

Electronic Supplementary Information

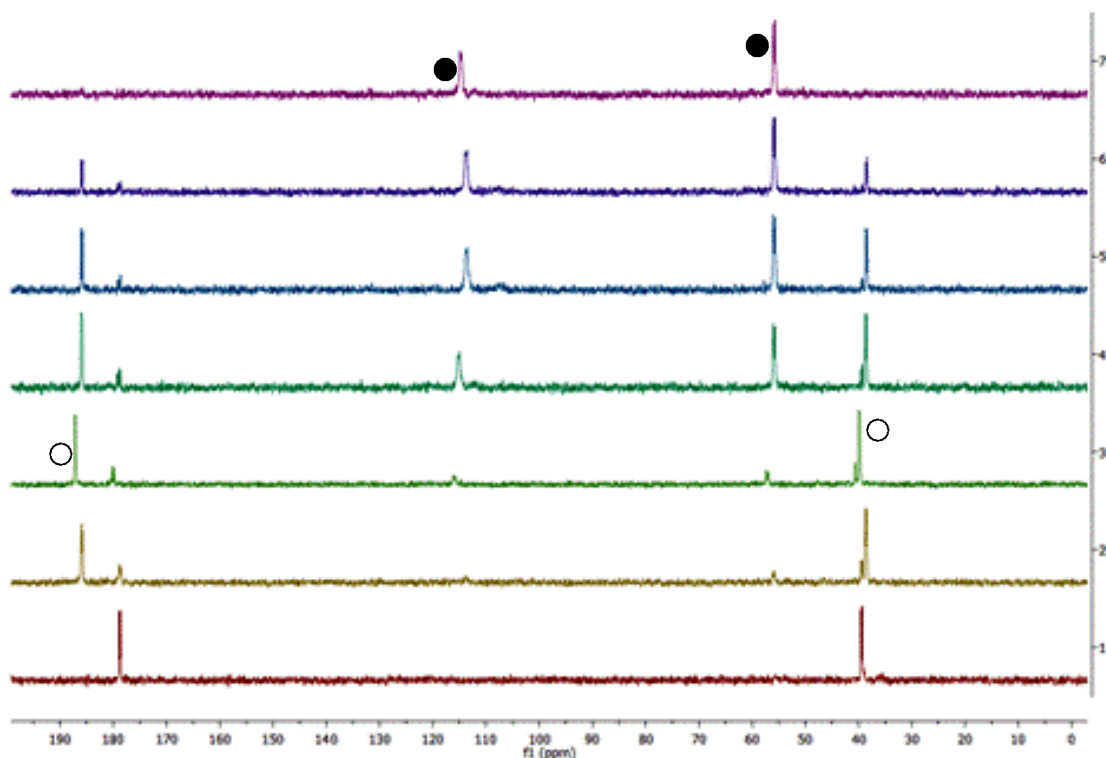
Investigation of Binap-based hydroxyphosphine arene-ruthenium(II) complexes as catalysts for nitrile hydration

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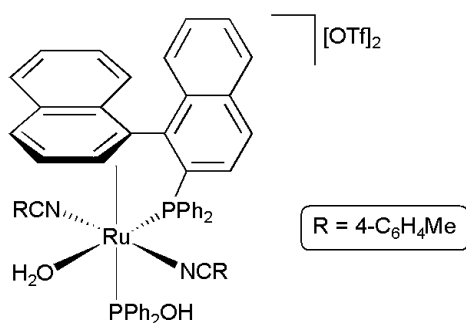
^b *WestCHEM, University of Strathclyde, Department of Pure and Applied Chemistry, 295 Cathedral Street, Glasgow, G1, 1XL, UK.*

Fig. S1 Behaviour of the metallacyclic complex **6** towards water.



1) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex **6** in acetone- d_6 . 2) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex **6** in acetone- d_6 in the presence of 25 μL of H_2O . Spectrum recorded after 1 min at r.t. 3) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex **6** in acetone- d_6 in the presence of 25 μL of H_2O . Spectrum recorded after 30 min at r.t. 4) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex **6** in acetone- d_6 in the presence of 25 μL of H_2O . Spectrum recorded after 16 h at r.t. 5) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex **6** in acetone- d_6 in the presence of 25 μL of H_2O . Spectrum recorded after 5 min at 70 $^\circ\text{C}$. 6) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex **6** in acetone- d_6 in the presence of 25 μL of H_2O . Spectrum recorded after 15 min at 70 $^\circ\text{C}$. 7) $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of complex **6** in acetone- d_6 in the presence of 25 μL of H_2O . Spectrum recorded after 1 h at 70 $^\circ\text{C}$.

● Signals corresponding to:



○ Signals tentatively assigned to:

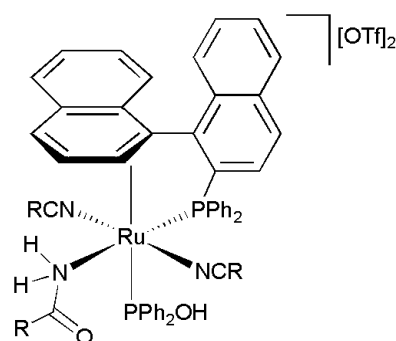
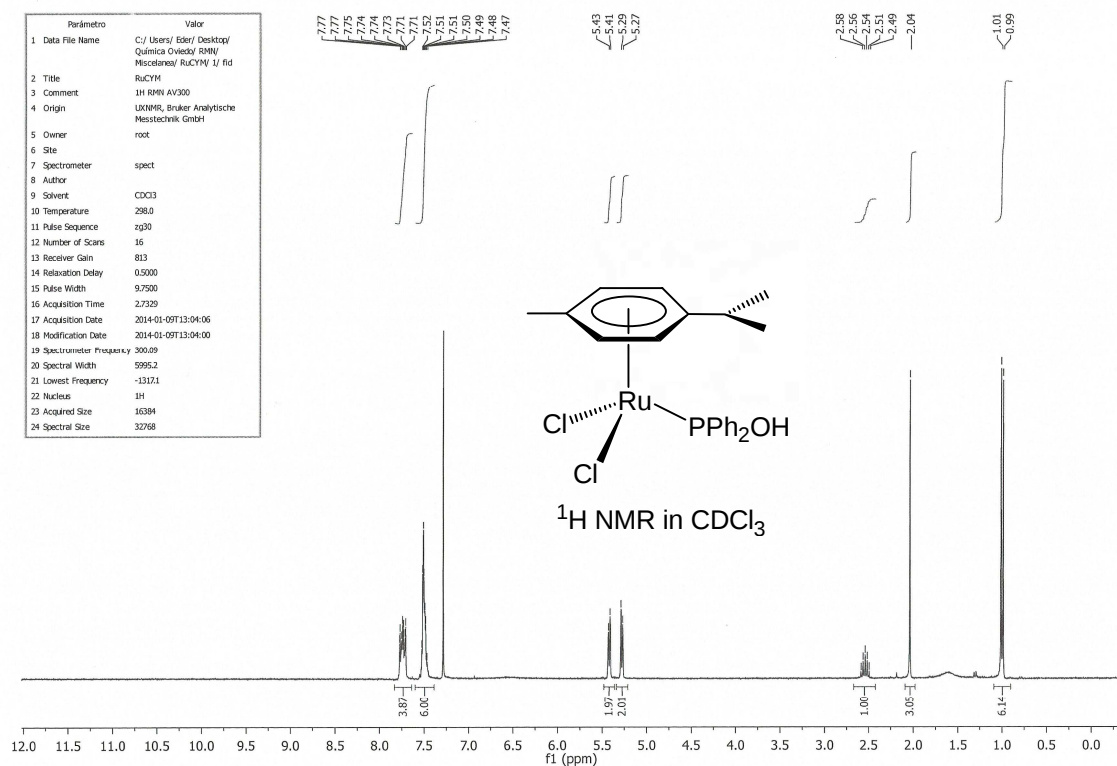
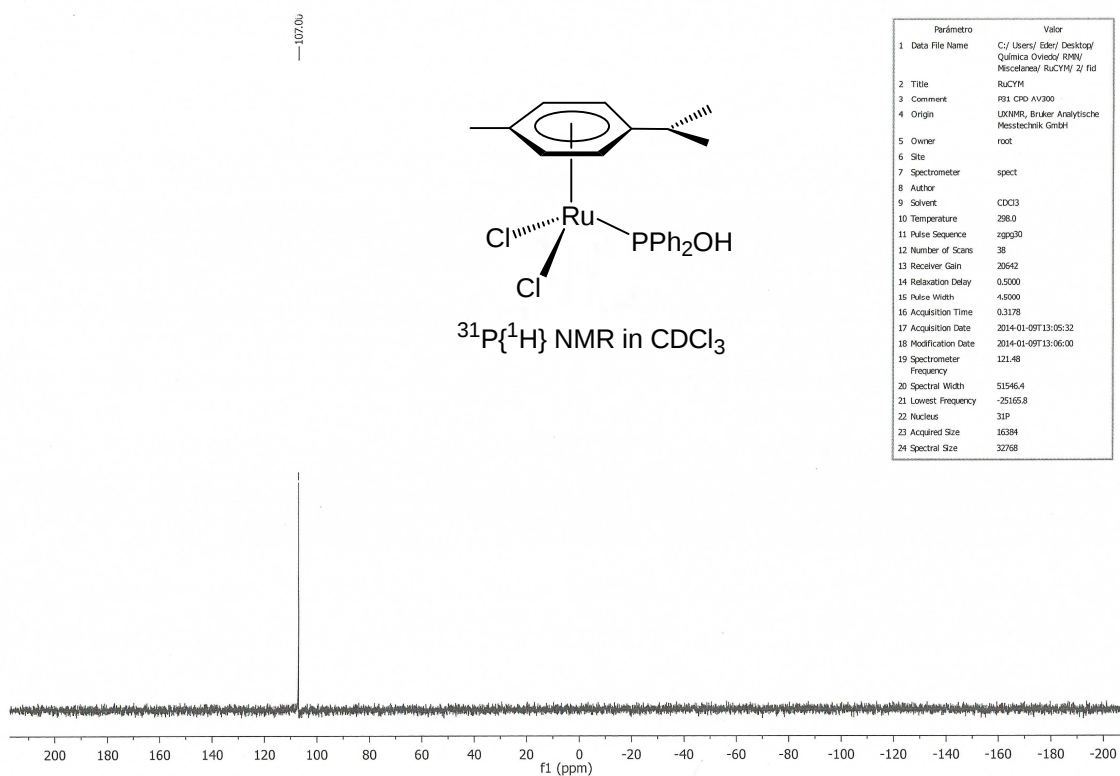


Fig. S2 NMR spectra of complex $[\text{RuCl}_2(\eta^6\text{-}p\text{-cymene})\{\text{PPh}_2(\text{OH})\}]$ (**2b**).



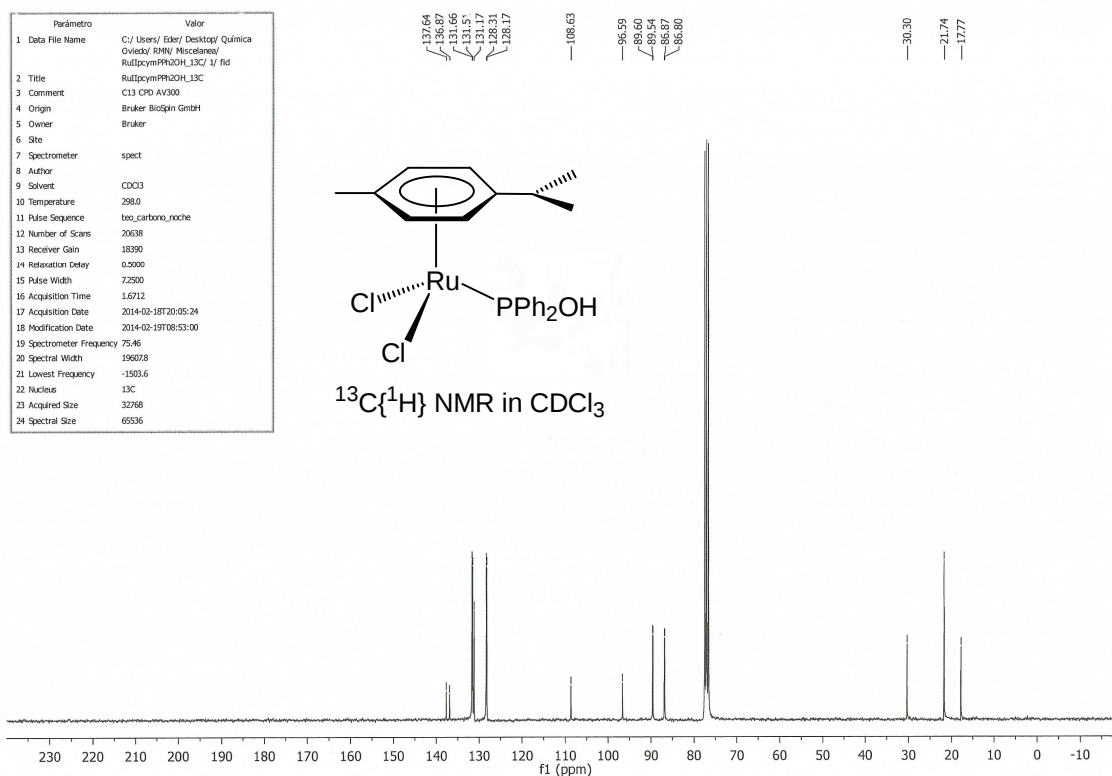
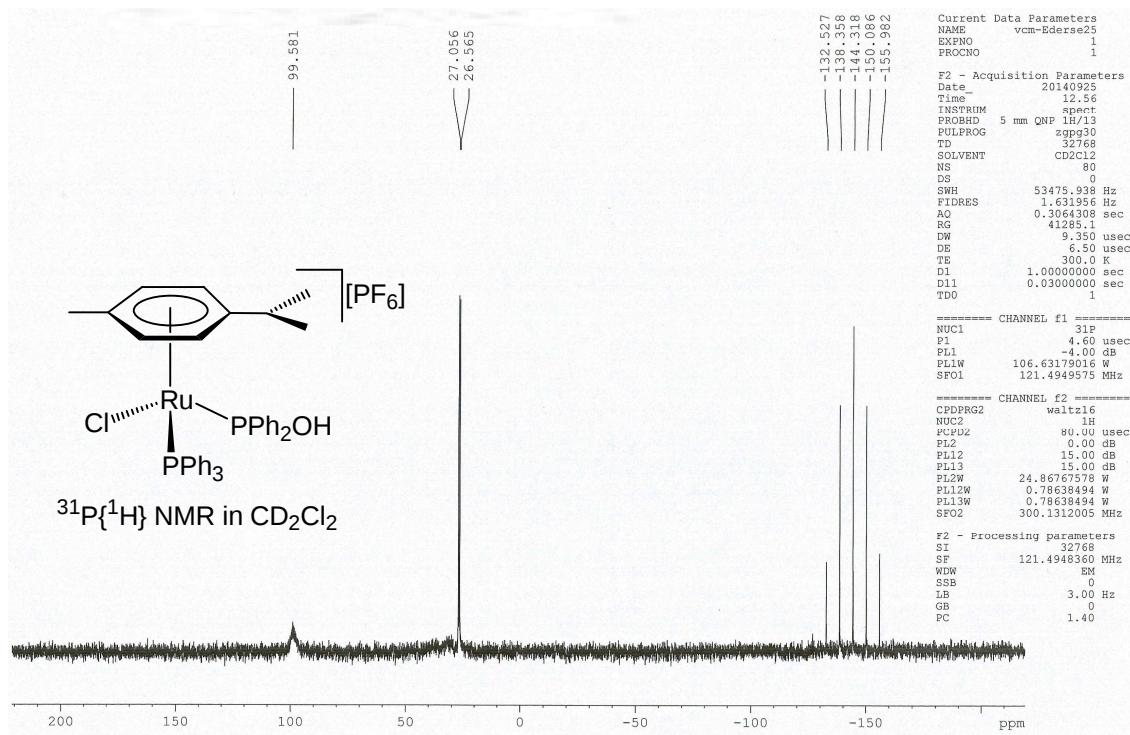


Fig. S3 NMR spectra of complex $[\text{RuCl}(\eta^6\text{-}p\text{-cymene})\{\text{PPh}_2(\text{OH})\}(\text{PPh}_3)][\text{PF}_6]$ (7).



