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Rhodium-Catalyzed Asymmetric Hydrogenation of β-Cyanocinnamic Esters with the Assistance of a Single Hydrogen bond in a Precise Position

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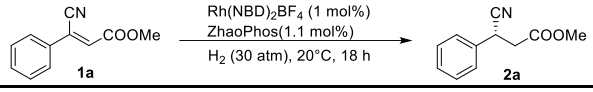
Contents

1. General Information

Unless otherwise noted, all reagents and solvents were purchased from commercial suppliers and used without further purification. NMR spectra were recorded on Bruker ADVANCE III (400 MHz) spectrometers for ^{1}H NMR and ^{13}C NMR. $CDCl_3$ was the solvent used for the NMR analysis, with tetramethylsilane as the internal standard. Chemical shifts were reported upfield to TMS (0.00 ppm) for ^{1}H NMR and relative to $CDCl_3$ (77.3 ppm) for ^{13}C NMR. Optical rotation was determined using a Perkin Elmer 343 polarimeter. HPLC analysis was conducted on an Agilent 1260 Series instrument. Column Chromatography was performed with silica gel Merck 60 (300-400 mesh). All new products were further characterized by HRMS. A positive ion mass spectrum of sample was acquired on a Thermo LTQ-FT mass spectrometer with an electrospray ionization source.

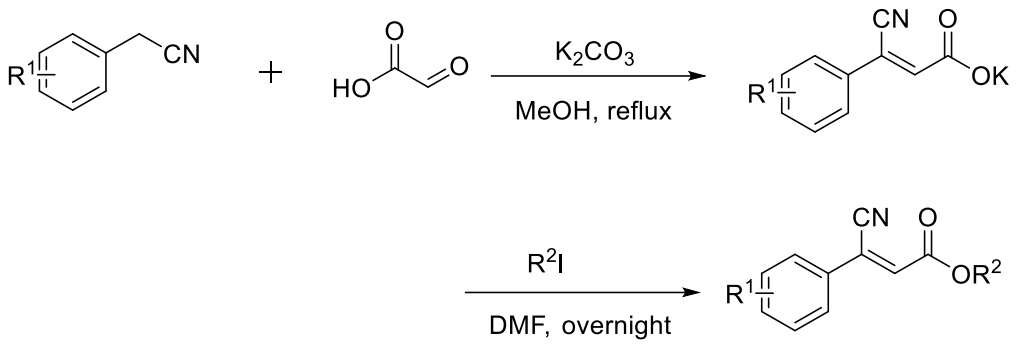
Table S1. Solvent screening for the Rh-catalyzed asymmetric hydrogenation of **1a**.[a]



Entry	Solvent	Conv. [%][b]	ee [%][c]
1	CH_3OH	28	84
2	CH_3CH_2OH	14	80
3	CF_3CH_2OH	68	95
4	EtOAc	20	96
5	toluene	14	97
6	1,4-dioxane	17	97
7	CH_2Cl_2	27	98
8	$CHCl_3$	11	98
9	$ClCH_2CH_2Cl$	20	97
10[d]	CF_3CH_2OH	99	95

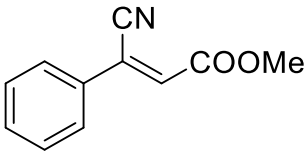
[a] Unless otherwise mentioned, all reactions were carried out with a $[Rh(NBD)_2]BF_4$/ZhaoPhos/substrate ratio of 1:1.1:100, in 1 mL of solvent, at 20 °C, under hydrogen (30 atm) for 18 h. [b] Determined by ^{1}H NMR spectroscopy. [c] Determined by HPLC analysis using a chiral stationary phase. [d] 35 °C, 50 atm H_2.

2. General procedure for the synthesis of compound 1

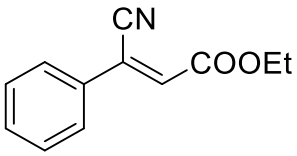


Preparation of **1a~1s** according to the literature [1]: To a solution of the commercial nitrile (21.0 mmol) and glyoxylic acid monohydrate (21.0 mmol, 1.58 g) in methanol (100 mL), K_2CO_3 (32.0 mmol, 4.42 g) was added. The mixture was heated under reflux for 3 hours, and monitored by TLC, until consumption of the starting material. The white precipitate was filtered, washed with dichloromethane, and recrystallized from water. The potassium salt thus obtained (9.48 mmol) was converted into the ester by reaction with R^2I (14.2 mmol) in dimethylformamide (10 mL) at 40℃ overnight. The reaction mixture was poured into water, and extracted with EtOAc. The organic layer was dried over Na_2SO_4 and the solvent was removed under reduced pressure, to afford, after purification by column chromatography eluting with hexane and an increasing amount of ethyl acetate, the corresponding cyanoester.

Preparation of **1t** based on the literature [2].

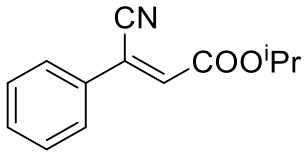


methyl (Z)-3-cyano-3-phenylacrylate (1a): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.82-7.67 (m, 2H), 7.59-7.42 (m, 3H), 6.89 (s, 1H), 3.90 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.94, 131.94, 131.88, 129.56, 129.12, 127.25, 126.57, 115.25, 52.78.

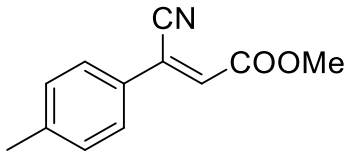


ethyl (Z)-3-cyano-3-phenylacrylate (1b): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ:

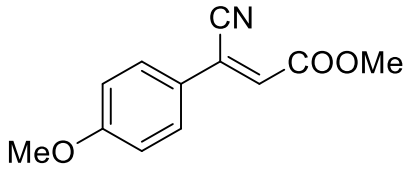
7.80-7.66 (m, 2H), 7.60-7.40 (m, 3H), 6.88 (s, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.48, 132.05, 131.79, 129.67, 129.54, 127.22, 126.28, 115.30, 62.02, 14.31. **HRMS** calculated $[M+H]^+$ for $C_{12}H_{12}O_2N$ = 202.0863, found: 202.0856.



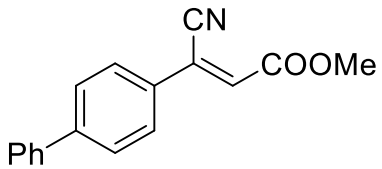
isopropyl (Z)-3-cyano-3-phenylacrylate (1c): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.83-7.63 (m, 2H), 7.56-7.40 (m, 3H), 6.86 (s, 1H), 5.21 (dt, *J*=12.5, 6.3 Hz, 1H), 1.36 (d, *J*=6.3 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.02, 132.16, 131.72, 130.26, 129.53, 127.22, 126.02, 115.38, 69.99, 21.98. **HRMS** calculated $[M+H]^+$ for $C_{13}H_{14}O_2N$ = 216.1019, found: 216.1015.



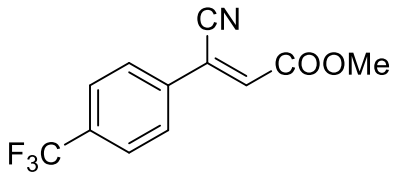
methyl (Z)-3-cyano-3-(p-tolyl)acrylate (1d): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.61 (d, *J*=8.3 Hz, 2H), 7.30-7.25 (m, 2H), 6.84 (s, 1H), 3.89 (s, 3H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 164.14, 142.69, 130.29, 129.25, 127.84, 127.23, 126.56, 115.37, 52.73, 21.69.



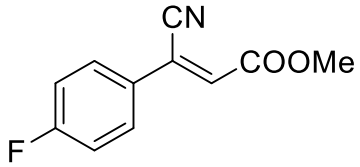
methyl (Z)-3-cyano-3-(4-methoxyphenyl)acrylate (1e): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ:7.68 (d, *J* = 8.8 Hz, 2H), 6.97 (d, *J* = 8.8 Hz, 2H), 6.77 (s, 1H), 3.88 (s, 3H), 3.87 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 164.27, 162.66, 128.99, 126.14, 126.07, 124.39, 115.42, 114.96, 55.81, 52.62.



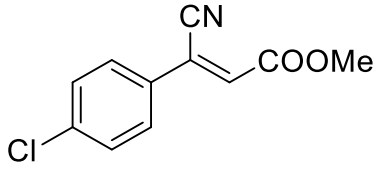
methyl (Z)-3-([1,1'-biphenyl]-4-yl)-3-cyanoacrylate (1f): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.82-7.76 (m, 2H), 7.72-7.67 (m, 2H), 7.64-7.59 (m, 2H), 7.51-7.44 (m, 2H), 7.44-7.38 (m, 1H), 6.92 (s, 1H), 3.90 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 164.03, 144.73, 139.58, 130.77, 129.28, 128.60, 128.49, 128.12, 127.79, 127.35, 126.21, 115.28, 52.82. **HRMS** calculated $[M+H]^+$ for $C_{17}H_{14}O_2N$ = 264.1019, found: 264.1016.



methyl (Z)-3-cyano-3-(4-(trifluoromethyl)phenyl)acrylate (1g): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.3 Hz, 2H), 7.75 (d, *J* = 8.4 Hz, 2H), 6.98 (s, 1H), 3.92 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.47, 135.37, 133.48 (q, *J* = 33.1 Hz), 131.47, 127.73, 126.61 (q, *J* = 3.7 Hz), 125.19, 123.67 (q, *J* = 275.1 Hz), 114.80, 53.03. **HRMS** calculated $[M+H]^+$ for $C_{12}H_9O_2NF_3$ = 256.0580, found: 256.0575.

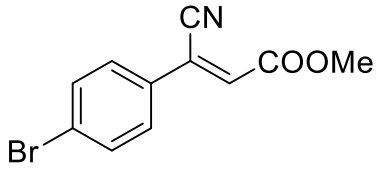


methyl (Z)-3-cyano-3-(4-fluorophenyl)acrylate (1h): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.81-7.67 (m, 2H), 7.24-7.13 (m, 2H), 6.85 (s, 1H), 3.90 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 166.07, 163.66 (d, *J* = 24.1 Hz), 129.43 (d, *J* = 8.9 Hz), 128.88 (d, *J* = 2.2 Hz), 128.13 (d, *J* = 3.4 Hz), 125.35, 116.80 (d, *J* = 22.3 Hz), 115.11, 52.78.

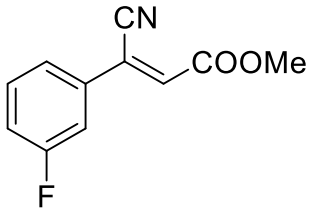


methyl (Z)-3-(4-chlorophenyl)-3-cyanoacrylate (1i): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.71-7.61 (m, 2H), 7.50-7.41 (m, 2H), 6.89 (s, 1H), 3.90 (s, 3H). ^{13}C

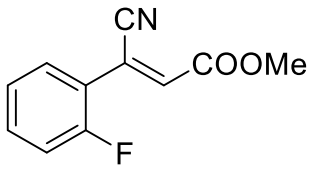
NMR (101 MHz, $CDCl_3$) δ: 163.69, 138.17, 130.37, 129.82, 129.40, 128.48, 125.32, 114.93, 52.85.



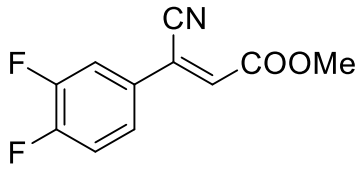
methyl (Z)-3-(4-bromophenyl)-3-cyanoacrylate (1j): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.66-7.54 (m, 4H), 6.90 (s, 1H), 3.89 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.64, 132.75, 130.81, 129.44, 128.61, 126.54, 125.37, 114.82, 52.82. **HRMS** calculated $[M+H]^+$ for $C_{11}H_9O_2NBr$ = 265.9811, found: 265.9805.



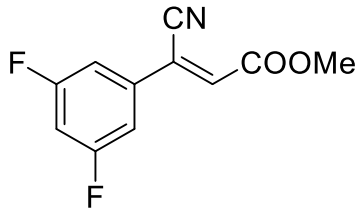
methyl (Z)-3-cyano-3-(3-fluorophenyl)acrylate (1k): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.59-7.38 (m, 3H), 7.24-7.19 (m, 1H), 6.90 (s, 1H), 3.91 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.64, 163.22 (d, J = 248.8 Hz), 134.09 (d, J = 7.9 Hz), 131.34 (d, J = 8.3 Hz), 130.35, 125.41 (d, J = 2.9 Hz), 123.19 (d, J = 3.0 Hz), 118.94 (d, J = 21.2 Hz), 114.92, 114.27 (d, J = 23.9 Hz), 52.97. **HRMS** calculated $[M+H]^+$ for $C_{11}H_9O_2NF$ = 206.0612, found: 206.0608.



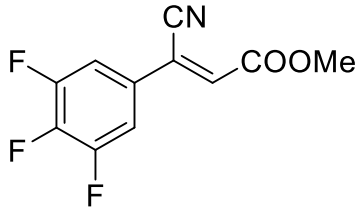
methyl (Z)-3-cyano-3-(2-fluorophenyl)acrylate (1l): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.75-7.71 (m, 1H), 7.52-7.44 (m, 1H), 7.33-7.27 (m, 1H), 7.22-7.17 (m, 1H), 7.05 (s, 1H), 3.91 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.97, 160.58 (d, J = 255.0 Hz), 134.15 (d, J = 12.5 Hz), 133.13 (d, J = 9.1 Hz), 131.09, 125.33 (d, J = 3.8 Hz), 121.17 (d, J = 3.0 Hz), 120.47 (d, J = 10.2 Hz), 117.18 (d, J = 22.4 Hz), 114.98, 52.90. **HRMS** calculated $[M+H]^+$ for $C_{11}H_9O_2NF$ = 206.0612, found: 206.0608.



methyl (Z)-3-cyano-3-(3,4-difluorophenyl)acrylate (1m): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.58-7.50 (m, 2H), 7.41-7.19 (m, 1H), 6.85 (s, 1H), 3.91 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.51, 153.00 (dd, *J* = 173.6, 13.0 Hz), 150.48 (dd, *J* = 168.7, 12.9 Hz), 130.09 (d, *J* = 2.3 Hz), 129.03 (dd, *J* = 6.0, 3.9 Hz), 124.48 (t, *J* = 2.0 Hz), 124.13 (dd, *J* = 6.9, 3.7 Hz), 118.73 (d, *J* = 18.0 Hz), 116.51 (d, *J* = 19.5 Hz), 114.76, 52.99. **HRMS** calculated $[M+H]^+$ for $C_{11}H_8O_2NF_2$ = 224.0518, found: 224.0515.

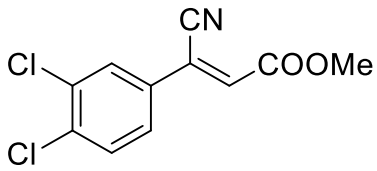


methyl (Z)-3-cyano-3-(3,5-difluorophenyl)acrylate (1n): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.32-7.22 (m, 2H), 7.00-6.96 (m, 1H), 6.92 (s, 1H), 4.13-3.76 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.59 (dd, *J* = 251.4, 12.9 Hz), 163.32, 135.04 (t, *J* = 9.8 Hz), 131.45, 124.37 (t, *J* = 3.2 Hz), 114.54, 110.59 (d, *J* = 27.8 Hz), 107.28 (t, *J* = 25.3 Hz), 53.10. **HRMS** calculated $[M+H]^+$ for $C_{11}H_8O_2NF_2$ = 224.0518, found: 224.0516.

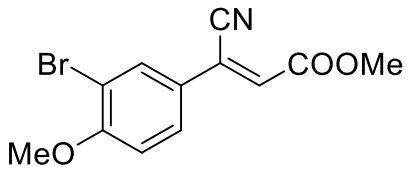


methyl (Z)-3-cyano-3-(3,4,5-trifluorophenyl)acrylate (1o): white solid;^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41 (dd, *J* = 7.9, 6.3 Hz, 2H), 6.86 (s, 1H), 3.92 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.6, 152.23 (ddd, *J* = 253.2, 11.9, 4.1 Hz), 142.34 (dt, *J*

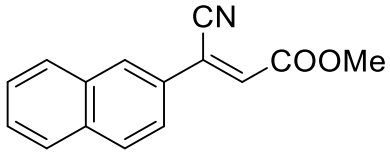
= 259.7, 15.2 Hz), 131.59 (d, *J* = 2.4 Hz), 128.49 (d, *J* = 4.8 Hz), 124.07 (d, *J* = 2.6 Hz), 114.76, 112.40 (d, *J* = 23.6 Hz). 53.5. **HRMS** calculated $[M+H]^+$ for $C_{11}H_7O_2NF_3$ = 242.0423, found: 242.0419.



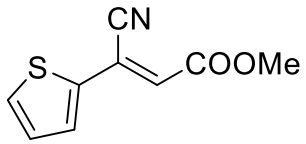
methyl (Z)-3-cyano-3-(3,4-dichlorophenyl)acrylate (1p): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.81 (t, *J* = 1.2 Hz, 1H), 7.57 (d, *J* = 1.2 Hz, 2H), 6.90 (s, 1H), 3.91 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.47, 136.44, 134.23, 131.80, 131.58, 130.53, 129.00, 126.32, 124.31, 114.63, 53.05.



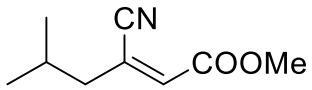
methyl (Z)-3-(3-bromo-4-methoxyphenyl)-3-cyanoacrylate (1q): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.91 (d, *J* = 2.4 Hz, 1H), 7.69 (dd, *J* = 8.7, 2.4 Hz, 1H), 6.97 (d, *J* = 8.7 Hz, 1H), 6.78 (s, 1H), 3.97 (s, 3H), 3.89 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.98, 158.82, 131.84, 128.40, 127.49, 125.61, 124.84, 115.08, 113.09, 112.21, 56.84, 52.84. **HRMS** calculated $[M+H]^+$ for $C_{12}H_{11}O_3NBr$ = 295.9917, found: 295.9914.



methyl (Z)-3-cyano-3-(naphthalen-2-yl)acrylate (1r): yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.18 (d, *J* = 1.5 Hz, 1H), 7.84-7.78 (m, 3H), 7.62-7.48 (m, 3H), 6.91 (s, 1H), 3.88 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.85, 134.43, 132.83, 129.31, 129.07, 129.02, 128.80, 128.49, 128.37, 127.80, 127.41, 126.12, 122.03, 115.14, 52.60. **HRMS** calculated $[M+H]^+$ for $C_{15}H_{12}O_2N$ = 238.0863, found: 238.0859.



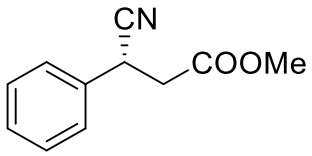
methyl (E)-3-cyano-3-(thiophen-2-yl)acrylate (1s): white solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.63 (dd, *J* = 3.8, 1.0 Hz, 1H), 7.49 (dd, *J* = 5.0, 1.0 Hz, 1H), 7.14 (dd, *J* = 5.0, 3.8 Hz, 1H), 6.68 (s, 1H), 3.88 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.90, 136.92, 132.25, 130.42, 128.97, 125.43, 120.46, 114.31, 52.74. **HRMS** calculated $[M+H]^+$ for $C_9H_8O_2NS$ = 194.0270, found: 194.0266.



methyl (Z)-3-cyano-5-methylhex-2-enoate (1t): colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 6.35 (t, *J* = 1.2 Hz, 1H), 3.83 (s, 3H), 2.29 (dd, *J* = 7.3, 1.2 Hz, 2H), 2.17-1.99 (m, 1H), 0.98 (d, *J* = 6.7 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.32, 132.75, 127.59, 116.08, 52.31, 44.78, 27.14, 21.91.

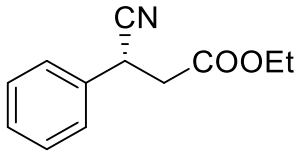
3. General Procedure for Asymmetric Hydrogenation of compound 1

A stock solution was made by mixing $[Rh(NBD)_2]BF_4$ with ZhaoPhos in a 1:1.1 molar ratio in CF_3CH_2OH at room temperature for 30 min in a nitrogen-filled glovebox. An aliquot of the catalyst solution (0.1mL, 0.001 mmol) was transferred by syringe into the vials charged with different substrates (0.1 mmol for each) in anhydrous CF_3CH_2OH (1.0 mL). The vials were subsequently transferred into an autoclave into which hydrogen gas was charged. The reaction was then stirred under H_2 (50 atm) at room temperature for 18-20 h. The hydrogen gas was released slowly and carefully. The solution was concentrated and passed through a short column of silica gel (eluant: EtOAc) to remove the metal complex. The ee values of all compounds **2** were determined by HPLC or GC analysis on a chiral stationary phase.

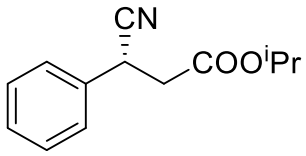


methyl (R)-3-cyano-3-phenylpropanoate (2a): colorless oil; Isolated yield: 97%; 98%

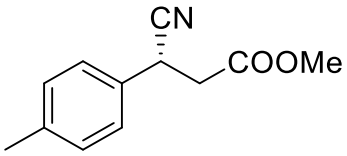
ee; $[\alpha]_{20}^{D}$ = 16.1 (c = 1.0, MeOH);(Lit [1] $[\alpha]_D$ = 14.9 (c = 1.1, MeOH) for (R)-2a with ee = 94%); The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 92:8; flow rate = 0.8 mL/min; UV detection at 210 nm; t_R = 16.7 min (major), 24.6 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.43-7.31 (m, 5H), 4.30 (dd, *J* = 8.3, 6.6 Hz, 1H), 3.71 (s, 3H), 2.94 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.83, 134.57, 129.48, 128.77, 127.51, 120.14, 52.54, 39.95, 33.30.



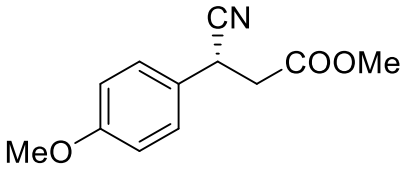
ethyl (R)-3-cyano-3-phenylpropanoate (2b): colorless oil; Isolated yield: 98%; 98% ee; $[\alpha]_{20}^{D}$ = 15.9 (c = 1.0, MeOH); The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 13.3 min (major), 17.3 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.44-7.32 (m, 5H), 4.29 (dd, *J* = 8.3, 6.7 Hz, 1H), 4.16 (qd, *J* = 7.1, 1.3 Hz, 2H), 2.91 (m, 2H), 1.23 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.23, 134.55, 129.31, 128.59, 127.42, 120.08, 61.46, 39.99, 33.19, 14.13. **HRMS** calculated $[M+H]^+$ for $C_{12}H_{14}O_2N$ = 204.1019, found: 204.1017.



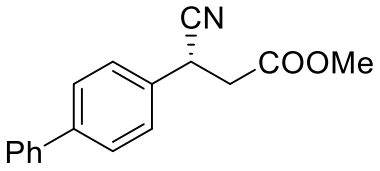
isopropyl (R)-3-cyano-3-phenylpropanoate (2c): colorless oil; Isolated yield: 98%; 96% ee; $[\alpha]_{20}^{D}$ = 14.3 (c = 1.0, MeOH); The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 9.4 min (major), 10.6 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.47-7.30 (m, 5H), 5.03 (hept, *J* = 6.3 Hz, 1H), 4.28 (dd, *J* = 8.3, 6.8 Hz, 1H), 3.07-2.73 (m, 2H), 1.21 (dd, *J* = 19.3, 6.3 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 168.84, 134.64, 129.42, 128.72, 127.55, 120.17, 69.39, 40.44, 33.41, 21.90, 21.84. **HRMS** calculated $[M+H]^+$ for $C_{13}H_{16}O_2N$ = 218.1176, found: 218.1172.



methyl (R)-3-cyano-3-(p-tolyl)propanoate (2d): colorless oil; Isolated yield: 98%; 98% ee; $[\alpha]_{20}^{D}$ = 8.2 (c = 1.0, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 14.7 min (major), 17.1 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.14 (dd, *J* = 24.9, 8.1 Hz, 4H), 4.28-4.10 (m, 1H), 3.63 (s, 3H), 2.84 (m, 2H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.90, 138.66, 131.56, 130.11, 127.37, 120.30, 52.51, 40.02, 32.95, 21.26.

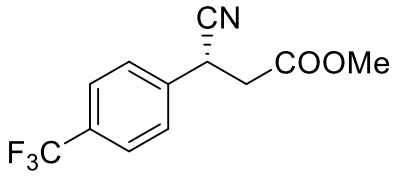


methyl (R)-3-cyano-3-(4-methoxyphenyl)propanoate (2e): colorless oil; Isolated yield: 99%; 97% ee; $[\alpha]_{20}^{D}$ = 10.6 (c = 1.0, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 22.5 min (major), 27.0 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.28 (d, *J* = 8.6 Hz, 2H), 6.90 (d, *J* = 8.7 Hz, 2H), 4.25 (t, *J* = 7.5 Hz, 1H), 3.80 (s, 3H), 3.71 (s, 3H), 2.91 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.92, 159.82, 128.72, 126.48, 120.40, 114.79, 55.53, 52.52, 40.09, 32.57

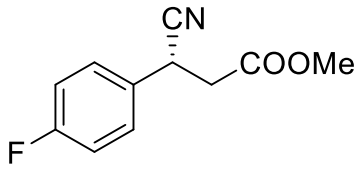


methyl (R)-3-([1,1'-biphenyl]-4-yl)-3-cyanopropanoate (2f): white solid; Isolated yield: 98%; 98% ee; $[\alpha]_{20}^{D}$ = -16.0 (c = 1.0, MeOH); The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 27.7 min (major), 36.1 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.62-7.55 (m, 4H), 7.46-7.42 (m, 4H), 7.39-7.33 (m,

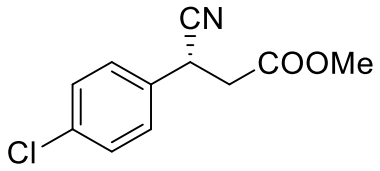
1H), 4.40-4.30 (m, 1H), 3.72 (s, 3H), 2.97 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.84, 141.77, 140.23, 133.51, 129.10, 128.16, 127.99, 127.94, 127.28, 120.12, 52.60, 39.94, 33.04. **HRMS** calculated $[M+H]^+$ for $C_{17}H_{16}O_2N$ = 266.1176, found: 266.1171.



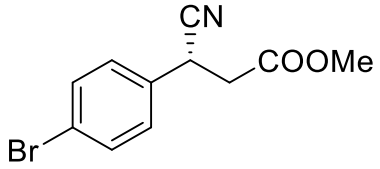
methyl (R)-3-cyano-3-(4-(trifluoromethyl)phenyl)propanoate (2g): white solid; Isolated yield: 97%; 98% ee; $[\alpha]_{20}^{D}$ = 8.8 (c = 1.0, MeOH); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 12.8 min (major), 14.1 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.66 (d, *J* = 8.2 Hz, 2H), 7.52 (d, *J* = 8.2 Hz, 2H), 4.38 (t, *J* = 7.3 Hz, 1H), 3.72 (s, 3H), 2.96 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.31, 138.35, 130.99 (q, *J* = 32.8 Hz), 127.99, 126.34 (q, *J* = 3.7 Hz), 122.35 (q, *J* = 271.0 Hz), 119.23, 52.53, 39.42, 32.92. **HRMS** calculated $[M+H]^+$ for $C_{12}H_{11}O_2NF_3$ = 258.0736, found: 258.0726.



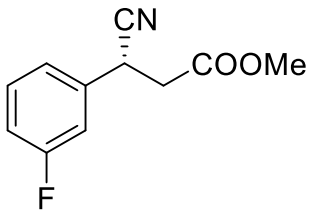
methyl (R)-3-cyano-3-(4-fluorophenyl)propanoate (2h): colorless oil; Isolated yield: 96%; 97% ee; $[\alpha]_{20}^{D}$ = 6.3(c = 1.0, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 23.2 min (major), 15.0 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41-7.32 (m, 2H), 7.13-7.04 (m, 2H), 4.30 (t, *J* = 7.4 Hz, 1H), 3.72 (s, 3H), 2.93 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.70, 162.82 (d, *J* = 248.2 Hz), 130.42 (d, *J* = 3.3 Hz), 129.42 (d, *J* = 8.4 Hz), 119.98, 116.51 (d, *J* = 21.9 Hz), 52.62, 39.96, 32.62.



methyl (R)-3-(4-chlorophenyl)-3-cyanopropanoate (2i): colorless oil; Isolated yield: 97%; 97% ee; $[\alpha]_{20}^{D}$ = 9.7(c = 1.0, MeOH); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 14.4 min (major), 15.8 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.42-7.29 (m, 4H), 4.29 (t, *J* = 7.4 Hz, 1H), 3.72 (s, 3H), 2.93 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.61, 134.86, 133.09, 129.69, 129.01, 119.74, 52.65, 39.77, 32.74.

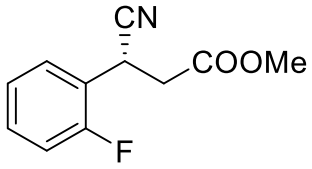


methyl (R)-3-(4-bromophenyl)-3-cyanopropanoate (2j): colorless oil; Isolated yield: 98%; 96% ee; $[\alpha]_{20}^{D}$ = 11.4(c = 1.0, MeOH); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 15.0 min (major), 16.4 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.51 (dd, *J* = 8.5, 2.2 Hz, 2H), 7.30-7.21 (m, 2H), 4.28 (t, *J* = 7.4 Hz, 1H), 3.71 (d, *J* = 2.3 Hz, 3H), 2.93 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.54, 133.55, 132.55, 129.26, 122.84, 119.64, 52.59, 39.57, 32.72. **HRMS** calculated $[M+H]^+$ for $C_{11}H_{11}O_2NBr$ = 267.9968, found: 267.9960.

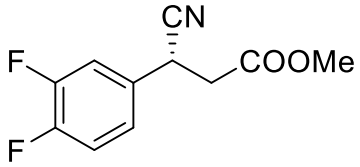


methyl (R)-3-cyano-3-(3-fluorophenyl)propanoate (2k): colorless oil; Isolated yield: 97%; 97% ee; $[\alpha]_{20}^{D}$ = 12.4(c = 1.0, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95:5; flow rate = 1.0

mL/min; UV detection at 210 nm; t_R = 11.8 min (major), 14.3 min (minor).^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.43-7.33 (m, 1H), 7.18-7.16 (m, 1H), 7.12-7.04 (m, 2H), 4.31 (t, *J* = 7.4 Hz, 1H), 3.73 (s, 3H), 2.95 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.62, 163.14 (d, *J* = 248.1 Hz), 136.84 (d, *J* = 7.4 Hz), 131.20 (d, *J* = 8.3 Hz), 123.31 (d, *J* = 3.1 Hz), 119.62, 115.95 (d, *J* = 21.0 Hz), 114.87 (d, *J* = 22.9 Hz), 52.68, 39.72, 33.00 (d, *J* = 1.8 Hz). **HRMS** calculated $[M+H]^+$ for $C_{11}H_{11}O_2NF$ = 208.0768, found: 208.0764.

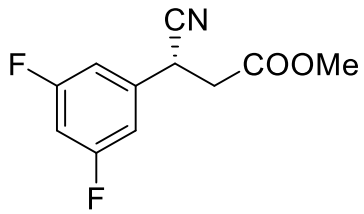


methyl (R)-3-cyano-3-(2-fluorophenyl)propanoate (2l): colorless oil; Isolated yield: 98%; 99% ee; $[\alpha]_{20}^D$ = 27.9(c = 1.0, $CHCl_3$); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 10.9 min (major), 11.6 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.51-7.47 (m, 1H), 7.39-7.34 (m, 1H), 7.20-7.18 (m, 1H), 7.15-7.08 (m, 1H), 4.53 (dd, *J* = 8.6, 6.0 Hz, 1H), 3.74 (s, 3H), 2.97 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.65, 160.04 (d, *J* = 248.4 Hz), 130.89 (d, *J* = 8.3 Hz), 129.50 (d, *J* = 3.0 Hz), 125.14 (d, *J* = 3.7 Hz), 121.66 (d, *J* = 13.7 Hz), 119.14, 116.29 (d, *J* = 21.0 Hz), 52.61, 38.03 (d, *J* = 1.4 Hz), 27.77 (d, *J* = 3.3 Hz). **HRMS** calculated $[M+H]^+$ for $C_{11}H_{11}O_2NF$ = 208.0768, found: 208.0764.

