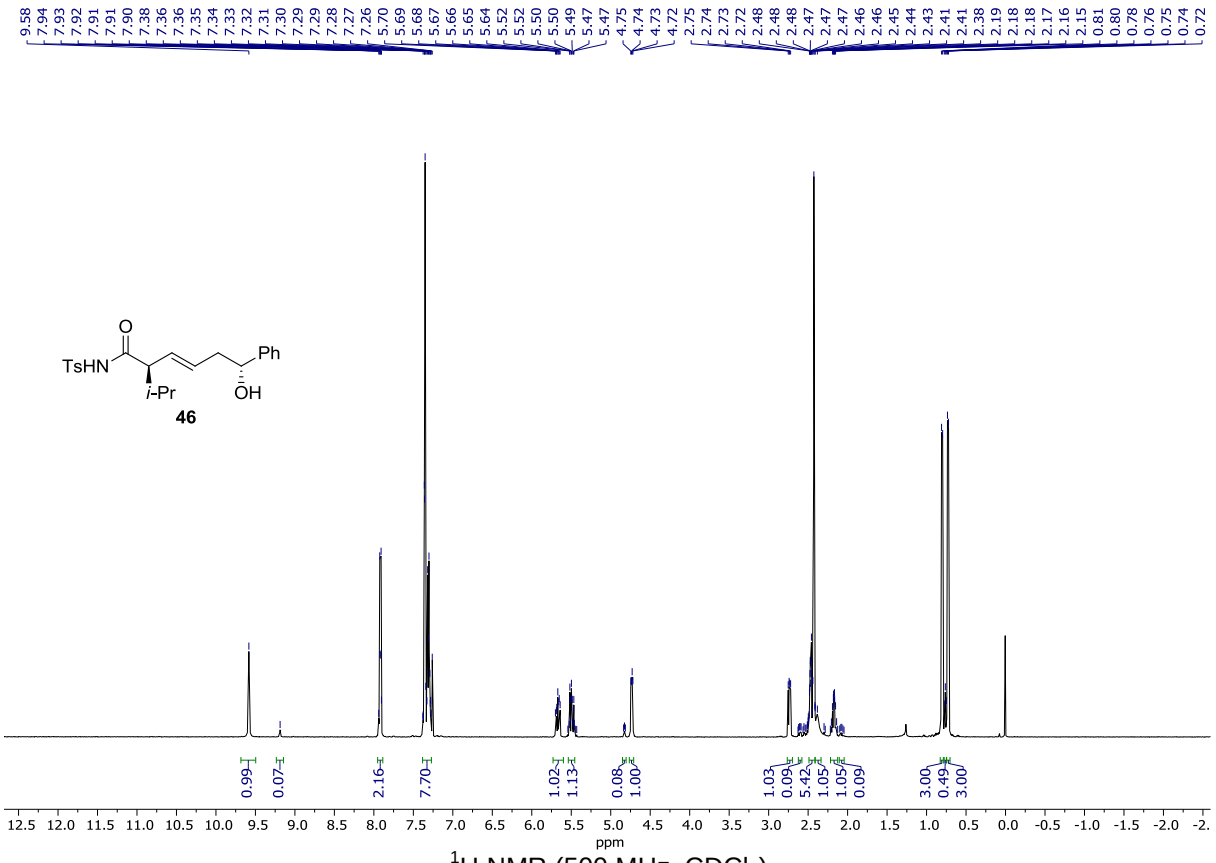
^{1}H NMR (400 MHz, C_6D_6)



