

Supporting Information

The Goldilocks Principle in Phase Labelling. Minimalist and Orthogonal Phase Tagging for Chromatography-free Mitsunobu Reaction

Mariann Szigeti, Zoltán Dobi, Tibor Soós*

Institute of Organic Chemistry, Research Centre of Natural Sciences, Hungarian Academy of Sciences

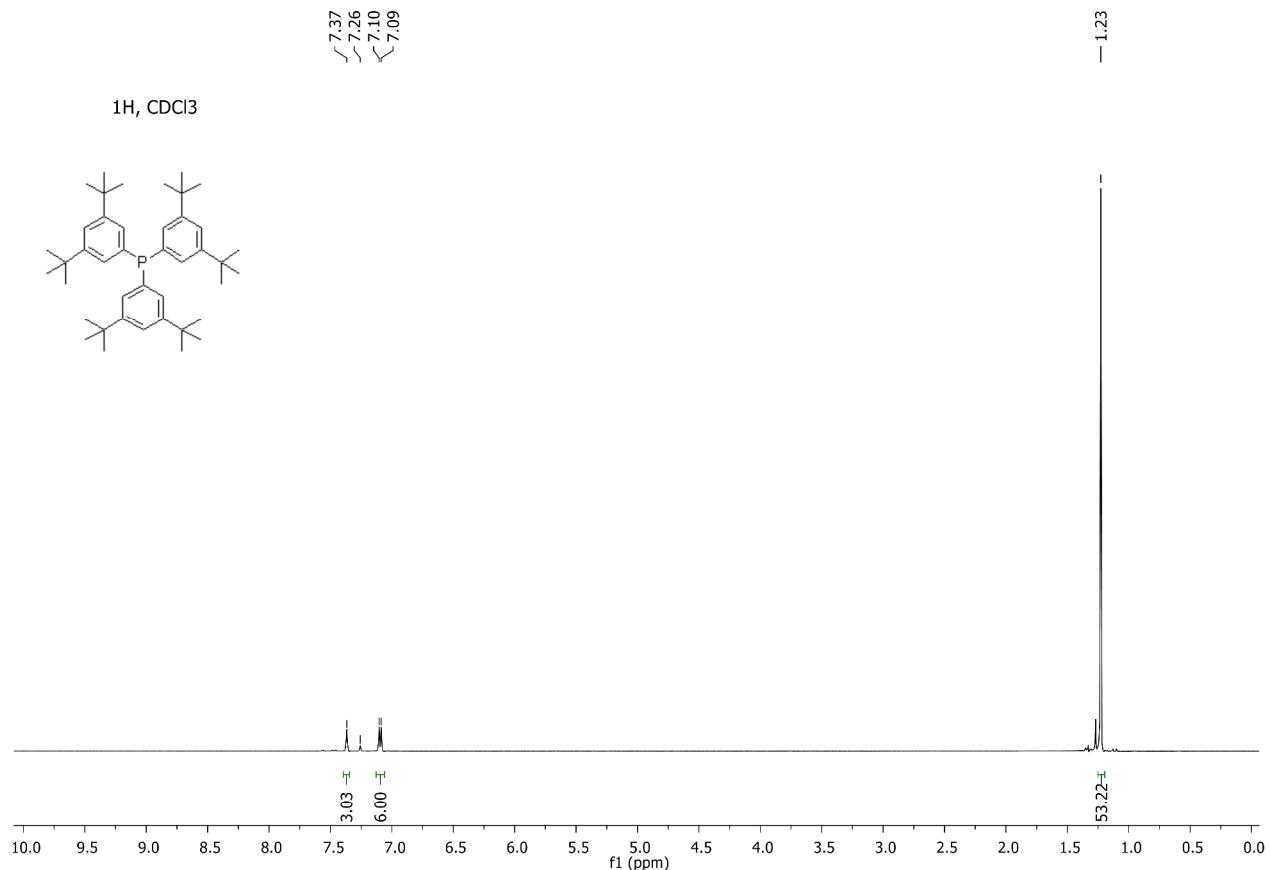
Magyar tudósok körútja 2., H-1117, Budapest, Hungary

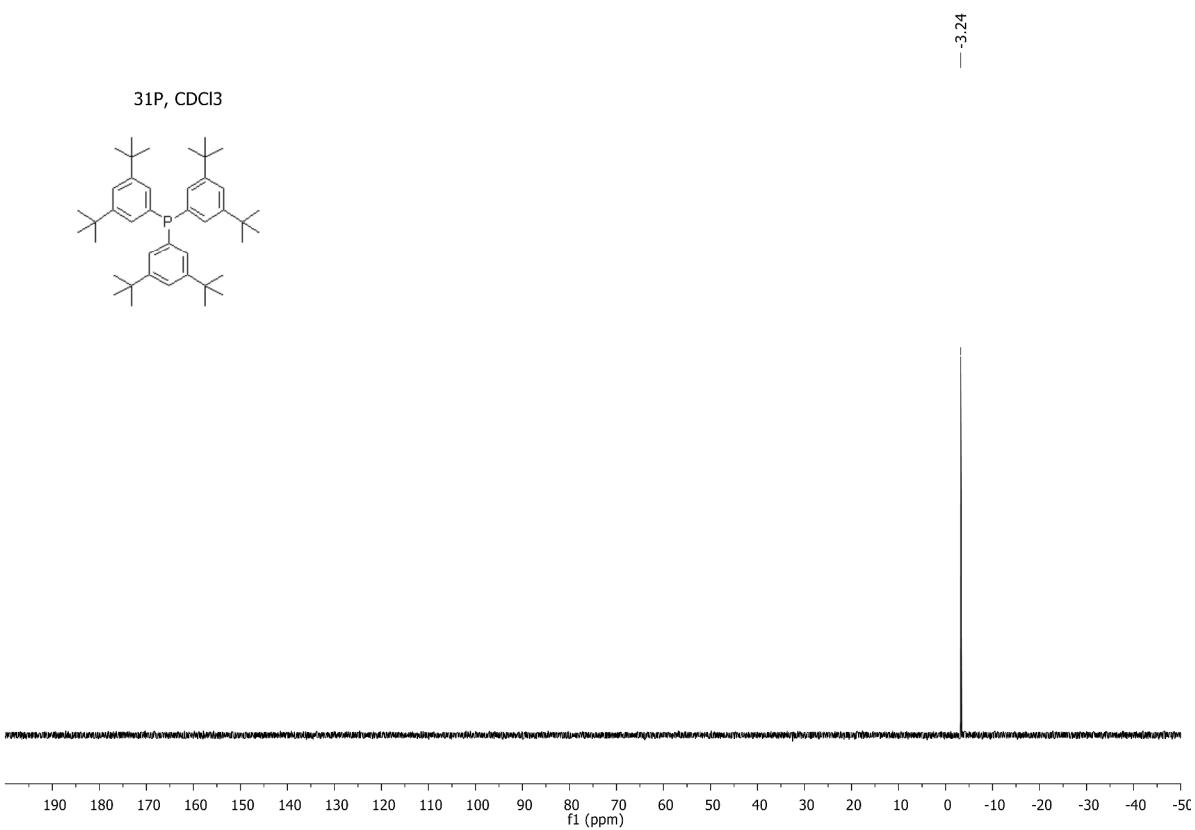
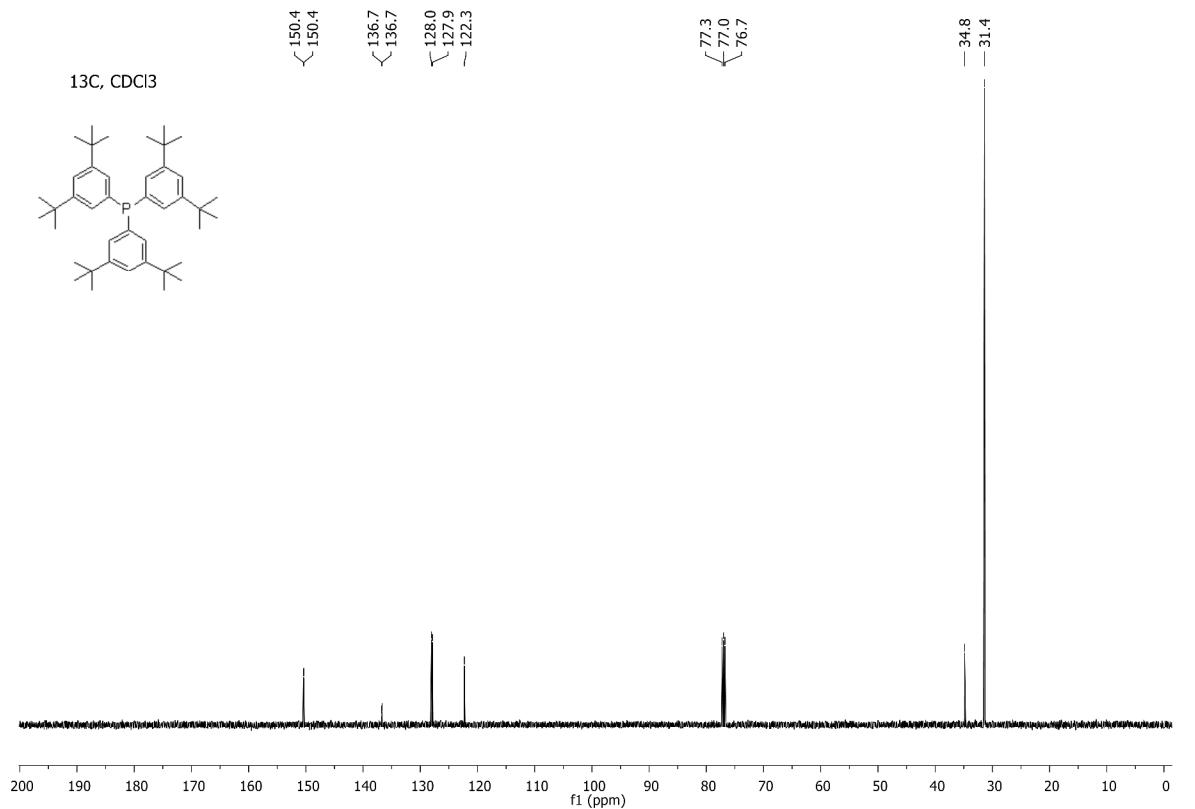
*Corresponding author: soos.tibor@ttk.mta.hu

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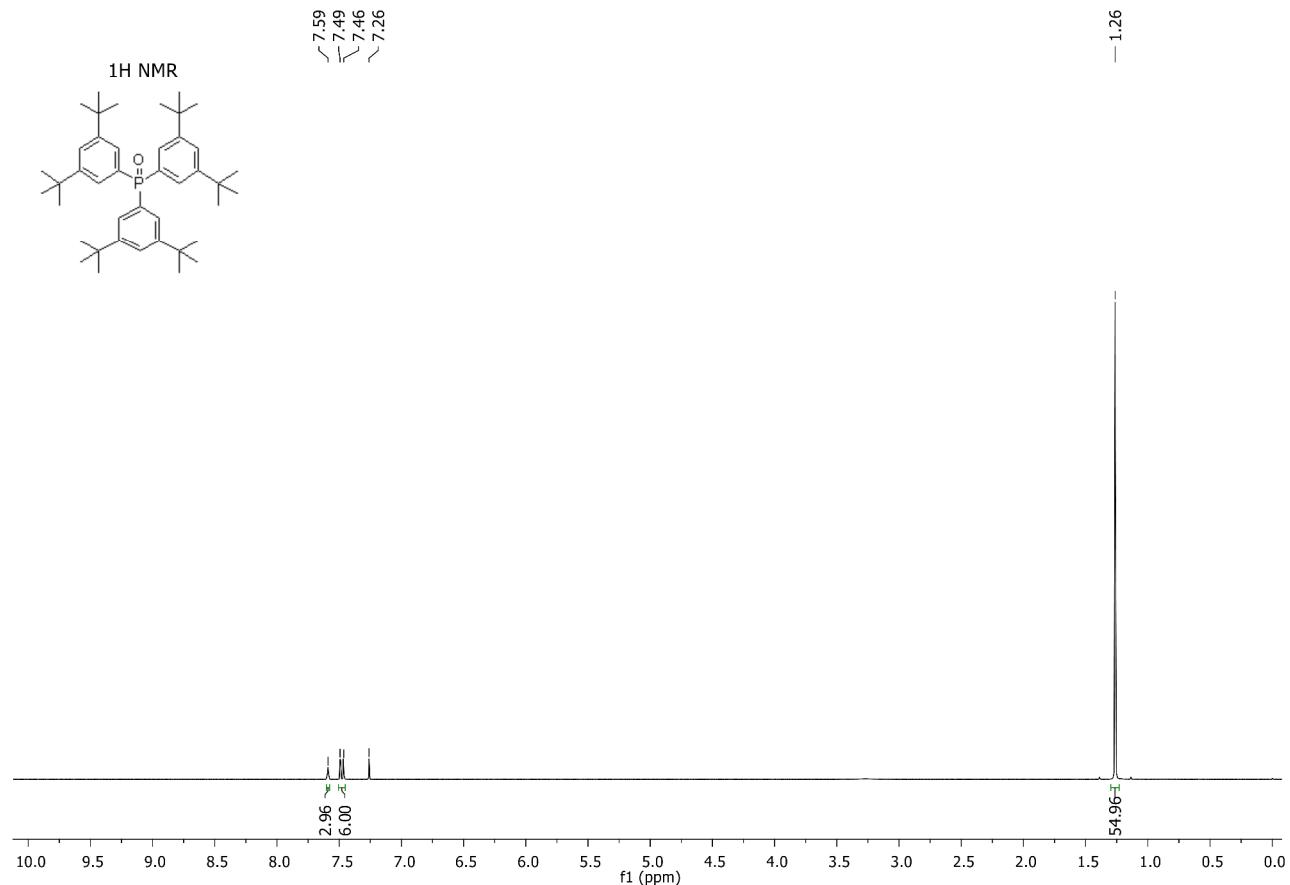
I. NMR Spectra (^1H , ^{13}C , ^{31}P) and HPLC analysis of compounds	2
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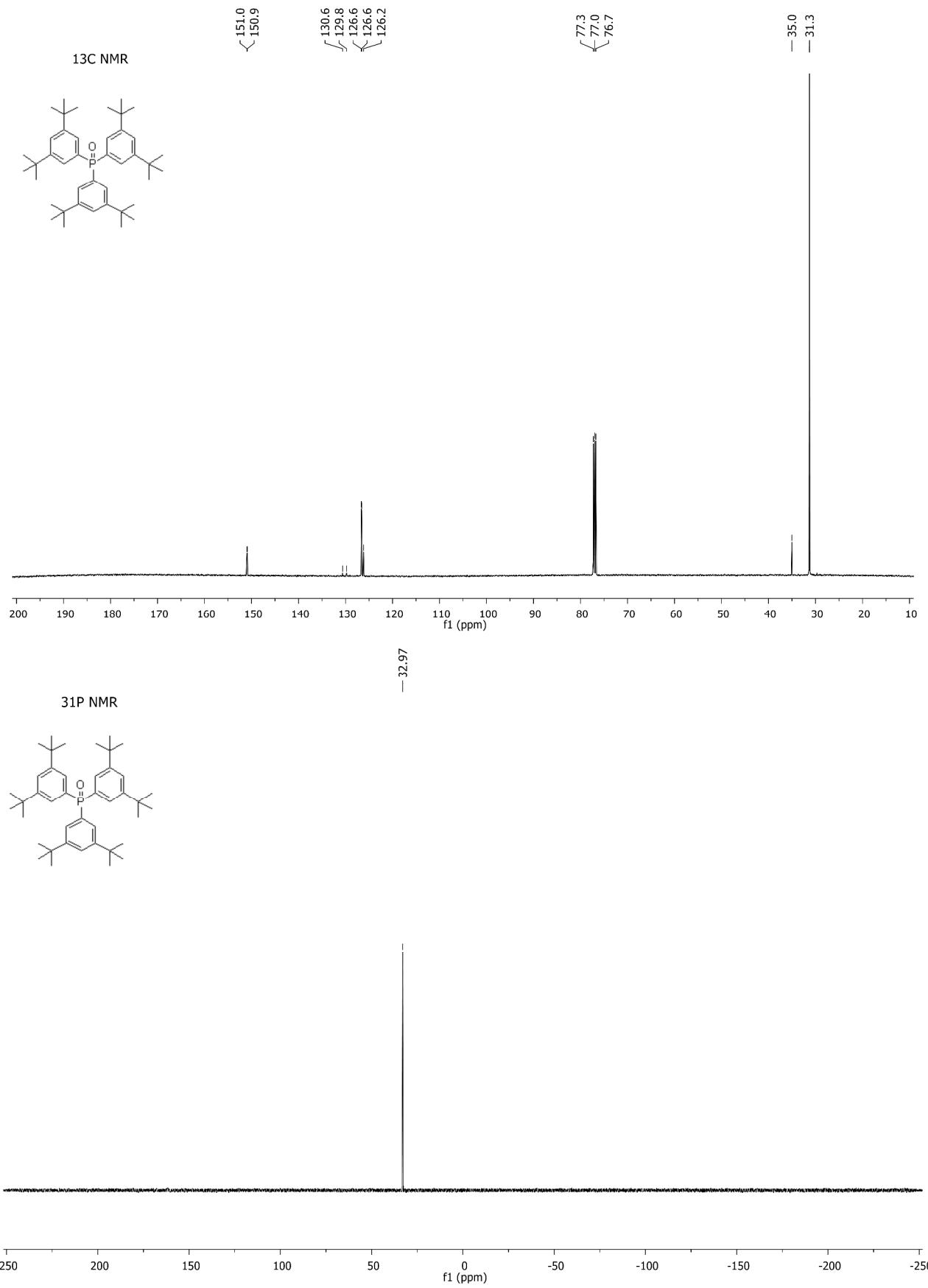
I. NMR Spectra (^1H , ^{13}C , ^{31}P) and HPLC analysis of compounds
Tris(3,5-di-*tert*-butylphenyl)phosphine (C)





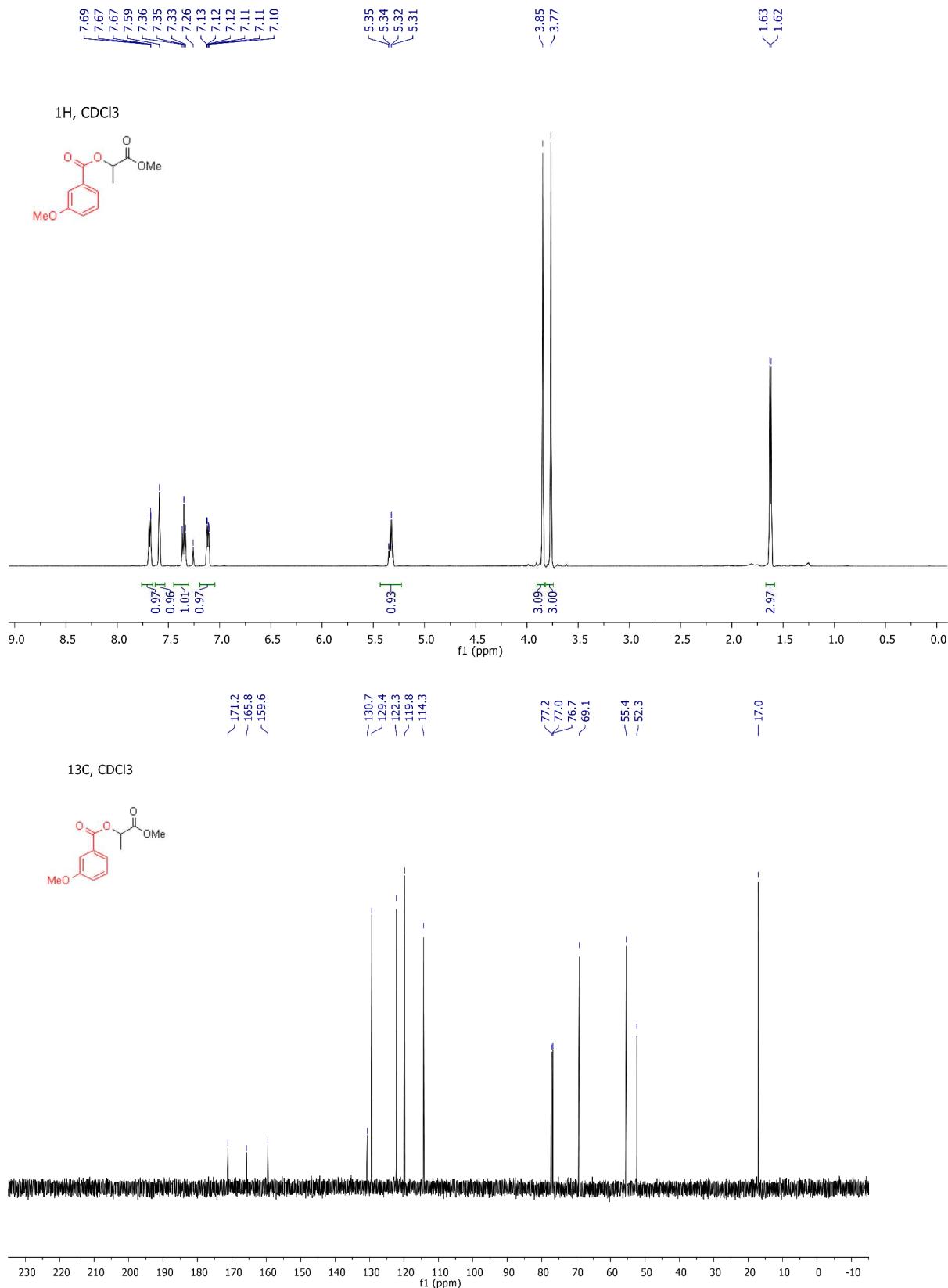
Tris(3,5-di-*tert*-butylphenyl)phosphine oxide (C-oxide)



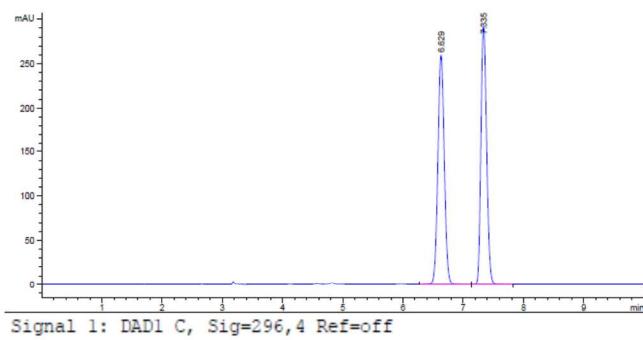
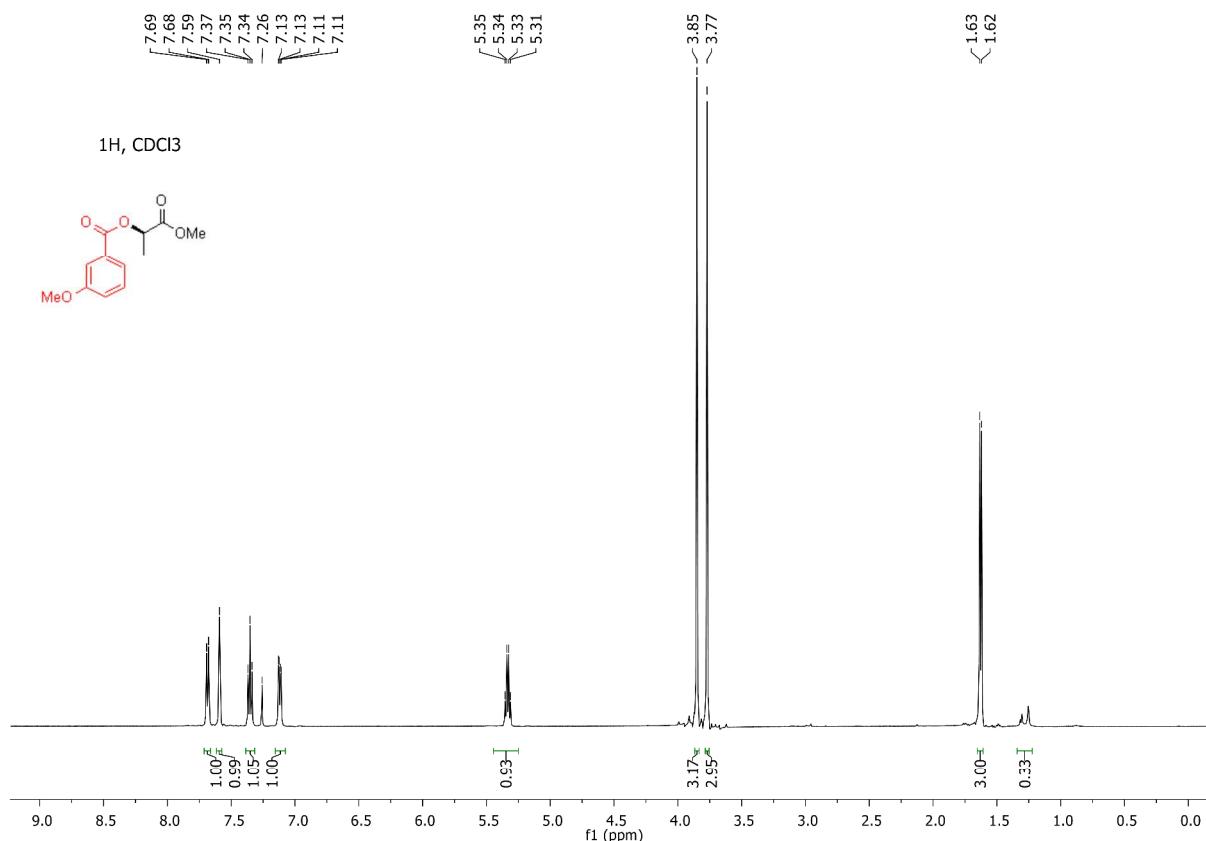


