Supporting Information:

NHC Catalyzed Oxidations of Aldehydes to Esters – Chemoselective Acylation of Alcohols in Presence of Amines

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Experimental Section:

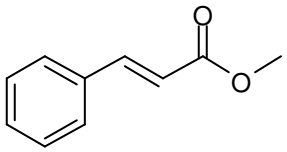
General: All reactions involving air or moisture-sensitive reagents or intermediates were carried out in heat-gun-dried glassware under an argon atmosphere. THF was freshly distilled from potassium under argon. All aldehydes, alcohols and amines were purified by distillation prior to use. All other solvents and reagents were purified according to standard procedures or were used as received from Aldrich, Acros or Fluka. 1,3-dimethyltriazolium iodide[1] and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone[2] were synthesized according to known procedures. ^{1}H and ^{13}C NMR spectroscopy: *Bruker dpx 300* (at 300 K). Chemical shifts, δ (in ppm), are reported relative to TMS (δ(^{1}H) 0.0 ppm, δ(^{13}C) 0.0 ppm) which was used as the inner reference. Otherwise the solvents residual proton resonance and carbon resonance ($CHCl_3$, δ(^{1}H) 7.26 ppm, δ(^{13}C) 77.0 ppm were used for calibration. TLC: Merck silica gel 60 F 254 plates; detection with UV light or by dipping into a solution of $KMnO_4$ (1.5 g in 400 mL H_2O, 5 g $NaHCO_3$) or a solution of $Ce(SO_4)_2$ x H_2O (10 g), phosphormolybdic acid hydrate (25 g), and conc. H_2SO_4 (60 mL) in H_2O (940 mL), followed by heating. Flash column chromatography (FC): Merck or Fluka silica gel 60 (40-63 μm) at approximately 0.4 bar. IR: Spectra were recorded on a *Bruker IFS-28* spectrophotometer. MS: Mass spectra were recorded on a *Finnigan MAT 4200S*, a *Bruker Daltonics MicroTof*, a *Waters Micromass Quatro LCZ* (ESI); and peaks are given in *m/z* (% of basis peak). GC analyses were carried out on a Hewlett Packard HP 6890 Series GC system equipped with a HP 5 column (30 m x 0.32 mm, film thickness 0.25 μm) using hydrogen as carrier gas. Full characterization is provided for unknown compounds.

General Procedure for the NHC-Catalyzed Oxidation of Aldehydes RCHO to the Corresponding Esters RCO_2R' (GP 1):

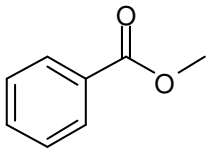
DBU (3 mol% or 1.1 equiv) was added to a solution of 1,3-dimethyltriazolium iodide (2 mol%) and alcohol R'OH (0.5 mL) in THF (2.0 mL) under argon atmosphere. The mixture was stirred for 5 minutes, followed by the addition of aldehyde RCHO (1.0 equiv) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (1.0 equiv). The reaction mixture was stirred at room temperature for 2-6 hours until consumption of starting aldehyde as checked by TLC. The solvent was removed under vacuum and the residue was purified by flash silica gel column chromatography by using a mixture of pentane and diethyl ether as eluent.

Entry	R	R'	Yield [%]
1	$C_6H_5CH=CH$	Me	99
2[a]	C_6H_5	Me	94
3	4-$NO_2C_6H_4$	Me	89
4[a]	4-$CH_3OC_6H_4$	Me	95
5	4-BrC_6H_4	Me	97
6	4-$CH_3OC(O)C_6H_4$	Me	97
7	2-$CF_3C_6H_4$	Me	96
8	3-ClC_6H_4	Me	99
9[a]	β-naphthyl	Me	99
10[a]	α-naphthyl	Me	99
11	2-thienyl	Me	97
12	4-$(CH_2=CH)C_6H_4$	Me	92
13	4-([1,3]dithiolan-2-yl)C_6H_4	Me	93
14	4-$([EtO]_2CH)C_6H_4$	Me	96
15[b]	$C_6H_5CH=CH$	Et	99
16[b]	$C_6H_5CH=CH$	$CH_2=CHCH_2$	99
17[b]	$C_6H_5CH=CH$	$C_6H_5CH_2$	95
18[b]	$C_6H_5CH=CH$	$(CH_3)_2CH$	92
19[b,c]	$C_6H_5CH=CH$	C_6H_{11}	92
20[b,c,d]	$C_6H_5CH=CH$	C_6H_5	96
21[b,e]	$C_6H_5CH=CH$	farnesyl	95

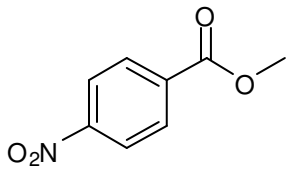
[a] Reaction conducted for 6h. [b] 1.1 equiv of DBU was used. [c] With 1.5 equiv of alcohol. [d] Product contains 2% of phenyl 3-phenylpropionate. [e] With 0.9 equiv of farnesol.



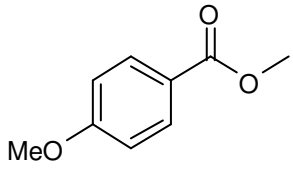
(*E*)-Cinnamic acid methyl ester: According to GP 1 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (2.3 mg, 15 µmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and methanol (0.5 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 50:1) to afford the corresponding ester (81 mg, 99%).



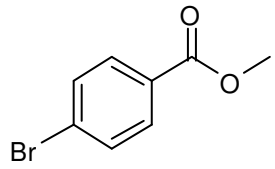
Benzoic acid methyl ester: According to GP 1 with benzaldehyde (53 mg, 0.5 mmol), DBU (2.3 mg, 15 µmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and methanol (0.5 mL) for 6 h and SiO_2-chromatography (pentane:Et_2O, 100:1) to afford the corresponding ester (64 mg, 94%).



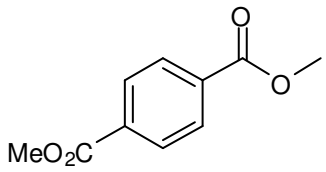
4-Nitro-benzoic acid methyl ester: According to GP 1 with 4-nitro-benzaldehyde (76 mg, 0.5 mmol), DBU (2.3 mg, 15 µmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and methanol (0.5 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 30:1) to afford the corresponding ester (81 mg, 89%).



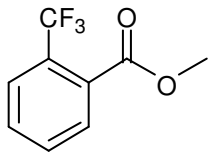
4-Methoxy-benzoic acid methyl ester: According to GP 1 with 4-methoxy-benzaldehyde (68 mg, 0.5 mmol), DBU (2.3 mg, 15 µmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and methanol (0.5 mL) for 6 h and SiO_2-chromatography (pentane:Et_2O, 30:1) to afford the corresponding ester (79 mg, 95%).



4-Bromo-benzoic acid methyl ester: According to GP 1 with 4-bromo-benzaldehyde (93 mg, 0.5 mmol), DBU (2.3 mg, 15 µmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and methanol (0.5 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 80:1) to afford the corresponding ester (104 mg, 97%).

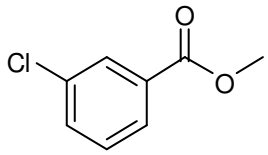


Terephthalic acid dimethyl ester: According to GP 1 with 4-formyl-benzoic acid methyl ester (82 mg, 0.5 mmol), DBU (2.3 mg, 15 µmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and methanol (0.5 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 30:1) to afford the corresponding ester (94 mg, 97%).

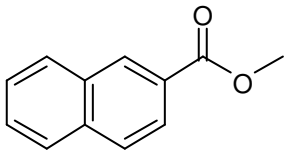


2-Trifluoromethyl-benzoic acid methyl ester: According to GP 1 with 2-trifluoromethyl-benzaldehyde (87 mg, 0.5 mmol), DBU (2.3 mg, 15 µmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg,

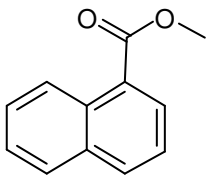
0.5 mmol) in THF (2.0 mL) and methanol (0.5 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 80:1) to afford the corresponding ester (98 mg, 96%).



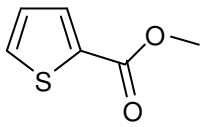
3-Chloro-benzoic acid methyl ester: According to GP 1 with 3-chloro-benzaldehyde (70 mg, 0.5 mmol), DBU (2.3 mg, 15 µmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and methanol (0.5 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 50:1) to afford the corresponding ester (85 mg, 99%).



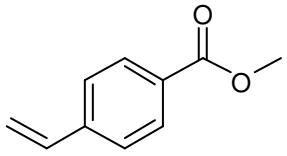
Naphthalene-2-carboxylic acid methyl ester: According to GP 1 with naphthalene-2-carbaldehyde (78 mg, 0.5 mmol), DBU (2.3 mg, 15 µmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and methanol (0.5 mL) for 6 h and SiO_2-chromatography (pentane:Et_2O, 80:1) to afford the corresponding ester (92 mg, 99%).



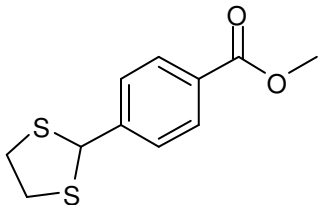
Naphthalene-1-carboxylic acid methyl ester: According to GP 1 with naphthalene-1-carbaldehyde (78 mg, 0.5 mmol), DBU (2.3 mg, 15 µmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and methanol (0.5 mL) for 6 h and SiO_2-chromatography (pentane:Et_2O, 80:1) to afford the corresponding ester (92 mg, 99%).



Thiophene-2-carboxylic acid methyl ester: According to GP 1 with 2-thiophenecarboxaldehyde (56 mg, 0.5 mmol), DBU (2.3 mg, 15 µmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and methanol (0.5 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 80:1) to afford the corresponding ester (69 mg, 97%).

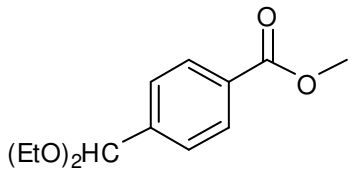


4-Vinyl-benzoic acid methyl ester: According to GP 1 with 4-vinyl-benzaldehyde[3] (66 mg, 0.5 mmol), DBU (2.3 mg, 15 µmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and methanol (0.5 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 60:1) to afford the corresponding ester (75 mg, 92%).



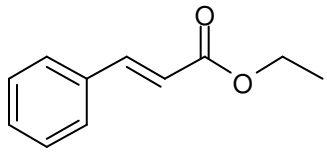
4-[1,3]Dithiolan-2-yl-benzoic acid methyl ester: According to GP 1 with 4-[1,3]dithiolan-2-yl-benzaldehyde[4] (105 mg, 0.5 mmol), DBU (2.3 mg, 15 µmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and methanol (0.5 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 50:1) to afford the corresponding ester (112 mg, 93%).

FTIR (neat): $\tilde{\nu}$ = 2933, 1717, 1295, 1092, 942 cm^{-1}. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.97 (d, *J*=8.4, 2H), 7.57 (d, *J*=8.2, 2H), 5.64 (s, 1H), 3.90 (s, 3H), 3.55 – 3.44 (m, 2H), 3.43 – 3.31 (m, 2H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.6, 146.0, 129.8, 129.5, 127.9, 55.6, 52.1, 40.3. HRMS (ESI) Exact mass calculated for $C_{11}H_{12}O_2S_2$ Na ([M + Na]$^+$): 263.0171. Found: 263.0178.

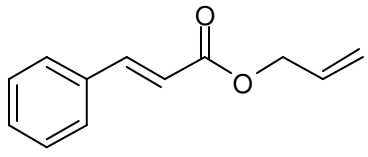


4-Diethoxymethyl-benzoic acid methyl ester: According to GP 1 with 4-diethoxymethyl-benzaldehyde (104 mg, 0.5 mmol), DBU (2.3 mg, 15 µmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and methanol (0.5 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 30:1) to afford the corresponding ester (114 mg, 96%).

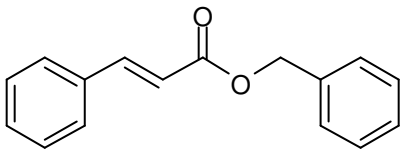
FTIR (neat): $\tilde{\nu}$ = 2977, 2883, 1723, 1436, 1274, 1051 cm^{-1}. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.03 (d, *J*=8.4, 2H), 7.55 (d, *J*=8.1, 2H), 5.54 (s, 1H), 3.91 (s, 3H), 3.57 (q, *J*= 7.1, 4H), 1.24 (t, *J*=7.1, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.9, 144.0, 130.0, 129.5, 126.7, 100.8, 61.1, 52.1, 15.1. HRMS (ESI) Exact mass calculated for $C_{13}H_{18}O_4$ Na ([M + Na]$^+$): 261.1097. Found: 261.1080.



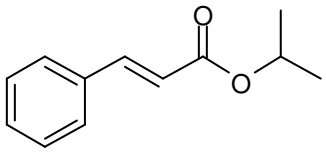
(*E*)-Cinnamic acid ethyl ester: According to GP 1 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and ethanol (0.5 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 50:1) to afford the corresponding ester (87 mg, 99%).



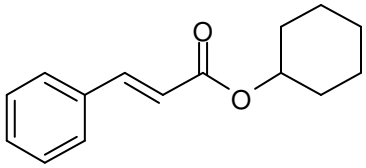
(*E*)-Cinnamic acid allyl ester: According to GP 1 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and allyl alcohol (0.5 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 60:1) to afford the corresponding ester (93 mg, 99%).



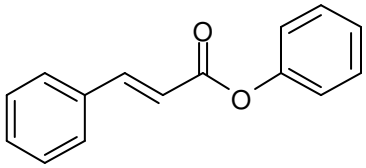
(*E*)-Cinnamic acid benzyl ester: According to GP 1 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and benzyl alcohol (0.5 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 60:1) to afford the corresponding ester (113 mg, 95%).



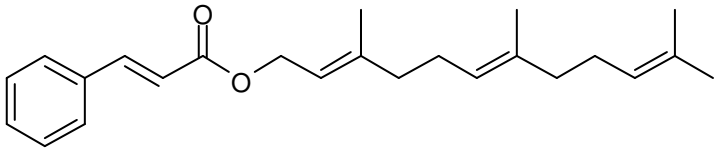
(*E*)-Cinnamic acid isopropyl ester: According to GP 1 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (2.0 mL) and isopropanol (0.5 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 80:1) to afford the corresponding ester (90 mg, 92%).



(*E*)-Cinnamic acid cyclohexyl ester: According to GP 1 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) and cyclohexanol (75 mg, 0.75 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 80:1) to afford the corresponding ester (106 mg, 92%).



(*E*)-Cinnamic acid phenyl ester: According to GP 1 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) and phenol (71 mg, 0.75 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 60:1) to afford the corresponding ester (107 mg, 96%, contains 2% of phenyl 3-phenylpropionate).



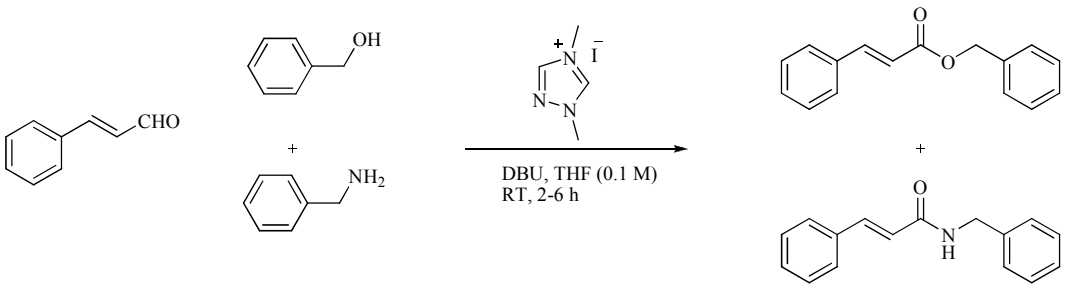
(*E*)-Cinnamic acid (2*E*,6*E*)-3,7,11-trimethyl-dodeca-2,6,10-trienyl ester: According to GP 1 with *(E)*-cinnamaldehyde (73 mg, 0.55 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) and (*E*,*E*)-farnesol (111 mg,

0.5 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 80:1) to afford the corresponding ester (167 mg, 95%).
FTIR (neat): $\tilde{\nu}$ = 2919, 1712, 1638, 1450, 1306, 1202 cm^{-1}. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.70 (d, *J*=16.0, 1H), 7.56 – 7.47 (m, 2H), 7.43 – 7.32 (m, 3H), 6.45 (d, *J*=16.0, 1H), 5.43 (td, *J*=7.1, 1.0, 1H), 5.17 – 5.05 (m, 2H), 4.74 (d, *J*=7.1, 2H), 2.17 – 1.95 (m, 8H), 1.76 (s, 3H), 1.68 (s, 3H), 1.61 (s, 3H), 1.60 (s, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 167.0, 144.6, 142.3, 135.4, 134.5, 131.3, 130.1, 128.8, 128.0, 124.3, 123.6, 118.4, 118.3, 61.4, 39.7, 39.5, 26.7, 26.2, 25.6, 17.6, 16.5, 16.0. HRMS (ESI) Exact mass calculated for $C_{24}H_{32}O_2$ Na ($[M + Na]^+$): 375.2295. Found: 375.2296.

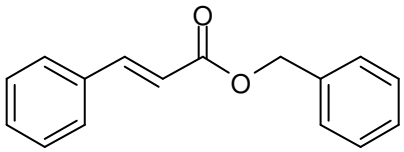
General Procedure for the NHC-Catalyzed Chemoselective Acylation Reactions (GP 2):

DBU (3 mol% or 1.1 equiv) was added to a solution of 1,3-dimethyltriazolium iodide (2 mol%), alcohol (1.0 or 1.5 equivalents) and amine (1.0 or 1.5 equivalents) [otherwise amino alcohol (1.5 or 3.0 equivalents)] in THF (5.0 mL) under argon atmosphere. The mixture was stirred for 5 minutes, followed by the addition of aldehyde (1.5 equivalents or 1.0 equivalent) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (1.0 equiv). The reaction mixture was stirred at room temperature for 2-6 hours. The solvent was removed under vacuum and the residue was purified by flash silica gel column chromatography by using a mixture of pentane-diethyl ether or MTBE-methanol as eluent.

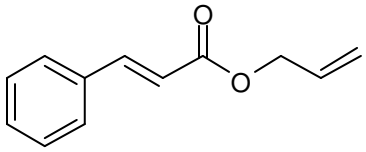
Effect of DBU on Chemoselective Acylation Reactions:



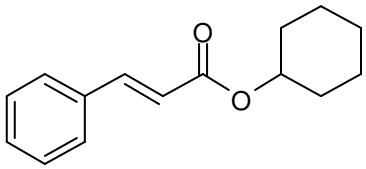
Entry	Aldehyde (mmol)	Alcohol (mmol)	Amine (mmol)	Catalyst (mol%)	DBU (mol%)	Ester [Yield %]	Amide [Yield %]
1	0.50	0.75	0.75	2	3	73	<1%
2	0.50	0.75	0.75	3	2	71	<1%
3	0.75	0.50	0.50	2	3	98	<1%
4	0.50	0.75	0.75	2	110	96	<1%



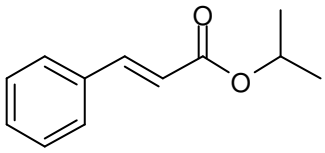
(*E*)-Cinnamic acid benzyl ester: According to GP 2 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), benzyl alcohol (81 mg, 0.75 mmol), benzyl amine (80 mg, 0.75 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 60:1) to afford the corresponding ester (114 mg, 96%).



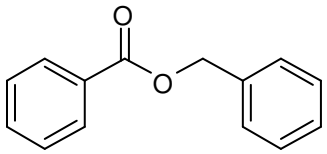
(*E*)-Cinnamic acid allyl ester: According to GP 2 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), allyl alcohol (44 mg, 0.75 mmol), allyl amine (43 mg, 0.75 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 60:1) to afford the corresponding ester (83 mg, 88%).



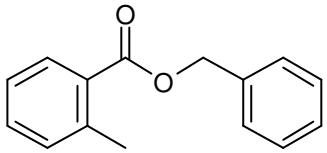
(*E*)-*N*-Cyclohexayl-cinnamamide: According to GP 2 with *(E)*-cinnamaldehyde (99 mg, 0.75 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), cyclohexanol (50 mg, 0.5 mmol), cyclohexayl amine (50 mg, 0.5 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 80:1) to afford the corresponding ester (105 mg, 91%).



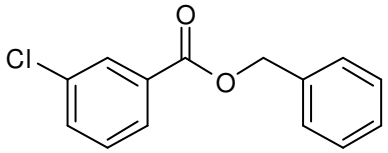
(*E*)-Cinnamic acid isopropyl ester: According to GP 2 with *(E)*-cinnamaldehyde (99 mg, 0.75 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), isopropanol (30 mg, 0.5 mmol), benzyl amine (54 mg, 0.5 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 80:1 to pentane:MTBE 1.5:1) to afford the corresponding ester (75 mg, 79%).and (*E*)-N-Benzyl-cinnamamide (16 mg, 13%).



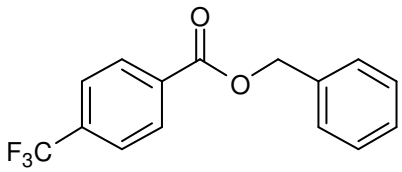
Benzyl benzoate: According to GP 2 with benzaldehyde (80 mg, 0.75 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), benzyl alcohol (54 mg, 0.5 mmol), benzyl amine (54 mg, 0.5 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 6 h and SiO_2-chromatography (pentane:Et_2O, 100:1) to afford the corresponding ester (86 mg, 81%).



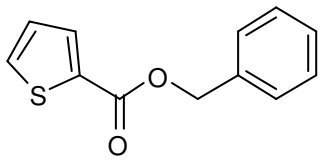
2-Methyl-benzoic acid benzyl ester: According to GP 2 with 2-methyl-benzaldehyde (90 mg, 0.75 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), benzyl alcohol (54 mg, 0.5 mmol), benzyl amine (54 mg, 0.5 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 6 h and SiO_2-chromatography (pentane:Et_2O, 100:1) to afford the corresponding ester (88 mg, 78%).
FTIR (neat): $\tilde{\nu}$ = 2959, 2361, 1716, 1601, 1456, 1247, 1072, 735 cm^{-1}. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.02 – 7.91 (m, 1H), 7.50 – 7.32 (m, 6H), 7.27 – 7.20 (m, 2H), 5.35 (s, 2H), 2.61 (s, 3H).^{13}C-NMR (75 MHz, $CDCl_3$): δ = 167.4, 140.3, 136.2, 132.0, 131.7, 130.7, 129.5, 128.6, 128.2, 125.7, 66.5, 21.8. HRMS (ESI) Exact mass calculated for $C_{15}H_{14}O_2$ Na ($[M + Na]^+$): 249.0886. Found: 249.0885.



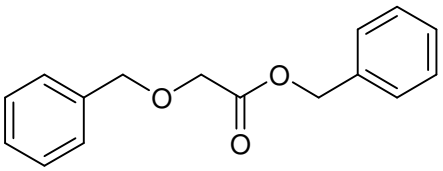
3-Chloro-benzoic acid benzyl ester: According to GP 2 with 3-chloro-benzaldehyde (71 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), benzyl alcohol (81 mg, 0.75 mmol), benzyl amine (80 mg, 0.75 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 100:1) to afford the corresponding ester (114 mg, 92%).
FTIR (neat): $\tilde{\nu}$ = 2956, 2360, 1720, 1575, 1426, 1282, 1249, 1124, 956, 696 cm^{-1}. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.05 (t, *J*=1.8, 1H), 8.01 – 7.88 (m, 1H), 7.53 (ddd, *J*=8.0, 2.1, 1.1, 1H), 7.48 – 7.32 (m, 6H), 5.37 (s, 2H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 165.2, 135.7, 134.6, 133.1, 131.9, 129.8, 129.7, 128.7, 128.4, 128.3, 127.9, 67.1. HRMS (ESI) Exact mass calculated for $C_{14}H_{11}ClO_2$ Na ($[M + Na]^+$): 269.0340. Found: 269.0331.



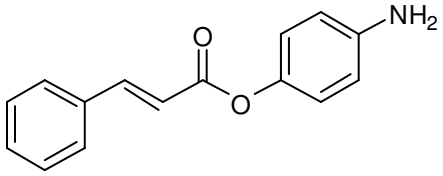
4-Trifluoromethyl-benzoic acid benzyl ester: According to GP 2 with 4-trifluoromethyl-benzaldehyde (87 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), benzyl alcohol (81 mg, 0.75 mmol), benzyl amine (80 mg, 0.75 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 100:1) to afford the corresponding ester (129 mg, 92%).



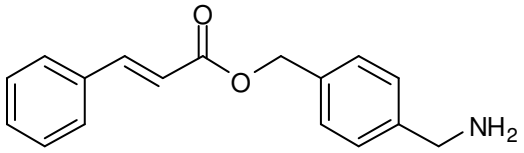
Thiophene-2-carboxylic acid benzyl ester: According to GP 2 with thiophene-2-carbaldehyde (56 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), benzyl alcohol (81 mg, 0.75 mmol), benzyl amine (80 mg, 0.75 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:Et_2O, 100:1) to afford the corresponding ester (107 mg, 98%).



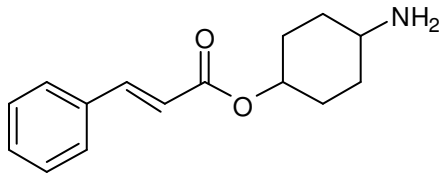
***O*-Benzylglycolic acid benzyl ester:** According to GP 2 with benzyloxy acetaldehyde (75 mg, 0.5 mmol), DBU (83 mg, 0.55 mmmol), 1,3-dimethyl triazolium iodide (2.25 mg, 0.01 mmol), benzyl alcohol (81 mg, 0.75 mmol), benzyl amine (80.3 mg,0.75 mmol) and 3,3',5,5'-tetra-tert-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.00 ml) for 13 hours and (SiO_2-chromatography (pentane:MTBE,50:1) to afford the ester (64 mg, 50%).
^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.30 – 7.19 (m, 10H), 5.13 (s, 2H), 4.57 (s, 2H), 4.07 (s, 2H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 170.2, 137.0, 135.4, 128.6, 128.5(0), 128.4(7), 128.4, 128.1(1), 128.0(5), 73.4, 67.2, 66.6. HRMS (ESI) Exact mass calculated for $C_{16}H_{16}O_3$ Na([M + Na]$^+$): 279.0983. Found: 279.0992.



(*E*)-Cinnamic acid 4-amino-phenyl ester (7): According to GP 2 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 4-amino-phenol (81 mg, 0.75 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:MTBE, 1.5:1) to afford **7** (111 mg, 93%).
FTIR (neat): $\tilde{\nu}$ = 3444, 3366, 3022, 1712, 1637, 1507, 1312, 1150 cm^{-1}. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.85 (d, *J*=16.0, 1H), 7.63 – 7.53 (m, 2H), 7.48 – 7.35 (m, 3H), 7.01 – 6.91 (m, 2H), 6.74 – 6.66 (m, 2H), 6.62 (d, *J*=16.0, 1H), 3.65 (s, 2H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 165.9, 146.1, 144.2, 143.0, 134.3, 130.5, 128.9, 128.21, 122.2, 117.6, 115.6. HRMS (ESI) Exact mass calculated for $C_{15}H_{13}NO_2$ H ([M + H]$^+$): 240.1019. Found: 240.1016.

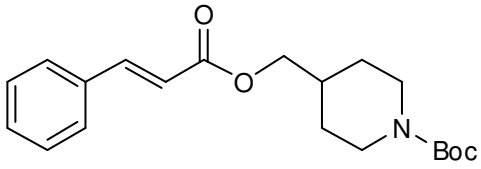


(*E*)-Cinnamic acid 4-aminomethyl-benzyl ester (8): According to GP 2 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), (4-aminomethyl-phenyl)-methanol[5] (103 mg, 0.75 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:MTBE, 1:1 to MTBE:methanol 3:1) to afford **8** (116 mg, 87%).
FTIR (neat): $\tilde{\nu}$ = 3354, 3028, 1709, 1636, 1450, 1309, 1162 cm^{-1}. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.72 (d, *J*=16.0, 1H), 7.59 – 7.46 (m, 2H), 7.47 – 7.31 (m, 7H), 6.47 (d, *J*=16.0, 1H), 5.23 (s, 2H), 3.88 (s, 2H), 2.12 (s, 2H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.8, 145.2, 142.6, 134.8, 134.3, 130.3, 128.9, 128.6, 128.1, 127.5, 117.9, 66.1, 45.9. HRMS (ESI) Exact mass calculated for $C_{17}H_{17}NO_2$ H ([M + H]$^+$): 268.1332. Found: 268.1320.



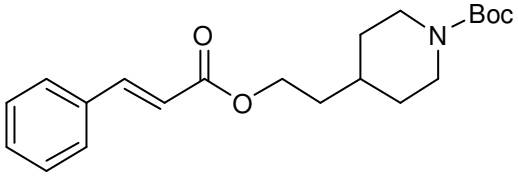
(*E*)-Cinnamic acid 4-amino-cyclohexyl ester (9): According to GP 2 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 4-amino-cyclohexanol (86 mg, 0.75 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:MTBE, 1:1 to MTBE:methanol 3:1) to afford **9** (87 mg, 71%).

FTIR (neat): $\tilde{\nu}$ = 3341, 2940, 2864, 1705, 1637, 1450, 1331, 1024 cm^{-1}. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.66 (d, *J*=16.0, 1H), 7.57 – 7.45 (m, 2H), 7.42 – 7.32 (m, 3H), 6.41 (d, *J*=16.0, 1H), 4.99 – 4.66 (m, 1H), 3.07 (bs, 2H), 2.93 – 2.75 (m, 1H), 2.16 – 1.89 (m, 4H), 1.58 – 1.24 (m, 4H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.4, 144.6, 134.5, 130.2, 128.9, 128.0, 118.5, 72.2, 49.4, 32.8, 30.0. HRMS (ESI) Exact mass calculated for $C_{15}H_{19}NO_2$ H ($[M + H]^+$): 246.1489. Found: 246.1481.



4-[(*E*)-(Cinnamoyl)oxymethyl]-piperidine-1-carboxylic acid *tert*-butyl ester (10): According to GP 2 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), piperidin-4-yl-methanol (86 mg, 0.75 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 2 h. The reaction mixture was then treated with di-*tert*-butyl dicarbonate (218 mg, 1.00 mmol) and triethylamine (101 mg, 1.00 mmol). After Boc protection, the resulting mixture was purified by SiO_2-chromatography (pentane:MTBE, 1:5) to afford **10** (141 mg, 82%).

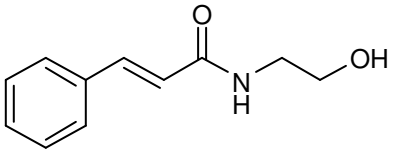
FTIR (neat): $\tilde{\nu}$ = 2974, 2937, 2361, 1687, 1637, 1420, 1311, 1234, 1143, 864, 685 cm^{-1}. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.68 (d, *J*=16.0, 1H), 7.56 – 7.47 (m, 2H), 7.44 – 7.33 (m, 3H), 6.43 (d, *J*=16.0, 1H), 4.16 – 4.12 (m, 2H), 4.07 (d, *J*=6.5, 2H), 2.82 – 2.63 (m, 2H), 1.96 – 1.81 (m, 1H), 1.76 – 1.72 (m, 2H), 1.46 (s, 9H), 1.24 (qd, *J*=12.5, 4.4, 2H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.9, 154.8, 144.9, 134.4, 130.3, 128.9, 128.1, 117.9, 79.4, 68.5, 43.5, 35.7, 28.8, 28.4, 28.0. HRMS (ESI) Exact mass calculated for $C_{20}H_{27}NO_4$ Na ($[M + Na]^+$): 368.1832. Found: 368.1834.



