

Electronic Supporting Information

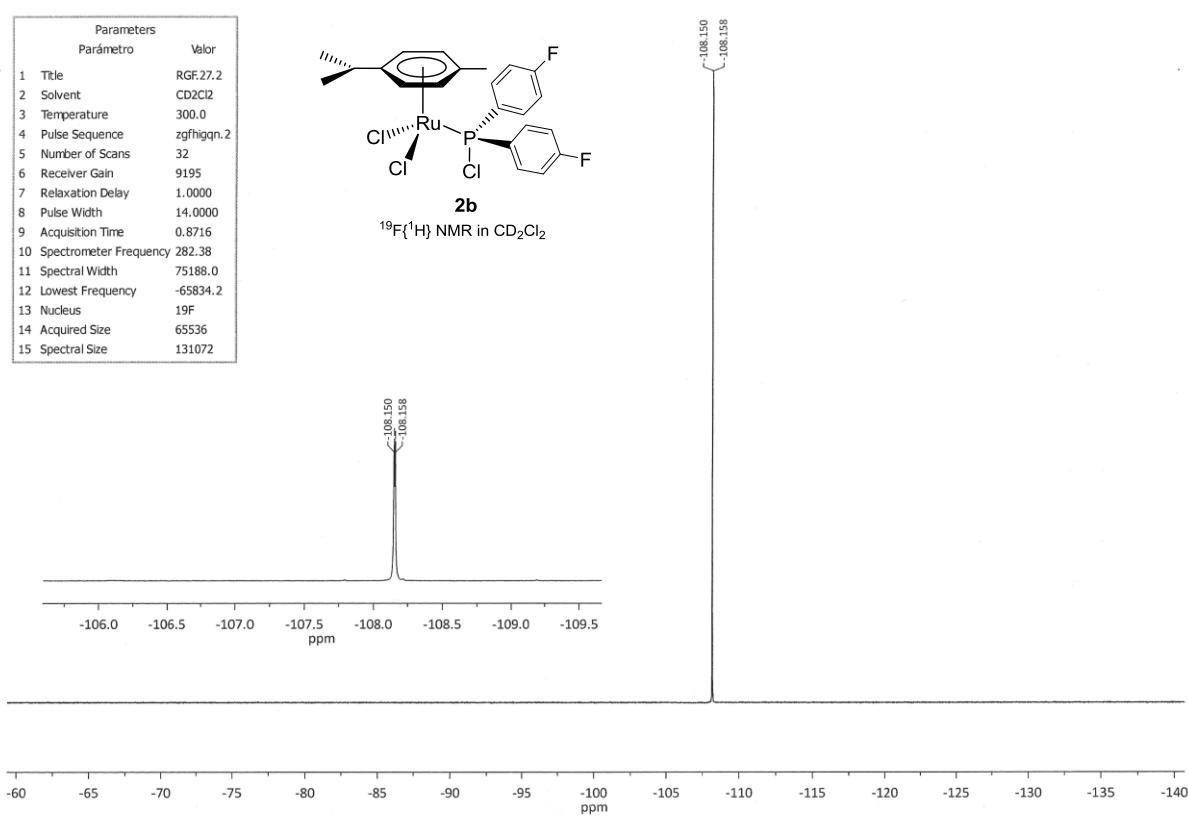
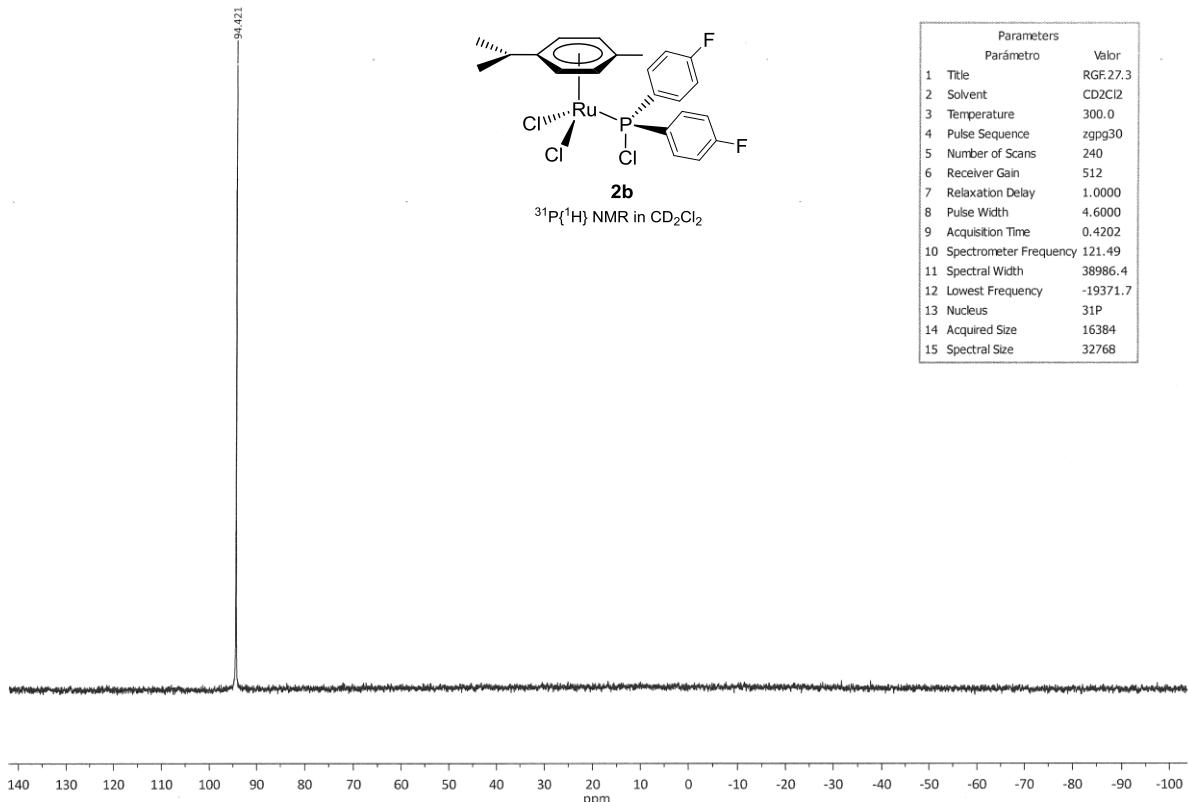
Chlorophosphines as auxiliary ligands in ruthenium-catalyzed nitrile hydration reactions: Application to the preparation of β -ketoamides

Rebeca González-Fernández,^a Pedro J. González-Liste,^a Javier Borge,^b Pascale Crochet^{*a} and Victorio Cadierno^{*a}

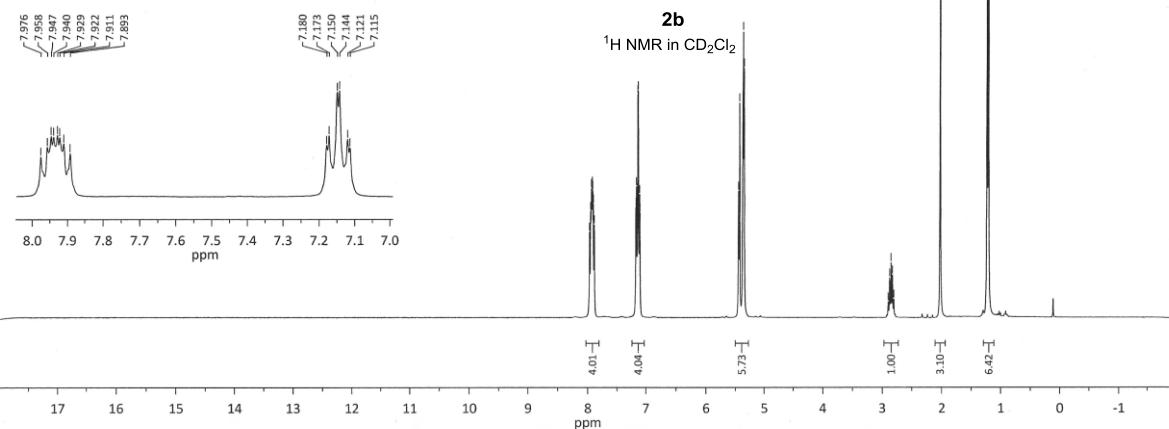
^a Laboratorio de Compuestos Organometálicos y Catálisis (Unidad Asociada al CSIC), Centro de Innovación en Química Avanzada (ORFEO-CINQA), Departamento de Química Orgánica e Inorgánica, IUQOEM, Universidad de Oviedo, Julián Clavería 8, E-33006 Oviedo, Spain. E-mail: crochetpascale@uniovi.es (P.C.), vcm@uniovi.es (V.C.); Fax: +(34) 985103446; Tel.: +(34) 985103453.

^b Departamento de Química Física y Analítica, Centro de Innovación en Química Avanzada (ORFEO-CINQA), Universidad de Oviedo, Julián Clavería 8, E-33006 Oviedo, Spain.

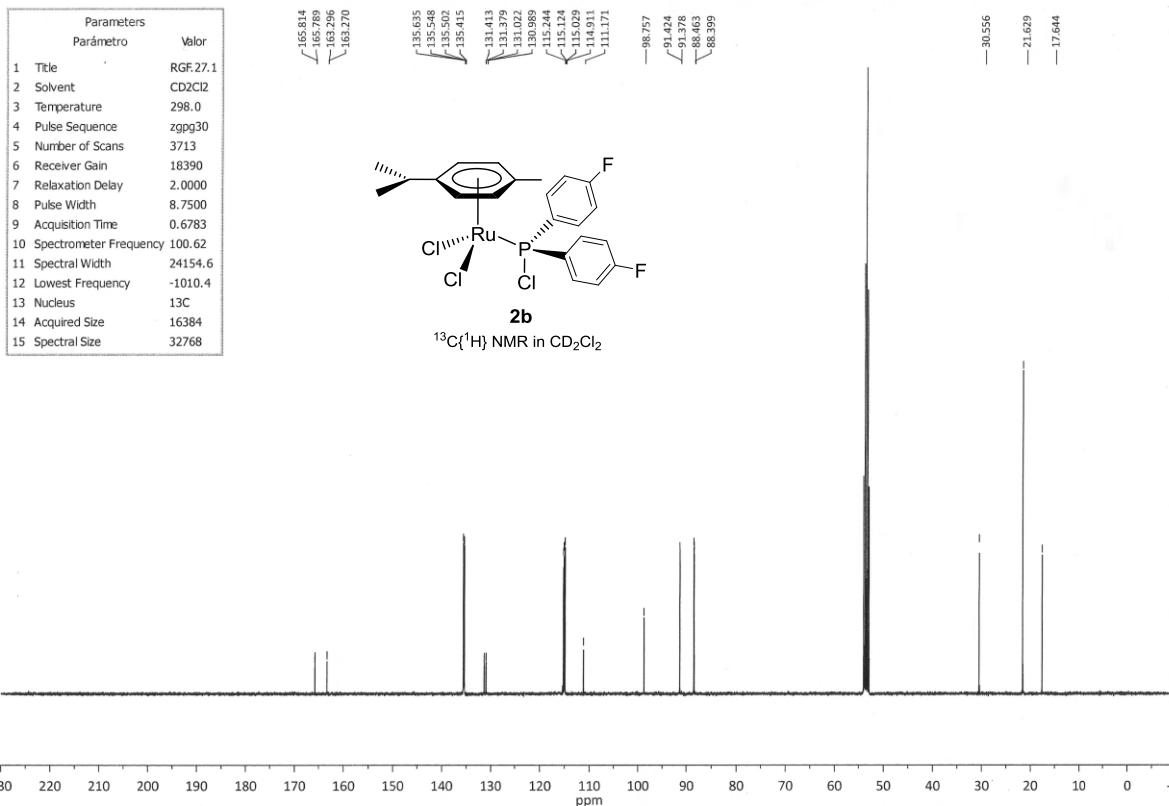
Copies of the NMR spectra of complexes 2b, 3 and 4b, and all the amides generated in this work



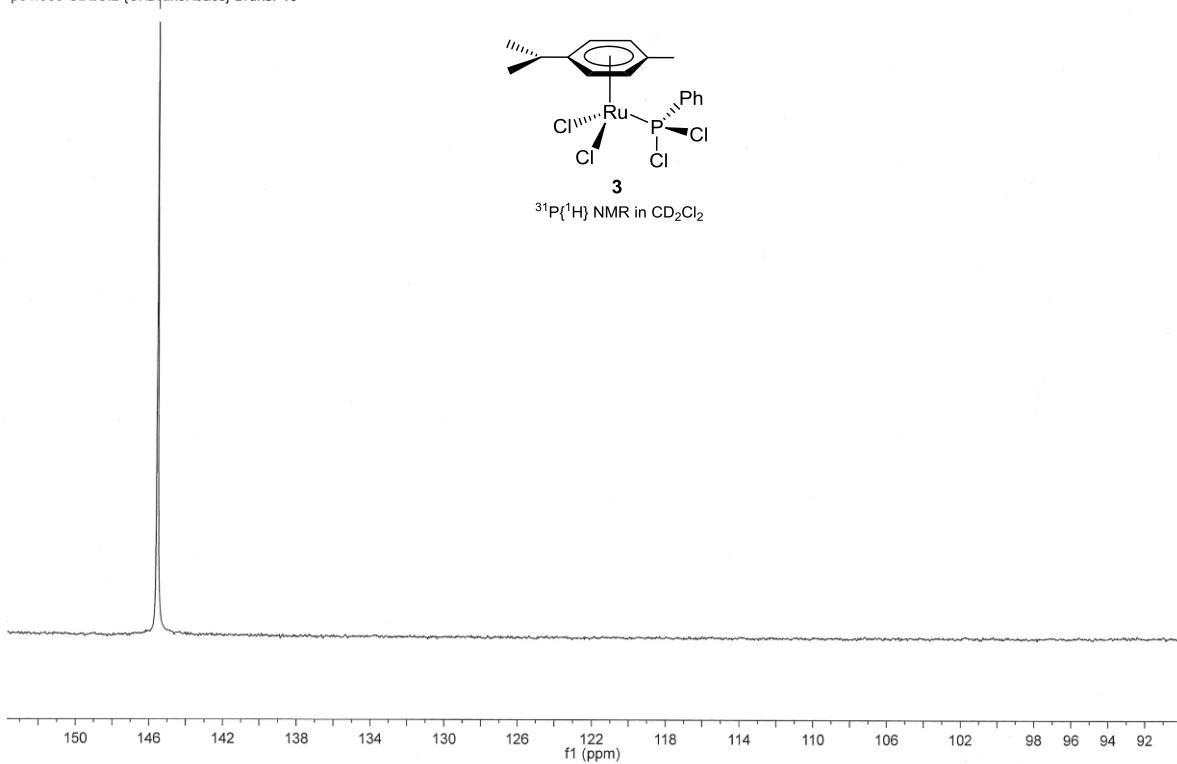
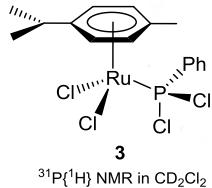
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8 Pulse Width	14.0000
9 Acquisition Time	2.7329
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11 Spectral Width	5995.2
12 Lowest Frequency	-596.6
13 Nucleus	1H
14 Acquired Size	16384
15 Spectral Size	32768



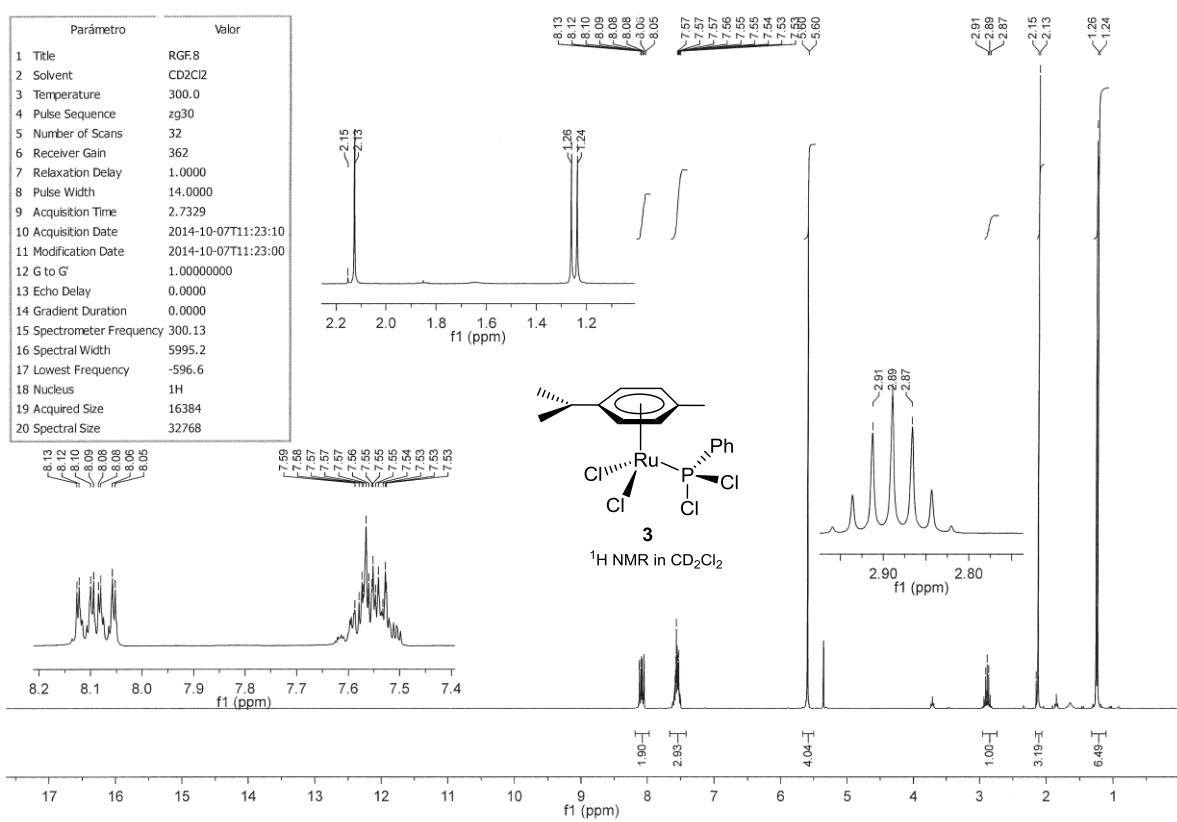
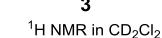
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6 Receiver Gain	18390
7 Relaxation Delay	2.0000
8 Pulse Width	8.7500
9 Acquisition Time	0.6783
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12 Lowest Frequency	-1010.4
13 Nucleus	13C
14 Acquired Size	16384
15 Spectral Size	32768



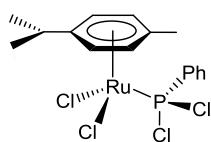
RGF.8
facturar a VCM
p31.300 CD2Cl2 {C:\Bruker\bacs} Bruker 19
145.57



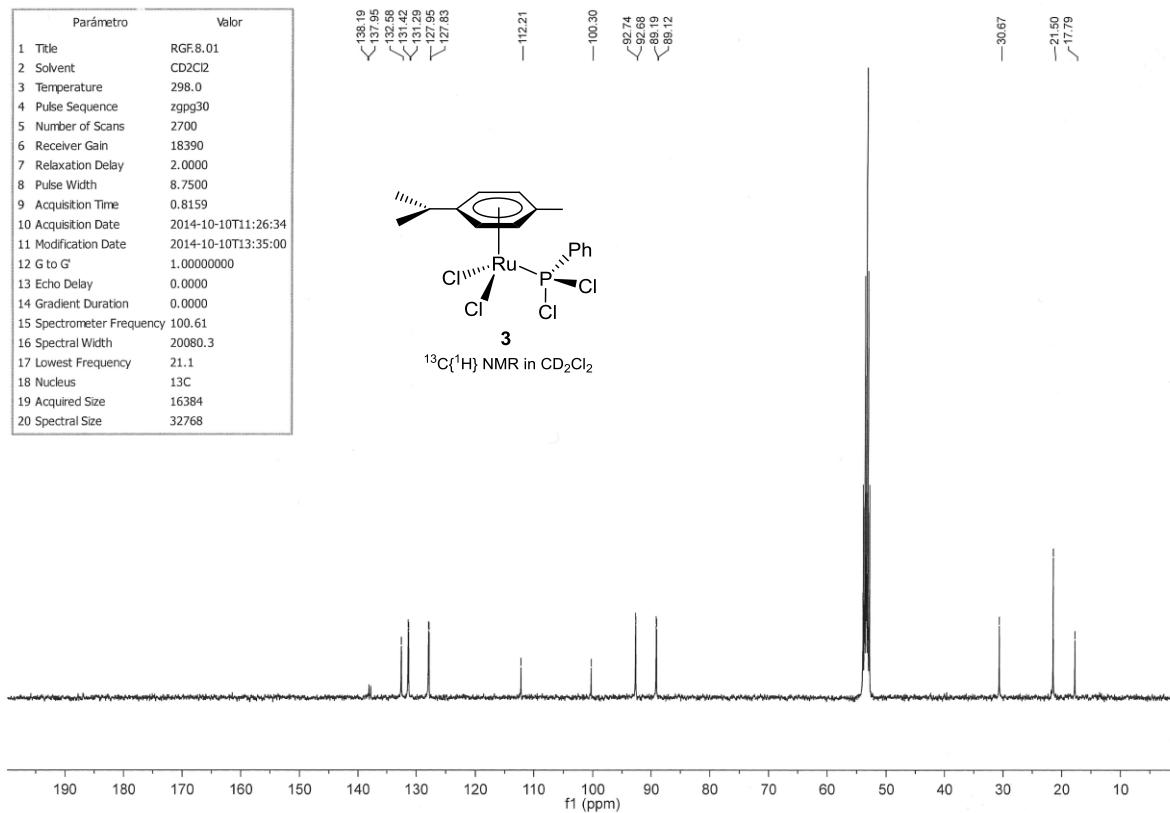
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16 Spectral Width	5995.2
17 Lowest Frequency	-596.6
18 Nucleus	1H
19 Acquired Size	16384
20 Spectral Size	32768



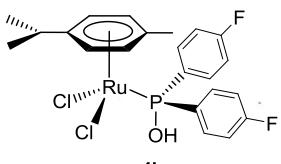
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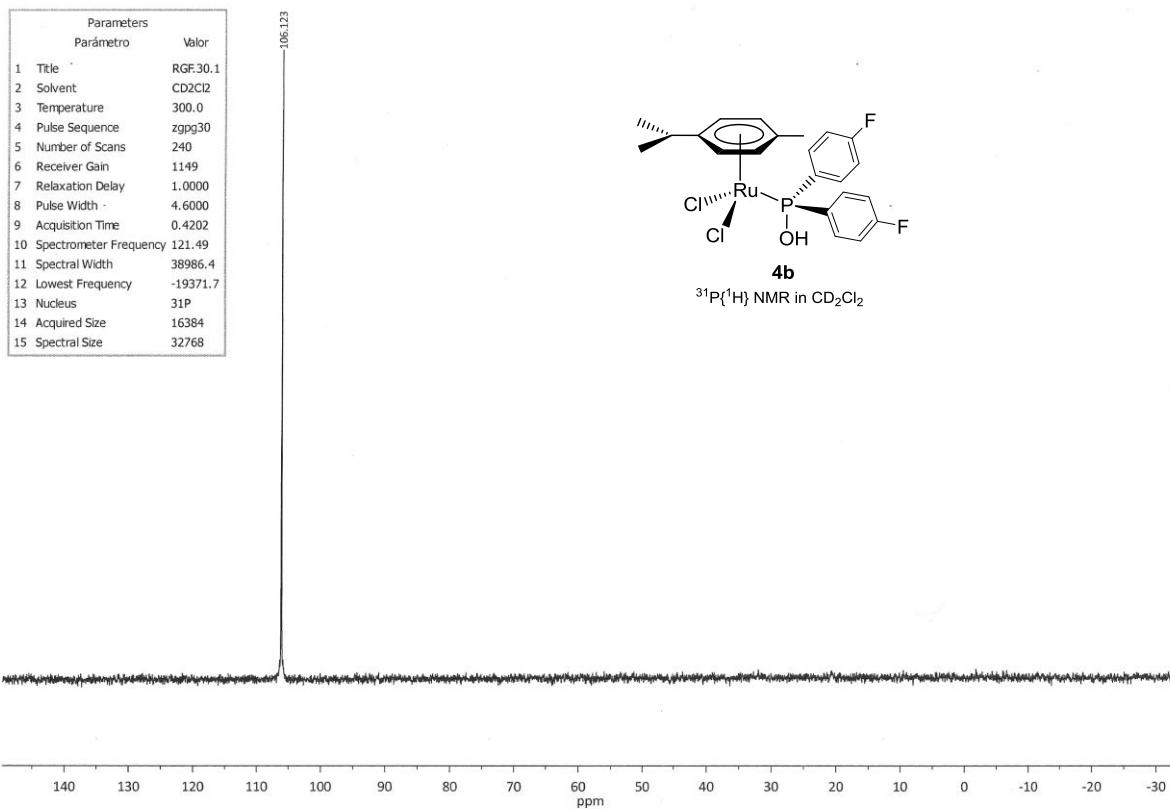
¹³C/{¹H} NMR in CD₂Cl₂



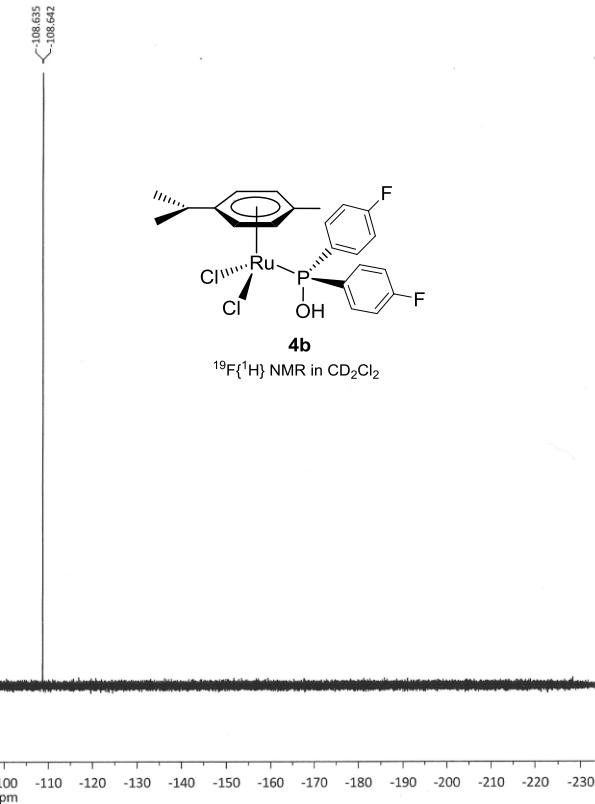
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1 Title	RGF.30.1
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3 Temperature	300.0
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6 Receiver Gain	1149
7 Relaxation Delay	1.0000
8 Pulse Width	4.6000
9 Acquisition Time	0.4202
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11 Spectral Width	38986.4
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13 Nucleus	31P
14 Acquired Size	16384
15 Spectral Size	32768



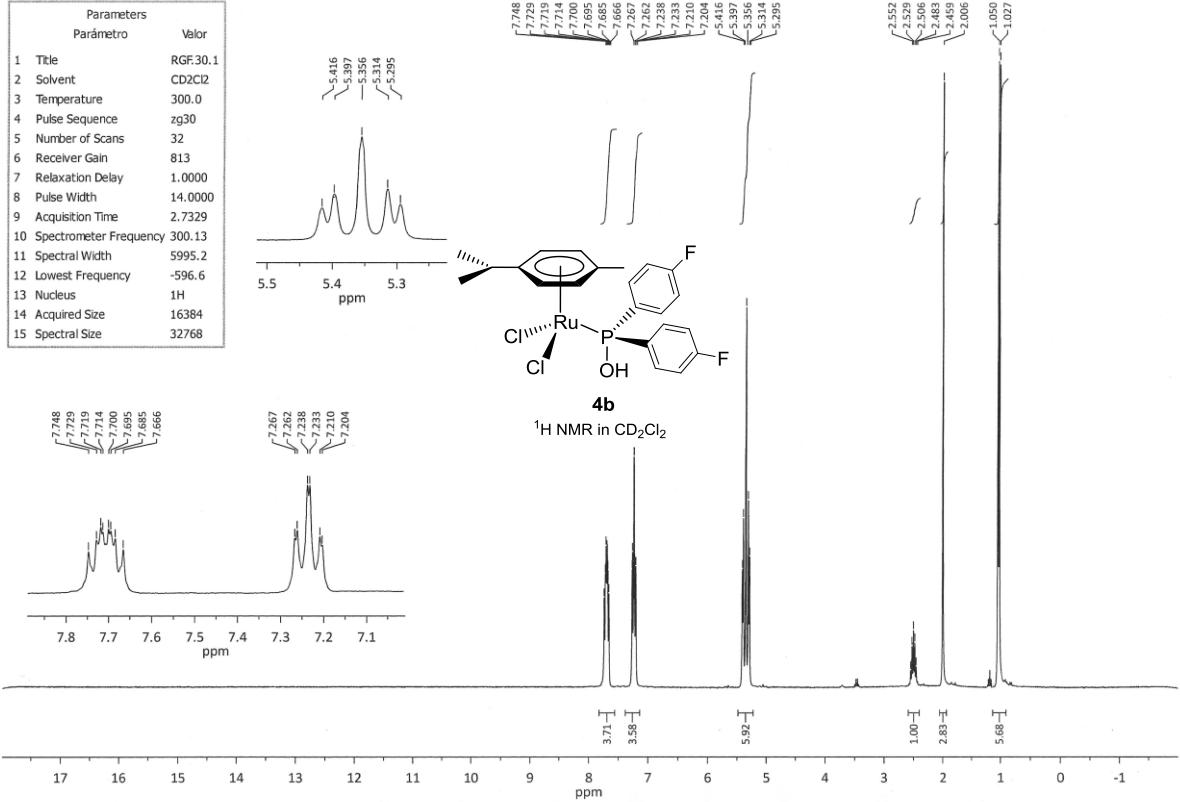
³¹P{¹H} NMR in CD₂Cl₂



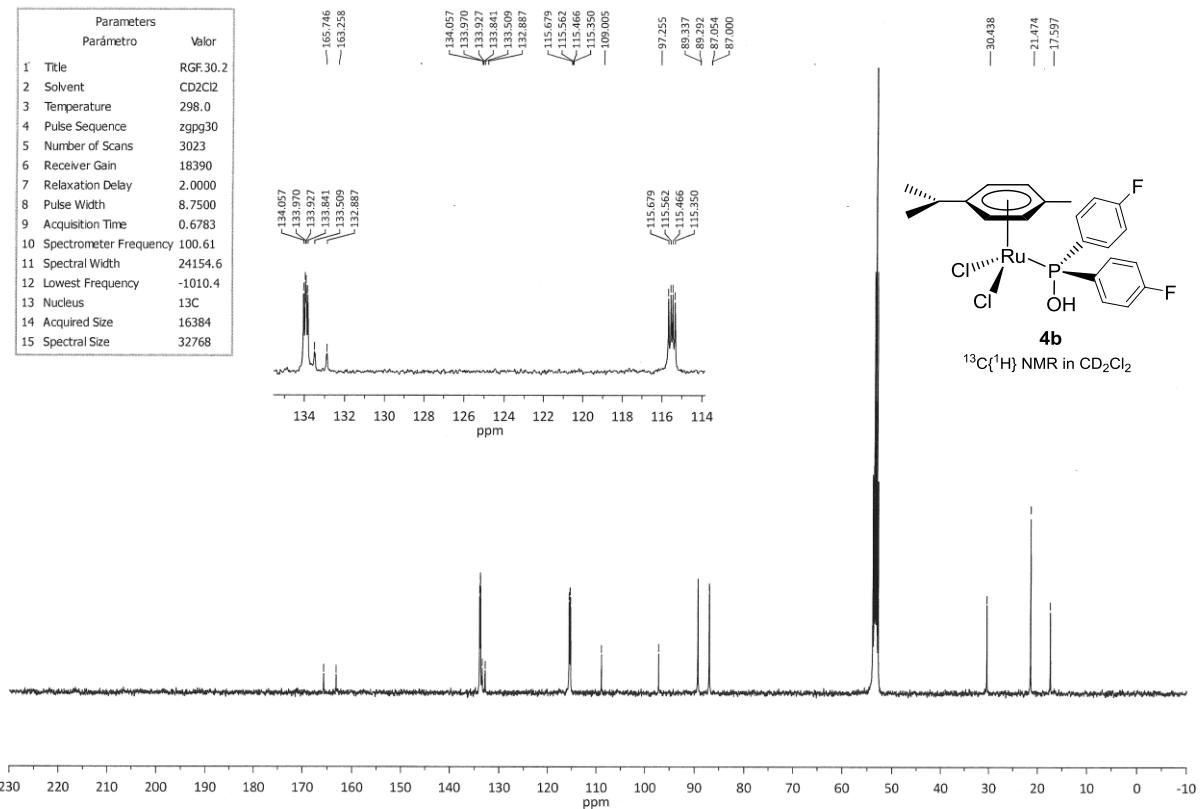
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5 Number of Scans		32
6 Receiver Gain		7298
7 Relaxation Delay		1.0000
8 Pulse Width		14.0000
9 Acquisition Time		0.8716
10 Spectrometer Frequency		282.38
11 Spectral Width		75188.0
12 Lowest Frequency		-65834.2
13 Nucleus		¹⁹ F
14 Acquired Size		65536
15 Spectral Size		131072