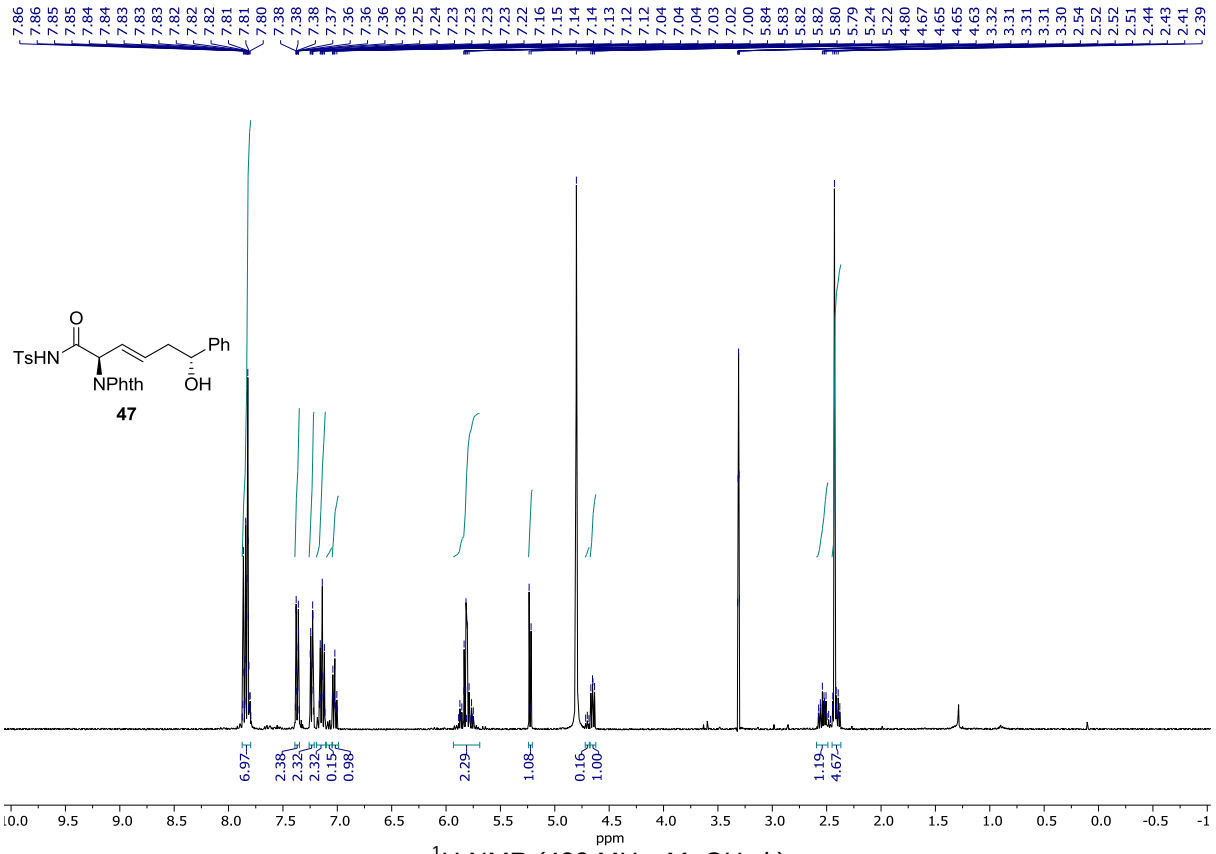
^{1}H NMR (400 MHz, $CDCl_3$)



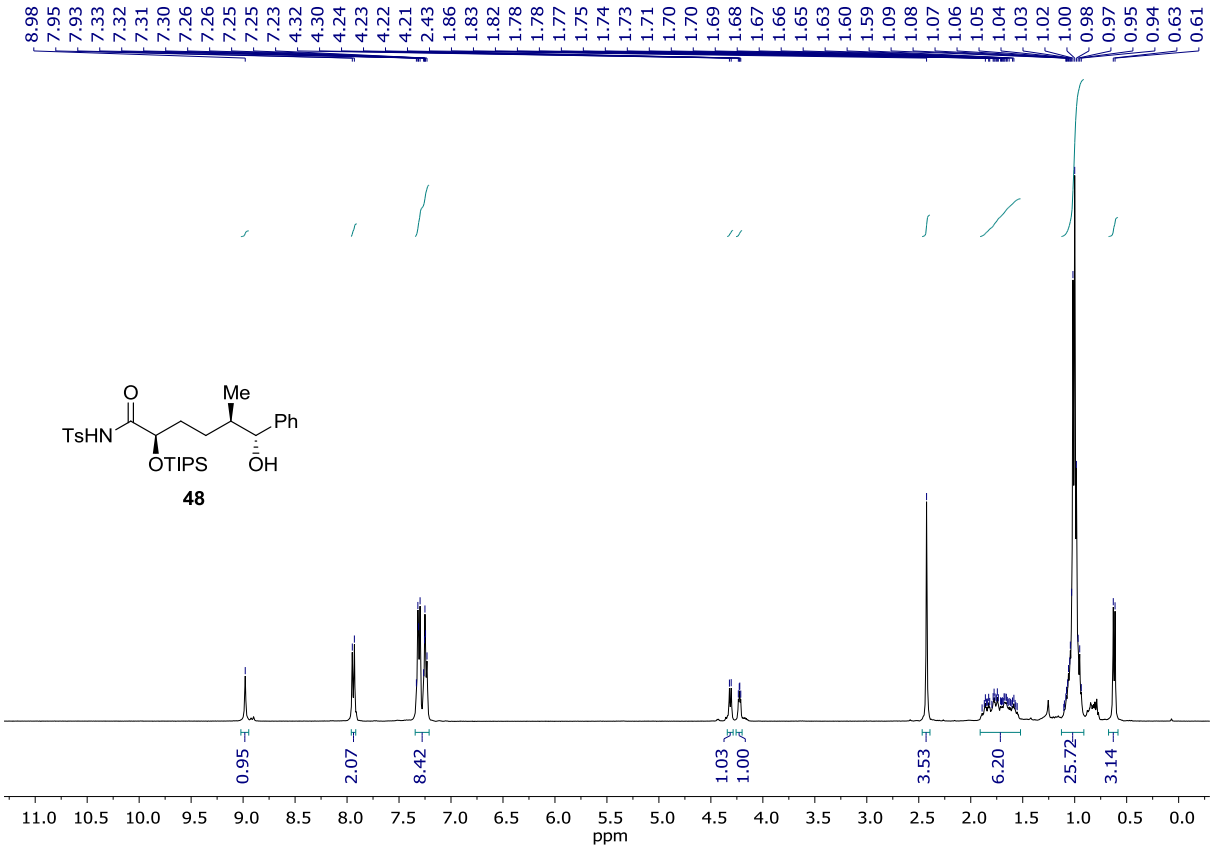
^{1}H NMR (400 MHz, $CDCl_3$)