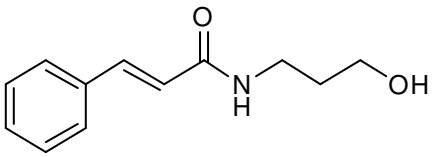
4-{2-[(*E*)-(Cinnamoyl)oxy]-ethyl}-piperidine-1-carboxylic acid *tert*-butyl ester (11): According to GP 2 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 2-piperidin-4-yl-ethanol (97 mg, 0.75 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 2 h. The reaction mixture was then treated with di-*tert*-butyl dicarbonate (218 mg, 1.00 mmol) and triethylamine (101 mg, 1.00 mmol). After Boc protection, the resulting mixture was purified by SiO_2-chromatography (pentane:MTBE, 1:5) to afford **11** (138 mg, 77%).

FTIR (neat): $\tilde{\nu}$ = 2929, 2380, 1688, 1637, 1420, 1278, 1164, 978, 685 cm^{-1}. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.67 (d, *J*=16.0, 1H), 7.52 (d, *J*=9.6, 2H), 7.37 (d, *J*=6.4, 3H),

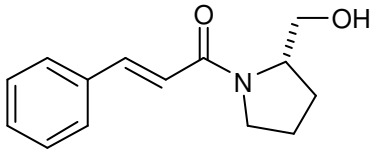
6.43 (d, *J*=16.0, 1H), 4.25 (t, *J*=6.5, 2H), 4.14 – 4.02 (m, 2H), 2.73 – 2.65 (m, 2H), 1.72 – 1.62 (m, 4H), 1.61 – 1.54 (m, 1H), 1.45 (s, 9H), 1.22 – 1.09 (m, 2H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.9, 154.8, 144.8, 134.4, 130.3, 128.9, 128.0, 118.1, 79.3, 62.2, 43.9, 35.3, 33.1, 32.0, 28.4, 28.0. HRMS (ESI) Exact mass calculated for $C_{21}H_{29}NO_4$ Na ([M + Na]$^+$): 382.1989. Found: 382.1993.



(*E*)-*N*-(2-Hydroxy-ethyl)-cinnamide (12): According to GP 2 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 2-amino-ethanol (92 mg, 1.50 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:MTBE, 1:1 to MTBE:methanol 20:1) to afford **12** (60 mg, 63%).
FTIR (neat): $\tilde{\nu}$ = 3284, 2935, 2361, 1655, 1617, 1545, 1340, 1225, 1065, 976, 764 cm^{-1}. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.62 (d, *J*=15.6, 1H), 7.53 – 7.42 (m, 2H), 7.39 – 7.28 (m, 3H), 6.45 (bs, 1H), 6.44 (d, *J*=15.6, 2H), 3.90 – 3.70 (m, 2H), 3.61 – 3.48 (m, 2H), 1.94 (bs, 1H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 167.1, 141.5, 134.7, 129.8, 128.8, 127.8, 120.29, 62.3, 42.7. HRMS (ESI) Exact mass calculated for $C_{11}H_{13}NO_2$ Na ([M + Na]$^+$): 214.0838. Found: 214.0833.



(*E*)-*N*-(3-Hydroxy-propyl)-cinnamide (13): According to GP 2 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), 3-amino-propan-1-ol (113 mg, 1.50 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:MTBE, 1:1 to MTBE:methanol 20:1) to afford **13** (57 mg, 55%).
FTIR (neat): $\tilde{\nu}$ = 3295, 2944, 2360, 1656, 1614, 1547, 1340, 1225, 907, 646 cm^{-1}. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.61 (d, *J*=15.6, 1H), 7.47 – 7.44 (m, 2H), 7.32 – 7.29 (m, 3H), 6.78 (s, 1H), 6.46 (d, *J*=15.6, 1H), 3.84 (bs, 1H), 3.67 (t, *J*=5.6, 2H), 3.53 (dd, *J*=12.3, 6.2, 2H), 1.84 – 1.68 (m, 2H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 167.2, 141.1, 134.7, 129.7, 128.8, 127.7, 120.4, 59.4, 36.6, 32.2. HRMS (ESI) Exact mass calculated for $C_{12}H_{15}NO_2$ Na ([M + Na]$^+$): 228.0995. Found: 228.0987.



(*E*)-1-((*S*)-2-Hydroxymethyl-pyrrolidin-1-yl) -cinnamide (14): According to GP 2 with *(E)*-cinnamaldehyde (66 mg, 0.5 mmol), DBU (83 mg, 0.55 mmol), 1,3-dimethyltriazolium iodide (2.3 mg, 10 µmol), (*S*)-1-pyrrolidin-2-yl-methanol (152 mg, 1.50 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (205 mg, 0.5 mmol) in THF (5.0 mL) for 2 h and SiO_2-chromatography (pentane:MTBE, 1:1 to MTBE:methanol 20:1) to afford **14** (61 mg, 53%).

FTIR (neat): $\tilde{\nu}$ = 3368, 2953, 2877, 2361, 1645, 1585, 1422, 1192, 1050, 764 cm^{-1}. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.72 (d, *J*=15.4, 1H), 7.59 – 7.45 (m, 2H), 7.44 – 7.29 (m, 3H), 6.73 (d, *J*=15.4, 1H), 5.22 (bs, 1H), 4.45 – 4.17 (m, 1H), 3.84 – 3.52 (m, 4H), 2.11 – 1.88 (m, 3H), 1.74 – 1.58 (m, 1H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 167.2, 143.1, 135.0, 129.9, 128.8, 127.9, 118.3, 67.3, 61.5, 48.1, 28.2, 24.4. HRMS (ESI) Exact mass calculated for $C_{14}H_{17}NO_2$ Na ($[M + Na]^+$): 254.1151. Found: 254.1136.

Procedure for the NHC-Catalyzed Kinetic experiments:

DBU (166 mg, 1.10 mmol) was added to a solution of 1,3-dimethyltriazolium iodide (1.1-22.5 mg, 5-100 µmol), isopropanol (90 mg, 1.50 mmol) and allyl amine (86 mg, 1.50 mmol) in THF (10.0 mL) under argon atmosphere. The mixture was stirred for 5 minutes, followed by the addition of *(E)*-cinnamaldehyde (132 mg, 1.0 mmol) and 3,3´,5,5´-tetra-*tert*-butyldiphenoquinone (410 mg, 1.0 mmol). The reaction mixture was stirred at room temperature for 1 hour and then subjected to GC analysis using decane as internal standard.

Catalyst Loading [mol%]	Yield Ester [%][a]	Yield Amide [%][a]	Ratio Ester/Amide
0.5	15.13	8.59	1.80
1.0	37.35	18.80	1.99
1.5	49.59	23.70	2.09
2.0	53.59	24.93	2.16
2.5	49.71	22.96	2.17
3.0	52.15	25.30	2.06
4.0	52.38	27.14	1.93
5.0	50.33	26.99	1.87
10.0	39.14	27.73	1.41

[a] GC yield using decane as internal standard. [b] Results represent average of three experiments.

Theoretical Methods and Technical Details of the Computations:

The quantum chemical calculations have been performed with the TURBOMOLE suite of programs.[6] As Gaussian AO basis for the structure optimizations, large triple-zeta (denoted as TZVPP) sets of Ahlrichs et al.[7] have been employed. In standard notation these are [5*s*3*p*2*d*1*f*] for C, N, O, and [3*s*2*p*1*d*] for H. All geometries have been fully optimized at the DFT level using the B97-D semi-local GGA density functional[8] that also includes an empirical correction for London dispersion (also called van der Waals) interactions[8,9]. For a detailed description of this dispersion correction, that is of great importance in studies of large molecules, including many illustrative examples see Ref.[9,10,11] In all DFT treatments, the RI-approximation has been used[12] for the Coulomb integrals which speeds the computations up significantly without any significant loss of accuracy. These structures were used in subsequent single-point computations of the interaction energy using MP2 which provides a rather accurate description of hydrogen

bonds. In all the perturbation treatments and also for the HF part (dubbed RI-K and RI-MP2, respectively), the RI-approximation using corresponding optimized auxiliary basis sets[13] have been used. These calculations employ the Dunning[14] basis sets cc-pVTZ and cc-pVQZ extrapolated to the AO basis set limt (CBS)[15] in both, the MP2 as well as the HF part. In all calculations the basis sets used are so large that the remaining incompleteness effects for the energies (called basis set super-position error, BSSE) are so small (typically <5% of the interaction energy) so that approximate counter-poise corrections are unnecessary (and furthermore inconsistent at the CBS level). For a detailed discussion of this point see refs.[8,16]

