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Supporting Information

Studies on cyclization reactions of 3-amino-2,4-dihydroxybutanoic acid derivatives

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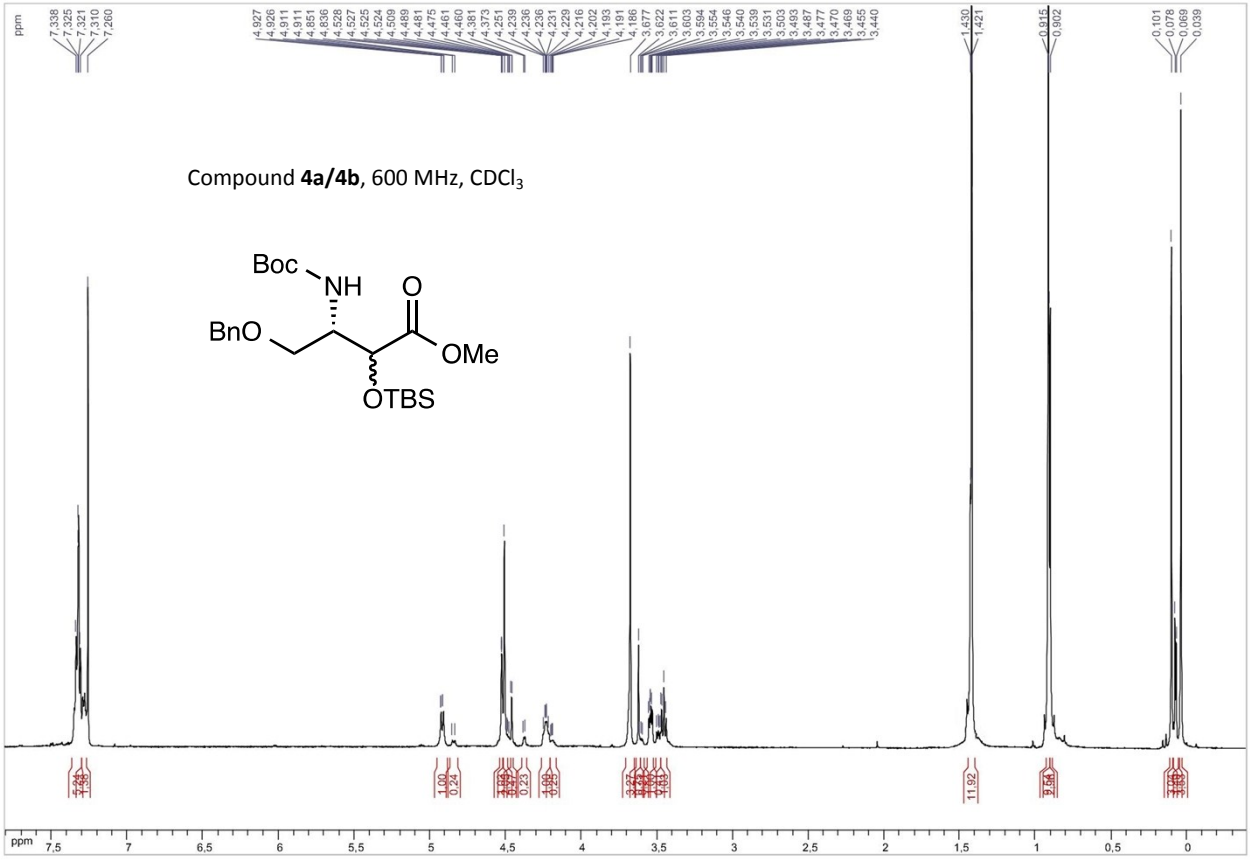
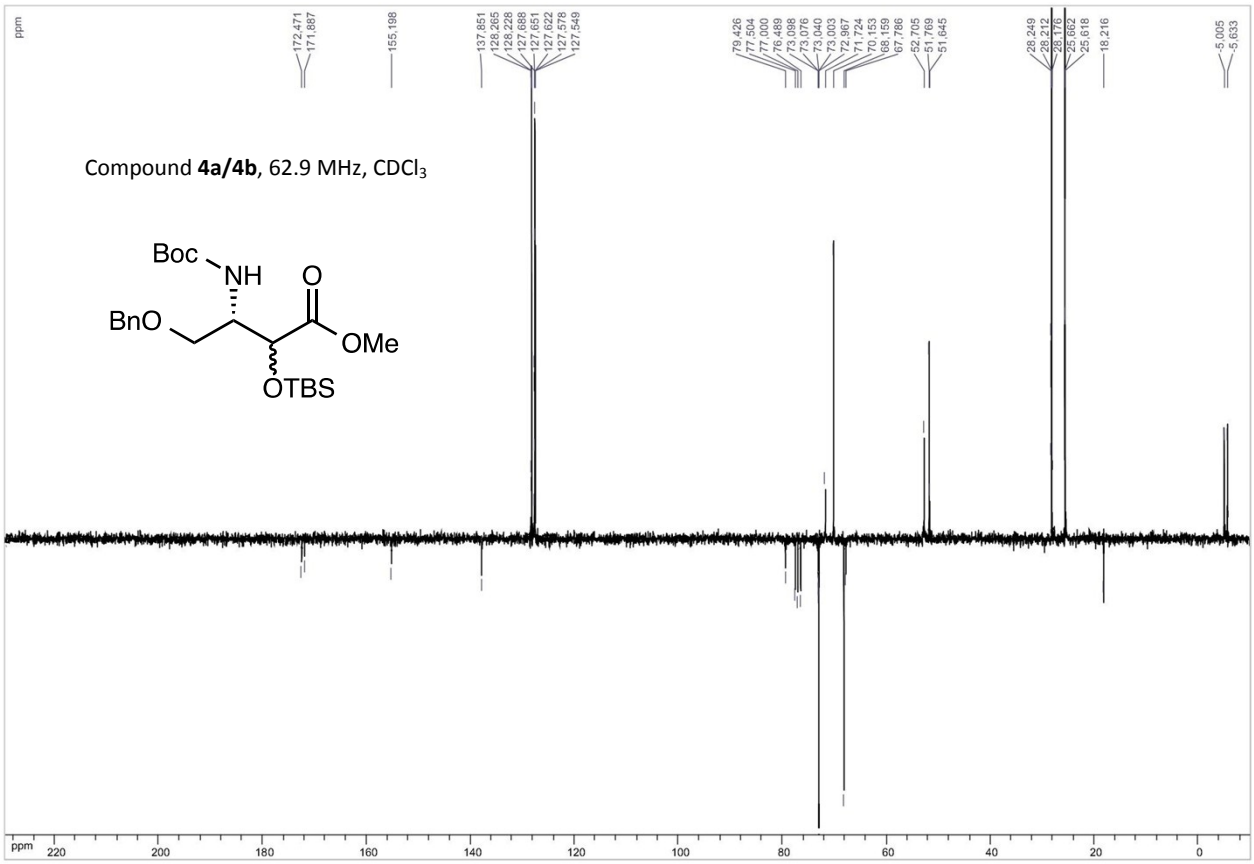
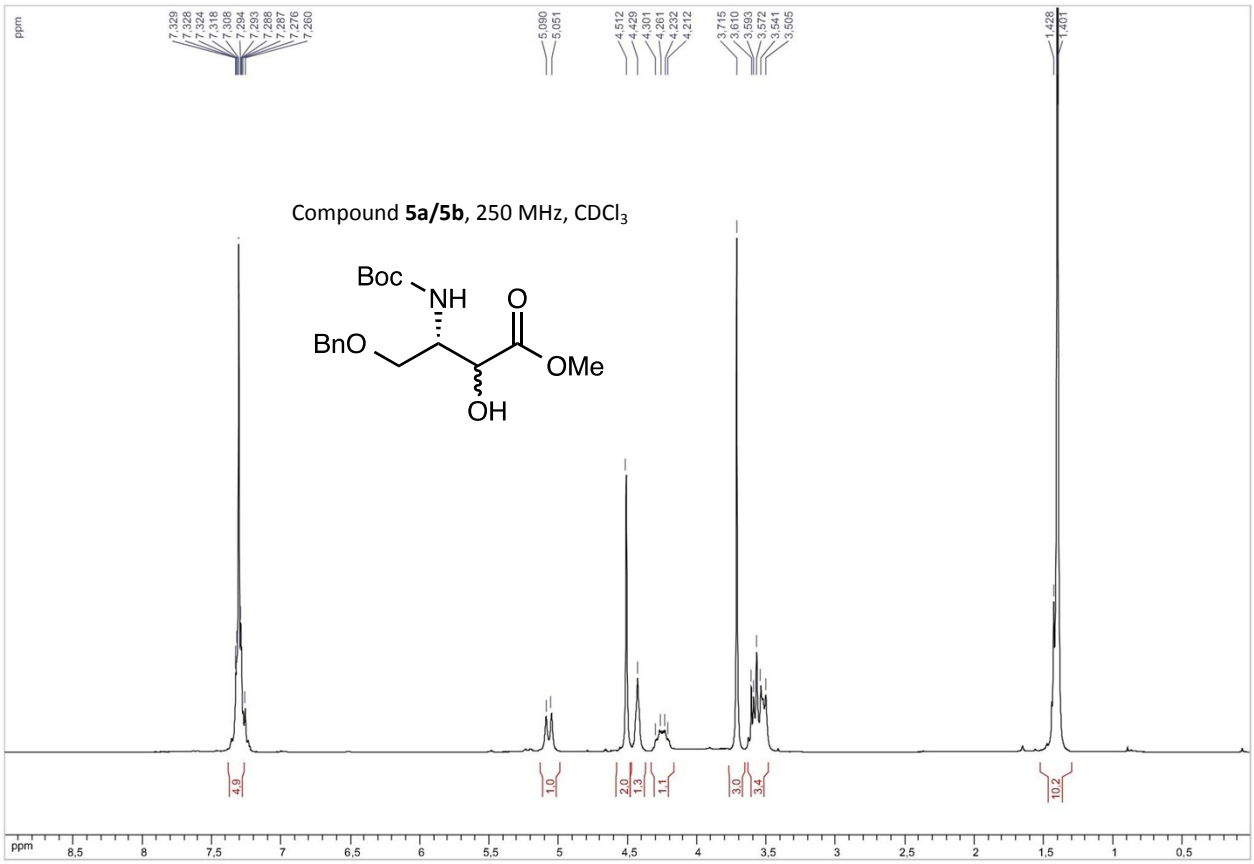
Copies of ^{1}H and ^{13}C NMR spectra