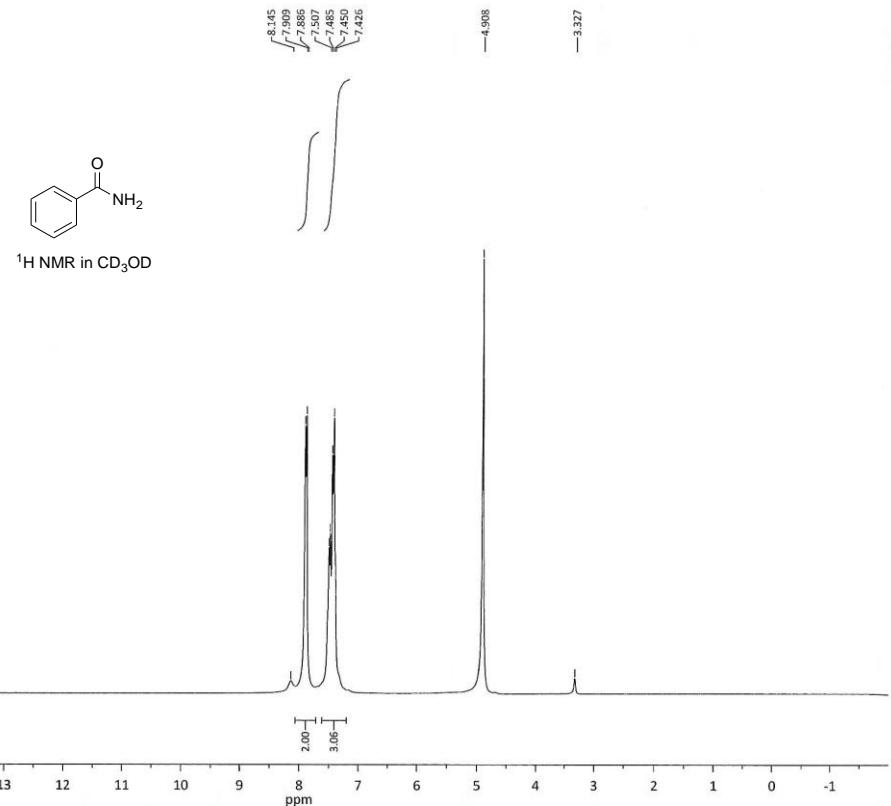
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1 Title		RGF.30.1
2 Solvent		CD ₂ Cl ₂
3 Temperature		300.0
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6 Receiver Gain		813
7 Relaxation Delay		1.0000
8 Pulse Width		14.0000
9 Acquisition Time		2.7329
10 Spectrometer Frequency		300.13
11 Spectral Width		5995.2
12 Lowest Frequency		-596.6
13 Nucleus		¹ H
14 Acquired Size		16384
15 Spectral Size		32768



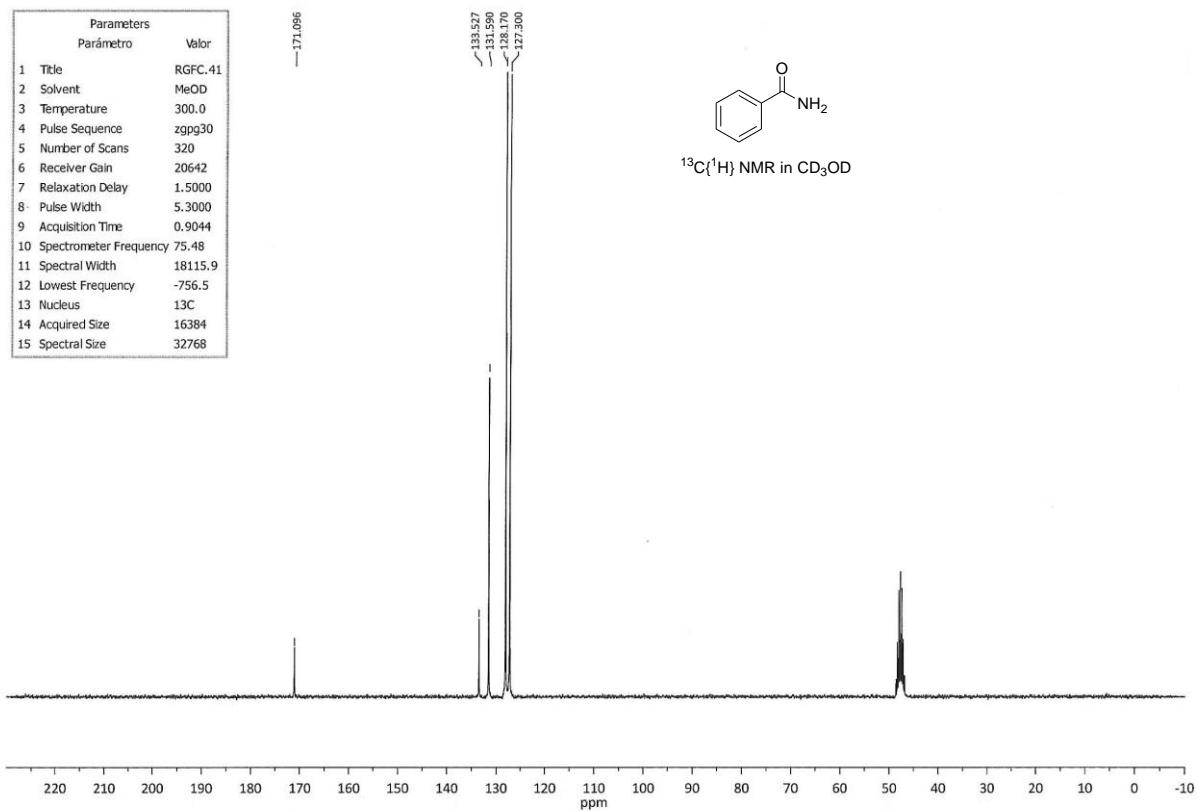
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	Parámetro
	Valor
1	Title
2	Solvent
3	Temperature
4	Pulse Sequence
5	Number of Scans
6	Receiver Gain
7	Relaxation Delay
8	Pulse Width
9	Acquisition Time
10	Spectrometer Frequency
11	Spectral Width
12	Lowest Frequency
13	Nucleus
14	Acquired Size
15	Spectral Size



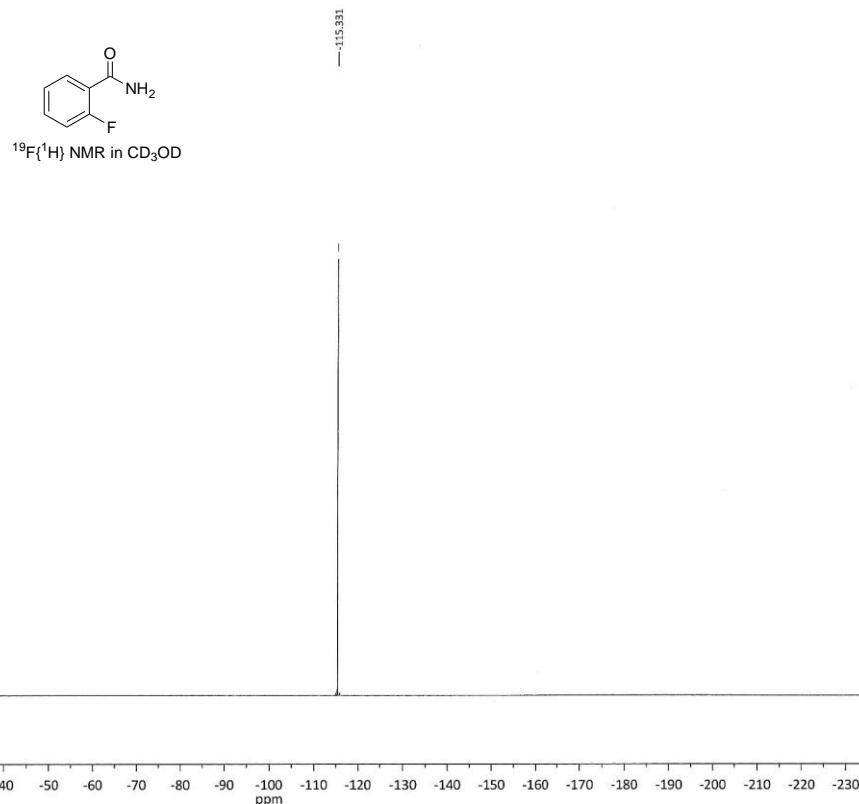
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2 Solvent	MeOD	
3 Temperature	300.0	
4 Pulse Sequence	zg30	
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7 Relaxation Delay	1.0000	
8 Pulse Width	14.0000	
9 Acquisition Time	2.7329	
10 Spectrometer Frequency	300.13	
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12 Lowest Frequency	-596.6	
13 Nucleus	1H	
14 Acquired Size	16384	
15 Spectral Size	32768	



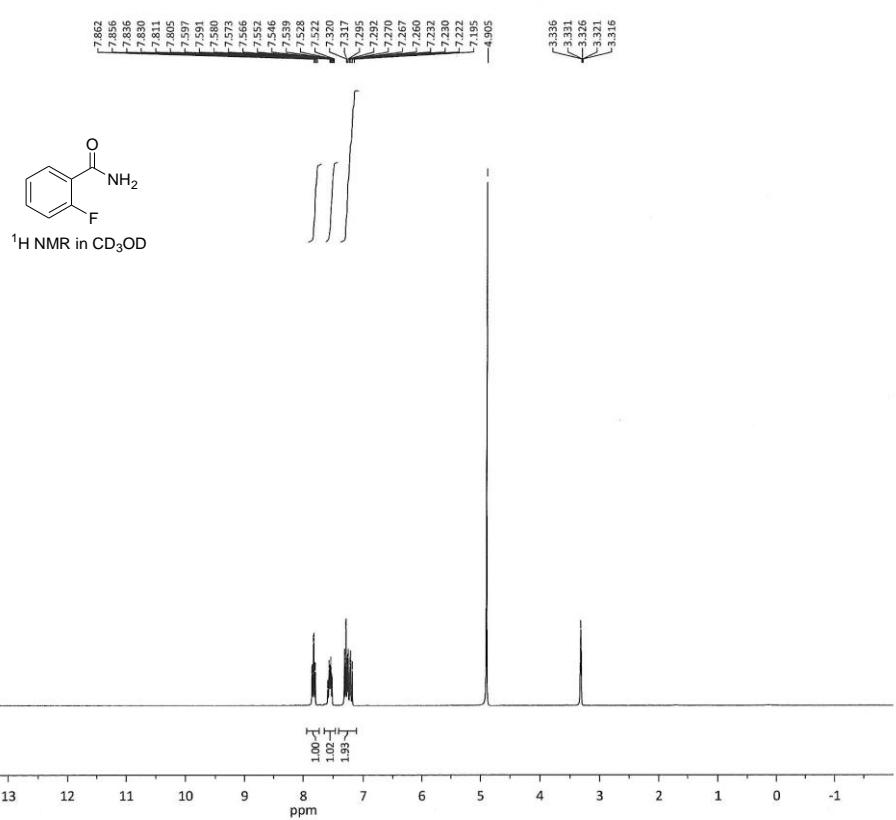
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6 Receiver Gain	20642	
7 Relaxation Delay	1.5000	
8 Pulse Width	5.3000	
9 Acquisition Time	0.9044	
10 Spectrometer Frequency	75.48	
11 Spectral Width	18115.9	
12 Lowest Frequency	-756.5	
13 Nucleus	13C	
14 Acquired Size	16384	
15 Spectral Size	32768	



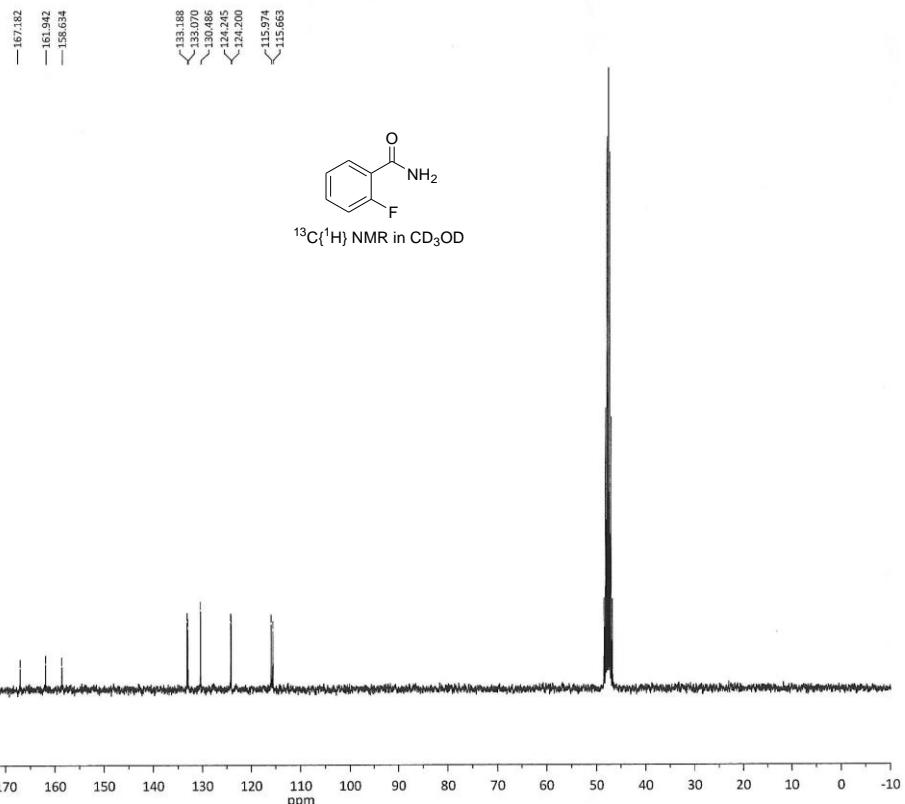
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1 Title	RGFC.47
2 Solvent	MeOD
3 Temperatura	300.0
4 Pulse Sequence	zgfhigg.n.2
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6 Receiver Gain	9195
7 Relaxation Delay	1.0000
8 Pulse Width	14.0000
9 Acquisition Time	0.8716
10 Spectrometer Frequency	282.38
11 Spectral Width	75188.0
12 Lowest Frequency	-65834.2
13 Nucleus	¹⁹ F
14 Acquired Size	65536
15 Spectral Size	131072



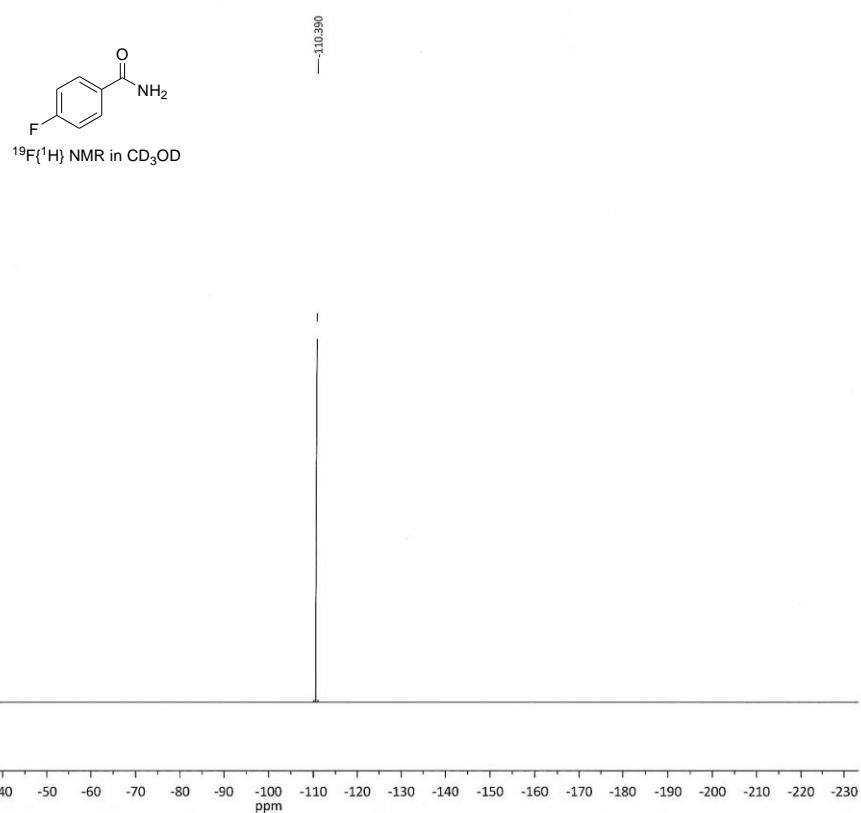
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2 Solvent	MeOD
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4 Pulse Sequence	zg30
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7 Relaxation Delay	1.0000
8 Pulse Width	14.0000
9 Acquisition Time	2.7329
10 Spectrometer Frequency	300.13
11 Spectral Width	5995.2
12 Lowest Frequency	-596.6
13 Nucleus	¹ H
14 Acquired Size	16384
15 Spectral Size	32768



Parámetro	Valor
1 Title	RGFC.47
2 Solvent	MeOD
3 Temperatura	300.0
4 Pulse Sequence	zpgg30
5 Number of Scans	300
6 Receiver Gain	32768
7 Relaxation Delay	1.5000
8 Pulse Width -	5.3000
9 Acquisition Time	0.9044
10 Spectrometer Frequency	75.48
11 Spectral Width	18115.9
12 Lowest Frequency	-756.5
13 Nucleus	13C
14 Acquired Size	16384
15 Spectral Size	32768



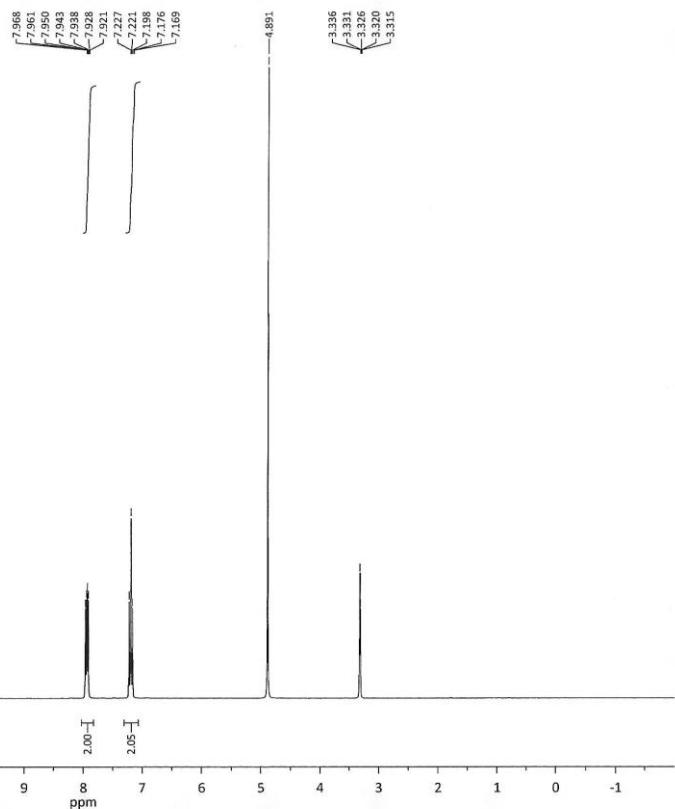
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5 Number of Scans	64
6 Receiver Gain	7298
7 Relaxation Delay	1.0000
8 Pulse Width	14.0000
9 Acquisition Time	0.8716
10 Spectrometer Frequency	282.38
11 Spectral Width	75188.0
12 Lowest Frequency	-65834.2
13 Nucleus	19F
14 Acquired Size	65536
15 Spectral Size	131072



Parameters	
Parámetro	Valor
1 Title	RGFC.44.1
2 Solvent	MeOD
3 Temperature	300.0
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	362
7 Relaxation Delay	1.0000
8 Pulse Width	14.0000
9 Acquisition Time	2.7329
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11 Spectral Width	5995.2
12 Lowest Frequency	-596.6
13 Nucleus	1H
14 Acquired Size	16384
15 Spectral Size	32768



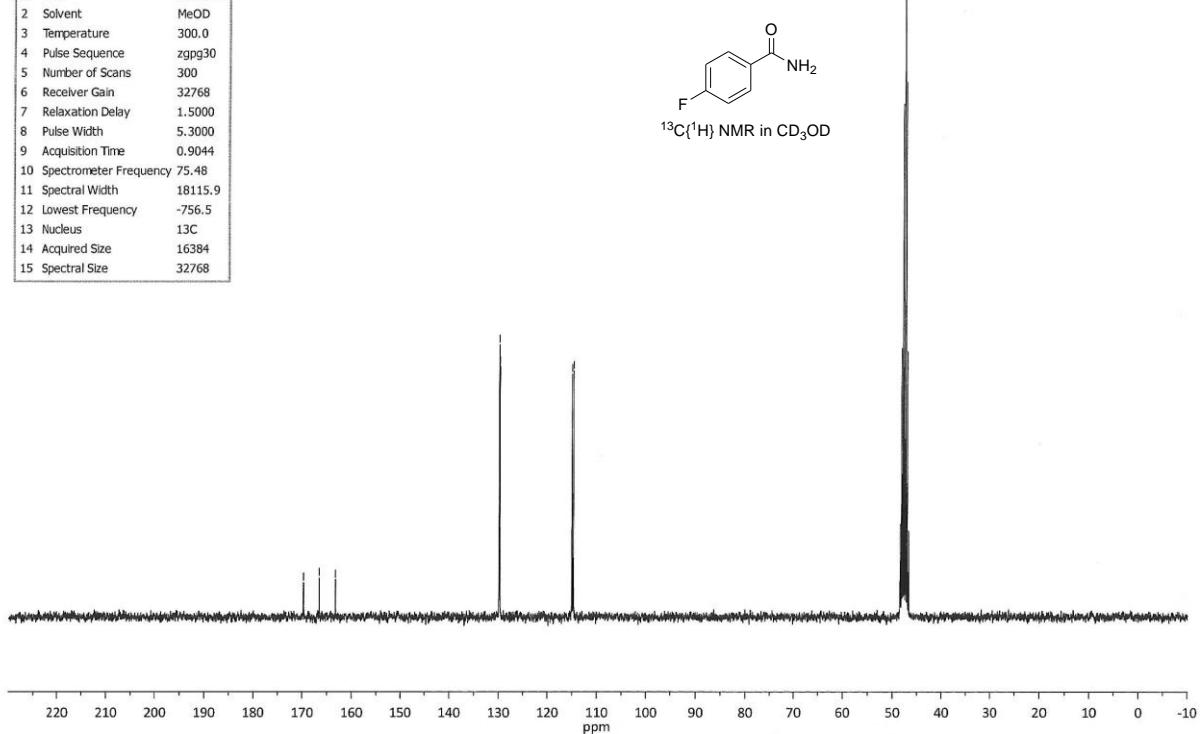
¹H NMR in CD₃OD



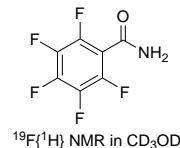
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7 Relaxation Delay	1.5000
8 Pulse Width	5.3000
9 Acquisition Time	0.9044
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13 Nucleus	13C
14 Acquired Size	16384
15 Spectral Size	32768



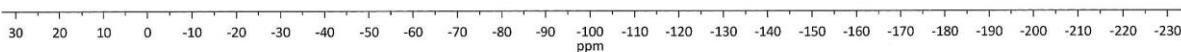
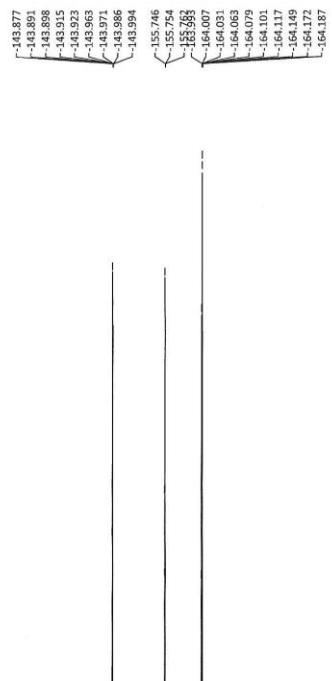
¹³C{¹H} NMR in CD₃OD



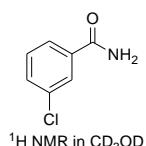
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6 Receiver Gain	4096
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8 Pulse Width	14.0000
9 Acquisition Time	0.8716
10 Spectrometer Frequency	282.38
11 Spectral Width	75188.0
12 Lowest Frequency	-65834.2
13 Nucleus	19F
14 Acquired Size	65536
15 Spectral Size	131072



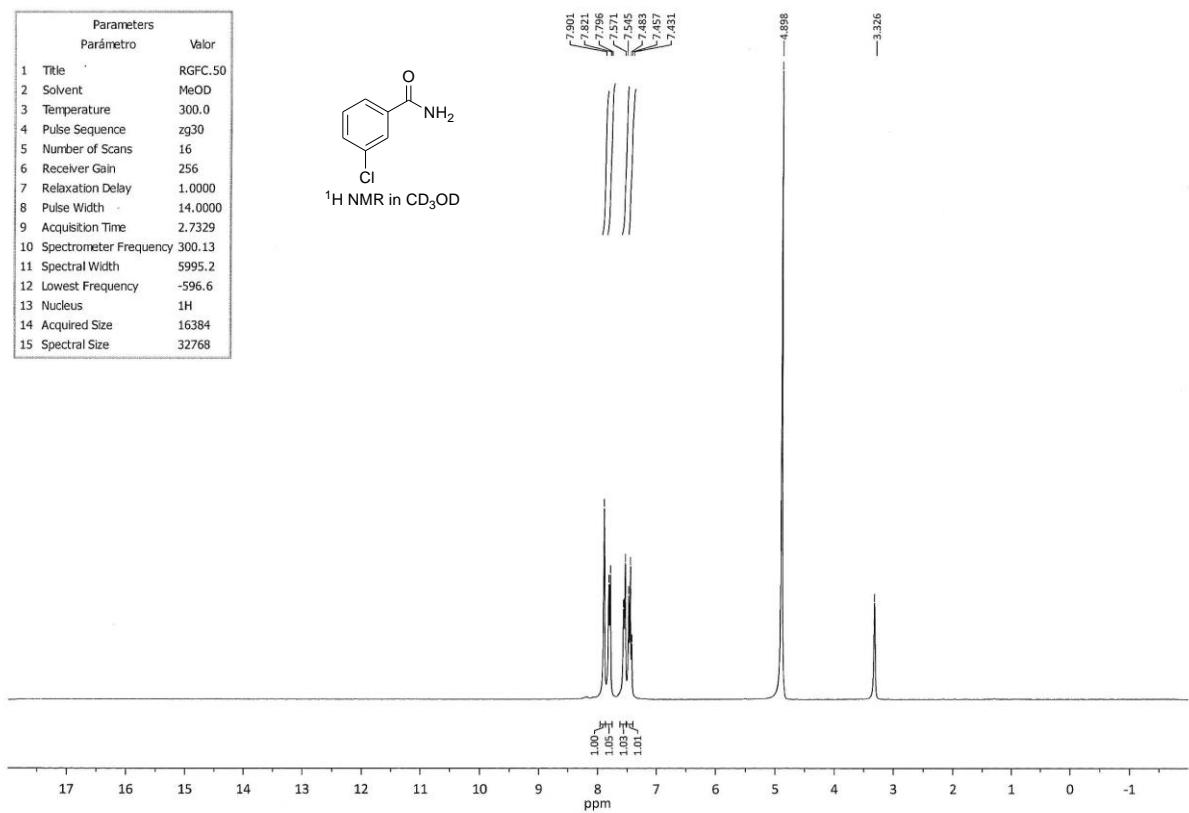
¹⁹F(¹H) NMR in CD₃OD



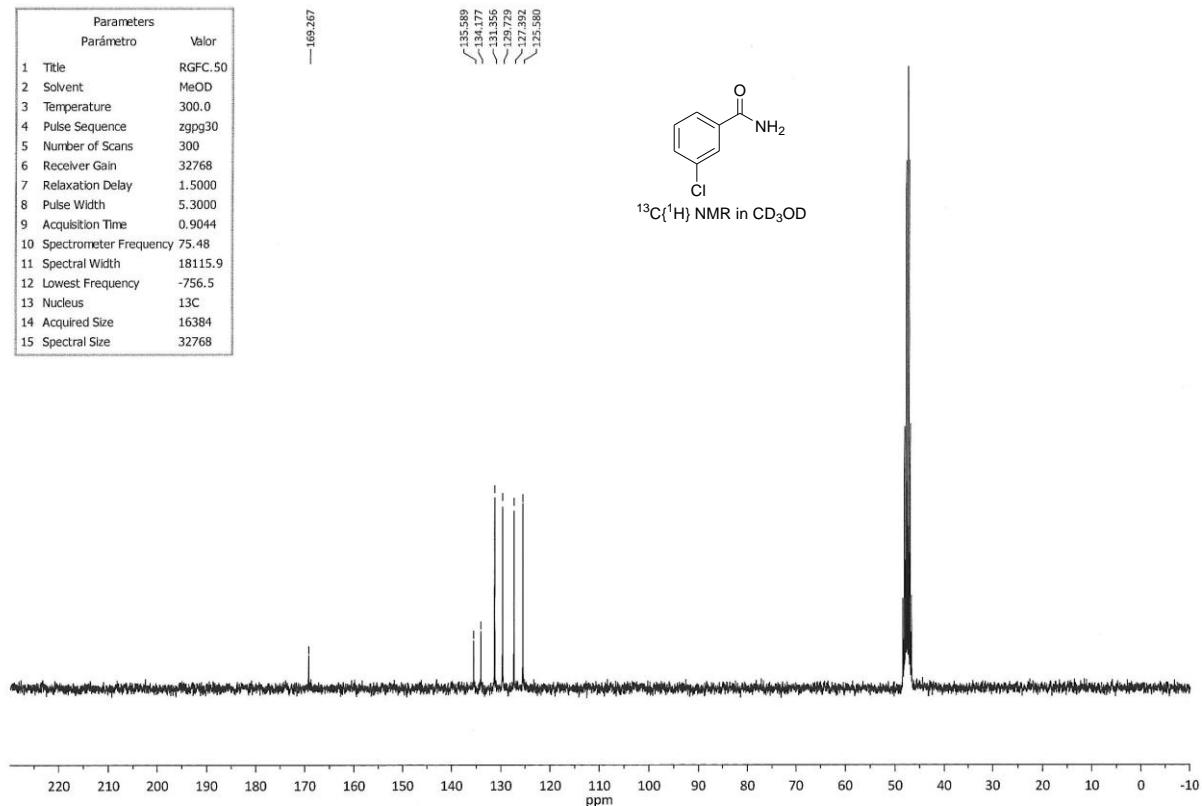
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8 Pulse Width	14.0000
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12 Lowest Frequency	-596.6
13 Nucleus	1H
14 Acquired Size	16384
15 Spectral Size	32768



