Supplementary Material

Synthetic studies toward eleganine A

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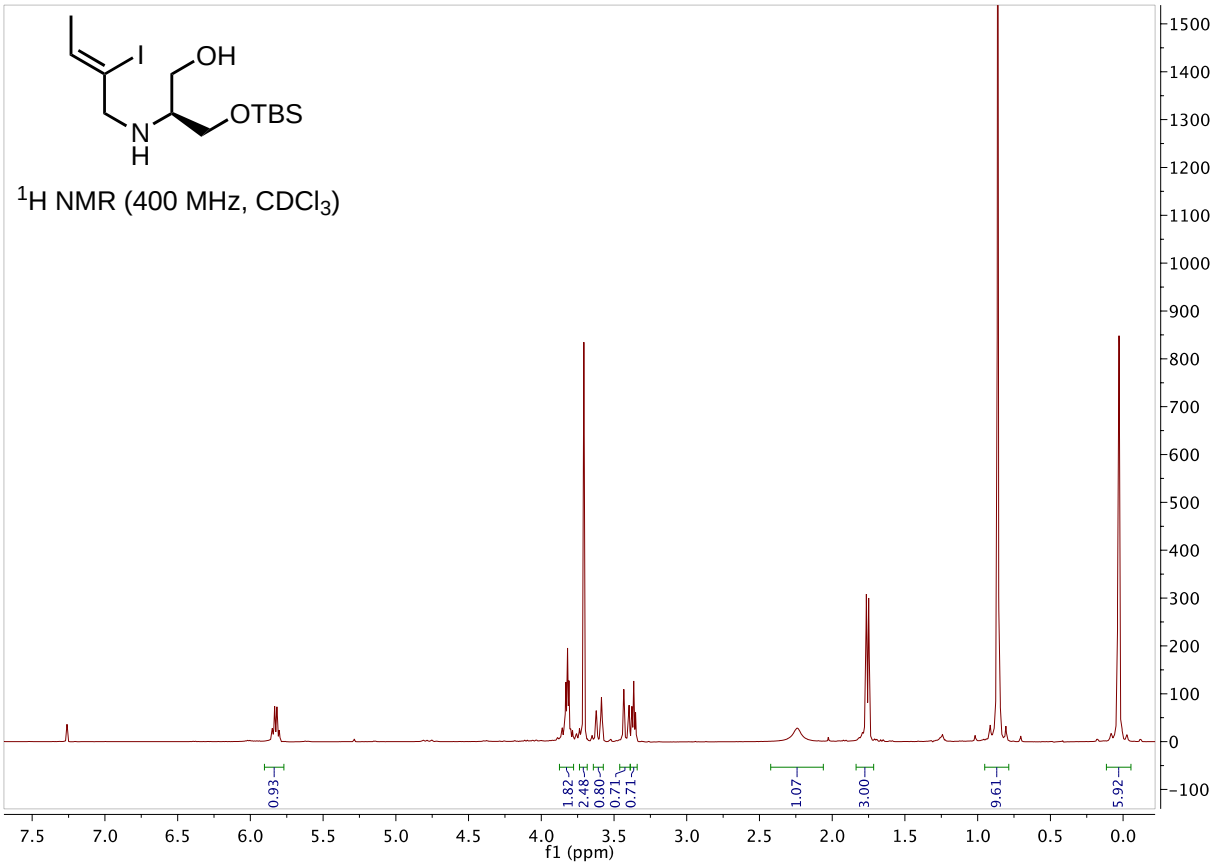
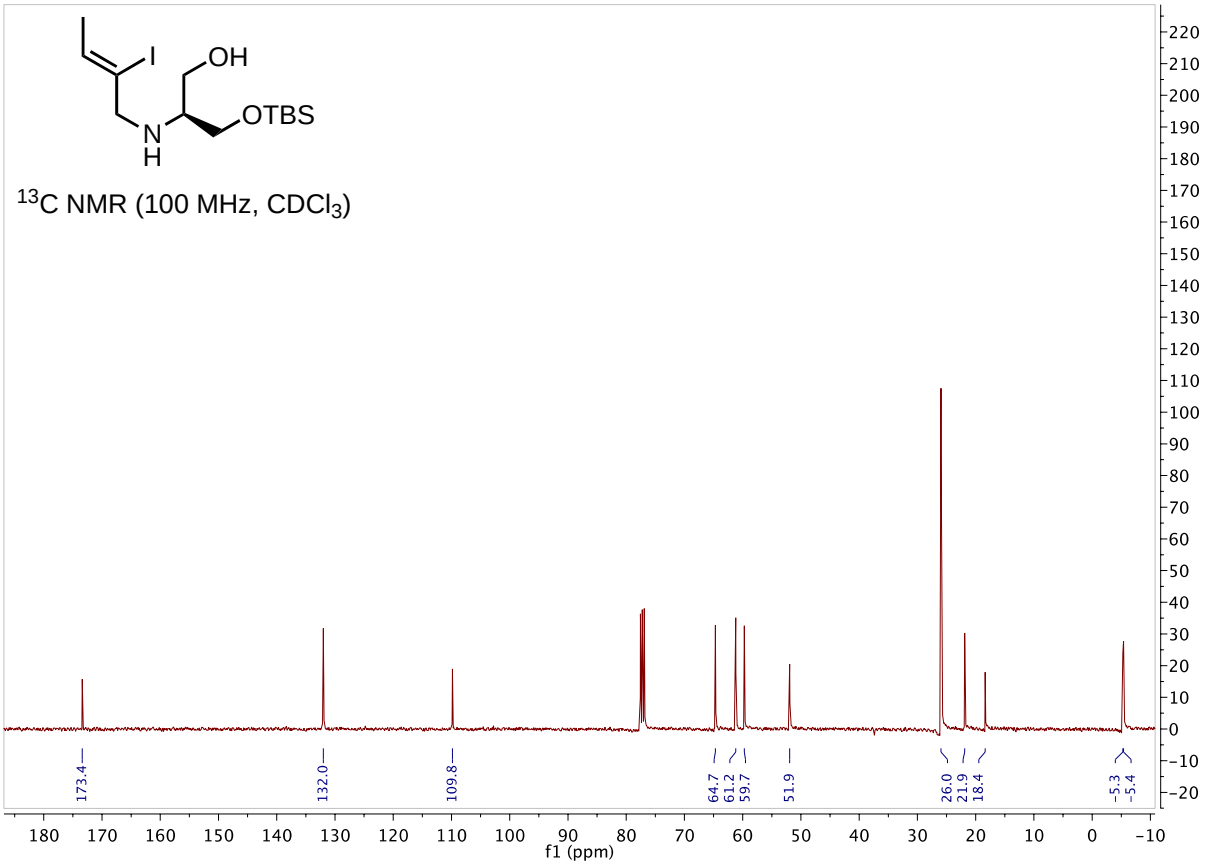


^{1}H NMR (400 MHz, $CDCl_3$)



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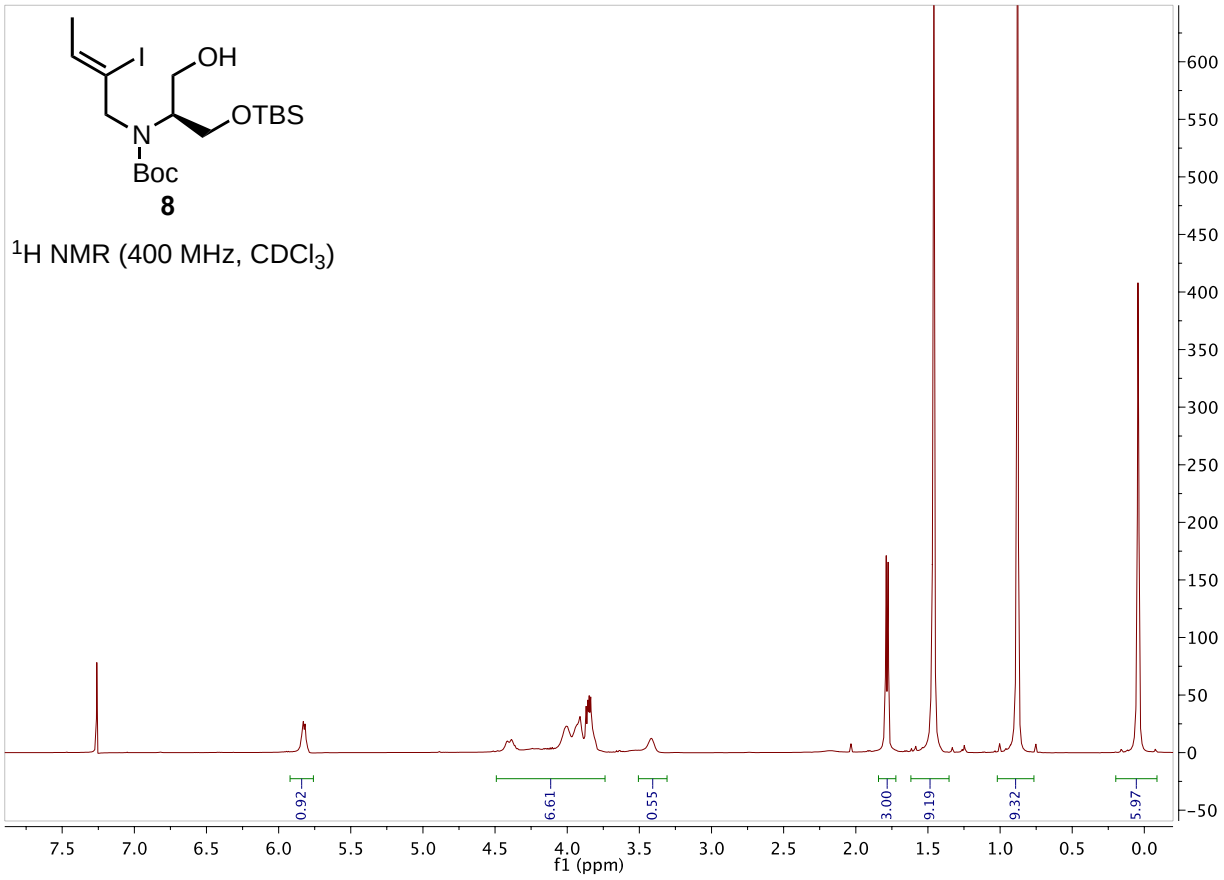

