

SUPPORTING INFORMATION

Common Strategy for the Synthesis of Some Strychnos Indole Alkaloids

Gaetan Maertens, Elsa Deruer, Maxime Denis and Sylvain Canesi*

Laboratoire de Méthodologie et Synthèse de Produit Naturels

*Université du Québec à Montréal, C.P.8888, Succ. Centre-Ville,
Montréal. H3C 3P8, Québec, Canada.*

*E-mail: canesi.sylvain@uqam.ca; Fax: (+1) 514-987-4054

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II. Circular dichroism spectroscopy of (-)-Strychnopivotine

Circular dichroism experiments were carried out on a Jasco J-815 spectropolarimeter at 25°C in a 0.0019 M methanol solution at 1.0 mm pathlength. Spectra were corrected from a baseline (pure solvent) that was collected the same number of times as the spectra.

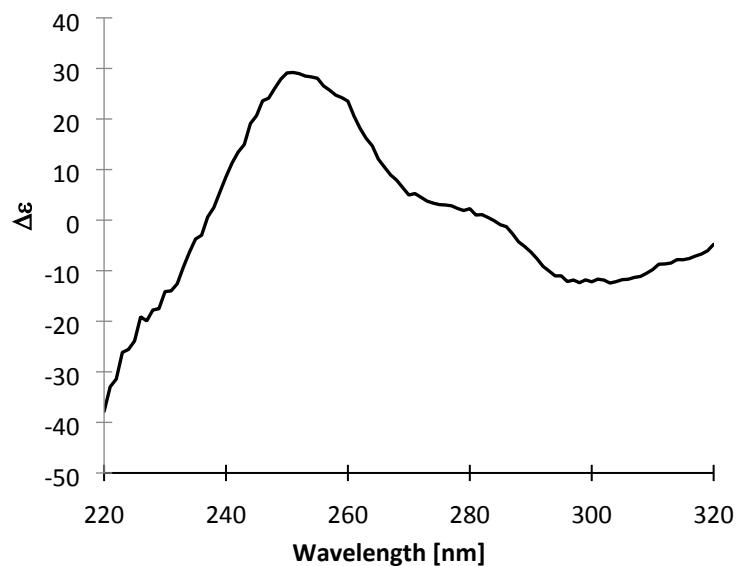


Figure S1. CD spectrum of (-)-Strychnopivotine ($c = 0.0019$ M in MeOH).

III. X-Ray crystal structure analysis of 16

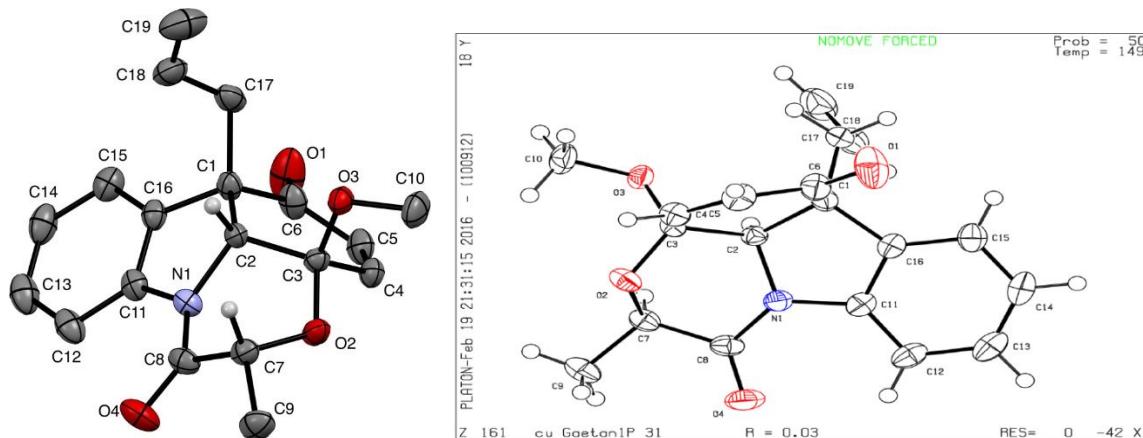


Figure S2. ORTEP representation at 50% ellipsoid probability of **16**. Hydrogen atoms were omitted for clarity, except on asymmetric carbon atoms (C2 and C7).

Crystals were directly obtained after silica gel chromatography (15:85 EtOAc/n-Hex), a recrystallization can be promoted in presence of methanol if necessary.

Crystallographic analysis was performed on a Bruker APEX-DUO diffractometer. A colorless needle-like specimen of $C_{19}H_{19}NO_4$, approximate dimensions 0.155 mm x 0.161 mm x 0.359 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. A total of 5856 frames were collected. The total exposure time was 10.98 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a trigonal unit cell yielded a total of 18370 reflections to a maximum θ angle of 68.27° (0.83 Å resolution), of which 3007 were independent (average redundancy 6.109, completeness = 100.0%, $R_{\text{int}} = 7.34\%$, $R_{\text{sig}} = 4.61\%$) and 2906 (96.64%) were greater than $2\sigma(F^2)$. The final cell constants of $a = b = 8.6520(2)$ Å, $c = 19.0082(6)$ Å, volume = 1232.27(7) Å³, are based upon the refinement of the XYZ-centroids of 6230 reflections above 20 $\sigma(I)$ with $11.81^\circ < 2\theta < 136.5^\circ$. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.891. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6560 and 0.7360.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 3₁, with $Z = 3$ for the formula unit, $C_{19}H_{19}NO_4$. The final anisotropic full-matrix least-squares refinement on F^2 with 220 variables converged at $R_1 = 3.19\%$, for the observed data and $wR_2 = 8.07\%$ for all data. The goodness-of-fit was 1.049. The largest peak in the final difference electron density synthesis was 0.189 e⁻/Å³ and the largest hole was -0.126 e⁻/Å³ with an RMS deviation of 0.035 e⁻/Å³. On the basis of the final model, the calculated density was 1.315 g/cm³ and $F(000)$, 516 e⁻.

The absolute structure was assigned using C7, which *R* configuration remains intact during synthesis. In addition, absolute structure was also determined using anomalous scatterers, which led to a Flack parameter of 0.16(12). Despite the large uncertainty due

to the lack of heavy atoms, this value is sufficient close to zero to corroborate the absolute structure assignment.

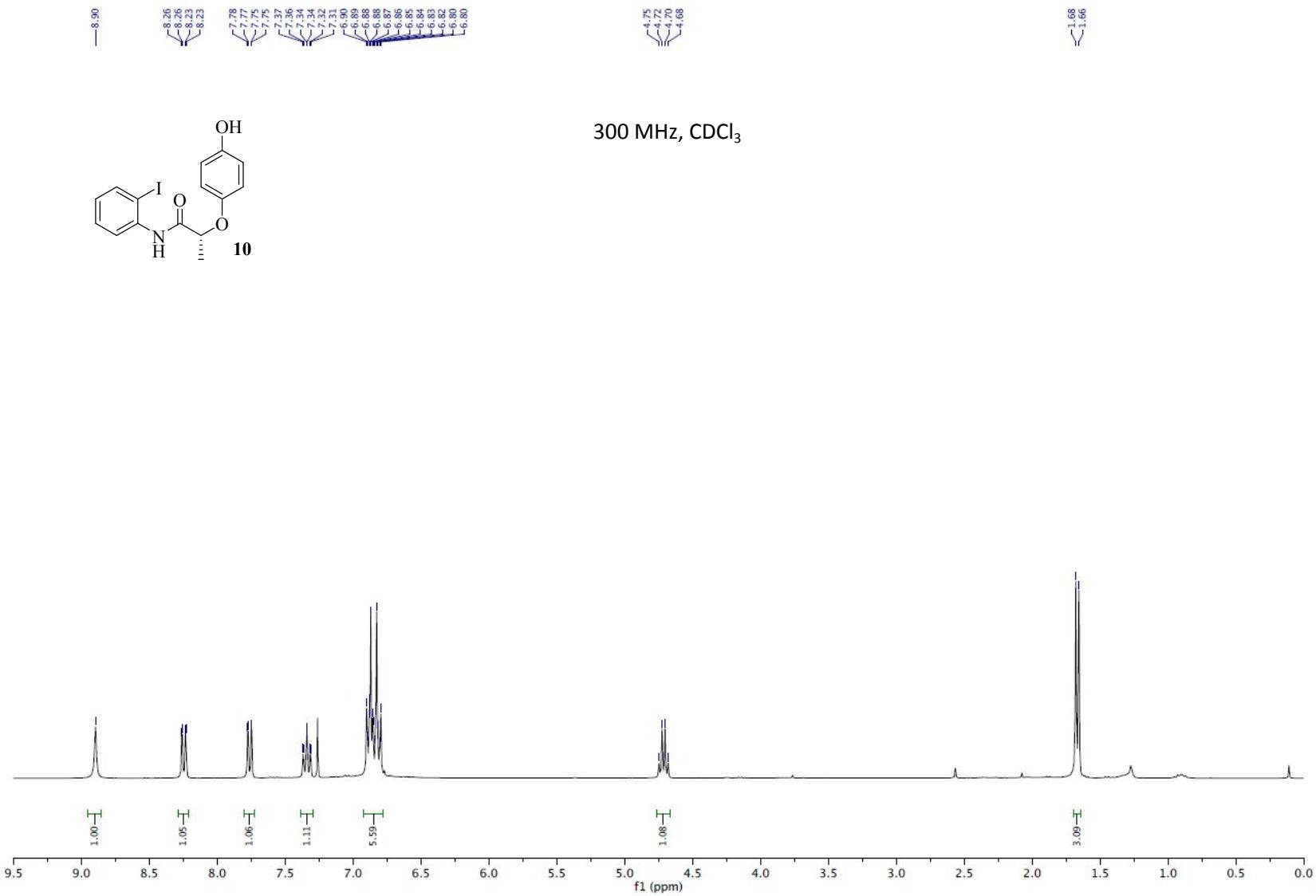
Bond precision: C-C = 0.0039 Å Wavelength=1.54178
Cell: a=8.6520(2) b=8.6520(2) c=19.0082(6)
alpha=90 beta=90 gamma=120
Temperature: 149 K

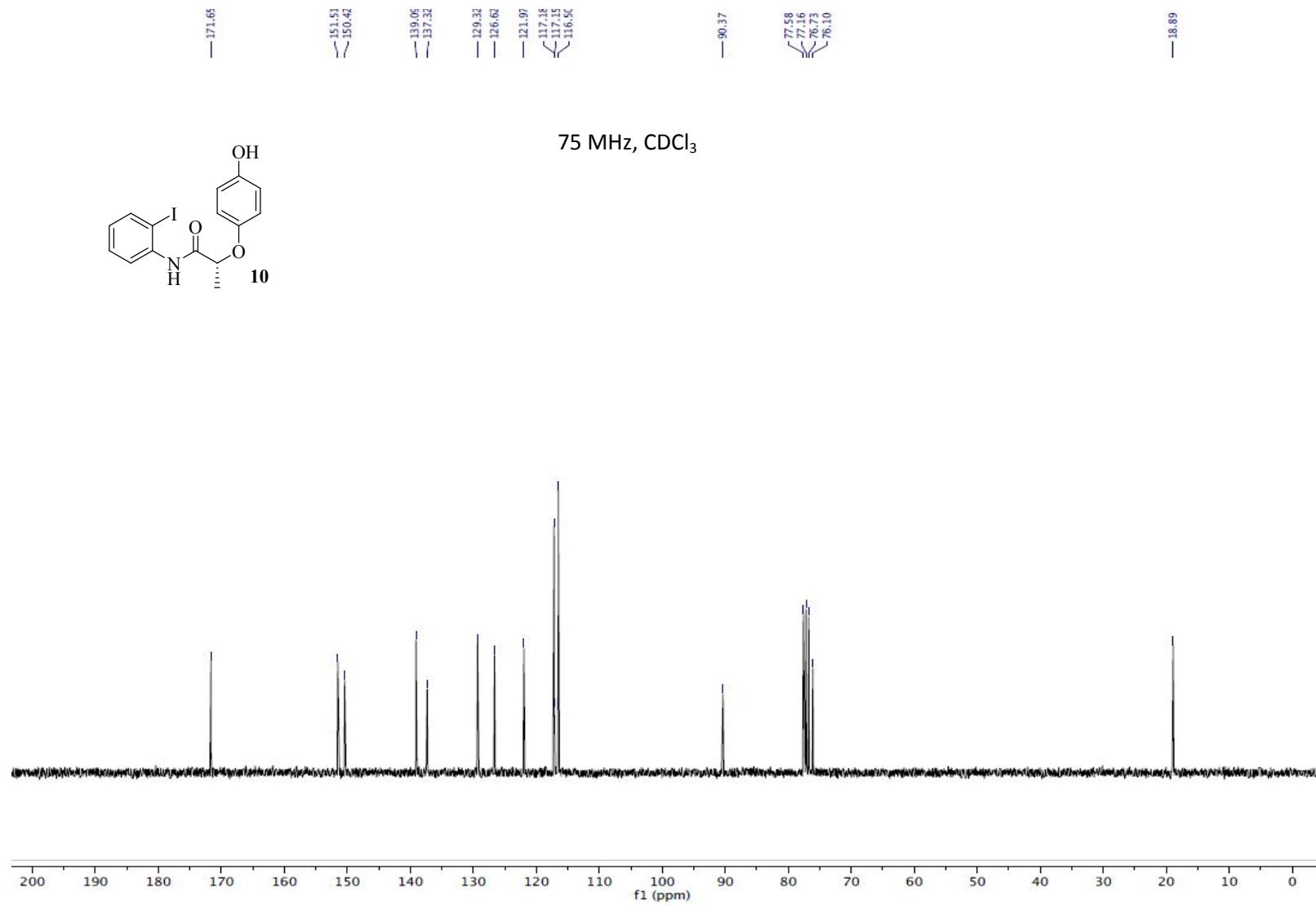
	Calculated	Reported
Volume	1232.27(8)	1232.27(7)
Space group	P 31	?
Hall group	P 31	P 31
Moiety formula	C ₁₉ H ₁₉ N O ₄	C ₁₉ H ₁₉ N O ₄
Sum formula	C ₁₉ H ₁₉ N O ₄	C ₁₉ H ₁₉ N O ₄
Mr	325.35	325.35
D _x , g cm ⁻³	1.315	1.315
Z	3	3
μ (mm ⁻¹)	0.757	0.757
F ₀₀₀	516.0	516.0
F _{000'}	517.64	
h, k, lmax	10,10,22	10,10,22
Nref	3006 [1503]	3007
Tmin, Tmax	0.864, 0.889	0.656, 0.736
Tmin'	0.762	
Correction method=	# Reported T Limits: Tmin=0.656	
Tmax=0.736	AbsCorr = MULTI-SCAN	
Data completeness=	2.00/1.00	Theta(max)= 68.271
R(reflections)=	0.0319(2906)	wR2(reflections)= 0.0807(3007)
S = 1.049	Npar= 220	

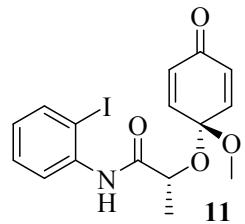
Table S1. Crystallographic parameters and data

Crystallographic parameters and data are provided in the CIF file which can be retrieved from the Cambridge Crystallographic Data Centre using deposition number 1454833 at the following URL:

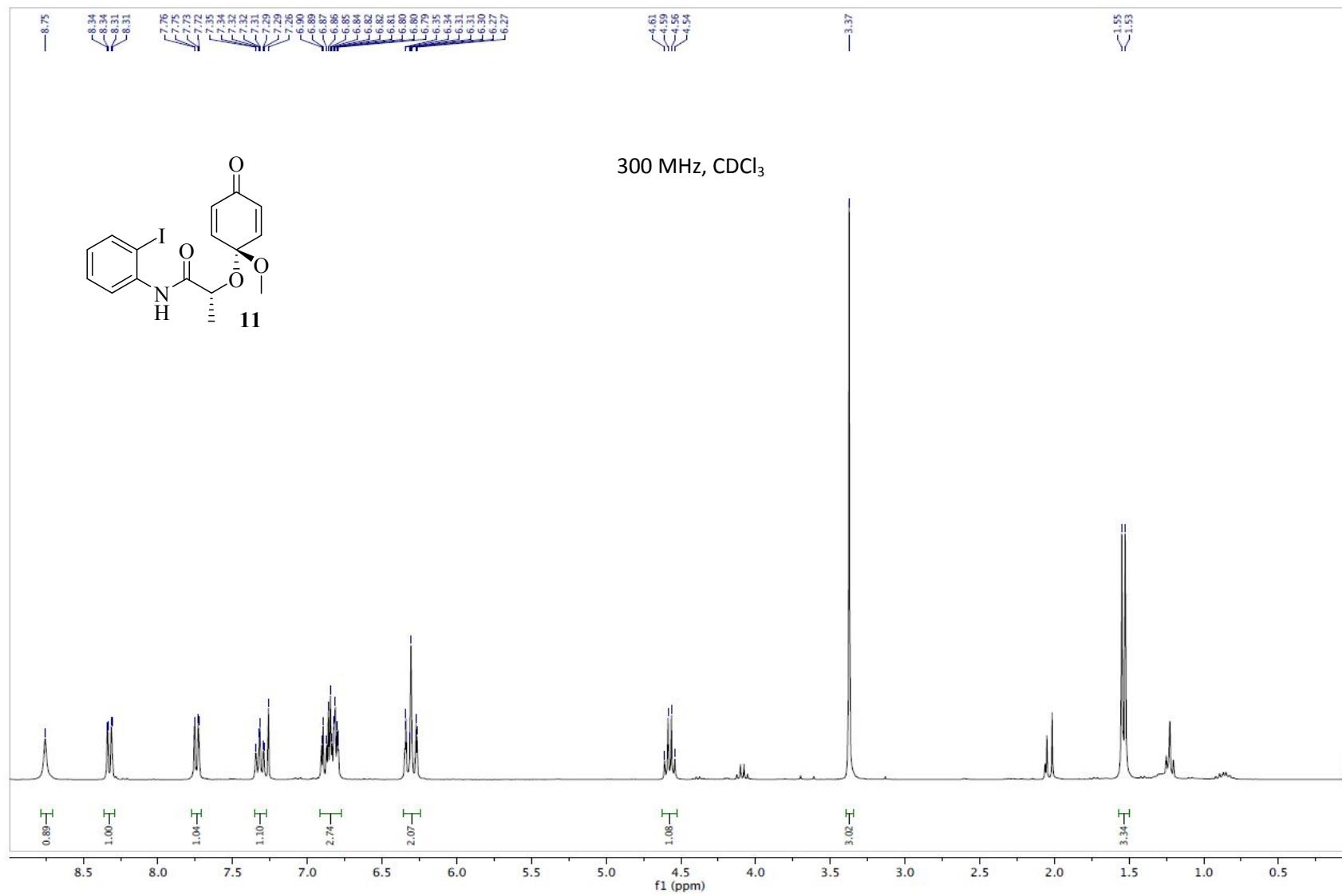
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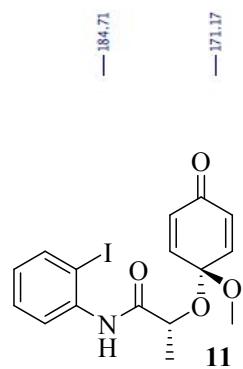