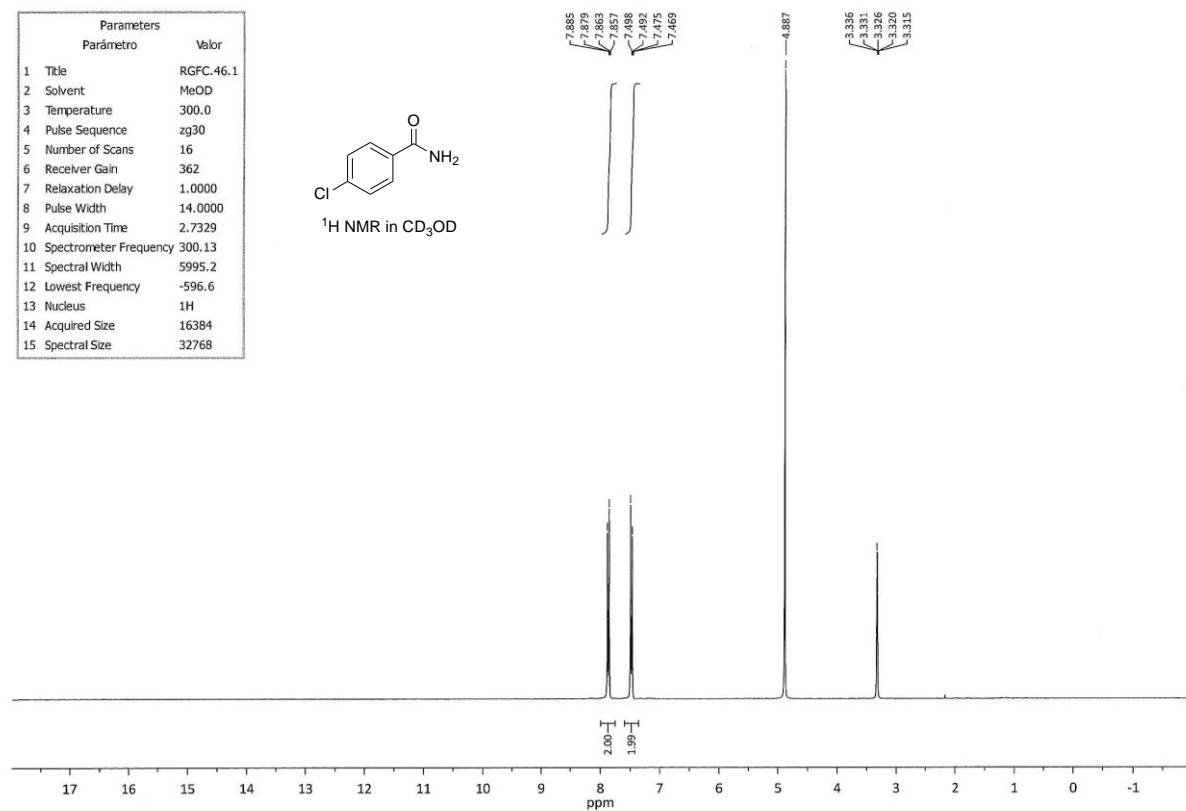
¹H NMR in CD₃OD



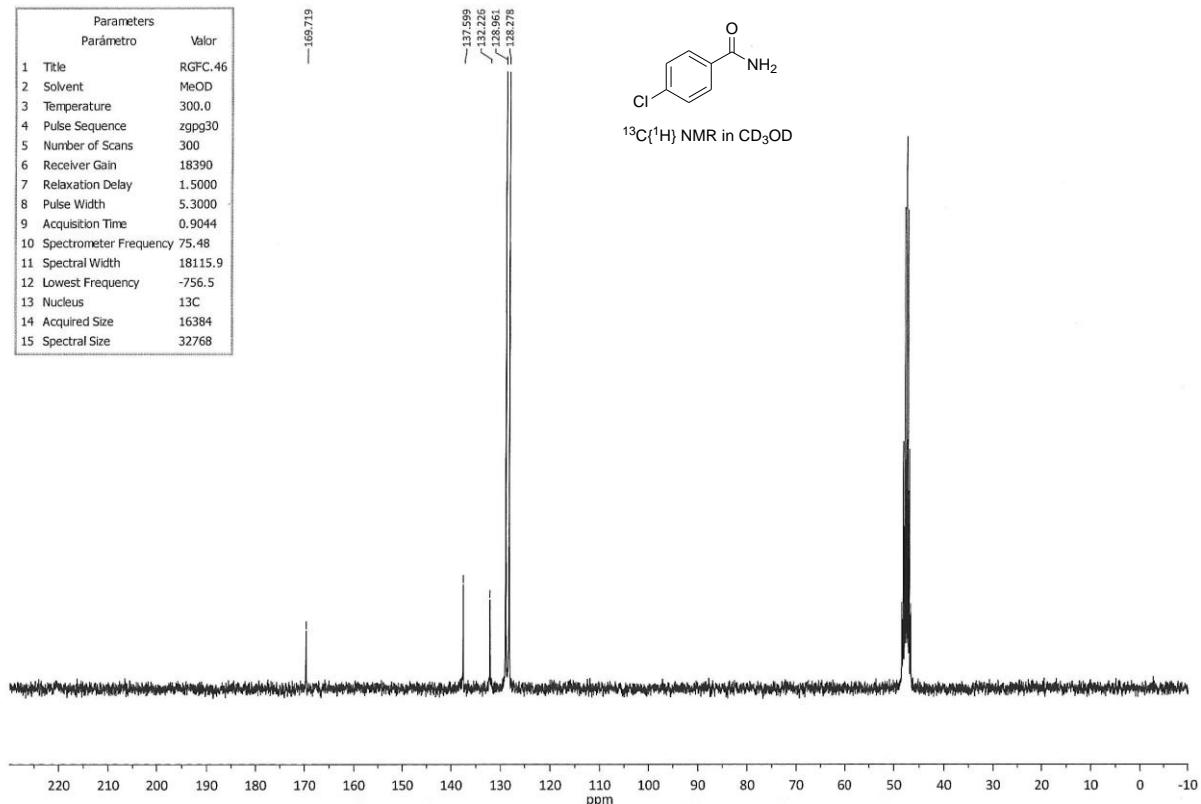
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8 Pulse Width	5.3000
9 Acquisition Time	0.9044
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12 Lowest Frequency	-756.5
13 Nucleus	¹³ C
14 Acquired Size	16384
15 Spectral Size	32768



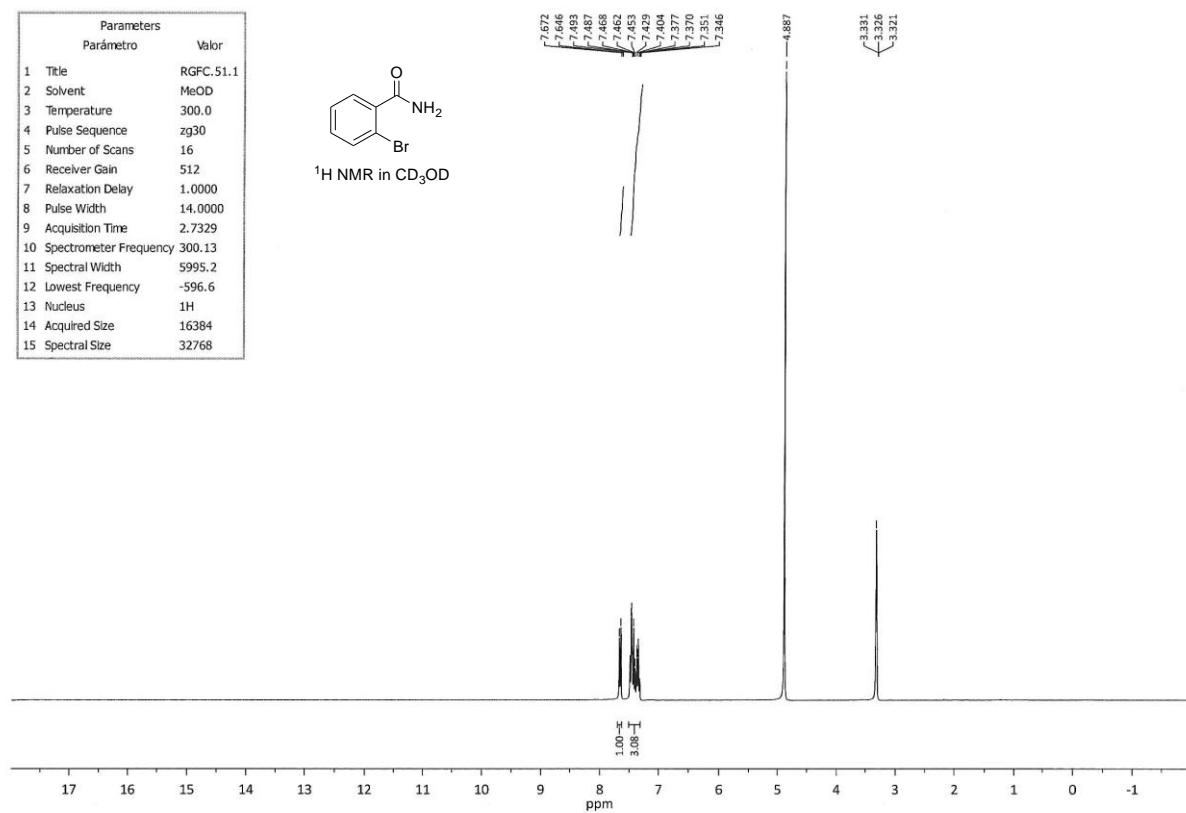
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9 Acquisition Time	2.7329
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12 Lowest Frequency	-596.6
13 Nucleus	¹ H
14 Acquired Size	16384
15 Spectral Size	32768



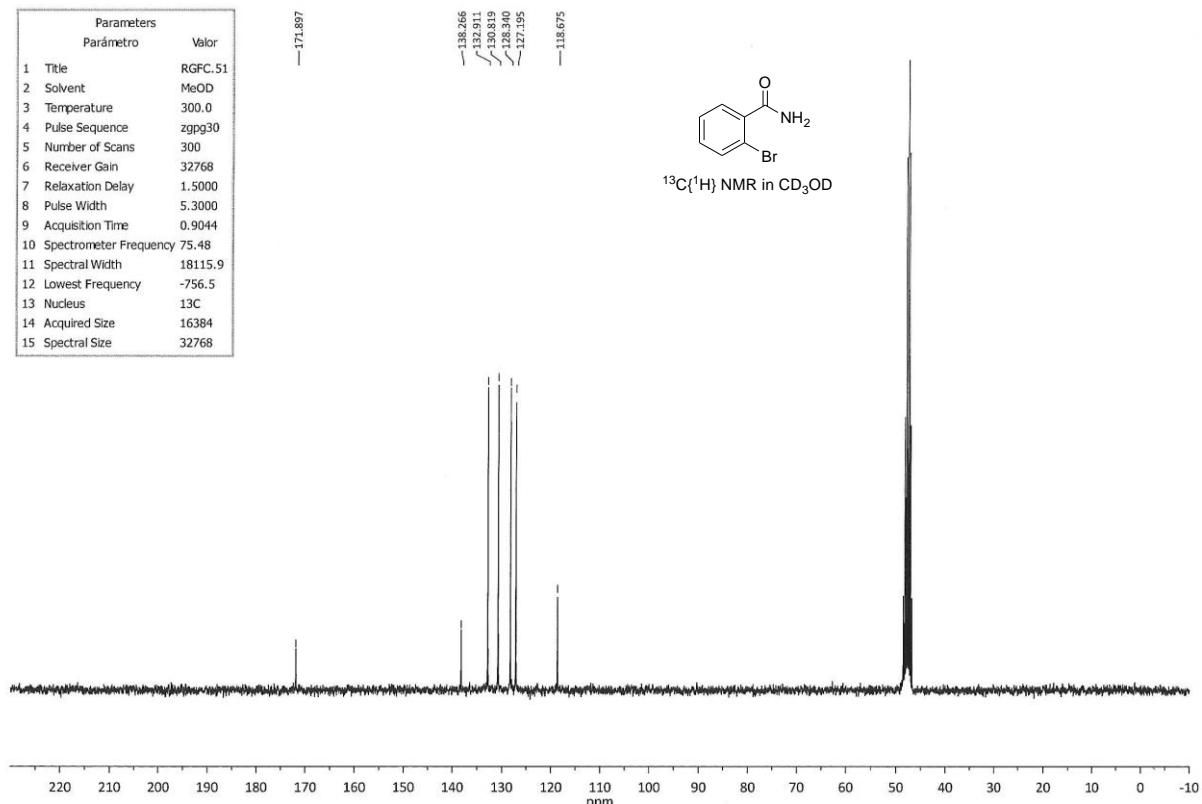
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8 Pulse Width	5.3000
9 Acquisition Time	0.9044
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11 Spectral Width	18115.9
12 Lowest Frequency	-756.5
13 Nucleus	¹³ C
14 Acquired Size	16384
15 Spectral Size	32768



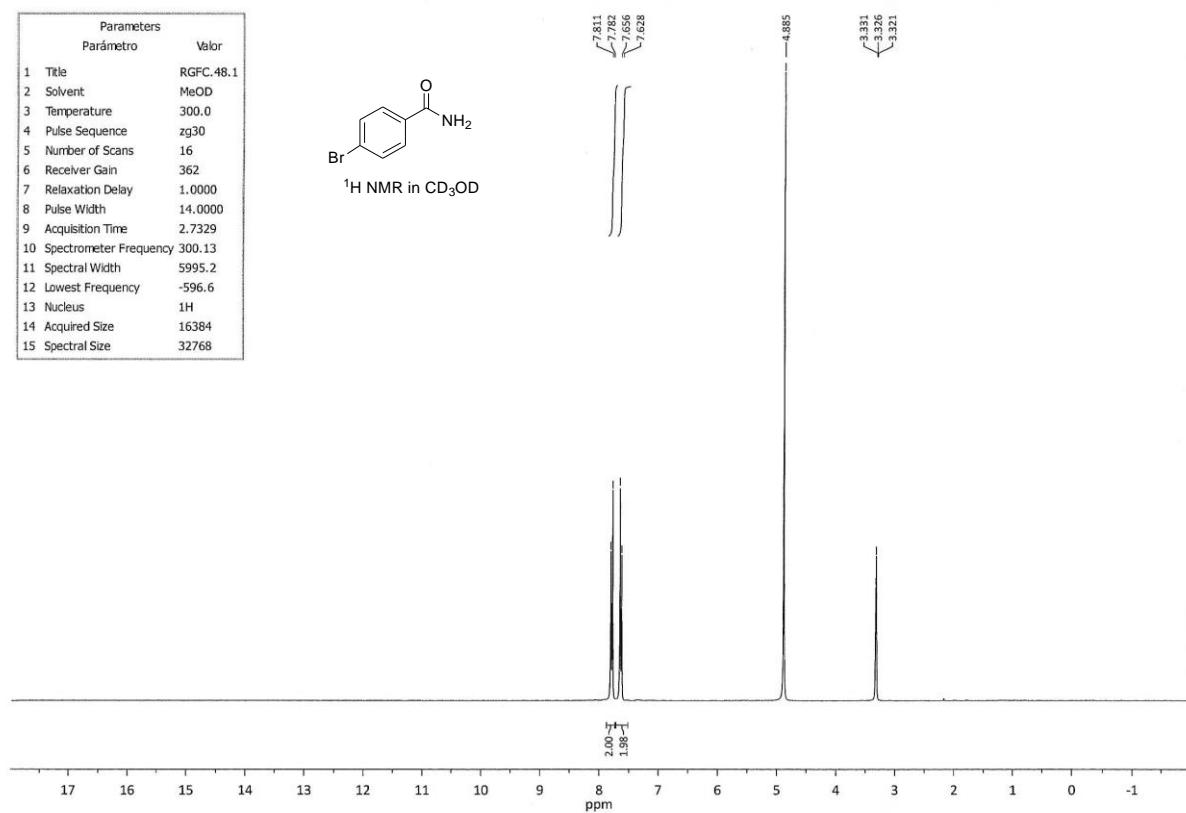
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9 Acquisition Time	2.7329
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12 Lowest Frequency	-596.6
13 Nucleus	¹ H
14 Acquired Size	16384
15 Spectral Size	32768



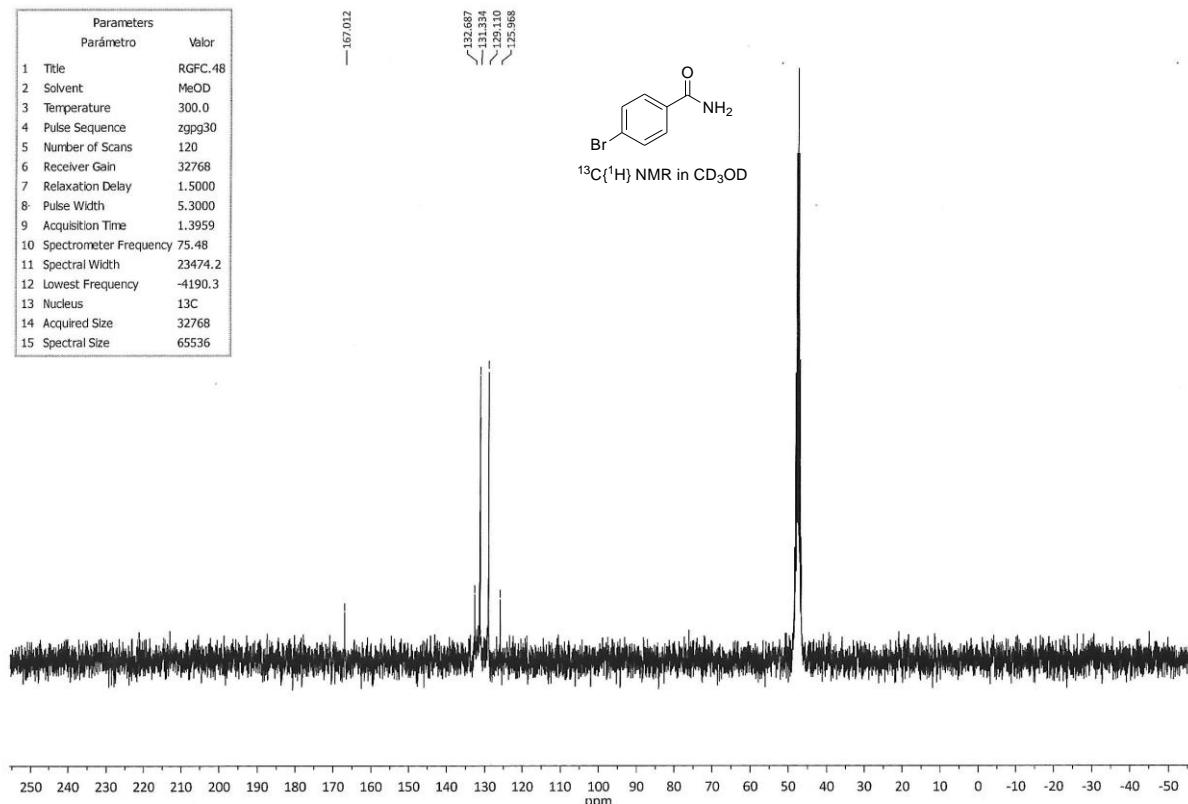
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1 Title	RGFC.51
2 Solvent	MeOD
3 Temperatura	300.0
4 Pulse Sequence	zpg30
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6 Receiver Gain	32768
7 Relaxation Delay	1.5000
8 Pulse Width	5.3000
9 Acquisition Time	0.9044
10 Spectrometer Frequency	75.48
11 Spectral Width	18115.9
12 Lowest Frequency	-756.5
13 Nucleus	¹³ C
14 Acquired Size	16384
15 Spectral Size	32768



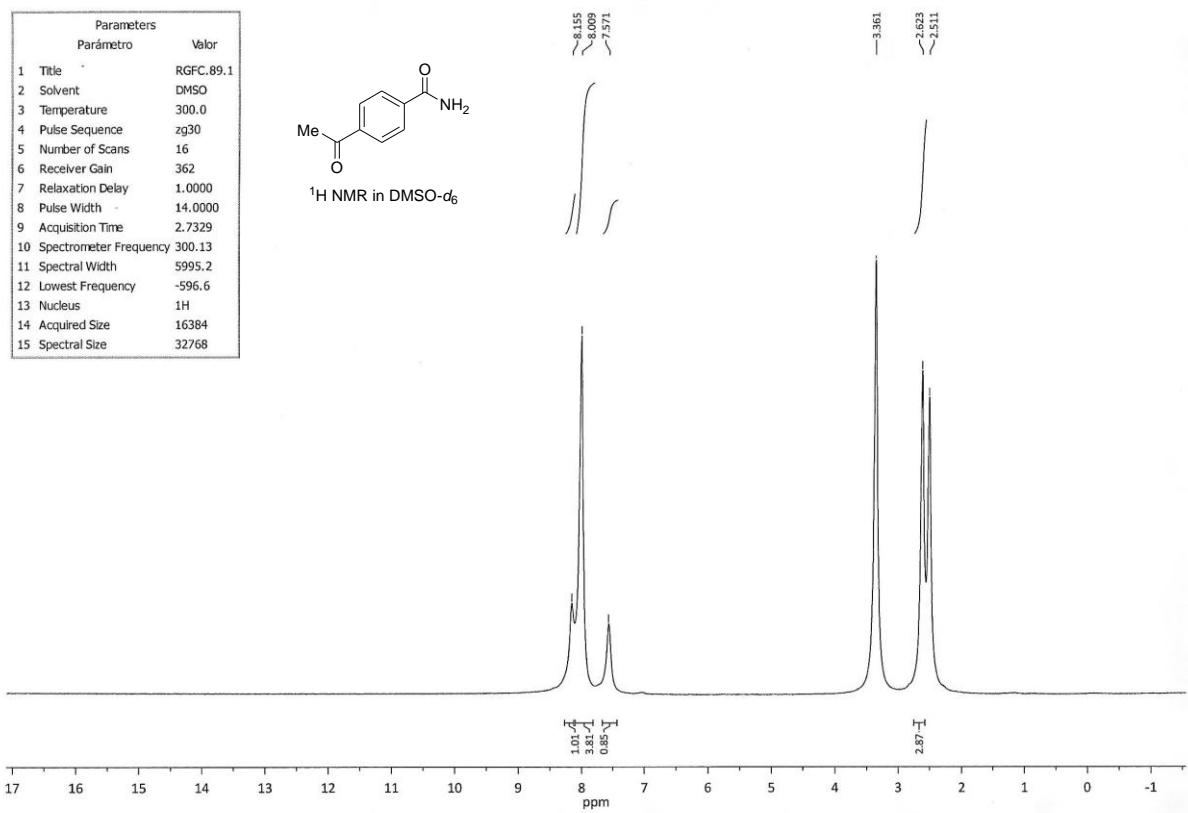
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5 Number of Scans	16
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9 Acquisition Time	2.7329
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11 Spectral Width	5995.2
12 Lowest Frequency	-596.6
13 Nucleus	¹ H
14 Acquired Size	16384
15 Spectral Size	32768

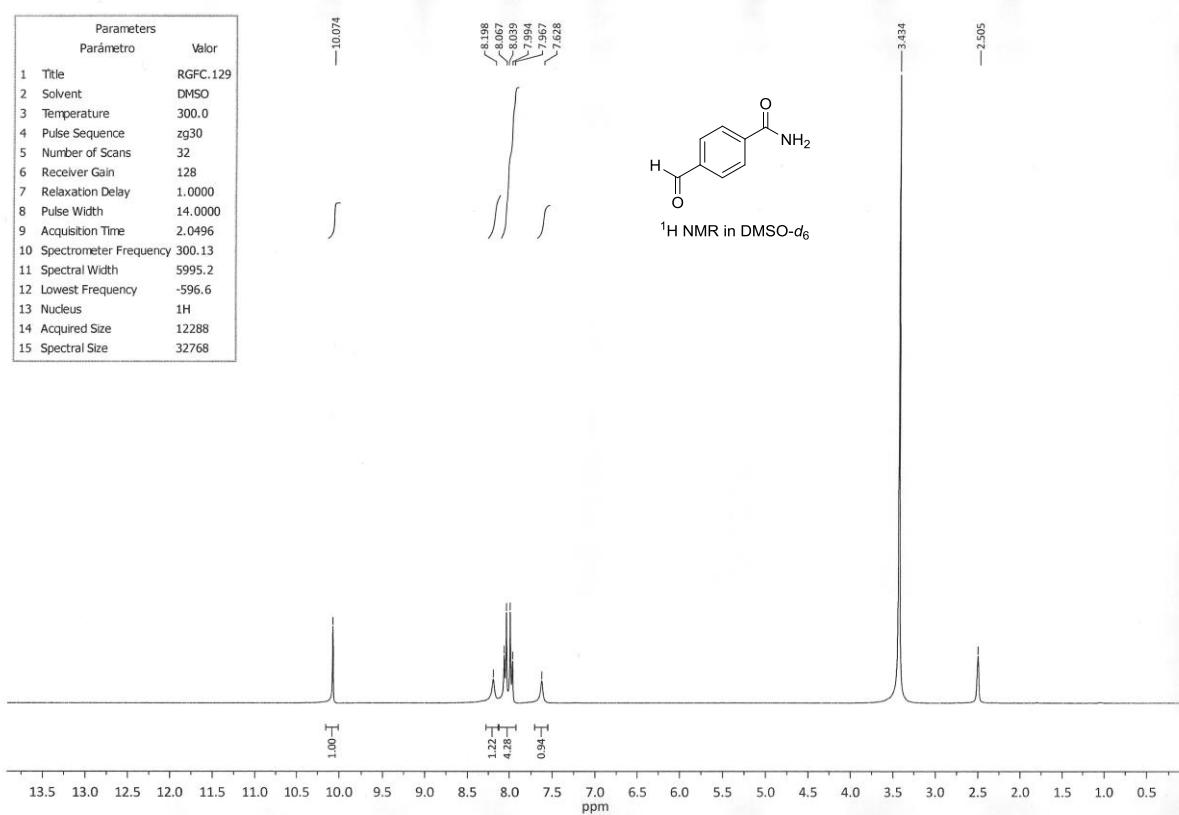
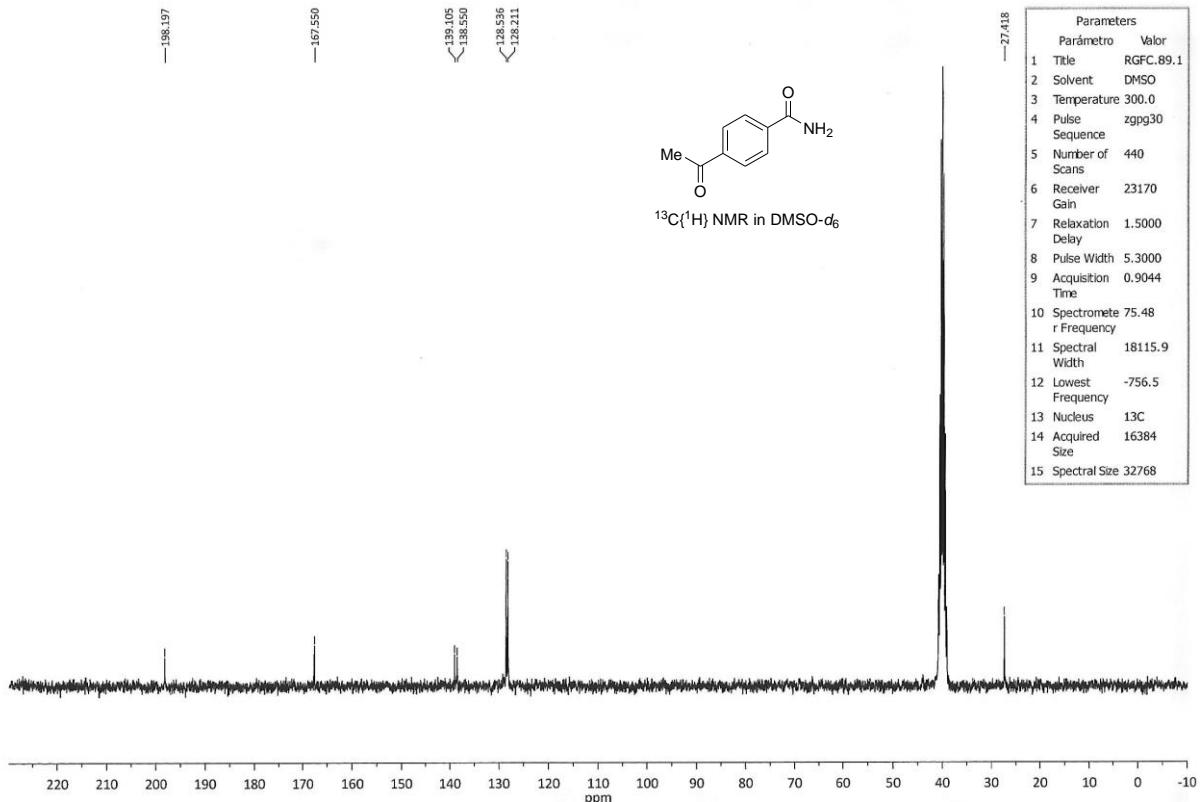