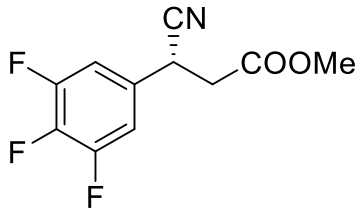


methyl (R)-3-cyano-3-(3,4-difluorophenyl)propanoate (2m): white solid; Isolated yield: 97%; 95% ee; $[\alpha]_{20}^D$ = 10.3(c = 1.0, MeOH); The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 92:8; flow rate = 0.8 mL/min; UV detection at 210 nm; t_R = 21.4 min (major), 27.3 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.13 (m, 3H), 4.29 (t, *J* = 7.3 Hz, 1H), 3.73 (s, 3H),

2.94 (m, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.50, 150.63 (dt, *J* = 250.6, 12.3 Hz,), 131.47 (dd, *J* = 5.6, 4.1 Hz), 123.97 (dd, *J* = 6.6, 3.8 Hz), 119.47, 118.45 (d, *J* = 17.7 Hz), 117.07 (d, *J* = 18.5 Hz), 52.73, 39.69, 32.53 (d, *J* = 1.2 Hz). **HRMS** calculated $[M+H]^+$ for $C_{11}H_{10}O_2NF_2$ = 226.0674, found: 226.0667.

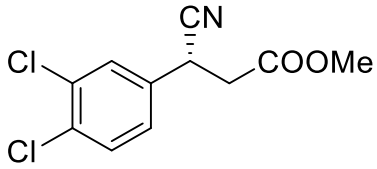


methyl (R)-3-cyano-3-(3,5-difluorophenyl)propanoate (2n): white solid; Isolated yield: 96%; 96% ee; $[\alpha]_{20}^{D}$ = 10.4(c = 1.0, MeOH); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95:5, flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 10.9 min (major), 13.8 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.00-6.92 (m, 2H), 6.85-6.79 (m, 1H), 4.32 (t, *J* = 7.3 Hz, 1H), 3.74 (s, 3H), 2.96 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.41, 163.47 (dd, *J* = 250.9 Hz, 13.0 Hz), 138.12 (t, *J* = 9.4 Hz), 119.09, 111.02 (d, *J* = 26.8 Hz), 104.59 (t, *J* = 25.1 Hz), 52.78, 39.42, 32.91 (t, *J* = 2.1 Hz). **HRMS** calculated $[M+H]^+$ for $C_{11}H_{10}O_2NF_2$ = 226.0674, found: 226.0666.

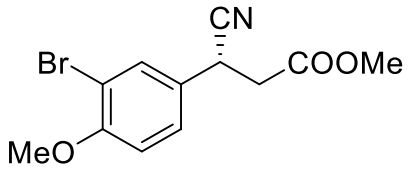


methyl (R)-3-cyano-3-(3,4,5-trifluorophenyl)propanoate (2o): white solid; Isolated yield: 98%; 90% ee; $[\alpha]_{20}^{D}$ = 9.6(c = 1.0, MeOH); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95:5, flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 10.1 min (major), 13.9 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.07 (dd, *J* = 7.6, 6.3 Hz, 2H), 4.28 (t, *J* = 7.3 Hz, 1H), 3.74 (s, 3H), 2.95 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.30, 151.68 (ddd, *J* = 252.5, 10.2, 4.1 Hz), 140.07 (dt, *J* = 254.1, 15.0 Hz, 2C), 130.80 (td, *J* = 7.6, 4.9 Hz),

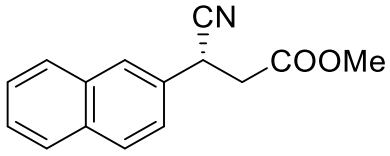
118.94, 112.38 (d, J = 22.8 Hz), 52.84, 39.42, 32.58. **HRMS** calculated $[M+H]^+$ for $C_{11}H_9O_2NF_3$ = 244.0580, found: 244.0573.



methyl (R)-3-cyano-3-(3,4-dichlorophenyl)propanoate (2p): colorless oil; Isolated yield: 97%; 90% ee; $[\alpha]_{20}^{D}$ = 5.2(c = 1.0, MeOH); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95:5, flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 13.5 min (major), 15.2 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.50-7.47 (m, 2H), 7.25 (dd, J = 8.3, 2.2 Hz, 1H), 4.29 (t, J = 7.3 Hz, 1H), 3.73 (s, 3H), 2.95 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.42, 134.63, 133.66, 133.31, 131.46, 129.72, 127.04, 119.25, 52.77, 39.53, 32.46.

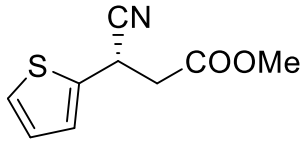


methyl (R)-3-(3-bromo-4-methoxyphenyl)-3-cyanopropanoate (2q): yellow solid; Isolated yield: 99%; 94% ee; $[\alpha]_{20}^{D}$ = 6.3(c = 1.0, MeOH); The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5, flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 33.8 min (major), 38.1 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.55 (d, J = 2.3 Hz, 1H), 7.30 (dd, J = 8.6, 2.4 Hz, 1H), 6.90 (d, J = 8.5 Hz, 1H), 4.24 (t, J = 7.4 Hz, 1H), 3.90 (s, 3H), 3.72 (s, 3H), 2.92 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.66, 156.22, 132.37, 127.86, 127.82, 119.88, 112.42, 56.53, 52.62, 39.85, 32.13. **HRMS** calculated $[M+H]^+$ for $C_{12}H_{13}O_3NBr$ = 298.0073, found: 298.0067.

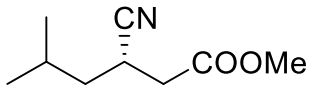


methyl (R)-3-cyano-3-(naphthalen-2-yl)propanoate (2r): yellow solid; Isolated

yield: 99%; 93% ee; $[\alpha]_{20}^{D}$ = 9.2 (c = 1.0, MeOH); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95:5, flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 17.6 min (major), 19.3 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.87-7.81 (m, 4H), 7.54-7.48 (m, 2H), 7.42 (dd, *J* = 8.5, 1.9 Hz, 1H), 4.46 (dd, *J* = 8.2, 6.7 Hz, 1H), 3.71 (s, 3H), 3.01 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.86, 133.42, 133.14, 131.80, 129.56, 128.14, 127.94, 127.07, 126.99, 126.87, 124.74, 120.18, 52.61, 39.94, 33.50. **HRMS** calculated $[M+H]^+$ for $C_{15}H_{14}O_2N$ = 240.1019, found: 240.1015.



methyl (S)-3-cyano-3-(thiophen-2-yl)propanoate (2s): colorless oil; Isolated yield: 96%; 94% ee; $[\alpha]_{20}^{D}$ = 6.9 (c = 1.0, MeOH); The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5, flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 18.4 min (major), 24.4 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.29 (dd, *J* = 5.2, 1.2 Hz, 1H), 7.14-7.10 (m, 1H), 6.99 (dd, *J* = 5.1, 3.6 Hz, 1H), 4.65-4.55 (m, 1H), 3.75 (s, 3H), 3.02 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.51, 136.21, 127.44, 126.95, 126.33, 119.25, 52.69, 40.08, 28.62. **HRMS** calculated $[M+H]^+$ for $C_9H_{10}O_2NS$ = 196.0427, found: 196.0425.



methyl (S)-3-cyano-5-methylhexanoate (2t): colorless oil; Isolated yield: 96%; 98% ee; $[\alpha]_{20}^{D}$ = -11.8(c = 1.0, MeOH); Enantiomeric excess was determined by GC with a Supelco's Beta Dex 225 column; Temperature program: 100 °C, stay 5 mins, 2 °C/min to 140 °C, Flow rate = 1.0 mL/min, t_R = 21.7 min (minor), 21.9 min (major). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 3.75 (s, 3H), 3.14-3.01 (m, 1H), 2.64 (m, 2H), 1.93-1.83 (m, 1H), 1.65 (ddd, *J* = 13.5, 10.7, 4.8 Hz, 1H), 1.34 (ddd, *J* = 13.6, 9.5, 5.1 Hz, 1H), 0.98 (d, *J* = 4.8 Hz, 3H), 0.96 (d, *J* = 4.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 170.44, 121.32, 52.43, 40.88, 37.08, 26.29, 25.96, 23.08, 21.38.

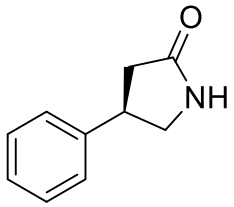
4. General procedures for gram-scale asymmetric hydrogenation and the synthesis of compound 3.

Gram-scale transformation of 1a:

A stock solution was made by mixing $[Rh(NBD)_2]BF_4$ with ZhaoPhos in a 1:1.1 molar ratio in CF_3CH_2OH at room temperature for 30 min in a nitrogen-filled glovebox. An aliquot of the catalyst solution (0.6 mL, 0.006 mmol) was transferred by syringe into the vials charged with substrate **1a** (6 mmol, 1.12g) in anhydrous CF_3CH_2OH (12 mL). The vials were subsequently transferred into an autoclave into which hydrogen gas was charged. The reaction was then stirred under H_2 (80 atm) at 30°C for 48 h. The hydrogen gas was released slowly and carefully. The solution was concentrated and passed through a short column of silica gel (eluant: EtOAc) to remove the metal complex. The ee values of all compounds **2a** were determined by HPLC analysis on Chiralpak OD-H column.

General procedure for the synthesis of compound 3 according to the literature [1]：

$NiCl_2·6H_2O$ (2 equiv, 2.6 mmol) followed by $NaBH_4$ (10 equiv, 14 mmol) were added to a solution of 2a (1.3mmol) in MeOH (8 mL). During addition, evolution of H_2 was observed and the reaction mixture turned black. The mixture was stirred at r.t. for 1 h, filtered through a Celite bed, concentrated, and extracted with EtOAc (2 × 20 mL). The solvent was evaporated to afford the desired product.



(R)-4-Phenylpyrrolidin-2-one [(R)-3]: colorless oil; Isolated yield: 85%; 98% ee; $[\alpha]_{20}^{D}$ = -33.8(c = 1.0, MeOH); The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 90:10, flow rate = 1.0 mL/min; UV detection at 210 nm; t_R = 9.8 min (major), 11.6 min (minor). ^{1}H NMR (400 MHz, $CDCl_3$) δ:7.40-7.30 (m, 5H), 3.72 (m, 1H), 3.65(m, 1H), 3.36 (dd, *J* = 9.0, 7.1 Hz,

1H), 2.68 (dd, *J* = 17.0, 8.9 Hz, 1H), 2.45 (dd, *J* = 17.0, 9.0 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ:177.31, 142.14, 128.88, 127.22, 126.72, 49.29, 40.40, 37.71.

5. General procedure for Job plot.

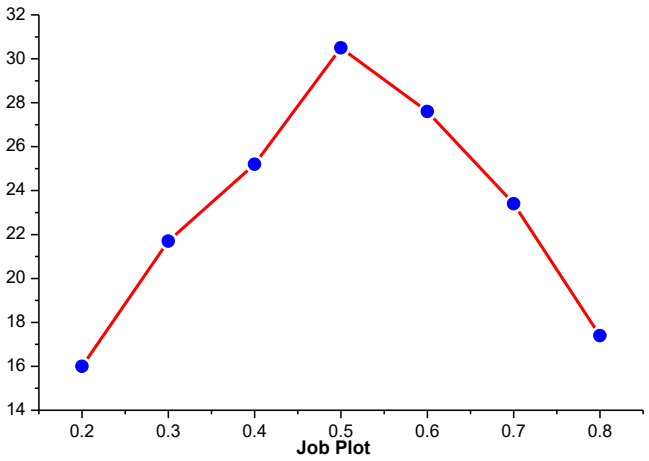
^{1}H NMR titration was conducted in chloroform-d, which was dried with potassium carbonate and degassed. The total concentration of the host (*N*-Me-ZhaoPhos or ZhaoPhos) and the guest (**1a**) was 0.02 M. The proportion of the concentration of the host vs the total concentration varied from 0.2 equivalent to 1.0. The chemical shifts of the two orho- protons on the 3,5-bis(trifluoromethyl)phenyl group were recorded. [Note: the other thiourea proton is buried in aromatic proton peaks and could not be measured when binding with low guest ratio]. A 1:1 binding pattern could also be observed in the Job plot.

Job plot of N-Me-ZhaoPhos

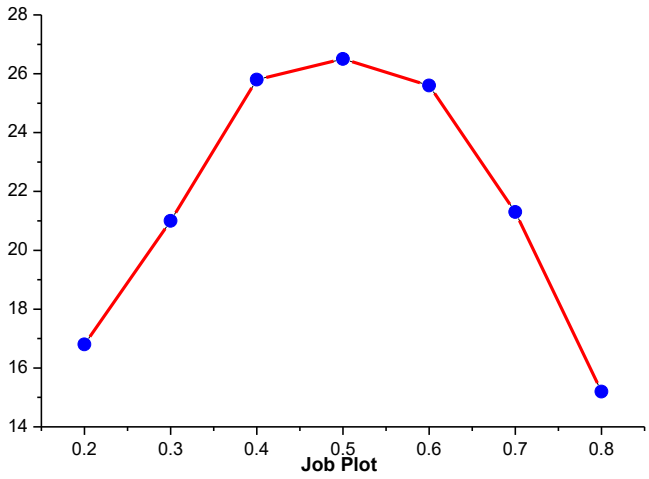
No.	C_1(host)	C_2(guest)	δ（Ar2H)	Δδ（Ar2H)	$\Delta\delta*10^4*C_1/0.02$
1	0.02	0	7.6488	0	0
2	0.016M	0.004M	7.6468	0.0020	16
3	0.014M	0.006M	7.6457	0.0031	21.7
4	0.012M	0.008M	7.6446	0.0042	25.2
5	0.01M	0.01M	7.6427	0.0061	30.5
6	0.008M	0.012M	7.6419	0.0069	27.6
7	0.006M	0.014M	7.6410	0.0078	23.4
8	0.04M	0.016M	7.6401	0.0087	17.4

Job plot of ZhaoPhos

No.	C_1(host)	C_2(guest)	δ（Ar2H)	Δδ（Ar2H)	$\Delta\delta*10^4*C_1/0.02$
1	0.02	0	7.7012	0	0
2	0.016M	0.004M	7.6991	0.0021	16.8
3	0.014M	0.006M	76982	0.0031	21.0
4	0.012M	0.008M	7.6969	0.0042	25.8
5	0.01M	0.01M	7.6959	0.0061	26.5
6	0.008M	0.012M	7.6948	0.0069	25.6
7	0.006M	0.014M	7.6941	0.0078	21.3
8	0.04M	0.016M	7.6936	0.0087	15.2



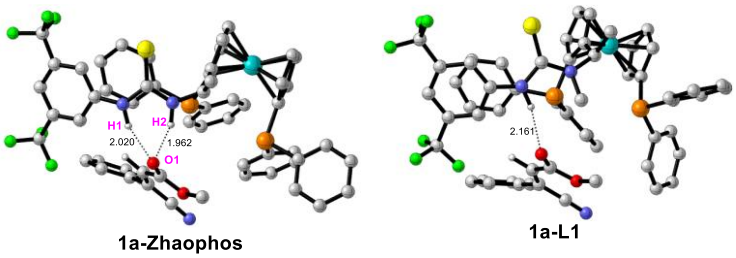
Job plot of **L1** and **1a**, x = c(**L1**)/[c(**L1**)+c(**1a**)], y = $\Delta\delta*10^4$*c(**L1**)/[c(**L1**)+c(**1a**)];



Job plot of ZhaoPhos and **1a**, x = c(ZhaoPhos)/[c(ZhaoPhos)+c(**1a**)], y = $\Delta\delta*10^4$*c(ZhaoPhos)/[c(ZhaoPhos)+c(**1a**)];

6. Computational details

Table S2. The absolute (in Hartree) and relative (in kcal/mol) energies for hydrogen bonds between different substrates with the ligand (Zhaophos or **L1** ligand) at 0 ºC, 20 ºC, 35 ºC and 60 ºC in gas phase by B3LYP-GD3BJ /6-31G** method.



1a-Zhaophos　　1a-L1

	G(0°C)	G(20°C)	G(35°C)	G(60°C)	ΔG(0°C)	ΔG(20°C)	ΔG(35°C)	ΔG(60°C)
1a	-629.681396	-629.684994	-629.687761	-629.692501				
Zp	-4789.270996	-4789.280107	-4789.287220	-4789.299608	0.0	0.0	0.0	0.0
substrates with Zhaophos(Zp) ligand								
1a-Zp	-5418.973685	-5418.984611	-5418.993159	-5419.008071	-13.4	-12.2	-11.4	-10.0
substrates with **L1** ligand								
L1	-4828.556698	-4828.566000	-4828.573264	-4828.585915	0.0	0.0	0.0	0.0
1a-L1	-5458.264252	-5458.275426	-5458.284168	-5458.299417	-16.4	-15.3	-14.5	-13.2

Cartesian coordinates of all optimized structures

ZhaoPhos(ZP)

C	-1.22835400	-2.49593300	-2.66017000
C	-1.02102600	-3.04491800	-1.36368400
H	-1.03465900	-4.09357400	-1.10757000
C	-0.83118800	-1.97490600	-0.44597900
C	-0.89336800	-0.73929300	-1.18934600
C	-1.15263600	-1.07986300	-2.55714700
H	-1.26953900	-0.37106400	-3.36339700
C	1.36291800	0.96345100	-0.78725800
C	2.10266100	1.90062400	-0.04769200
H	1.60925300	2.47587000	0.73293500
C	3.45547900	2.11782800	-0.31545500
H	4.01885800	2.84033100	0.26566300
C	4.09273400	1.37105600	-1.30542600
H	5.14974400	1.51157800	-1.50172600
C	3.38004700	0.39973600	-2.00898000

H	3.89084100	-0.21237800	-2.74508500
C	2.02227200	0.20067800	-1.75990000
H	1.47579600	-0.55085600	-2.31771700
C	-1.07458600	2.10774000	-1.67095000
C	-2.32916700	1.94534900	-2.27105600
H	-2.88216400	1.03774200	-2.08867400
C	-2.86749800	2.93642500	-3.08785000
H	-3.84441300	2.78687100	-3.53758300
C	-2.16399900	4.11912900	-3.31259000
H	-2.58344100	4.89611100	-3.94431500
C	-0.91420600	4.29380200	-2.71812400
H	-0.35192700	5.20680000	-2.89118900
C	-0.37154700	3.29818700	-1.90627300
H	0.60808300	3.44859300	-1.46678900
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C	-4.25175400	-3.09636300	-1.36254300
C	-4.03852800	-2.56399500	-0.05897300
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H	-6.31075900	3.61215100	-1.07937700

C	-4.40028000	4.23161100	-0.29196100
H	-4.47332100	5.23934000	-0.68858500
C	-3.28150300	3.85137600	0.44426200
H	-2.47721300	4.55855800	0.61884600
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C	-5.65066000	-0.33558000	2.14001000
C	-5.83442900	0.16013300	3.43948700
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F	7.90867000	2.04878500	2.44044500

F	6.52079800	-0.86669000	-2.24896400
F	6.61029500	-2.80855200	-1.27477100
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C	4.90827200	-1.37552200	0.38899800
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C	6.56188200	2.00488900	2.44360100
C	6.89271900	-1.50304700	-1.10528600
H	0.53210200	-0.49405500	1.77674500

1a-Zp

C	1.61556000	-3.56671200	2.45997400
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C	1.11971800	-1.64129800	1.26396200
C	1.36933300	-2.17262100	2.57428400
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C	-1.36975500	-0.29961000	1.34408700
C	-2.30495100	0.73262700	1.16024900
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C	5.57512300	2.85398900	1.41096000
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C	4.52220600	3.77178800	1.37165800
H	4.59760300	4.70861200	1.91516100
C	3.37768100	3.48832300	0.63190500
H	2.56258300	4.19935400	0.59184300
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H	2.37471200	2.05791900	-0.62172400
C	5.77966600	-0.25007000	-1.84589900
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H	7.13772900	1.09683300	-4.67200100
C	8.19302600	-0.17047700	-3.28267100
H	9.12568200	-0.14108900	-3.83762100
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F	-7.34849600	1.41419800	-2.16208000
F	-6.28835700	-2.99500300	1.69601500
F	-6.31732500	-4.38186900	0.02384700
F	-7.91498600	-2.91822400	0.25512300
C	1.12786500	-2.64112000	-1.17307400
H	1.85126400	-1.87975700	-1.48265700
C	1.46447700	-3.93596000	-1.91790000
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H	2.47382100	-4.26810900	-1.66338200
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C	-4.25932600	-0.23887000	-1.75888200
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C	-5.56332300	0.06174600	-1.39285400
C	-6.35231400	-0.87284500	-0.72096300
H	-7.36761200	-0.63850100	-0.42768200

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H	-4.50614200	5.66502300	2.41511200

L1

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F	7.97453600	1.93261400	2.36094000
F	6.46615700	-0.97395300	-2.38148000
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H	0.76267100	0.44521100	2.34888400

1a- L1

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C	3.65324500	1.61229400	-1.80096700
H	4.09453700	2.60293500	-1.82717900

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H	4.40987200	-1.65324300	-2.34393700
C	2.48806900	-0.91927300	-1.72645800
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C	-0.83044400	1.43294900	-1.44475500
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H	-4.66020700	4.13621900	2.31918800
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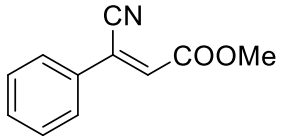
H	0.38974800	-1.98724100	3.27893500
H	-0.83465500	-1.03664100	2.40363600

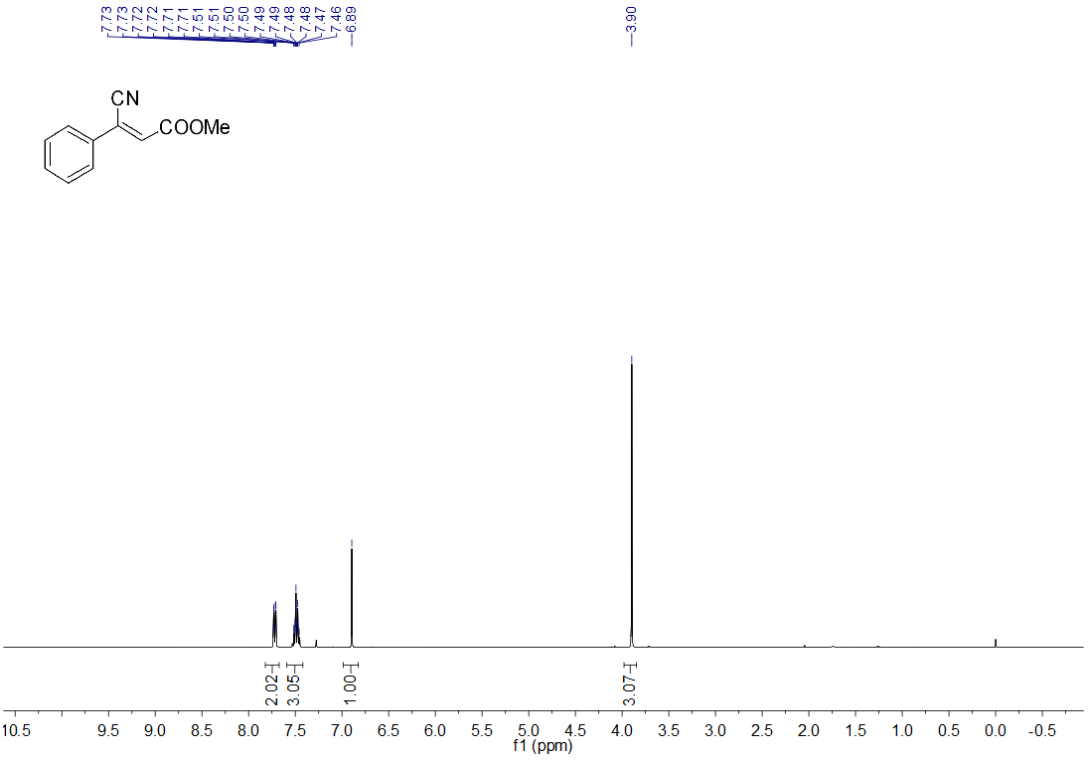
7. References

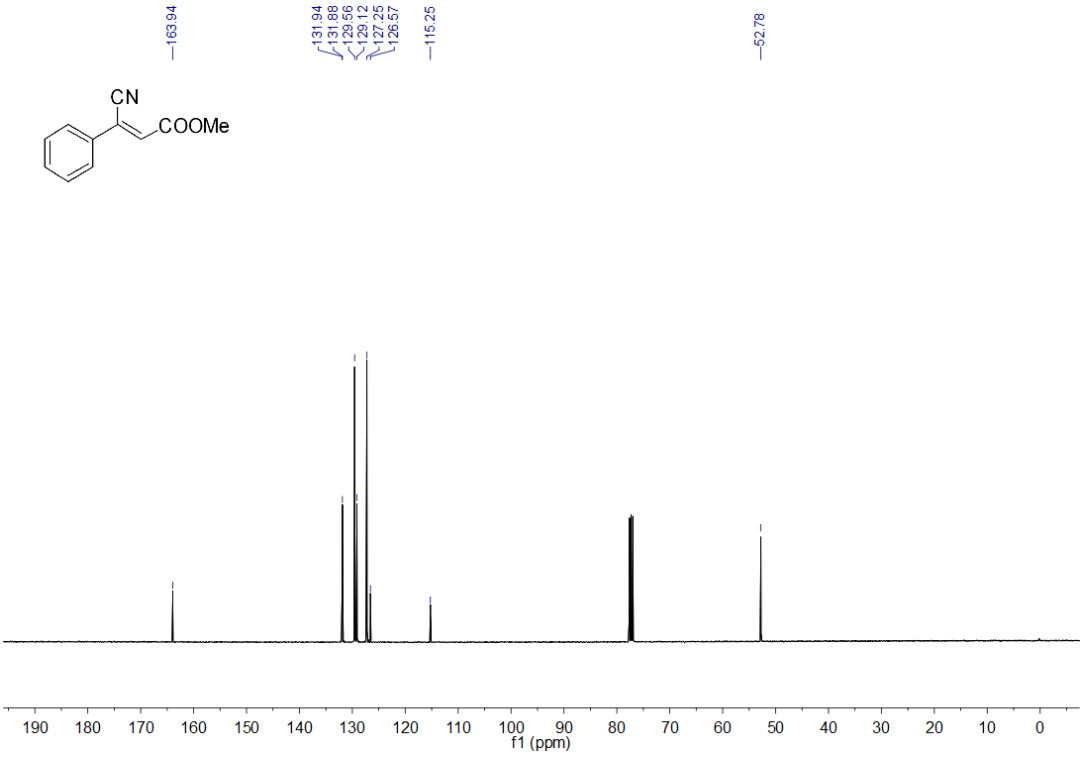
[1] E. Brenna, M. Crotti, F. G. Gatti, D. Monti, F. Parmeggiani, R. W. Powell III, S. Santangelo, J. D.Stewart, *Adv. Synth. Catal.* **2015**, *357*, 1849-1860.

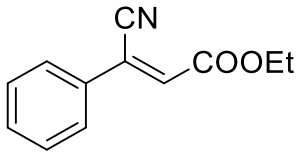
[2] C. K. Winkler, D. Clay, S. Davies, P. O'Neill, P. McDaid, S. Debarge, J. Steflik, M. Karmilowicz, J. W. Wong, K. Faber, *J. Org. Chem.* **2013**, *78*, 1525-1533.