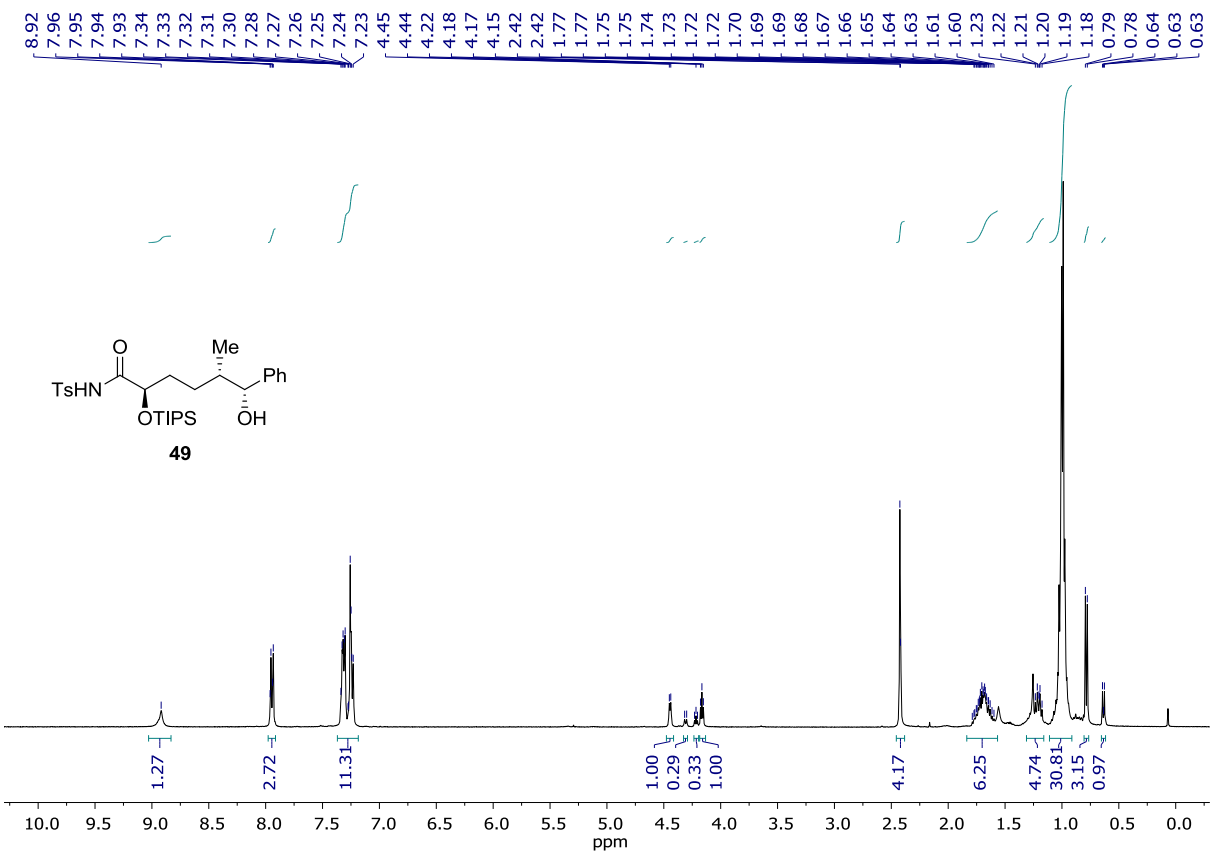
^{1}H NMR (500 MHz, $CDCl_3$)