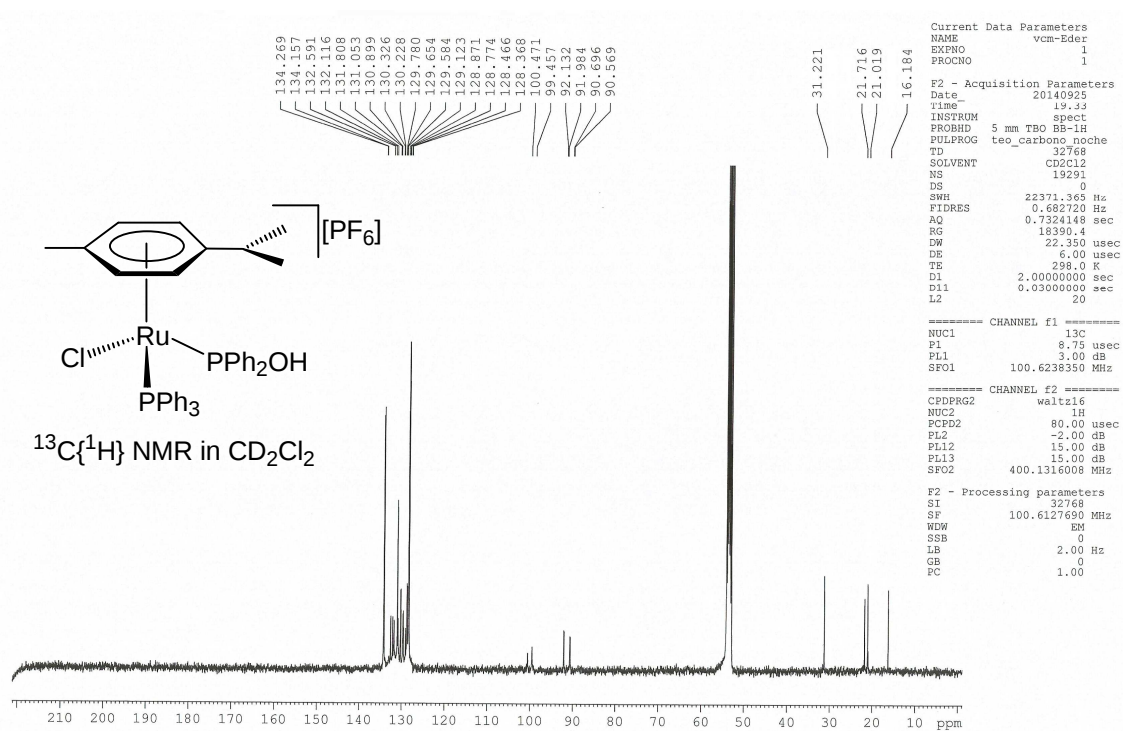
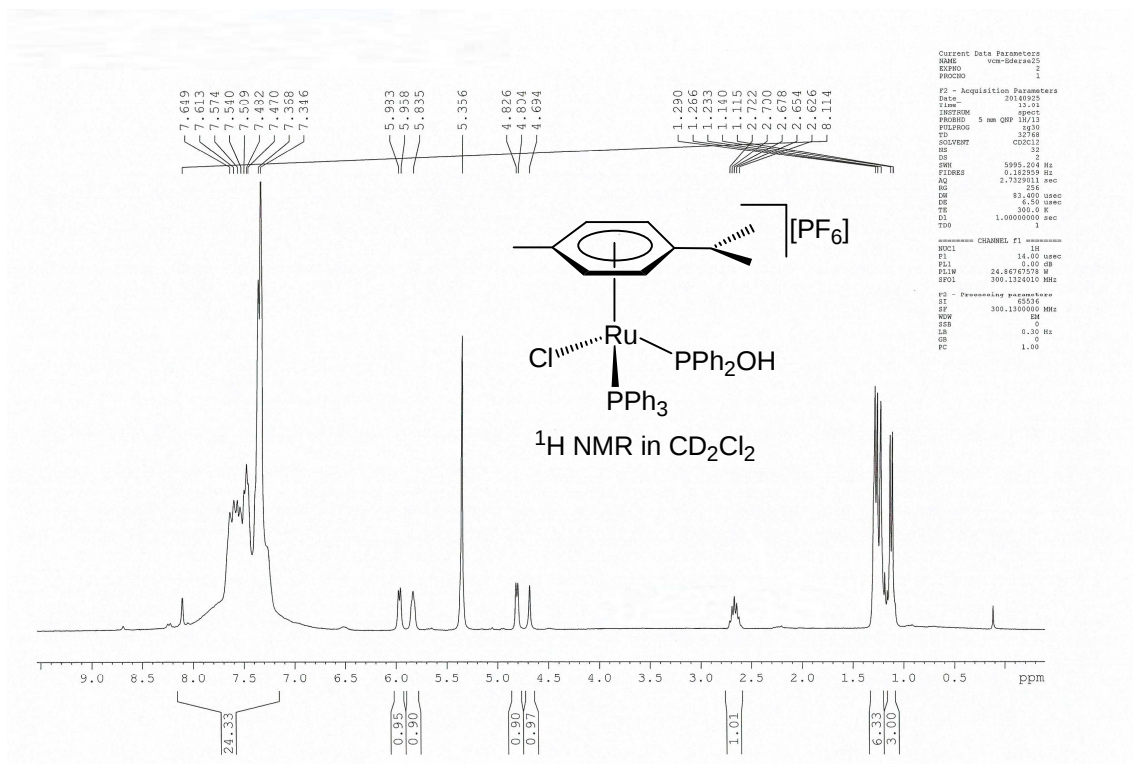
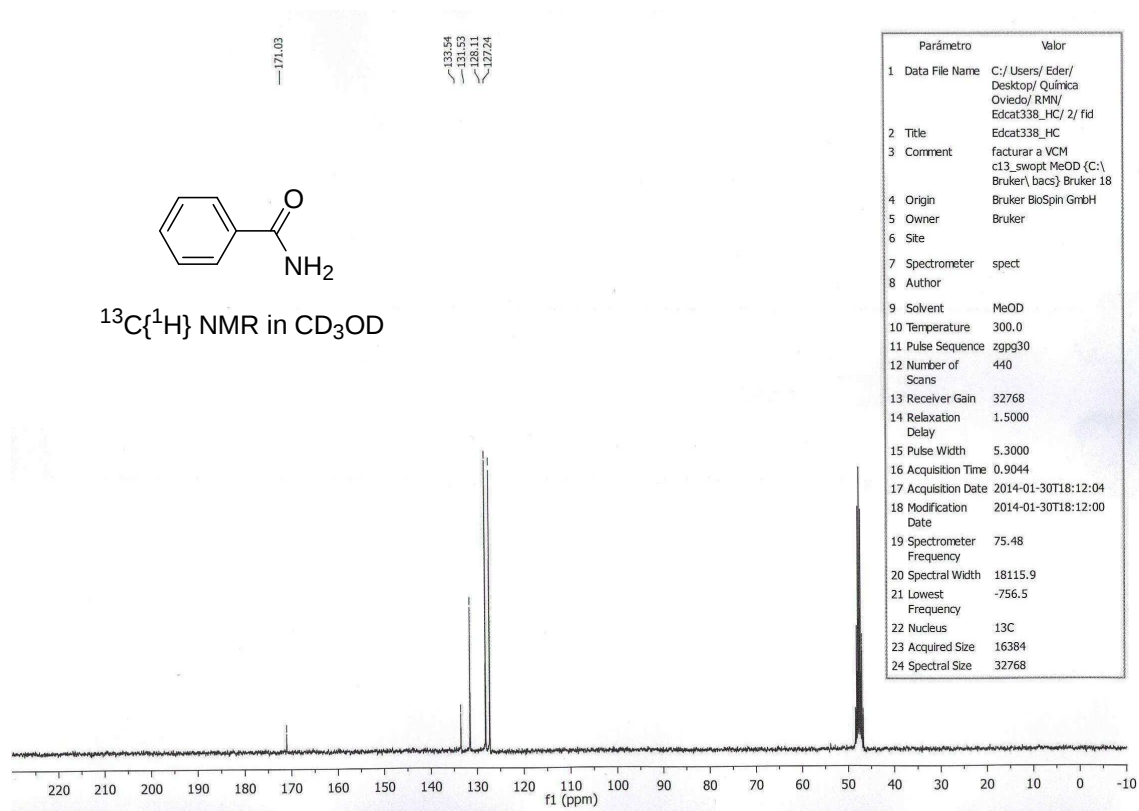
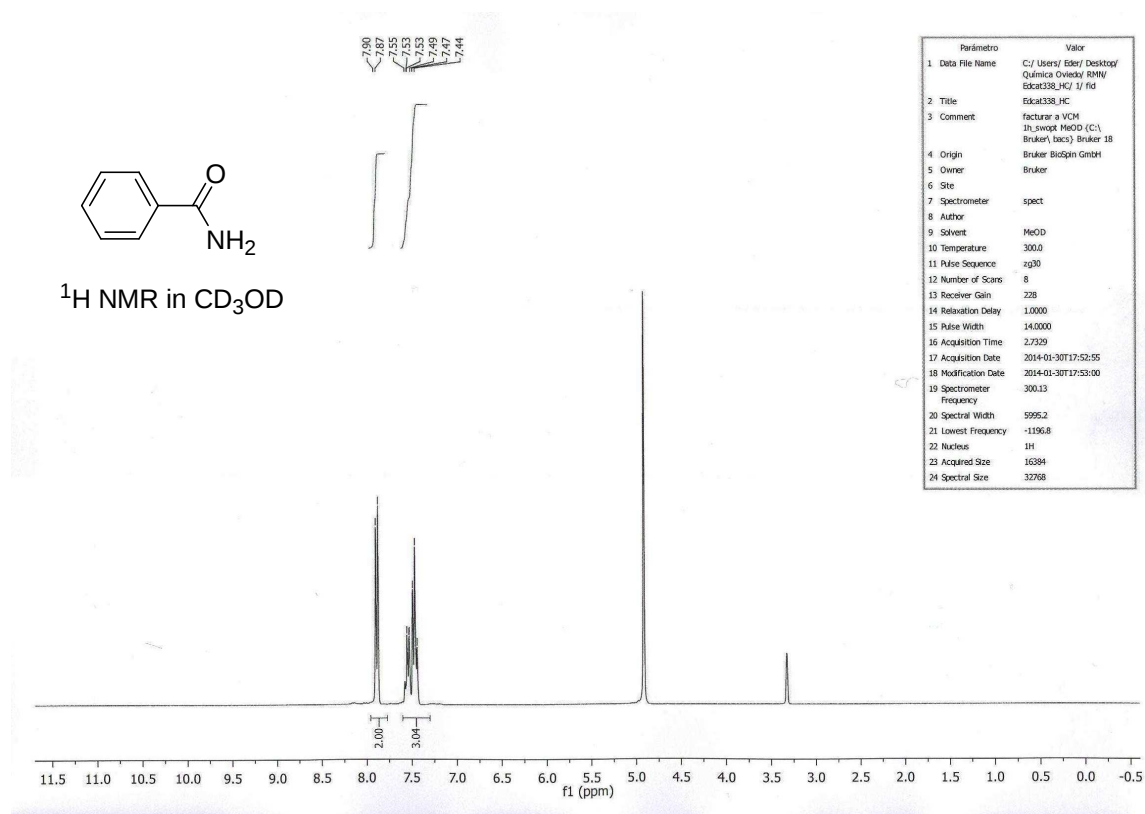
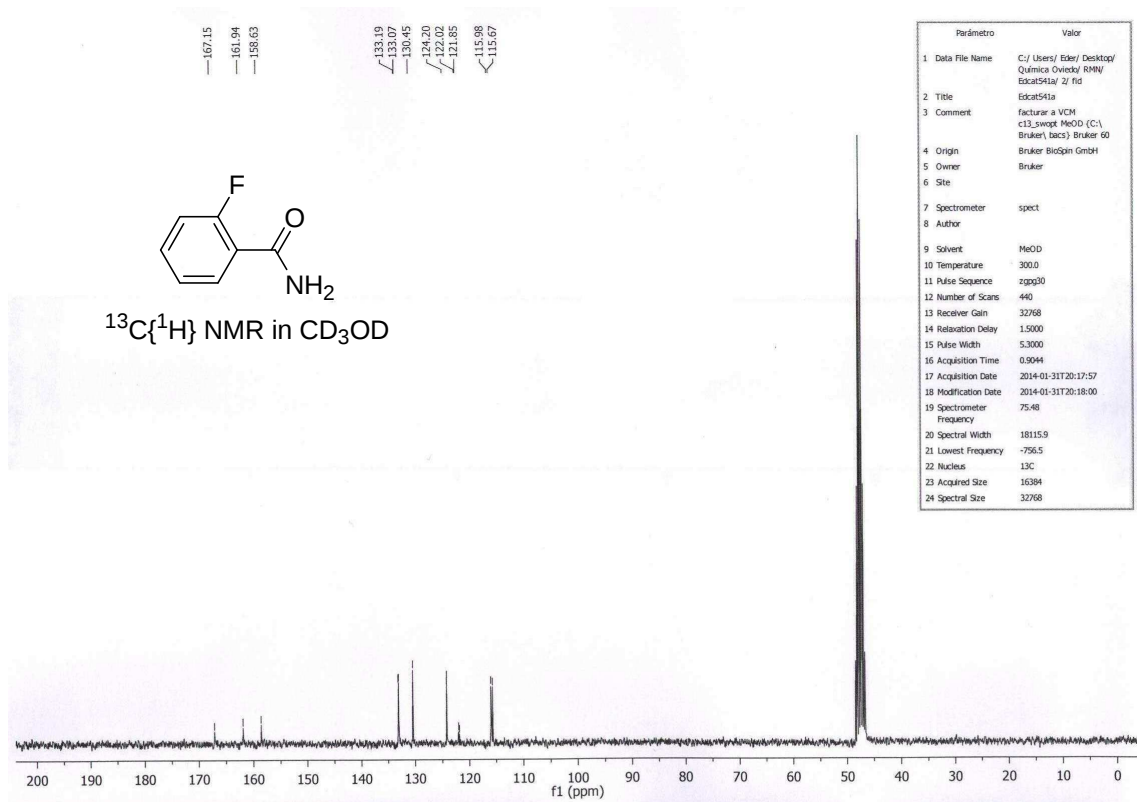
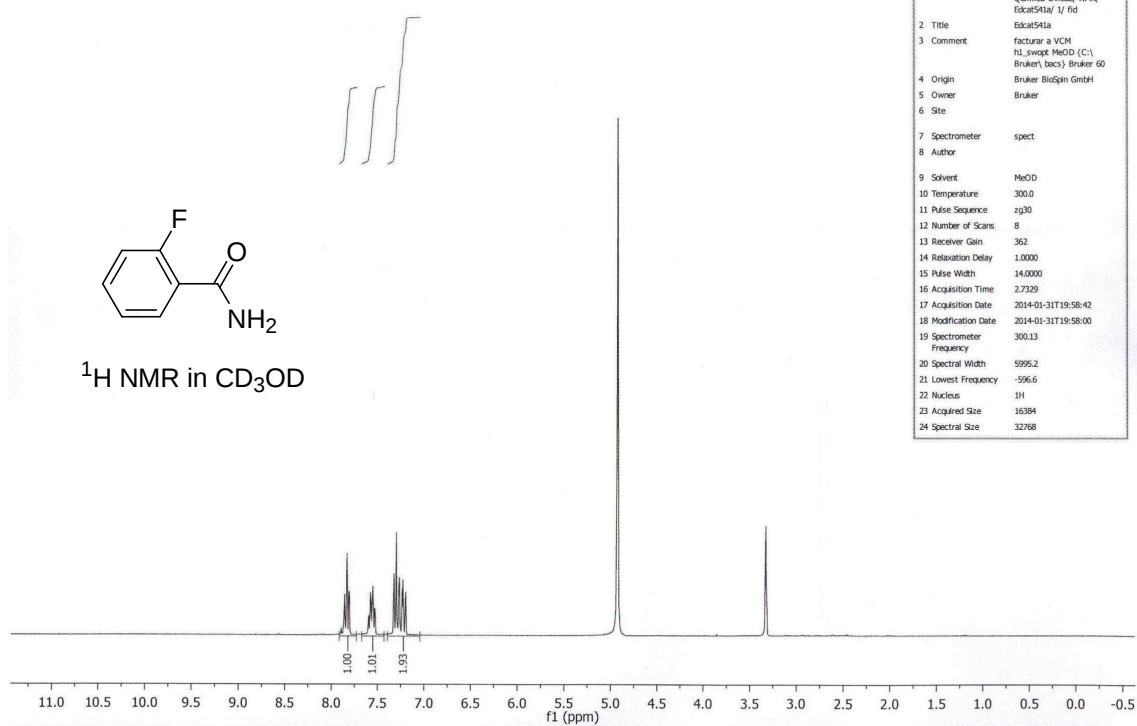
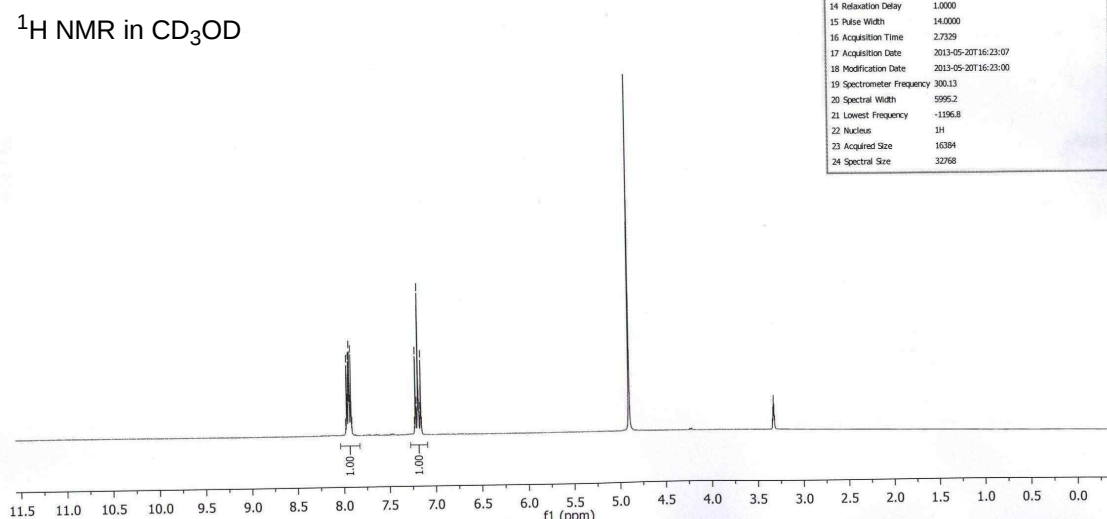
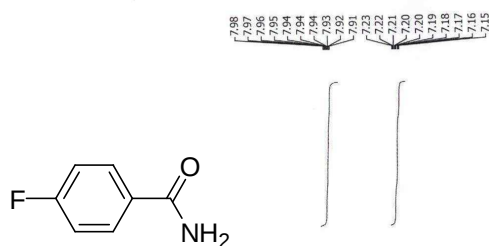
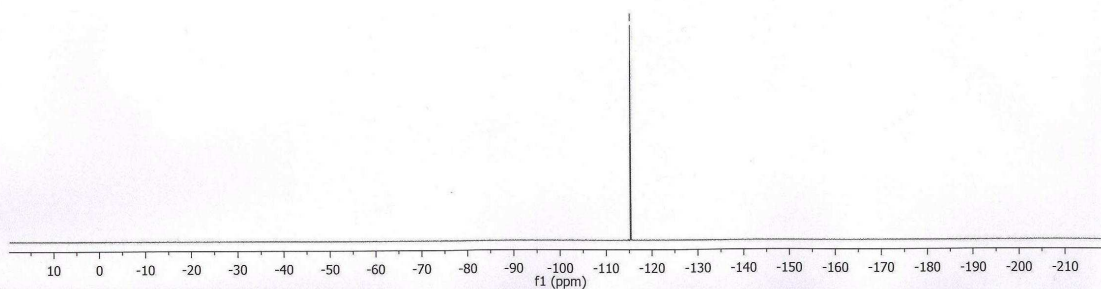
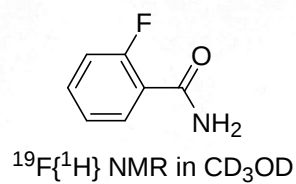


Fig. S4 NMR spectra of the primary amides generated by hydration of the corresponding nitrile with complex **4**.

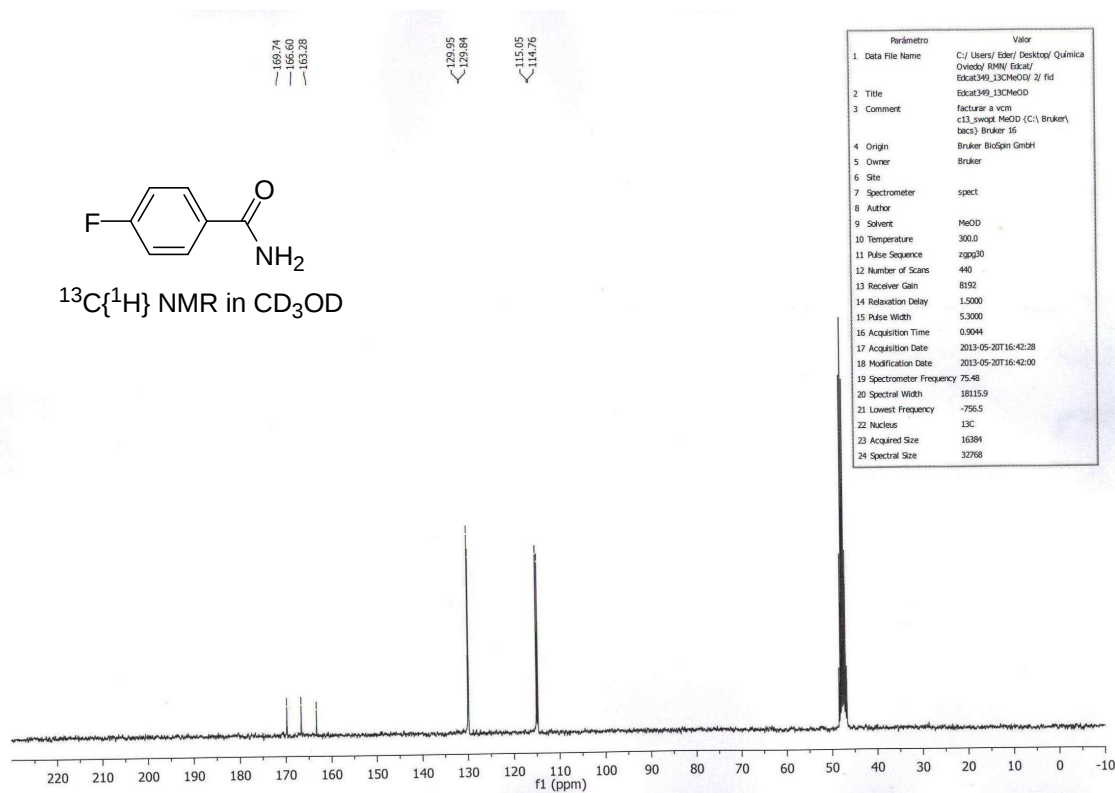
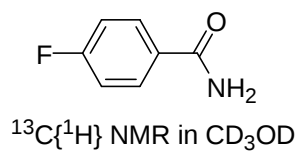




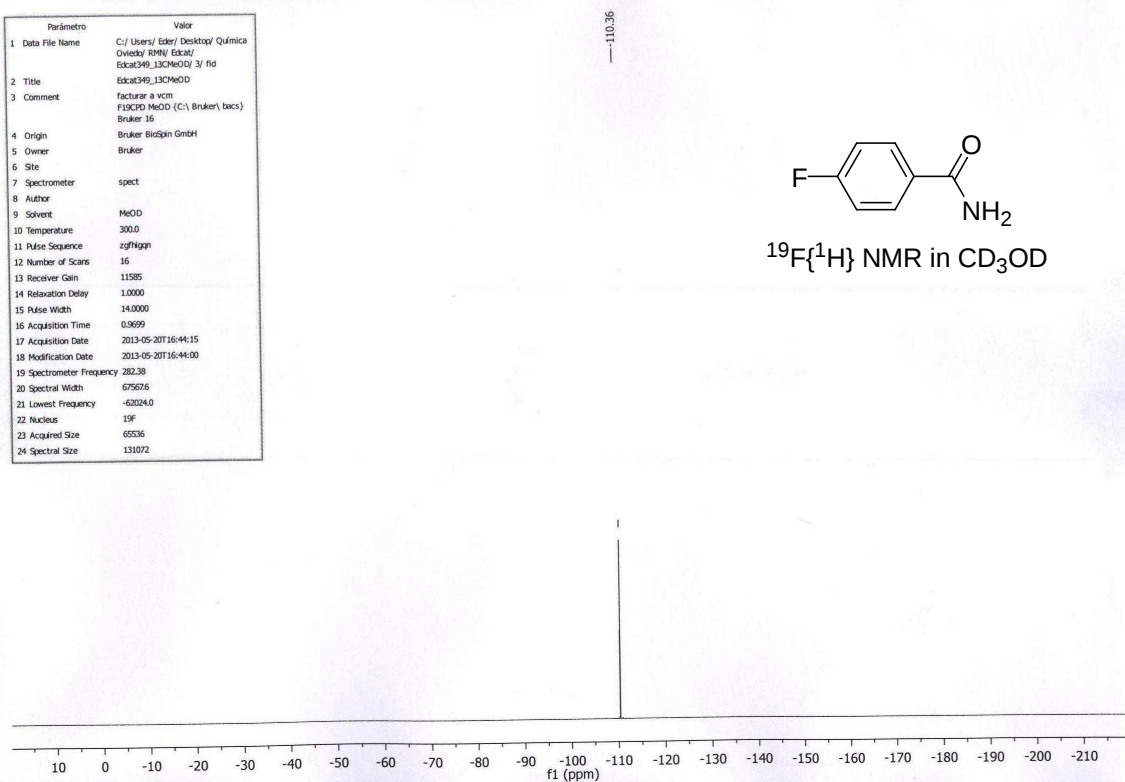
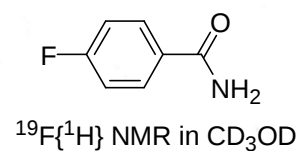
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5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	MeOD
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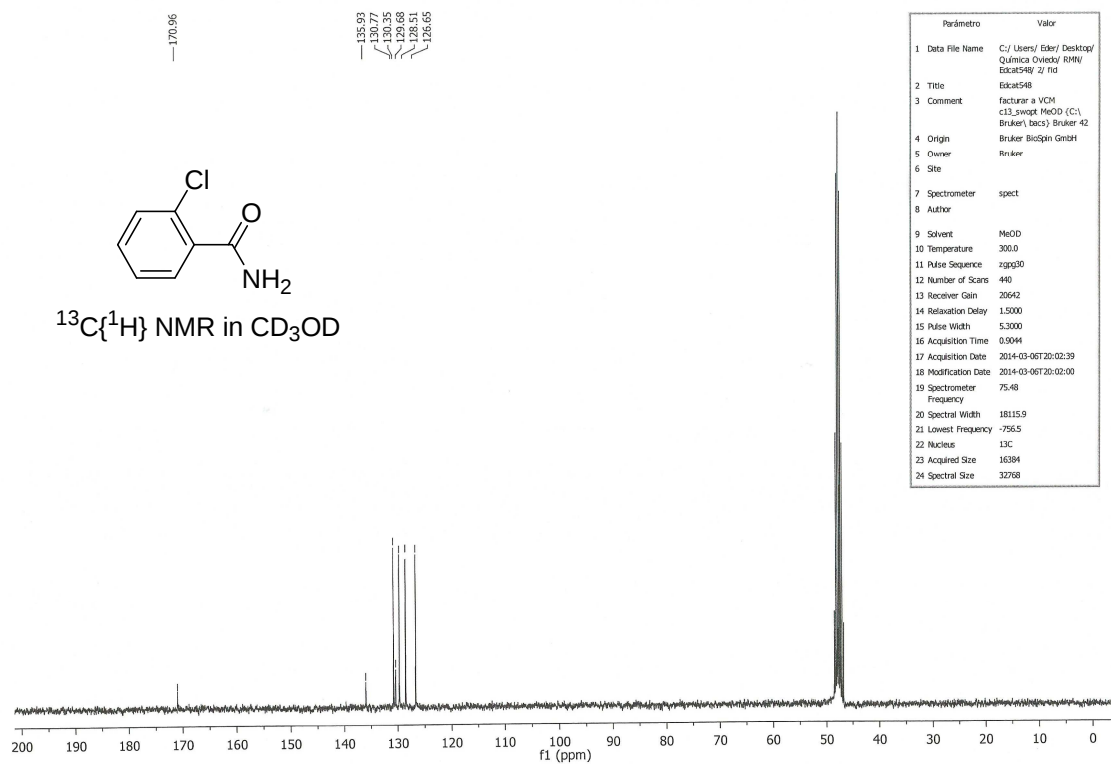
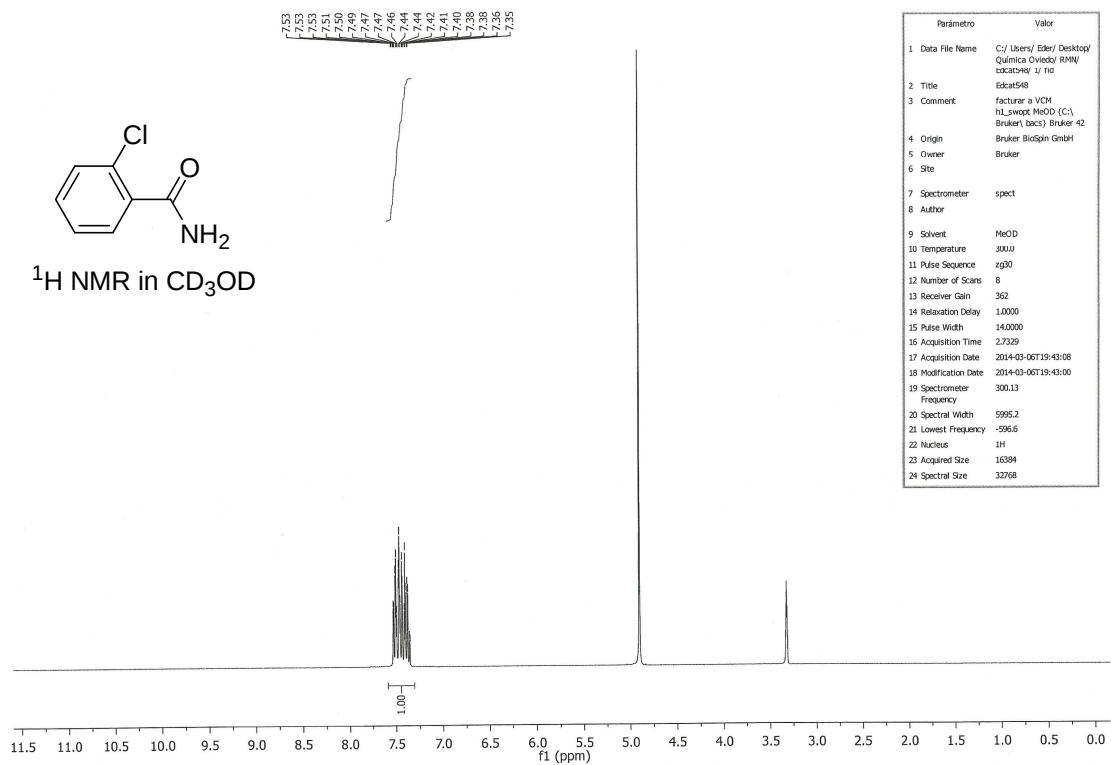