8. NMR spectra of 1 and 2








CN
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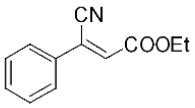
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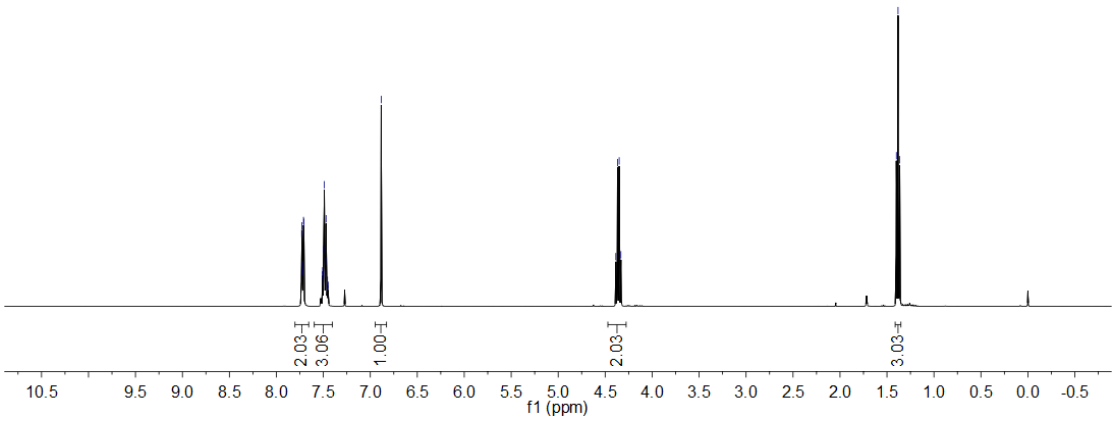
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5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


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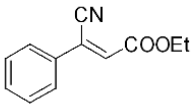
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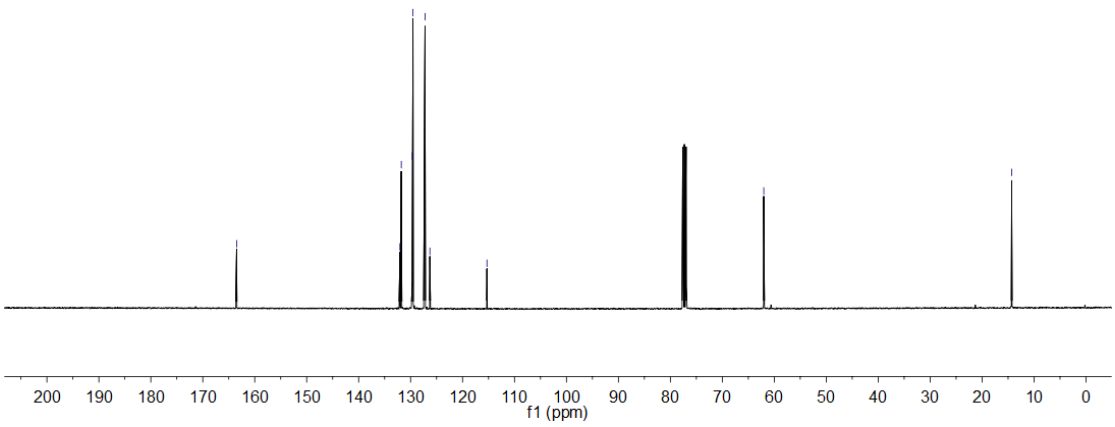
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10
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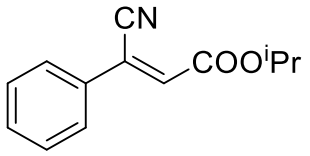
f1 (ppm)


CN
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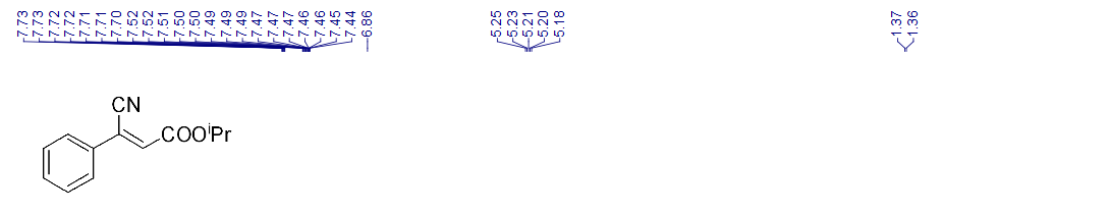
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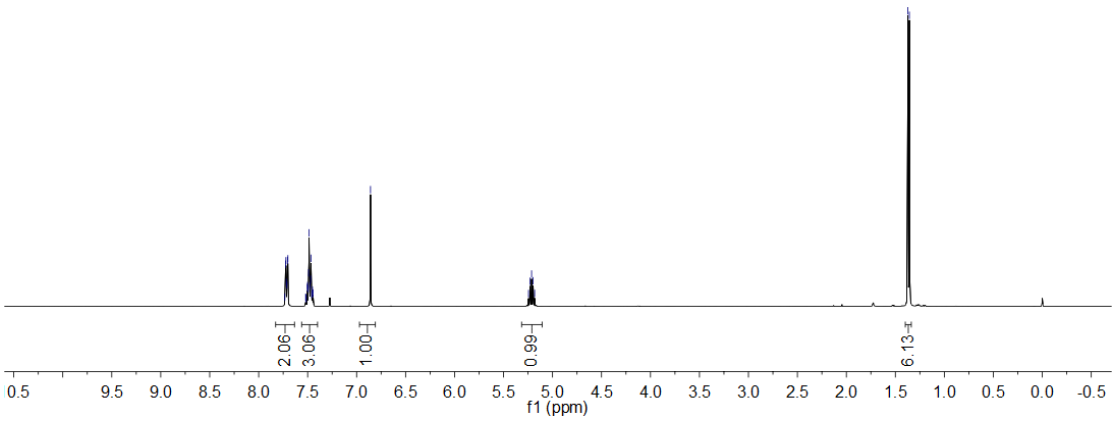
CN
COO^{i}Pr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2.5
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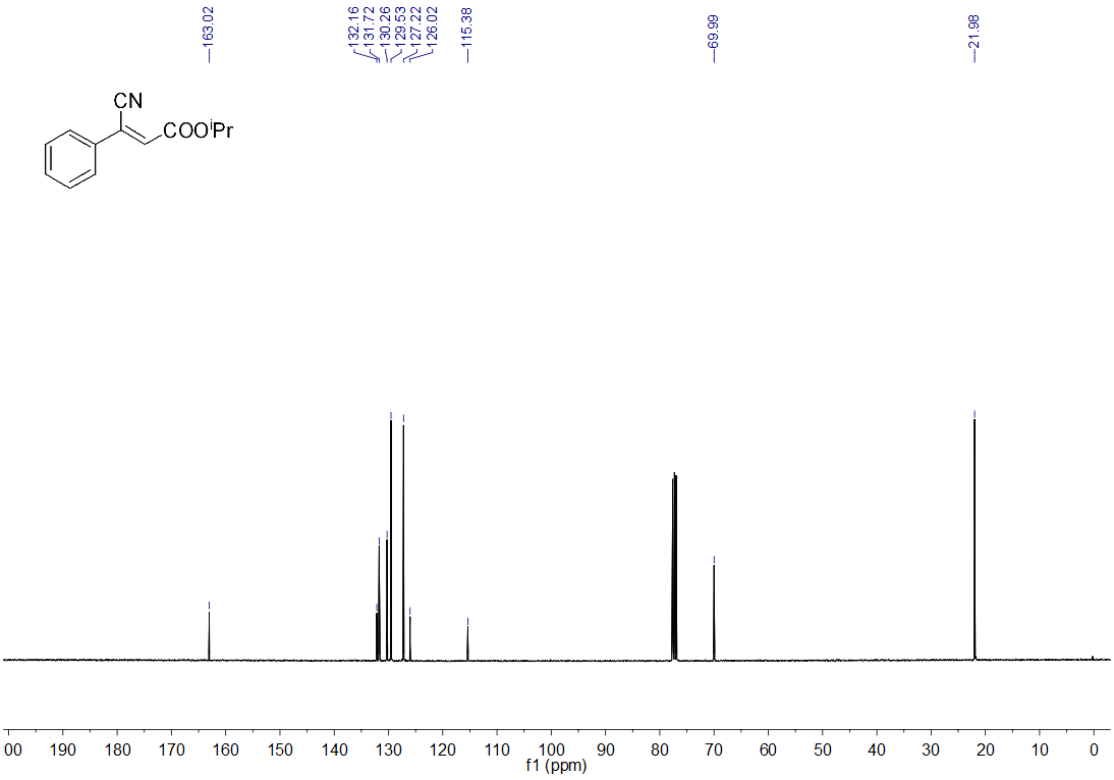
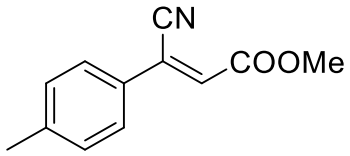
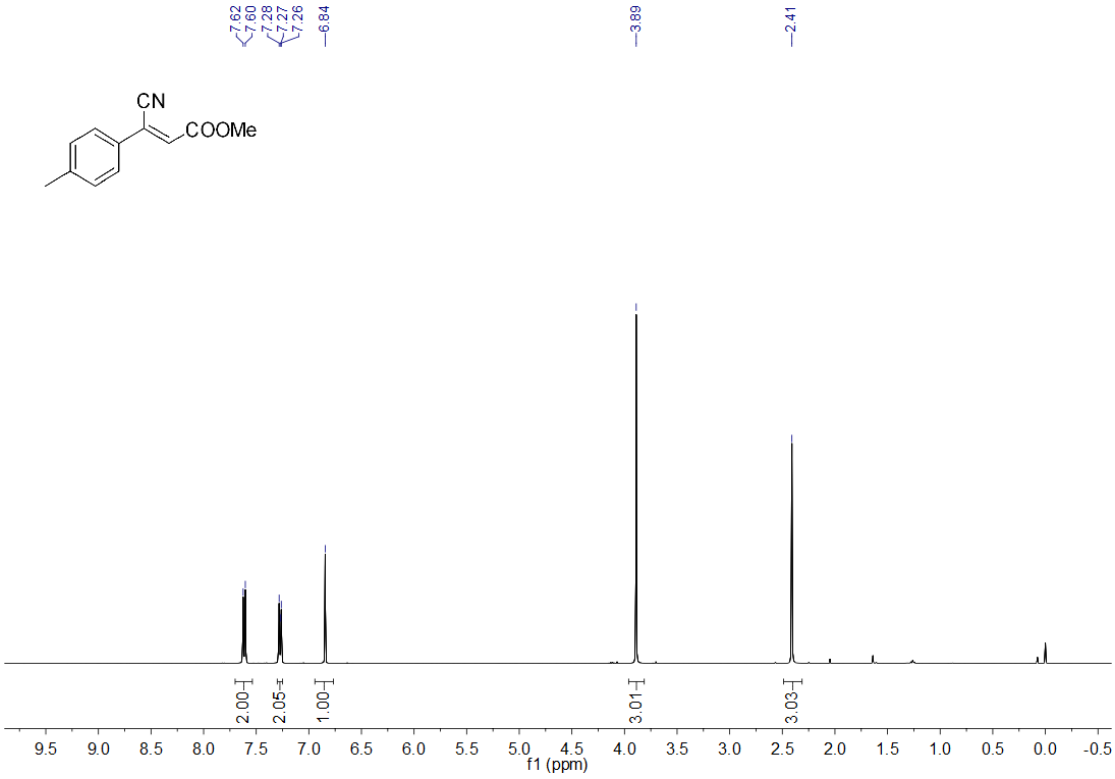
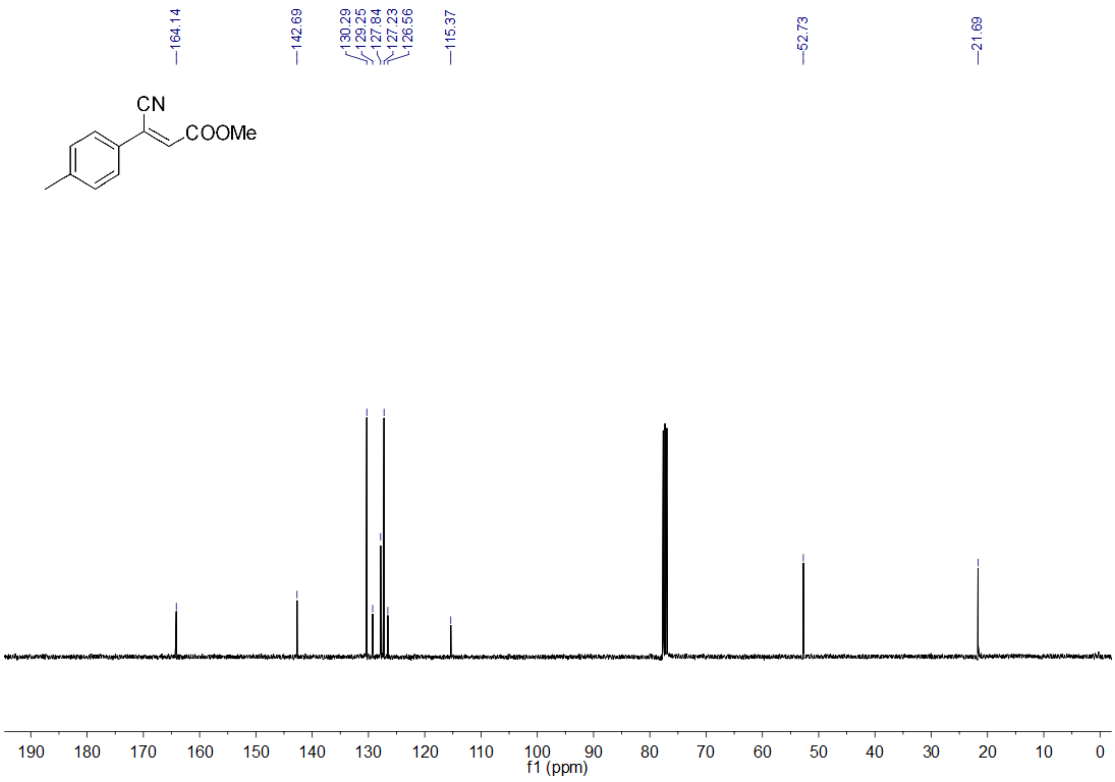
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


163.02
132.16
131.72
130.26
129.53
127.22
126.02
115.38
69.99
21.98
CN
COO^{i}Pr
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


CN
COOMe


7.62
7.60
7.28
7.27
7.26
6.84
3.89
2.41
CN
COOMe
2.00
2.05
1.00
3.01
3.03
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 -0.5
f1 (ppm)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142.69
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129.25
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127.23
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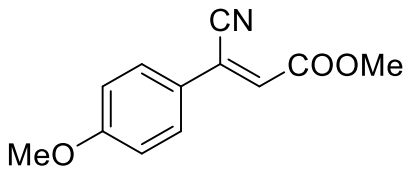
21.69
CN
COOMe
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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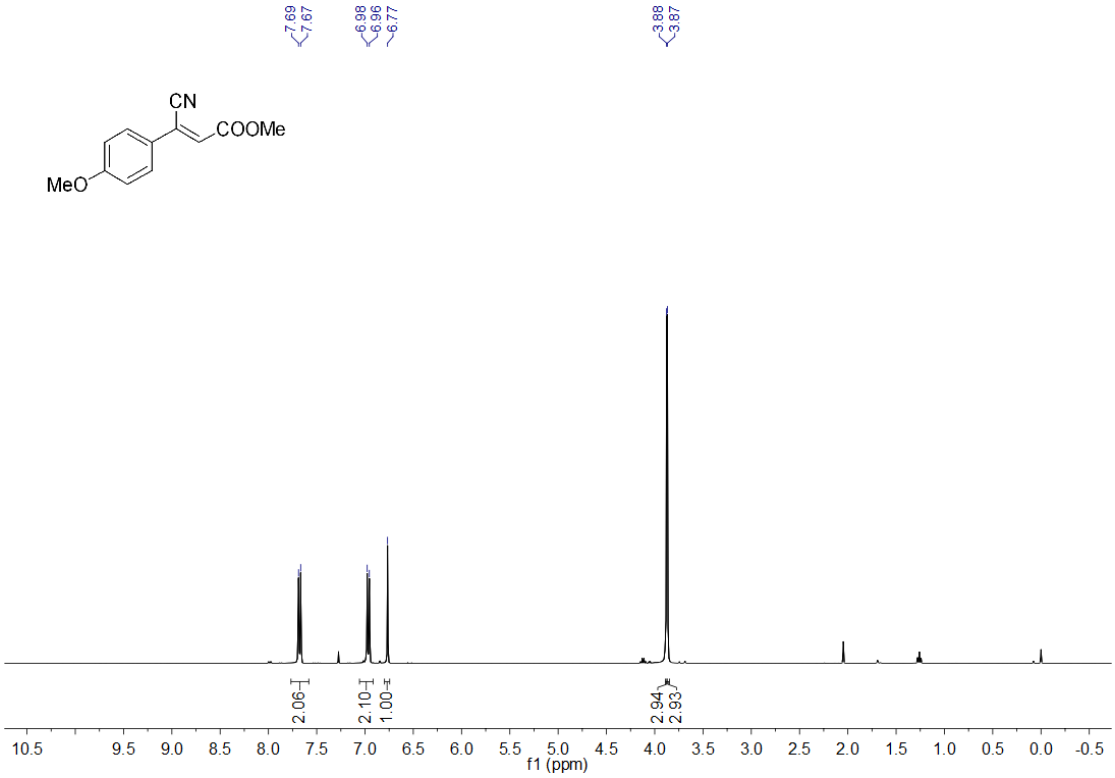
COOMe
MeO


7.69
7.67
6.98
6.96
6.77
3.88
3.87
CN
COOMe
MeO
2.06
2.10
1.00
2.94
2.93
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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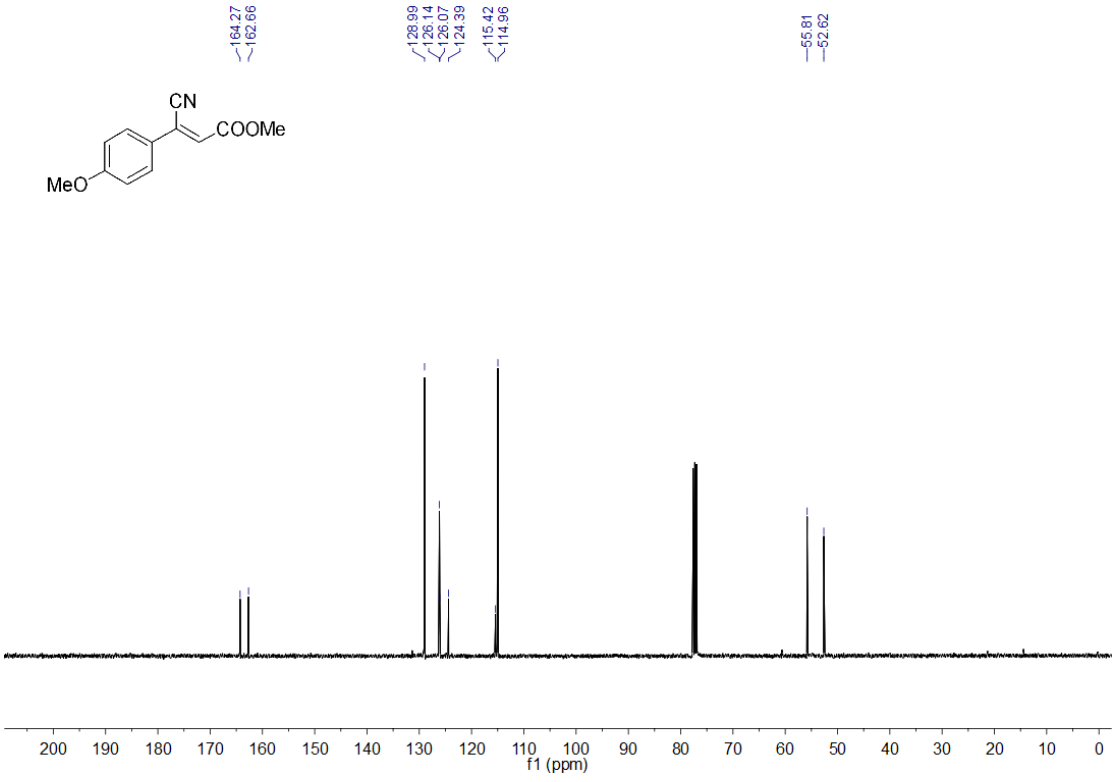
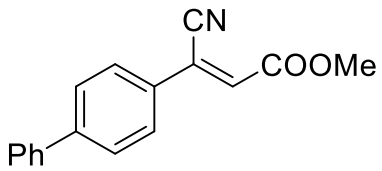
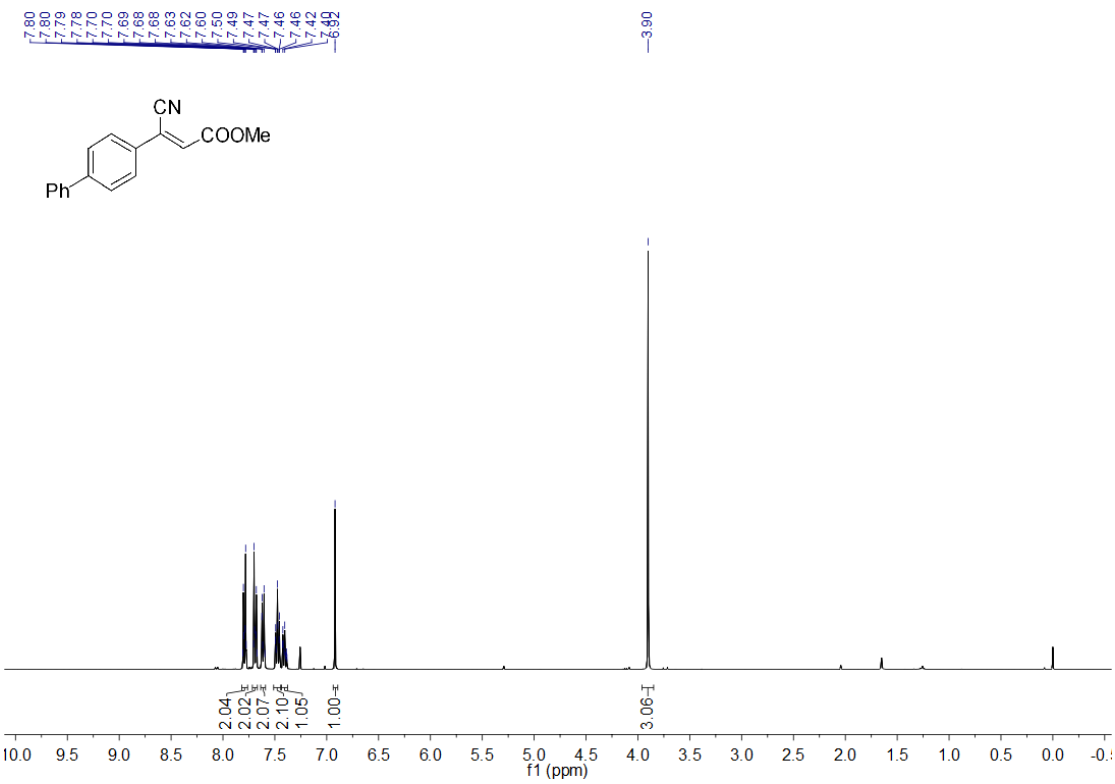
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


164.27
162.66
128.99
126.14
126.07
124.39
115.42
114.96
55.81
52.62
CN
COOMe
MeO
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


CN
COOMe
Ph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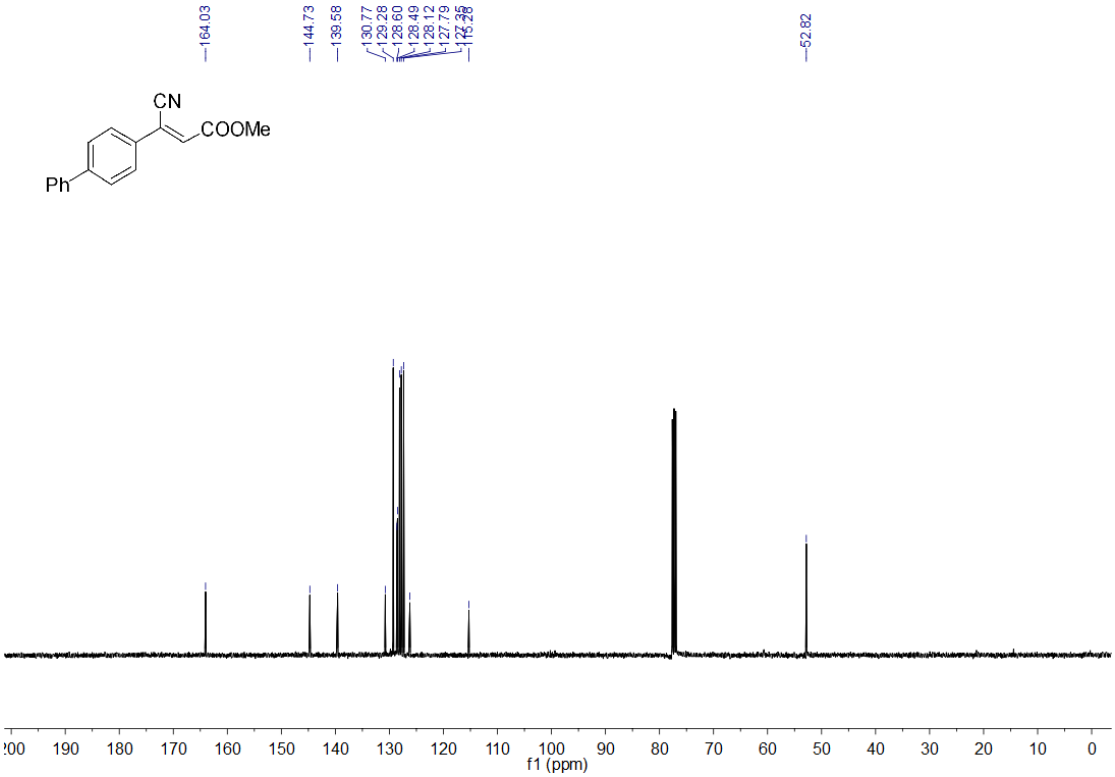
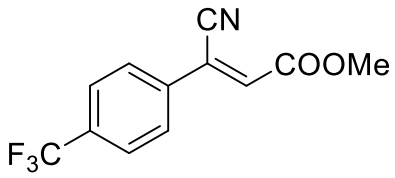
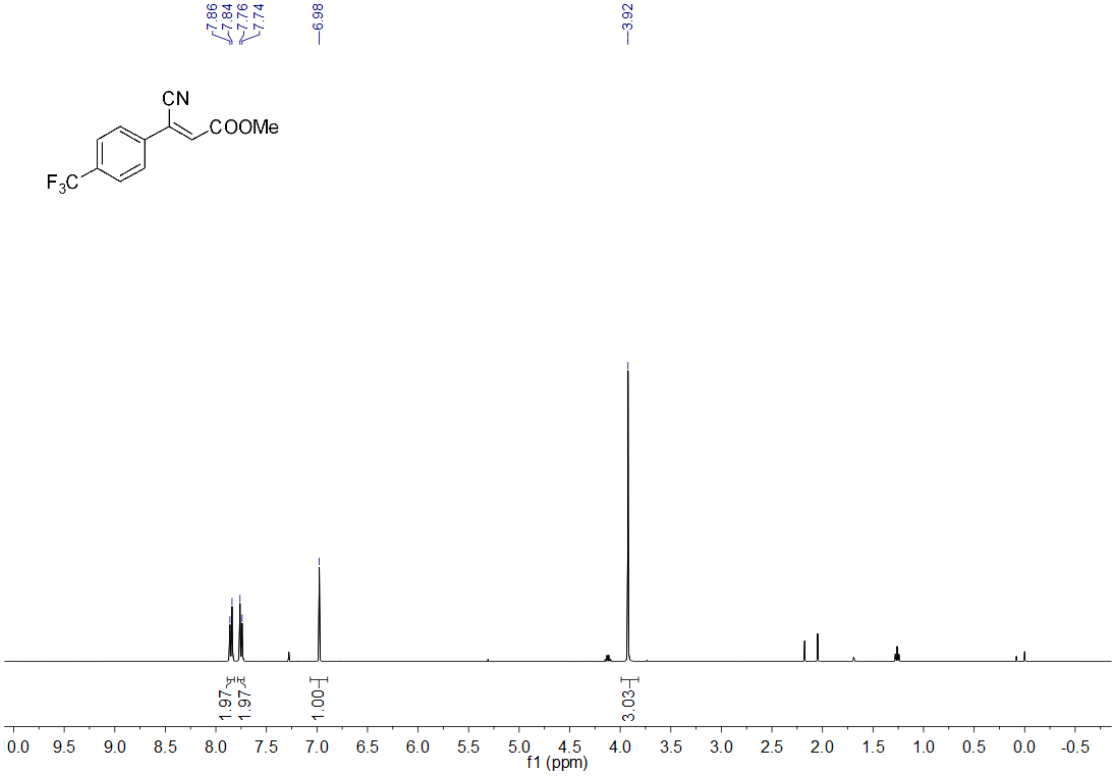
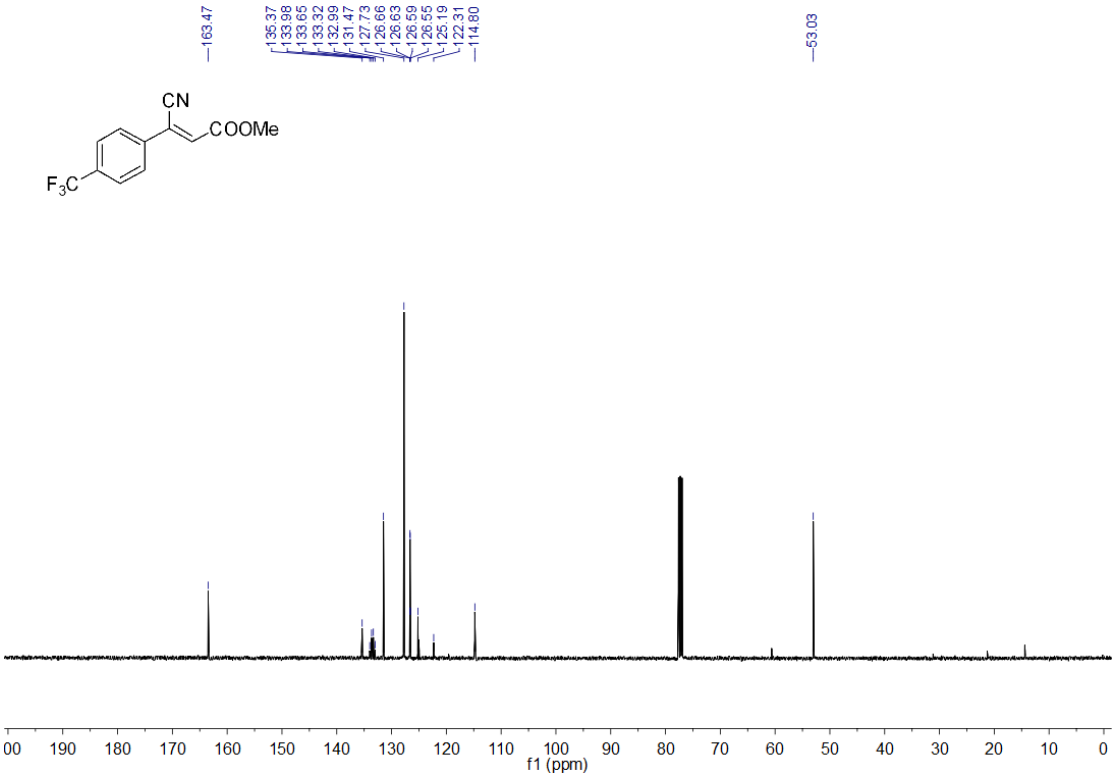
7.70
7.69
7.68
7.68
7.63
7.62
7.60
7.50
7.49
7.47
7.47
7.46
7.46
7.42
3.90
CN
COOMe
Ph
2.04
2.02
2.07
2.10
1.05
1.00
3.06
f1 (ppm)


164.03
144.73
139.58
130.77
129.28
128.60
128.49
128.12
127.79
52.82
CN
COOMe
Ph
f1 (ppm)


CN
COOMe
F3C


7.86
7.84
7.76
7.74
6.98
3.92
CN
COOMe
F3C
1.97
1.97
1.00
3.03
f1 (ppm)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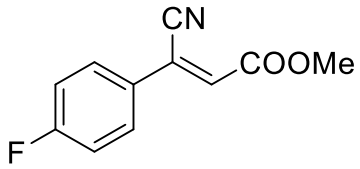
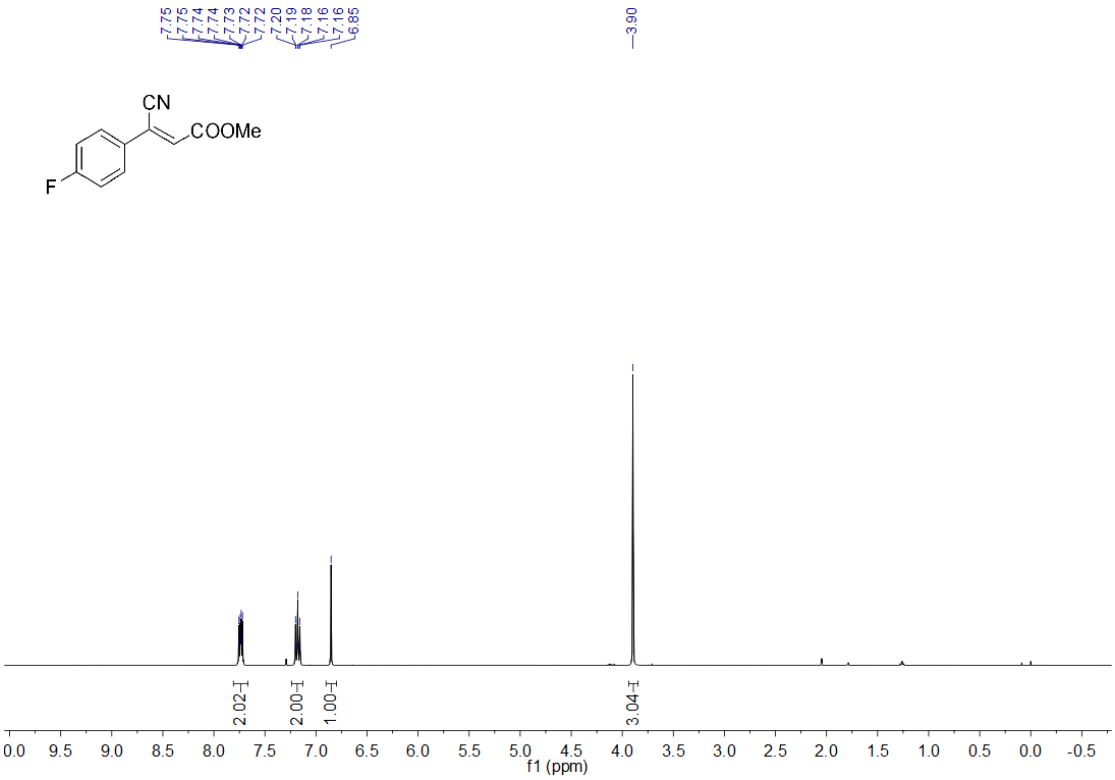
135.37
133.98
133.65
133.32
132.99
131.47
127.73
126.66
126.63
126.59
126.55
125.19
122.31
114.80
53.03
CN
COOMe
F3C
f1 (ppm)