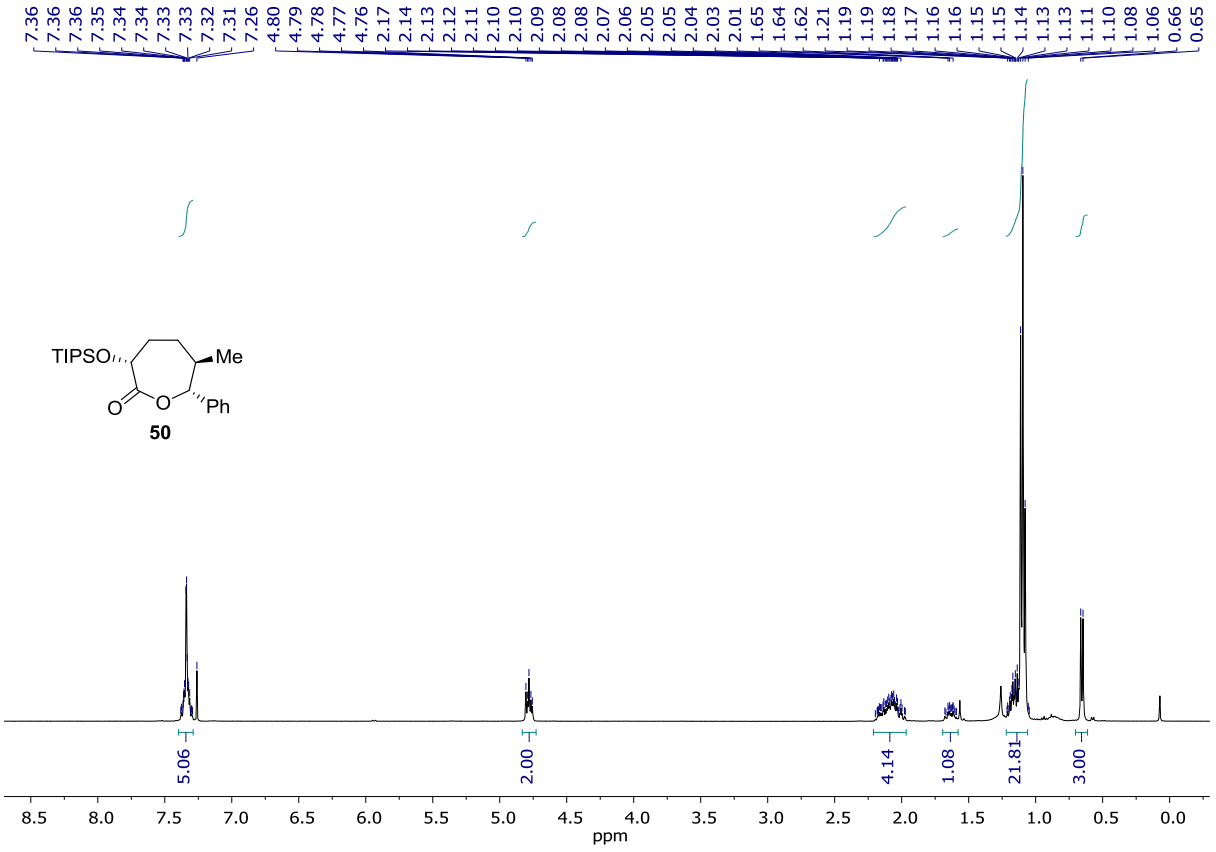
^{1}H NMR (400 MHz, MeOH-d_4)



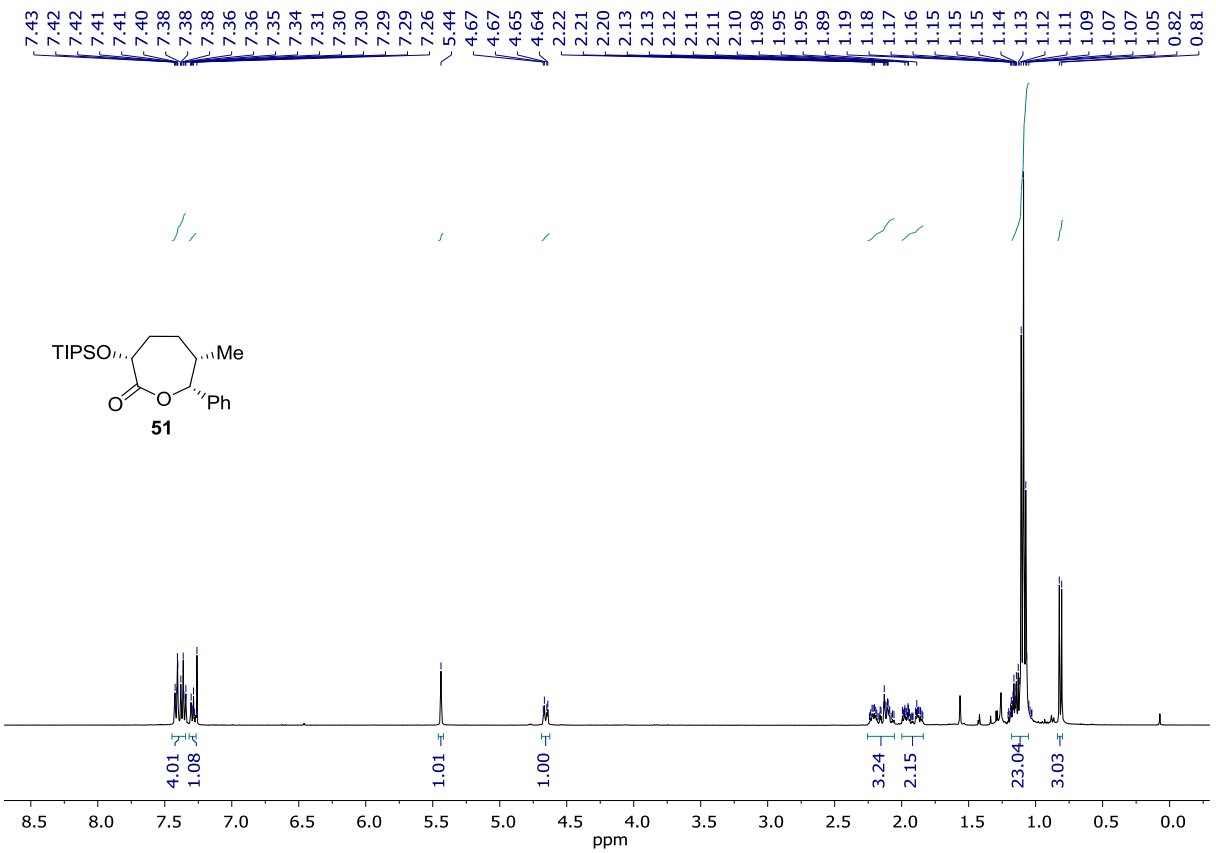
^{1}H NMR (400 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)