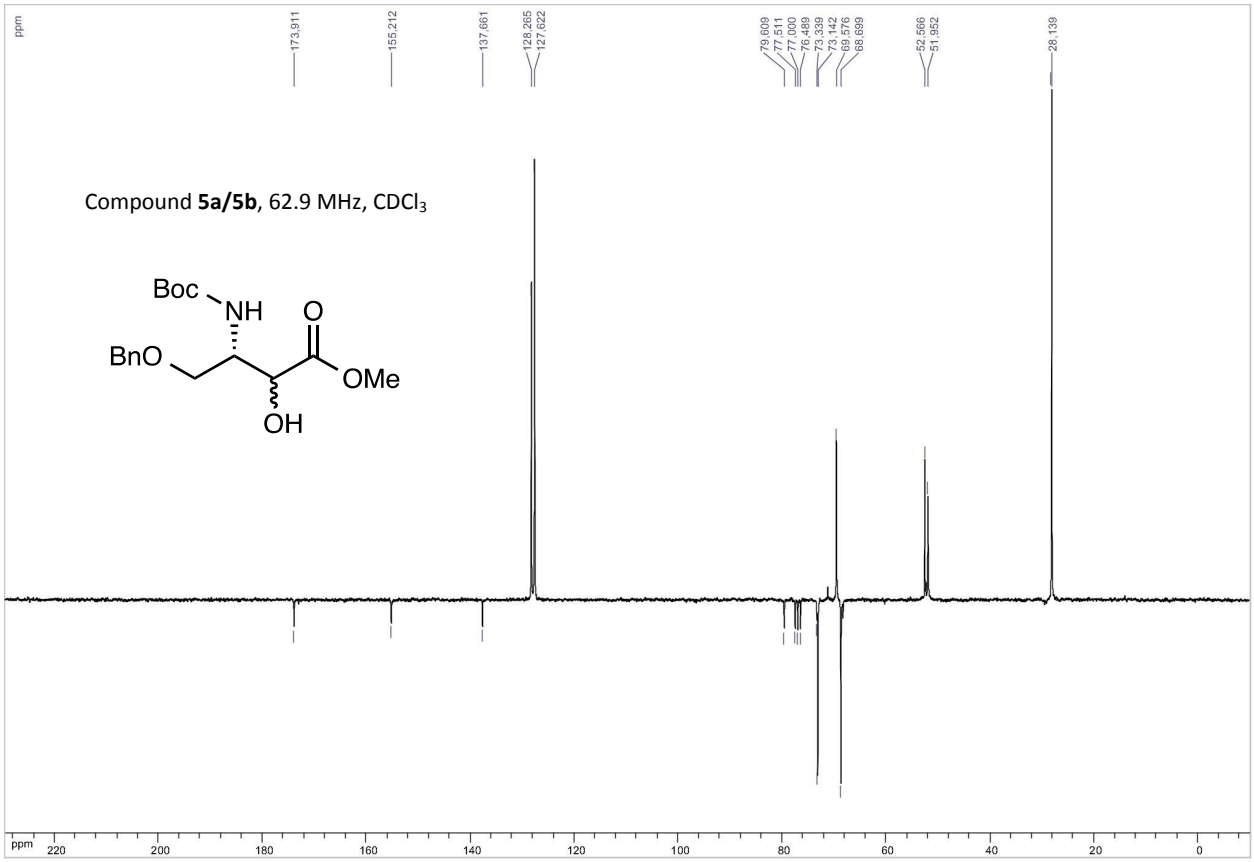
Compound **4a/4b**



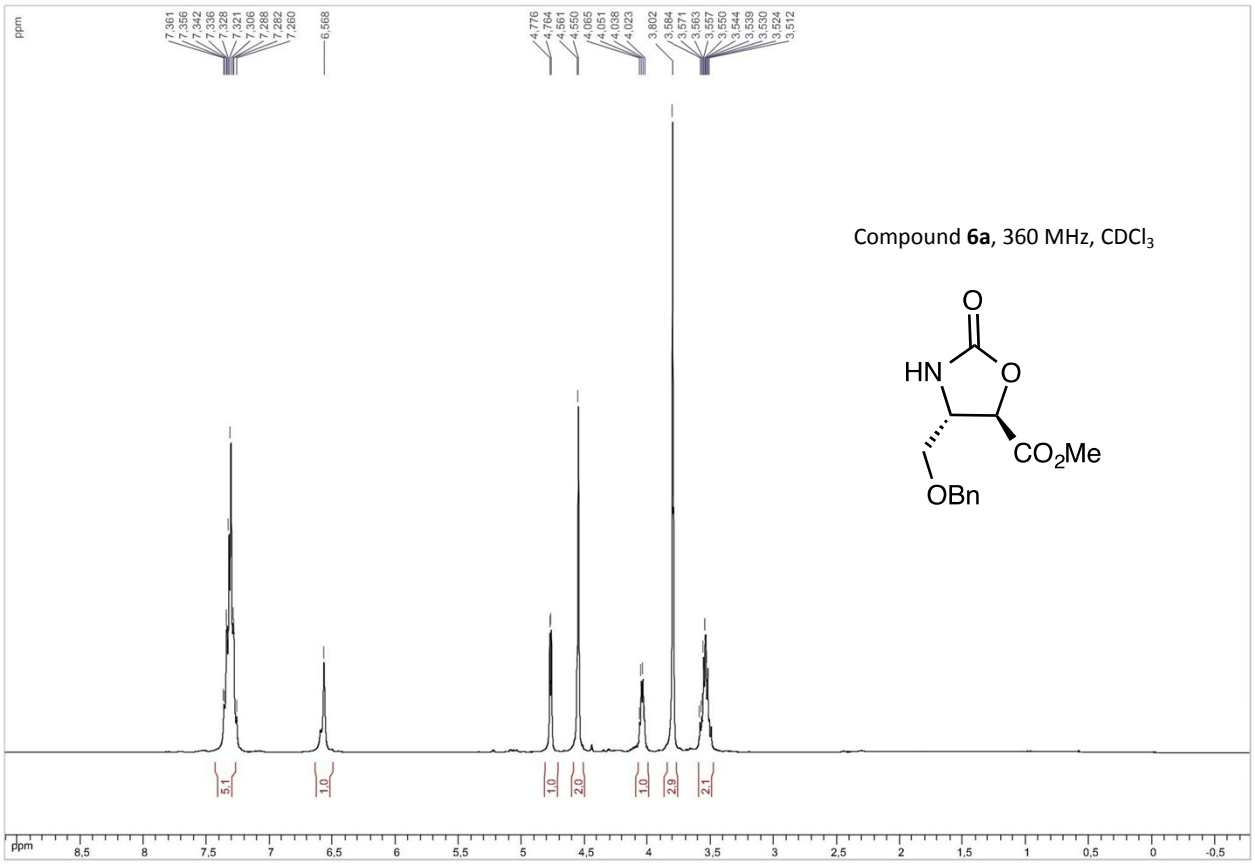


Compound **5a/5b**





Compound **6a**


Compound **6a**, 360 MHz, $CDCl_3$
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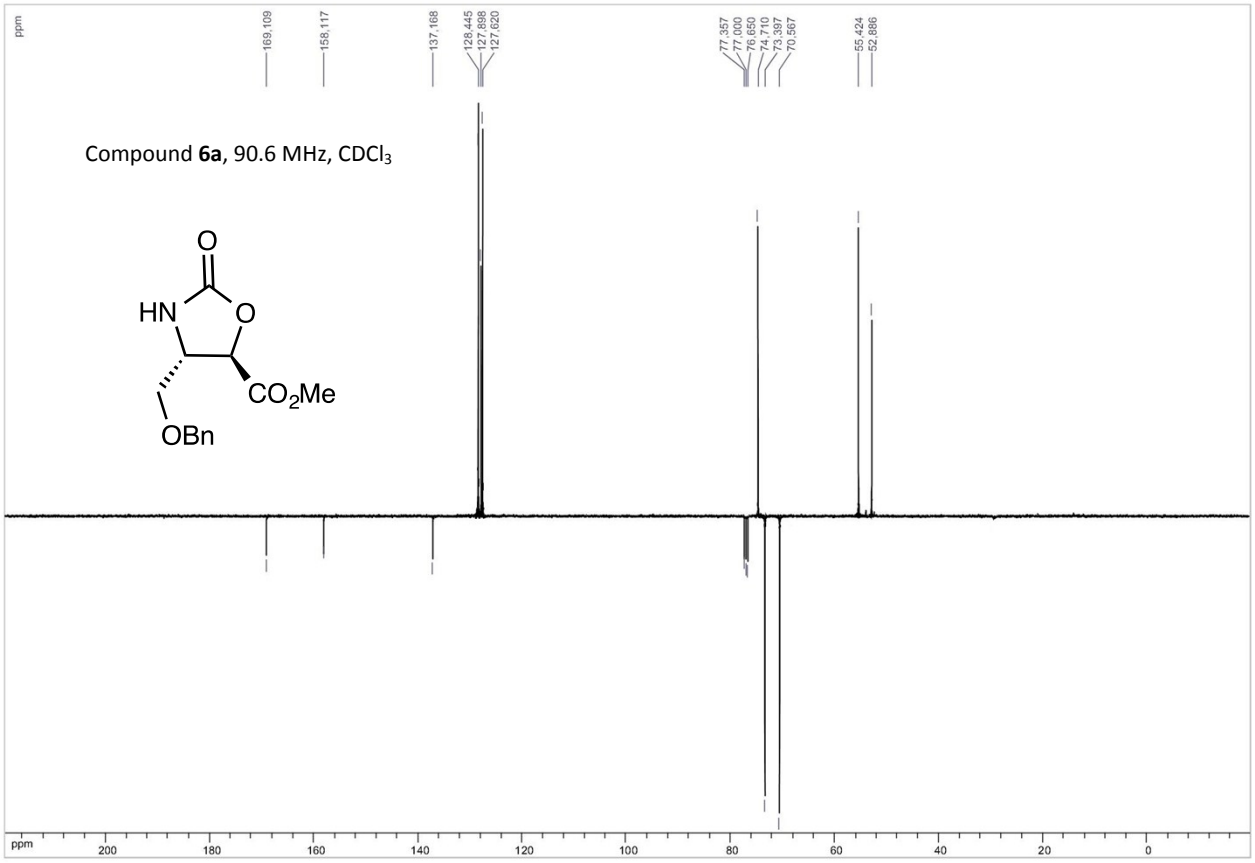
O
CO_2Me
OBn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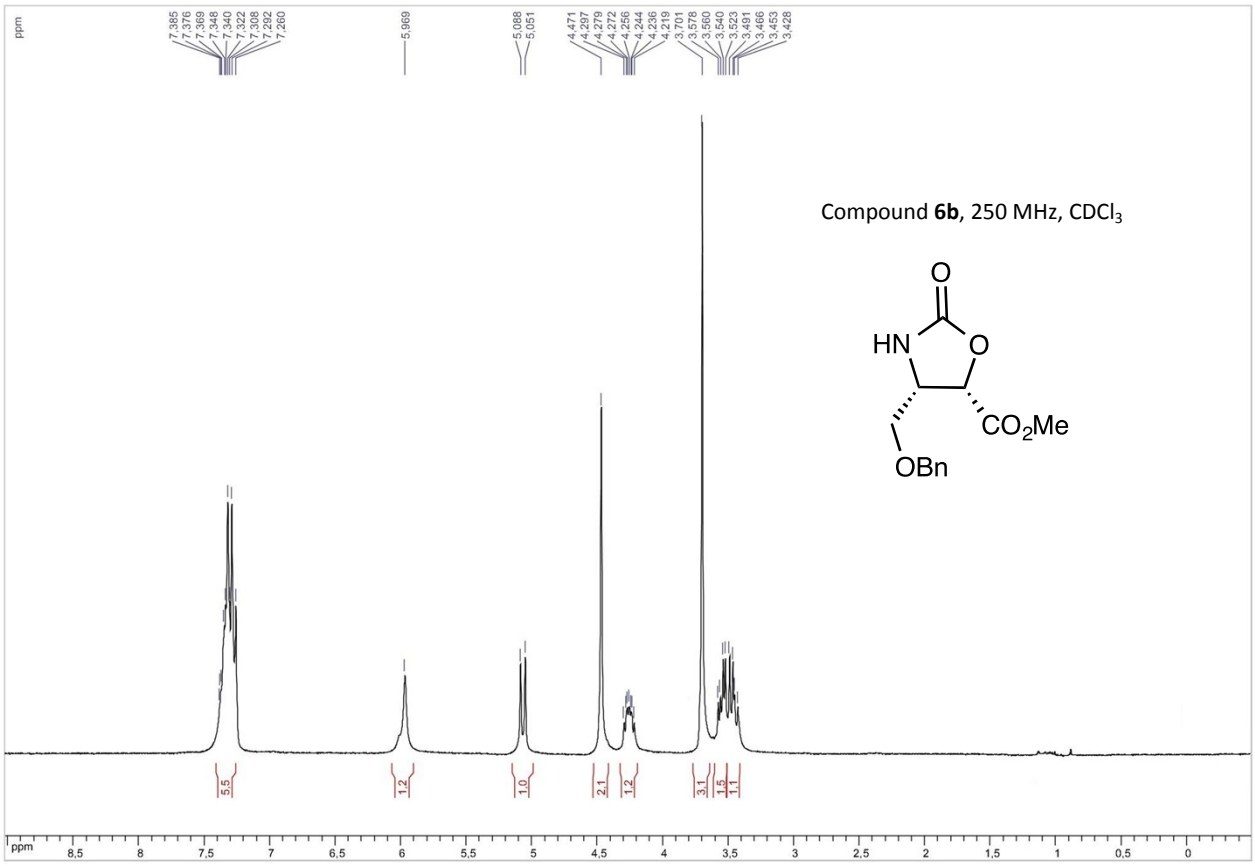
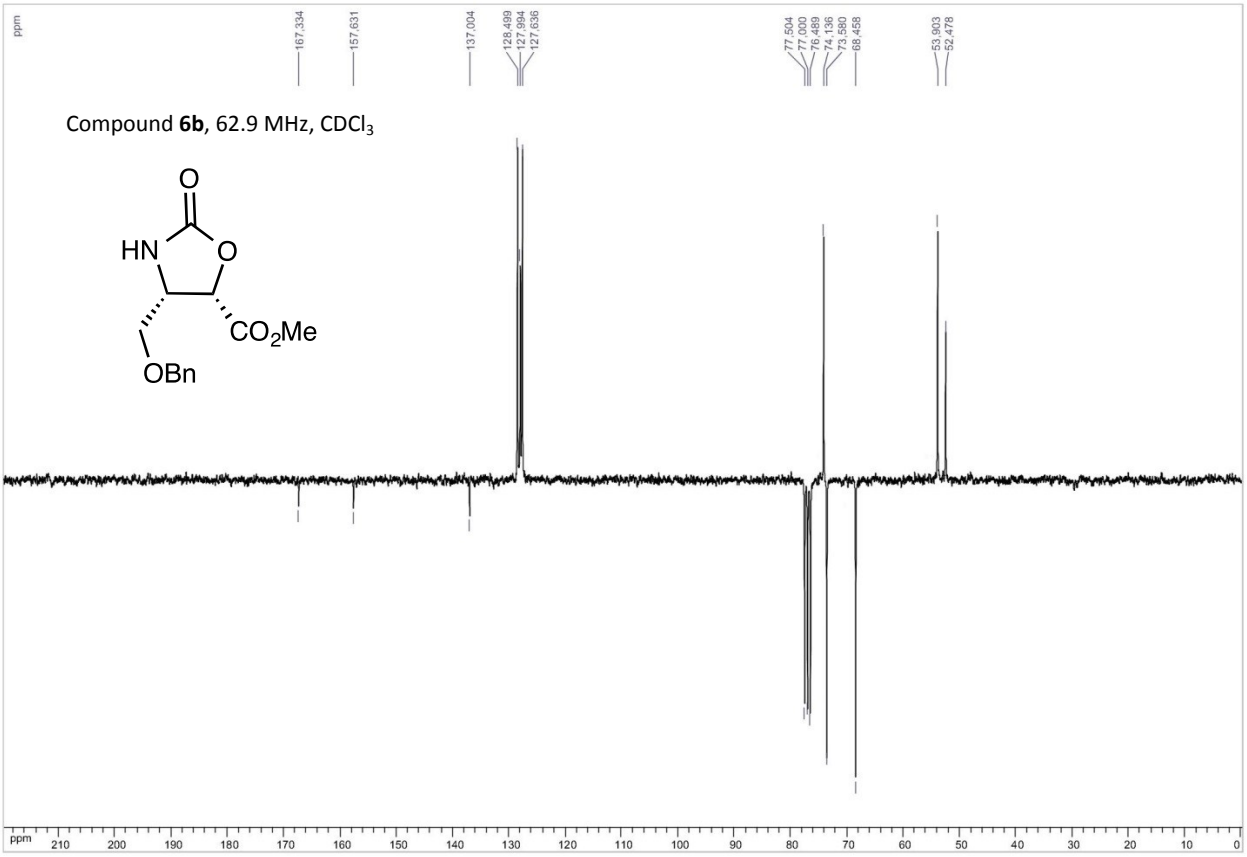
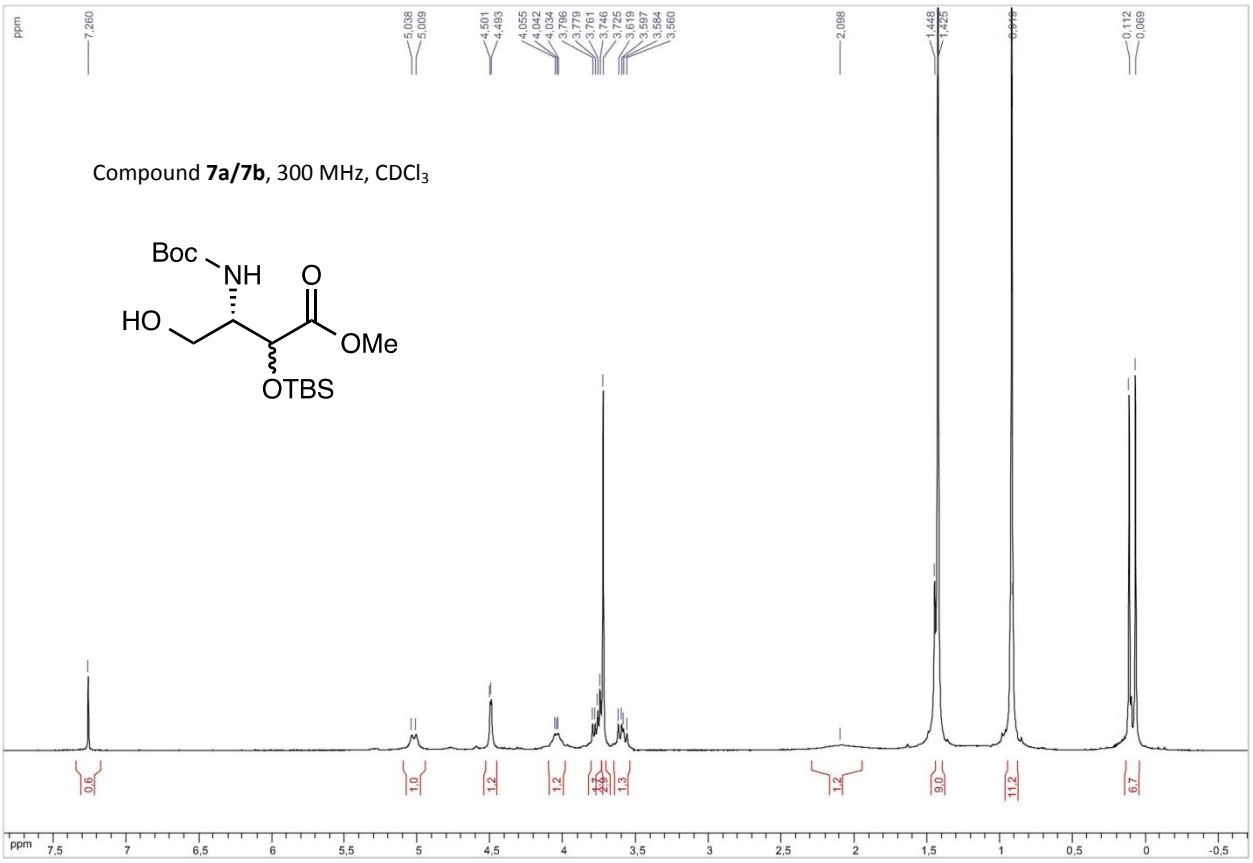
HN
O
CO_2Me
OBn