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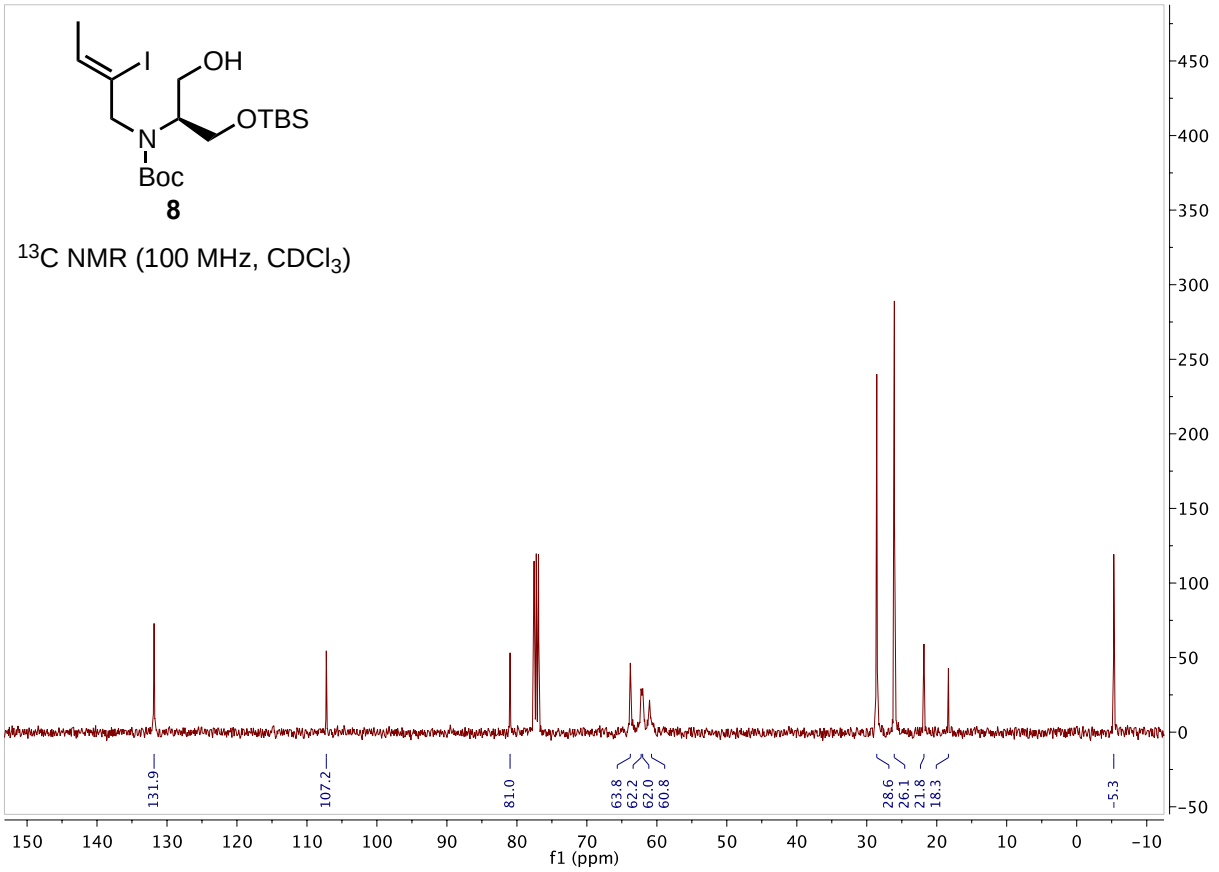

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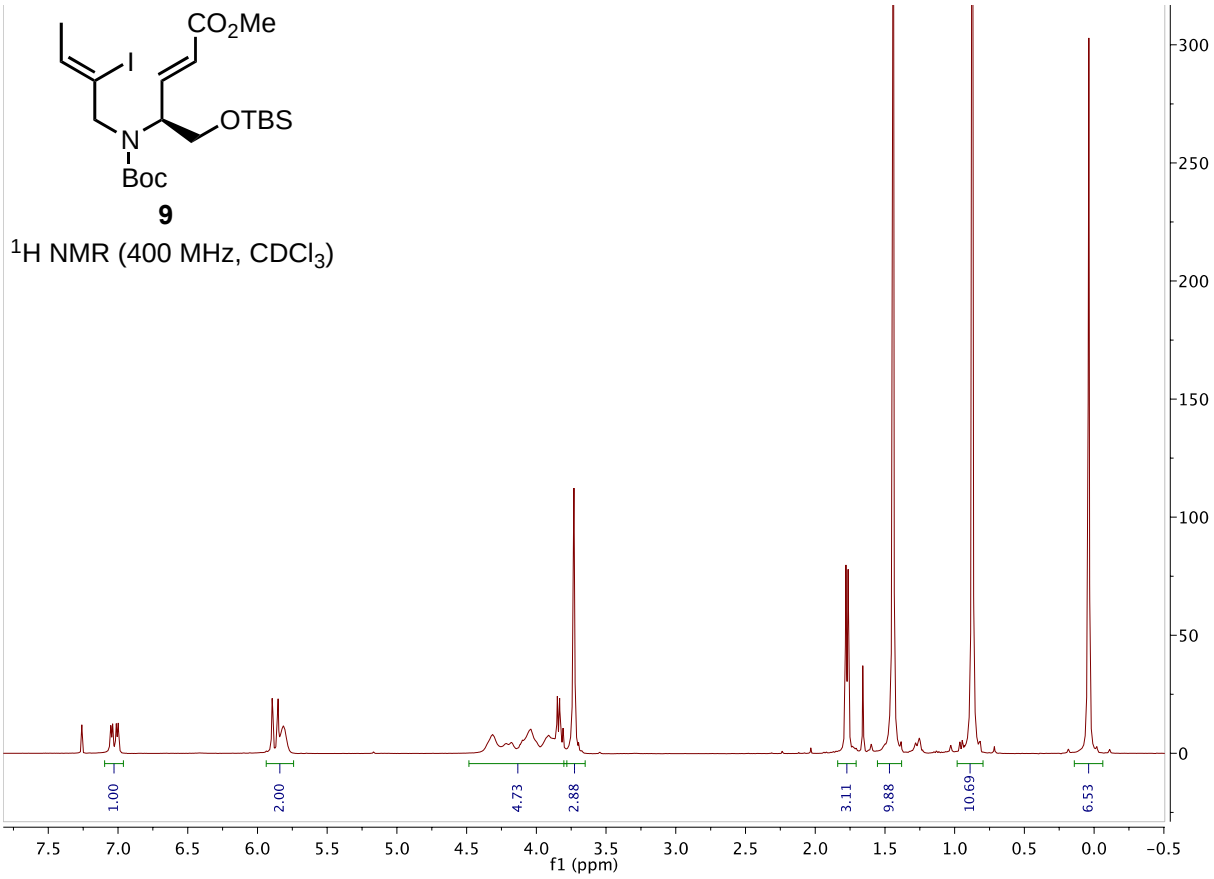