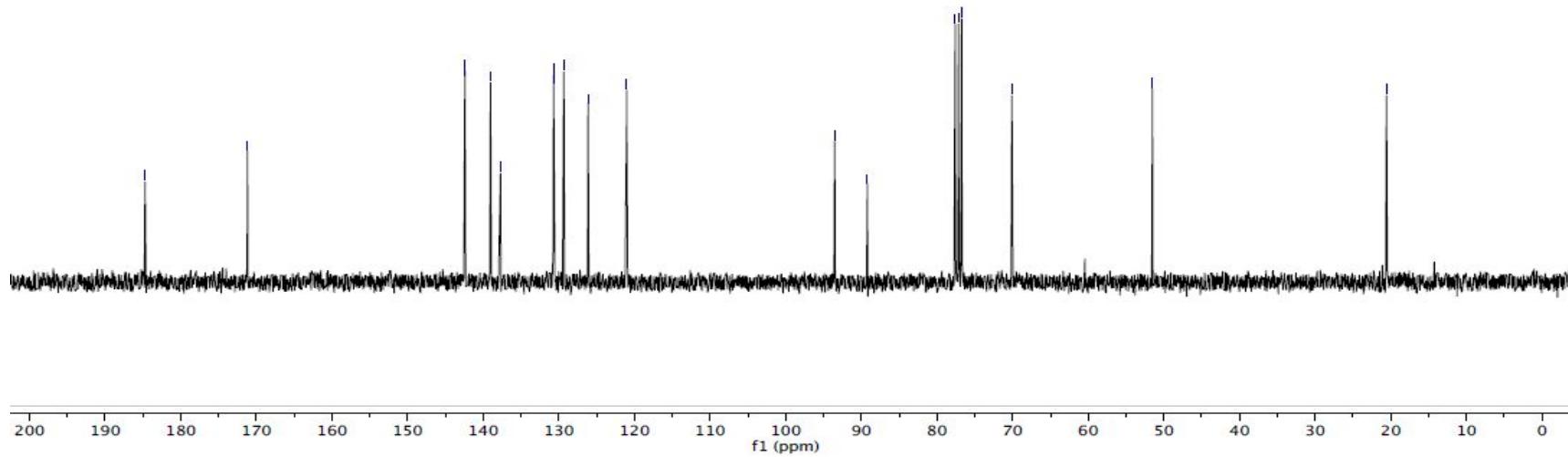


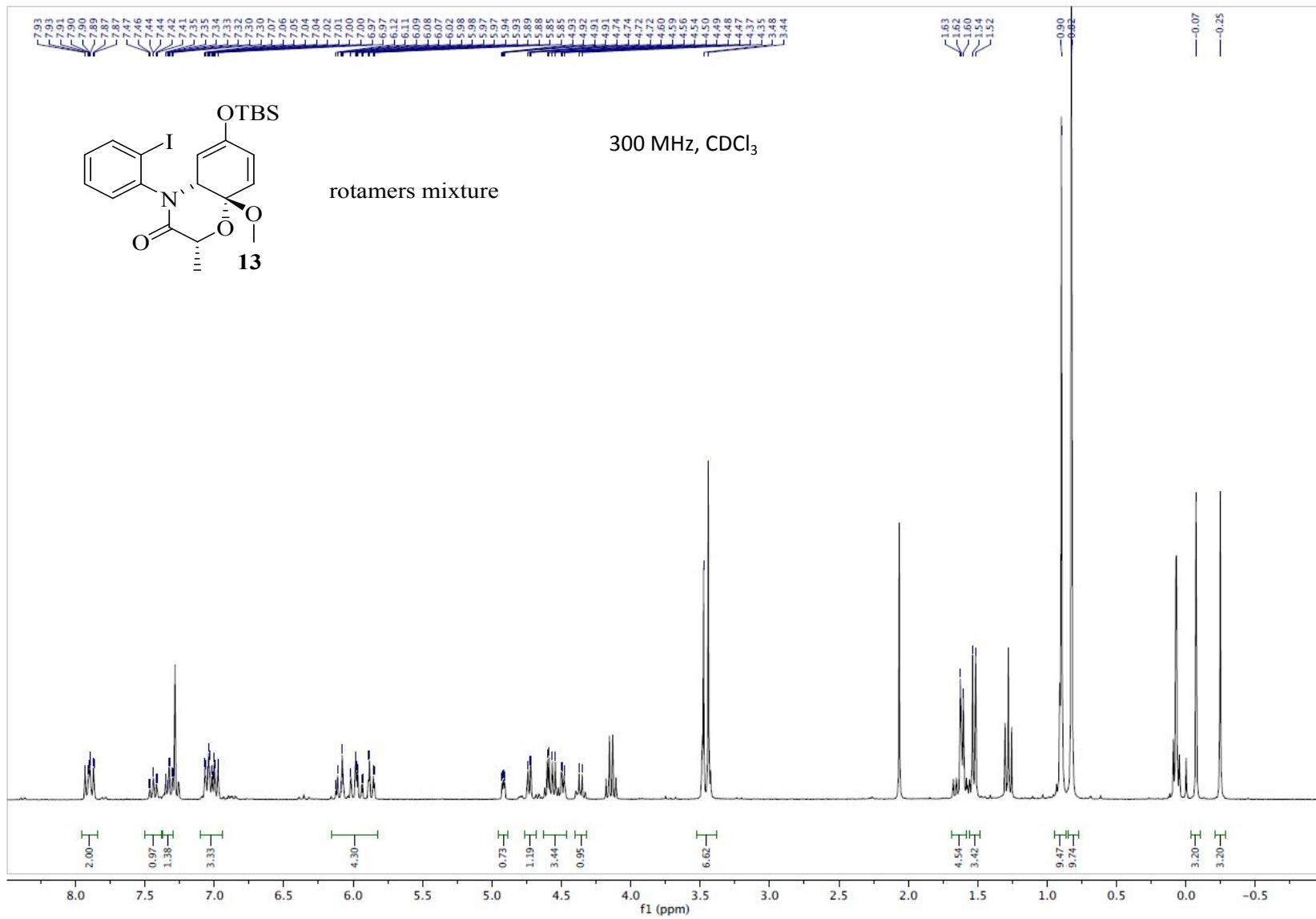
300 MHz, CDCl₃

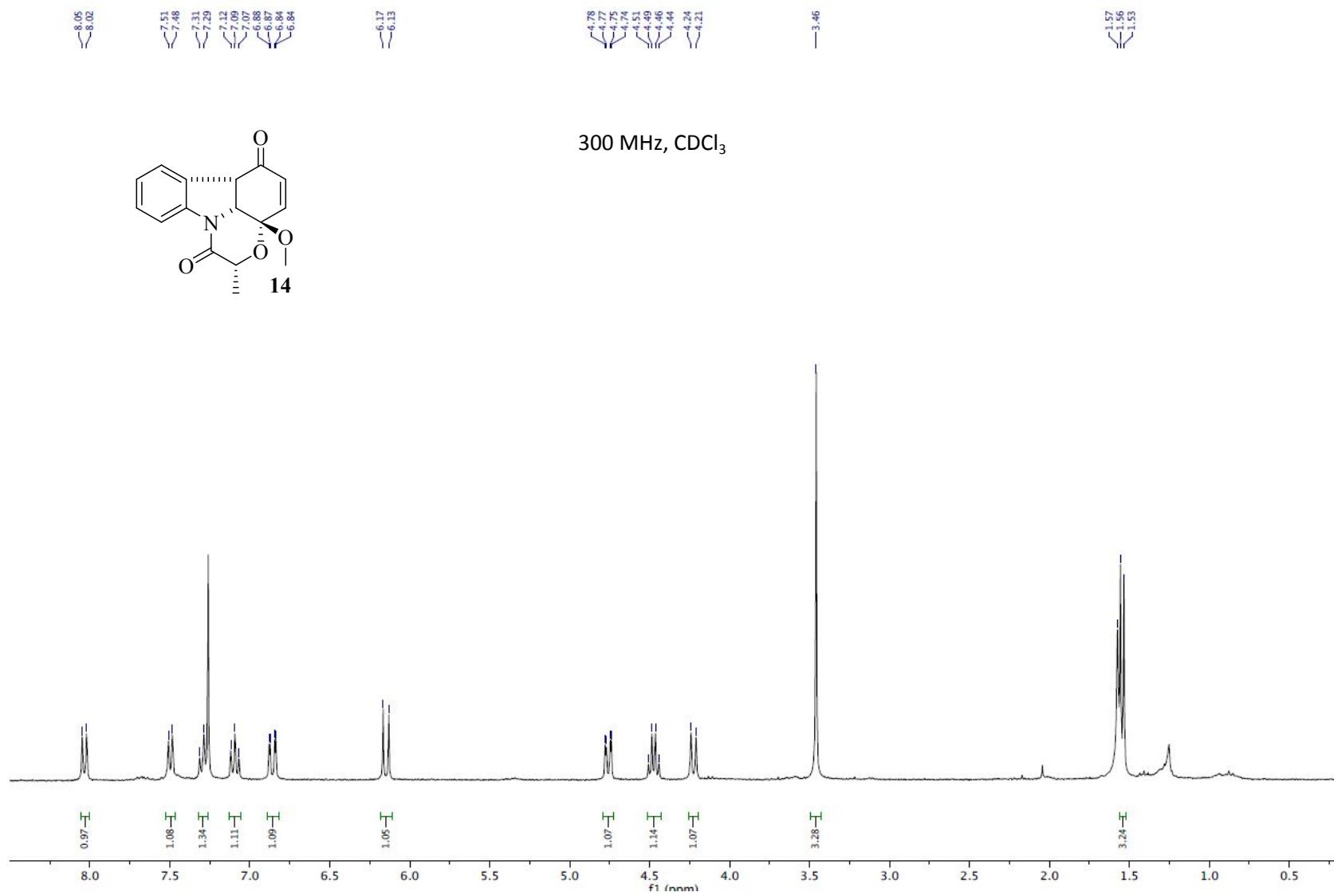


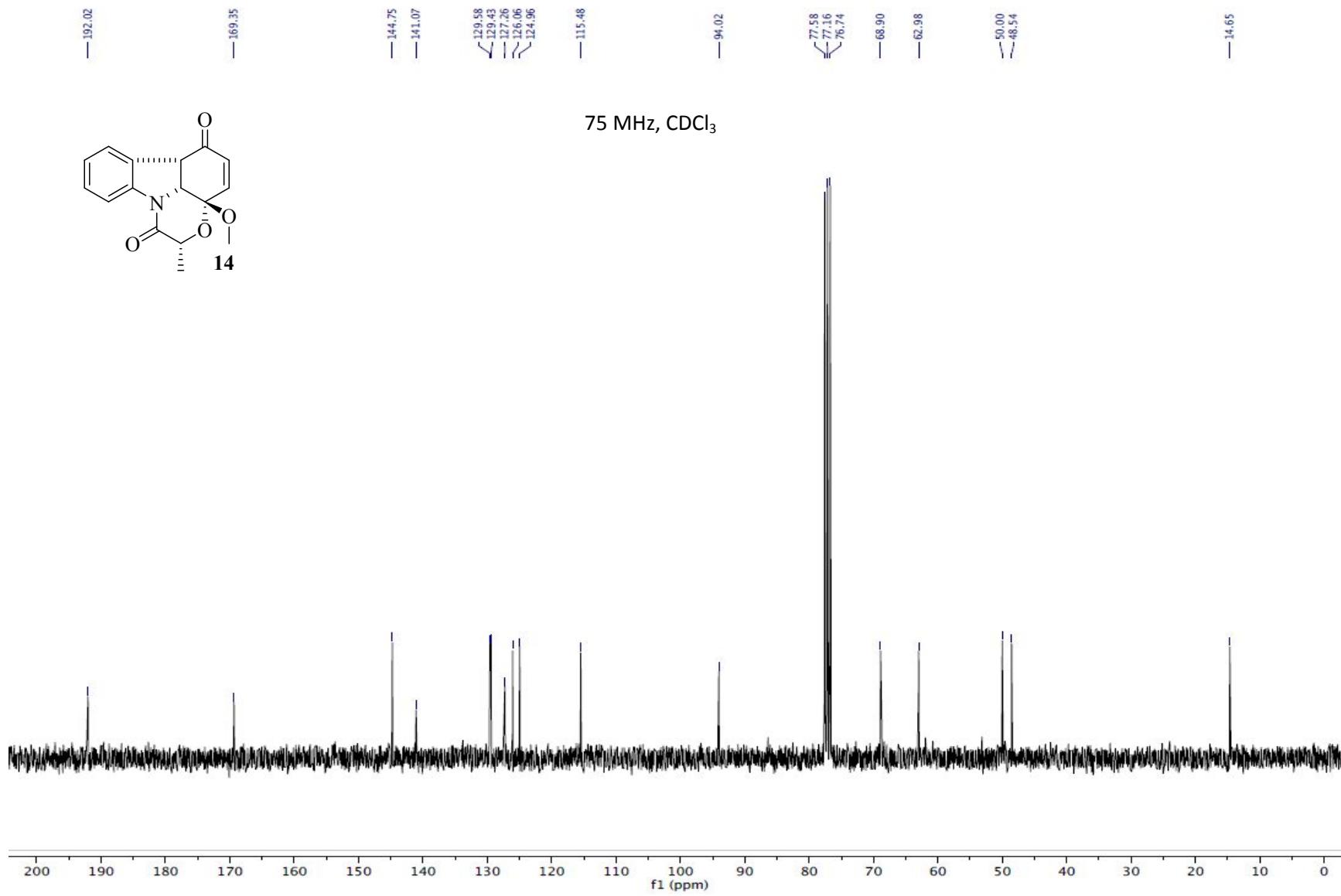


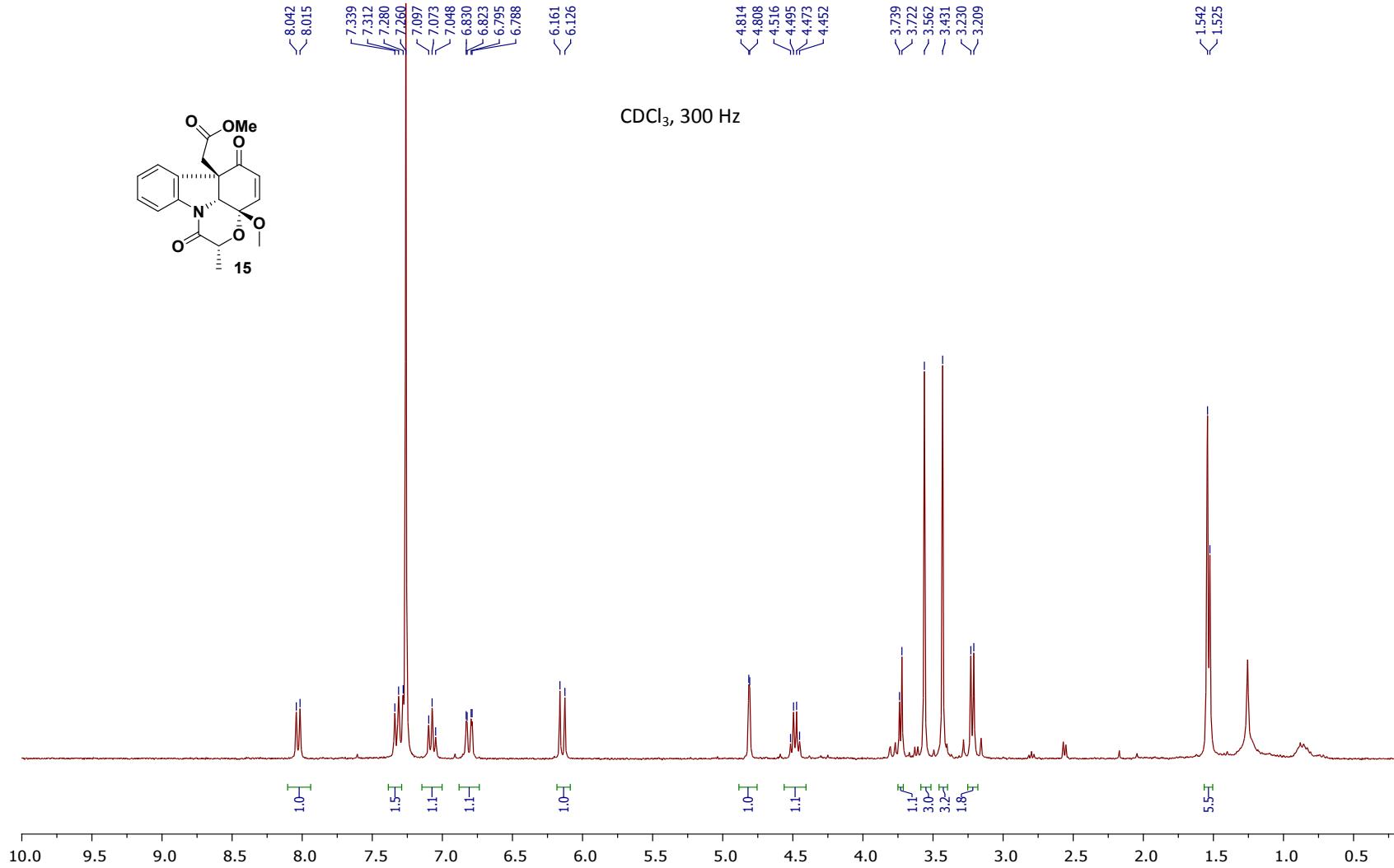
75 MHz, CDCl_3

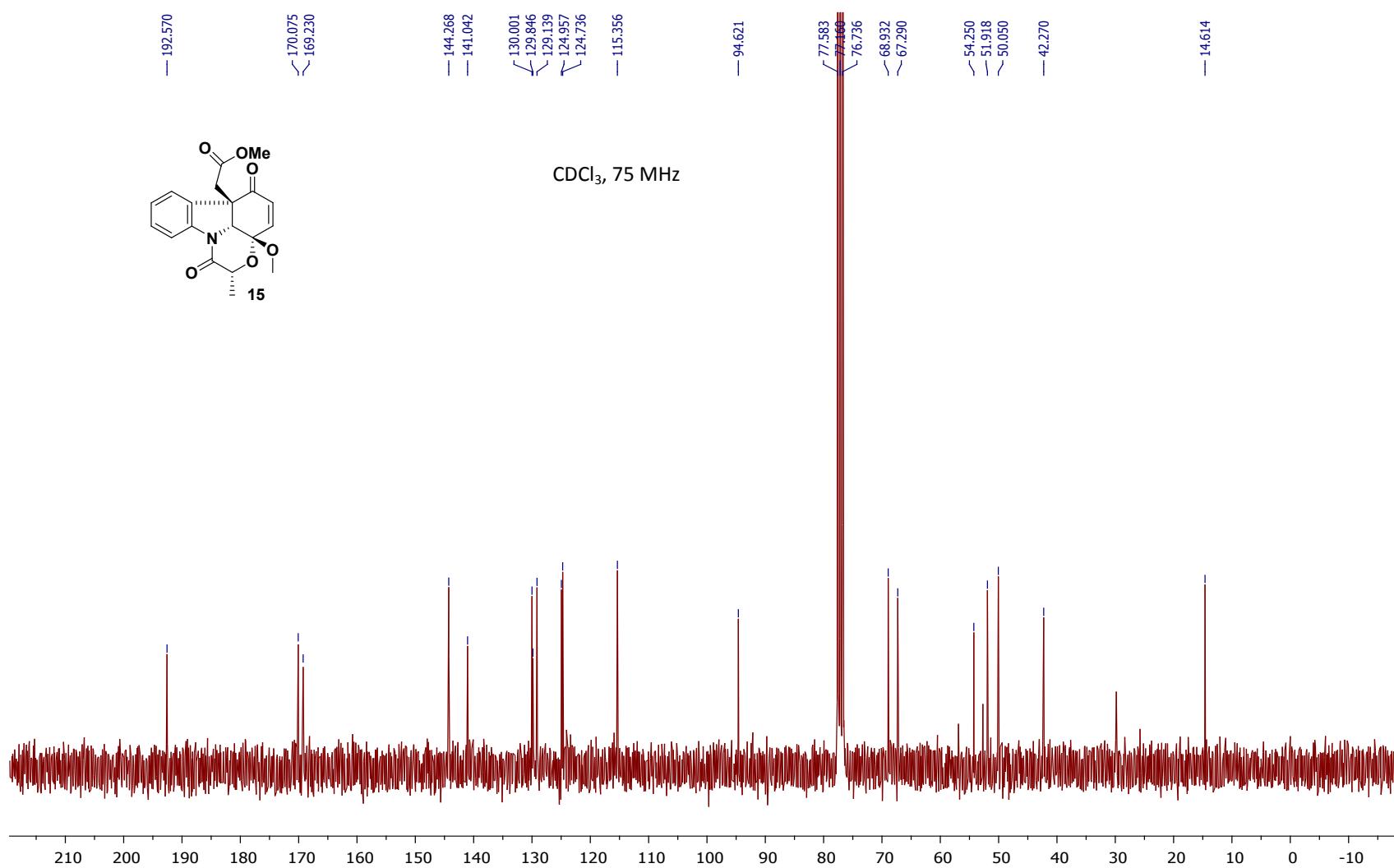


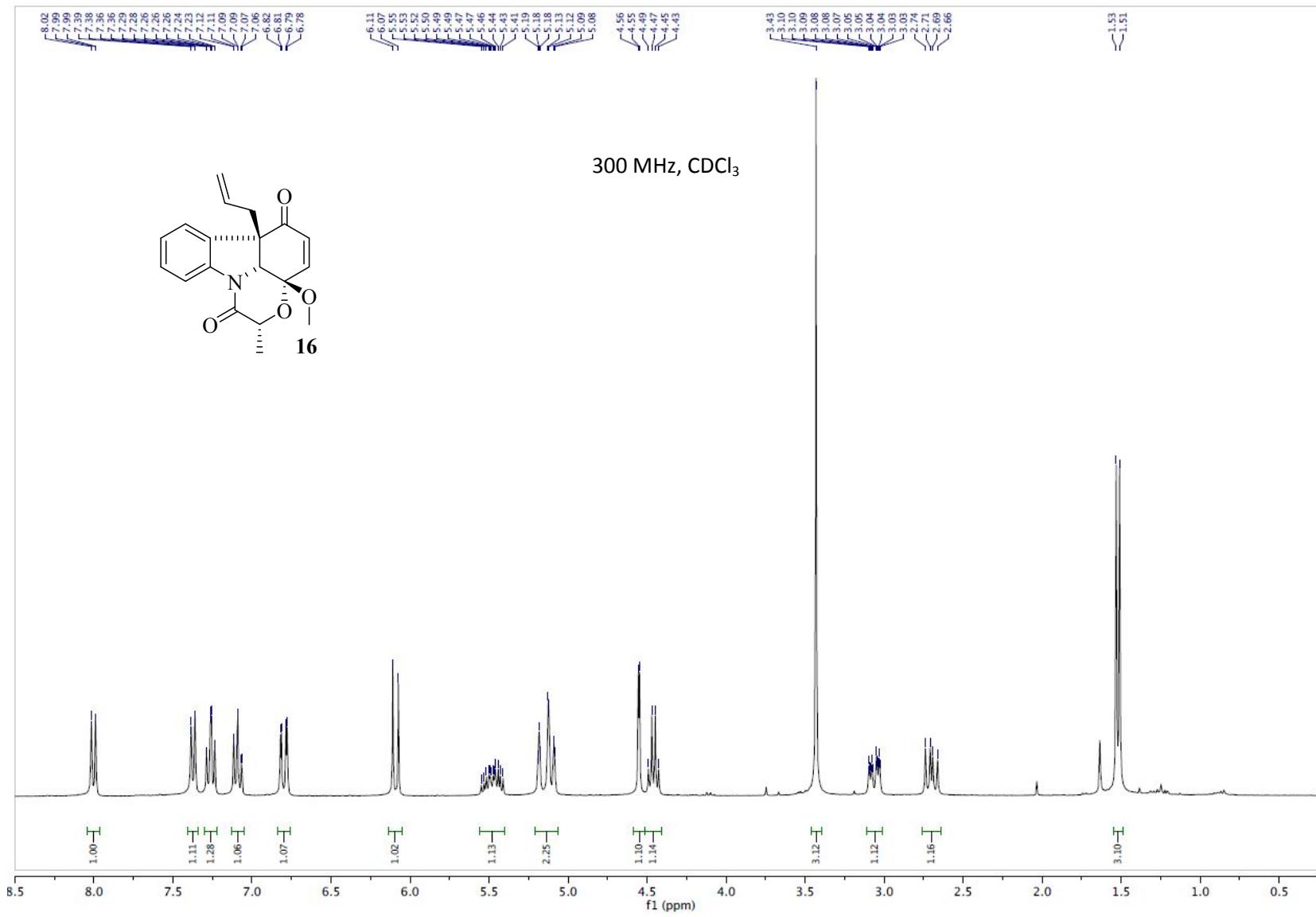


