Supporting Information

Development of Efficient Palladium Catalysts for Alkoxycarbonylation of Alkenes

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General information

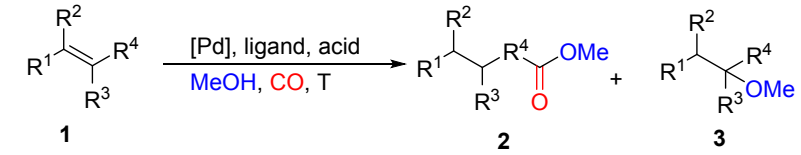
All commercial reagents were ordered from Alfa Aesar, Aldrich, TCI or Strem. Unless otherwise stated, commercial reagents were used without purification. Air- and moisture-sensitive syntheses were performed under argon atmosphere in heating gun vacuum dried glassware. Analytical data of literature known compounds were in agreement with reported data. NMR spectra were recorded on Bruker Avance 300 (300 MHz) NMR spectrometers. Multiplets were assigned as s (singlet), d (doublet), t (triplet), dd (doublet of doublet), m (multiplet) and br. s (broad singlet). All measurements were carried out at room temperature unless otherwise stated. Electron impact (EI) mass spectra were recorded on AMD 402 mass spectrometer (70 eV). High resolution mass spectra (HRMS) were recorded on Agilent 6210 Time-of-Flight LC/MS (Agilent) with electrospray ionization (ESI). The data are given as mass

units per charge (m/z) and intensities of signals are given in brackets. For GC analyses, HP 6890 chromatograph with a 29 m HP5 column was used.

Experimental sections

1. Palladium-catalysed alkoxycarbonylation of alkenes

1.1 General procedure

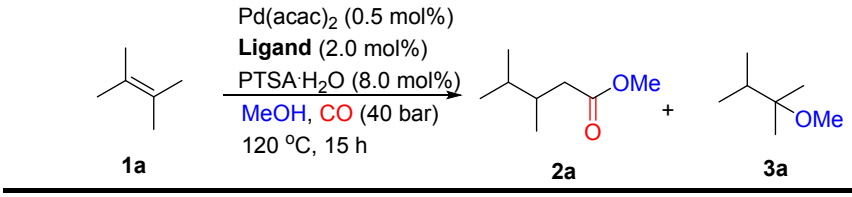


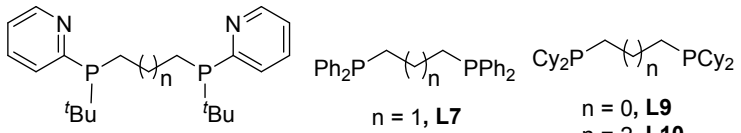
steric hindrance:$R^4 < R^1, R^2, R^3$

General procedure: A 4 mL screw-cap vial was charged with palladium salts, ligand, acid and an oven-dried stirring bar. The vial was closed by PTFE/white rubber septum (Wheaton 13 mm Septa) and phenolic cap and connected with atmosphere with a needle. Then, the vial was evacuated under vacuum and recharged with argon for three times. After MeOH and **1** were injected by syringe; the vial was fixed in an alloy plate and put into Paar 4560 series autoclave (300 mL) under argon atmosphere. At room temperature, the autoclave was flushed with carbon monoxide for three times and carbon monoxide was charged. The reaction was heated at the specified temperature. Afterwards, the autoclave was cooled to room temperature and the pressure was carefully released. Isooctane was added into the reaction as internal standard. A sample of the mixture was analysed by gas chromatography. Pure products were obtained by column chromatography on silica gel.

1.2 Optimisation of reaction conditions

Table *S1*. The effect of ligand [a]





n = 1, **L3**;n = 2, **L4**
n = 3, **L5**;n = 4, **L6**

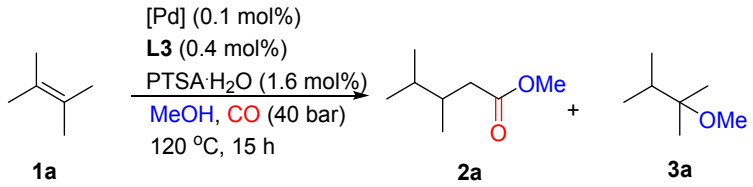
n = 1, **L7**
n = 2, **L8**

n = 0, **L9**
n = 2, **L10**

Entry	Ligand	Conv. (%)	GC yield of **2** (%)	*n*/*i*	GC yield of **3** (%)
1	**L3**	>99	99	>99/1	0
2	**L4**	92	84	>99/1	7
3	**L5**	49	4	>99/1	41
4	**L6**	52	2	>99/1	44
5	**L7**	48	2	>99/1	43
6	**L8**	63	22	>99/1	31
7	**L9**	54	<1	-/-	45
8	**L10**	48	0	-/-	45

[a]. Standard reaction conditions: **1a** (1.0 mmol), $Pd(acac)_2$ (0.005 mmol, 0.5 mol%), ligand (0.02 mmol, 2.0 mol%), PTSA·H_2O (16.0 mg, 8.0 mol%), MeOH (2.0 mL), CO (40 atm), 120 °C, 15 h; the conversion, GC yield of **2a** and **3a** were determined by GC analysis with isooctane as the internal standard

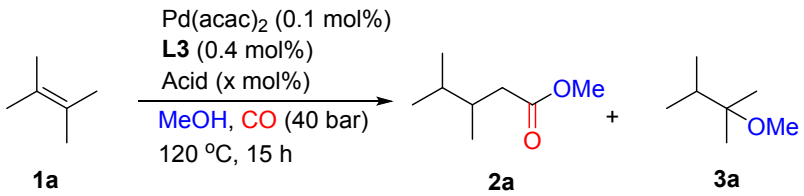
Table *S2*. The effect of palladium salts [a]



Entry	[Pd]	Conv.(%)	GC Yield of **2** (%)	*n*/*i*	GC yield of **3** (%)
1	$Pd(acac)_2$ (0.1 mol%)	>99	99	>99/1	<1
2	$Pd(OAc)_2$ (0.1 mol%)	98	93	>99/1	1
3	$PdCl_2$ (0.1 mol%)	>99	99	>99/1	<1
4	$Pd_2(dba)_3$ (0.05mol%)	97	92	>99/1	2
5	$Pd(TFA)_2$(0.1 mol%)	98	93	>99/1	1
6	$Pd(MeCN)_2Cl_2$(0.1 mol%)	98	97	>99/1	1

[a]. Standard reaction conditions: **1a** (4.0 mmol), palladium salt (0.004 mmol, 0.1 mol%), **L3** (0.016 mmol, 0.4 mol%), PTSA·H_2O (12.8 mg, 1.6 mol%), MeOH (2.0 mL), CO (40 atm), 120 °C, 15 h; the conversion, GC yield of **2a** and **3a** were determined by GC analysis with isooctane as the internal standard.

Table *S3*. The effect of acid [a]



Entry	Acid (x)	Conv.(%)	GC Yield of **2** (%)	*n*/*i*	GC yield of **3** (%)
1	AcOH(1.6)	0	0	-/-	0
2	CF_3SO_3H (1.6)	>99	96	>99/1	<1
3	H_2SO_4 (0.8)	87	72	>99/1	9
4	PTSA (1.6)	>99	99	>99/1	<1
5	PTSA (0.8)	91	87	>99/1	4
6	PTSA (3.2)	>99	99	>99/1	<1

[a]. Standard reaction conditions: **1a** (4.0 mmol), $Pd(acac)_2$ (0.004 mmol, 0.1 mol%), **L3** (0.016mmol, 0.4mol%), acid (0.064 mmol, 1.6mol%), MeOH (2.0 mL), CO (40 atm), 120 °C, 15 h; the conversion, GC yield of **2a** and **3a** were determined by GC analysis with isooctane as

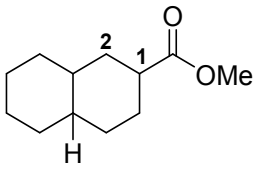
the internal standard.

1.3 Methoxycarbonylation of ethylene

A 100 mL steel autoclave was charged with $Pd(acac)_2$ (6.52 mg, 0.04 mol%), **L2-L6** (0.16 mol %), and PTSA·H_2O (61.1 mg, 0.6 mol%) under argon atmosphere. Methanol (20 mL) was injected into the autoclave via syringe. Then ethylene (1.5 g, 53.6 mmol) was introduced into the autoclave (mass control by balance). CO (30 bar) was introduced into the autoclave at 23 ^oC and the reaction was carried out for 20 h. The autoclave was depressurised slowly. The content was transferred to a 50 mL Schlenk flask and isooctane (internal standard, 3.0 mL) was added into the solution. The yield was measured by GC analysis.

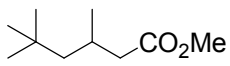
1.4 Characterization of the products 2b-2z

methyl decahydronaphthalene-2-carboxylate (2b) [1]



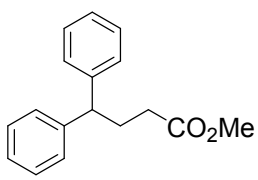
Colorless oil, 92% yield, **1/2** = 89/11. ^1H NMR (300 MHz, $CDCl_3$) δ 3.63-3.62 (m, 3H), 2.43-2.25 (m, 1H), 1.77-1.18 (m, 13H), 0.95-0.89 (m, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 176.32, 51.32, 43.41, 42.53, 42.34, 36.19, 33.68, 33.59, 32.95, 28.97, 26.47 ppm.

methyl 3,5,5-trimethylhexanoate (2c)



Colorless oil, 95% yield, >99/1 *n*/*iso*, ^1H NMR (300 MHz, $CDCl_3$) δ 3.66 (s, 3H), 2.32 (dd, J = 15.0, 6.0 Hz, 1H), 2.18-2.01 (m, 2H), 1.28-1.22 (m, 2H), 1.12 (d, J = 6.0 Hz, 3H), 0.91 (s, 9H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 173.54, 51.25, 50.52, 43.81, 31.03, 29.90, 26.99, 22.69 ppm. HRMS (ESI): Calcd. for $C_{10}H_{21}O_2$ $[M+H]^+$: 173,15361, Found: 173,15381.

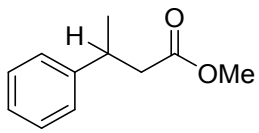
methyl 4,4-diphenylbutanoate (2d) [2]



White solid, 90% yield, *n*/*iso* = 97/3, ^1H NMR (300 MHz, $CDCl_3$) δ 7.43-7.29 (m, 8H), 7.28-7.25 (m, 2H), 4.05 (t, J = 6.0 Hz, 1H), 3.72 (s, 3H), 2.56-2.48 (m, 2H), 2.44-2.37 (m, 2H) ppm;

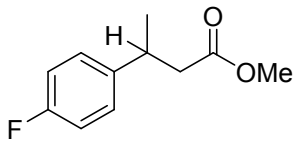
^{13}C NMR (75 MHz, $CDCl_3$) δ 173.83, 144.24, 128.65, 127.96, 126.48, 51.57, 50.61, 32.64, 30.71 ppm.

methyl 3-phenylbutanoate (2e) [1]



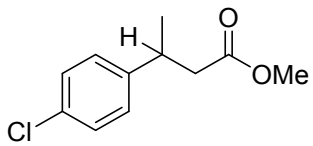
Colorless oil, 96% yield, >99/1 *n*/*iso*. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.23-7.07 (m, 5H), 3.51 (s, 3H), 3.25-3.13 (m, 1H), 2.57-2.41 (m, 2H), 1.21 (d, J = 6.0 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.80, 145.71, 128.53, 126.72, 126.43, 51.48, 42.74, 36.46, 21.80 ppm.

methyl 3-(4-fluorophenyl)butanoate (2f) [1]



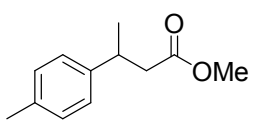
Colorless oil, 96% yield, >99/1 *n*/*iso*. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.10-7.05 (m, 2H), 6.90-6.82 (m, 2H), 3.50 (s, 3H), 3.21-3.11 (m, 1H), 2.52-2.38 (m, 2H), 1.18 (d, J = 9.0 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.52, 161.44 (d, J = 242.2 Hz, 1C), 141.33 (d, J = 3.0 Hz, 1C), 128.12 (d, J = 8.3 Hz, 1C), 115.19 (d, J = 21.0 Hz, 1C), 51.38, 42.77, 35.75, 21.87 ppm; ^{19}F NMR (282 MHz, $CDCl_3$) δ -116.85 ppm.

methyl 3-(4-chlorophenyl)butanoate (2g) [1]



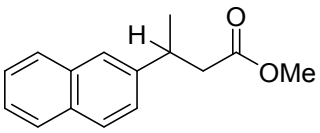
Colorless oil, 99% yield, >99/1 *n*/*iso*. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.16-7.12 (m, 2H), 7.06-7.03 (m, 2H), 3.50 (s, 3H), 3.19-3.12 (m, 1H), 2.52-2.38 (m, 2H), 1.17 (d, J = 6.0 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.40, 144.15, 132.02, 128.60, 128.12, 51.45, 42.51, 35.86, 21.75 ppm.

methyl 3-(p-tolyl)butanoate (2h) [3]



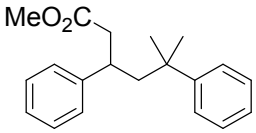
Colorless oil, 98% yield, >99/1 *n*/*iso*. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.18 (s, 4H), 3.68 (s, 3H), 3.36-3.29 (m, 1H), 2.72-2.55 (m, 2H), 2.38 (s, 3H), 1.35 (d, J = 6.0 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.86, 142.76, 135.86, 129.22, 126.60, 51.43, 42.58, 36.07, 21.89, 21.00 ppm.

methyl 3-(naphthalen-2-yl)butanoate (2i) [1]



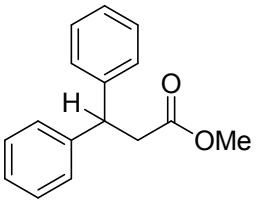
Colorless oil, 98% yield, >99/1 *n*/*iso*. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.93-7.88 (m, 3H), 7.78 (s, 1H), 7.60-7.47 (m, 3H), 3.72 (s, 3H), 3.65-3.54 (m, 1H), 2.90-2.71 (m, 2H), 1.52 (d, J = 9.0 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.79, 143.29, 133.76, 132.52, 128.33, 127.82, 127.74, 126.11, 125.57, 125.53, 125.06, 51.54, 42.72, 36.67, 21.91 ppm.

methyl 5-methyl-3,5-diphenylhexanoate (2j)



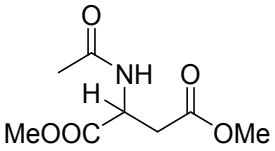
Colorless oil, 95% yield, *n*/*iso* = 97/3. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.16-7.02 (m, 8H), 6.97-6.89 (m, 2H), 3.32 (s, 3H), 2.90-2.84 (m, 1H), 2.26 (d, J = 6.0 Hz, 2H), 1.99-1.89 (m, 2H), 1.12 (s, 3H), 1.04 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.41, 148.78, 145.42, 128.38, 128.13, 127.65, 126.27, 126.04, 125.70, 51.33, 50.27, 43.44, 39.39, 38.32, 31.03, 28.13 ppm.

methyl 3,3-diphenylpropanoate (2k) [1]



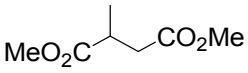
Colorless oil, 99% yield, >99/1 *n*/*iso*. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42-7.26 (m, 10H), 4.71 (t, J = 6.0 Hz, 1H), 3.66 (s, 3H), 3.19 (d, J = 6.0 Hz, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.29, 143.61, 128.69, 127.77, 126.67, 51.72, 47.09, 40.67 ppm.

dimethyl acetylaspartate (2l) [1]



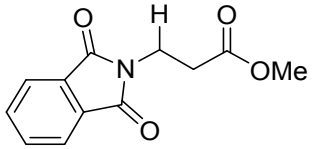
White solid, 95% yield, >99/1 *n*/*iso*. ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.81-6.79 (m, 1H), 4.83-4.77 (m, 1H), 3.68 (s, 3H), 3.62 (s, 3H), 2.97-2.75 (m, 2H), 1.96 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.38, 171.20, 169.95, 52.61, 51.88, 48.45, 35.02, 22.84 ppm.

dimethyl 2-methylsuccinate (2m) [4]



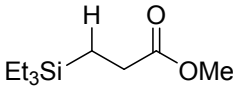
Colorless oil, 95% yield, >99/1 *n*/*iso*. ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.65 (s, 3H), 3.64 (s, 3H), 2.89-2.85 (m, 1H), 2.70 (dd, *J* = 12.0, 6.0 Hz, 1H), 2.37 (dd, *J* = 12.0, 6.0 Hz, 1H), 1.18 (d, *J* = 6.0 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 175.59, 172.17, 51.82, 51.60, 37.32, 35.64, 16.91 ppm.

methyl 3-(1,3-dioxoisoindolin-2-yl)propanoate (2n) [1]



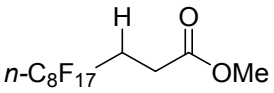
White solid, 94% yield, *n*/*iso* = 94/6. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.74-7.70 (m, 2H), 7.65-7.60 (m, 2H), 3.88 (t, *J* = 9.0 Hz, 2H), 3.58 (s, 3H), 2.63 (t, *J* = 9.0 Hz, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.11, 167.80, 133.96, 131.90, 123.19, 51.79, 33.66, 32.65 ppm.

methyl 3-(triethylsilyl)propanoate (2o) [1]



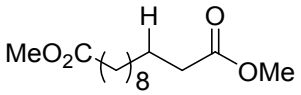
Colorless oil, 79% yield, *n*/*iso* = 94/6.^{1}H NMR (300 MHz, $CDCl_3$) δ 3.59 (s, 3H), 2.24-2.18 (m, 2H), 0.89-0.77 (m, 11H), 0.49-0.41 (m, 6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 175.53, 51.48, 28.57, 7.24, 6.54, 2.99 ppm.

methyl 4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-heptadecafluoroundecanoate (2p) [1]



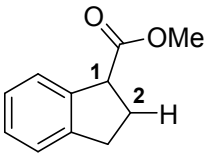
Colorless oil, 99% yield, *n*/*iso* = 99/1. ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.63 (s, 3H), 2.57-2.52 (m, 2H), 2.41-2.35 (m, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.39, 122.78-110.14 (broad, 8C), 51.80, 26.41 (t, *J* = 21.8 Hz, 1C), 25.02 (t, *J* = 3.8 Hz, 1C).

dimethyl dodecanedioate, dimethyl 2-methylundecanedioate (2q) [1]



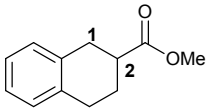
Colorless oil, 93% yield, *n*/*iso* = 55/45. ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.59-3.58 (m, 6H), 2.22 (t, *J* = 9.0 Hz, 4H), 1.56-1.49 (m, 4H), 1.21 (s, 12H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ = 174.01, 51.20, 33.91, 29.23, 29.09, 29.00, 24.81 ppm.

methyl 2,3-dihydro-1H-indene-1-carboxylate (2r) [1]



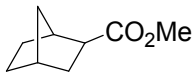
Colorless oil, 93% yield, **1**/**2** = 70/30. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.28-7.02 (m, 4H), 3.97-3.92 (m, 0.62H for minor isomer), 3.61-3.60 (m, 3H), 3.20-2.82 (m, 3H), 2.39-2.17 (m, 1.35 H for major isomer) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 175.73, 174.36, 144.13, 141.59, 140.74, 127.60, 126.66, 126.48, 124.94, 124.84, 124.73, 124.37, 52.02, 51.93, 50.15, 43.53, 36.25, 31.82, 28.82 ppm.

methyl 1,2,3,4-tetrahydronaphthalene-2-carboxylate (2s) [5]



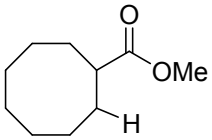
White solid, 95% yield, **1**/**2** = 6/94. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.23-7.14 (m, 4H), 3.81 (s, 3H), 3.10 (d, *J* = 6.0 Hz, 2H), 2.94-2.80 (m, 3H), 2.34-2.25 (m, 1H), 2.01-1.88 (m, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 175.86, 135.71, 134.92, 129.13, 128.91, 126.00, 125.89, 51.80, 40.00, 31.73, 28.61, 25.99 ppm.