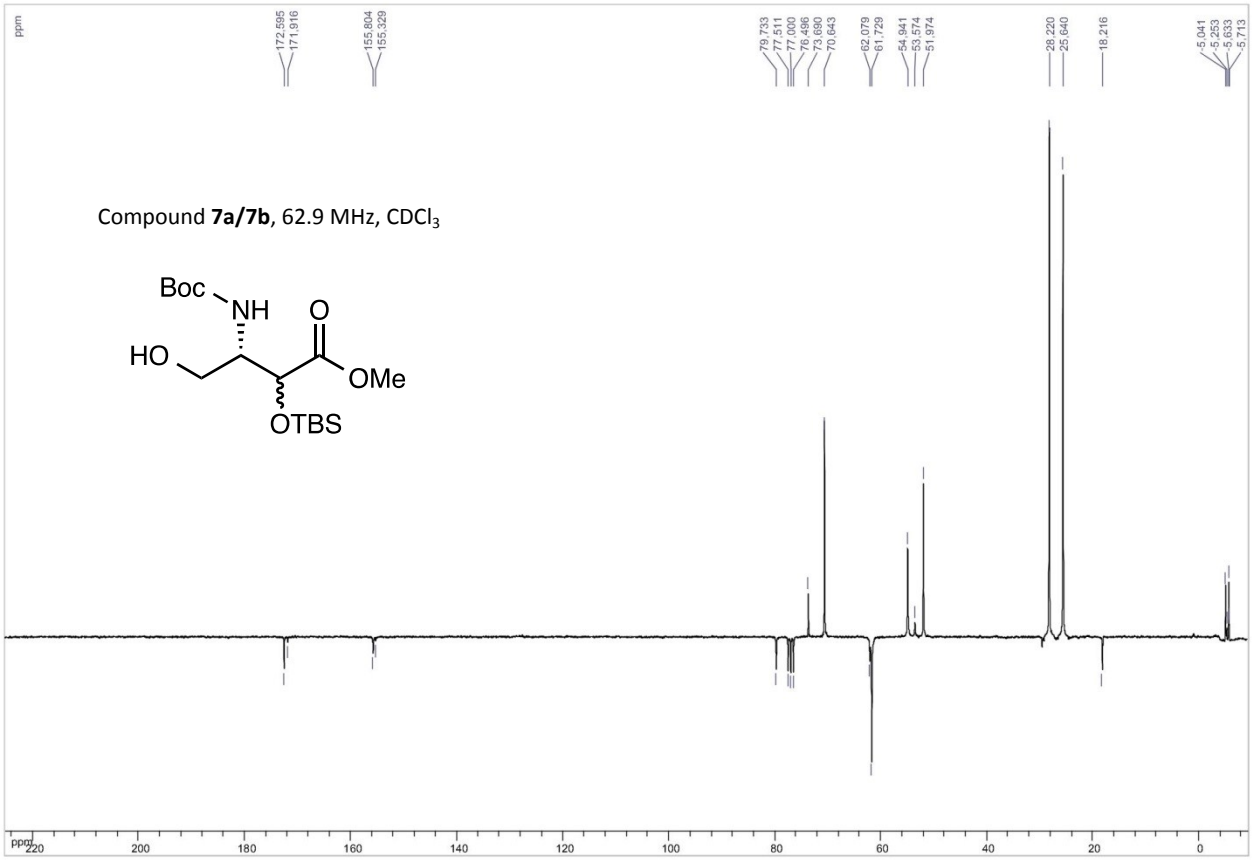
Compound **6b**


Compound **6b**, 250 MHz, $CDCl_3$
HN
O
CO_2Me
OBn

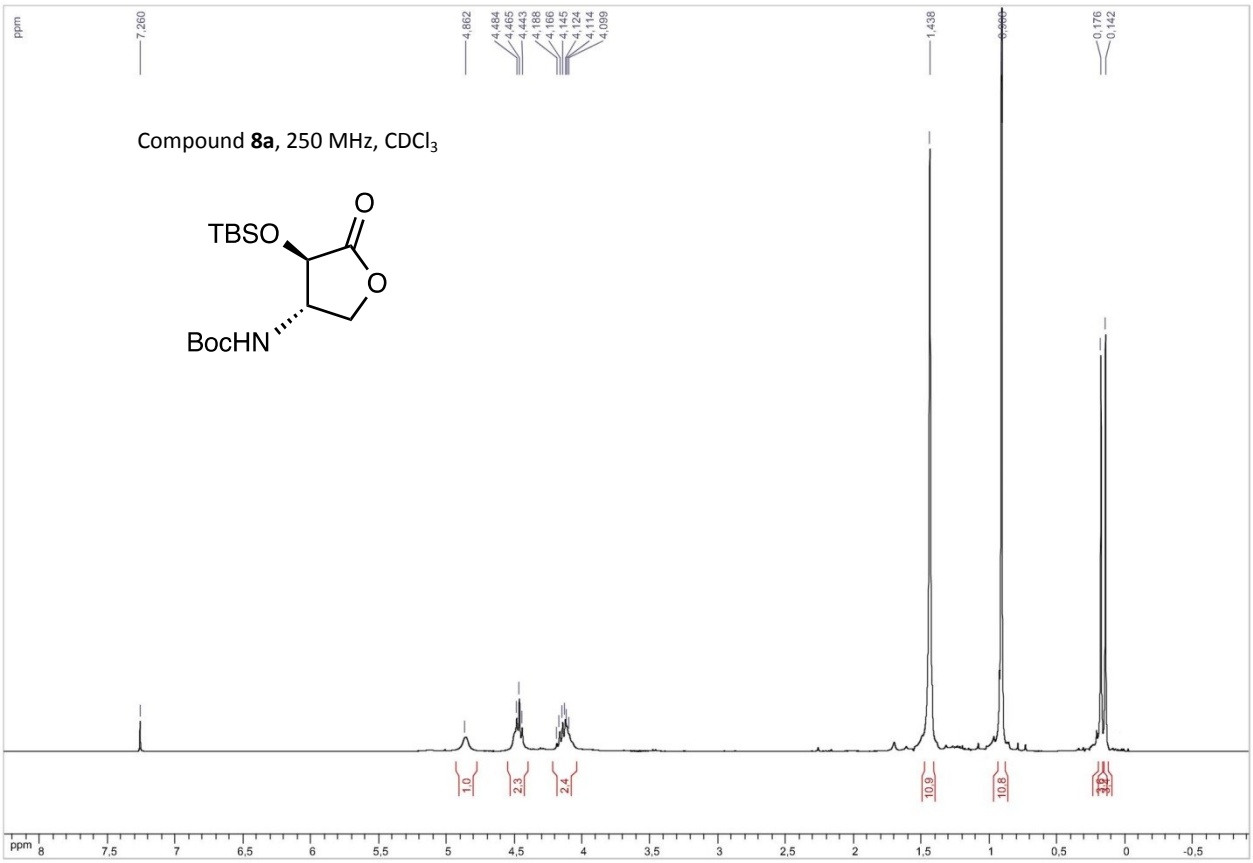

Compound **6b**, 62.9 MHz, $CDCl_3$
HN
O
CO_2Me
OBn

Compound **7a/7b**

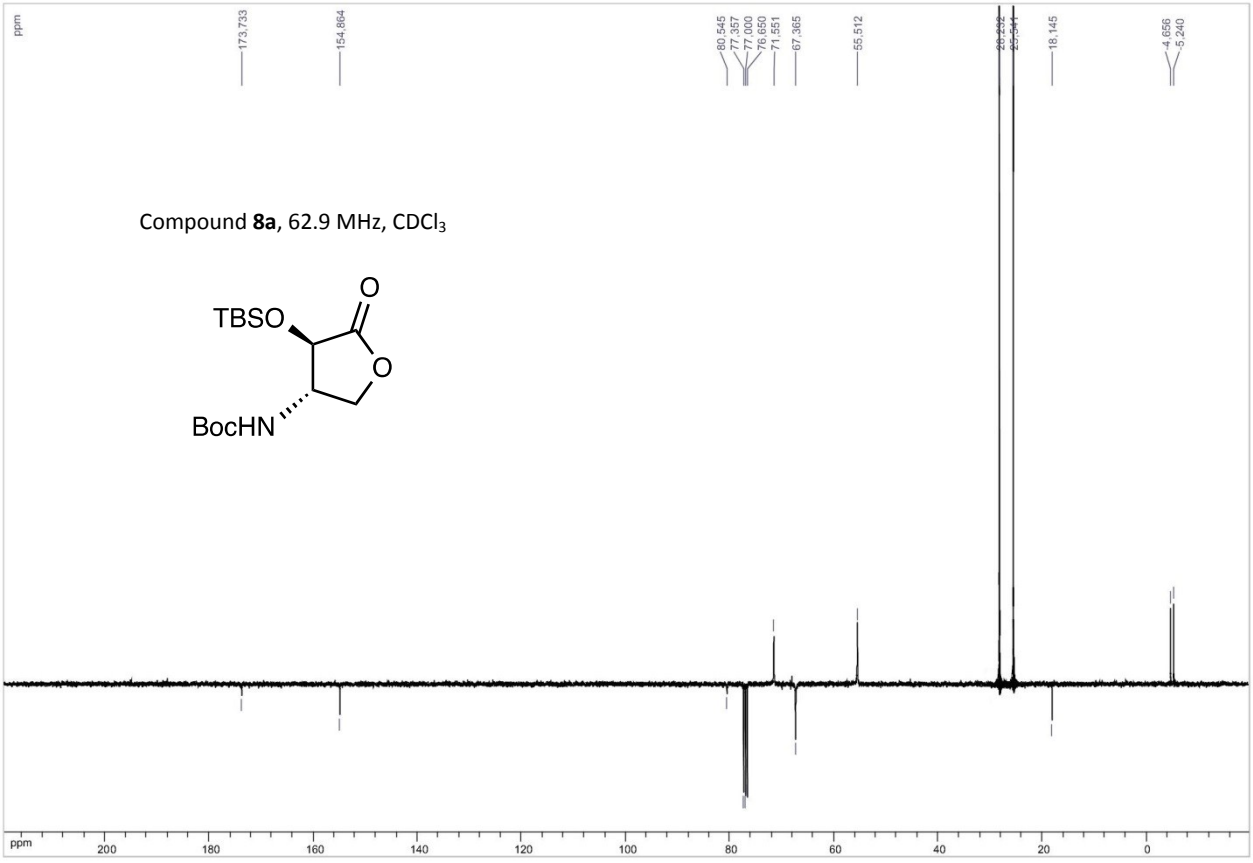




Compound **8a**

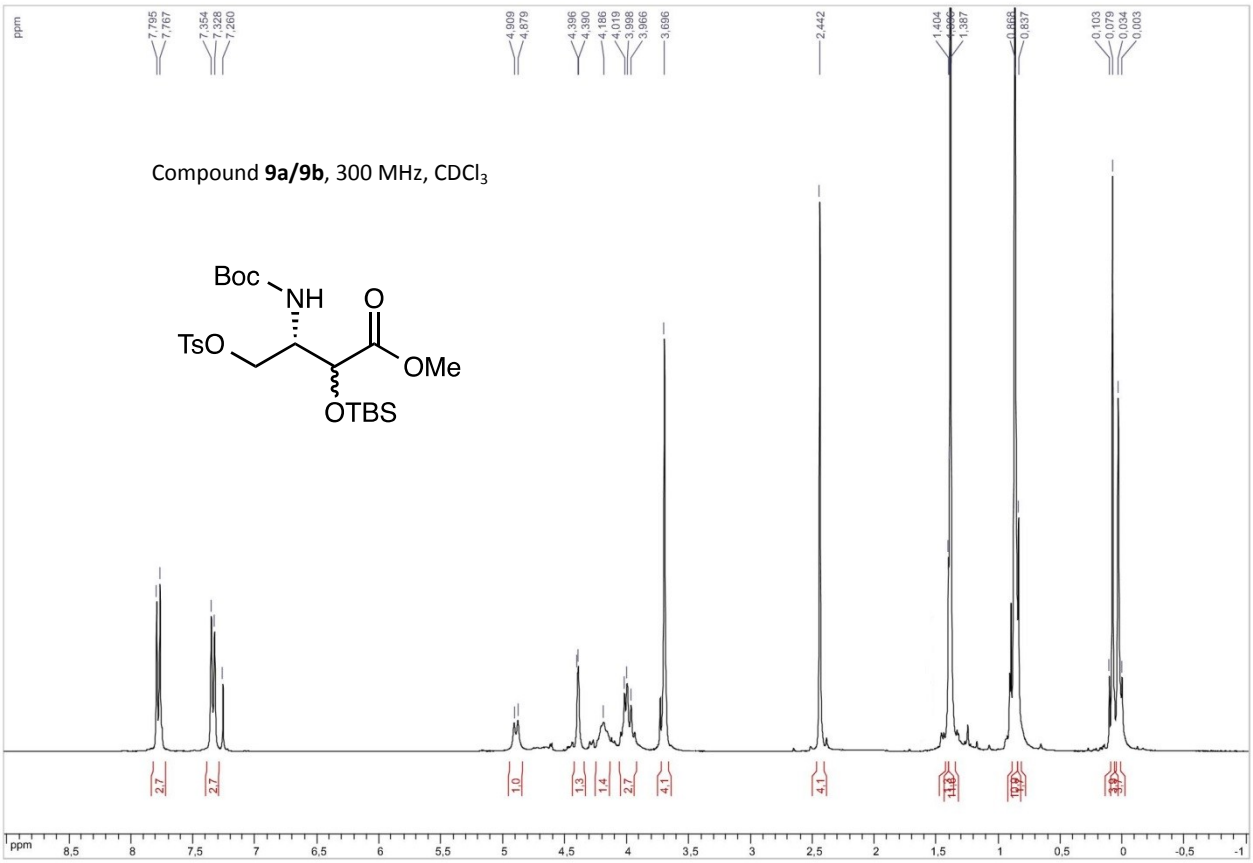


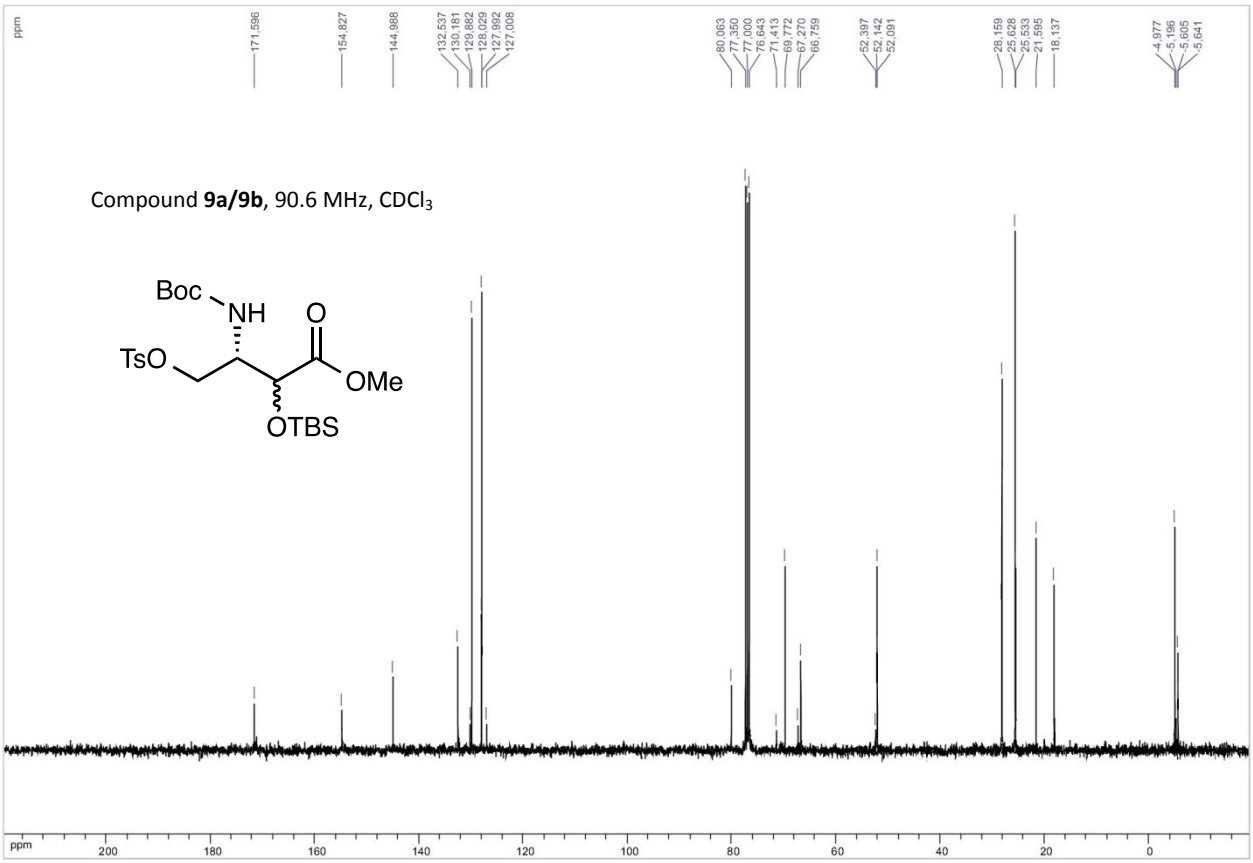
Compound **8a**, 250 MHz, $CDCl_3$



Compound **8a**, 62.9 MHz, $CDCl_3$

Compound **9a/9b**





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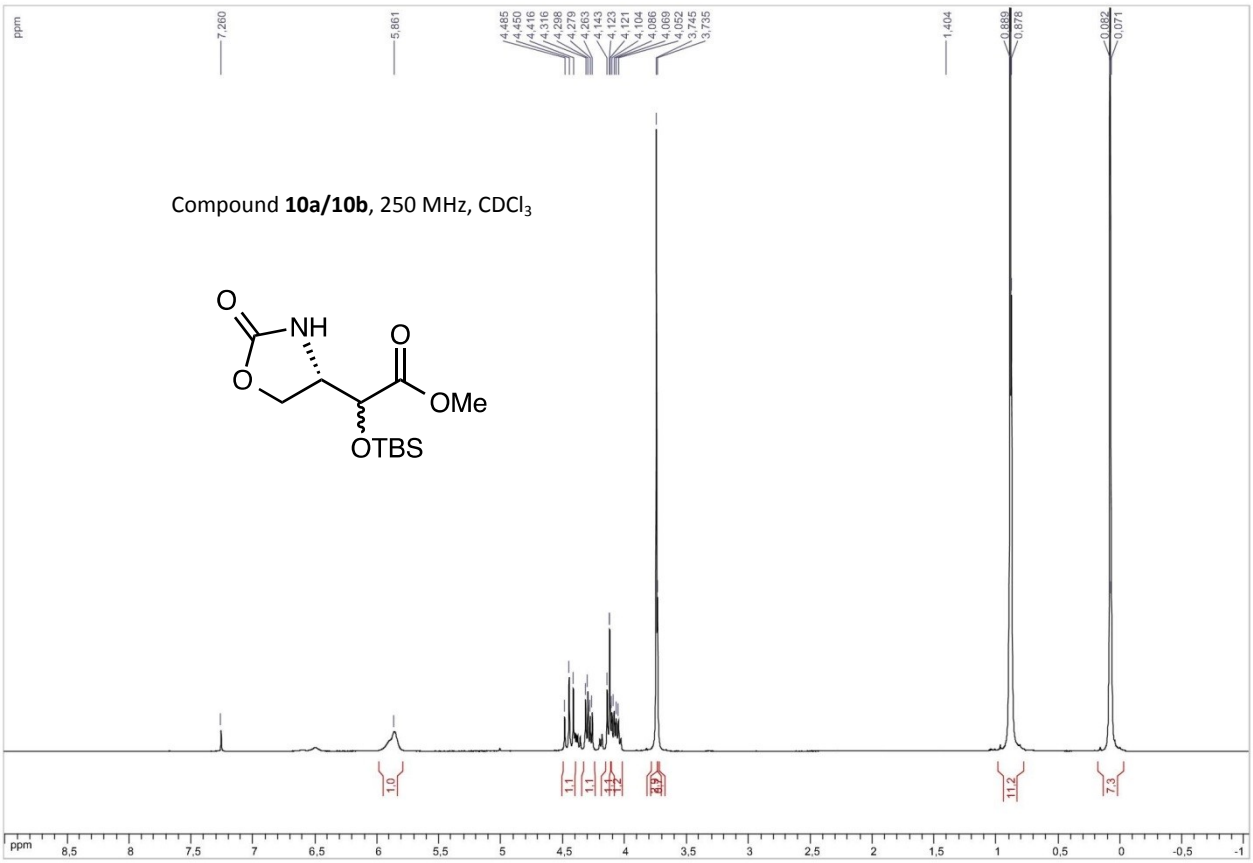