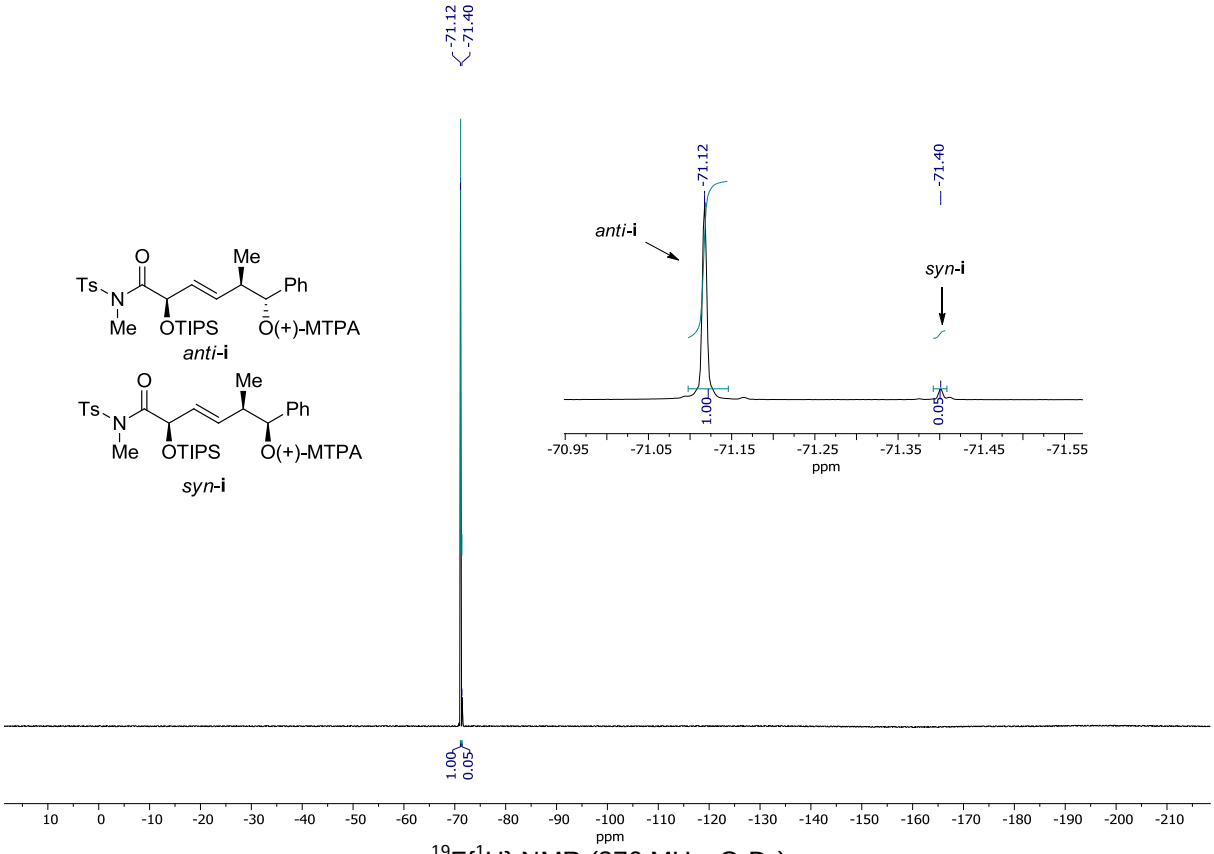


^{1}H NMR (400 MHz, $CDCl_3$)