methyl bicyclo[2.2.1]heptane-2-carboxylate (2t)[6]



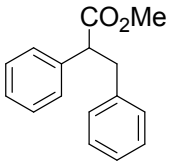
Colorless oil, 91% yield, *n*/*iso* = 94/6, ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.65 (s, 3H), 2.49-2.47 (m, 1H), 2.32-2.27 (m, 2H), 1.83-1.80 (m, 1H), 1.55-1.42 (m, 4H), 1.23-1.13 (m, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 176.50, 51.53, 46.32, 40.87, 36.43, 35.98, 34.13, 29.44, 28.60 ppm. DEPT 135 NMR (75 MHz, $CDCl_3$) δ 51.53 (-), 46.32 (-), 40.87 (-), 36.43 (+), 35.98 (-), 34.13 (+), 29.44 (+), 28.60 (+) (CH and CH_3: -, positive; CH_2: +, negative).

methyl cyclooctanecarboxylate (2u) [1]



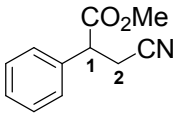
Colorless oil, 98% yield, ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.64 (s, 3H), 2.55-2.47 (m, 1H), 1.92-1.83 (m, 2H), 1.74-1.47 (m, 12H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 177.72, 51.45, 43.45, 28.70, 26.74, 26.09, 25.21 ppm.

methyl 2,3-diphenylpropanoate (2v) [7]



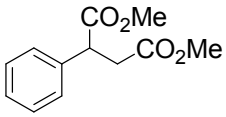
Colorless oil, 94% yield, ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47-7.24 (m, 10H), 4.02 (dd, *J* = 9.0, 6.0 Hz, 1H), 3.68 (s, 3H), 3.58 (dd, *J* = 12.0, 9.0 Hz, 1H), 3.17 (dd, *J* = 12.0, 6.0 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 173.89, 139.17, 138.79, 129.06, 128.78, 128.47, 128.08, 127.52, 126.52, 53.74, 52.04, 39.97 ppm.

methyl 3-cyano-2-phenylpropanoate (2w) [8]



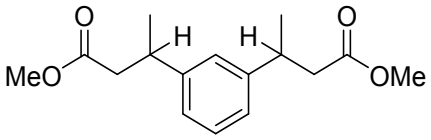
Colorless oil, 61% yield, **1**/**2** = 97/3, ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43-7.29 (m, 5H), 3.97 (t, *J* = 6.0 Hz, 1H), 3.74 (s, 3H), 3.05 (dd, *J* = 15.0, 6.0 Hz, 1H), 2.83 (dd, *J* = 15.0, 6.0 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.51, 135.83, 129.26, 128.56, 127.58, 117.60, 52.80, 47.58, 21.72 ppm.

dimethyl 2-phenylsuccinate (2x) [9]



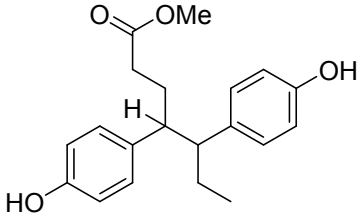
White solid, ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35-7.23 (m, 5H), 4.10 (dd, *J* = 9.0, 6.0 Hz, 1H), 3.65 (s, 3H), 3.22 (dd, *J* = 18.0, 9.0 Hz, 1H), 2.67 (dd, *J* = 18.0, 6.0 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 173.35, 171.88, 137.72, 128.86, 127.71, 127.65, 52.24, 51.76, 47.08, 37.60 ppm.

dimethyl 3,3'-(1,3-phenylene)dibutyrate (2y) [1]



Colorless oil, 99% yield, >99/1 *n*/*iso*. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.22-7.17 (m, 1H), 7.07-7.02 (m, 3H), 3.58 (s, 6H), 3.26-3.24 (m, 2H), 2.58-2.50 (m, 4H), 1.28 (d, *J* = 9.0 Hz, 6H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.60, 145.87, 128.61, 125.31, 124.63, 51.30, 42.70, 36.42, 21.67 ppm.

methyl 4,5-bis(4-hydroxyphenyl)heptanoate (2z) [1]



White solid, 75% yield, n/iso = 98/2, *dr* = 68/32. ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.93-6.89 (m, 2H), 6.72-6.68 (m, 2H), 6.62-6.53 (m, 4H), 6.32 (s, br, 2H, OH), 3.52 (s, 1H, OMe), 3.43 (s, 2H, OMe), 2.67-2.36 (m, 2H), 2.07-1.18 (m, 6H), 0.64 (t, *J* = 6.0 Hz, 1H, CH_3), 0.44 (t, *J* = 6.0 Hz, 2H, CH_3) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 175.53, 175.50, 154.16, 153.94, 153.80, 153.54, 135.59, 135.09, 134.18, 133.32, 130.02, 129.97, 129.24, 115.35, 115.20, 114.65, 114.49, 53.47, 52.64, 51.81, 51.73, 50.85, 49.92, 32.55, 32.45, 29.51, 28.61, 27.24, 25.99, 12.27, 12.12 ppm.

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Beller, *Nat. Commun.* 2017, **8**, 14117-14123;

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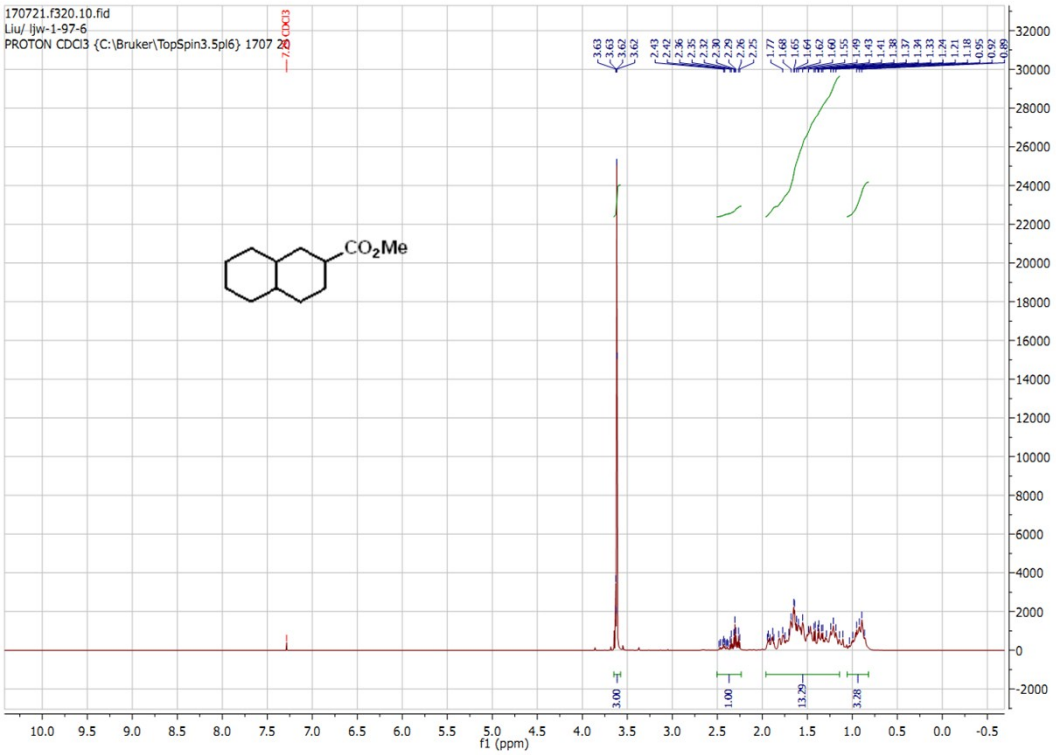
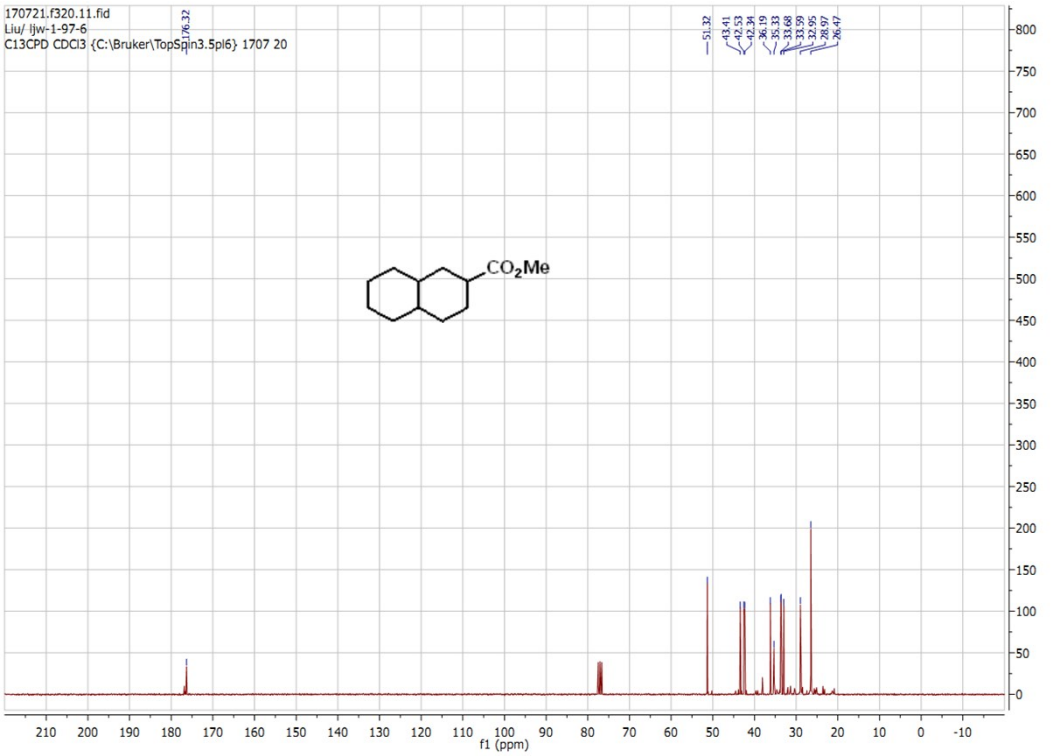
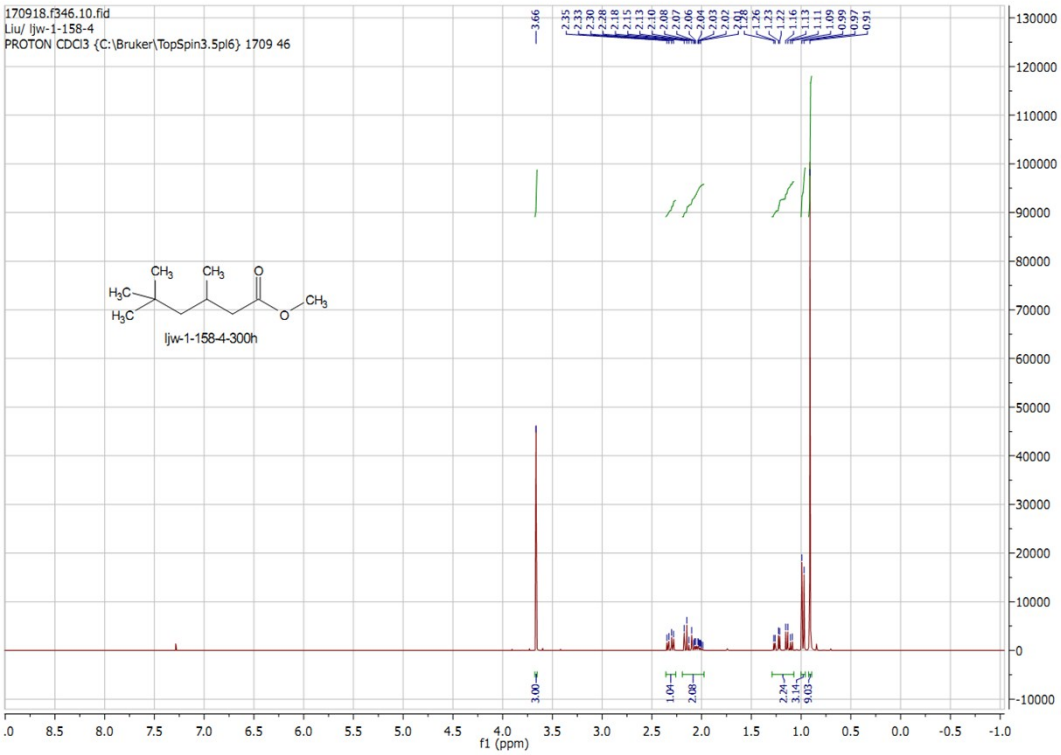
NMR spectra:

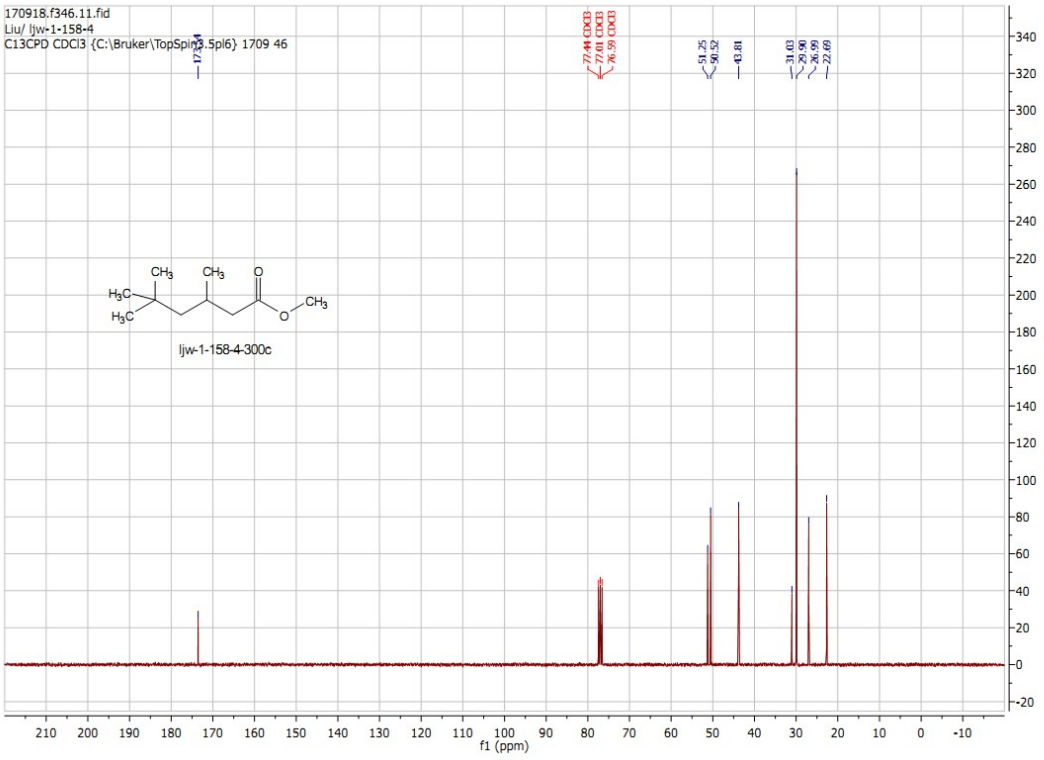
NMR spectra of **2b:**



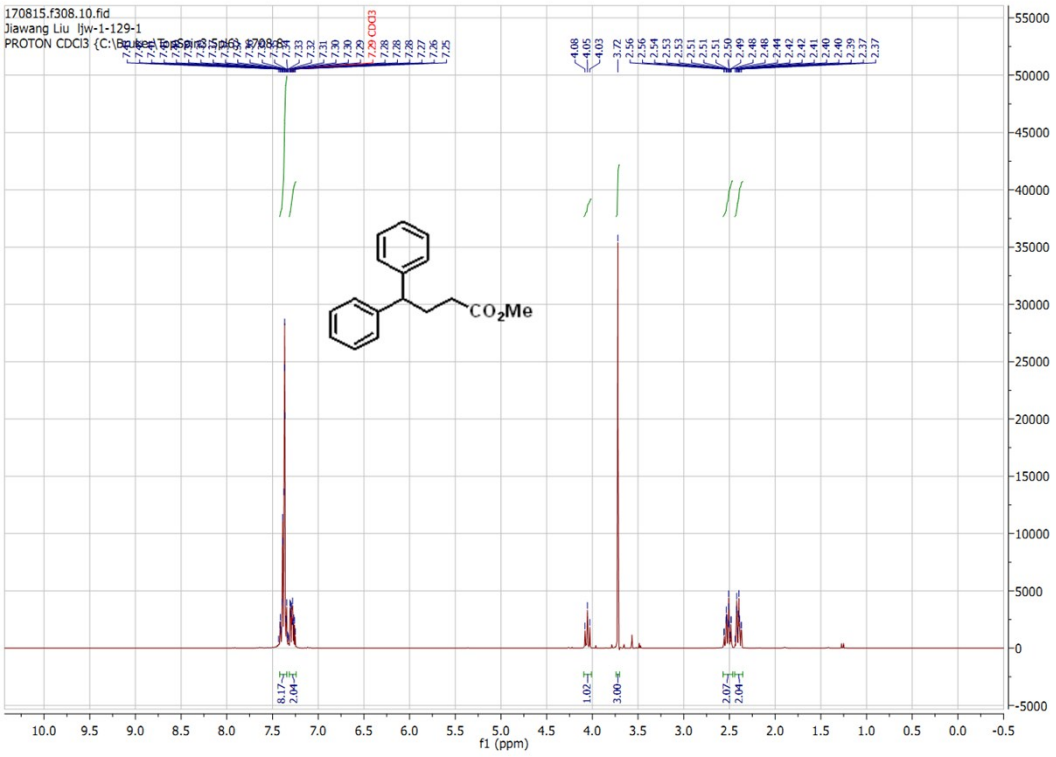


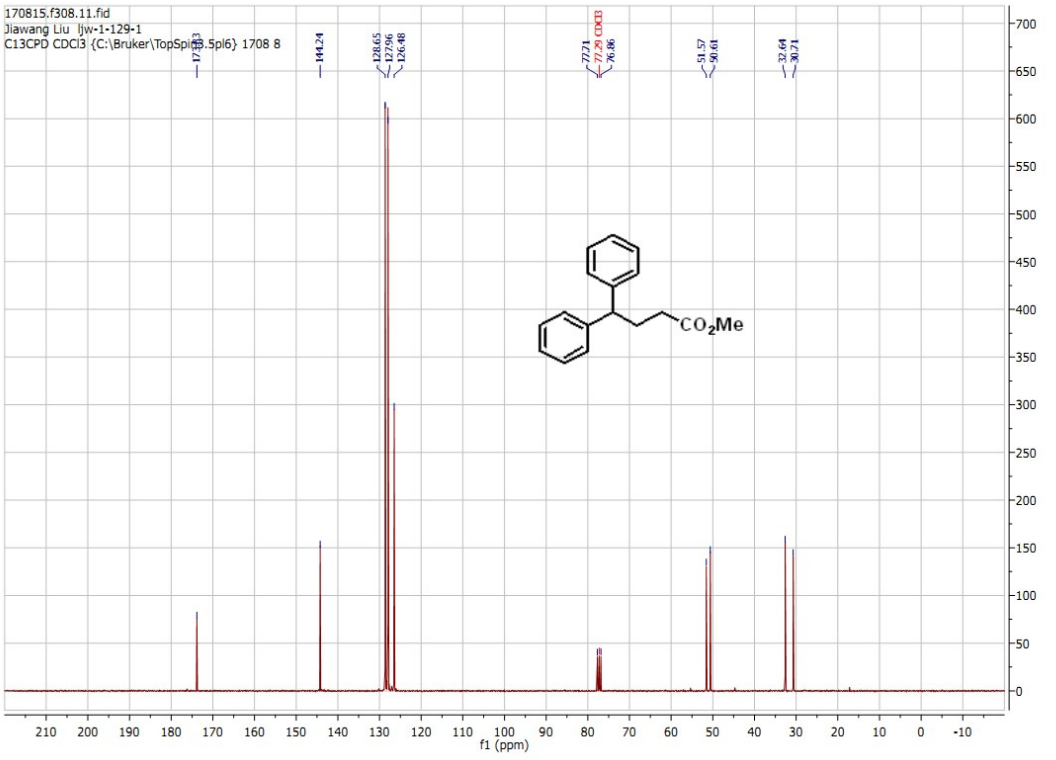
NMR spectra of **2c:**



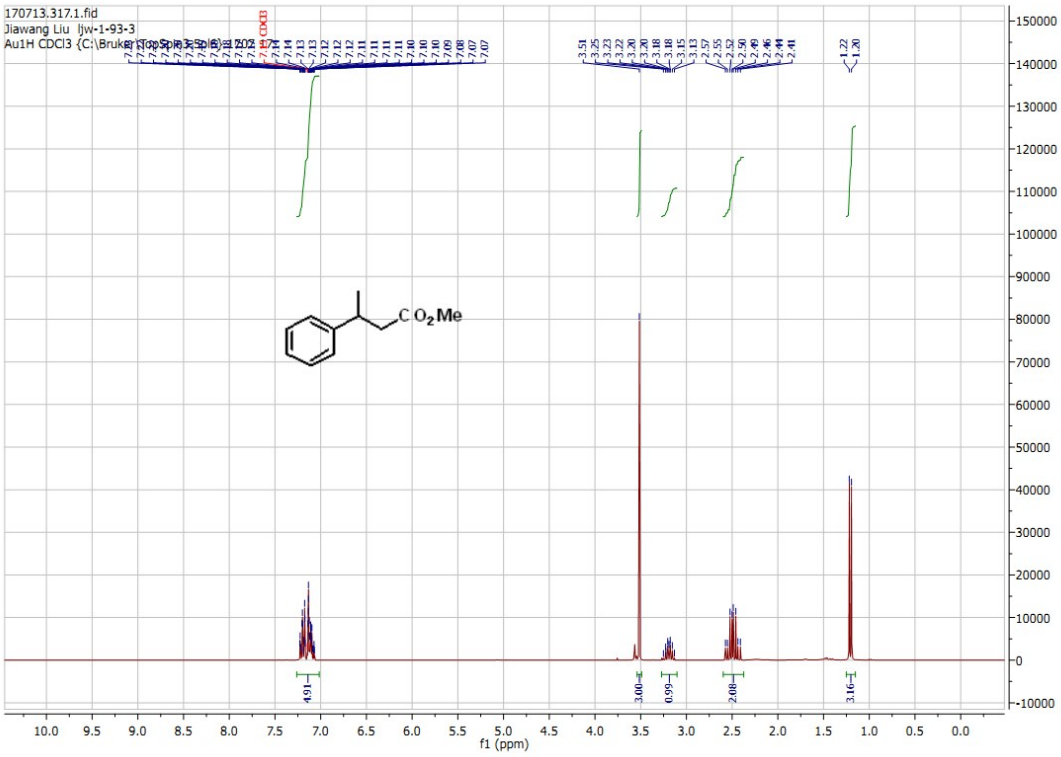


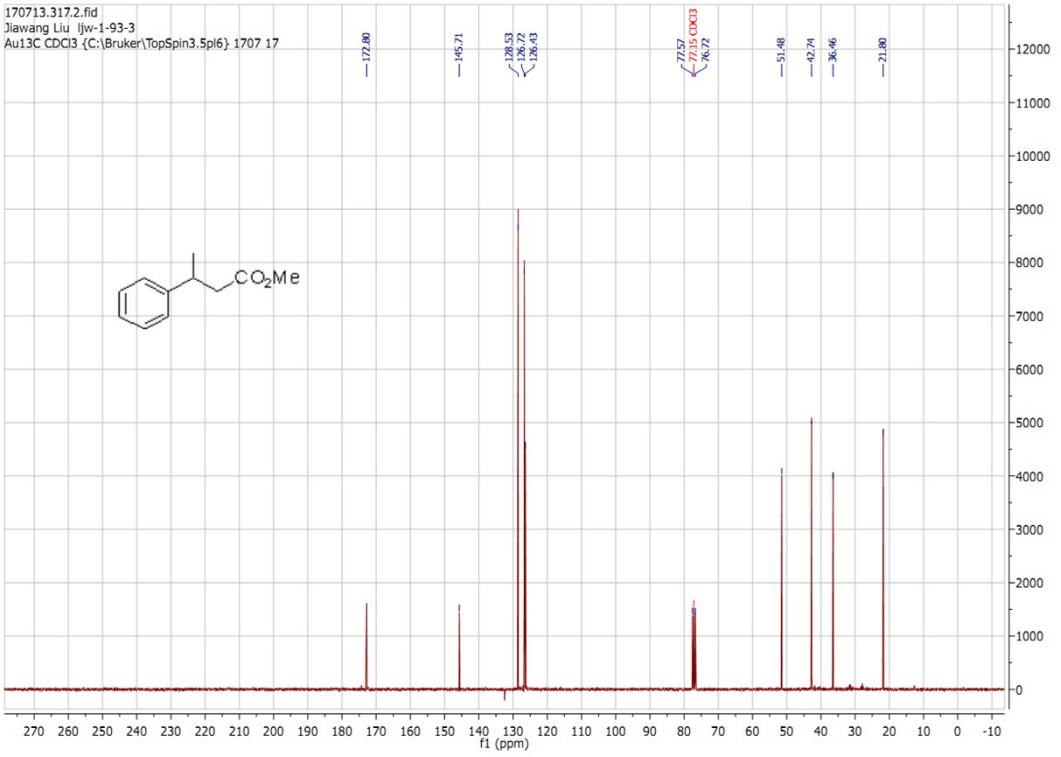
NMR spectra of **2d:**



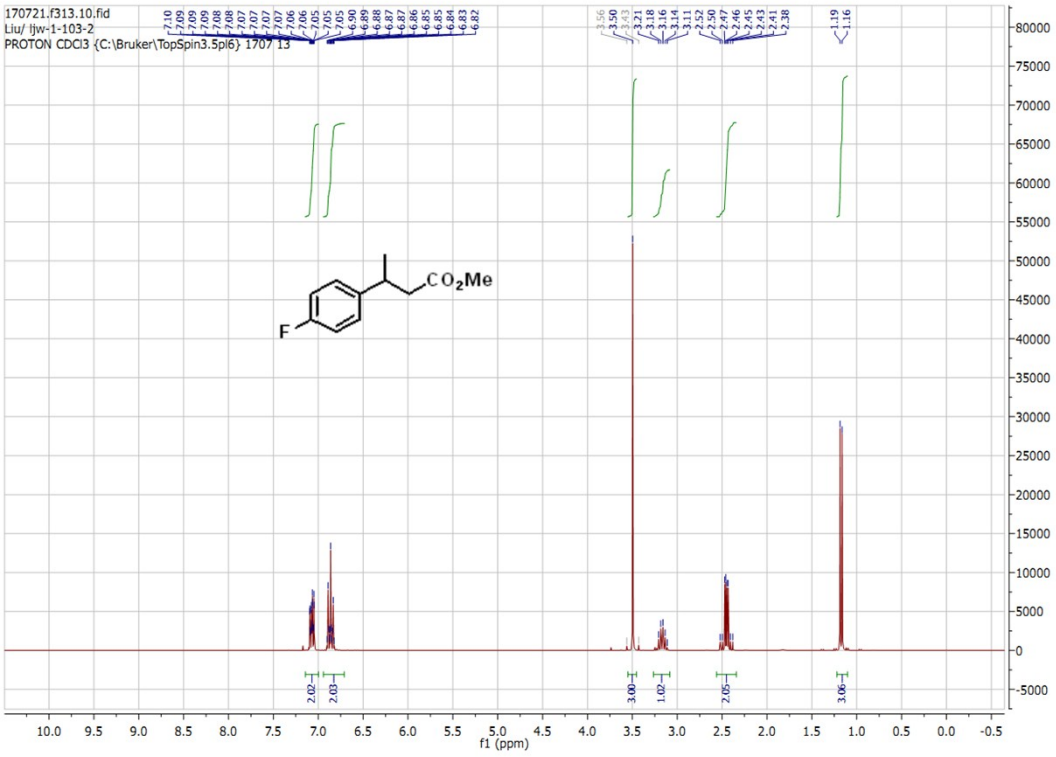


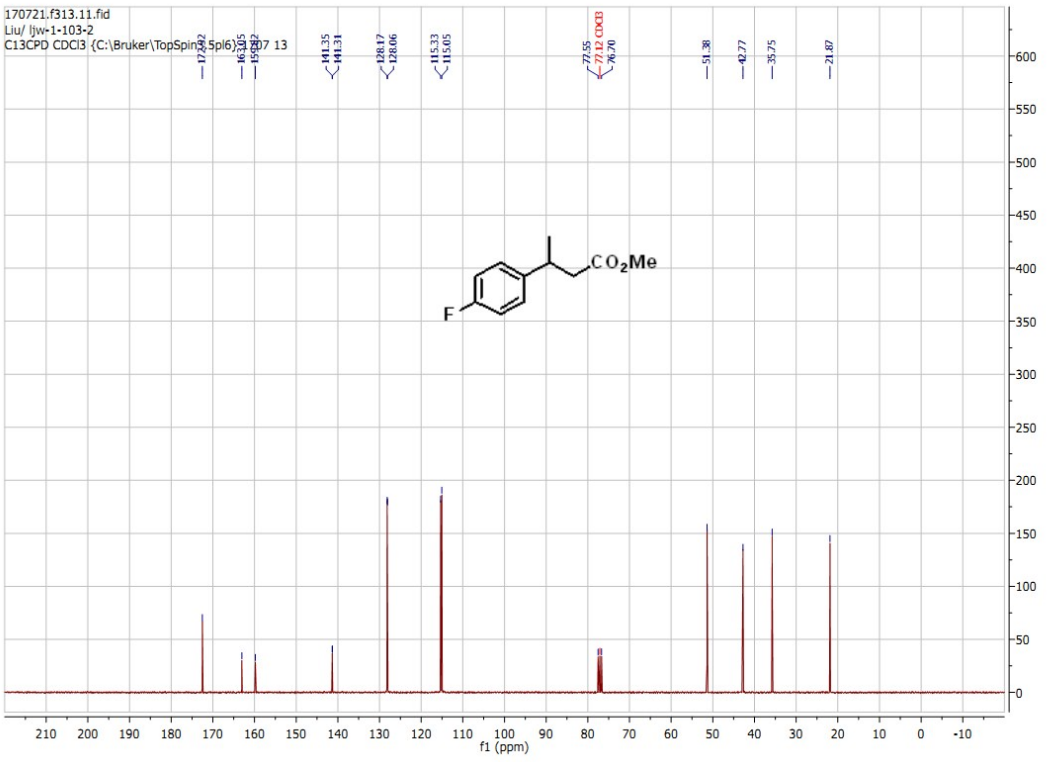
NMR spectra of **2e:**





NMR spectra of **2f:**


170721.f313.10.fid
Liu/ ljw-1-103-2
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 13
CO2Me
F
f1 (ppm)


170721.f313.11.fid
Liu/ ljw-1-103-2
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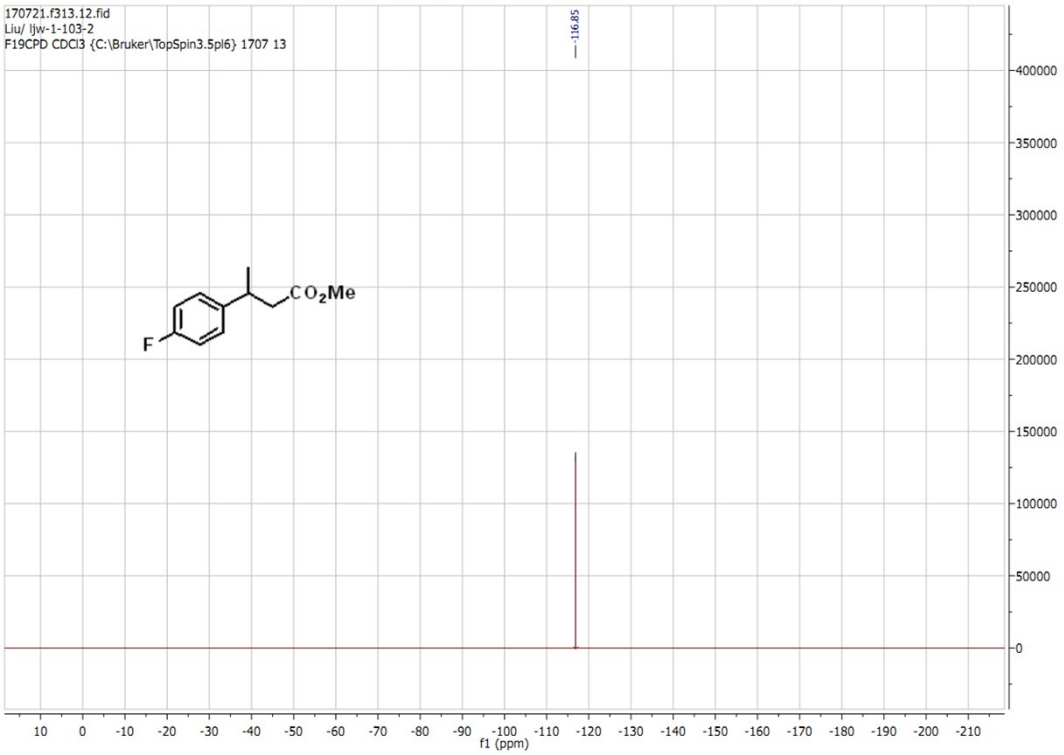
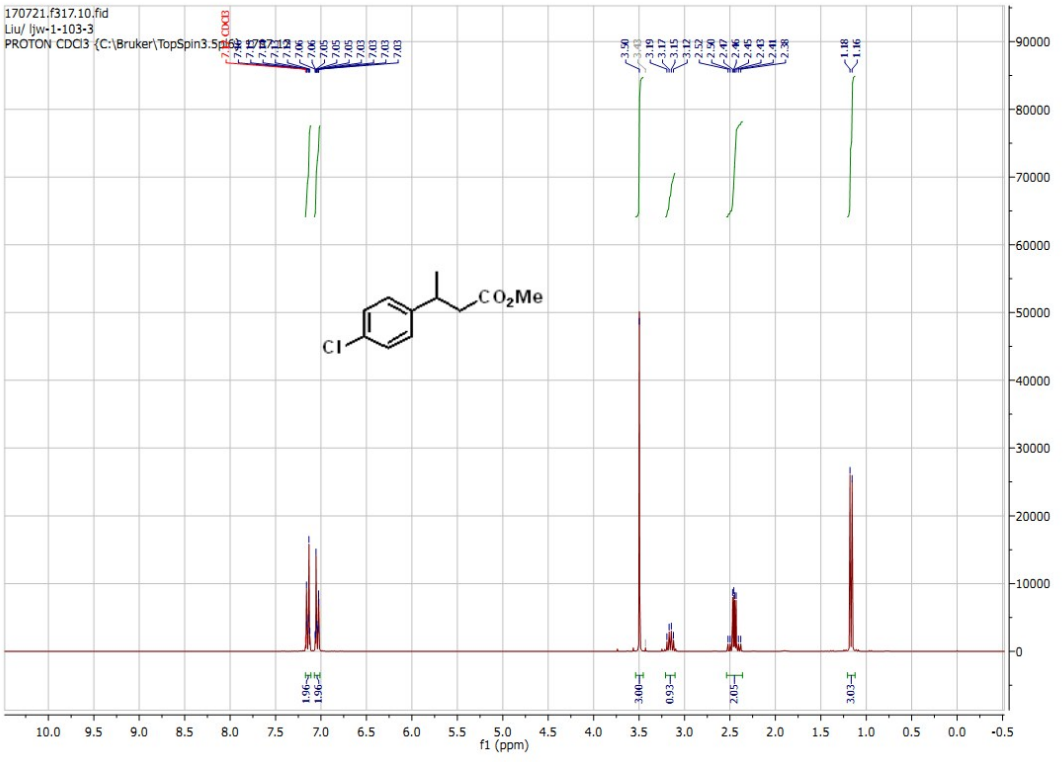
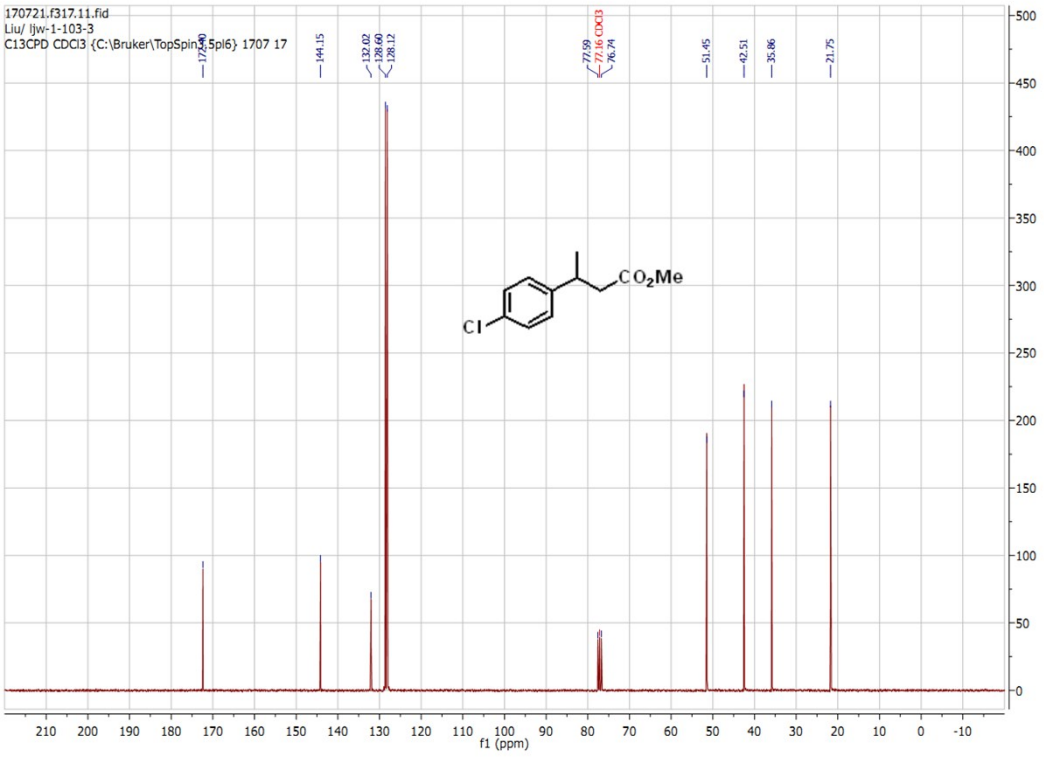
CO2Me
F
f1 (ppm)