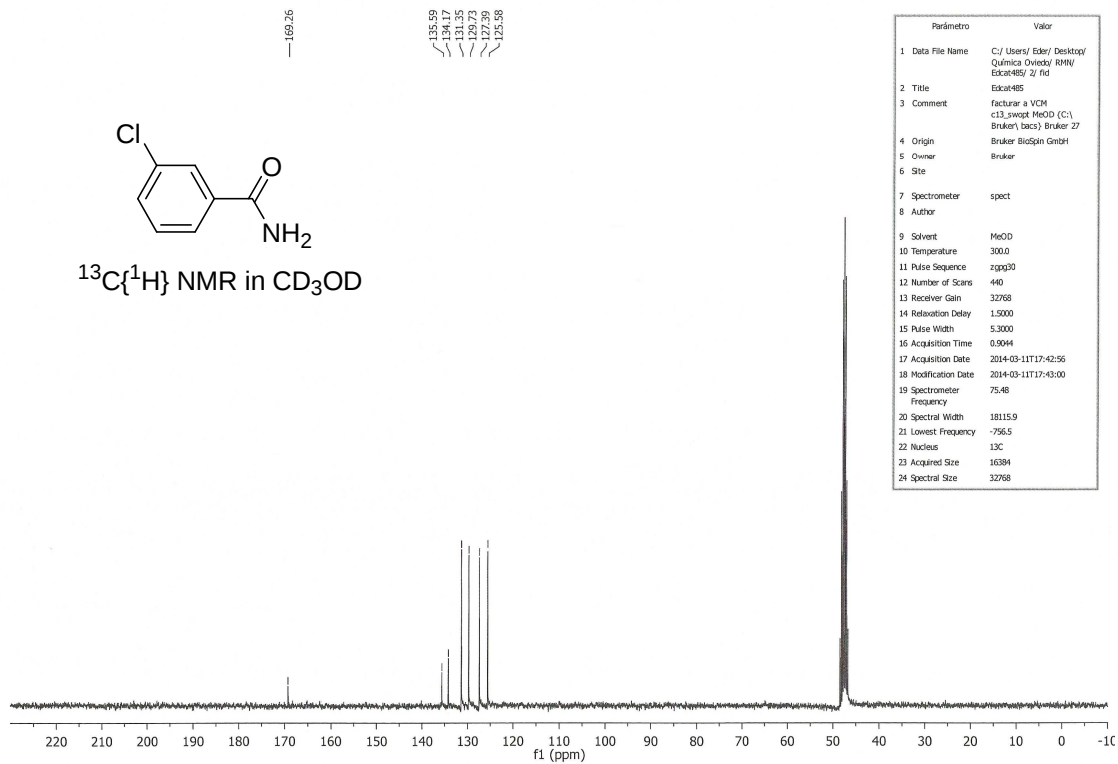
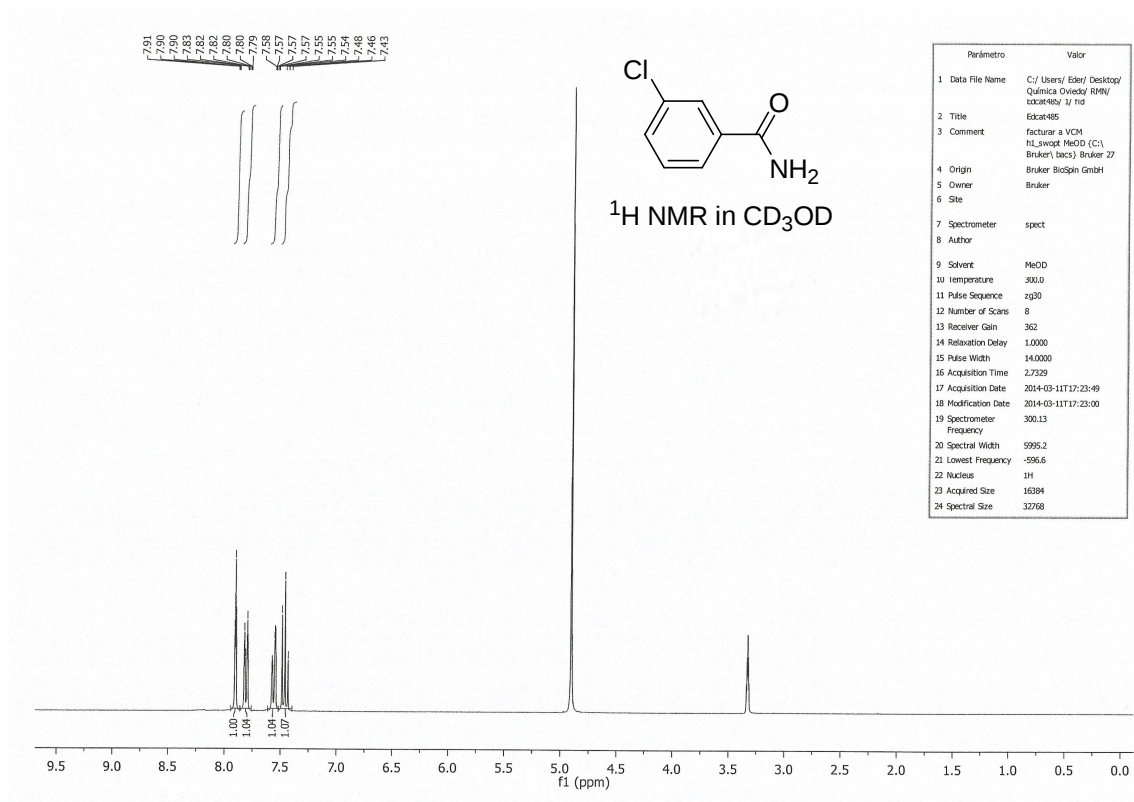
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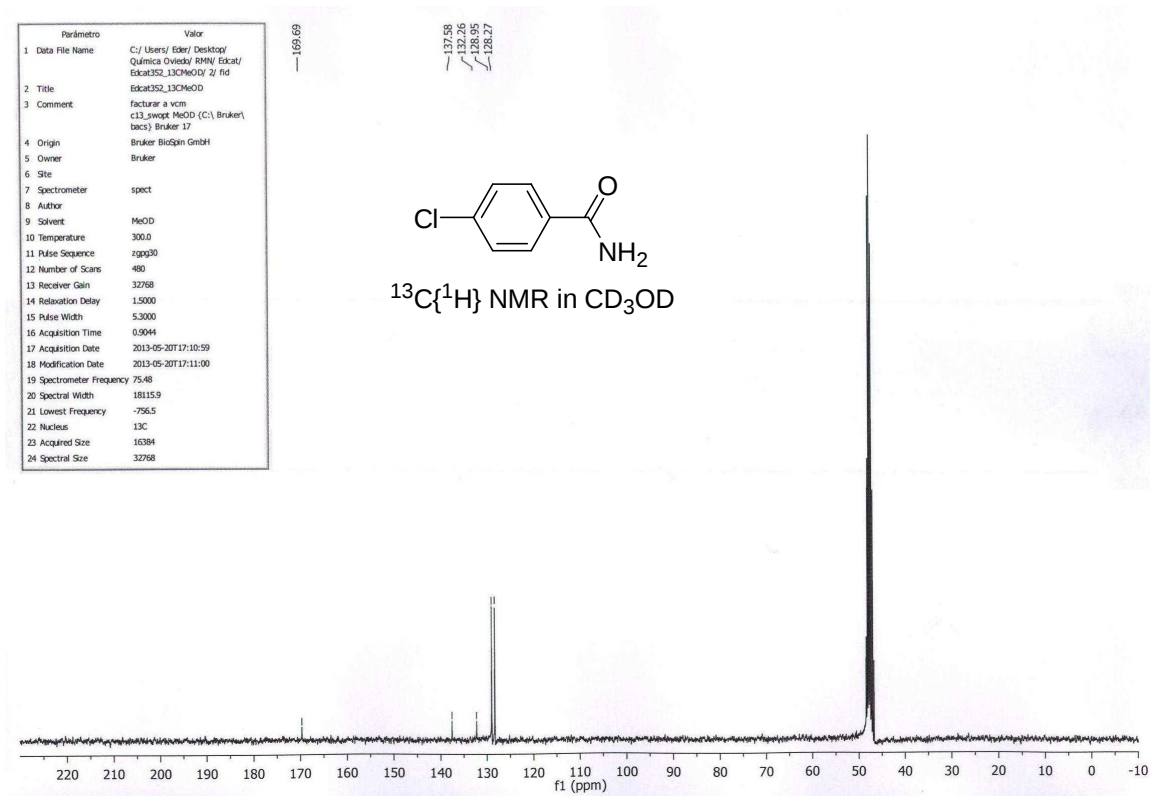
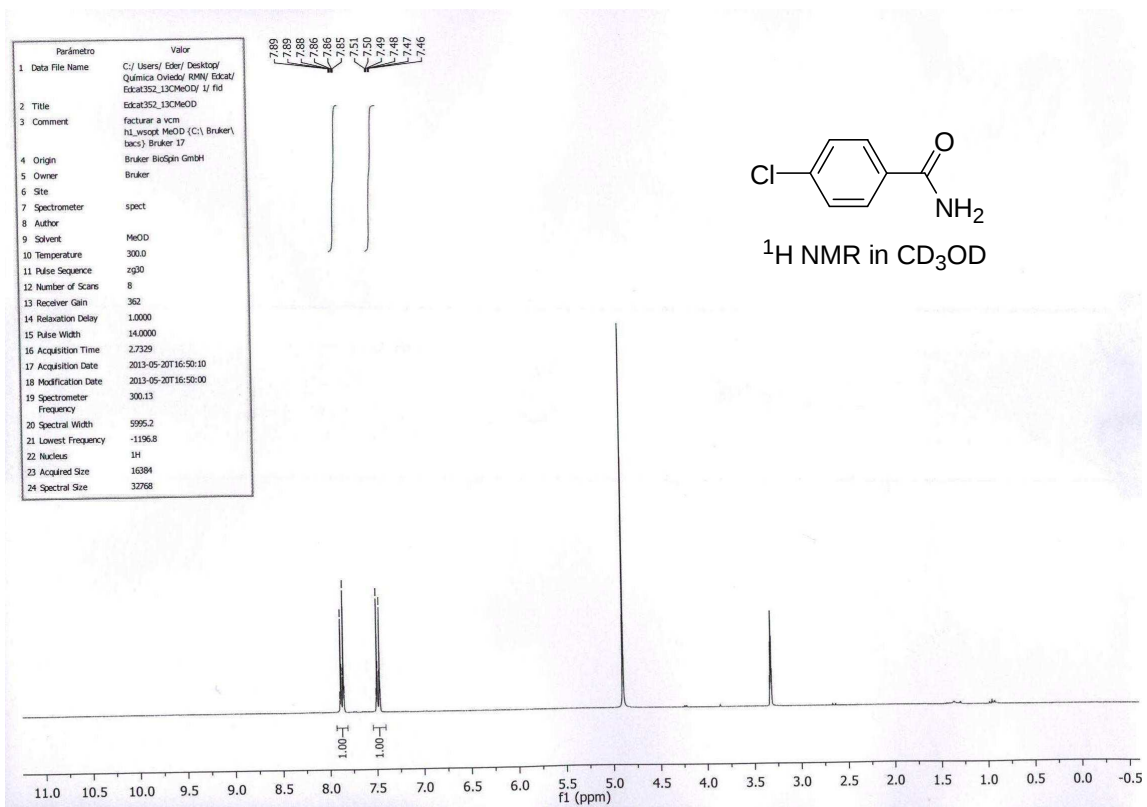


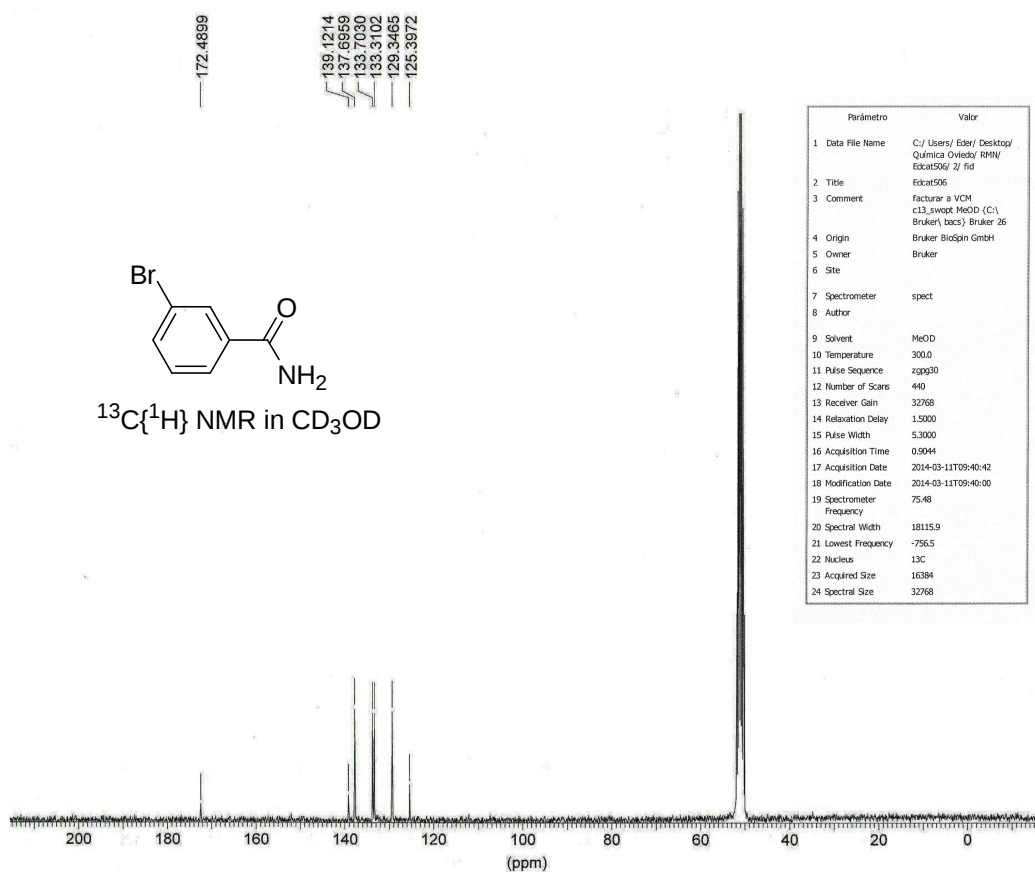
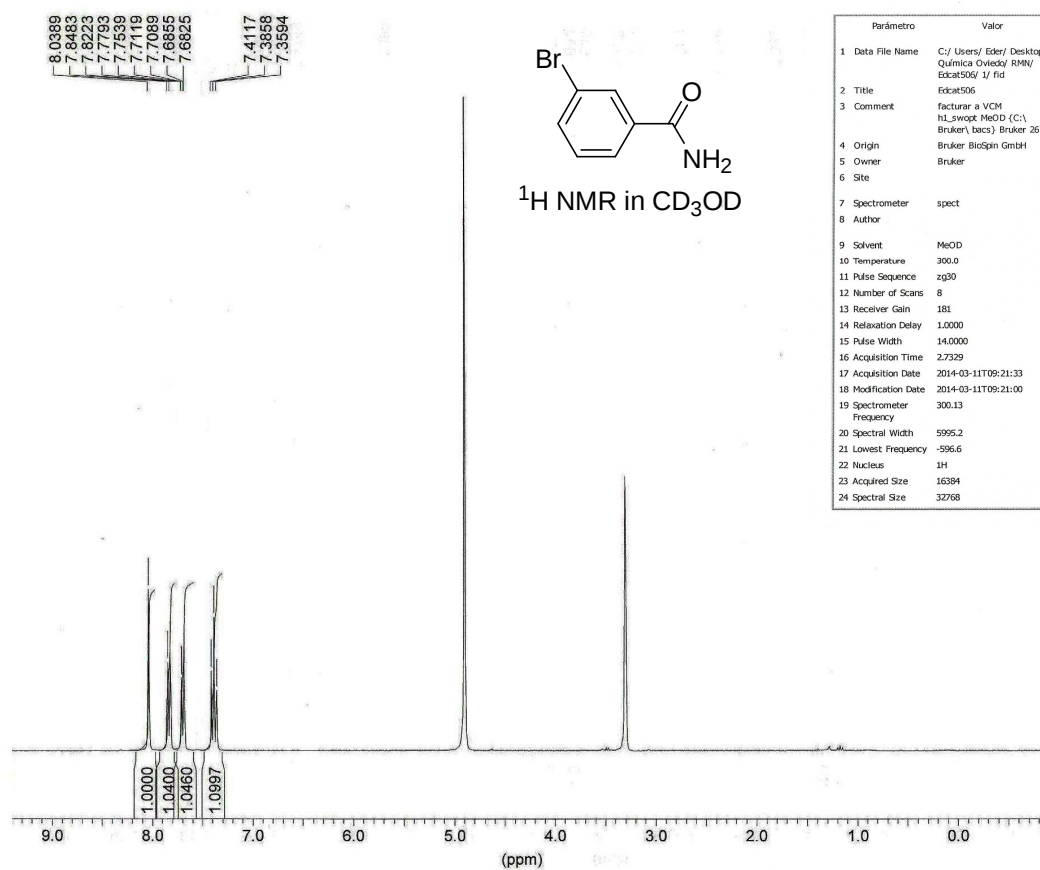
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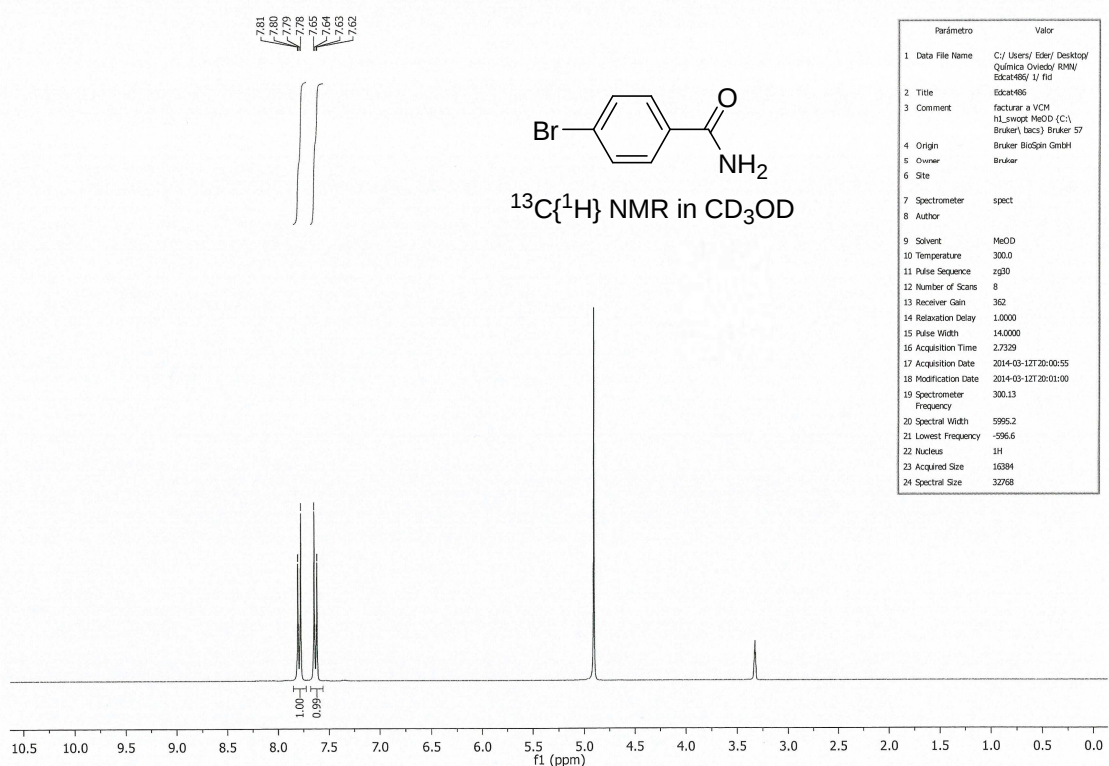
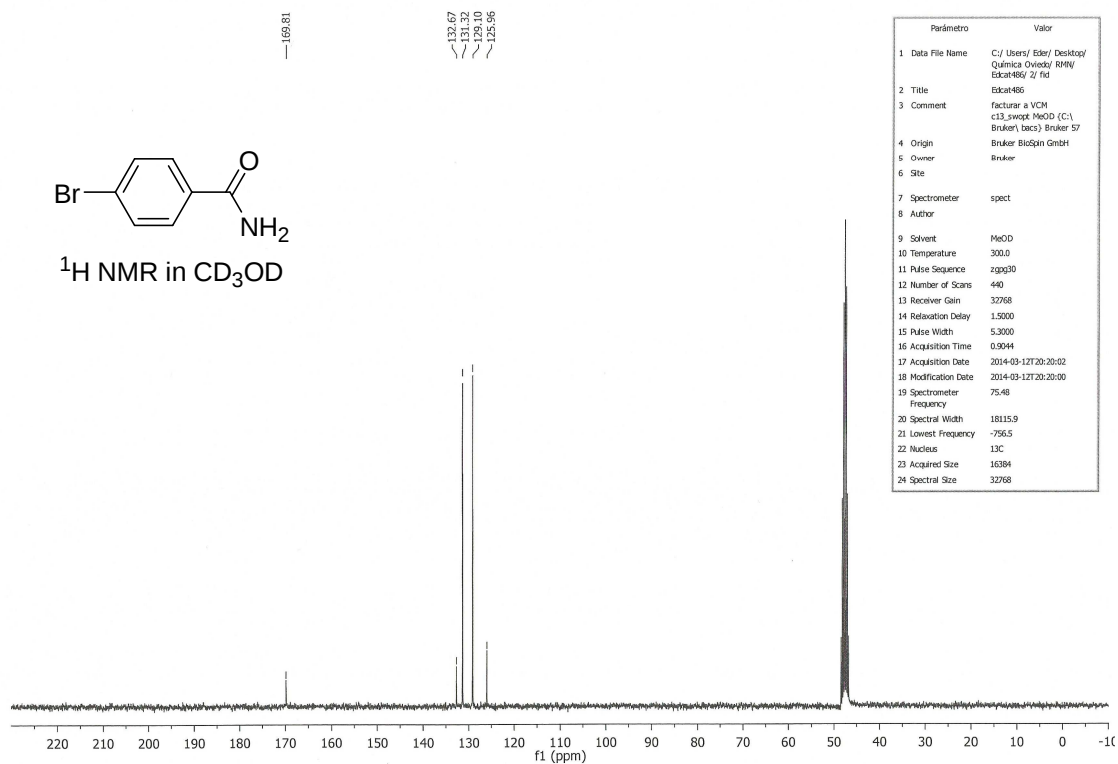