CN
COOMe
F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7.75
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7.74
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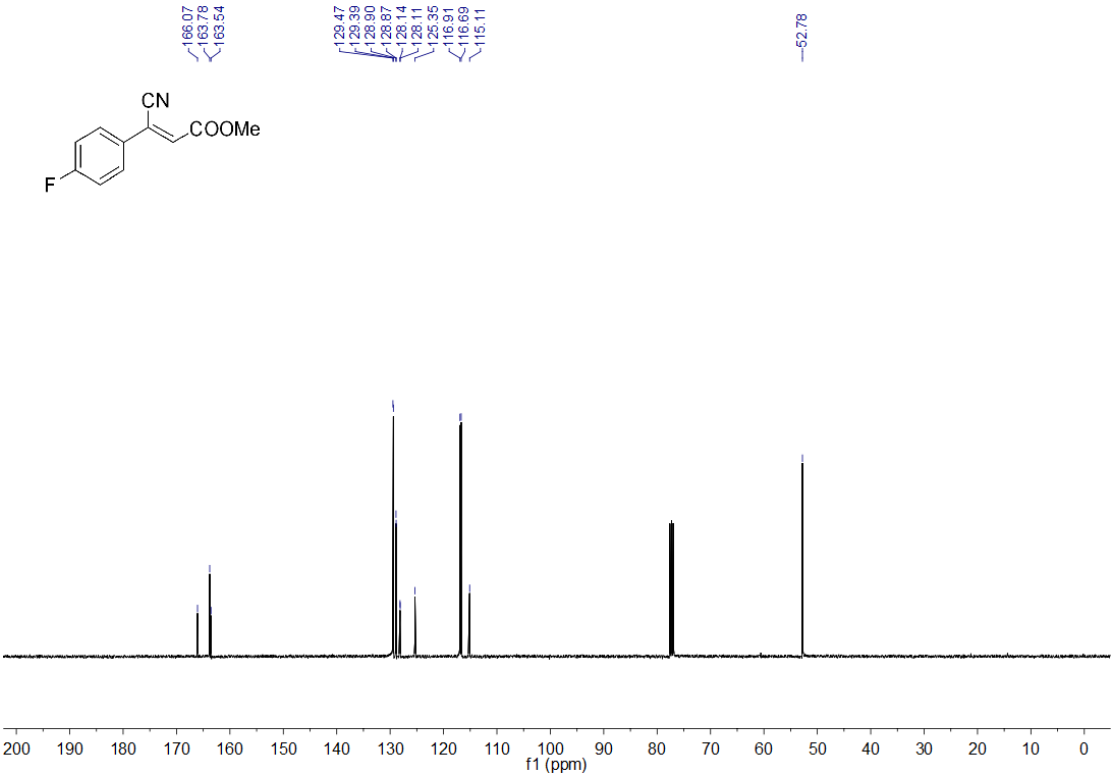
7.72
7.72
7.20
7.19
7.18
7.16
7.16
6.85
3.90
CN
COOMe
F
2.02
2.00
1.00
3.04
f1 (ppm)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163.78
163.54
129.47
129.39
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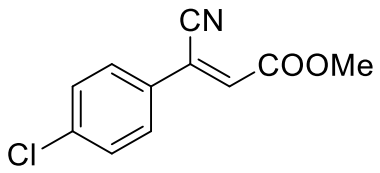
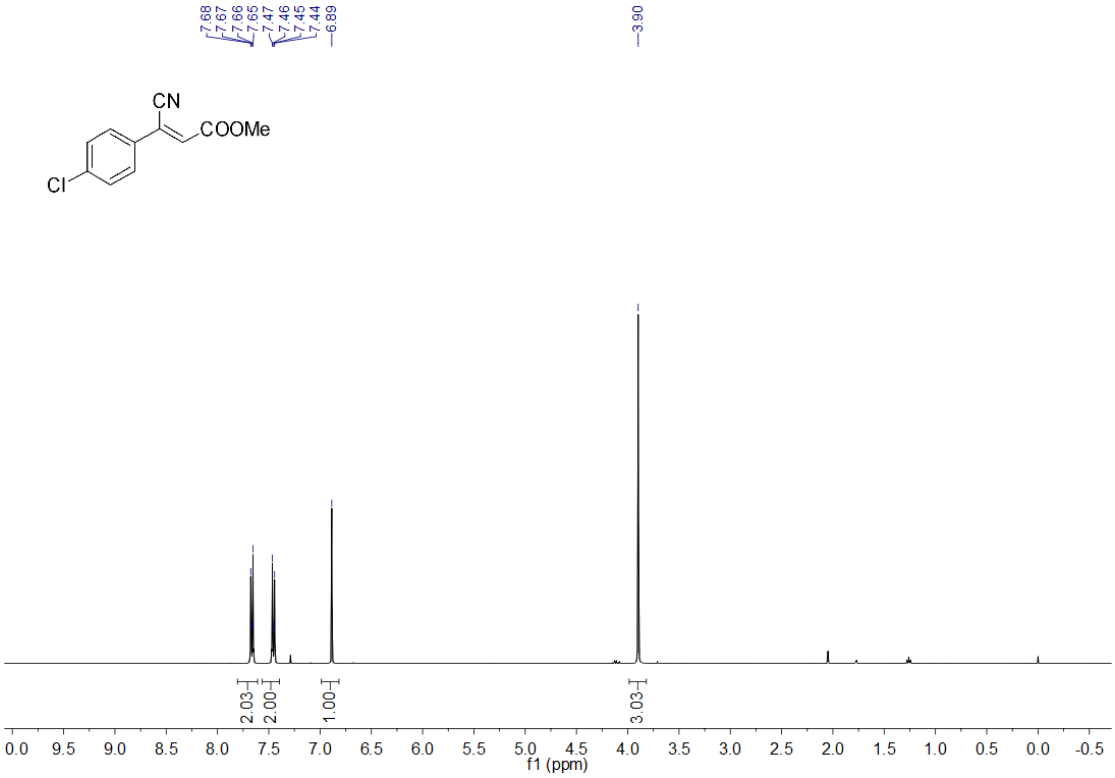
128.11
125.35
116.91
116.69
115.11
52.78
CN
COOMe
F
f1 (ppm)


CN
COOMe
Cl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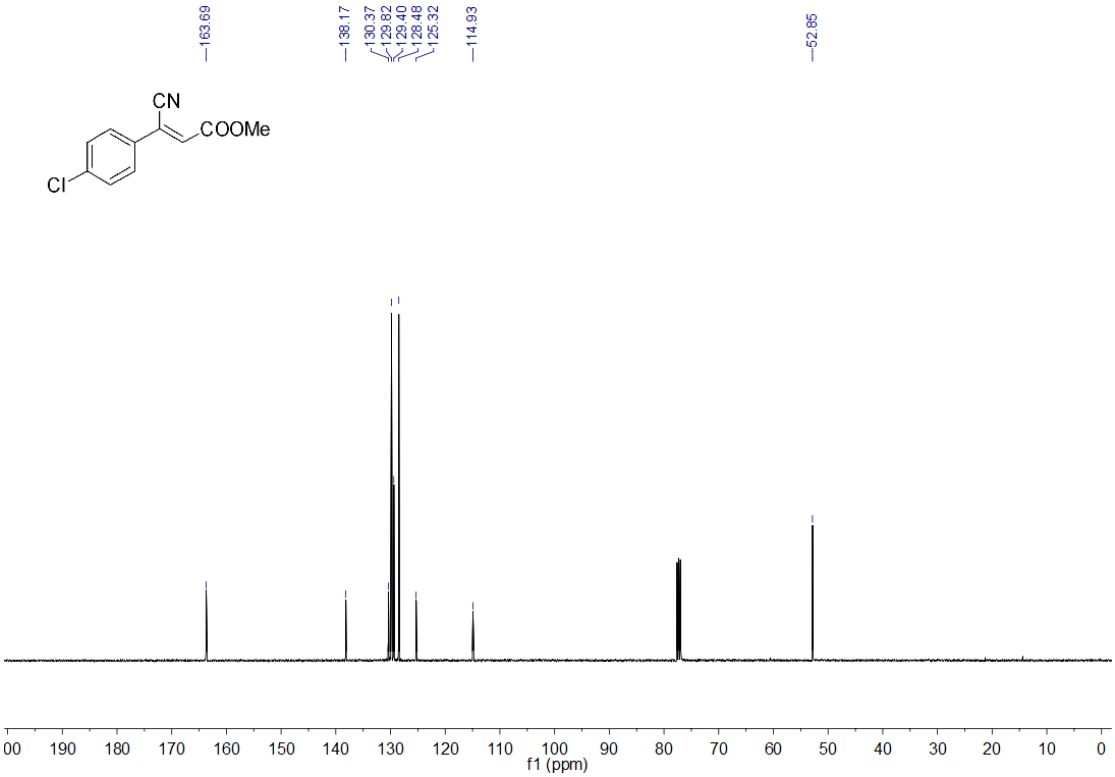
6.89
3.90
CN
COOMe
Cl
2.03
2.00
1.00
3.03
f1 (ppm)


163.69
138.17
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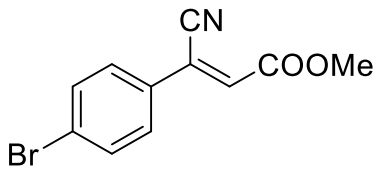
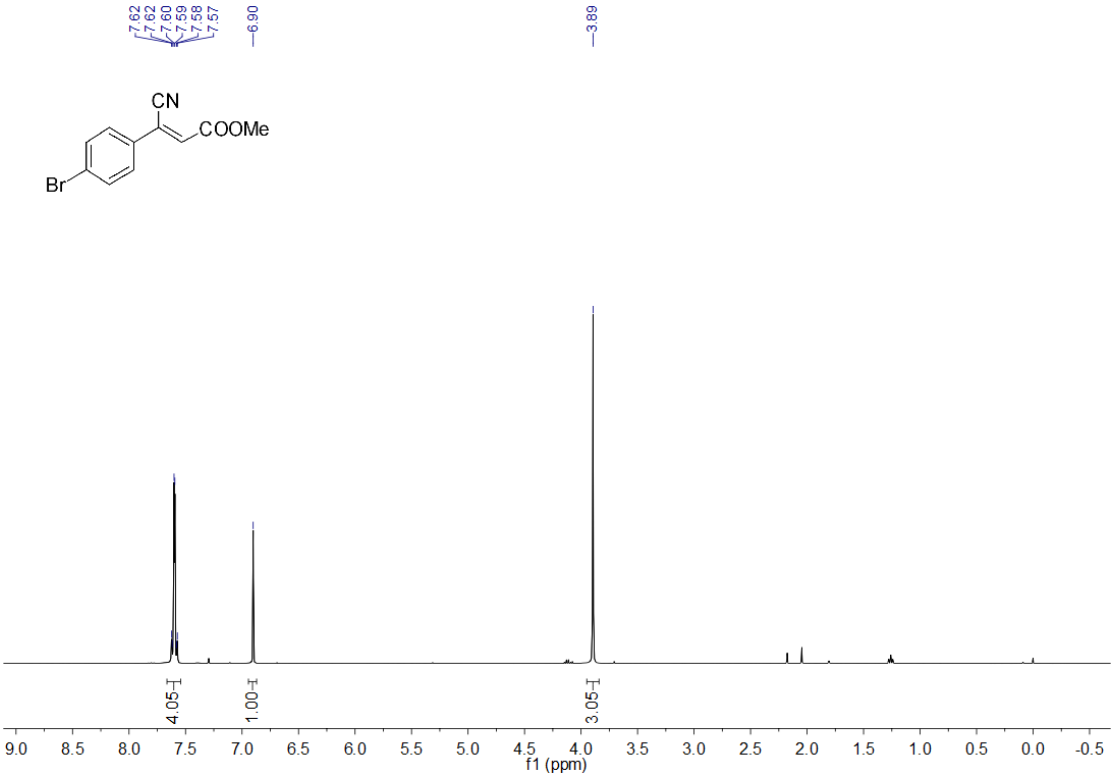
129.82
129.40
128.48
125.32
114.93
52.85
CN
COOMe
Cl
f1 (ppm)


CN
COOMe
Br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7.62
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7.57
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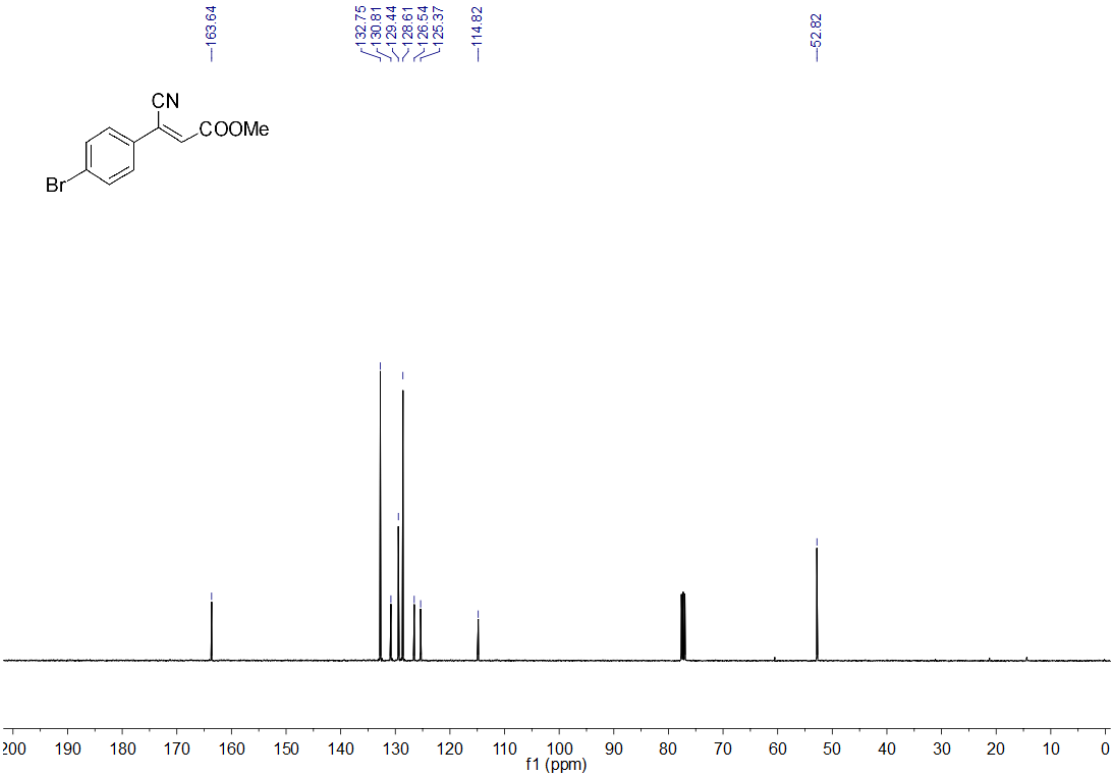
3.89
CN
COOMe
Br
4.05
1.00
3.05
f1 (ppm)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52.82
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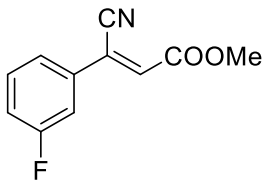
COOMe
Br
f1 (ppm)


CN
COOMe
F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7.50
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7.46
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7.40
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7.24
7.24
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7.20
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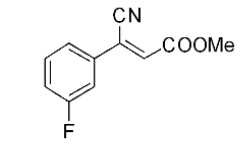
7.19
6.90
3.91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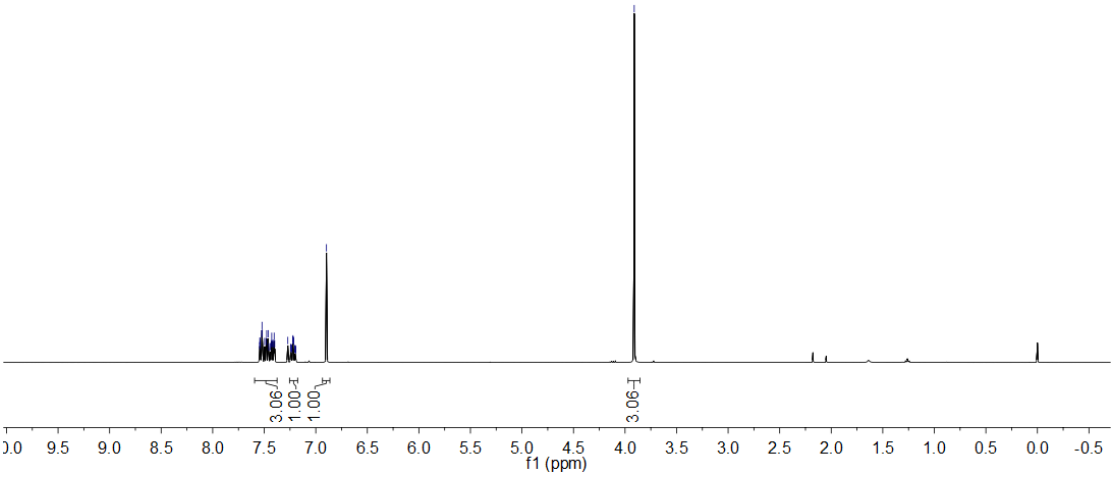
3.06
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1.00
3.06
f1 (ppm)


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134.05
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131.30
130.35
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125.40
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123.17
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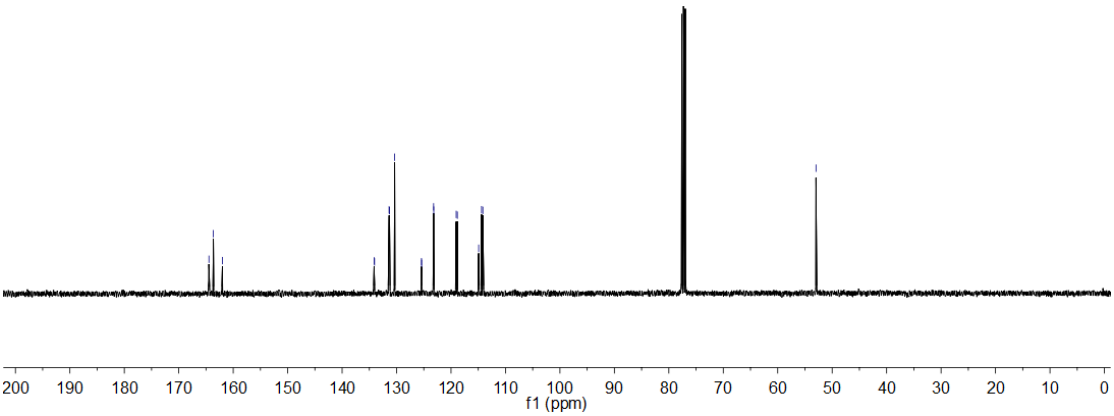
118.84
114.92
114.39
114.15
52.97

CN
COOMe
F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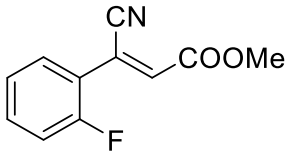
CN
COOMe
F


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7.71
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7.49
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7.48
7.47
7.47
7.47
7.46
7.45
7.45
7.31
7.29
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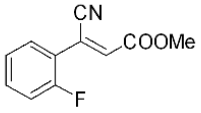
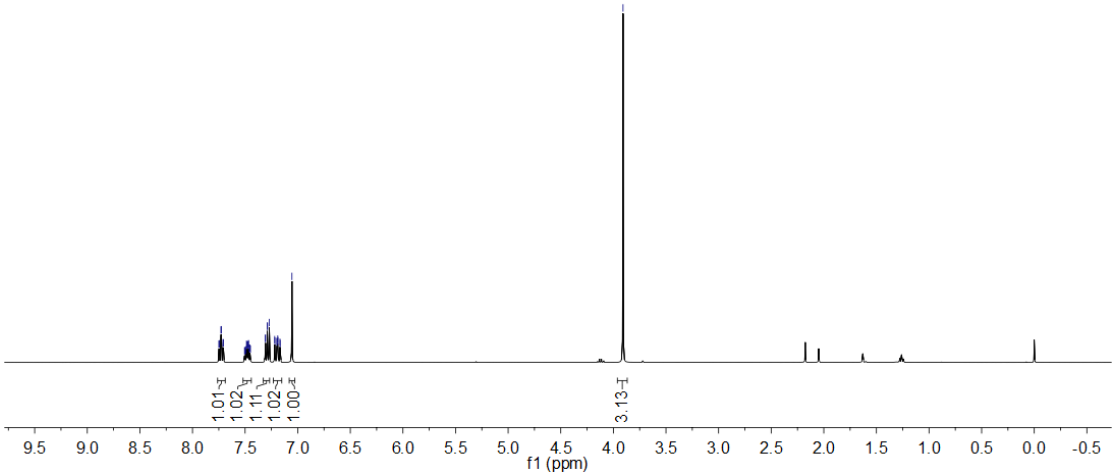
7.19
7.17
7.17
7.05
3.91


CN
COOMe
F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1.02
1.11
1.02
1.00
3.13
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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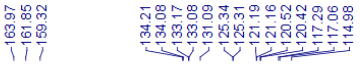
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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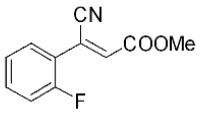
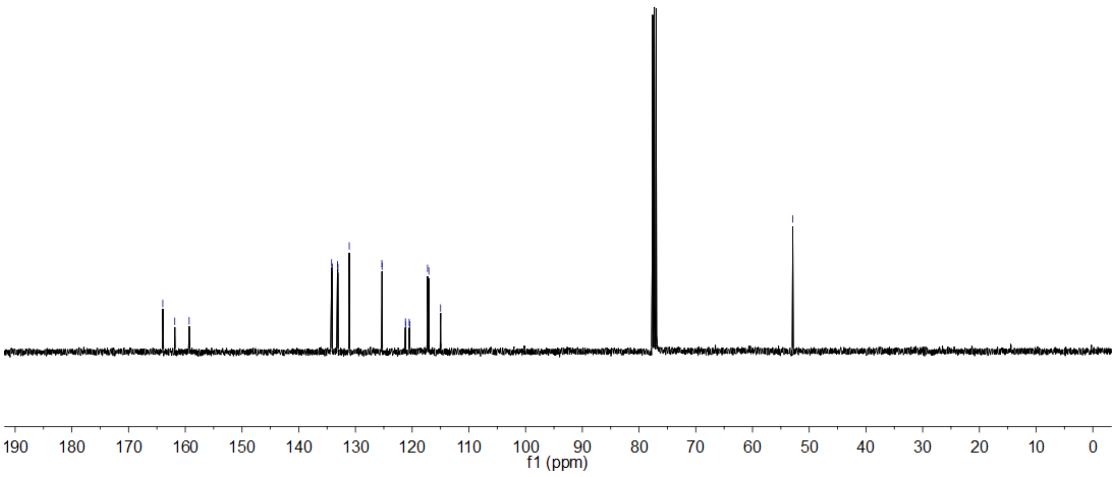
52.90


CN
COOMe
F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40
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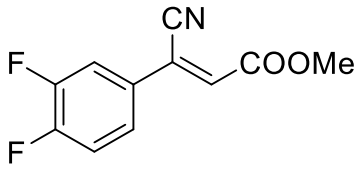
10
0
f1 (ppm)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COOMe
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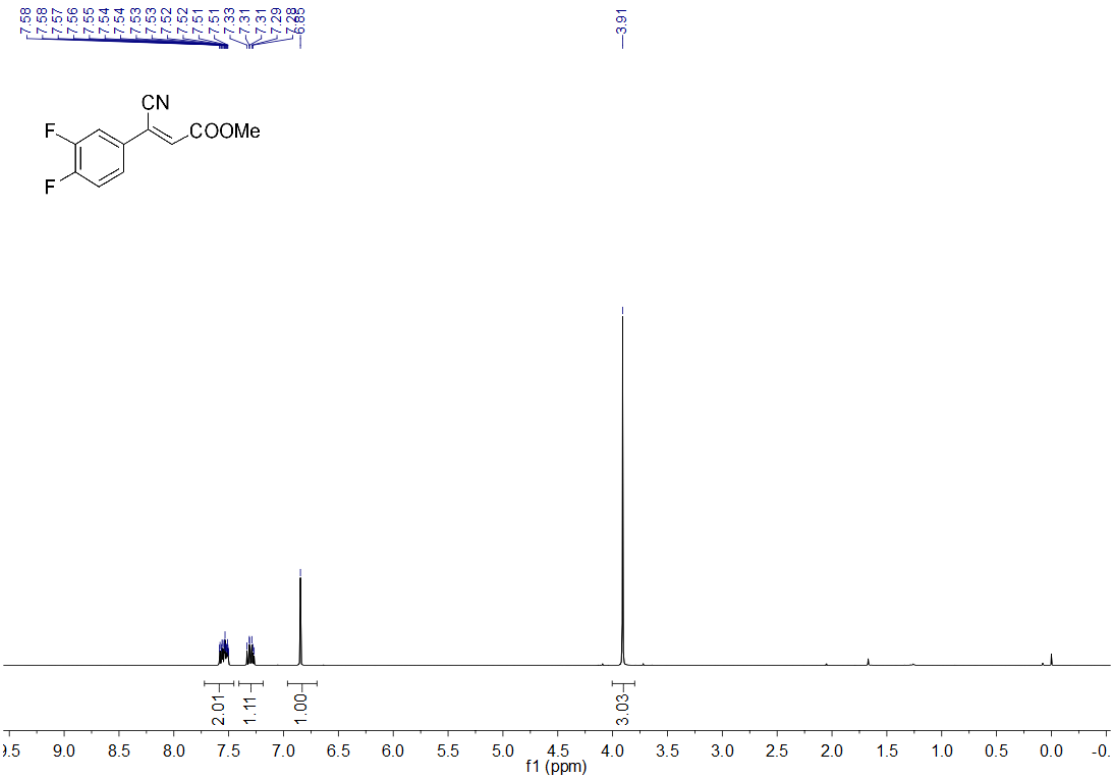
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7.51
7.33
7.31
7.31
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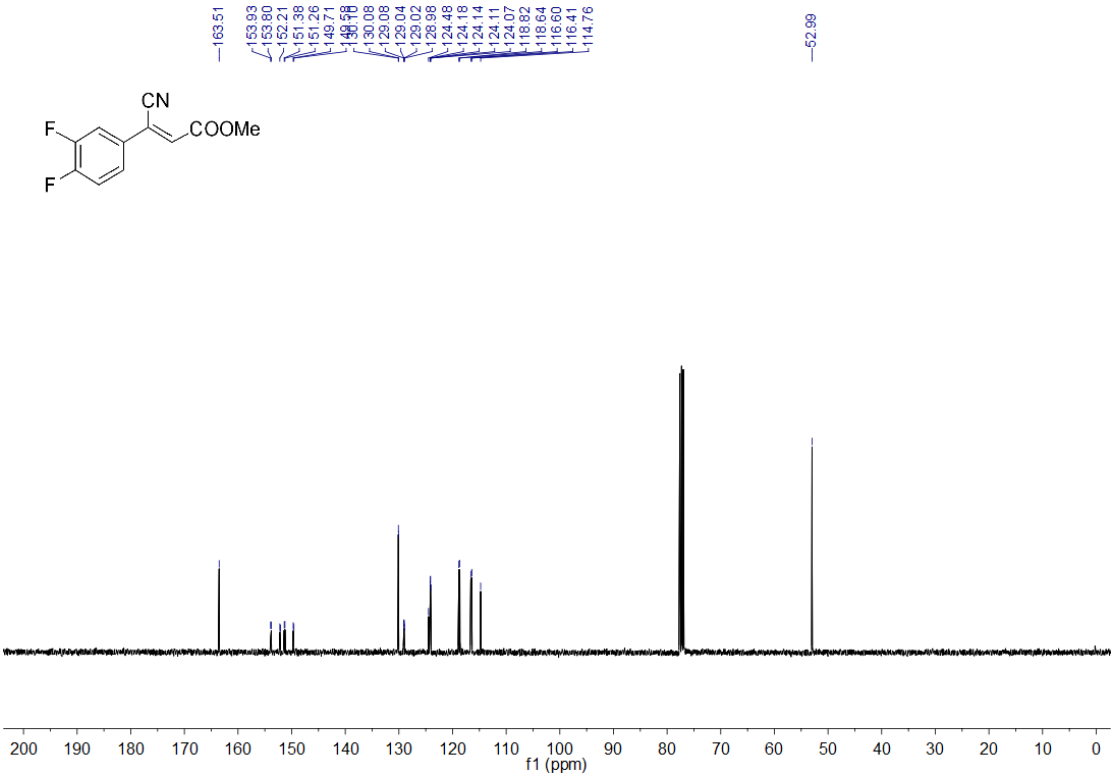
3.91
CN
F
COOMe
F
2.01
1.11
1.00
3.03
f1 (ppm)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129.02
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124.18
124.14
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124.07
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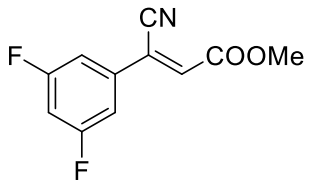
116.41
114.76
52.99
CN
F
COOMe
F
f1 (ppm)