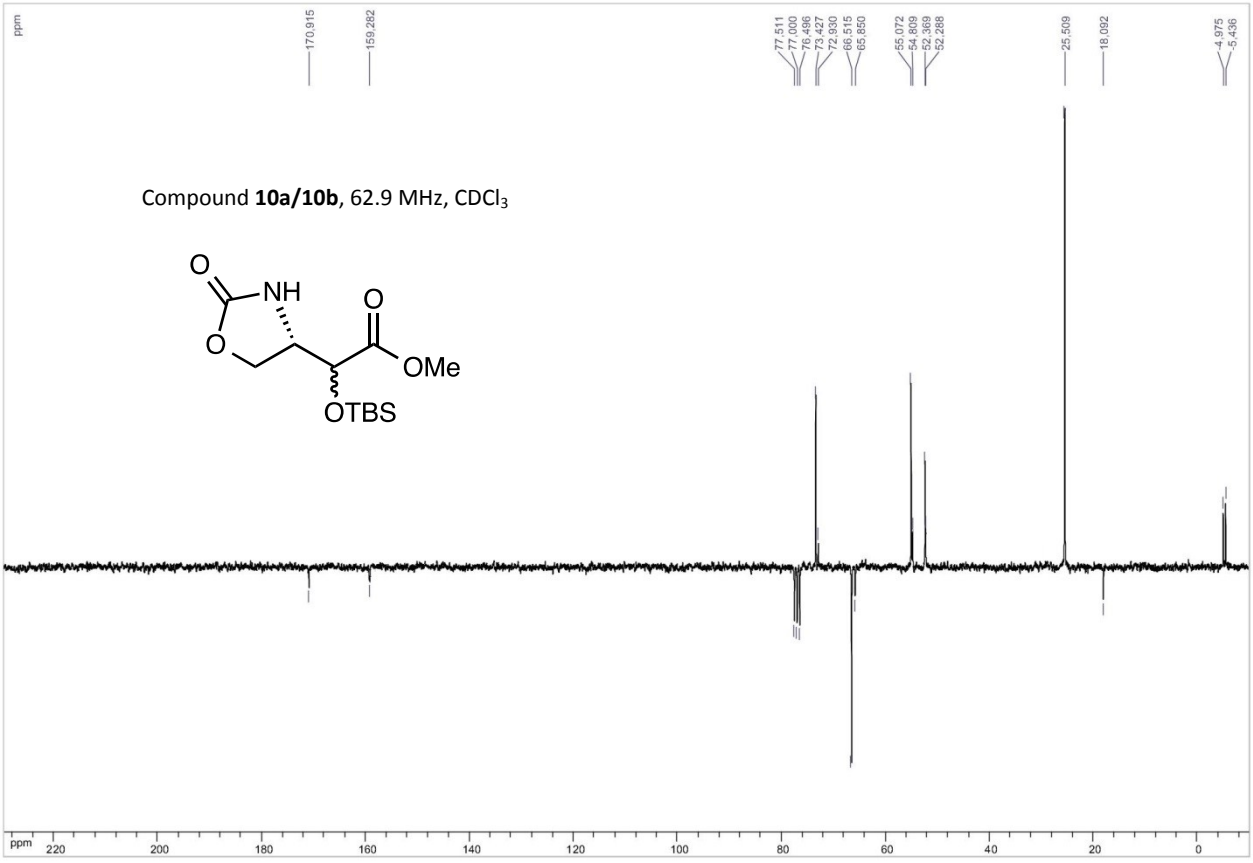

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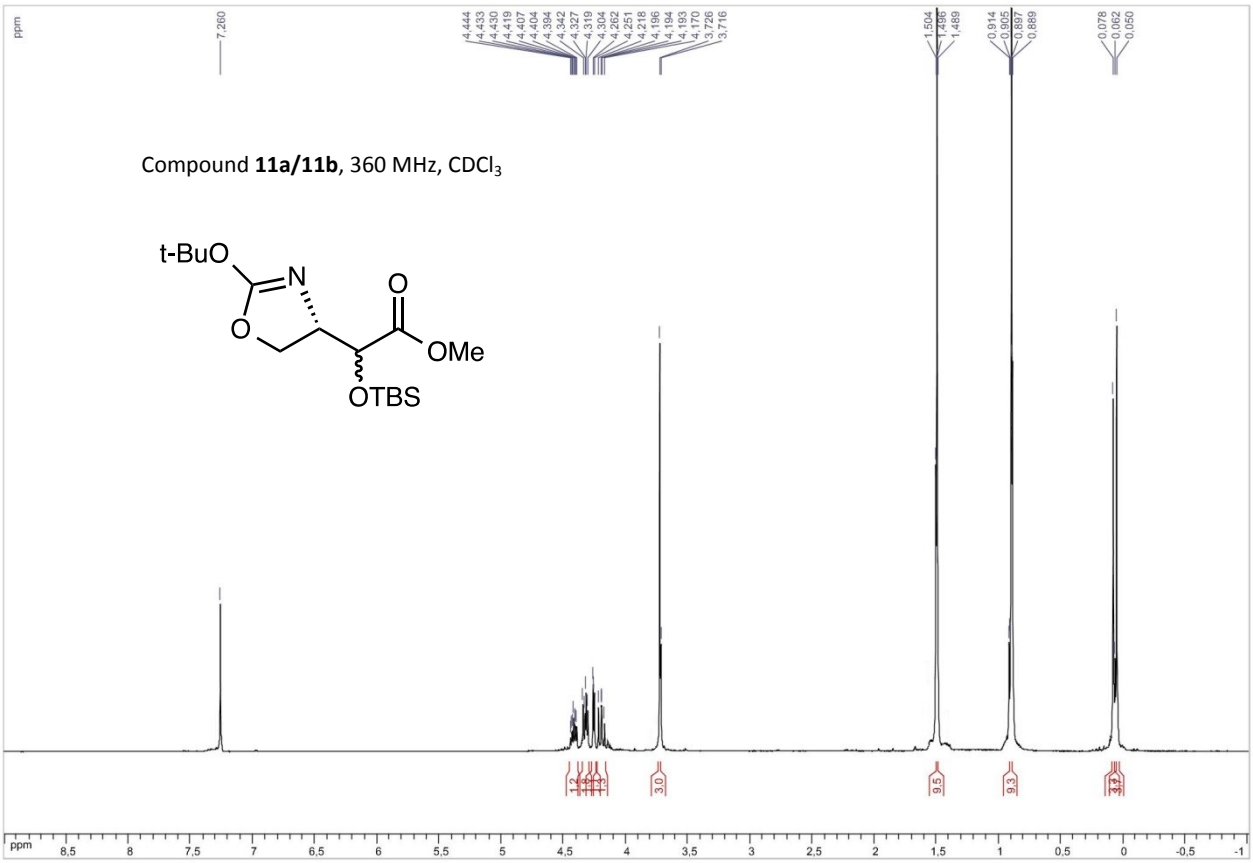

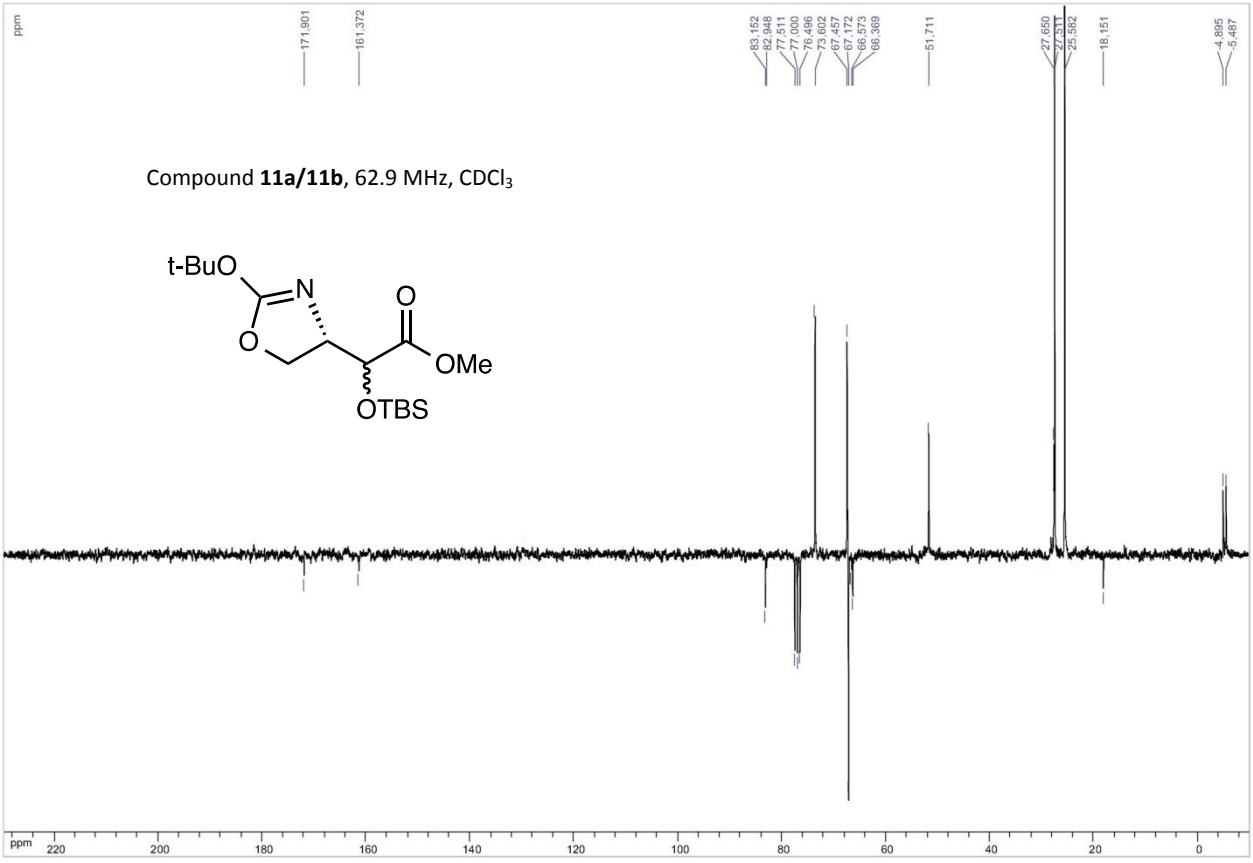

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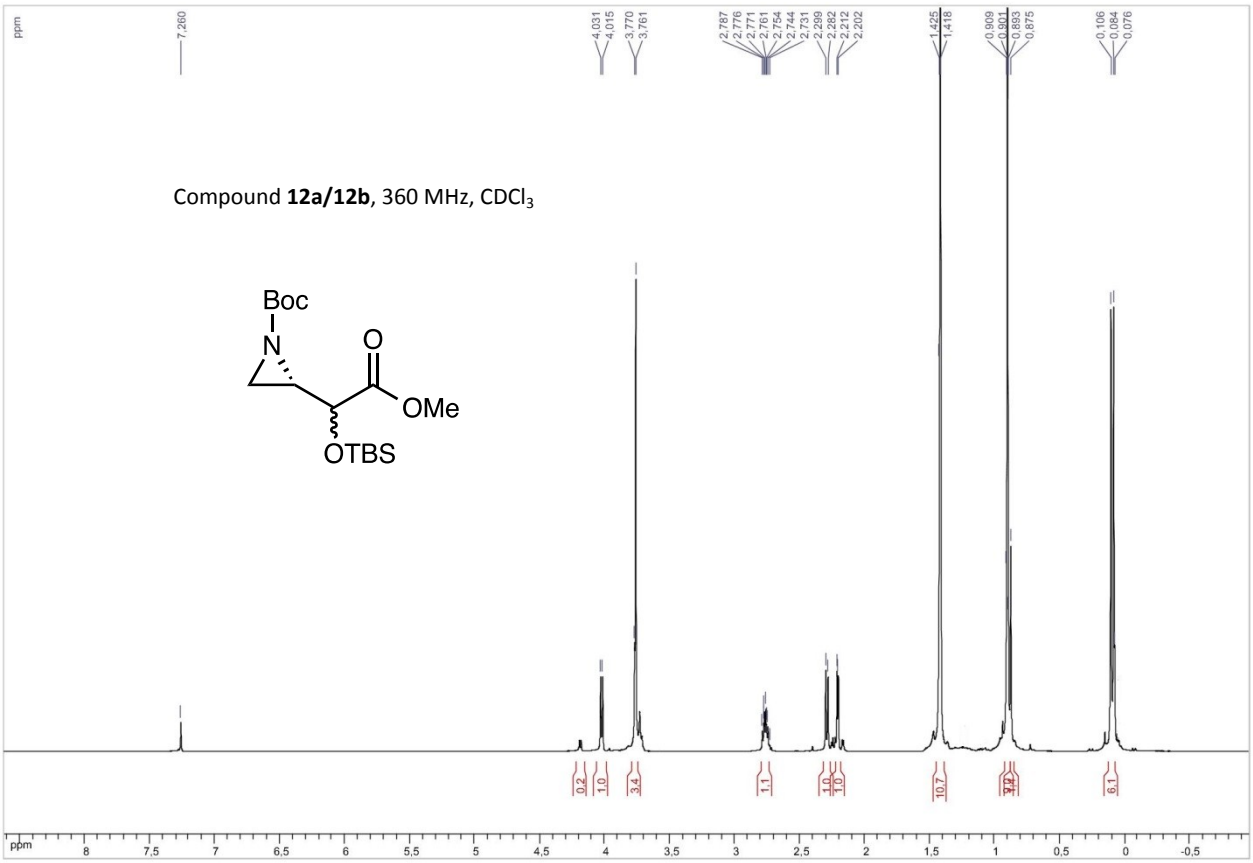
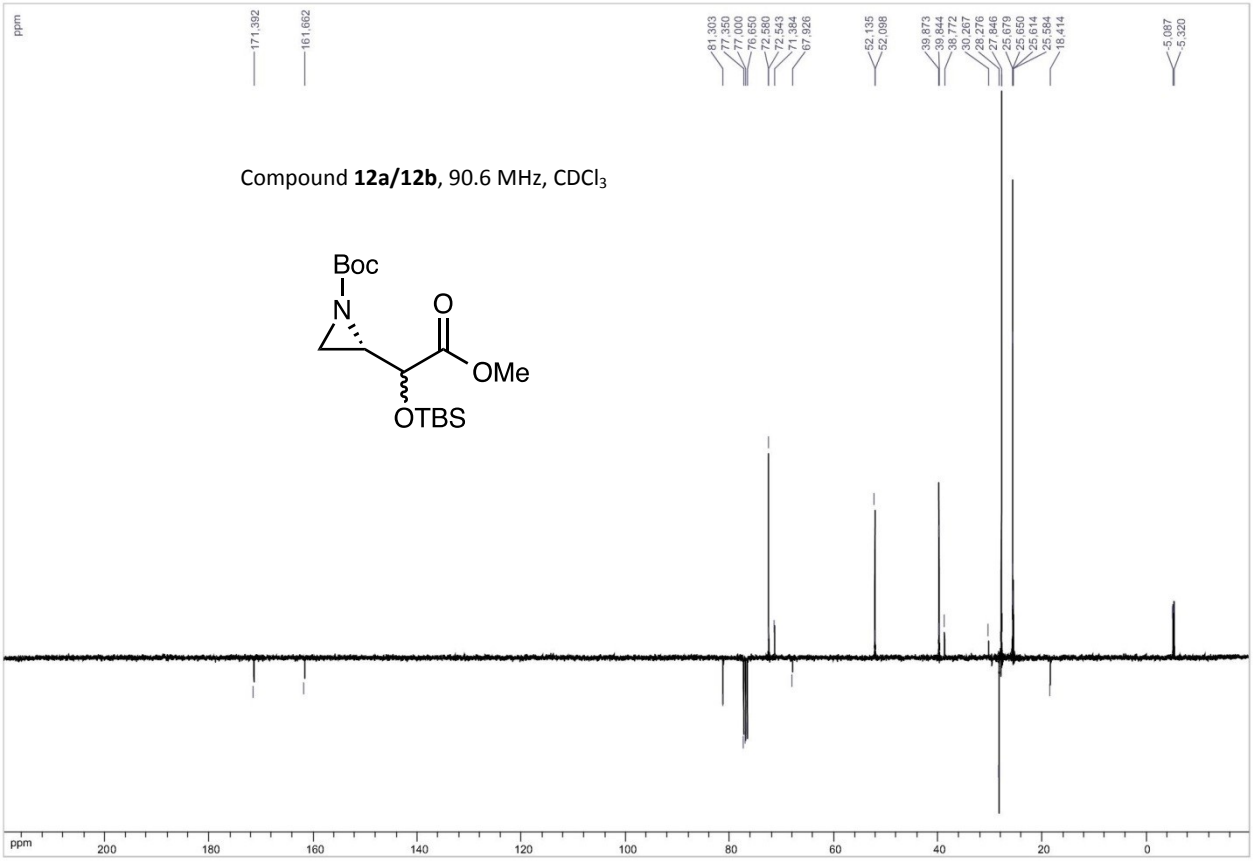
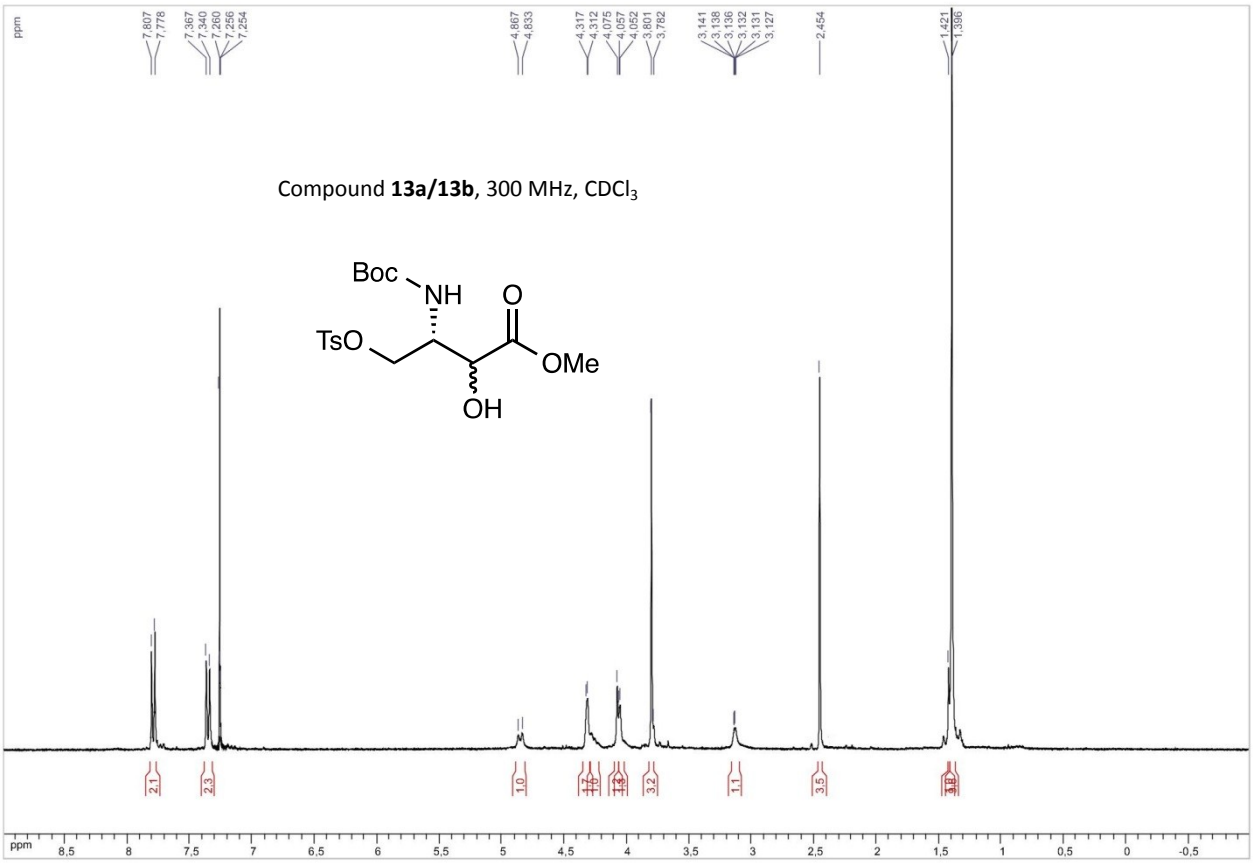
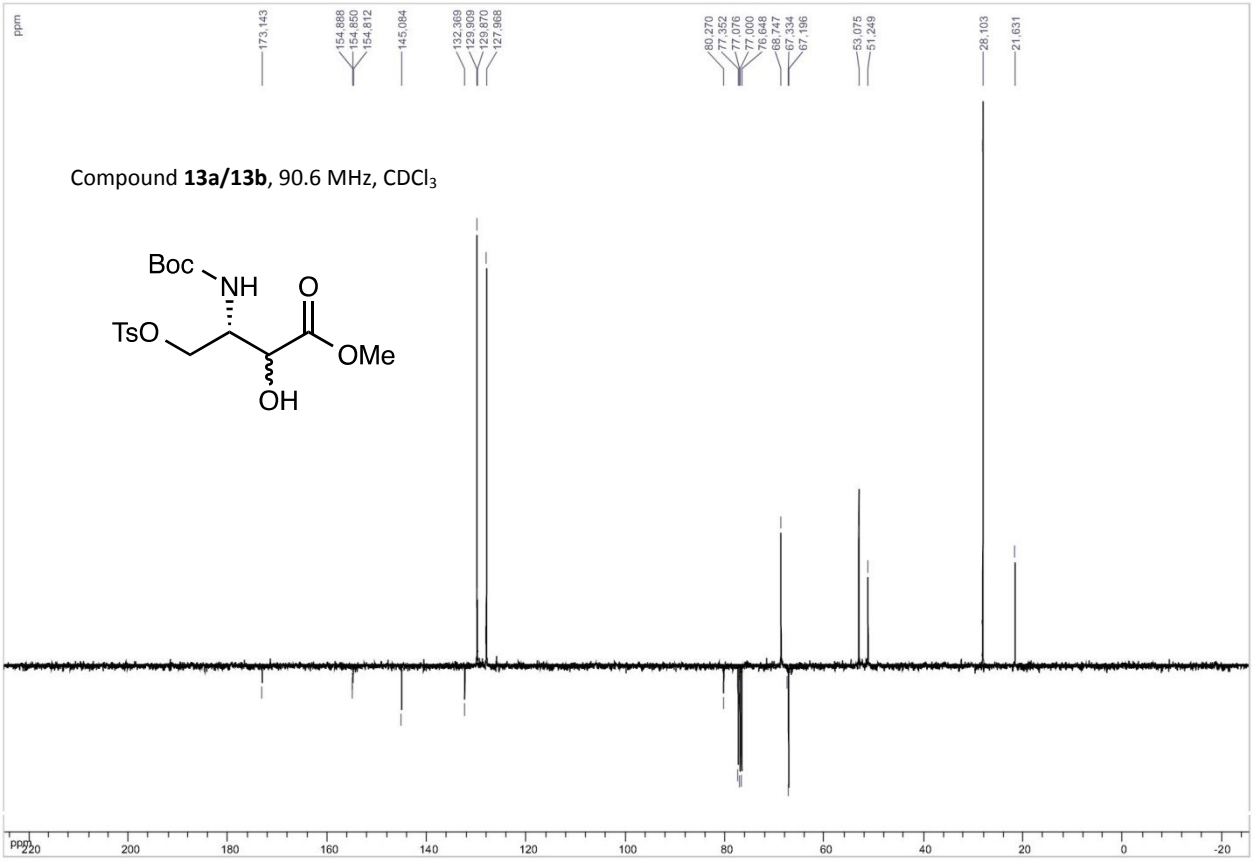