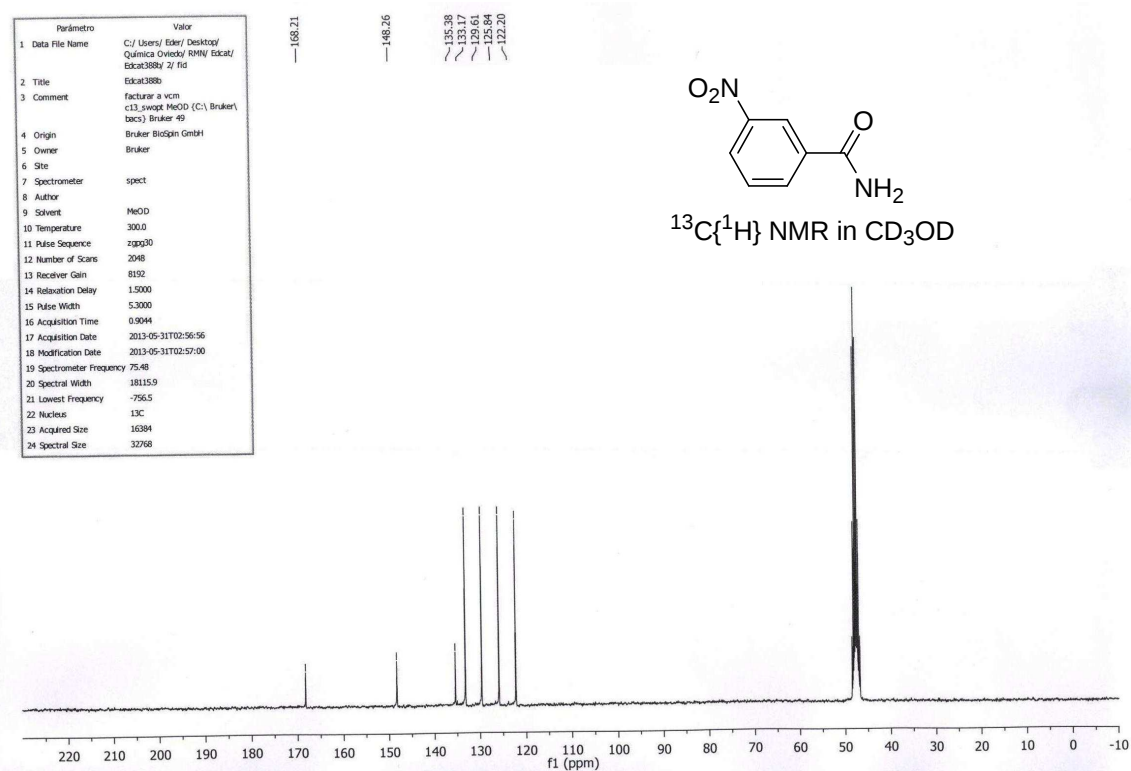
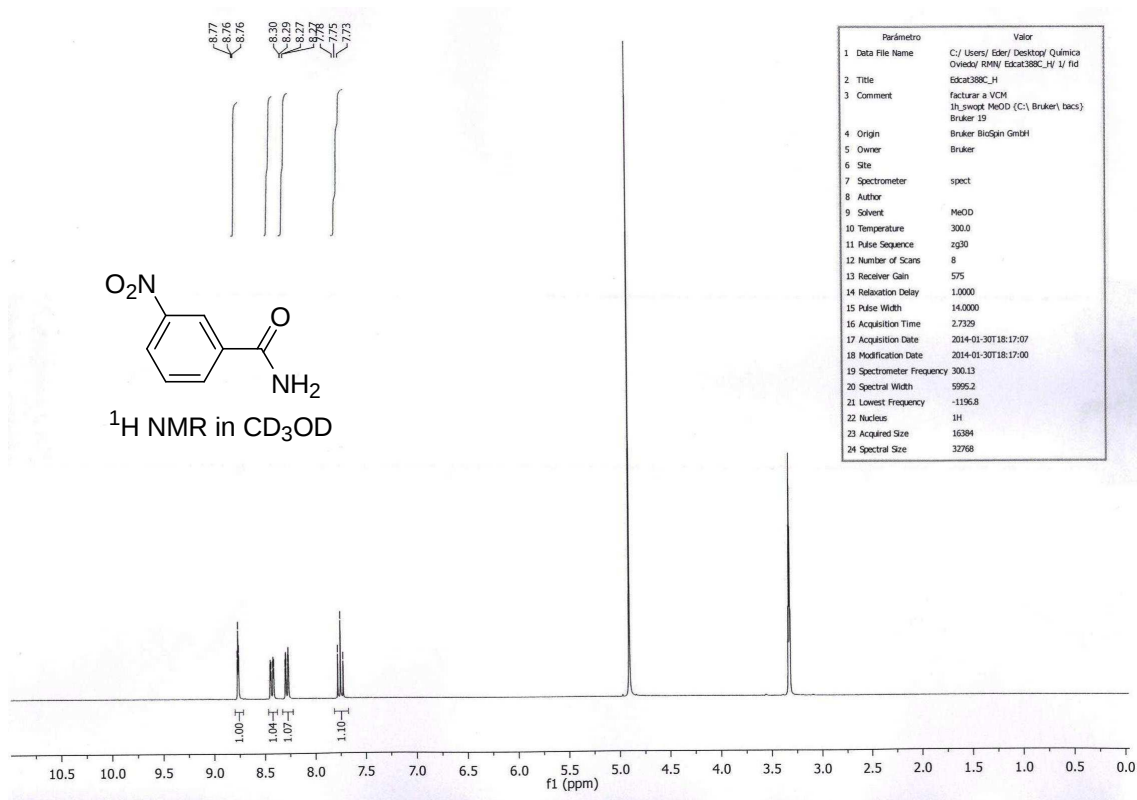




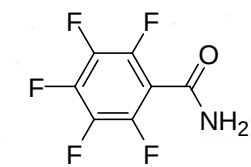




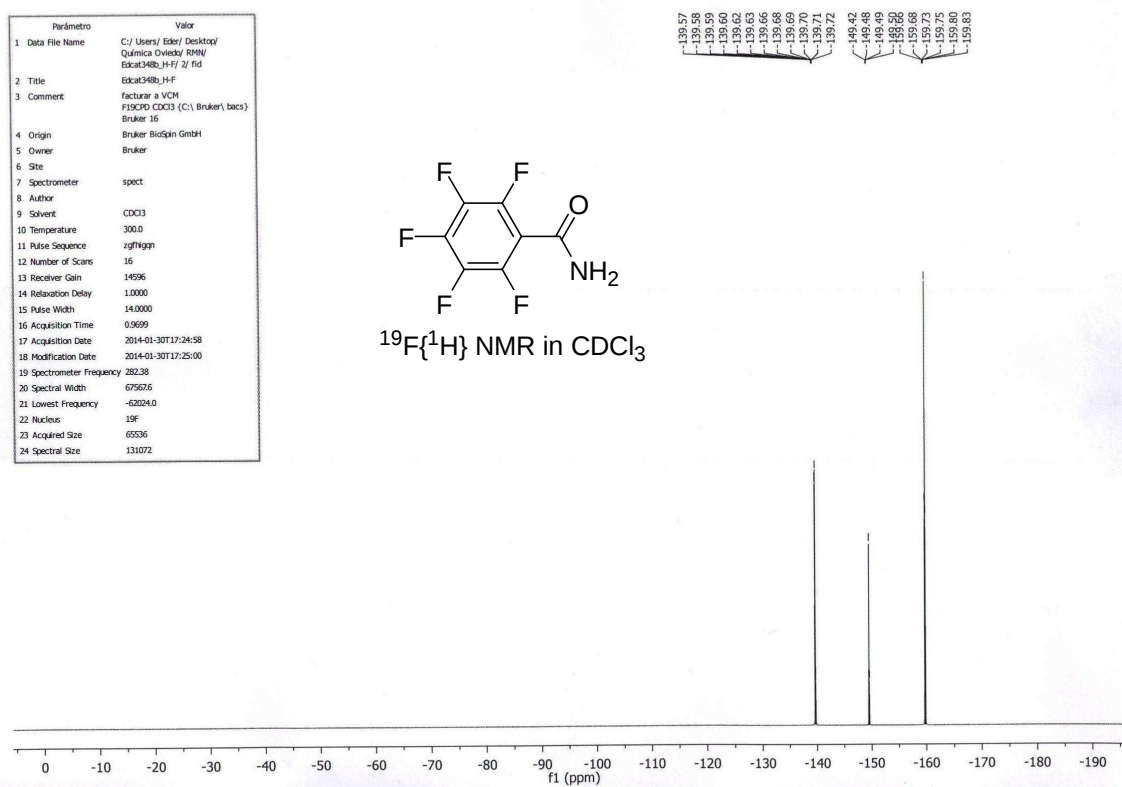




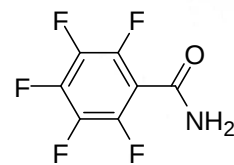
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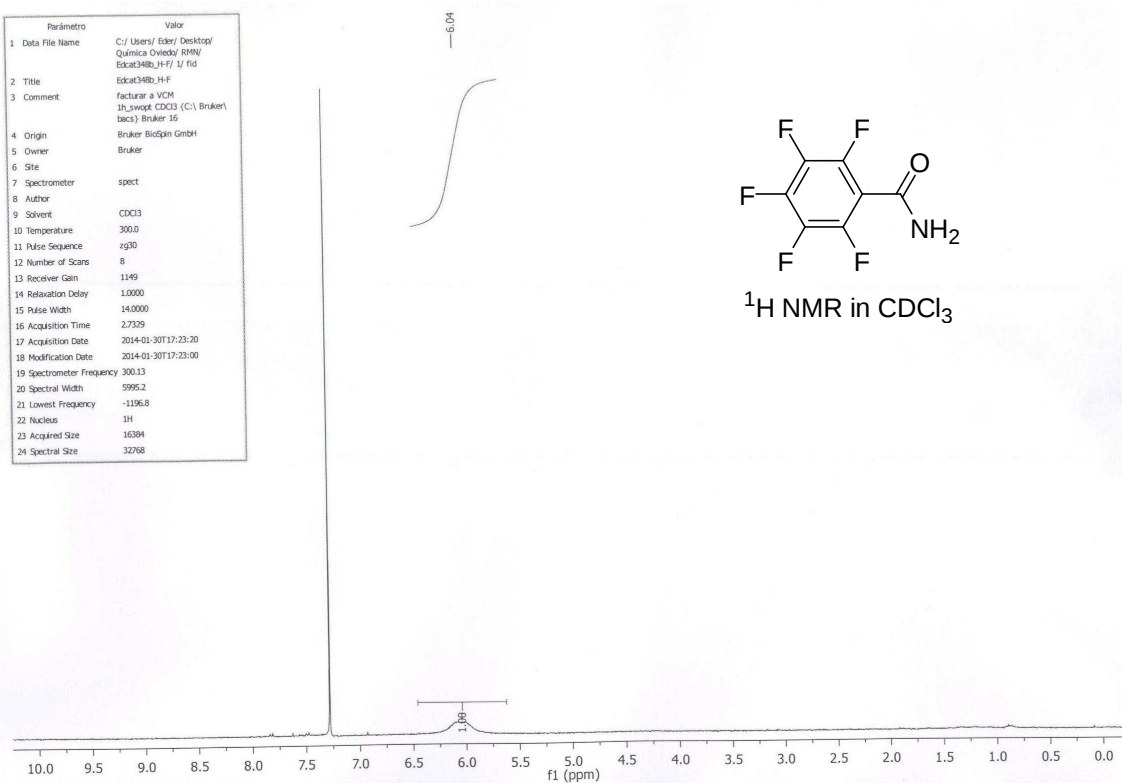
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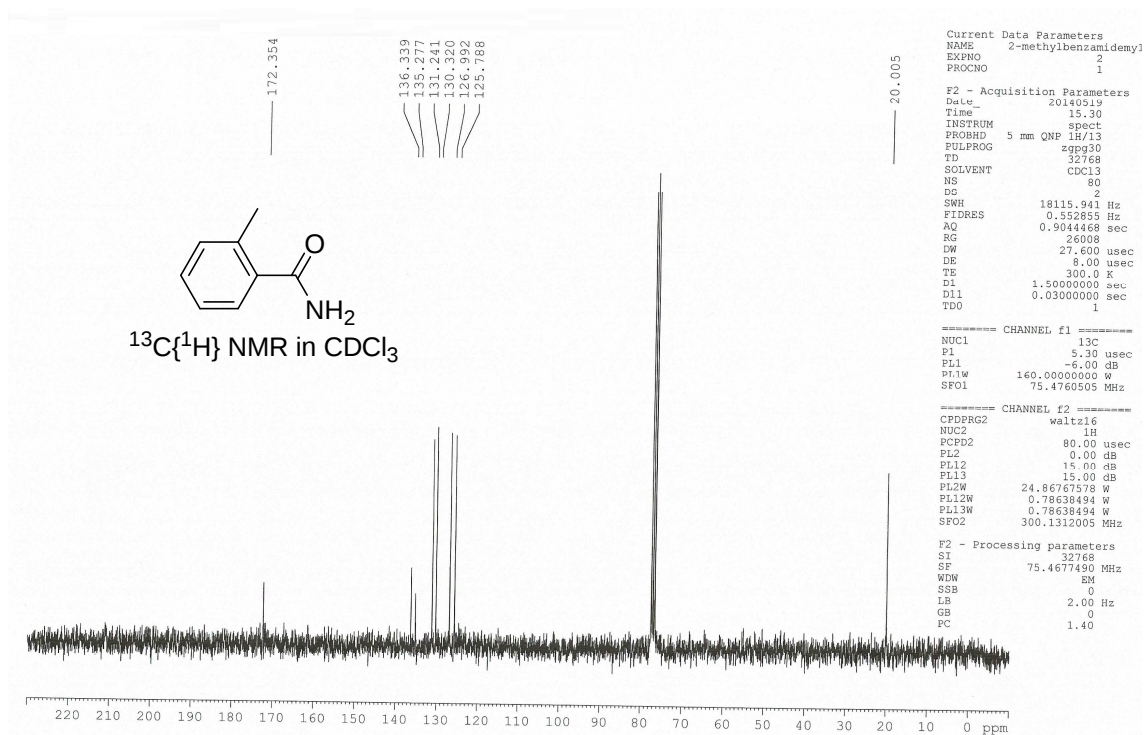
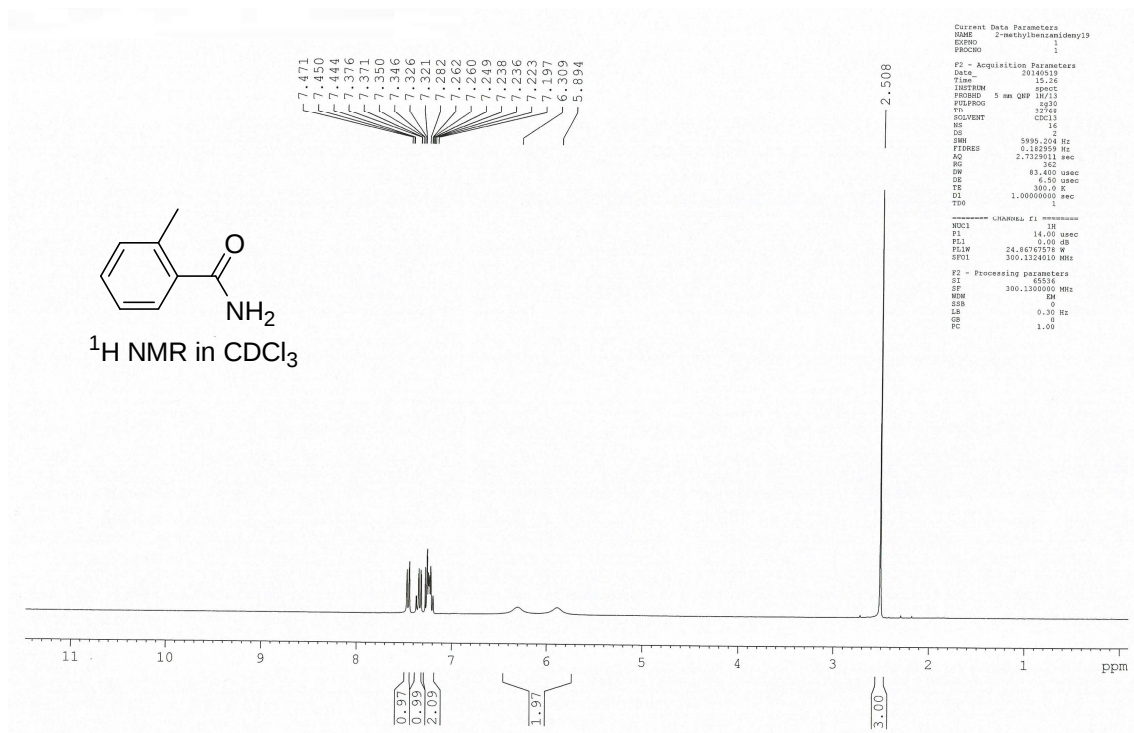


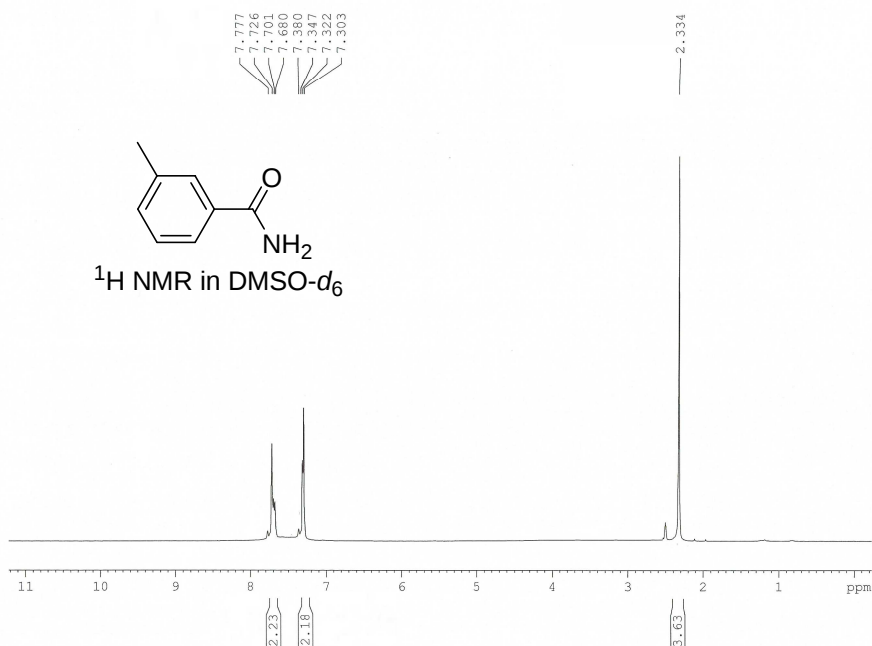
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^1H NMR in CDCl_3