S5

1-methoxy-1-oxopropan-2-yl 3-methoxybenzoate (3**, *Method B*)**

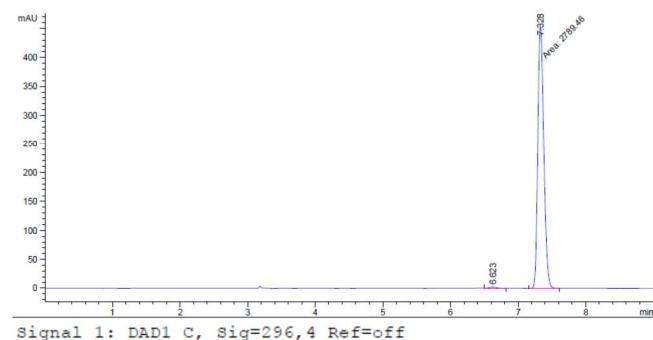


1-methoxy-1-oxopropan-2-yl 3-methoxybenzoate (3, Method A)



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.629	BB	0.1153	1920.99084	259.67642	50.0407
2	7.335	BB	0.1035	1917.86243	292.64941	49.9593

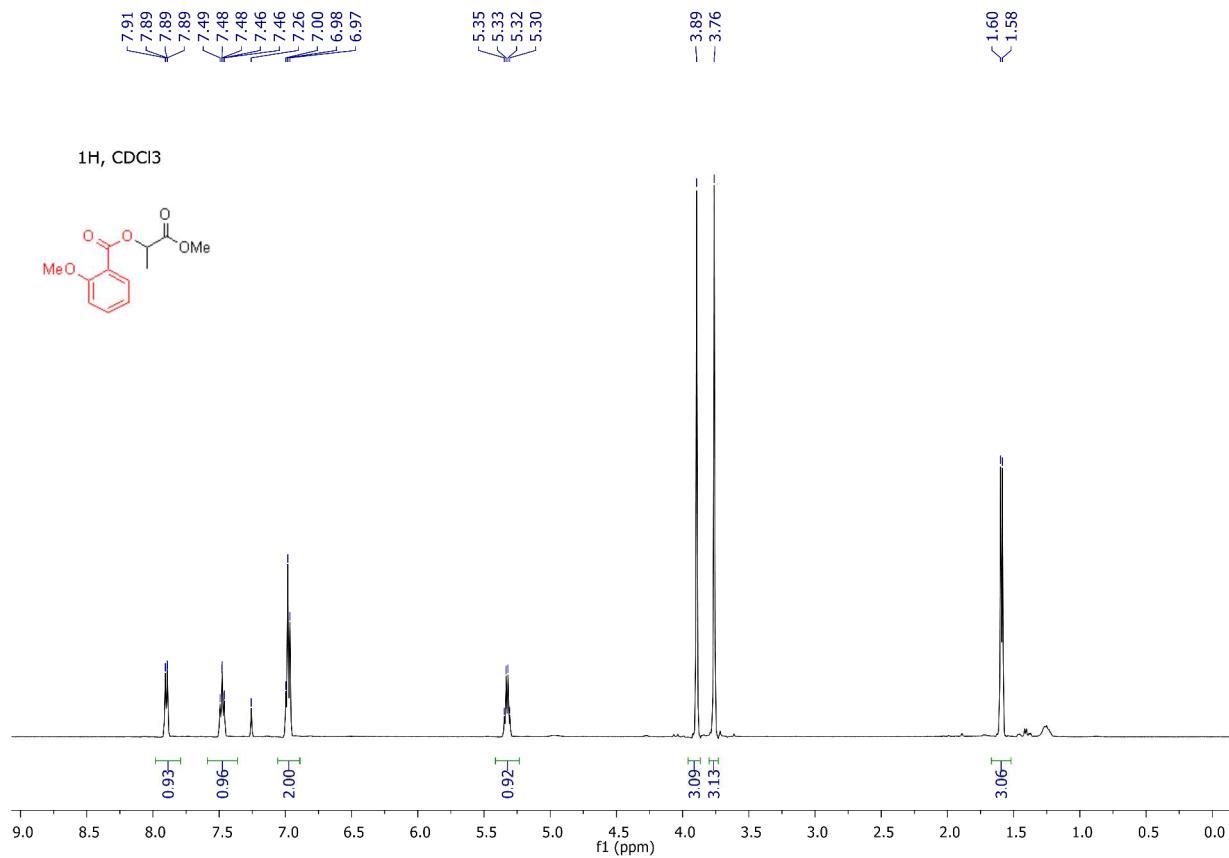
Totals : 3838.85327 552.32584

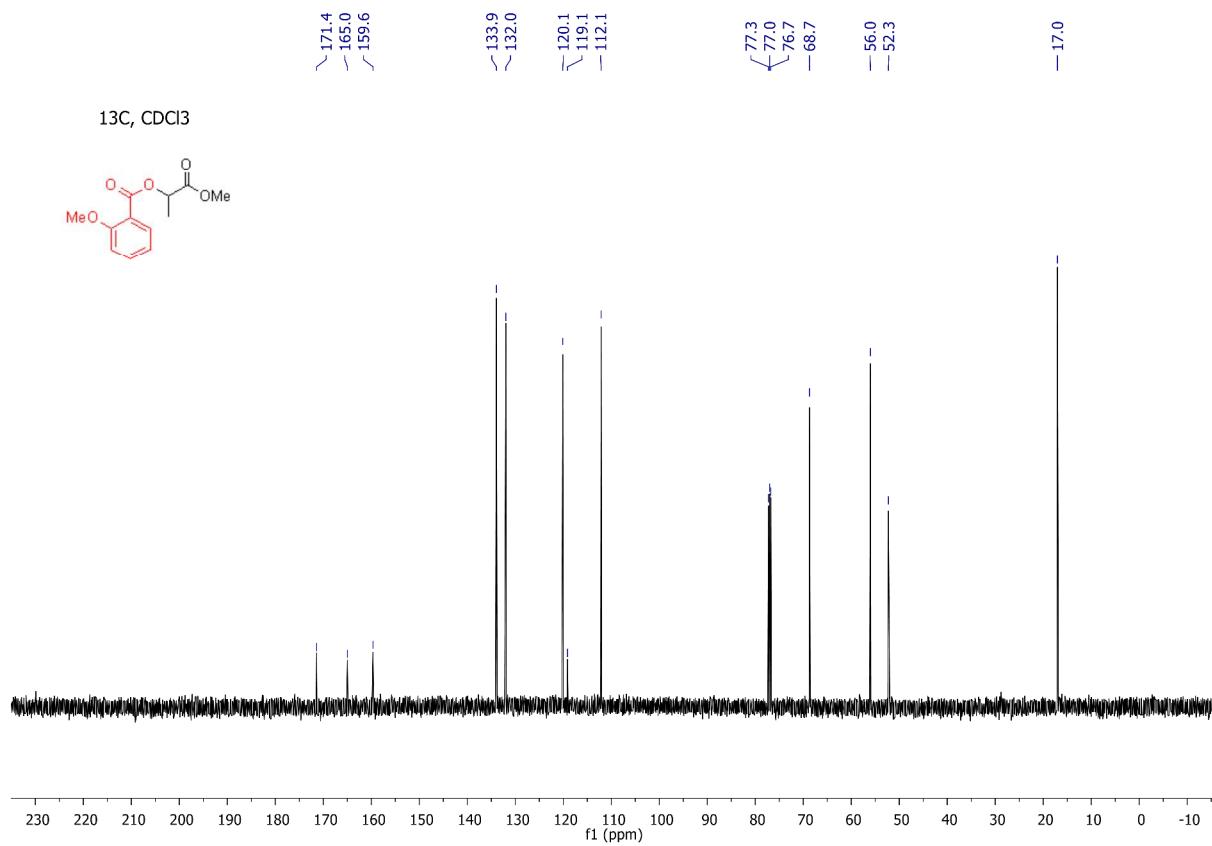


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.623	VB	0.1153	16.74639	2.23801	0.5968
2	7.328	MM	0.1025	2789.45825	453.61978	99.4032

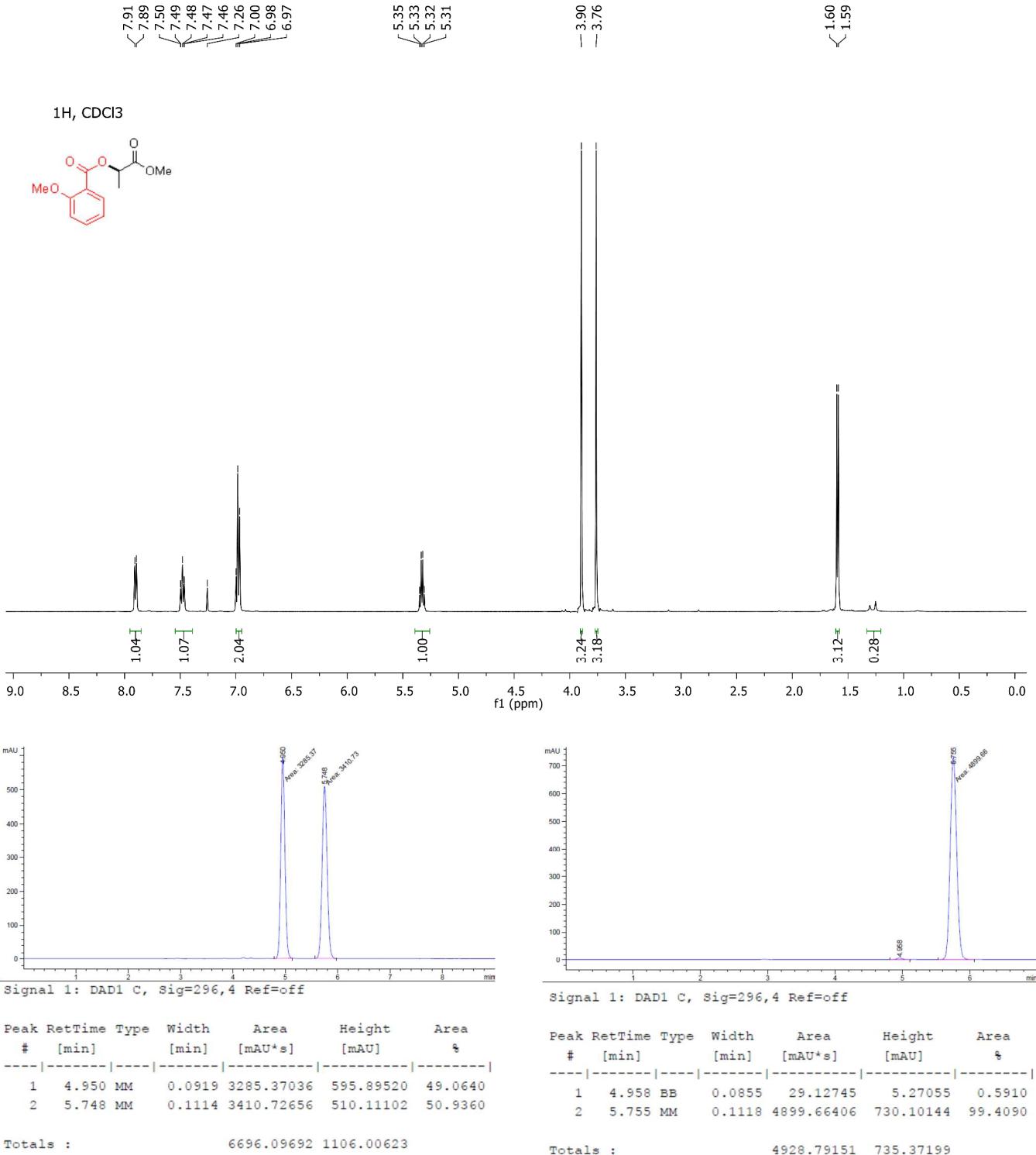
Totals : 2806.20464 455.85779

1-methoxy-1-oxopropan-2-yl 2-methoxybenzoate (4, Method B)

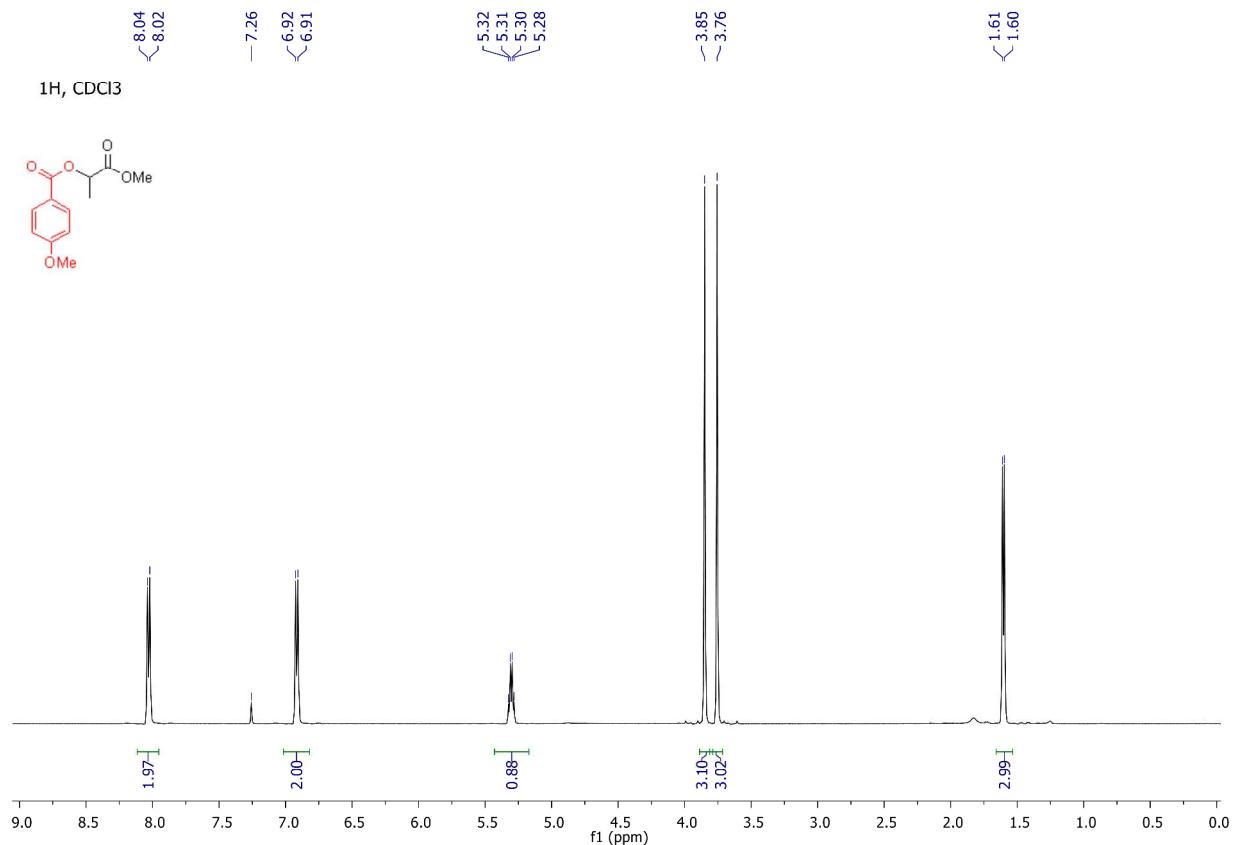


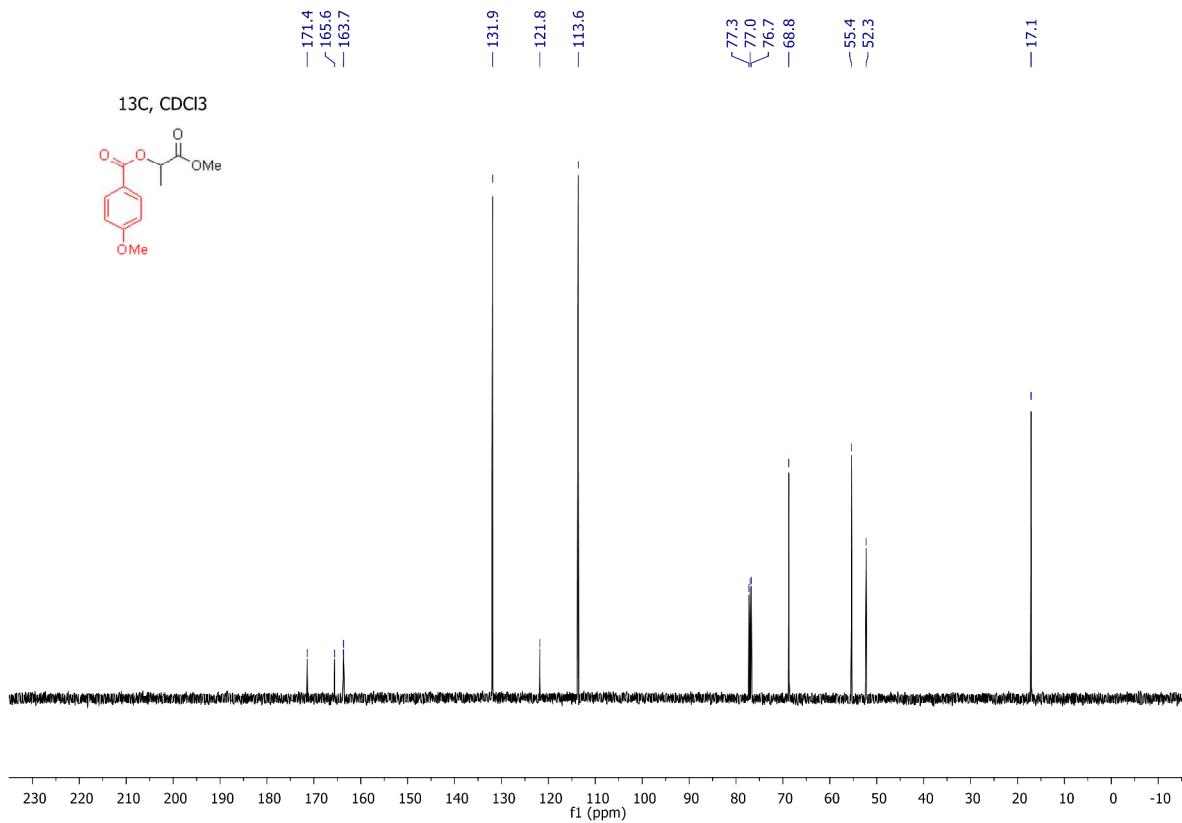


1-methoxy-1-oxopropan-2-yl 2-methoxybenzoate (4, *Method A*)

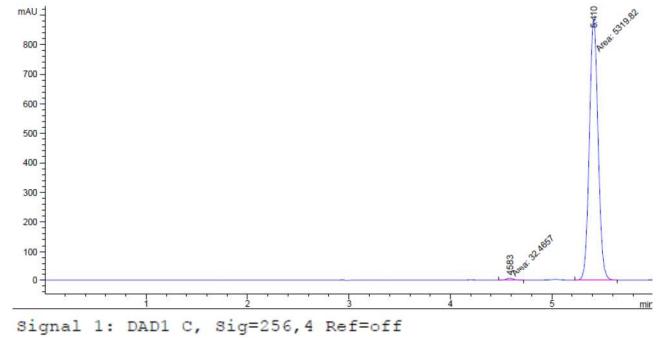
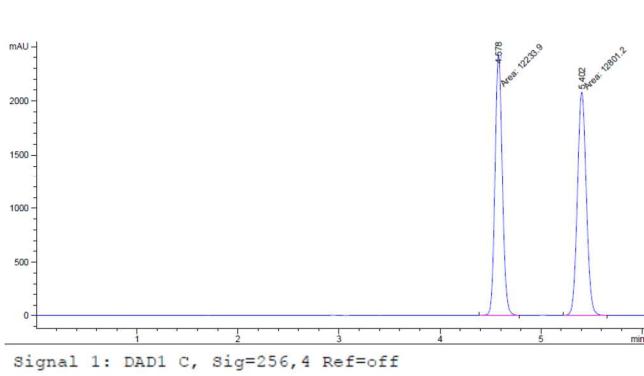
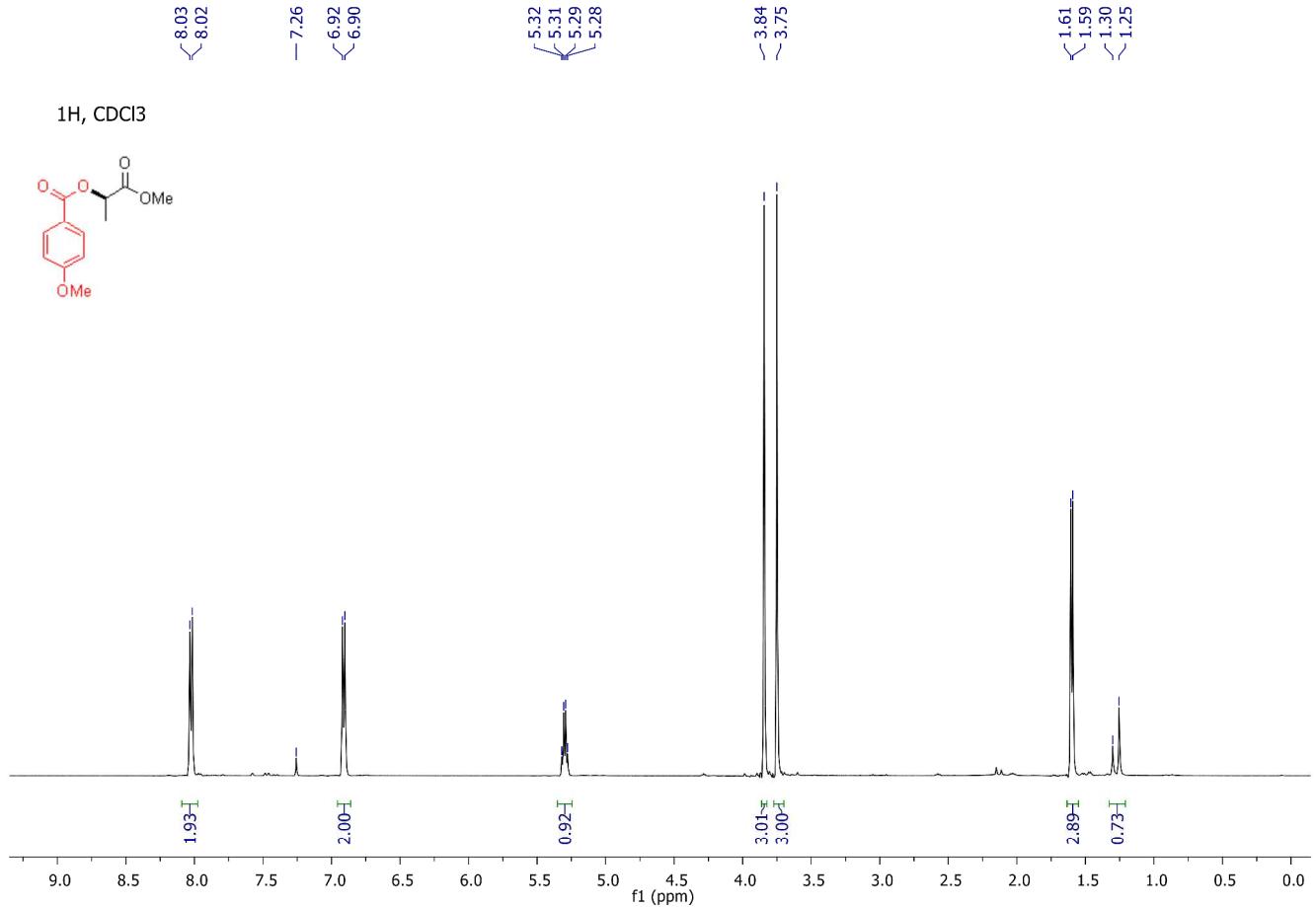