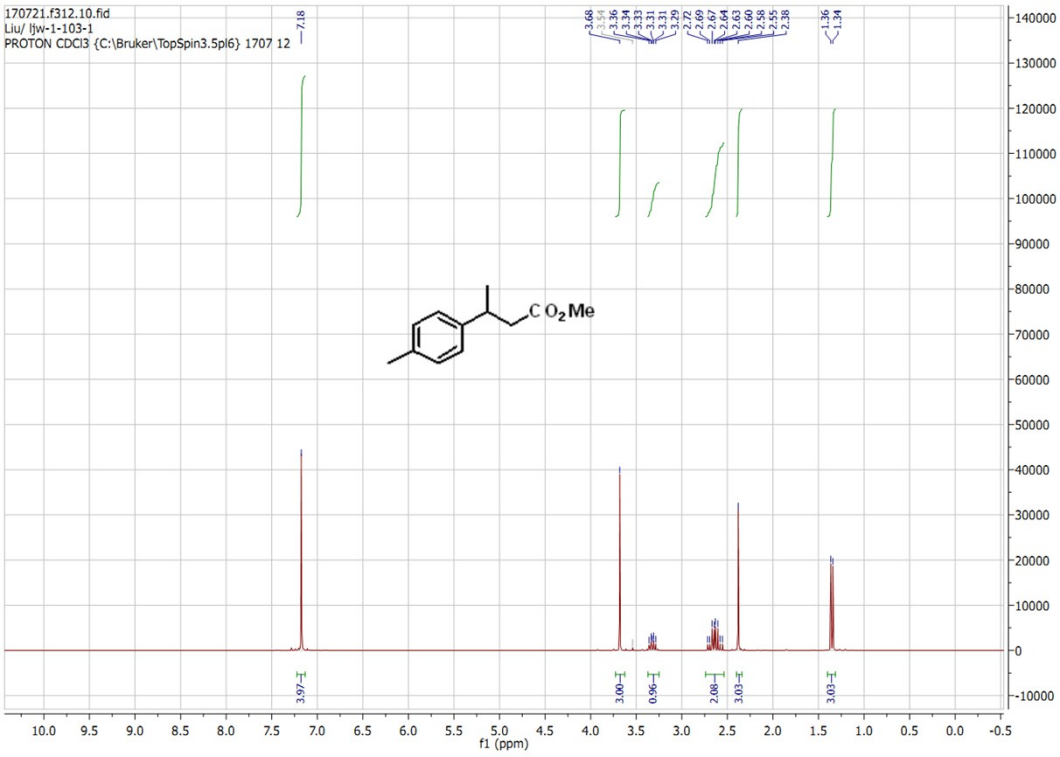


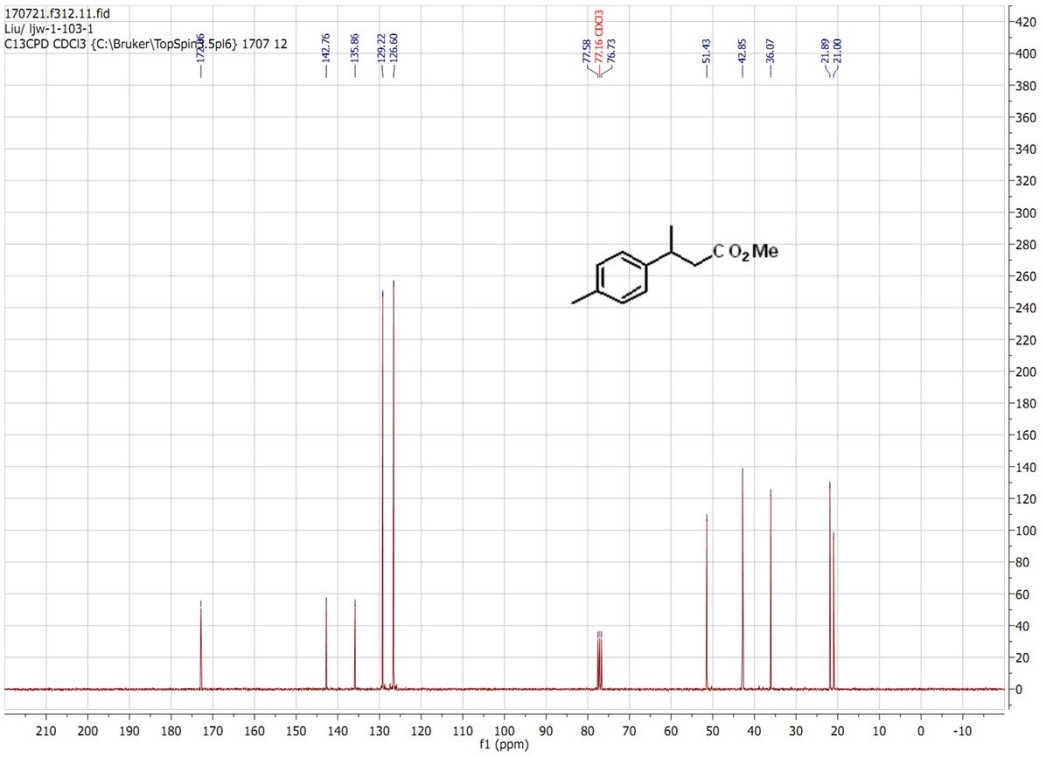
NMR spectra of **2g:**



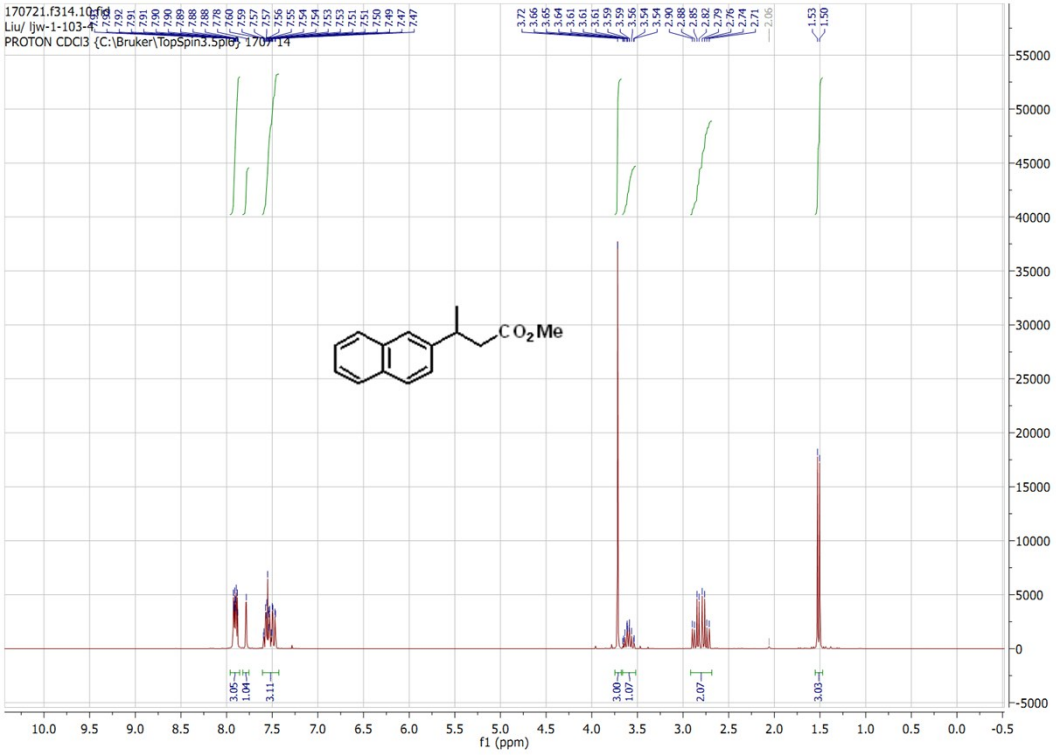


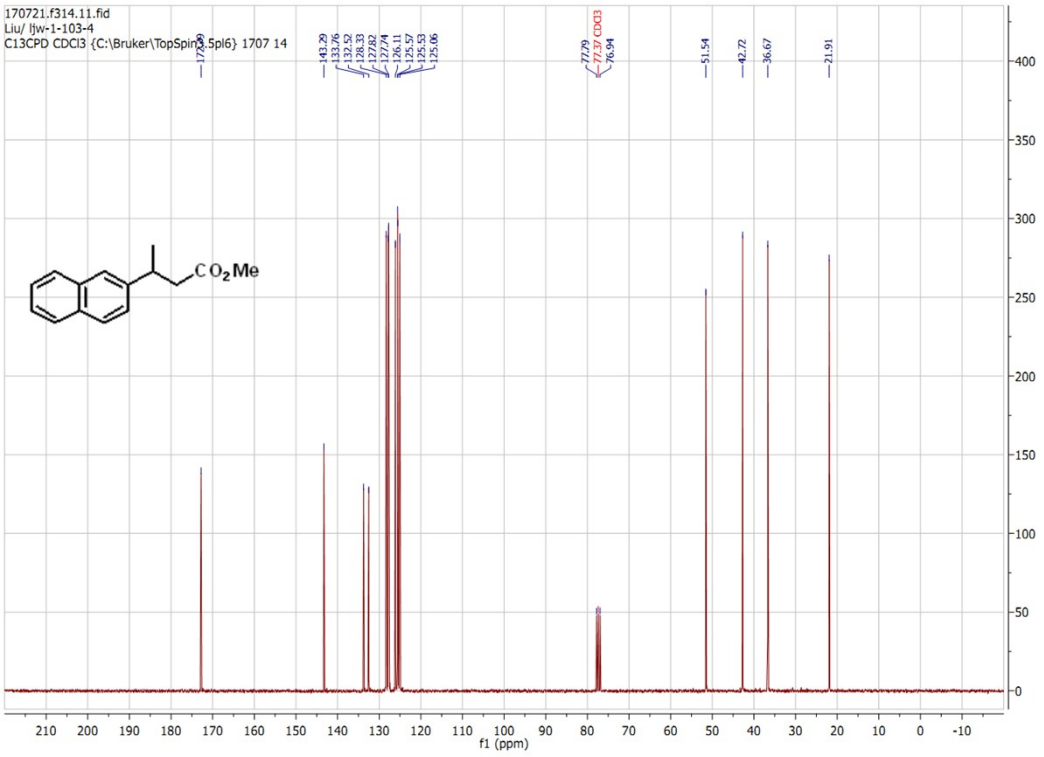
NMR spectra of **2h:**



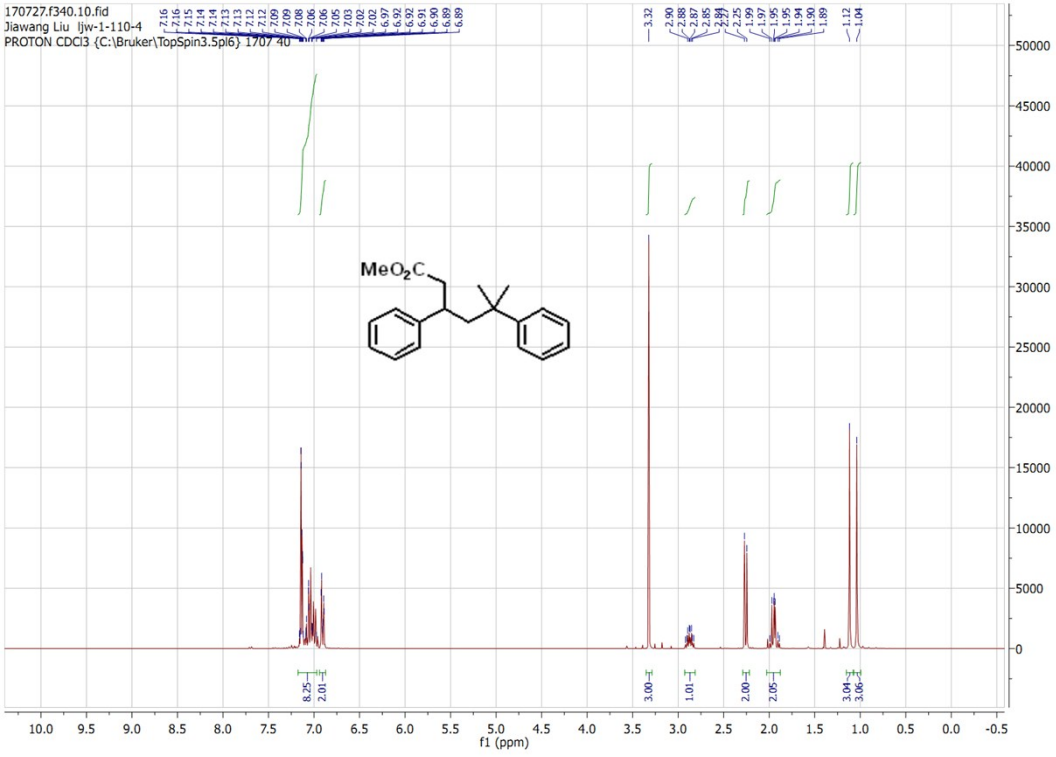


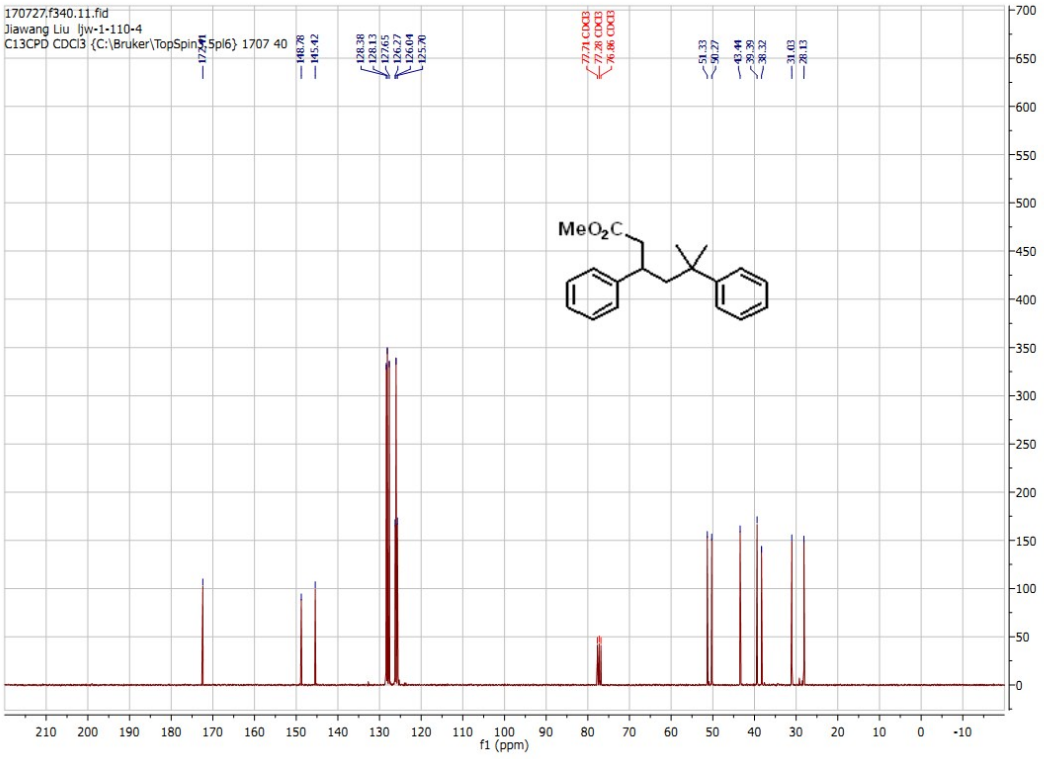
NMR spectra of **2i:**



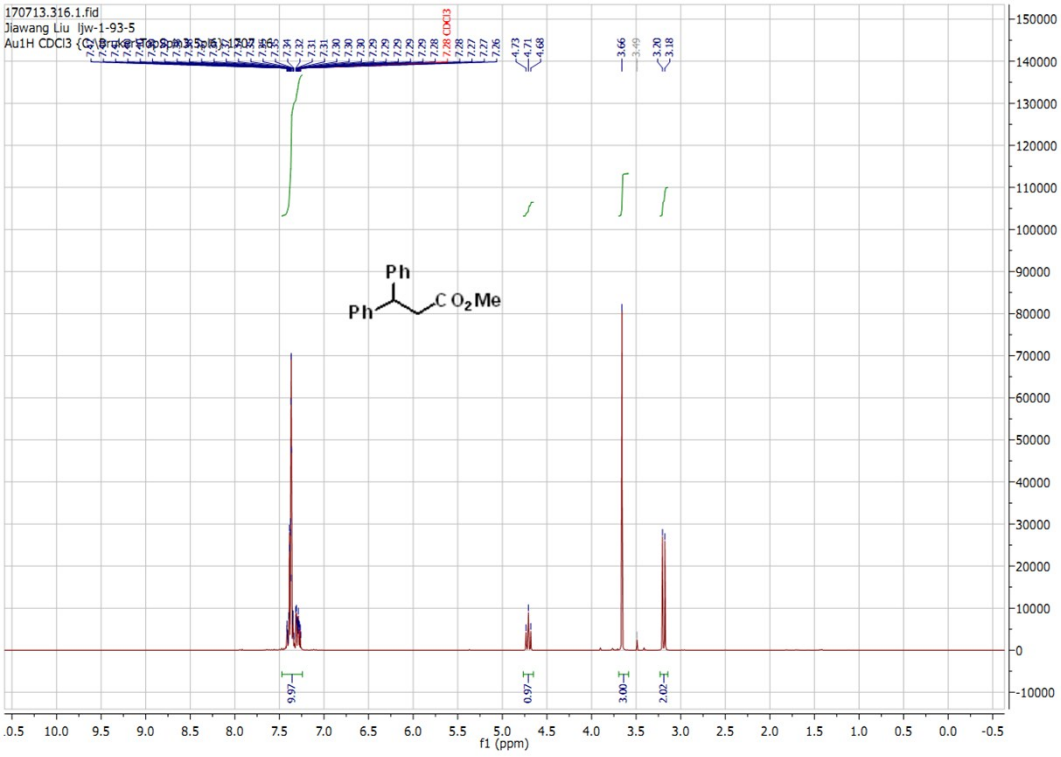


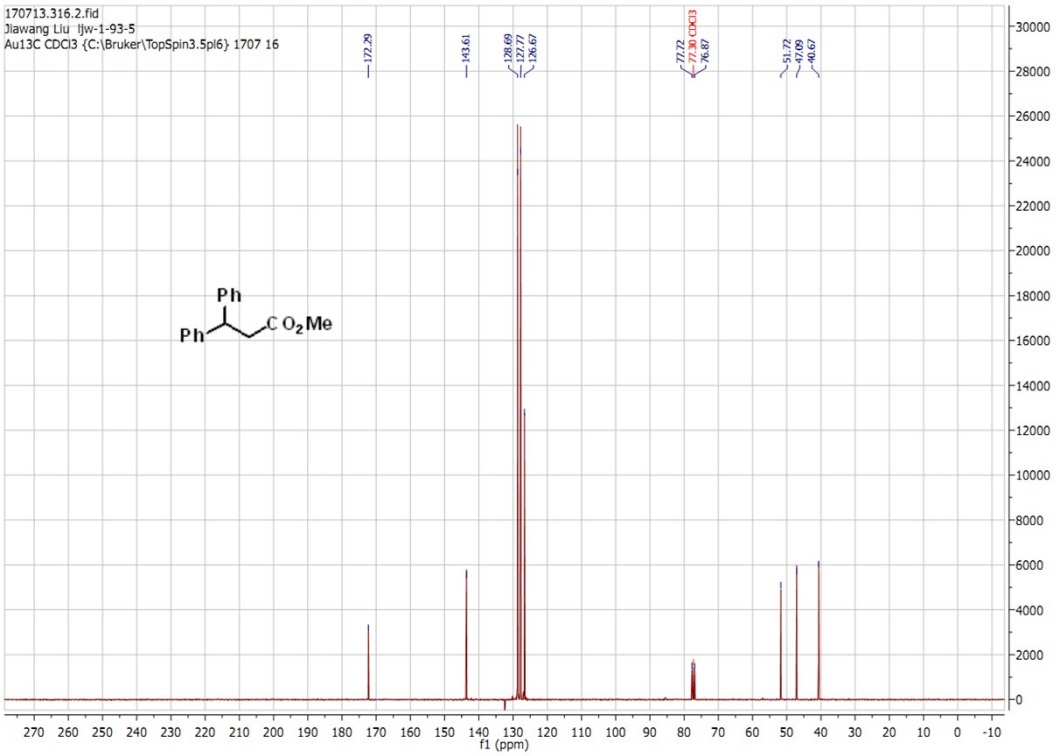