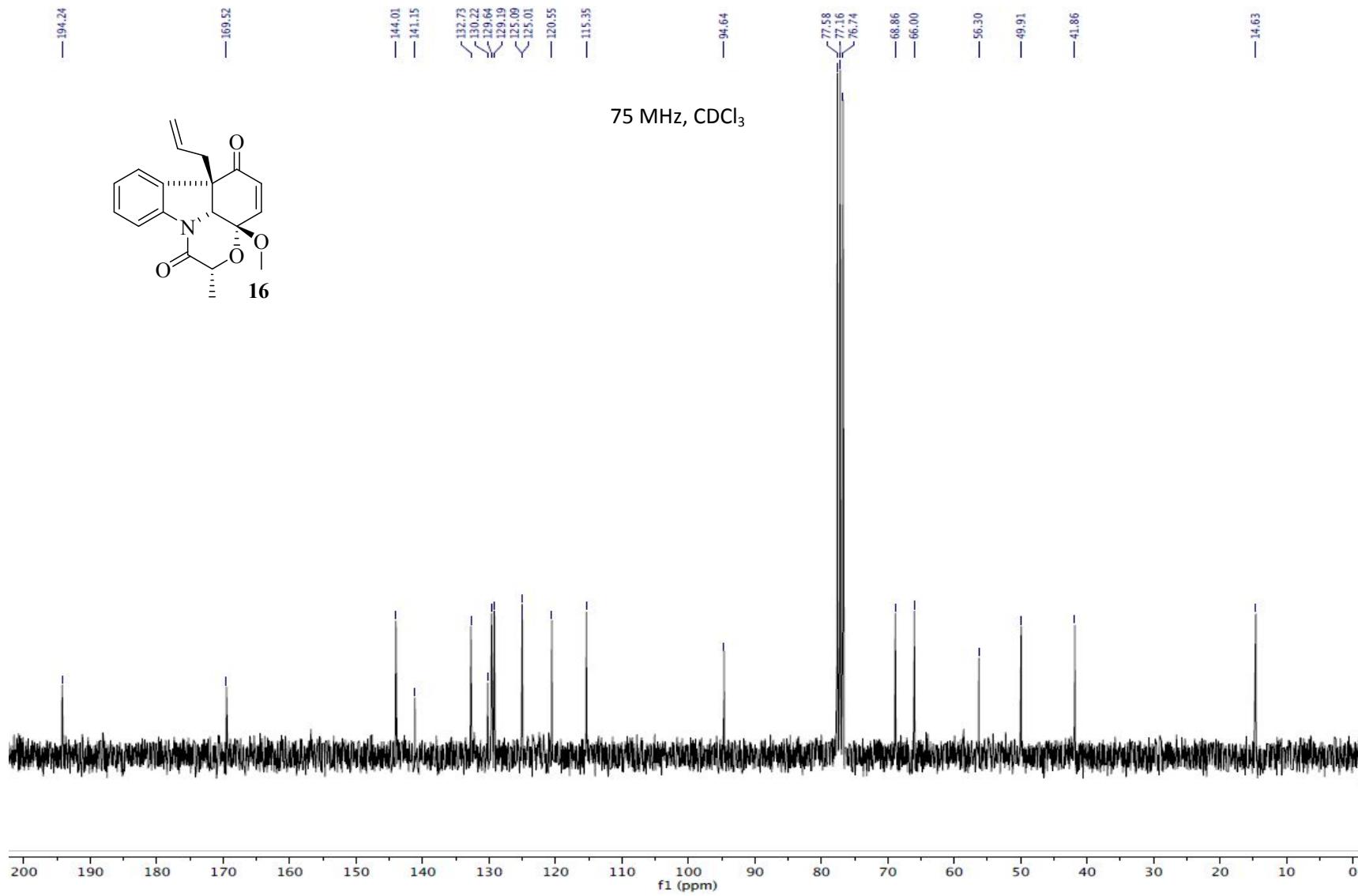


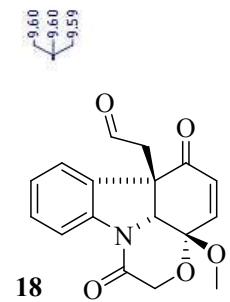




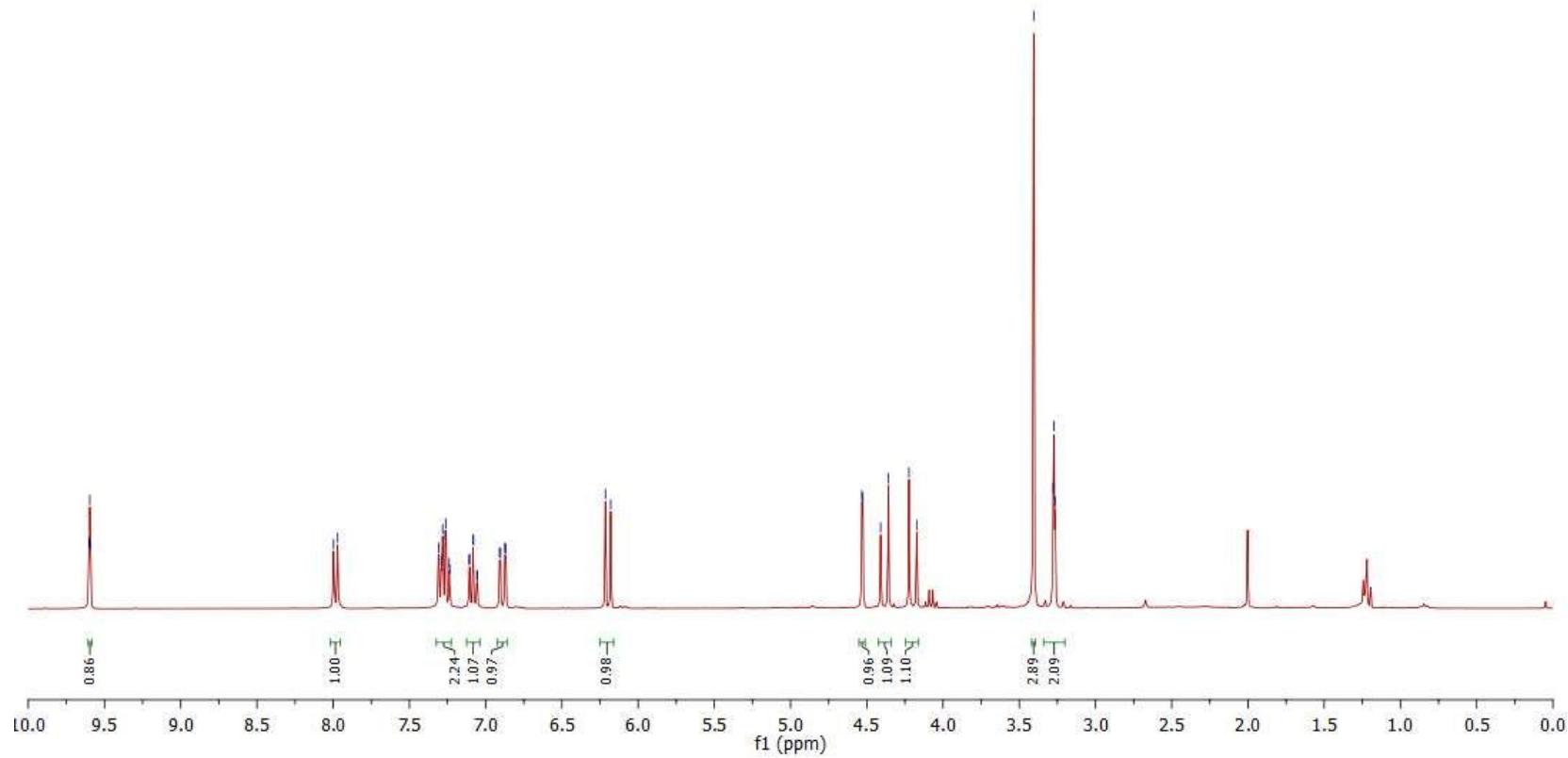


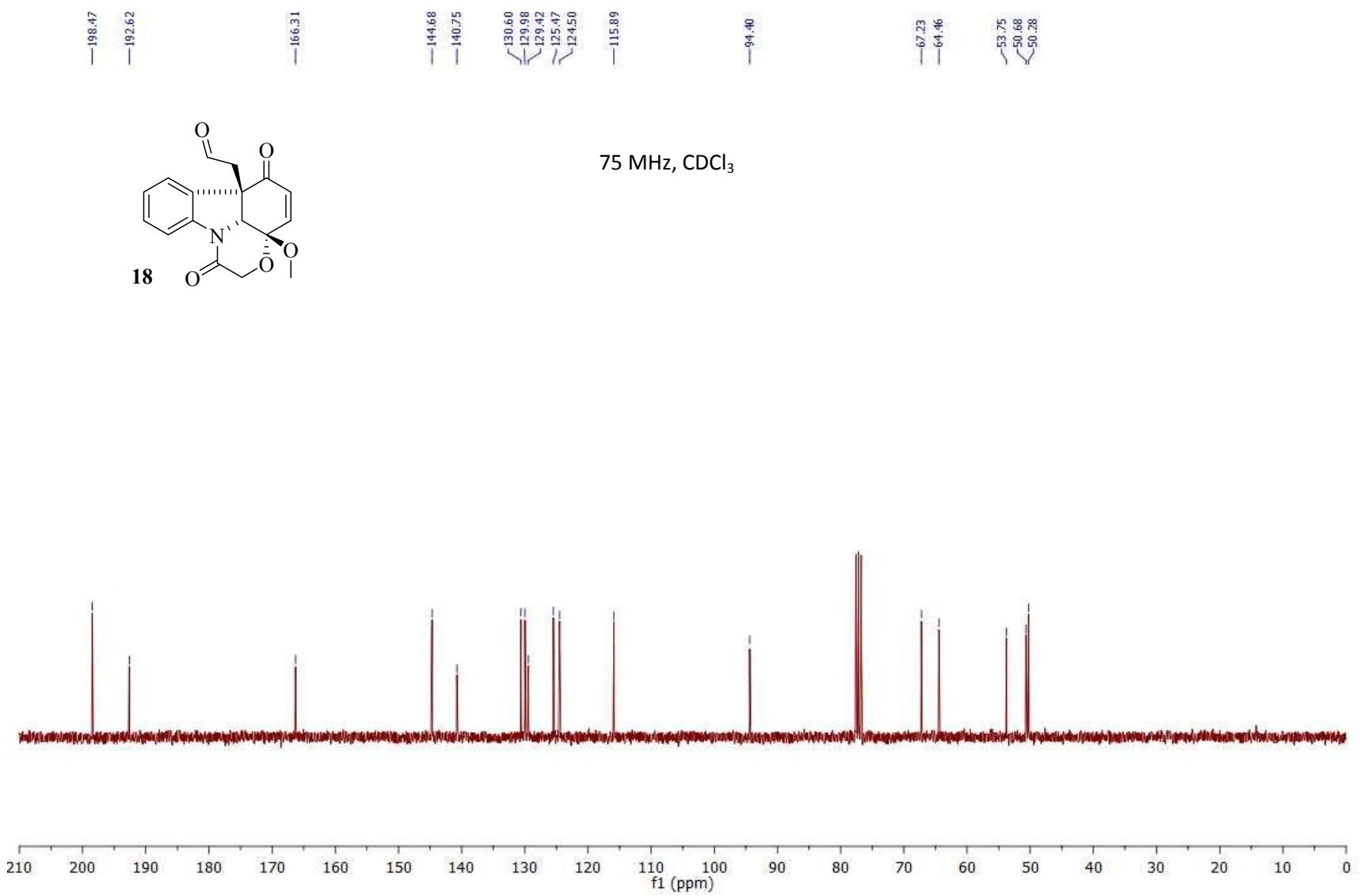


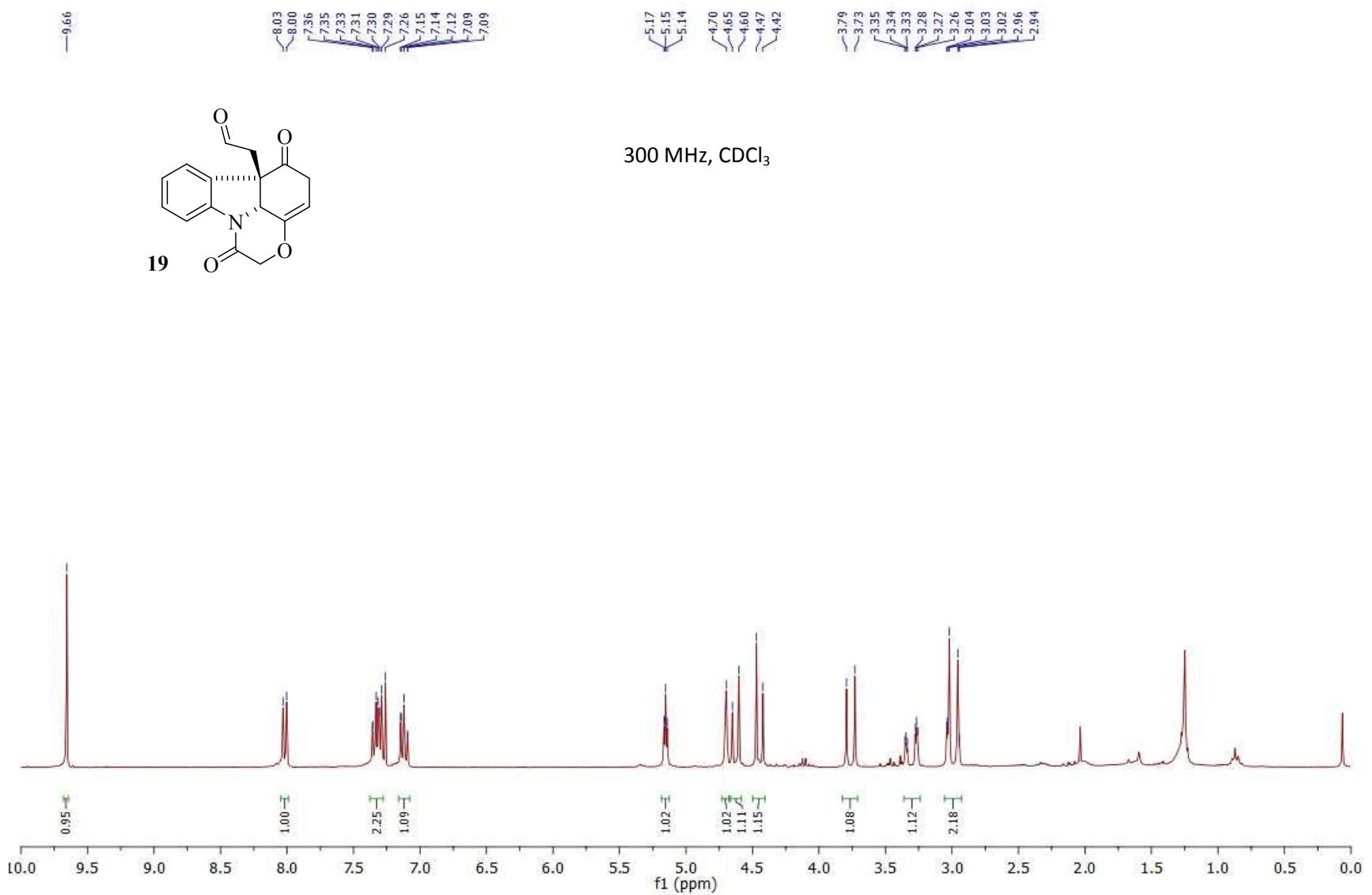


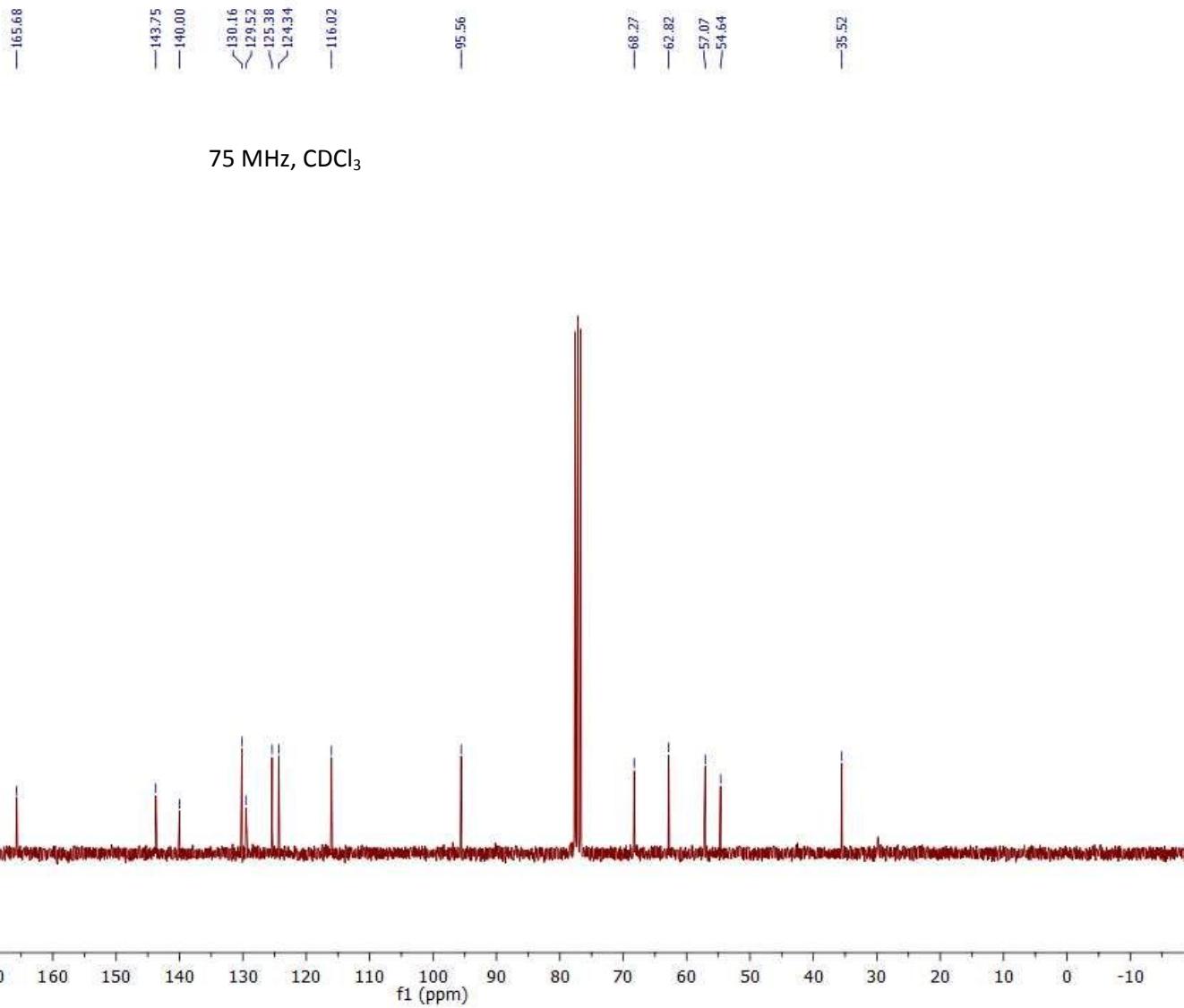
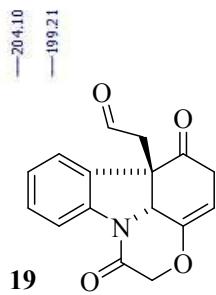