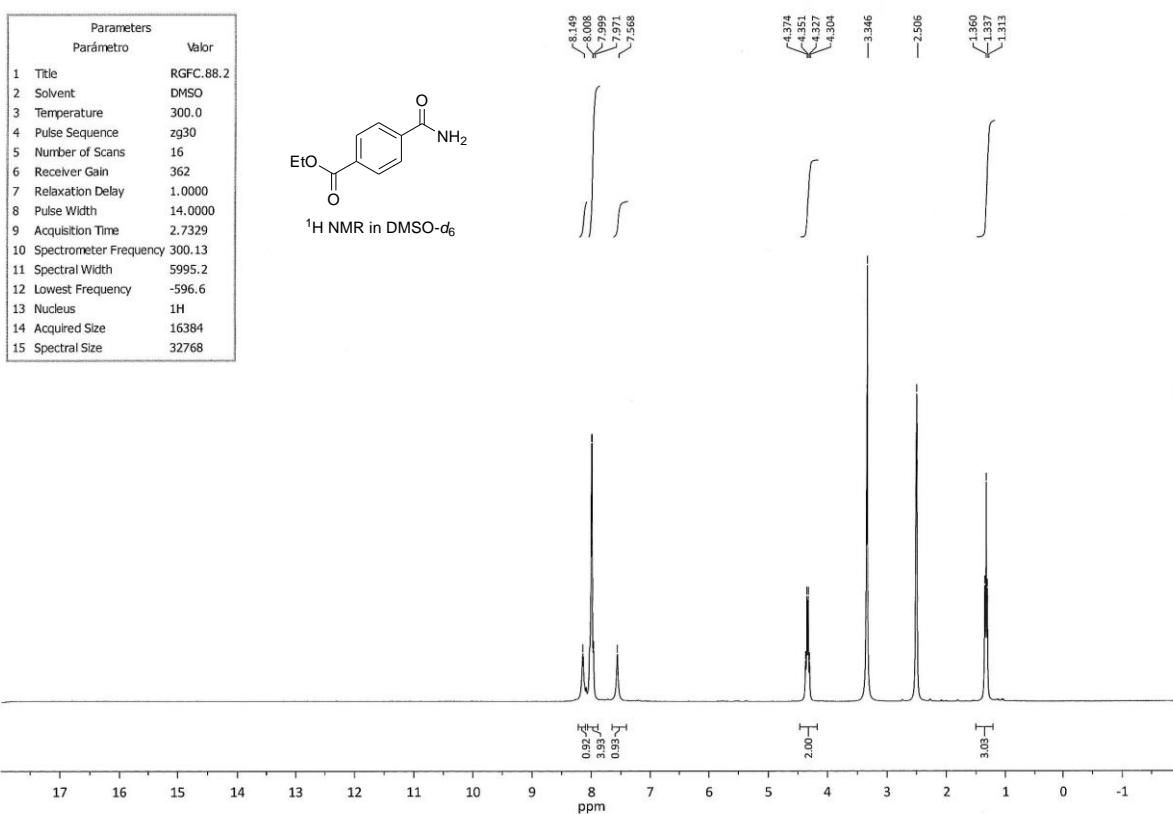
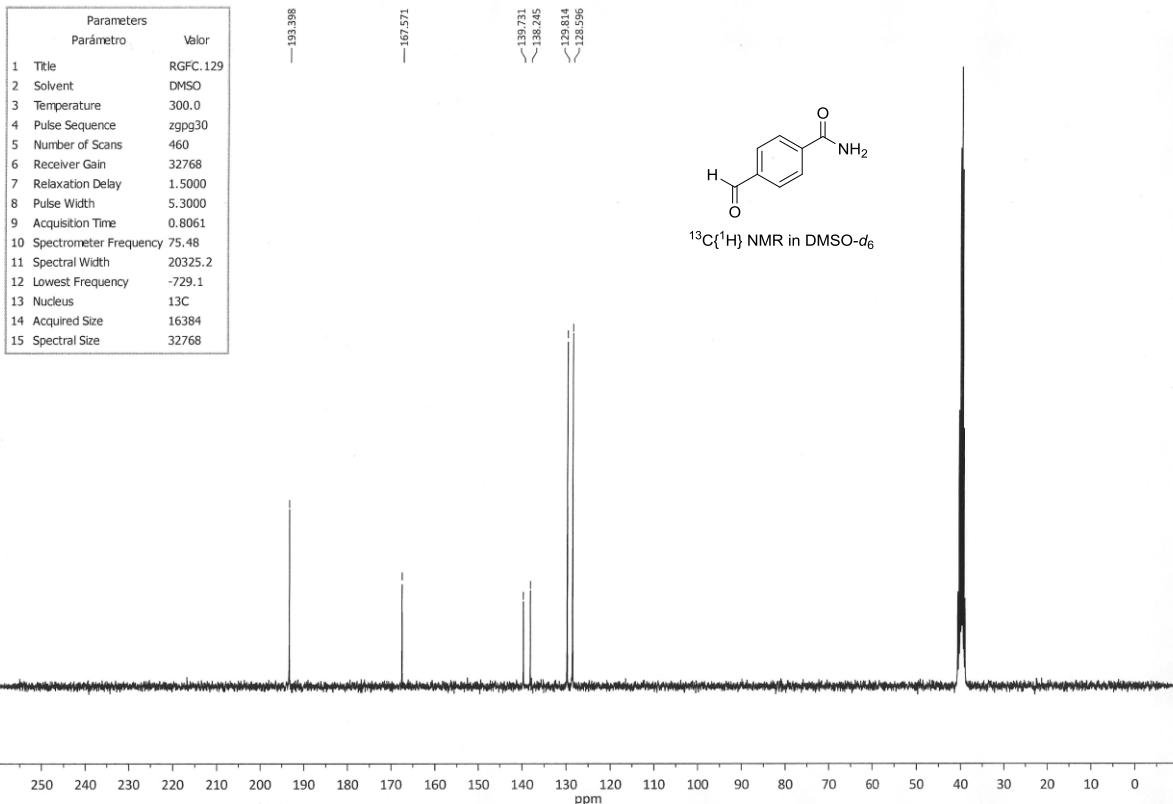
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1 Title	RGFC.48
2 Solvent	MeOD
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7 Relaxation Delay	1.5000
8 Pulse Width	5.3000
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14 Acquired Size	32768
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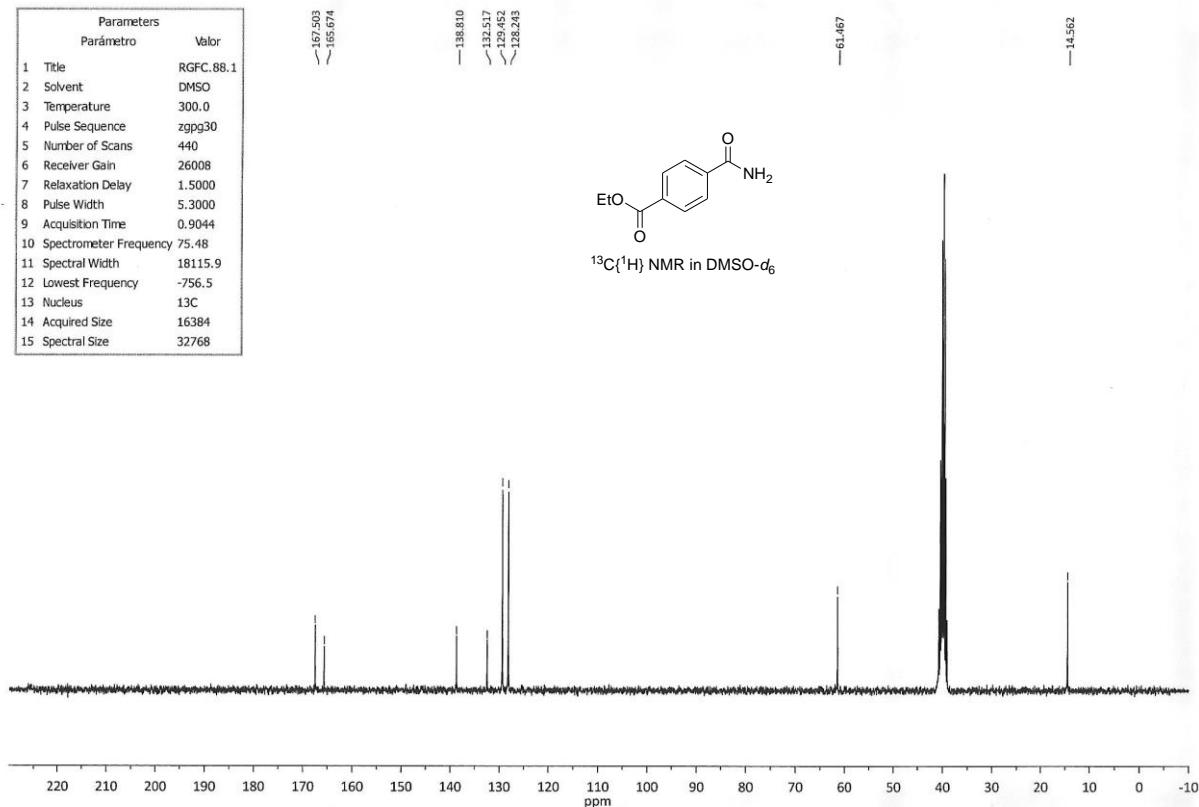
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5 Number of Scans	16
6 Receiver Gain	362
7 Relaxation Delay	1.0000
8 Pulse Width	14.0000
9 Acquisition Time	2.7329
10 Spectrometer Frequency	300.13
11 Spectral Width	5995.2
12 Lowest Frequency	-596.6
13 Nucleus	¹ H
14 Acquired Size	16384
15 Spectral Size	32768



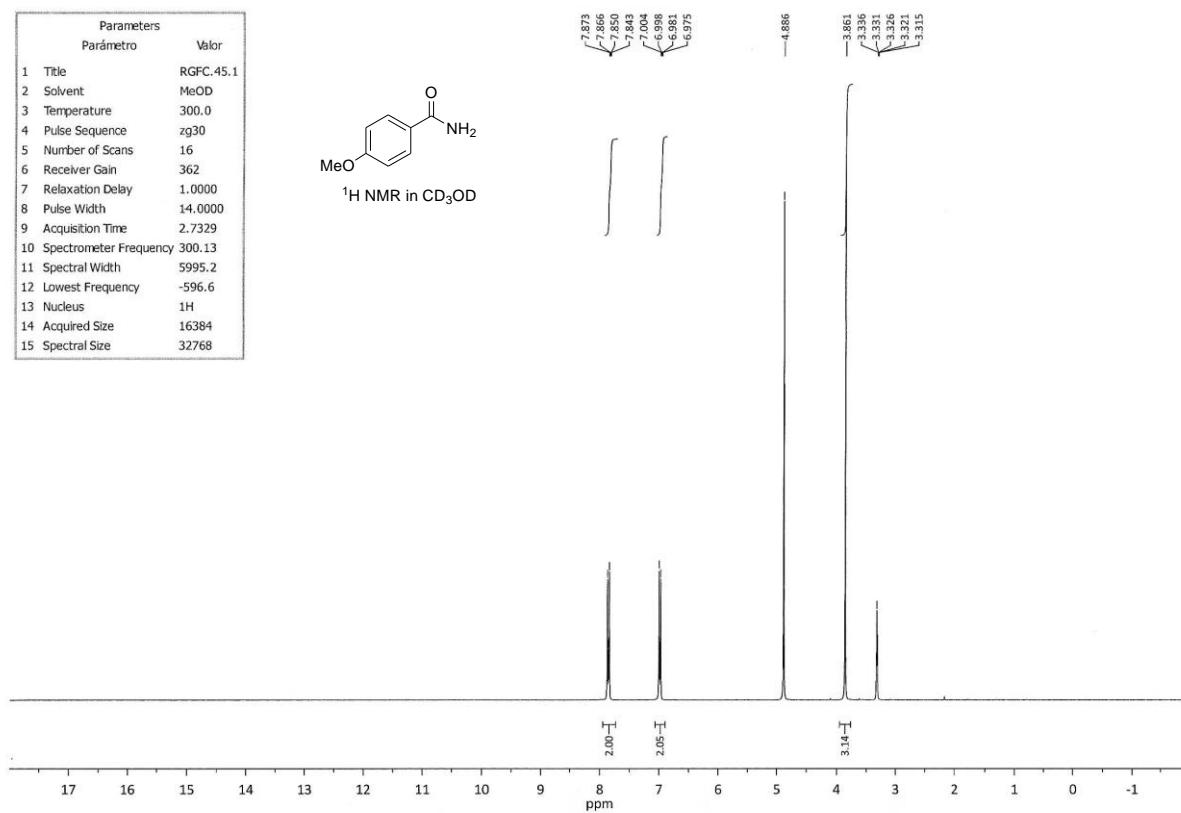




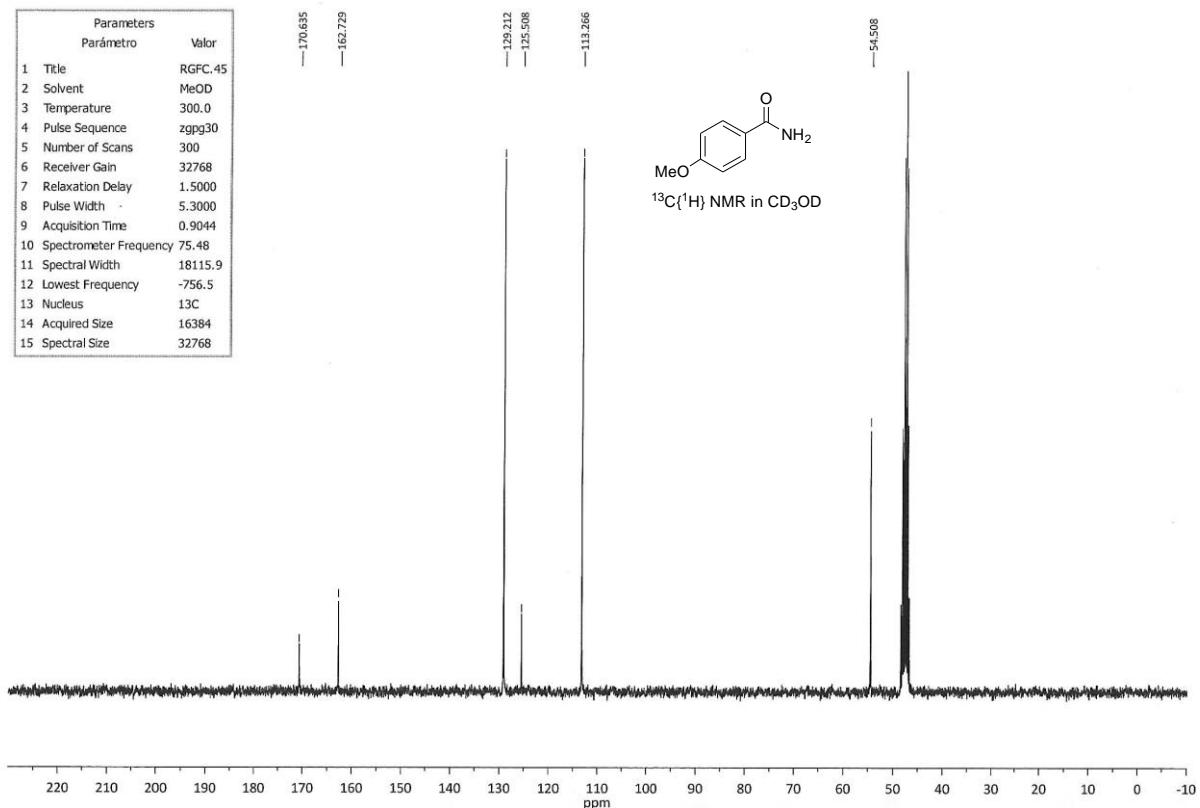
Parameters	
Parámetro	Valor
1 Title	RGFC.88.1
2 Solvent	DMSO
3 Temperature	300.0
4 Pulse Sequence	zpg30
5 Number of Scans	440
6 Receiver Gain	26008
7 Relaxation Delay	1.5000
8 Pulse Width	5.3000
9 Acquisition Time	0.9044
10 Spectrometer Frequency	75.48
11 Spectral Width	18115.9
12 Lowest Frequency	-756.5
13 Nucleus	¹³ C
14 Acquired Size	16384
15 Spectral Size	32768



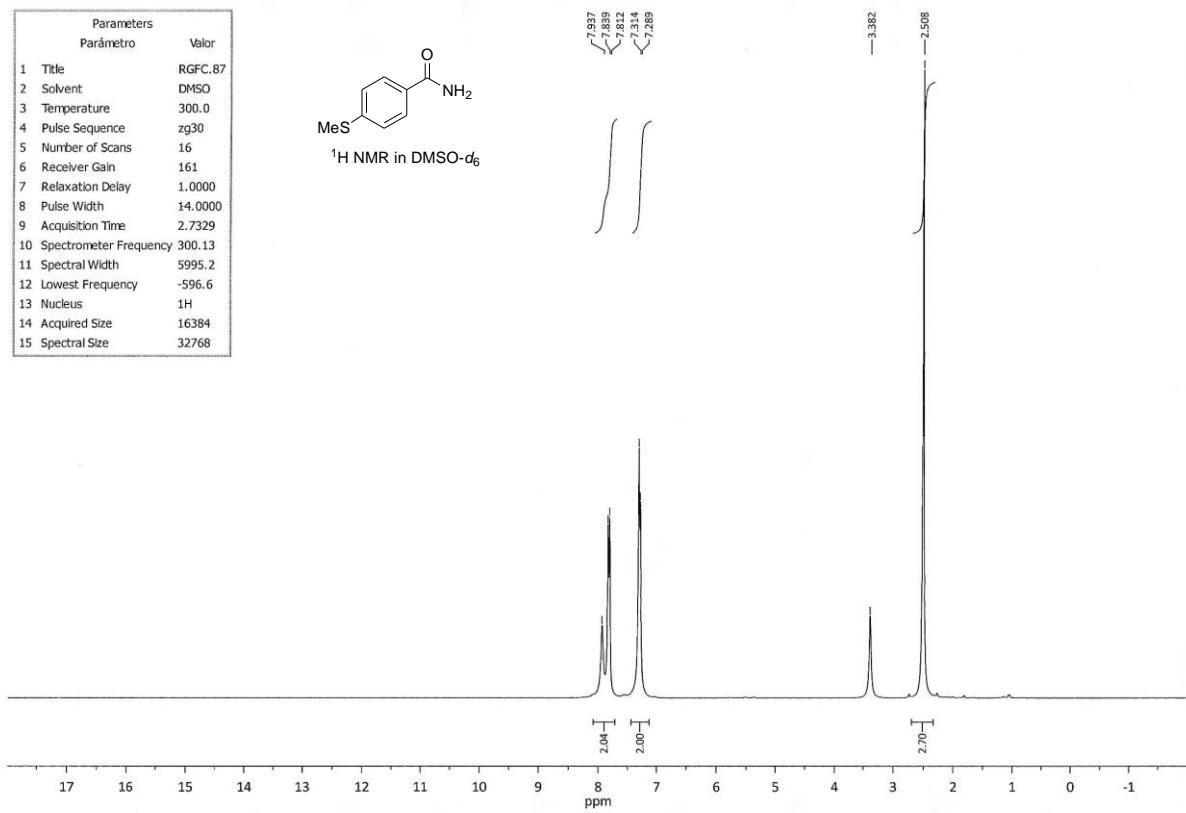
Parameters	
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1 Title	RGFC.45.1
2 Solvent	MeOD
3 Temperature	300.0
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	362
7 Relaxation Delay	1.0000
8 Pulse Width	14.0000
9 Acquisition Time	2.7329
10 Spectrometer Frequency	300.13
11 Spectral Width	5995.2
12 Lowest Frequency	-596.6
13 Nucleus	¹ H
14 Acquired Size	16384
15 Spectral Size	32768

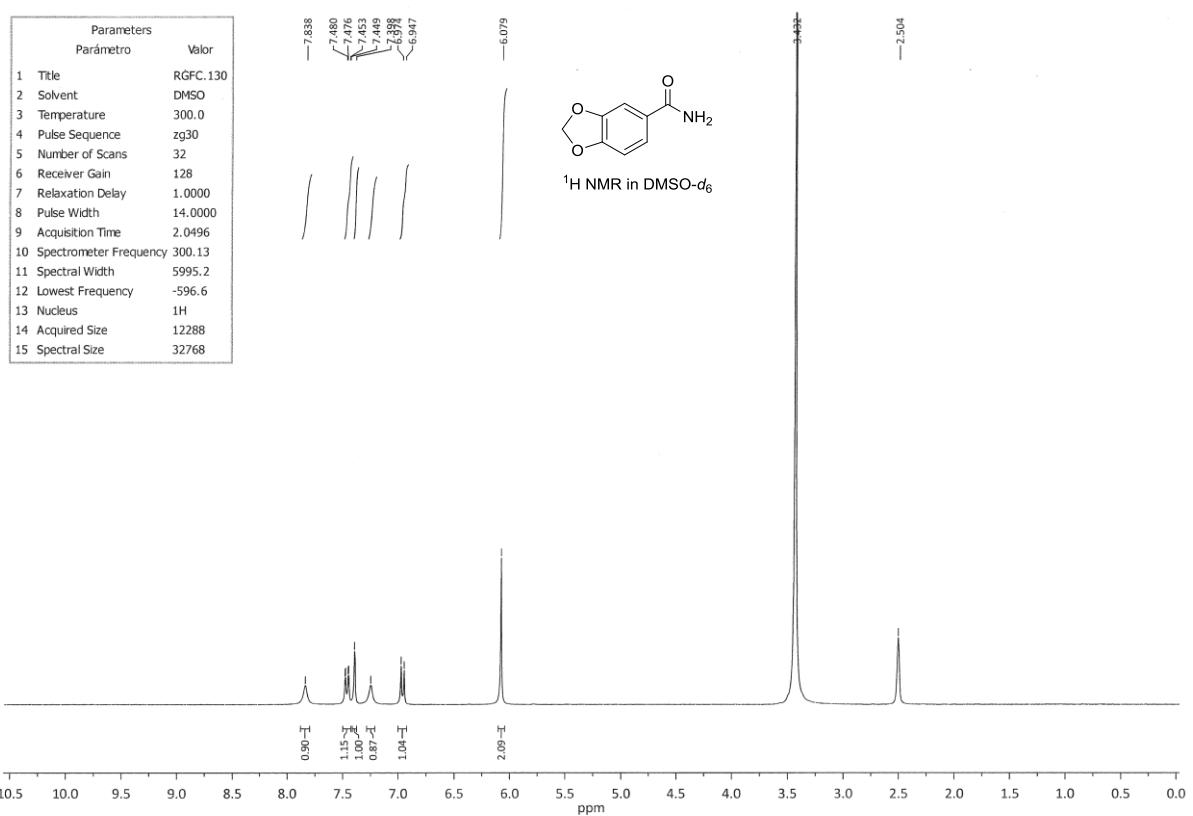
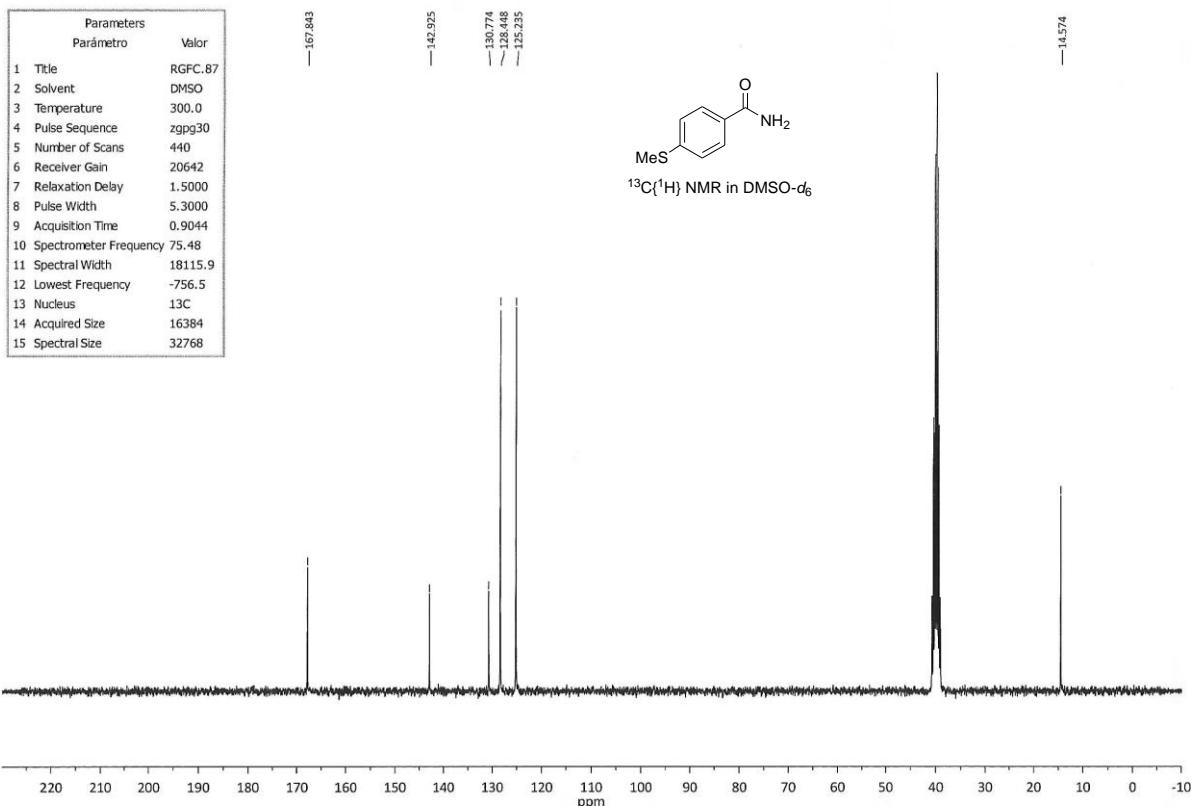


Parámetro	Valor
1 Title	RGFC.45
2 Solvent	MeOD
3 Temperatura	300.0
4 Pulse Sequence	zpg30
5 Number of Scans	300
6 Receiver Gain	32768
7 Relaxation Delay	1.5000
8 Pulse Width	5.3000
9 Acquisition Time	0.9044
10 Spectrometer Frequency	75.48
11 Spectral Width	18115.9
12 Lowest Frequency	-756.5
13 Nucleus	¹³ C
14 Acquired Size	16384
15 Spectral Size	32768

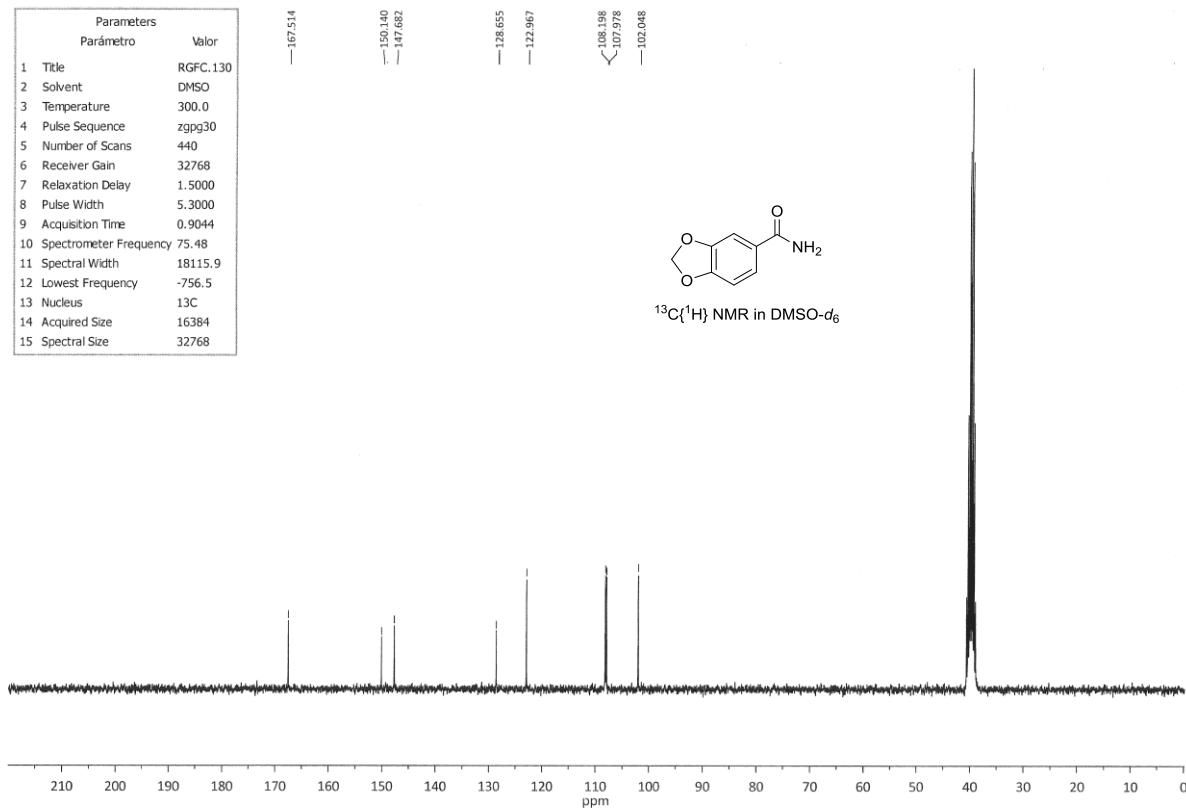


Parámetro	Valor
1 Title	RGFC.87
2 Solvent	DMSO
3 Temperatura	300.0
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	161
7 Relaxation Delay	1.0000
8 Pulse Width	14.0000
9 Acquisition Time	2.7329
10 Spectrometer Frequency	300.13
11 Spectral Width	5995.2
12 Lowest Frequency	-596.6
13 Nucleus	¹ H
14 Acquired Size	16384
15 Spectral Size	32768