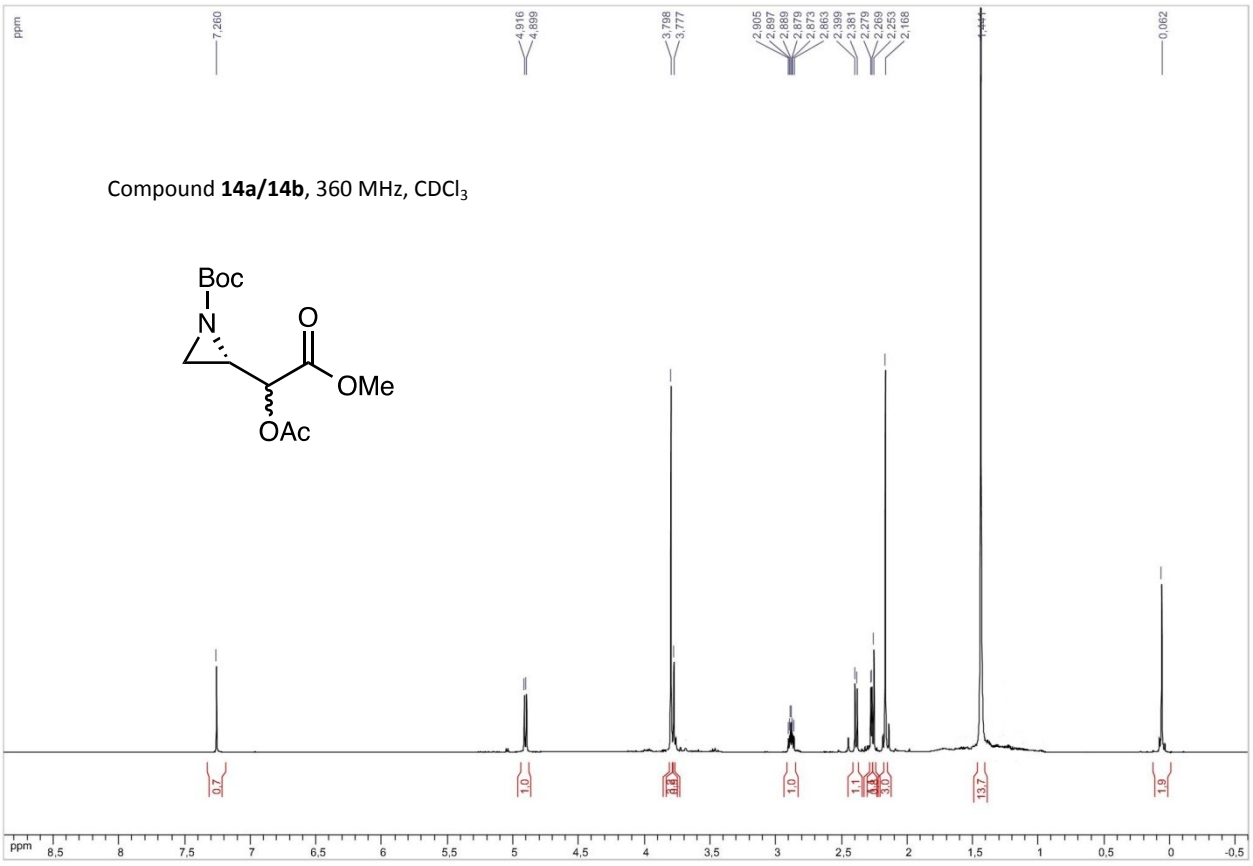


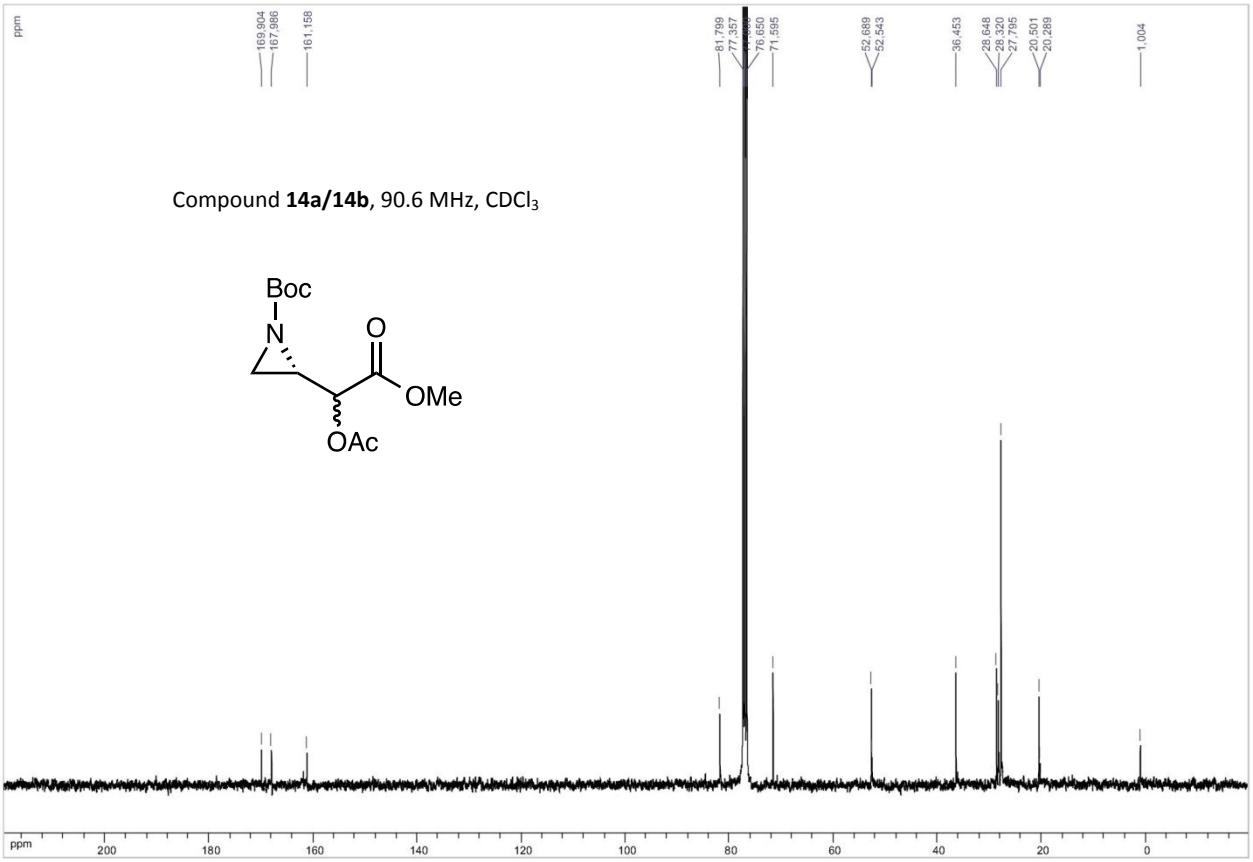
Compound **13a/13b**



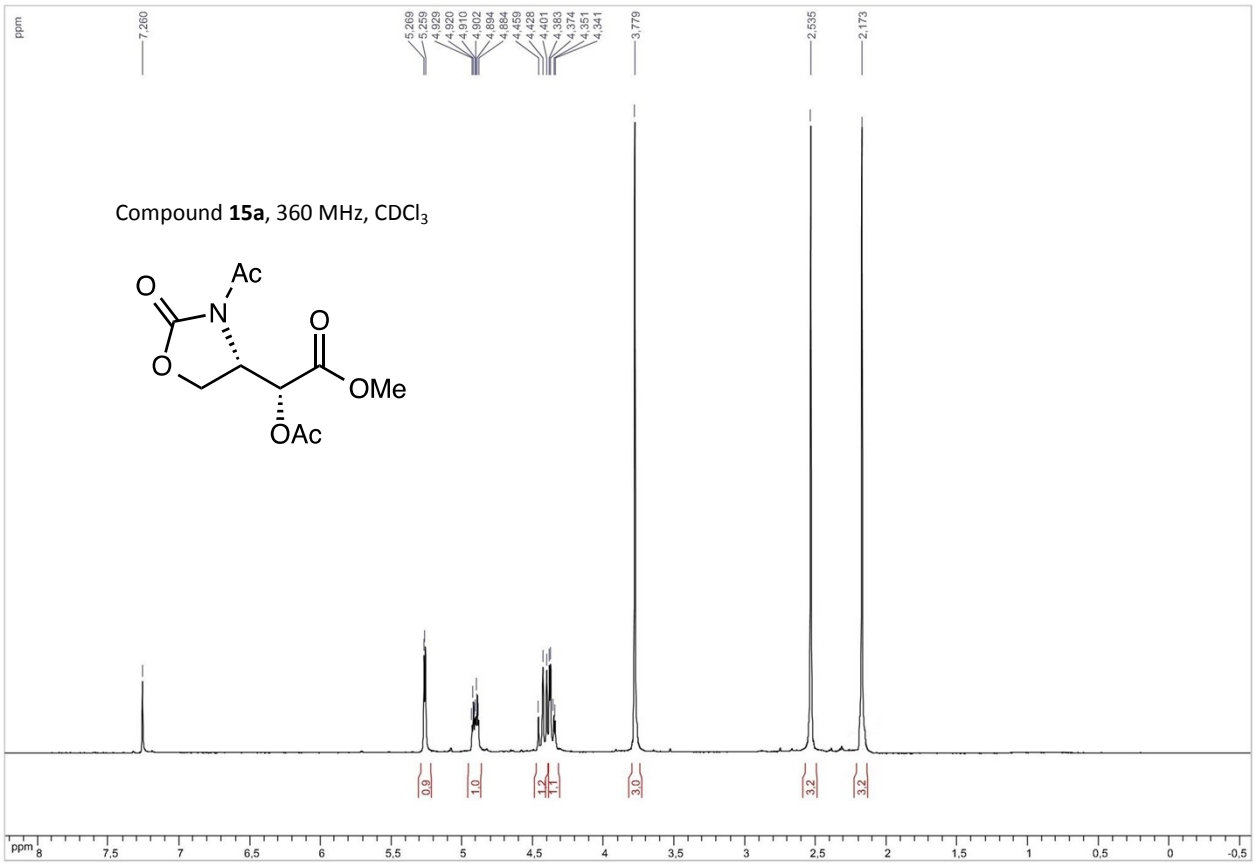


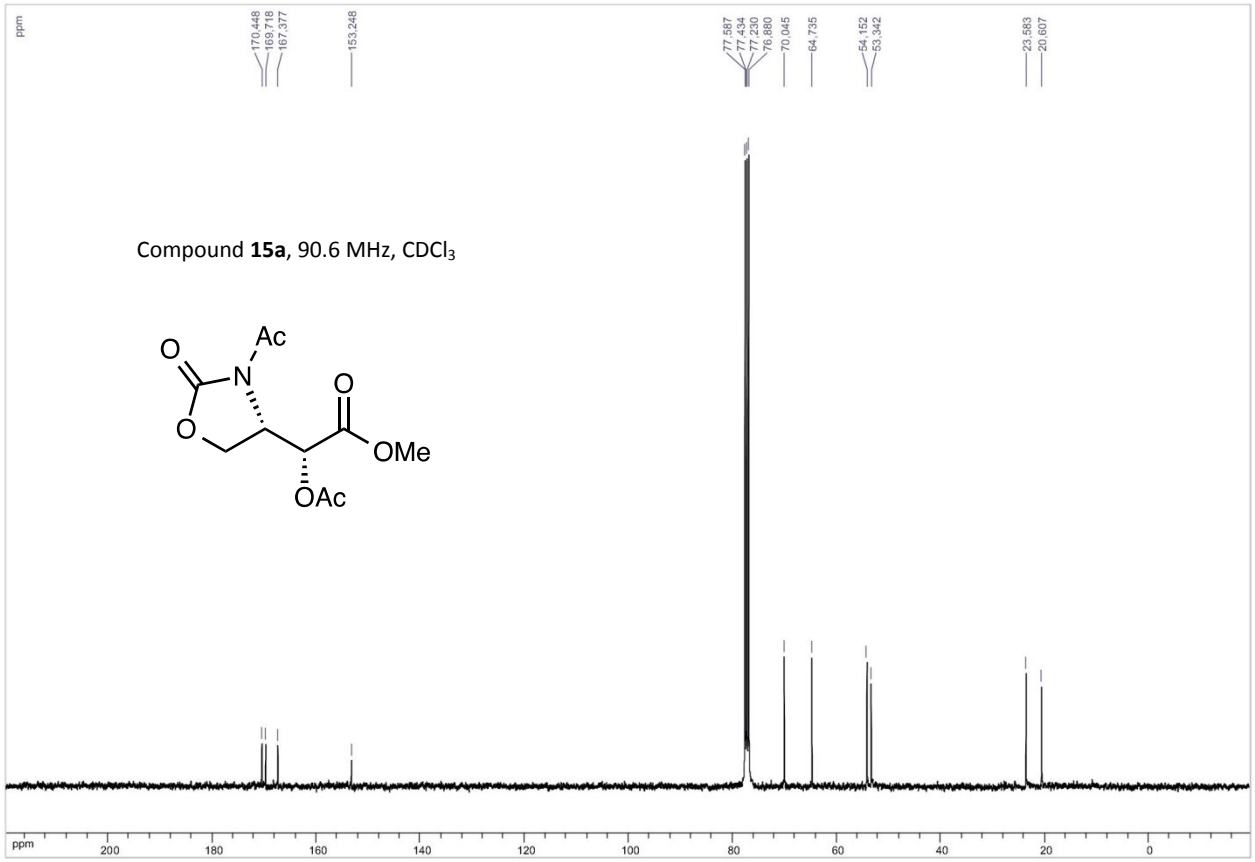
Compound **14a/14b**





Compound **15a**