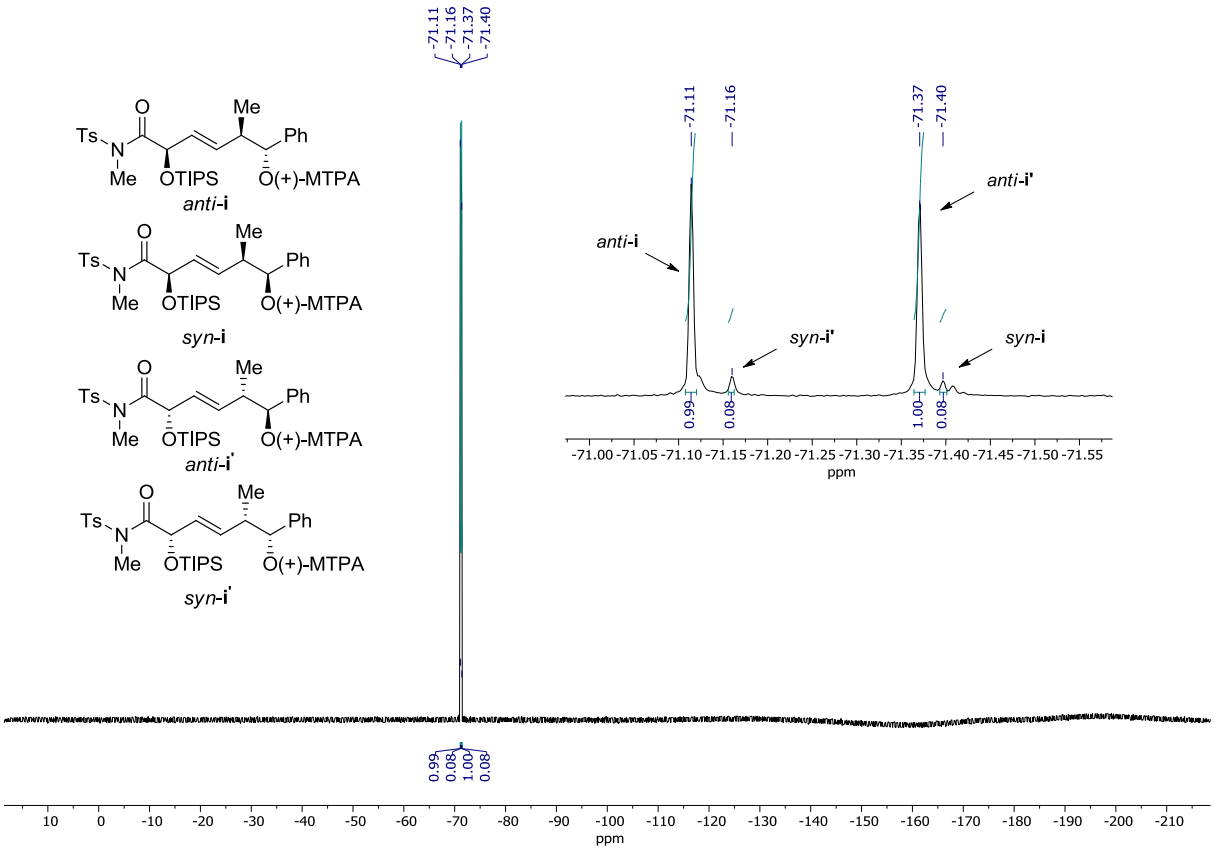


^{1}H NMR (400 MHz, $CDCl_3$)

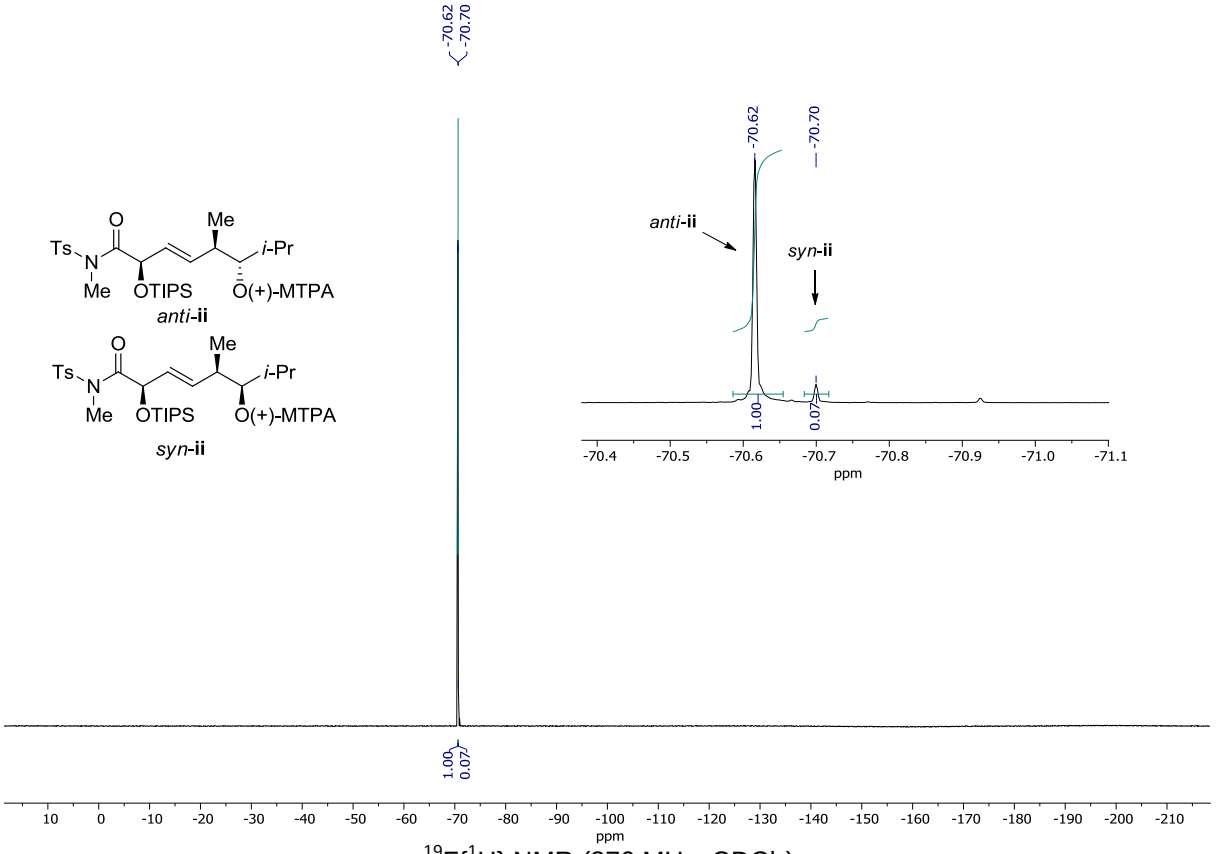
2. $^{19}F\{^{1}H\}$ NMR spectra of Mosher's esters i, i/i', ii and ii/ii'