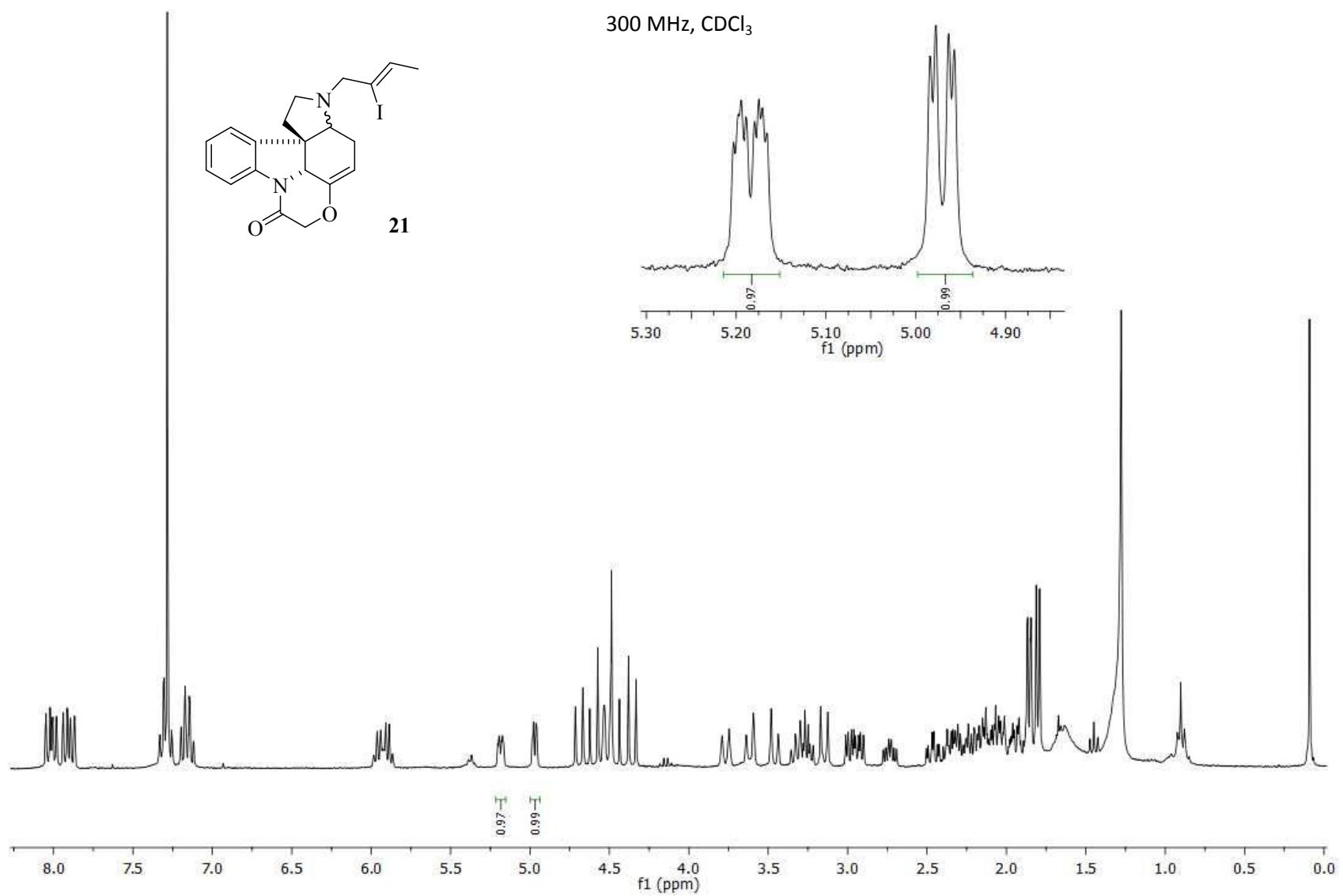
300 MHz, CDCl₃

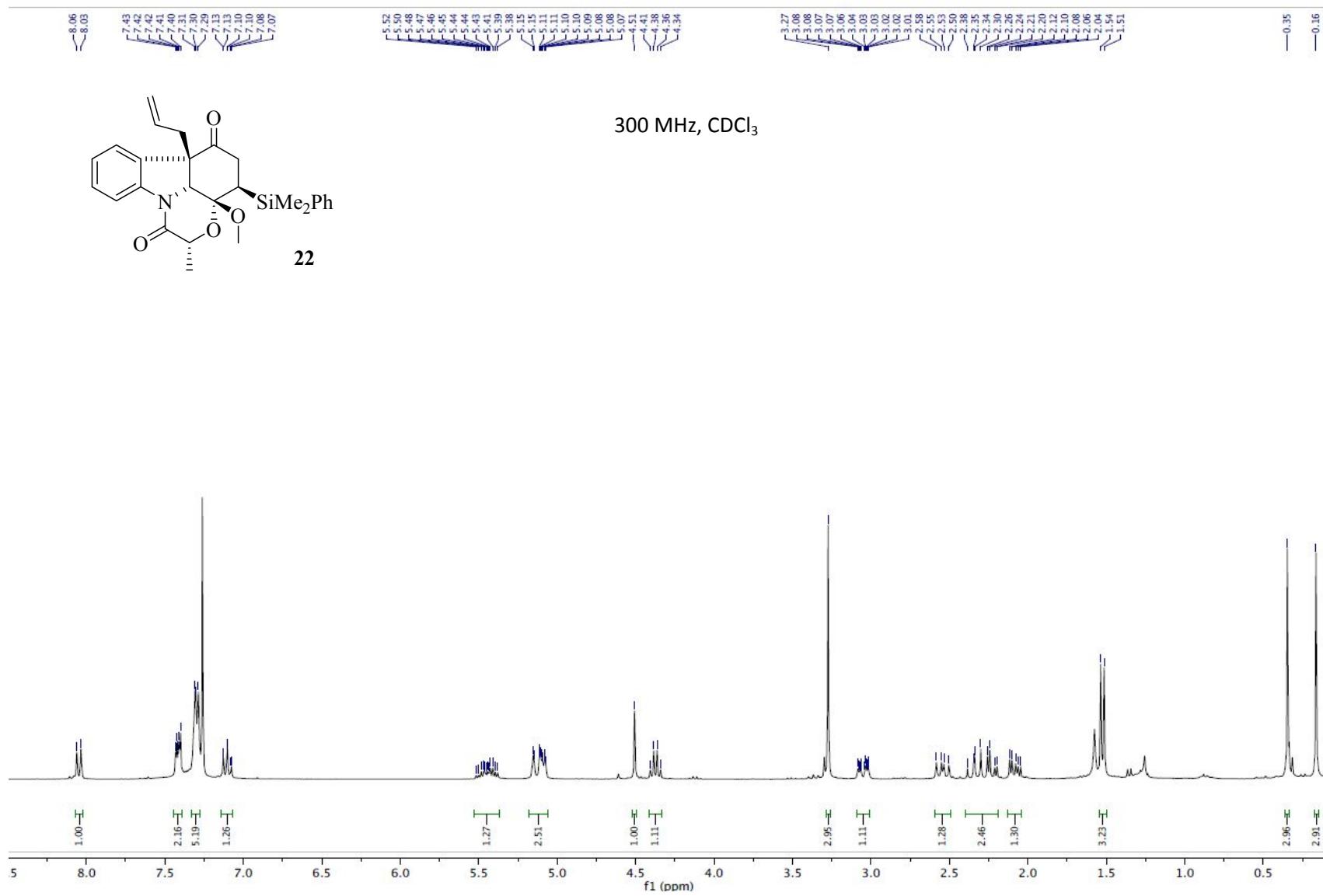


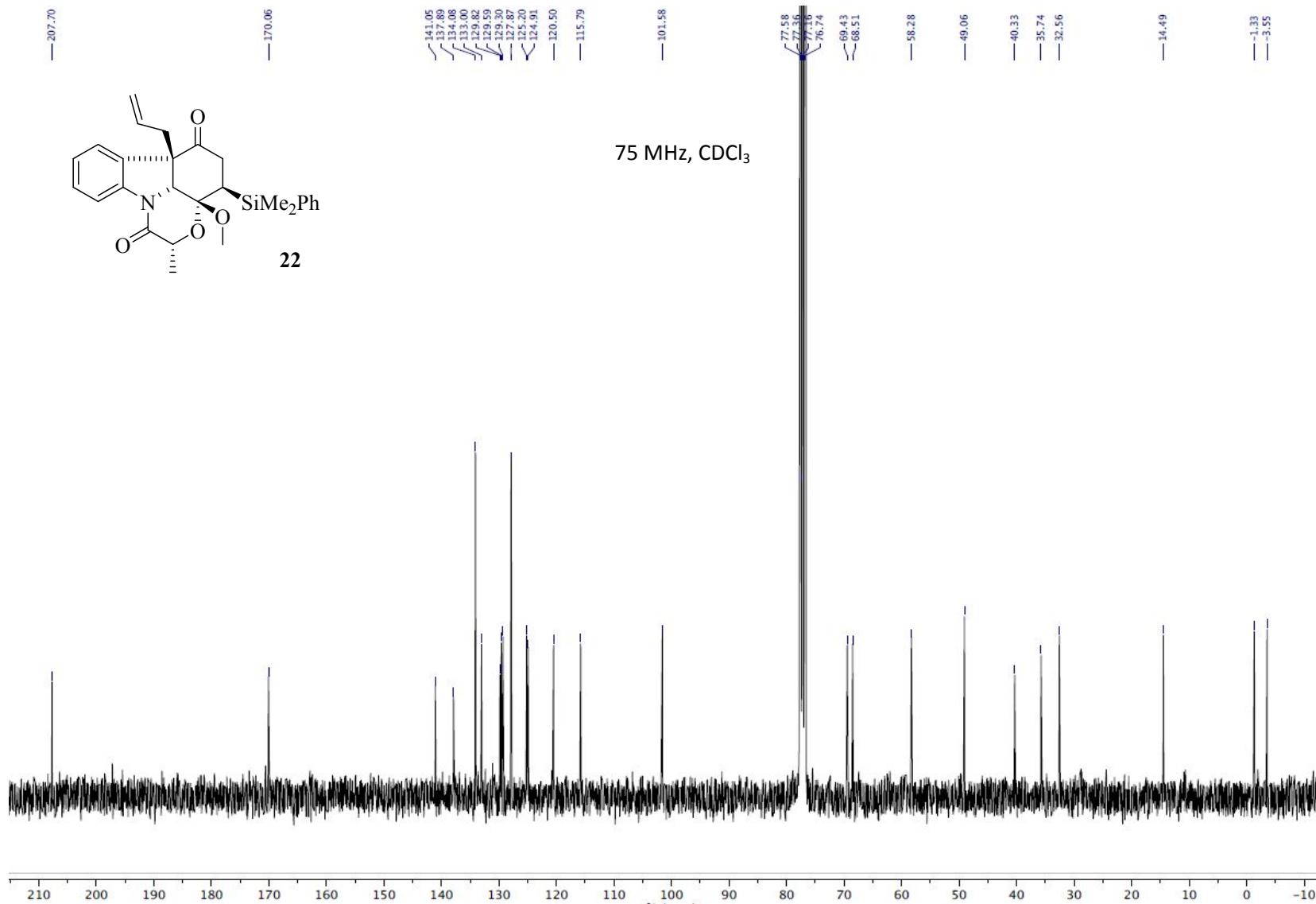


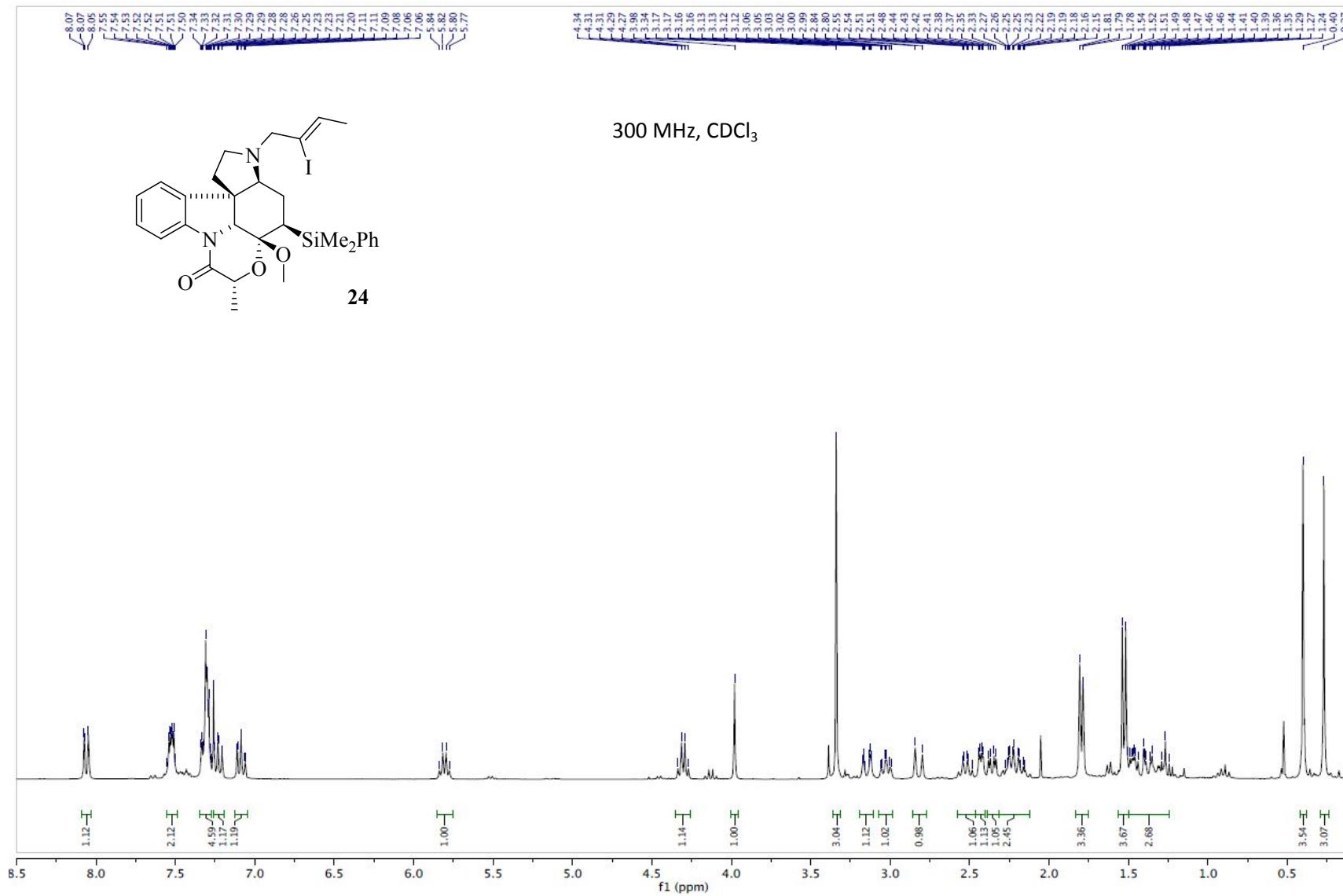


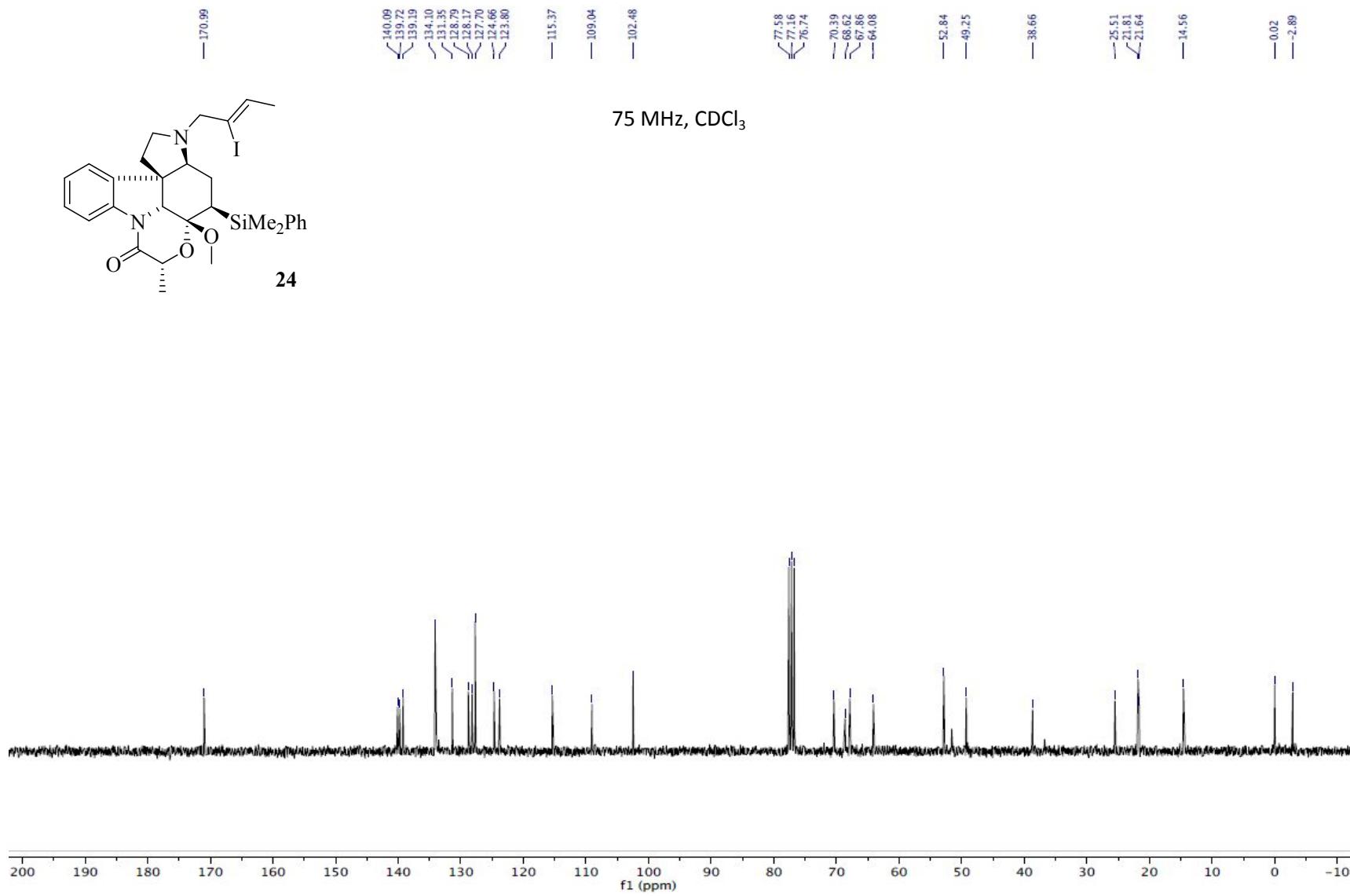


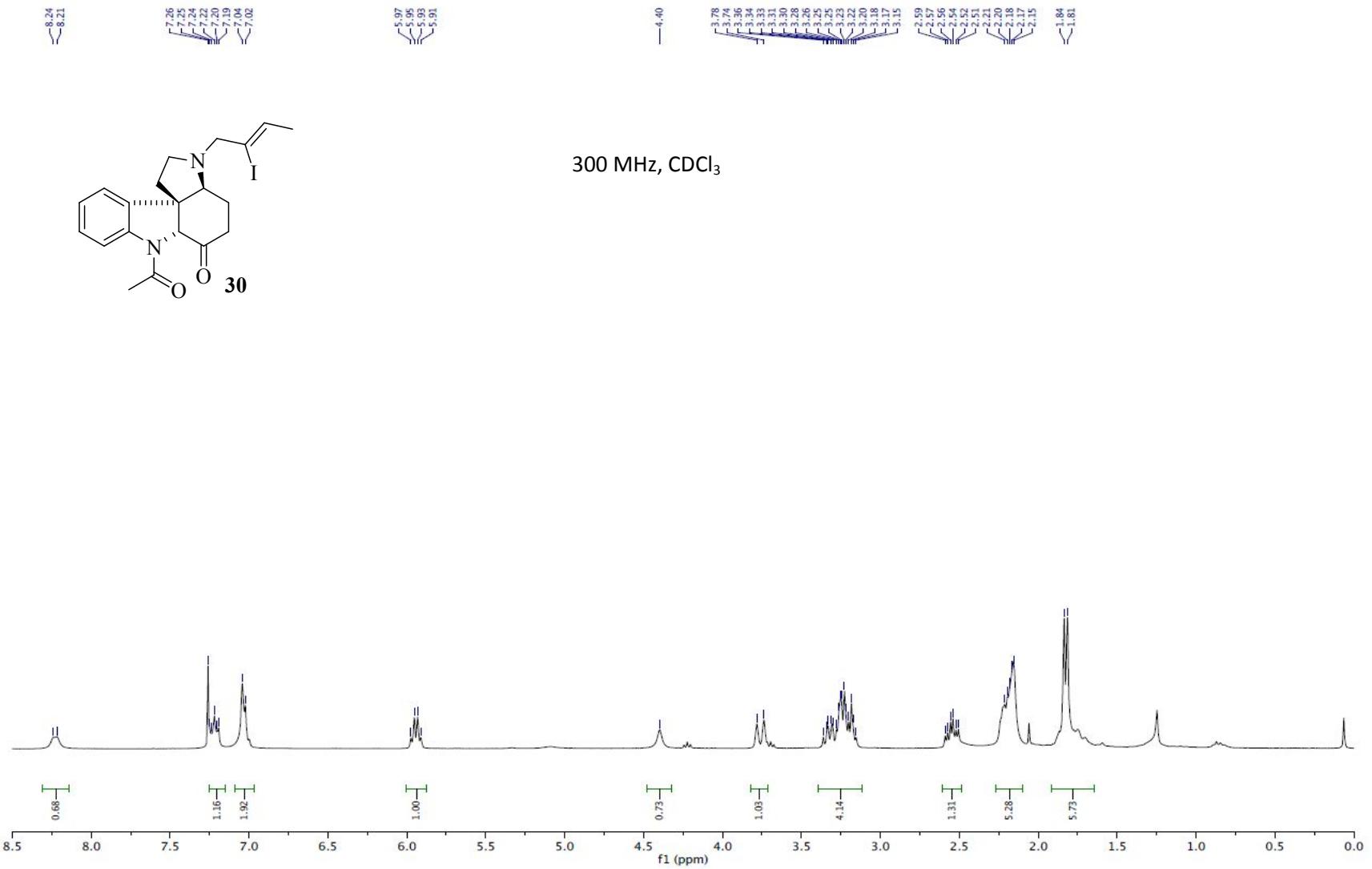


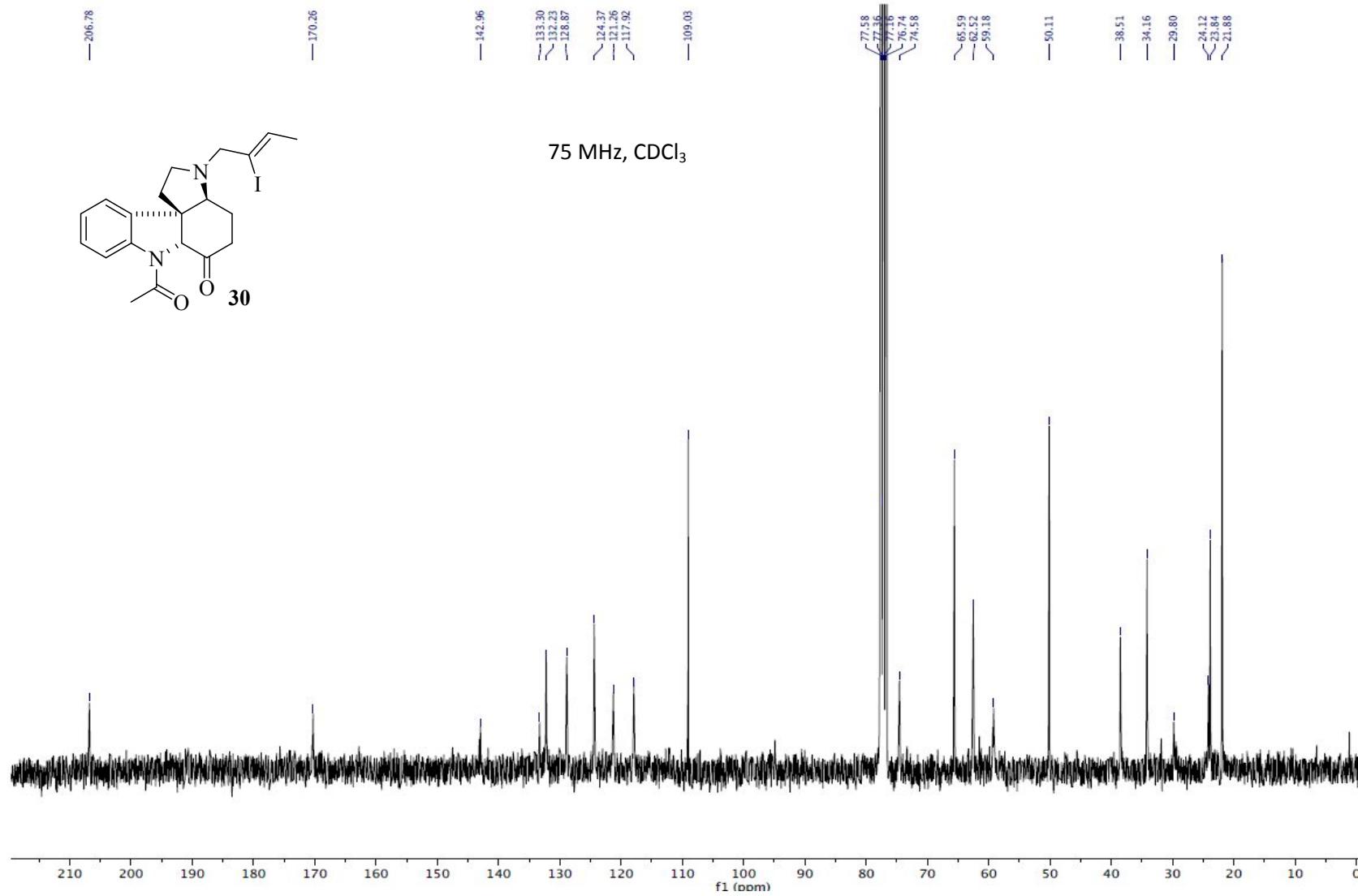


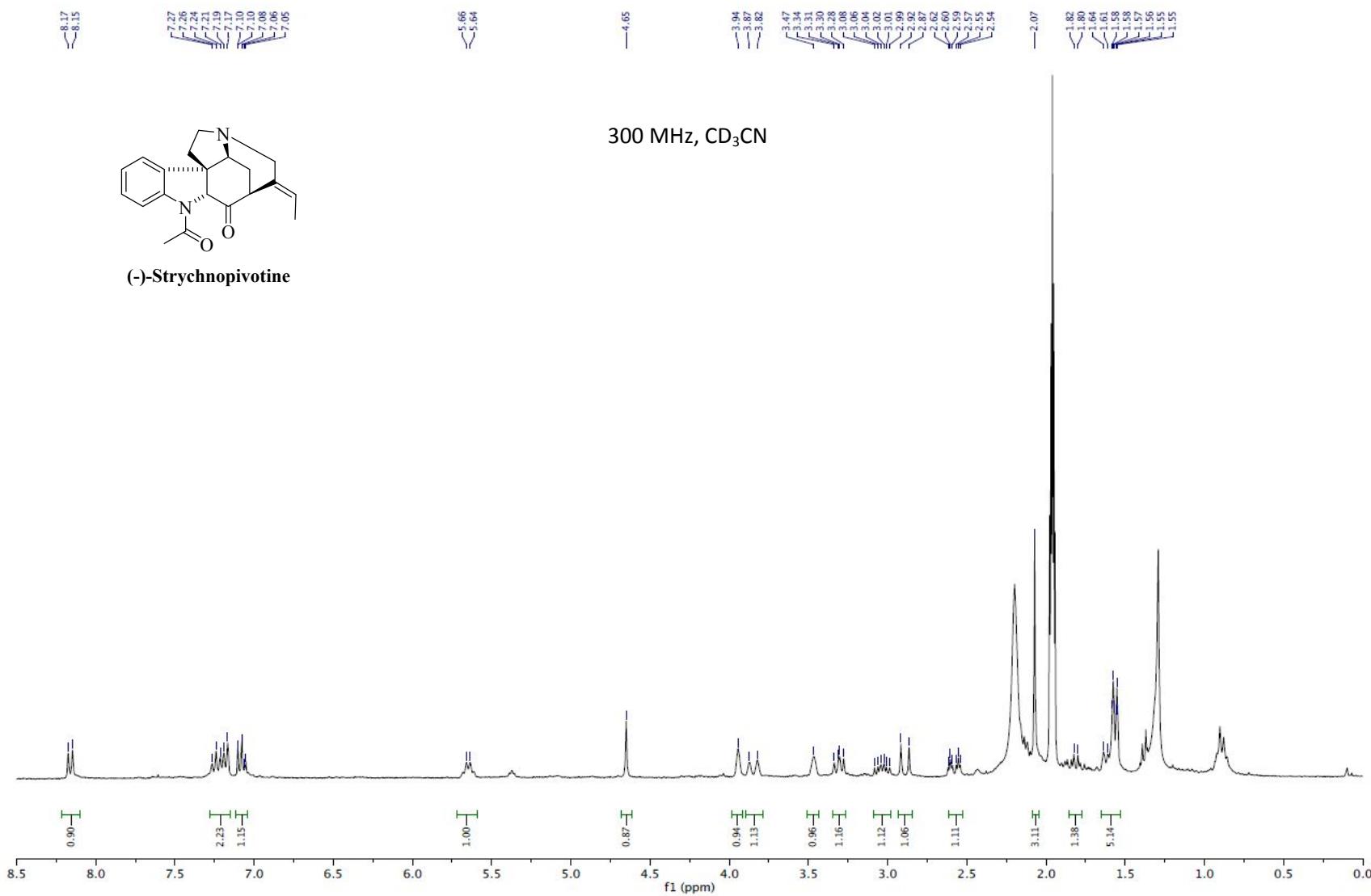


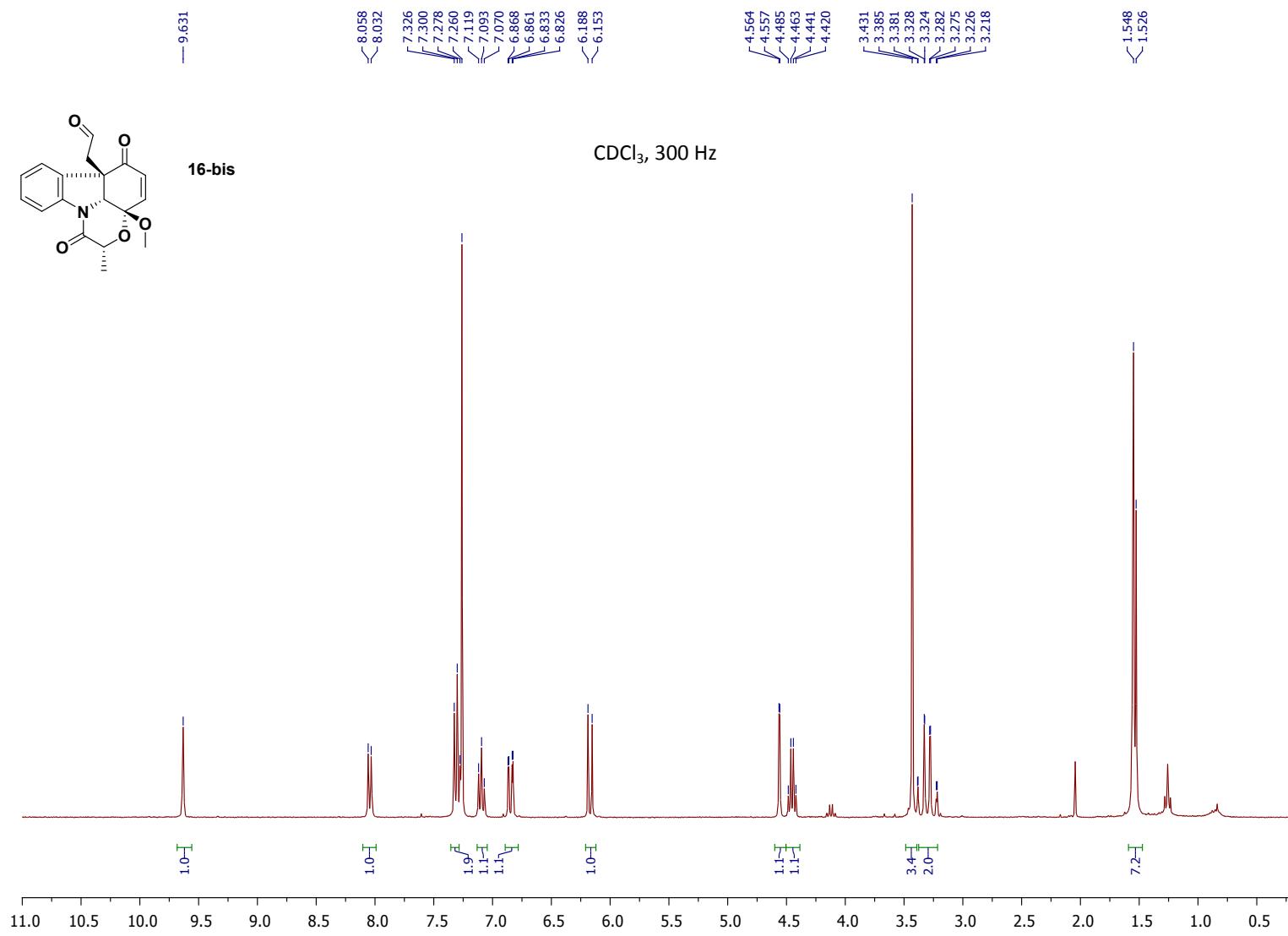