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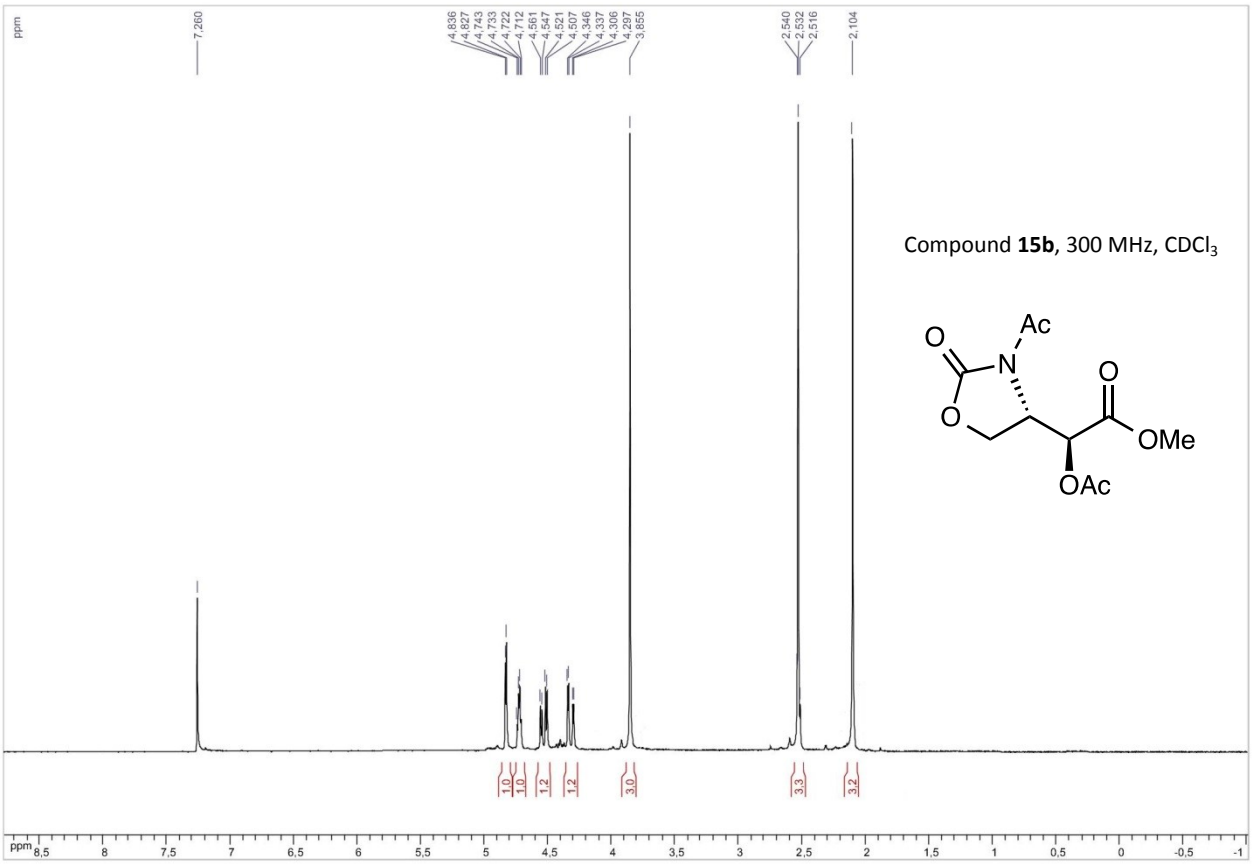

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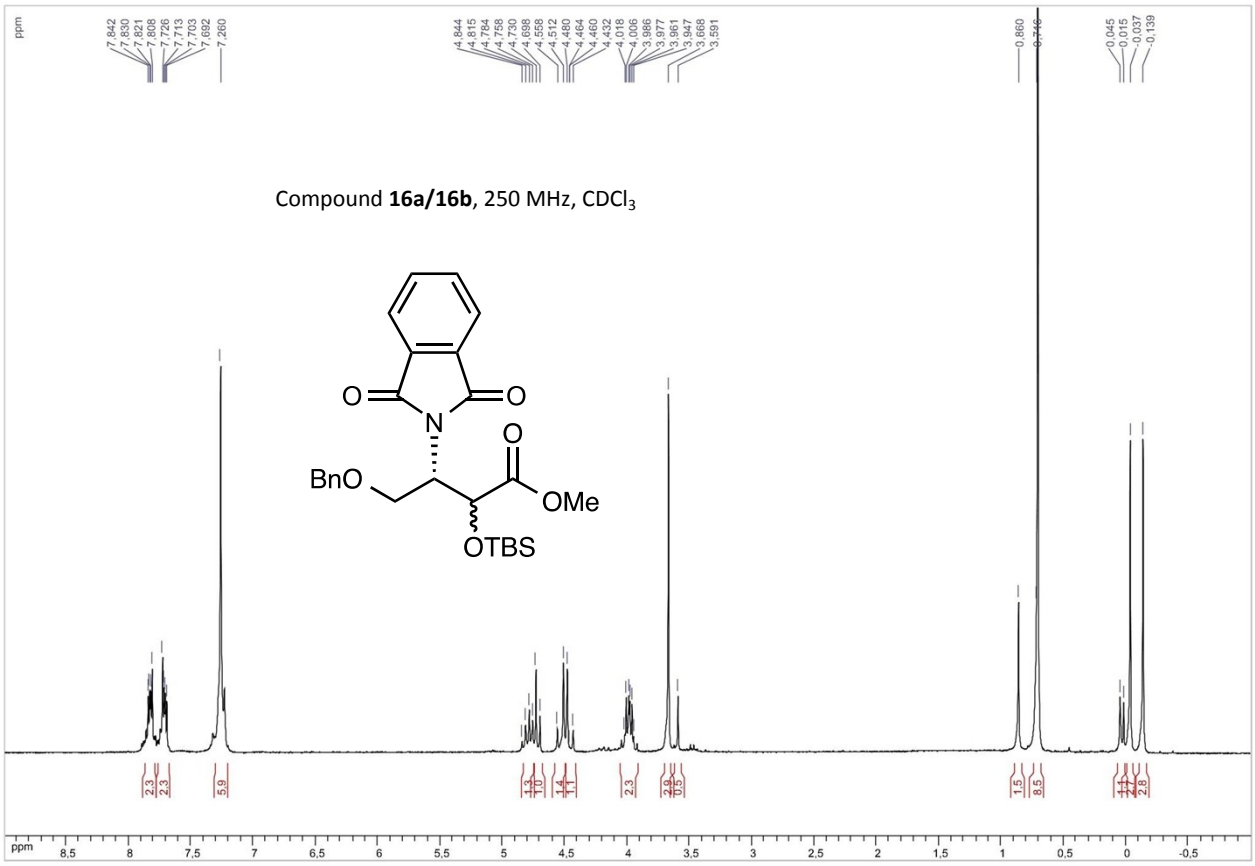
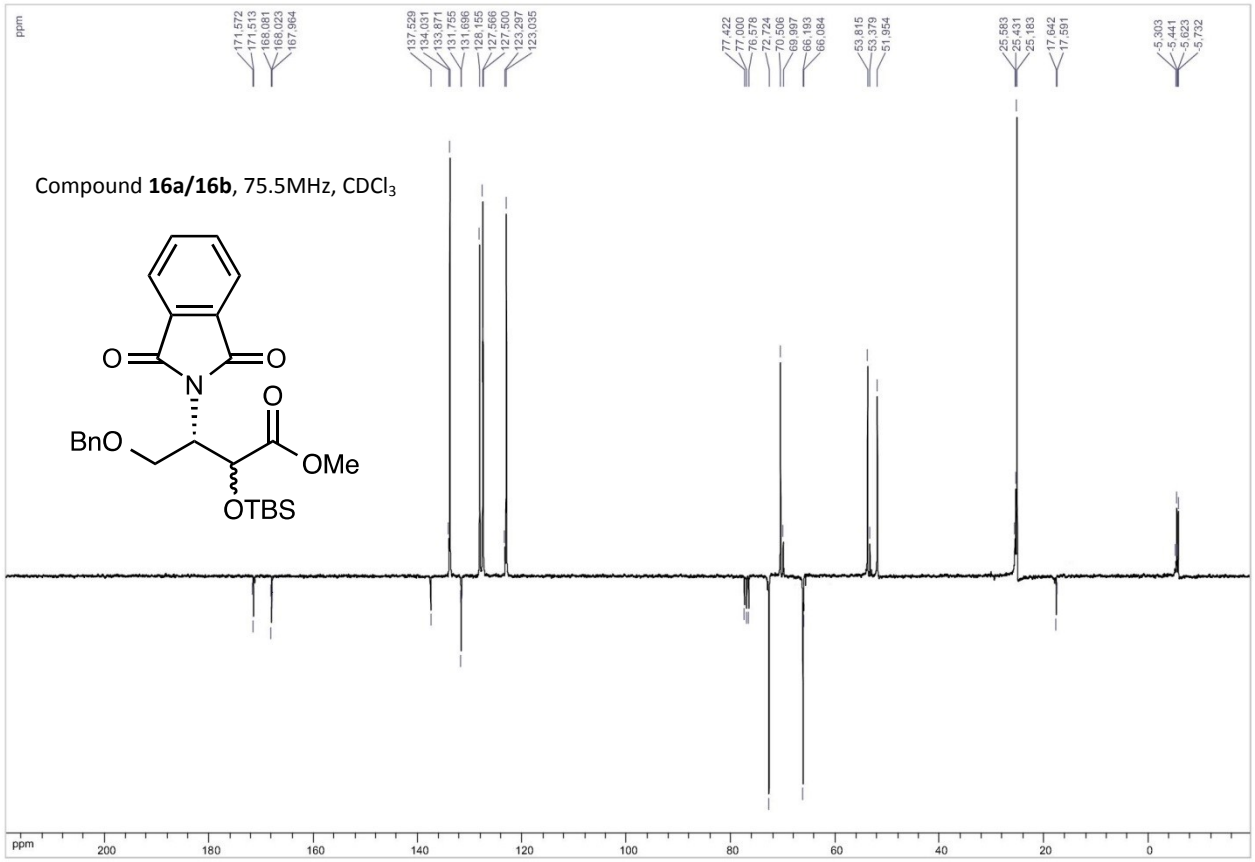
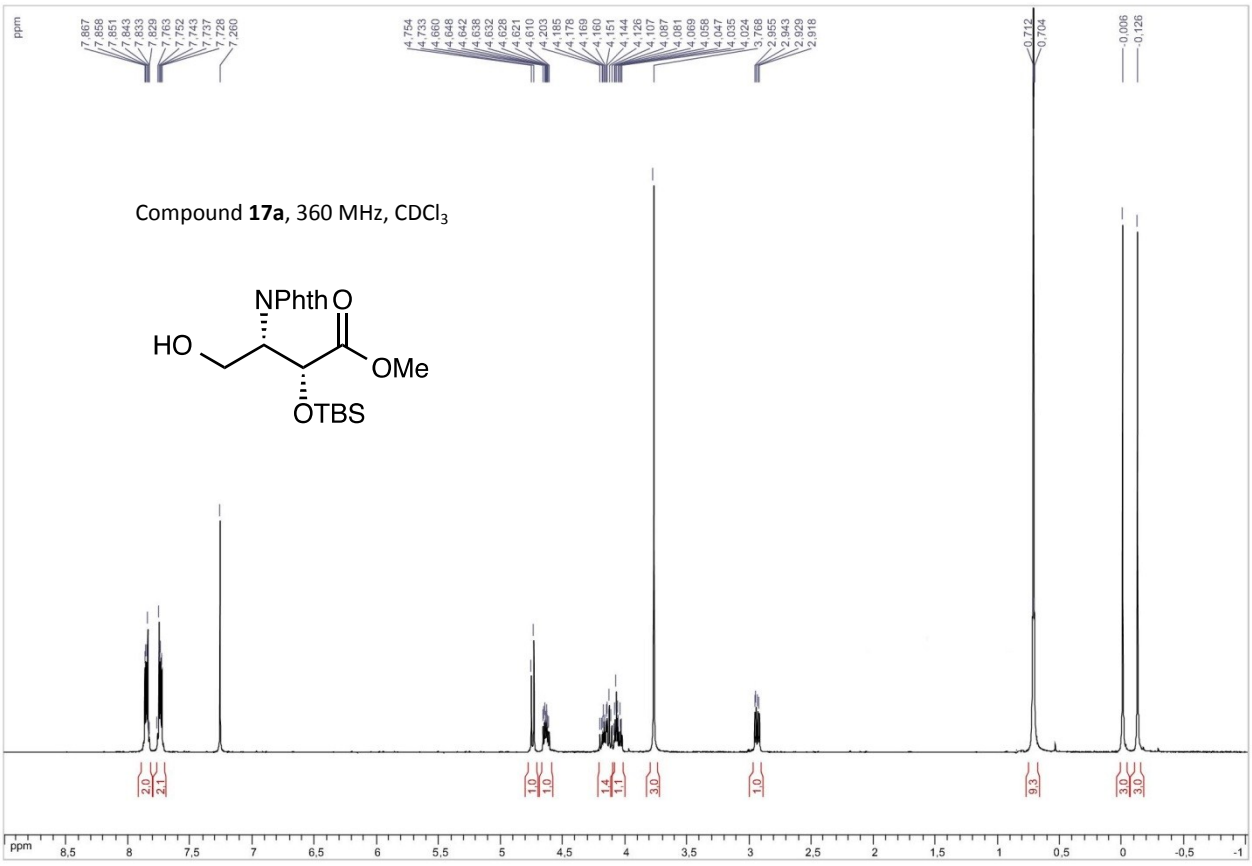
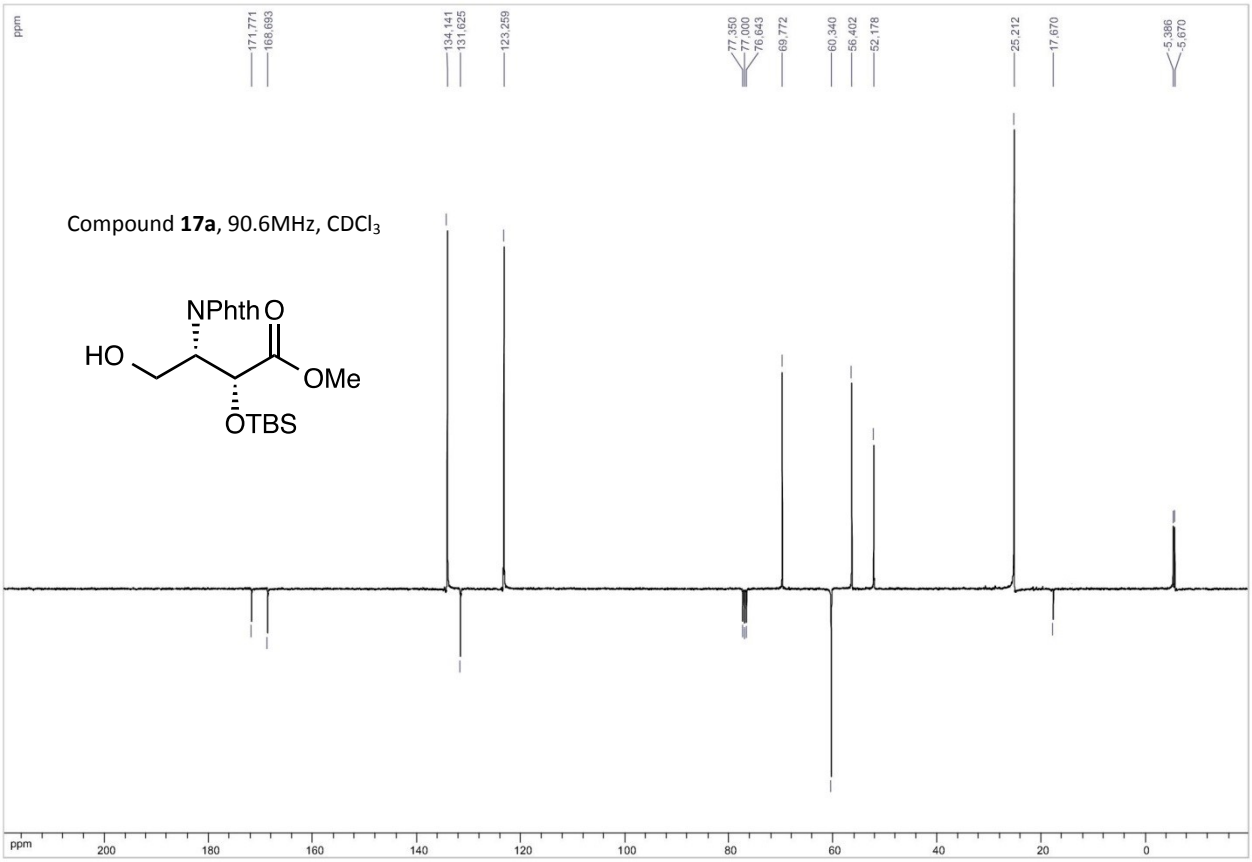