$^{19}F\{^{1}H\}$ NMR (376 MHz, C_6D_6)



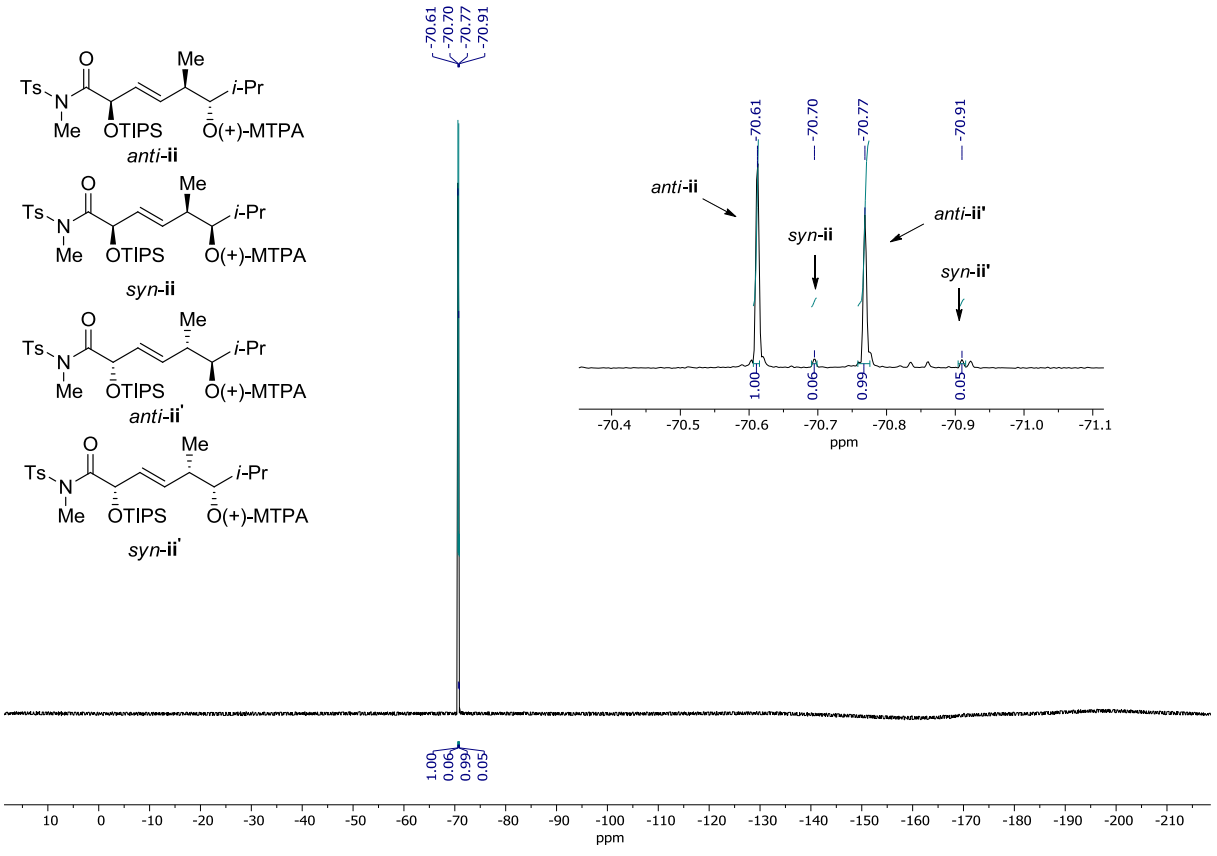
$^{19}F\{^{1}H\}$ NMR (376 MHz, C_6D_6)



anti-**ii**

syn-**ii**

$^{19}F\{^{1}H\}$ NMR (376 MHz, $CDCl_3$)



anti-**ii**'

syn-**ii**'

$^{19}F\{^{1}H\}$ NMR (376 MHz, $CDCl_3$)

3. X-ray crystallographic data for 12

Sample of **12** was prepared by crystallization from hexane. The measurements were performed on Bruker X8 APEXII diffractometer using Cu-Kα radiation (λ = 1.54178 Å). Frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm.[1] Data were corrected for absorption effects using the face-indexed numerical method (SADABS).[2] placed in calculated positions and refined as riding on their parent atoms with Uiso = 1.2 Ueq. The structure was solved by direct methods SHELXS-2014[3] and refined with full-matrix least-squares calculations on F2 using SHELX-2014[3]. All non-hydrogen atoms were refined anisotropically.

The structures presented in this article have been deposited with the Cambridge Crystallographic Data Centre. Copies of these data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html or from the Cambridge Crystallographic Data Centre,12 Union Road, Cambridge CB2 1EZ, UK; fax:(+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk.