1-methoxy-1-oxopropan-2-yl 4-methoxybenzoate (5**, *Method B*)**





1-methoxy-1-oxopropan-2-yl 4-methoxybenzoate (5**, *Method A*)**



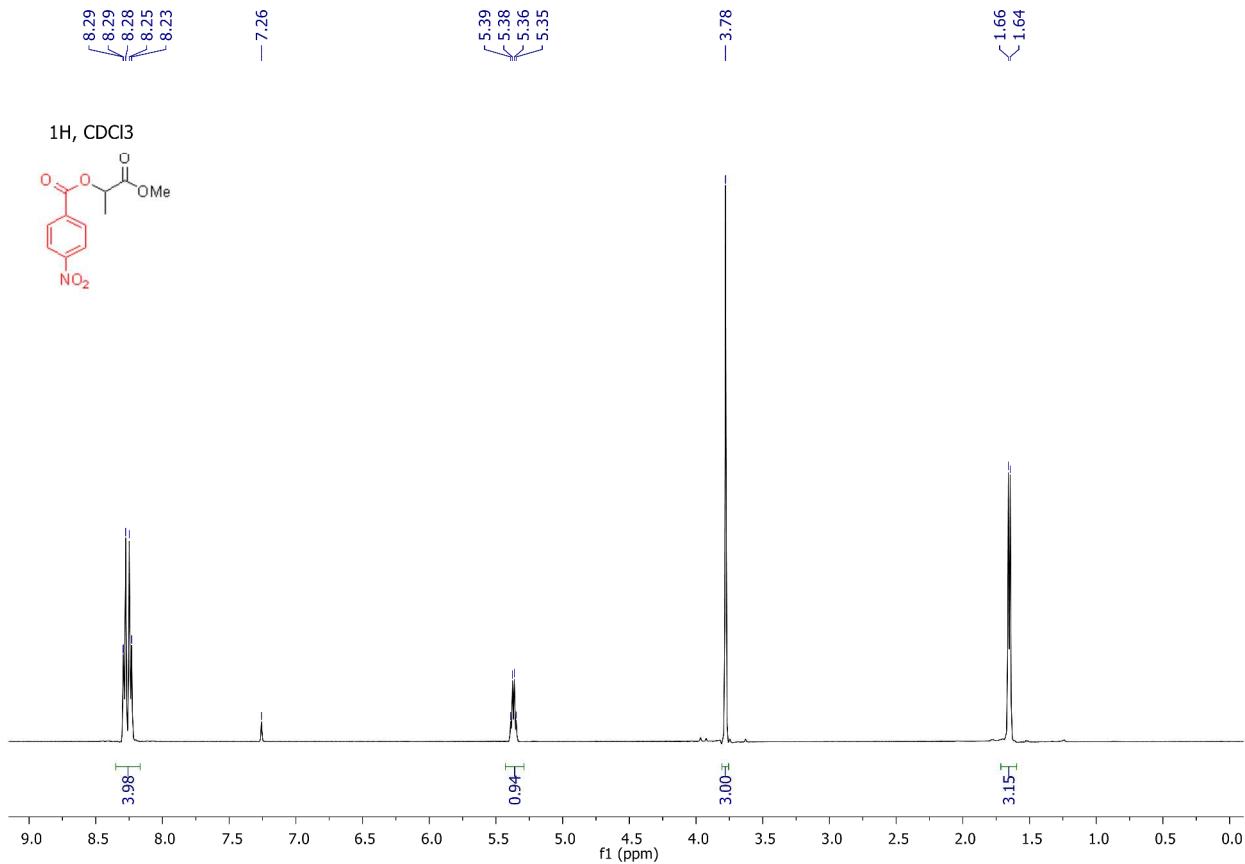
Peak	RetTime	Type	Width	Area	Height	Area %
#	[min]		[min]	[mAU*s]	[mAU]	%
1	4.578	MM	0.0840	1.22339e4	2426.58203	48.8668
2	5.402	MM	0.1024	1.28012e4	2083.00903	51.1332

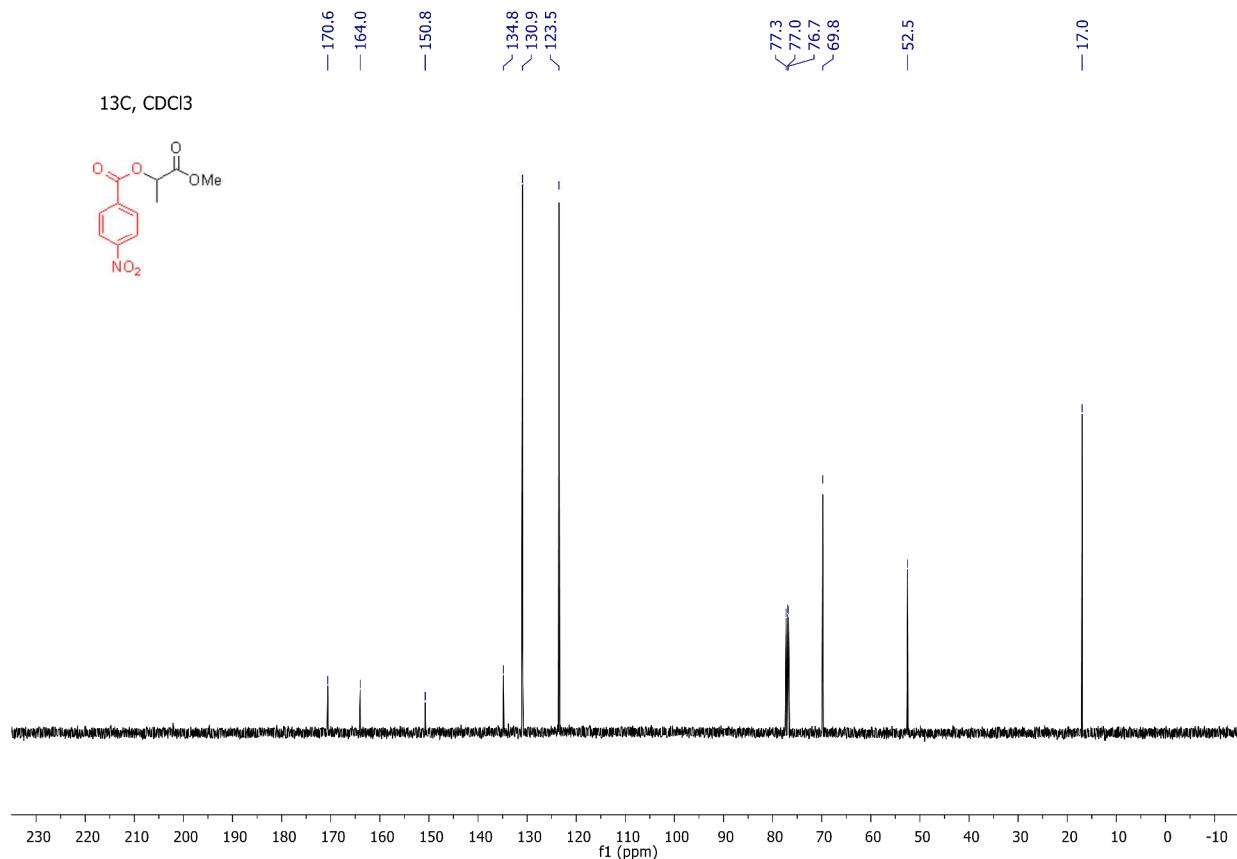
Totals : 2.50351e4 4509.59106

Peak	RetTime	Type	Width	Area	Height	Area %
#	[min]		[min]	[mAU*s]	[mAU]	%
1	4.583	MM	0.0794	32.46567	6.81307	0.6066
2	5.410	MM	0.1001	5319.81934	885.37927	99.3934

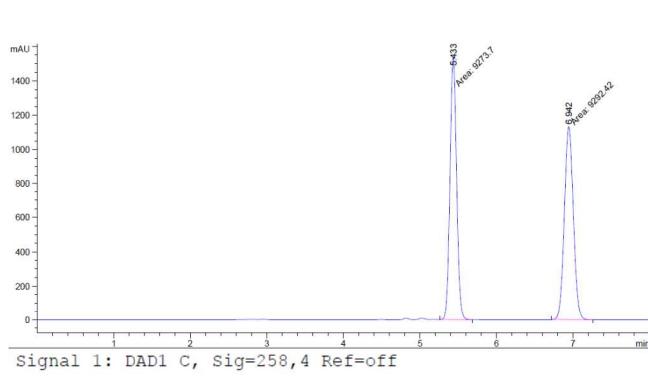
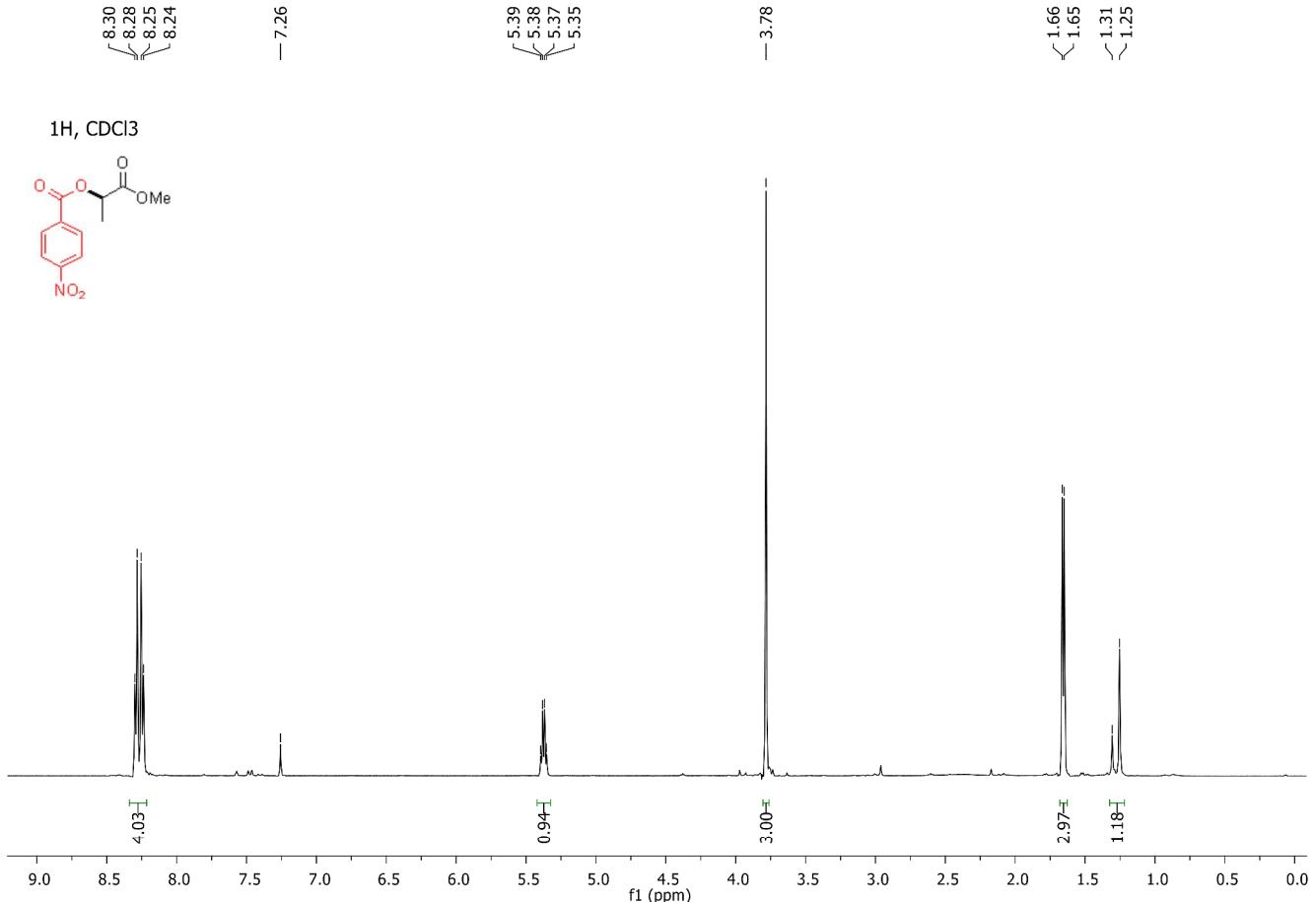
Totals : 5352.28500 892.19234

1-methoxy-1-oxopropan-2-yl 4-nitrobenzoate (6, Method B)



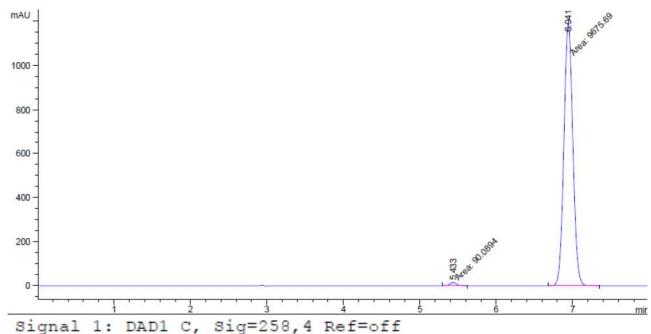


1-methoxy-1-oxopropan-2-yl 4-nitrobenzoate (6, *Method A*)



Peak	RetTime	Type	Width	Area	Height	Area %
#	[min]		[min]	[mAU*s]	[mAU]	%
1	5.433	MM	0.1004	9273.70020	1540.05481	49.9496
2	6.942	MM	0.1365	9292.42285	1134.63147	50.0504

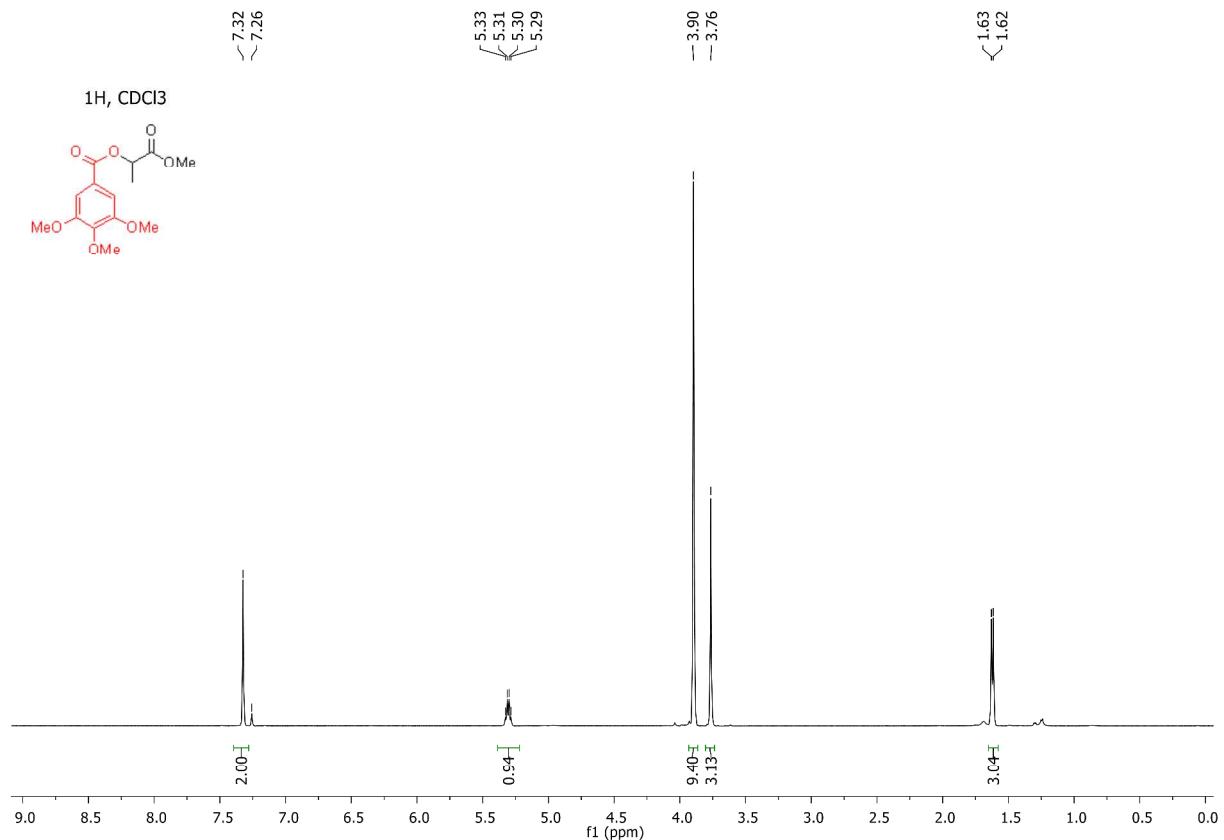
Totals : 1.85661e4 2674.68628

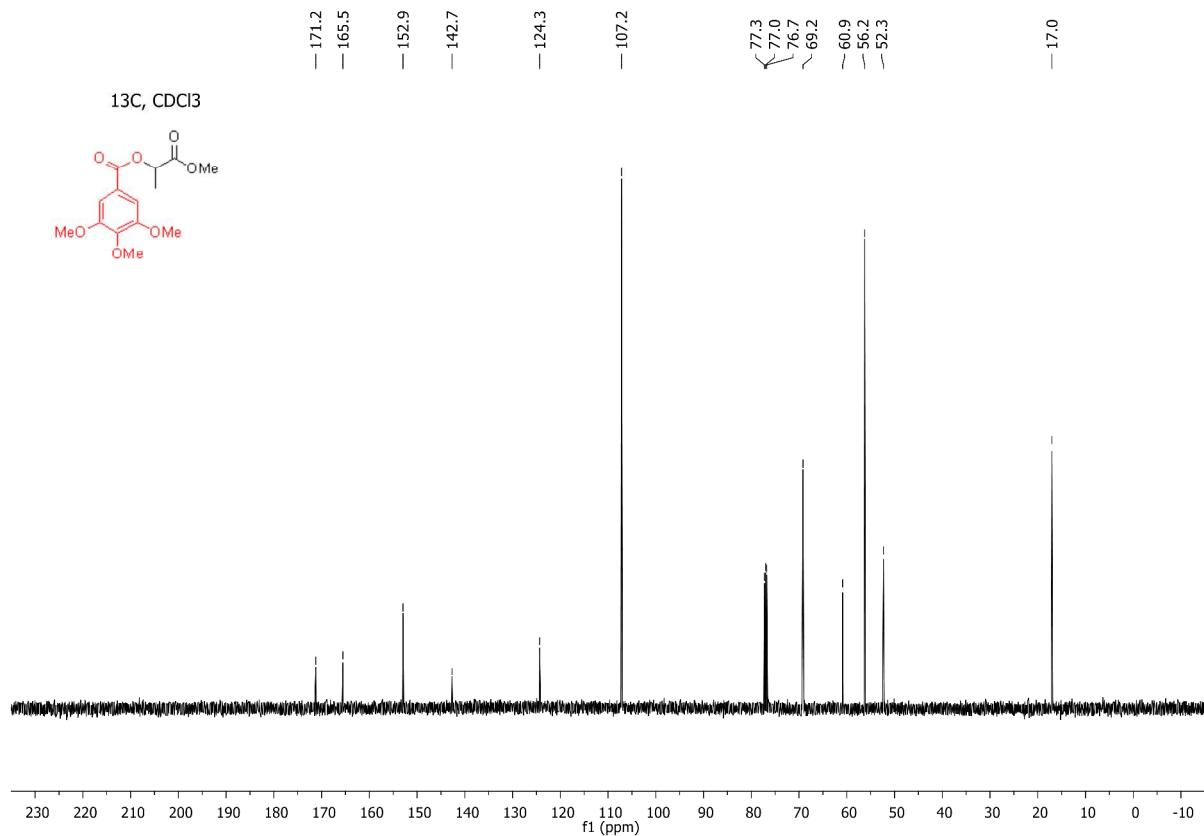


Peak	RetTime	Type	Width	Area	Height	Area %
#	[min]		[min]	[mAU*s]	[mAU]	%
1	5.433	MM	0.0985	90.08936	15.23748	0.9225
2	6.941	MM	0.1354	9675.68945	1190.59521	99.0775

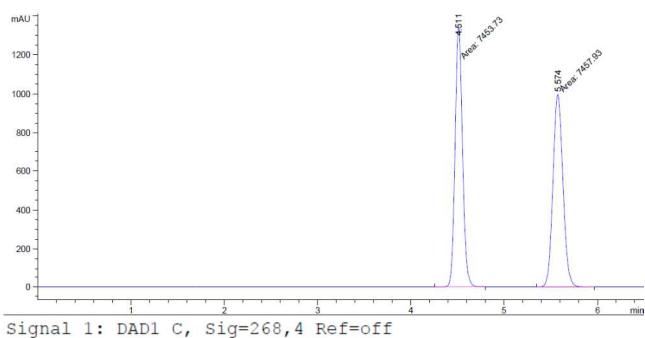
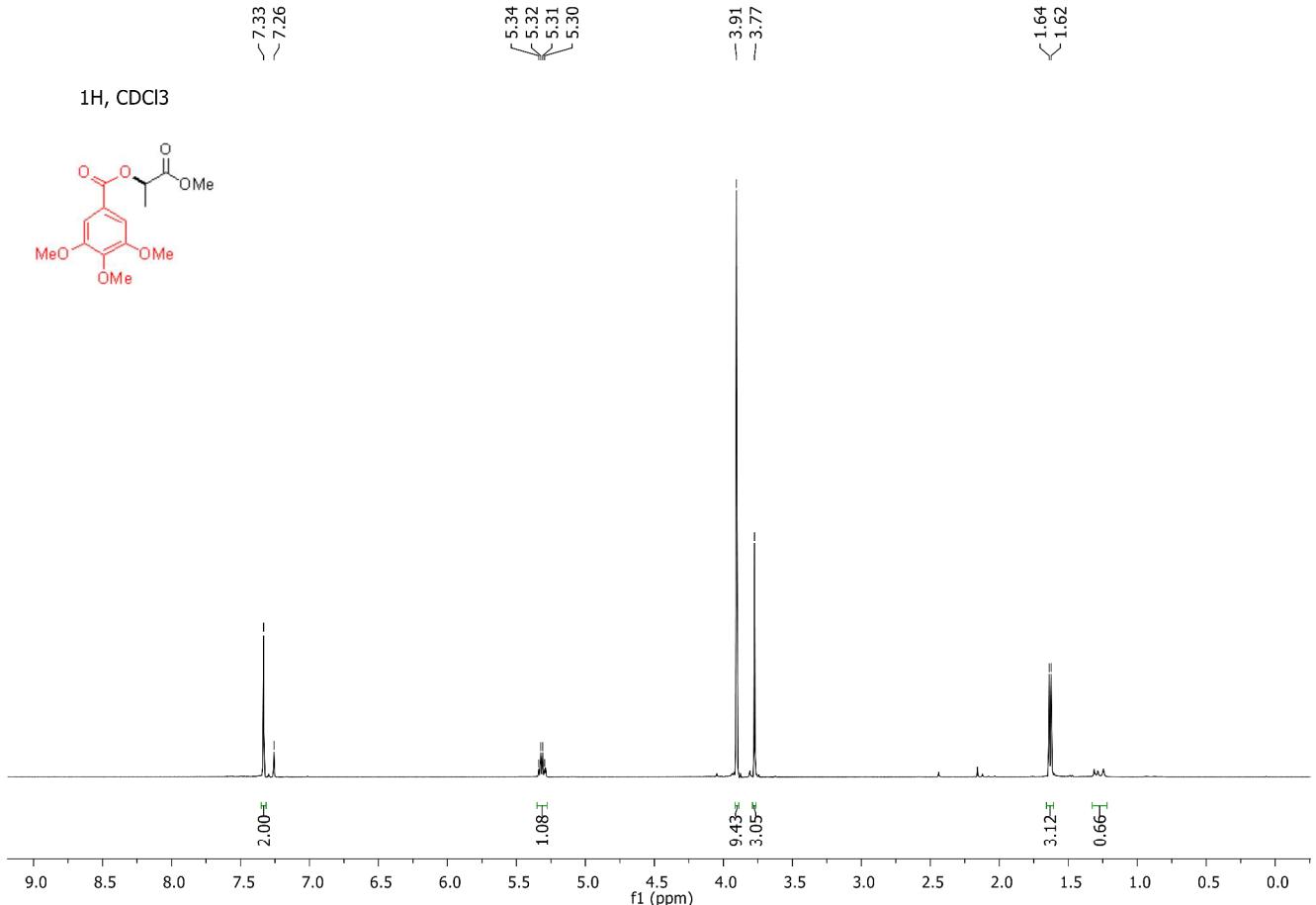
Totals : 9765.77881 1205.83270