NMR spectra of **2j:**



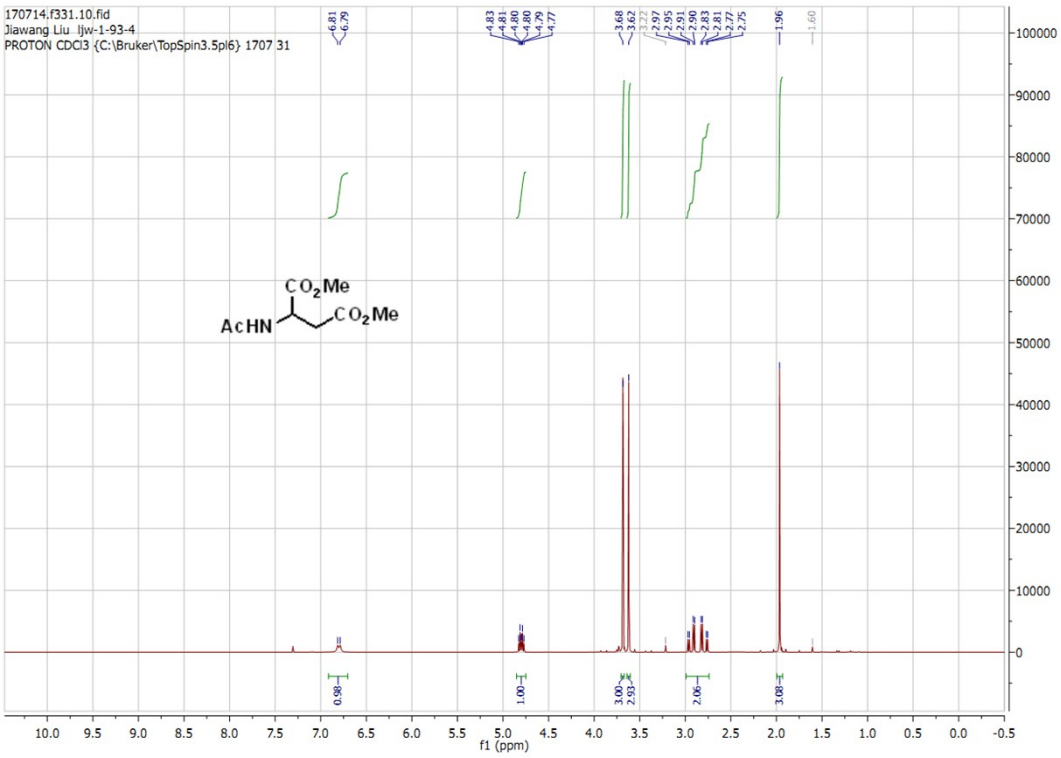


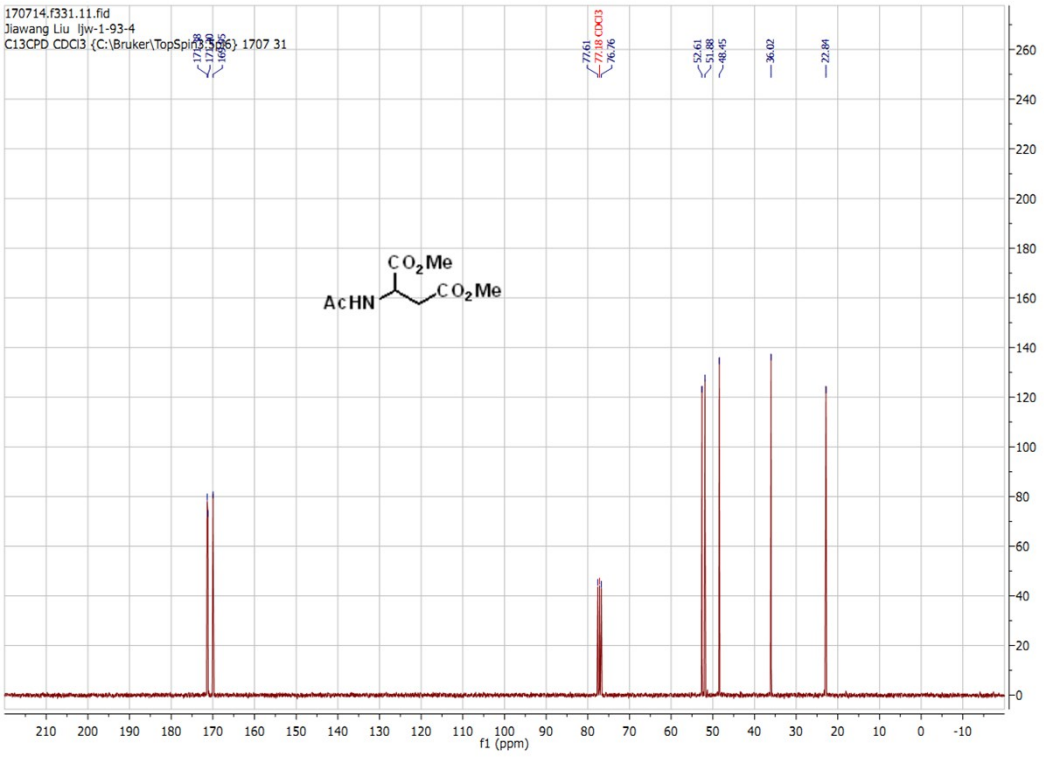
NMR spectra of **2k:**





NMR spectra of **2l:**





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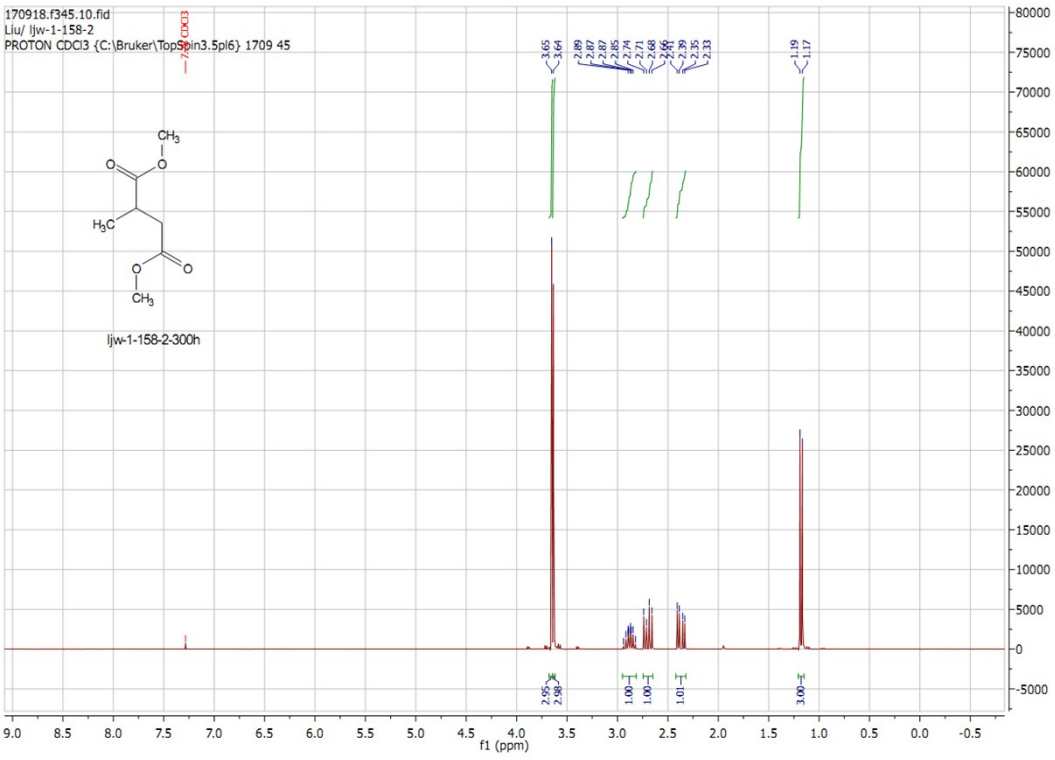
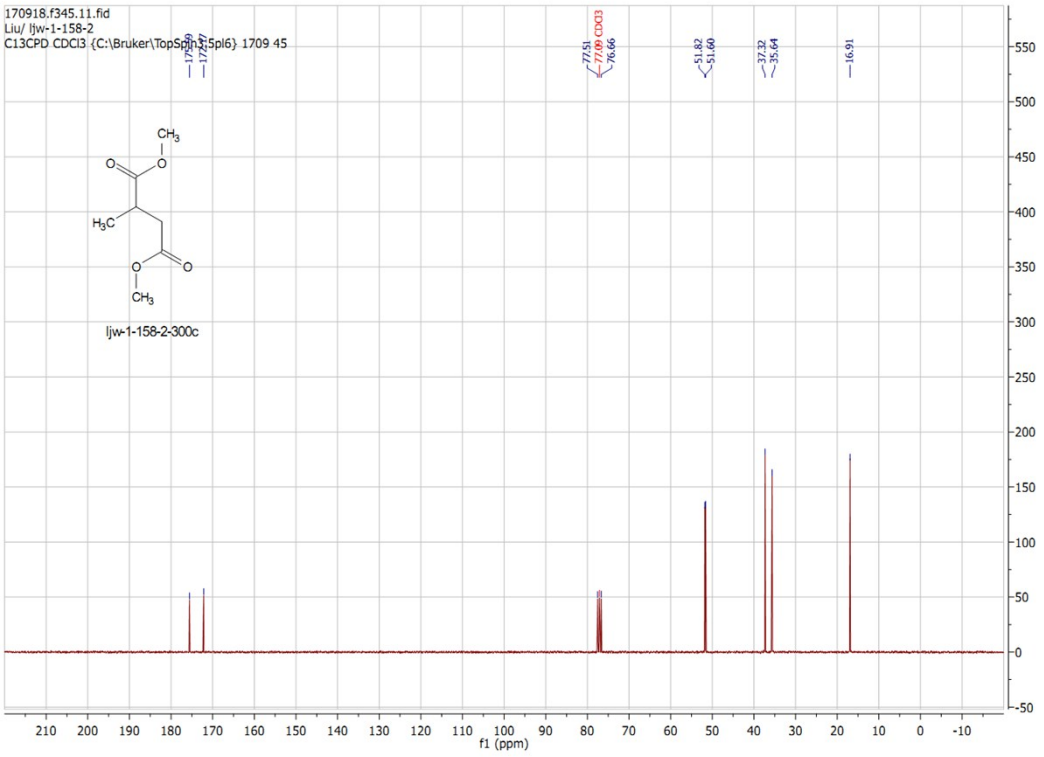
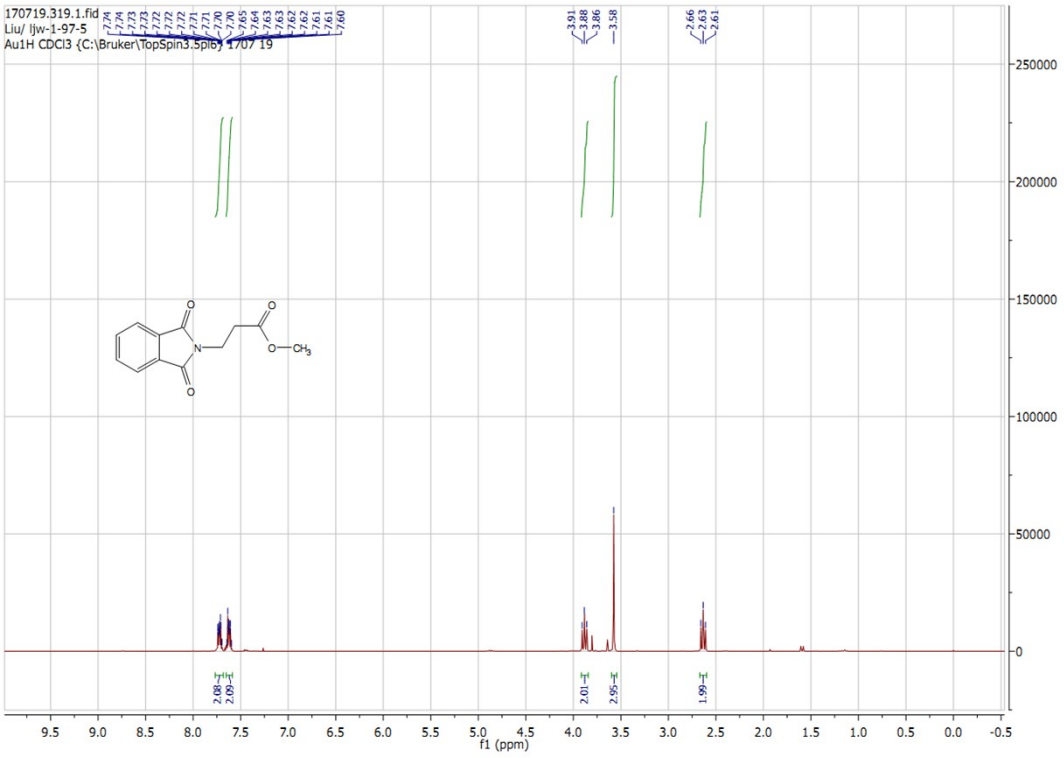
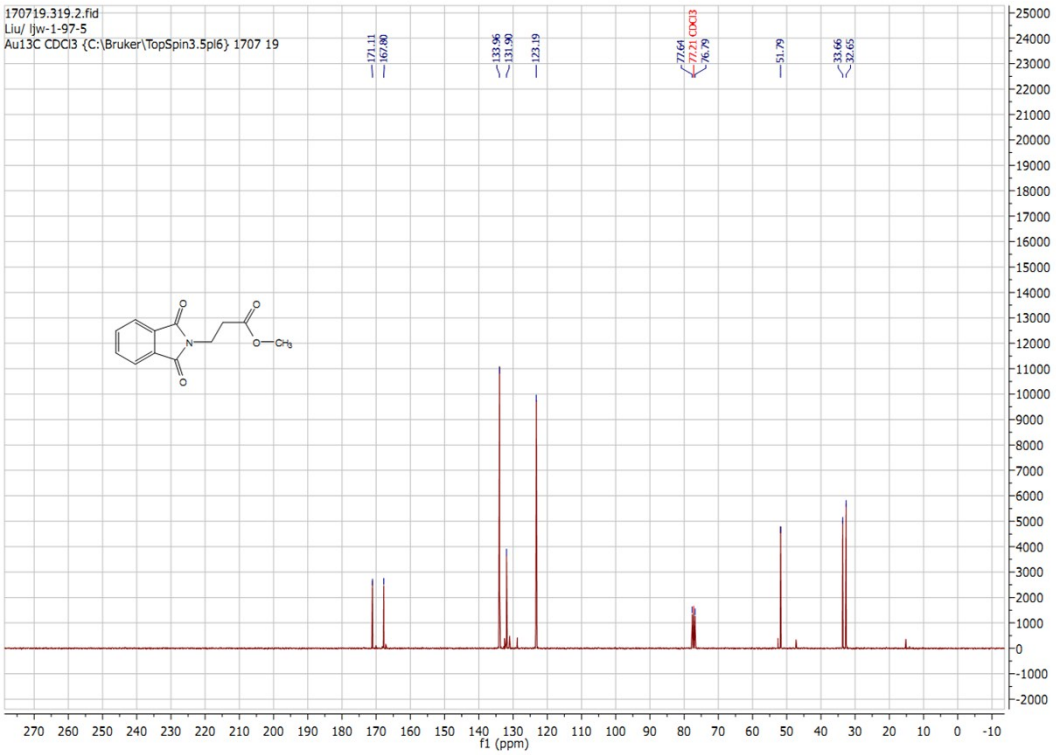