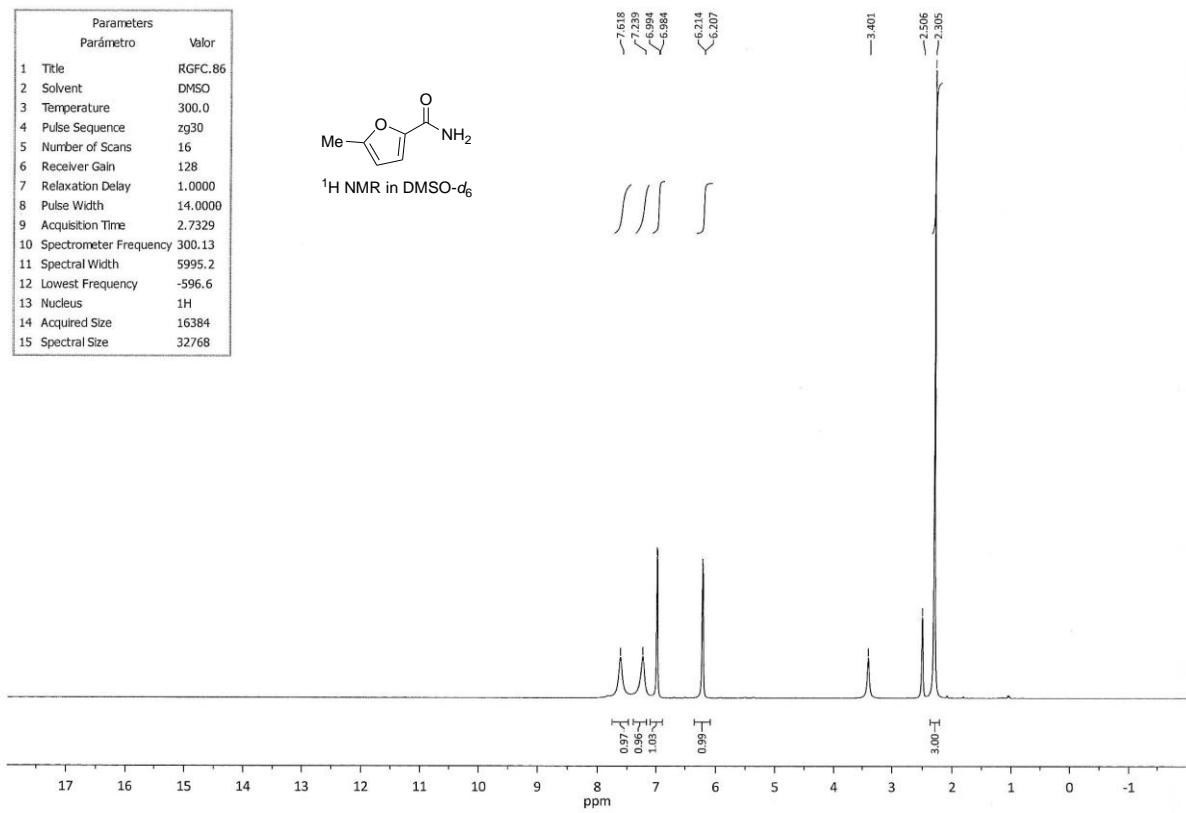




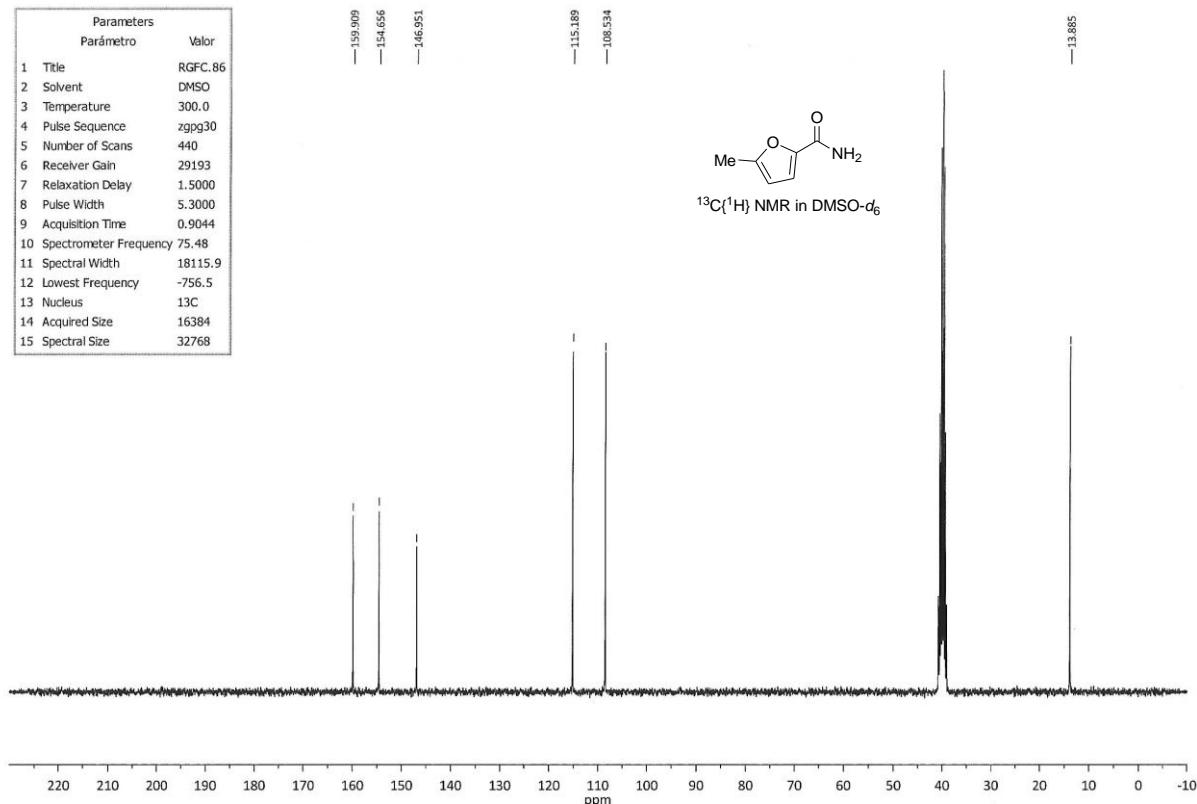
Parámetro	Valor
1 Title	RGFC.130
2 Solvent	DMSO
3 Temperatura	300.0
4 Pulse Sequence	zpg30
5 Number of Scans	440
6 Receiver Gain	32768
7 Relaxation Delay	1.5000
8 Pulse Width	5.3000
9 Acquisition Time	0.9044
10 Spectrometer Frequency	75.48
11 Spectral Width	18115.9
12 Lowest Frequency	-756.5
13 Nucleus	¹³ C
14 Acquired Size	16384
15 Spectral Size	32768



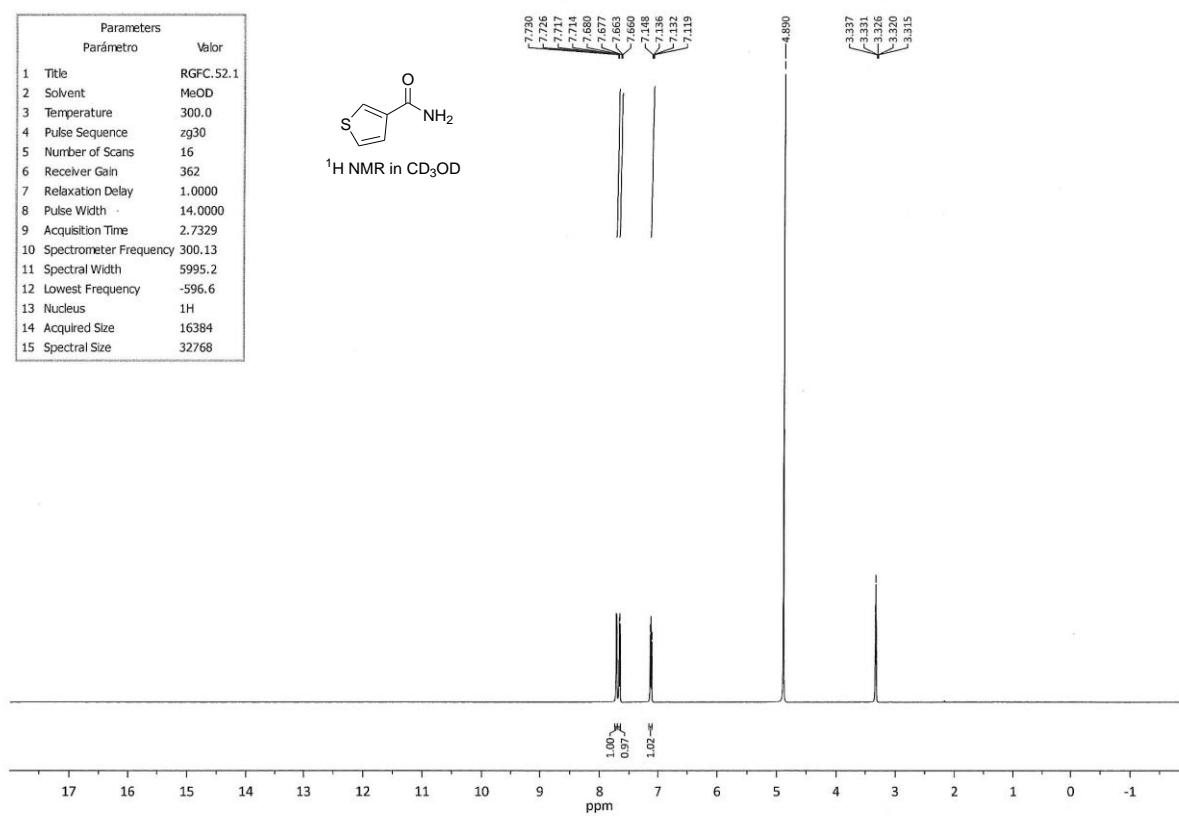
Parámetro	Valor
1 Title	RGFC.86
2 Solvent	DMSO
3 Temperatura	300.0
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	128
7 Relaxation Delay	1.0000
8 Pulse Width	14.0000
9 Acquisition Time	2.7329
10 Spectrometer Frequency	300.13
11 Spectral Width	5995.2
12 Lowest Frequency	-596.6
13 Nucleus	¹ H
14 Acquired Size	16384
15 Spectral Size	32768

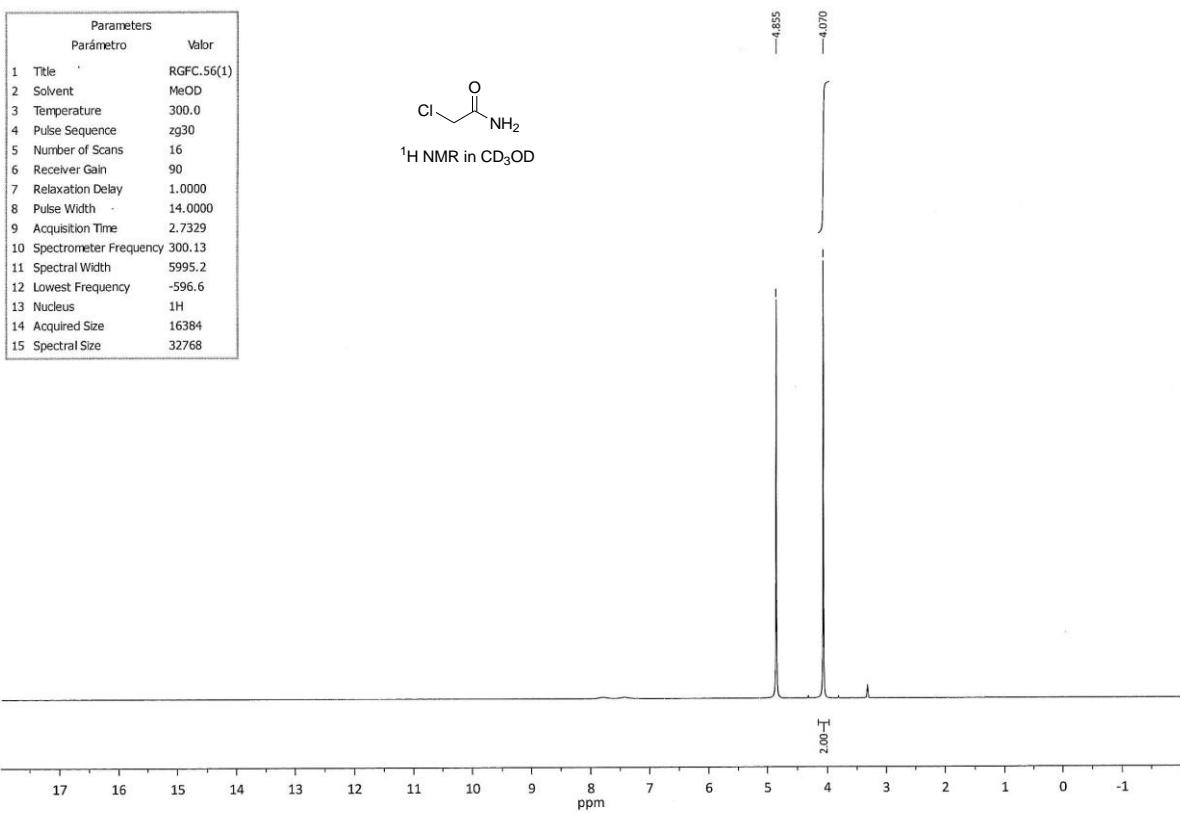
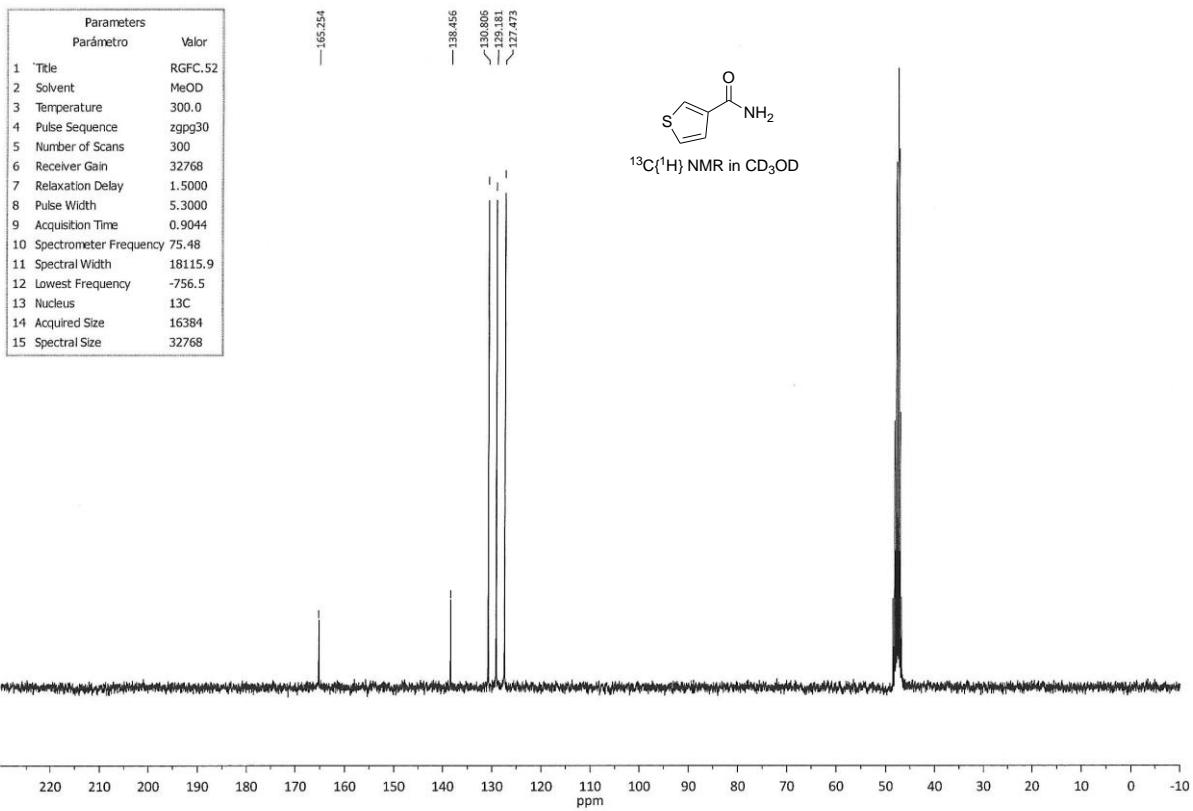


Parámetro	Valor
1 Title	RGFC.86
2 Solvent	DMSO
3 Temperatura	300.0
4 Pulse Sequence	zpg30
5 Number of Scans	440
6 Receiver Gain	29193
7 Relaxation Delay	1.5000
8 Pulse Width	5.3000
9 Acquisition Time	0.9044
10 Spectrometer Frequency	75.48
11 Spectral Width	18115.9
12 Lowest Frequency	-756.5
13 Nucleus	¹³ C
14 Acquired Size	16384
15 Spectral Size	32768

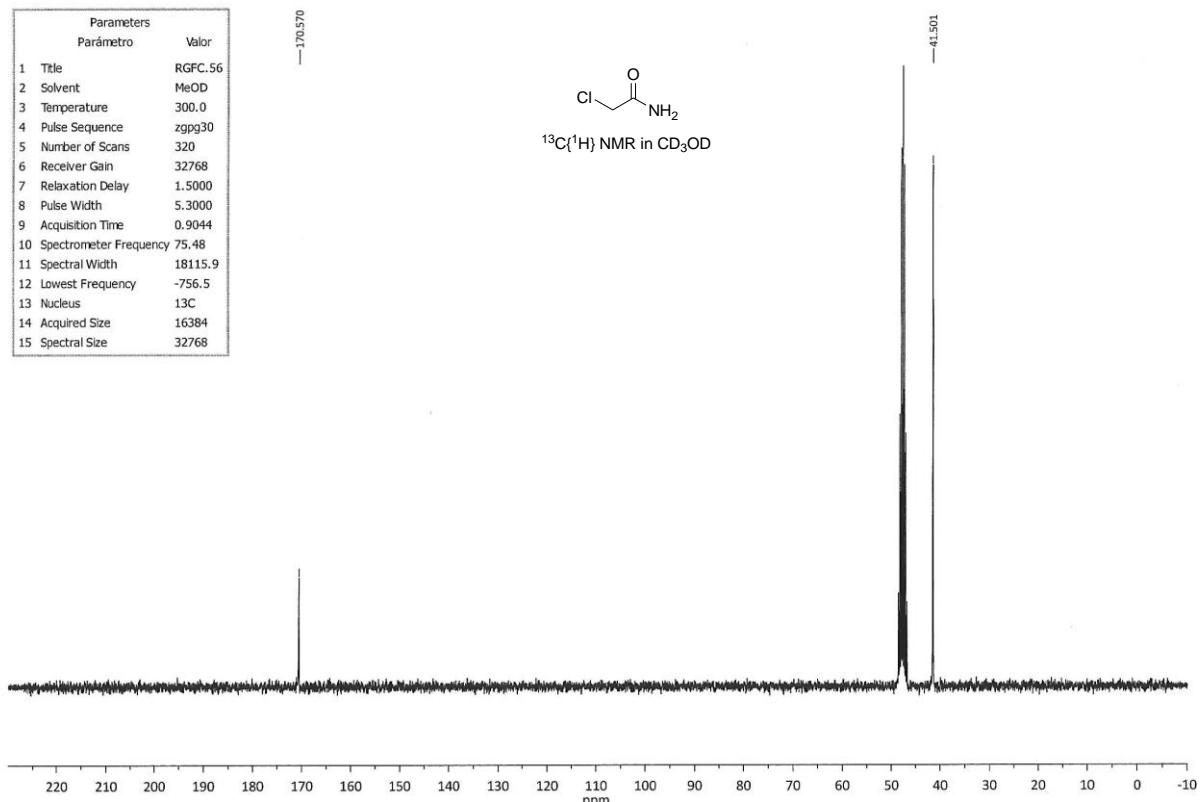


Parámetro	Valor
1 Title	RGFC.52.1
2 Solvent	MeOD
3 Temperatura	300.0
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	362
7 Relaxation Delay	1.0000
8 Pulse Width	14.0000
9 Acquisition Time	2.7329
10 Spectrometer Frequency	300.13
11 Spectral Width	5995.2
12 Lowest Frequency	-596.6
13 Nucleus	¹ H
14 Acquired Size	16384
15 Spectral Size	32768

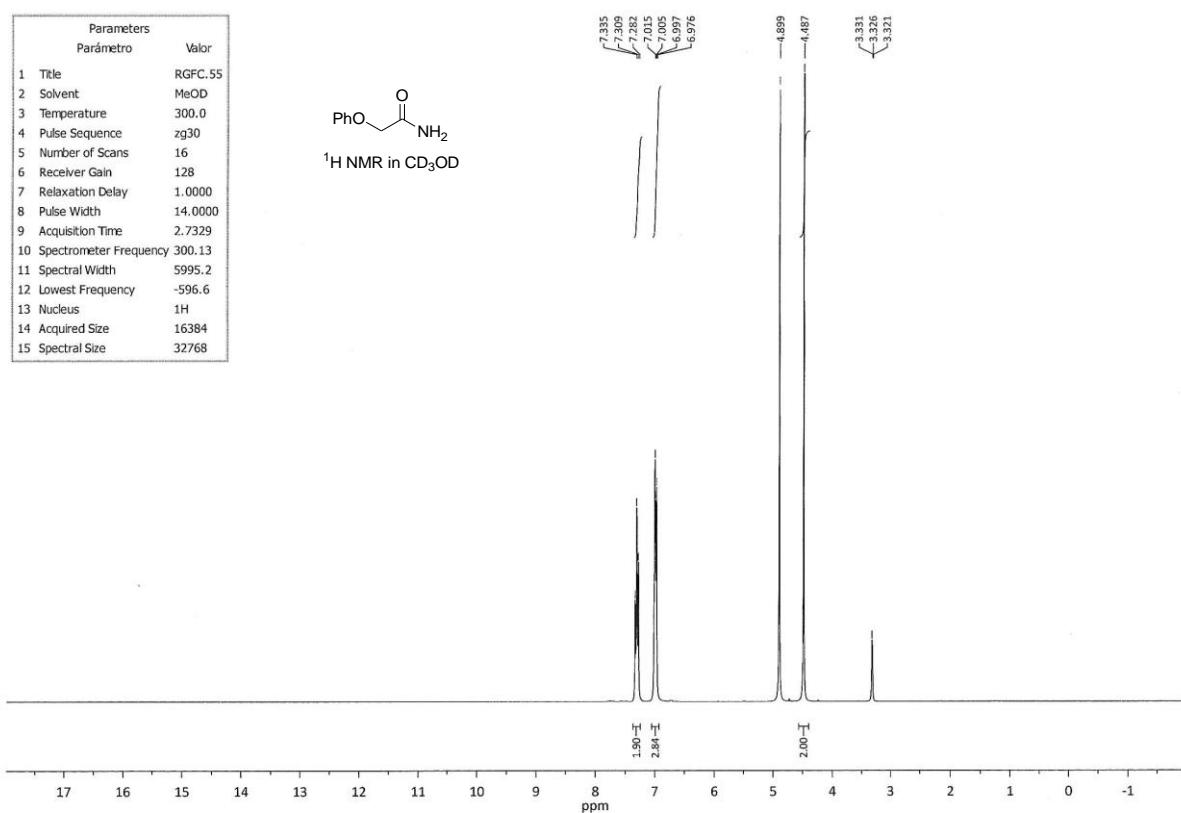


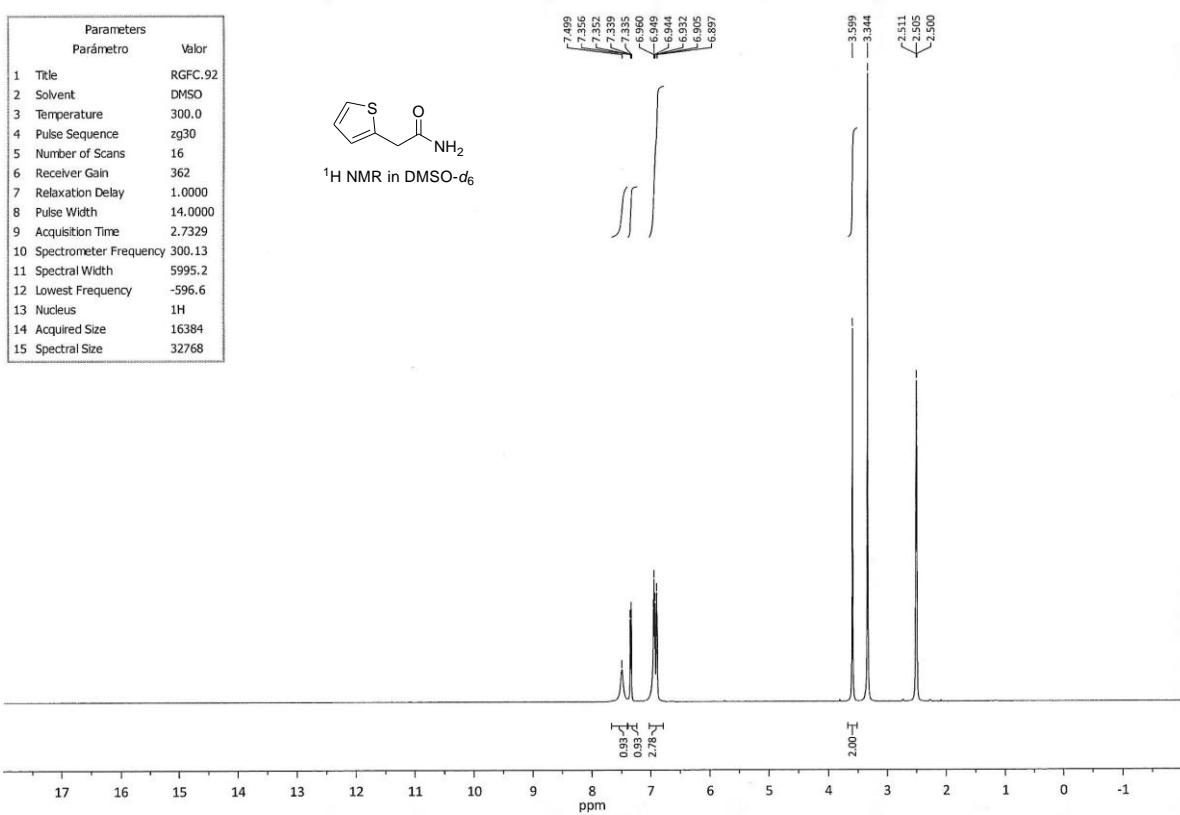
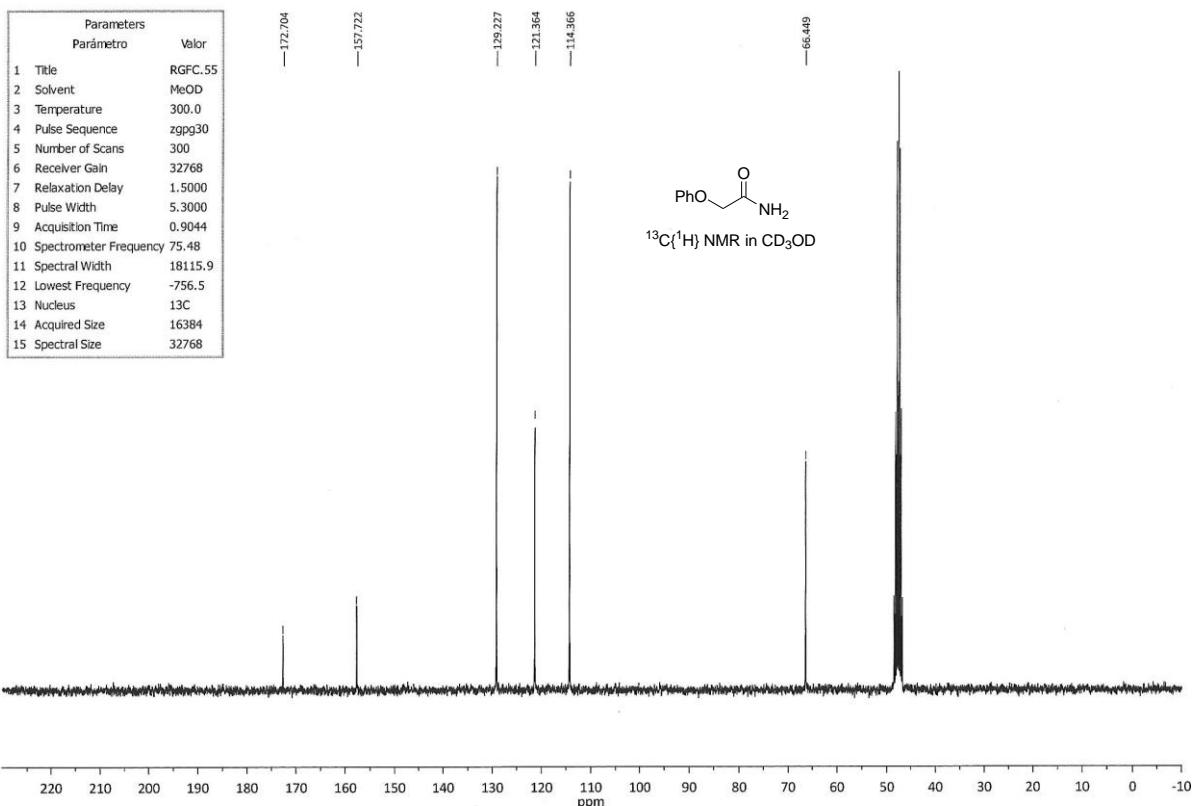