1-methoxy-1-oxopropan-2-yl 3,4,5-trimethoxybenzoate (7, Method B)

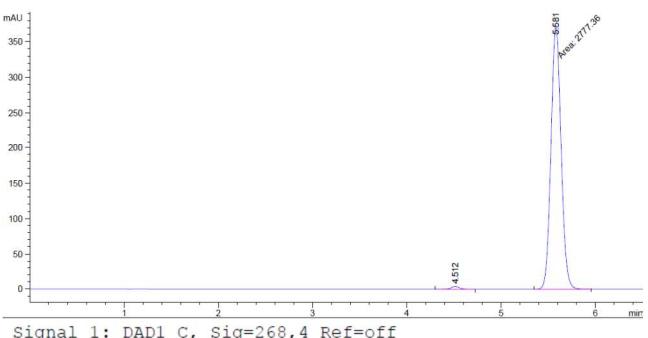




1-methoxy-1-oxopropan-2-yl 3,4,5-trimethoxybenzoate (7, Method A)

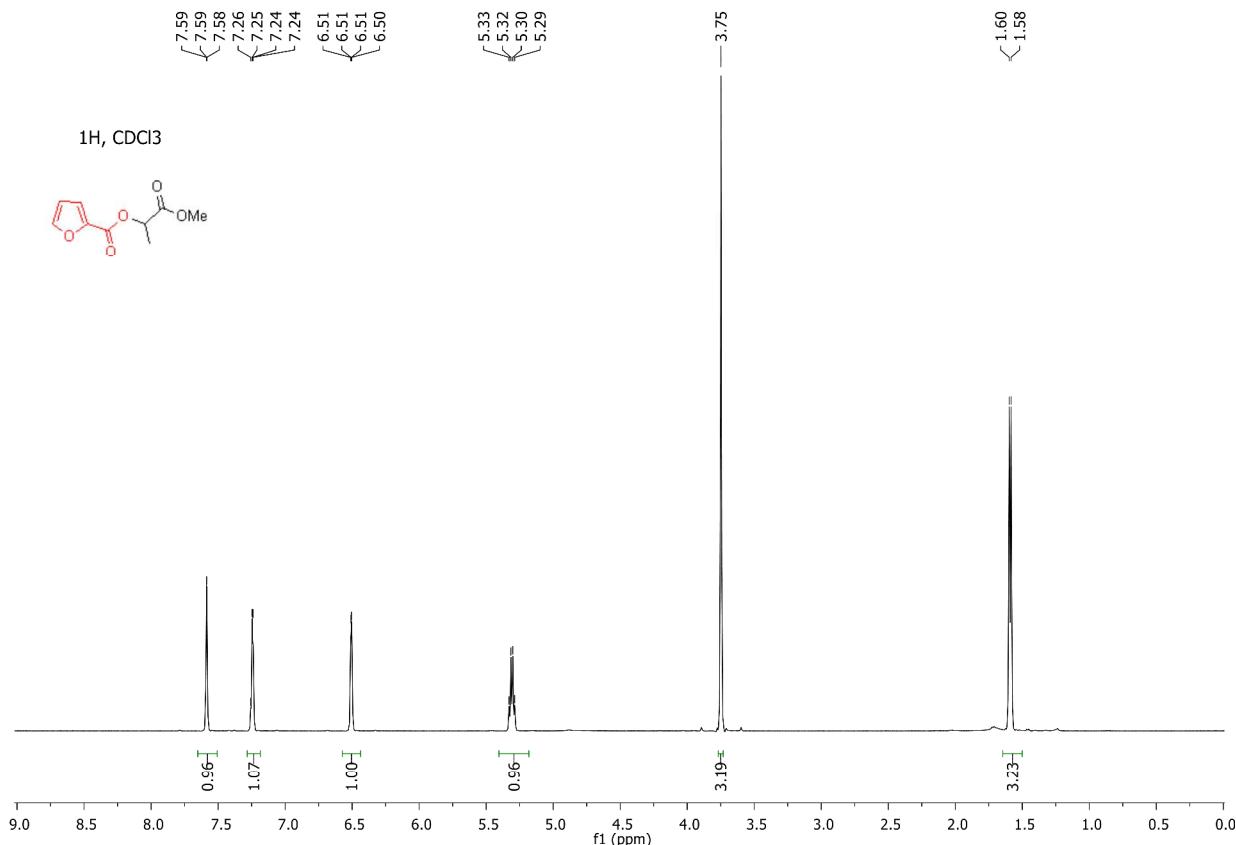


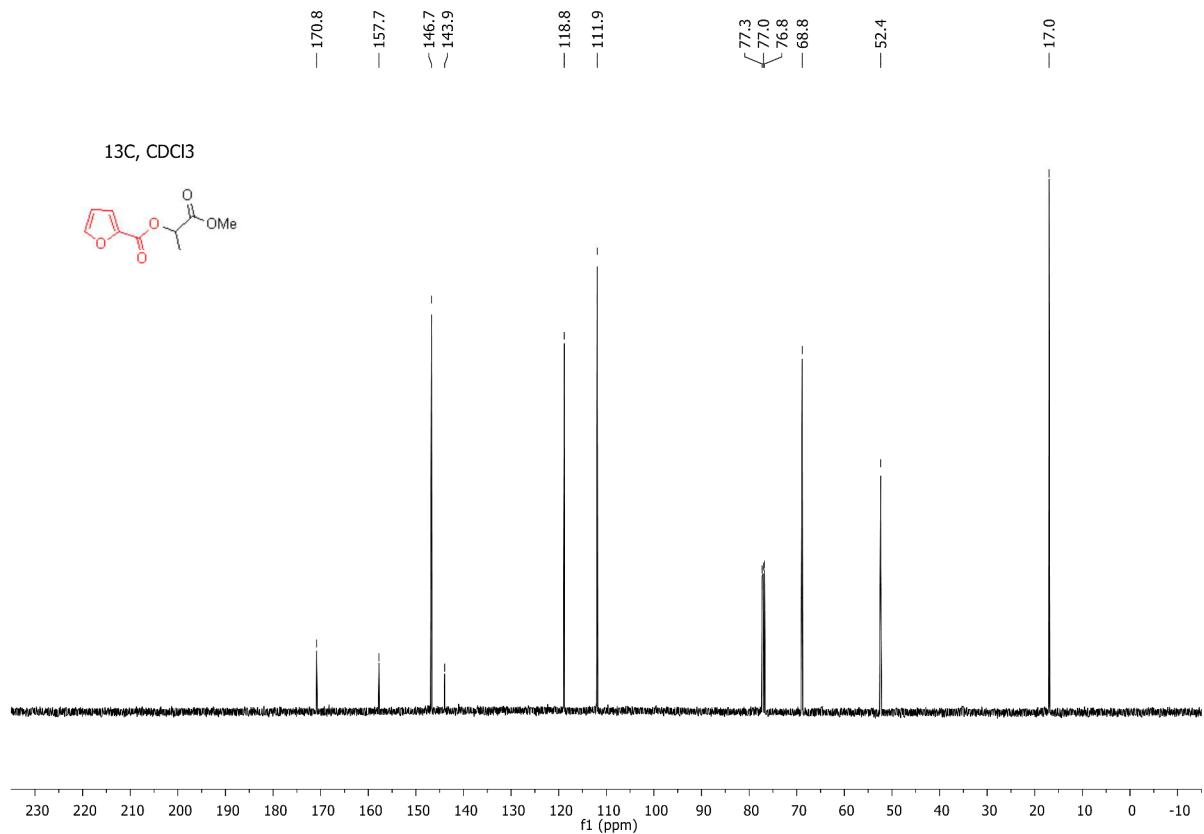
Totals : 1.49117e4 2341.77441



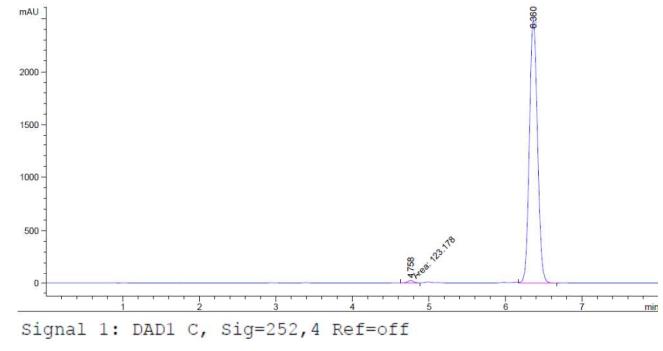
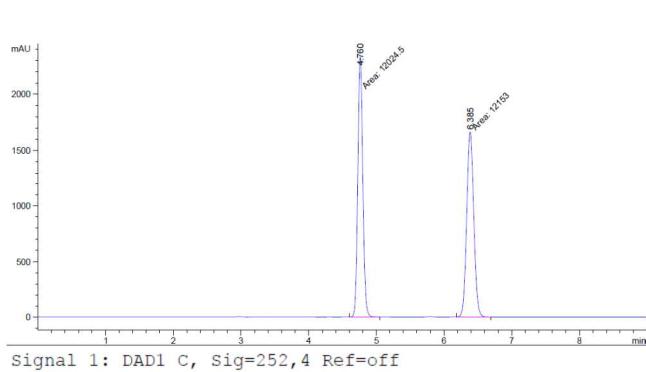
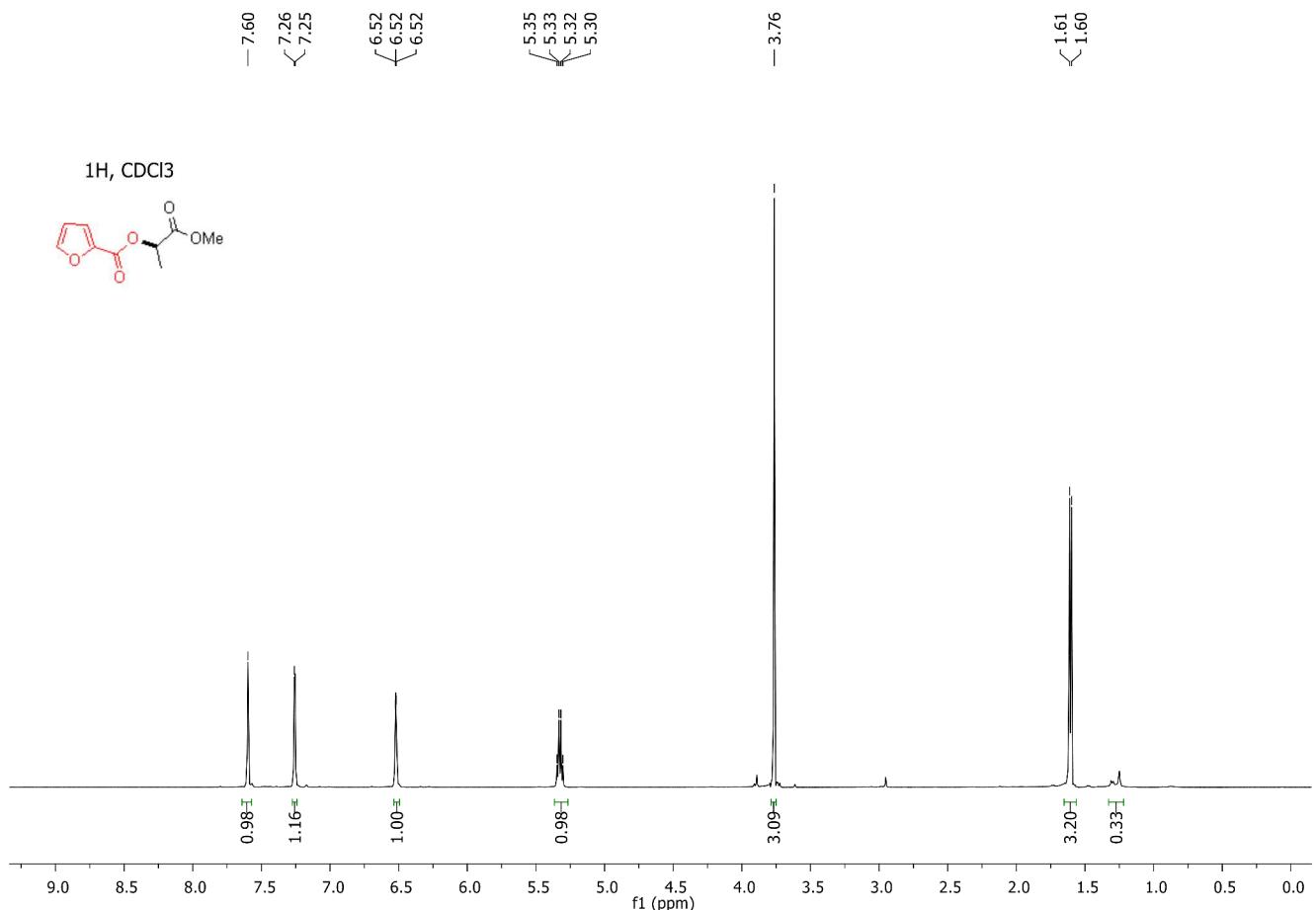
Totals : 2799.45997 376.64317

1-methoxy-1-oxopropan-2-yl furan-2-carboxylate (8**, *Method B*)**

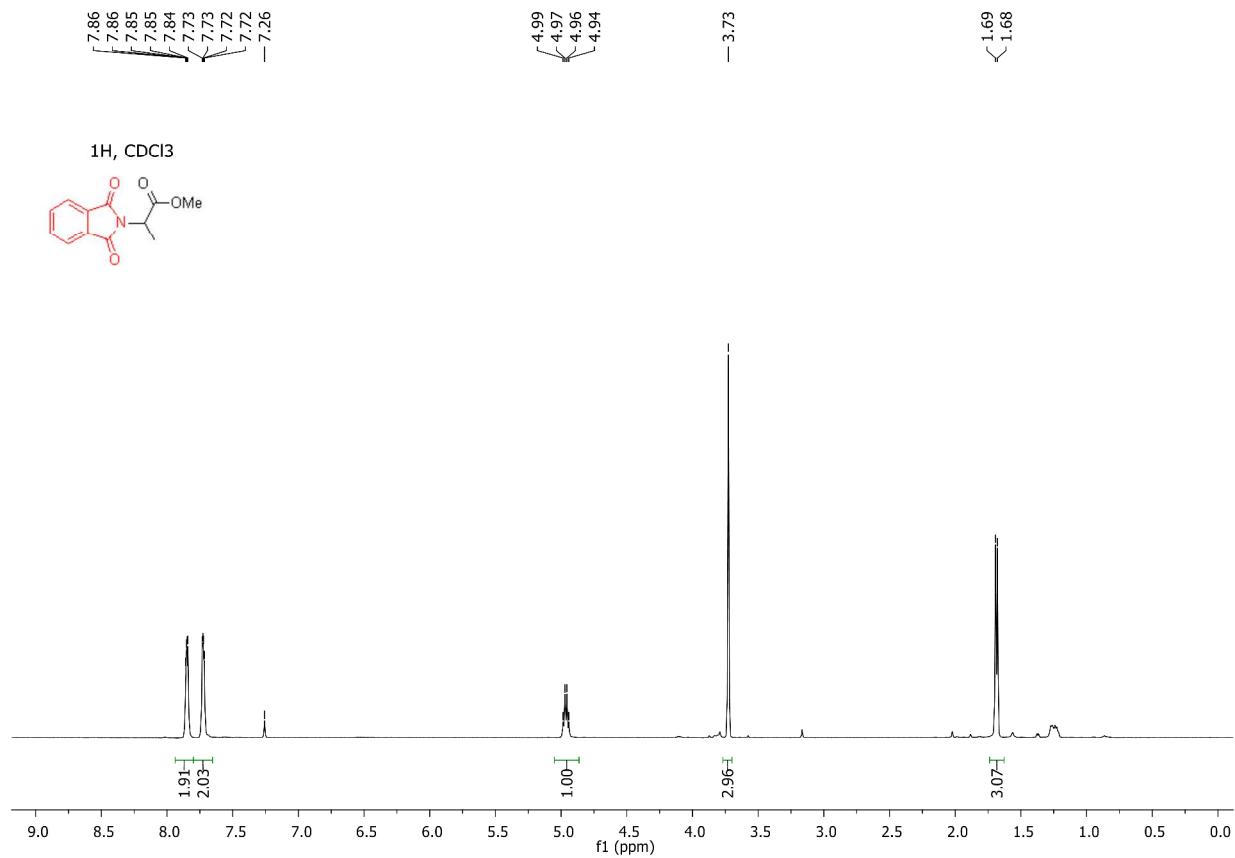


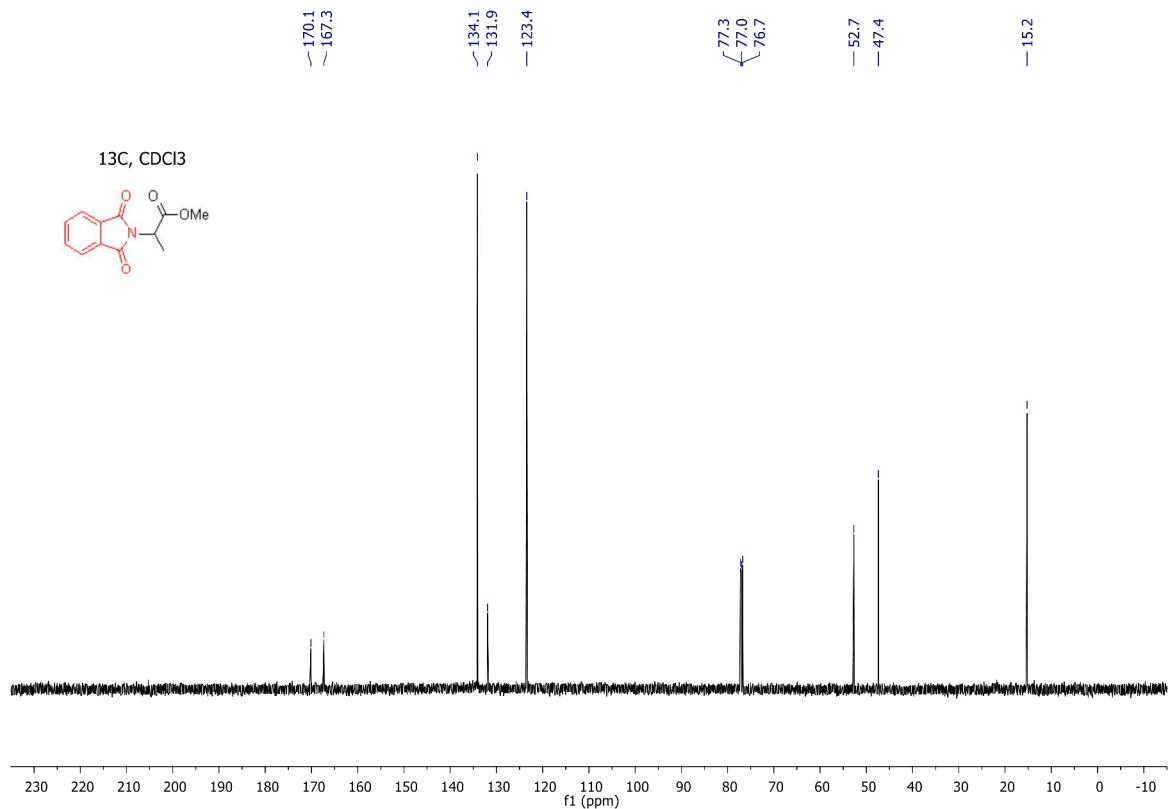


1-methoxy-1-oxopropan-2-yl furan-2-carboxylate (8, *Method B*)