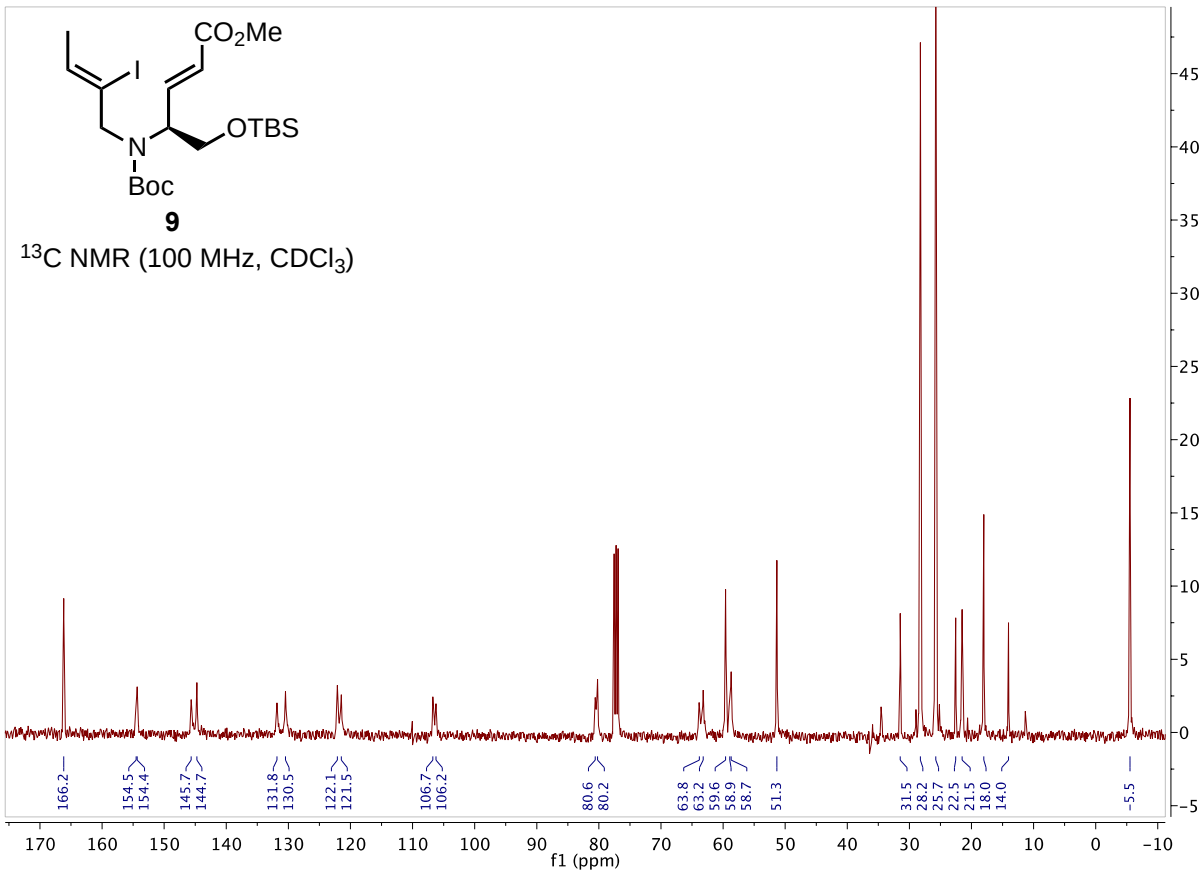

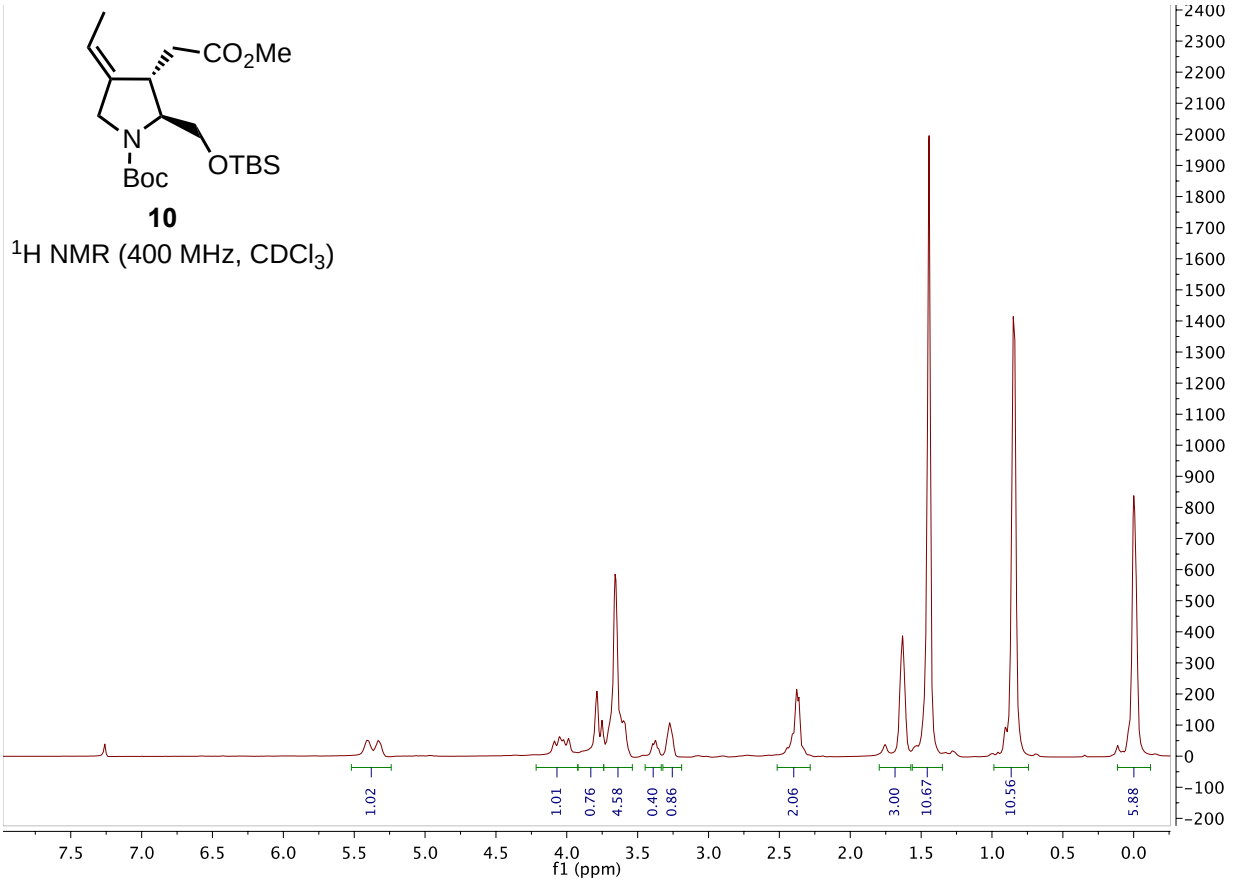

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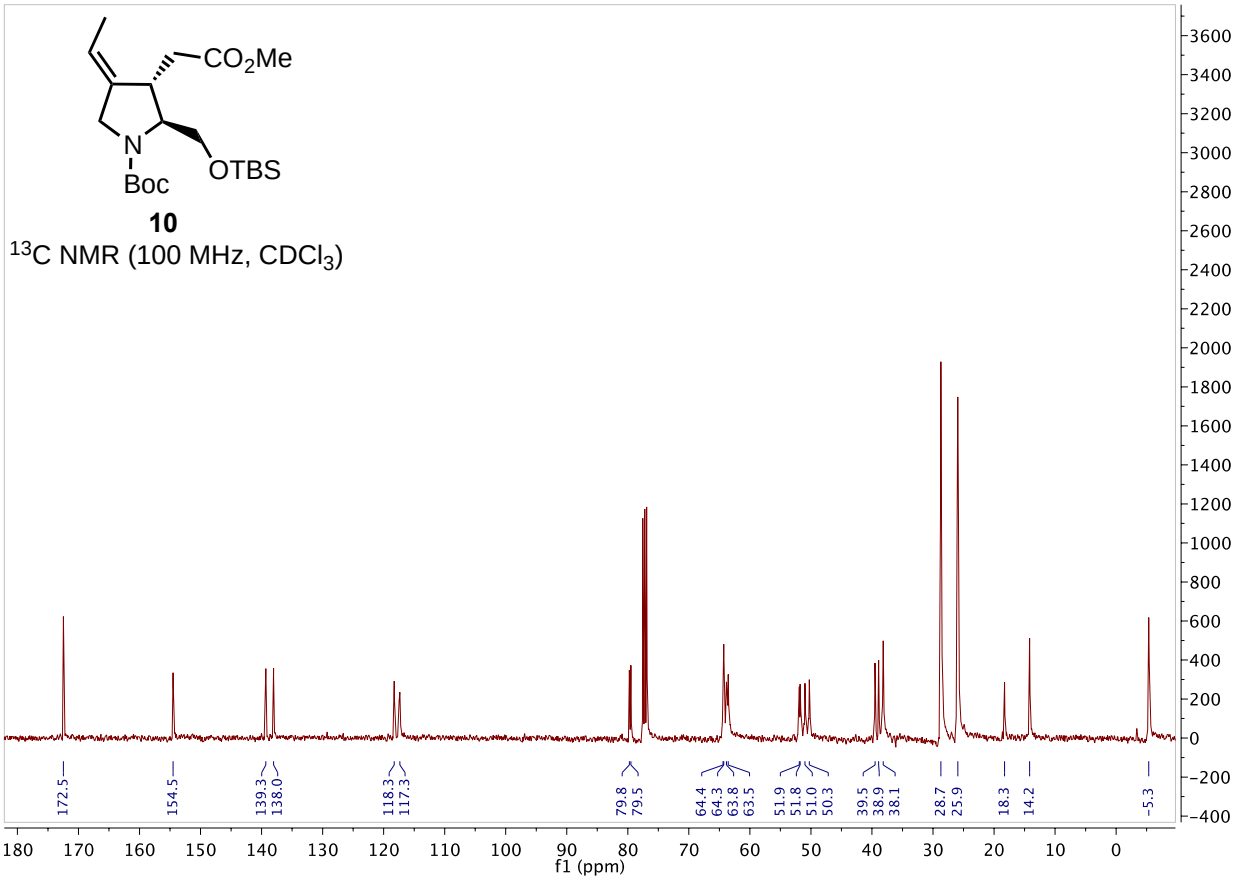