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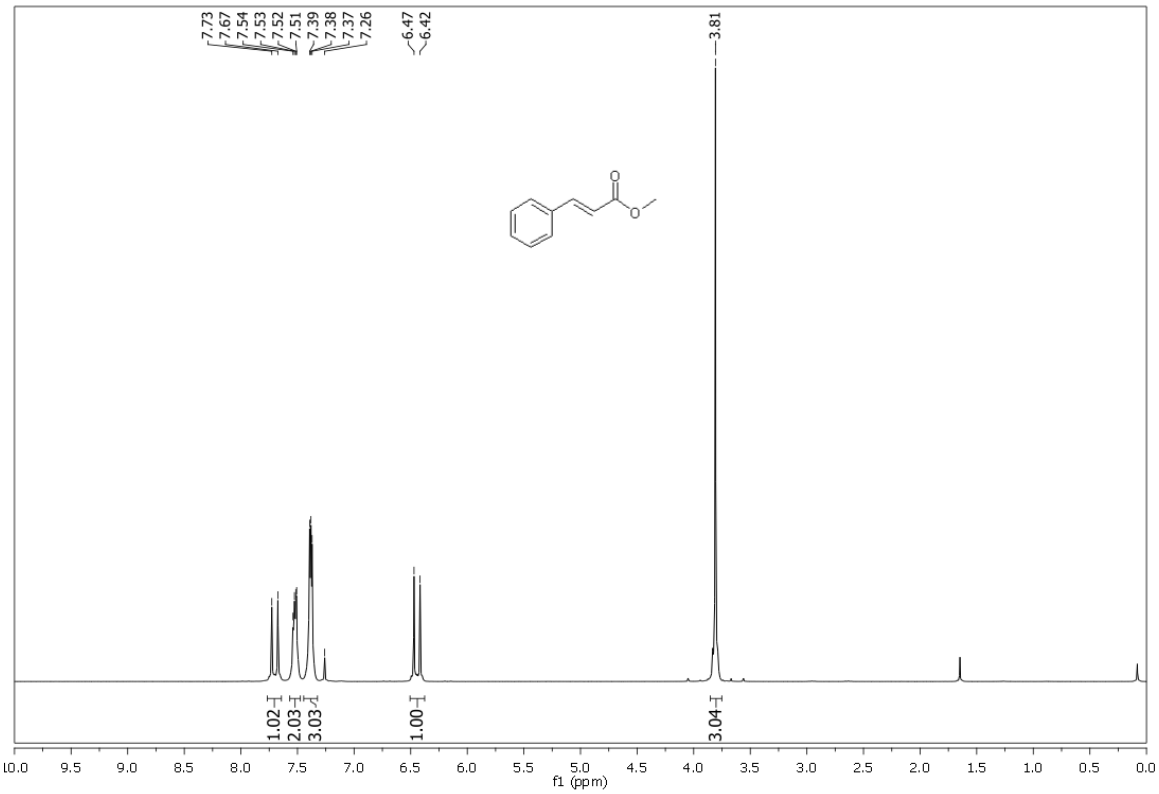
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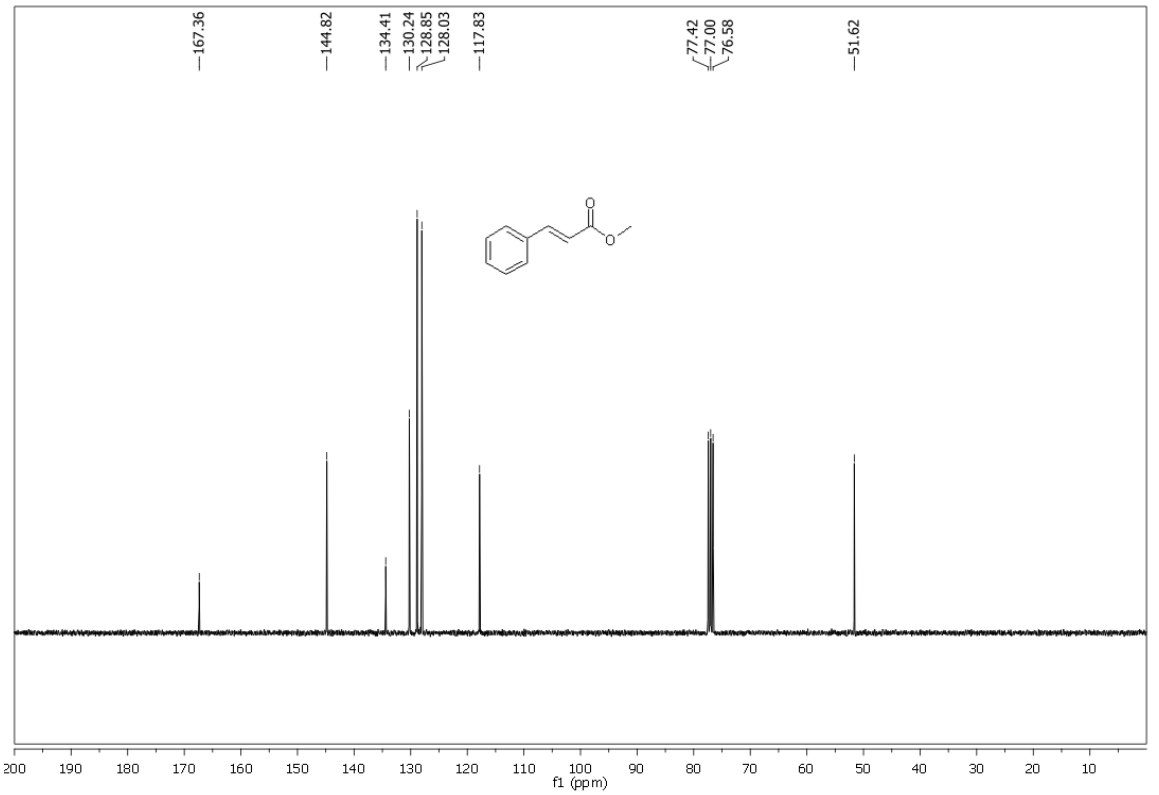
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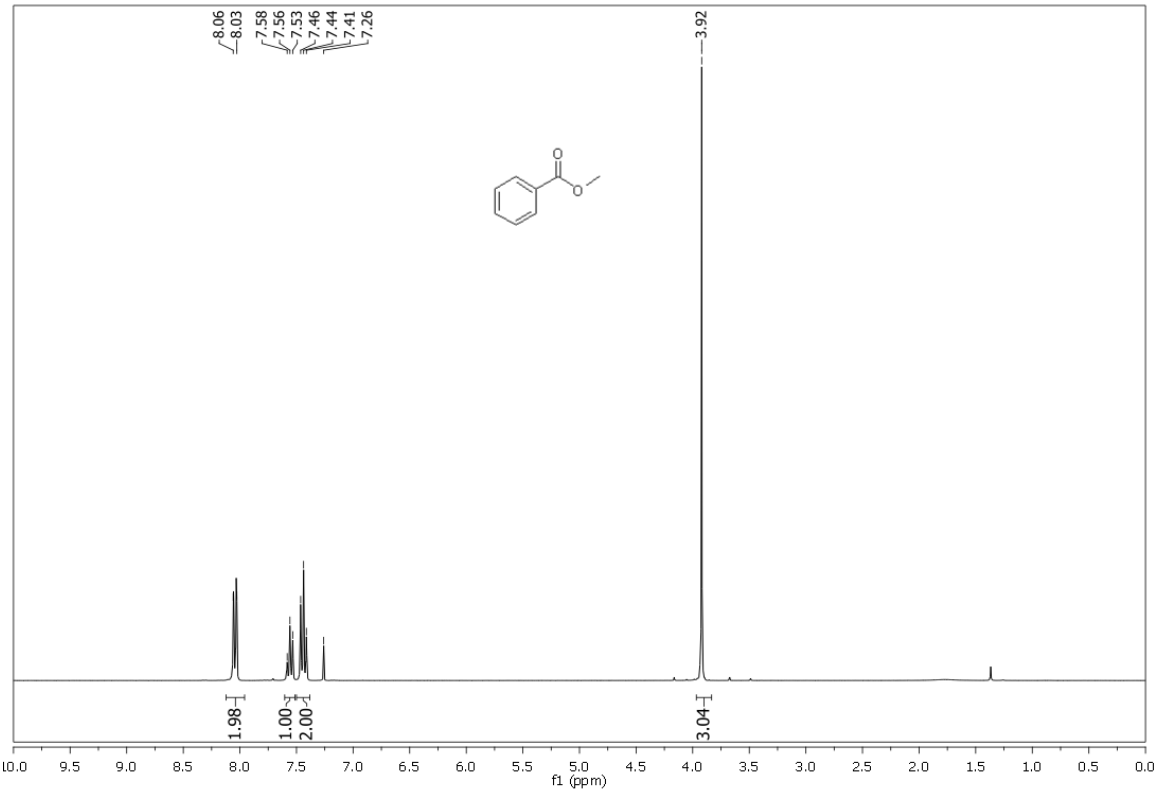
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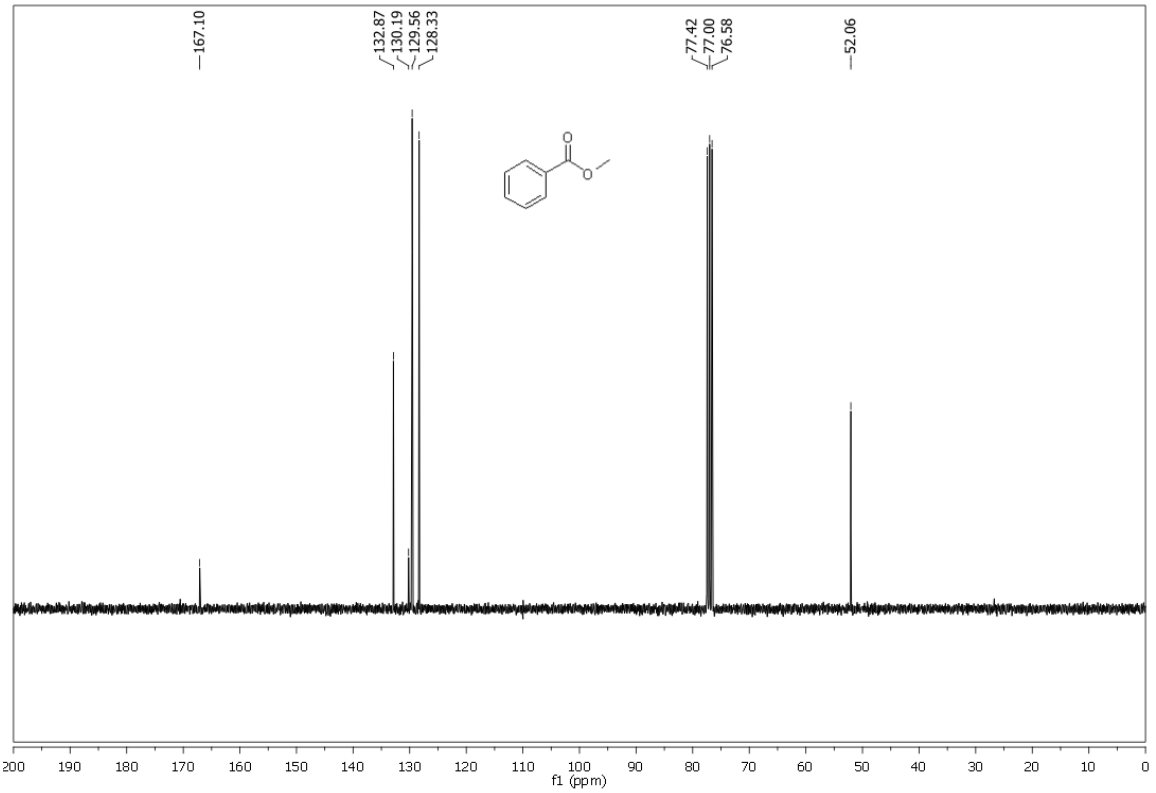
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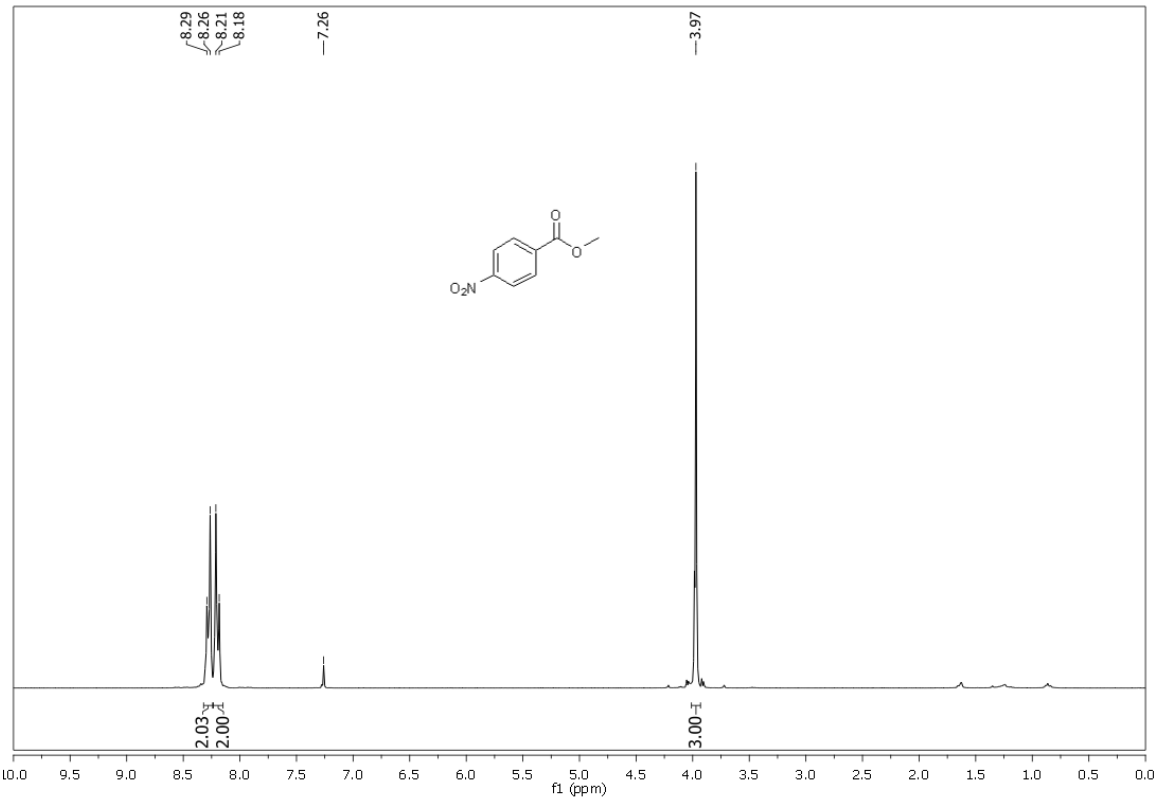
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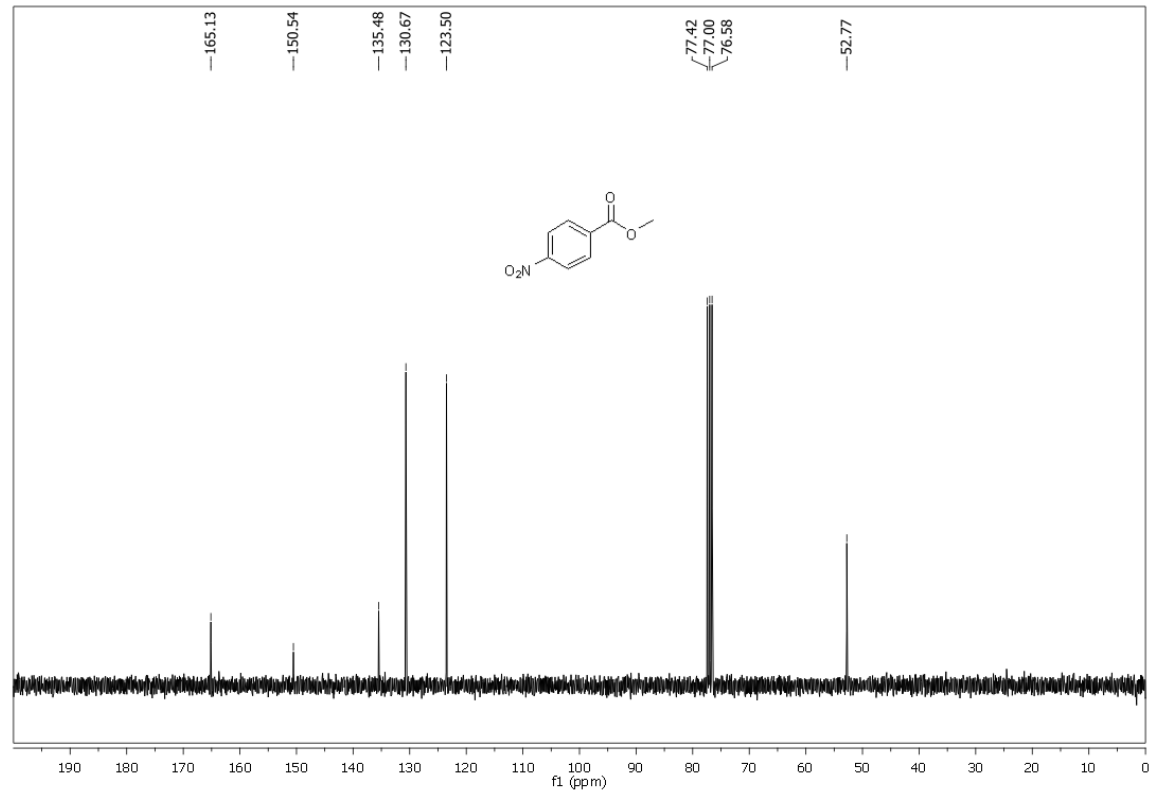
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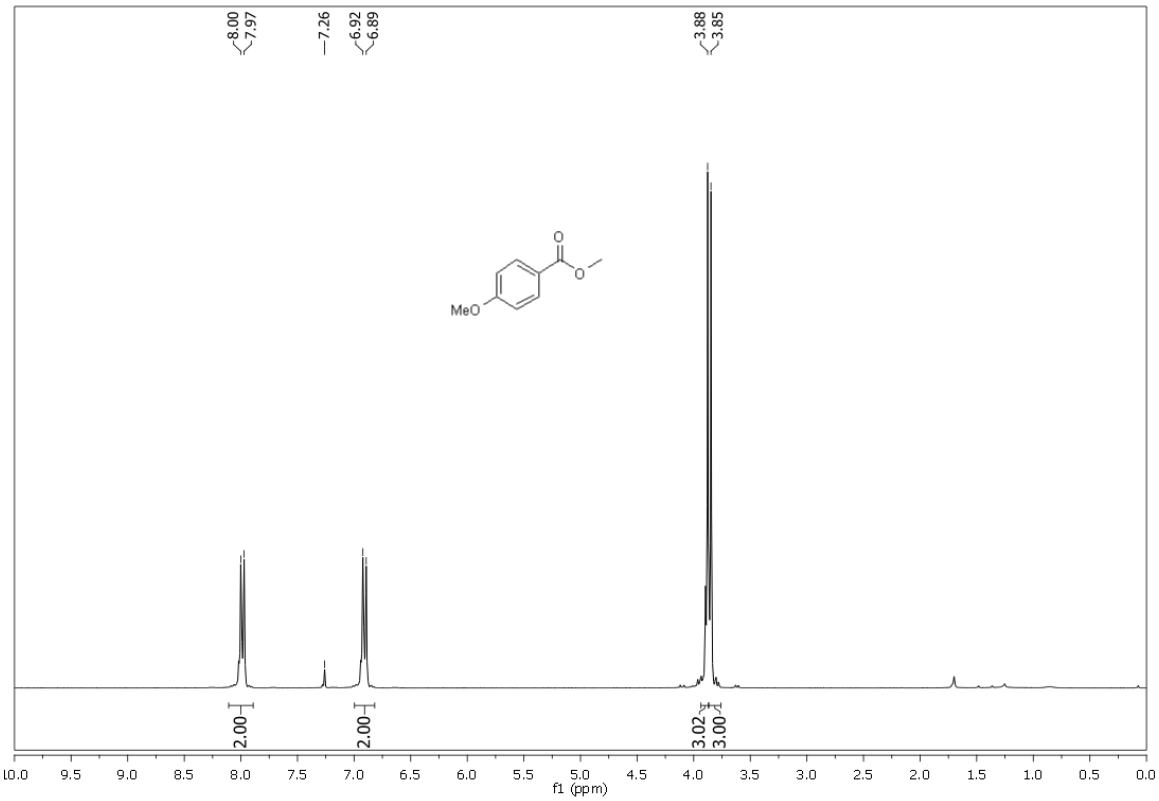
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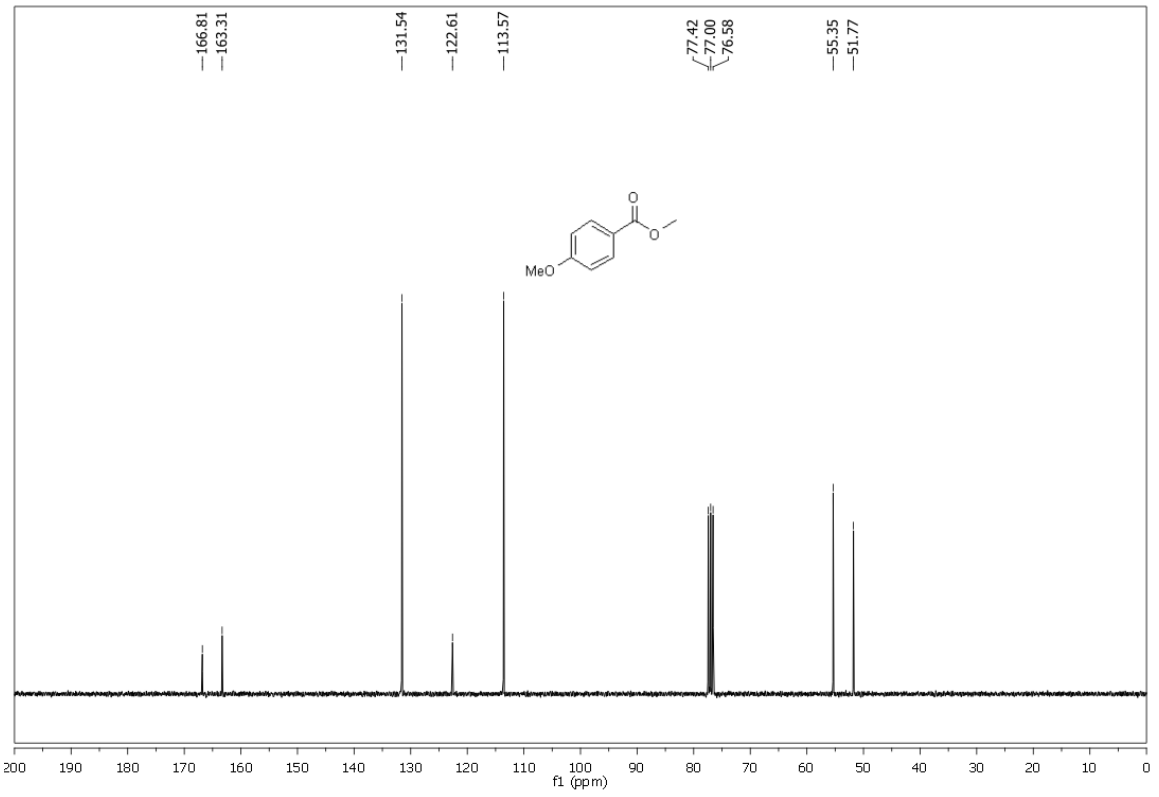
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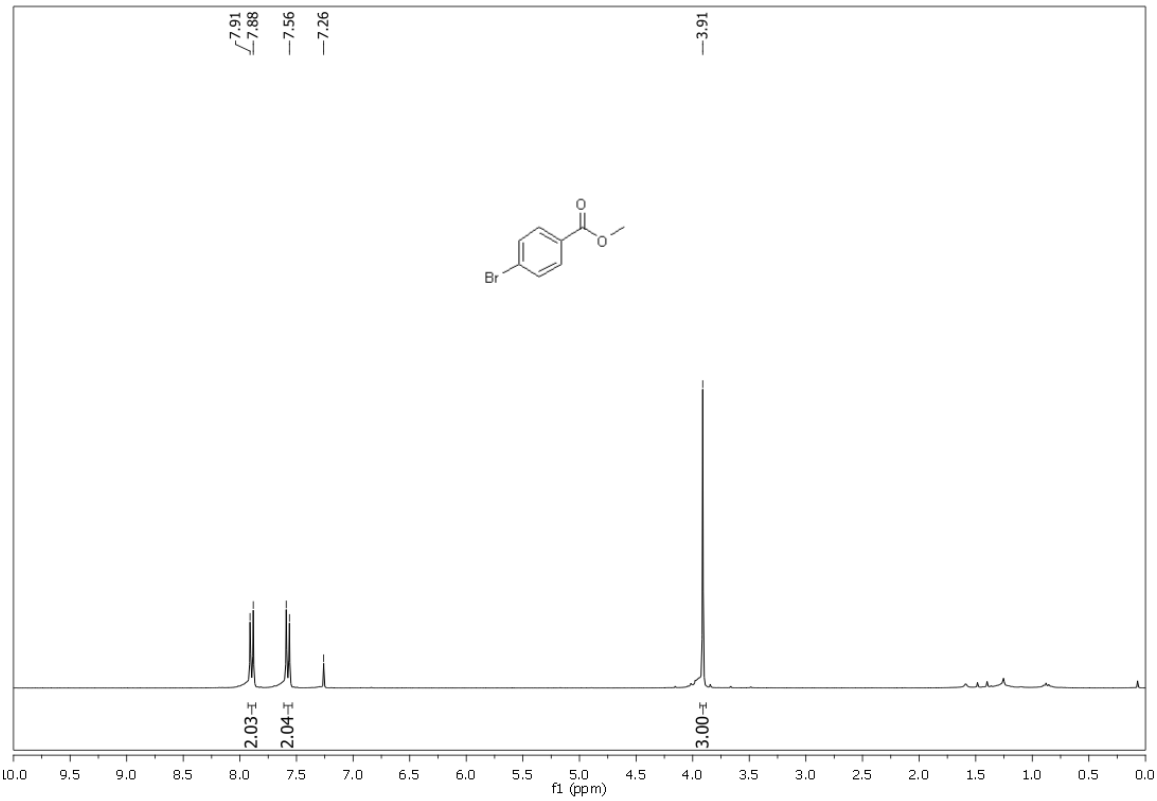
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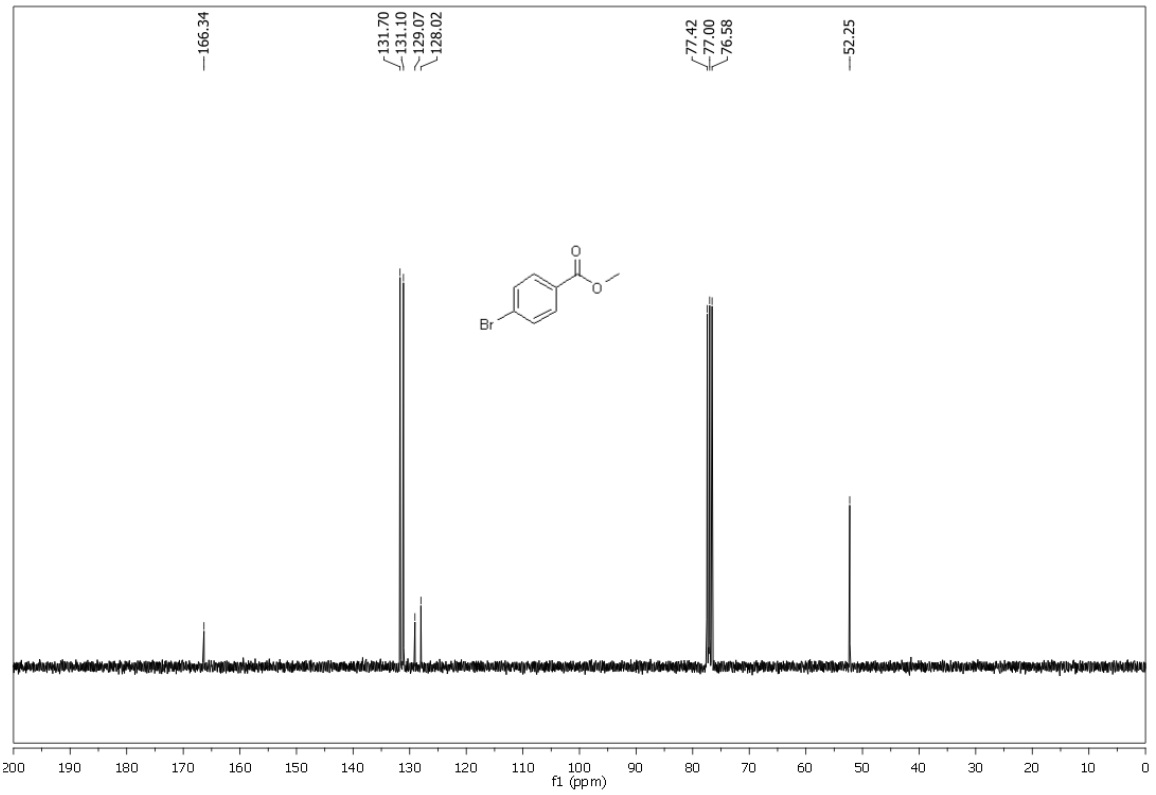
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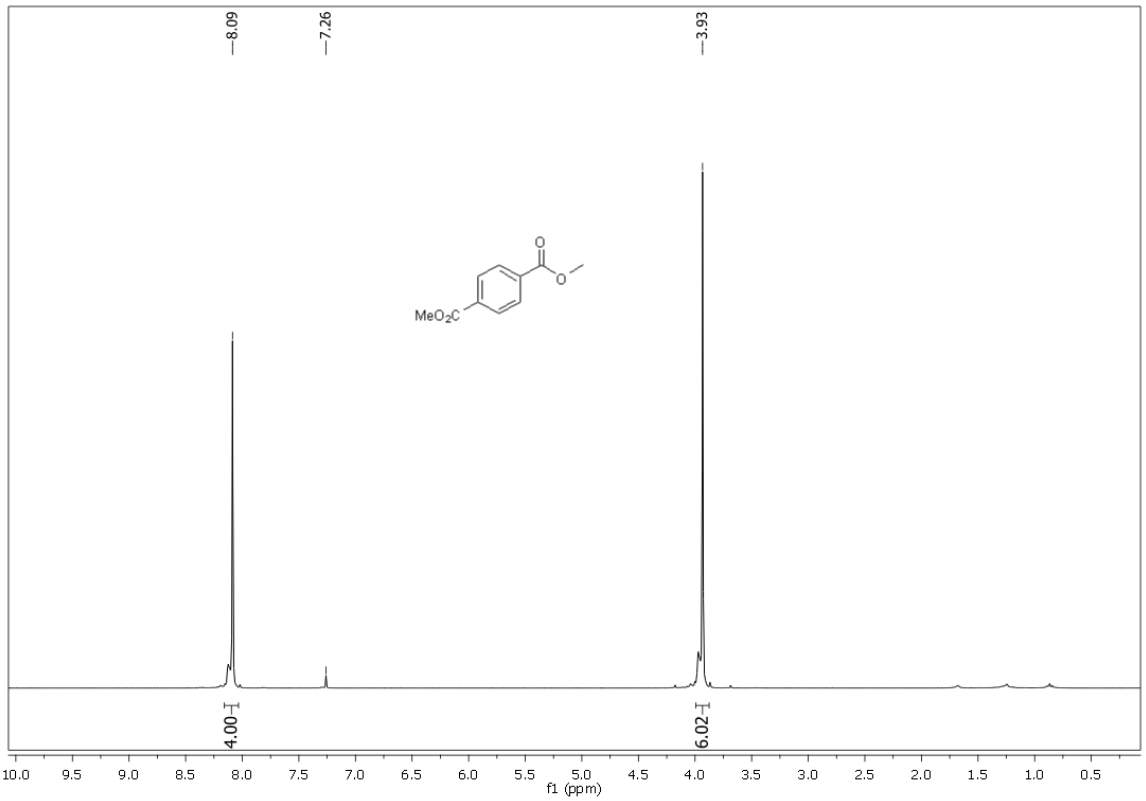
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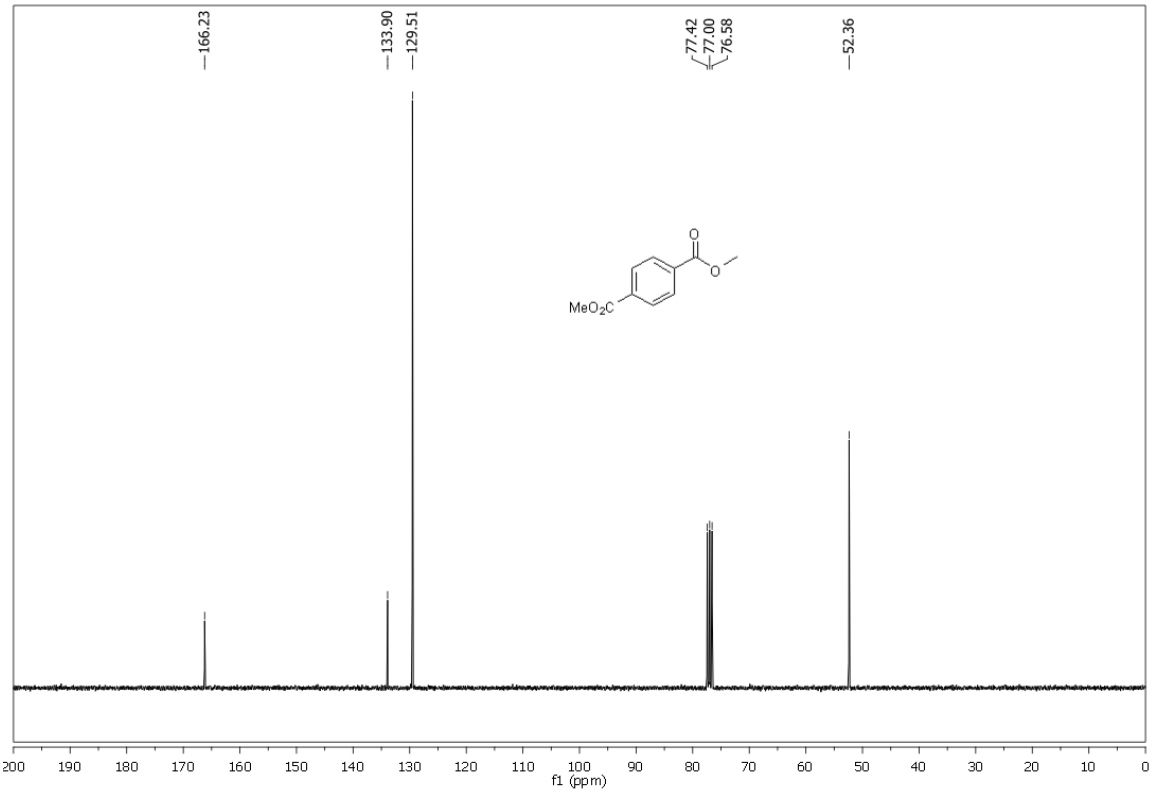
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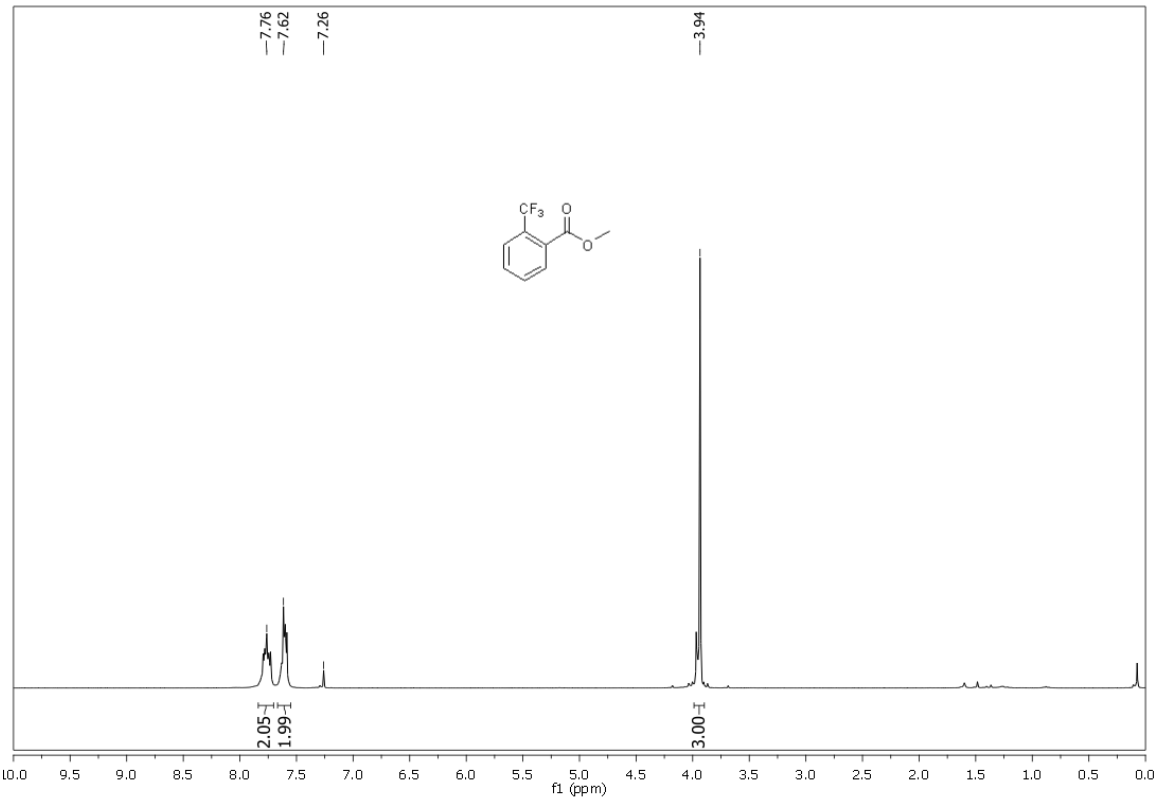
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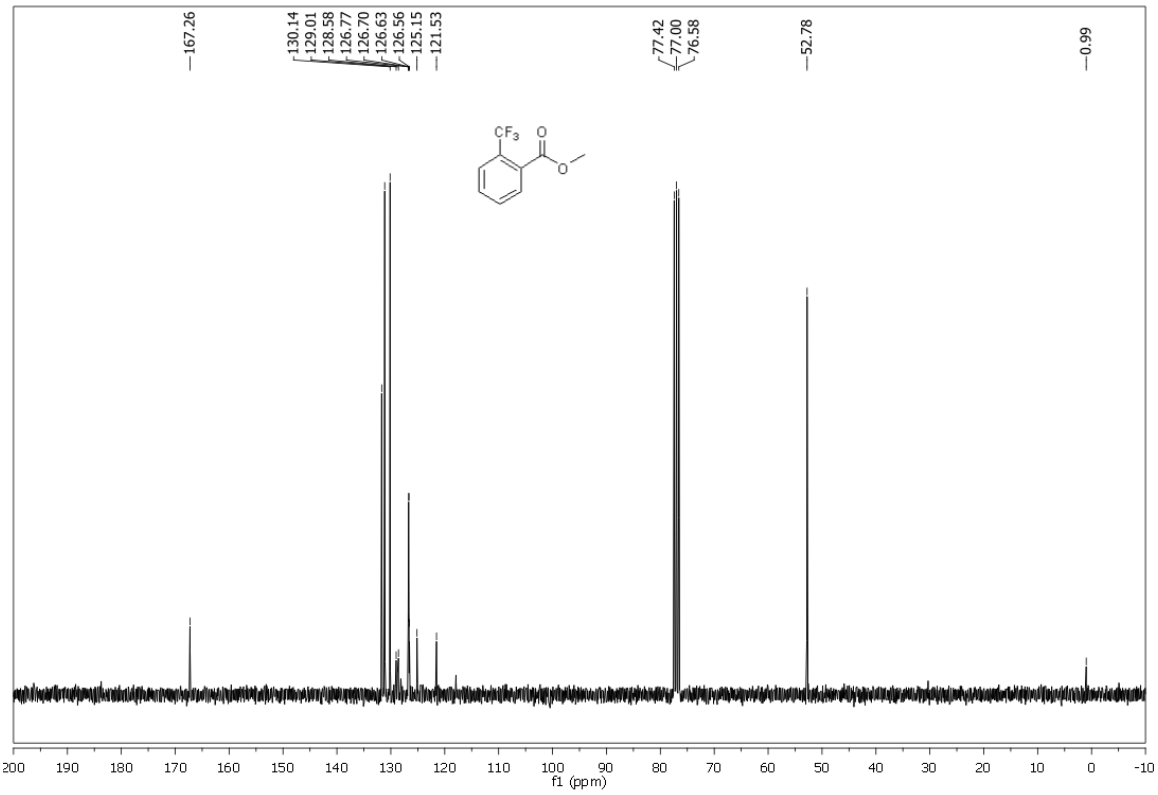
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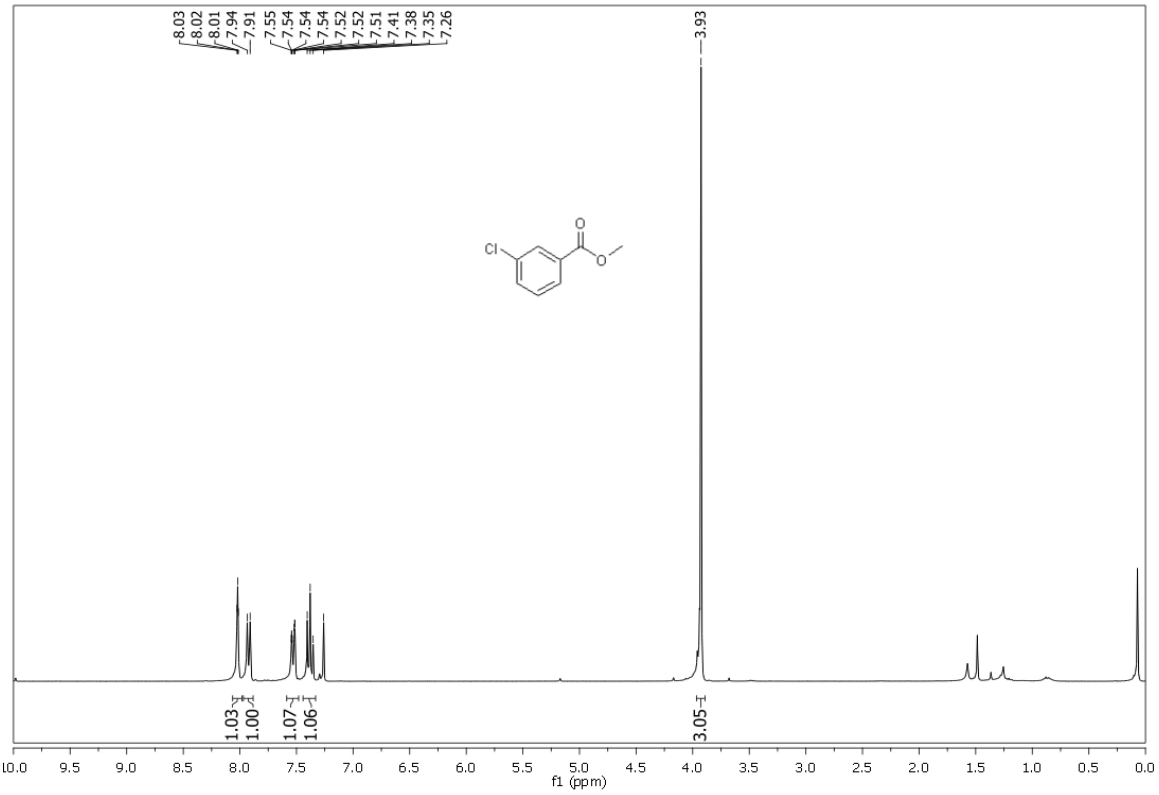
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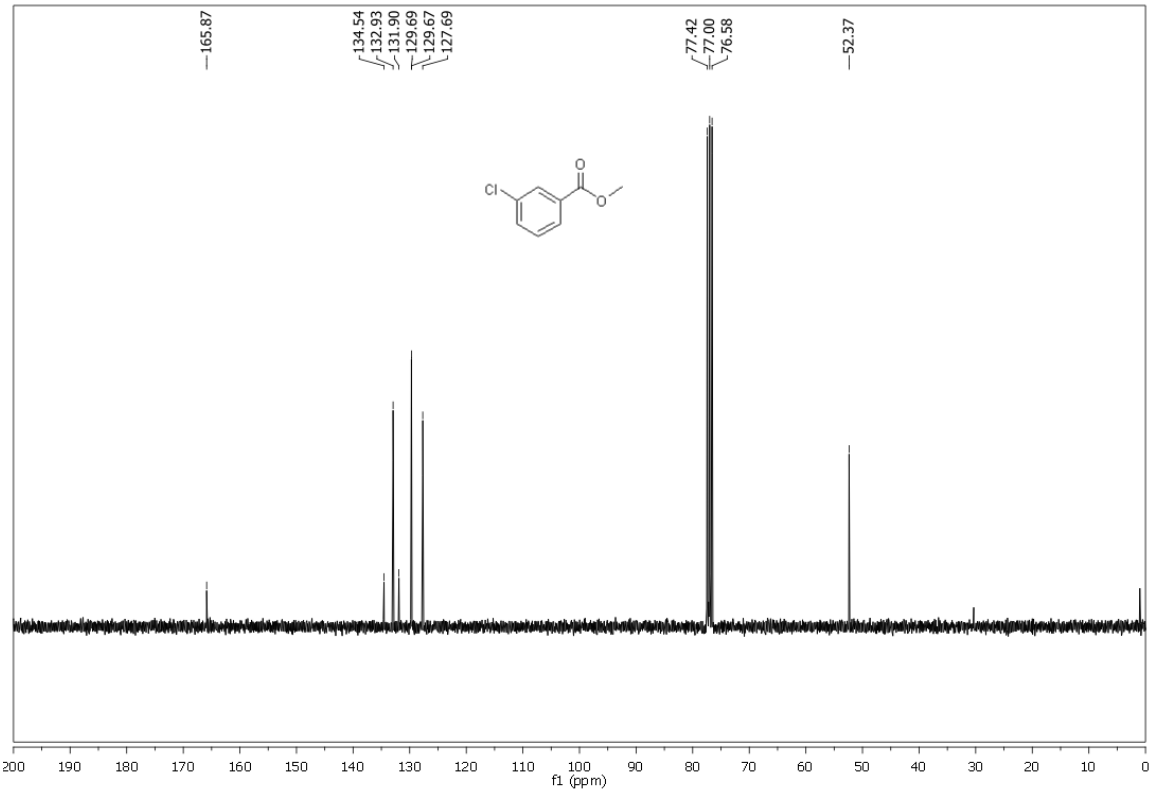
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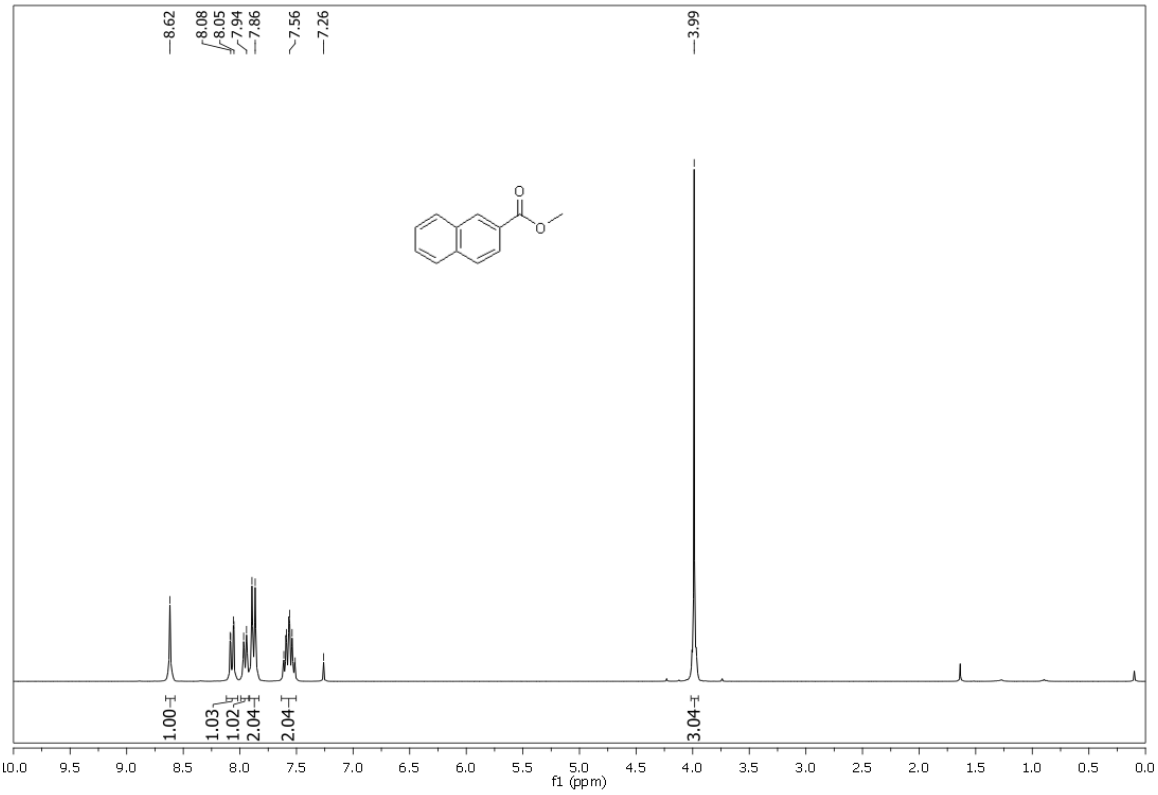
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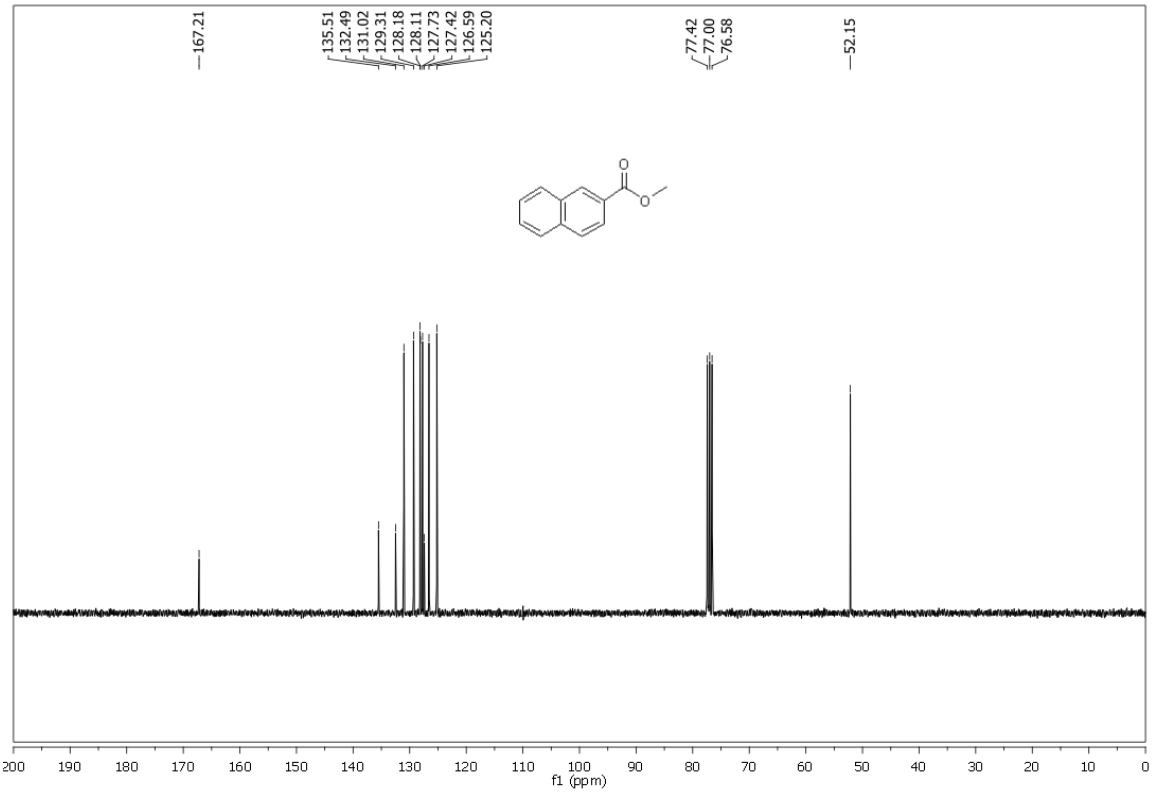
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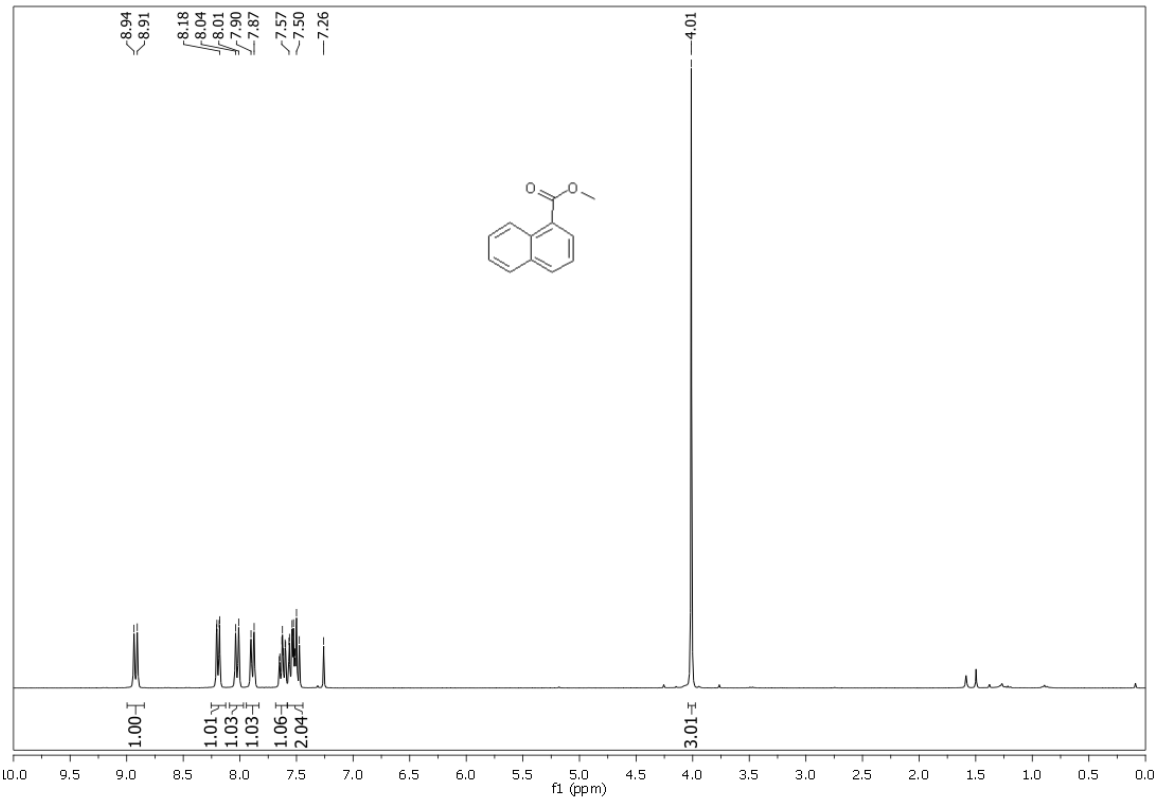
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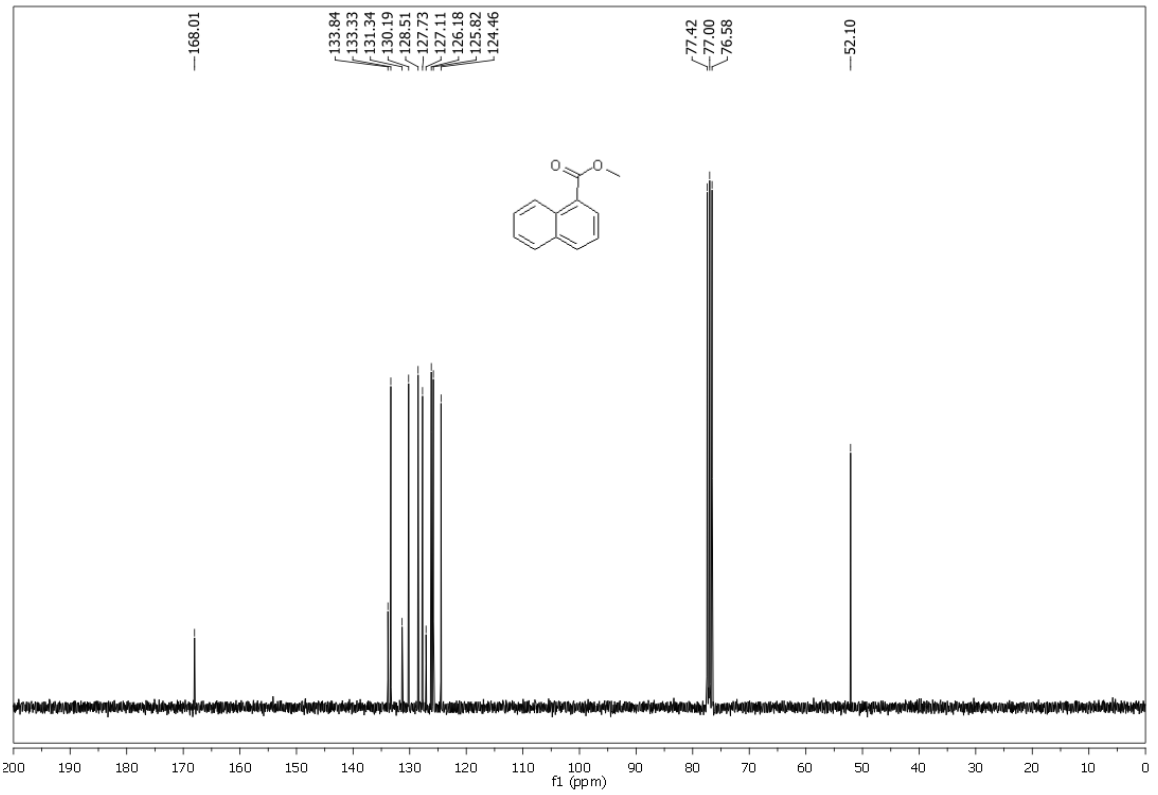
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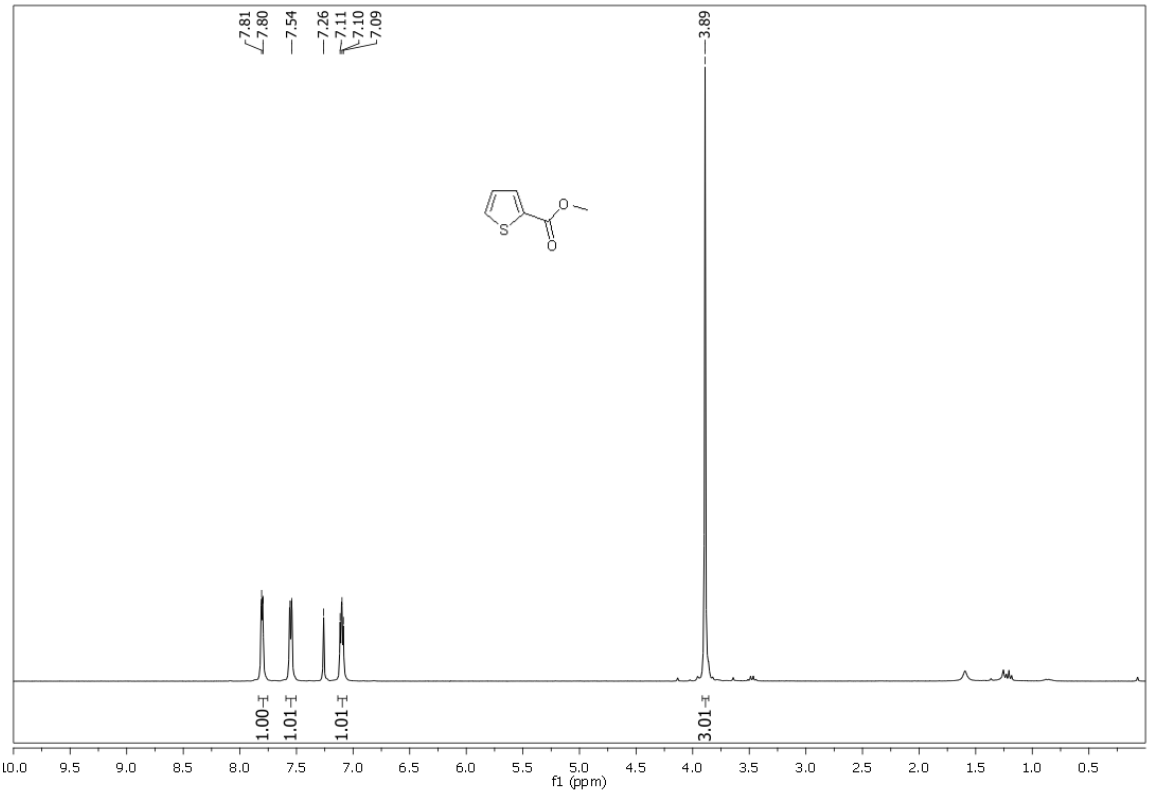
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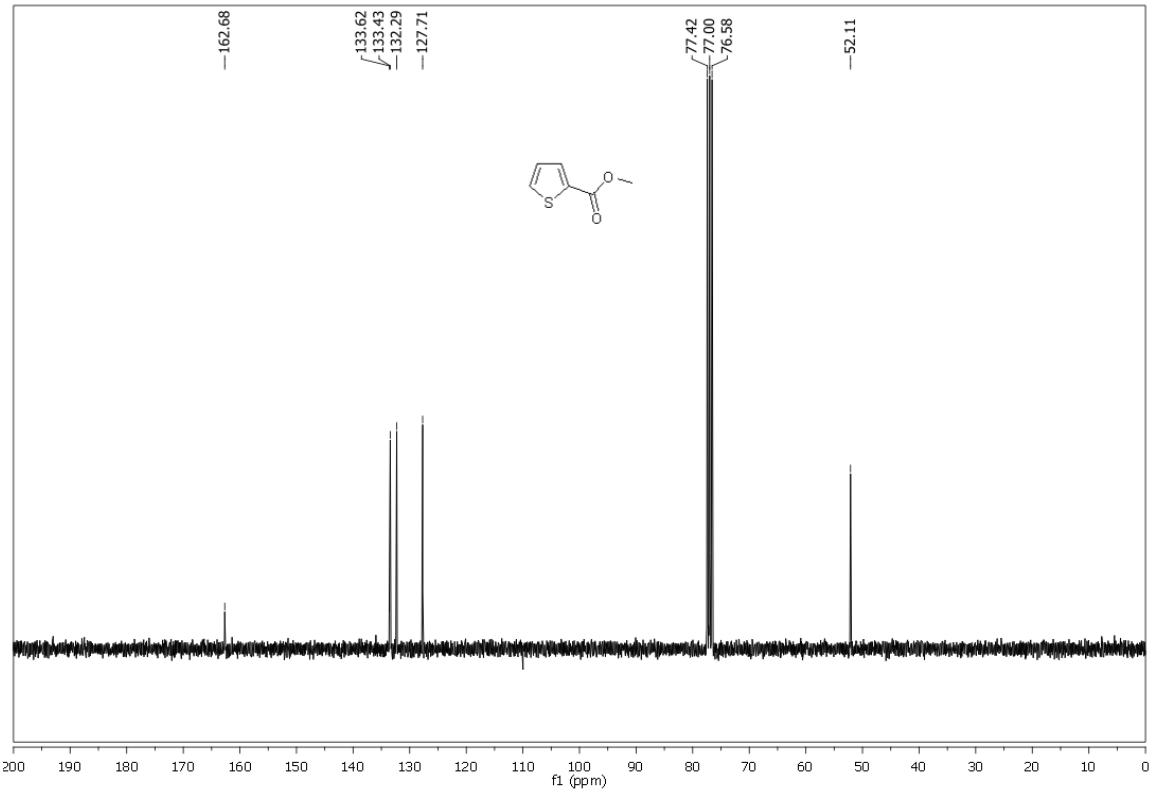
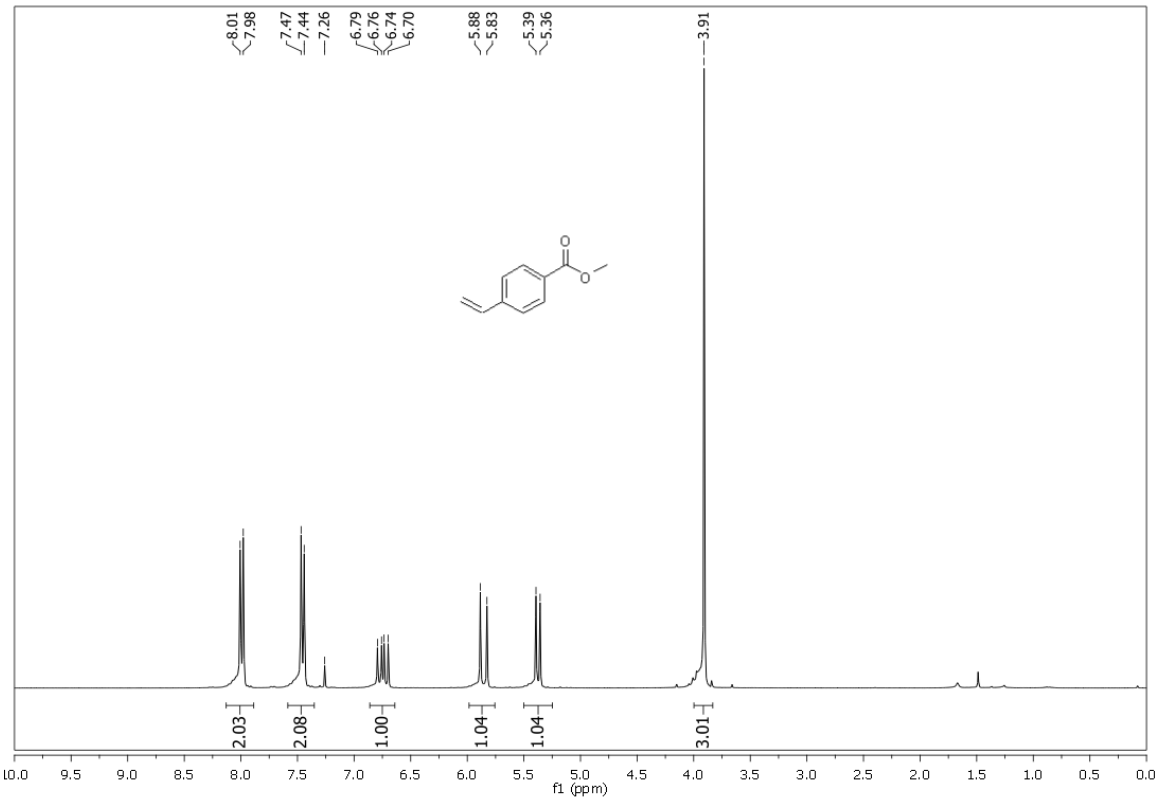
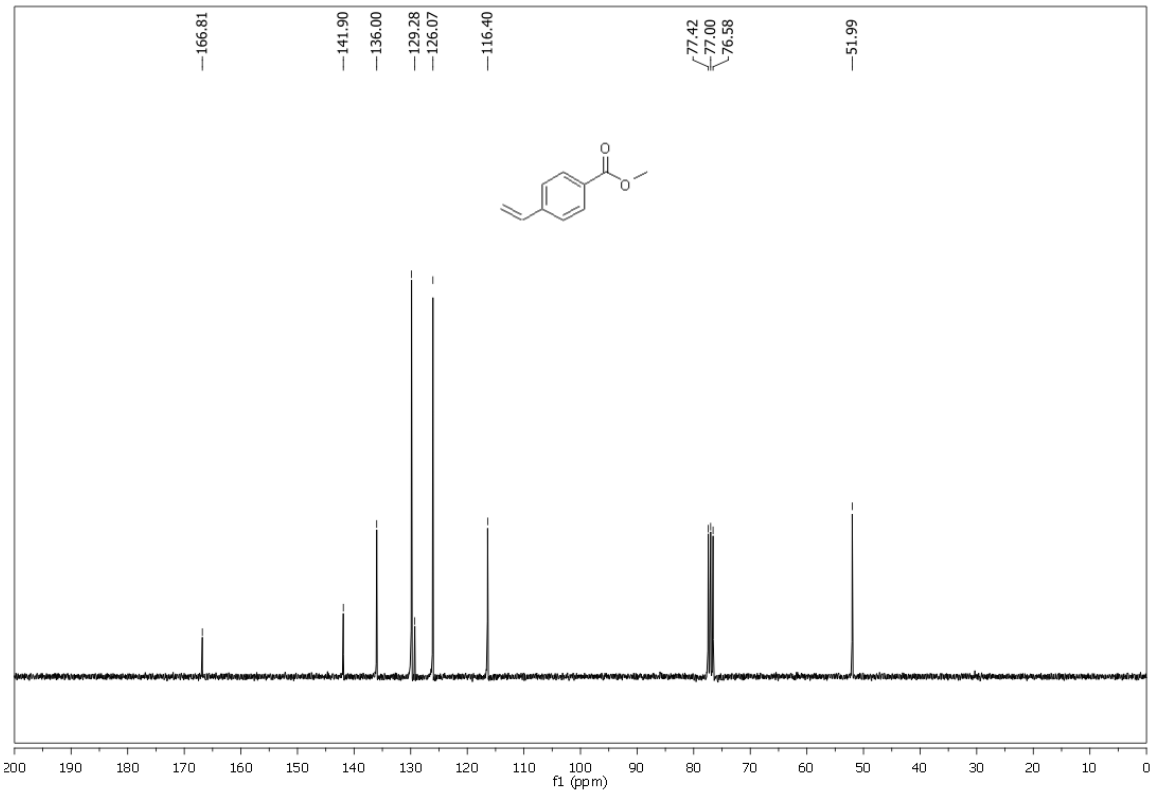
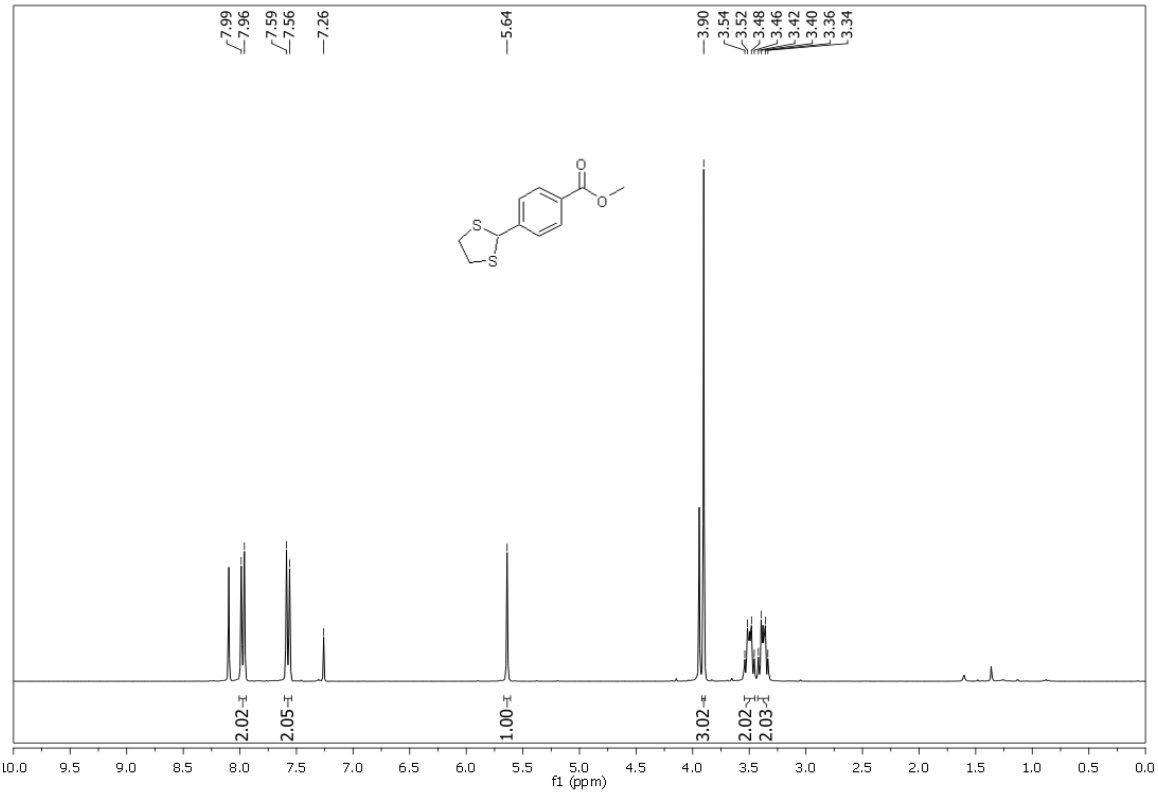
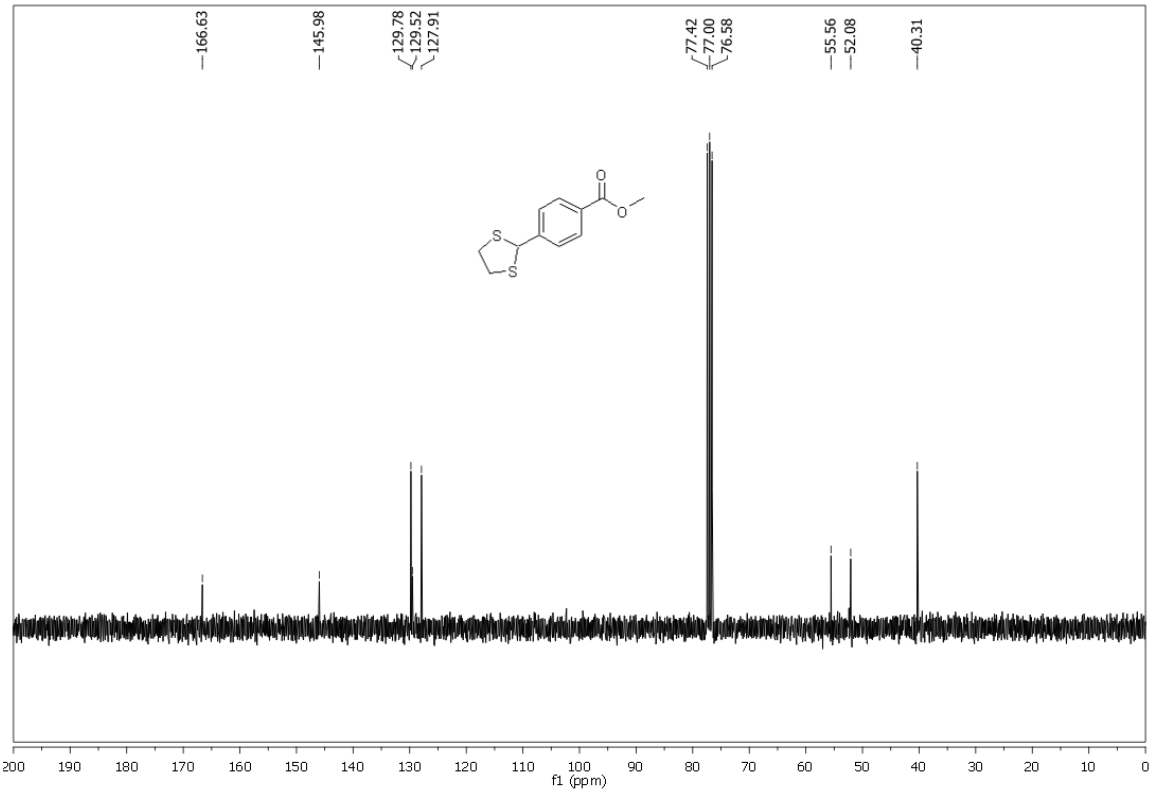
f1 (ppm)