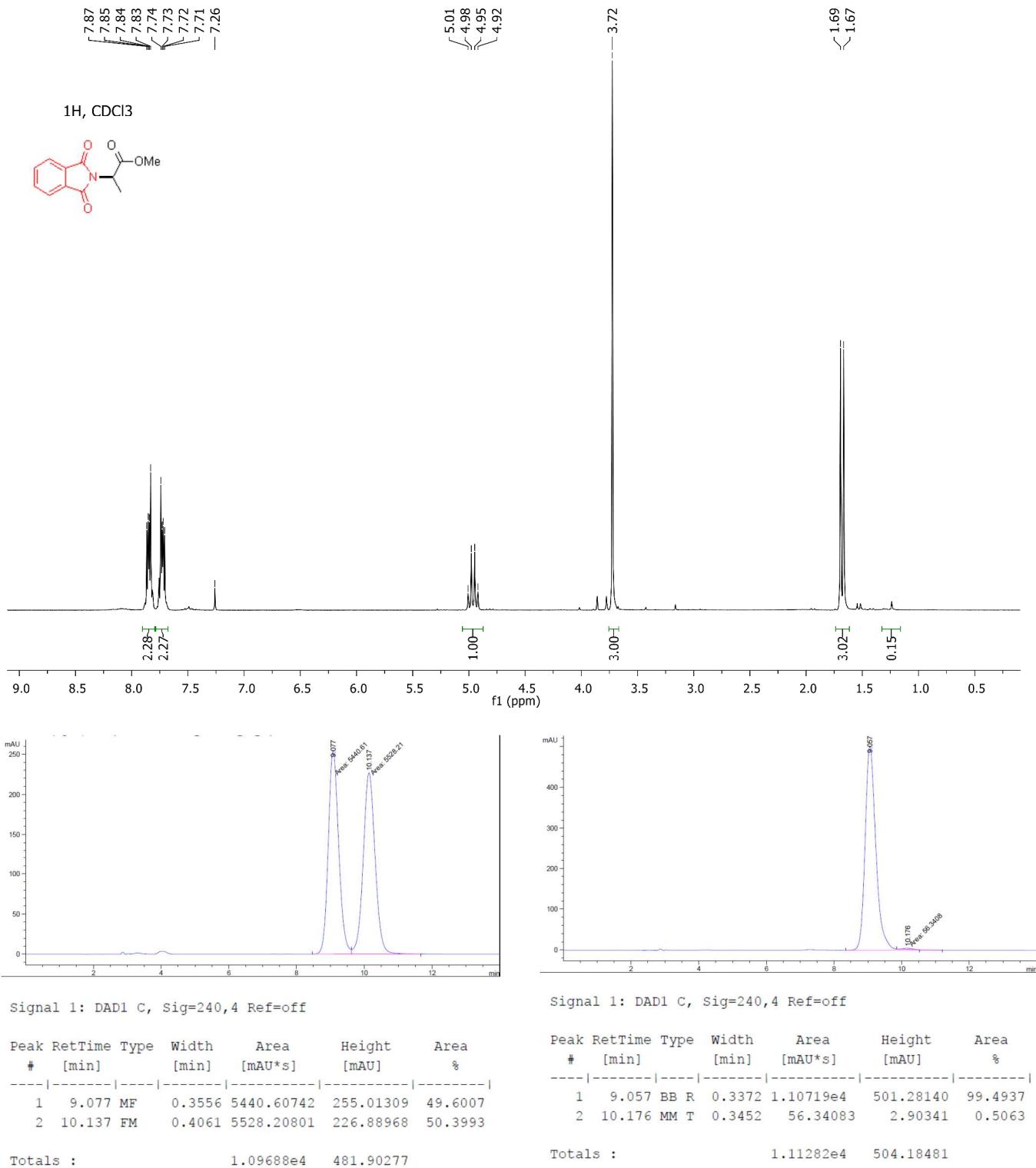


Methyl 2-(1,3-dioxoisindolin-2-yl)propanoate (9**, *Method B*)**

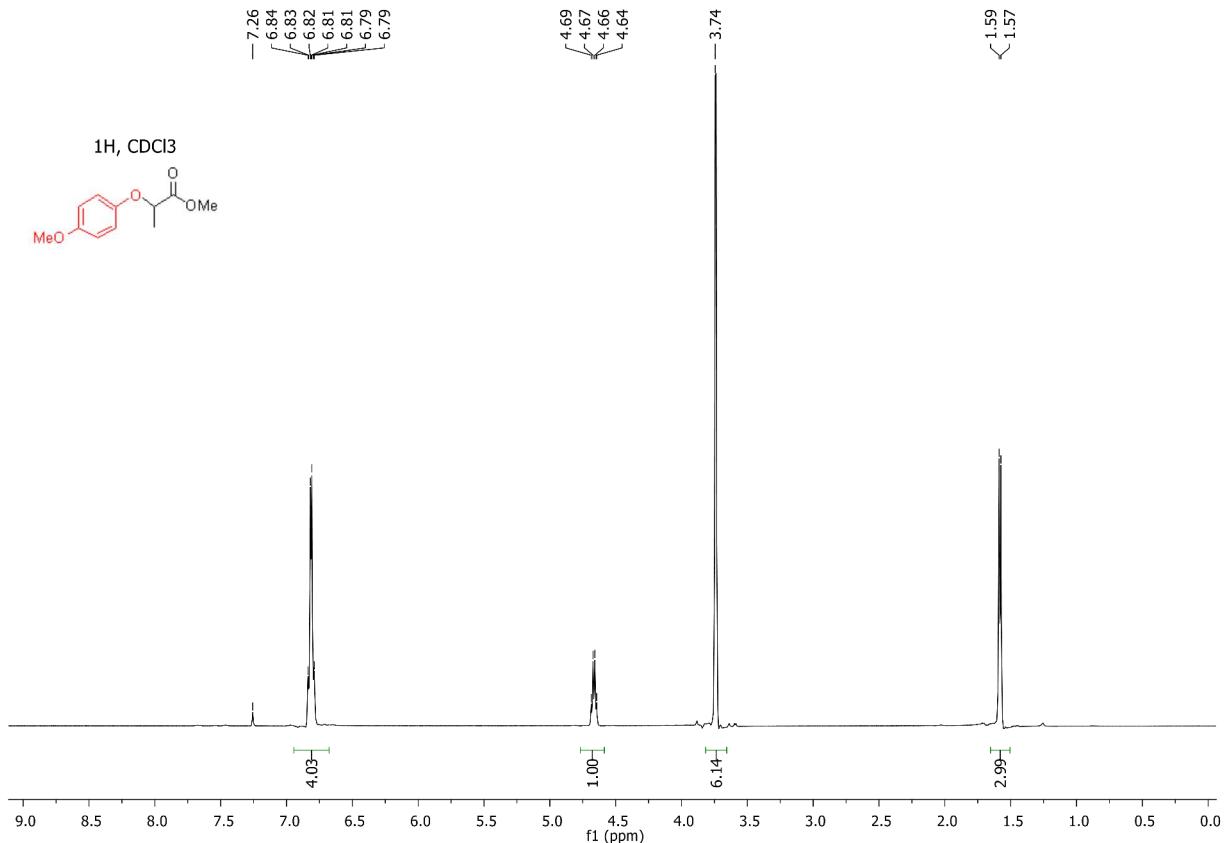


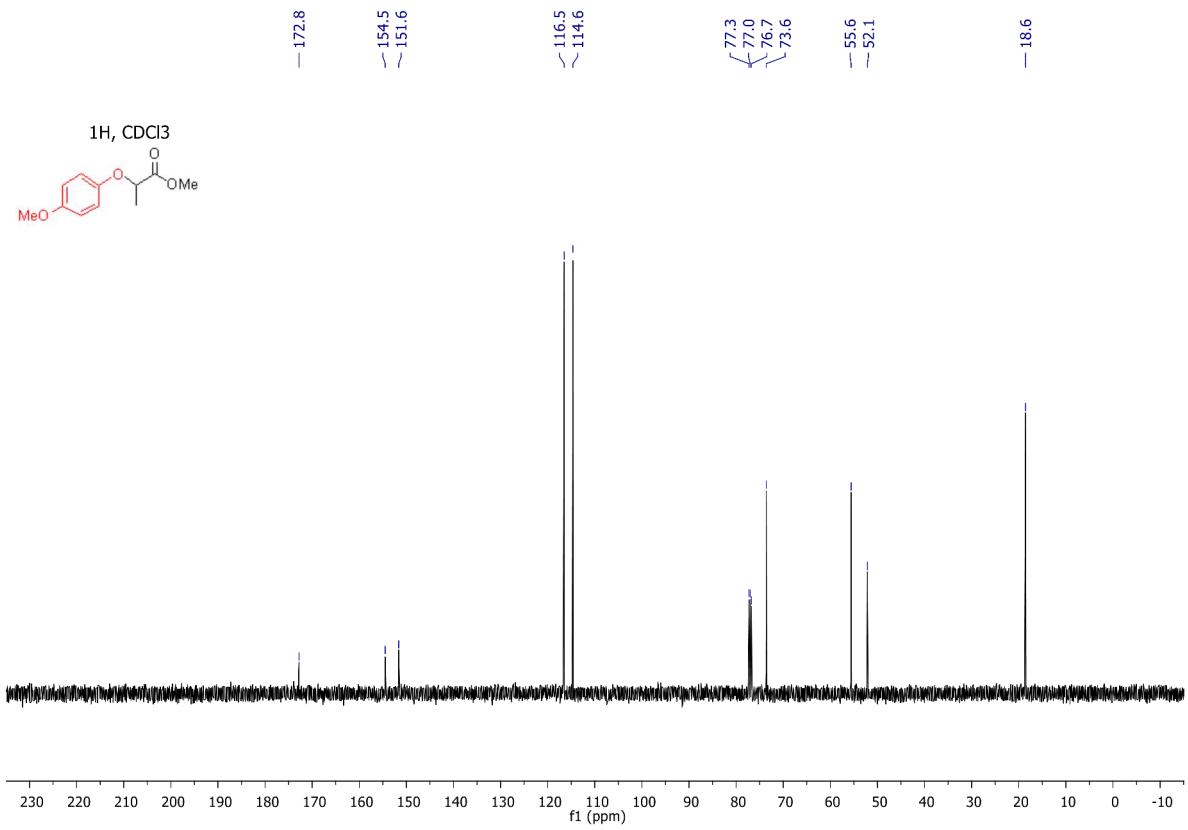


Methyl 2-(1,3-dioxoisooindolin-2-yl)propanoate (**9**, *Method A*)

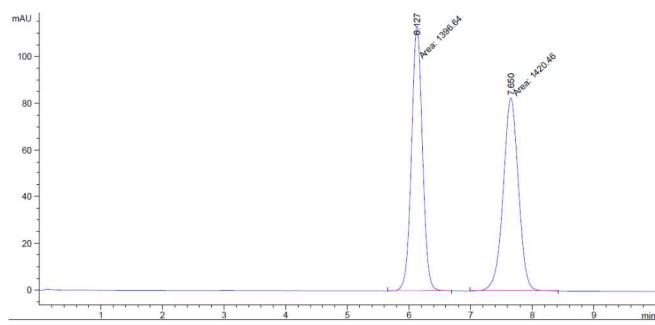
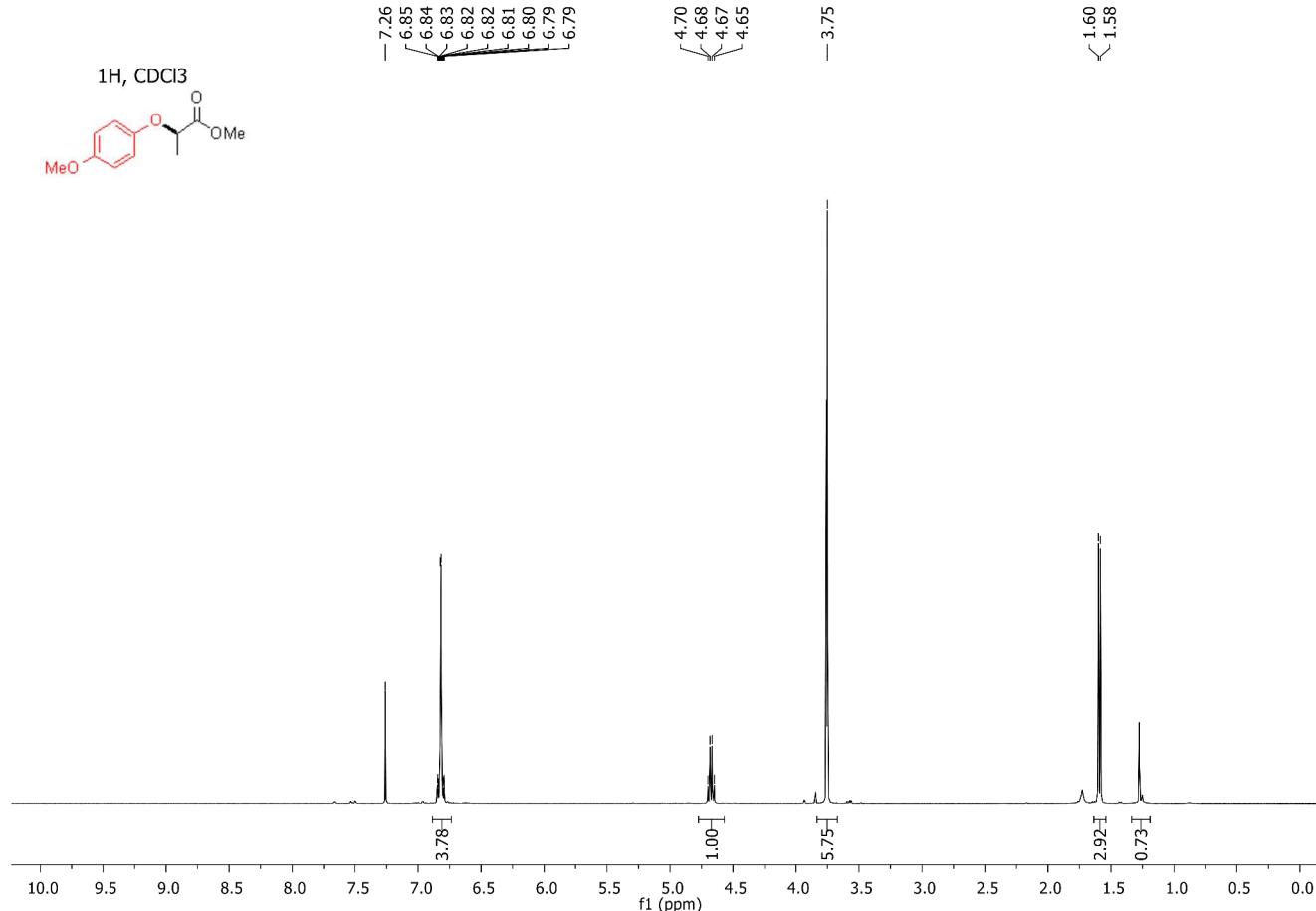


Methyl 2-(4-methoxyphenoxy)propanoate (10**, *Method B*)**





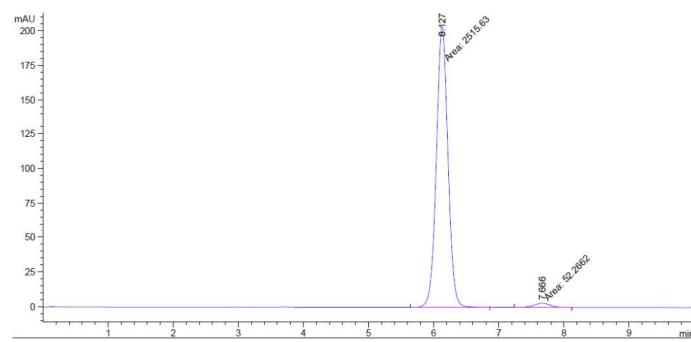
Methyl 2-(4-methoxyphenoxy)propanoate (10, *Method A*)



Signal 1: DAD1 D, Sig=288,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.127	MM	0.2056	1396.63916	113.20187	49.5773
2	7.650	MM	0.2868	1420.45618	82.55312	50.4227

Totals : 2817.09534 195.75500

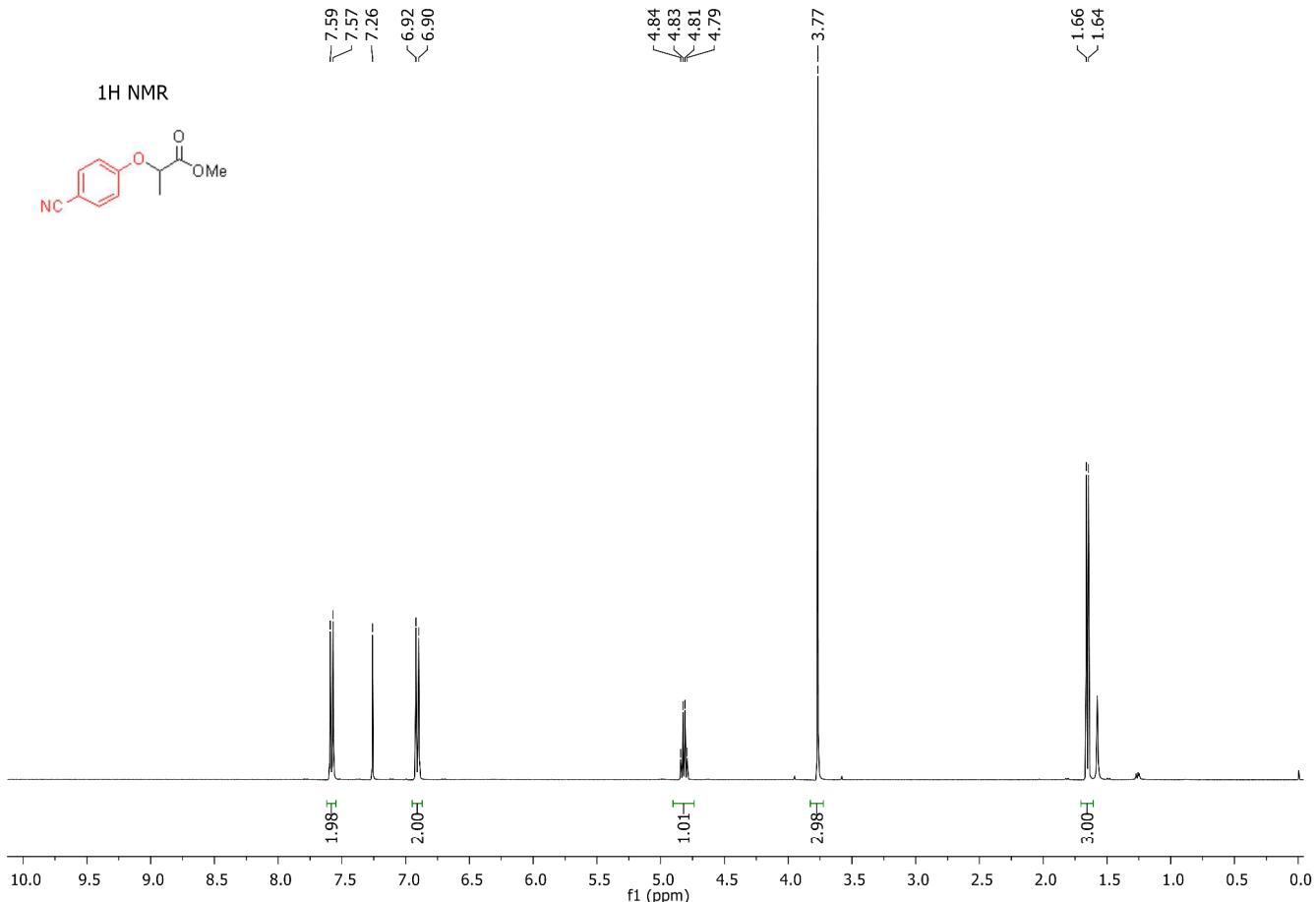


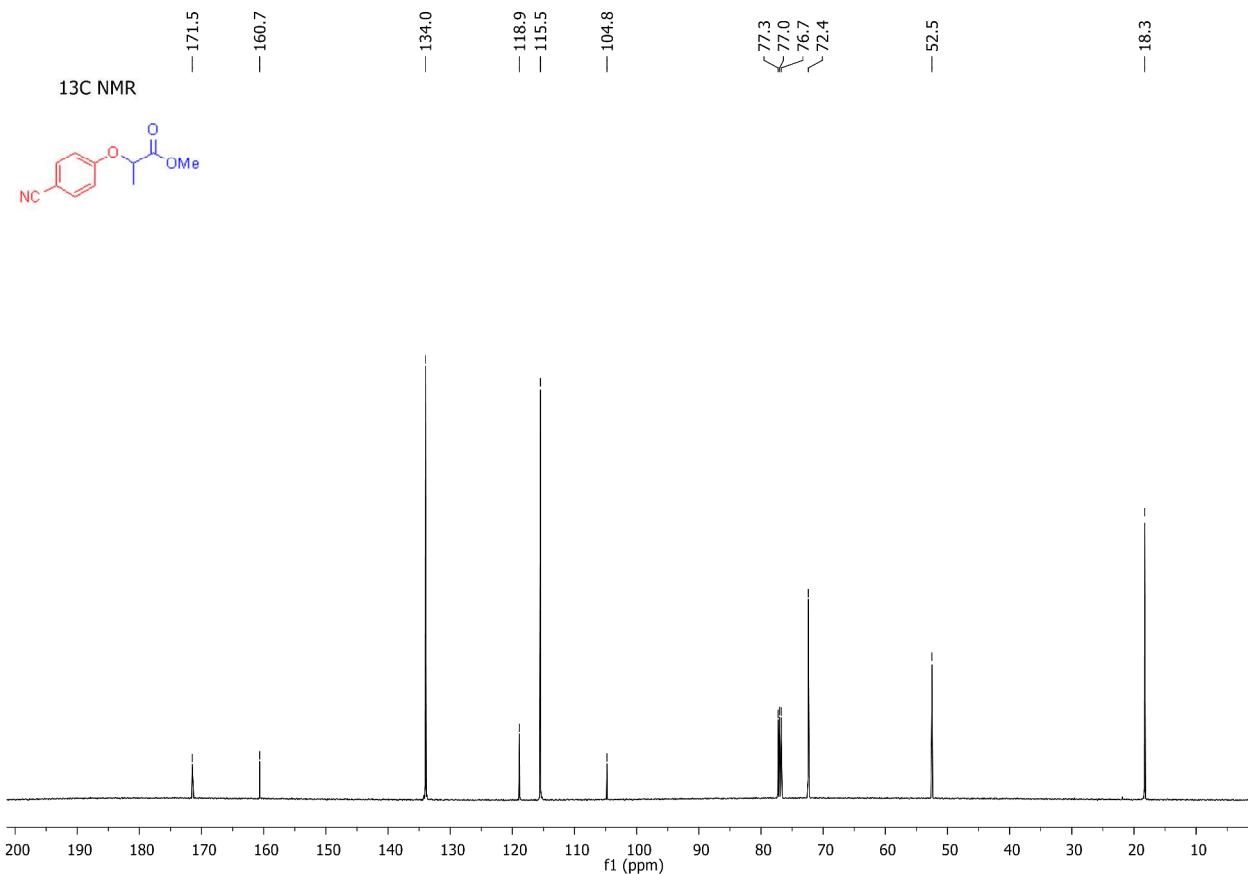
Signal 1: DAD1 D, Sig=288,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.127	MM	0.2065	2515.63379	203.08040	97.9646
2	7.666	MM	0.2841	52.26617	3.06593	2.0354

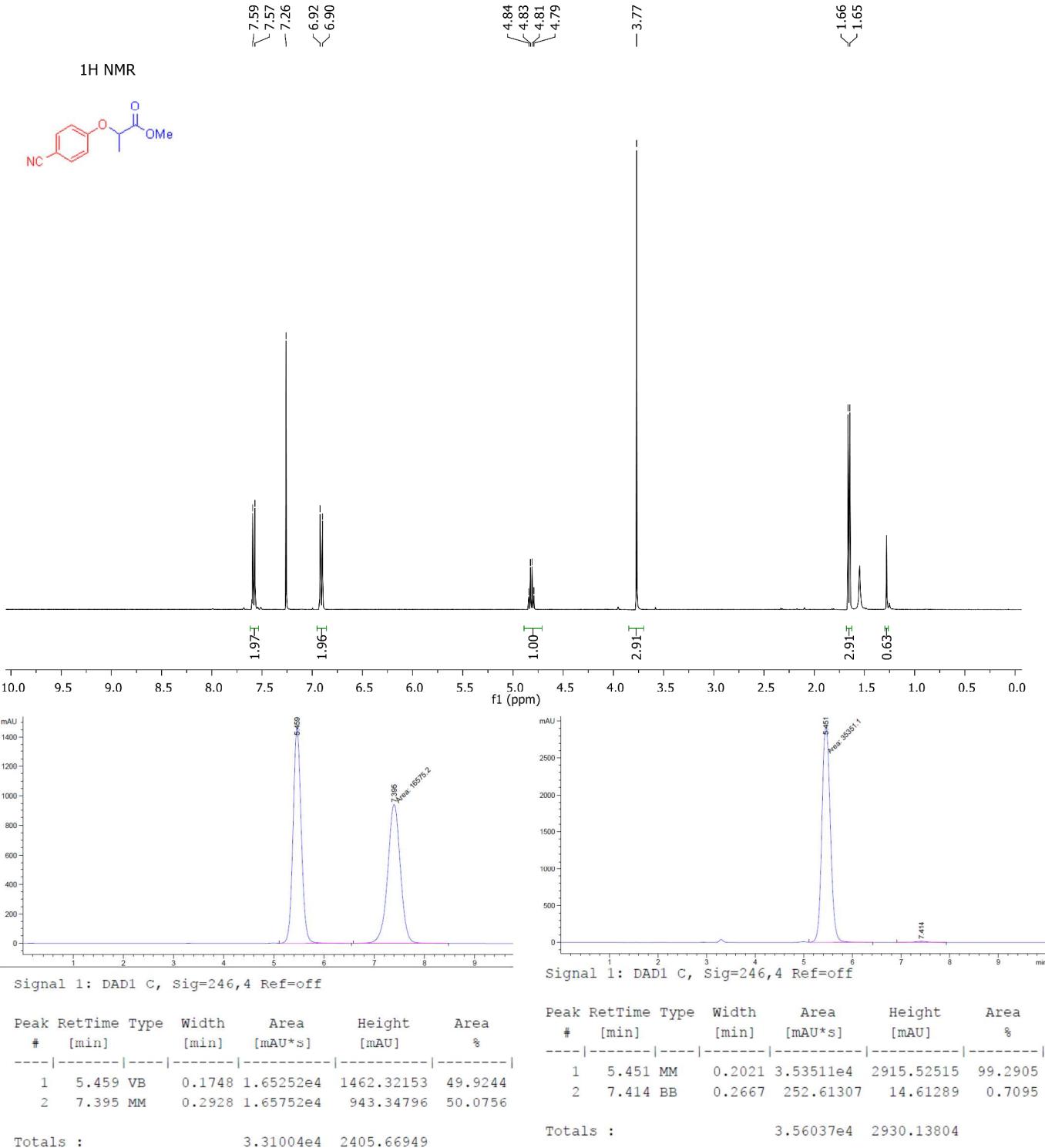
Totals : 2567.89996 206.14633

Methyl 2-(4-cyanophenoxy)propanoate (11, *Method B*)