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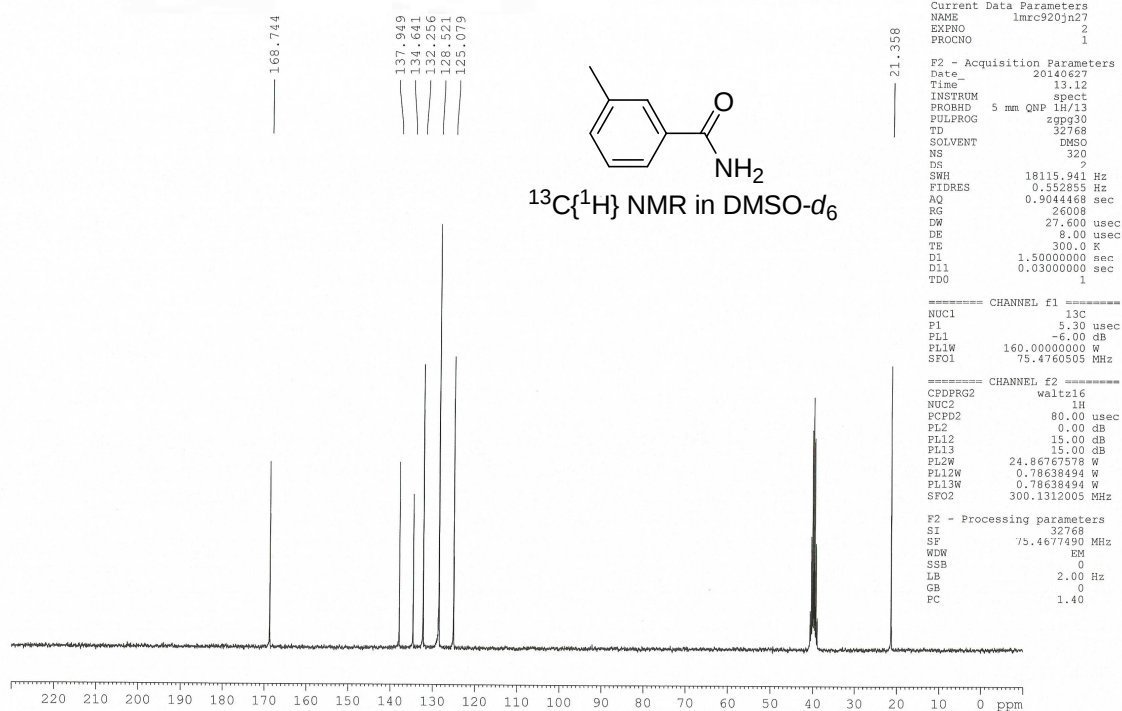
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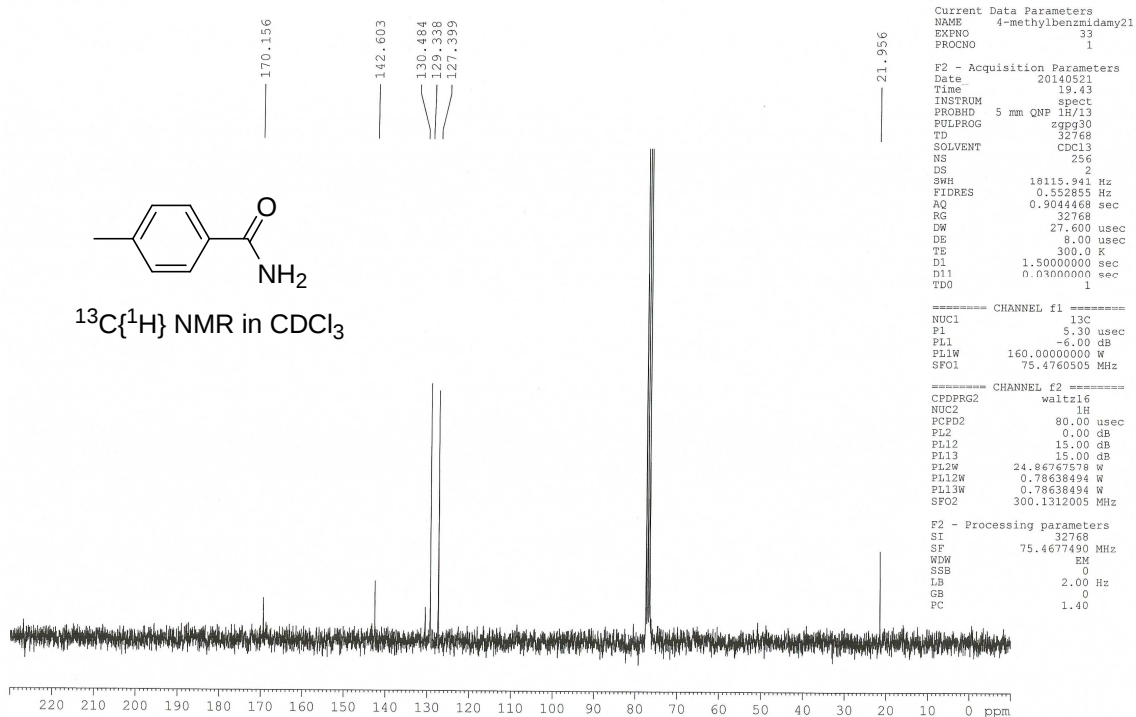
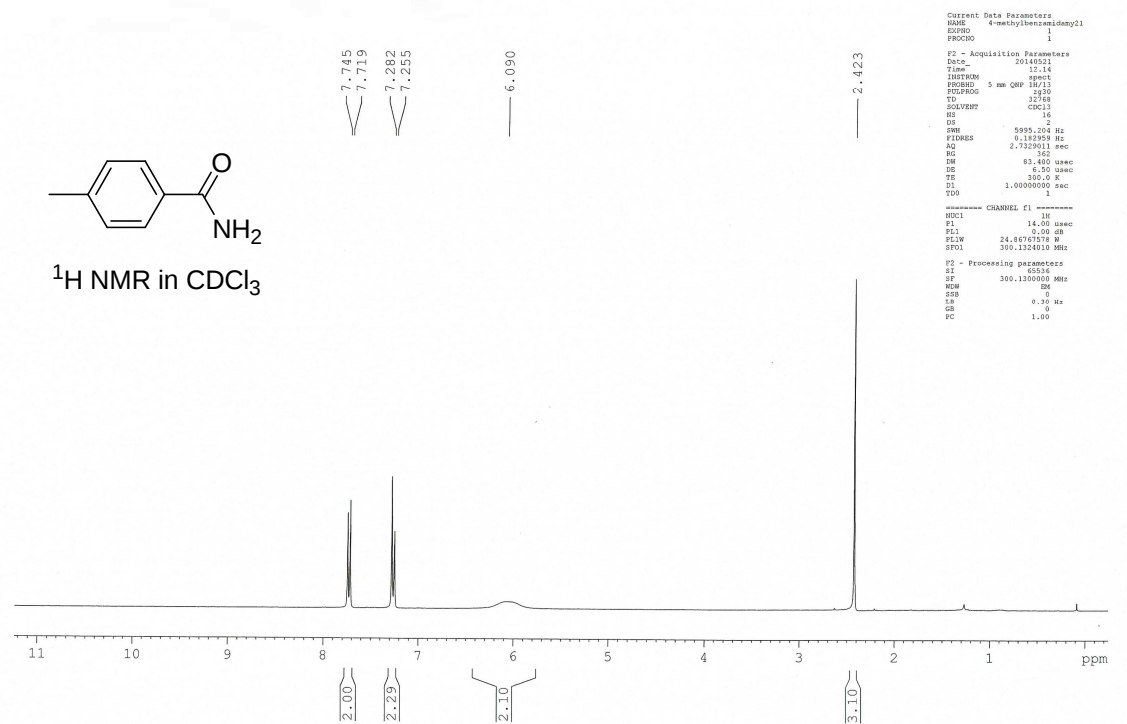
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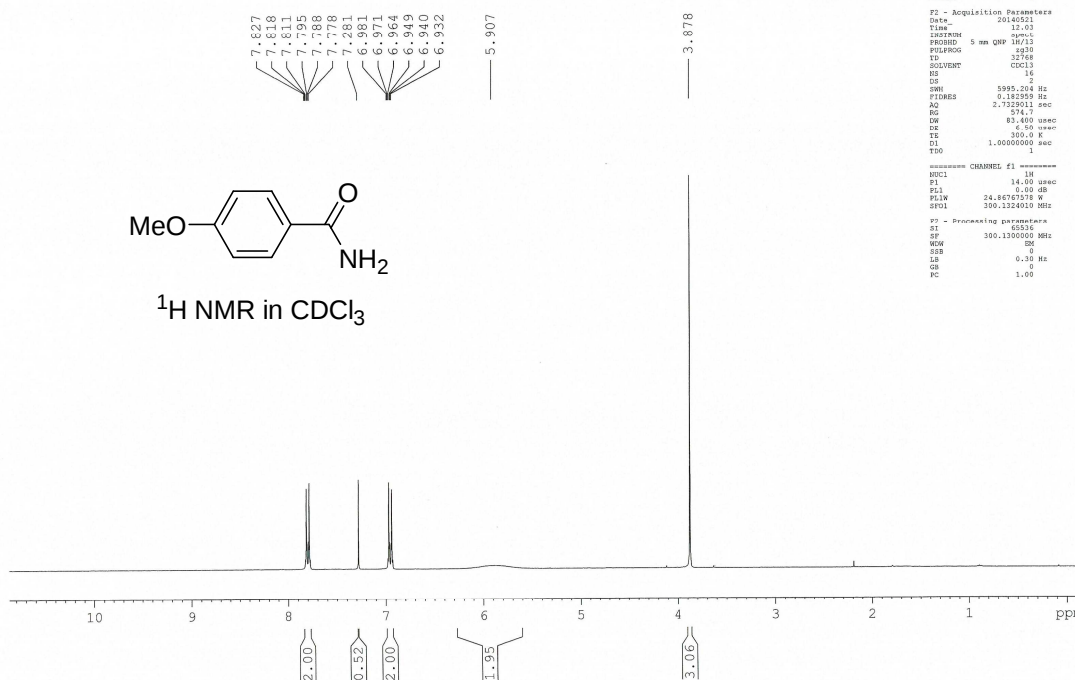
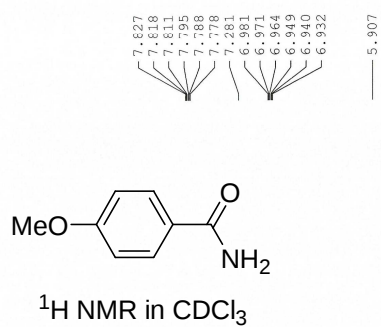
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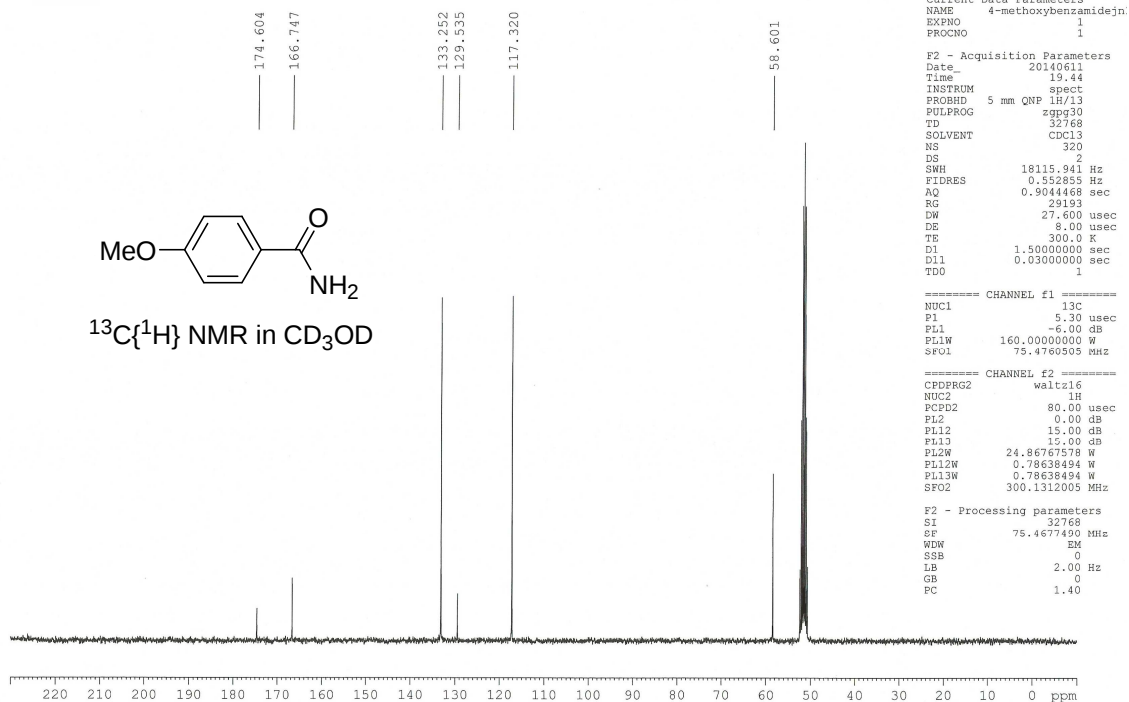
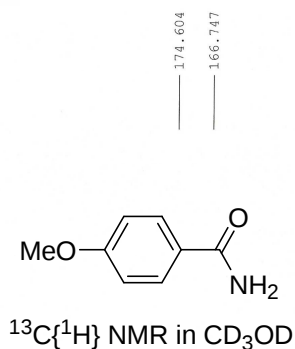




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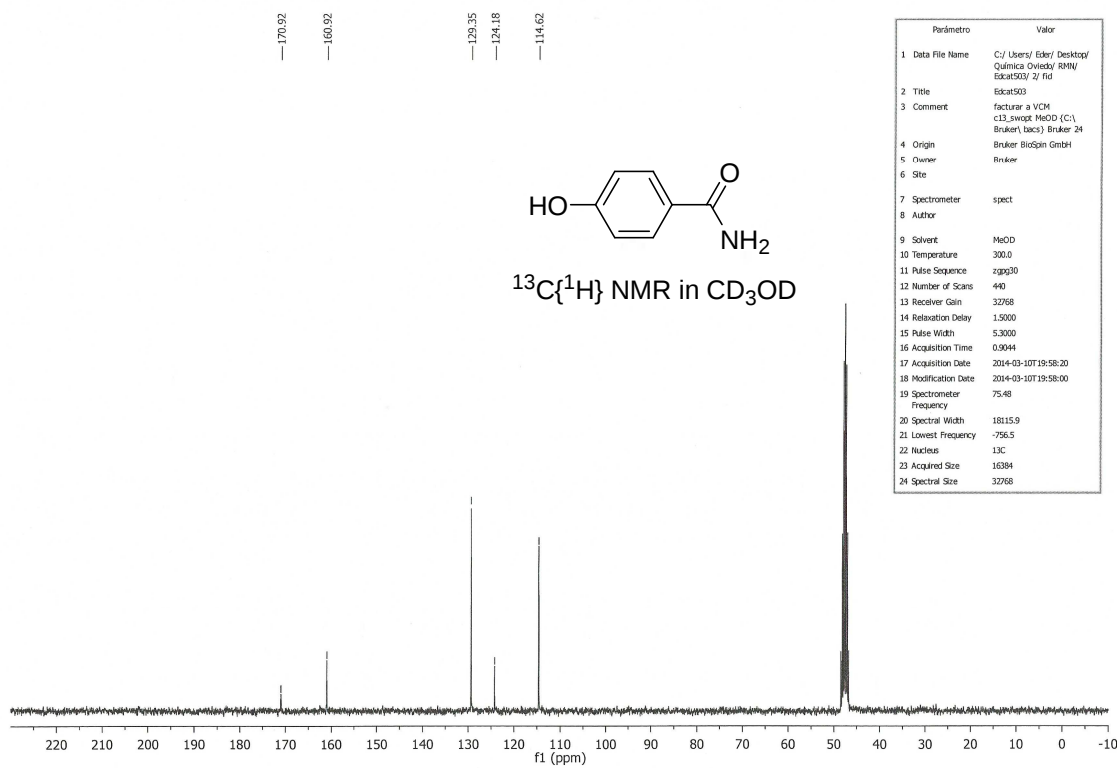
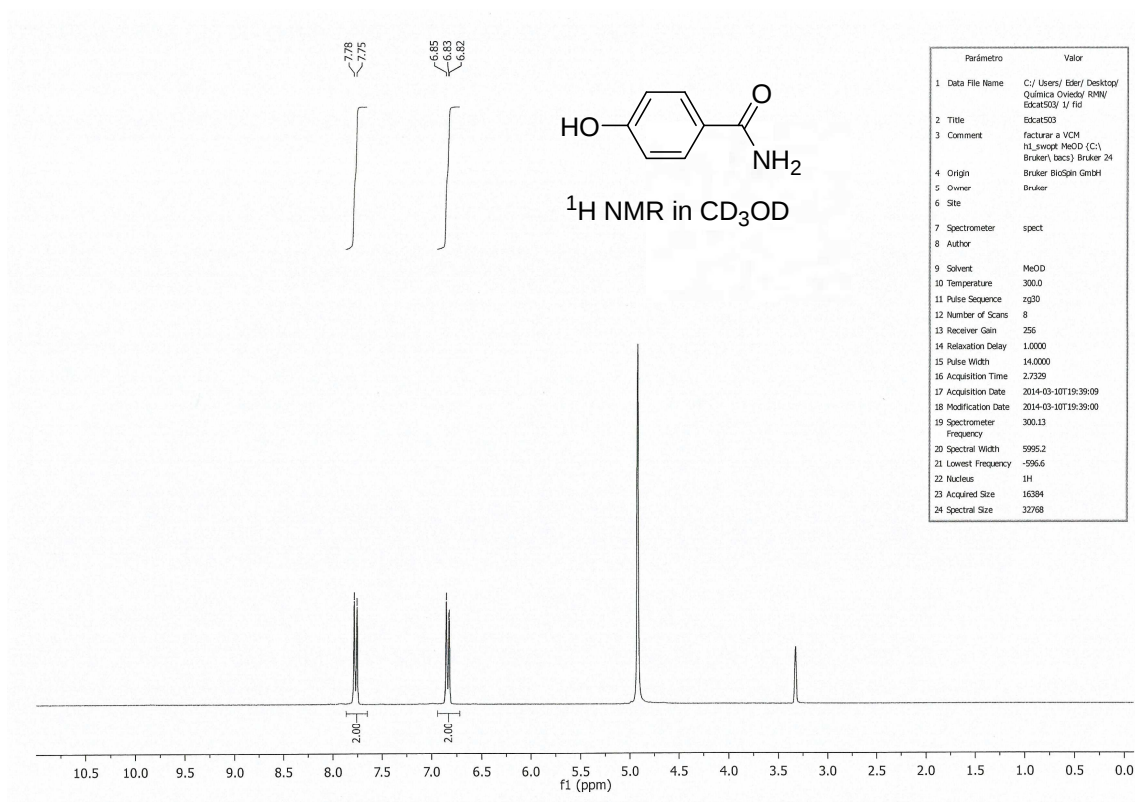
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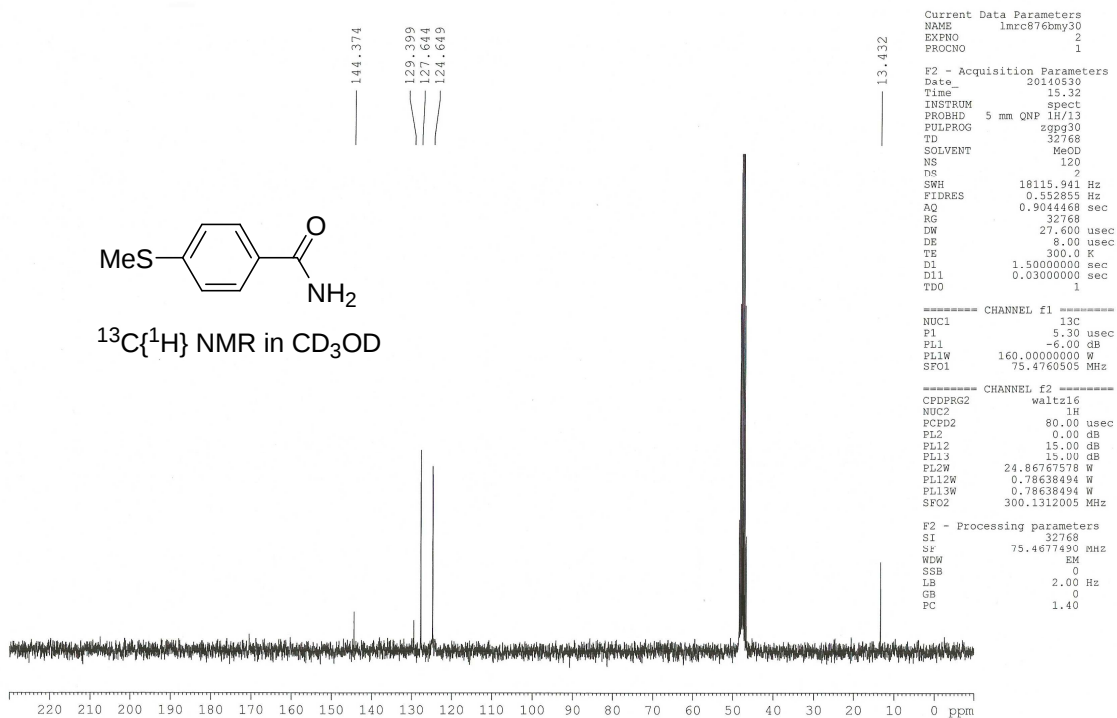
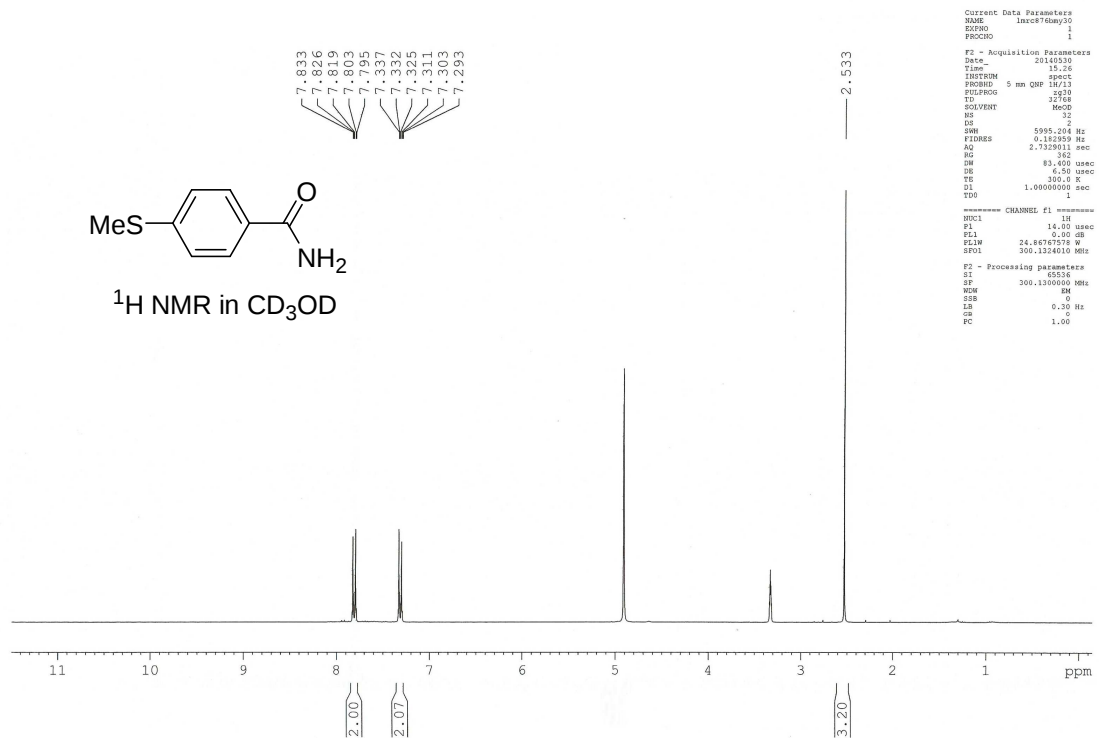
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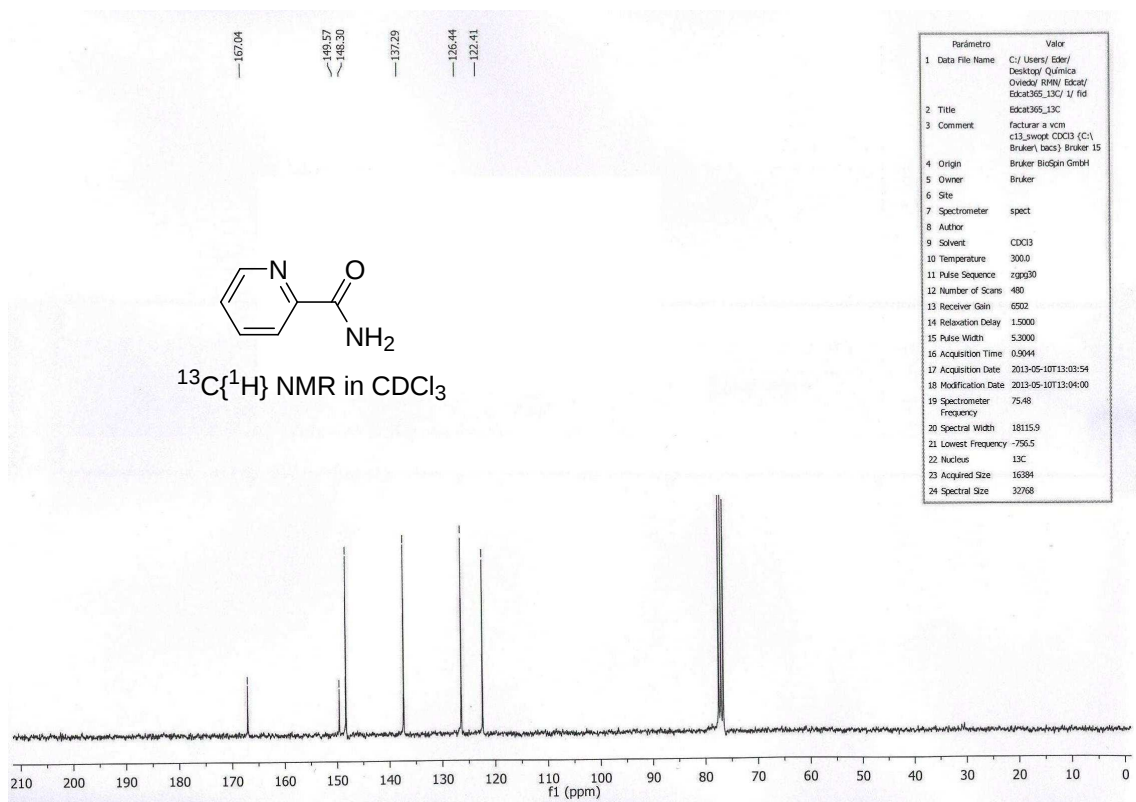
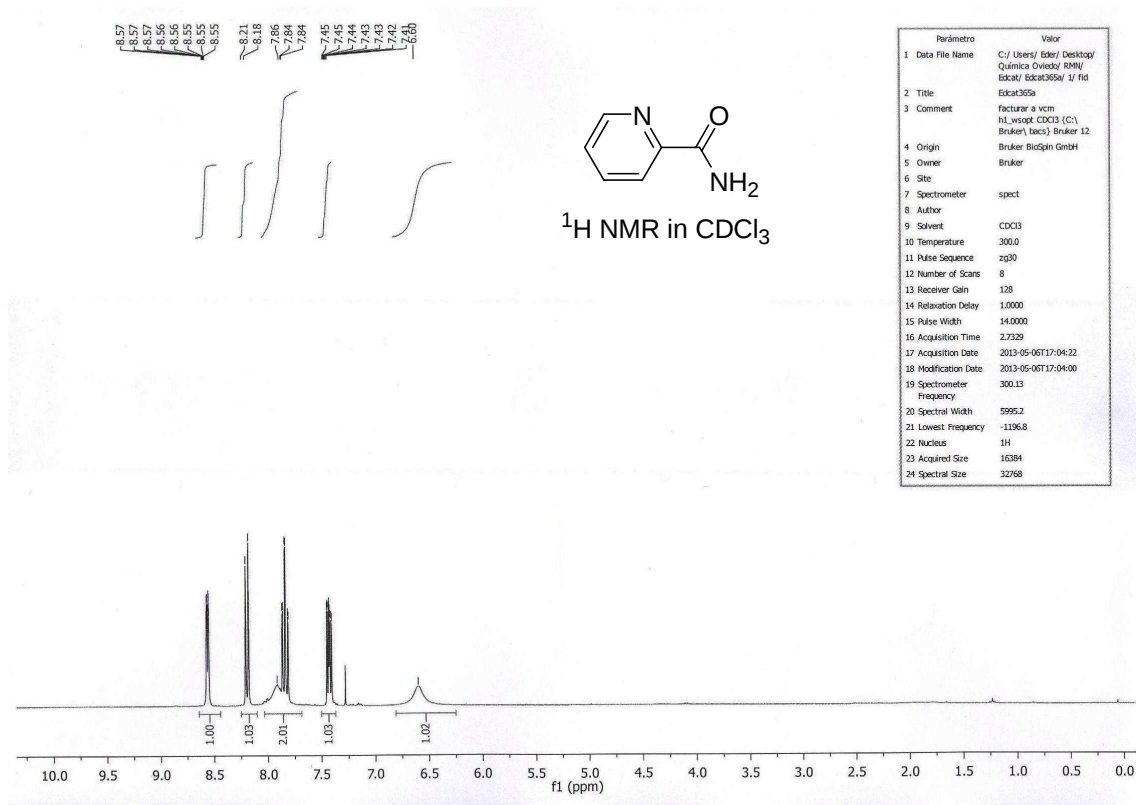
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SFO1 75.4760505 MHz