162.68
133.62
133.43
132.29
127.71
77.42
77.00
76.58
52.11
f1 (ppm)


8.01
7.98
7.47
7.44
7.26
6.79
6.76
6.74
6.70
5.88
5.83
5.39
5.36
3.91
2.03
2.08
1.00
1.04
1.04
3.01
f1 (ppm)


166.81
141.90
136.00
129.28
126.07
116.40
77.42
77.00
76.58
51.99
f1 (ppm)


7.99
7.96
7.59
7.56
7.26
5.64
3.90
3.54
3.52
3.48
3.46
3.42
3.40
3.36
3.34
2.02
2.05
1.00
3.02
2.02
2.03
f1 (ppm)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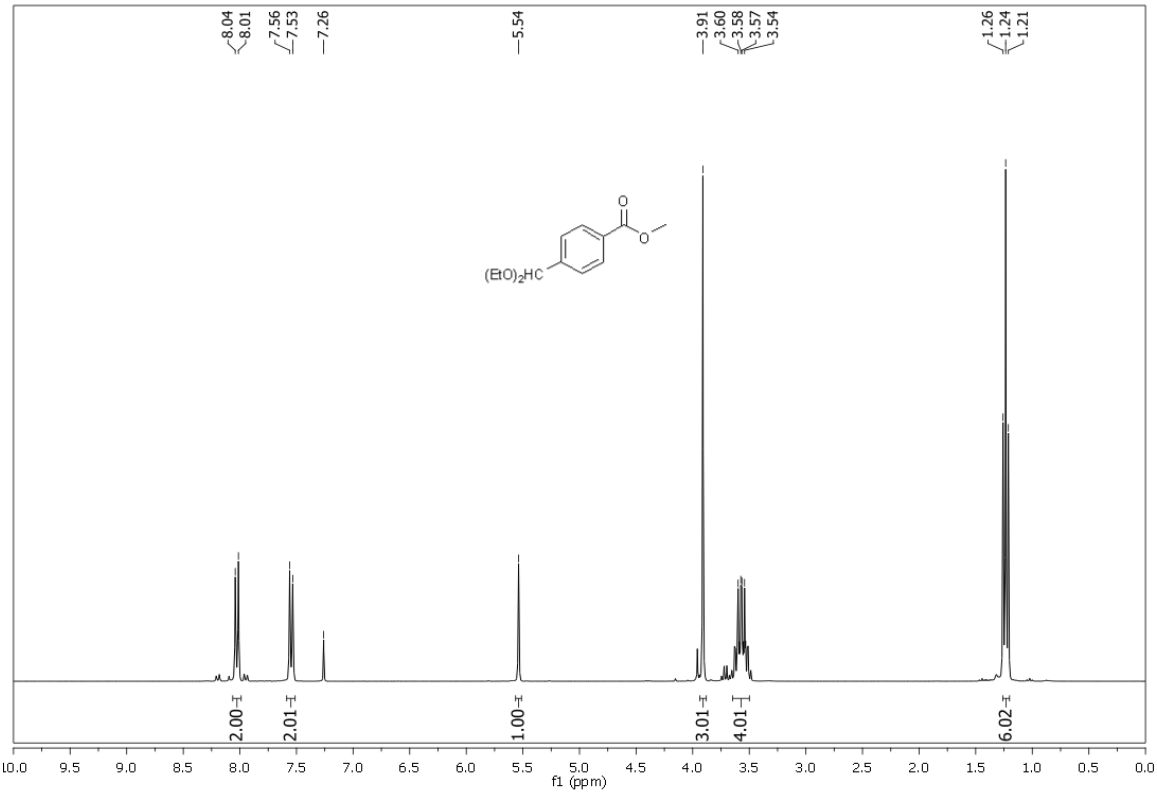
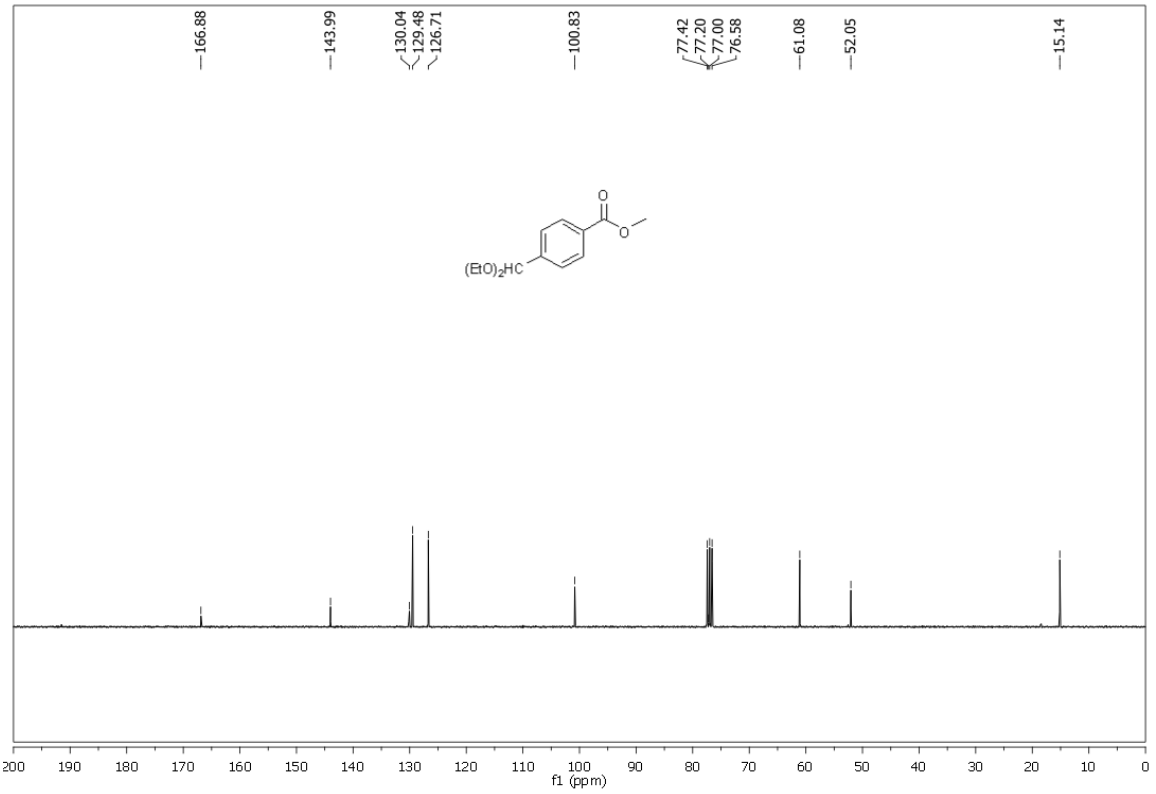
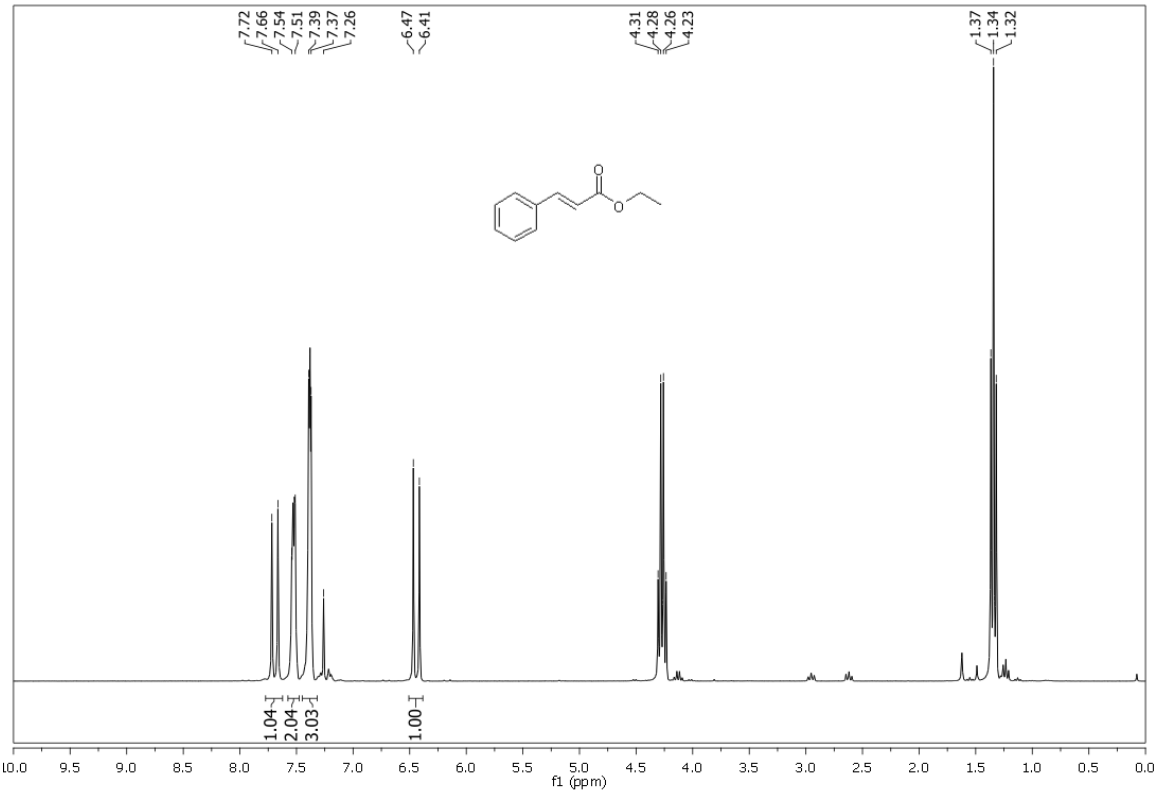
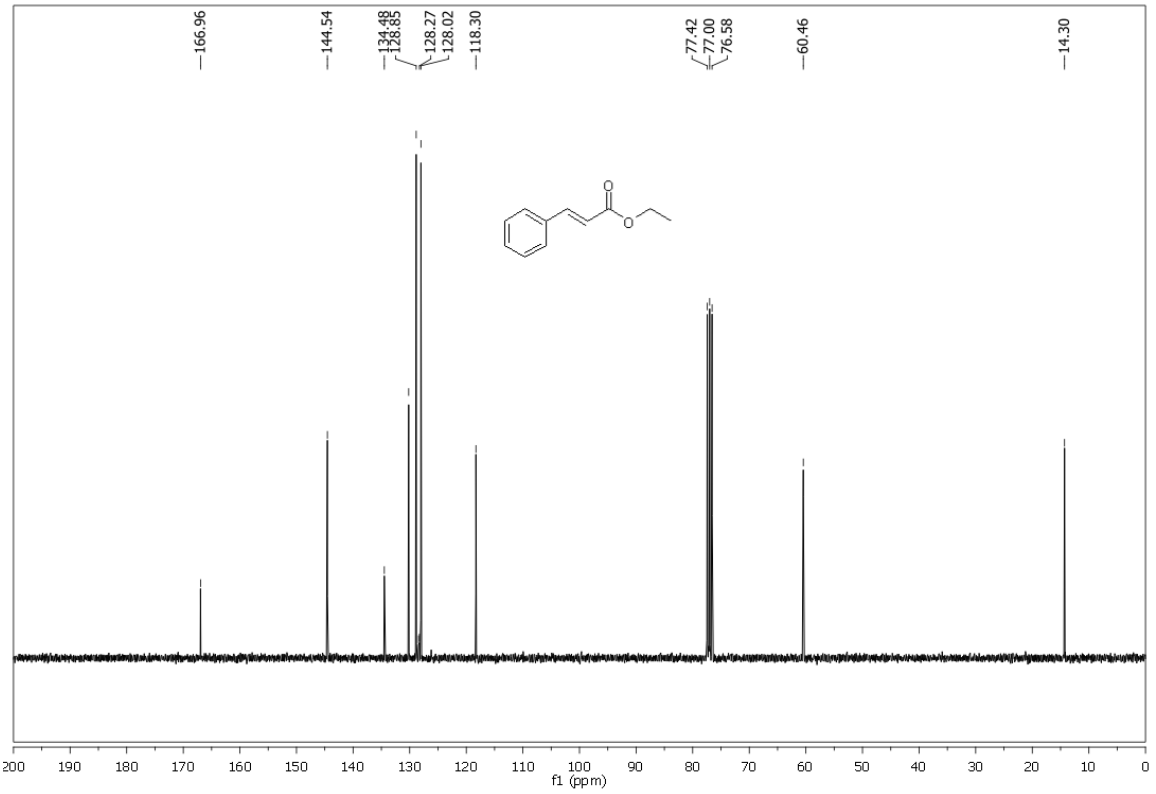
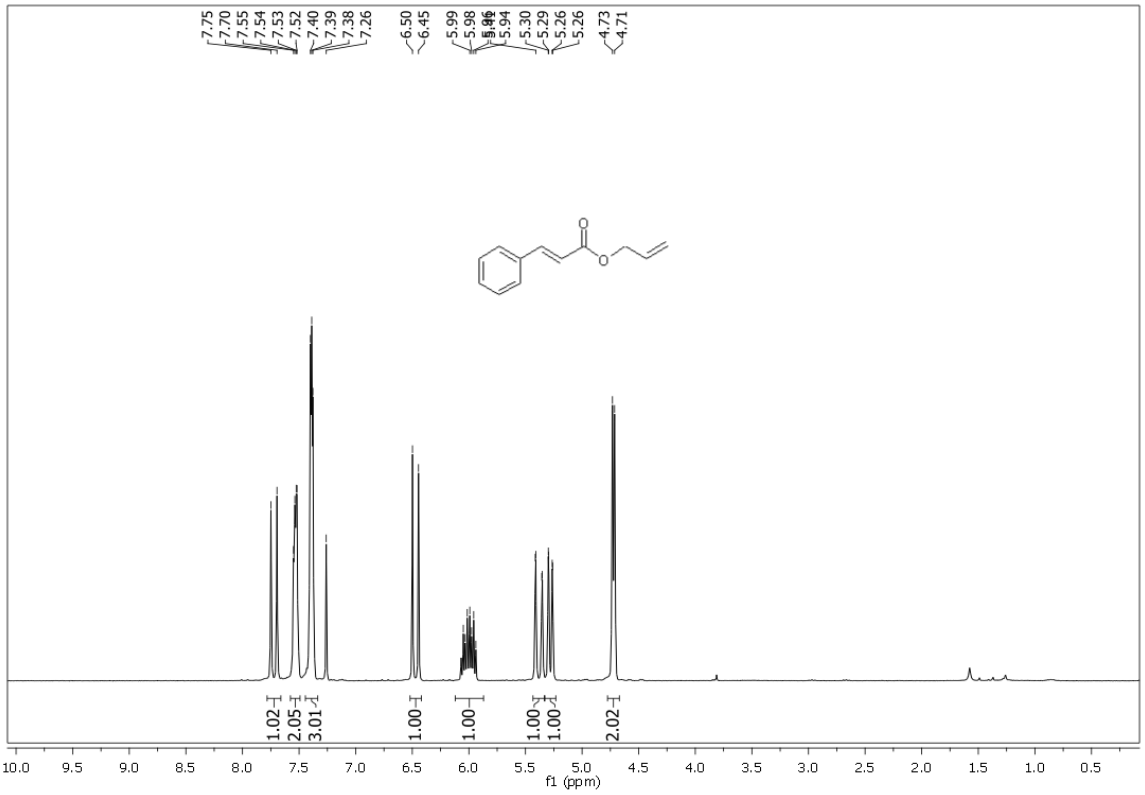
145.98
129.78
129.52
127.91
77.42
77.00
76.58
55.56
52.08
40.31
f1 (ppm)