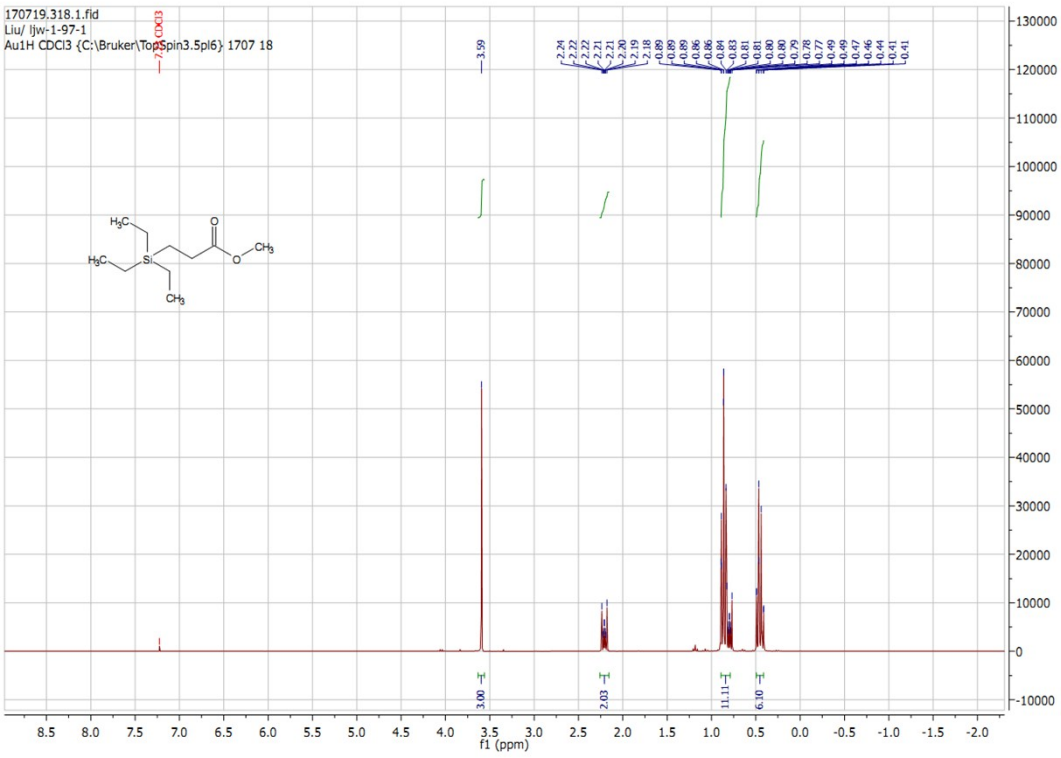


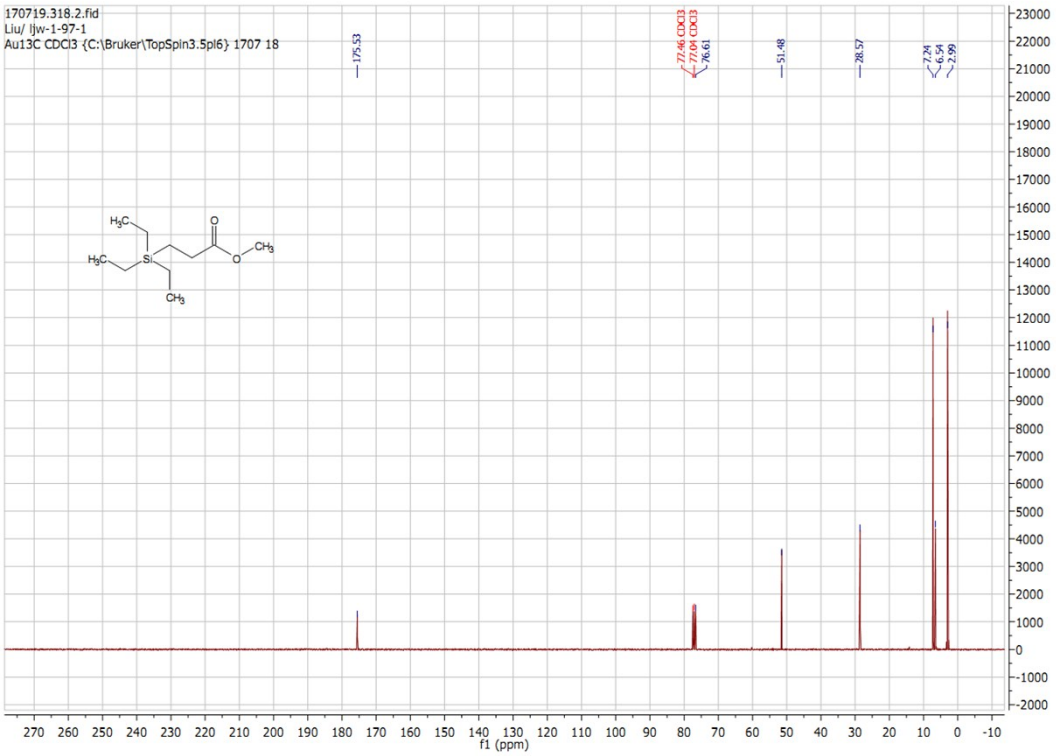
NMR spectra of **2n:**



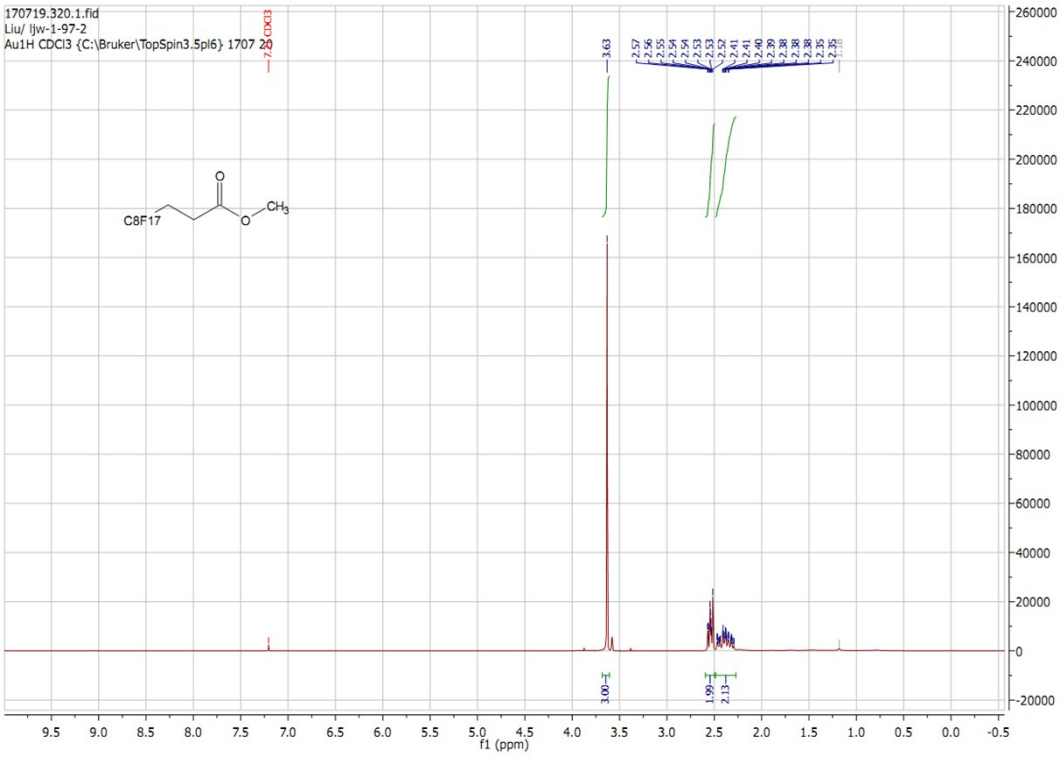


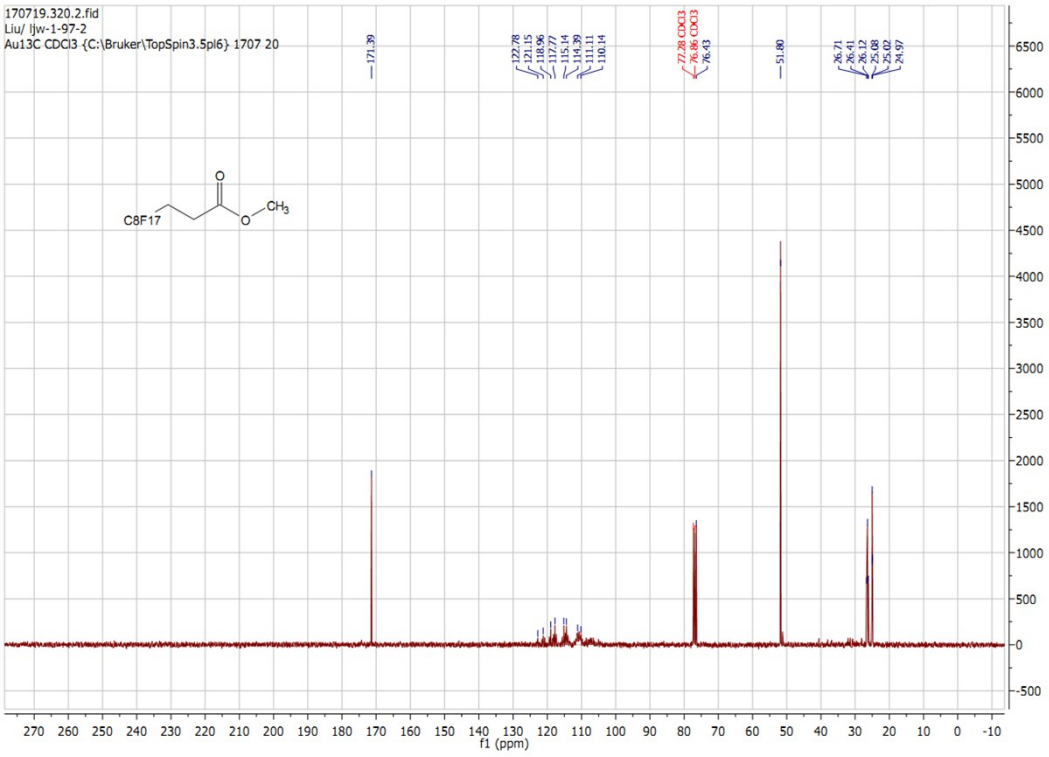
NMR spectra of **2o:**



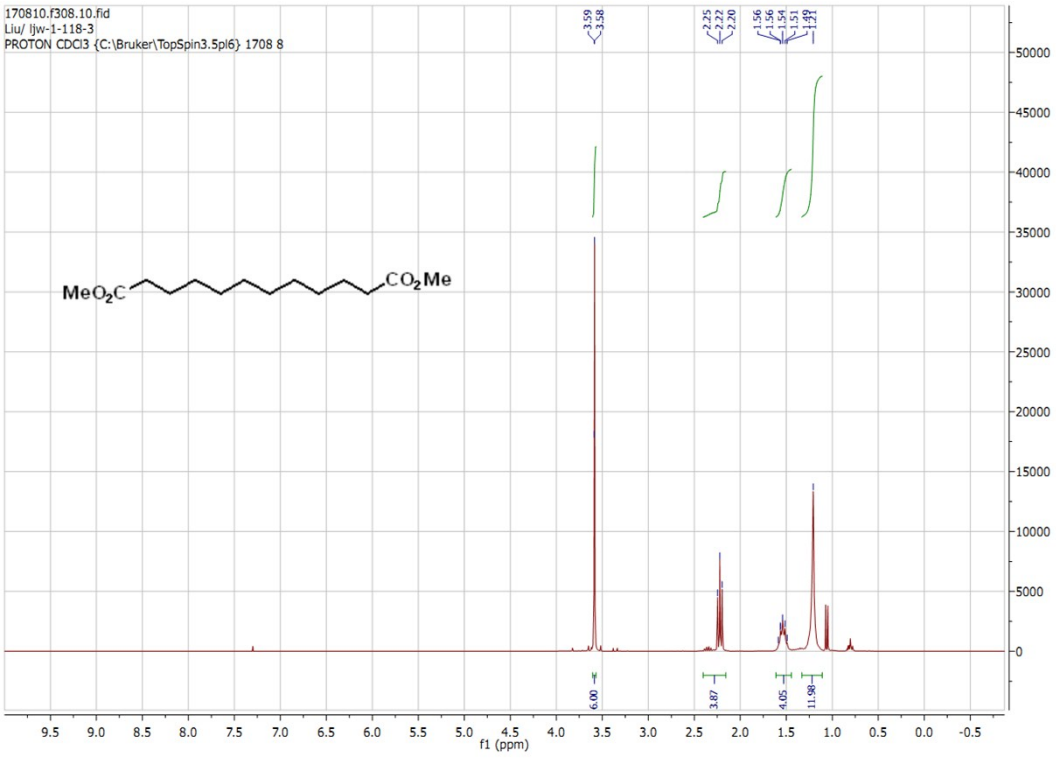


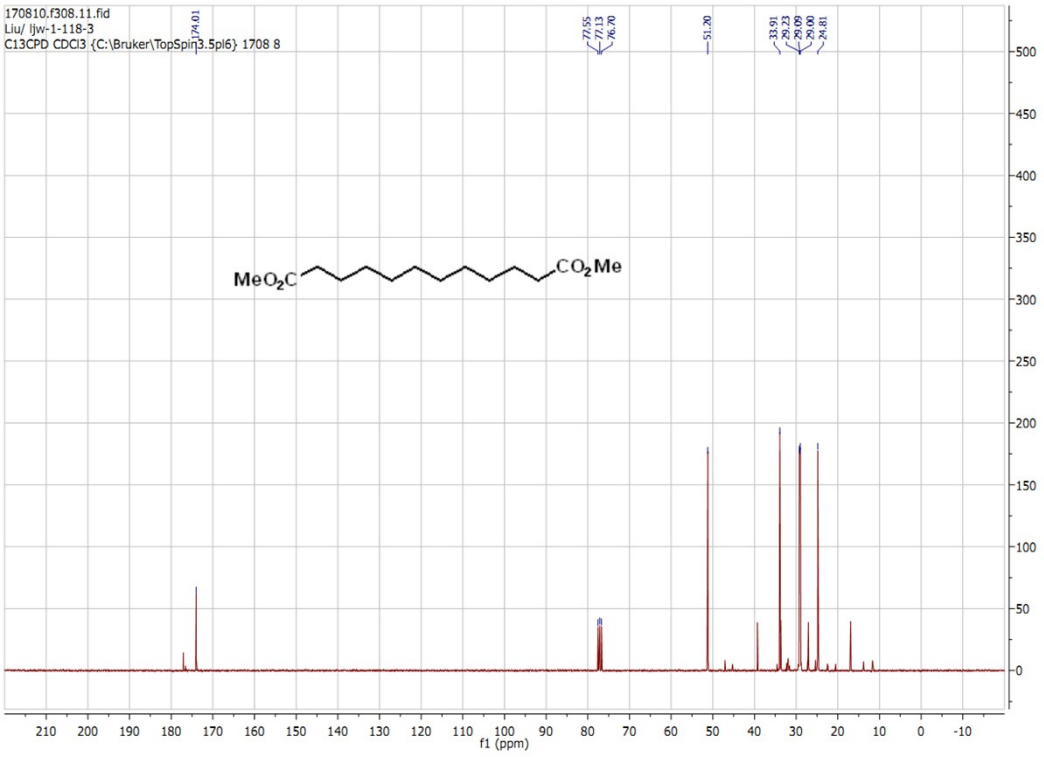
NMR spectra of **2p:**



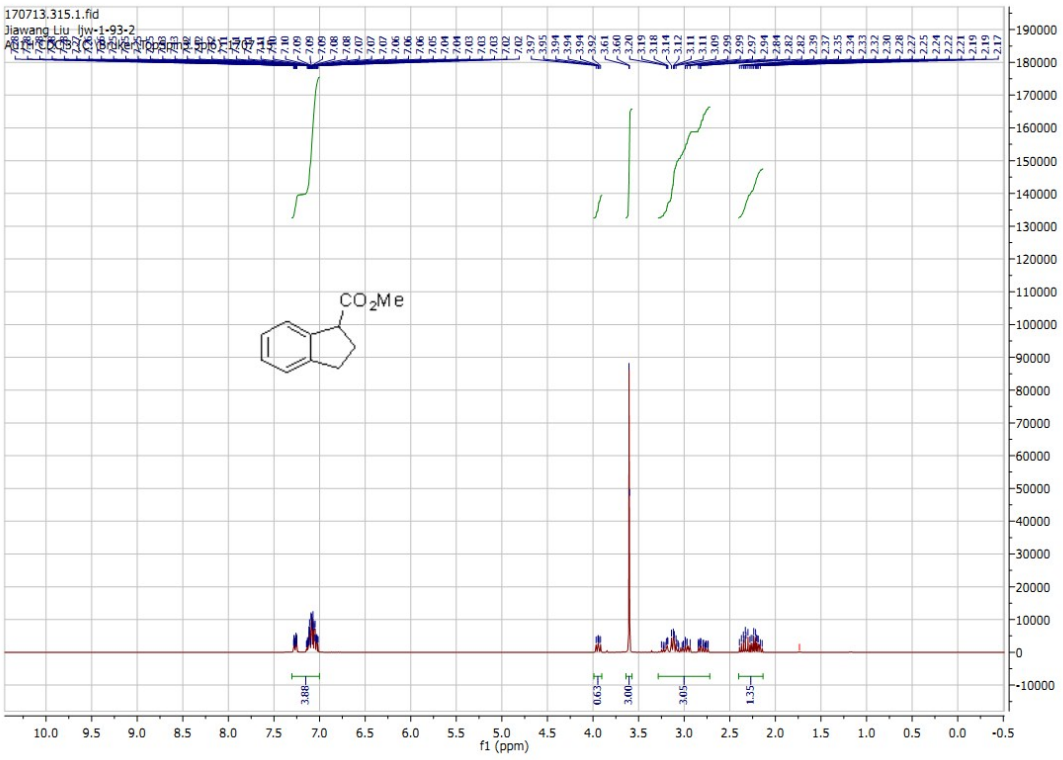


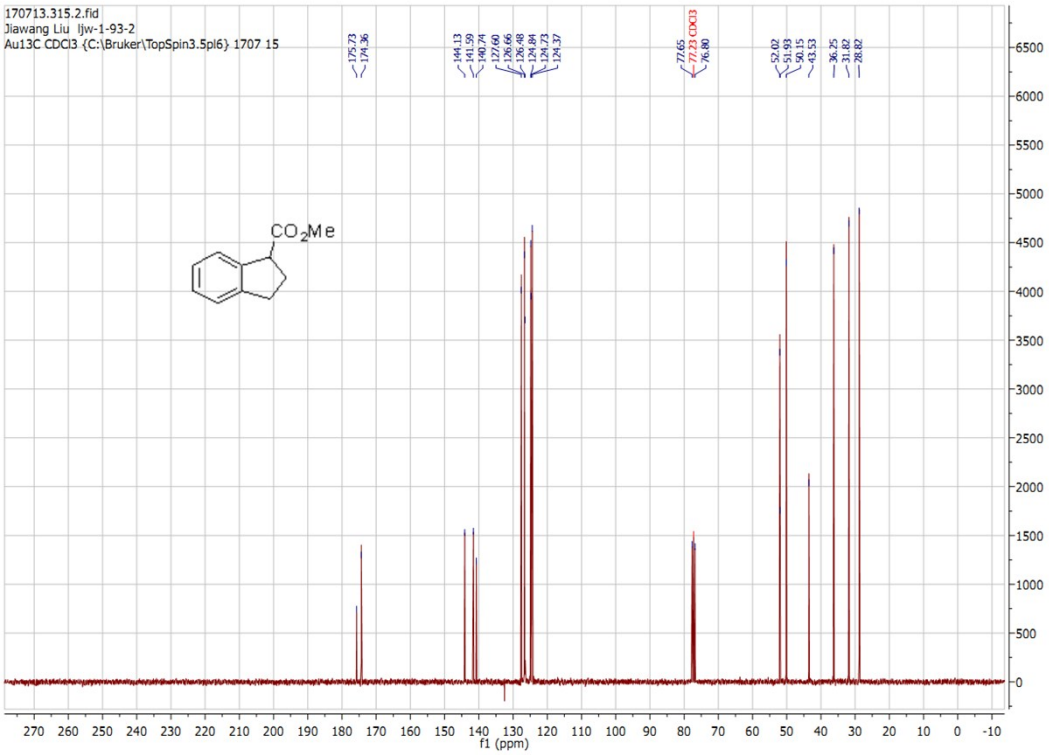
NMR spectra of **2q:**



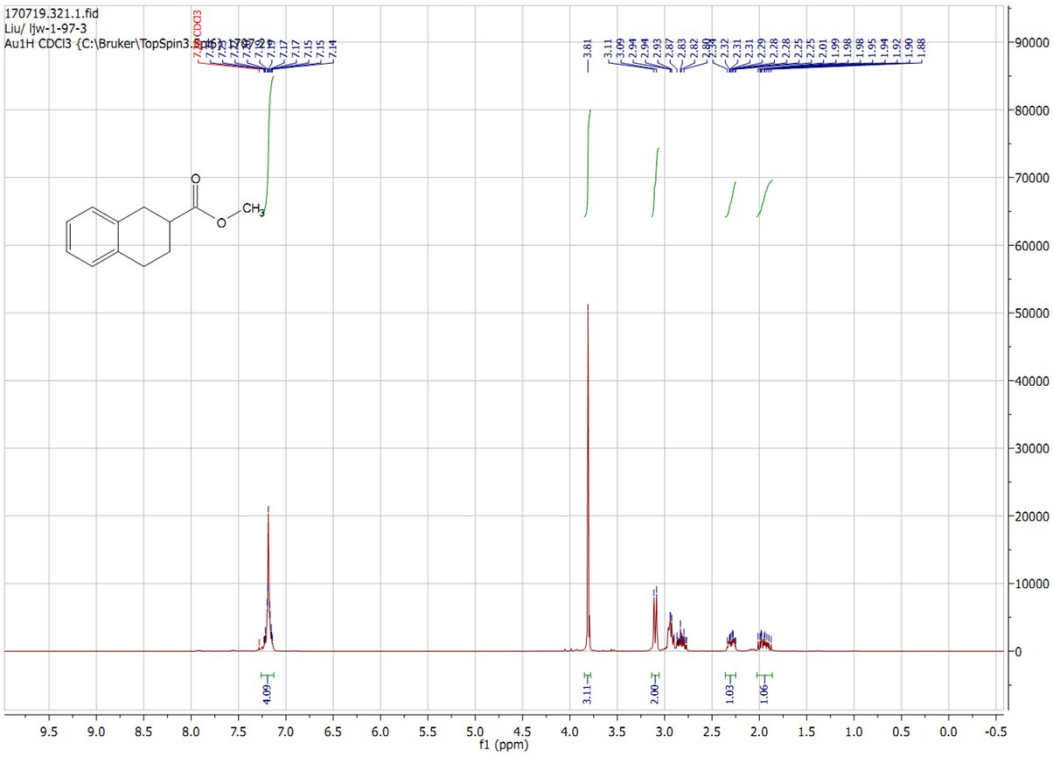


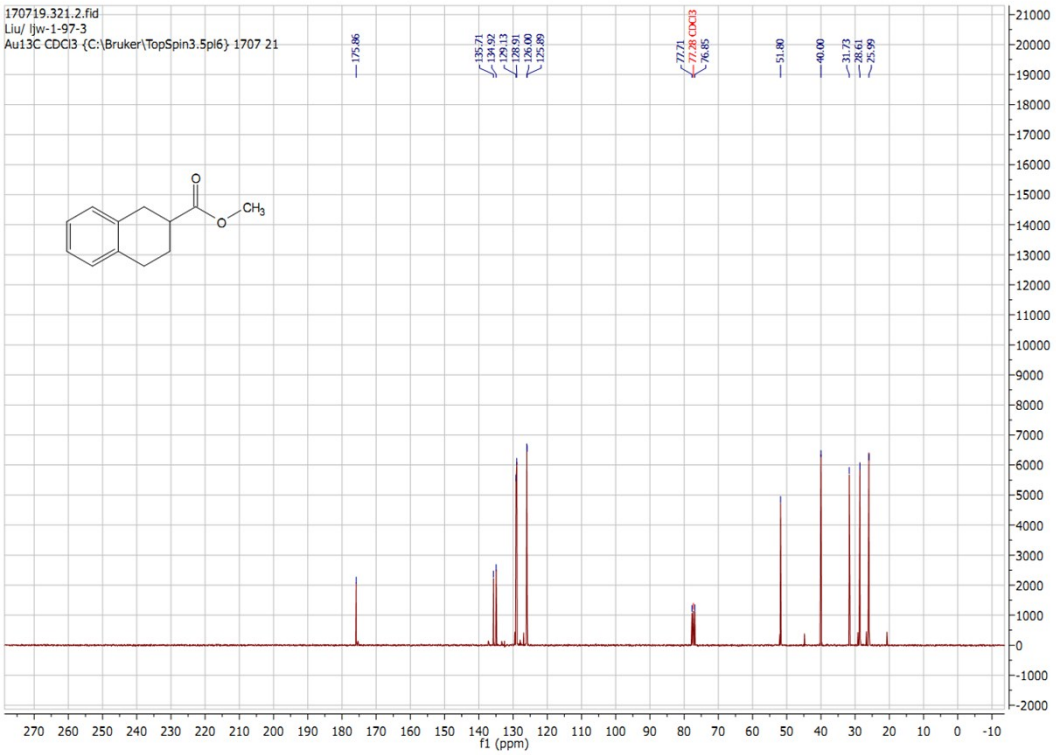
NMR spectra of **2r:**



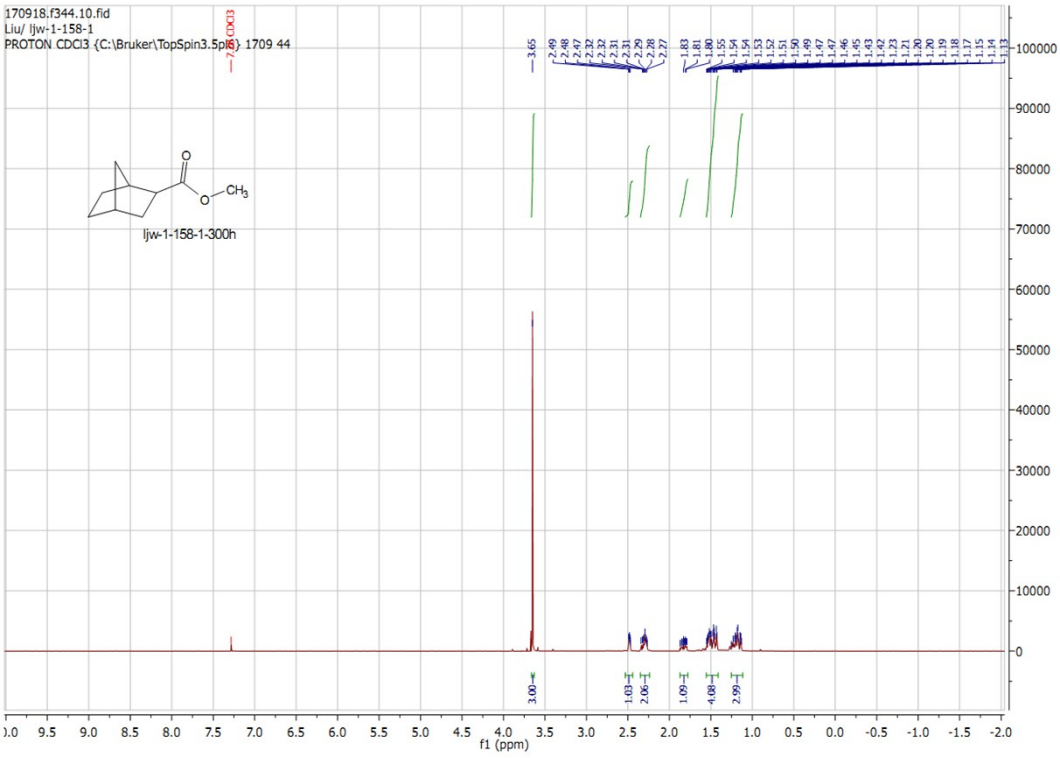