CN
F
COOMe
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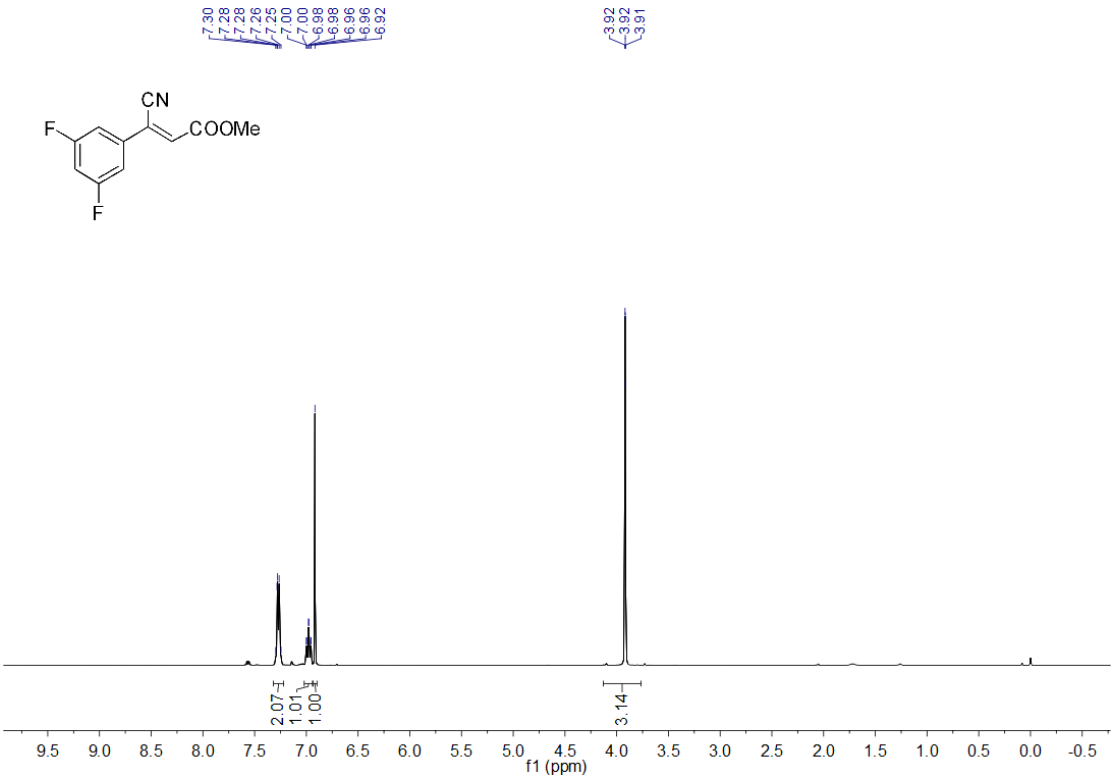
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6.98
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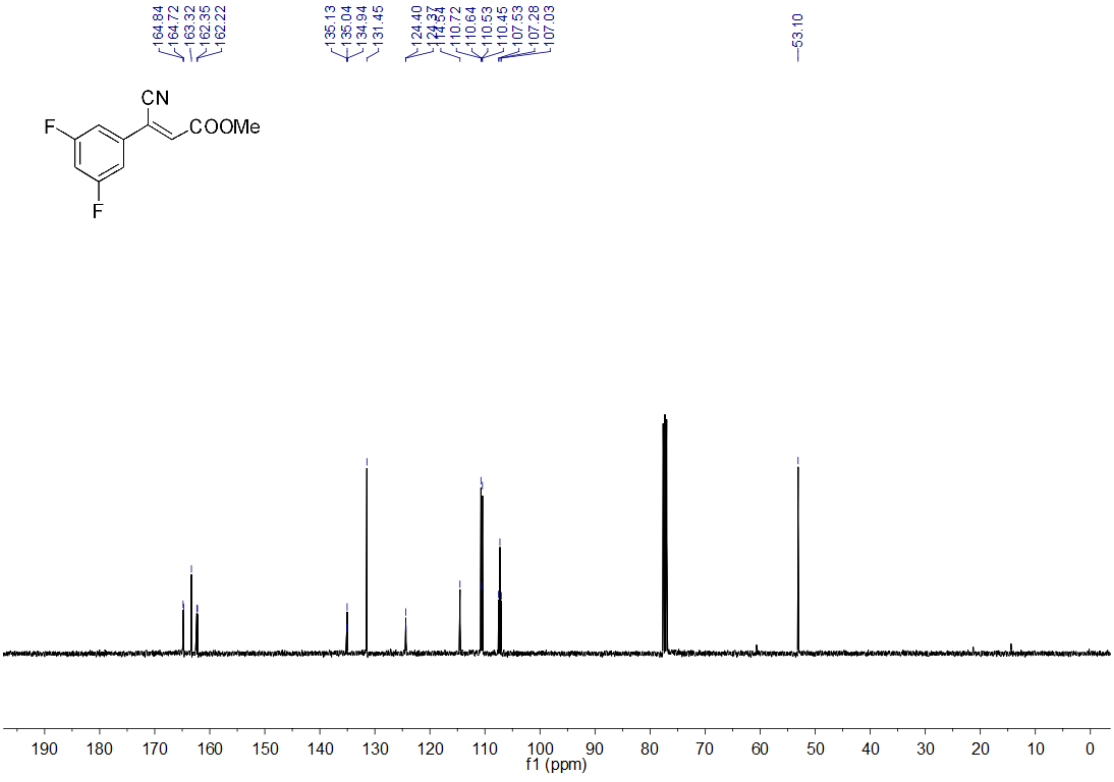
6.96
6.92
3.92
3.92
3.91
CN
F
COOMe
F
2.07
1.01
1.00
3.14
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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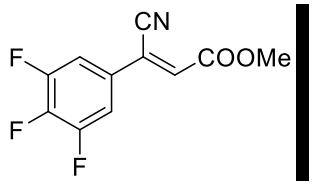
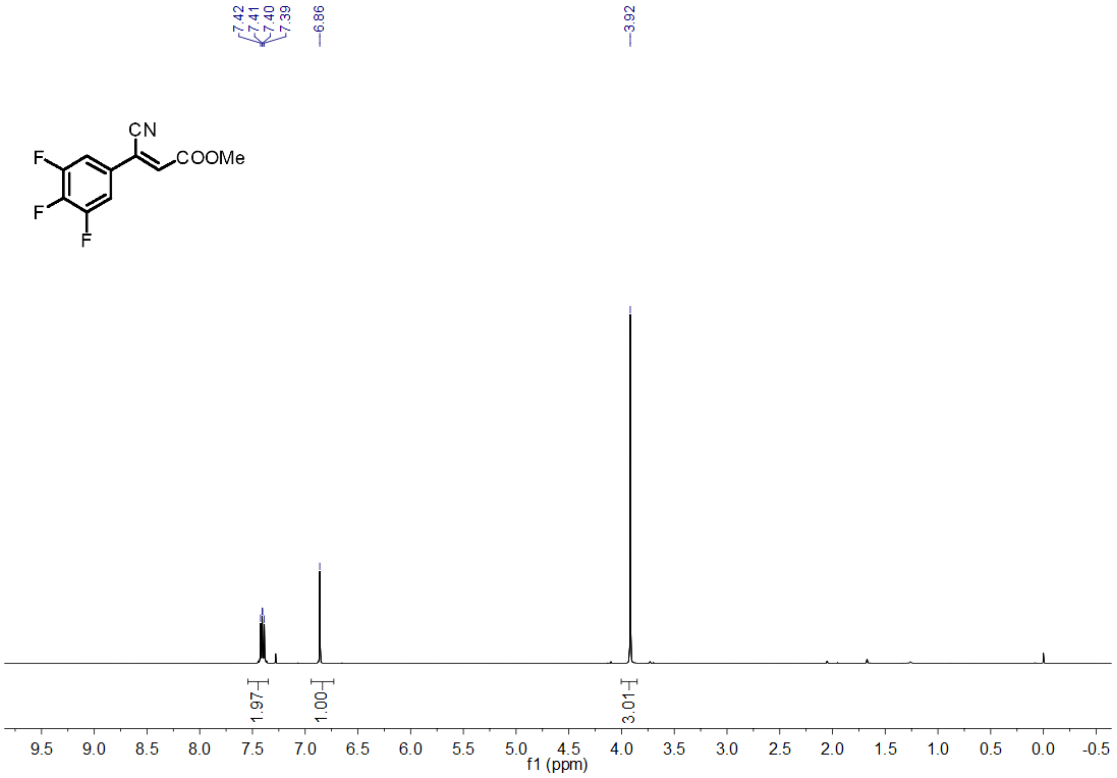
110.64
110.53
110.45
107.53
107.28
107.03
53.10
CN
F
COOMe
F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


CN
COOMe
F
F
F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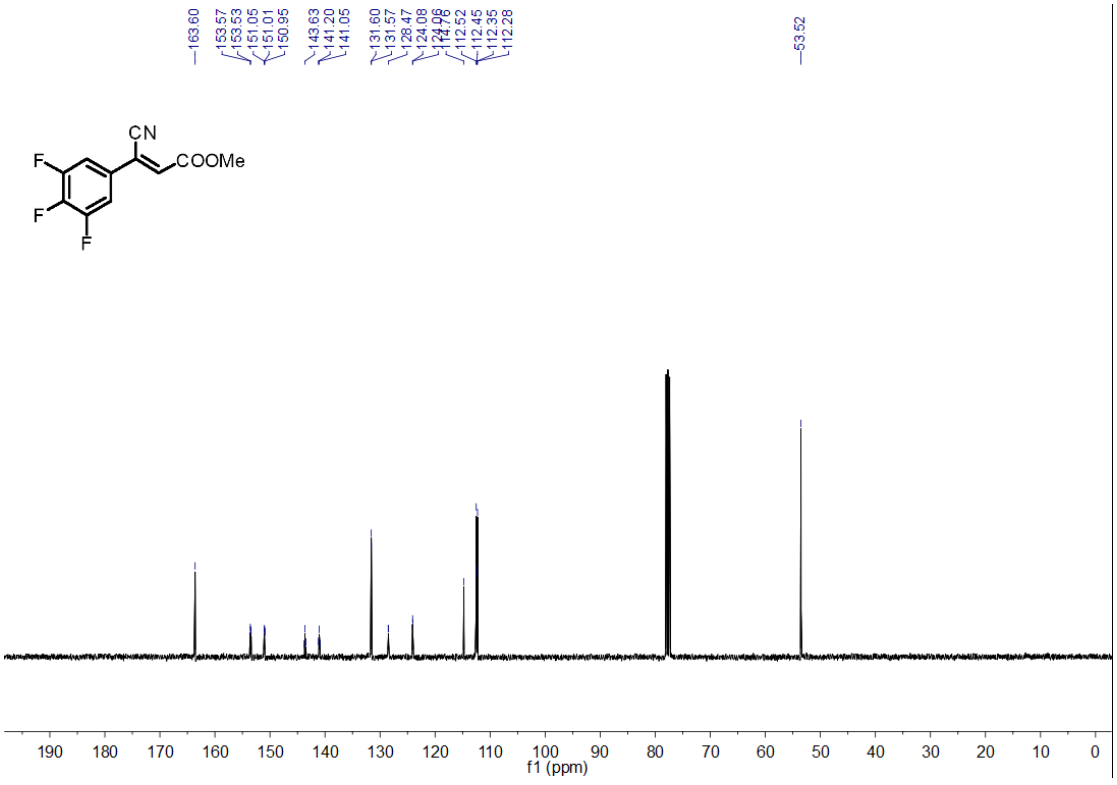
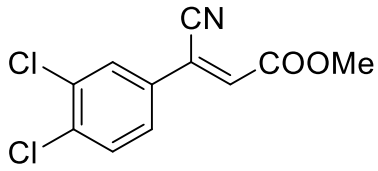
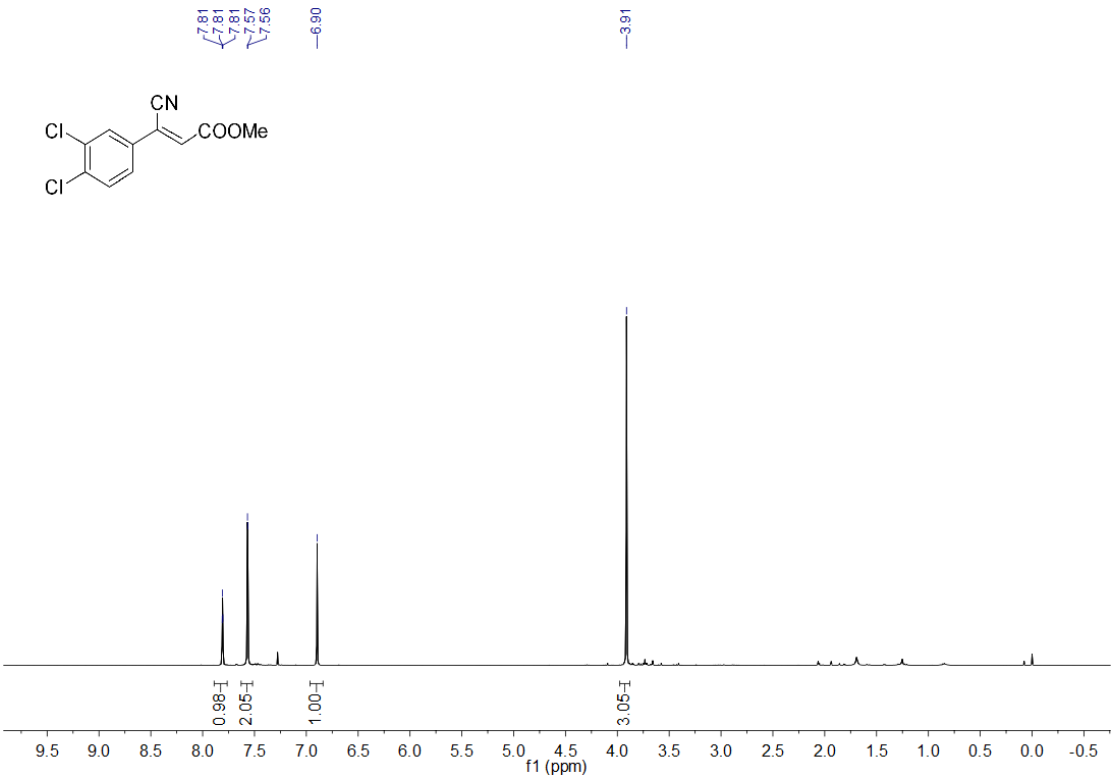
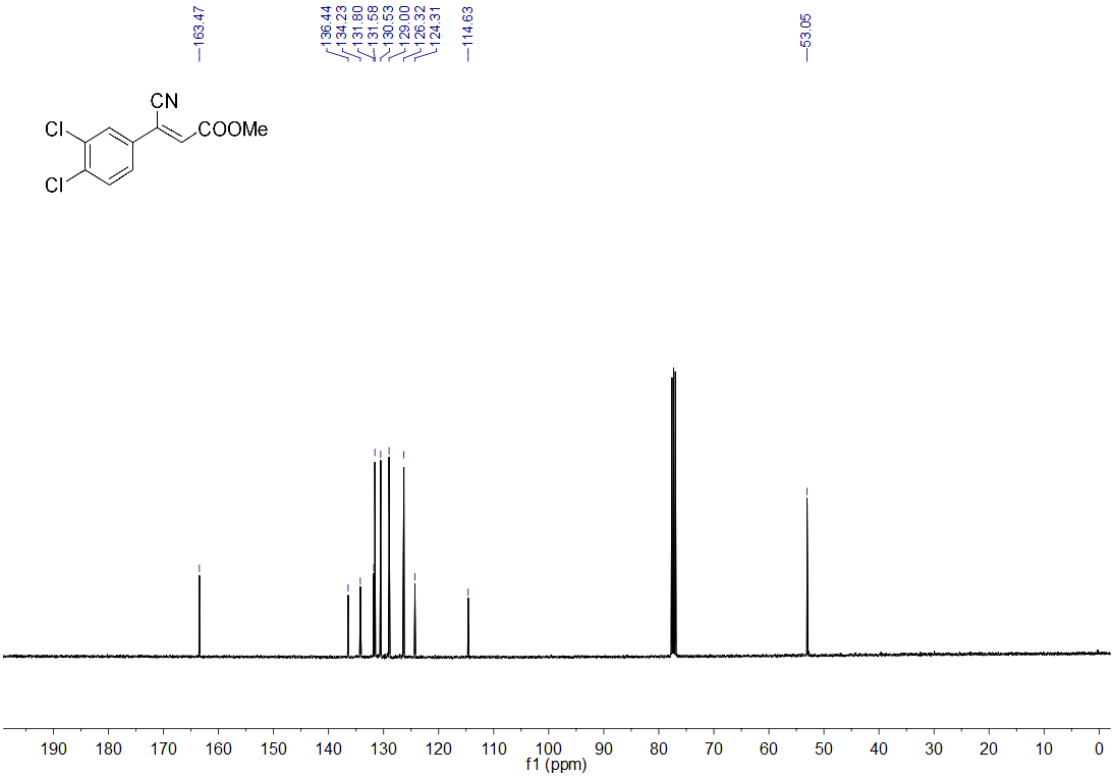
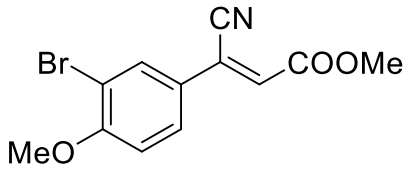
CN
COOMe
F
F
F
1.97
1.00
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

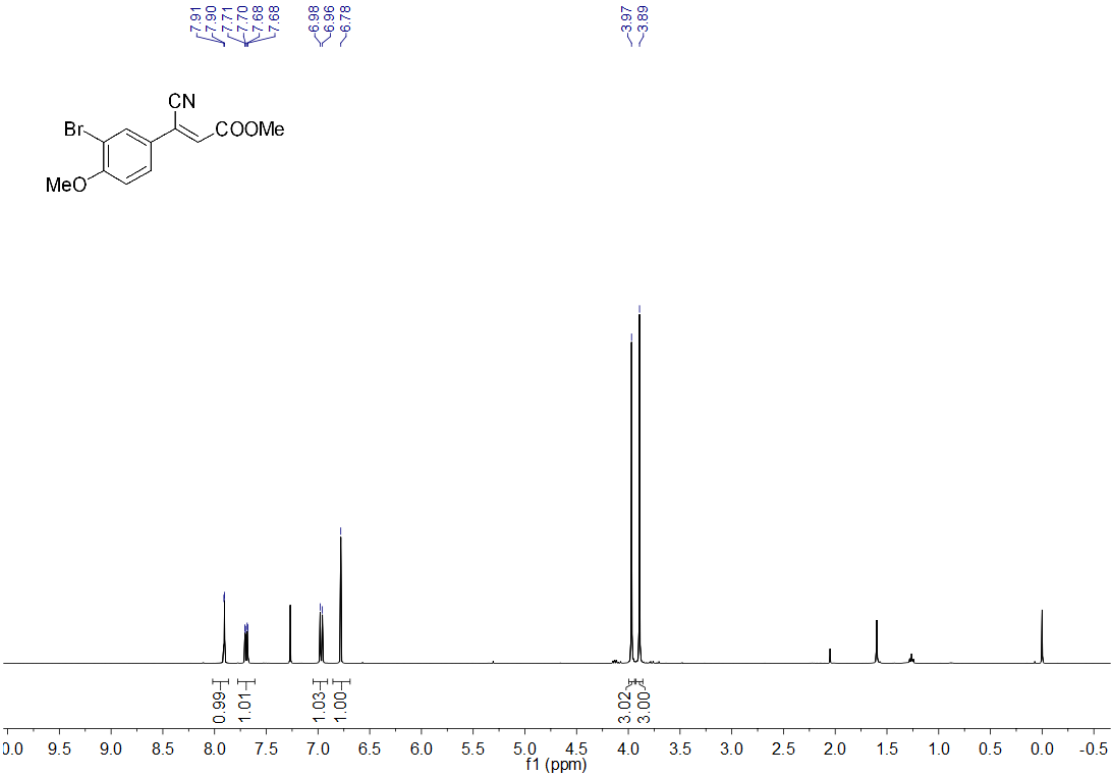

163.60
153.57
153.53
151.05
151.01
150.95
143.63
141.20
141.05
131.60
131.57
128.47
124.08
112.52
112.45
112.35
112.28
53.52
CN
COOMe
F
F
F
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

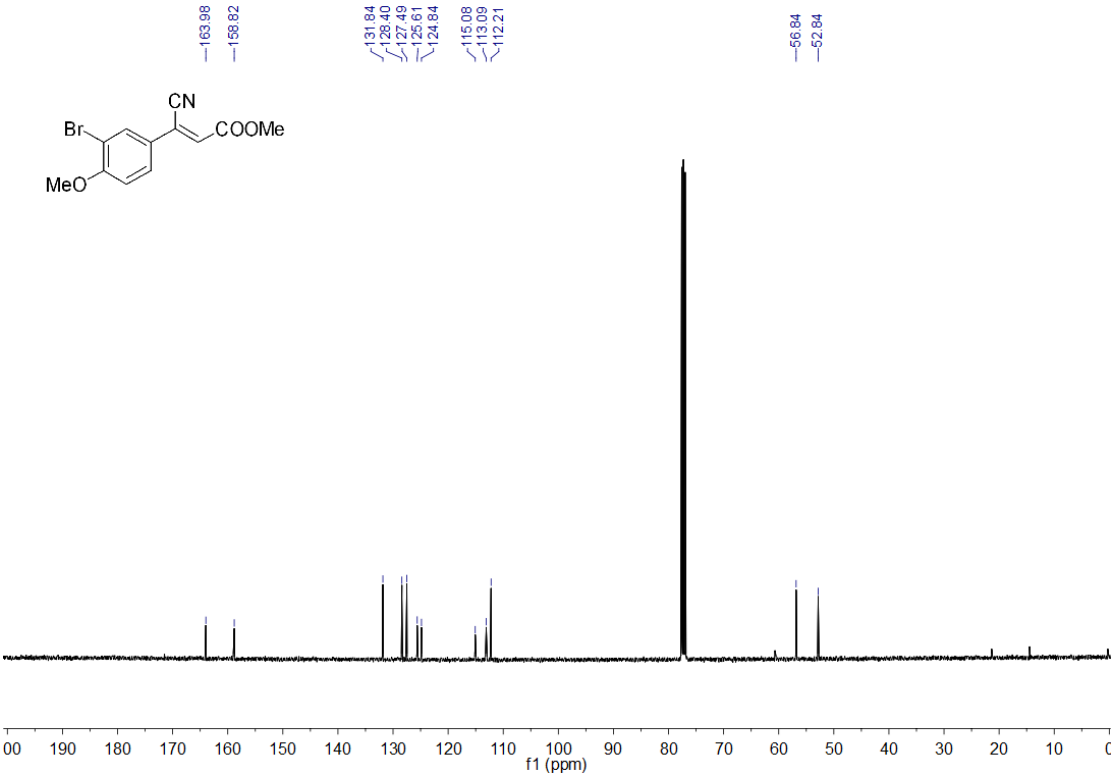

CN
Cl
COOMe
Cl

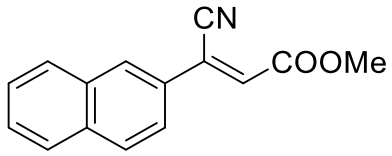

7.81
7.81
7.81
7.57
7.56
6.90
3.91
CN
Cl
COOMe
Cl
0.98
2.05
1.00
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


163.47
136.44
134.23
131.80
131.58
130.53
129.00
126.32
124.31
114.63
53.05
CN
Cl
COOMe
Cl
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


CN
Br
COOMe
MeO


7.91
7.90
7.71
7.70
7.68
7.68
6.98
6.96
6.78
3.97
3.89
CN
Br
COOMe
MeO
0.99
1.01
1.03
1.00
3.02
3.00
f1 (ppm)


163.98
158.82
131.84
128.40
127.49
125.61
124.84
115.08
113.09
112.21
56.84
52.84
CN
Br
COOMe
MeO
f1 (ppm)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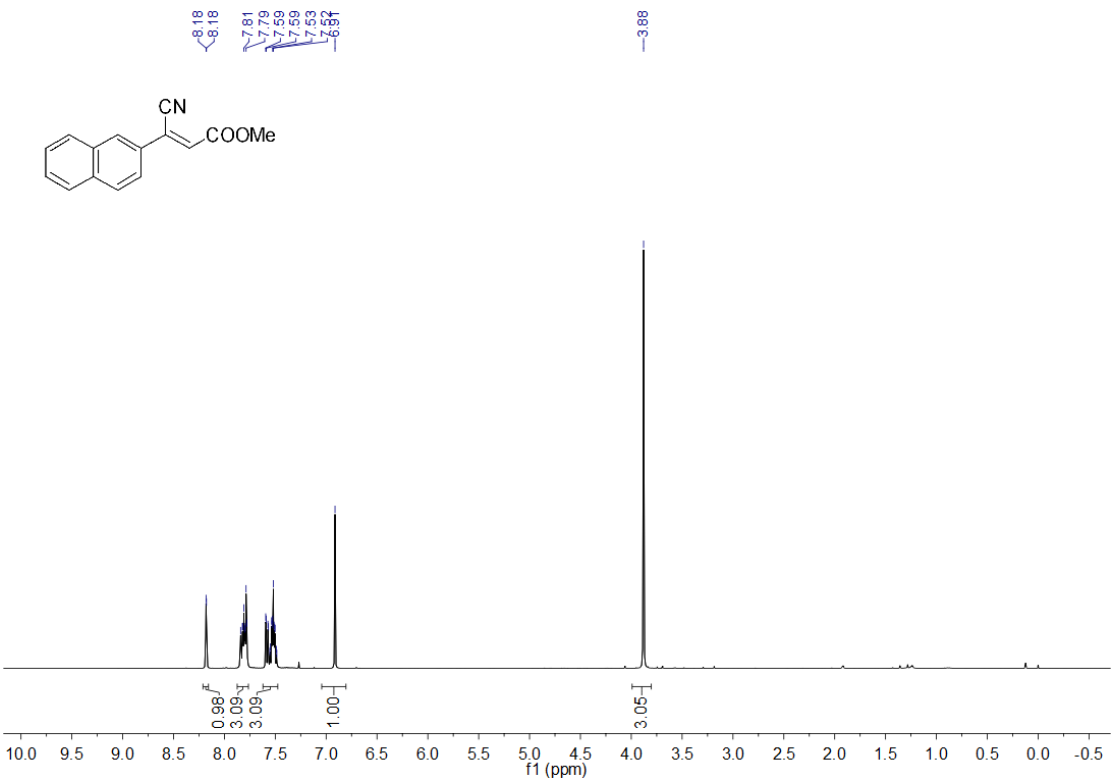
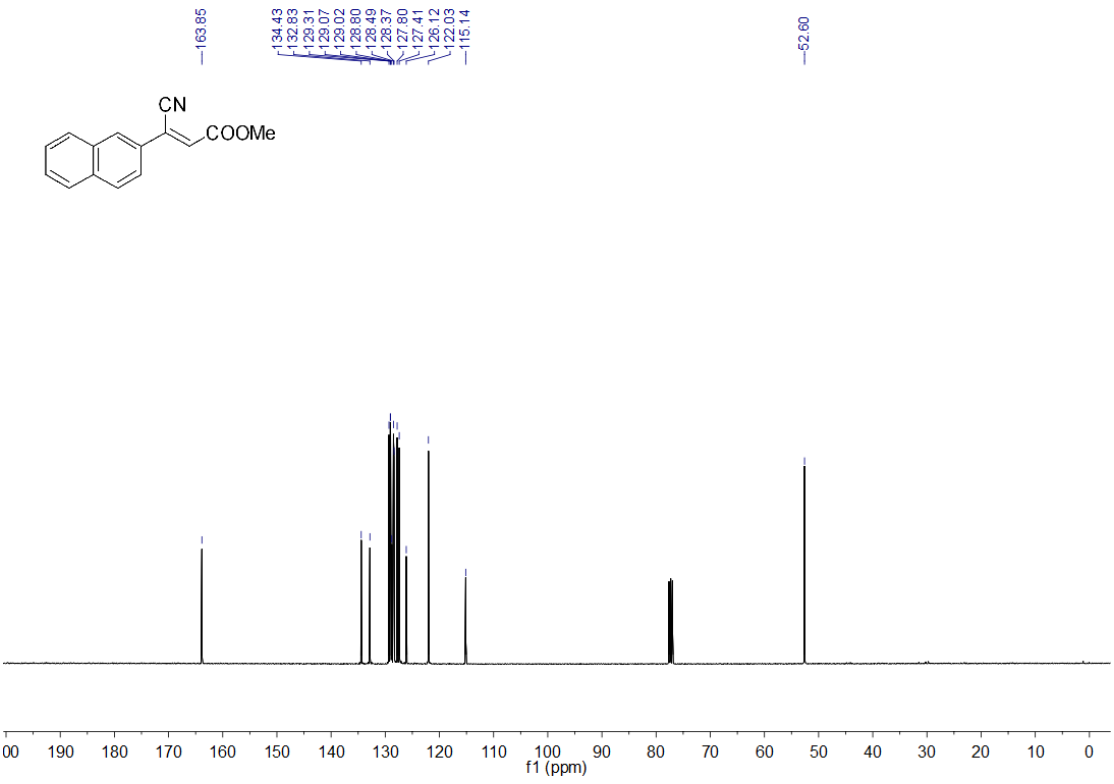
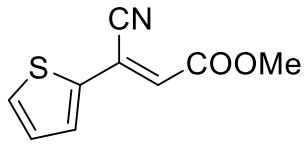
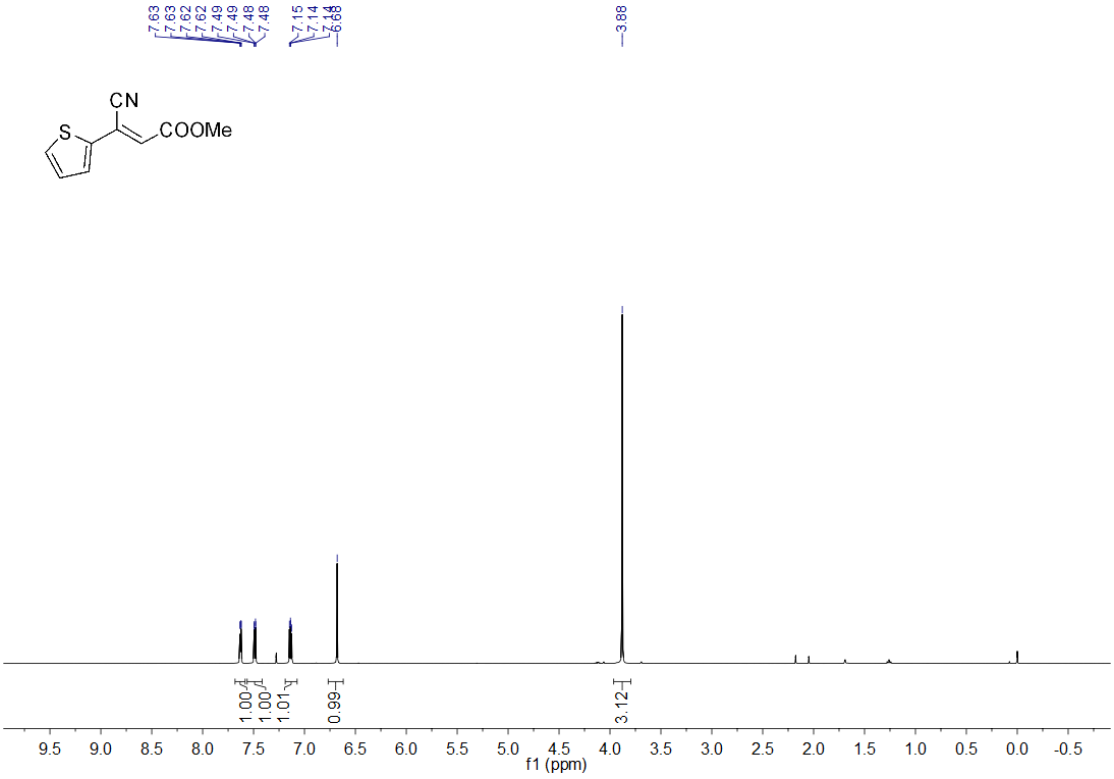
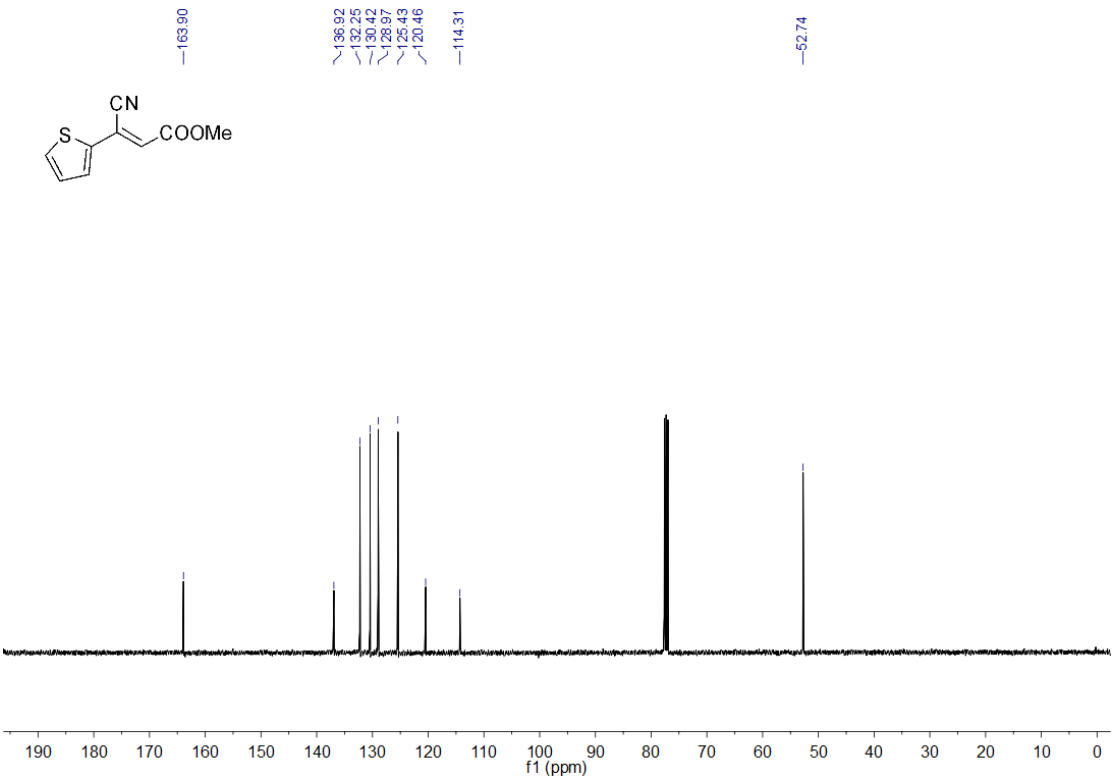
COOMe

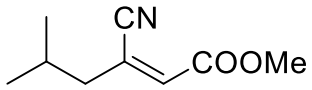

8.18
8.18
7.81
7.79
7.59
7.59
7.59
7.53
7.53
6.91
3.88
CN
COOMe
0.98
3.09
3.09
1.00
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