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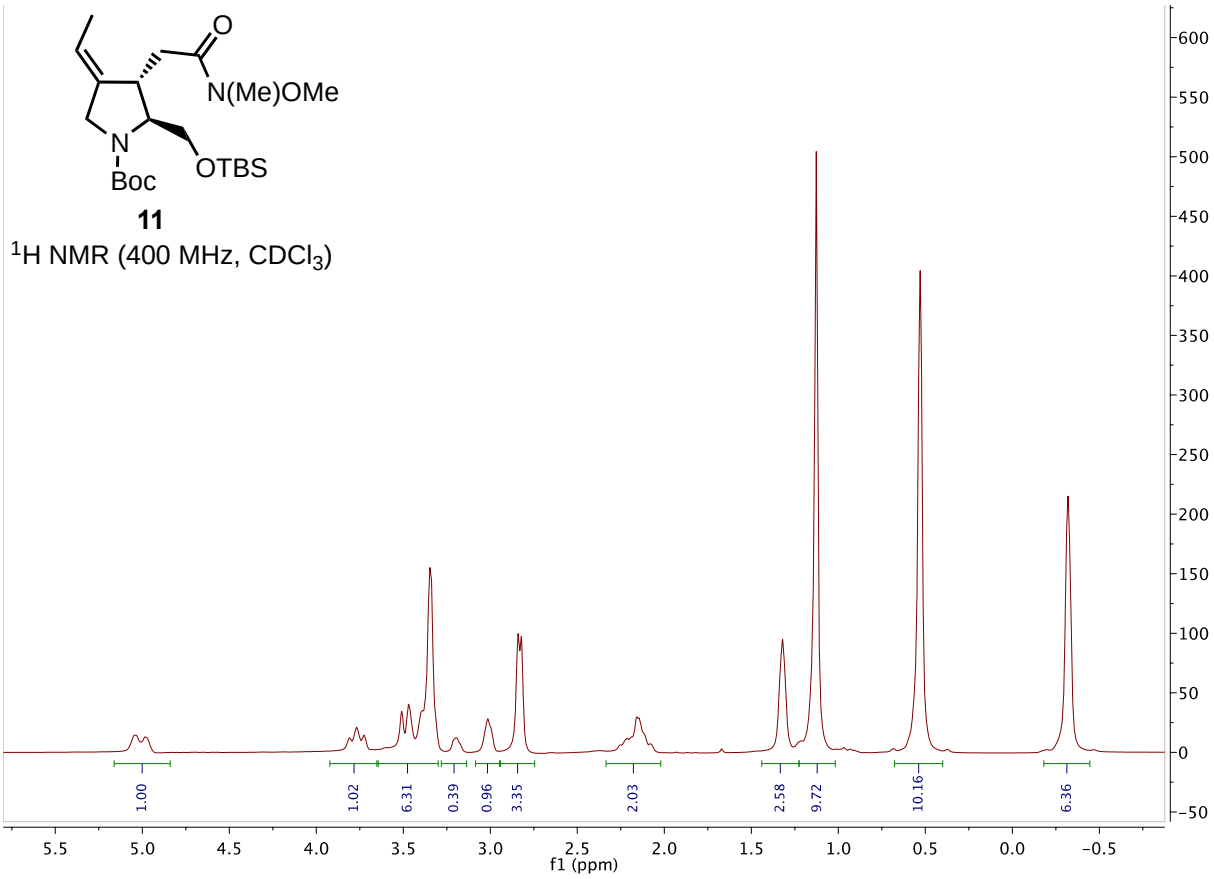

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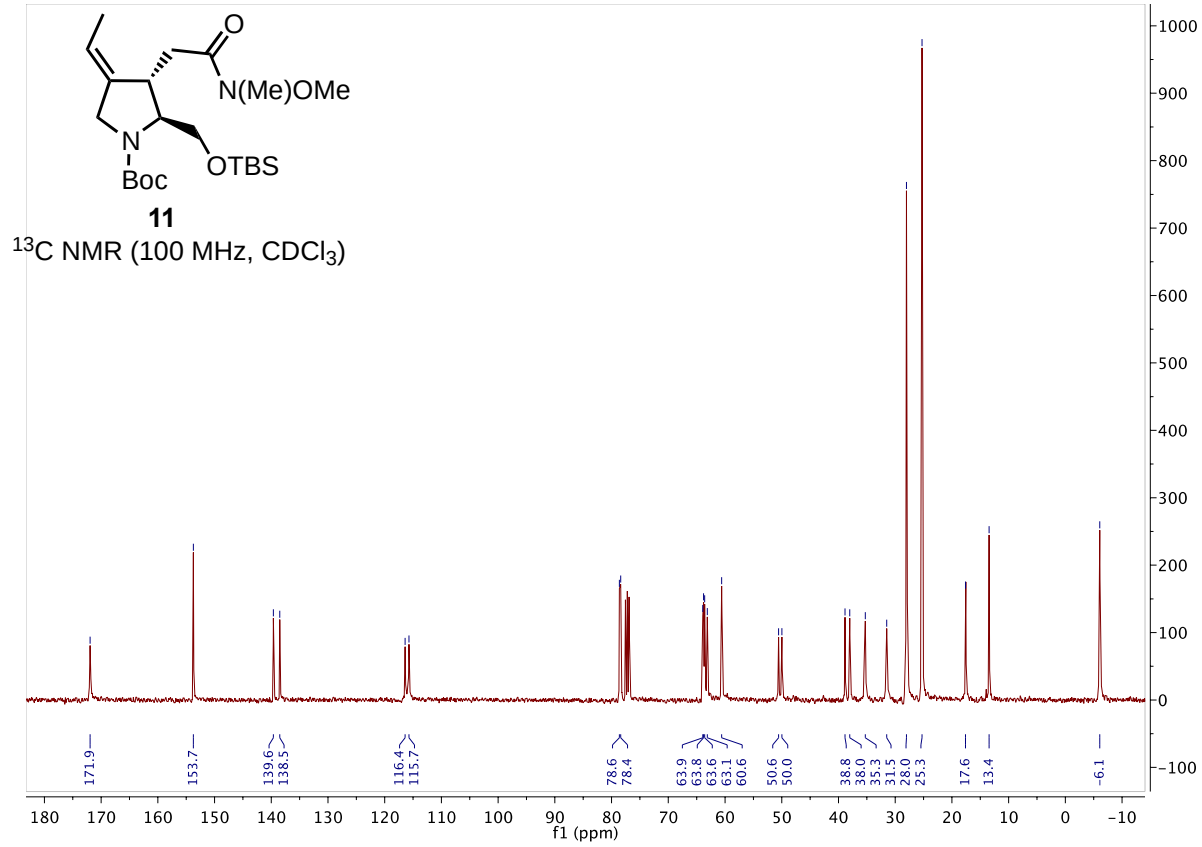