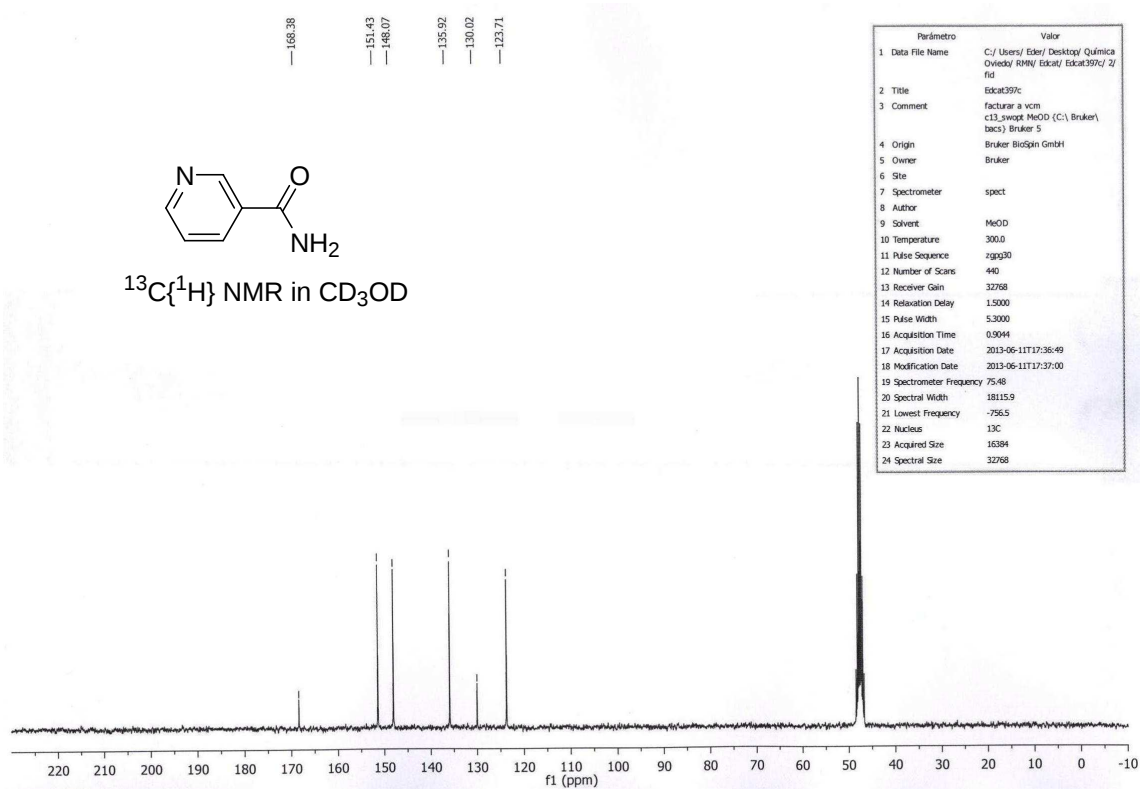
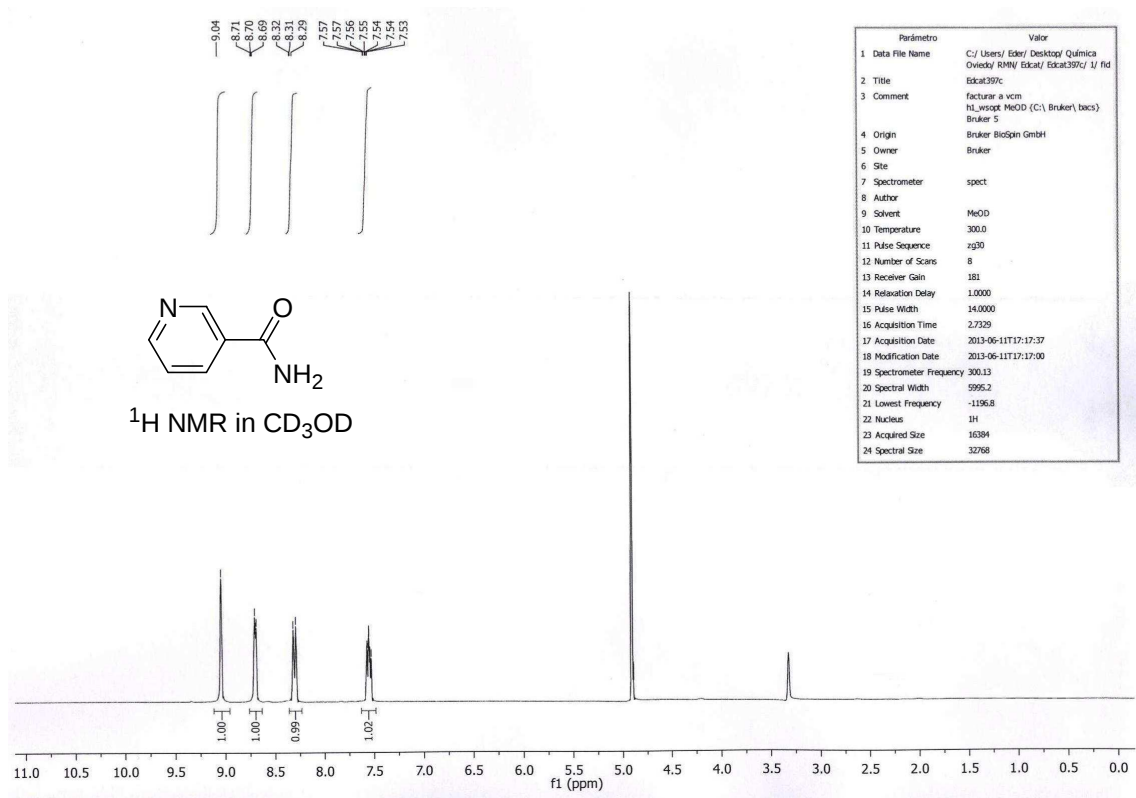
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 24.8676758 W
PL12W 0.78638494 W
PL13W 0.78638494 W
SFO2 300.1312005 MHz

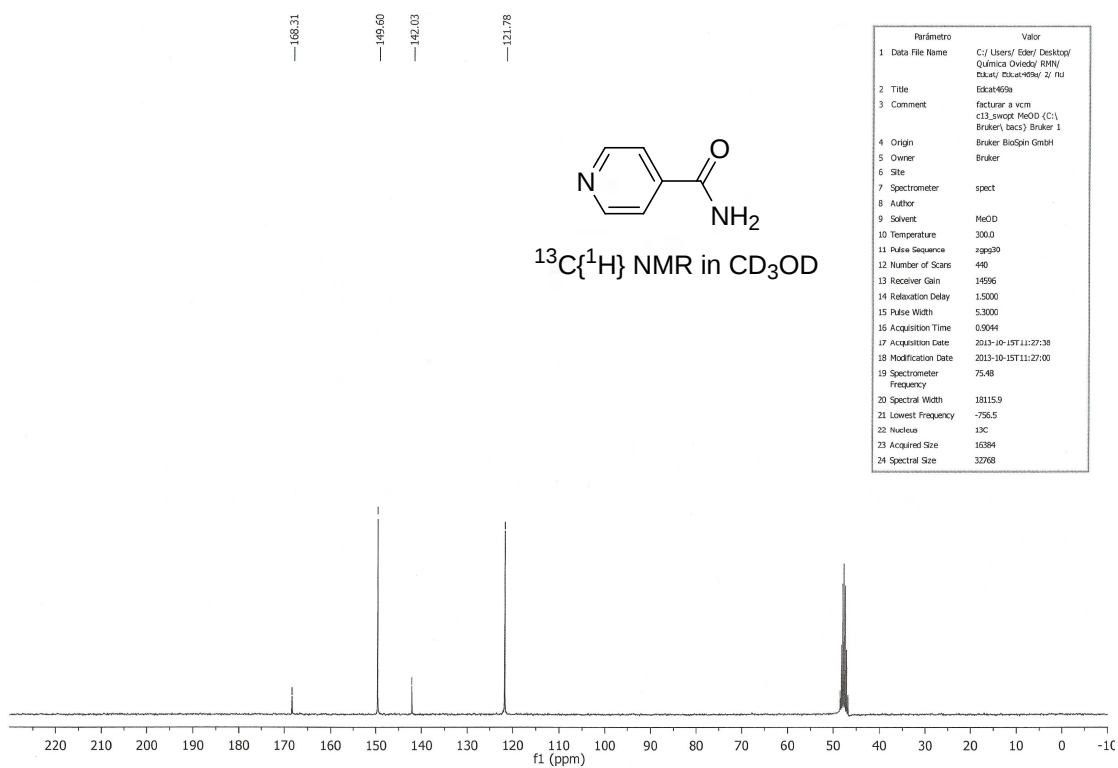
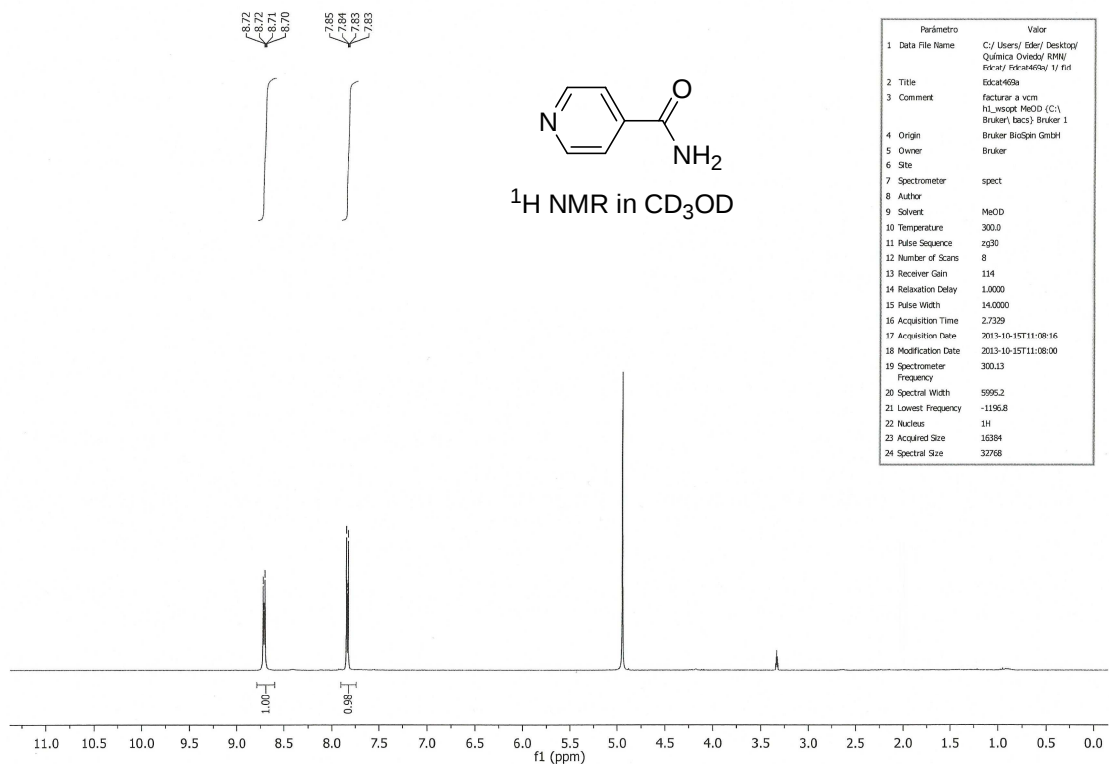
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

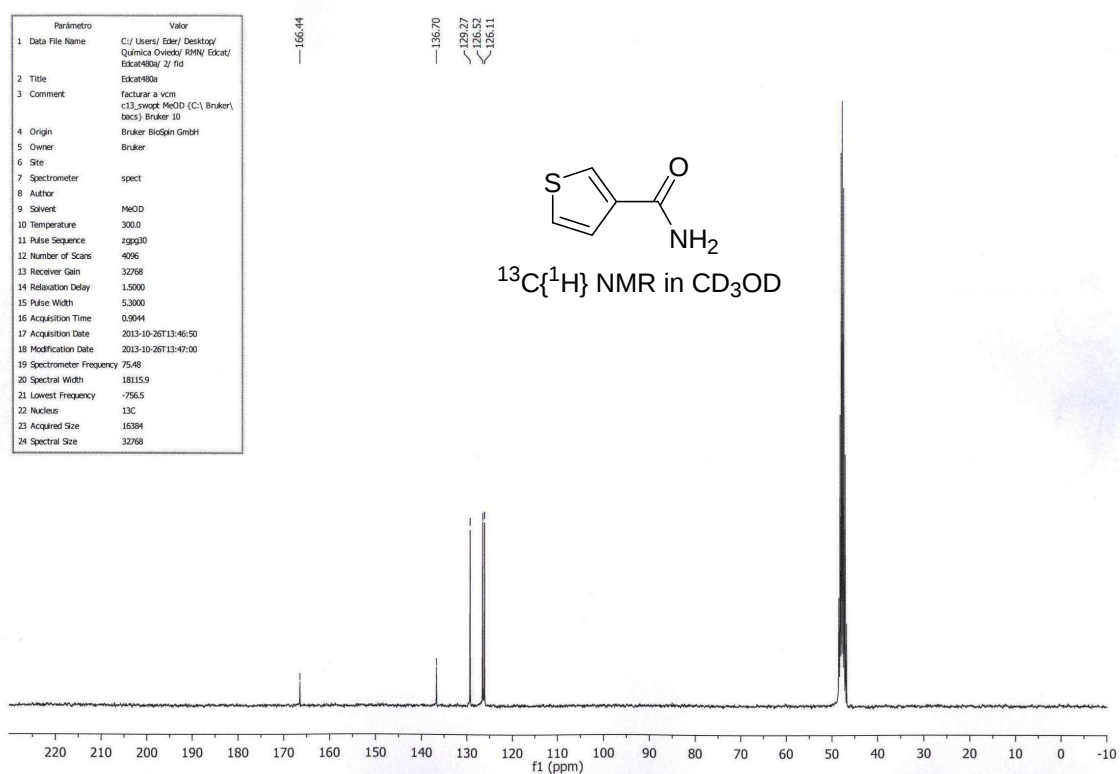
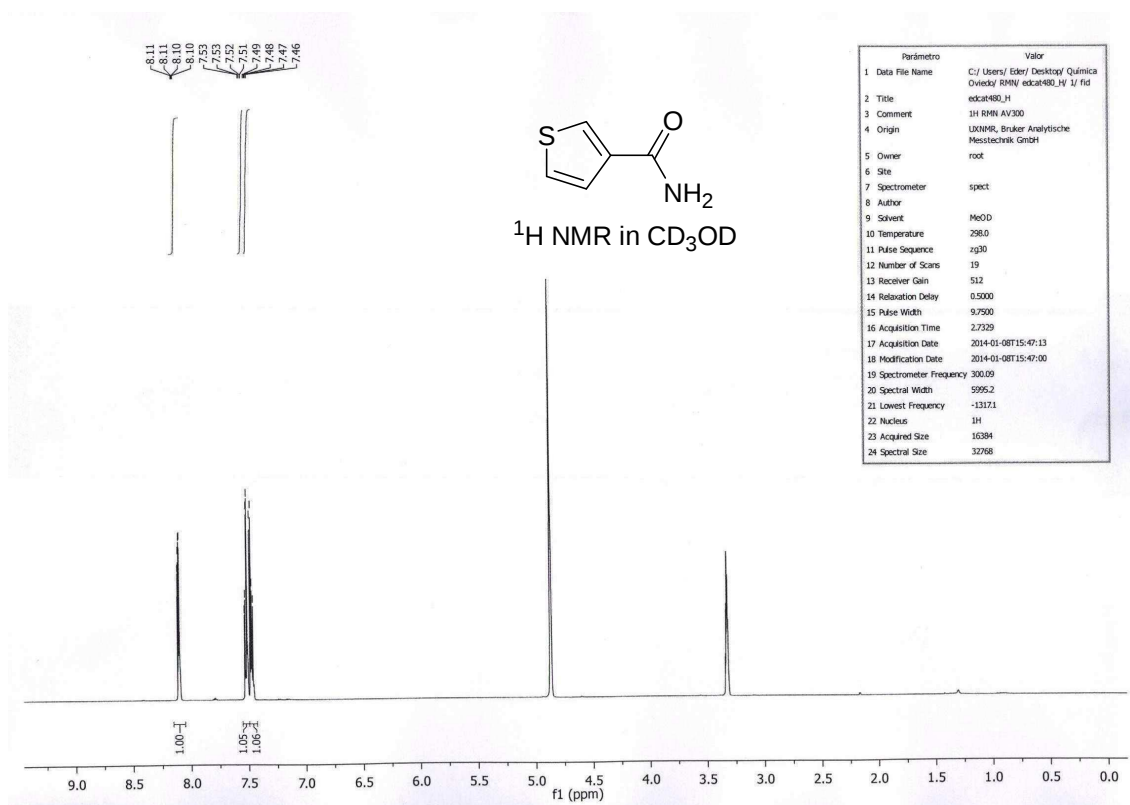


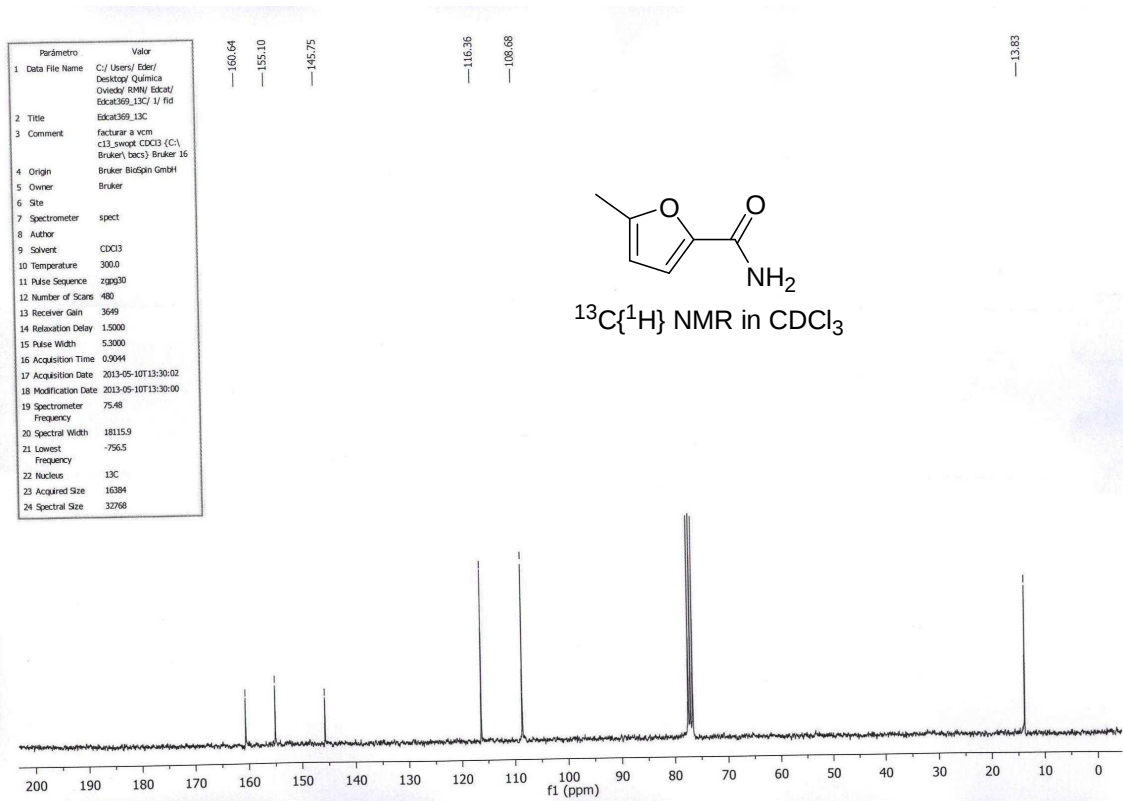
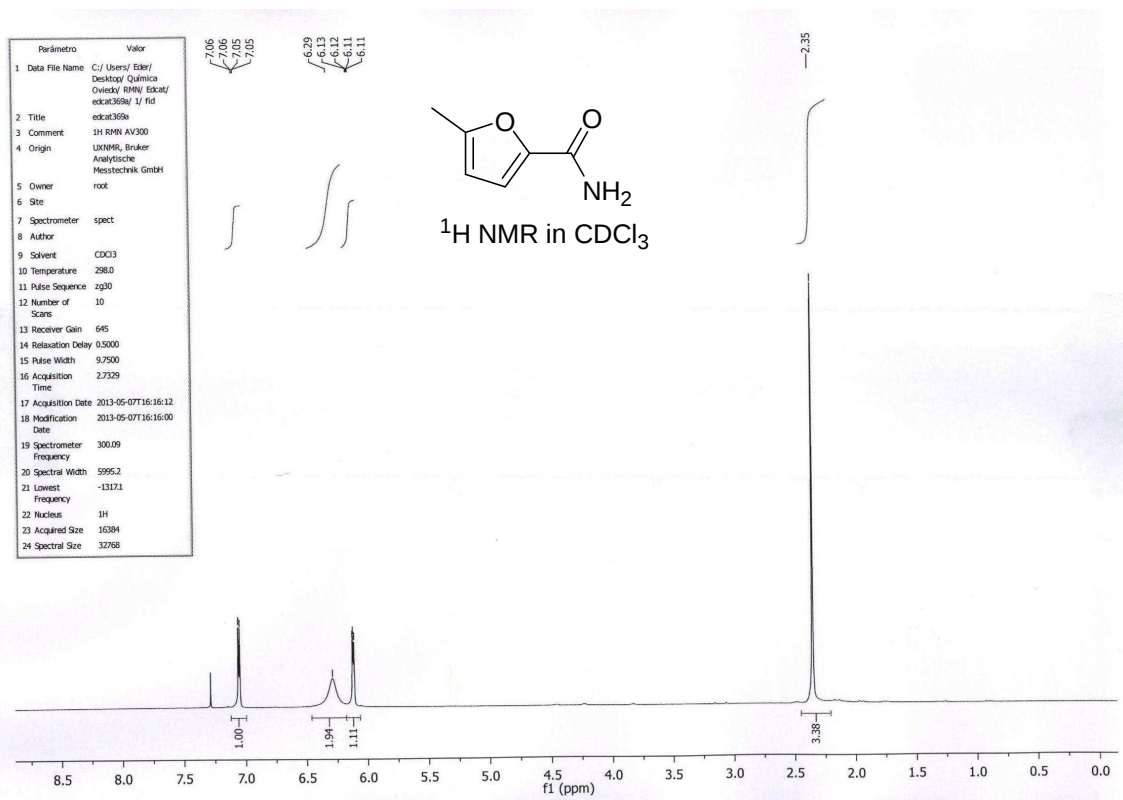