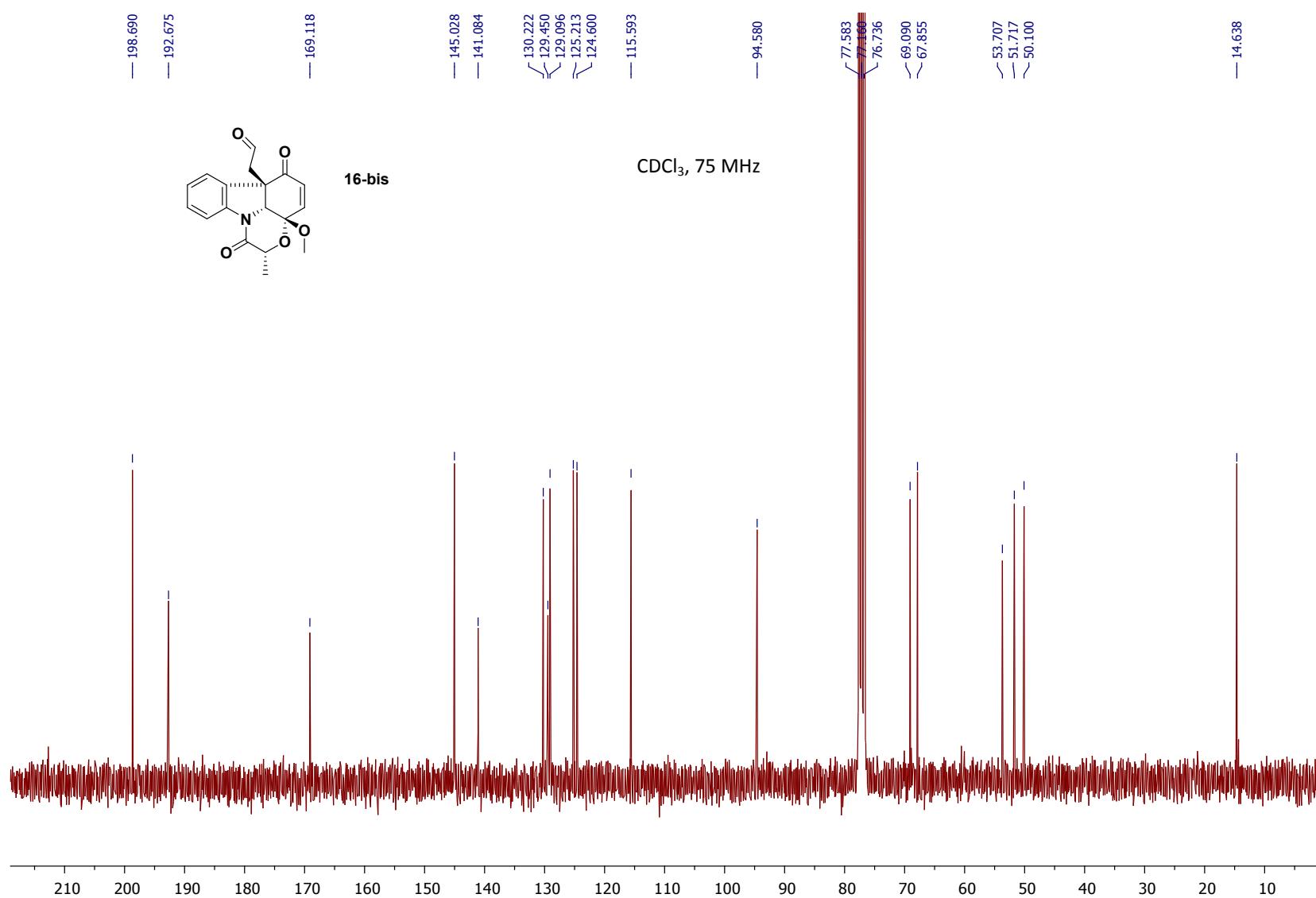


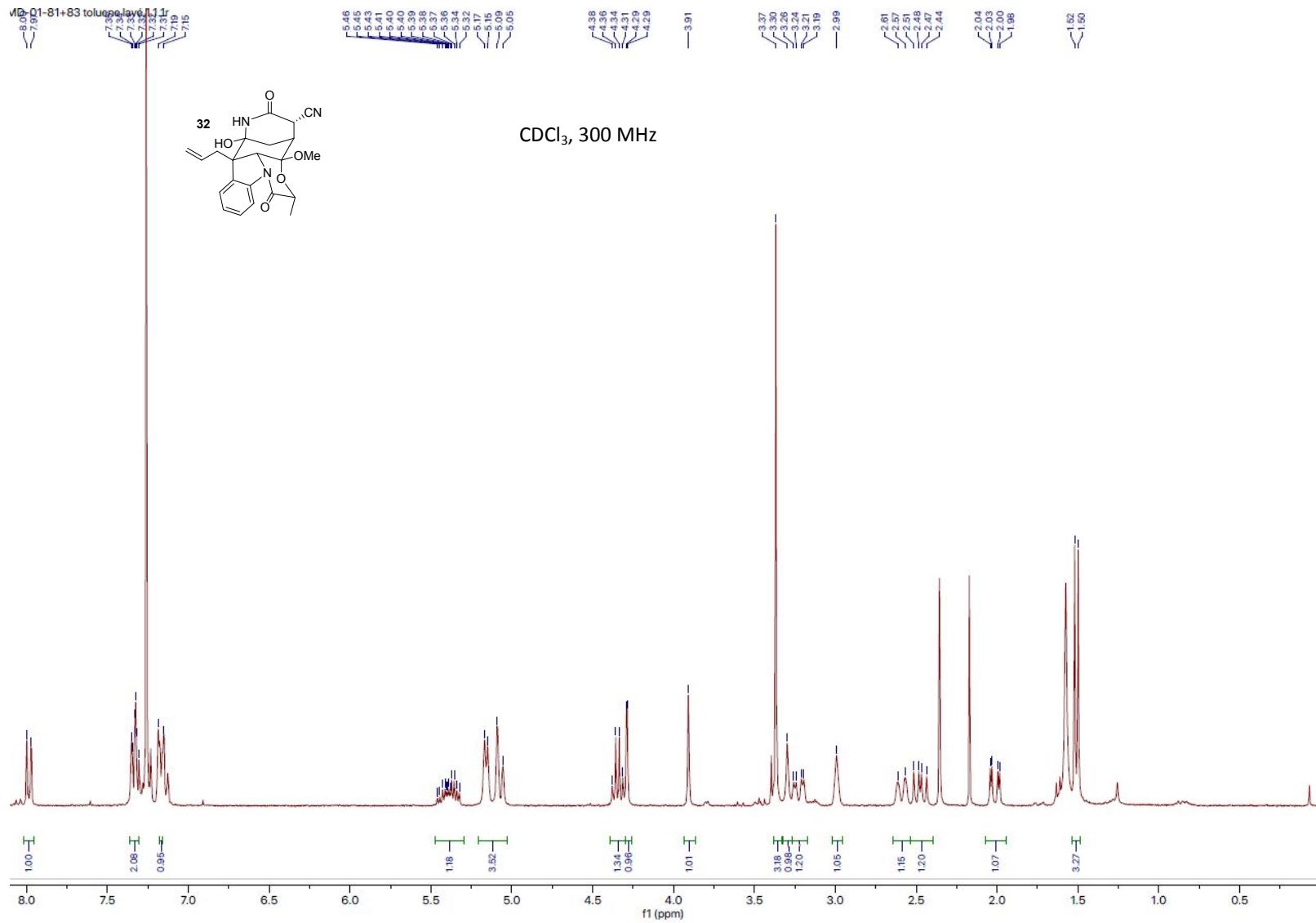






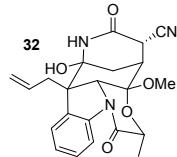




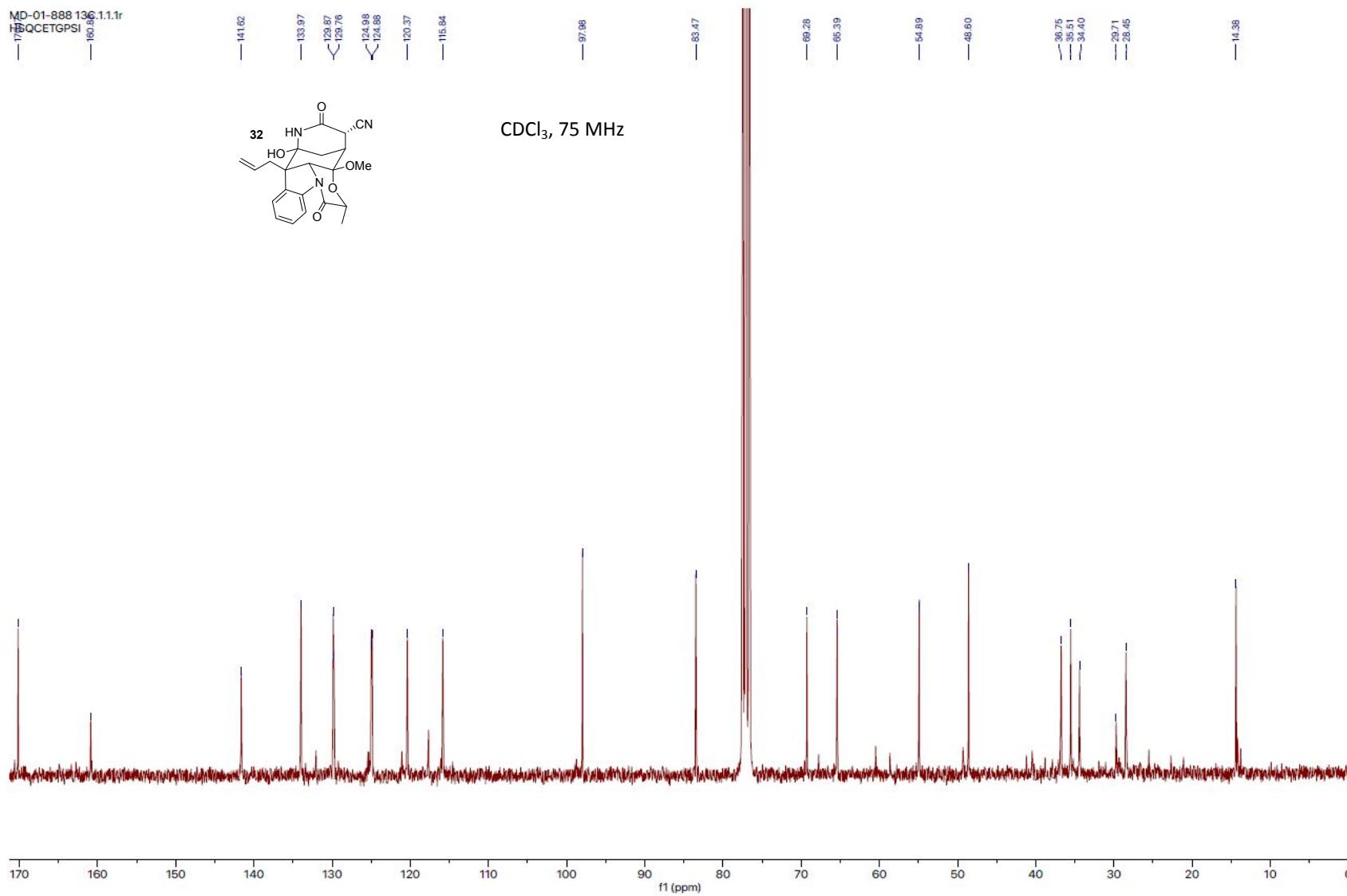


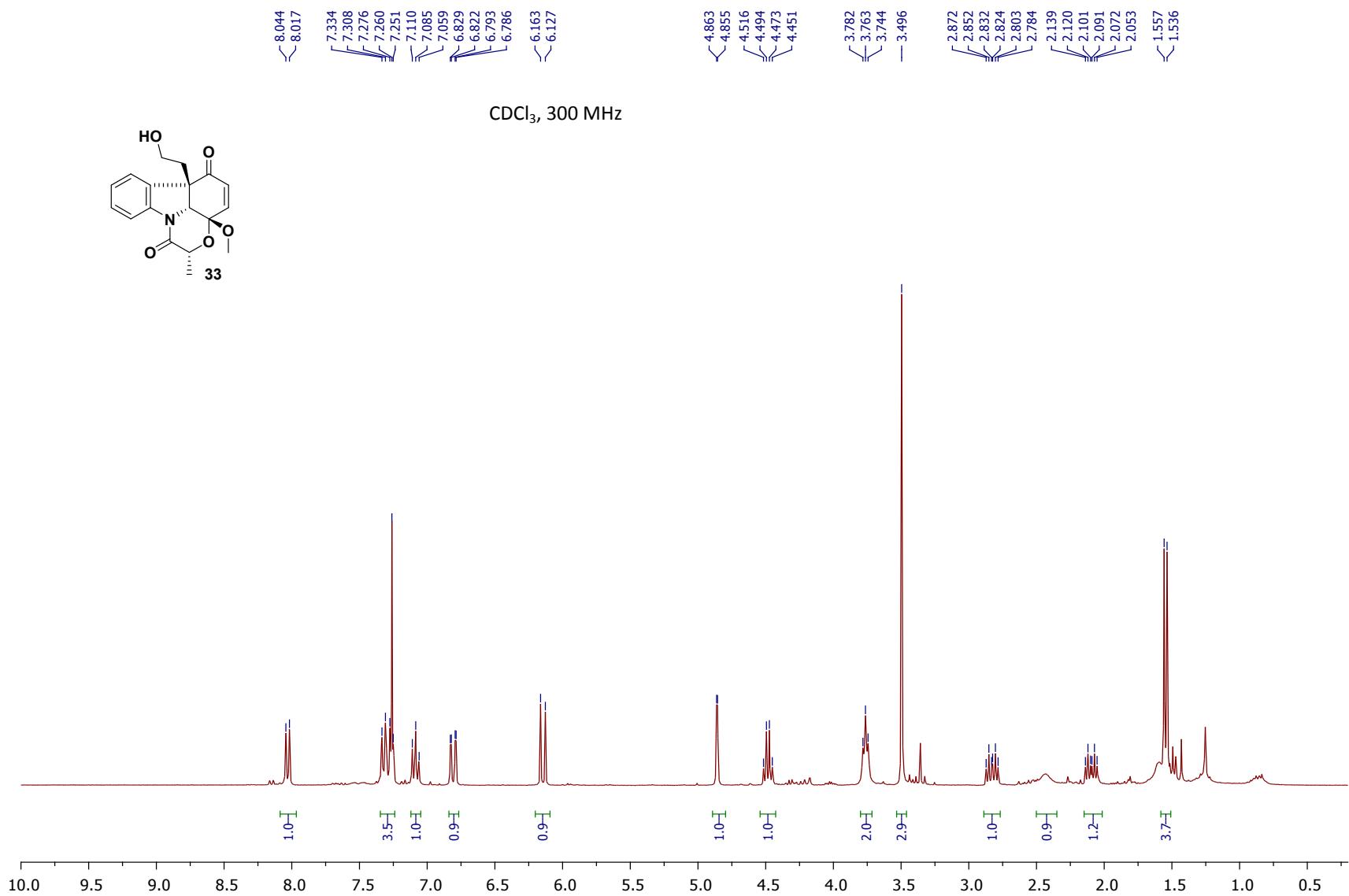
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¹³CQETGPSI
— 160.86

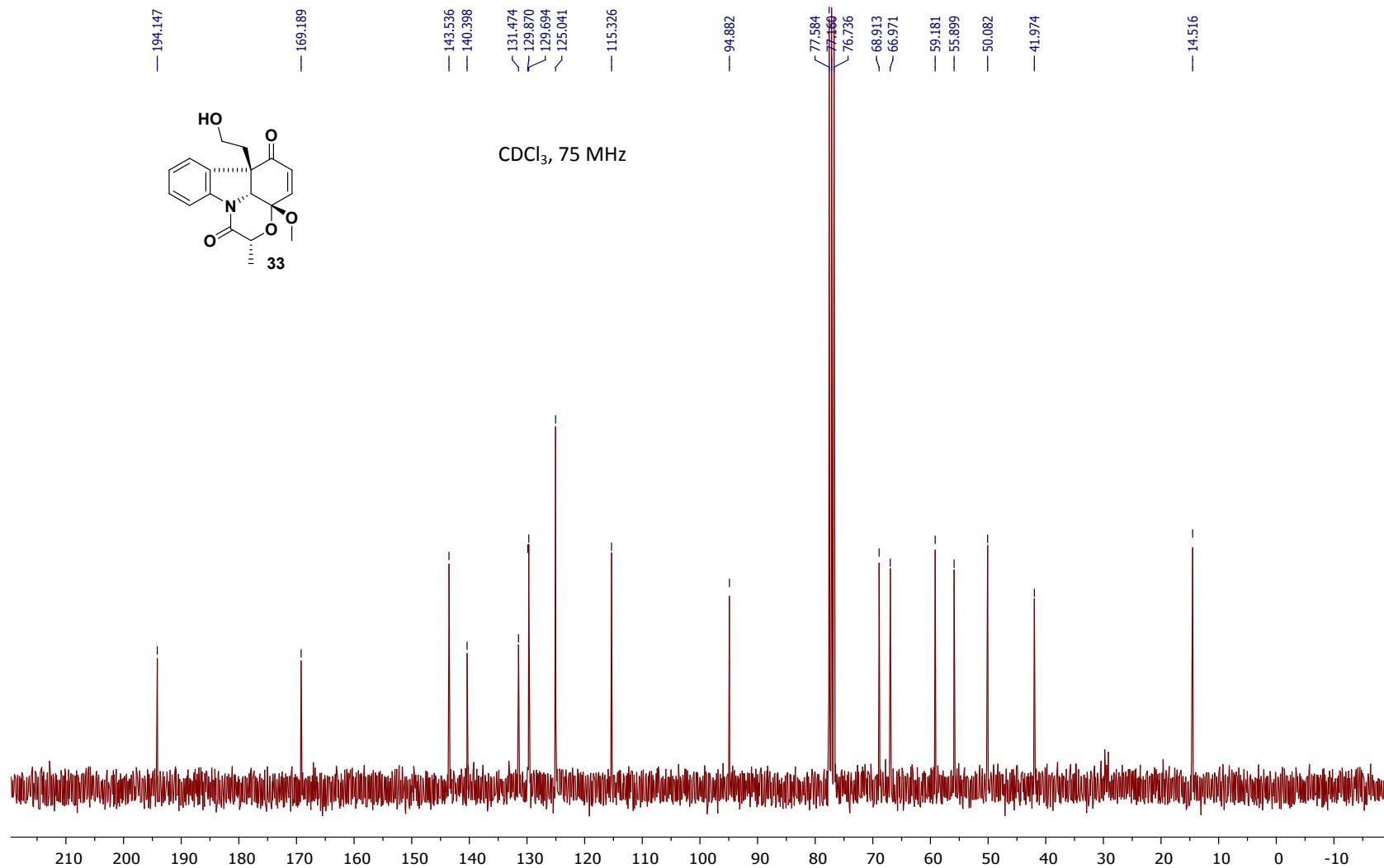
— 141.62
— 133.97
— 129.87
— 129.76
— 124.98
— 124.68
— 120.37
— 115.84