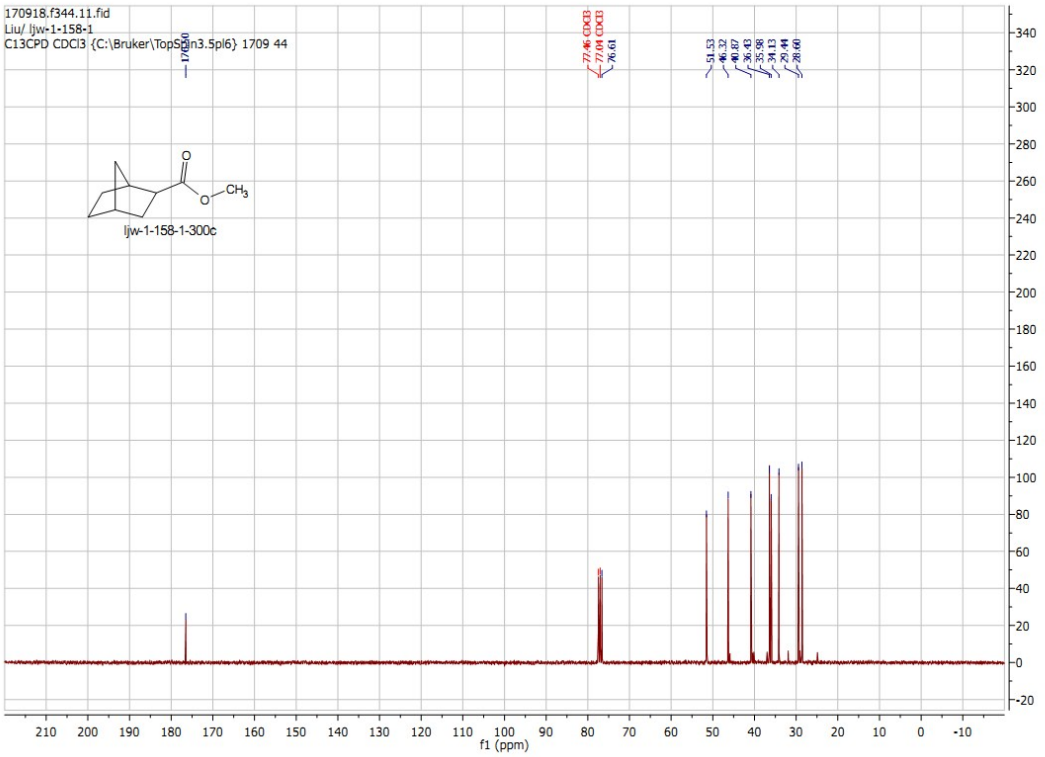
NMR spectra of **2s:**





NMR spectra of **2t:**

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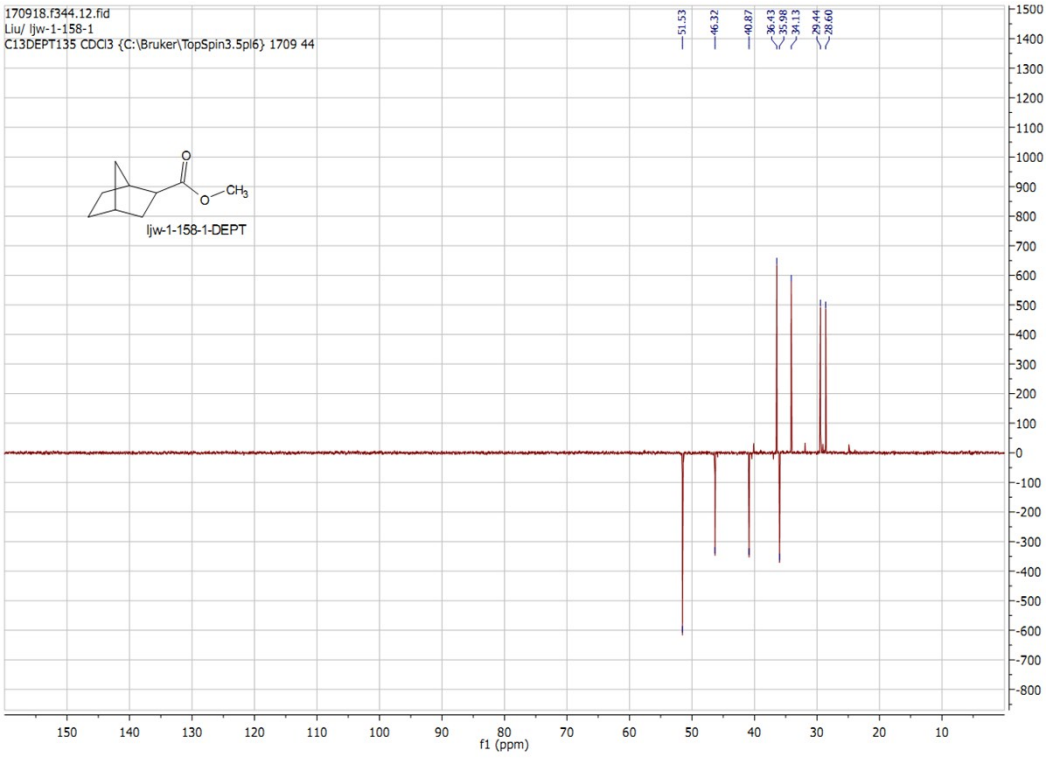
Liu/ ljw-1-158-1
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1709 44
77.46 CDCl3
77.04 CDCl3
76.61
51.53
46.32
40.87
36.43
35.98
34.13
29.44
28.60
O
O
CH3
ljw-1-158-1-300c
f1 (ppm)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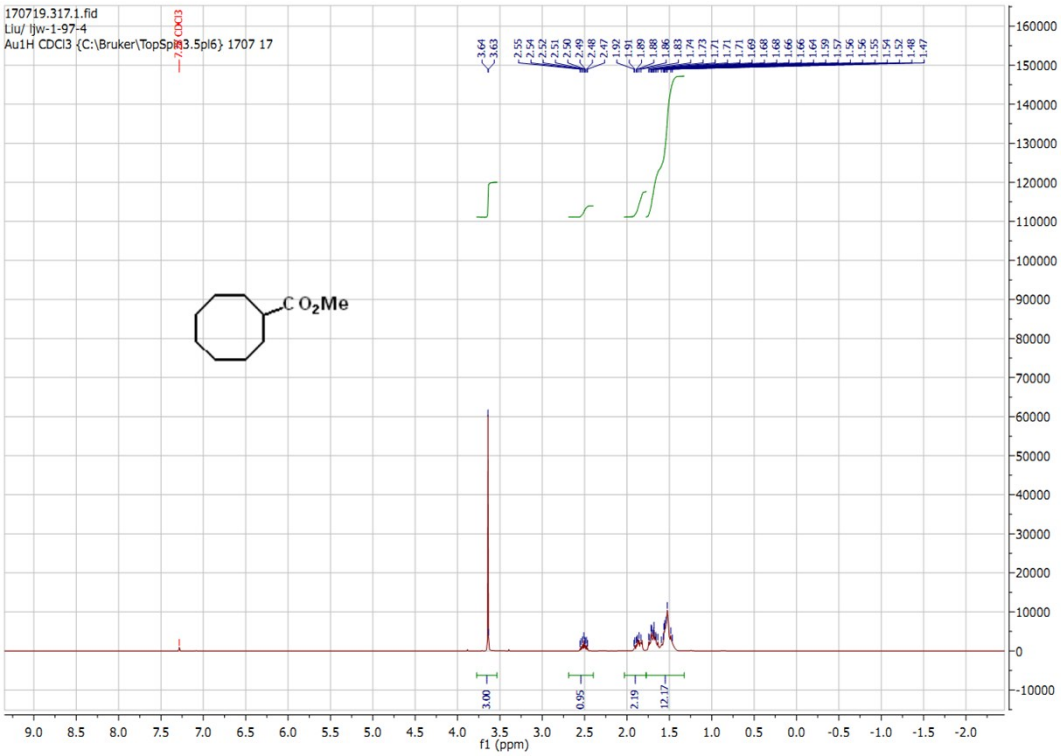
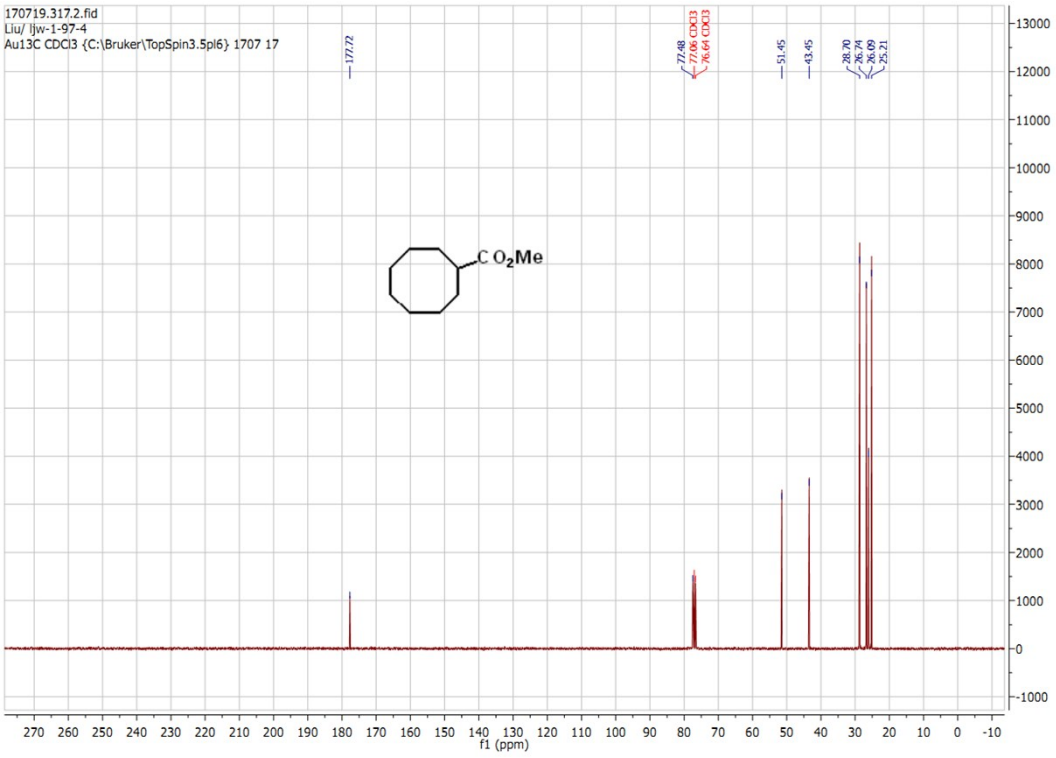
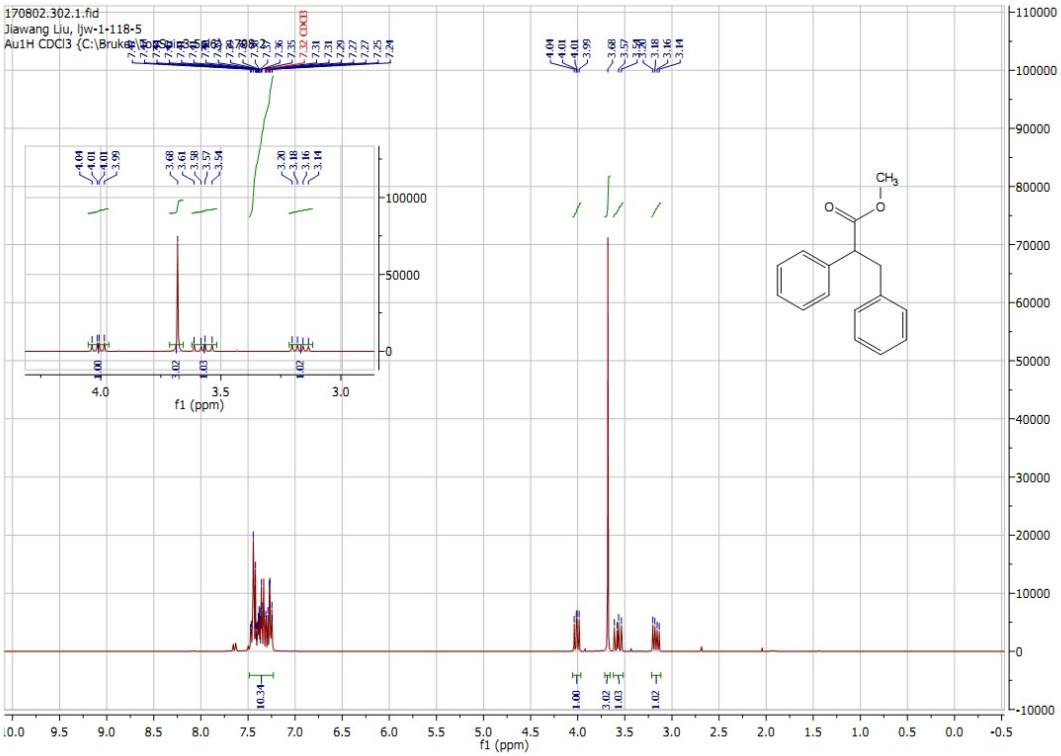
46.32
40.87
36.43
35.98
34.13
29.44
28.60
O
O
CH3
ljw-1-158-1-DEPT
f1 (ppm)