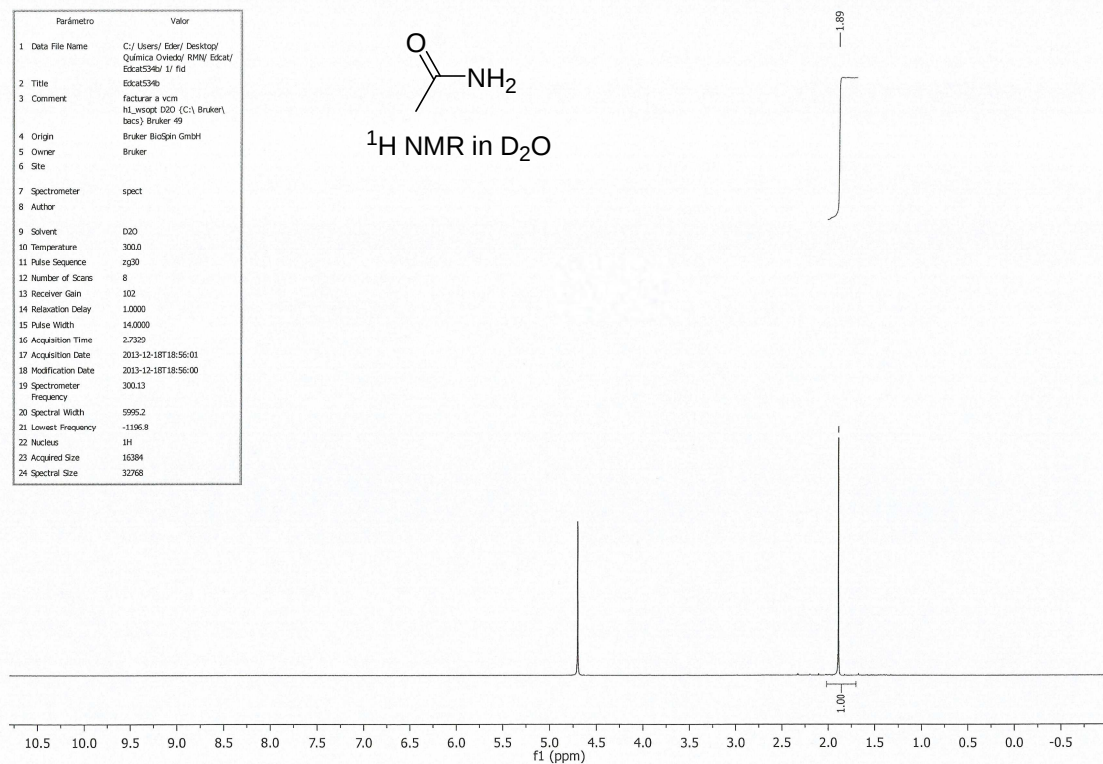
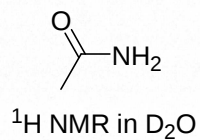




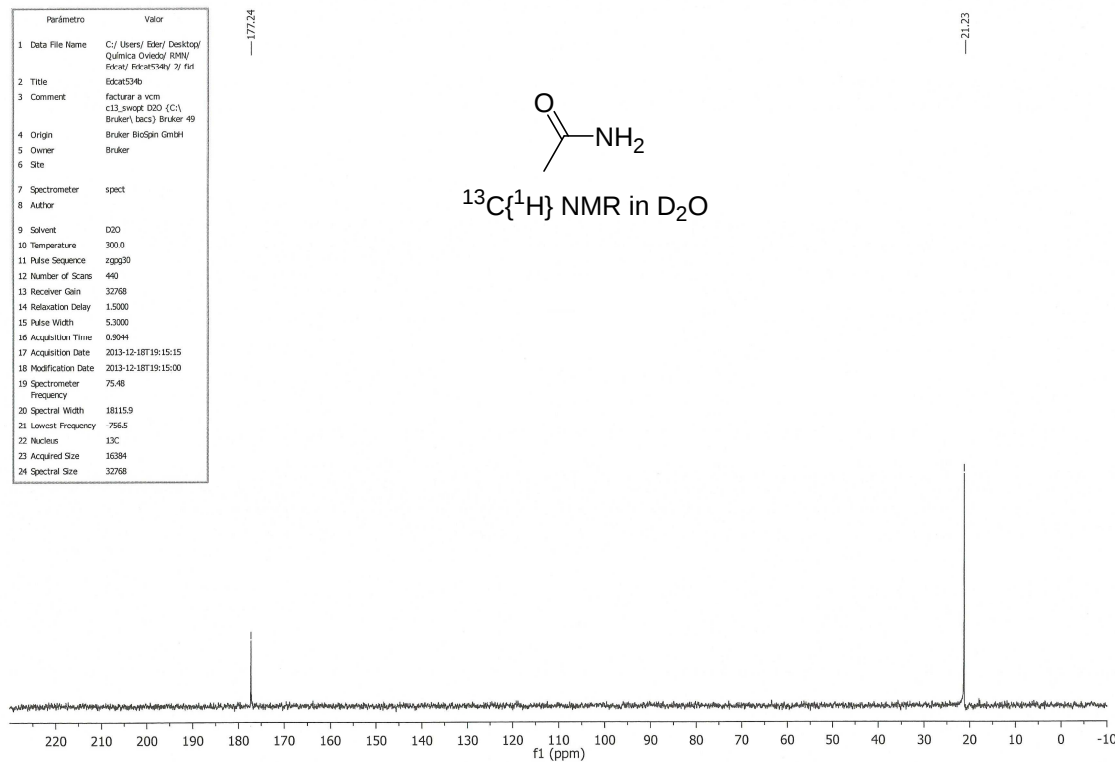
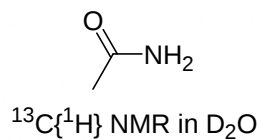


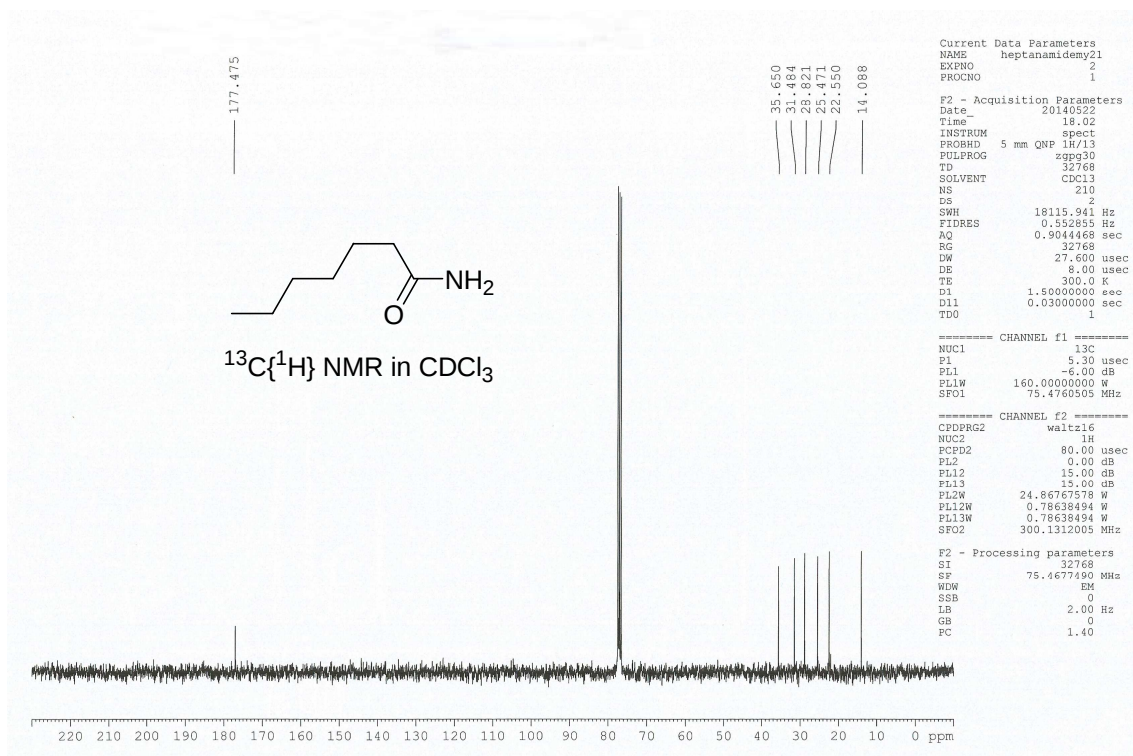
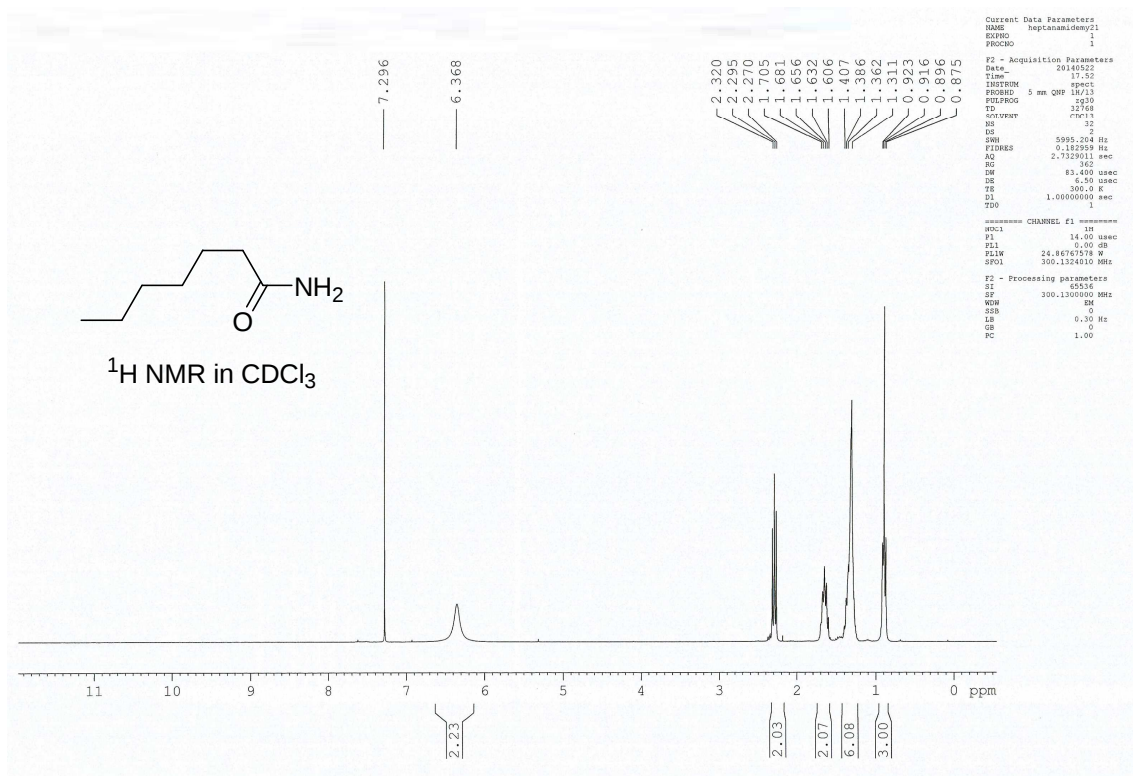


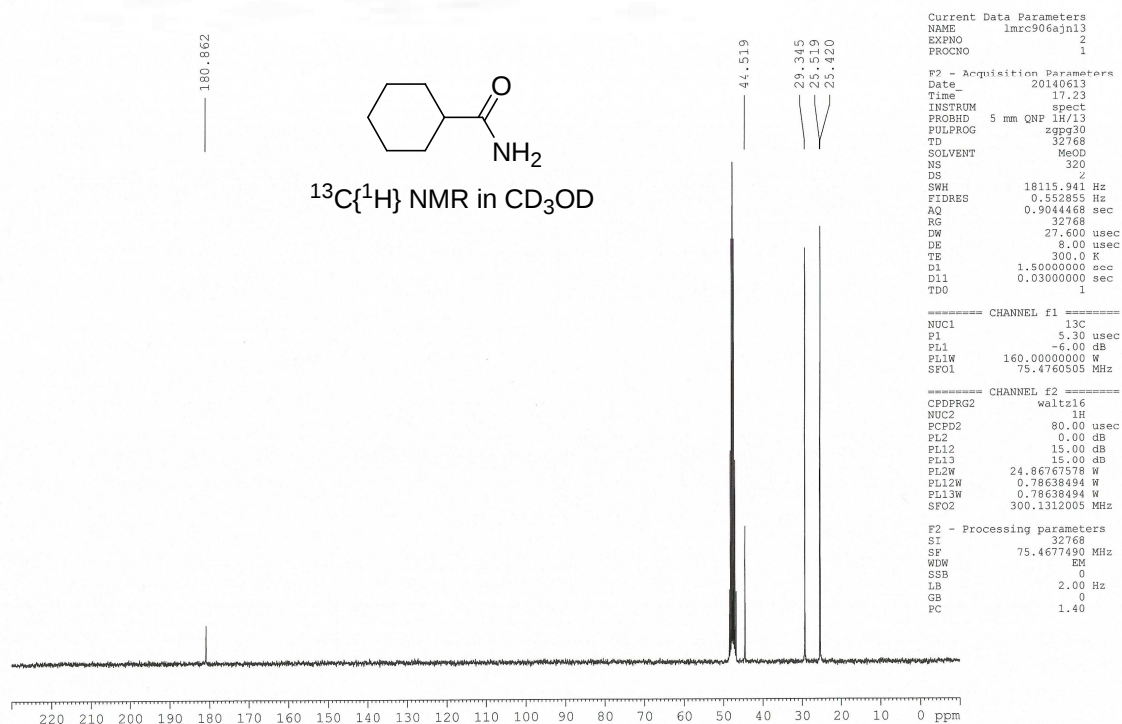
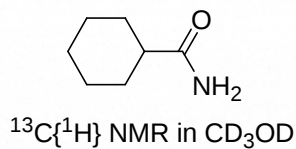
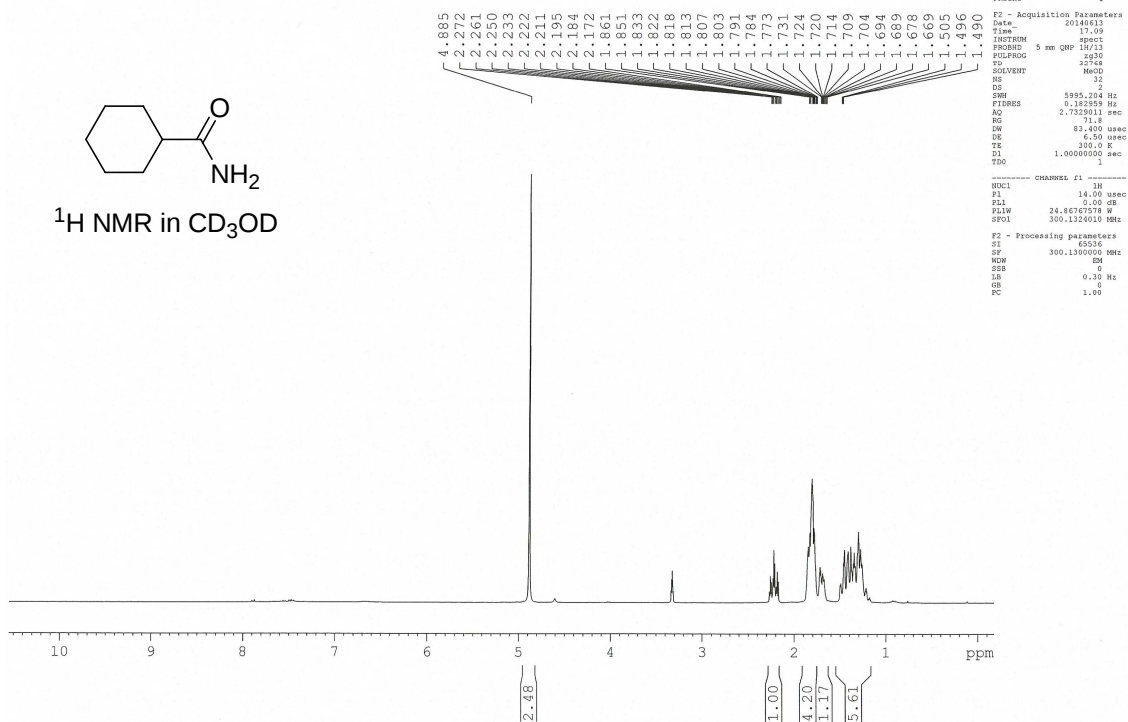
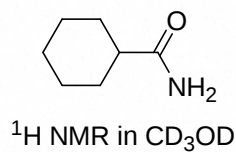
Parámetro	Valor
1 Data File Name	C:/Users/Eder/Desktop/Química Oviedo/ RMN/ Edcat/ Edcat539d/ 1/ fid
2 Title	Edcat539d
3 Comment	facturar a vcm hLvsopd D2O (C-1; Bruker/ bacs) Bruker 49
4 Origin	Bruker BioSpin GmbH
5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	D2O
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Number of Scans	8
13 Receiver Gain	102
14 Relaxation Delay	1.0000
15 Pulse Width	14.0000
16 Acquisition Time	2.7320
17 Acquisition Date	2013-12-18T18:56:01
18 Modification Date	2013-12-18T18:56:00
19 Spectrometer Frequency	300.13
20 Spectral Width	9995.2
21 Lowest Frequency	-1196.8
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	32768

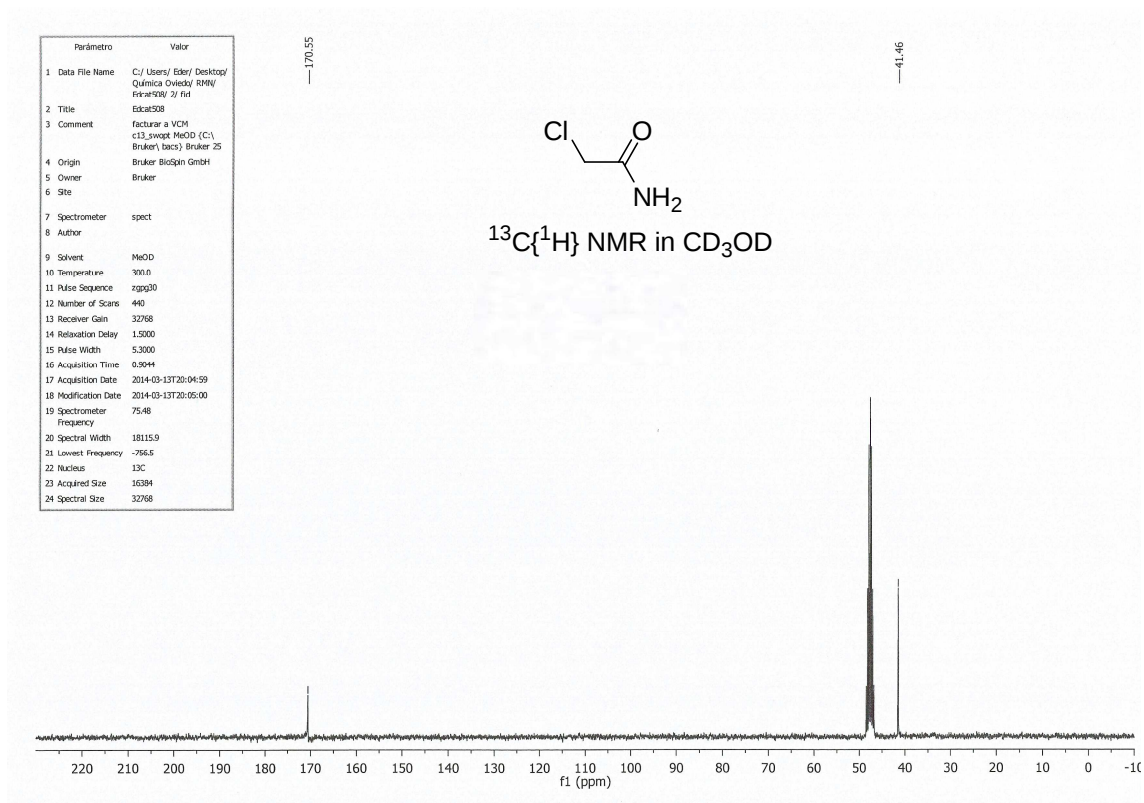
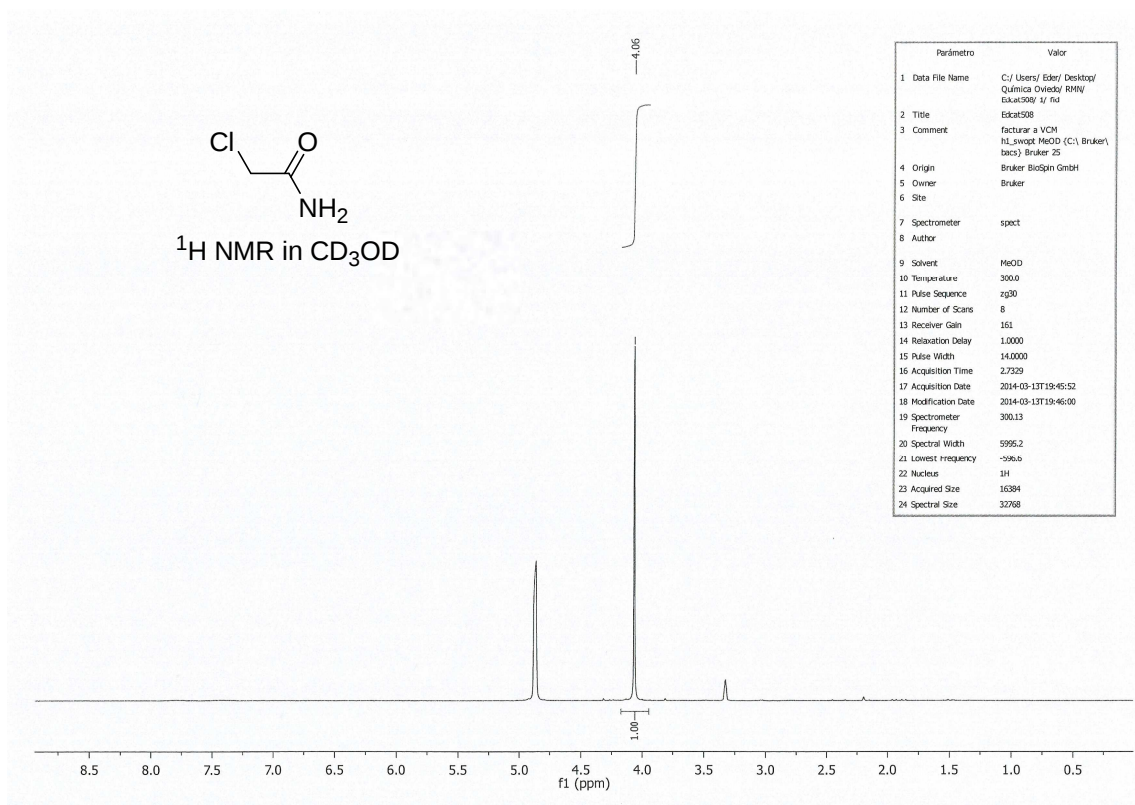