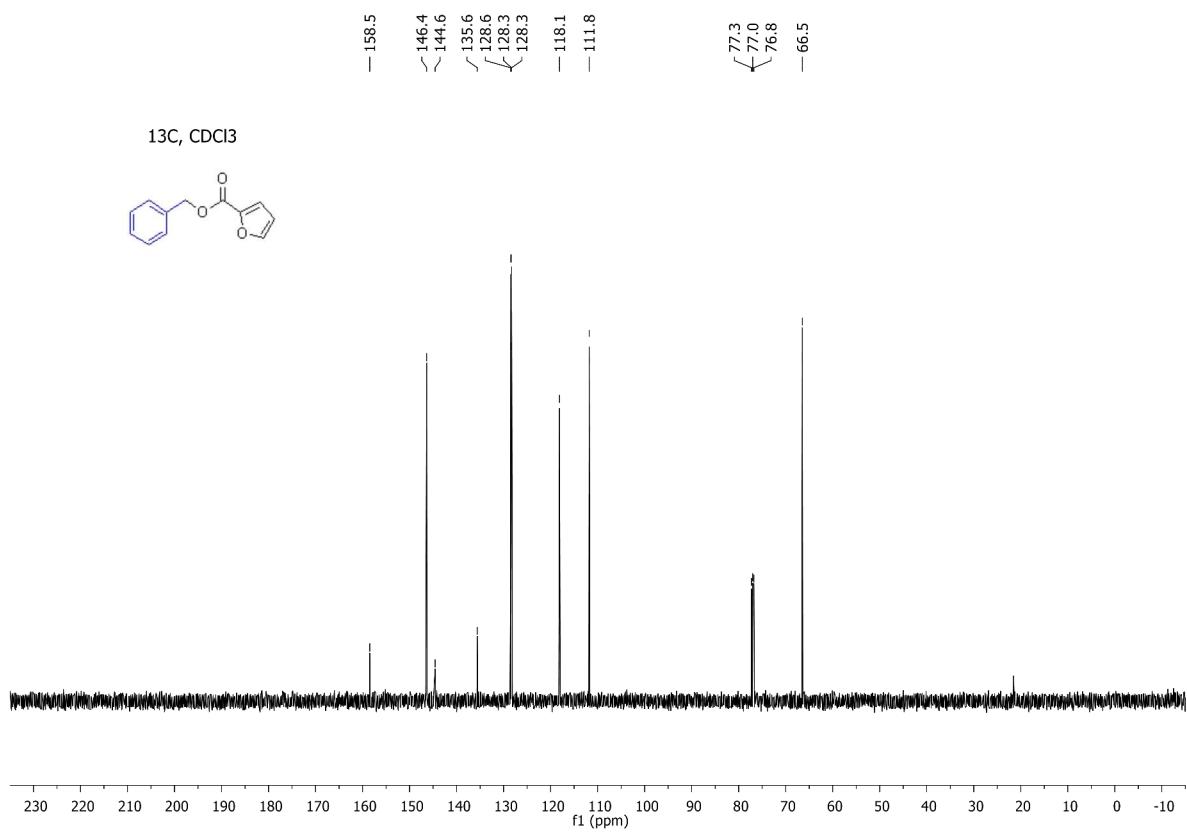
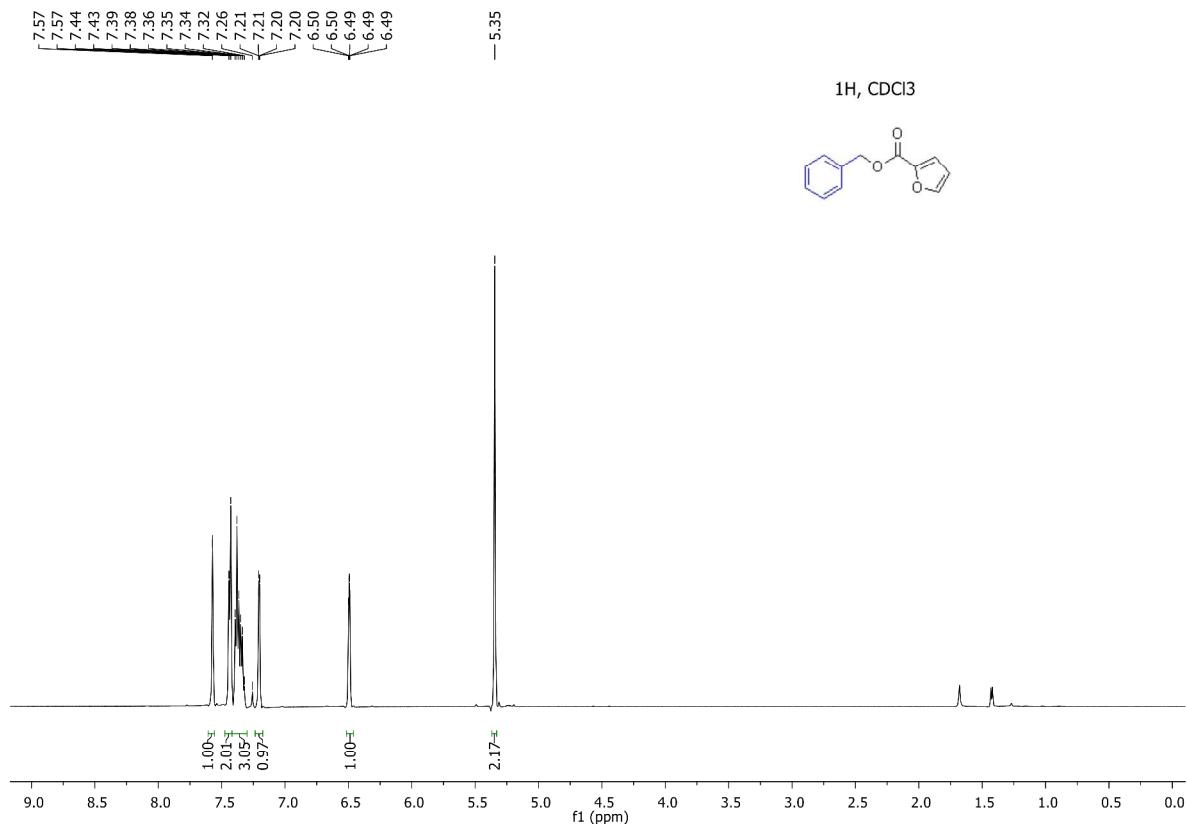




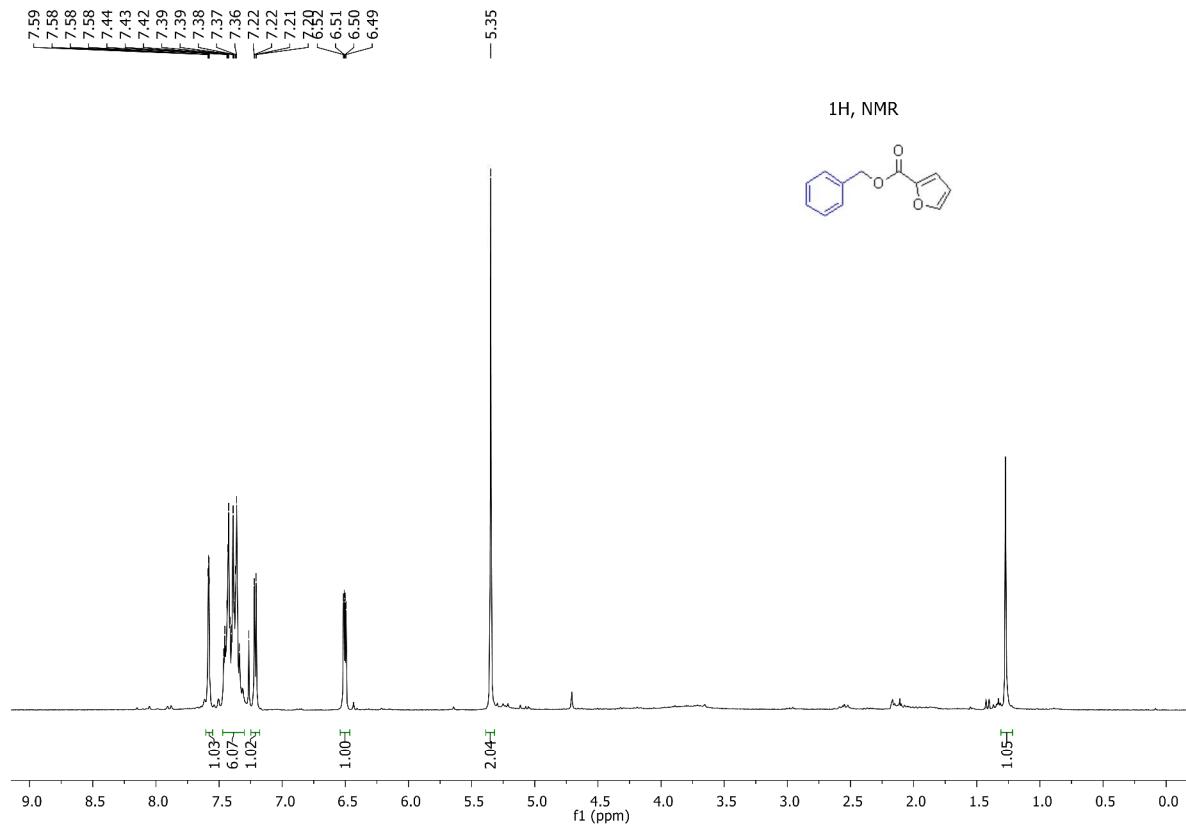
(*R*)-Methyl 2-(4-cyanophenoxy)propanoate (11**, *Method A*)**



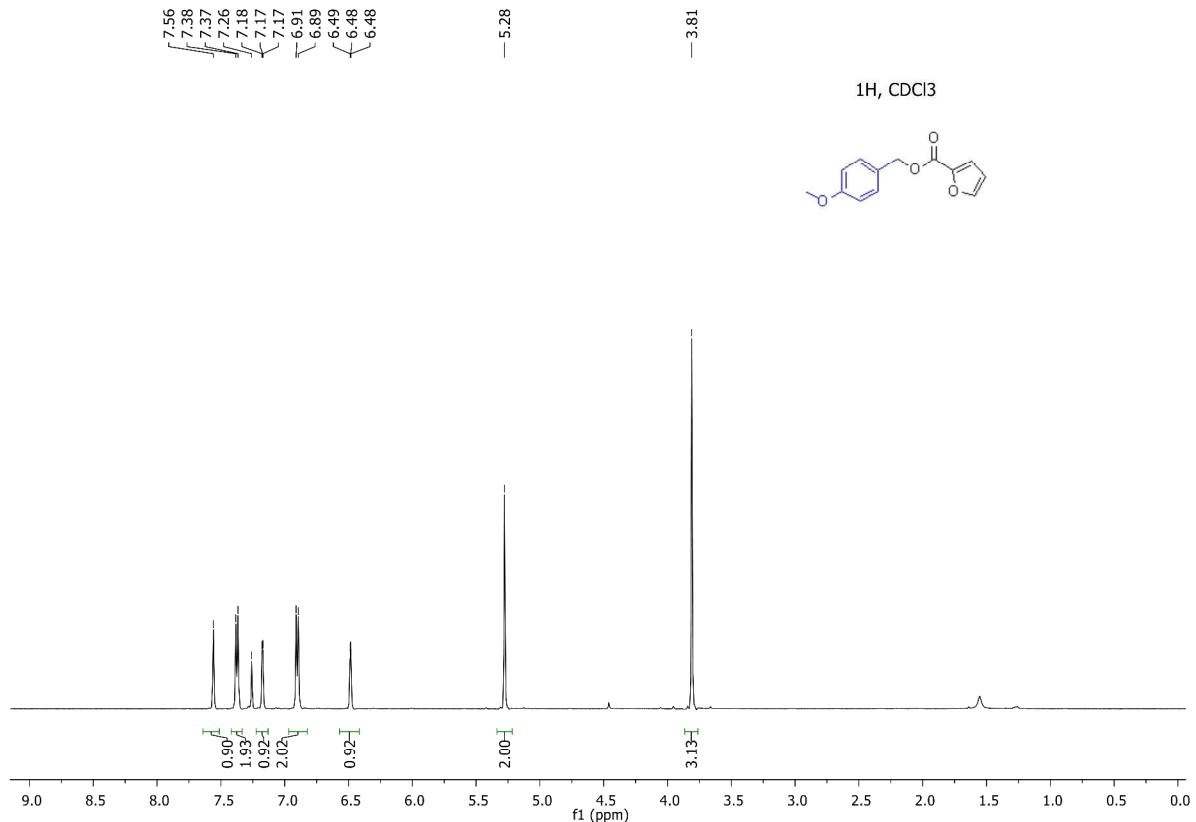
Benzyl furan-2-carboxylate (12, Method B)

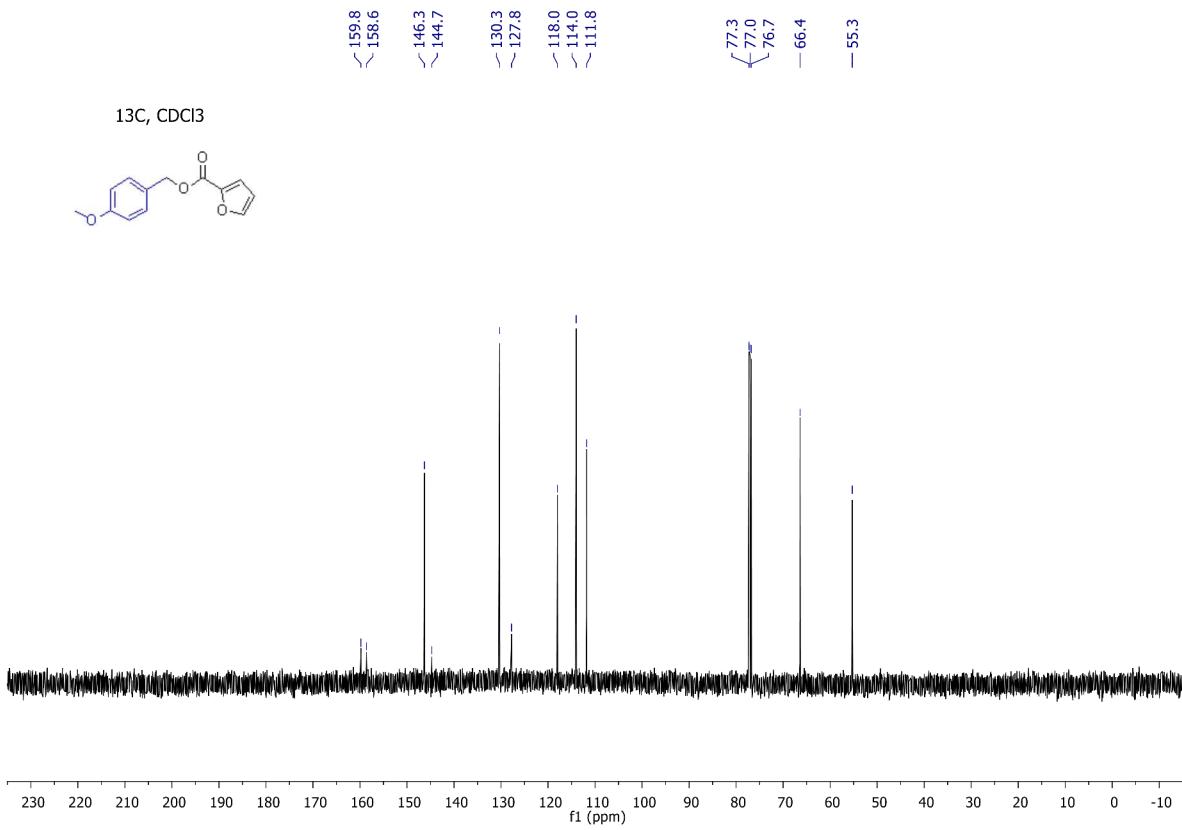


Benzyl furan-2-carboxylate (12, Method A)

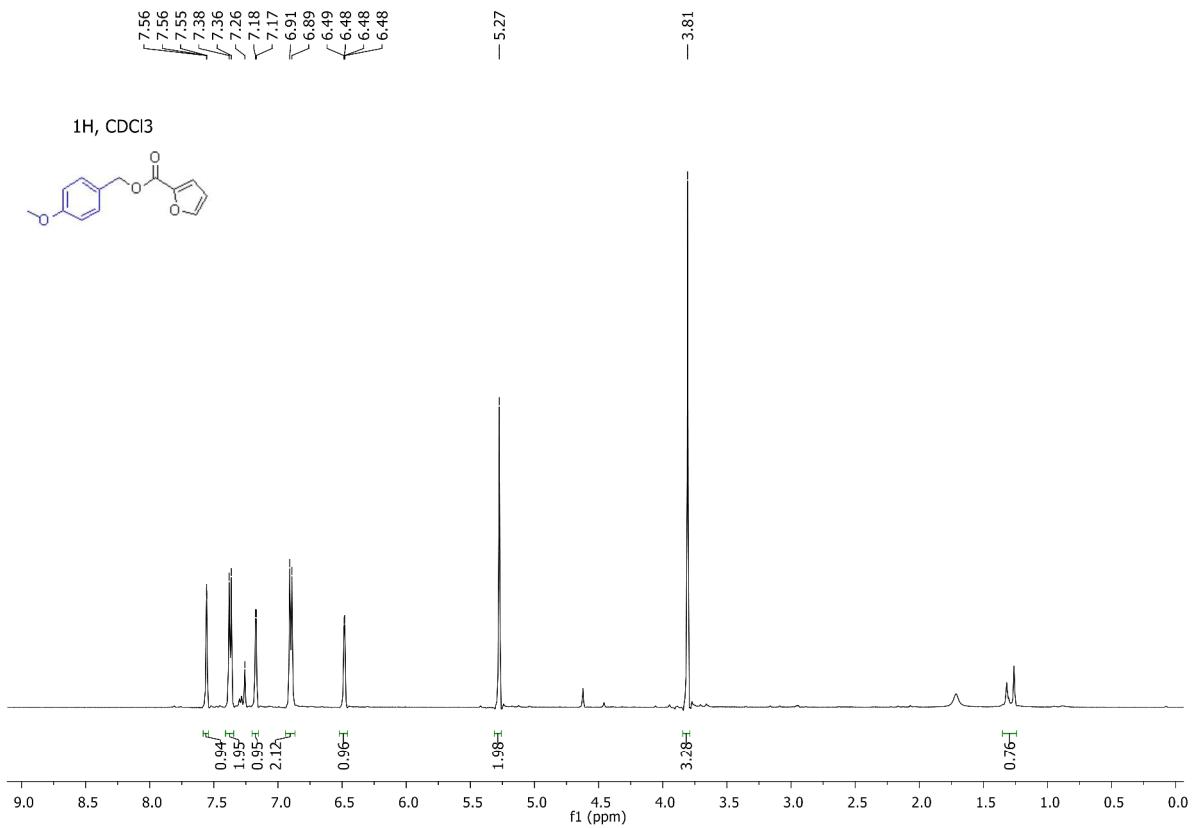


4-methoxybenzyl furan-2-carboxylate (13, Method B)

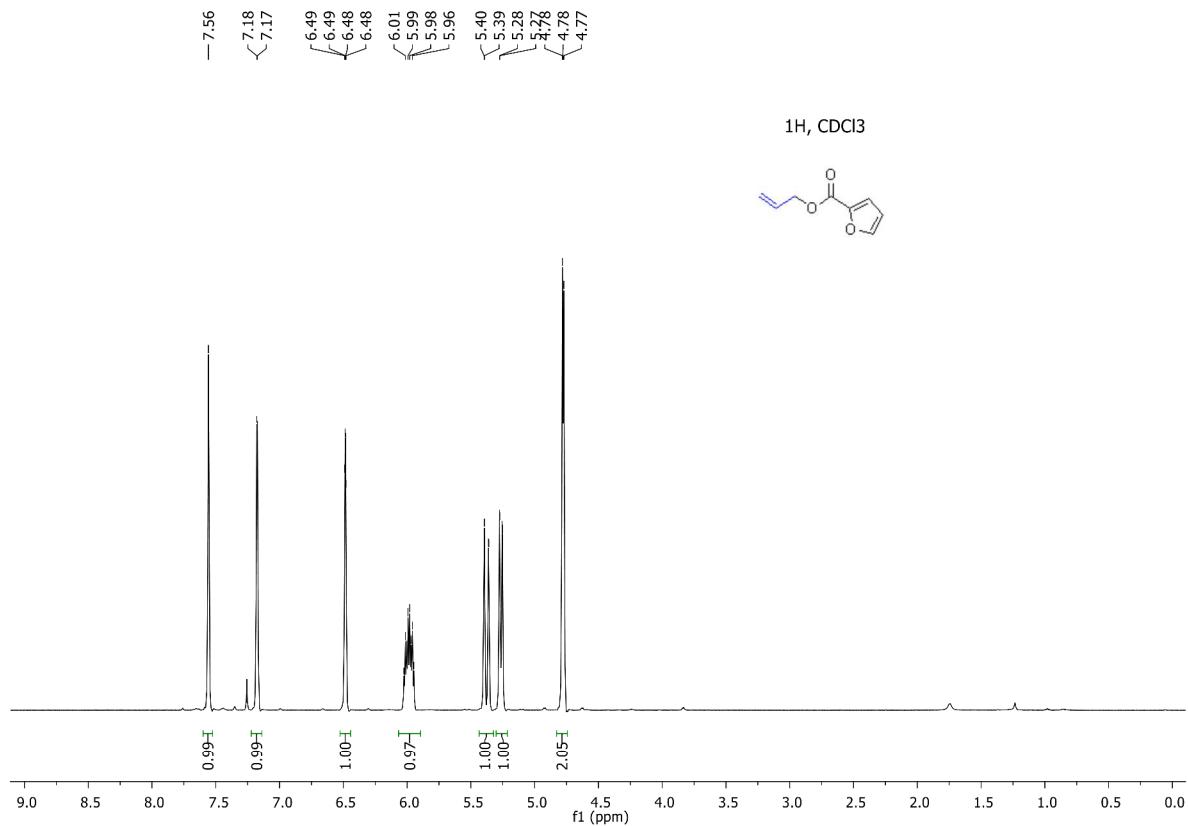


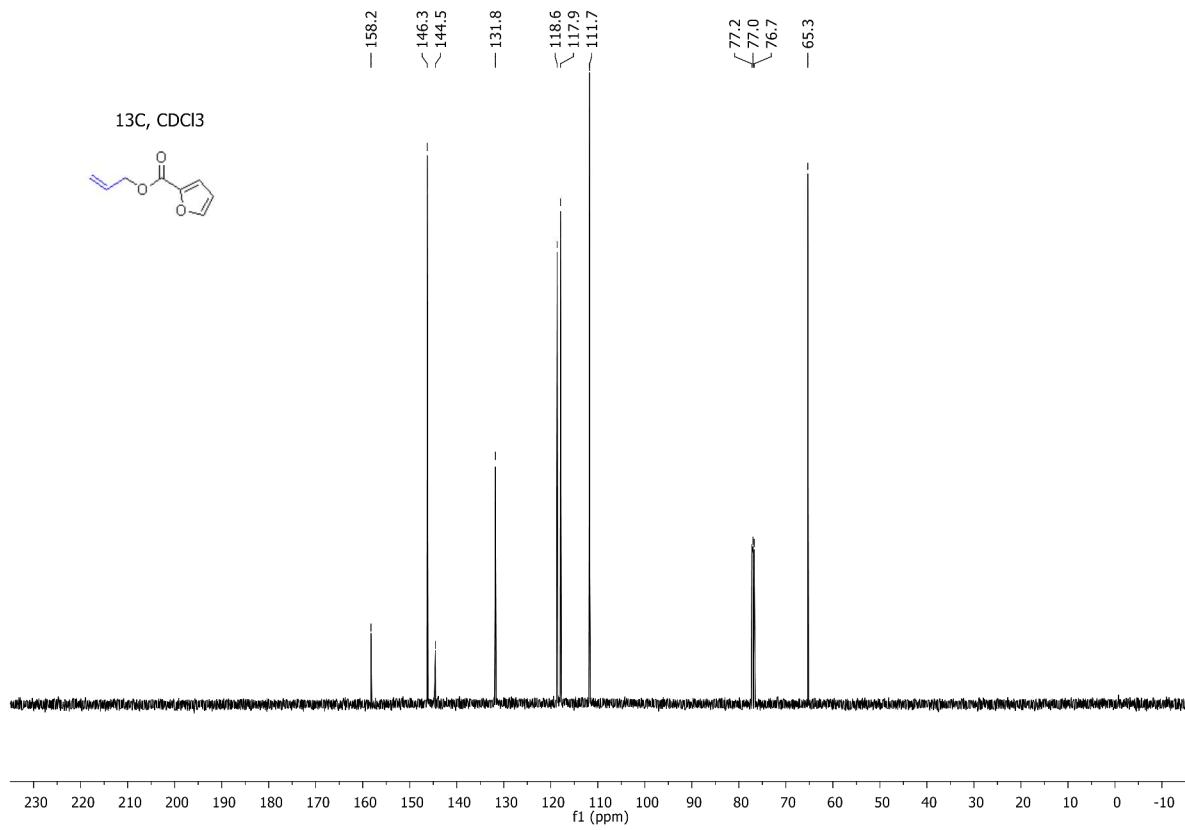


4-methoxybenzyl furan-2-carboxylate (13, Method A)