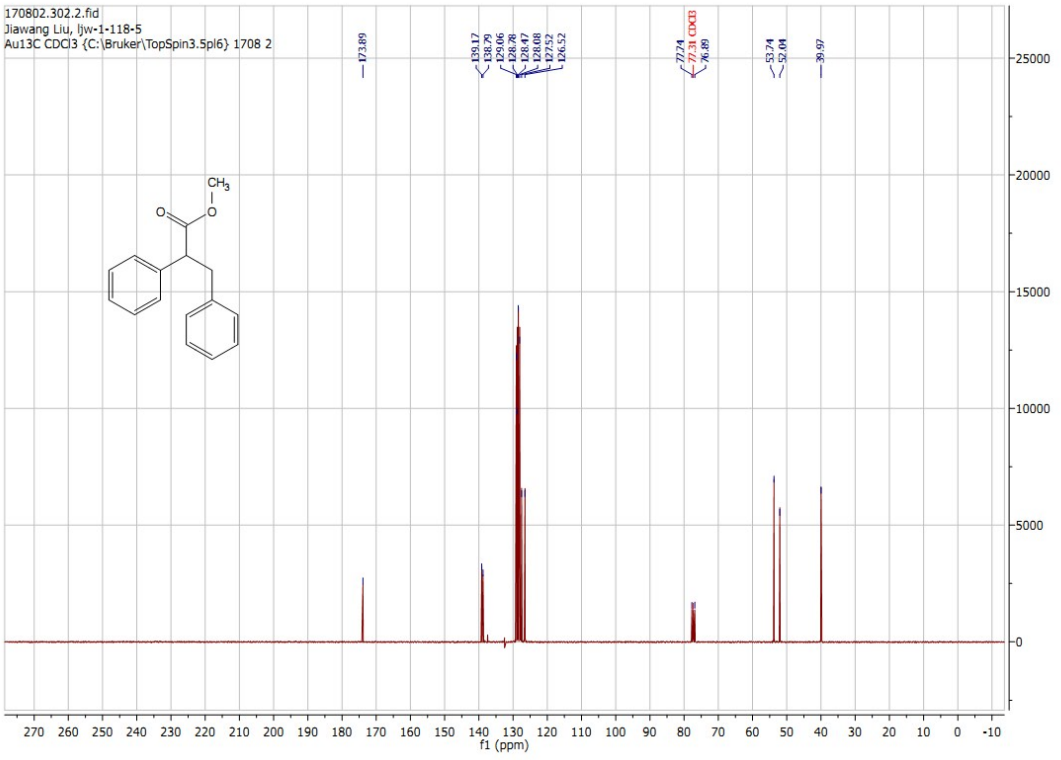
NMR spectra of **2u:**



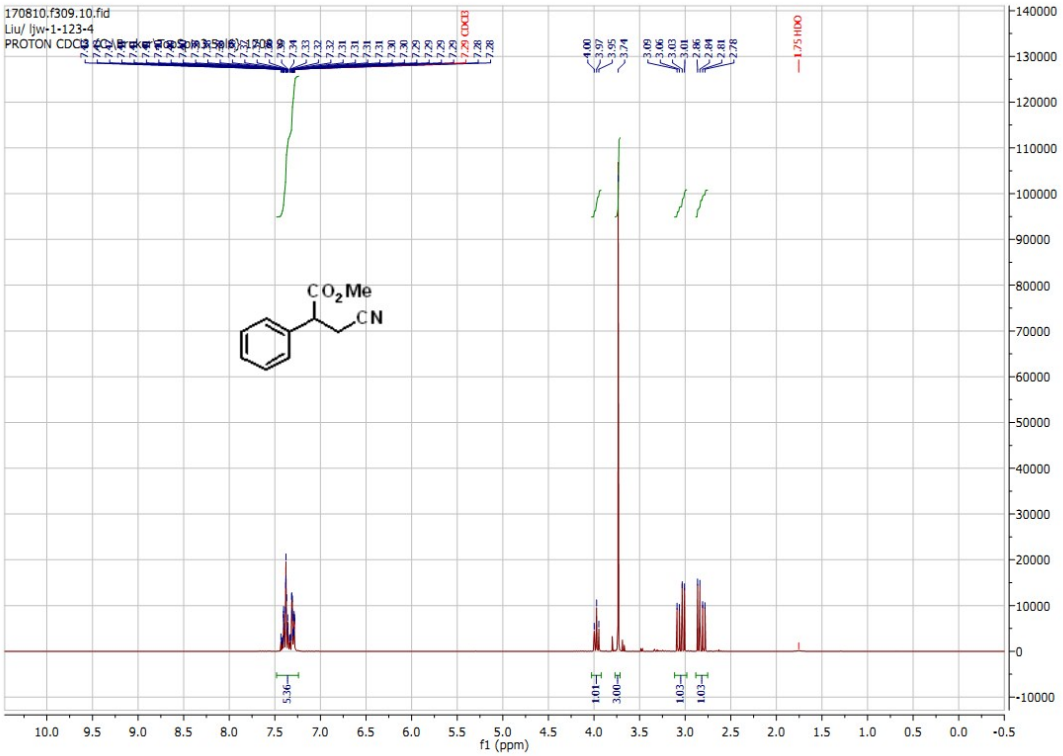


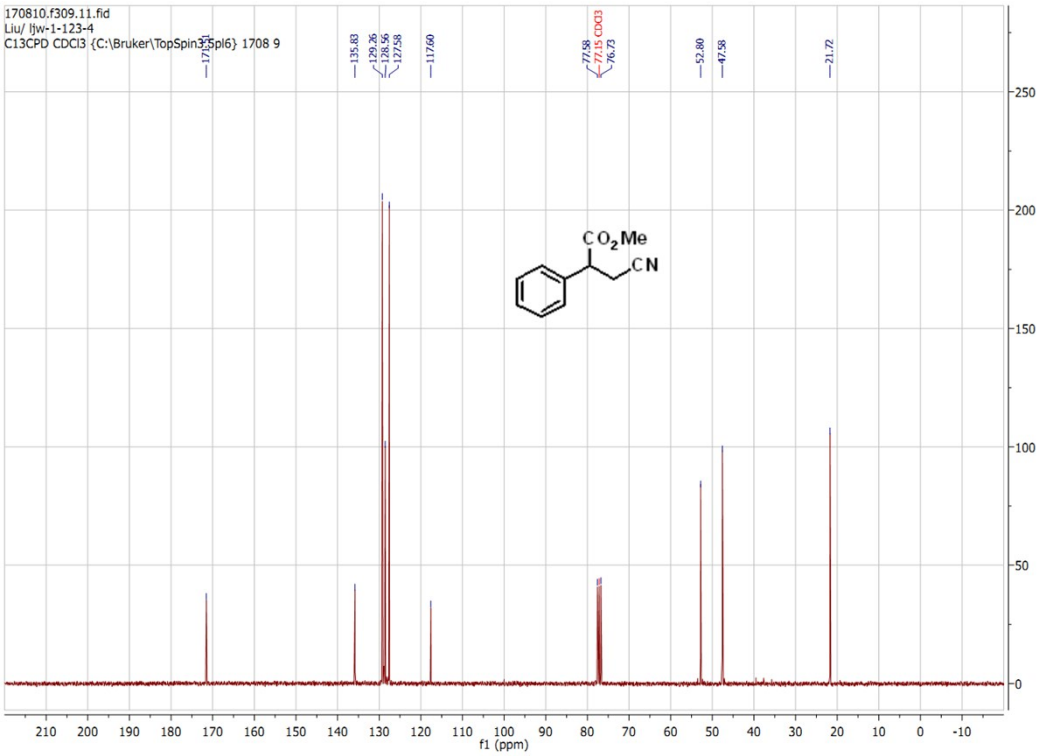
NMR spectra of **2v:**



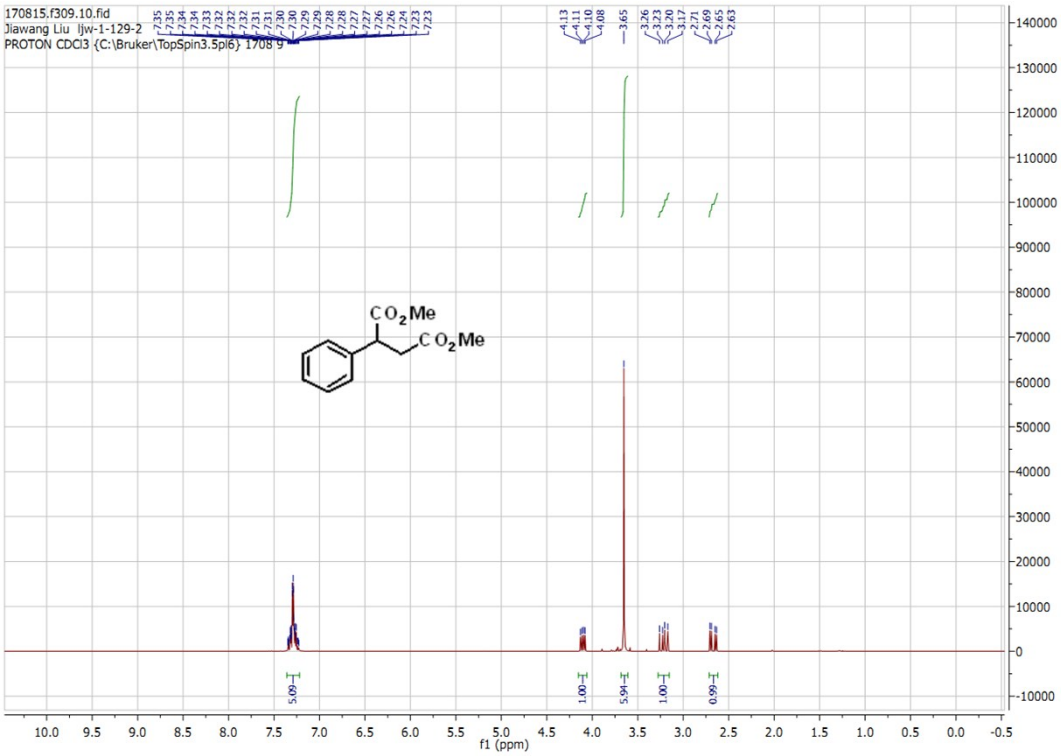


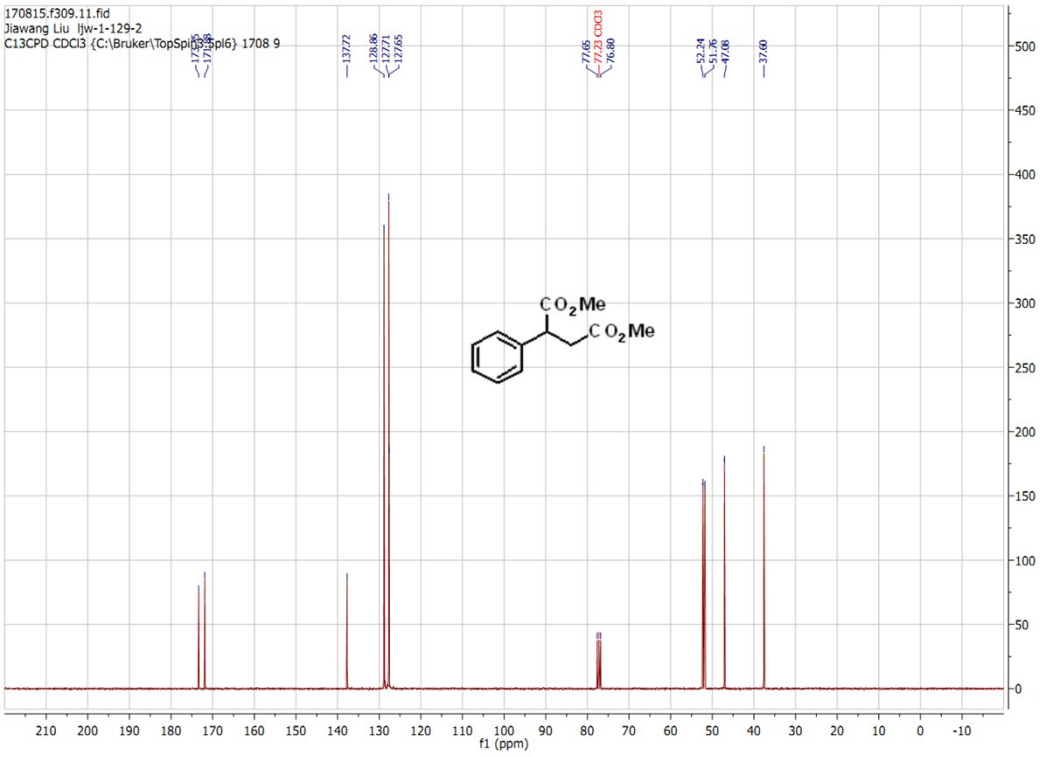
NMR spectra of **2w:**



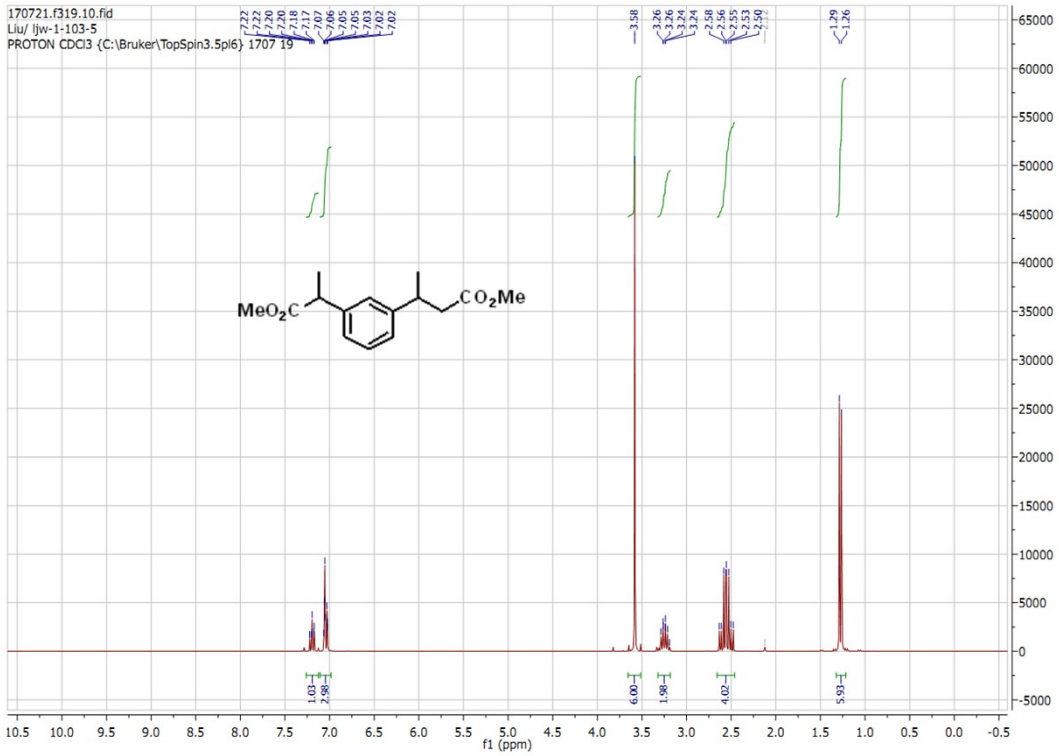


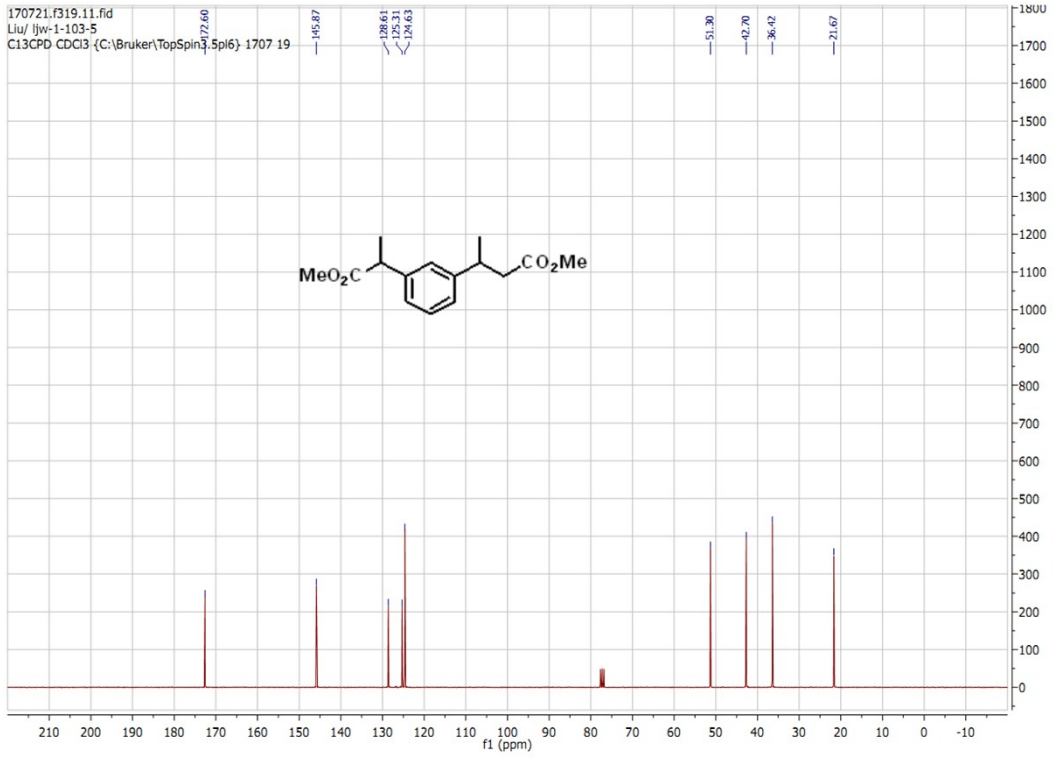
NMR spectra of **2x:**



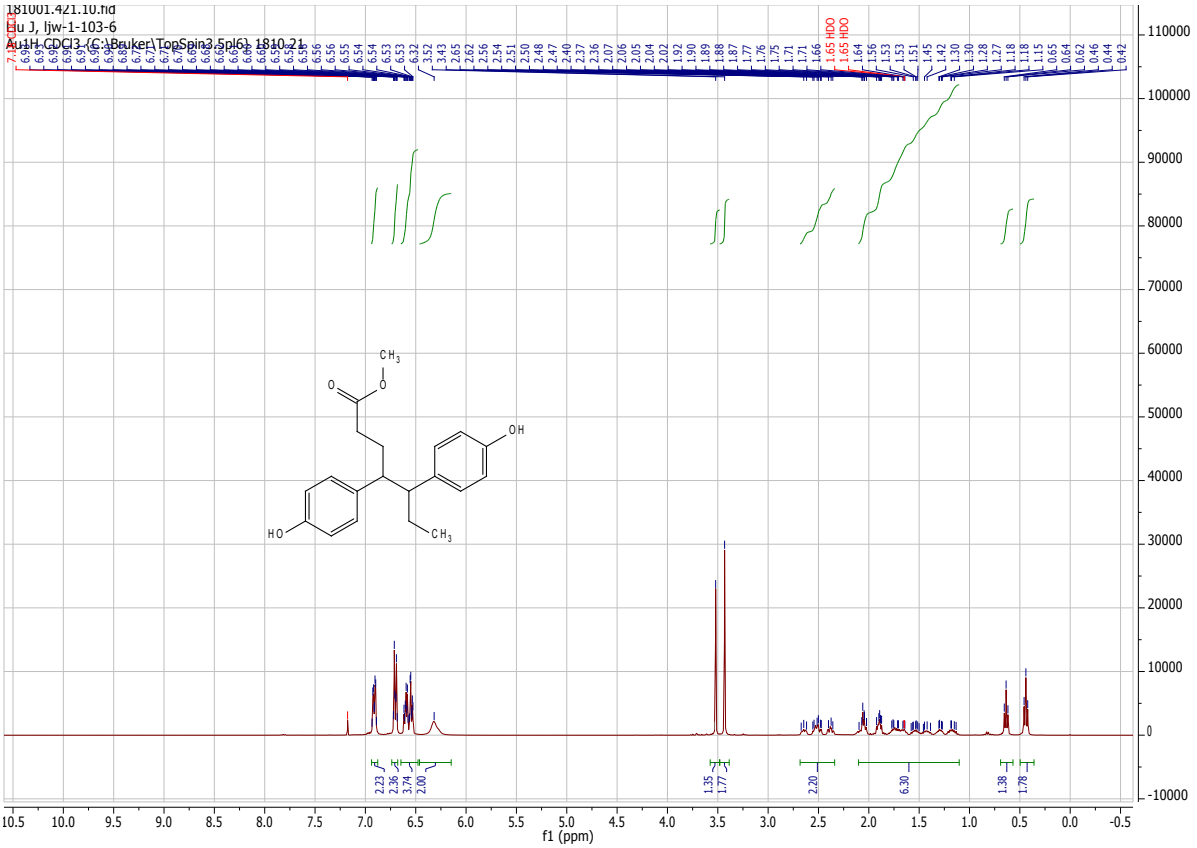


NMR spectra of **2y:**





NMR spectra of **2z:**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Liu J, ljw-1-103-6
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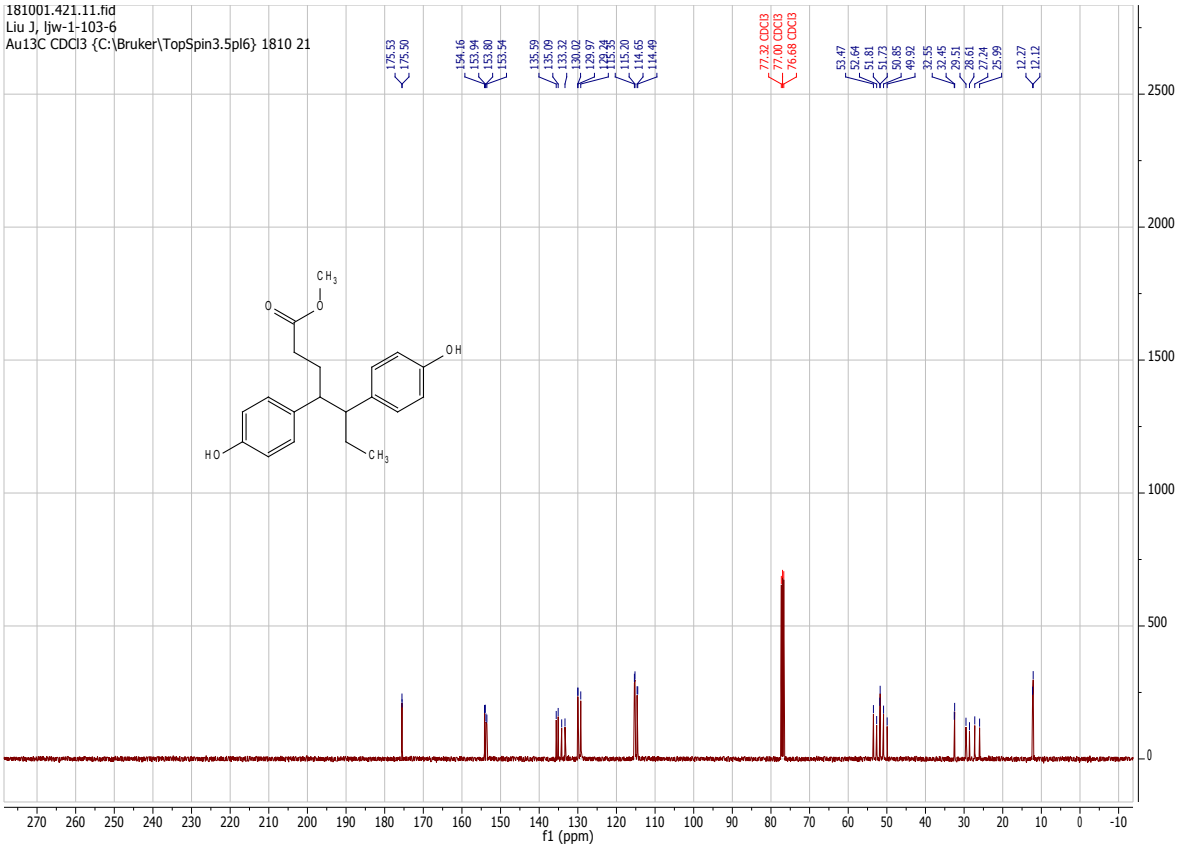
f1 (ppm)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Liu J, ljw-1-103-6
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 1810 21
f1 (ppm)