8.04
8.01
7.56
7.53
7.26
5.54
3.91
3.60
3.58
3.57
3.54
1.26
1.24
1.21
O
O
(EtO)2HC
2.00
2.01
1.00
3.01
4.01
6.02
f1 (ppm)


166.88
143.99
130.04
129.48
126.71
100.83
77.42
77.20
77.00
76.58
61.08
52.05
15.14
O
O
(EtO)2HC
f1 (ppm)


7.72
7.66
7.54
7.51
7.39
7.37
7.26
6.47
6.41
4.31
4.28
4.26
4.23
1.37
1.34
1.32
1.04
2.04
3.03
1.00
f1 (ppm)


166.96
144.54
134.48
128.85
128.27
128.02
118.30
77.42
77.00
76.58
60.46
14.30
f1 (ppm)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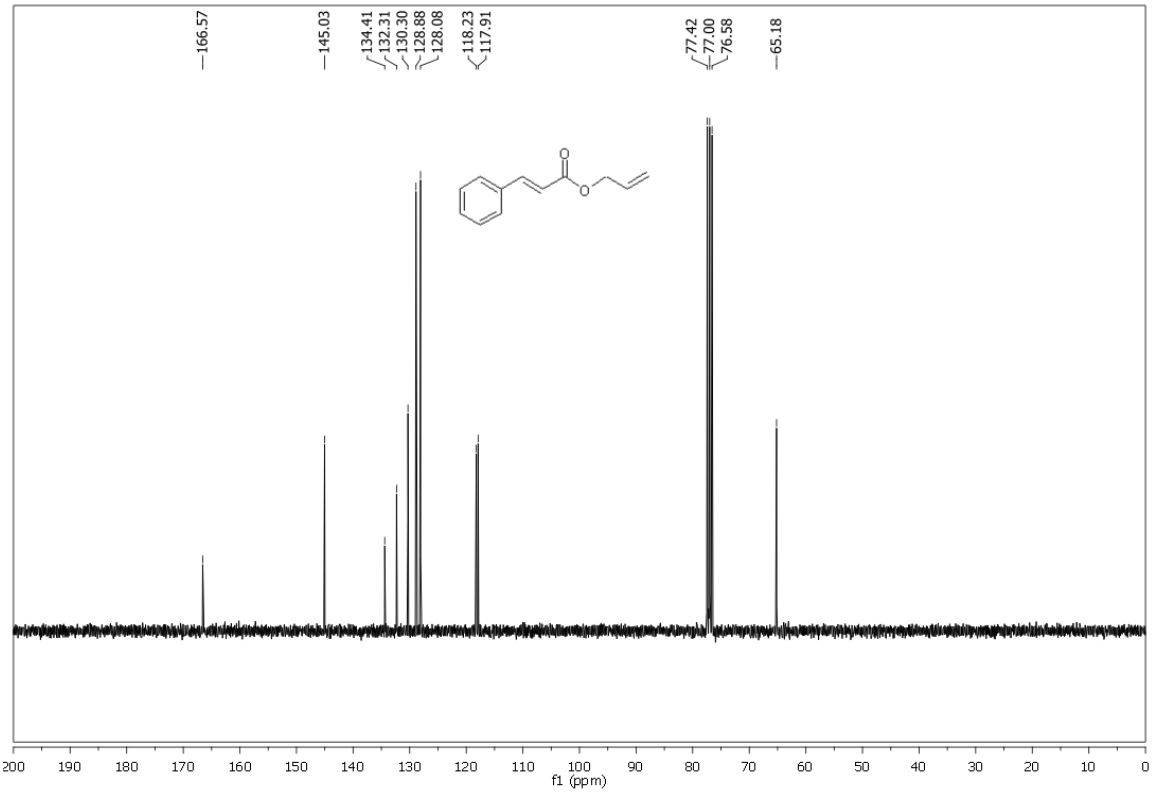
7.70
7.55
7.54
7.53
7.52
7.40
7.39
7.38
7.26
6.50
6.45
5.99
5.98
5.94
5.30
5.29
5.26
5.26
4.73
4.71
1.02
2.05
3.01
1.00
1.00
1.00
1.00
2.02
f1 (ppm)


166.57
145.03
134.41
132.31
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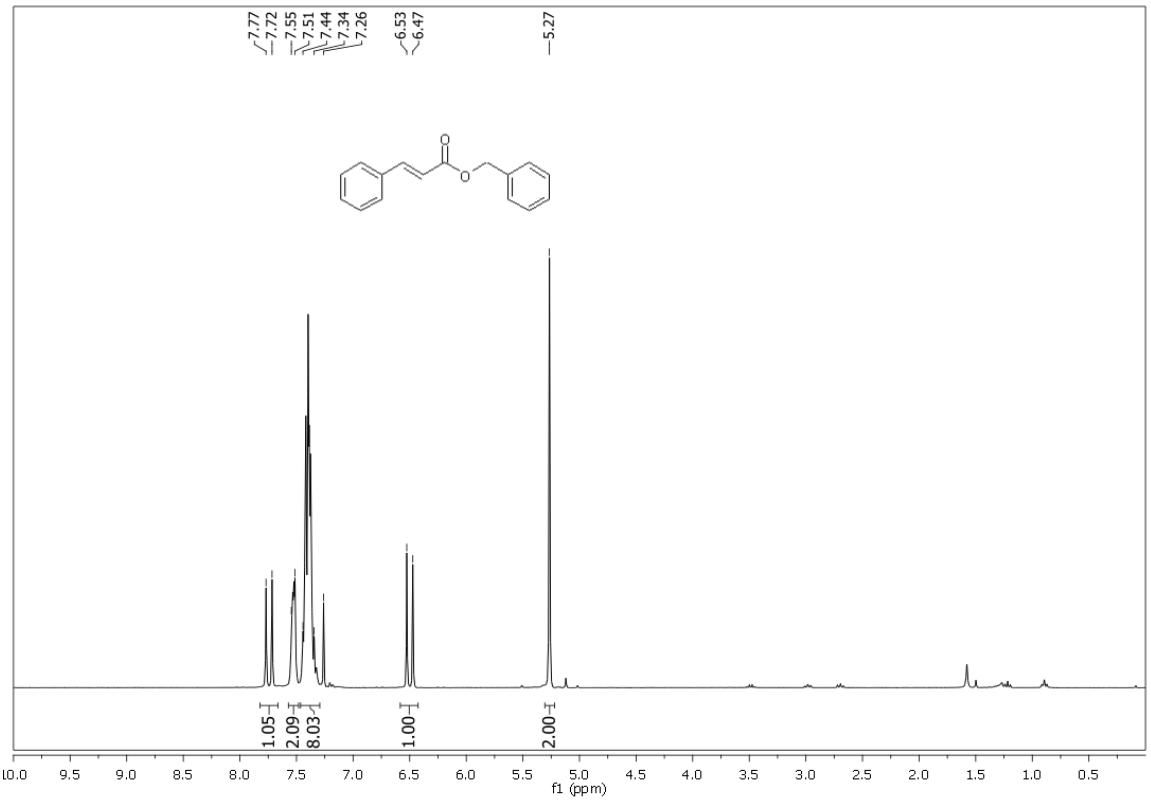
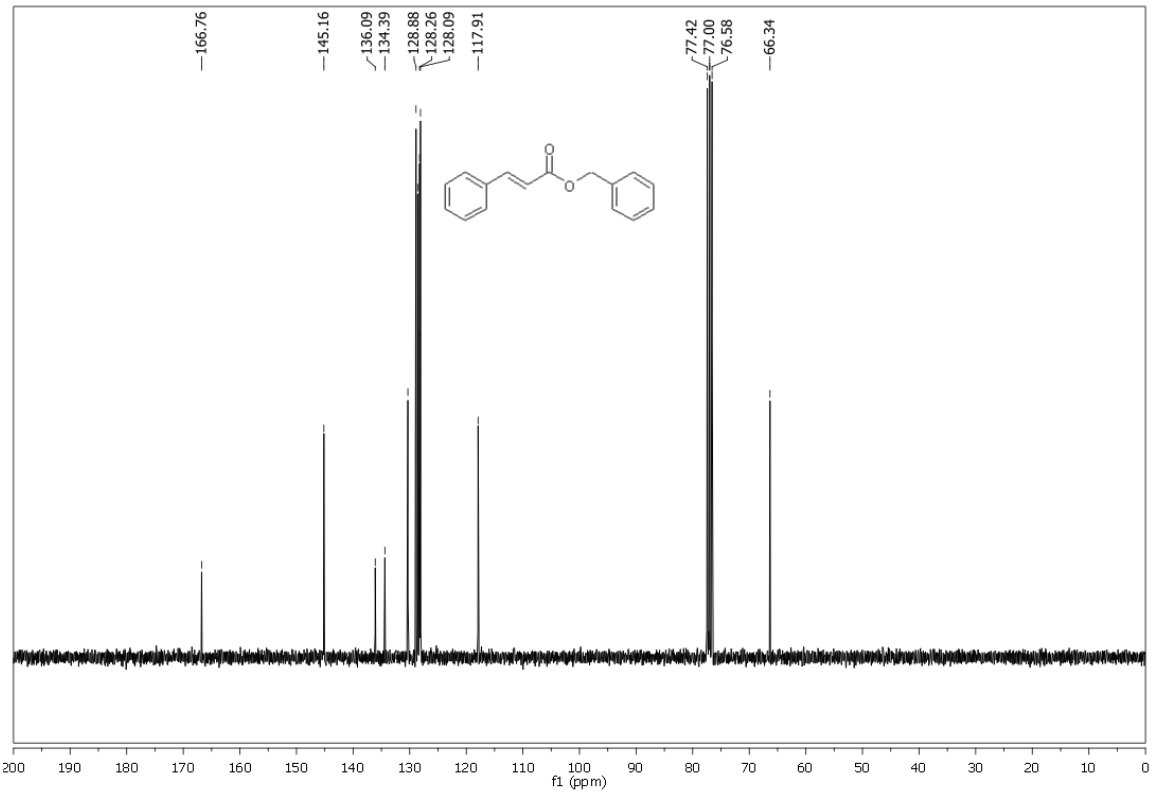
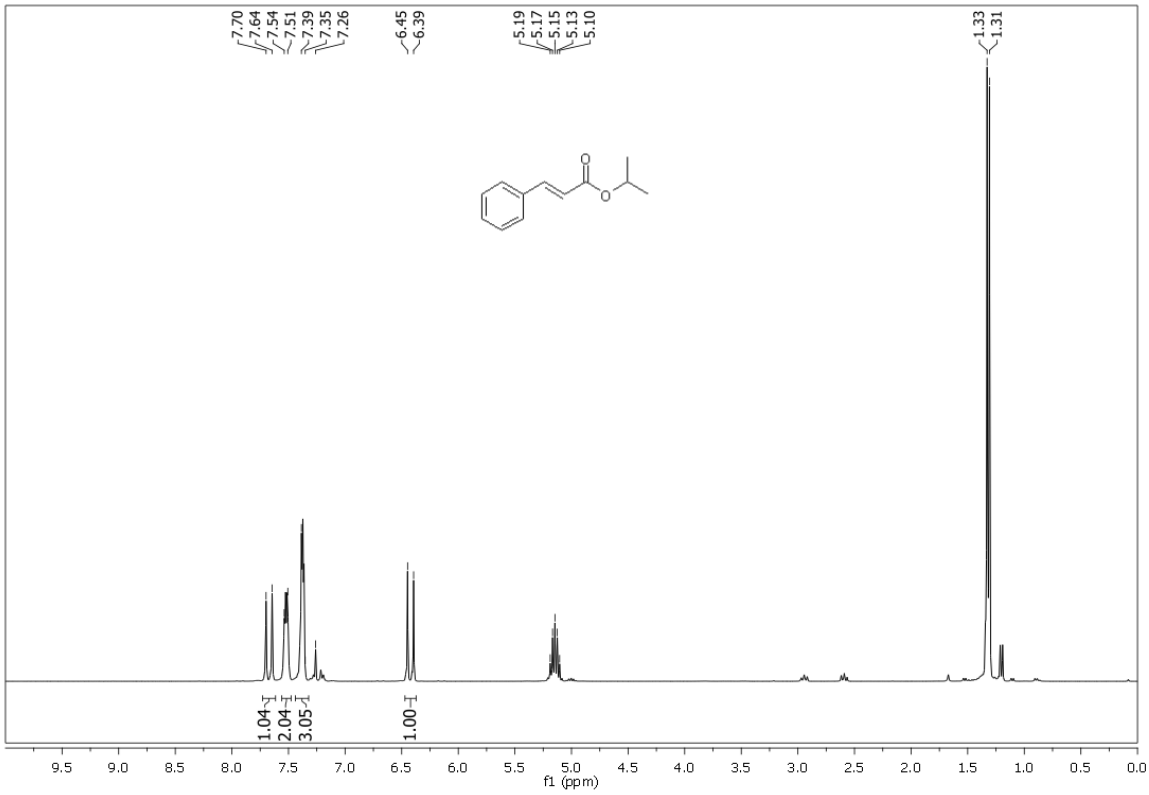
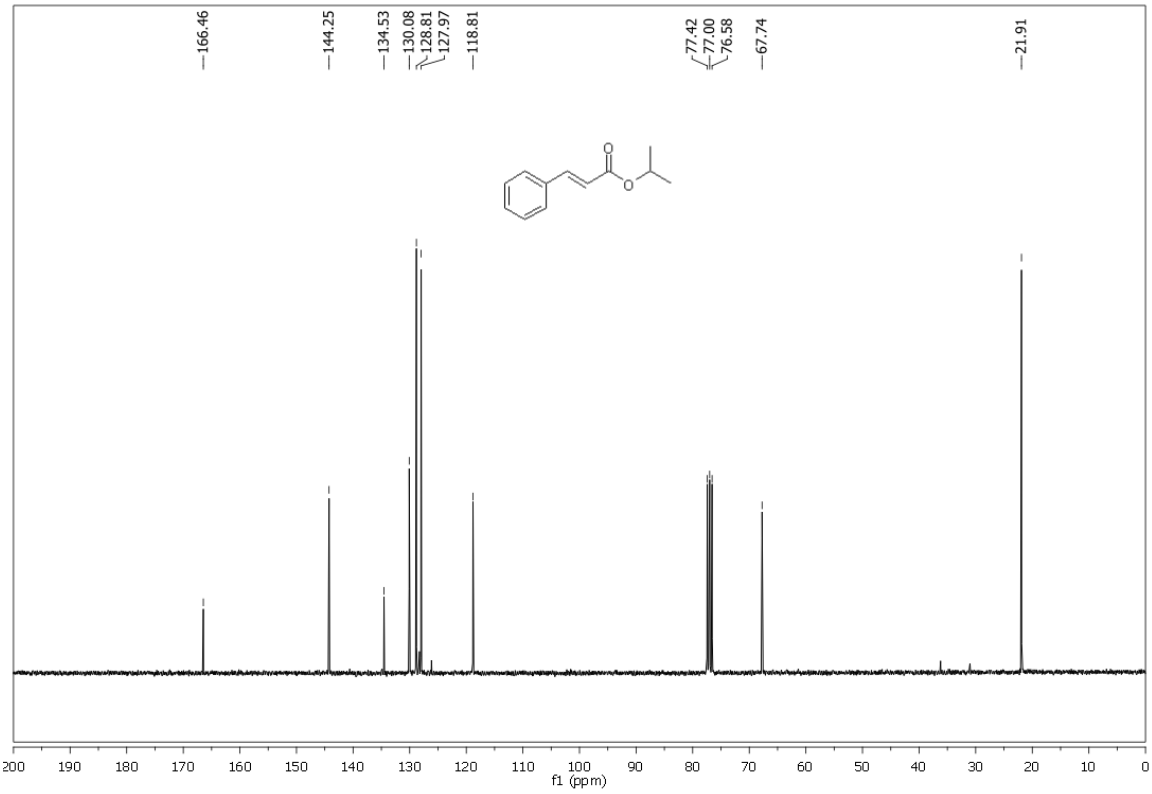
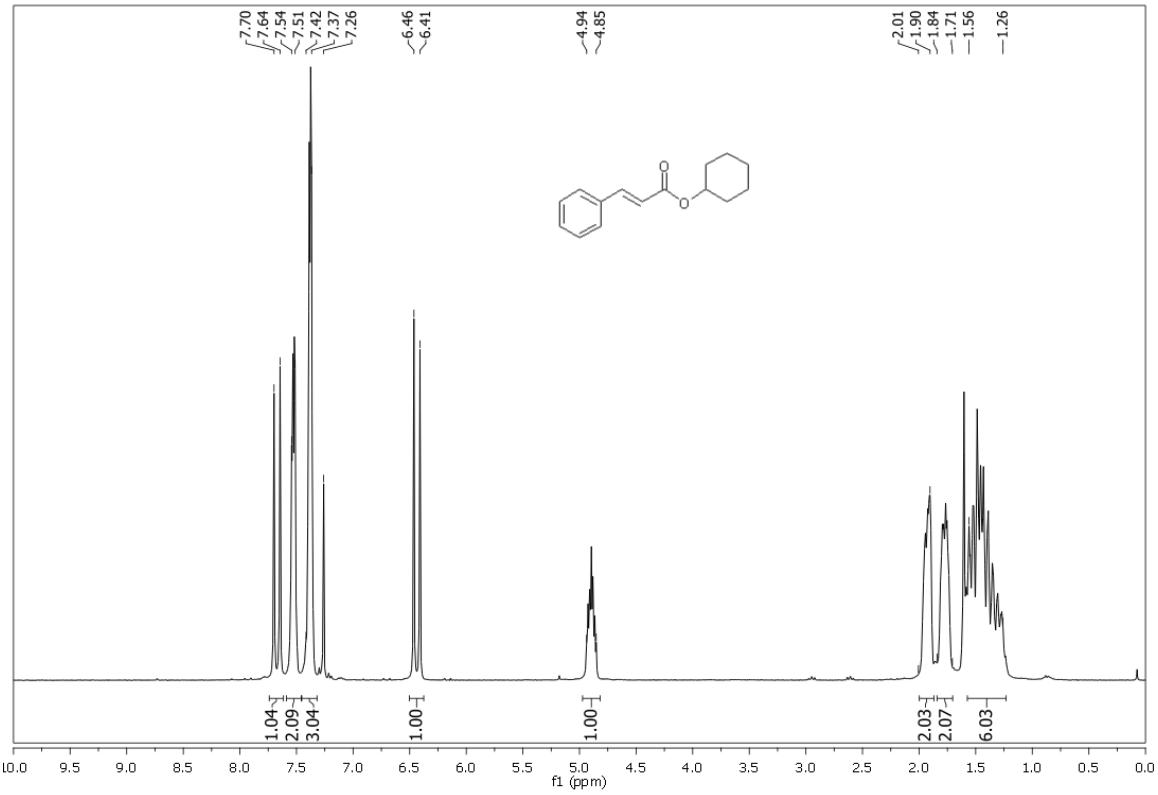
128.88
128.08
118.23
117.91
77.42
77.00
76.58
65.18
f1 (ppm)

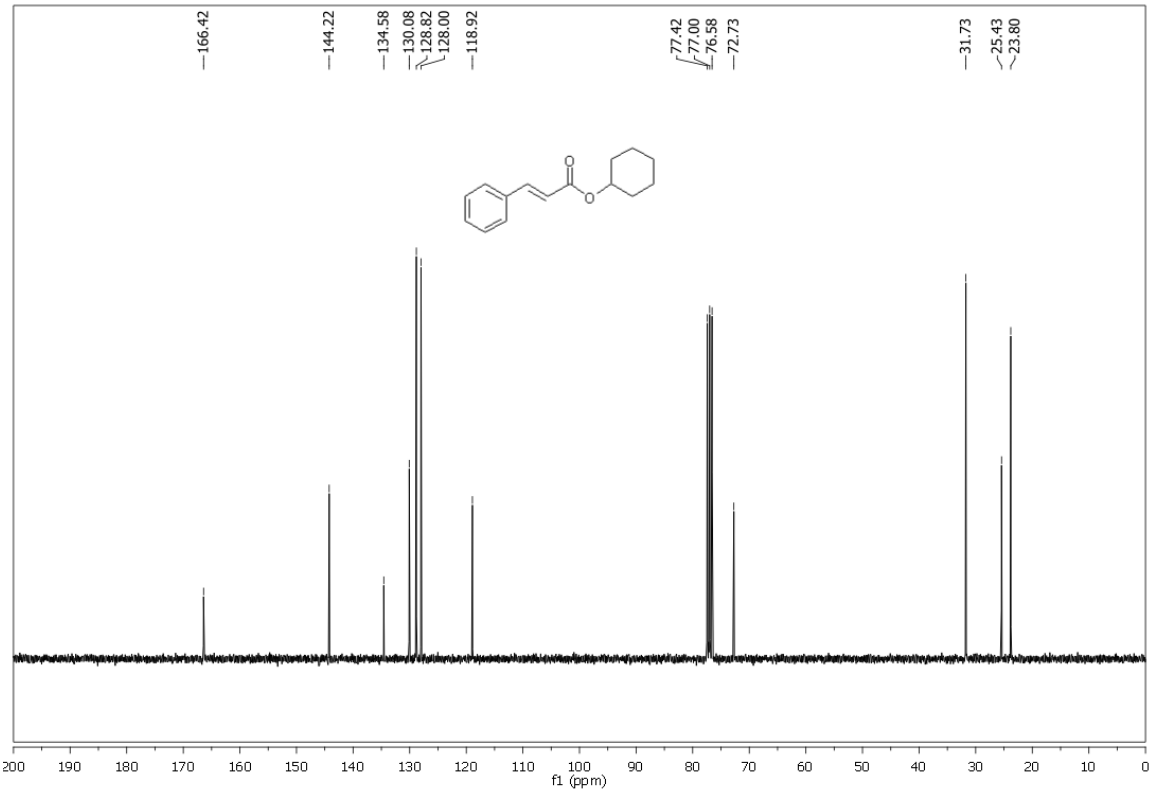

7.77
7.72
7.55
7.51
7.44
7.34
7.26
6.53
6.47
5.27
1.05
2.09
8.03
1.00
2.00
f1 (ppm)

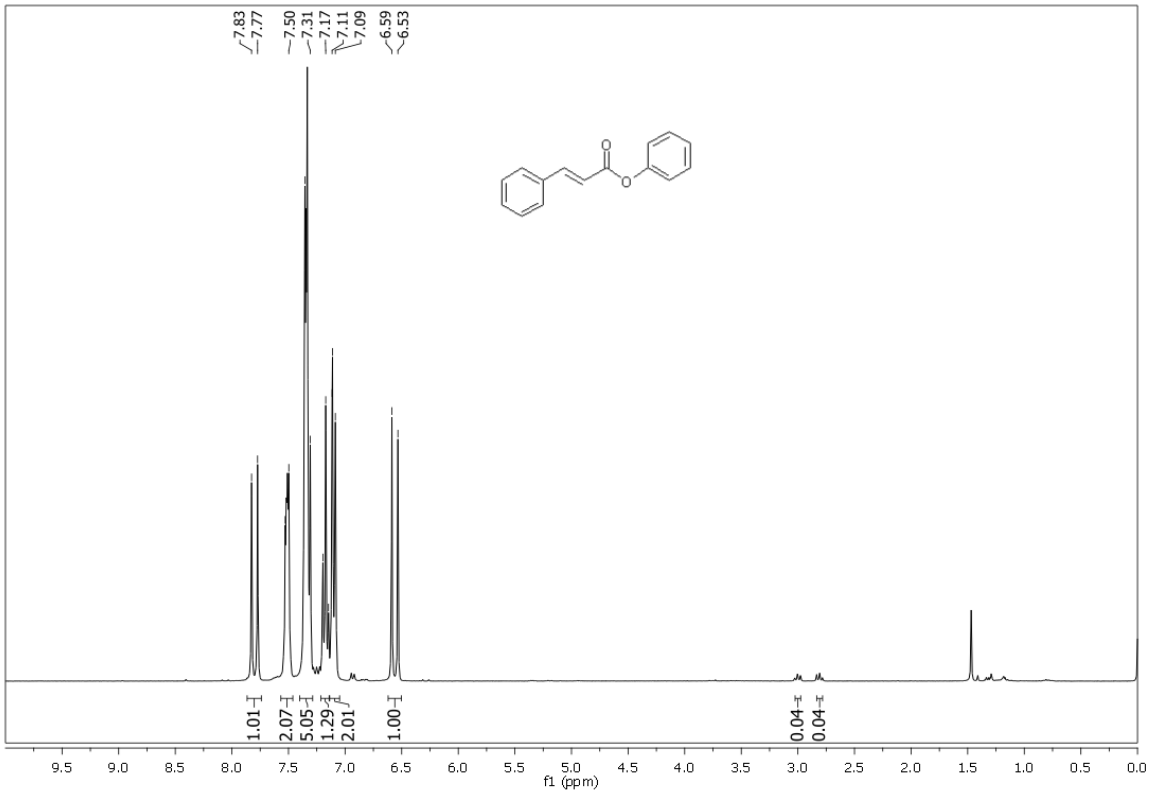

166.76
145.16
136.09
134.39
128.88
128.26
128.09
117.91
77.42
77.00
76.58
66.34
f1 (ppm)