References:

1. Bruker, 2004, APEX2 and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA
2. Bruker, 2008, SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
3. G. M. Sheldrick, SHELXL-2014. Program for the Refinement of Crystal Structures from Diffraction Data, University of Göttingen, Germany (2014).

Table S1. Crystal data and structure refinement details for 12

Empirical formula	$C_{27}H_{47}NO_5SSi$
Formula weight	525.80
Crystal color and habit	colorless plate
CCDC No.	1917839
Temperature /K	296(2)
Crystal system	triclinic
Space group	P -1
a /Å	11.3319(4)
b /Å	12.7598(5)
c /Å	12.8305(5)
α /°	110.192(2)
β /°	106.603(2)
γ /°	101.611(2)
Volume /Å^3	1573.10(11)
Z	2
ρ_{calc}/ g cm^{-3}	1.110
μ/mm^{-1}	1.537
F(000)	572.0
Crystal size /mm^3	0.066 x 0.167 x 0.245
Θ range for data collection /°	3.92 to 60.32
Index ranges	-12<=h<=11, -11<=k<=14, -14<=l<=11
Reflections collected (all/independent)	28870/ 3741
Data/restraints/parameters	3741 / 0 / 328
Goodness-of-fit on F^2	1.033
Final R indexes [I>2σ (I)]	R1 = 0.0549, wR2 = 0.1087
Final R indexes [all data]	R1 = 0.1349, wR2 = 0.1337
Largest diff. peak and hole /e Å^{-3}	0.174 and -0.157

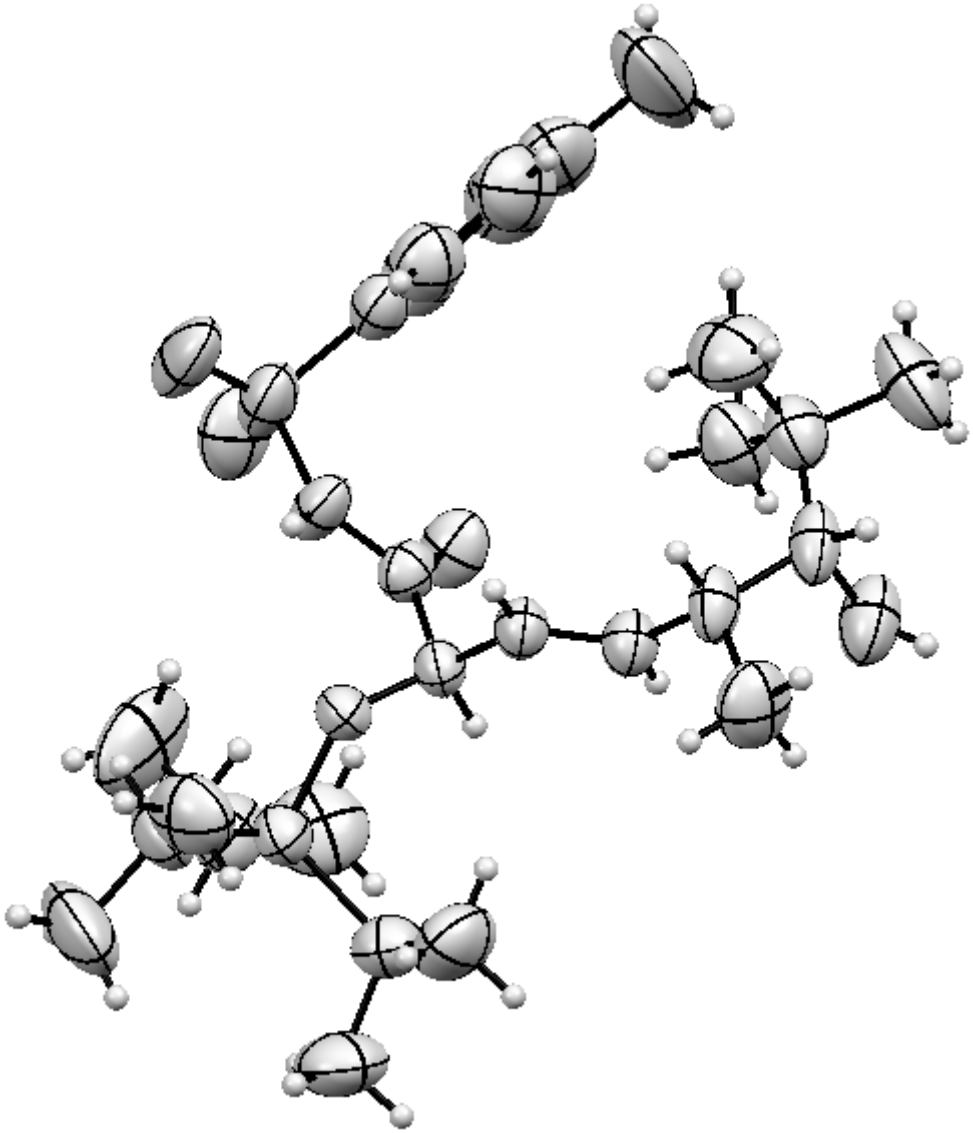


Figure S1. ORTEP diagram (50% probability) of **12.**