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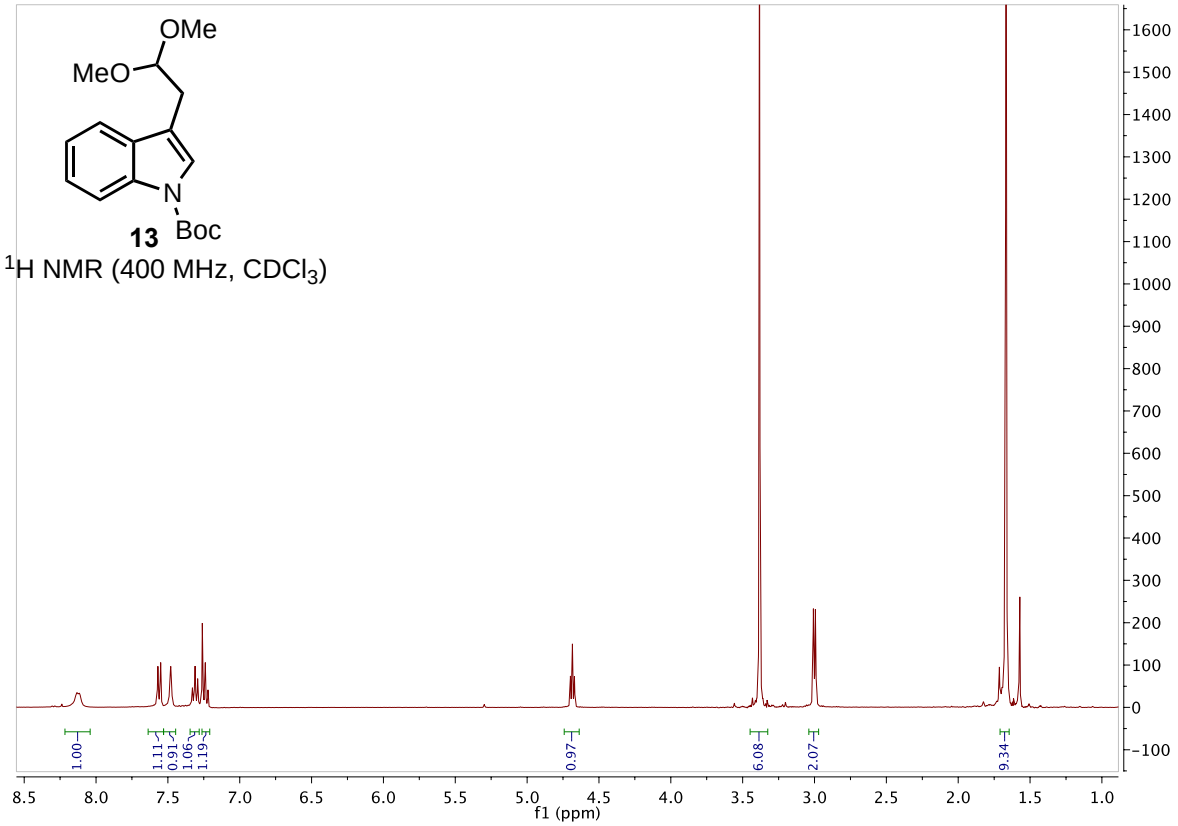

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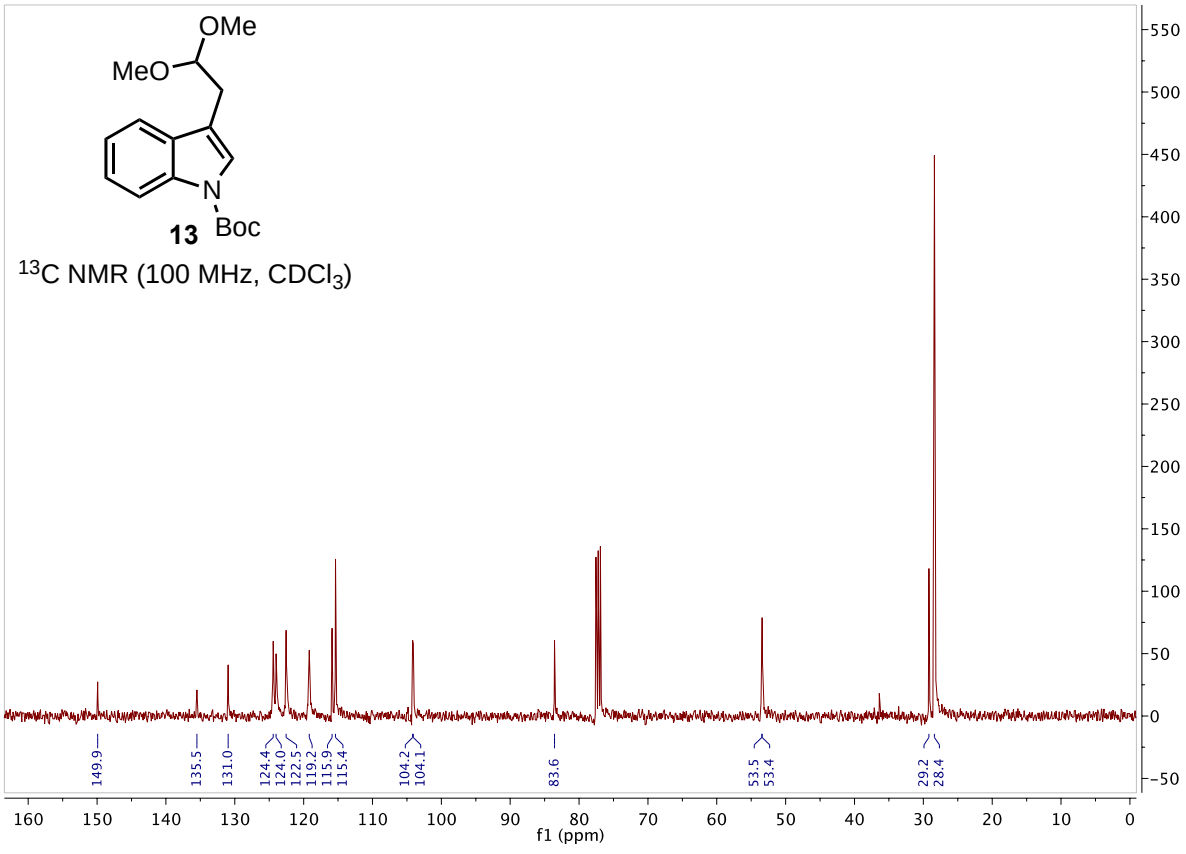

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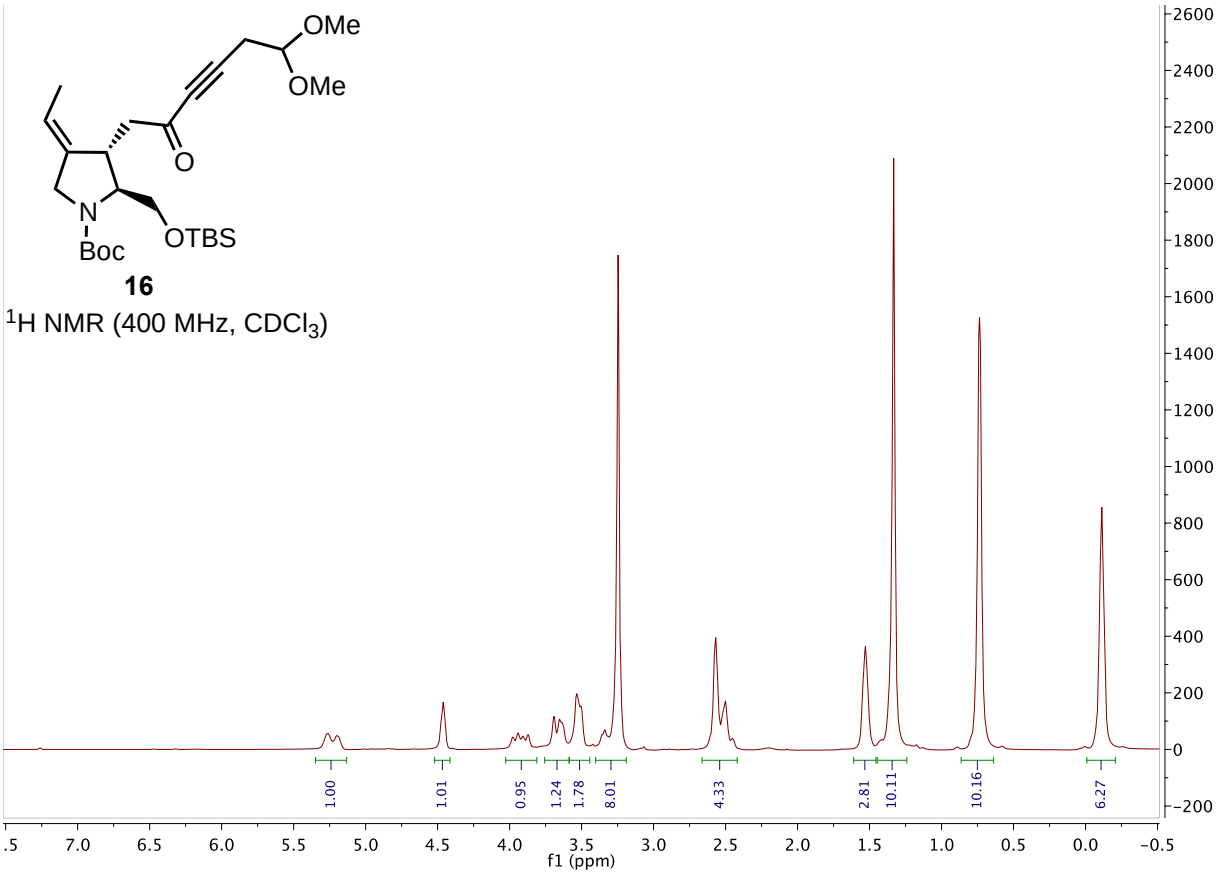