Allyl furan-2-carboxylate (14, Method B)

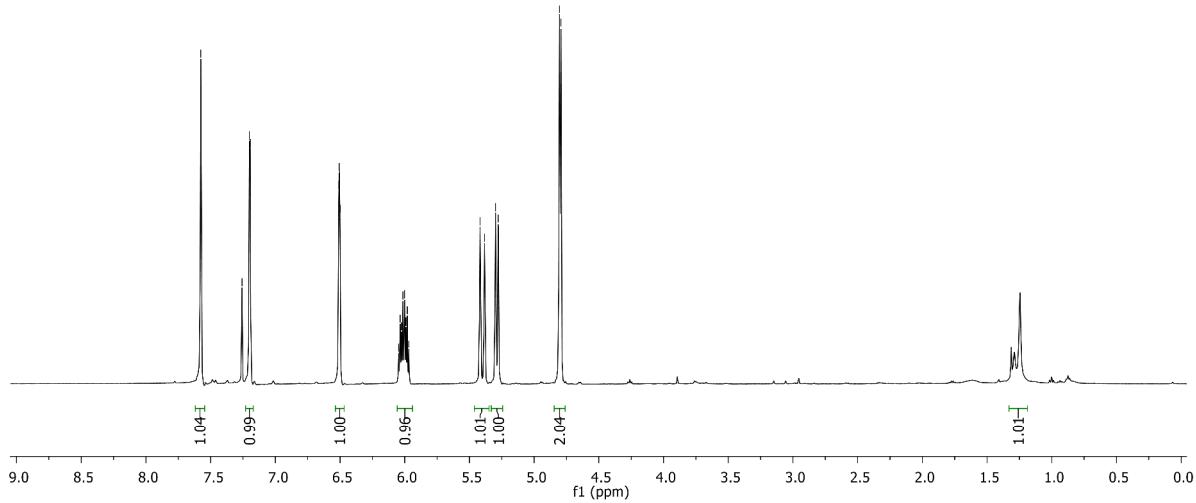
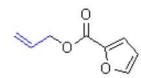




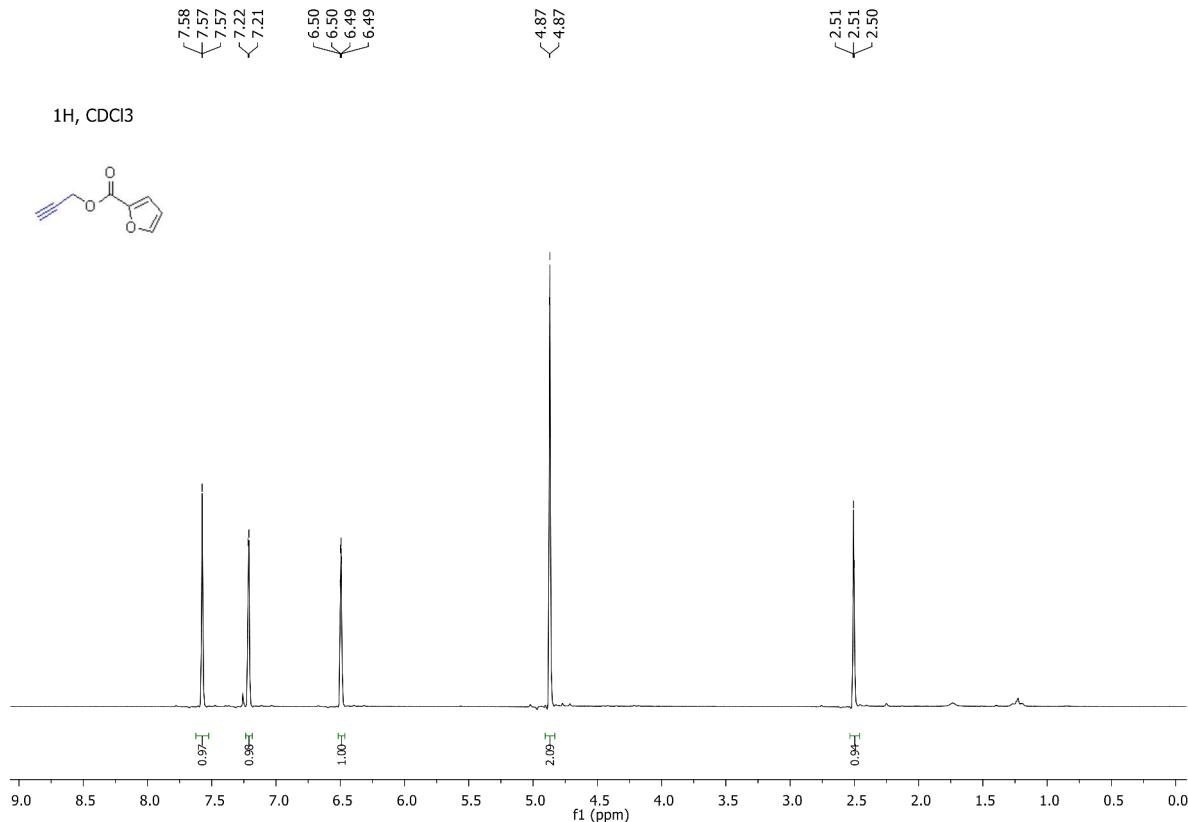
Allyl furan-2-carboxylate (14, Method A)

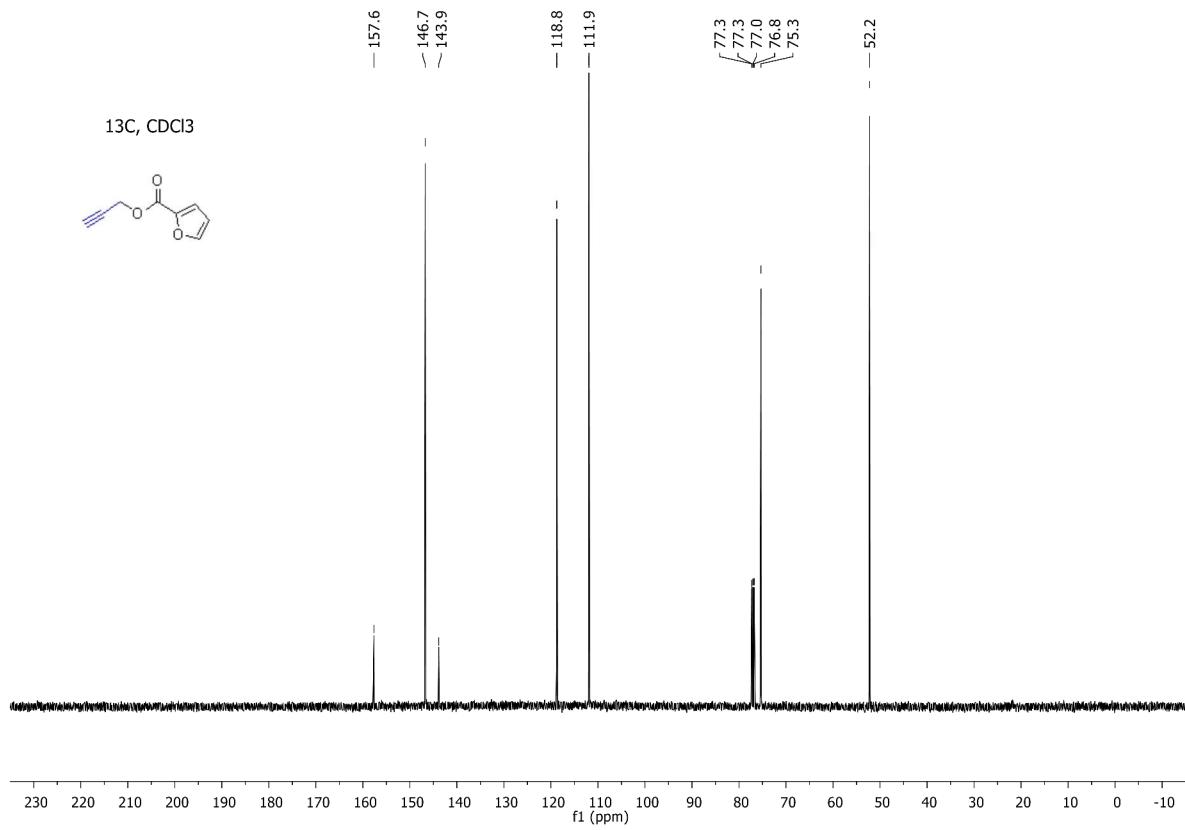
— 7.58
✓ 7.26
✓ 7.20
✓ 7.19
✓ 6.51
✓ 6.50
✓ 6.50
✓ 6.04
✓ 6.01
✓ 6.00
✓ 5.98
✓ 5.38
✓ 5.30
✓ 5.28
✓ 4.80
✓ 4.79

1H, CDCl₃

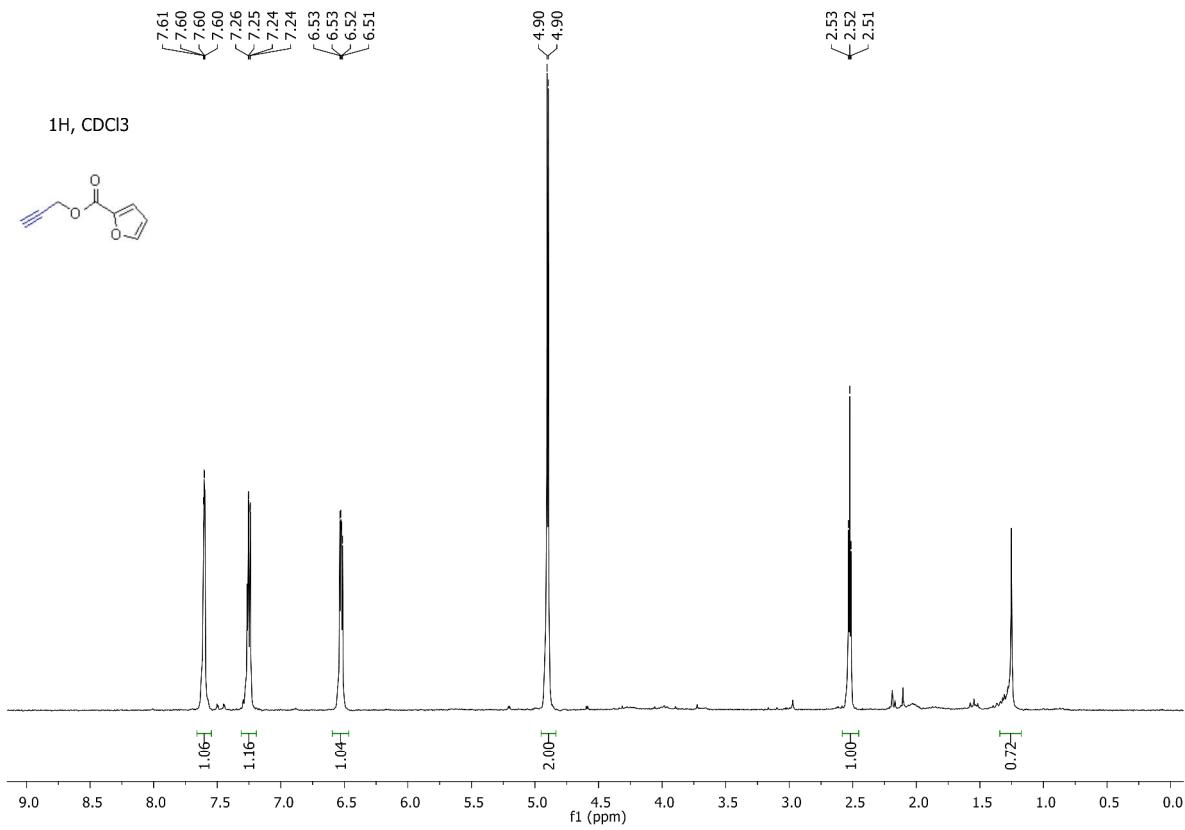


Prop-2-yn-1-yl furan-2-carboxylate (15, Method B)

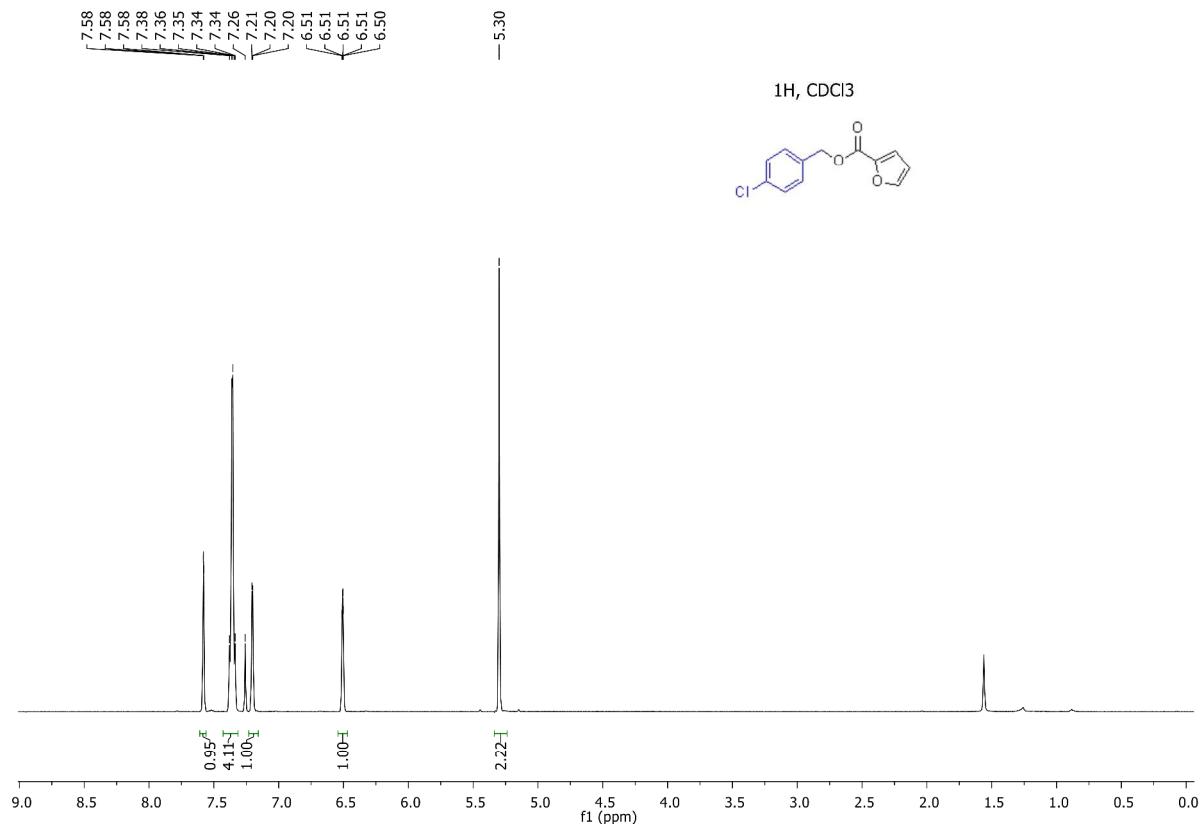


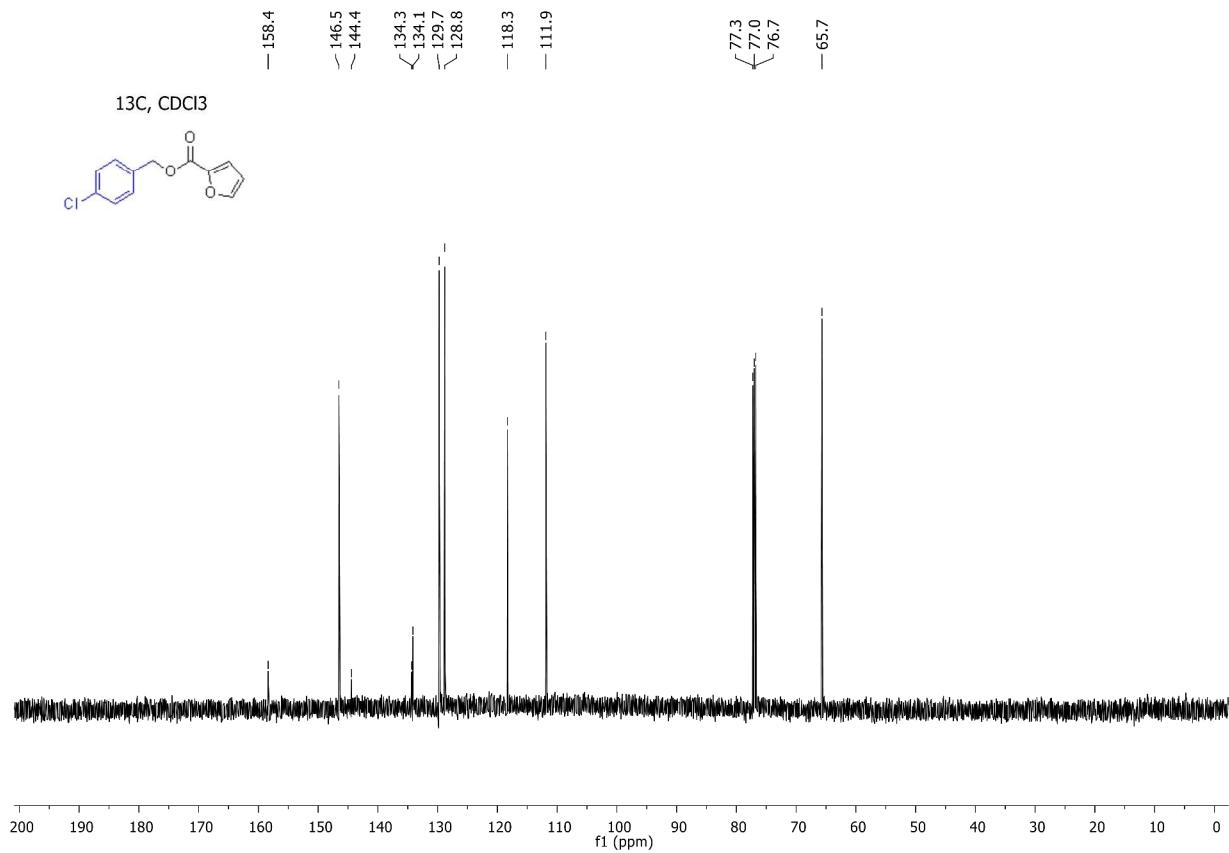


Prop-2-yn-1-yl furan-2-carboxylate (15, Method A)

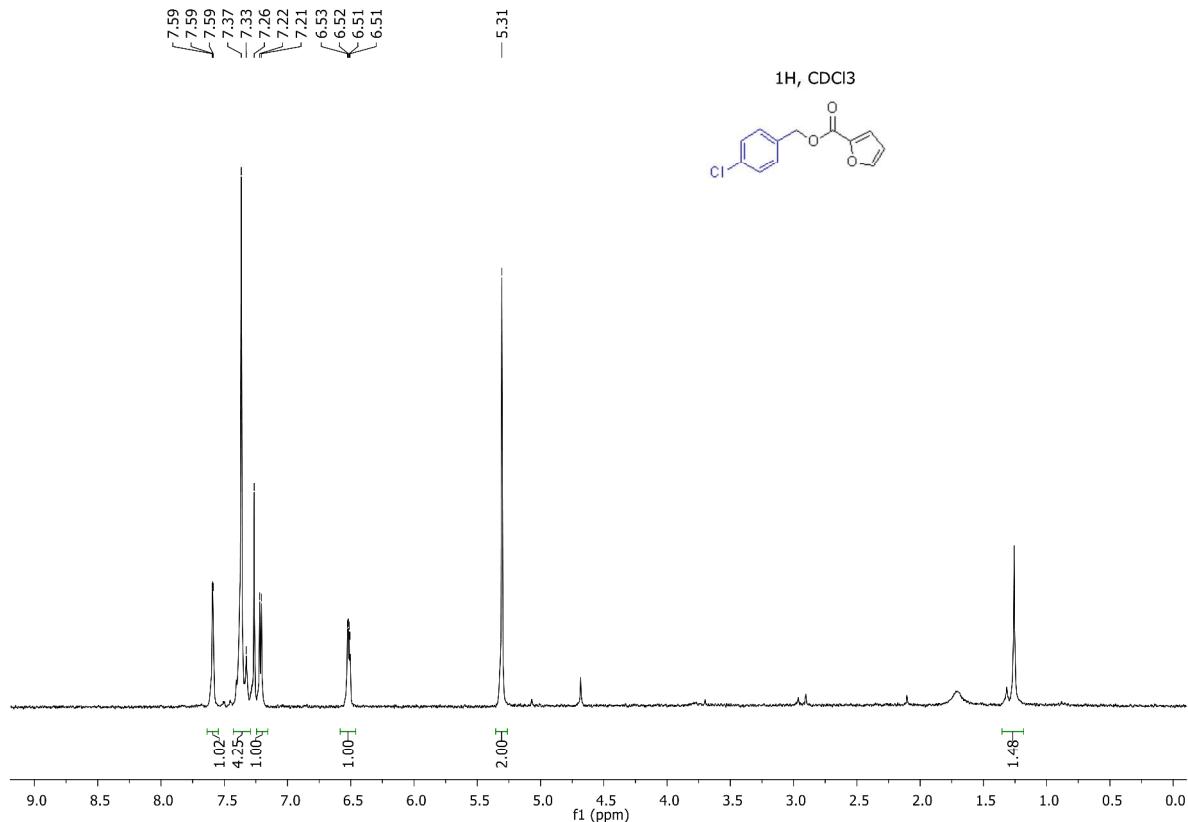


4-chlorobenzyl furan-2-carboxylate (16, Method B)