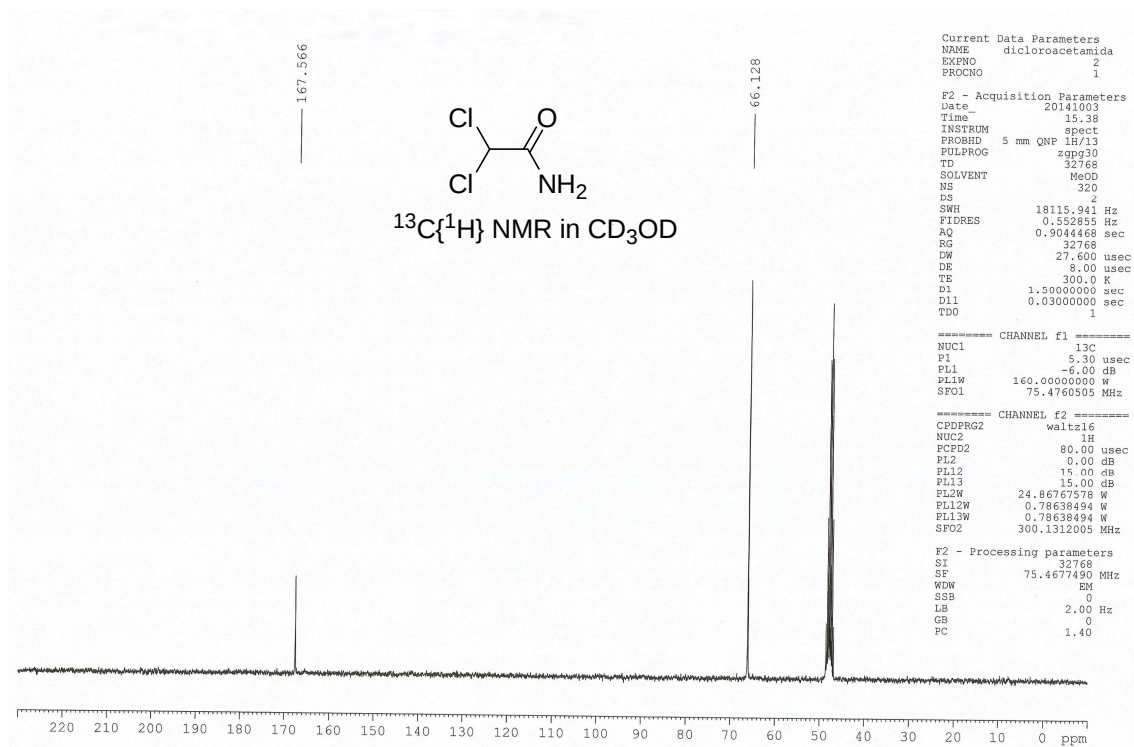
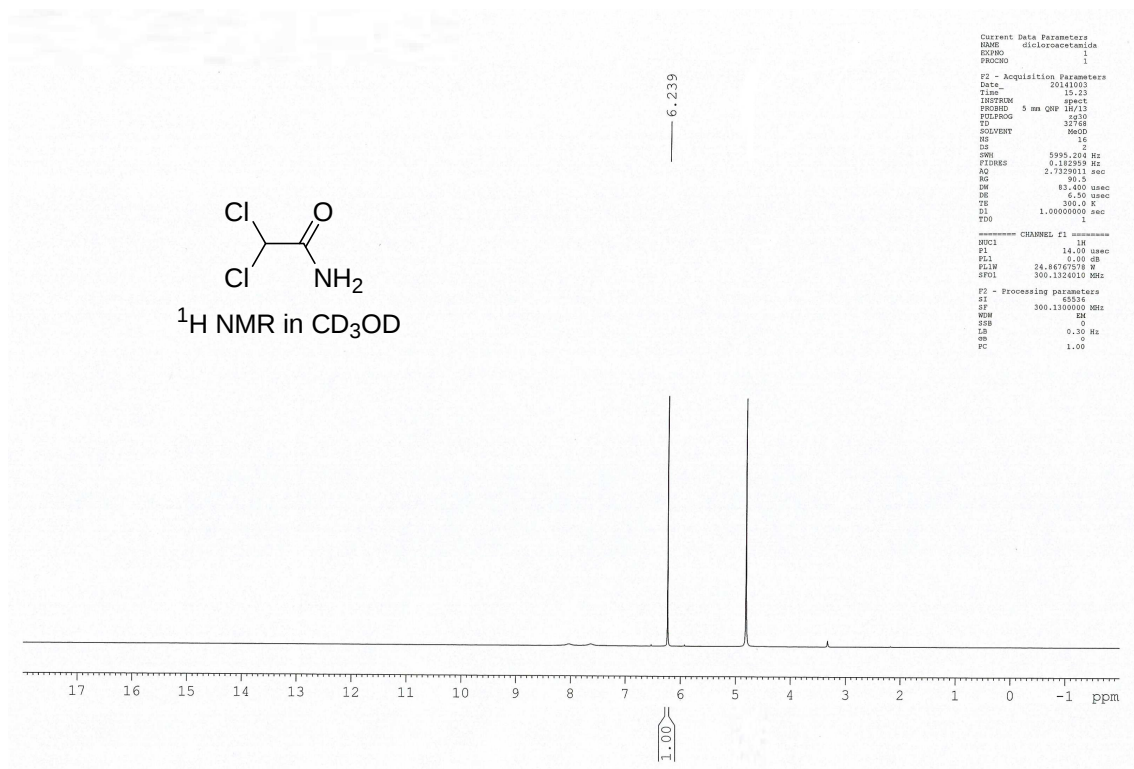
Parámetro	Valor
1 Data File Name	C:/Users/Eder/Desktop/Química Oviedo/ RMN/ Edcat/ Edcat539d/ 2/ fid
2 Title	Edcat539d
3 Comment	facturar a vcm c13_swpd D2O (C-1; Bruker/ bacs) Bruker 49
4 Origin	Bruker BioSpin GmbH
5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	D2O
10 Temperature	300.0
11 Pulse Sequence	zgpg30
12 Number of Scans	440
13 Receiver Gain	32768
14 Relaxation Delay	1.5000
15 Pulse Width	5.3000
16 Acquisition Time	0.9094
17 Acquisition Date	2013-12-18T19:15:15
18 Modification Date	2013-12-18T19:15:00
19 Spectrometer Frequency	75.46
20 Spectral Width	18115.9
21 Lowest Frequency	756.5
22 Nucleus	13C
23 Acquired Size	16384
24 Spectral Size	32768

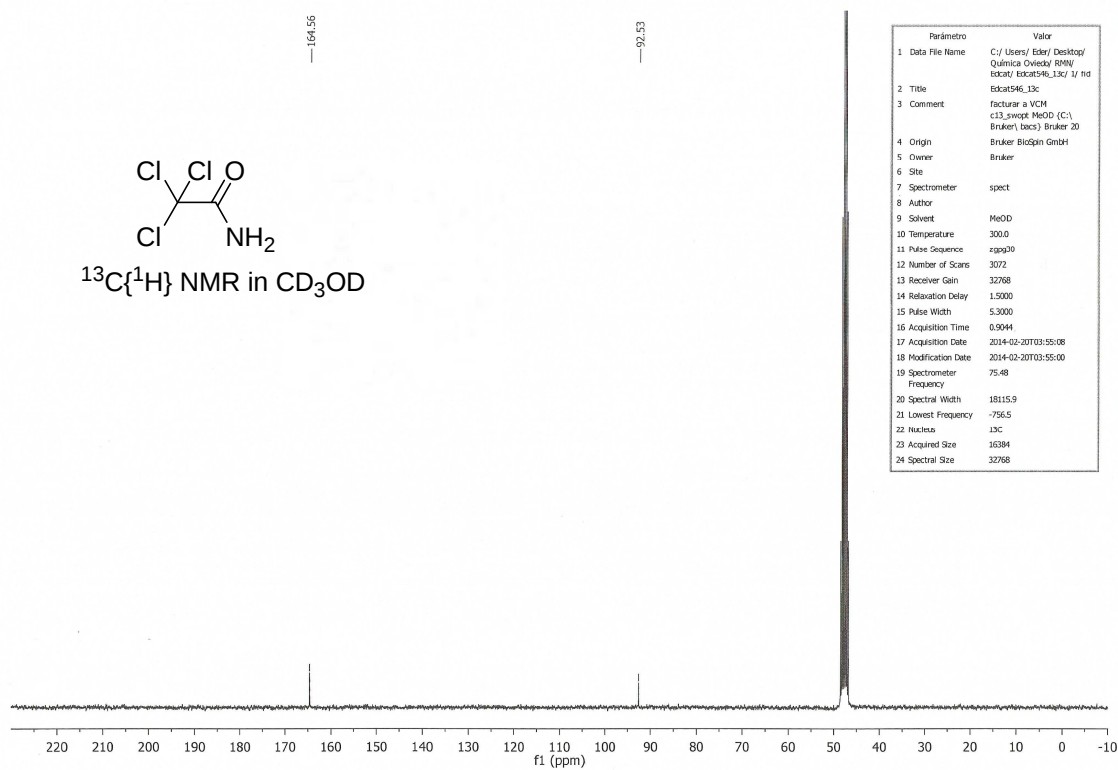
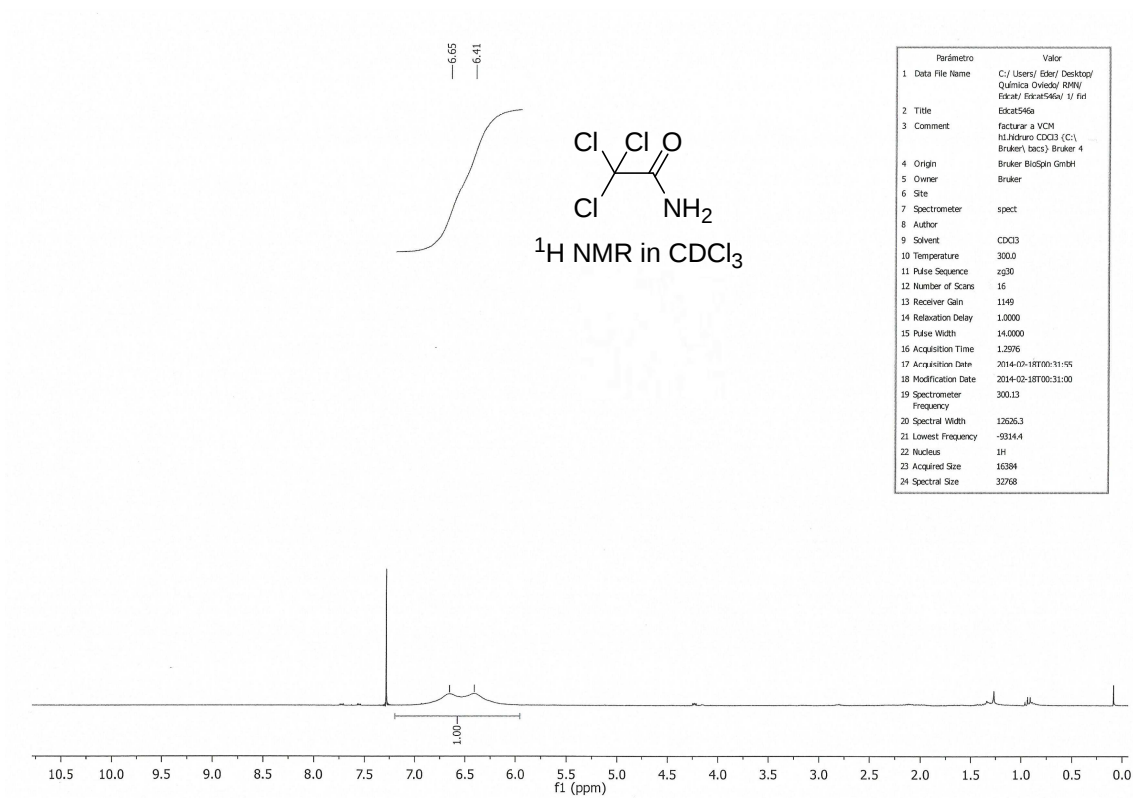


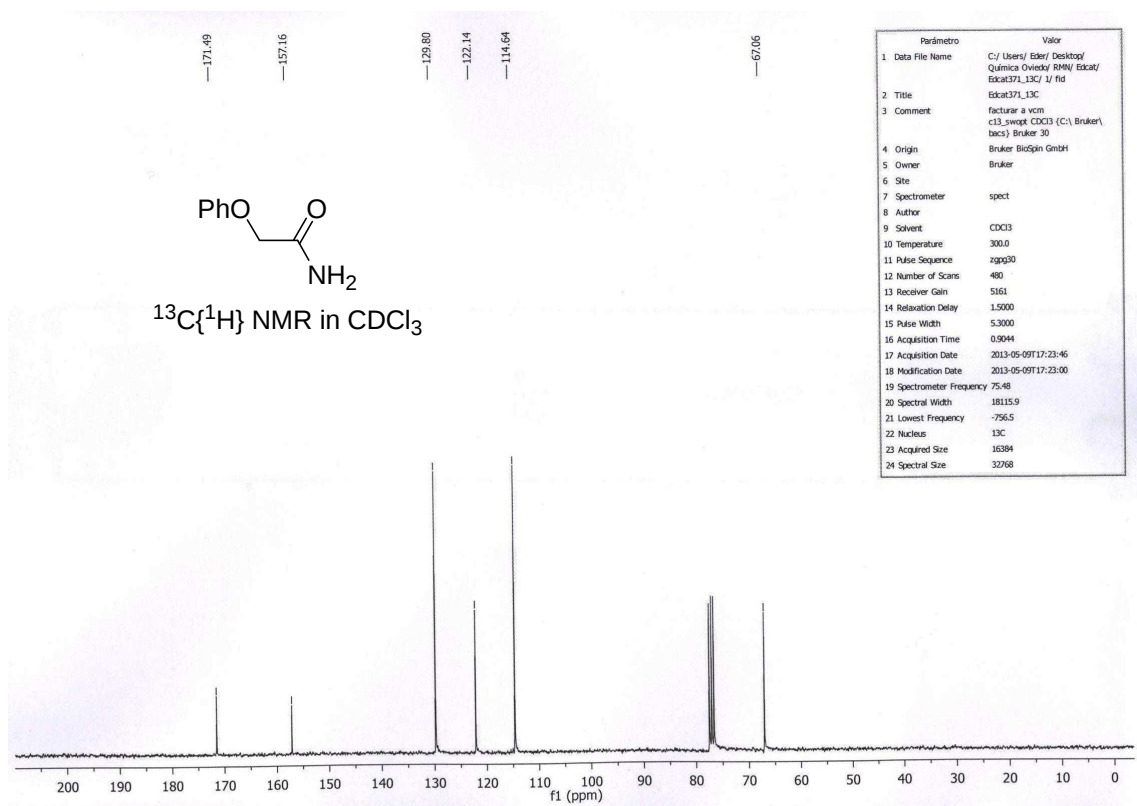
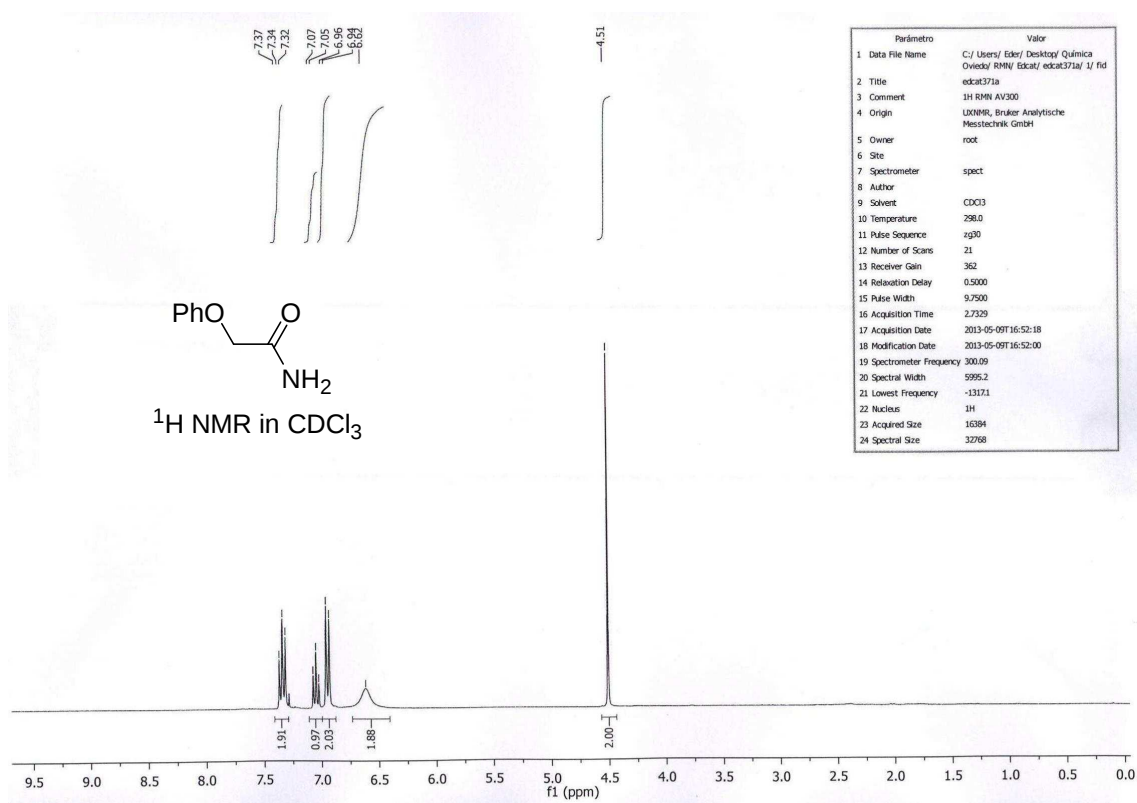


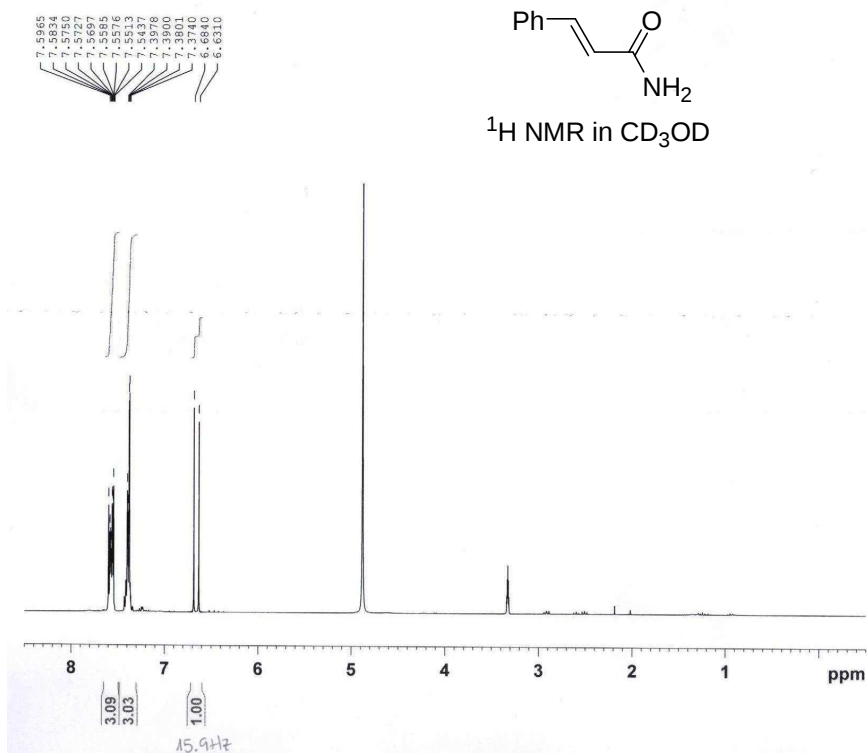












Current Data Parameters

NAME aeda541
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

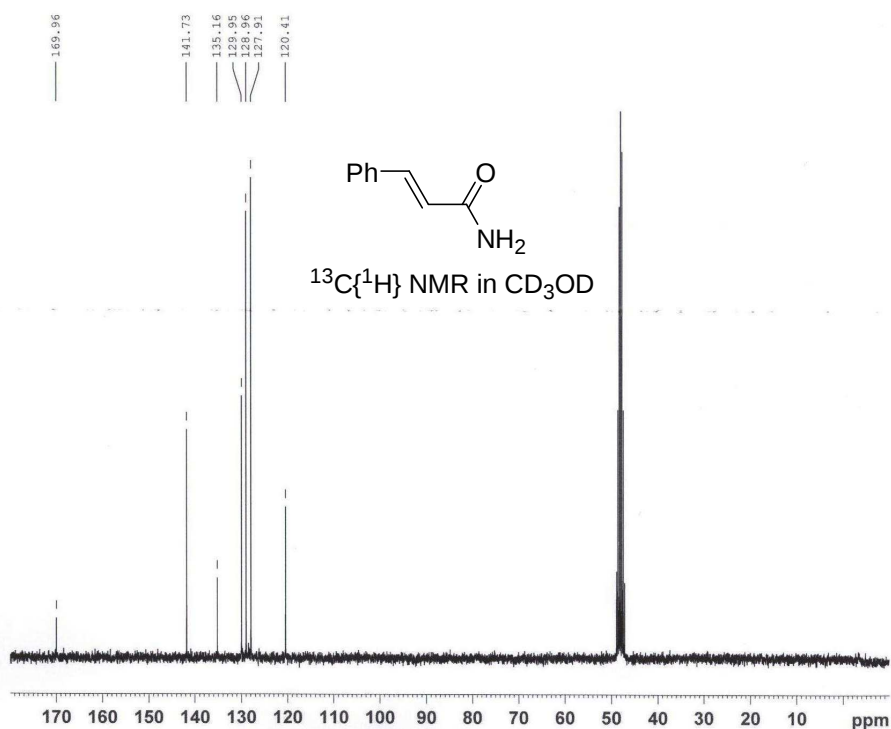
Date 20121019
Time 14.38
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 24576
SOLVENT
NS 56
DS 0
SWH 7183.908 Hz
FIDRES 0.292314 Hz
AQ 1.7106092 sec
RG 143.7
DW 69.600 usec
DE 7.00 usec
TE 298.2 K
D1 0.5000000 sec
TD0 1

===== CHANNEL f1 =====

NUC1 1H
P1 6.30 usec
PL1 -6.00 dB
SFO1 300.1315007 MHz

F2 - Processing parameters

SI 32768
SF 300.1300000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



Current Data Parameters

NAME aeda541
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date 20121019
Time 14.44
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT
NS 160
DS 4
SWH 20491.803 Hz
FIDRES 0.625360 Hz
AQ 0.7996136 sec
RG 11585.2
DW 24.400 usec
DE 20.00 usec
TE 298.2 K
D1 0.5000000 sec
d11 0.03000000 sec
DELTA 0.40000001 sec
TD0 1

===== CHANNEL f1 =====

NUC1 13C
P1 7.00 usec
PL1 -4.00 dB
SFO1 75.4771525 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 21.00 dB
PL13 120.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters

SI 32768
SF 75.4677190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40