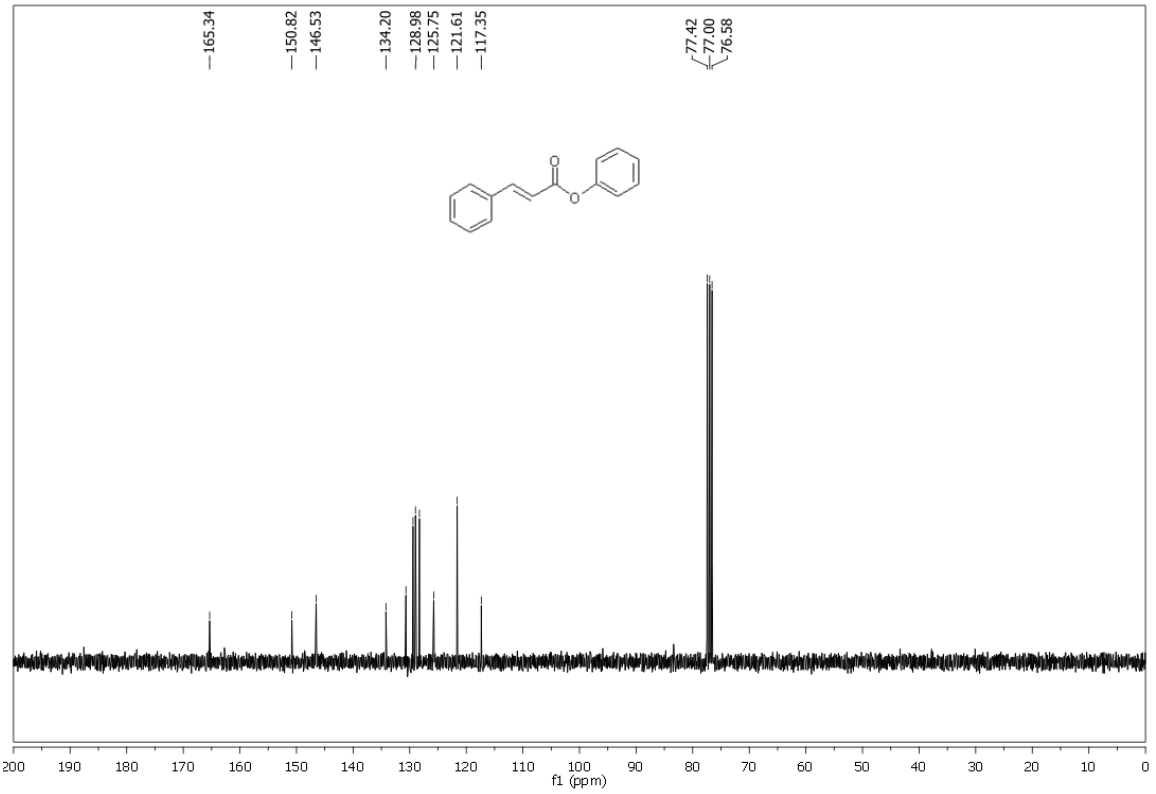

7.70
7.64
7.54
7.51
7.39
7.35
7.26
6.45
6.39
5.19
5.17
5.15
5.13
5.10
1.33
1.31
1.04
2.04
3.05
1.00
f1 (ppm)

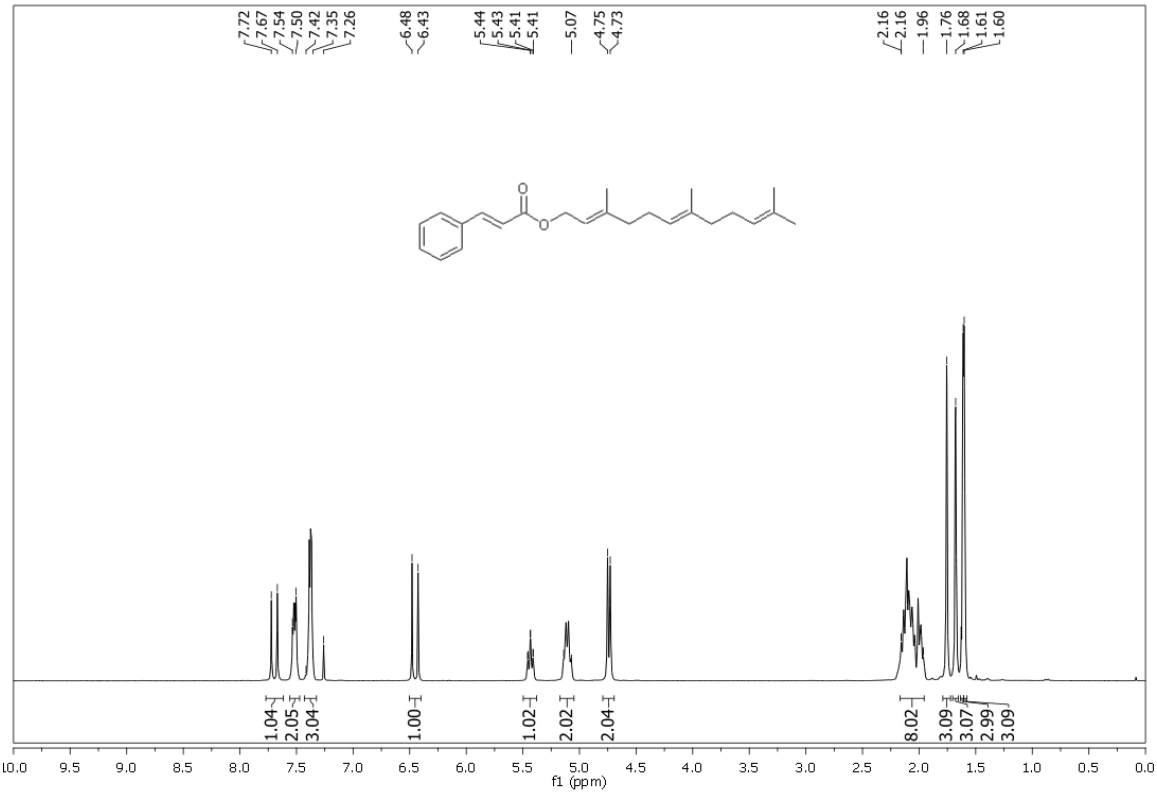

166.46
144.25
134.53
130.08
128.81
127.97
118.81
77.42
77.00
76.58
67.74
21.91
f1 (ppm)

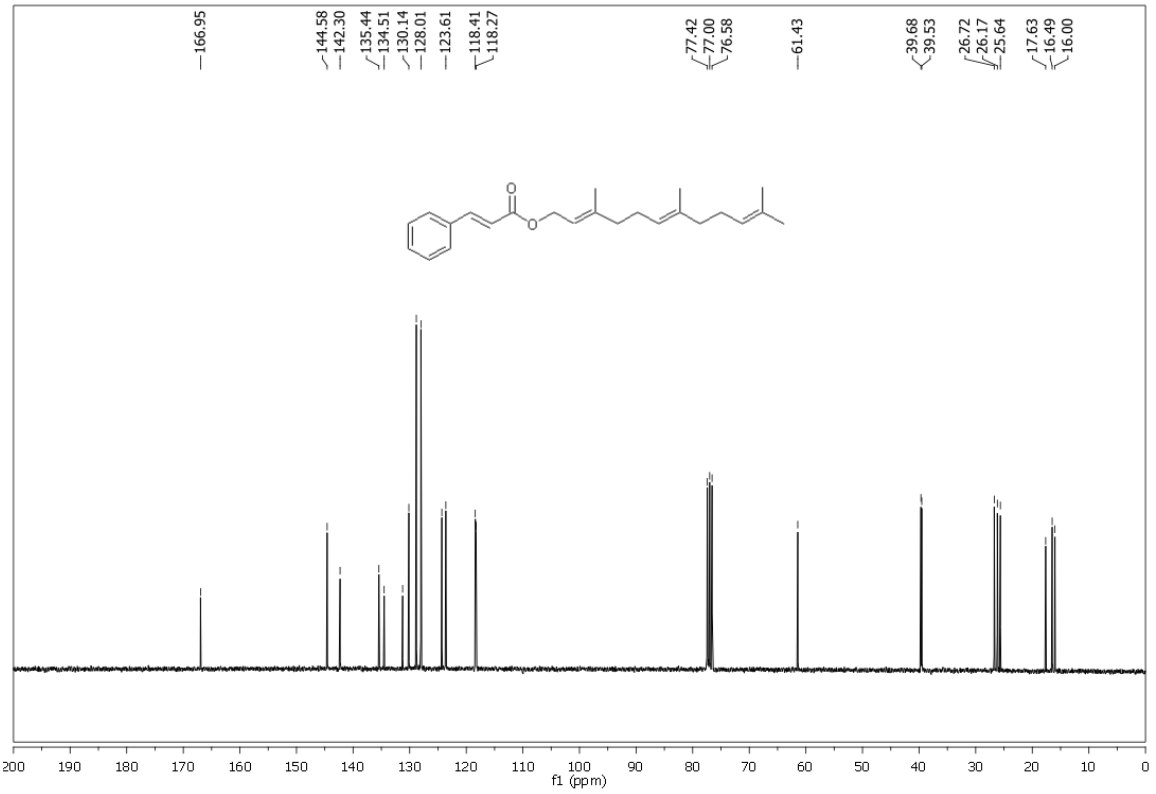

7.70
7.64
7.54
7.51
7.42
7.37
7.26
6.46
6.41
4.94
4.85
2.01
1.90
1.84
1.71
1.56
1.26
1.04
2.09
3.04
1.00
1.00
2.03
2.07
6.03
f1 (ppm)

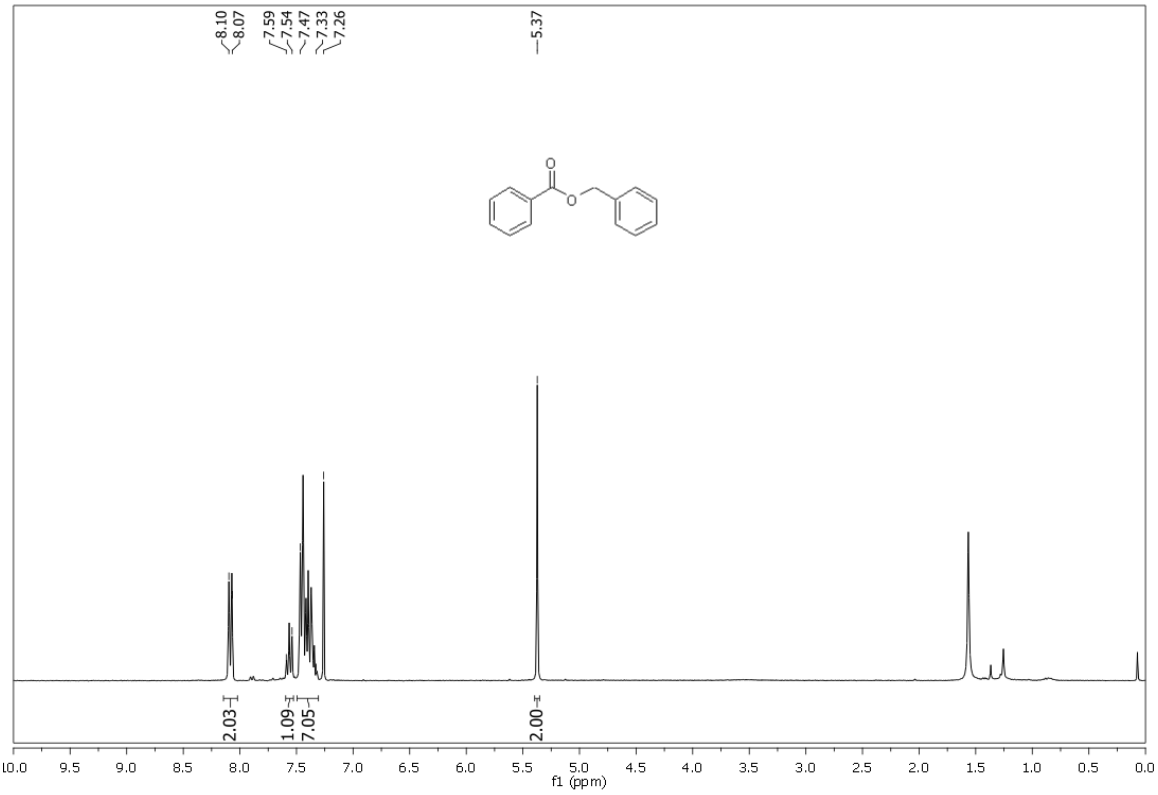

166.42
144.22
134.58
130.08
128.82
128.00
118.92
77.42
77.00
76.58
72.73
31.73
25.43
23.80
f1 (ppm)

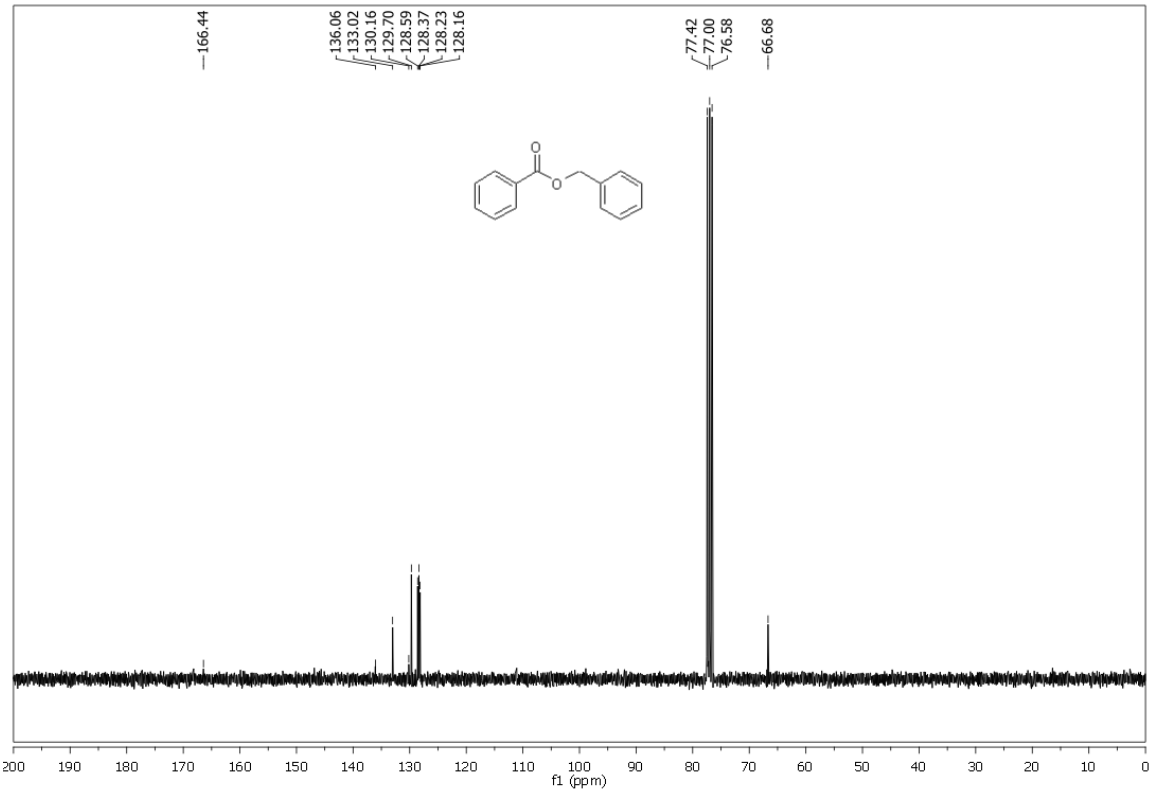

7.83
7.77
7.50
7.31
7.17
7.11
7.09
6.59
6.53
1.01
2.07
5.05
1.29
2.01
1.00
0.04
0.04
f1 (ppm)

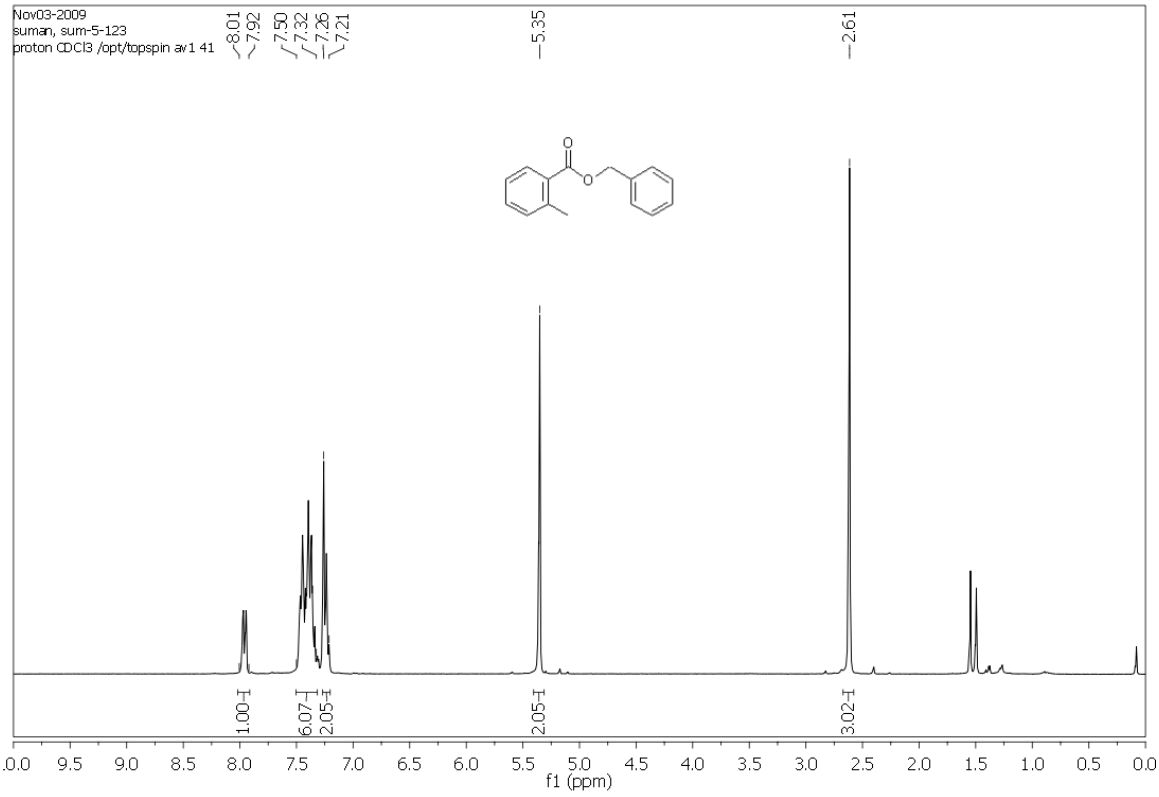

165.34
150.82
146.53
134.20
128.98
125.75
121.61
117.35
77.42
77.00
76.58
f1 (ppm)

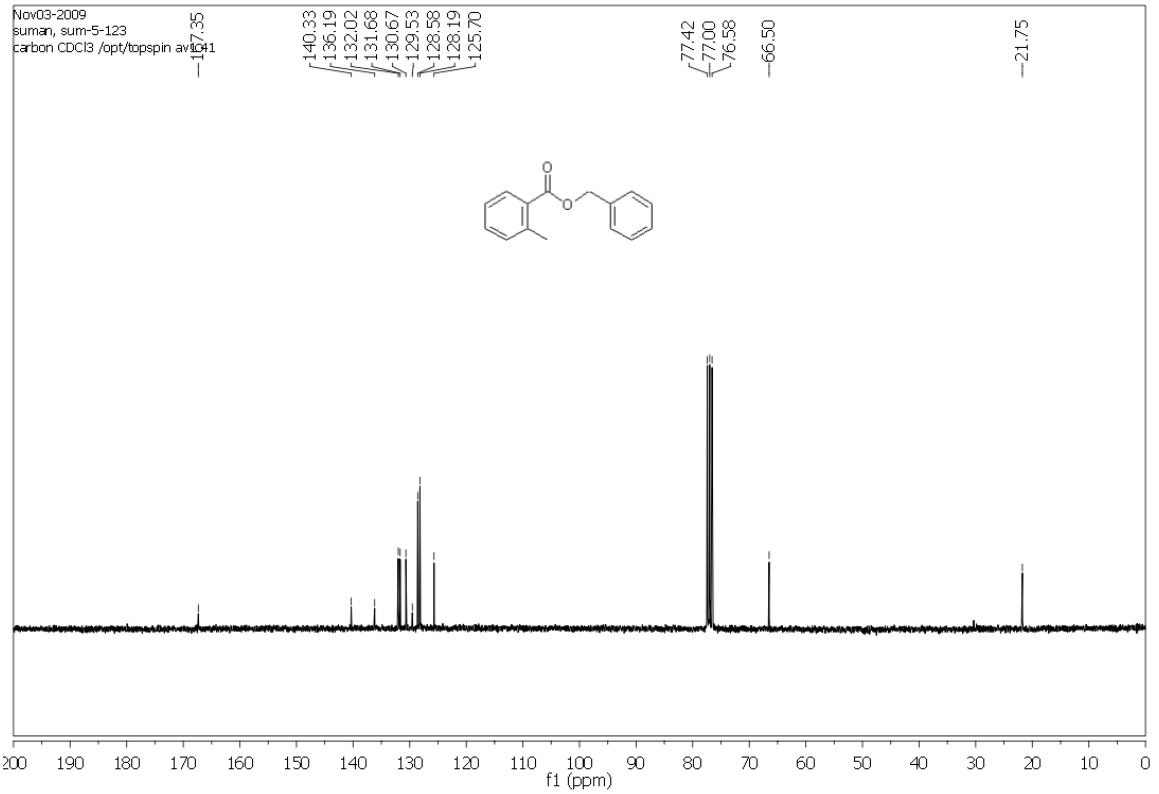

7.72
7.67
7.54
7.50
7.42
7.35
7.26
6.48
6.43
5.44
5.43
5.41
5.41
5.07
4.75
4.73
2.16
2.16
1.96
1.76
1.68
1.61
1.60
1.04
2.05
3.04
1.00
1.02
2.02
2.04
8.02
3.09
3.07
2.99
3.09
f1 (ppm)

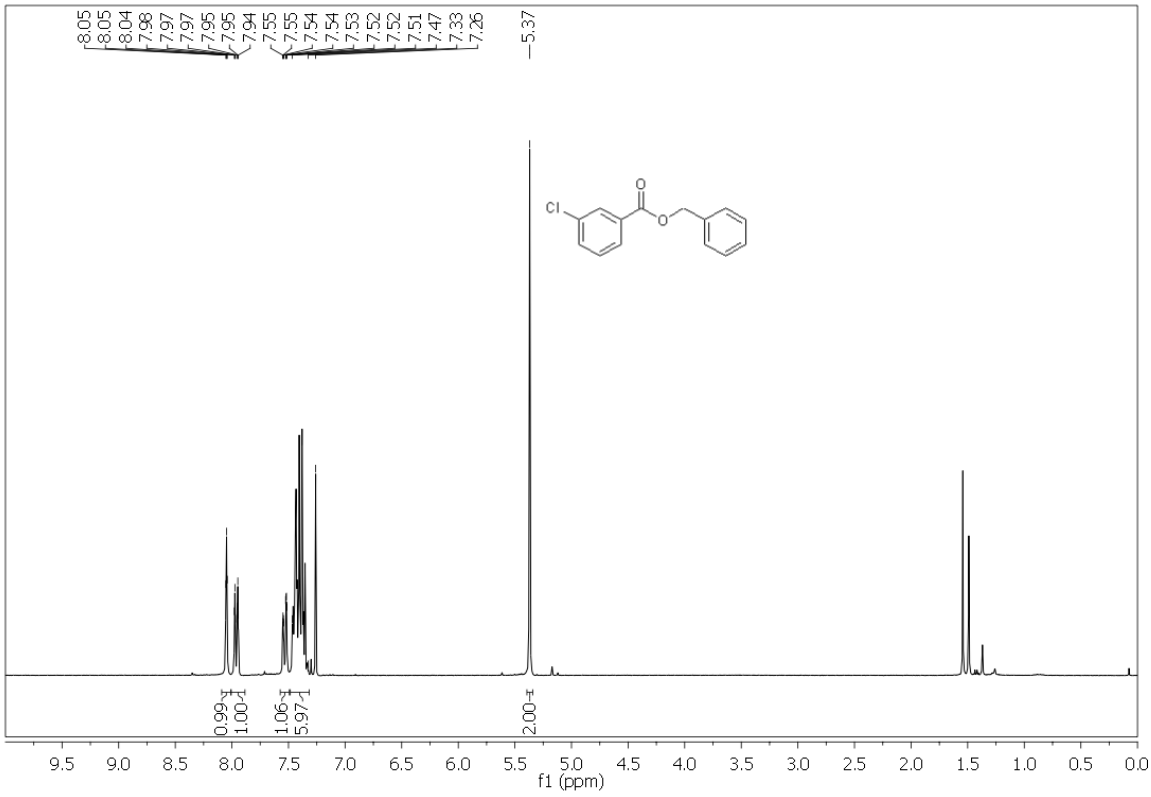

166.95
144.58
142.30
135.44
134.51
130.14
128.01
123.61
118.41
118.27
77.42
77.00
76.58
61.43
39.68
39.53
26.72
26.17
25.64
17.63
16.49
16.00
f1 (ppm)

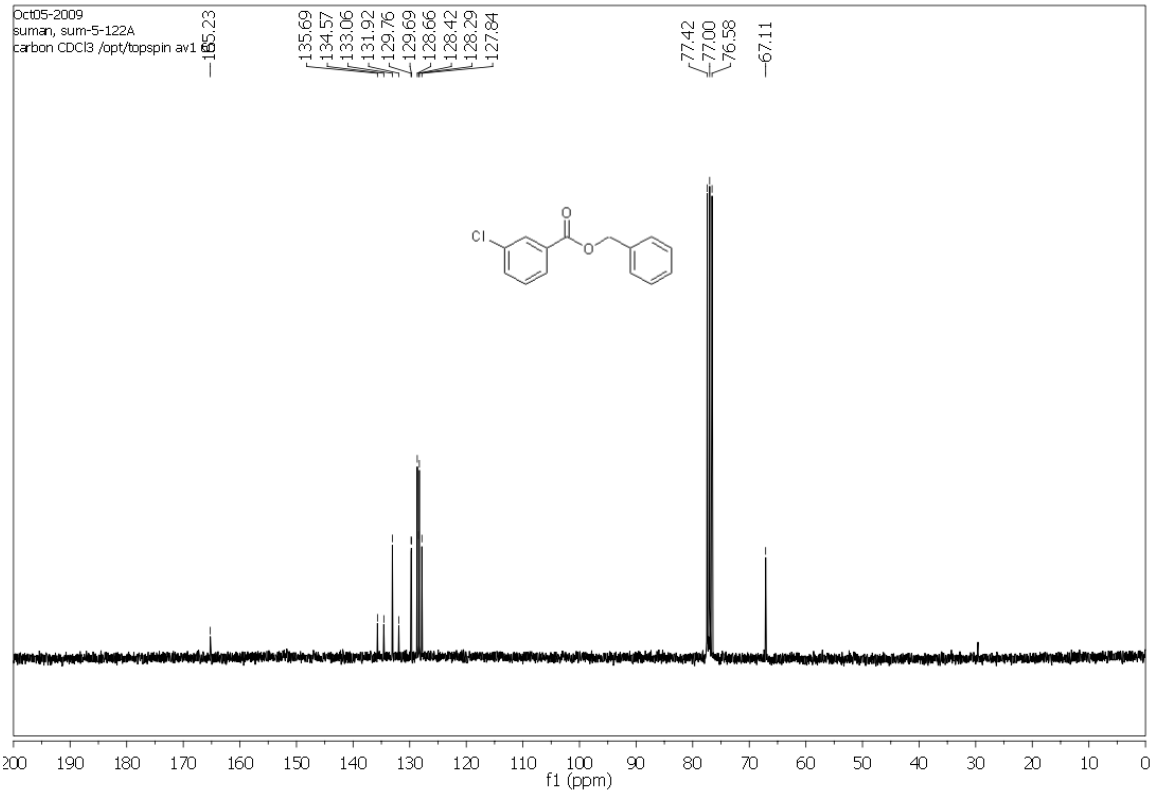

8.10
8.07
7.59
7.54
7.47
7.33
7.26
5.37
2.03
1.09
7.05
2.00
f1 (ppm)

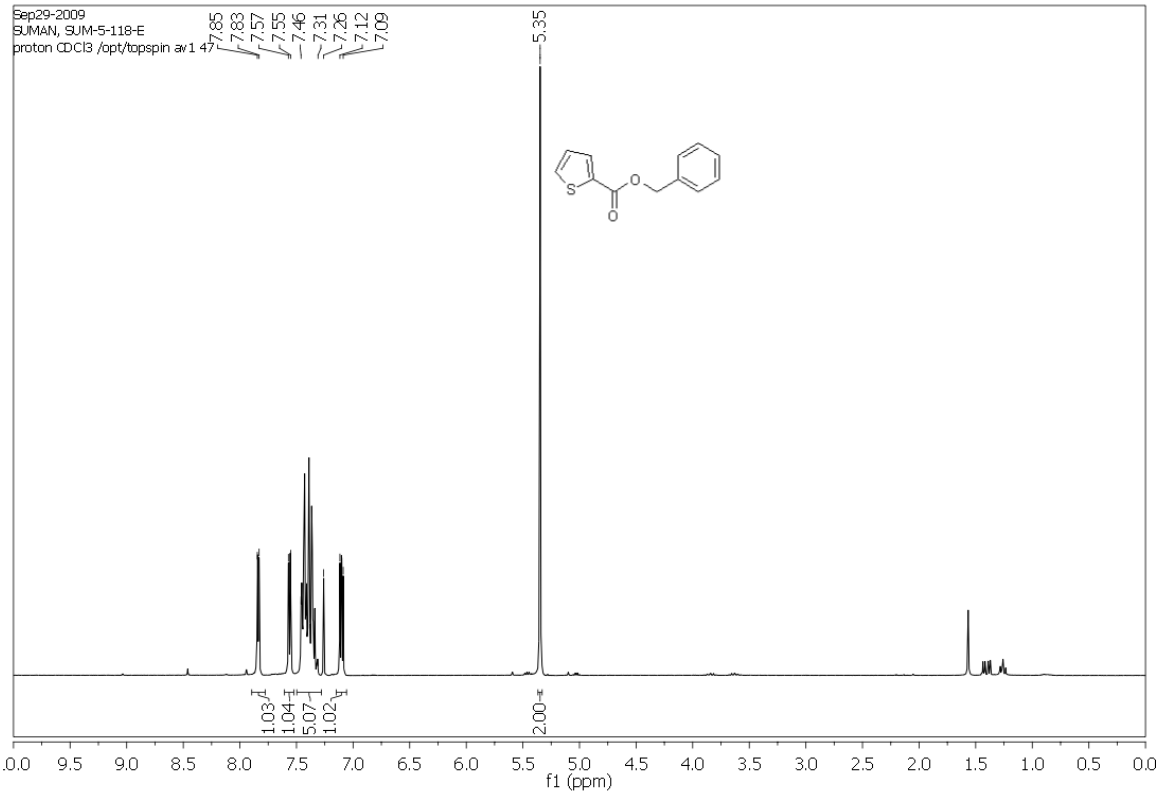

166.44
136.06
133.02
130.16
129.70
128.59
128.37
128.23
128.16
77.42
77.00
76.58
66.68
f1 (ppm)