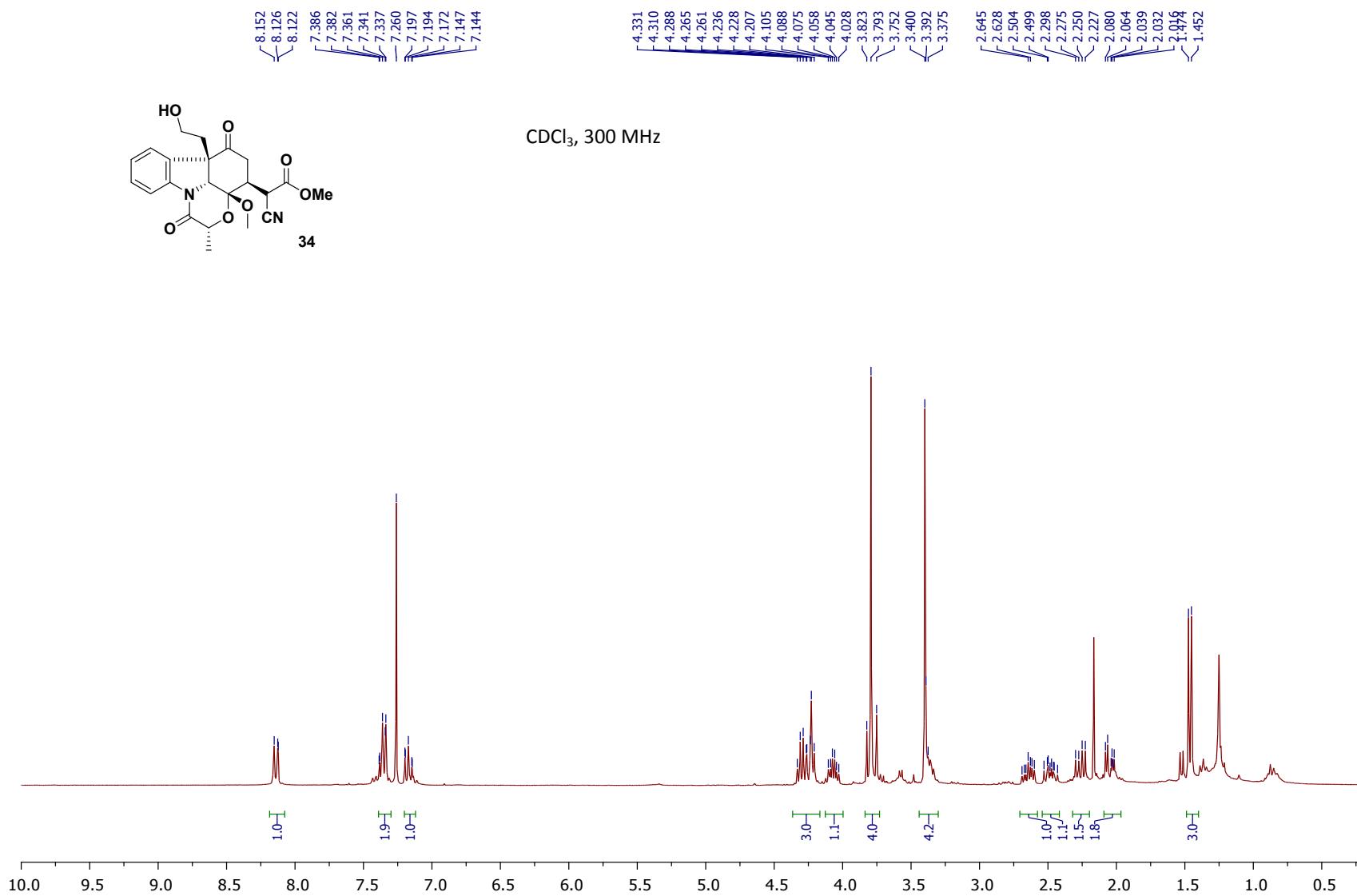


CDCl₃, 75 MHz

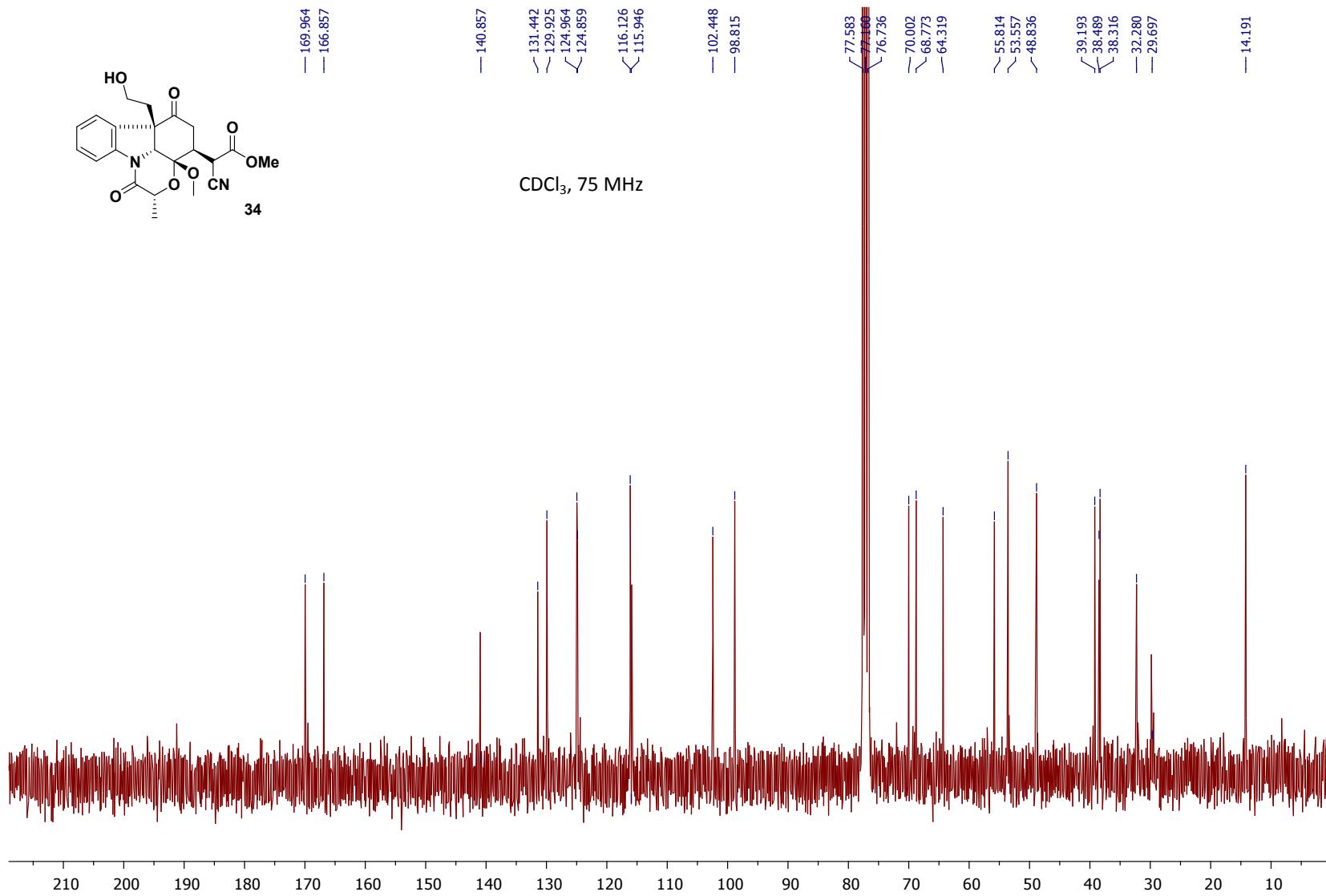


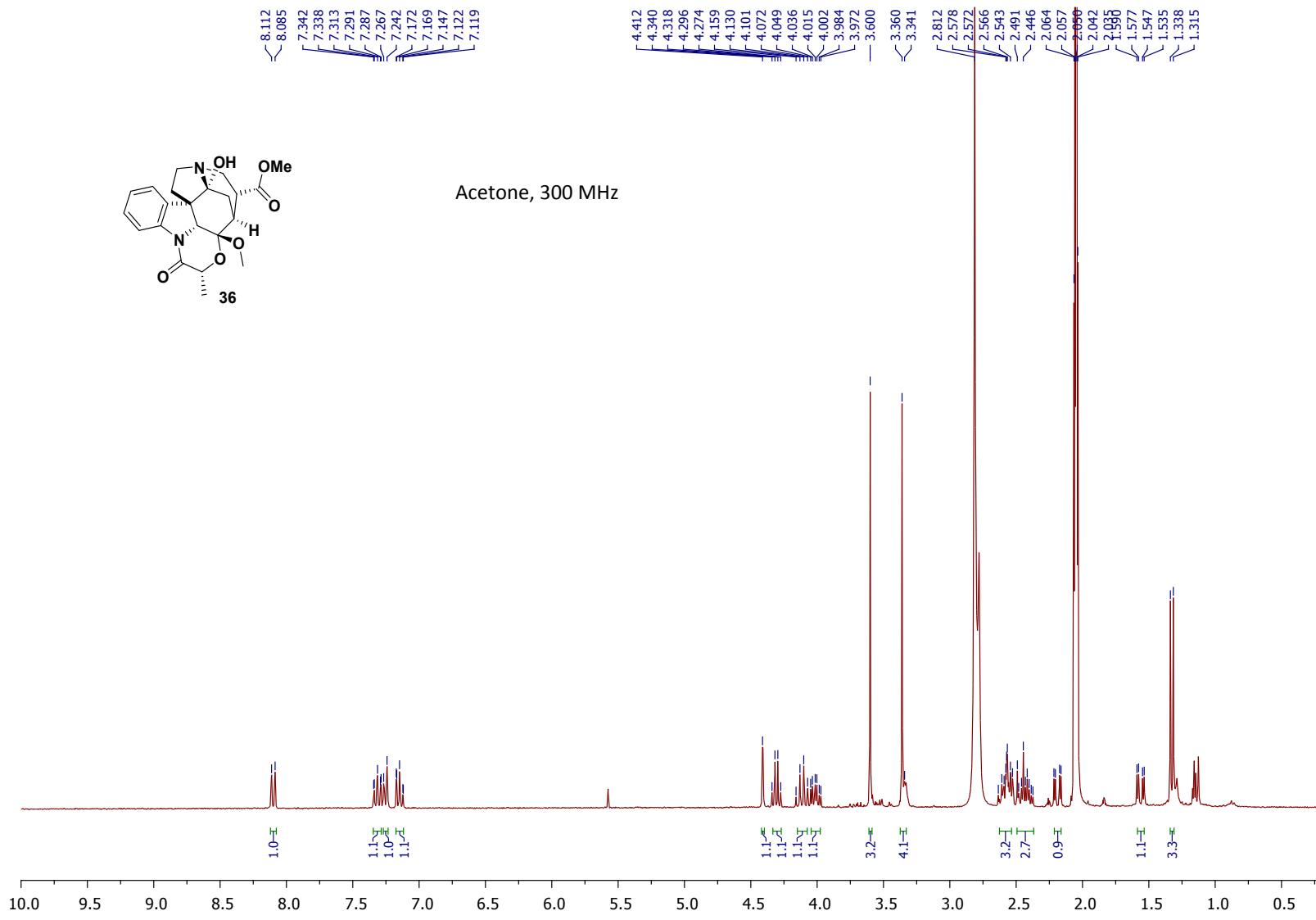


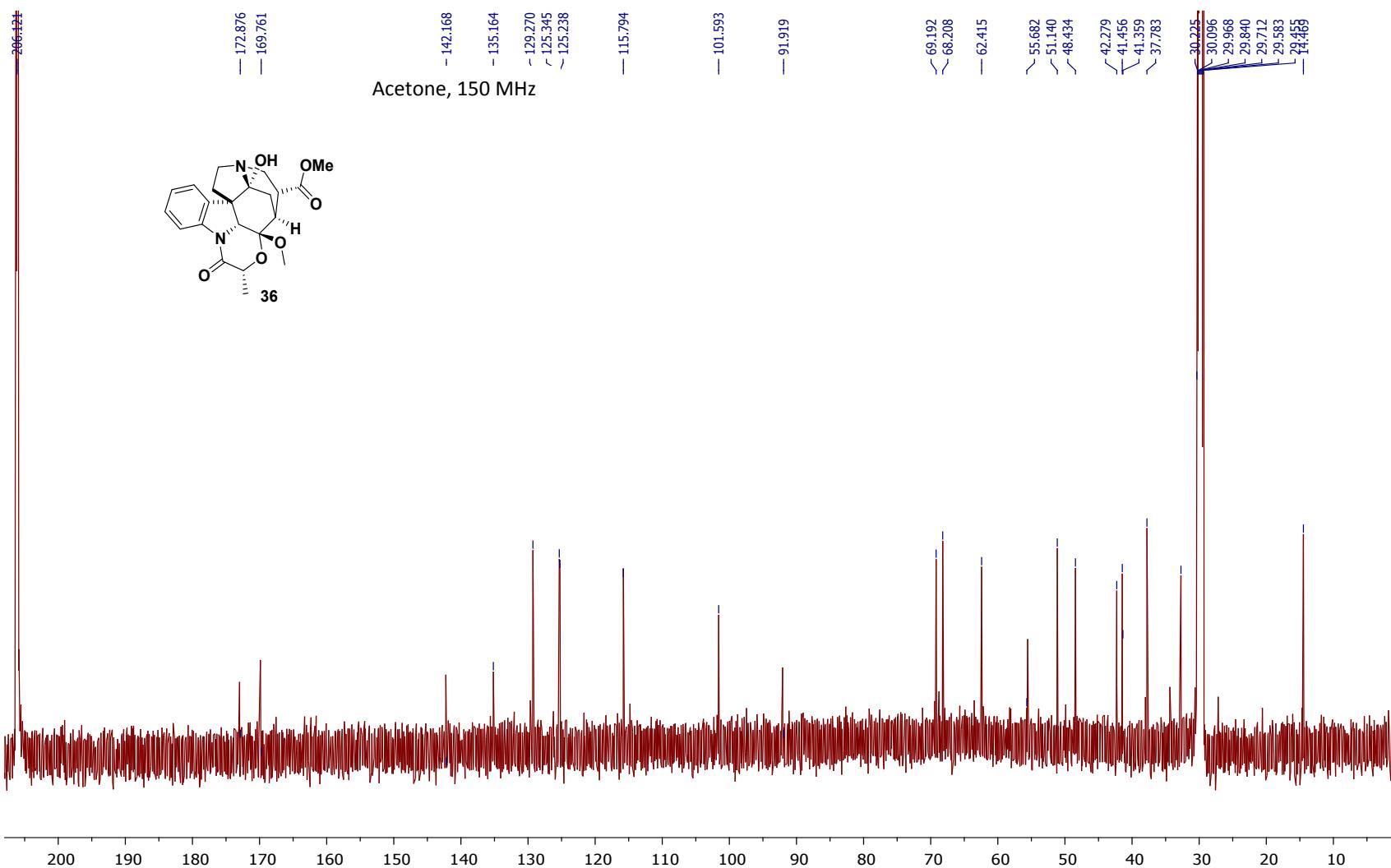




S34

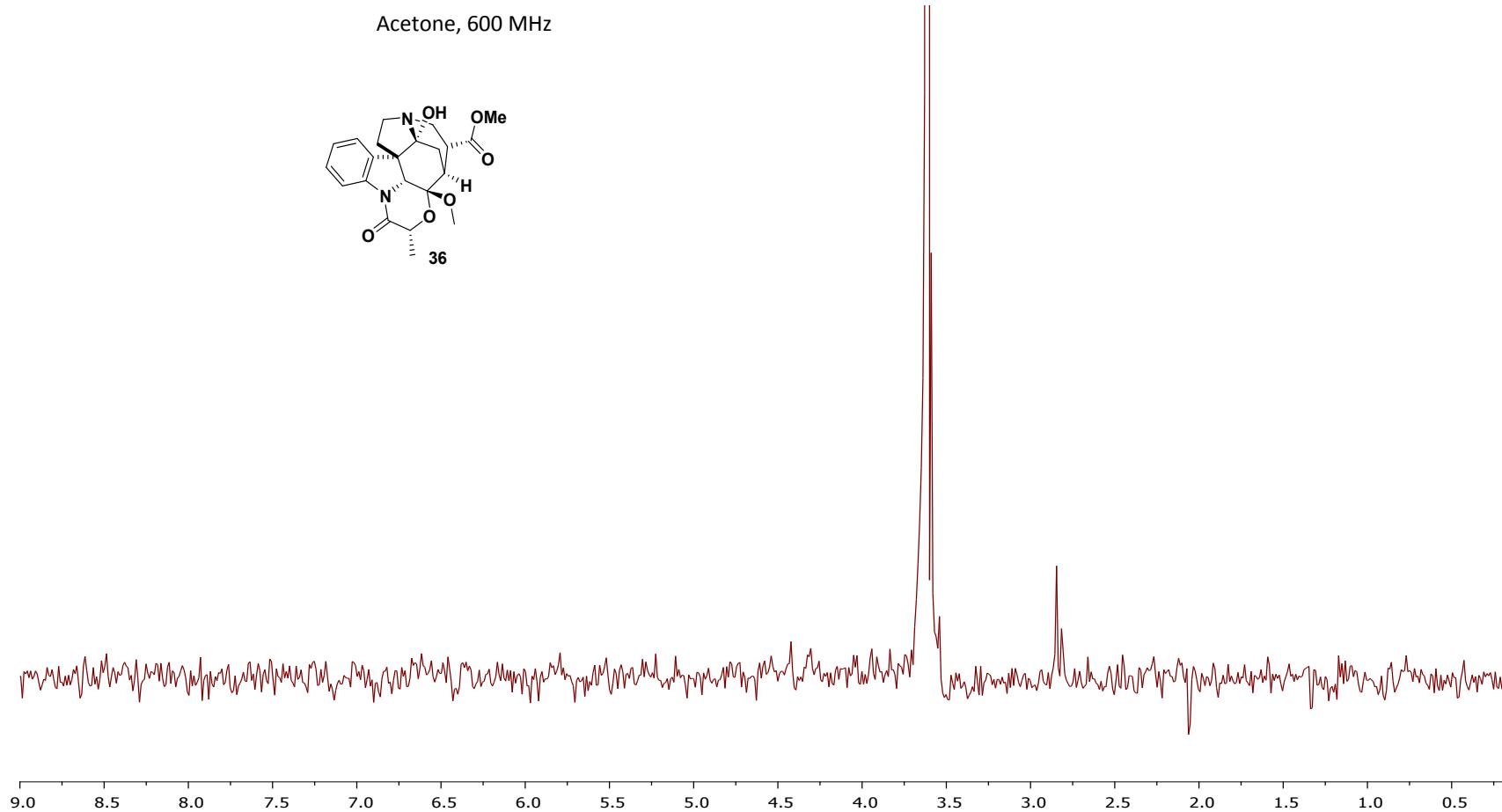
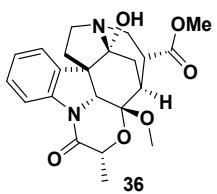




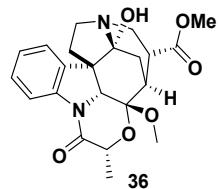


NOE ^1H - ^1H Peak at 3.60 ppm :

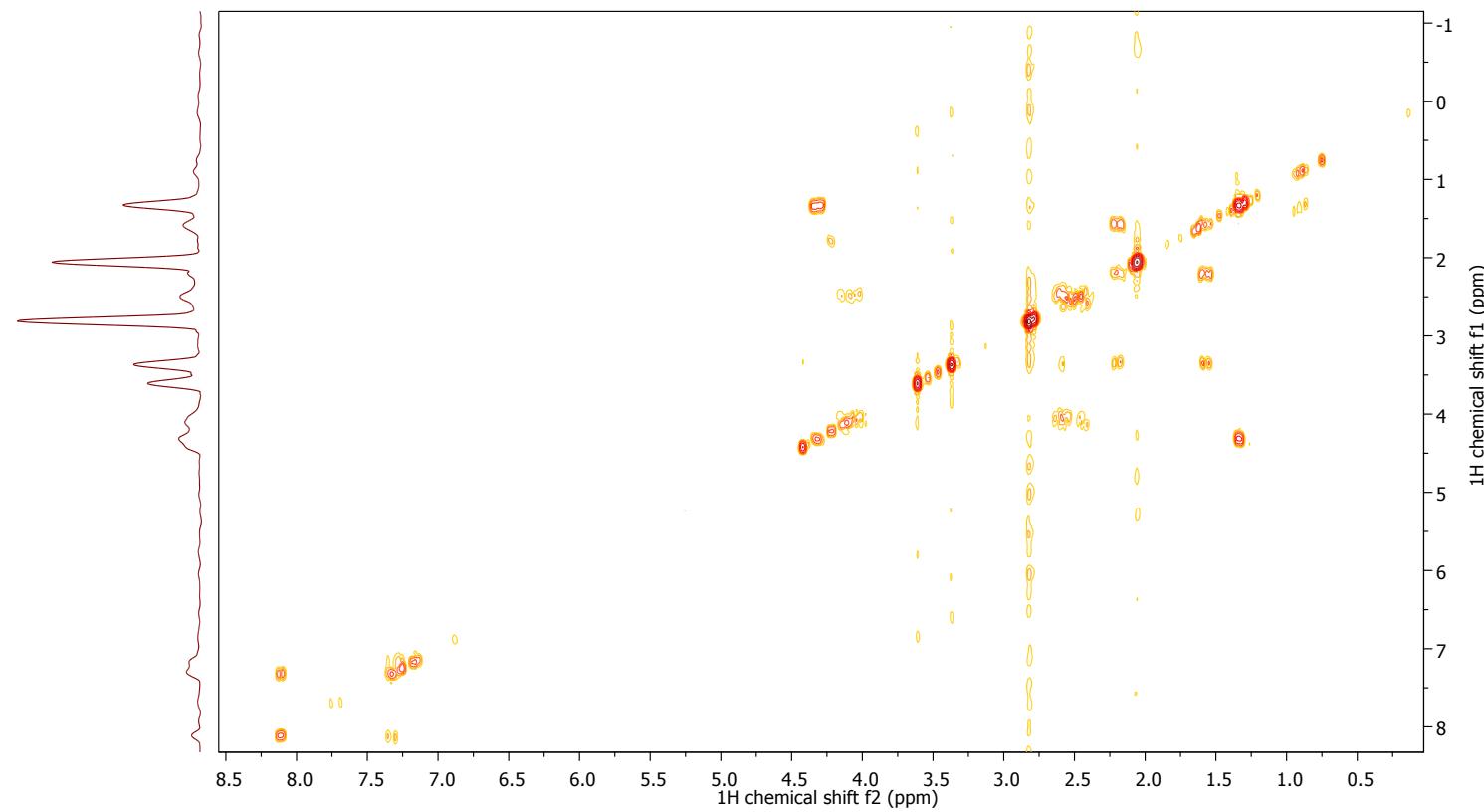
Acetone, 600 MHz

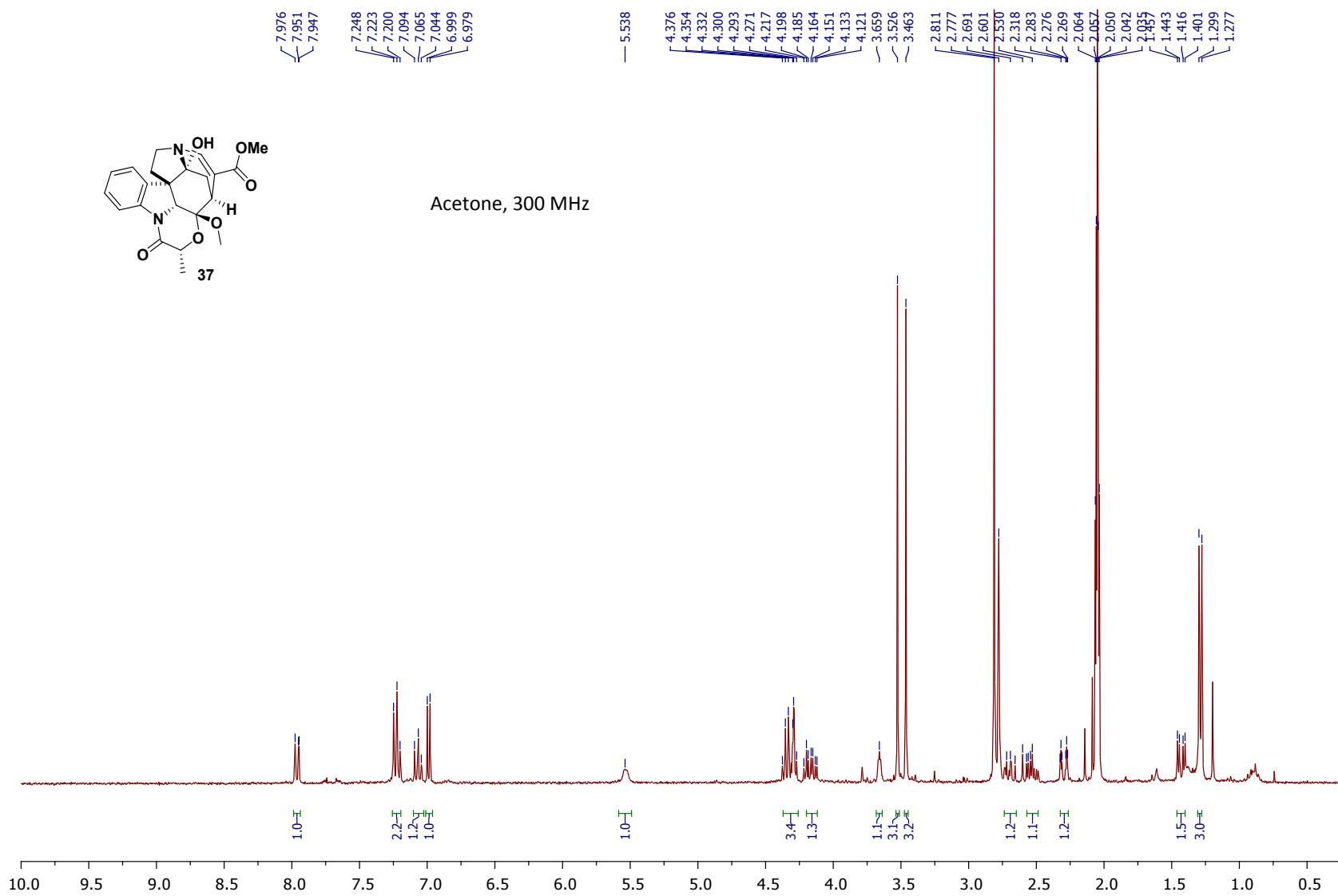


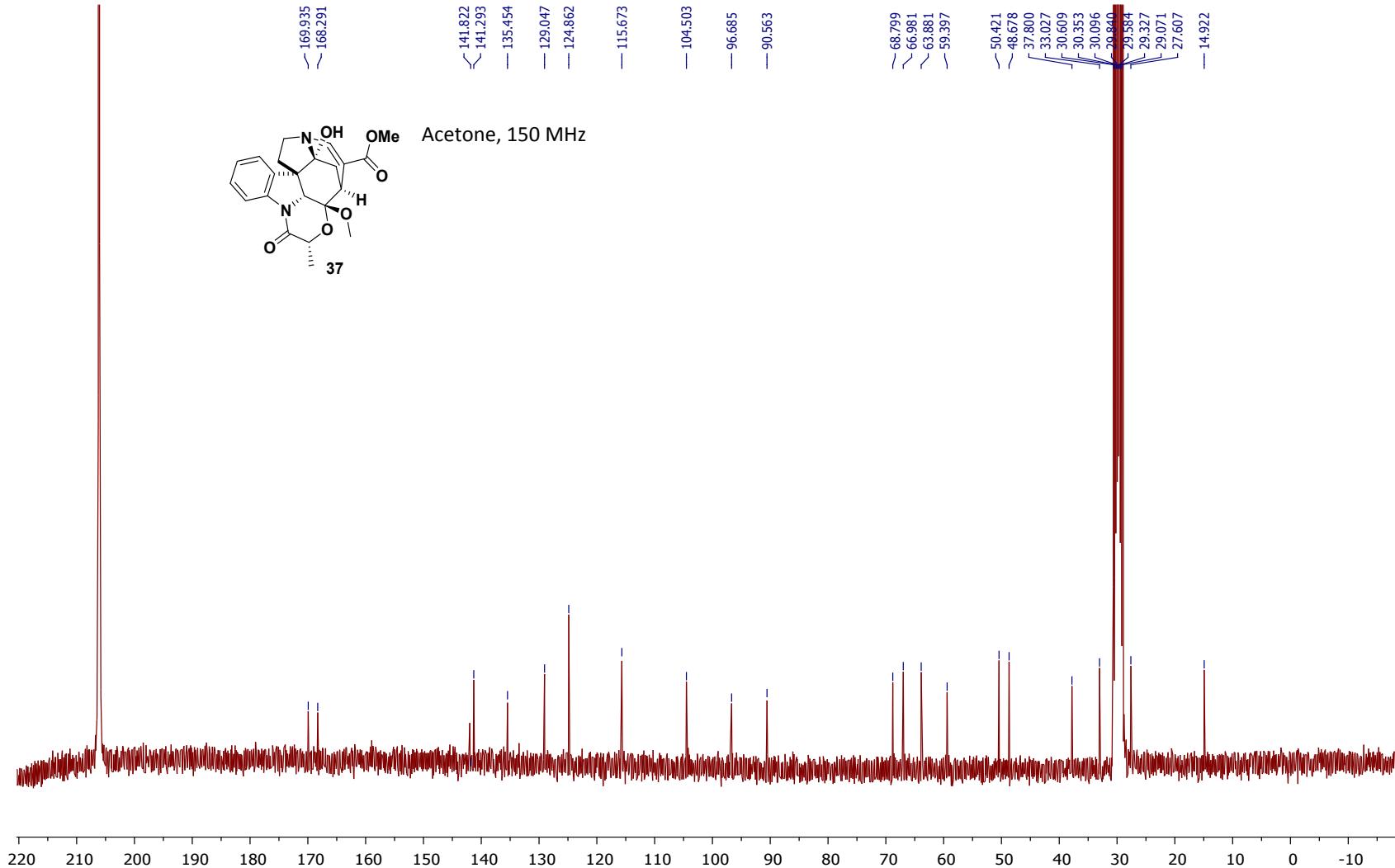
COSY ^1H - ^1H :



Acetone, 300 MHz

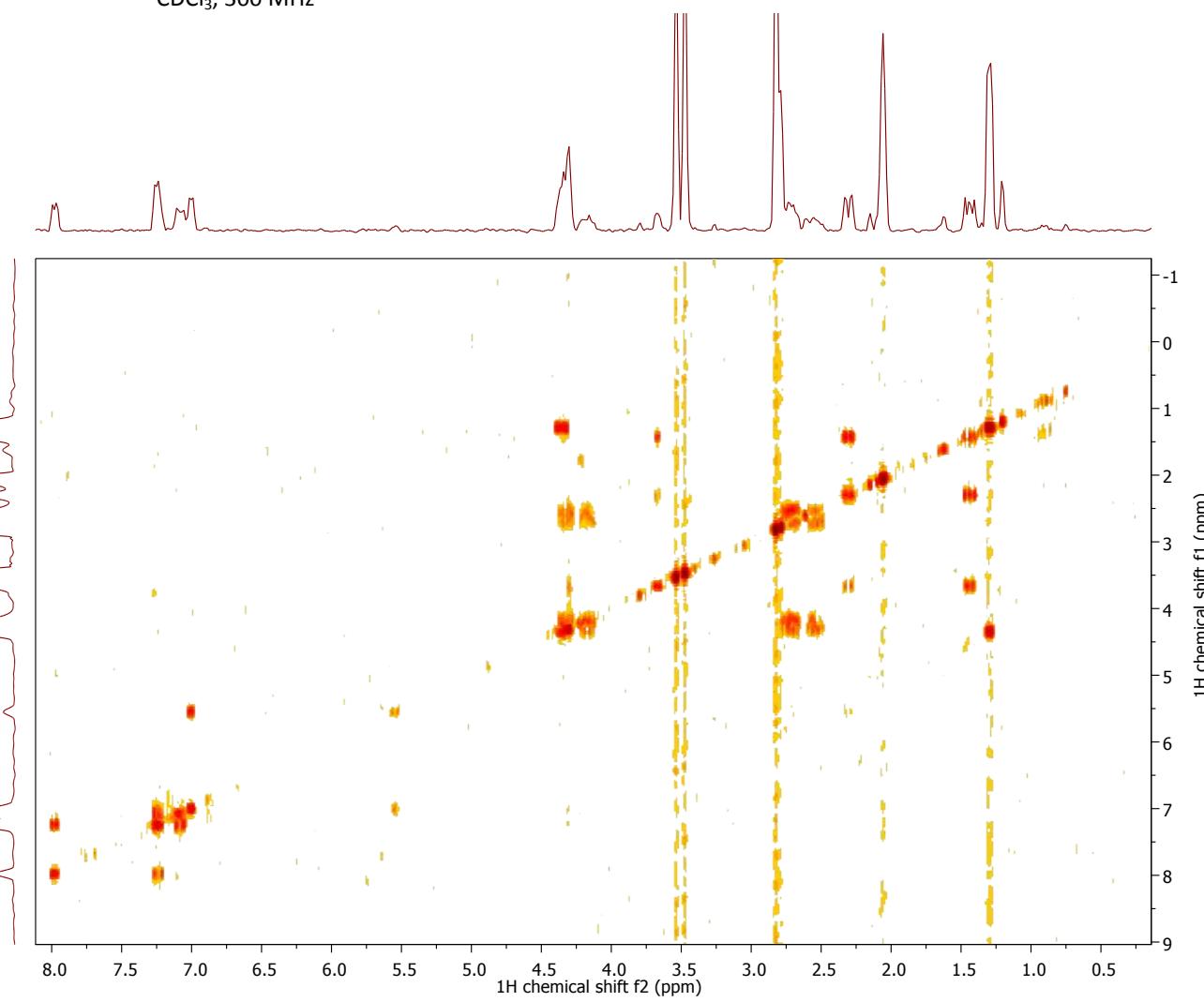
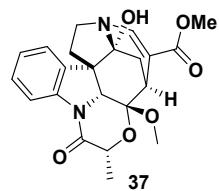