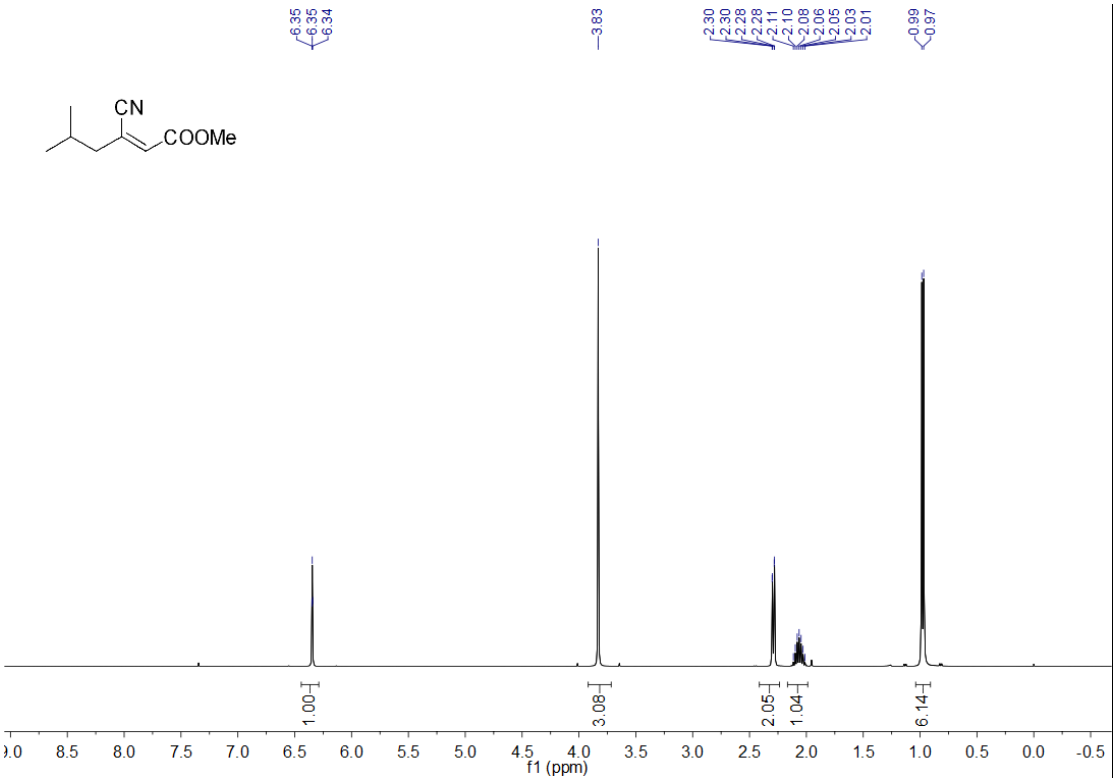

163.85
134.43
132.83
129.31
129.07
129.02
128.80
128.49
128.37
127.80
127.41
126.12
122.03
115.14
52.60
CN
COOMe
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

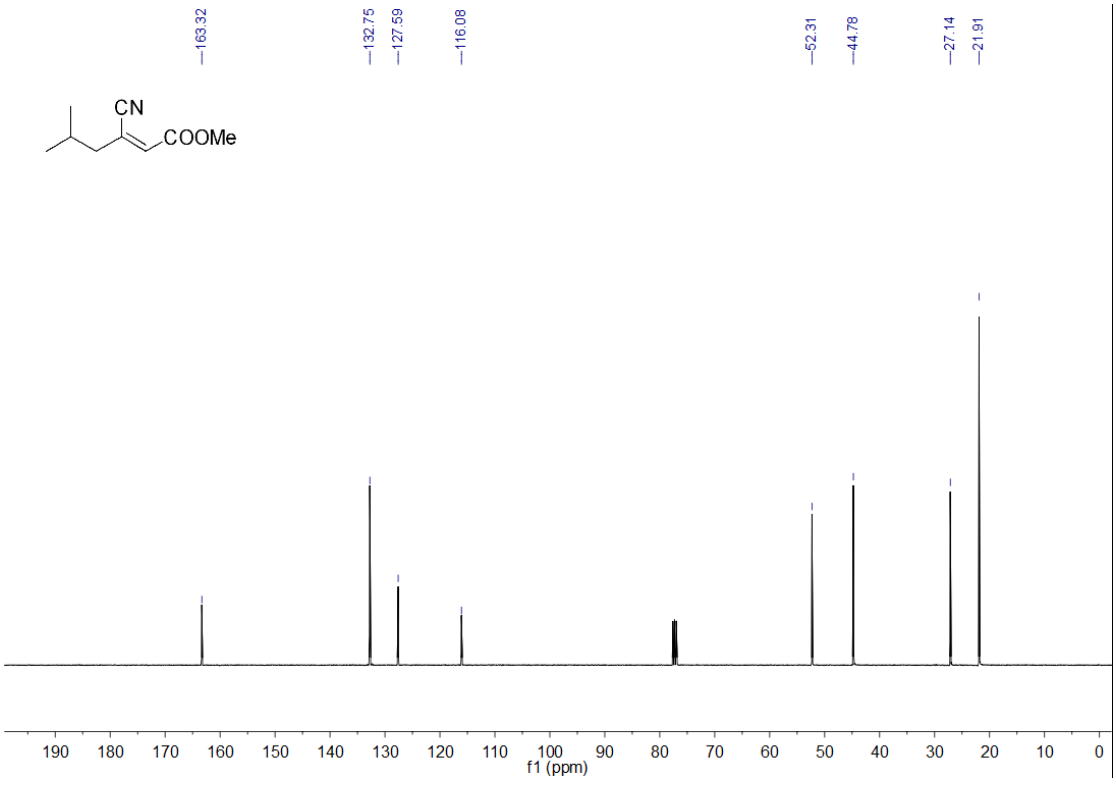

CN
S
COOMe

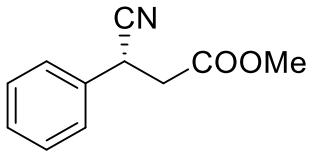

7.63
7.63
7.62
7.62
7.49
7.49
7.48
7.48
7.15
7.14
6.68
3.88
CN
S
COOMe
1.00
1.00
1.01
0.99
3.12
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


163.90
136.92
132.25
130.42
128.97
125.43
120.46
114.31
52.74
CN
S
COOMe
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


CN
COOMe


6.35
6.35
6.34
3.83
2.30
2.30
2.28
2.28
2.11
2.10
2.08
2.06
2.05
2.03
2.01
0.99
0.97
CN
COOMe
1.00
3.08
2.05
1.04
6.14
f1 (ppm)


163.32
132.75
127.59
116.08
52.31
44.78
27.14
21.91
CN
COOMe
f1 (ppm)


CN
COOMe


7.41
7.41
7.41
7.39
7.39
7.38
7.36
7.36
7.35
7.35
7.34
7.34
7.33
7.32
7.32
4.32
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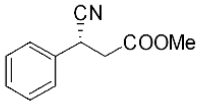
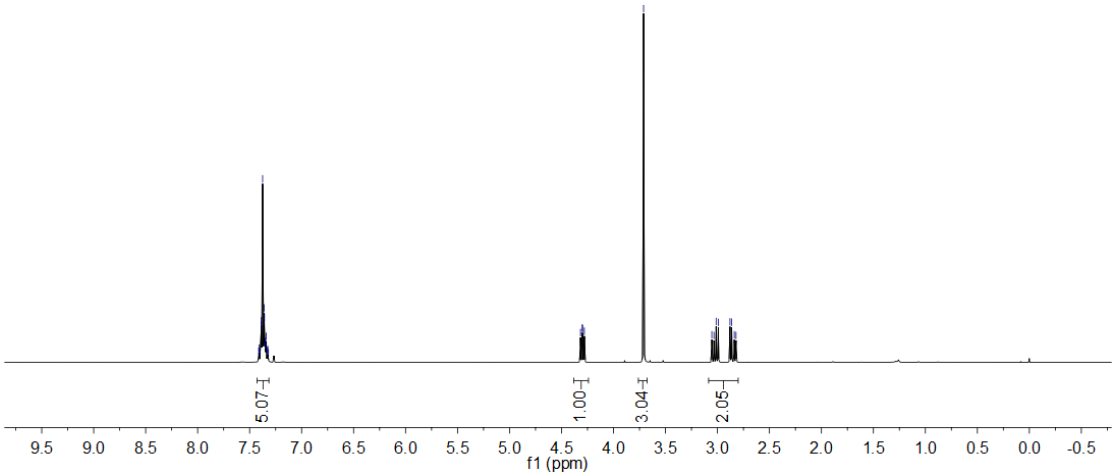
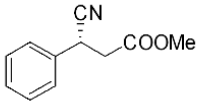
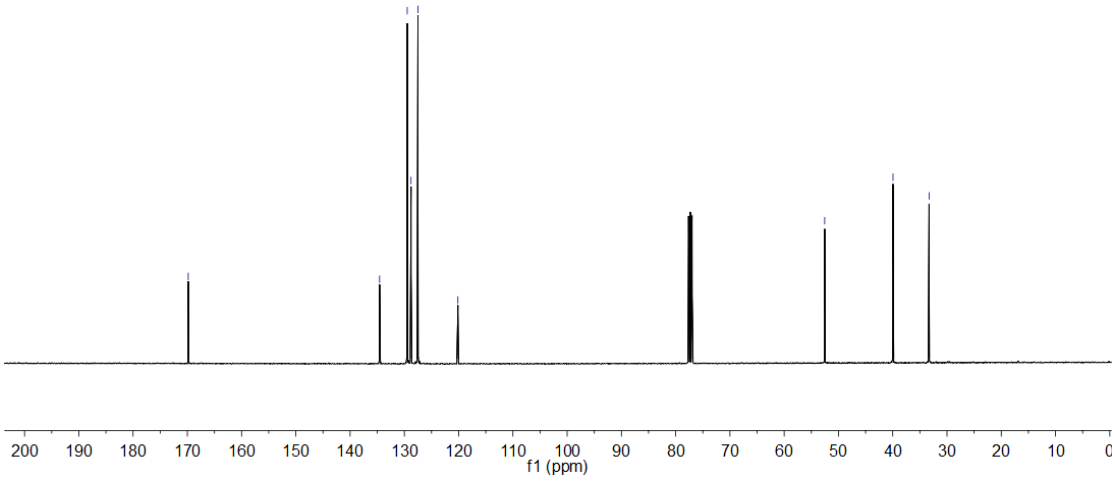
3.01
2.99
2.88
2.86
2.84
2.82

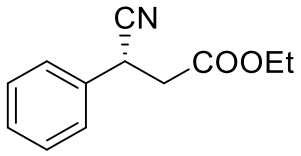

CN
COOMe

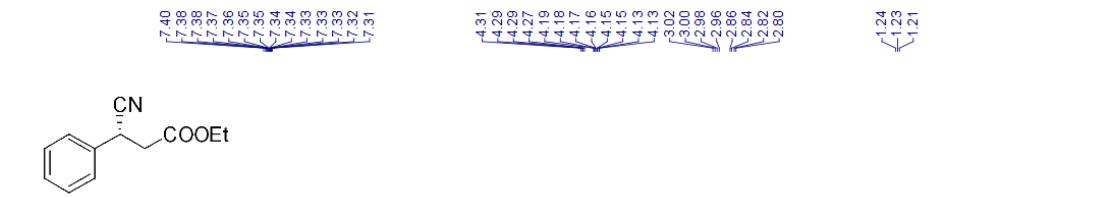

5.07
1.00
3.04
2.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


169.83
134.57
129.48
128.77
127.51
120.14
52.54
39.95
33.30


CN
COOMe


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


CN
COOEt


7.40
7.38
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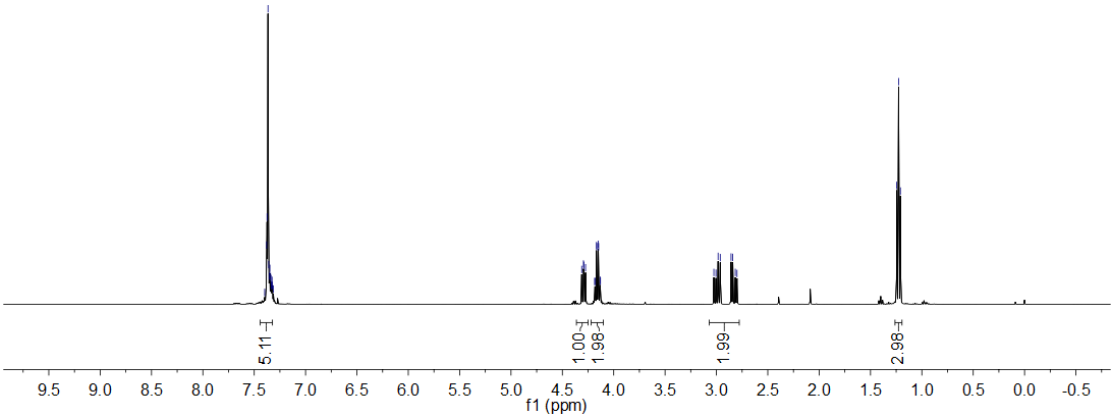
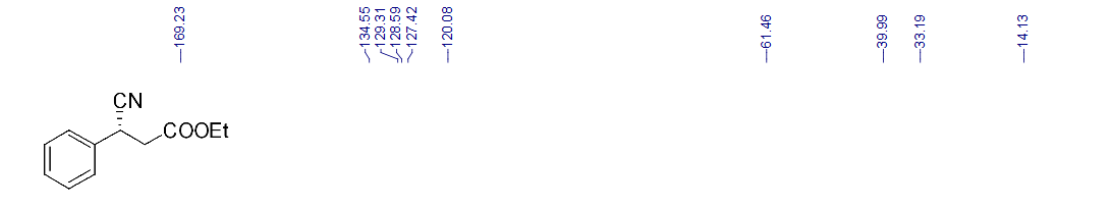
7.35
7.35
7.34
7.34
7.33
7.33
7.33
7.32
7.31
4.31
4.29
4.29
4.27
4.19
4.18
4.17
4.16
4.15
4.15
4.13
4.13
3.02
3.00
2.98
2.96
2.86
2.84
2.82
2.80
1.24
1.23
1.21

CN
COOEt


5.11
1.00
1.98
1.99
2.98
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 -0.5
f1 (ppm)


169.23
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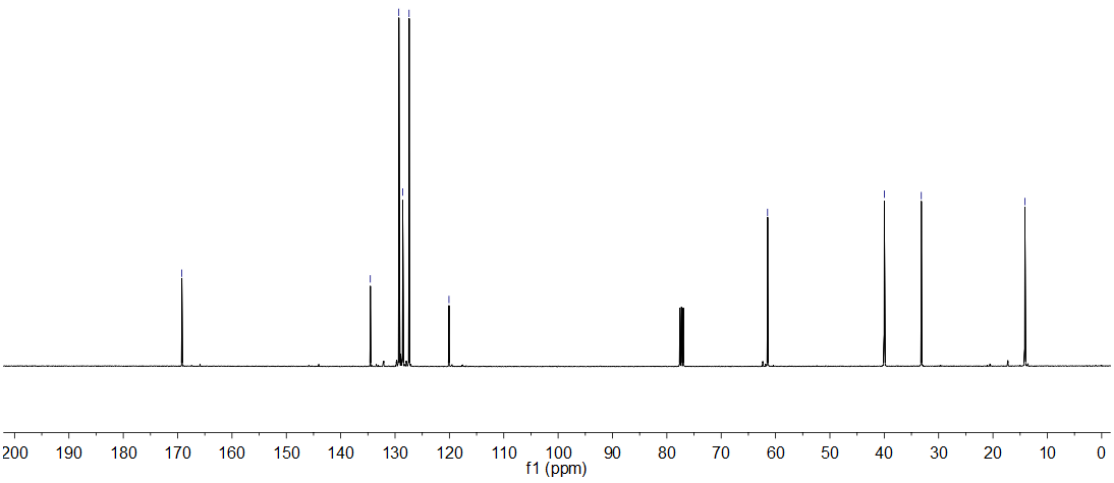
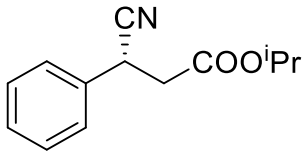
129.31
128.59
127.42
120.08
61.46
39.99
33.19
14.13

CN
COOEt


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


CN
COO^{i}Pr


7.41
7.40
7.40
7.39
7.38
7.38
7.37
7.36
7.36
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7.35
7.34
7.34
7.33
7.33
7.32
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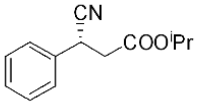
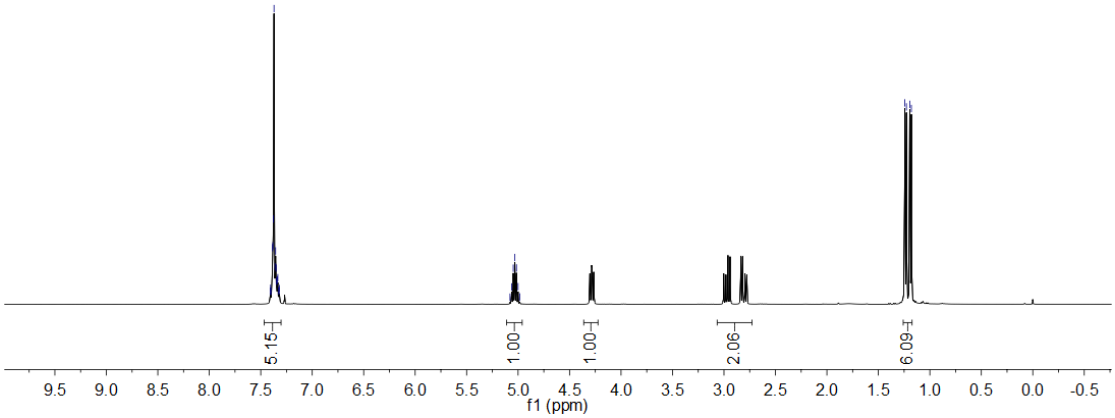
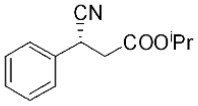
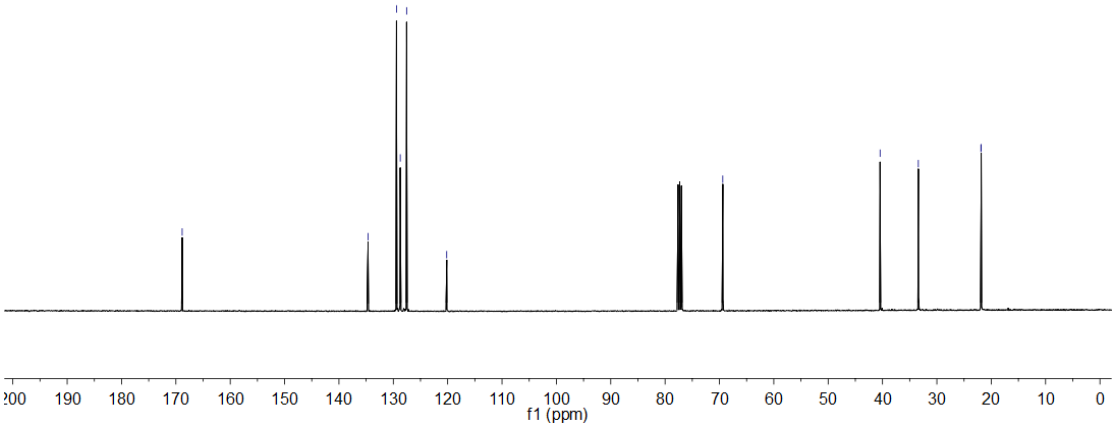
5.00
4.98
1.24
1.23
1.20
1.18

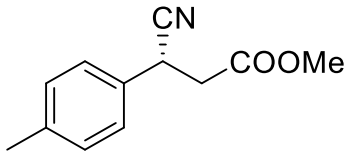

CN
COO^{i}Pr

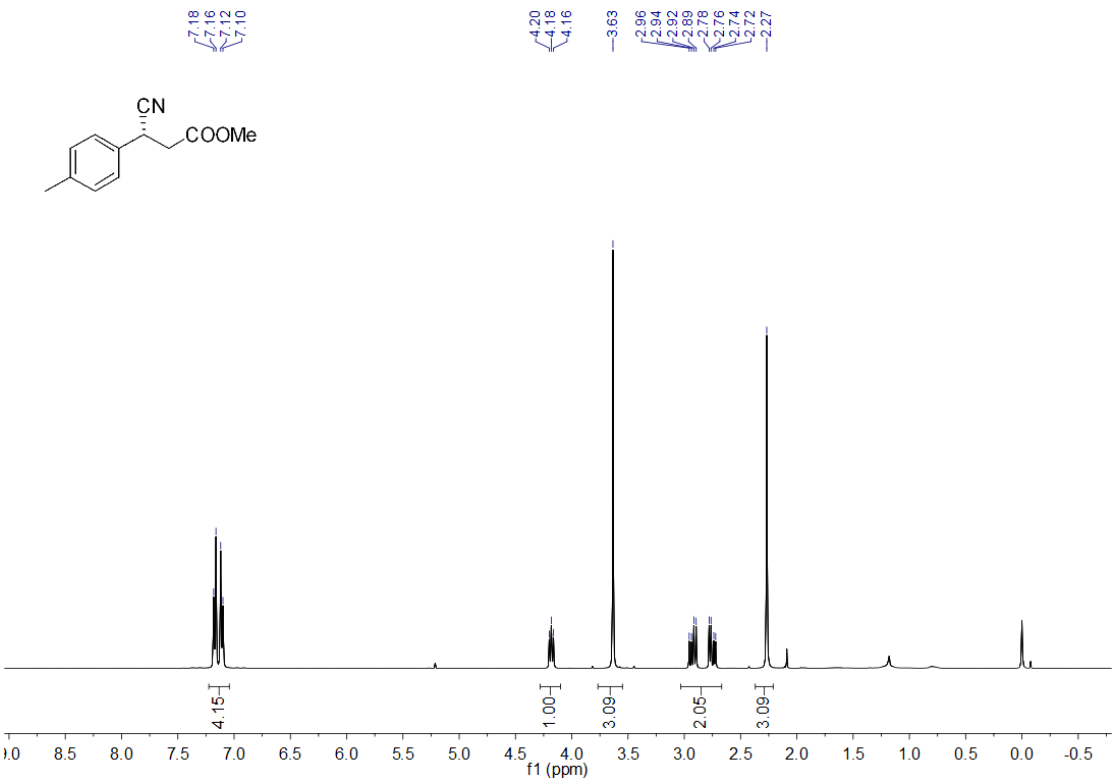

5.15
1.00
1.00
2.06
6.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


168.84
134.64
129.42
128.72
127.55
120.17
69.39
40.44
33.41
21.90
21.84


CN
COO^{i}Pr


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


CN
COOMe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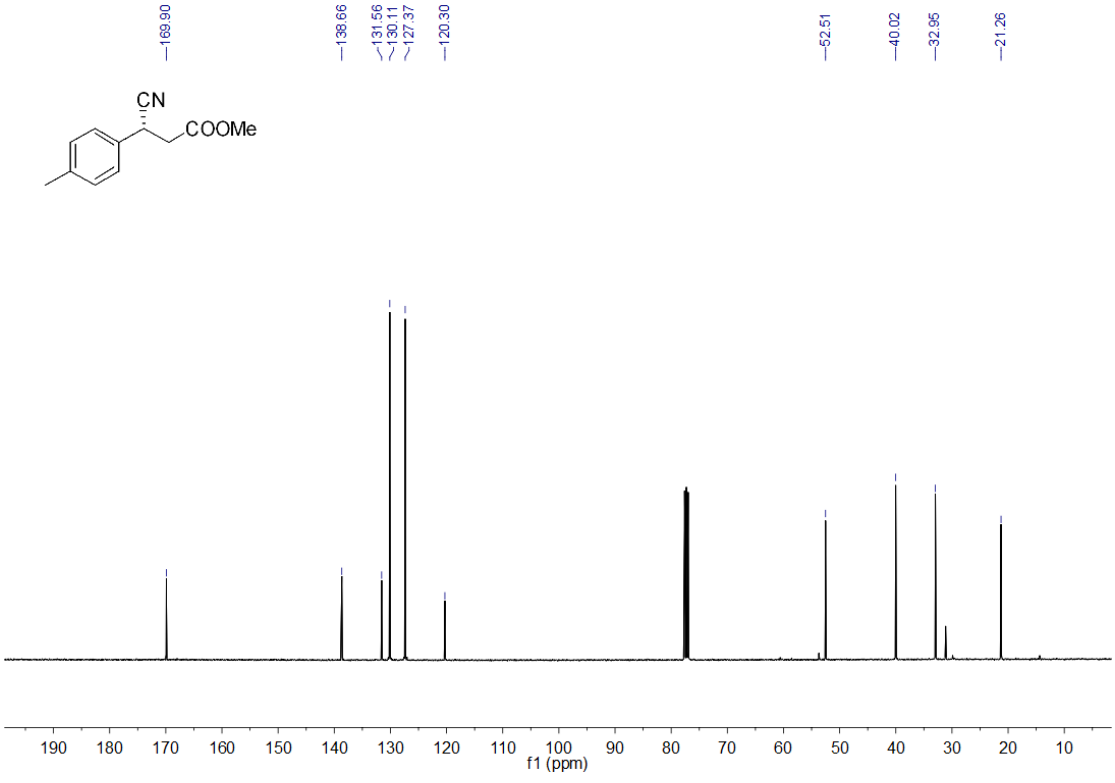
7.16
7.12
7.10
4.20
4.18
4.16
3.63
2.96
2.94
2.92
2.89
2.78
2.76
2.74
2.72
2.27
CN
COOMe
4.15
1.00
3.09
2.05
3.09
f1 (ppm)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138.66
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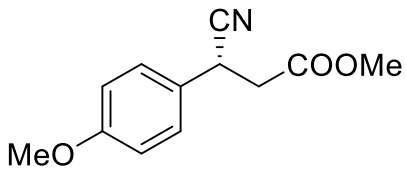
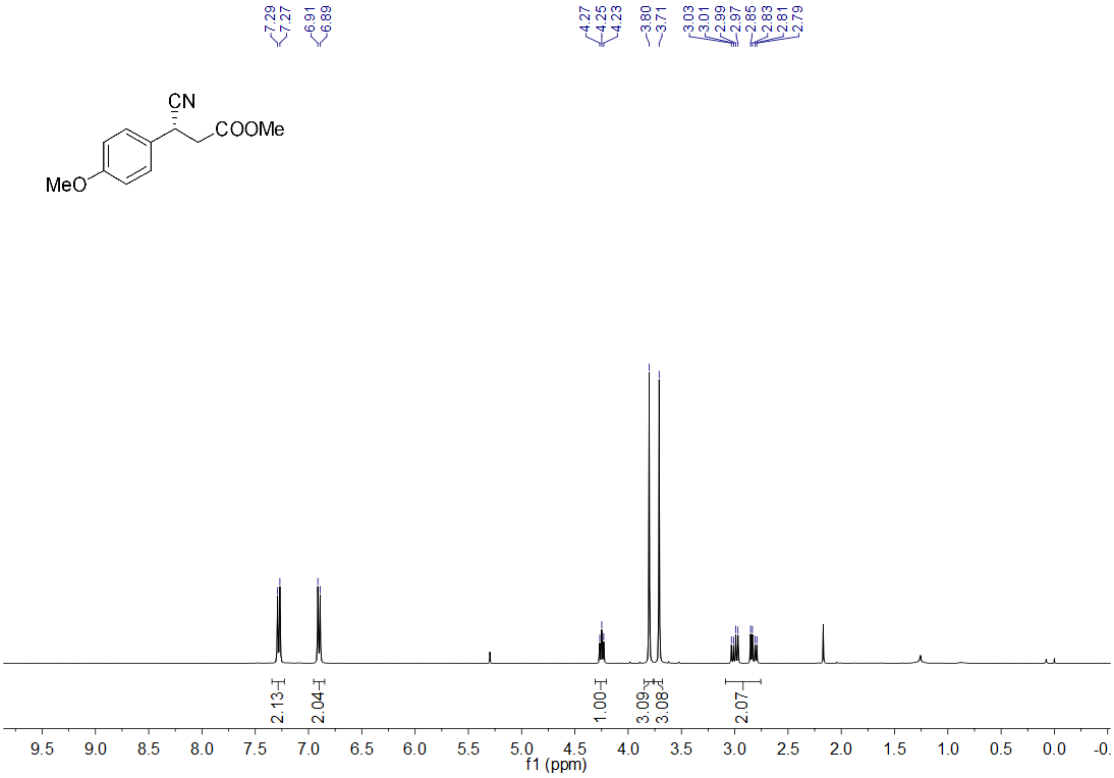
130.11
127.37
120.30
52.51
40.02
32.95
21.26
CN
COOMe
f1 (ppm)


CN
COOMe
MeO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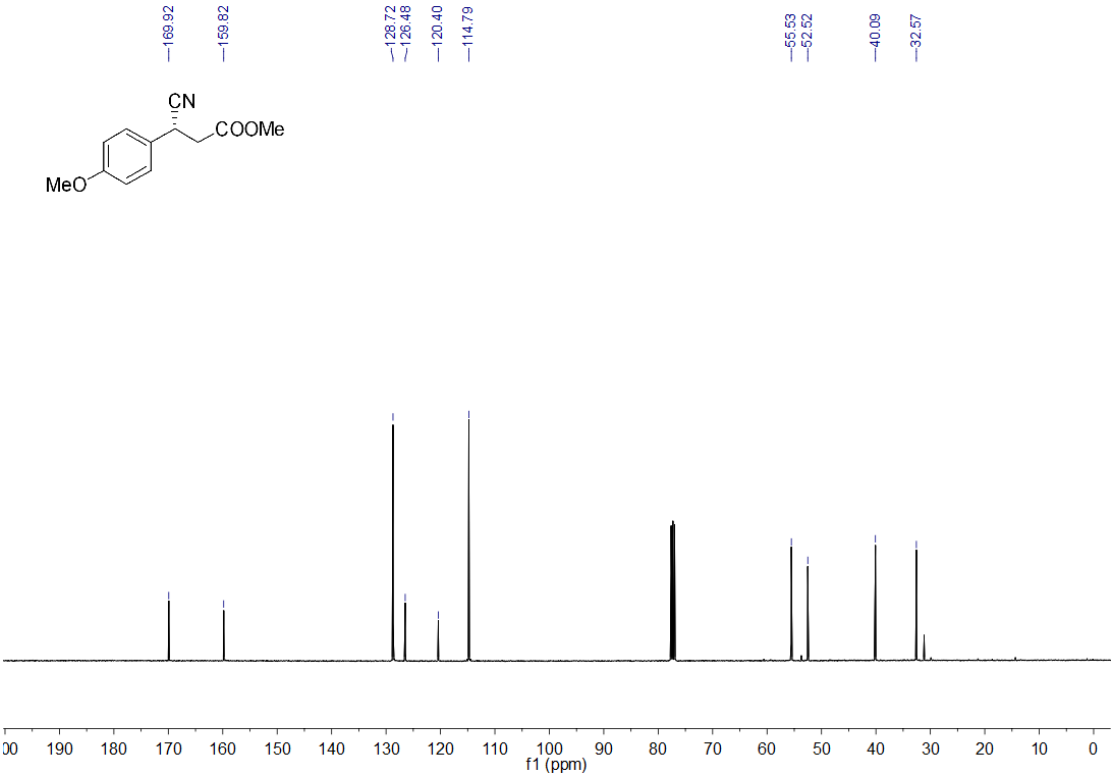
7.27
6.91
6.89
4.27
4.25
4.23
3.80
3.71
3.03
3.01
2.99
2.97
2.85
2.83
2.81
2.79
CN
COOMe
MeO
2.13
2.04
1.00
3.09
3.08
2.07
f1 (ppm)


169.92
159.82
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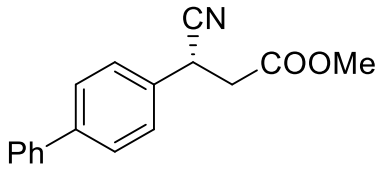
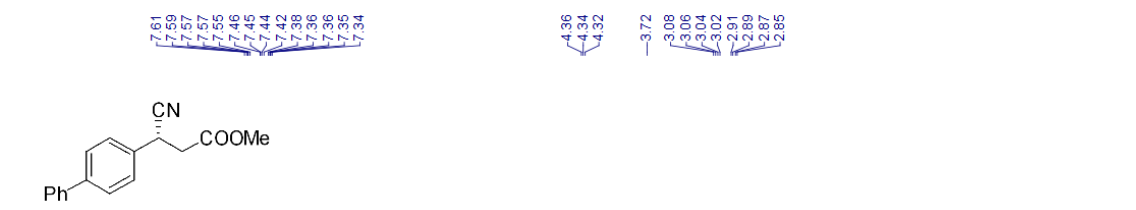
120.40
114.79
55.53
52.52
40.09
32.57
CN
COOMe
MeO
f1 (ppm)