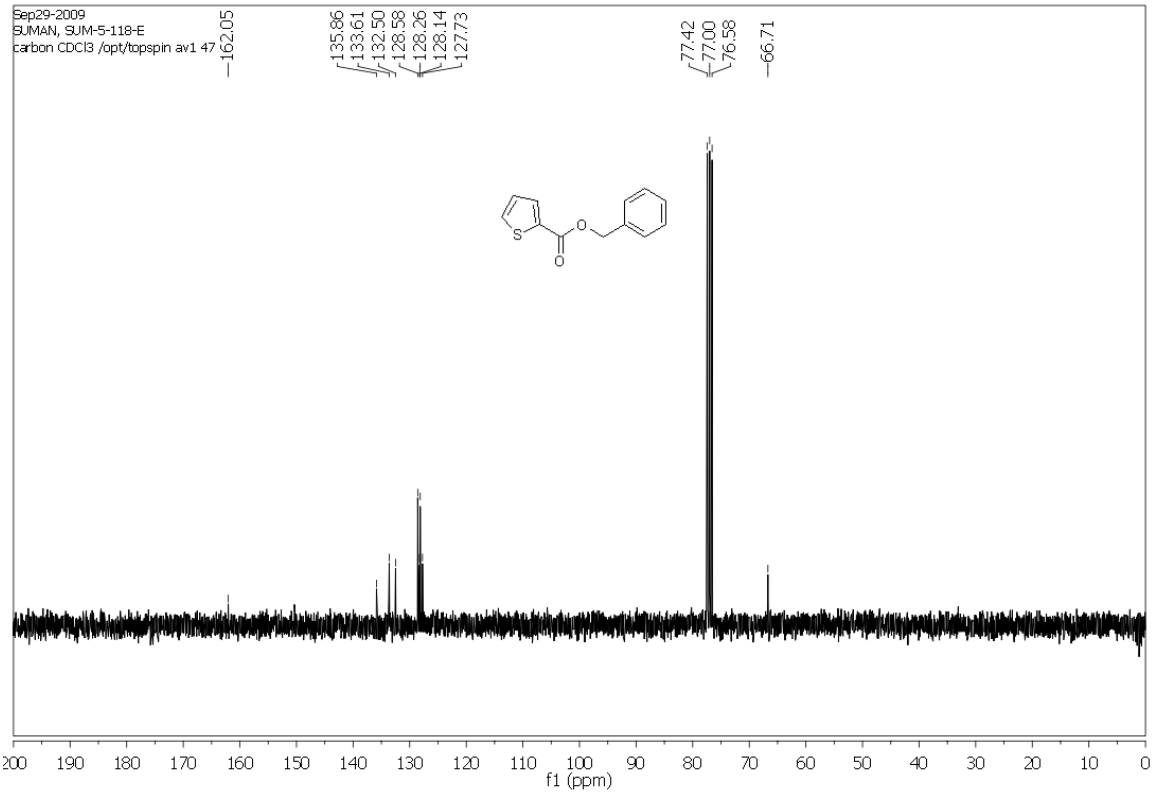

Nov03-2009
suman, sum-5-123
proton CDCl3 /opt/topspin av1 41
8.01
7.92
7.50
7.32
7.26
7.21
5.35
2.61
1.00
6.07
2.05
2.05
3.02
f1 (ppm)

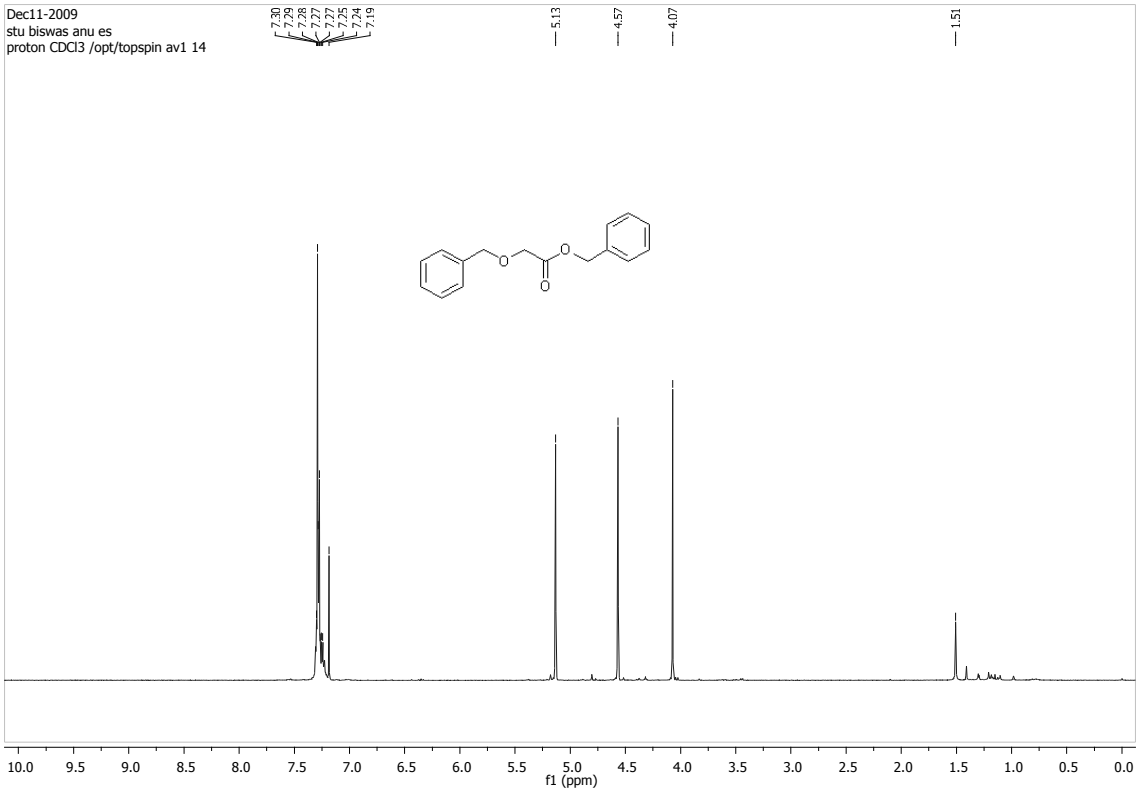

Nov03-2009
suman, sum-5-123
carbon CDCl3 /opt/topspin av1 41
167.35
140.33
136.19
132.02
131.68
130.67
129.53
128.58
128.19
125.70
77.42
77.00
76.58
66.50
21.75
f1 (ppm)

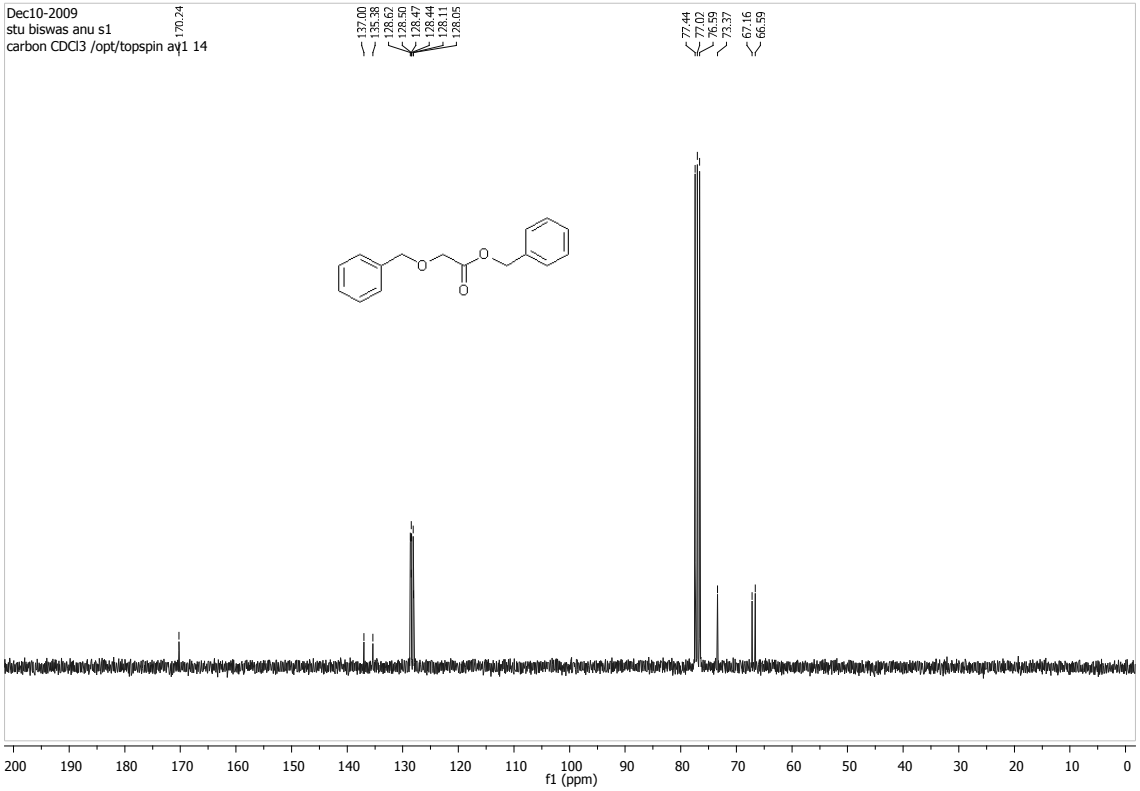

8.05
8.05
8.04
7.98
7.97
7.97
7.95
7.95
7.94
7.55
7.55
7.54
7.54
7.53
7.52
7.52
7.51
7.47
7.33
7.26
5.37
Cl
O
O
0.99
1.00
1.06
5.97
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

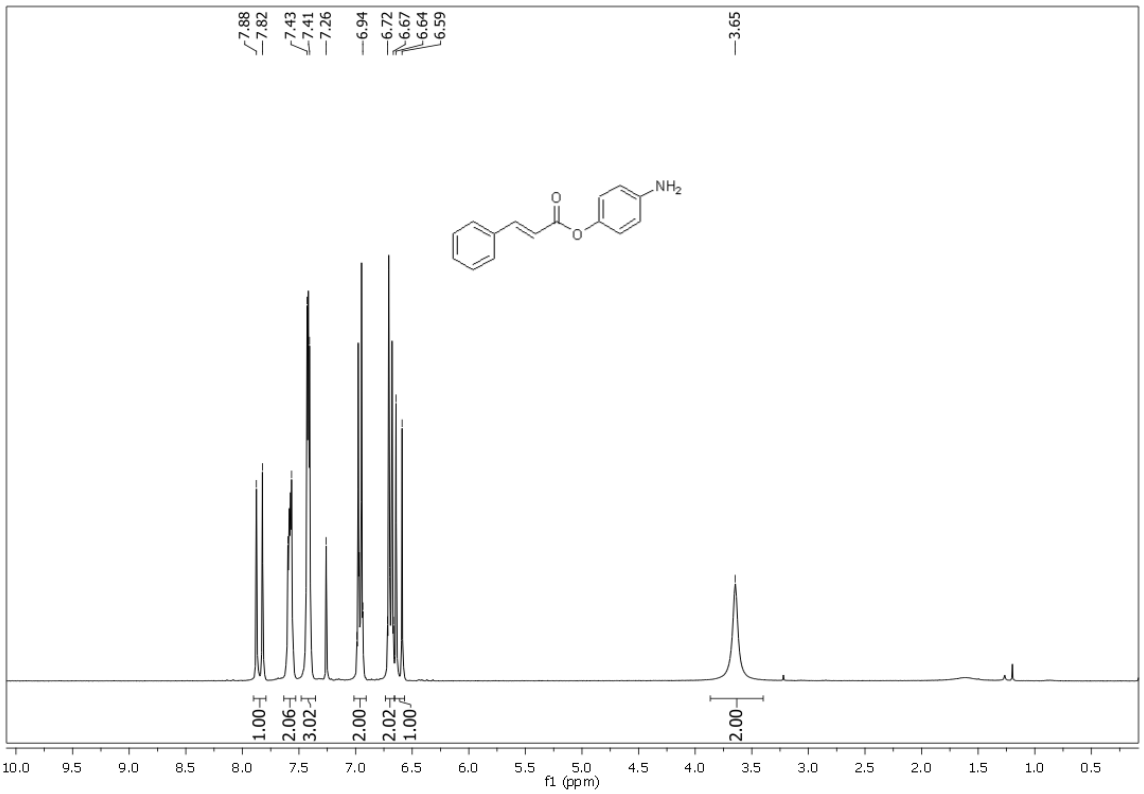

Oct05-2009
suman, sum-5-122A
carbon CDCl3 /opt/topspin av1
165.23
135.69
134.57
133.06
131.92
129.76
129.69
128.66
128.42
128.29
127.84
77.42
77.00
76.58
67.11
Cl
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

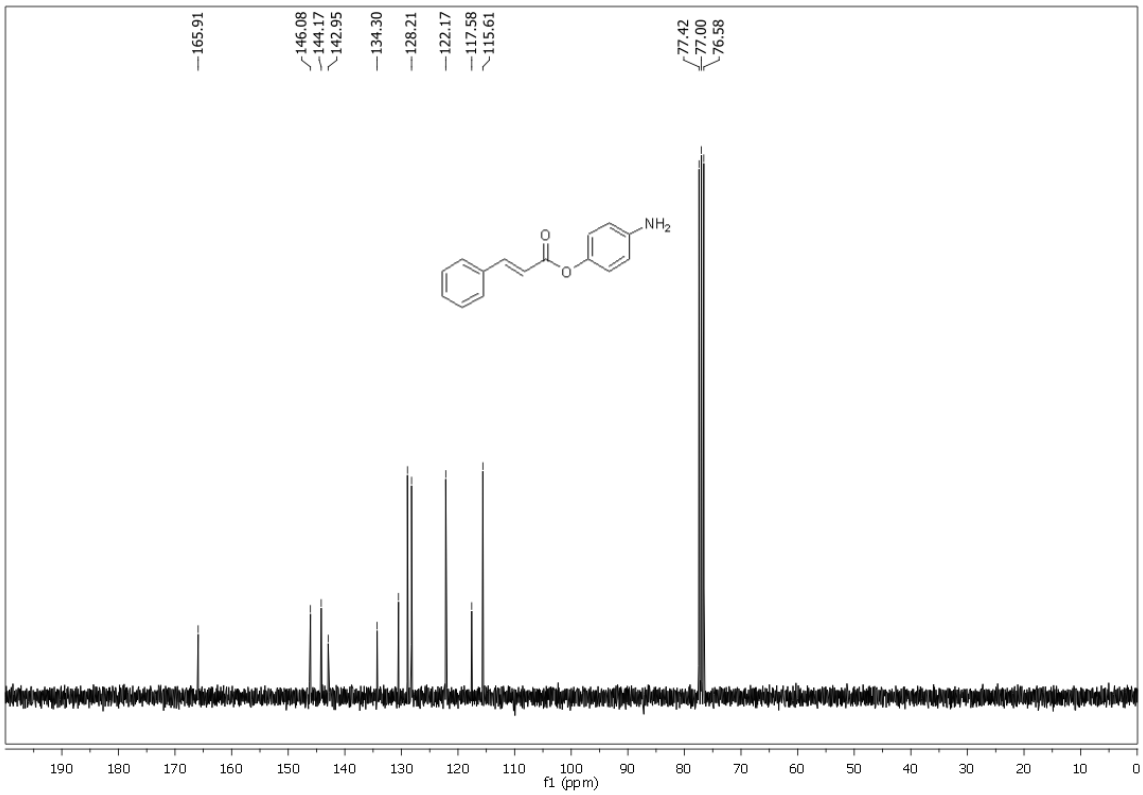

Sep29-2009
SUMAN, SUM-5-118-E
proton CDCl3 /opt/topspin av1 47
7.85
7.83
7.57
7.55
7.46
7.31
7.26
7.12
7.09
5.35
1.03
1.04
5.07
1.02
2.00
f1 (ppm)

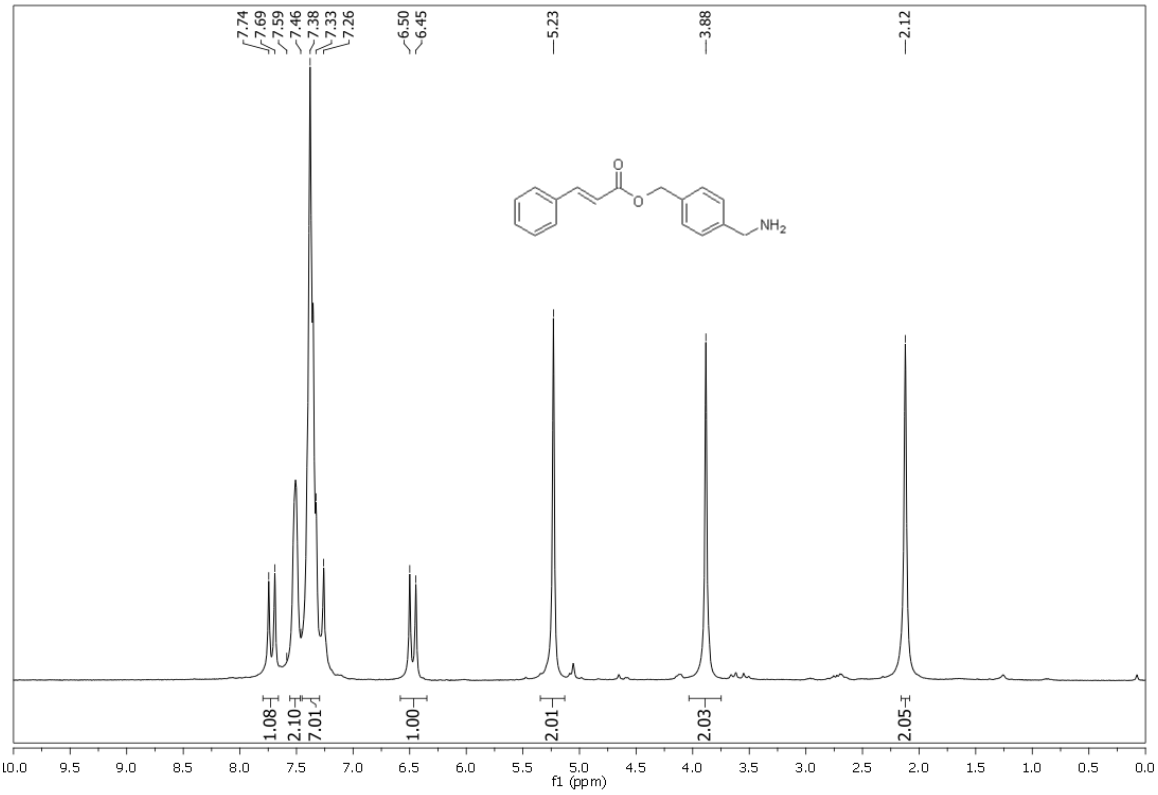

Sep29-2009
SUMAN, SUM-5-118-E
carbon CDCl3 /opt/topspin av1 47
162.05
135.86
133.61
132.50
128.58
128.26
128.14
127.73
77.42
77.00
76.58
66.71
f1 (ppm)

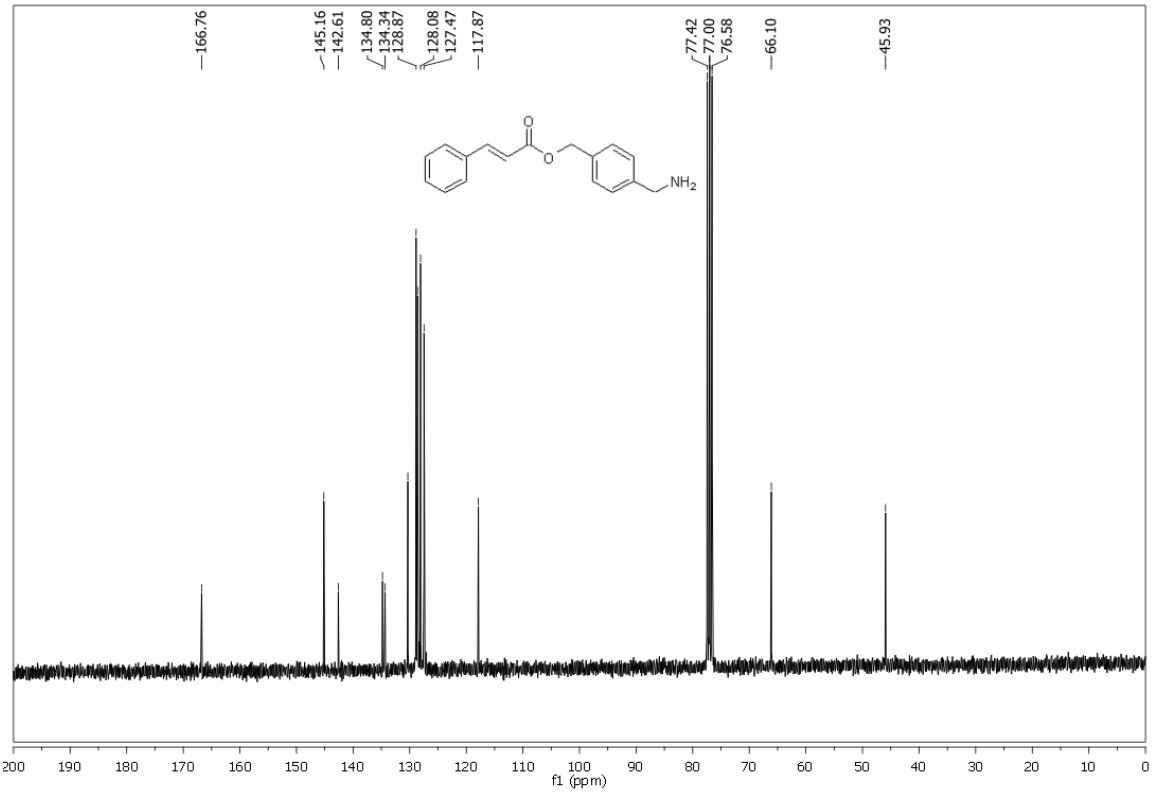

Dec11-2009
stu biswas anu es
proton CDCl3 /opt/topspin av1 14
7.30
7.29
7.28
7.27
7.27
7.25
7.24
7.19
5.13
4.57
4.07
1.51
O
O
O
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

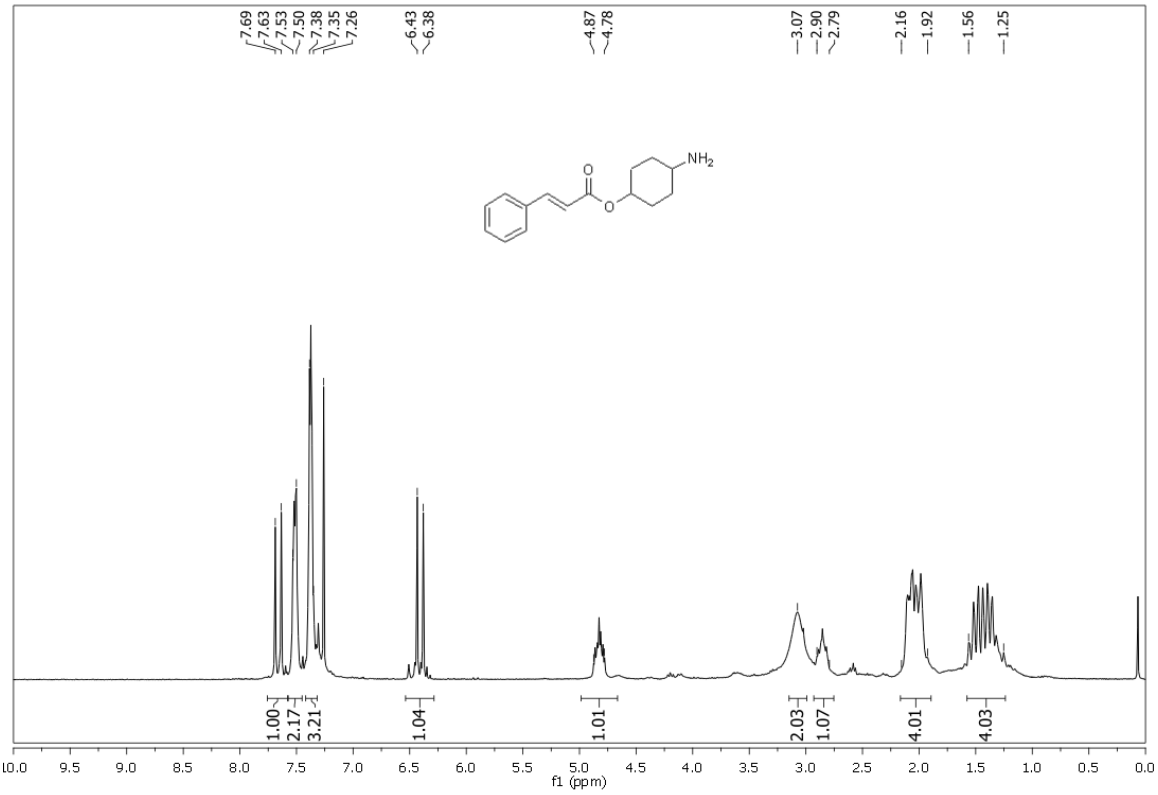

Dec10-2009
stu biswas anu s1
carbon CDCl3 /opt/topspin av1 14
170.24
137.00
135.38
128.62
128.50
128.47
128.44
128.11
128.05
77.44
77.02
76.59
73.37
67.16
66.59
O
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

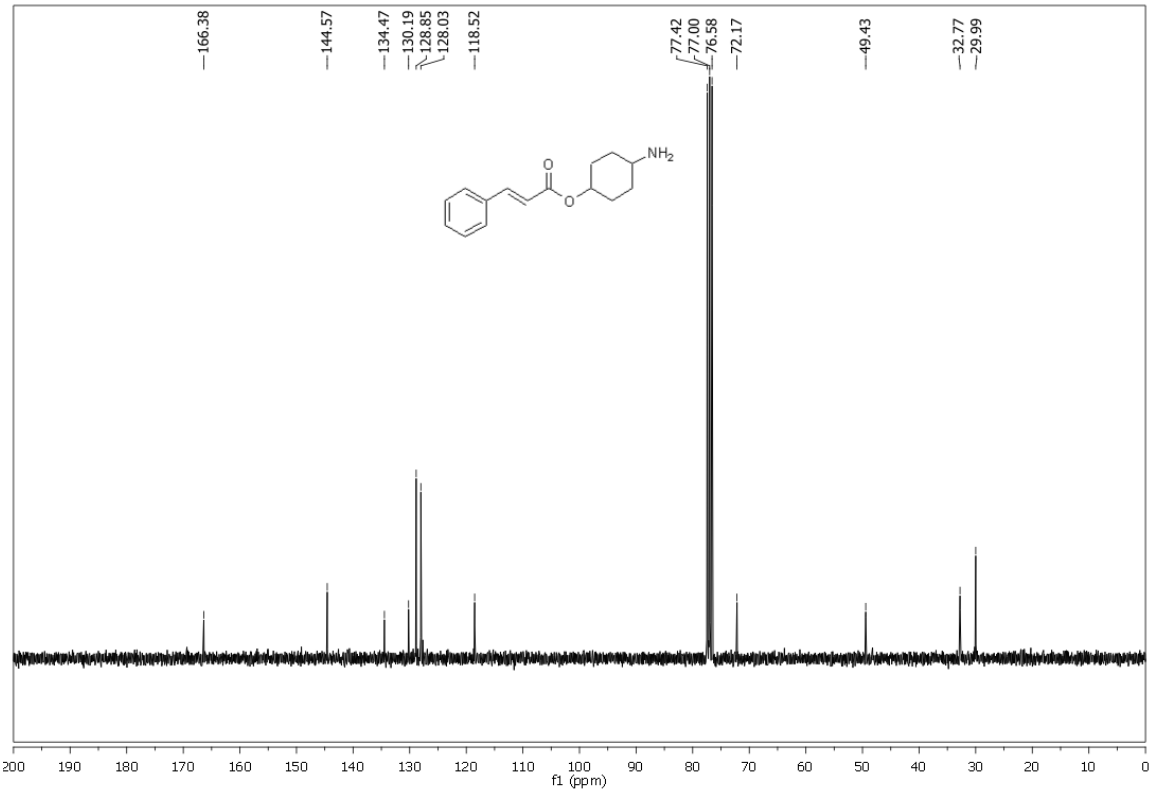

7.88
7.82
7.43
7.41
7.26
6.94
6.72
6.67
6.64
6.59
3.65
NH2
O
O
1.00
2.06
3.02
2.00
2.02
1.00
2.00
f1 (ppm)

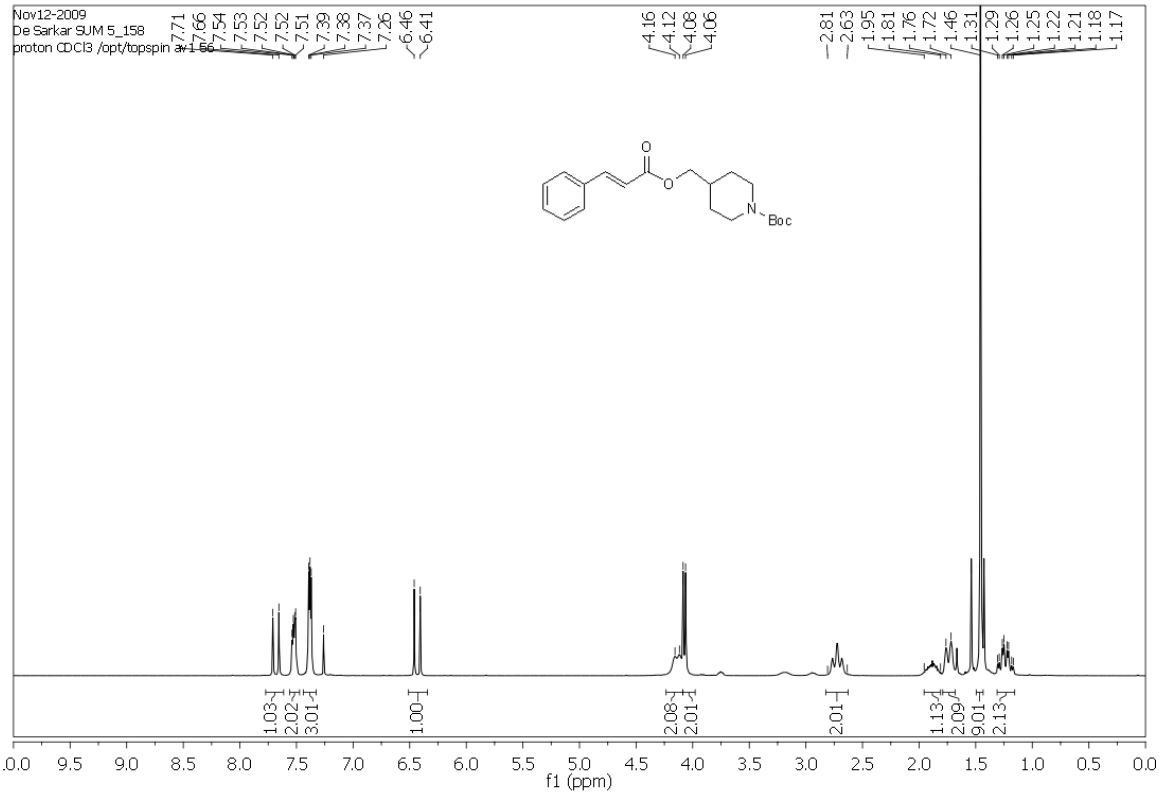

165.91
146.08
144.17
142.95
134.30
128.21
122.17
117.58
115.61
77.42
77.00
76.58
NH2
O
O
f1 (ppm)