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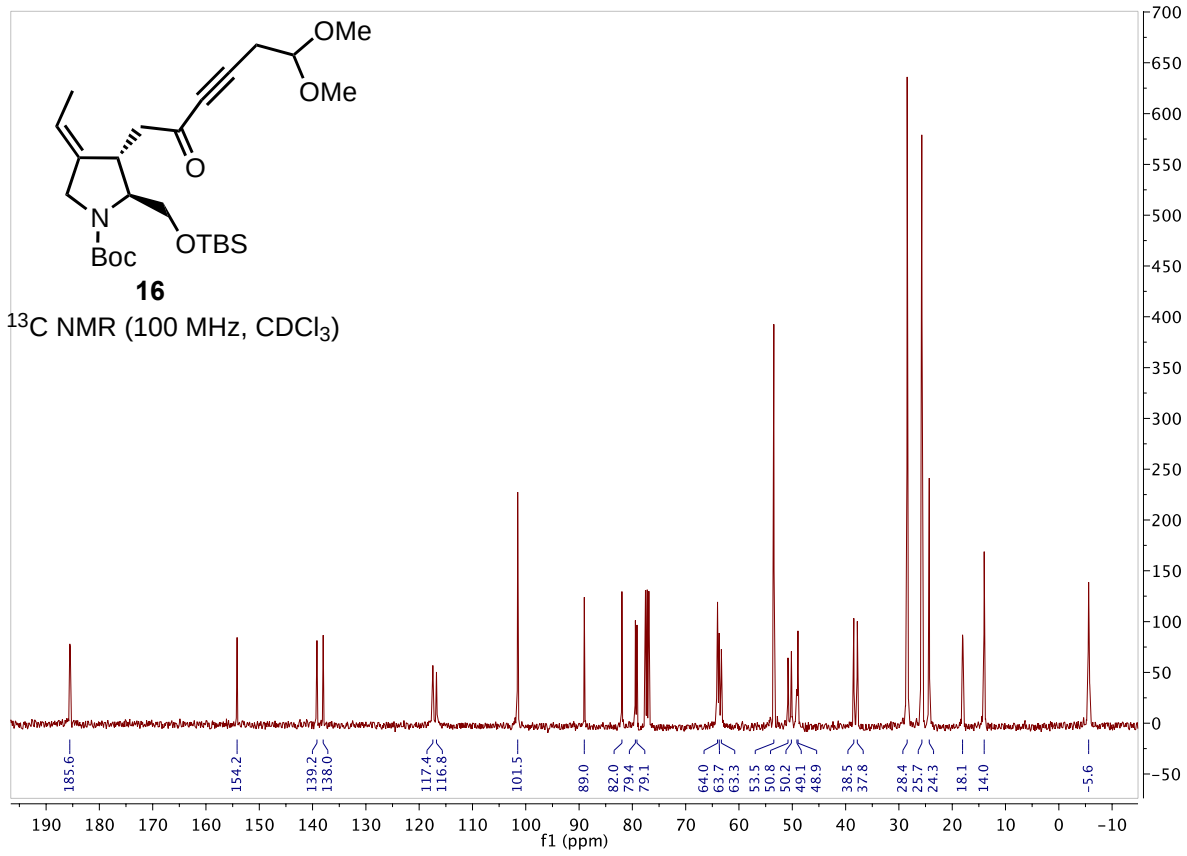

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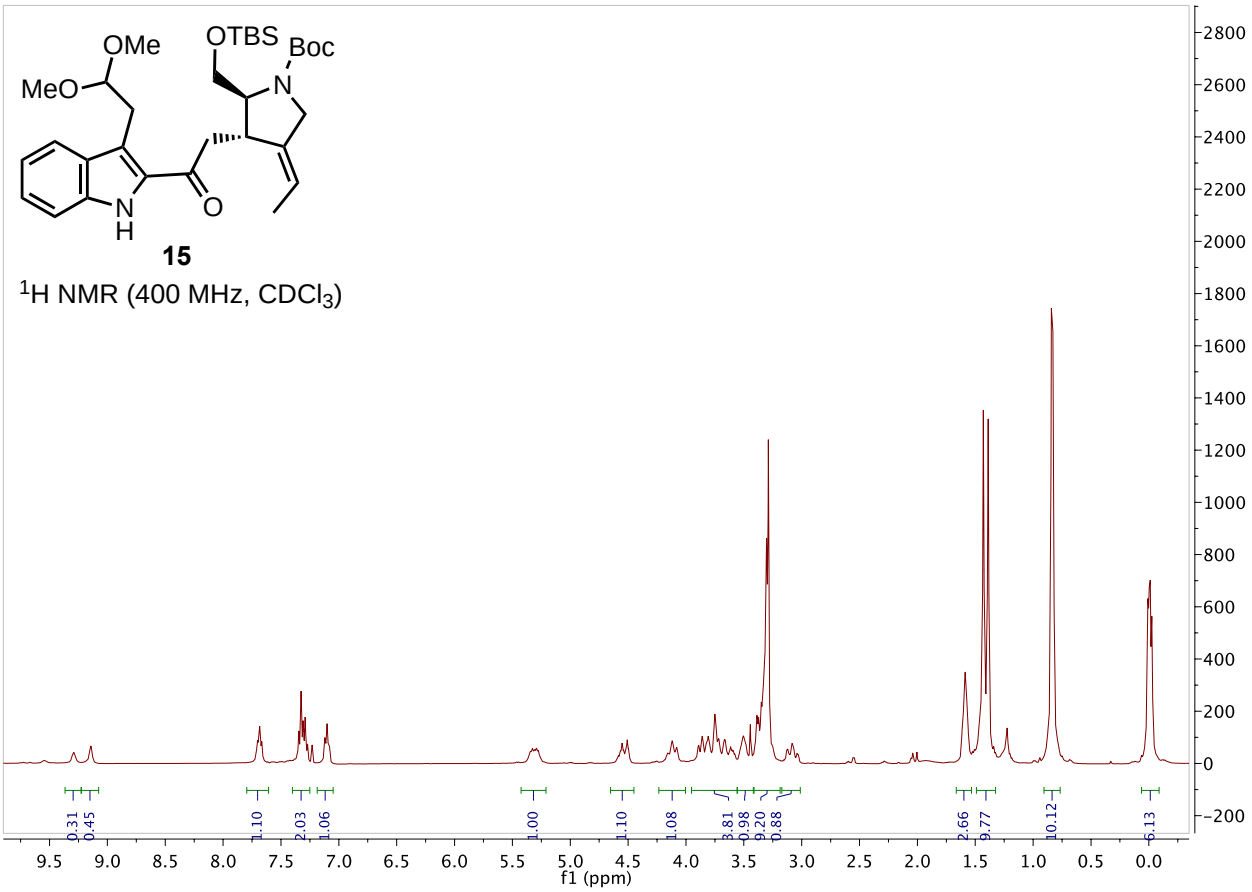

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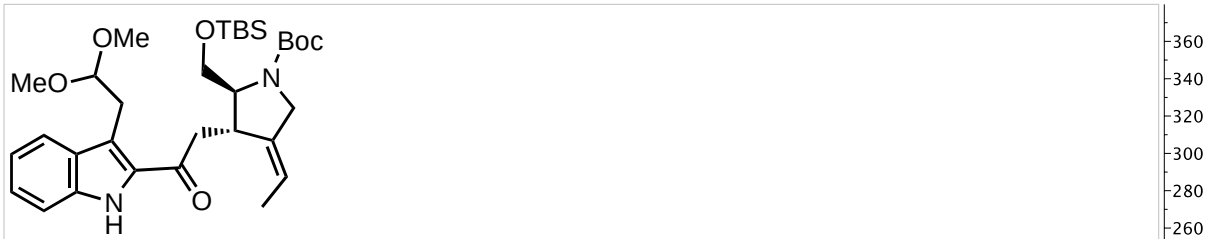