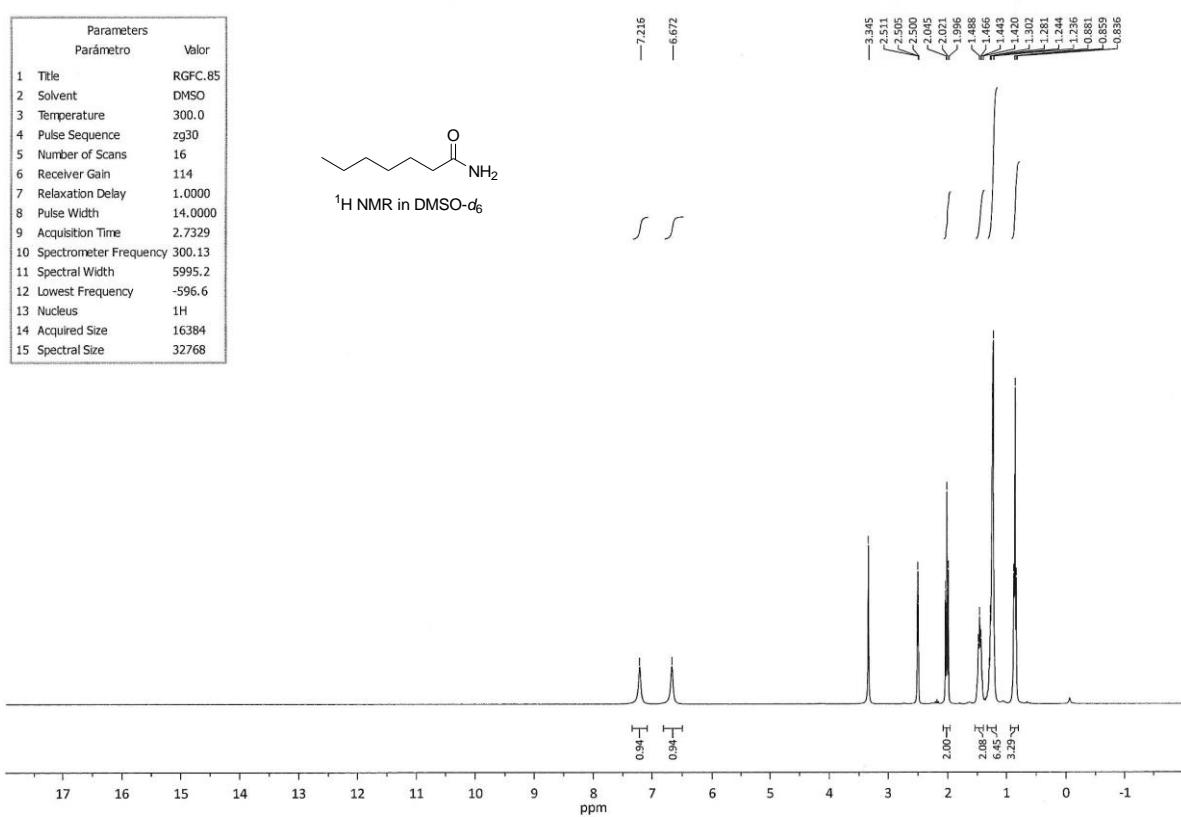
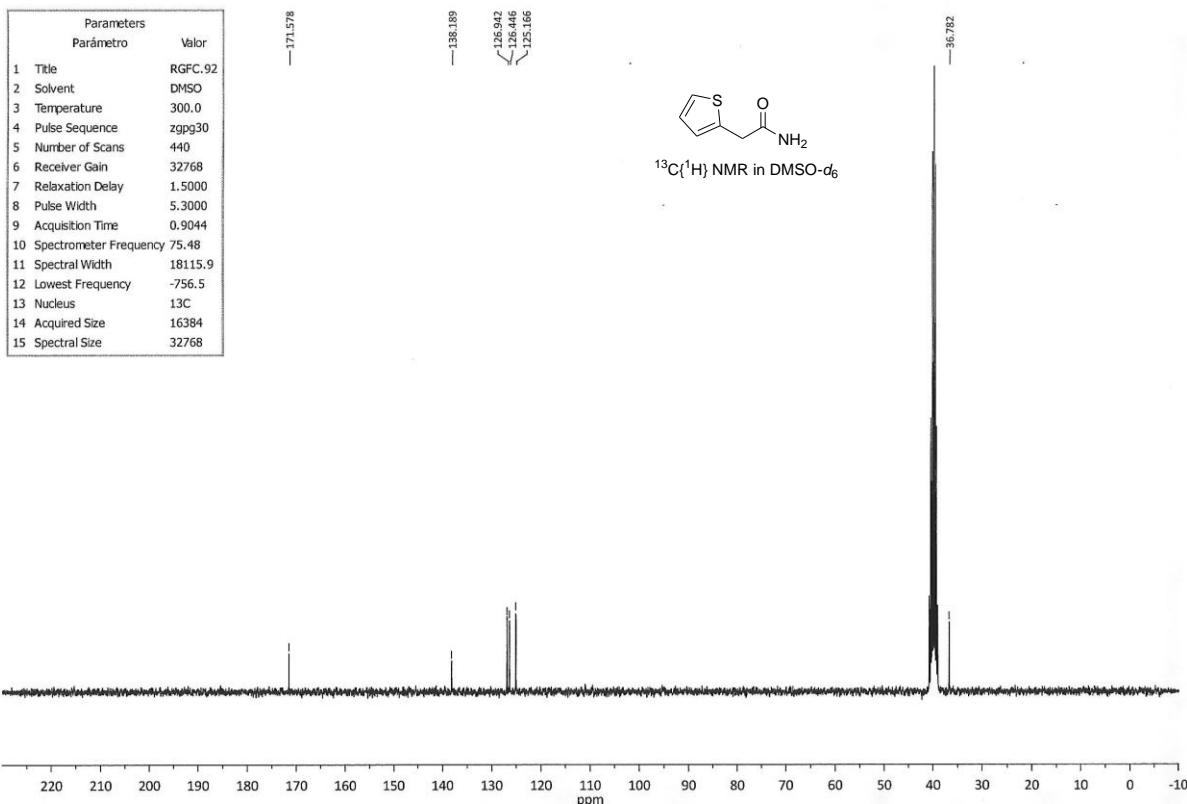
Parameters		
Parámetro	Valor	
1 Title	RGFC.56	
2 Solvent	MeOD	
3 Temperature	300.0	
4 Pulse Sequence	zpg30	
5 Number of Scans	320	
6 Receiver Gain	32768	
7 Relaxation Delay	1.5000	
8 Pulse Width	5.3000	
9 Acquisition Time	0.9044	
10 Spectrometer Frequency	75.48	
11 Spectral Width	18115.9	
12 Lowest Frequency	-756.5	
13 Nucleus	¹³ C	
14 Acquired Size	16384	
15 Spectral Size	32768	



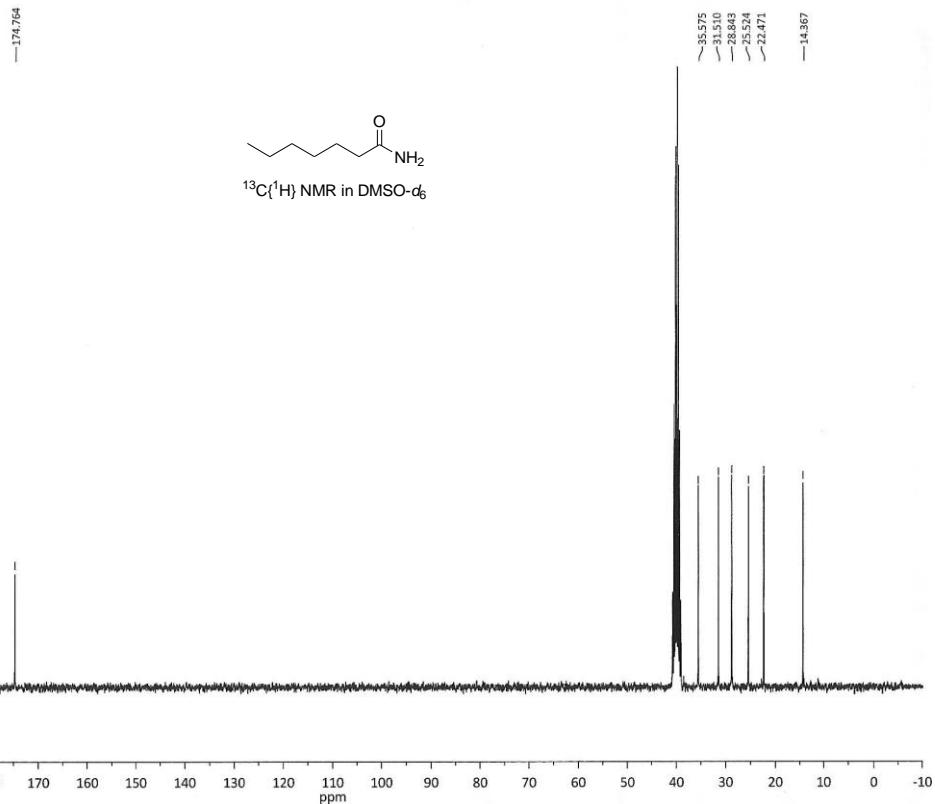
Parameters		
Parámetro	Valor	
1 Title	RGFC.55	
2 Solvent	MeOD	
3 Temperature	300.0	
4 Pulse Sequence	zg30	
5 Number of Scans	16	
6 Receiver Gain	128	
7 Relaxation Delay	1.0000	
8 Pulse Width	14.0000	
9 Acquisition Time	2.7329	
10 Spectrometer Frequency	300.13	
11 Spectral Width	5995.2	
12 Lowest Frequency	-596.6	
13 Nucleus	¹ H	
14 Acquired Size	16384	
15 Spectral Size	32768	



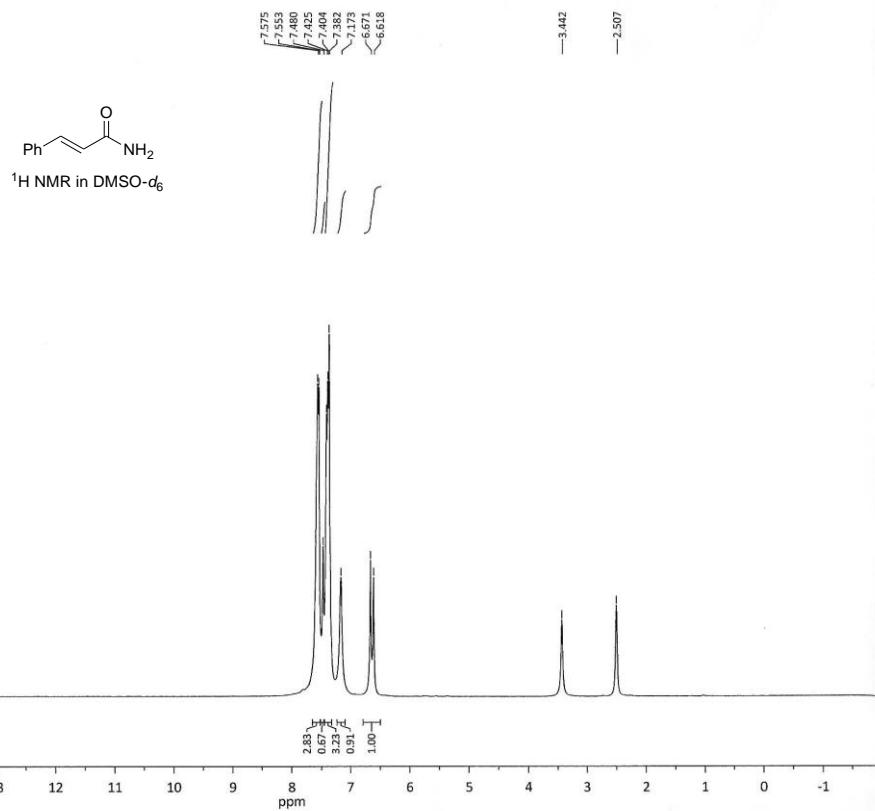




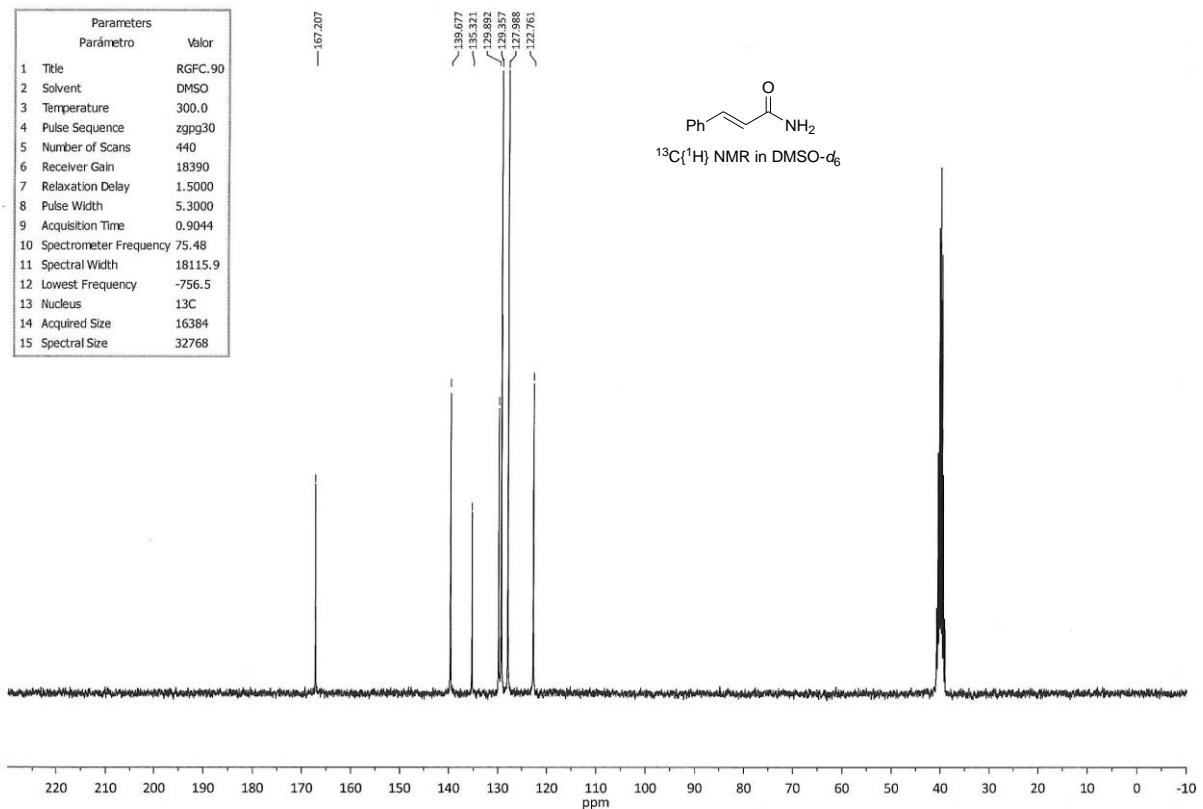
Parameters	
Parámetro	Valor
1 Title	RGFC.85
2 Solvent	DMSO
3 Temperature	300.0
4 Pulse Sequence	zgpg30
5 Number of Scans	440
6 Receiver Gain	32768
7 Relaxation Delay	1.5000
8 Pulse Width	5.3000
9 Acquisition Time	0.9044
10 Spectrometer Frequency	75.48
11 Spectral Width	18115.9
12 Lowest Frequency	-756.5
13 Nucleus	¹³ C
14 Acquired Size	16384
15 Spectral Size	32768

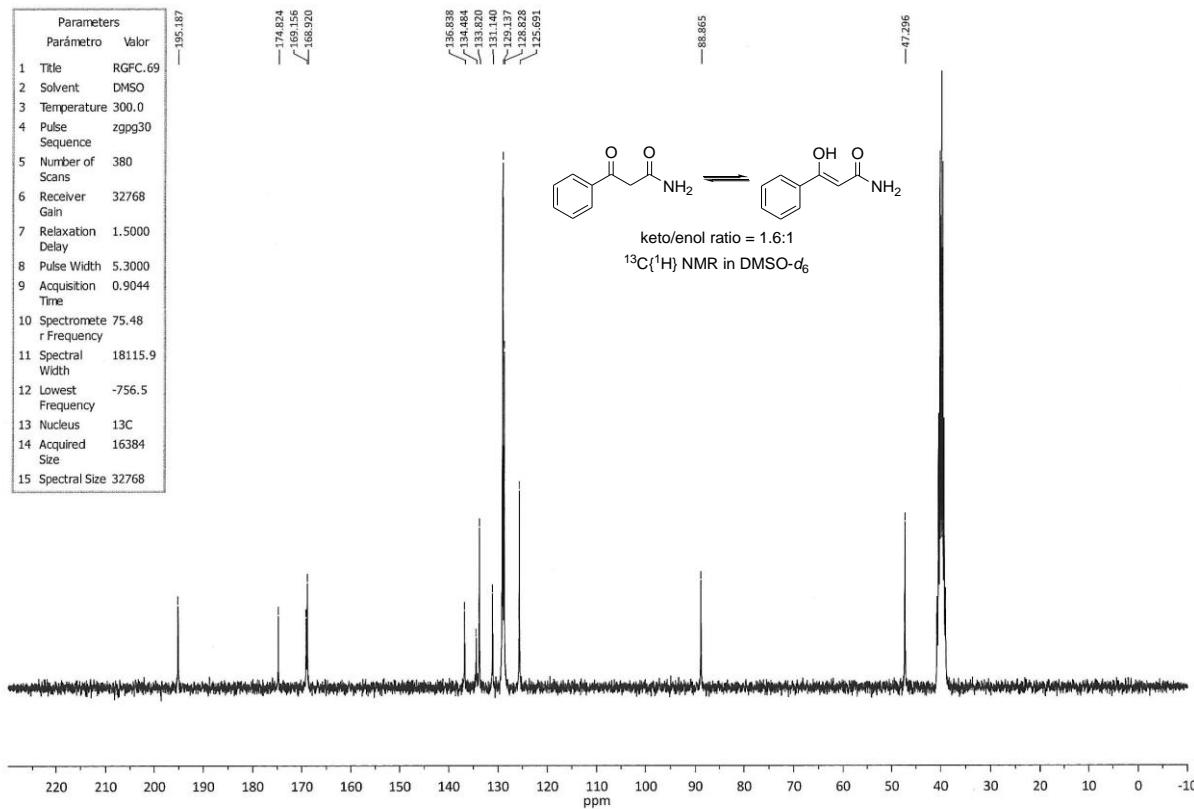
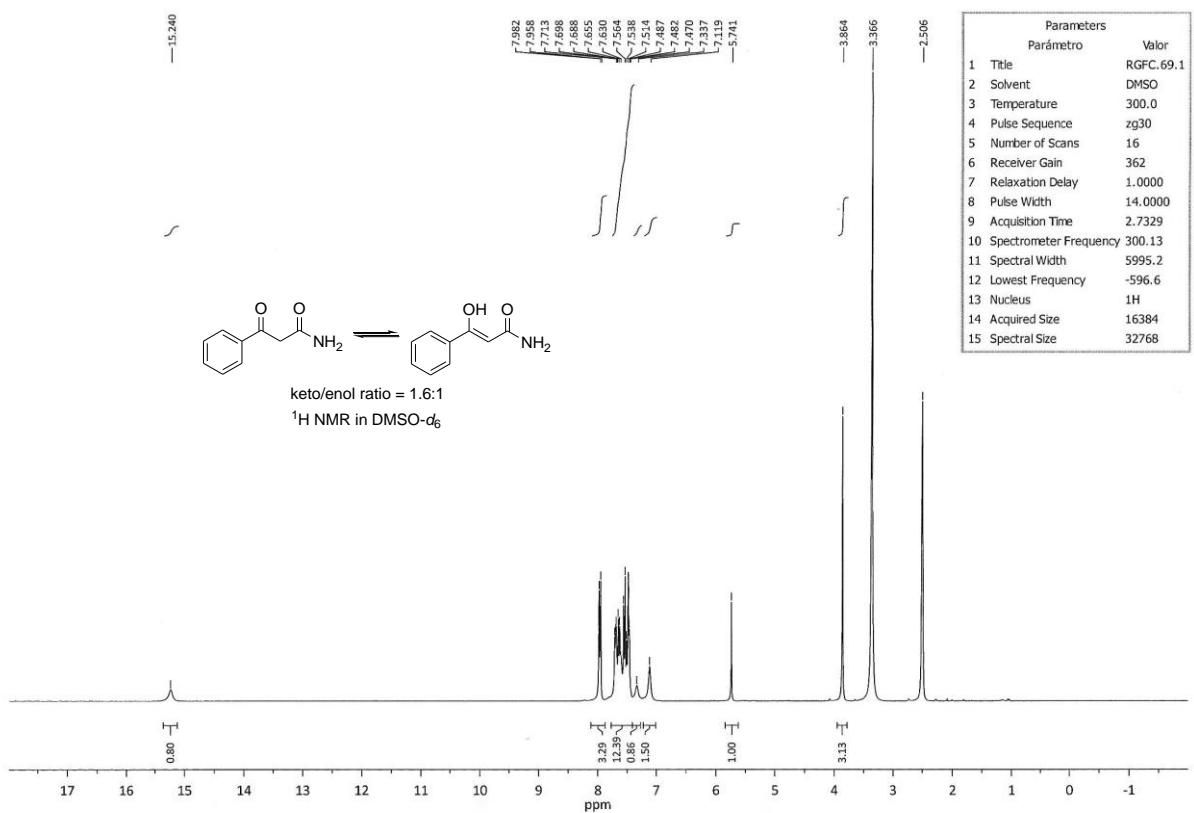


Parameters	
Parámetro	Valor
1 Title	RGFC.90
2 Solvent	DMSO
3 Temperature	300.0
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	90
7 Relaxation Delay	1.0000
8 Pulse Width	14.0000
9 Acquisition Time	2.7329
10 Spectrometer Frequency	300.13
11 Spectral Width	5995.2
12 Lowest Frequency	-596.6
13 Nucleus	¹ H
14 Acquired Size	16384
15 Spectral Size	32768

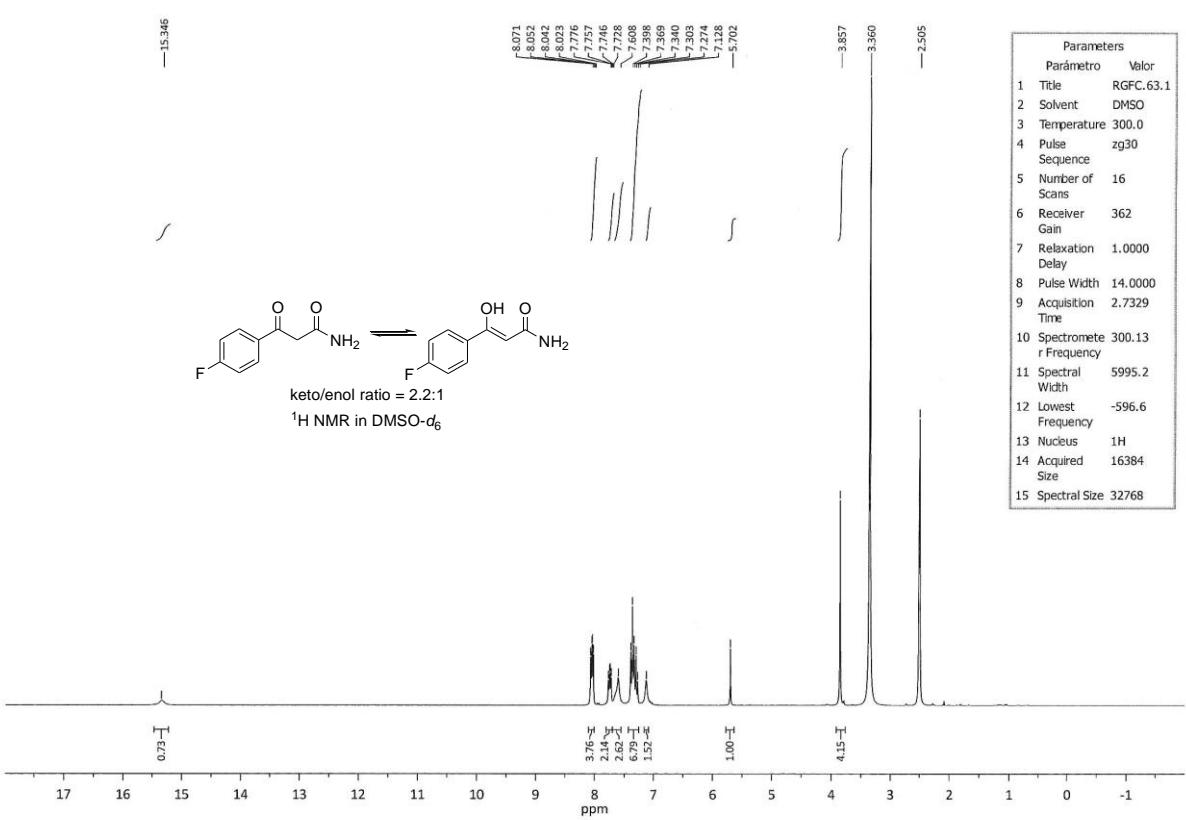
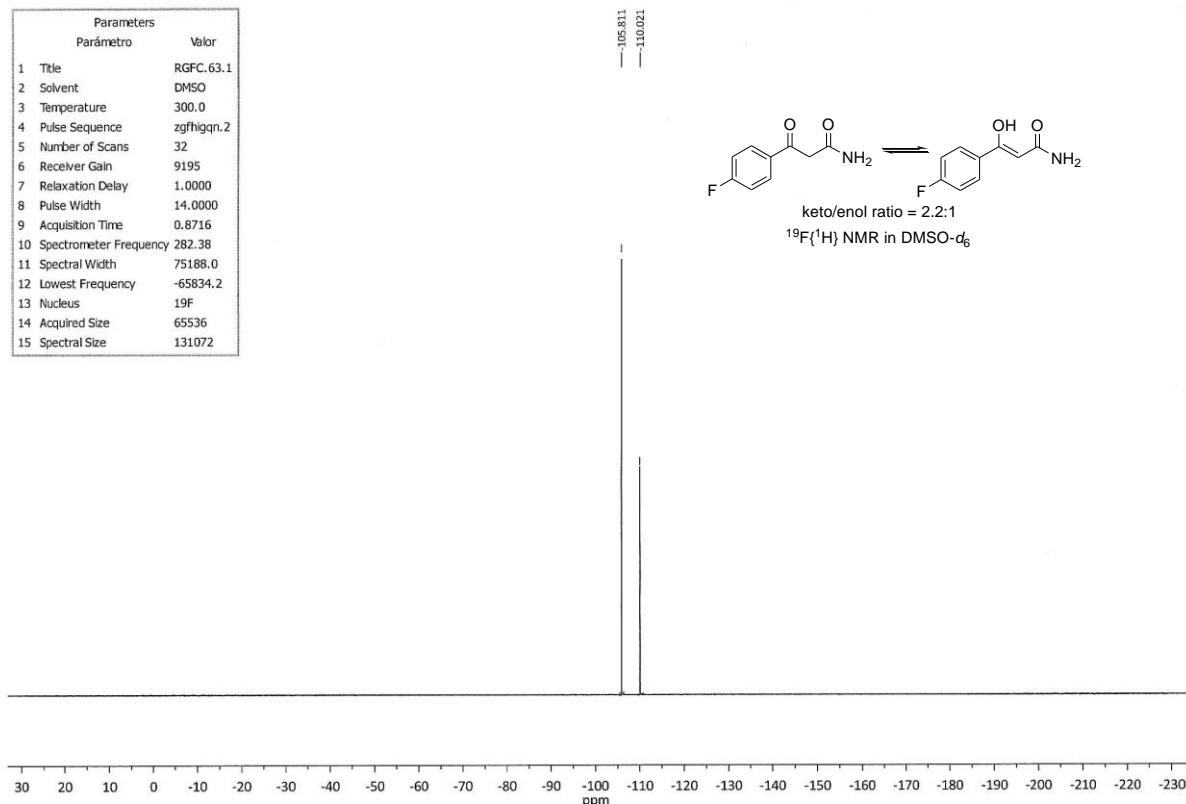