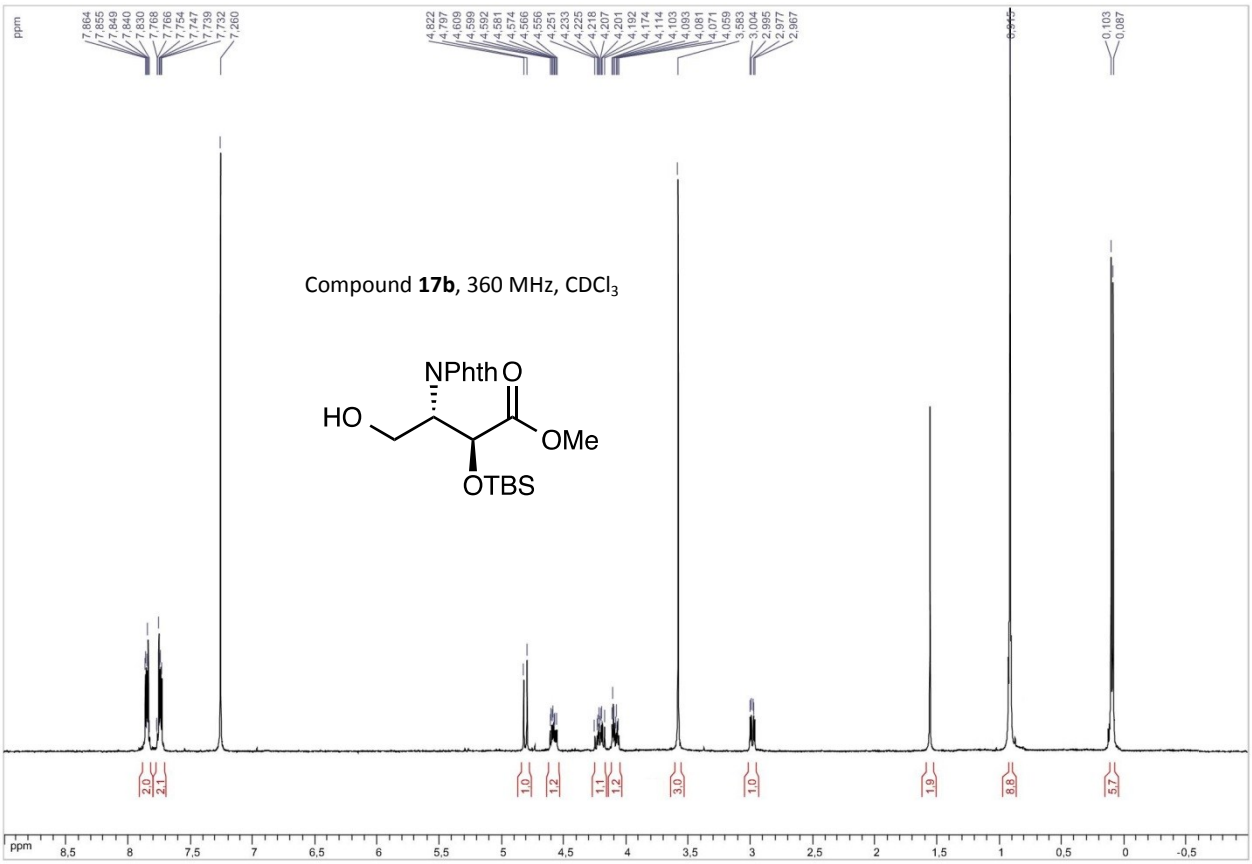


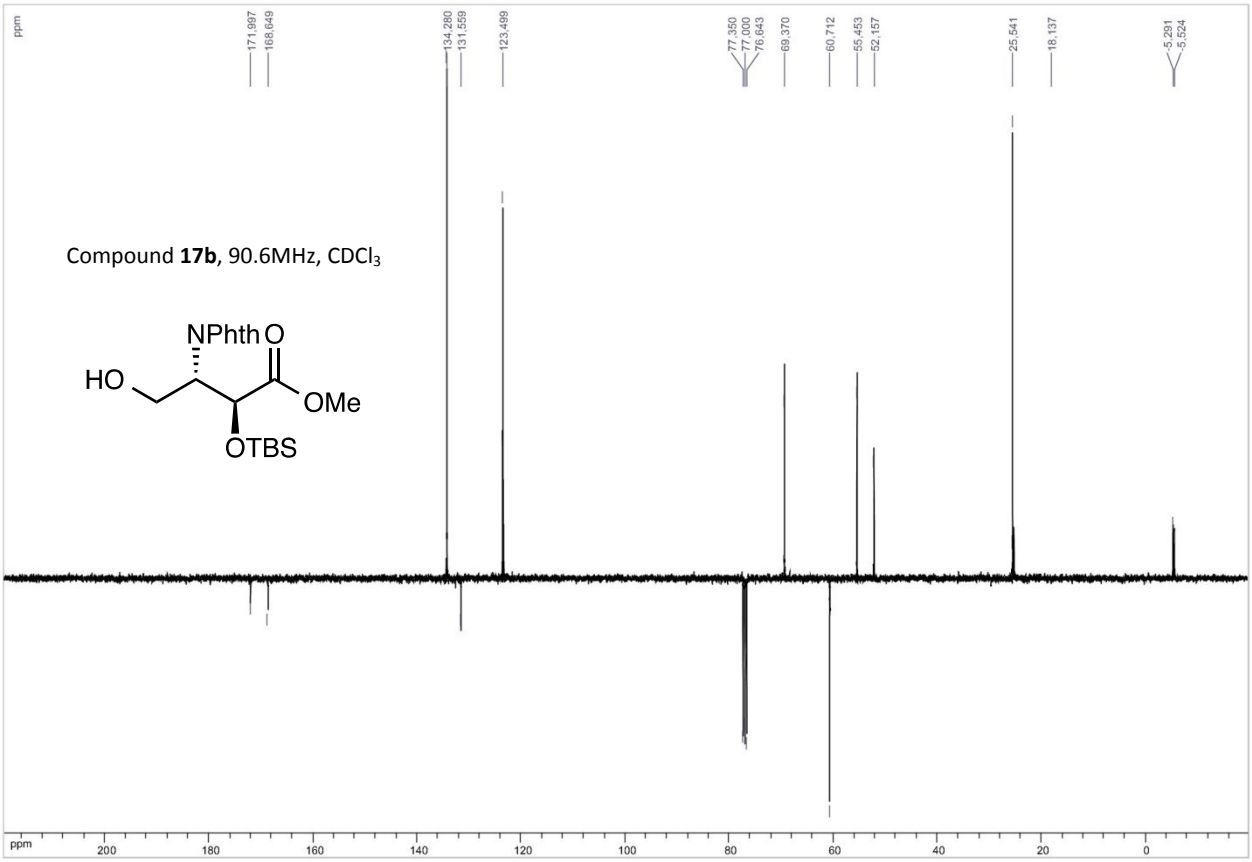
Compound 1**7a**



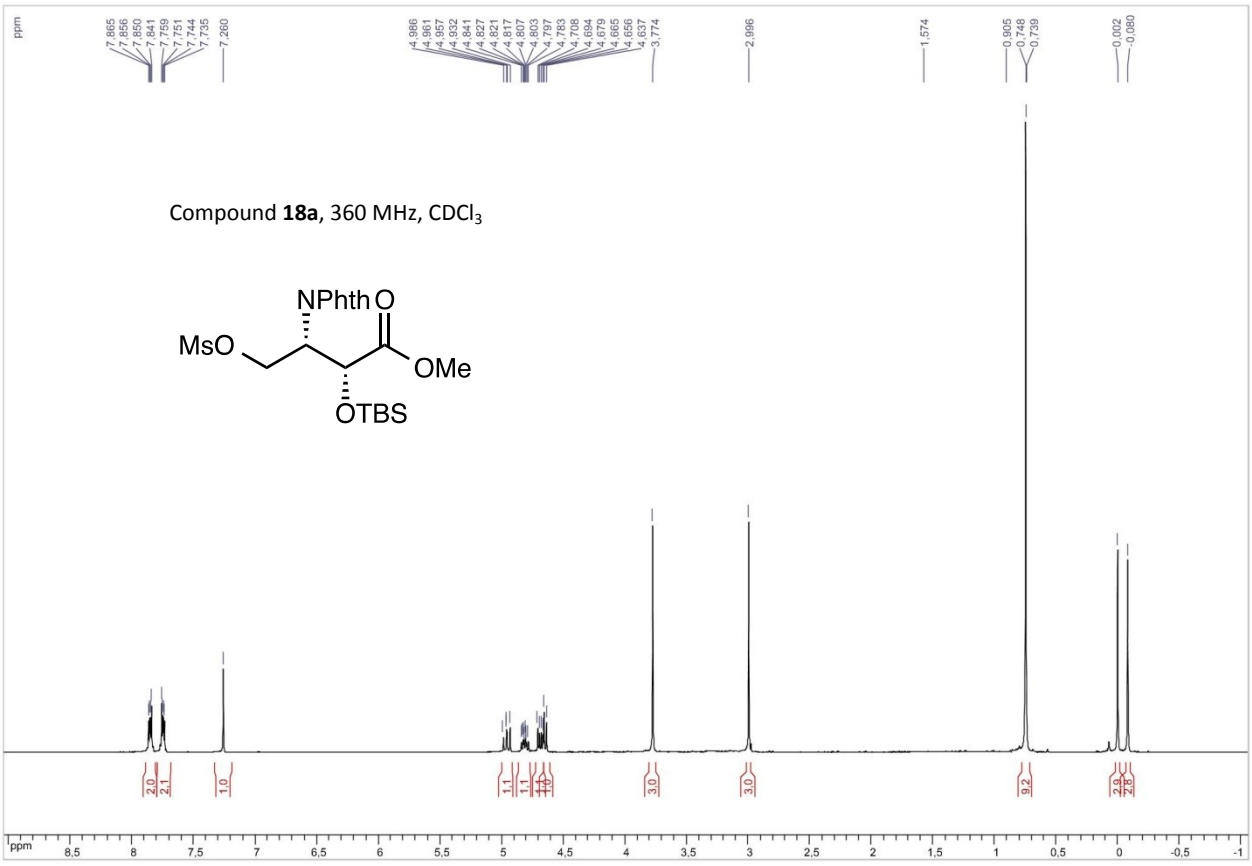


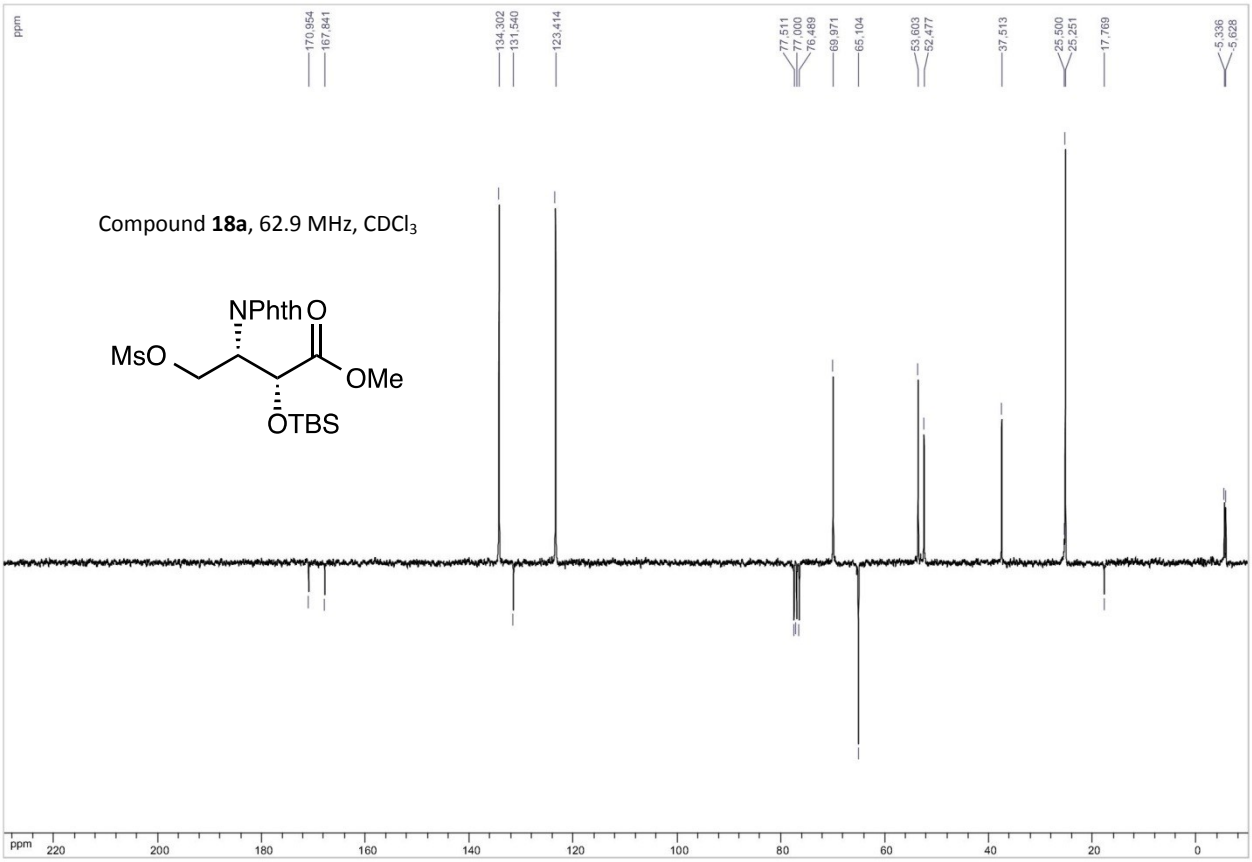
Compound **17b**



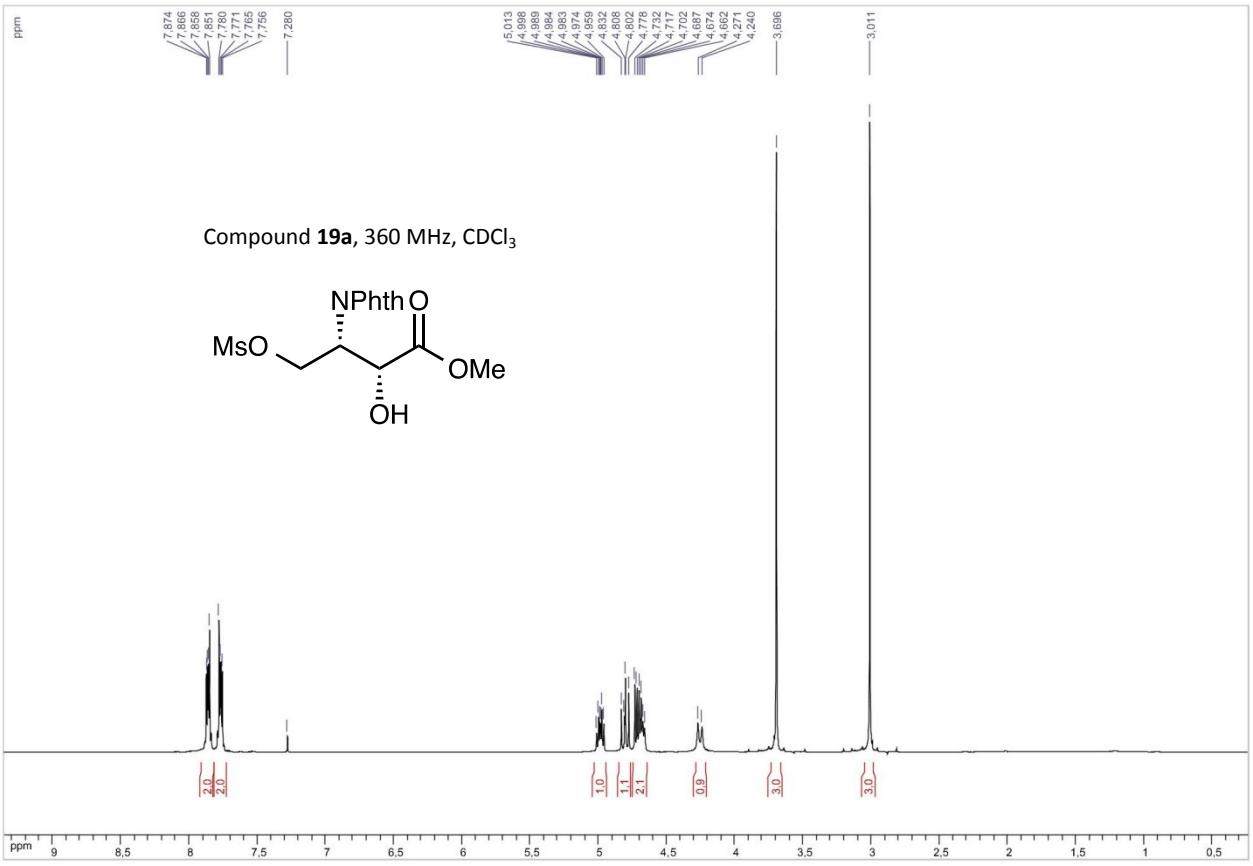


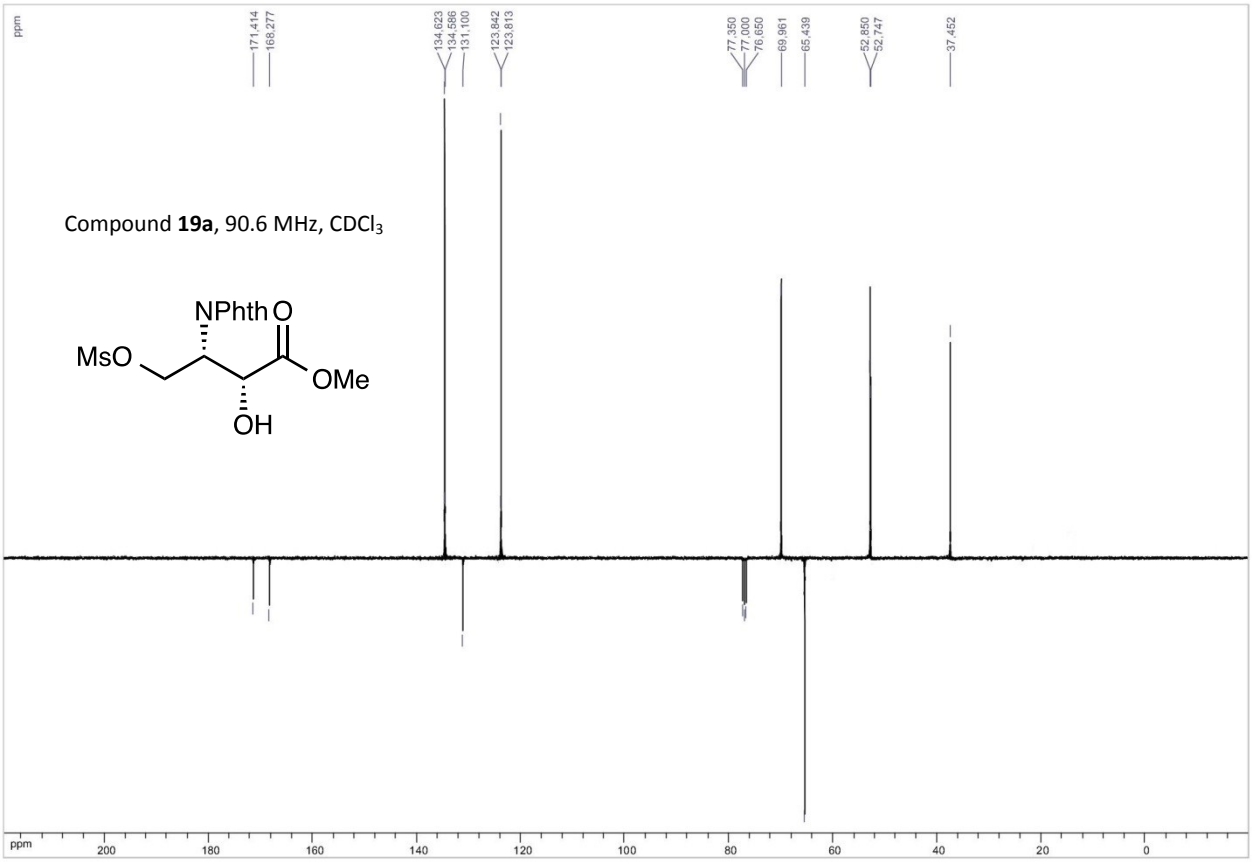
Compound **18a**



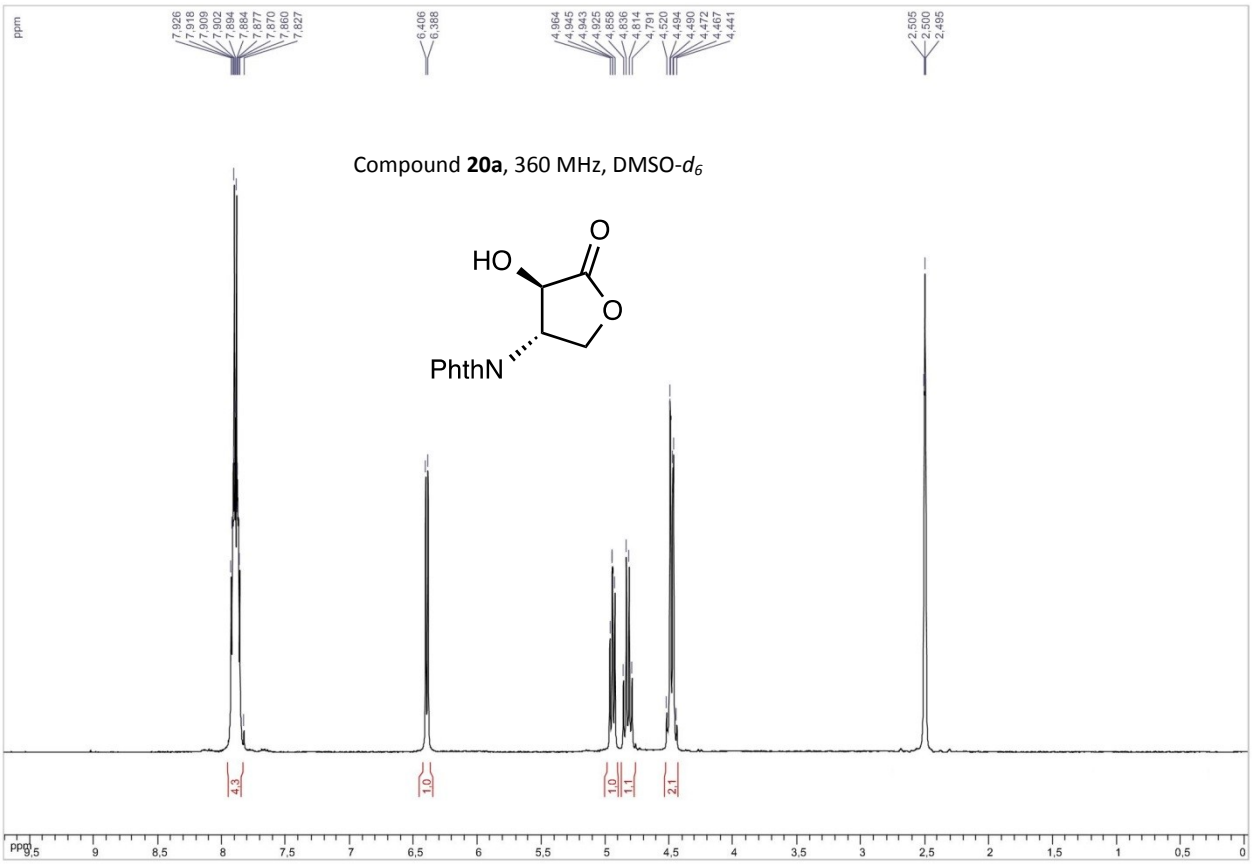


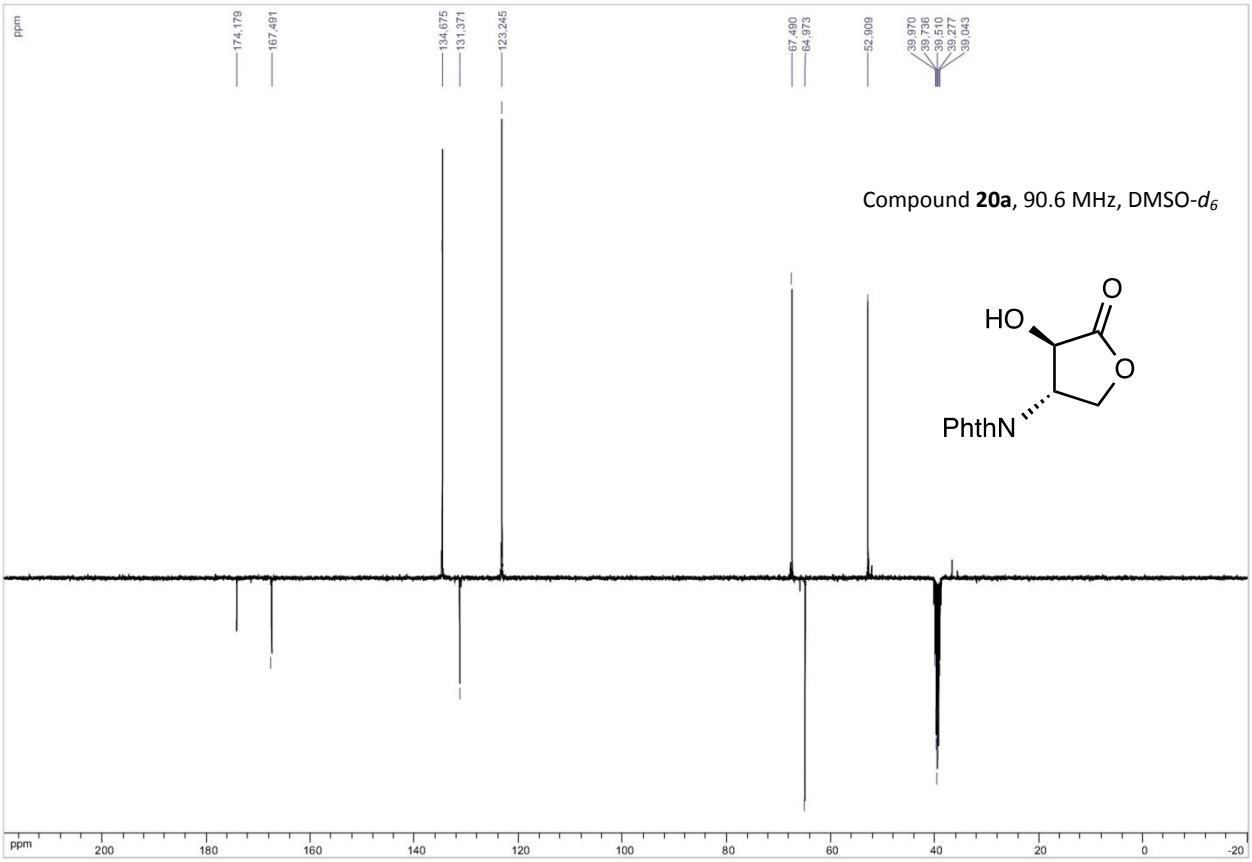
Compound **19a**





Compound **20a**





Crystallographic Data

X-ray diffraction data for compounds **15a**, **17a** and **20a** were collected by using a VENTURE PHOTON100 CMOS Bruker diffractometer with Micro-focus IuS source $Mo_{K\alpha}$ radiation. Crystals were mounted on a CryoLoop (Hampton Research) with Paratone-N (Hampton Research) as cryoprotectant and then flash-frozen in a nitrogen gas stream at 100 K. The temperature of the crystals was maintained at the selected value (100 K) by means of a N-Helix device cooling within an accuracy of ±1 K. The data were corrected for Lorentz polarization and absorption effects. The structures were solved by direct methods using SHELXS-97[1] and refined against F^2 by full-matrix least-squares techniques using SHELXL-2016[2] with anisotropic displacement parameters for all non-hydrogen atoms. Hydrogen atoms were located on a difference Fourier map and introduced into the calculations as a riding model with isotropic thermal parameters. All calculations were performed by using the Crystal Structure crystallographic software package WINGX.[3]

ORTEP drawings are shown in Figures S1, S2 and S3. The crystal data collection and refinement parameters are given in Table S1. CCDC 1520833, 1520834 and 1520835 contain the supplementary crystallographic data for this study. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/Community/Requestastructure.

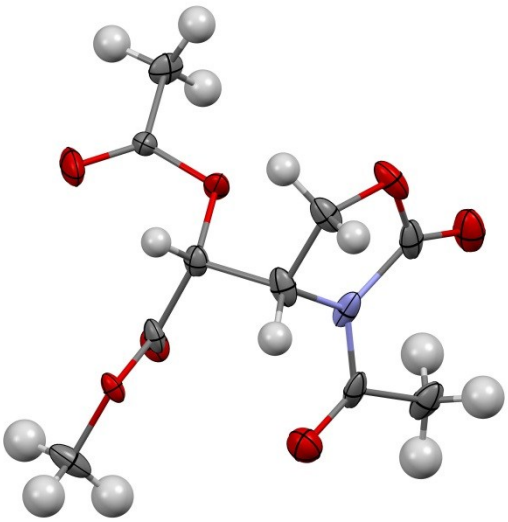