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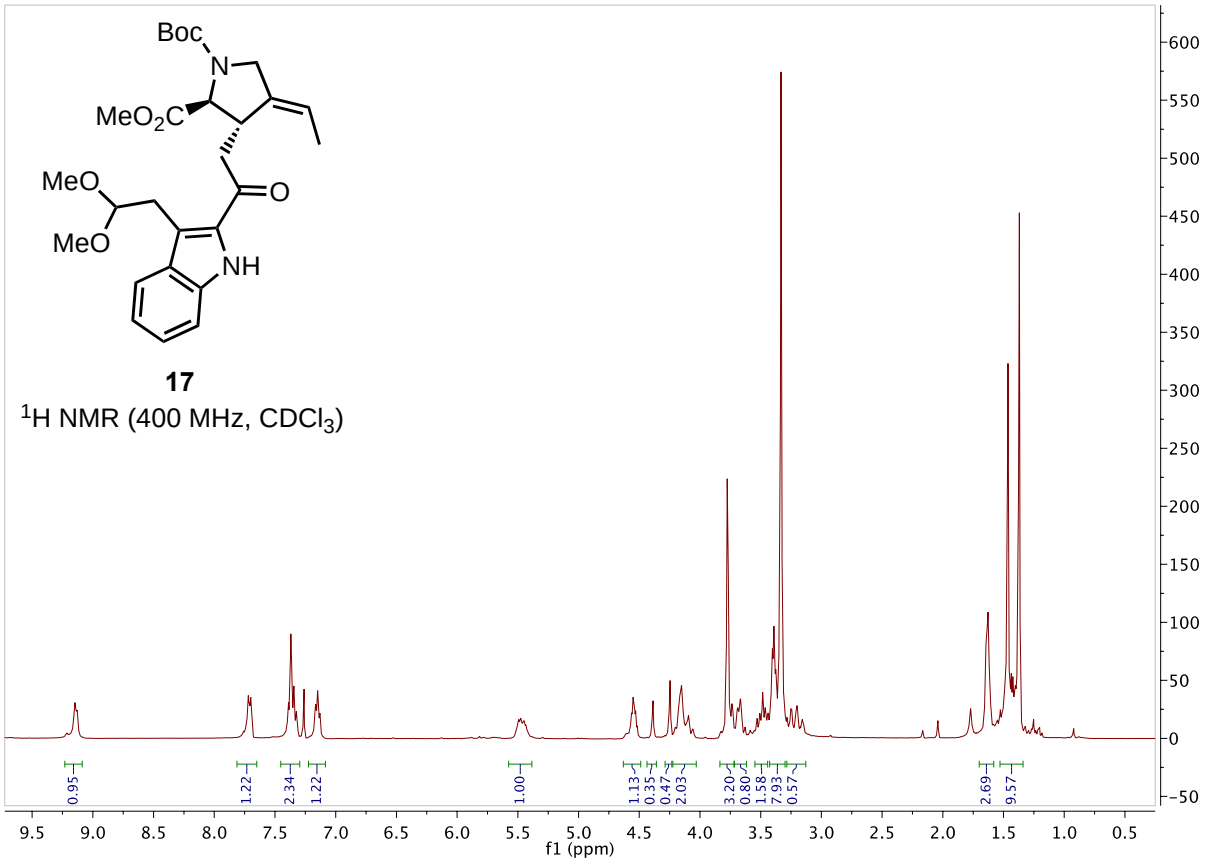

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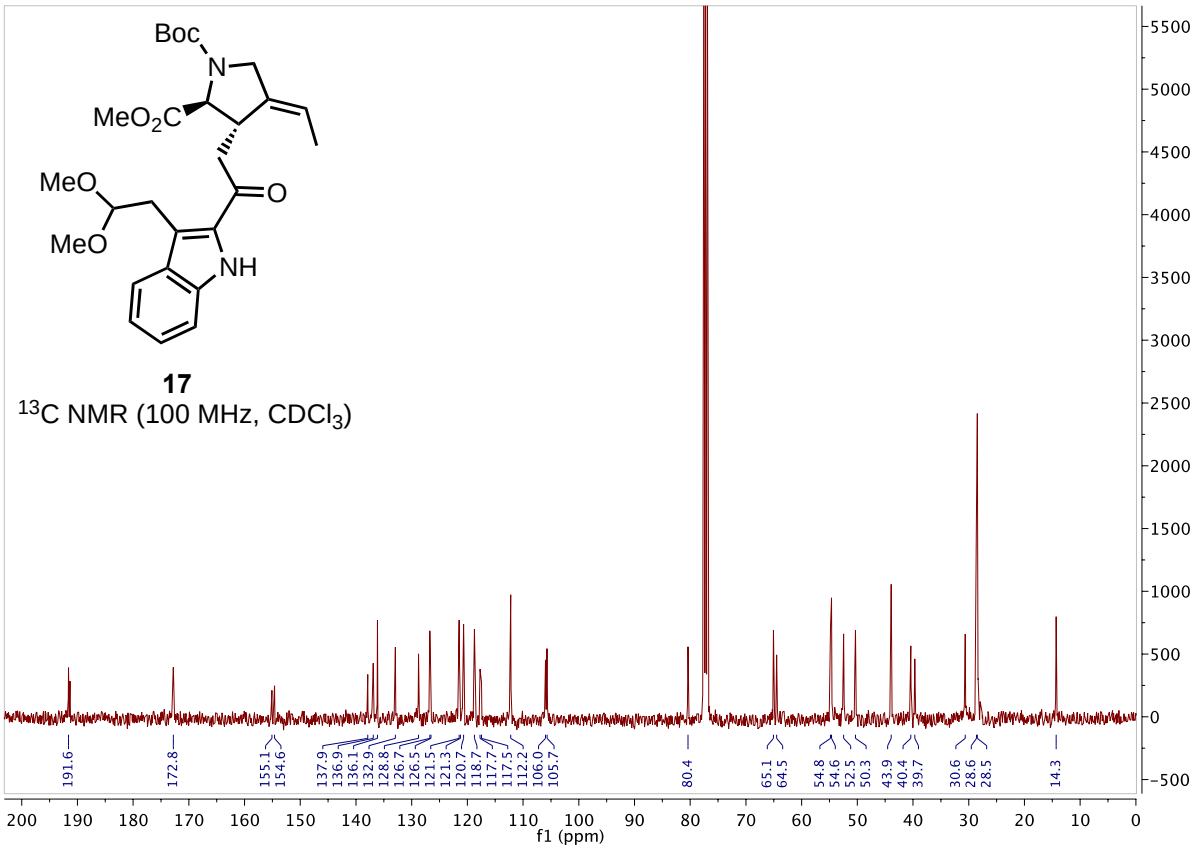

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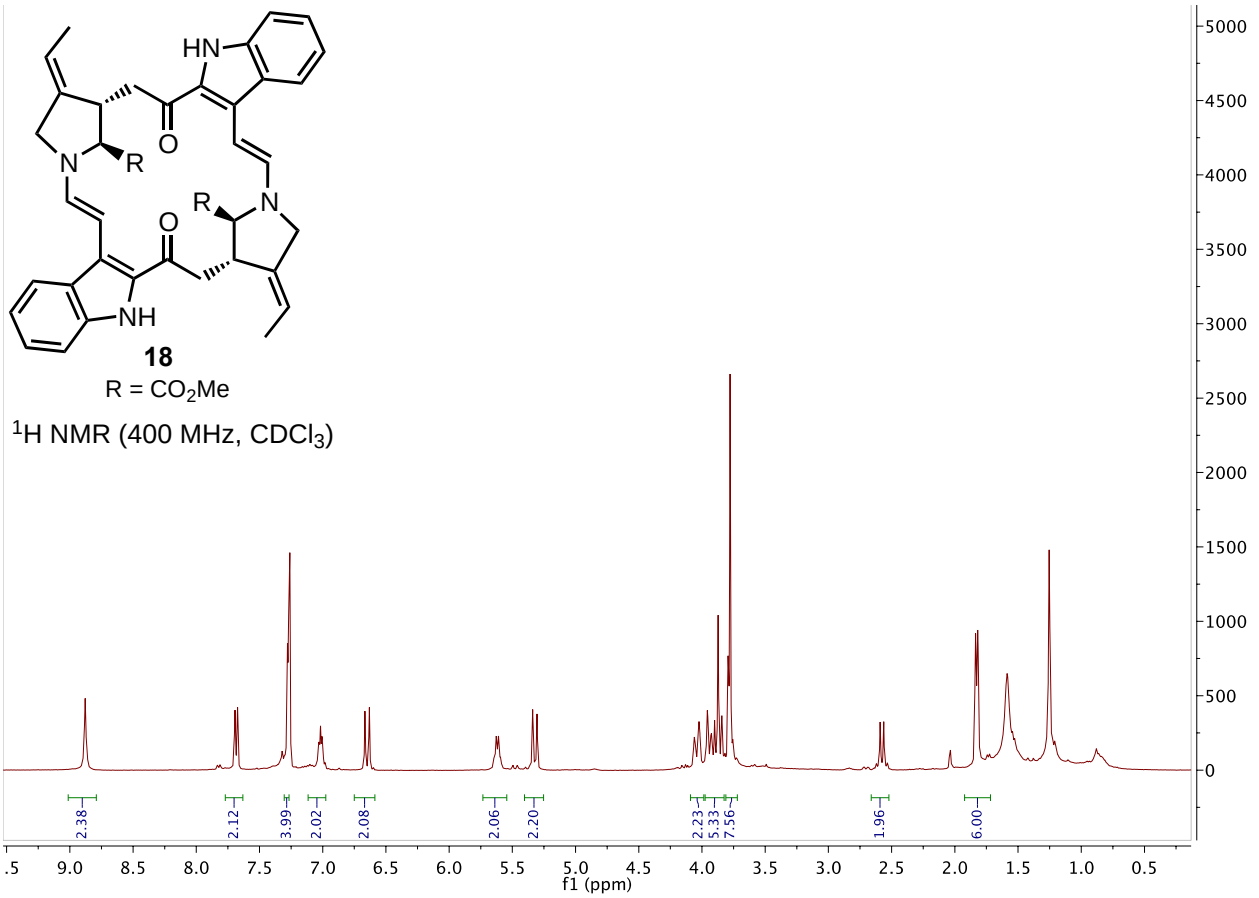