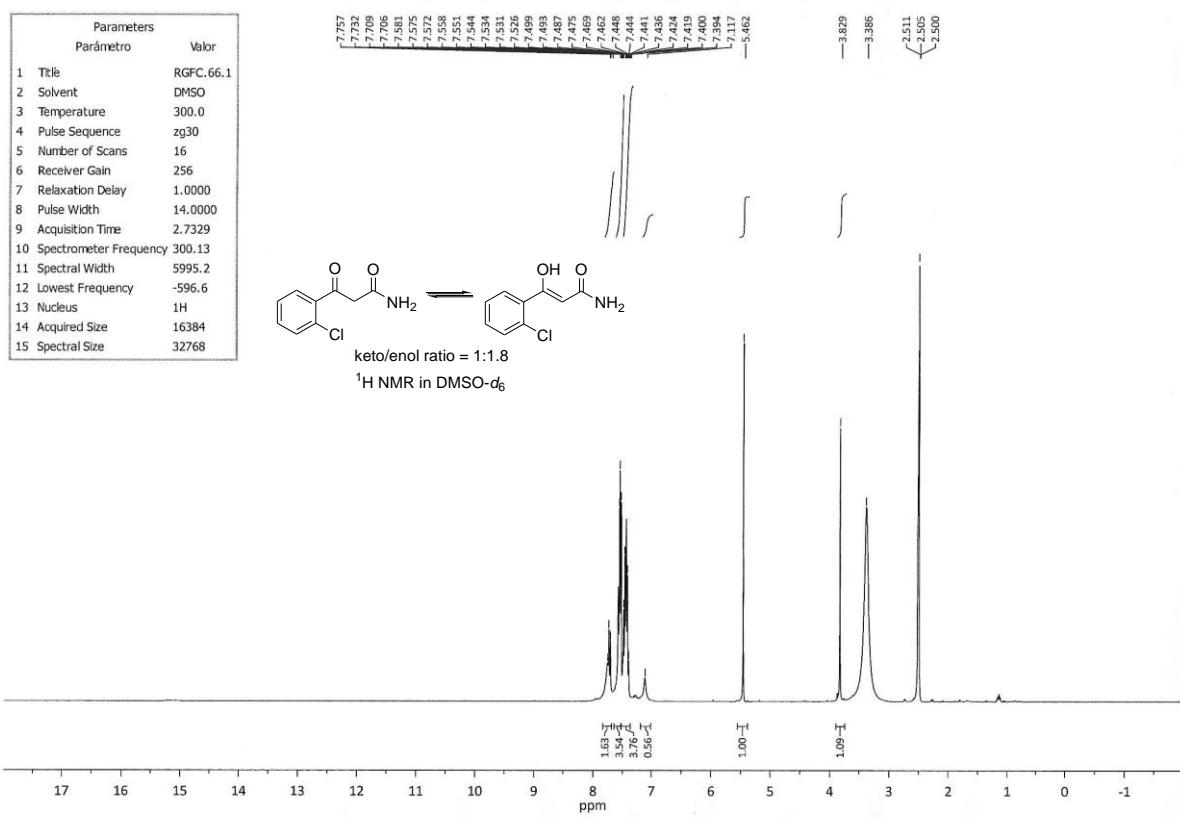
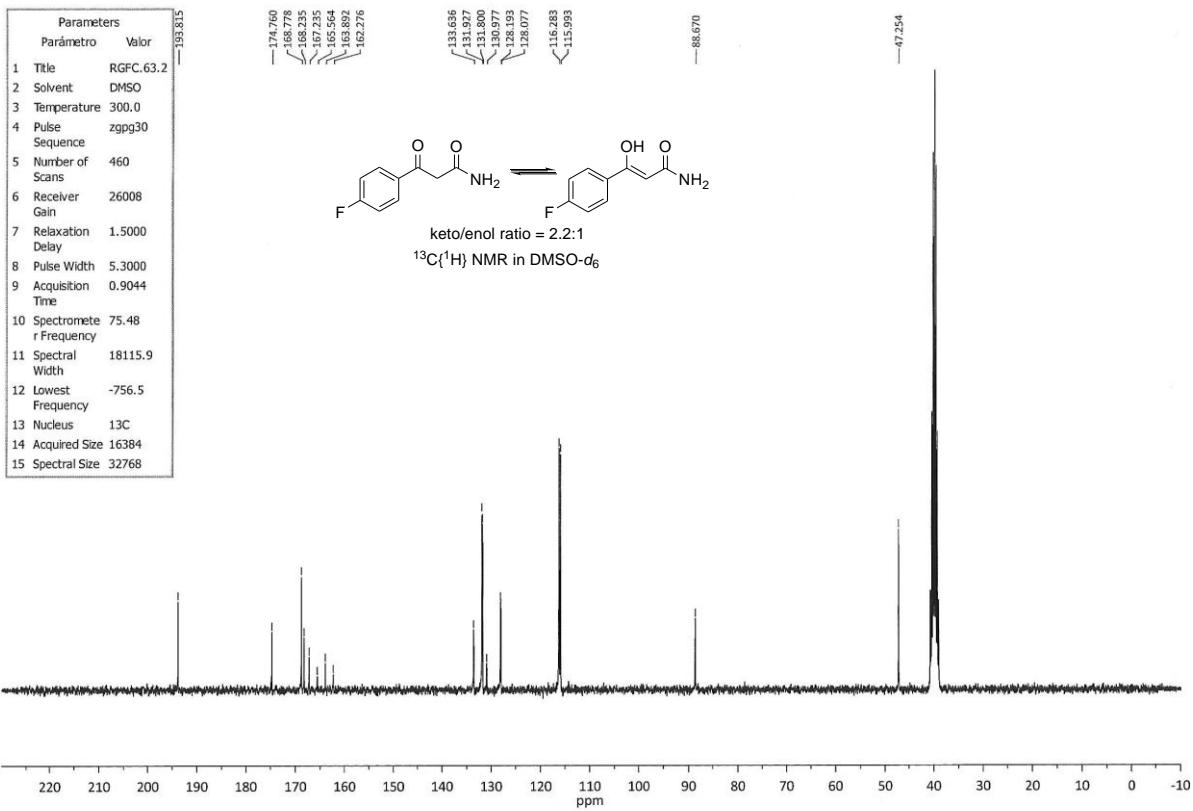
Parámetro	Valor
1 Title	RGFC.90
2 Solvent	DMSO
3 Temperatura	300.0
4 Pulse Sequence	zpg30
5 Number of Scans	440
6 Receiver Gain	18390
7 Relaxation Delay	1.5000
8 Pulse Width	5.3000
9 Acquisition Time	0.9044
10 Spectrometer Frequency	75.48
11 Spectral Width	18115.9
12 Lowest Frequency	-756.5
13 Nucleus	¹³ C
14 Acquired Size	16384
15 Spectral Size	32768

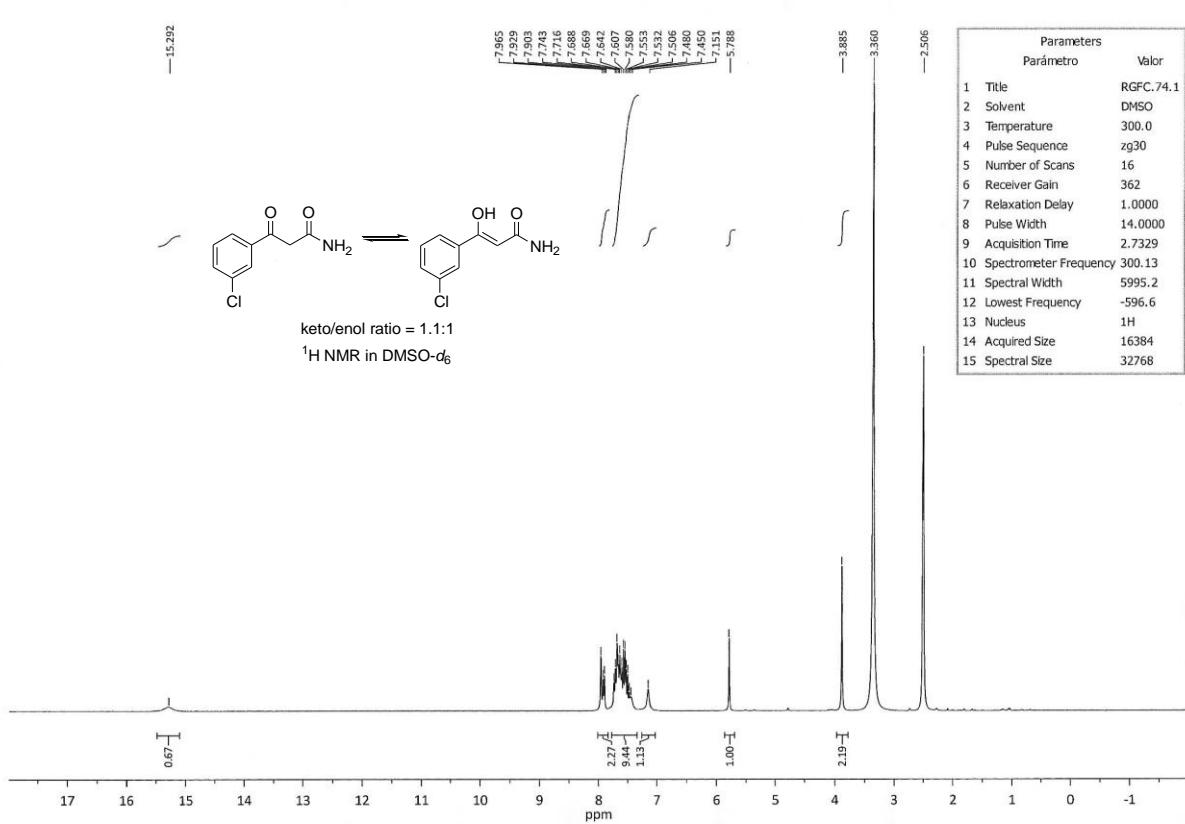
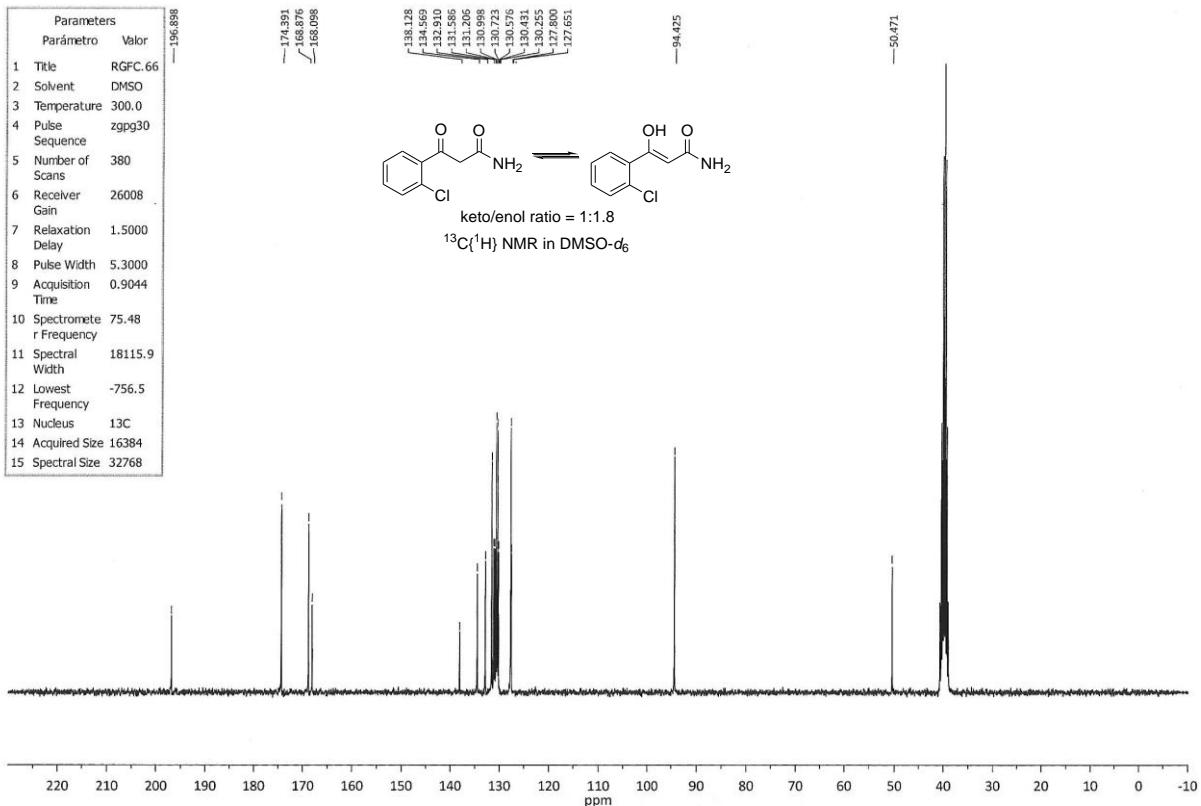


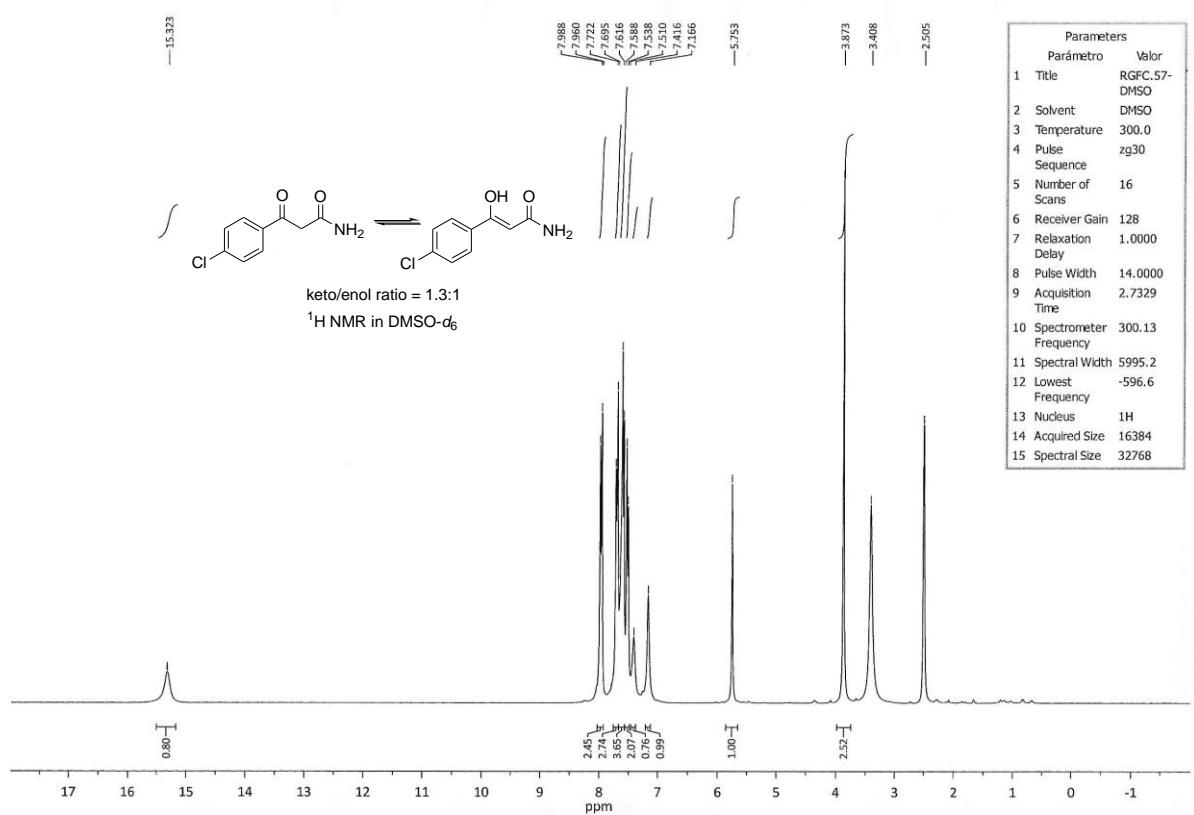
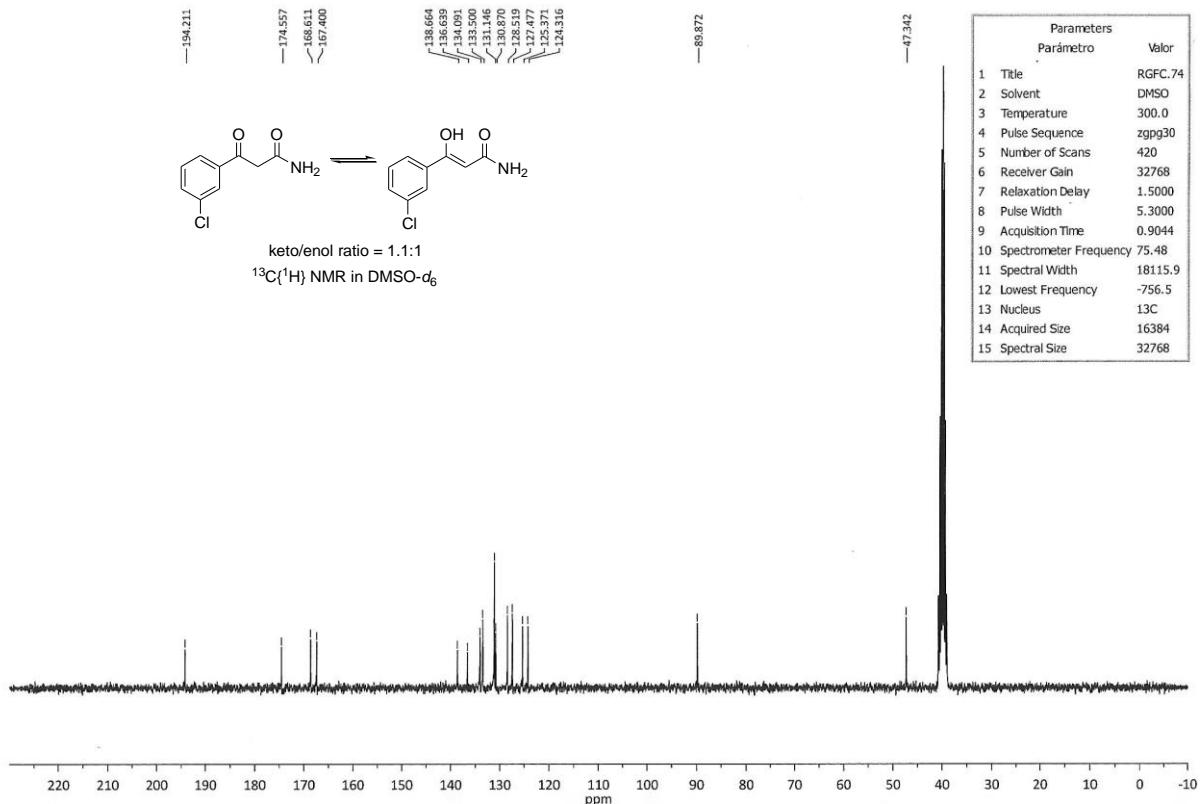


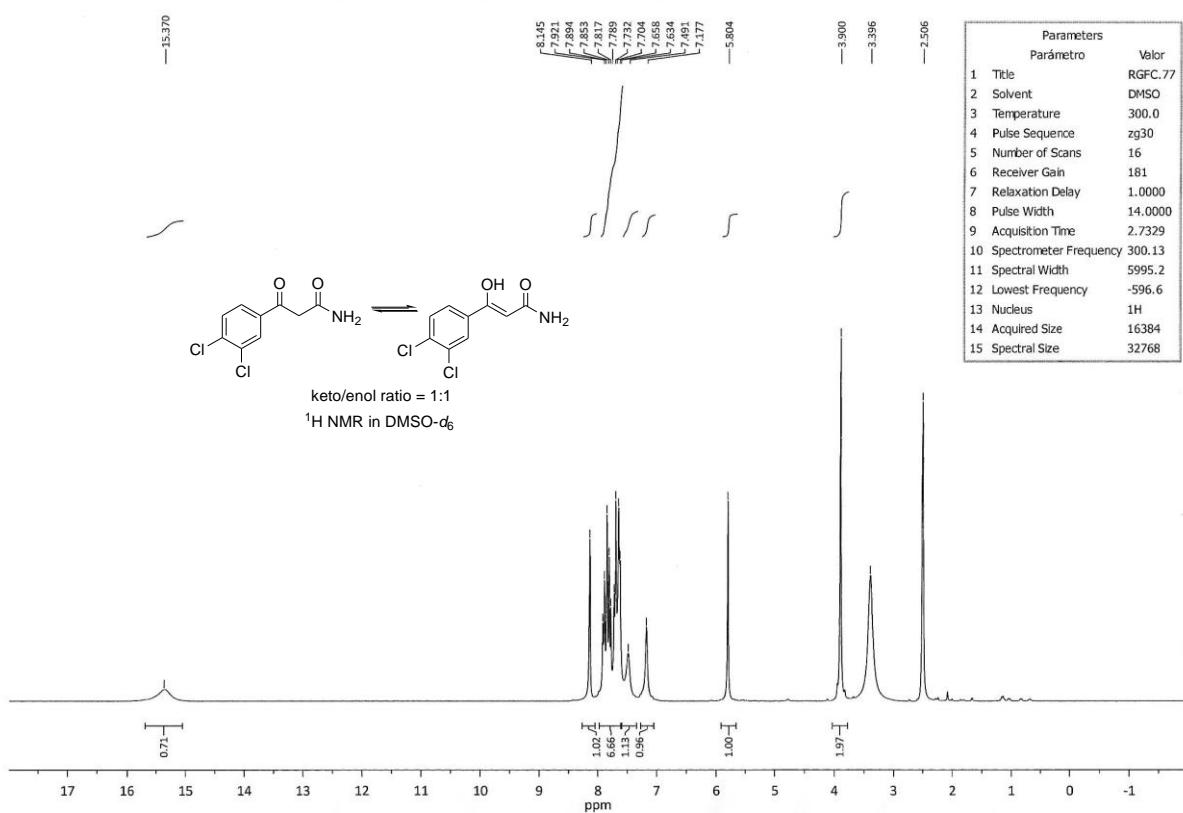
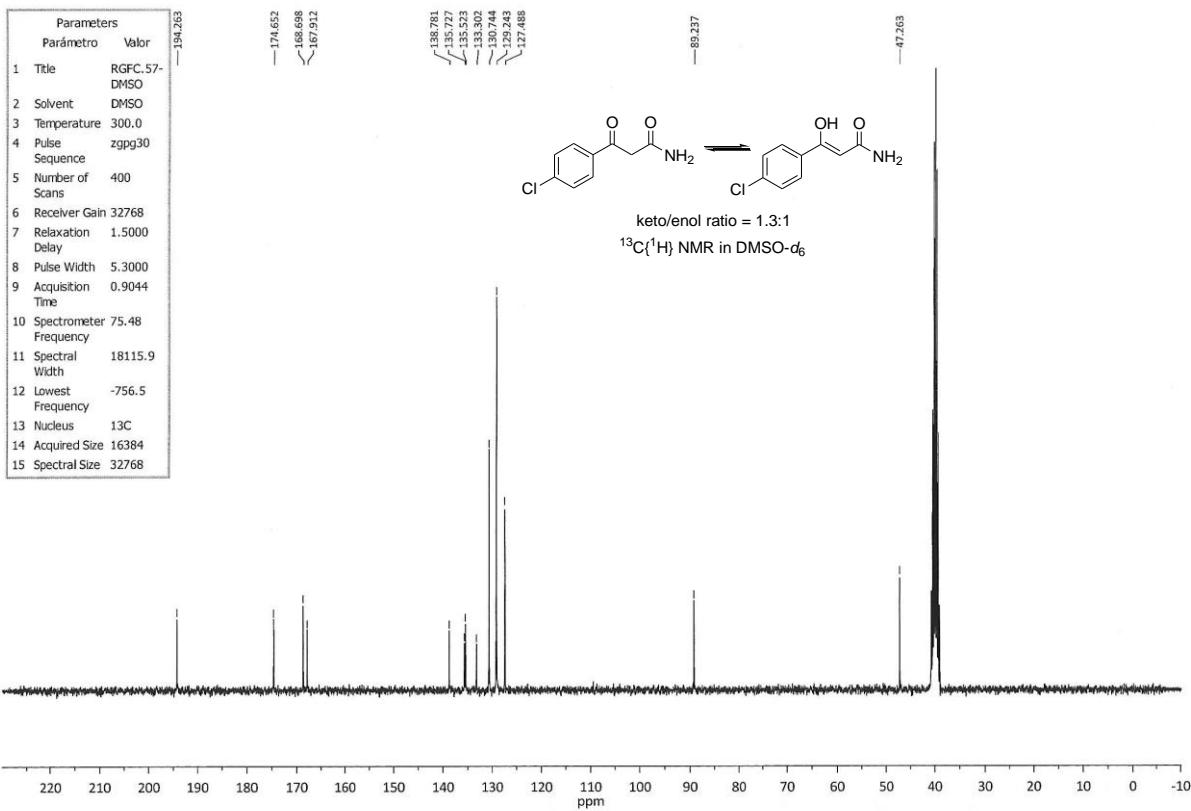
	Parámetro	Valor
1	Title	RGFC.63.1
2	Solvent	DMSO
3	Temperature	300.0
4	Pulse Sequence	zgfhqgn.2
5	Number of Scans	32
6	Receiver Gain	9195
7	Relaxation Delay	1.0000
8	Pulse Width	14.0000
9	Acquisition Time	0.6716
10	Spectrometer Frequency	282.38
11	Spectral Width	75188.0
12	Lowest Frequency	-65834.2
13	Nucleus	¹⁹ F
14	Acquired Size	65536
15	Spectral Size	131072

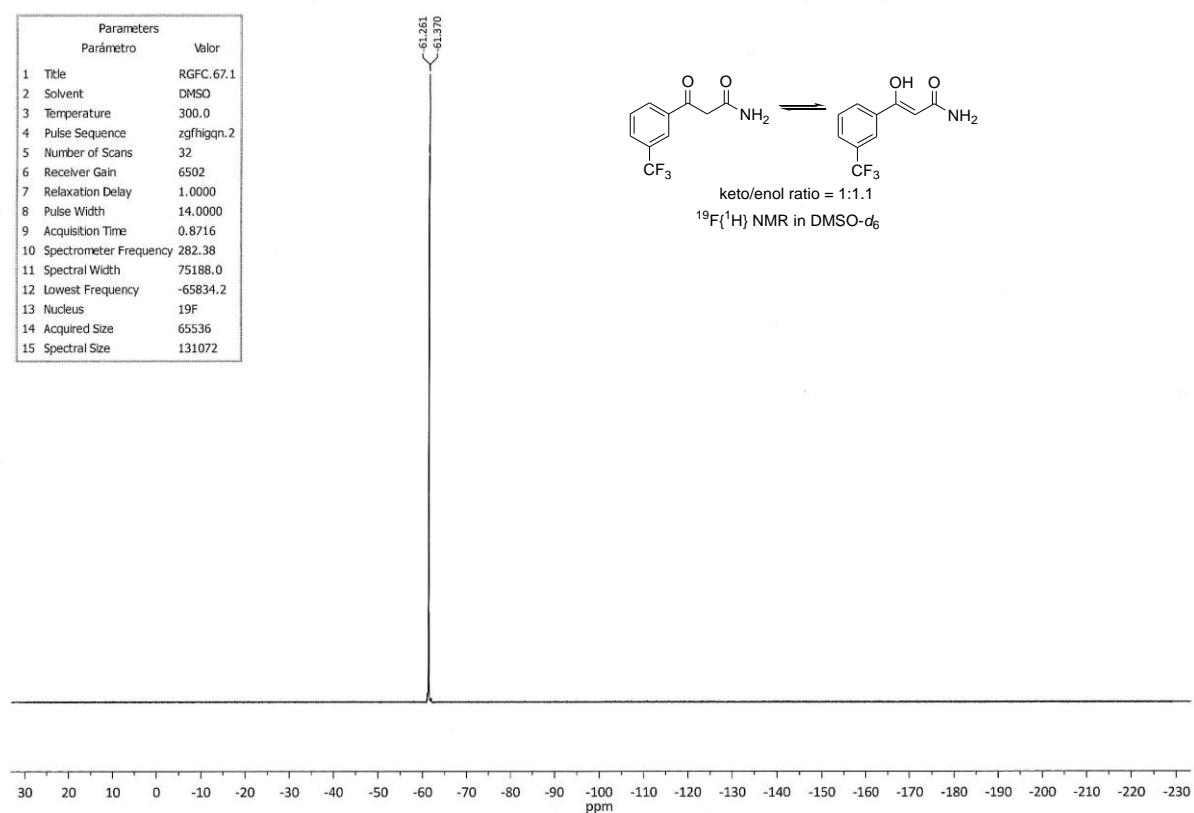
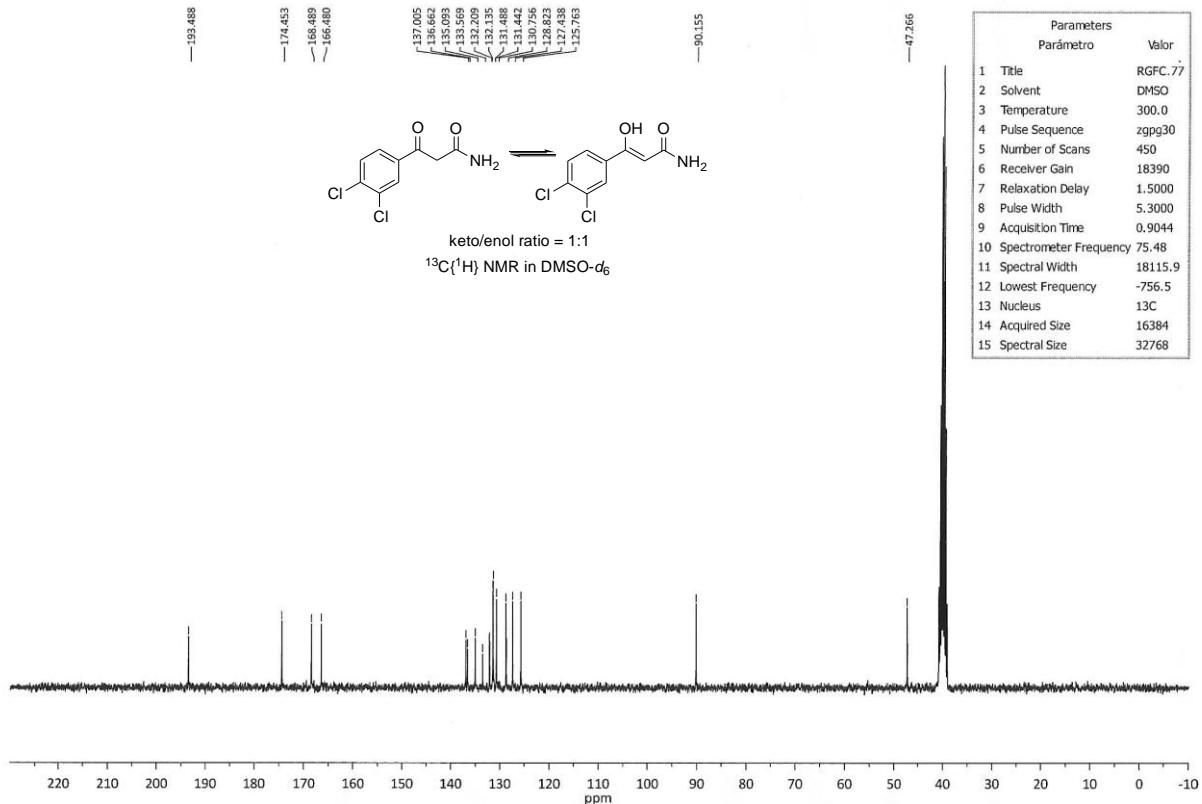