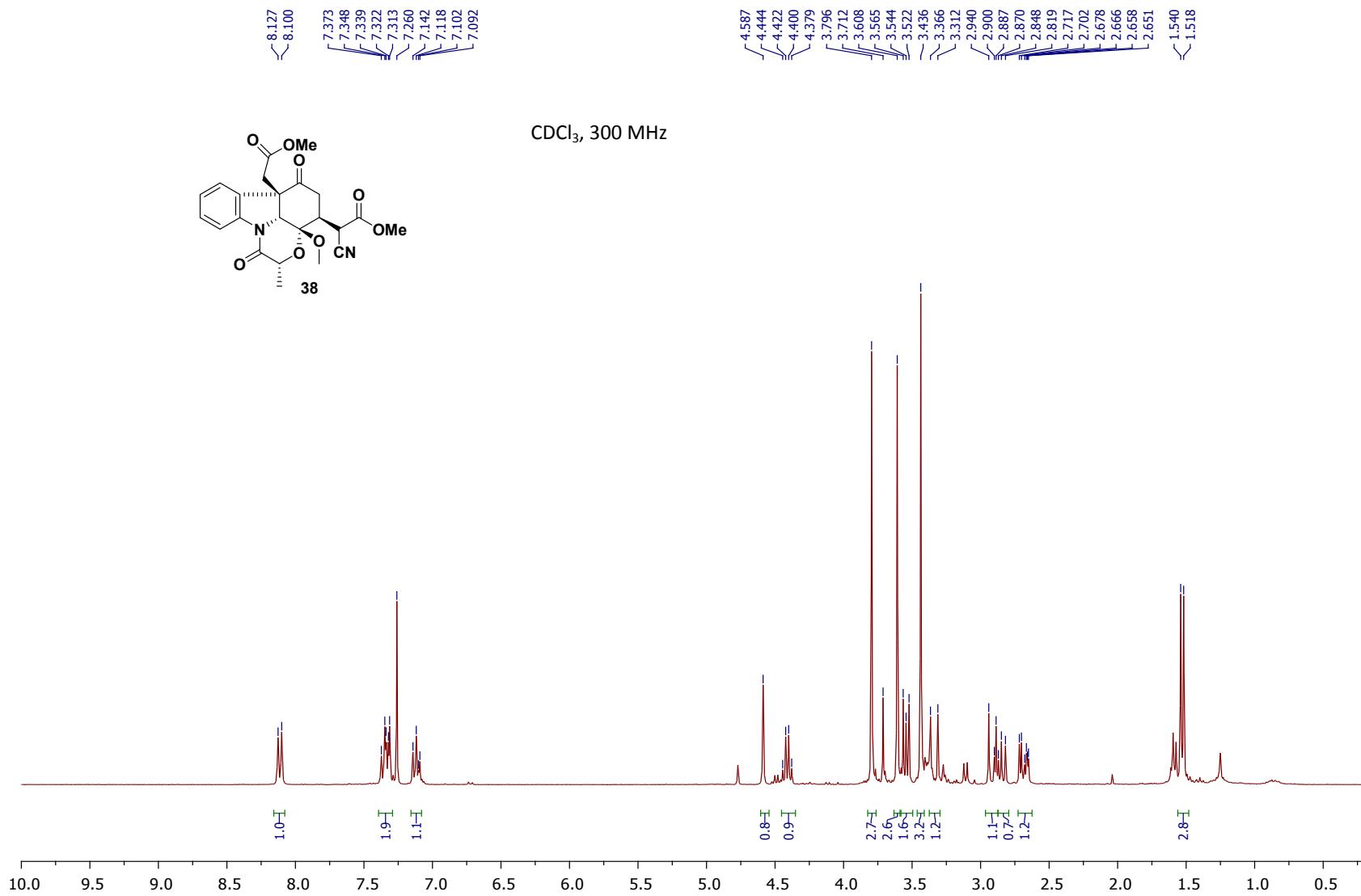


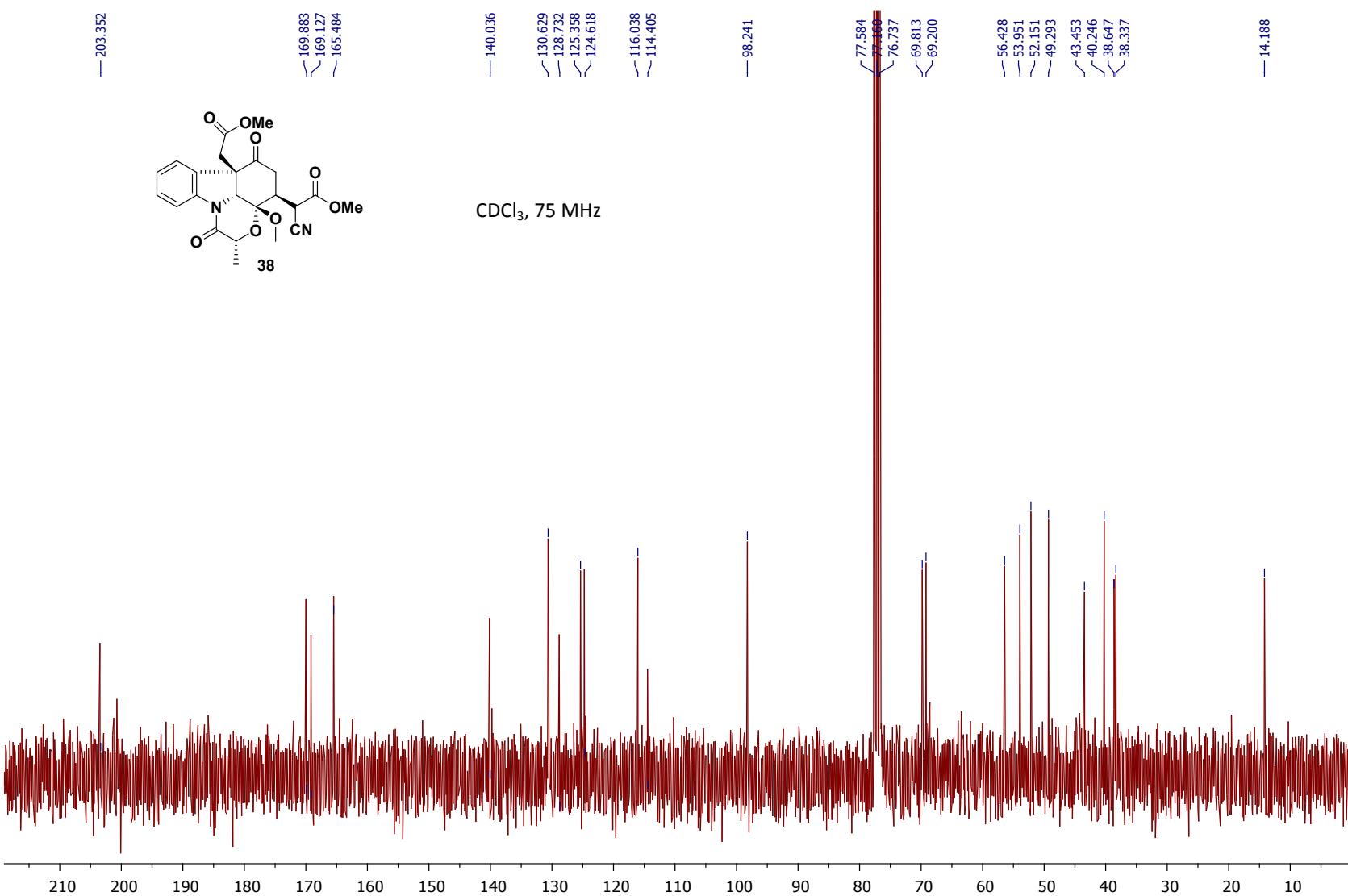


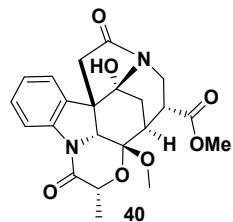
COSY ^1H - ^1H

CDCl_3 , 300 MHz

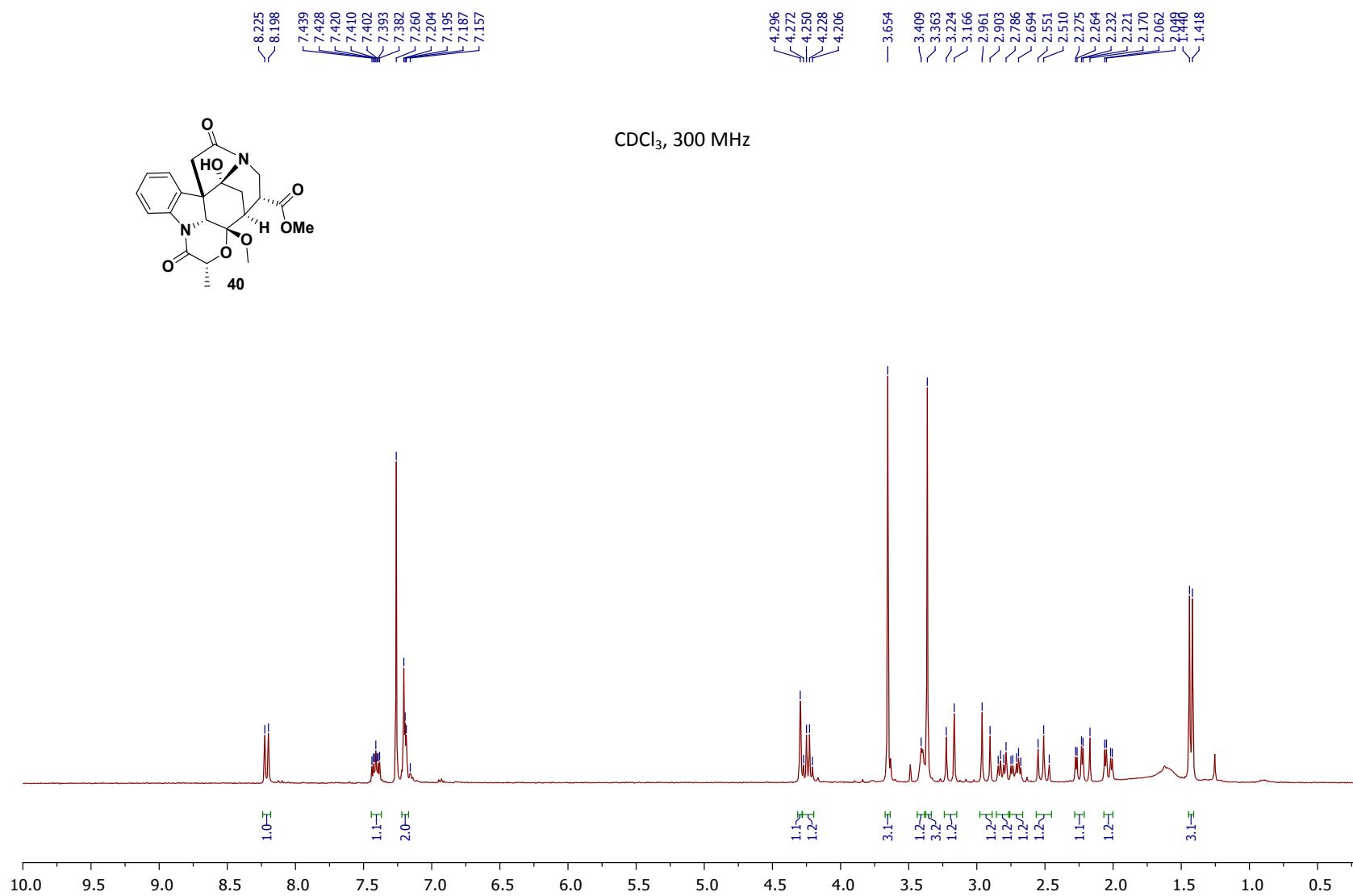


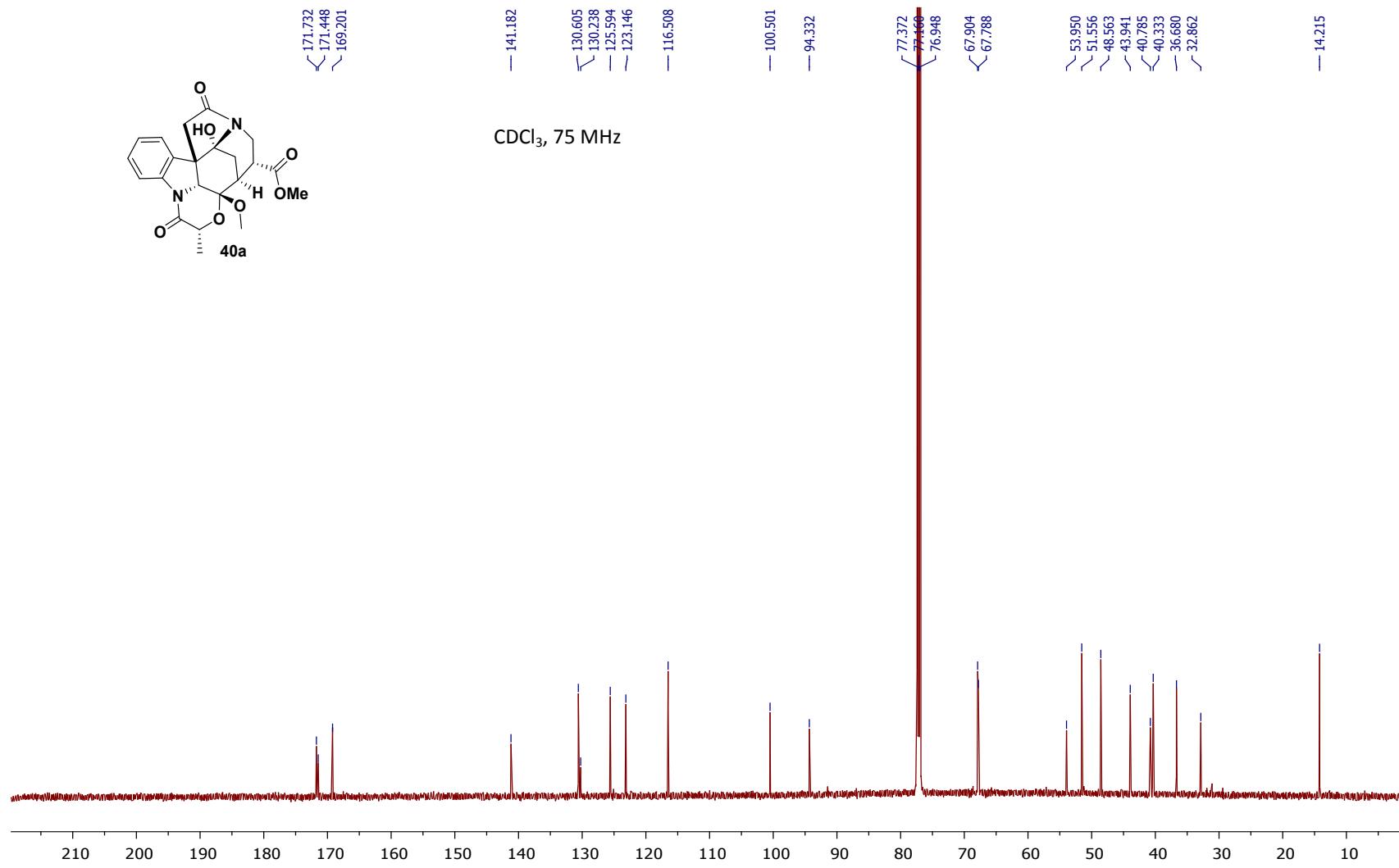






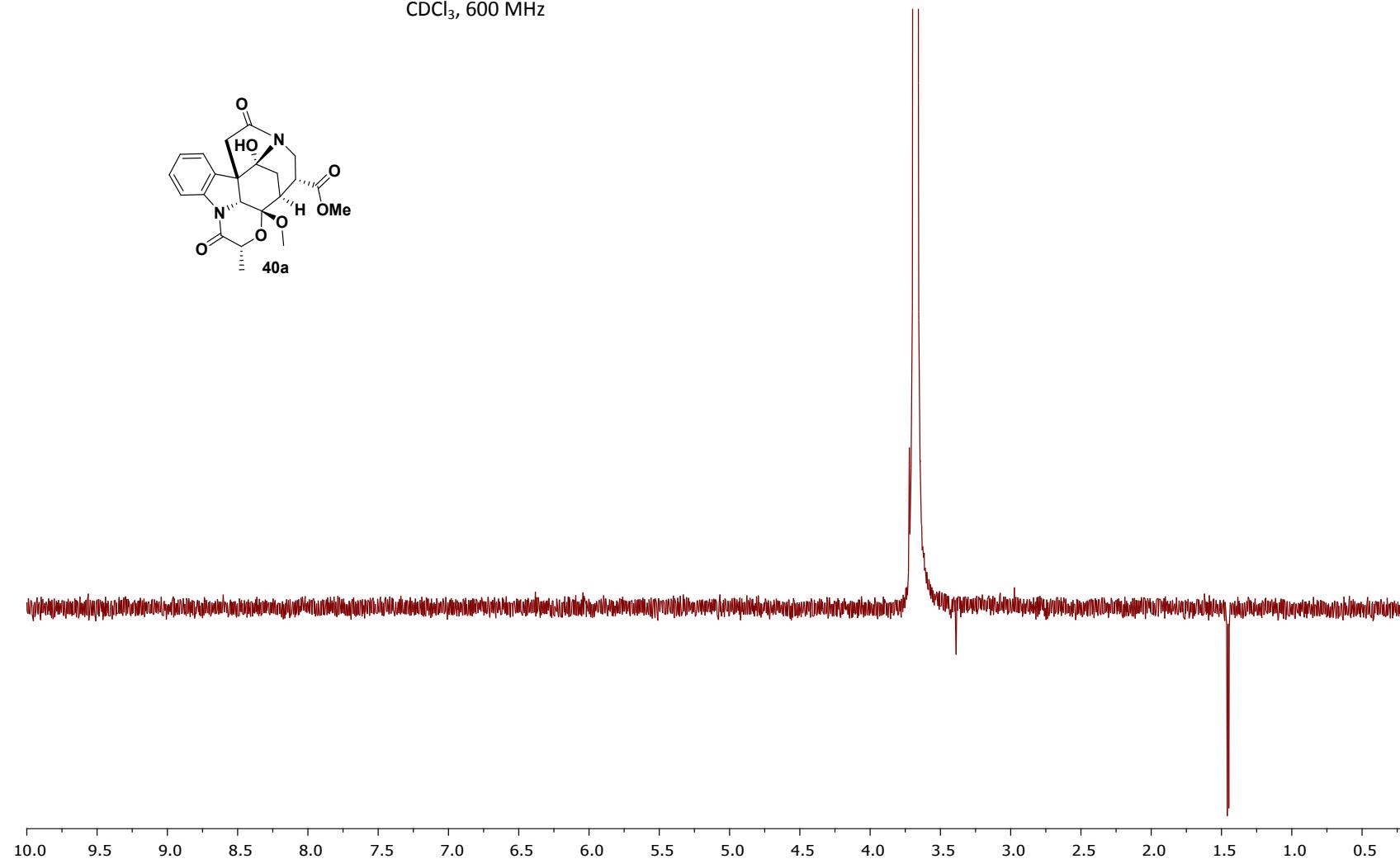
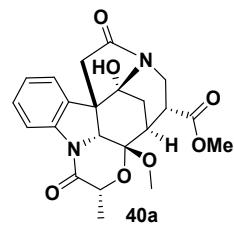
CDCl₃, 300 MHz



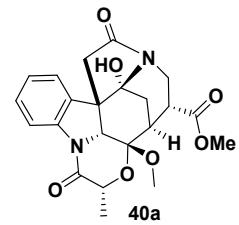


NOE ^1H - ^1H Peak at 3.65 ppm :

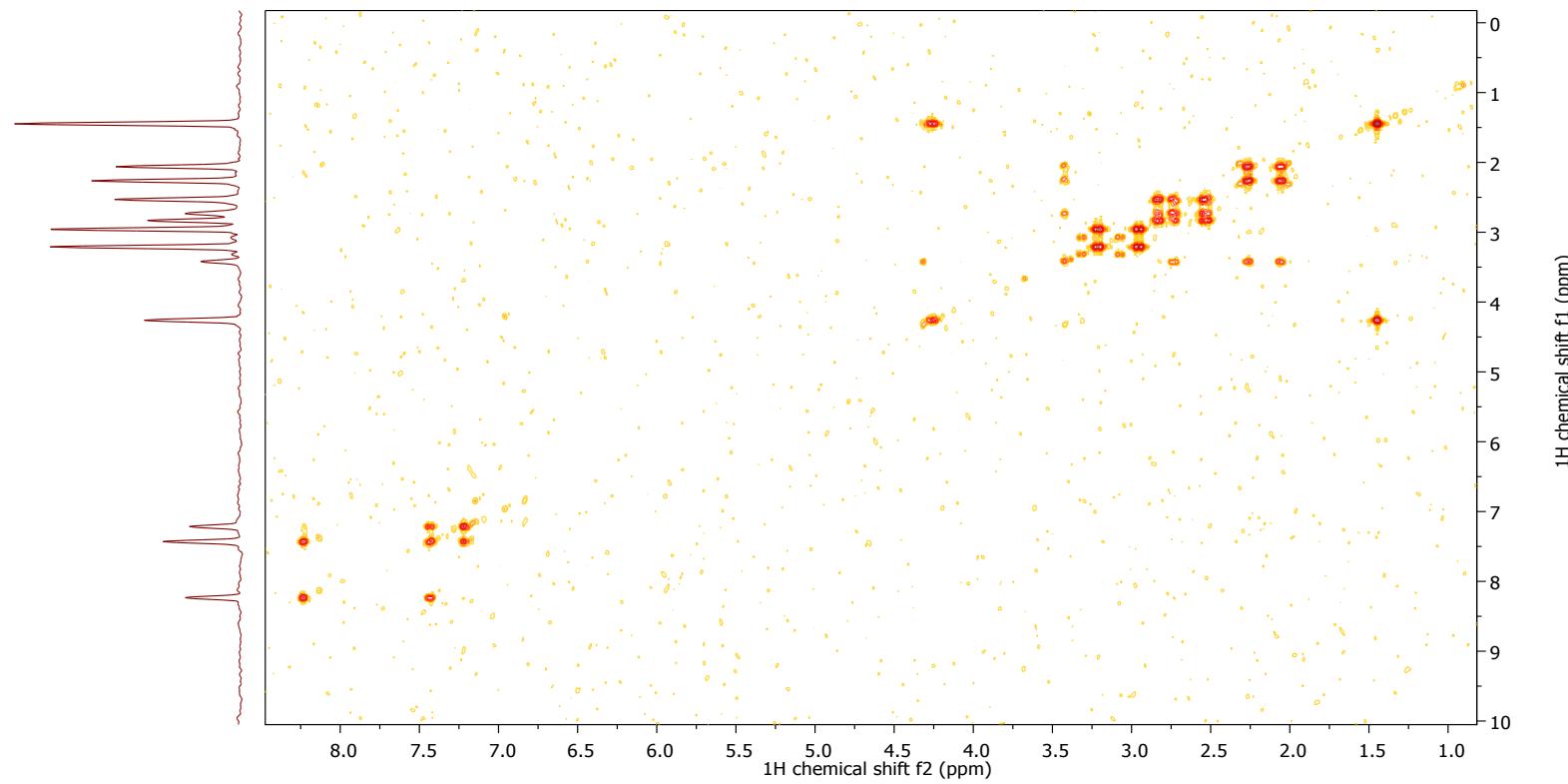
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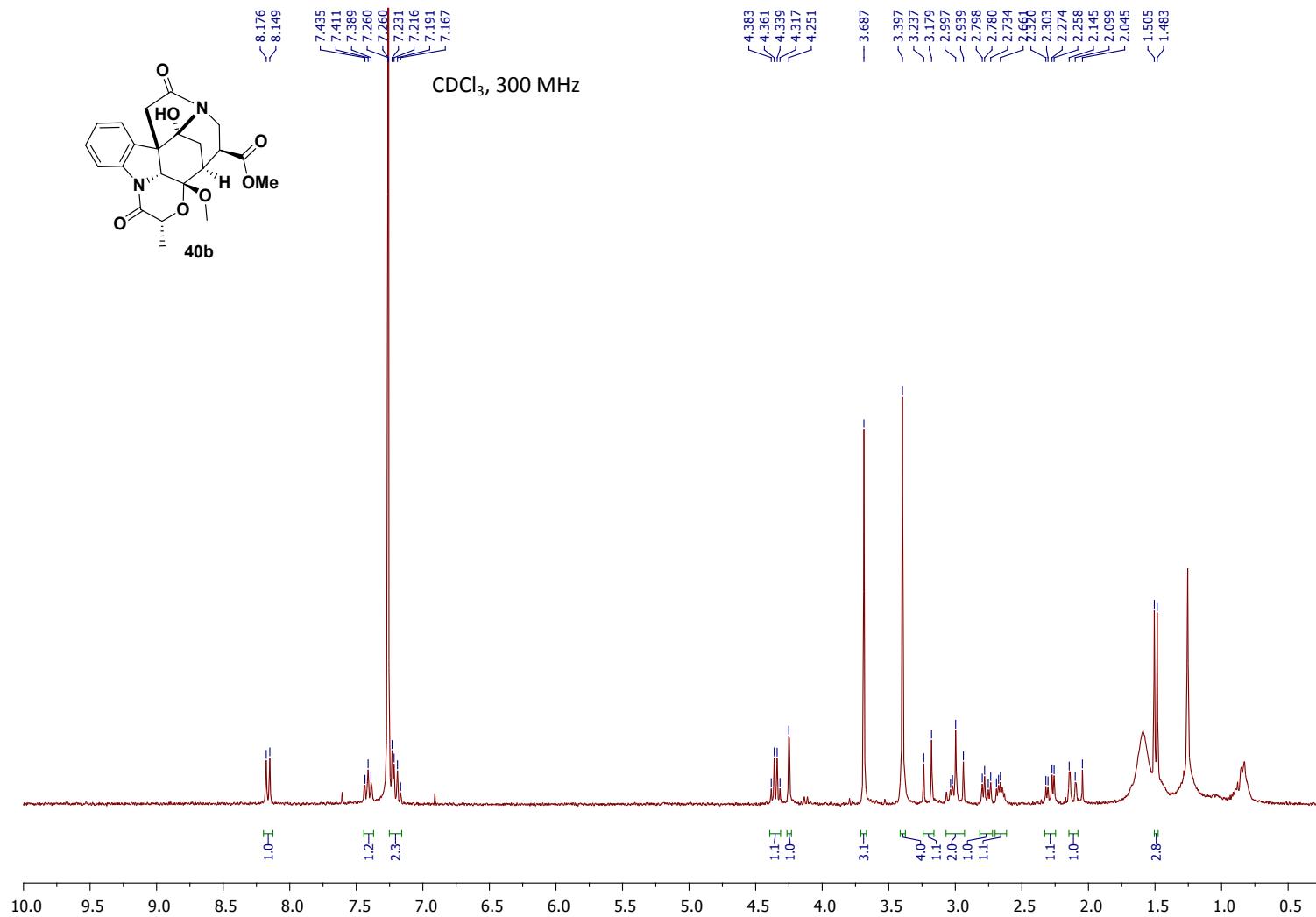