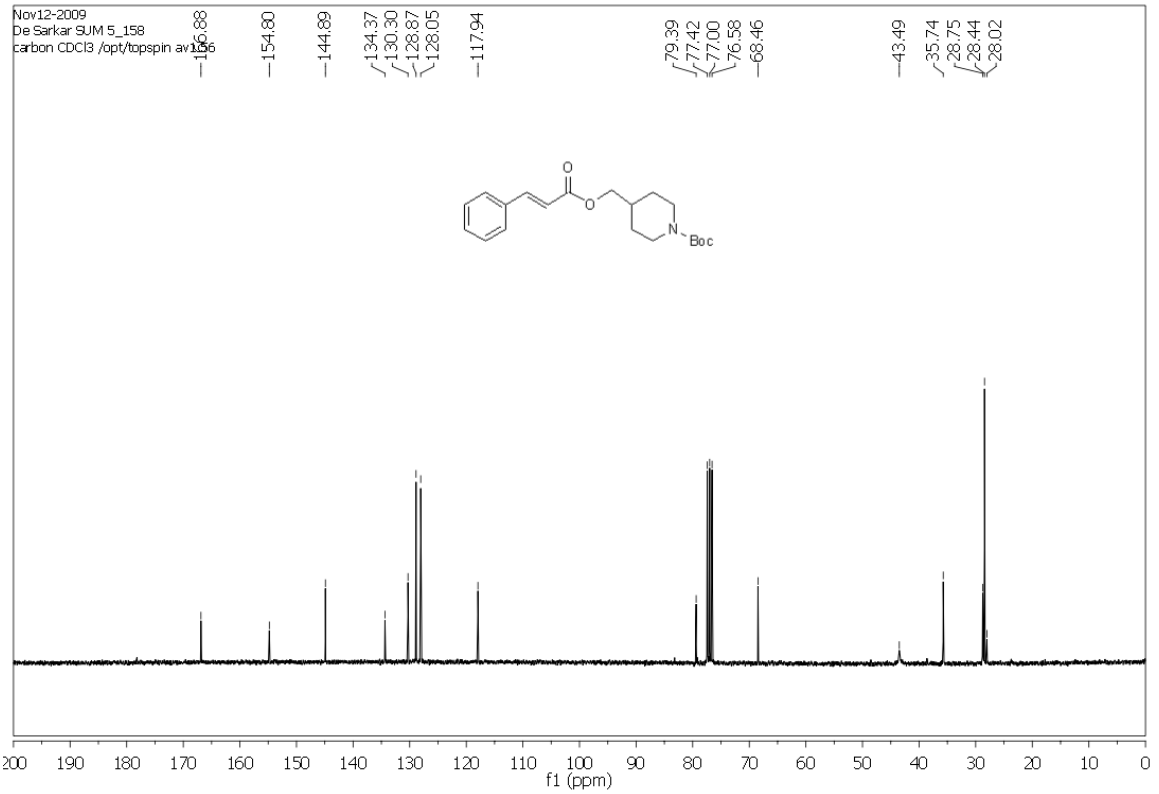

7.74
7.69
7.59
7.46
7.38
7.33
7.26
6.50
6.45
5.23
3.88
2.12
O
O
NH2
1.08
2.10
7.01
1.00
2.01
2.03
2.05
f1 (ppm)

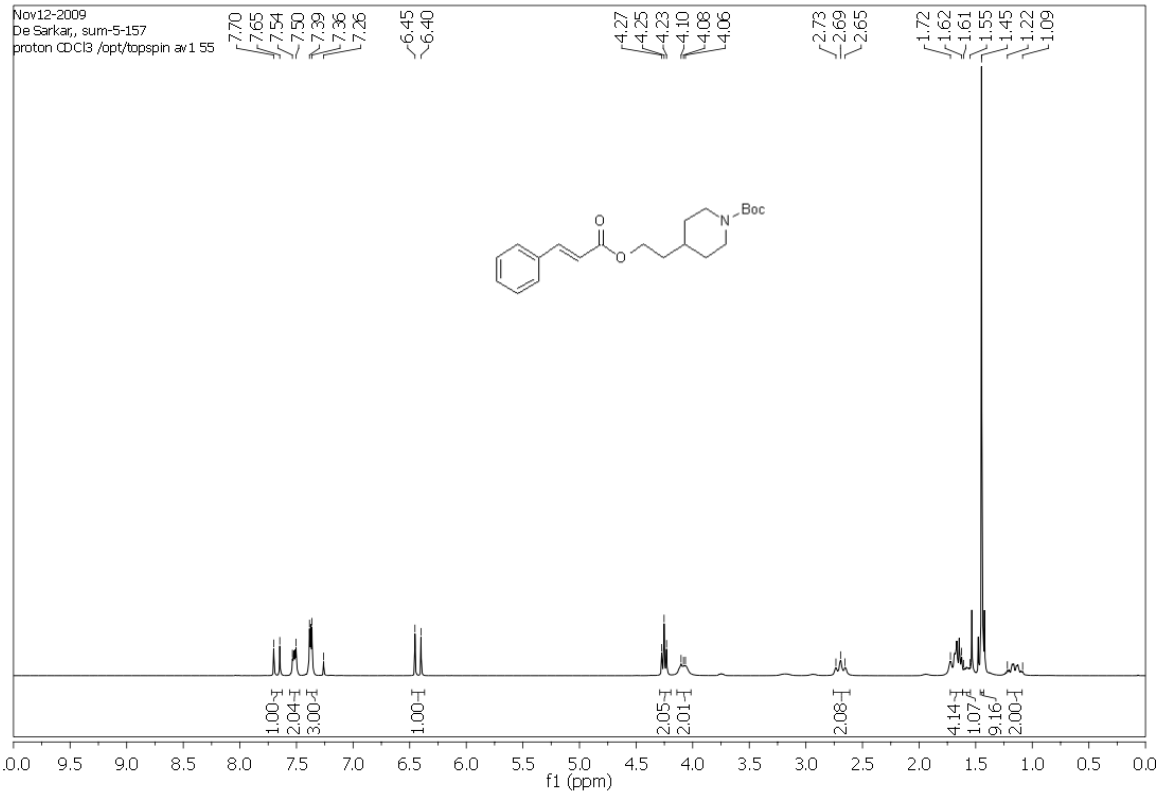

166.76
145.16
142.61
134.80
134.34
128.87
128.08
127.47
117.87
77.42
77.00
76.58
66.10
45.93
O
O
NH2
f1 (ppm)

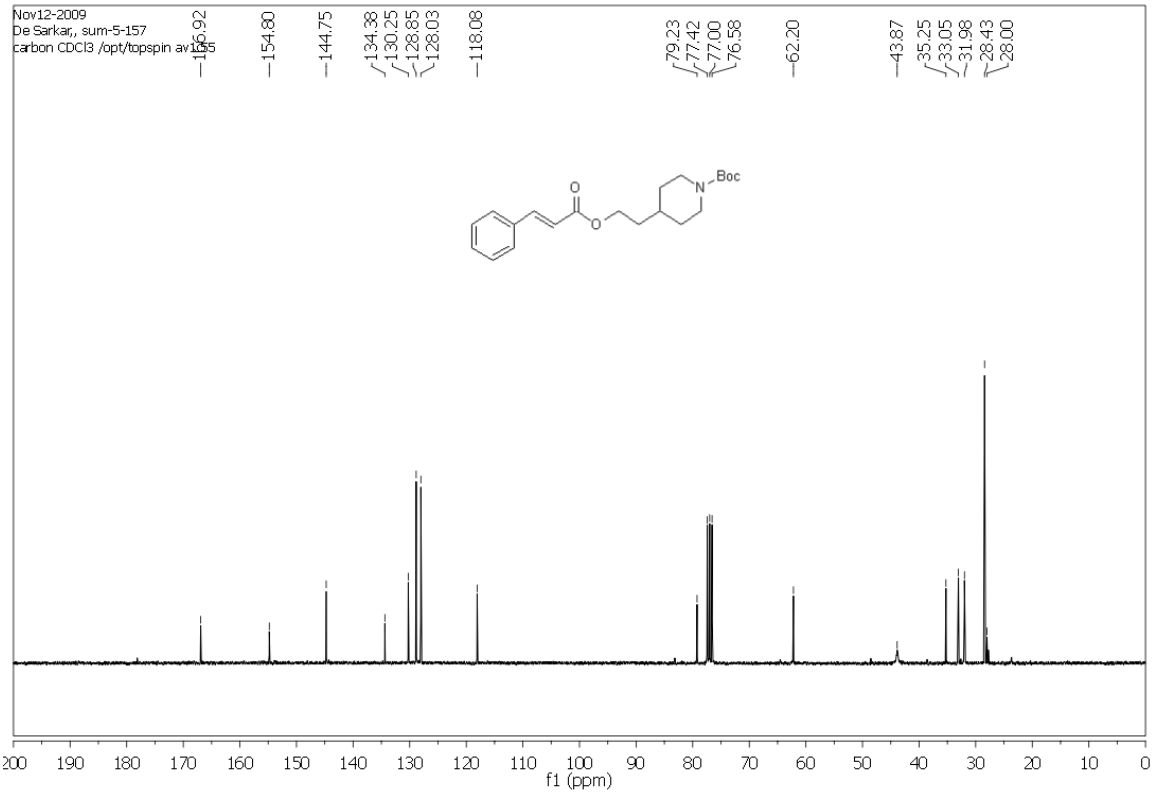

7.69
7.63
7.53
7.50
7.38
7.35
7.26
6.43
6.38
4.87
4.78
3.07
2.90
2.79
2.16
1.92
1.56
1.25
NH2
O
O
1.00
2.17
3.21
1.04
1.01
2.03
1.07
4.01
4.03
f1 (ppm)

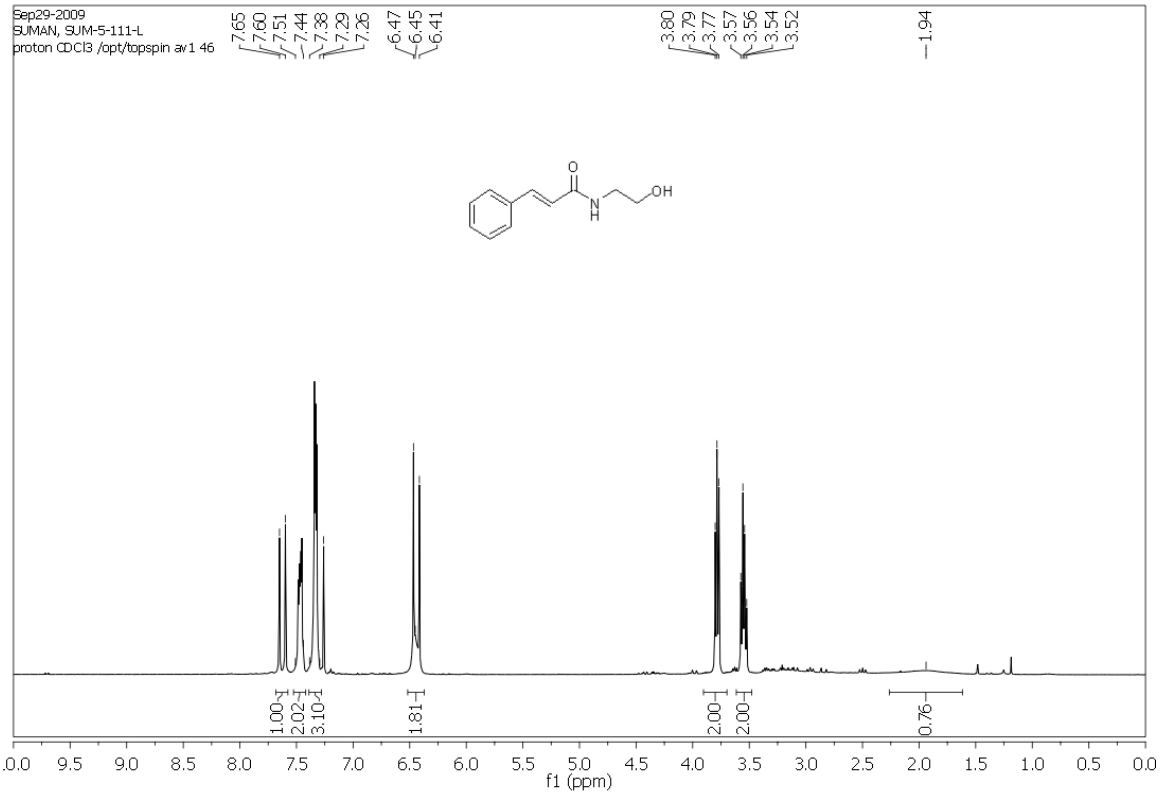

166.38
144.57
134.47
130.19
128.85
128.03
118.52
77.42
77.00
76.58
72.17
49.43
32.77
29.99
NH2
O
O
f1 (ppm)

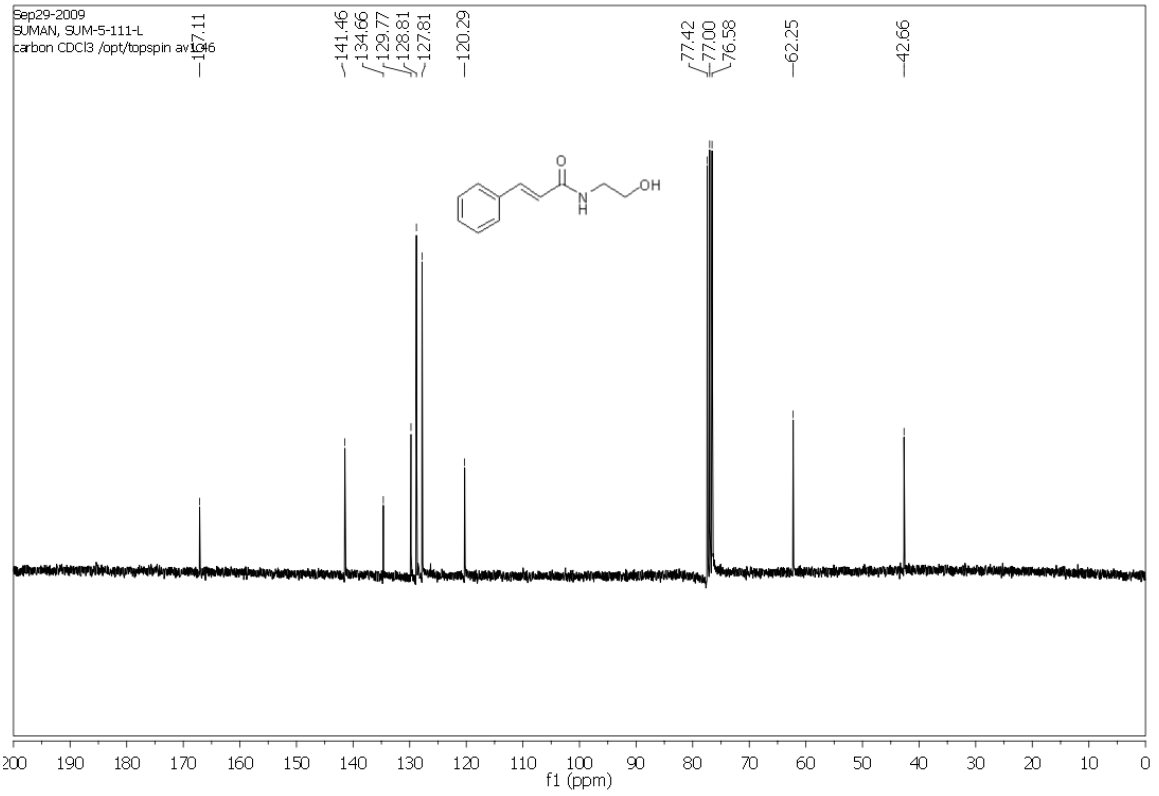

Nov12-2009
De Sarkar SUM 5_158
proton CDCl3 /opt/topspin av1 56
7.71
7.66
7.54
7.53
7.52
7.52
7.51
7.39
7.38
7.37
7.26
6.46
6.41
4.16
4.12
4.08
4.06
2.81
2.63
1.95
1.81
1.76
1.72
1.46
1.31
1.29
1.26
1.25
1.22
1.21
1.18
1.17
O
O
N
Boc
1.03
2.02
3.01
1.00
2.08
2.01
2.01
1.13
2.09
9.01
2.13
f1 (ppm)

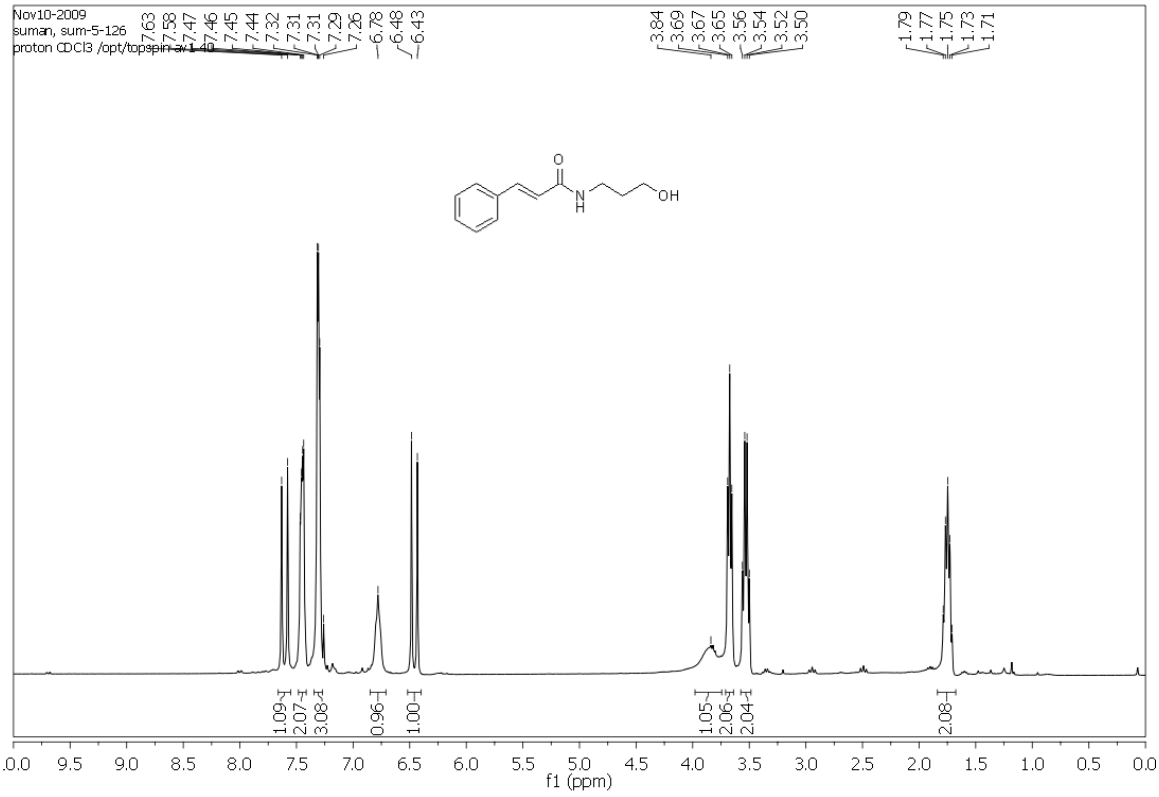

Nov12-2009
De Sarkar SUM 5_158
carbon CDCl3 /opt/topspin av1 56
166.88
154.80
144.89
134.37
130.30
128.87
128.05
117.94
79.39
77.42
77.00
76.58
68.46
43.49
35.74
28.75
28.44
28.02
O
O
N
Boc
f1 (ppm)

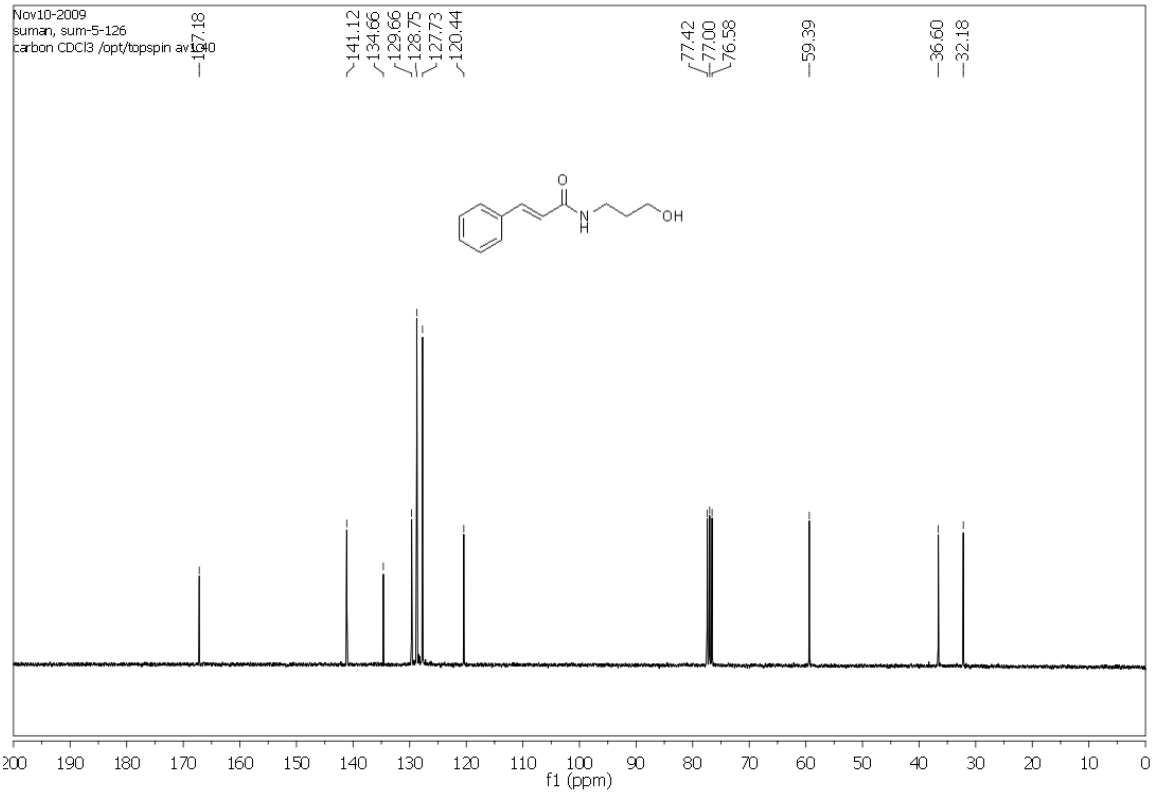

Nov12-2009
De Sarkar,, sum-5-157
proton CDCl3 /opt/topspin av1 55
7.70
7.65
7.54
7.50
7.39
7.36
7.26
6.45
6.40
4.27
4.25
4.23
4.10
4.08
4.06
2.73
2.69
2.65
1.72
1.62
1.61
1.55
1.45
1.22
1.09
Boc
1.00
2.04
3.00
1.00
2.05
2.01
2.08
4.14
1.07
9.16
2.00
f1 (ppm)

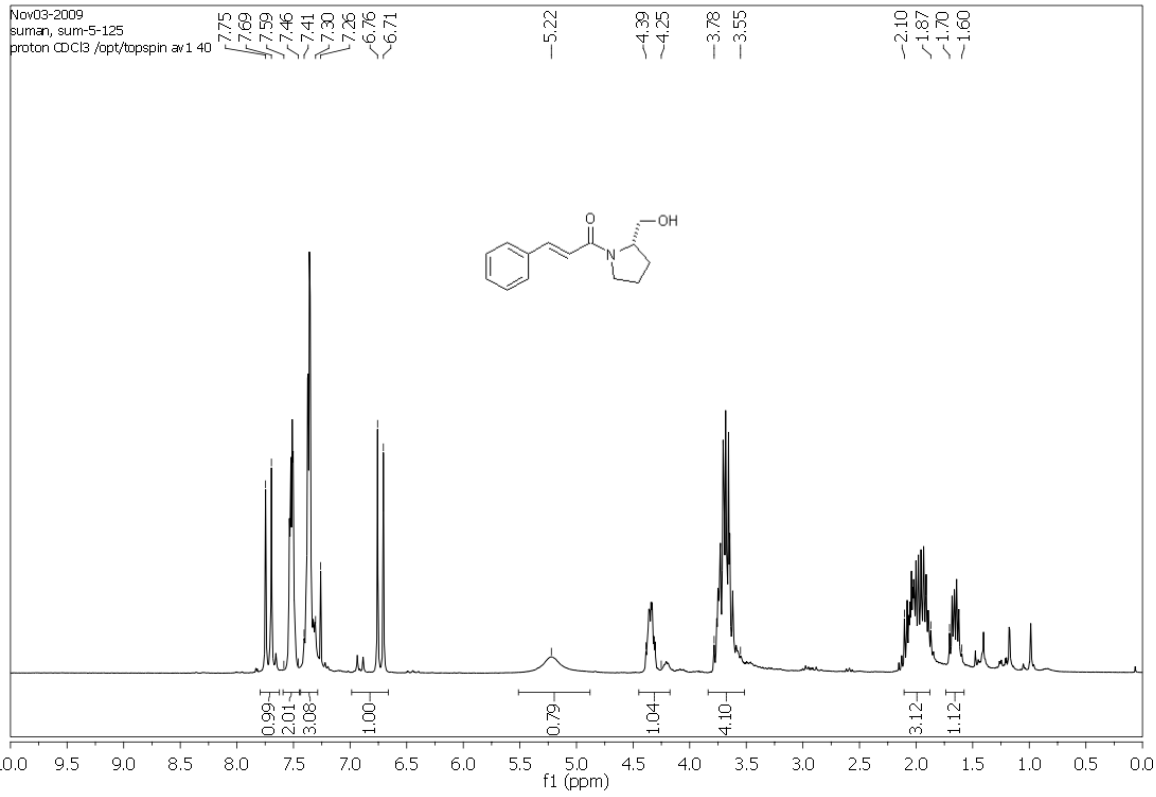

Nov12-2009
De Sarkar,, sum-5-157
carbon CDCl3 /opt/topspin av1
166.92
154.80
144.75
134.38
130.25
128.85
128.03
118.08
79.23
77.42
77.00
76.58
62.20
43.87
35.25
33.05
31.98
28.43
28.00
Boc
f1 (ppm)

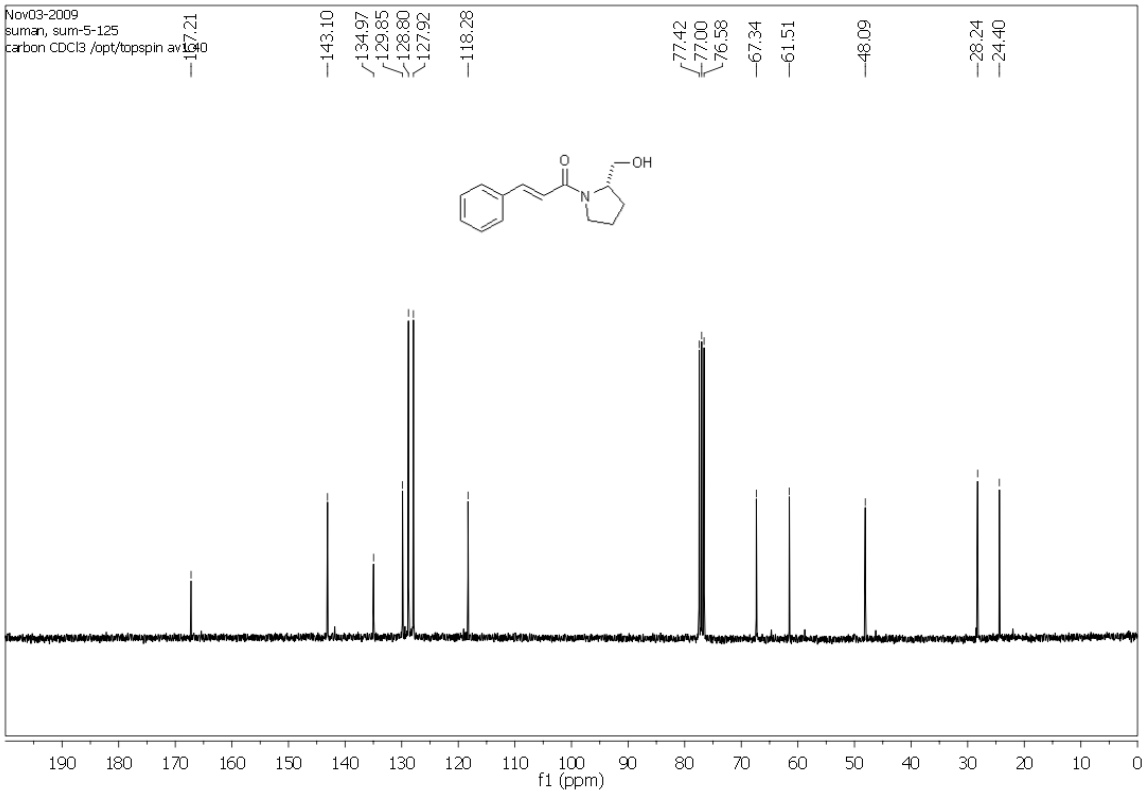

Sep29-2009
SUMAN, SUM-5-111-L
proton CDCl3 /opt/topspin av1 46
7.65
7.60
7.51
7.44
7.38
7.29
7.26
6.47
6.45
6.41
3.80
3.79
3.77
3.57
3.56
3.54
3.52
1.94
O
N
H
OH
1.00
2.02
3.10
1.81
2.00
2.00
0.76
f1 (ppm)


Sep29-2009
SUMAN, SUM-5-111-L
carbon CDCl3 /opt/topspin av1 46
167.11
141.46
134.66
129.77
128.81
127.81
120.29
77.42
77.00
76.58
62.25
42.66
O
N
H
OH
f1 (ppm)


Nov10-2009
suman, sum-5-126
proton CDCl3 /opt/topspin av1 40
7.63
7.58
7.47
7.46
7.45
7.44
7.32
7.31
7.31
7.29
7.26
6.78
6.48
6.43
3.84
3.69
3.67
3.65
3.56
3.54
3.52
3.50
1.79
1.77
1.75
1.73
1.71
O
N
H
OH
1.09
2.07
3.08
0.96
1.00
1.05
2.06
2.04
2.08
f1 (ppm)


Nov10-2009
suman, sum-5-126
carbon CDCl3 /opt/topspin av1 40
167.18
141.12
134.66
129.66
128.75
127.73
120.44
77.42
77.00
76.58
59.39
36.60
32.18
O
N
H
OH
f1 (ppm)


Nov03-2009
suman, sum-5-125
proton CDCl3 /opt/topspin av1 40
7.75
7.69
7.59
7.46
7.41
7.30
7.26
6.76
6.71
5.22
4.39
4.25
3.78
3.55
2.10
1.87
1.70
1.60
OH
0.99
2.01
3.08
1.00
0.79
1.04
4.10
3.12
1.12
f1 (ppm)


Nov03-2009
suman, sum-5-125
carbon CDCl3 /opt/topspin av1 40
167.21
143.10
134.97
129.85
128.80
127.92
118.28
77.42
77.00
76.58
67.34
61.51
48.09
28.24
24.40
OH
f1 (ppm)