CN
COOMe
Ph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7.57
7.55
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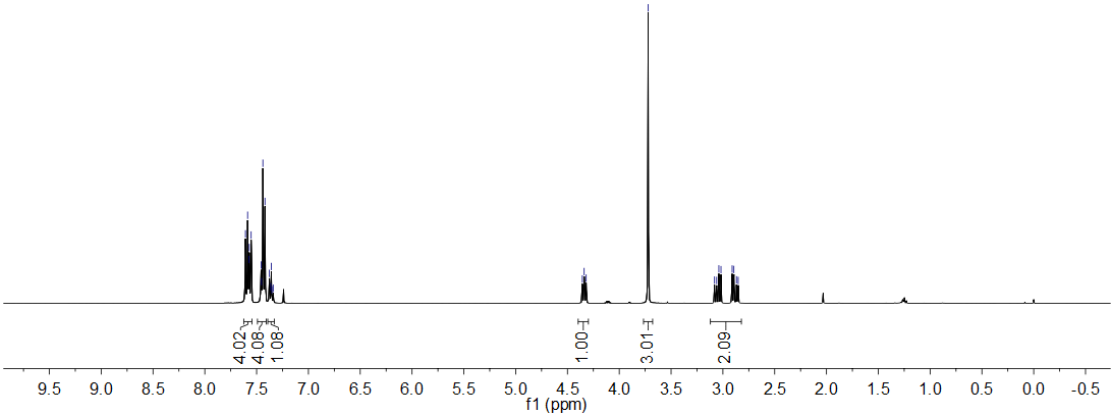
7.45
7.44
7.42
7.38
7.36
7.36
7.35
7.34
4.36
4.34
4.32
3.72
3.08
3.06
3.04
3.02
2.91
2.89
2.87
2.85

CN
COOMe
Ph


4.02
4.08
1.08
1.00
3.01
2.09
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 -0.5
f1 (ppm)


169.84
141.77
140.23
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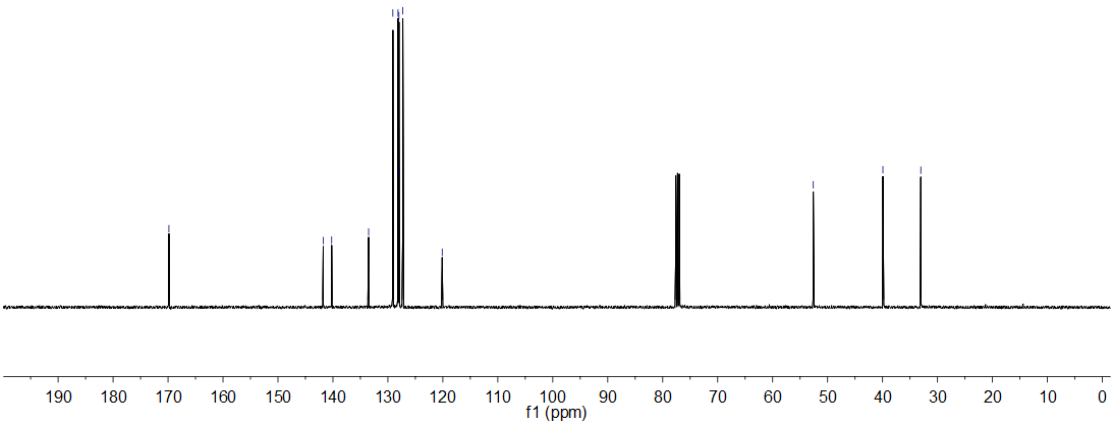
39.94
33.04

CN
COOMe
Ph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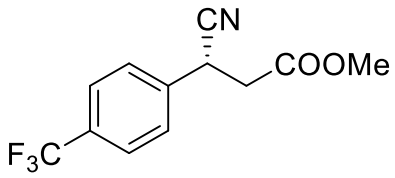
f1 (ppm)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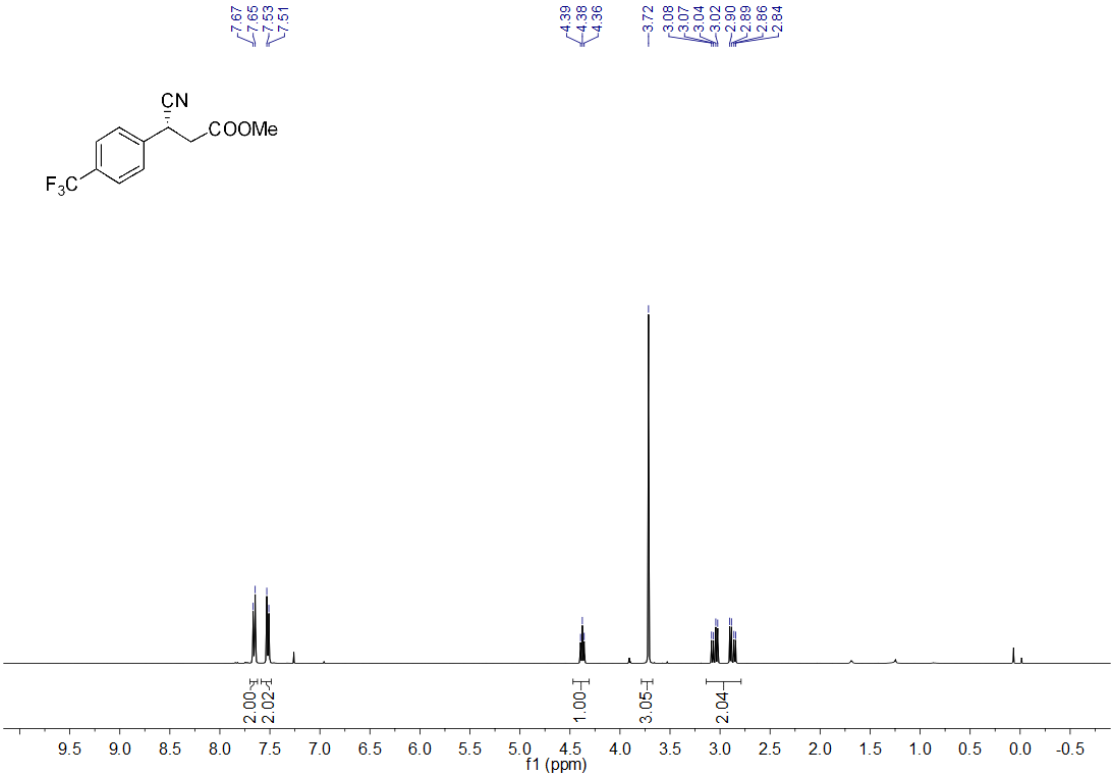
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3.02
2.90
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2.84
CN
COOMe
F3C
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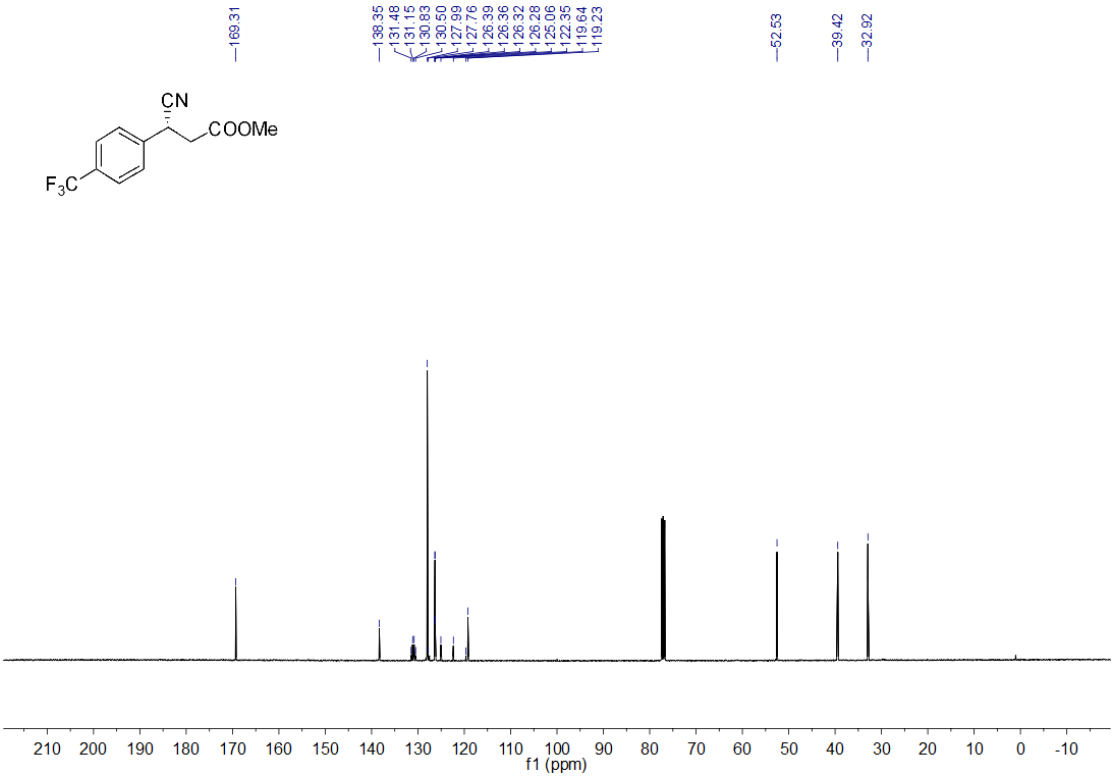
2.02
1.00
3.05
2.04
f1 (ppm)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39.42
32.92
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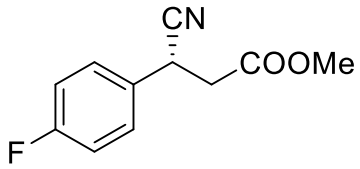
F3C
f1 (ppm)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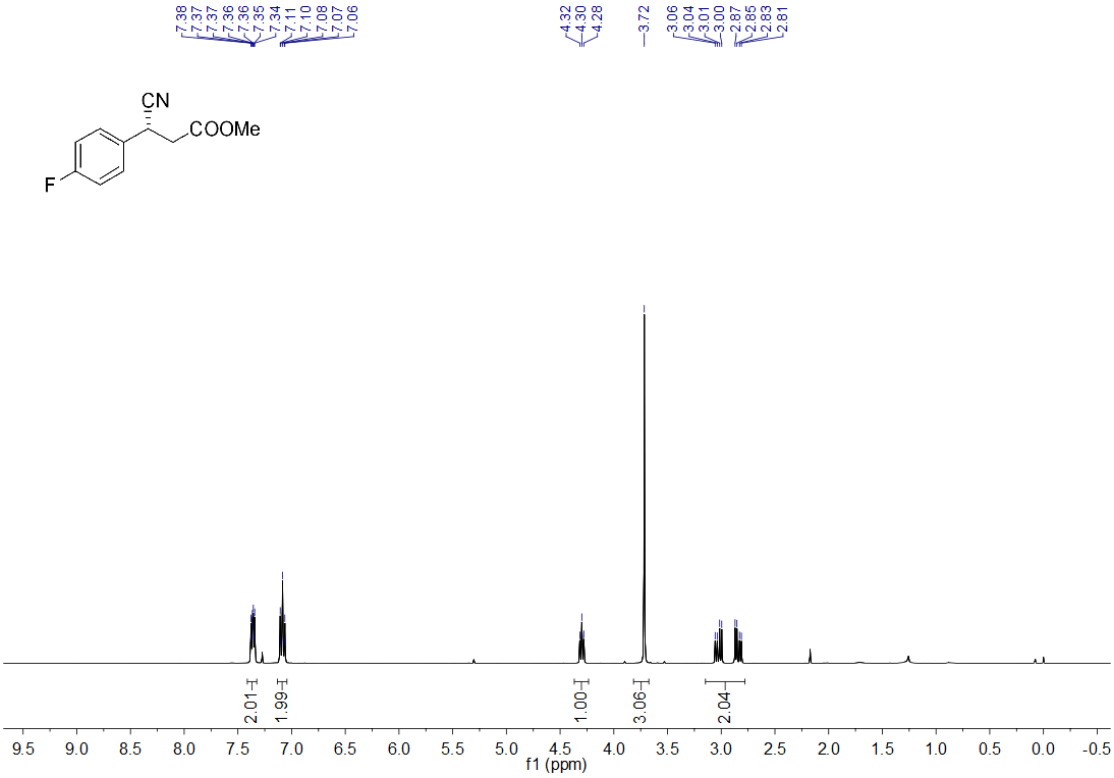
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7.08
7.07
7.06
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4.30
4.28
3.72
3.06
3.04
3.01
3.00
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2.81
CN
COOMe
F
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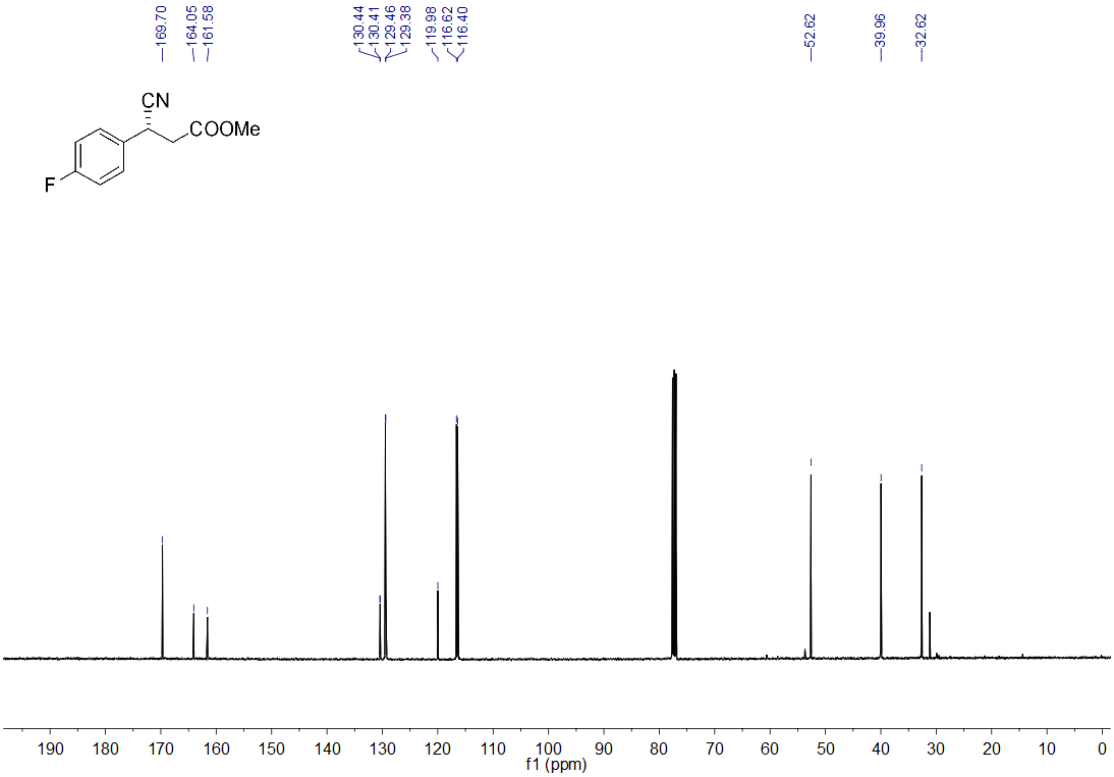
1.99
1.00
3.06
2.04
f1 (ppm)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32.62
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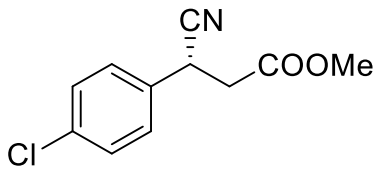
COOMe
F
f1 (ppm)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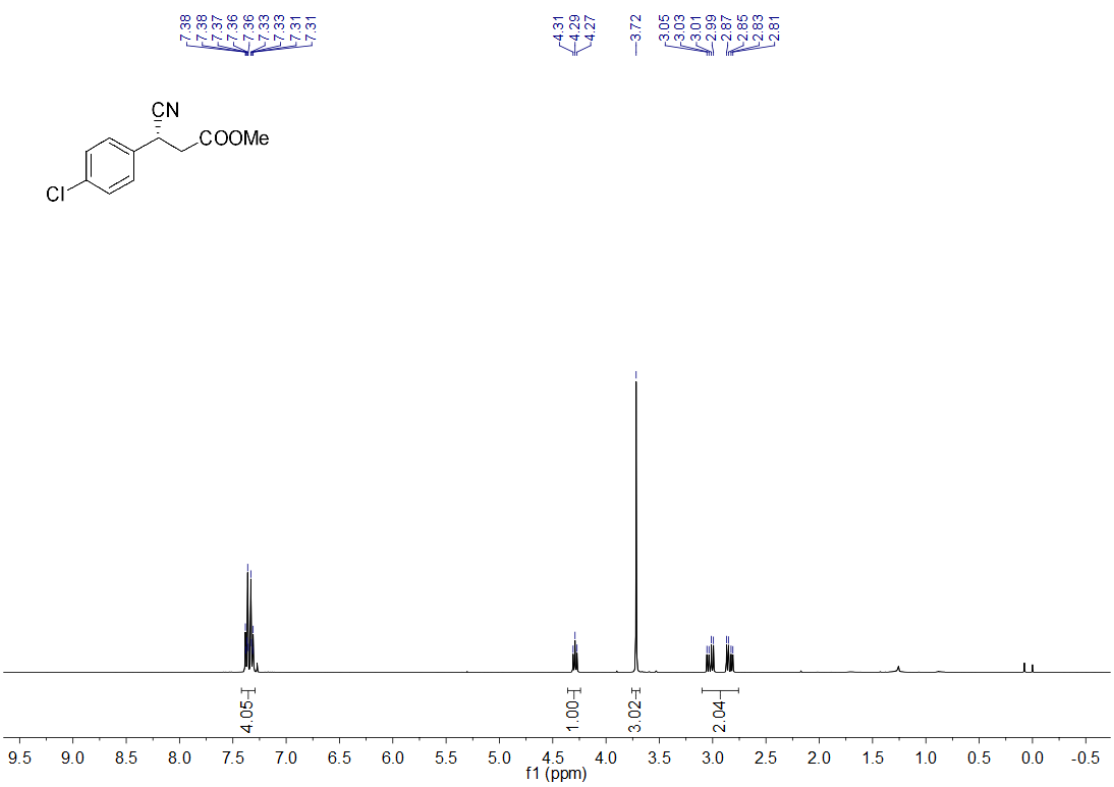
COOMe
Cl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3.72
3.05
3.03
3.01
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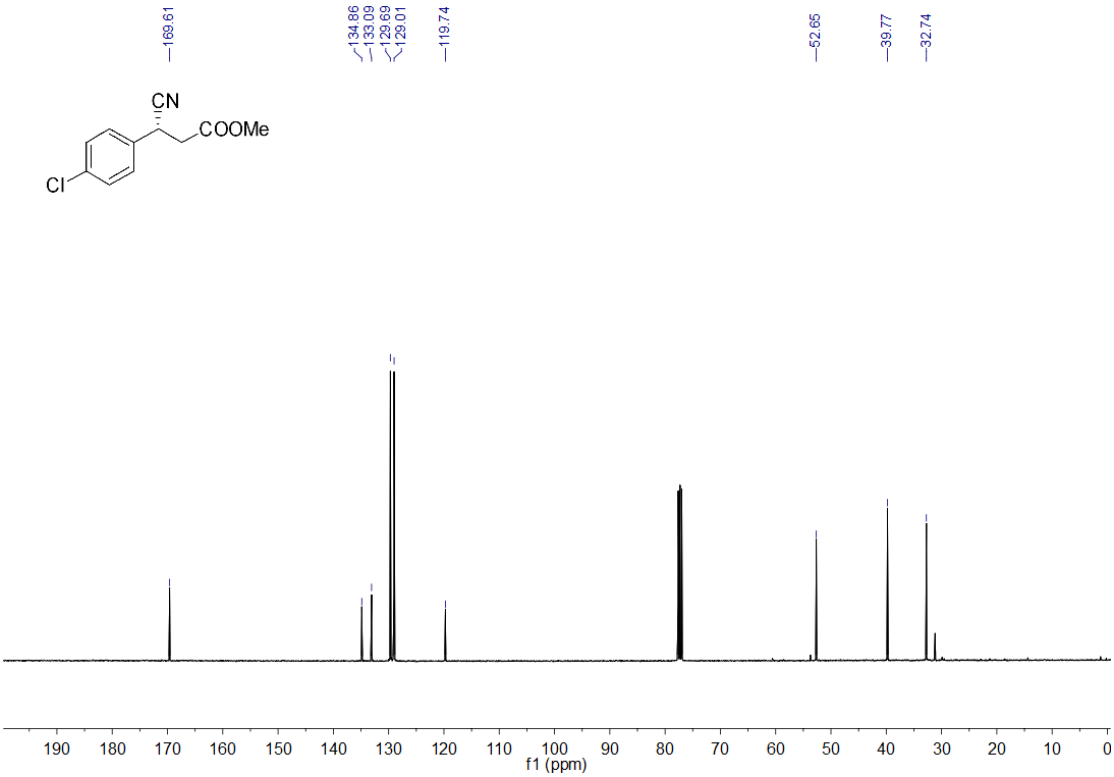
2.83
2.81
CN
COOMe
Cl
4.05
1.00
3.02
2.04
f1 (ppm)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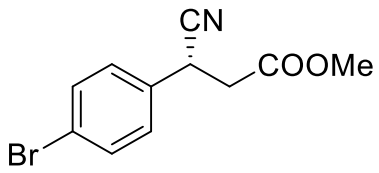
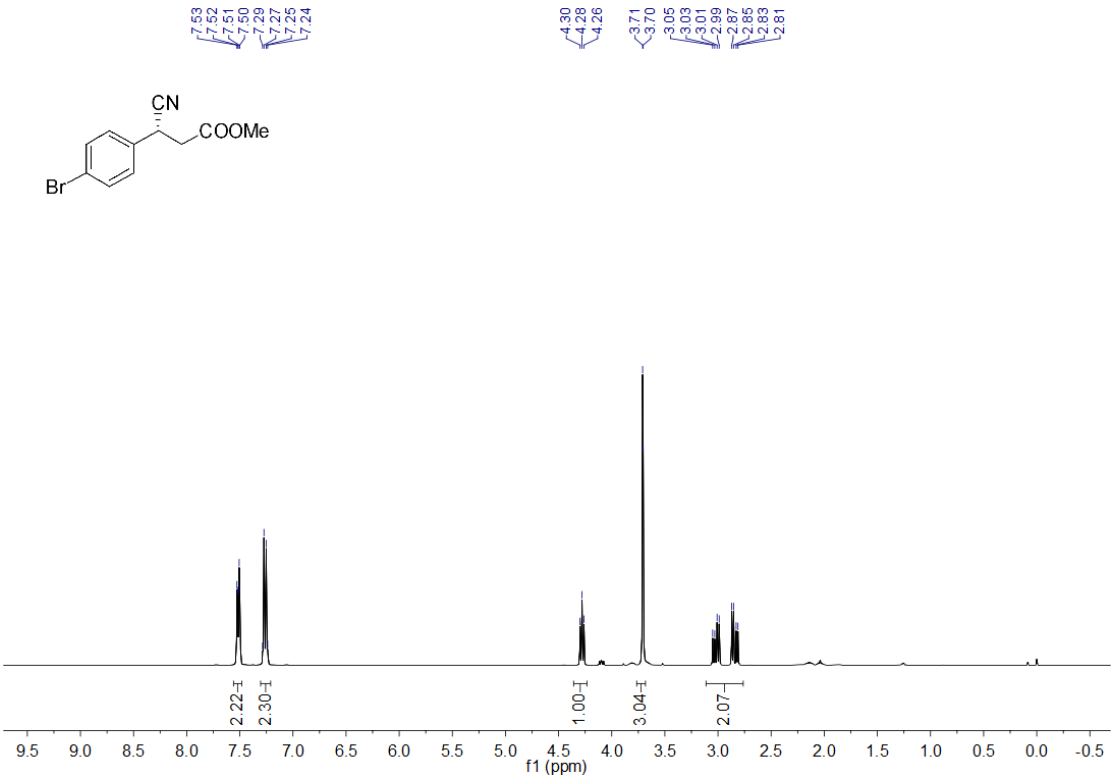
COOMe
Cl
f1 (ppm)


CN
COOMe
Br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7.24
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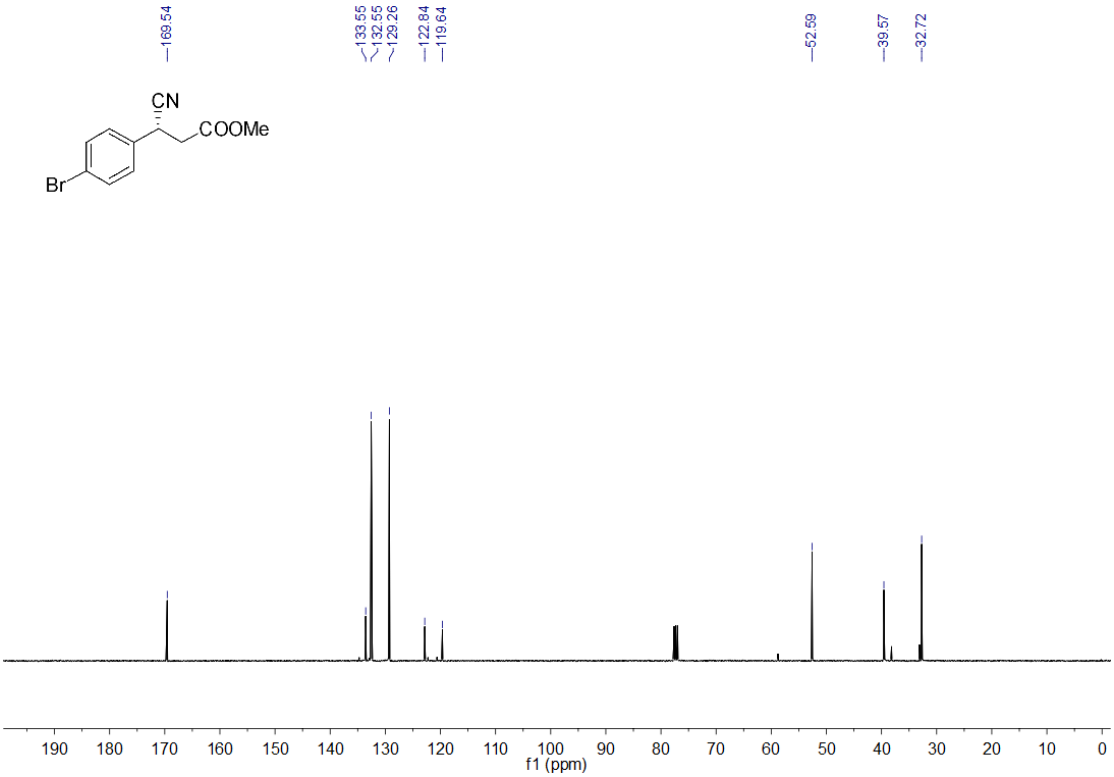
4.28
4.26
3.71
3.70
3.05
3.03
3.01
2.99
2.87
2.85
2.83
2.81
CN
COOMe
Br
2.22
2.30
1.00
3.04
2.07
f1 (ppm)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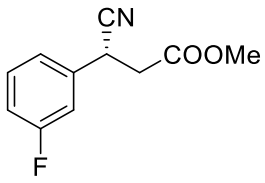
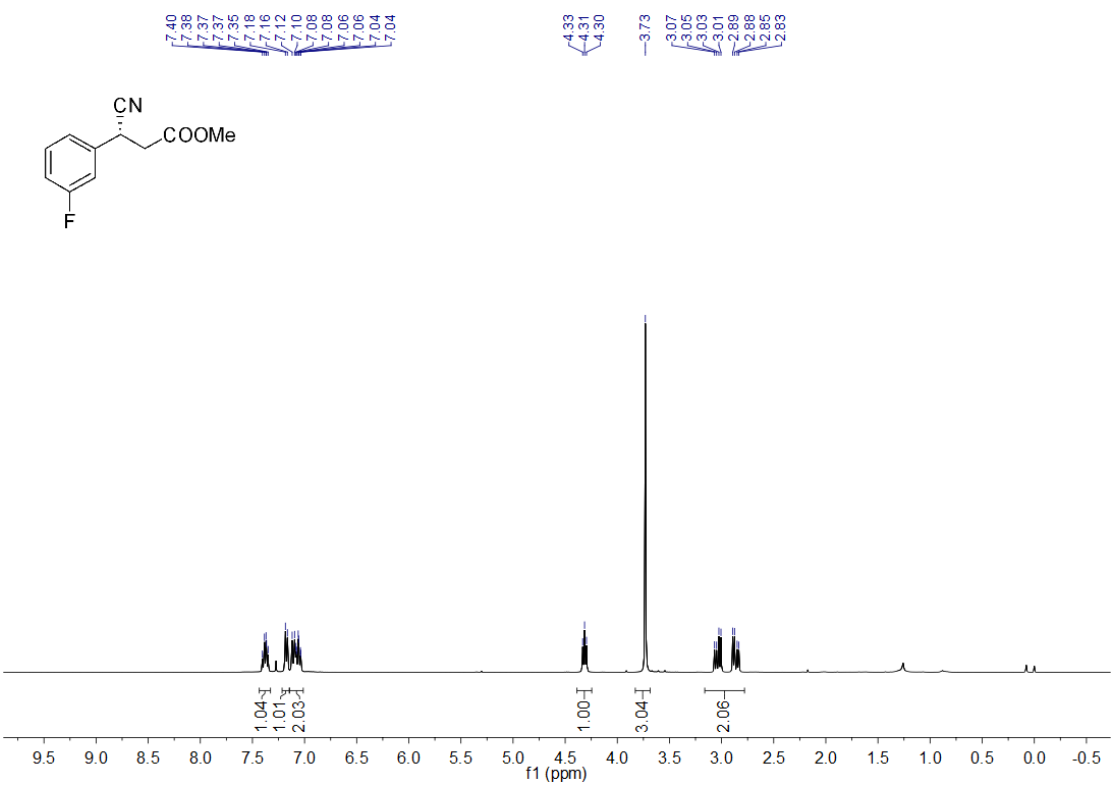
119.64
52.59
39.57
32.72
CN
COOMe
Br
f1 (ppm)


CN
COOMe
F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7.12
7.10
7.08
7.08
7.06
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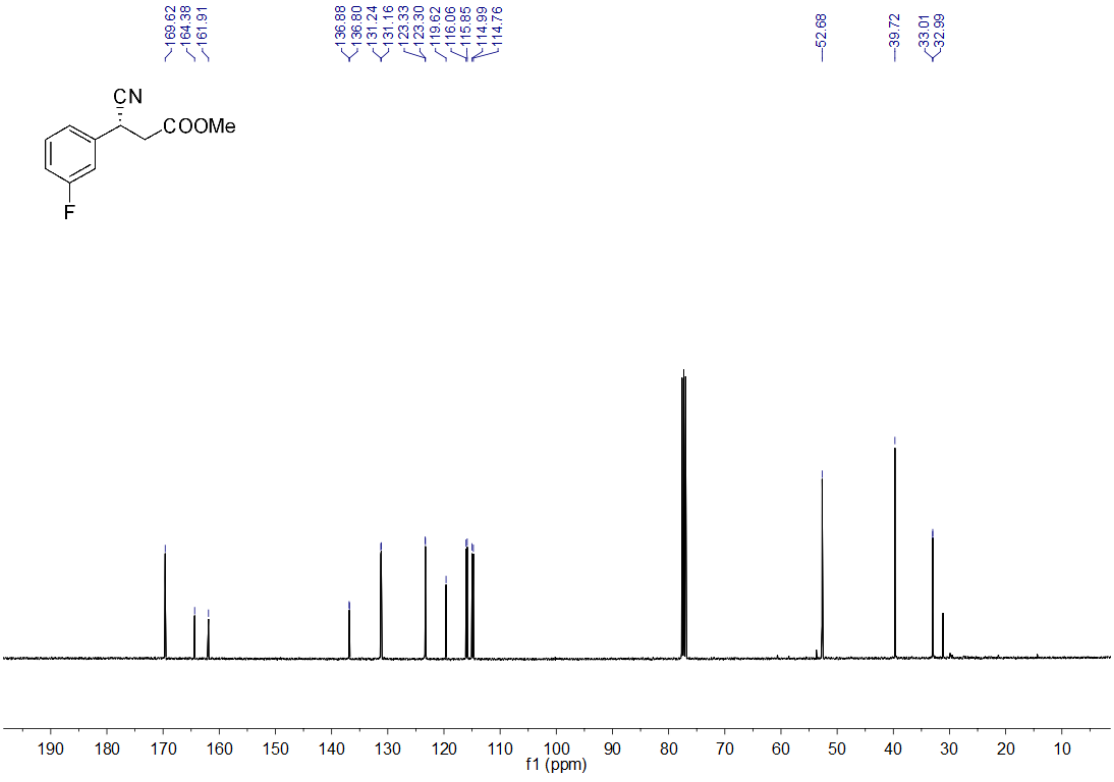
7.04
7.04
4.33
4.31
4.30
3.73
3.07
3.05
3.03
3.01
2.89
2.88
2.85
2.83
CN
COOMe
F
1.04
1.01
2.03
1.00
3.04
2.06
f1 (ppm)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123.30
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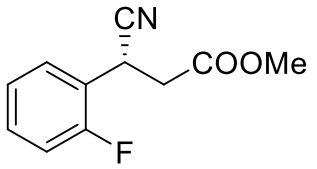
114.76
52.68
39.72
33.01
32.99
CN
COOMe
F
f1 (ppm)