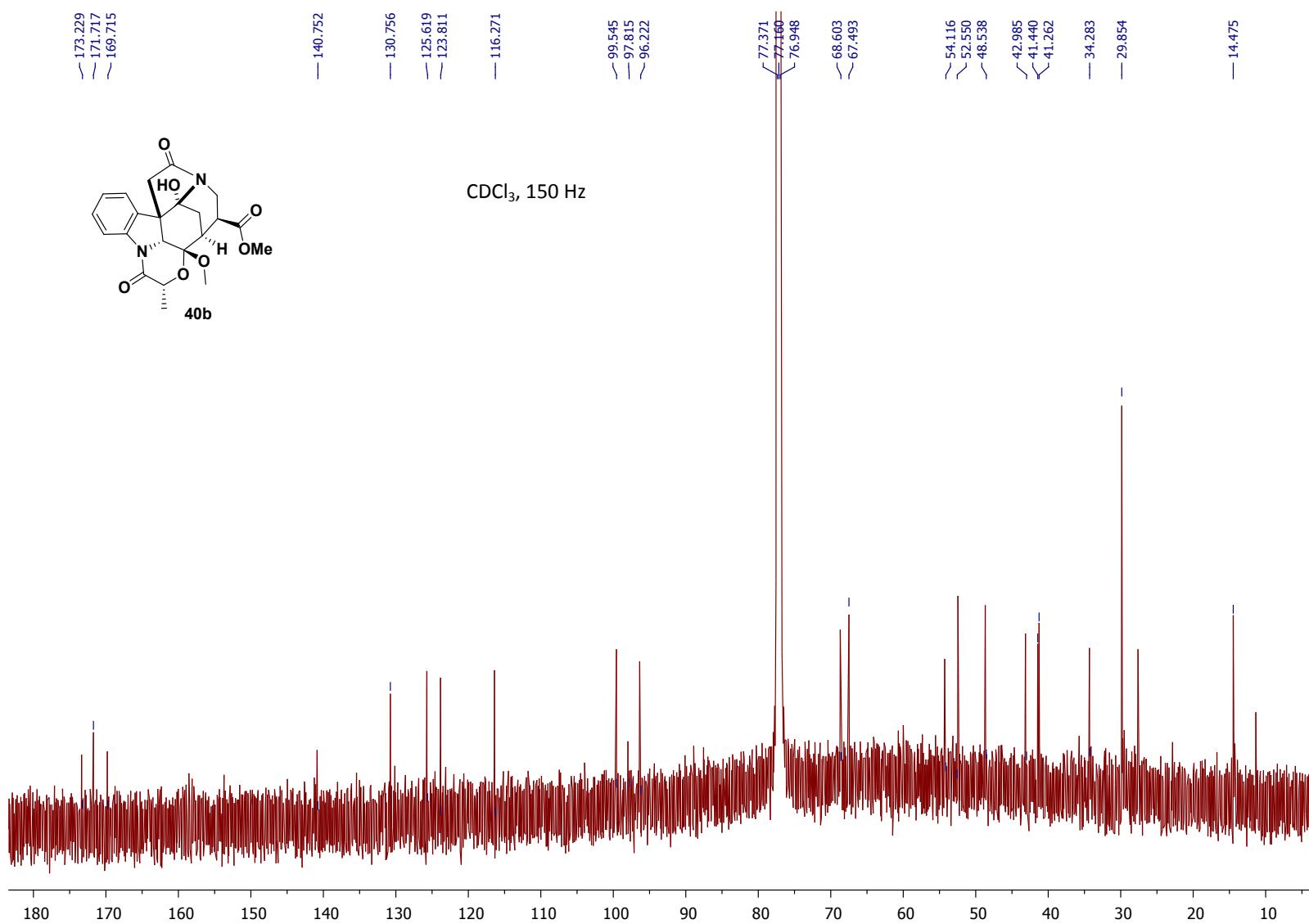
COSY ^1H - ^1H :



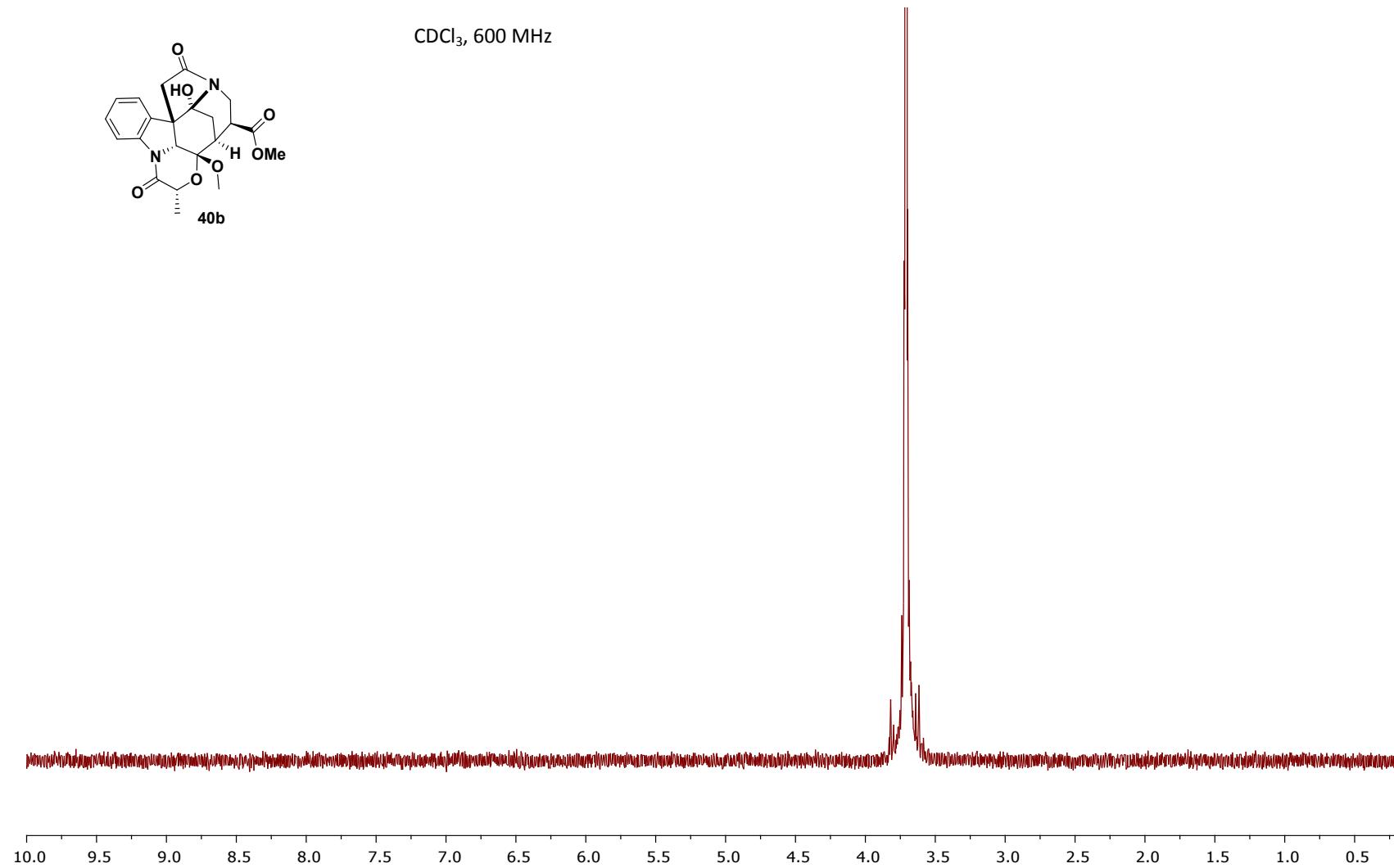
CDCl_3 , 600 MHz

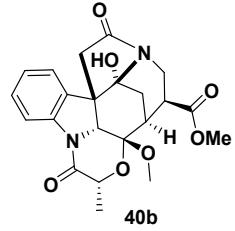




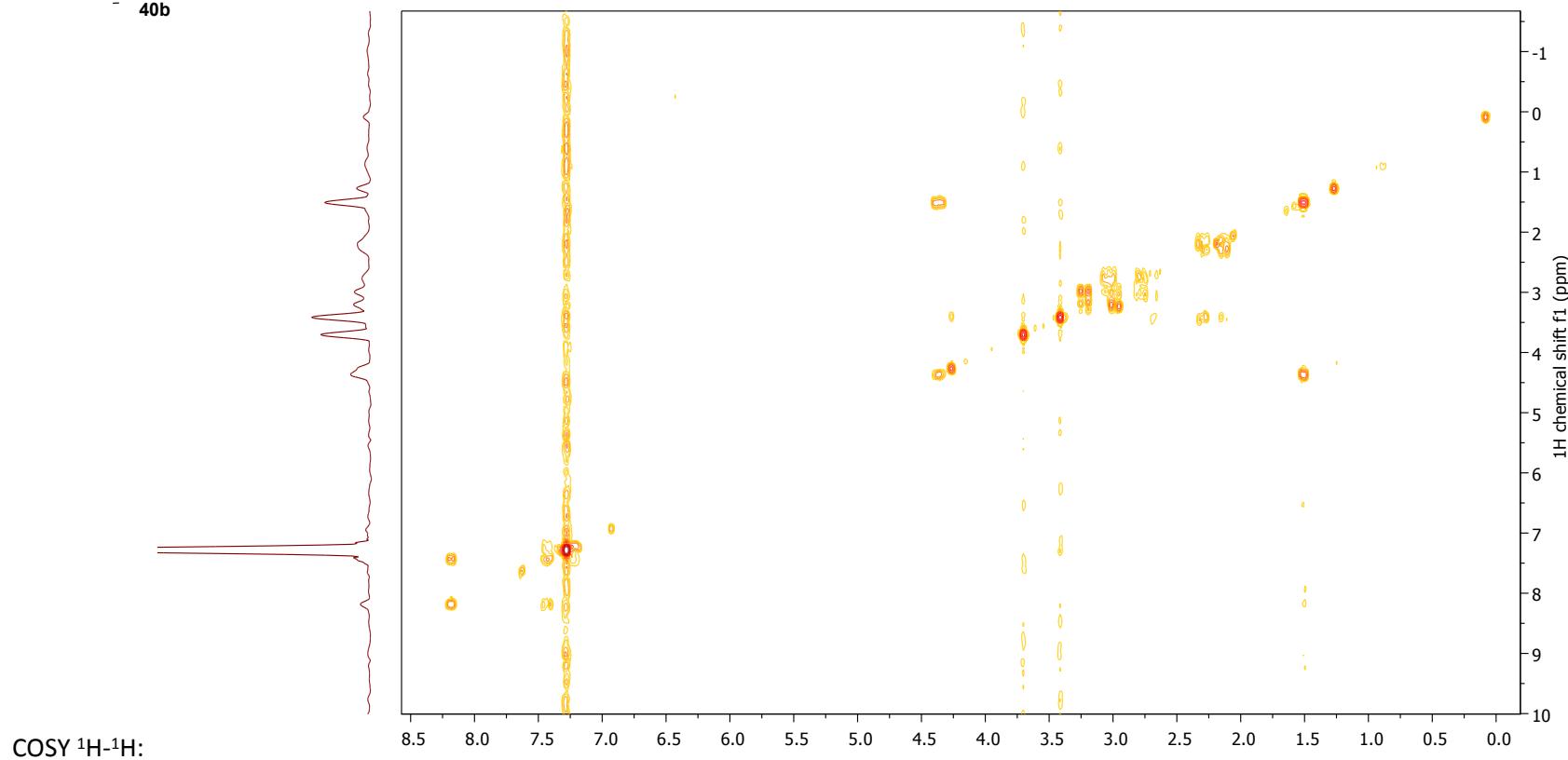


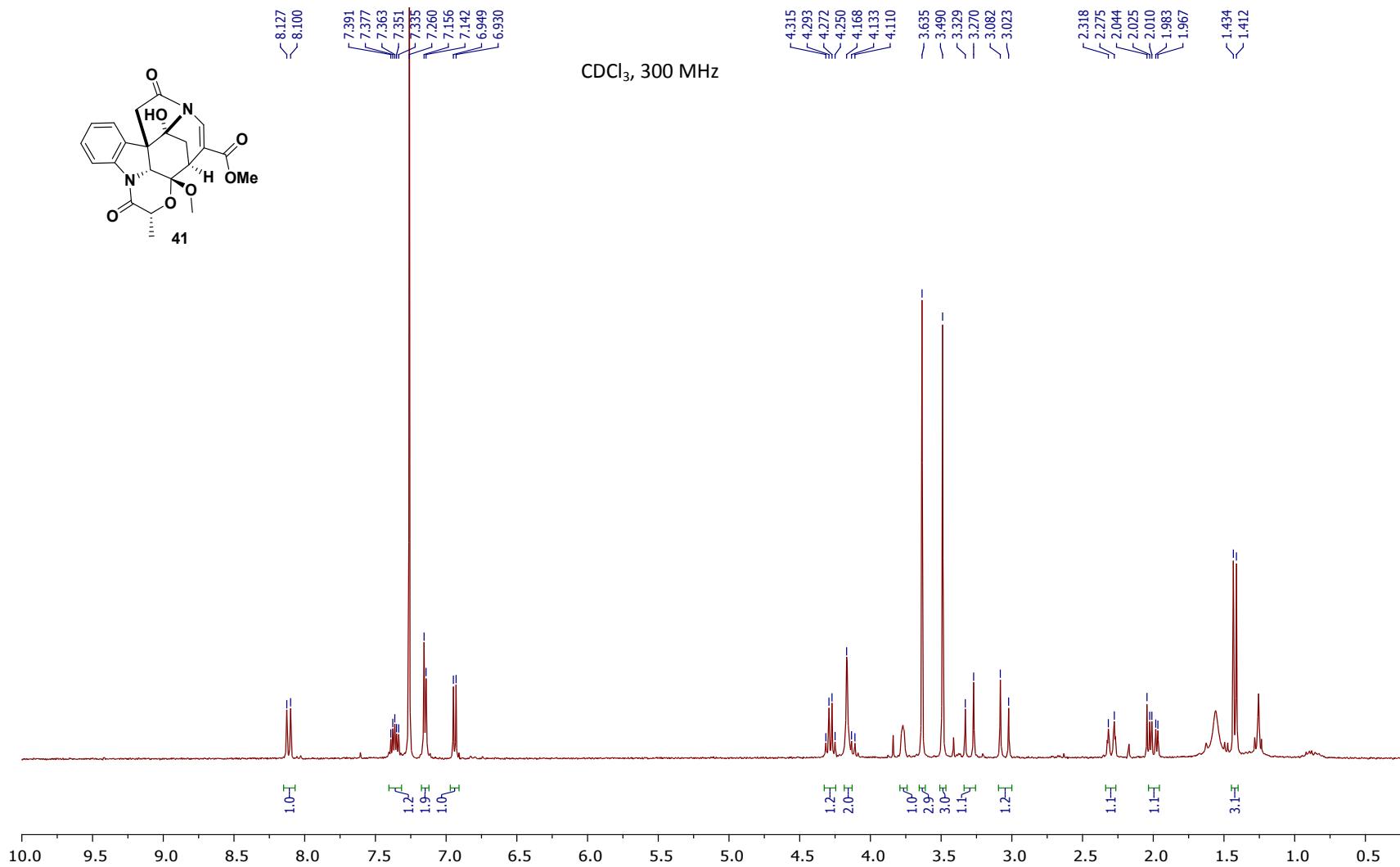
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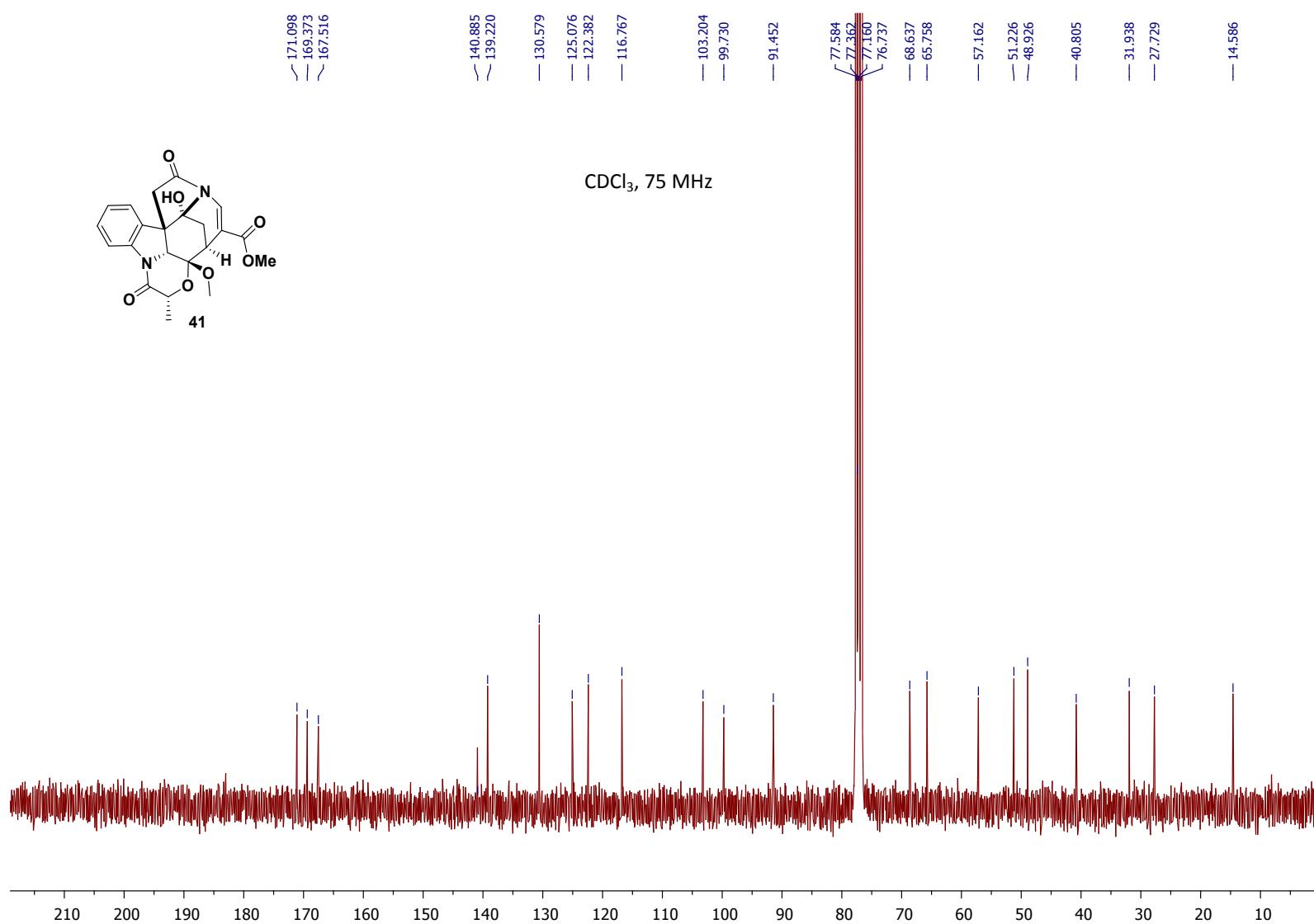




CDCl₃, 600 MHz

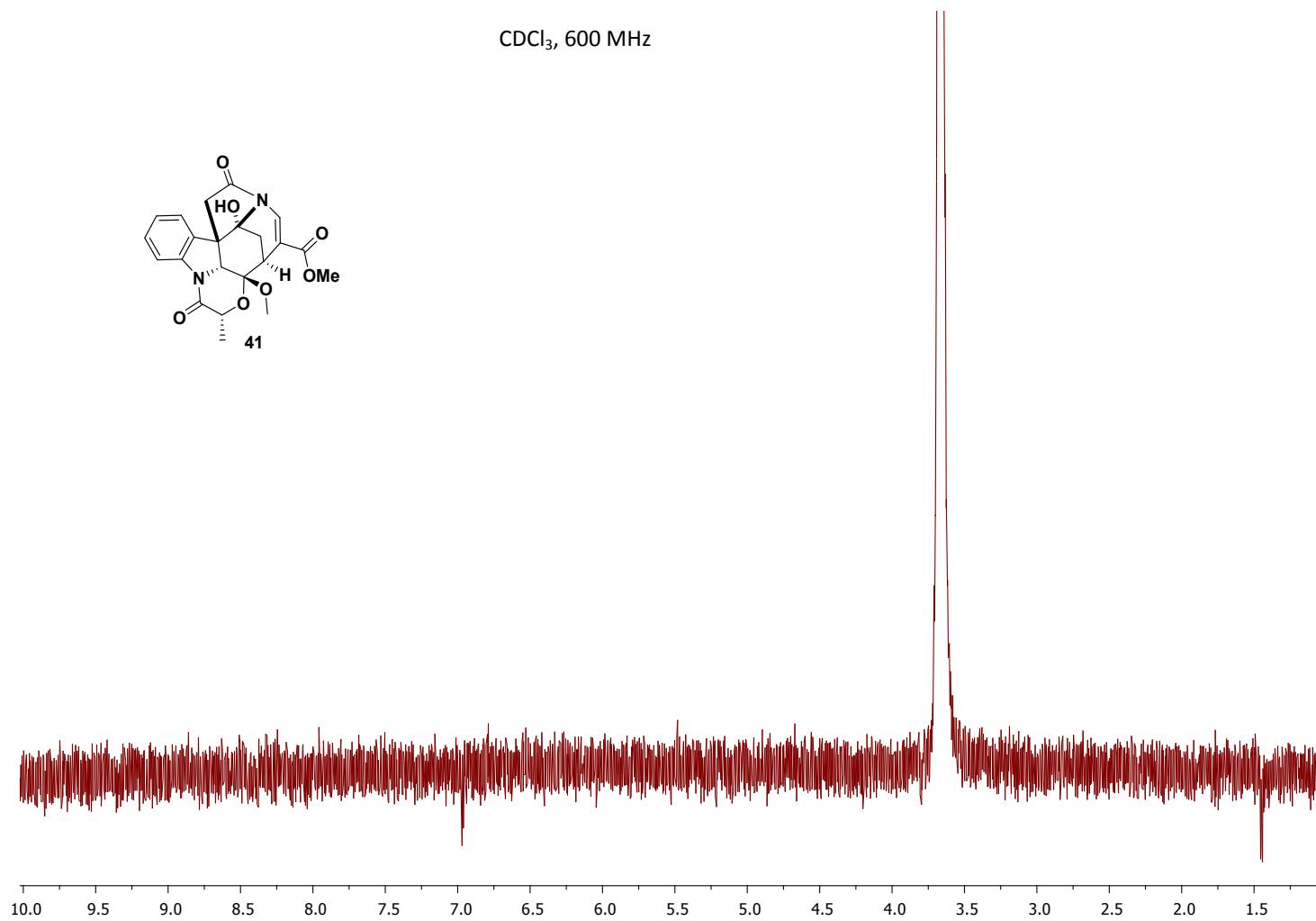
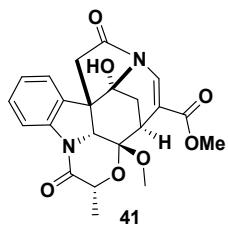




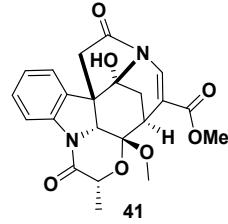


NOE ^1H - ^1H Peak at 3.63 ppm :

CDCl_3 , 600 MHz



COSY ^1H - ^1H :



CDCl₃, 600 MHz