Fig. S1. An ORTEP drawing of compound **15a**. Thermal ellipsoids are shown at the 30% level.

1) Sheldrick, G. M. SHELXS-97, Program for Crystal Structure Solution, University of Göttingen, Göttingen, Germany, **1997**.
2) G. M. Sheldrick, Acta Crystallogr., Sect. A: Found. Crystallogr., **2008**, 64, 112-122
3) Farrugia, L. J. *J. Appl. Cryst*., **1999**, *32*, 837.

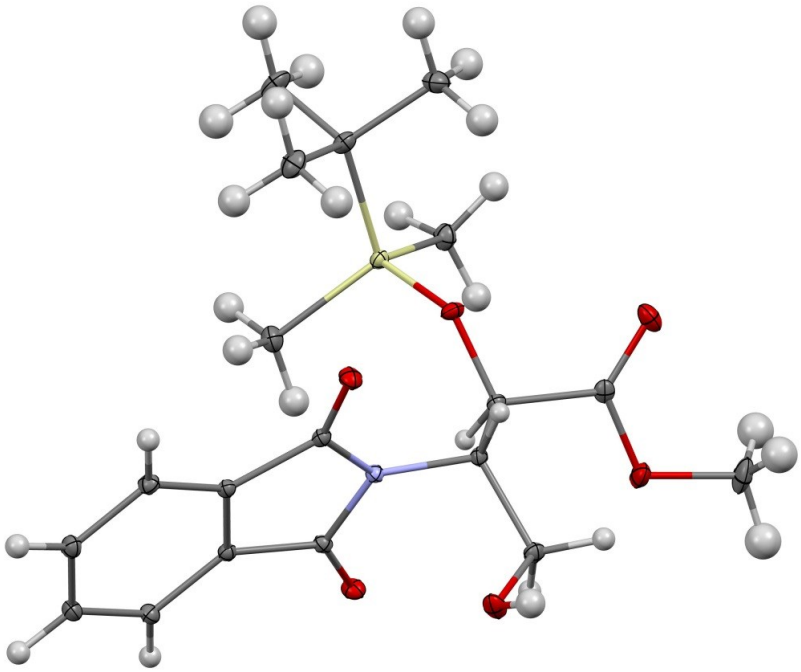


Fig. S2. An ORTEP drawing of compound **17a**. Thermal ellipsoids are shown at the 30% level.

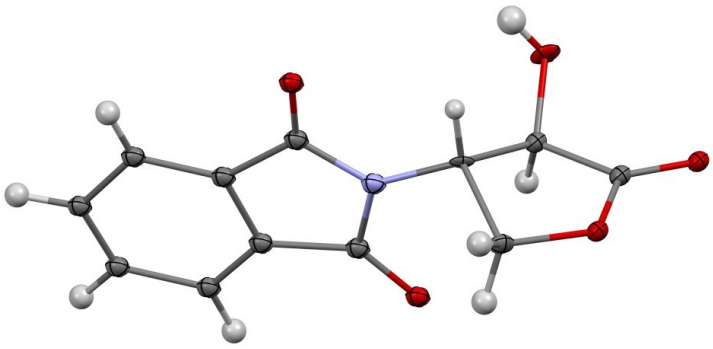


Fig. S3. An ORTEP drawing of compound **20a**. Thermal ellipsoids are shown at the 30% level.

Table S1. Crystallographic data and structure refinement details.

Compound	**15a**	**17a**	**20a**
Empirical formula	C_{10} H_{13} N O_7	C_{19} H_{27} N O_6 Si	C_{12} H_9 N O_5
M_r	259.21	393.50	247.20
Crystal size, mm	0.09 × 0.05 × 0.01	0.12 × 0.11 × 0.08	0.13 × 0.07 × 0.01
Crystal system	monoclinic	monoclinic	monoclinic
Space group	*P* 2_1	*P* 2_1	*P* 2_1
a, Å	6.0454(6)	8.1774(4)	8.2084(14)
b, Å	14.0347(14)	8.2158(3)	5.2477(8)
c, Å	7.1416(8)	15.0345(7)	24.351(4)
α, °	90	90	90
β, °	101.033(3)	98.231(2)	90.768(5)
γ, °	90	90	90
Cell volume, Å^3	594.73(11)	999.67(8)	1048.8(3)
Z ; Z’	2 ; 1	2 ; 1	4 ; 2
T, K	100(1)	100(1)	100(1)
Radiation type ; wavelength Å	MoKα ; 0.71073	MoKα ; 0.71073	MoKα ; 0.71073
F_{000}	272	420	512
μ, mm^{-1}	0.124	0.152	0.124
θ range, °	2.903 - 30.409	2.517 - 30.554	2.481 - 26.435
Reflection collected	20 042	42 103	20 958
Reflections unique	3 515	6 114	4 289
R_{int}	0.0943	0.0235	0.0587
GOF	1.062	1.055	1.159
Refl. obs. ($I > 2\sigma(I)$)	2 242	5 766	3 895
Parameters	166	252	202
Flack parameter	0.1(4)	0.03(2)	0.9(6)
wR_2 (all data)	0.3029	0.0635	0.3717
R value ($I > 2\sigma(I)$)	0.1101	0.0254	0.1518
Largest diff. peak and hole (e$^-$.Å^{-3})	1.060 ; –0.377	0.260 ; –0.226	1.245 ; –0.734