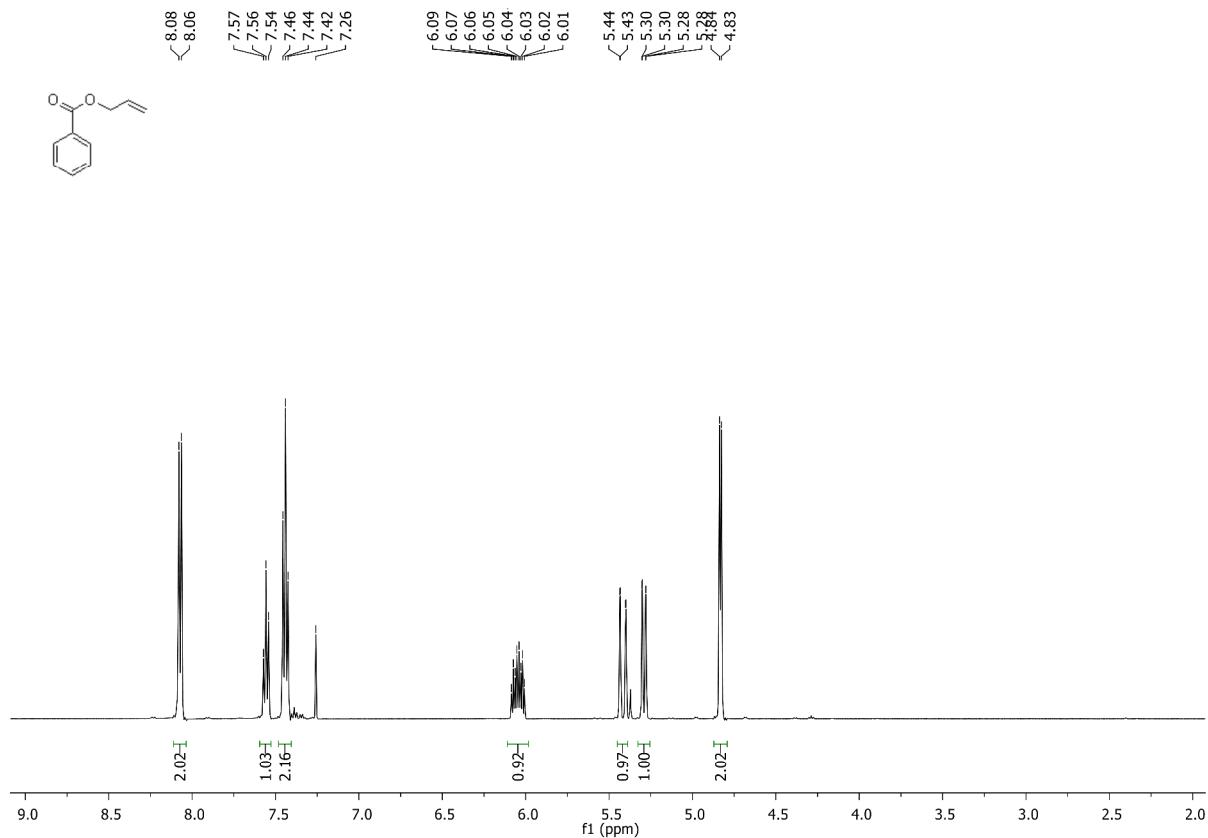


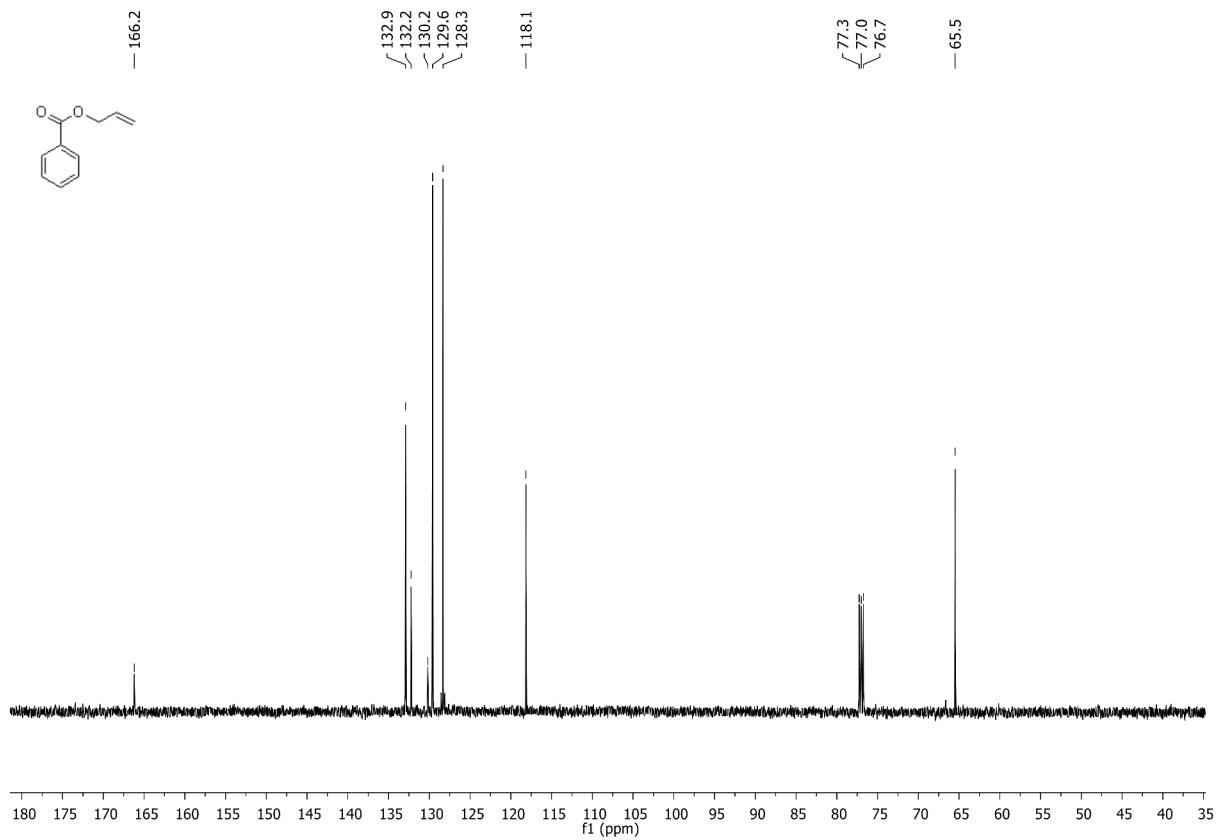


4-chlorobenzyl furan-2-carboxylate (16, Method A)

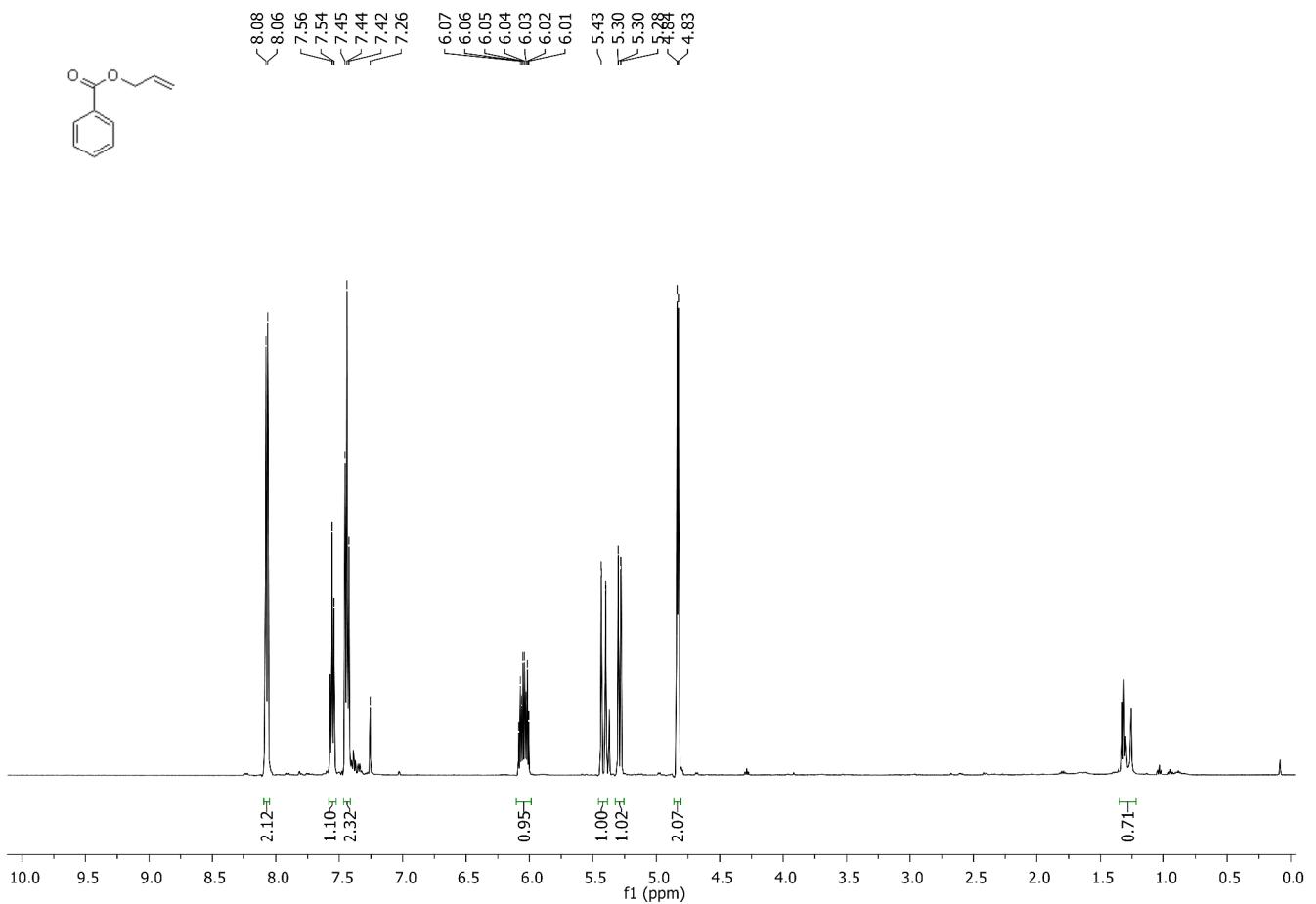


Allyl benzoate (17, Method B)

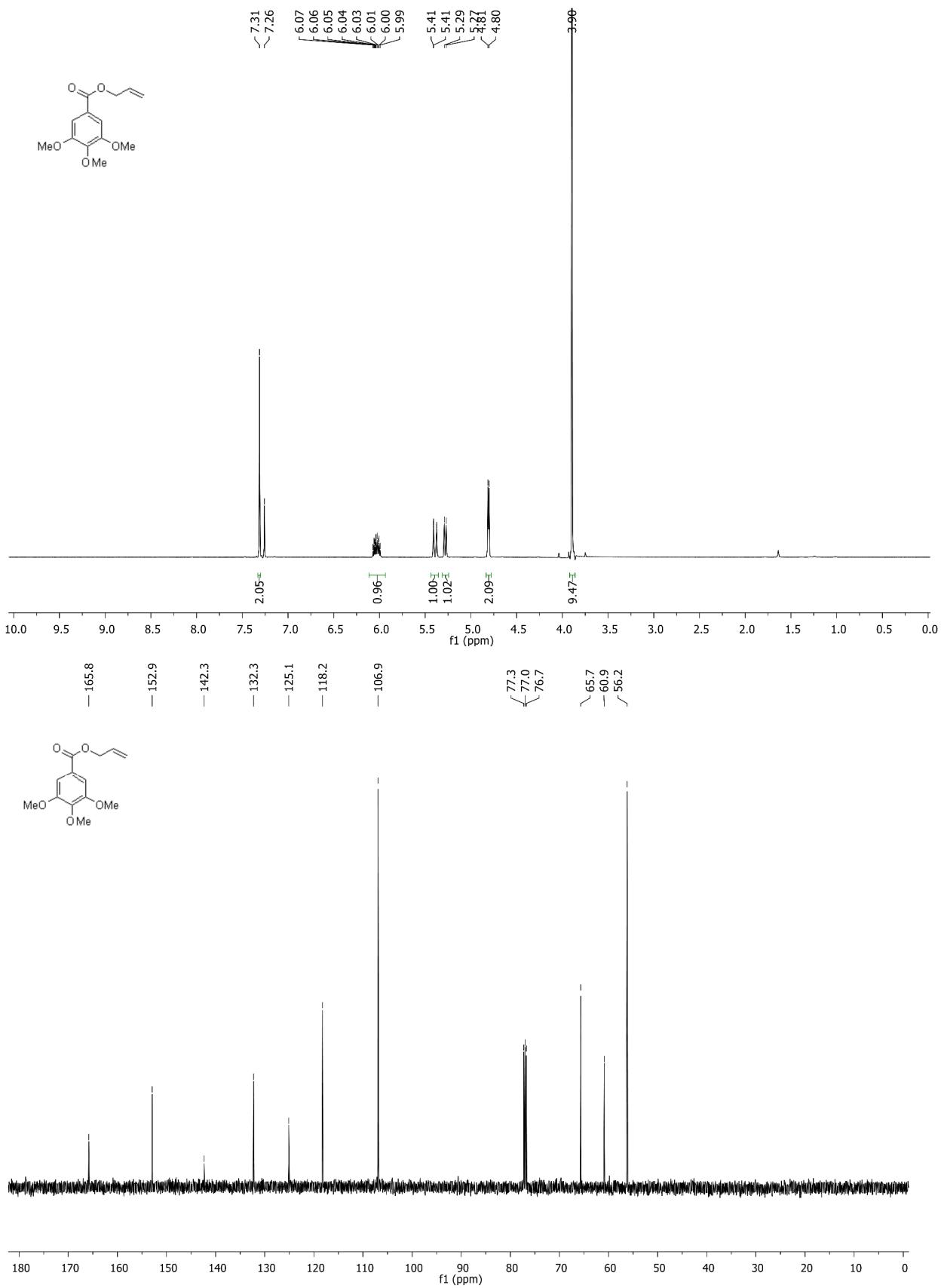




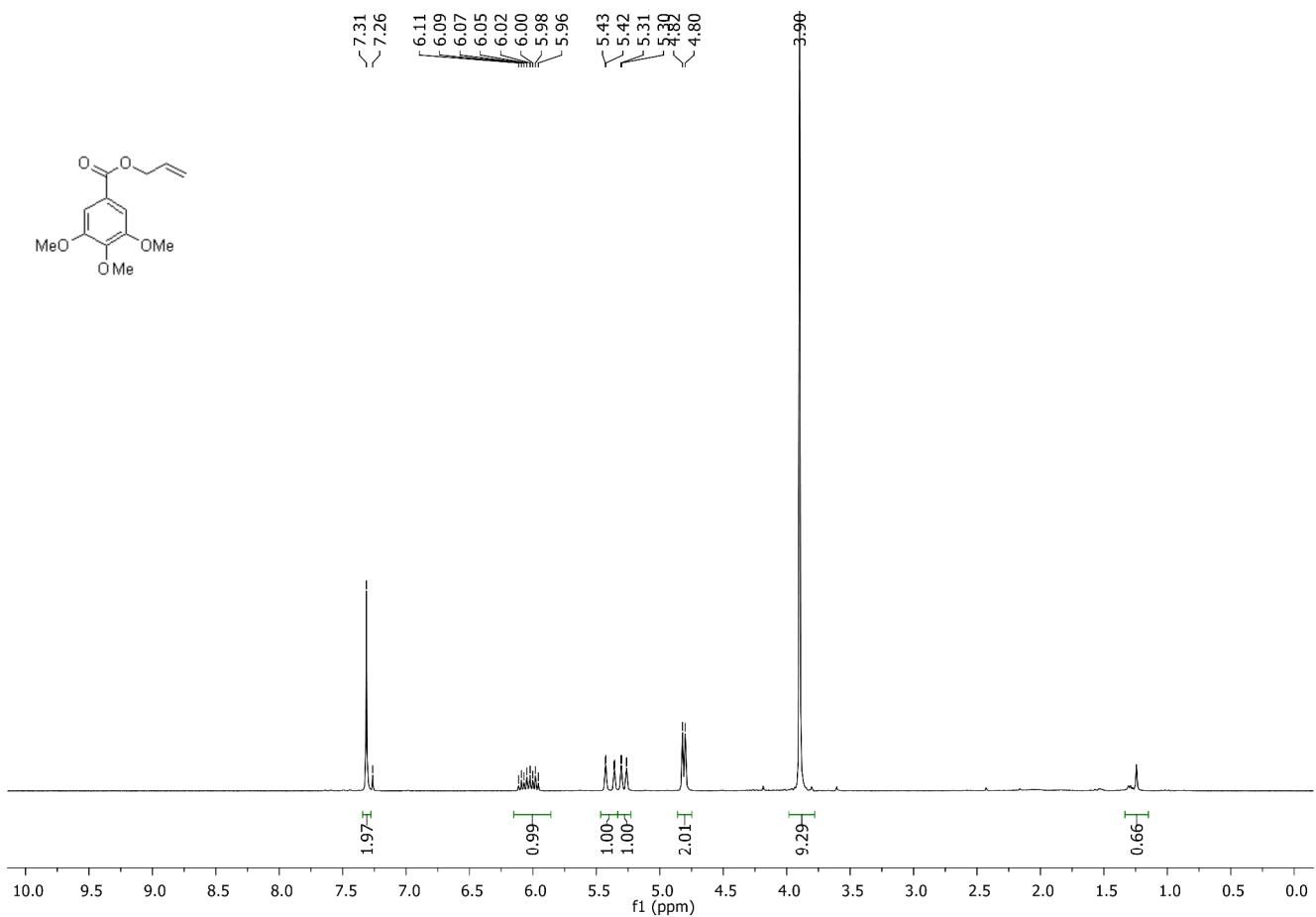
Allyl benzoate (17, Method A)



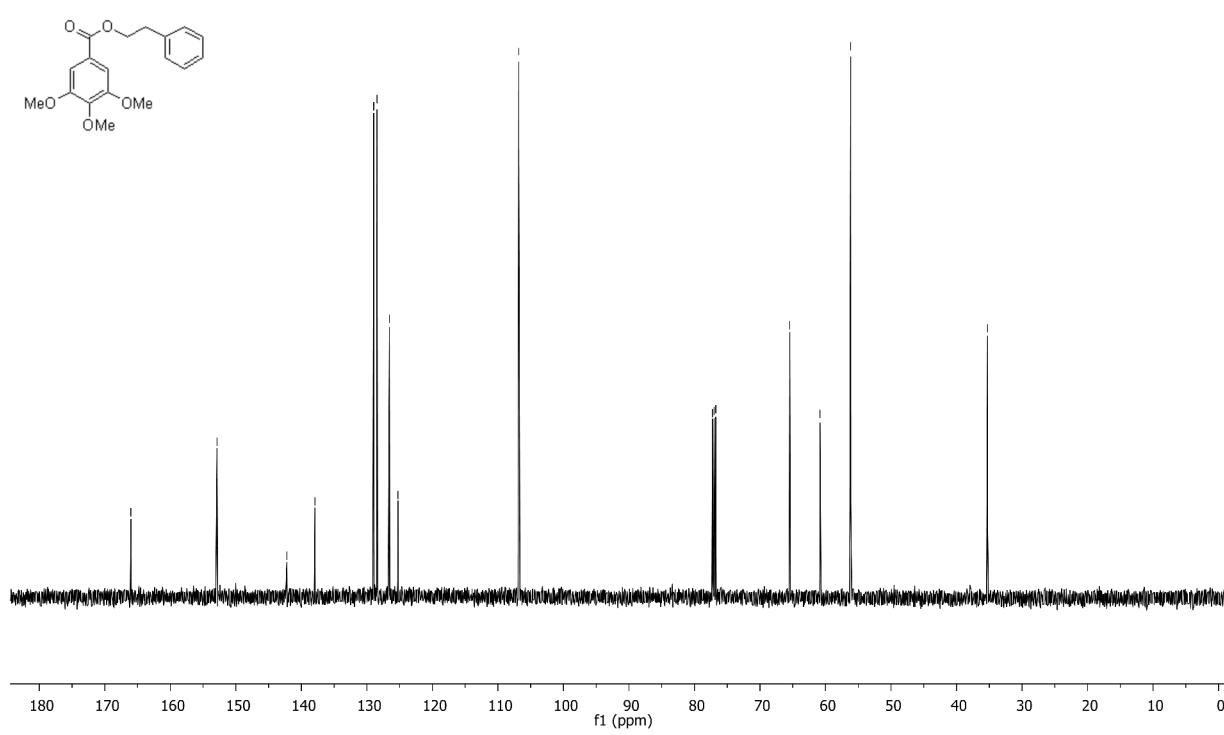
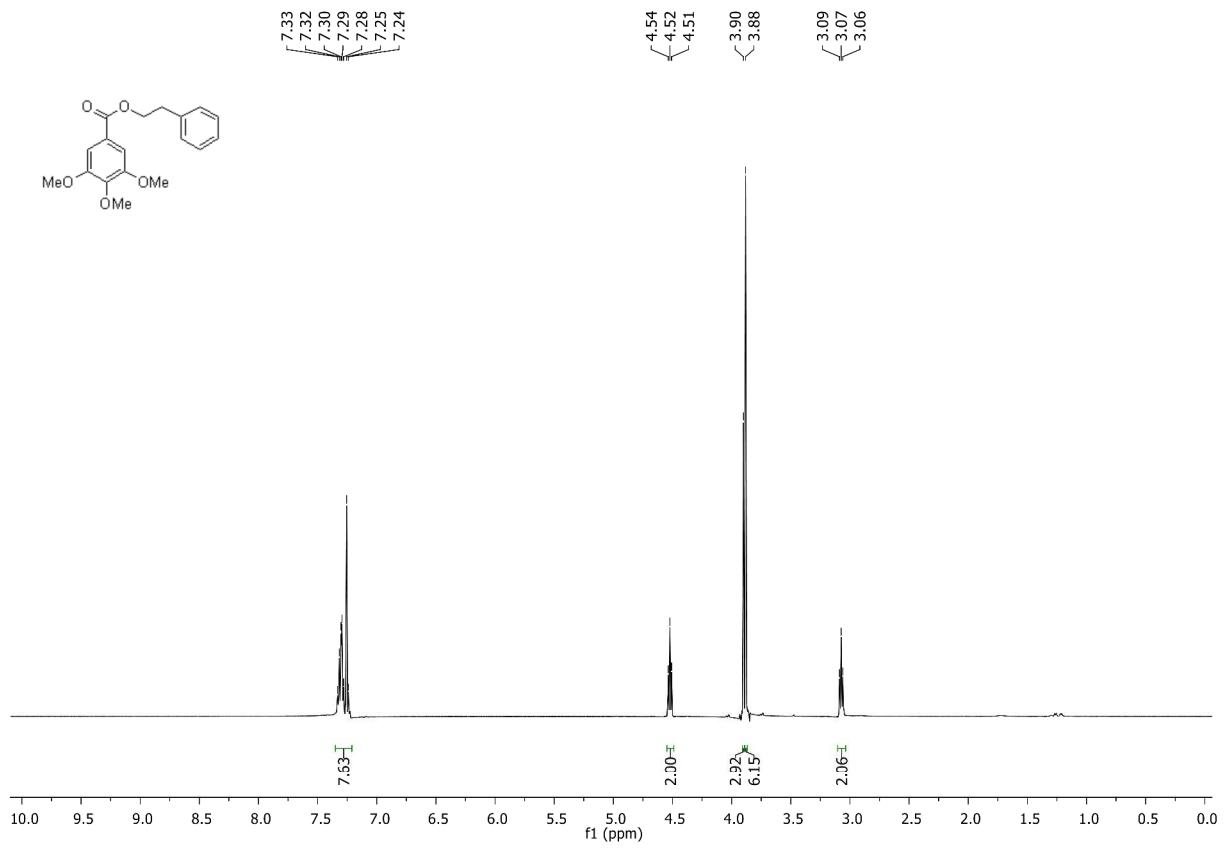
Allyl 3,4,5-trimethoxybenzoate (18, Method B)



Allyl 3,4,5-trimethoxybenzoate (18, Method A)



Phenethyl 3,4,5-trimethoxybenzoate (19, Method B)



Phenethyl 3,4,5-trimethoxybenzoate (19, Method A)