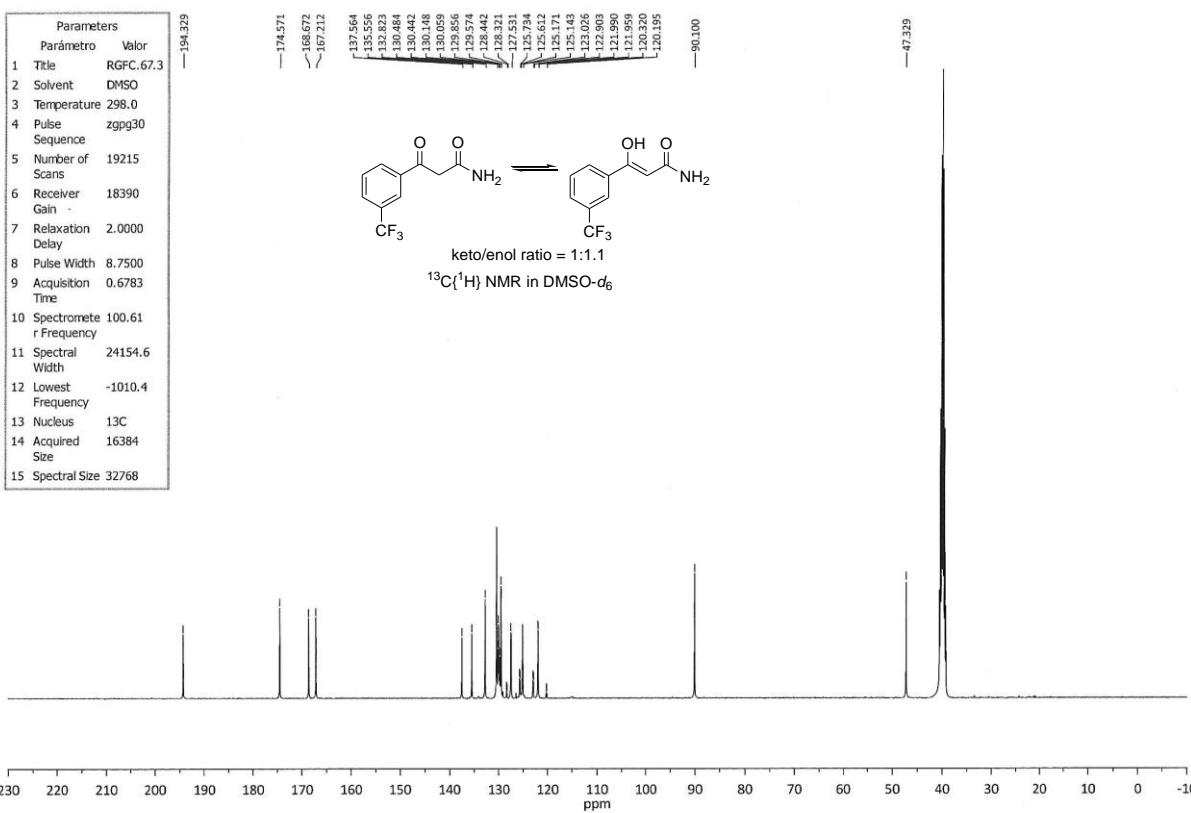
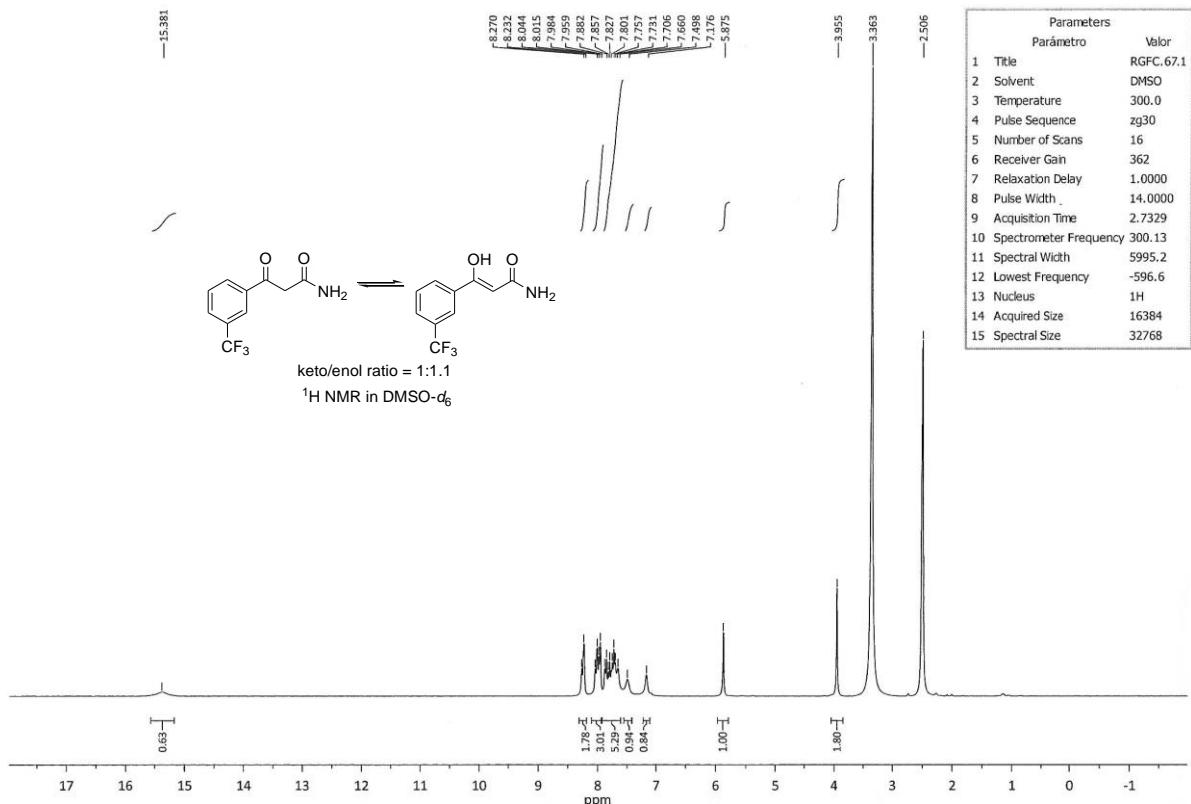


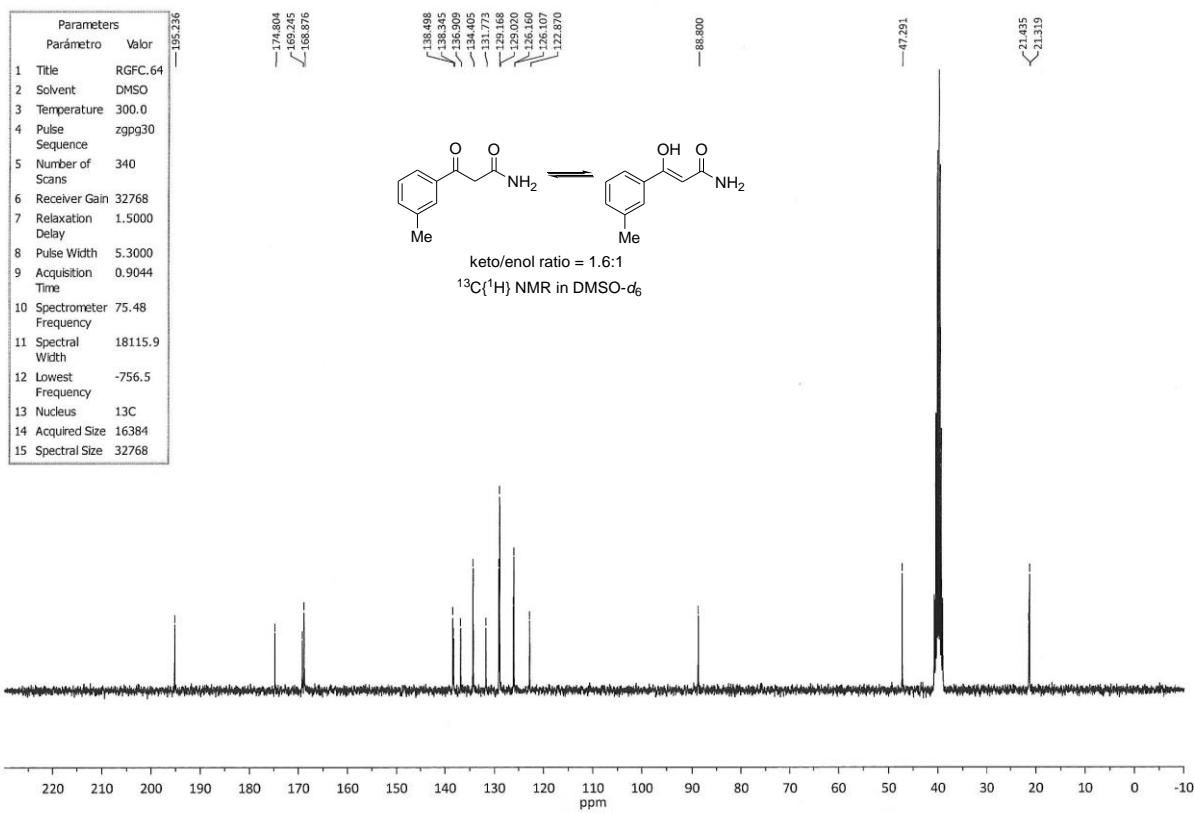
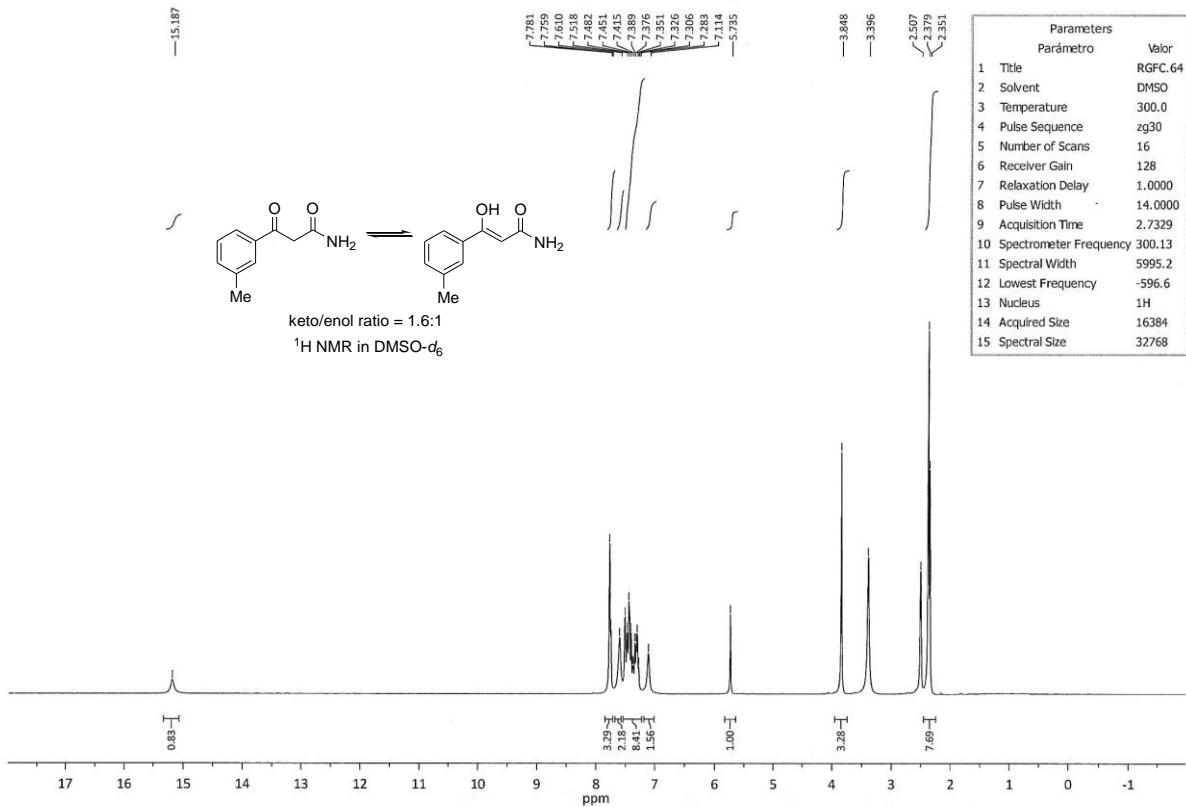


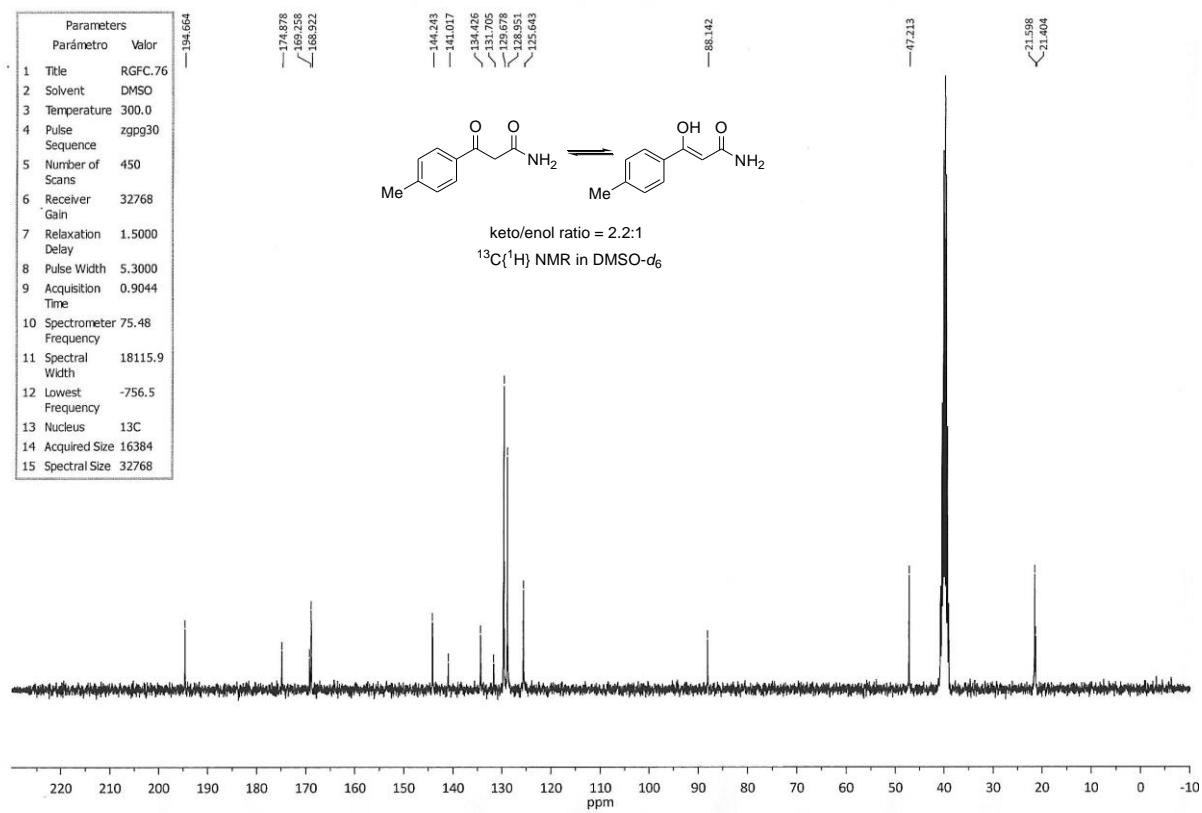
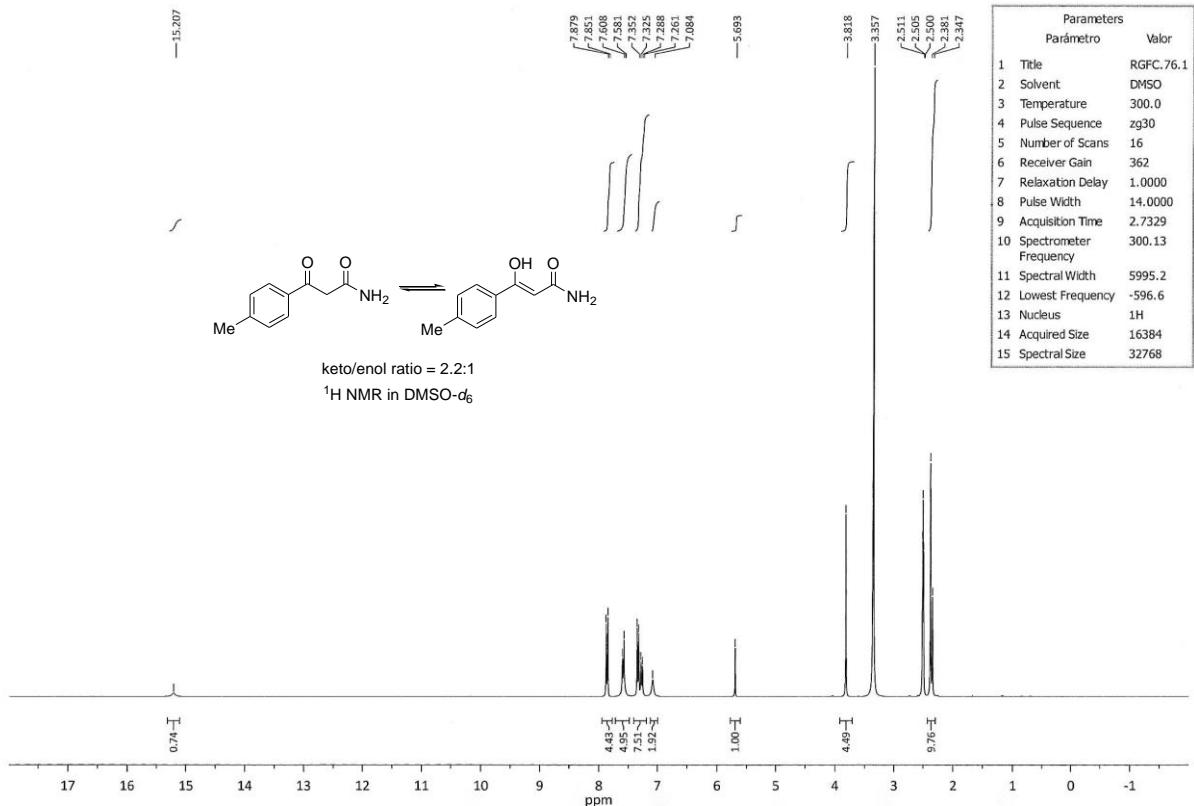


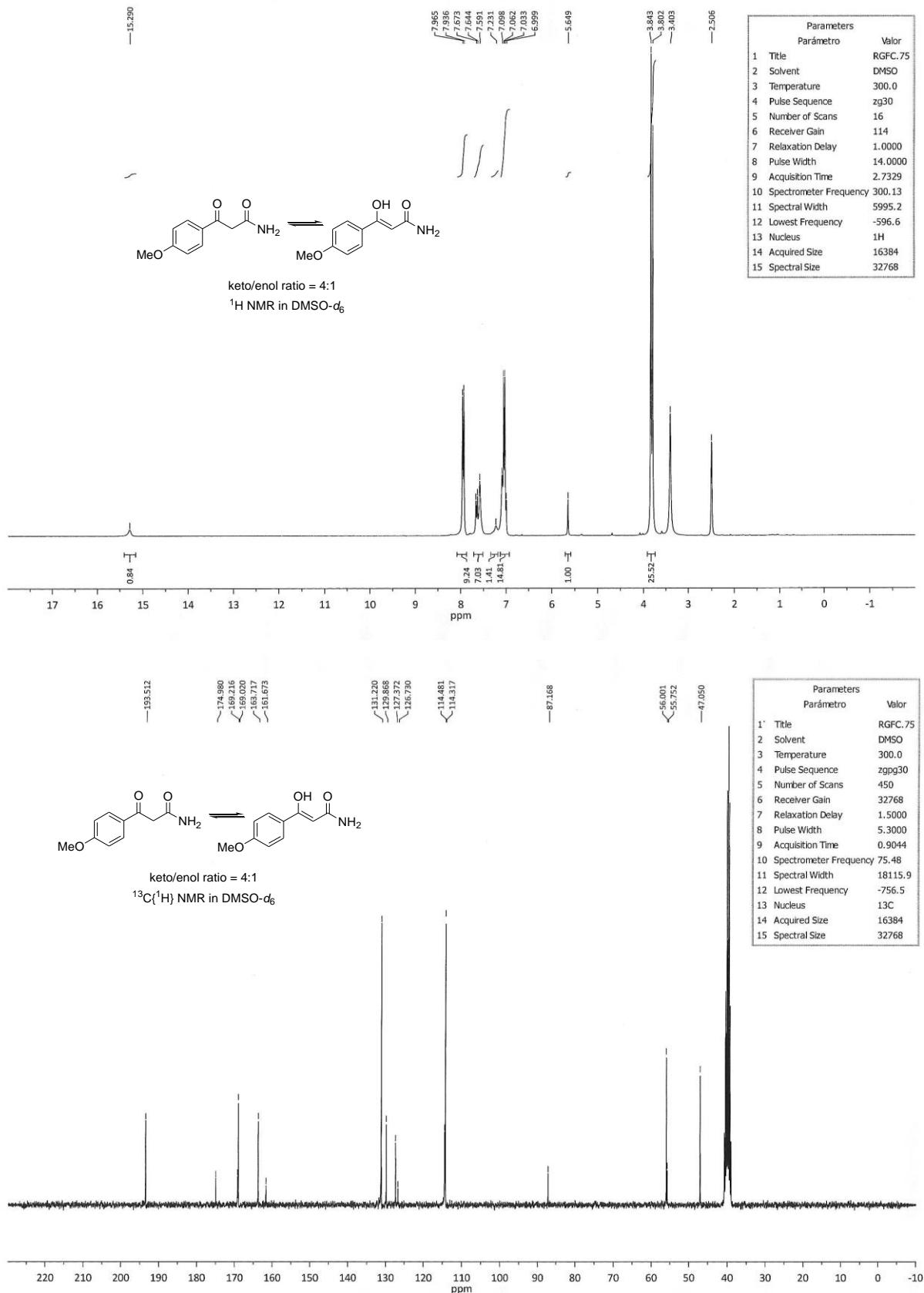


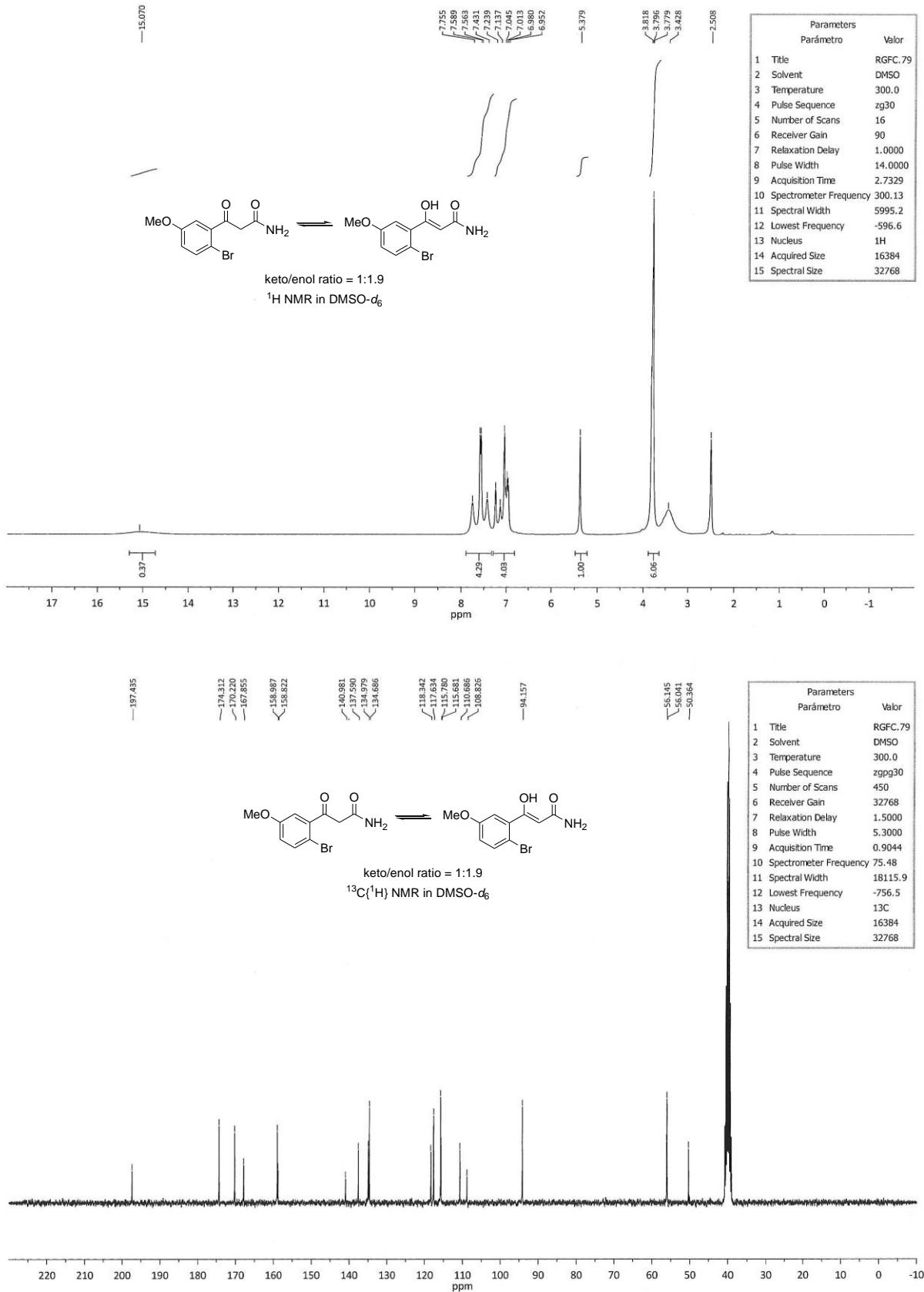




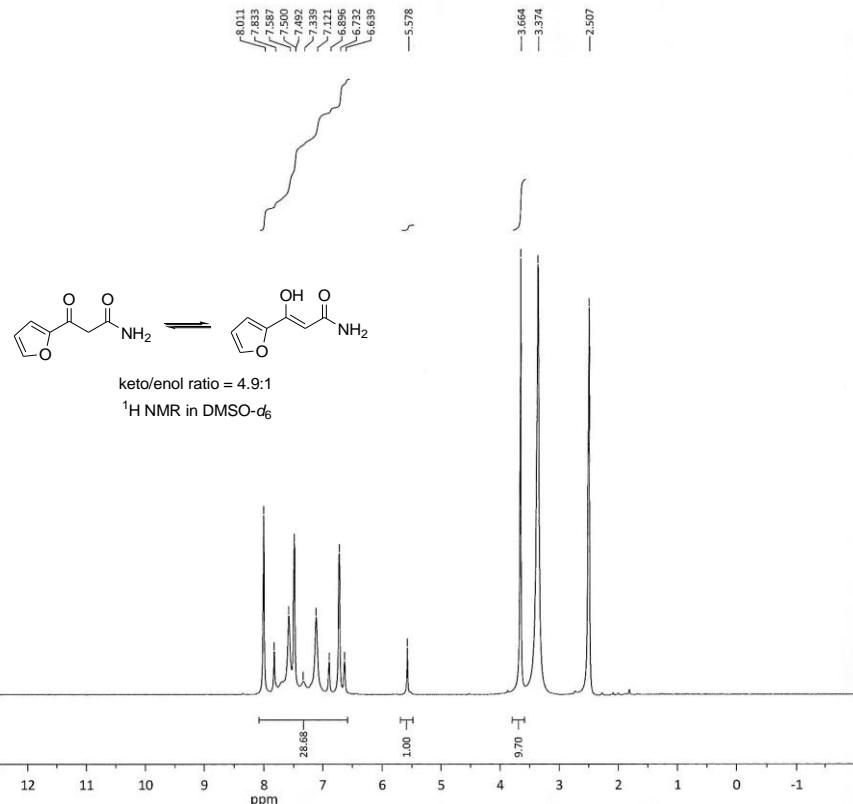




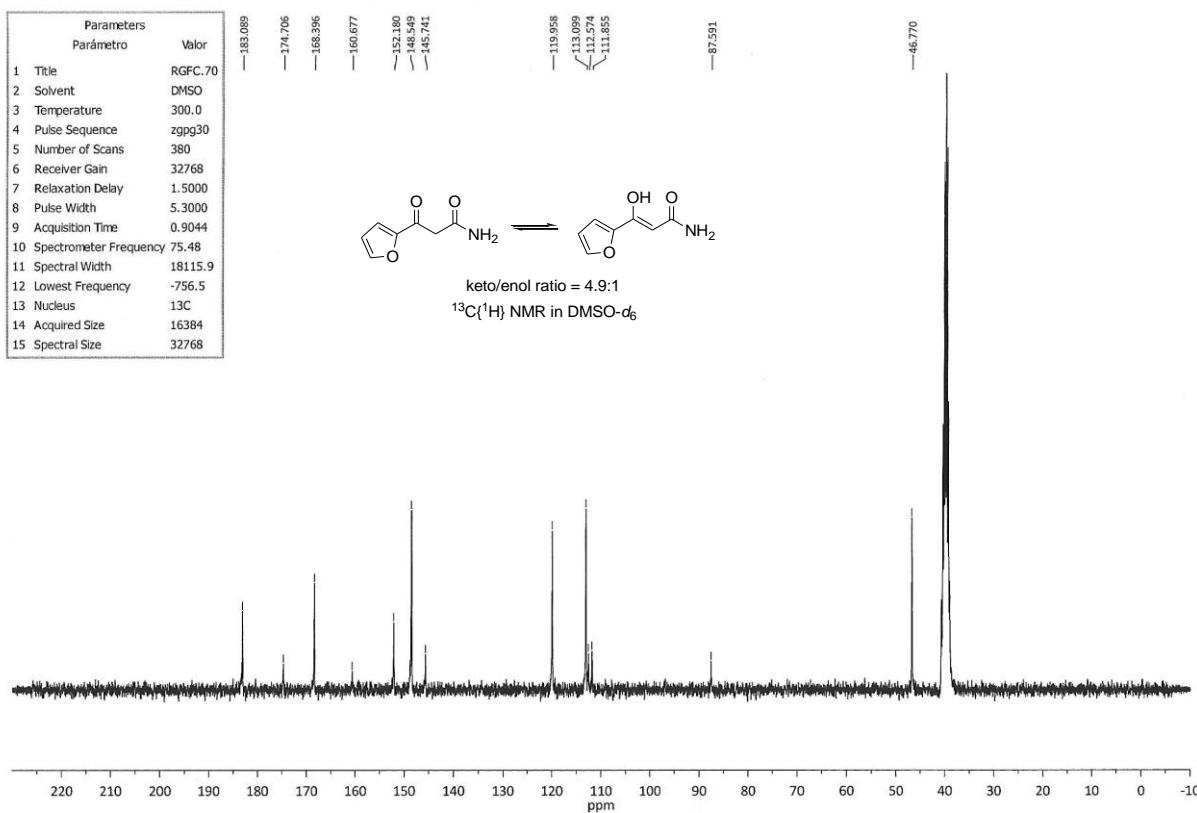




Parámetro	Valor
1 Title	RGFC.70.1
2 Solvent	DMSO
3 Temperatura	300.0
4 Pulse Sequence	zg30
5 Number of Scans	16
6 Receiver Gain	362
7 Relaxation Delay	1.0000
8 Pulse Width	14.0000
9 Acquisition Time	2.7329
10 Spectrometer Frequency	300.13
11 Spectral Width	5995.2
12 Lowest Frequency	-596.6
13 Nucleus	1H
14 Acquired Size	16384
15 Spectral Size	32768



Parámetro	Valor
1 Title	RGFC.70.1
2 Solvent	DMSO
3 Temperatura	300.0
4 Pulse Sequence	zgpg30
5 Number of Scans	380
6 Receiver Gain	32768
7 Relaxation Delay	1.5000
8 Pulse Width	5.3000
9 Acquisition Time	0.9044
10 Spectrometer Frequency	75.48
11 Spectral Width	18115.9
12 Lowest Frequency	-756.5
13 Nucleus	13C
14 Acquired Size	16384
15 Spectral Size	32768



Parameters	Parámetro	Valor
1 Title	RGFC.78	
2 Solvent	DMSO	
3 Temperature	300.0	
4 Pulse Sequence	zg30	
5 Number of Scans	16	
6 Receiver Gain	128	
7 Relaxation Delay	1.0000	
8 Pulse Width	14.0000	
9 Acquisition Time	2.7329	
10 Spectrometer Frequency	300.13	
11 Spectral Width	5995.2	
12 Lowest Frequency	-596.6	
13 Nucleus	1H	
14 Acquired Size	16384	
15 Spectral Size	32768	