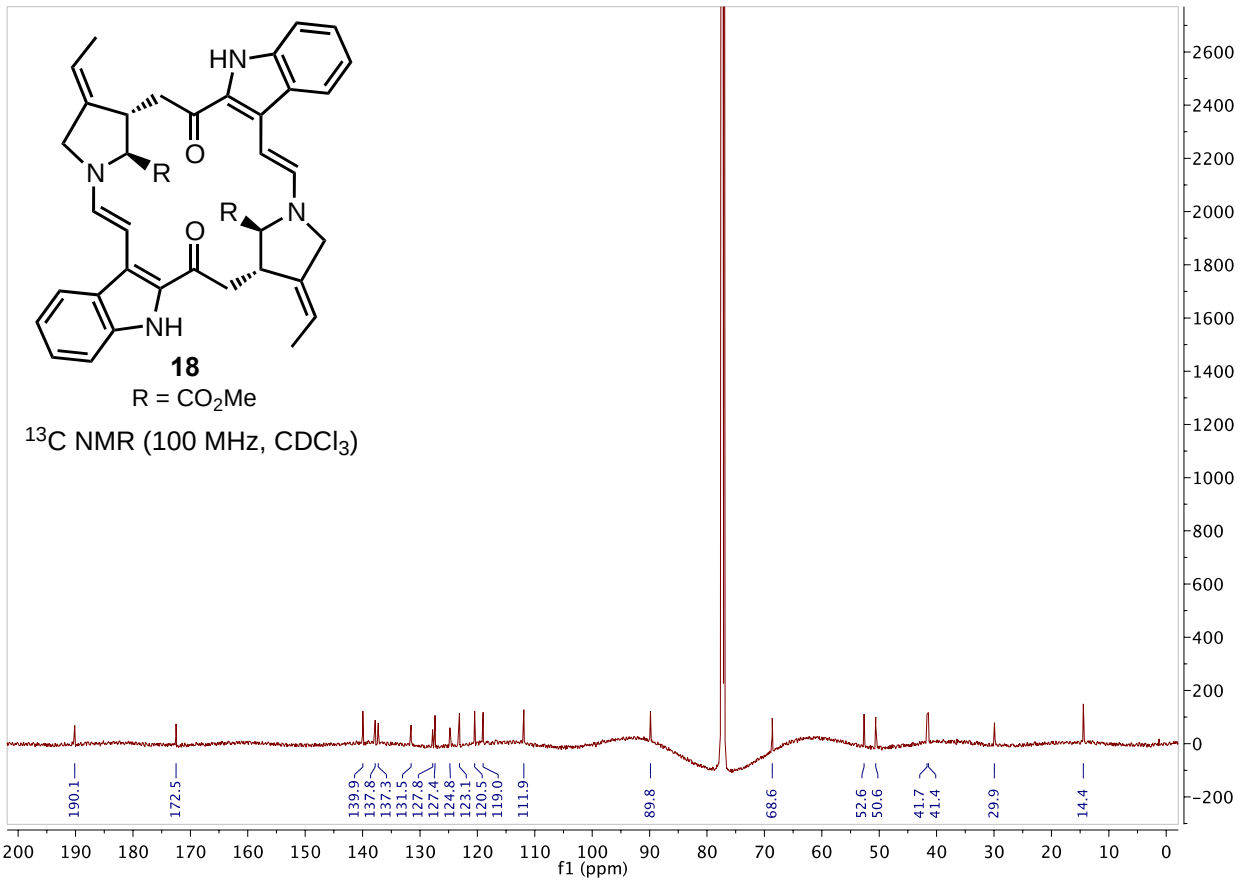

X-ray Crystallographic Data for 18

The X-ray diffraction data for compound **18** was measured on Bruker D8 Venture PHOTON 100 CMOS system equipped with a Cu K_α INCOATEC ImuS micro-focus source (λ = 1.54178 Å). Indexing was performed using *APEX3* [1] (Difference Vectors method). Data integration and reduction were performed using SaintPlus 6.01 [2]. Absorption correction was performed by multi-scan method implemented in SADABS [3]. Space groups were determined using XPREP implemented in APEX3 [1]. Structures were solved using SHELXT and refined using SHELXL-2016 [4-6] (full-matrix least-squares on F^2) through OLEX2 interface program [7]. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms of -CH, -CH_2, -CH_3 groups were placed in geometrically calculated positions and were included in the refinement process using riding model with isotropic thermal parameters: Uiso(H) = 1.2(1.5)Ueq(-CH,-CH_2, (-CH_3)). Hydrogen atom of NH group was found in difference Fourier map and was freely refined. Crystal data and refinement conditions are shown in Table 1. The CIF file was deposited in the Cambridge Crystallographic Data Centre (CCDC 1892734).

Table 1. Crystal data and structure refinement for 18.

Identification code	CFC_III_30_28_0m
Empirical formula	$C_{40}H_{40}N_4O_6$
Formula weight	672.76
Temperature/K	99.97
Crystal system	monoclinic
Space group	C2
a/Å	22.6240(6)
b/Å	7.3720(2)
c/Å	10.3718(3)
α/°	90
β/°	91.733(2)
γ/°	90
Volume/Å^3	1729.06(8)
Z	2
ρ_{calc}g/cm^3	1.292
μ/mm^{-1}	0.710
F(000)	712.0
Crystal size/mm^3	0.1 × 0.1 × 0.05
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	7.818 to 153.78
Index ranges	-28 ≤ h ≤ 28, -9 ≤ k ≤ 8, -13 ≤ l ≤ 12
Reflections collected	13239
Independent reflections	3351 [R_{int} = 0.0913, R_{sigma} = 0.0798]
Data/restraints/parameters	3351/1/231
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0470, wR_2 = 0.0886
Final R indexes [all data]	R_1 = 0.0659, wR_2 = 0.0948
Largest diff. peak/hole / e Å^{-3}	0.18/-0.24
Flack parameter	0.2(3)

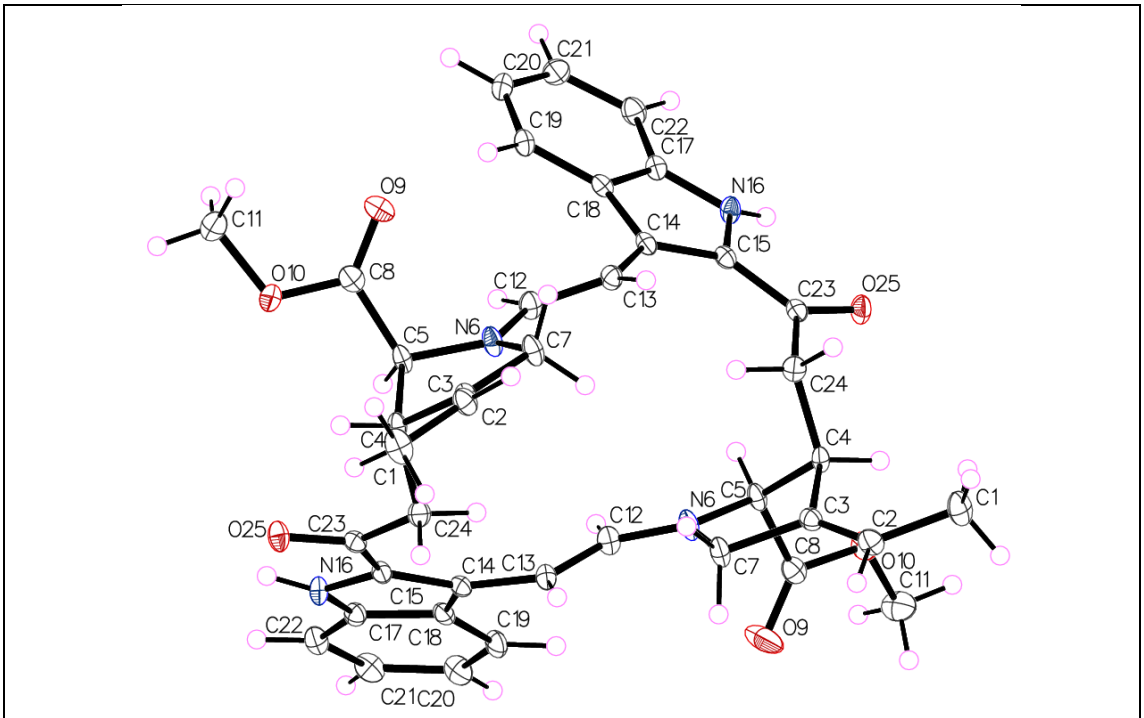

Figure S1. Conformation and numbering scheme of molecule in **18**. Thermal ellipsoids were drawn at 50% probability.

References:

1. Bruker (2016). *APEX3* (Version 2015.9). Bruker AXS Inc., Madison, Wisconsin, USA.
2. Bruker (2016) SAINT V8.35A. Data Reduction Software.
3. Sheldrick, G. M. (1996). *SADABS. Program for Empirical Absorption Correction.* University of Gottingen, Germany.
4. G.M. Sheldrick (2015) "Crystal structure refinement with SHELXL", Acta Cryst., C71, 3-8 (Open Access)
5. Sheldrick, G.M. (1990) Acta Cryst. A46, 467-473
6. Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
7. Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H., OLEX2: A complete structure solution, refinement and analysis program (2009). J. Appl. Cryst., 42, 339-341.