CN
COOMe
F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7.47
7.39
7.39
7.38
7.37
7.35
7.35
7.34
7.34
7.22
7.20
7.18
7.14
7.11
7.09
4.55
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3.74
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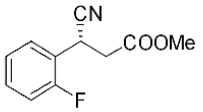
3.03
3.01
2.99
2.94
2.92
2.90
2.88


CN
COOMe
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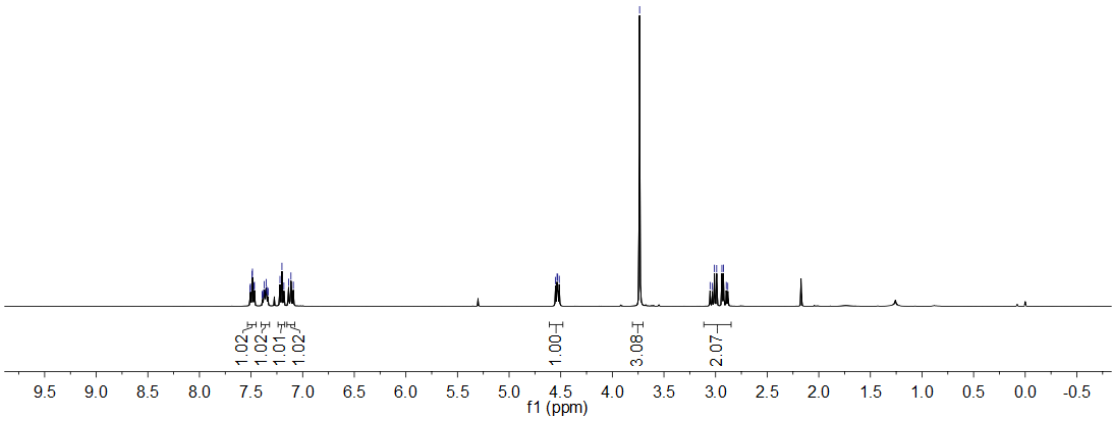
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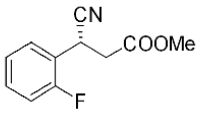
1.02
1.01
1.02
1.00
3.08
2.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


169.65
161.27
158.60
130.93
130.85
129.52
129.49
125.16
125.12
121.73
121.59
119.14
116.40
116.19
52.61
38.04
38.02
27.79
27.75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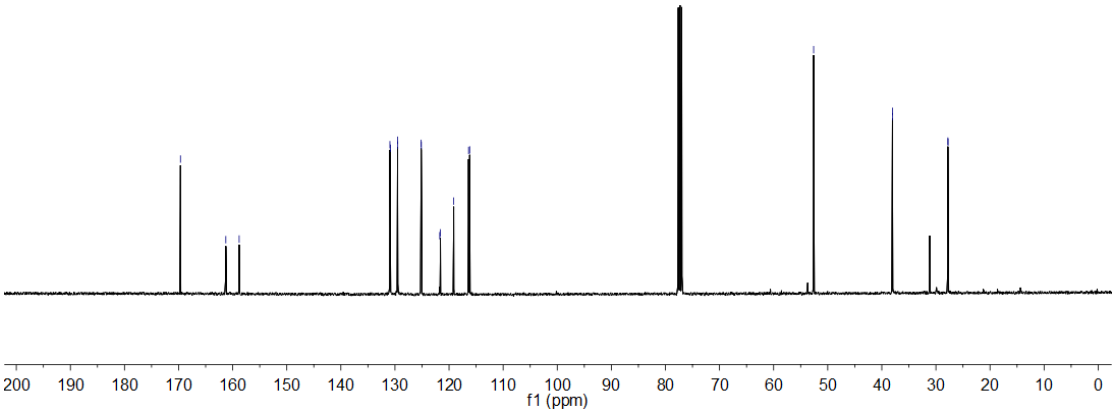
COOMe
F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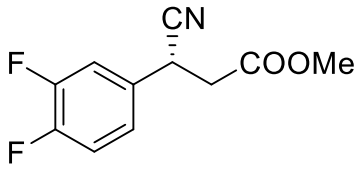
f1 (ppm)


CN
F
COOMe
F


7.28
7.26
7.26
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7.24
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7.22
7.20
7.19
7.17
7.16
7.16
7.16
7.15
7.14
7.13
7.13
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3.00
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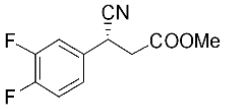
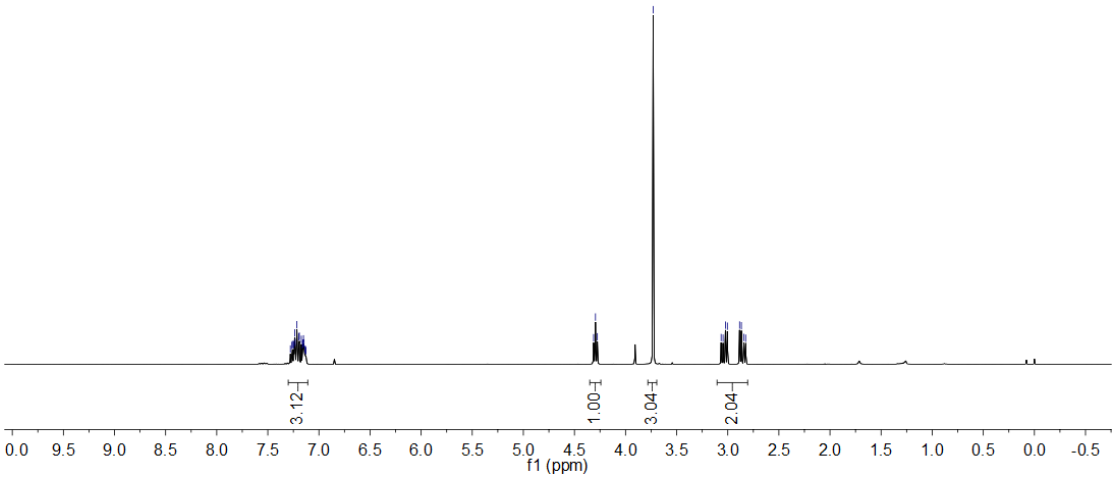
2.84
2.82


CN
F
COOMe
F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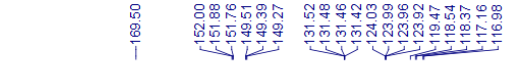
3.04
2.04
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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131.46
131.42
124.03
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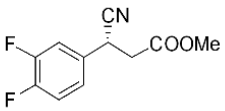
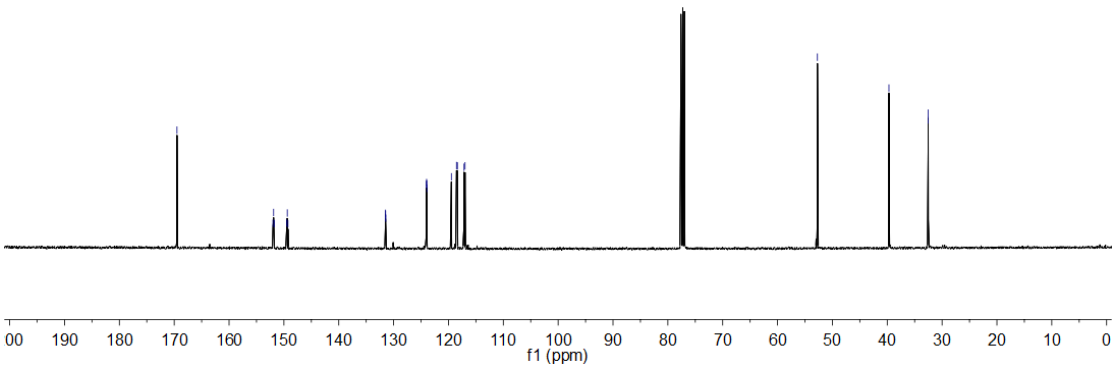
123.92
119.47
118.54
118.37
117.16
116.98
52.73
39.69
32.53
32.52


CN
F
COOMe
F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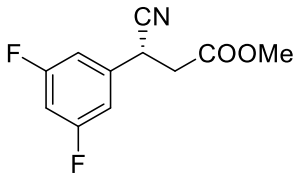
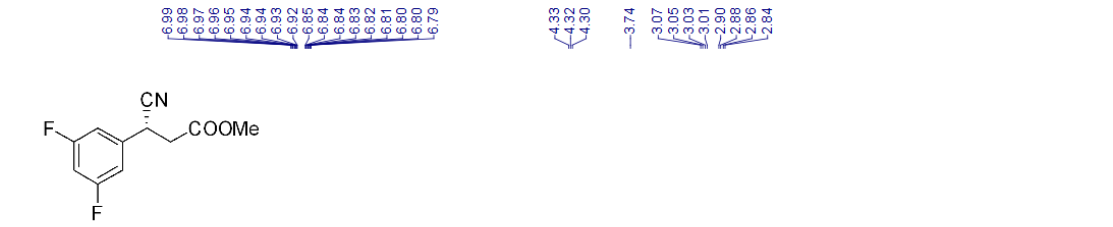
f1 (ppm)


CN
F
COOMe
F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6.98
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6.96
6.95
6.94
6.94
6.93
6.92
6.85
6.84
6.84
6.84
6.83
6.82
6.81
6.80
6.80
6.79
4.33
4.32
4.30
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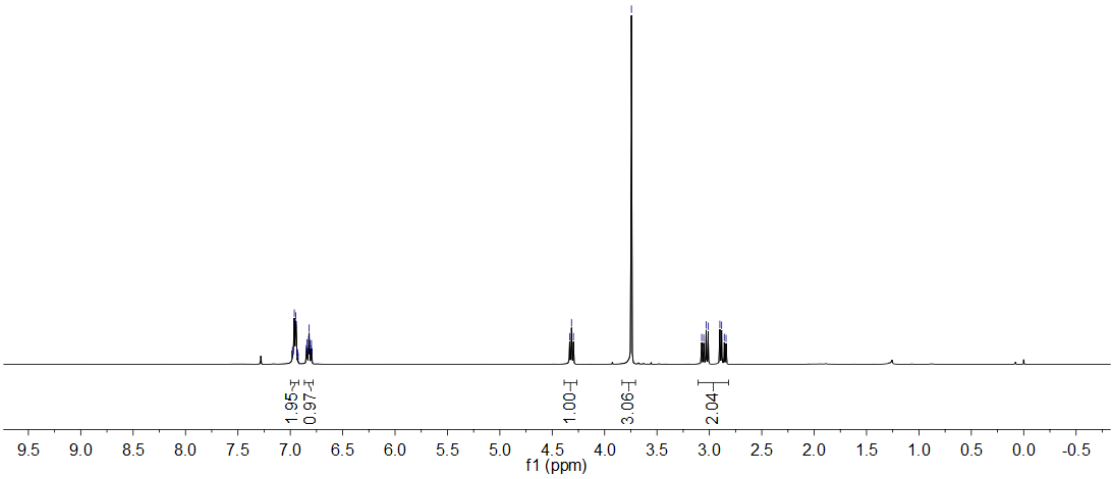
3.05
3.03
3.01
2.90
2.88
2.86
2.84

CN
F
COOMe
F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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
-0.5
f1 (ppm)


169.41
164.79
164.66
162.29
162.17
138.21
138.12
138.02
119.09
111.15
110.88
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104.34
52.78
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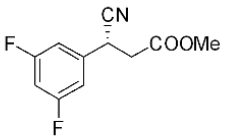
32.93
32.91
32.89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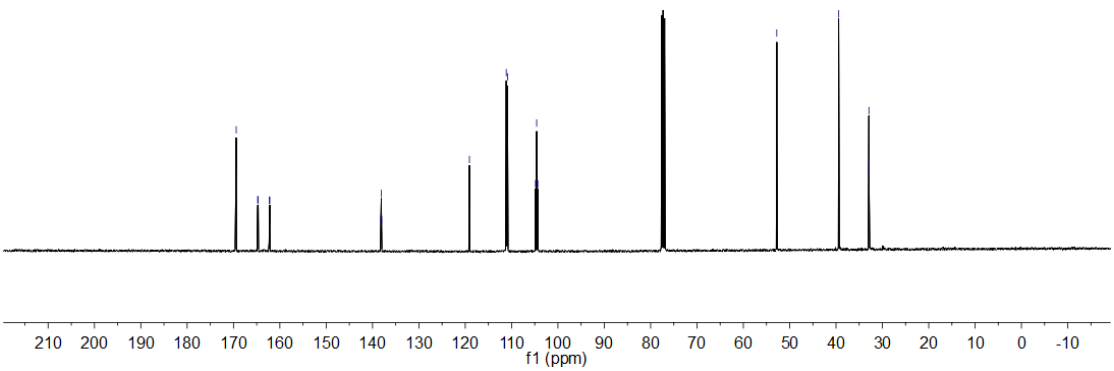
F
COOMe
F


210
200
190
180
170
160
150
140
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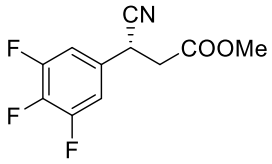
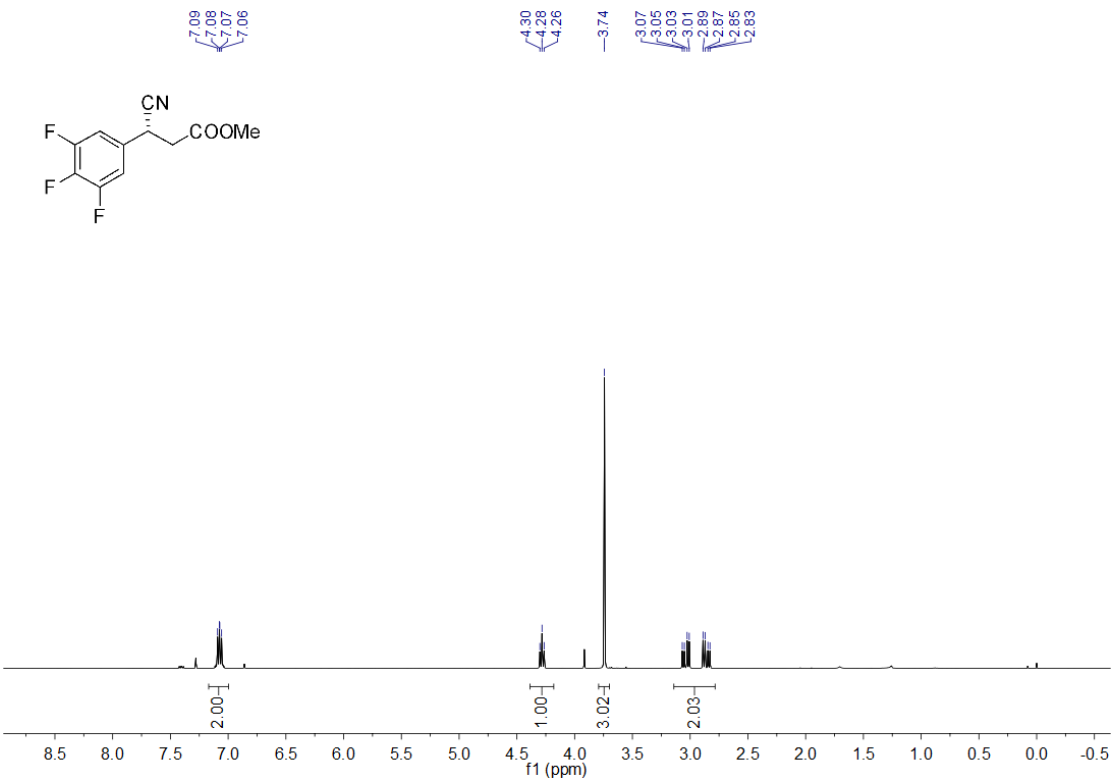
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


CN
COOMe
F
F
F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7.08
7.07
7.06
4.30
4.28
4.26
3.74
3.07
3.05
3.03
3.01
2.89
2.87
2.85
2.83
CN
COOMe
F
F
F
2.00
1.00
3.02
2.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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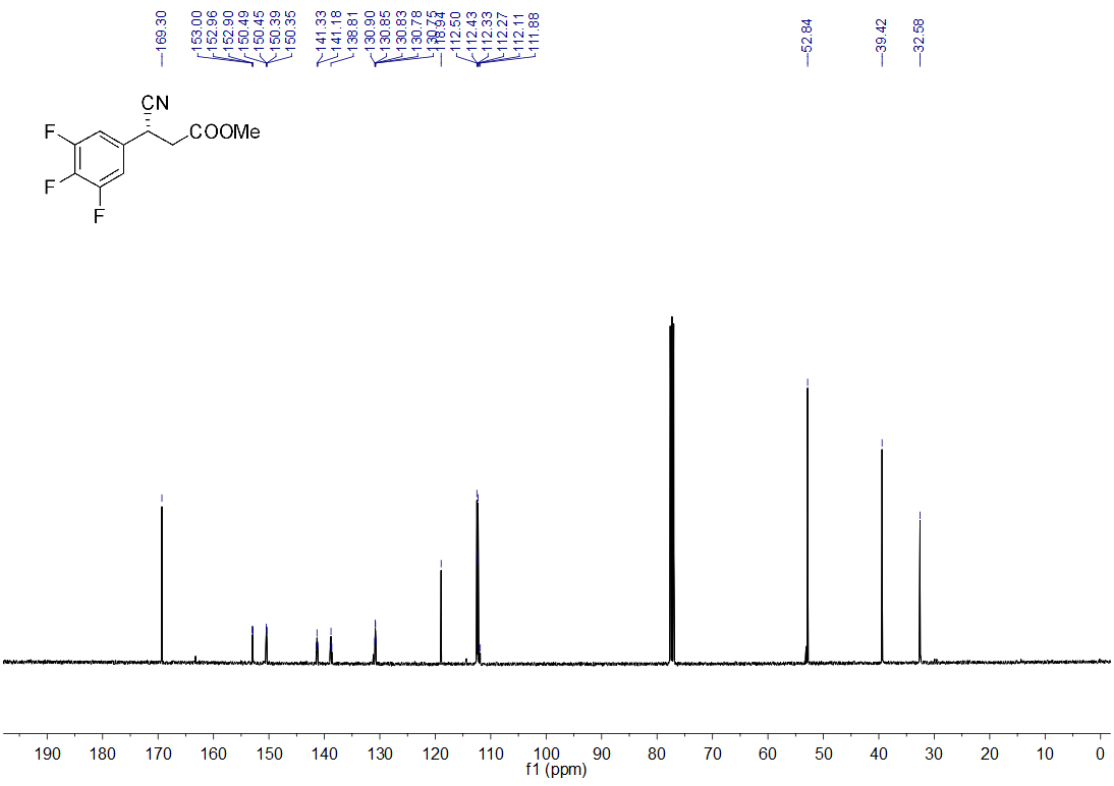
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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130.85
130.83
130.78
112.50
112.43
112.33
112.27
112.11
111.88
52.84
39.42
32.58
CN
COOMe
F
F
F
190
180
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130
120
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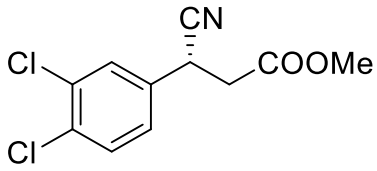
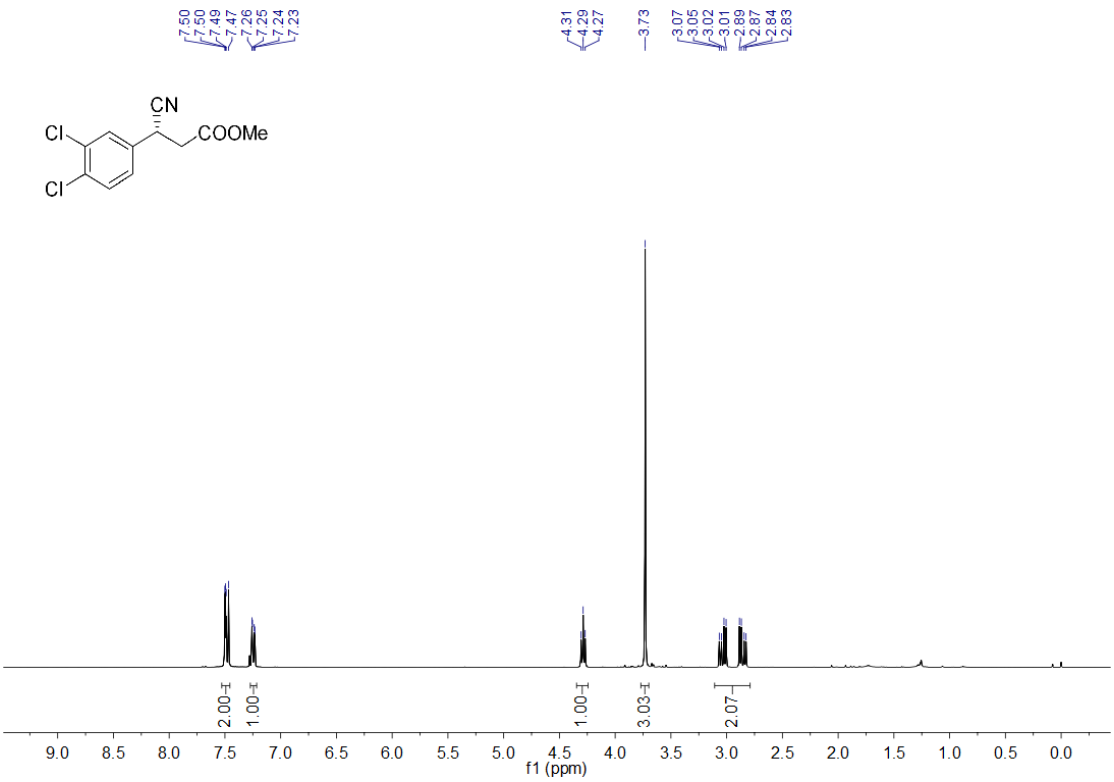
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


CN
Cl
COOMe
Cl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7.47
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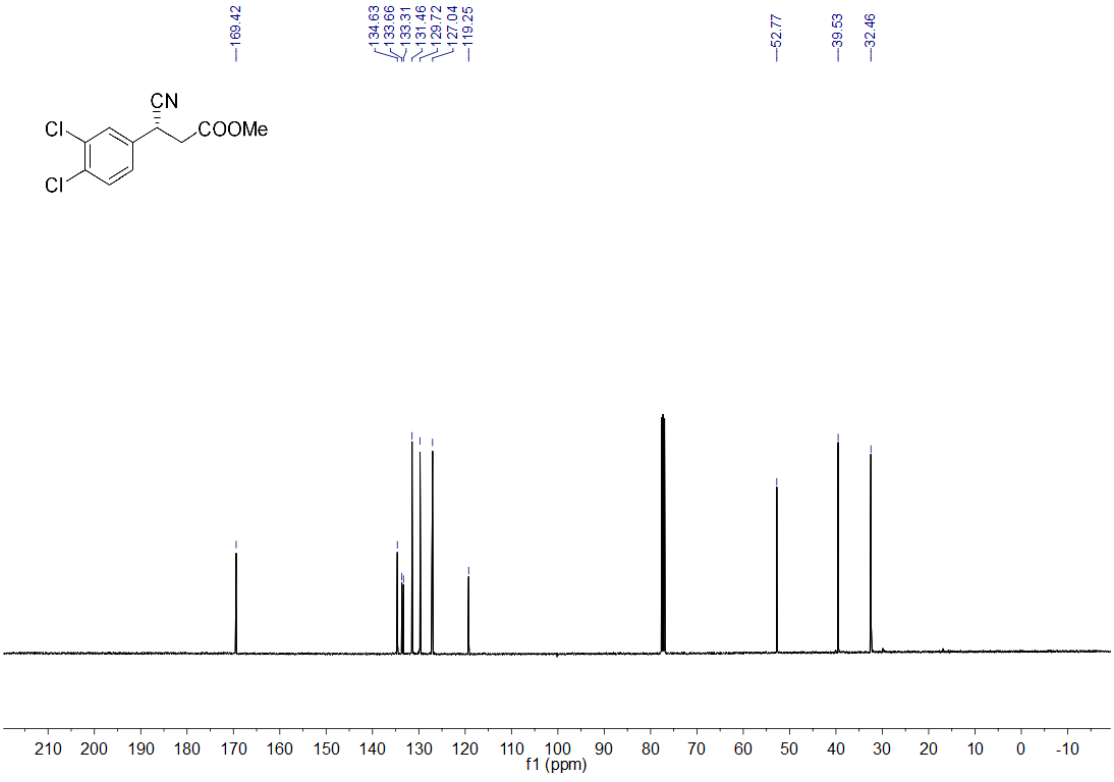
7.25
7.24
7.23
4.31
4.29
4.27
3.73
3.07
3.05
3.02
3.01
2.89
2.87
2.84
2.83
CN
Cl
COOMe
Cl
2.00
1.00
1.00
3.03
2.07
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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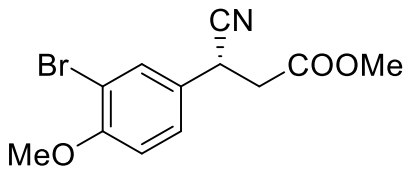
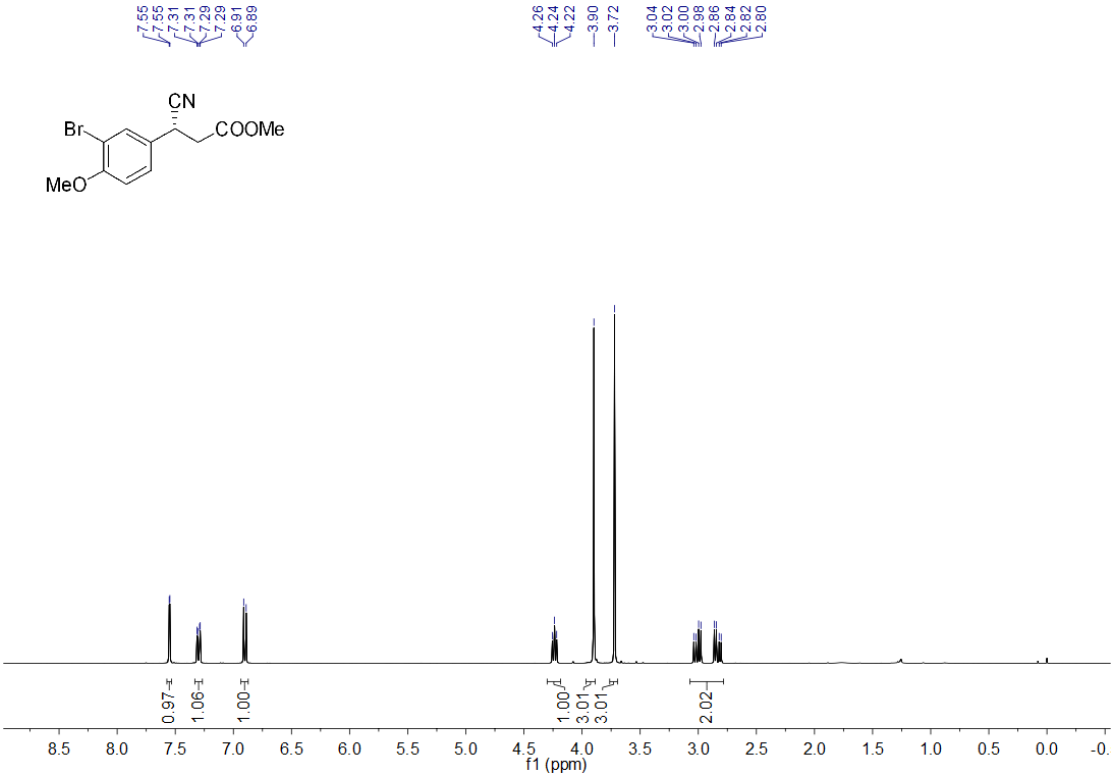
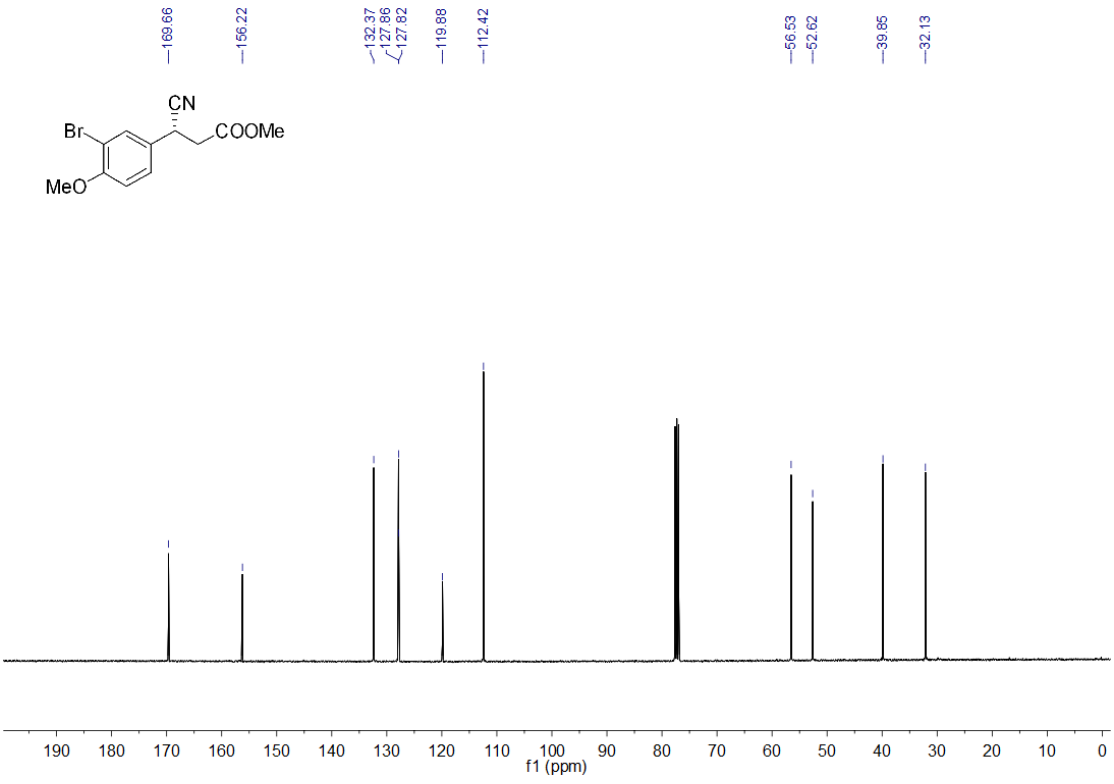
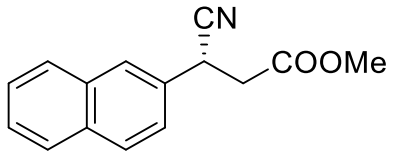
52.77
39.53
32.46
CN
Cl
COOMe
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

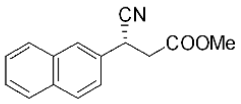

CN
Br
COOMe
MeO

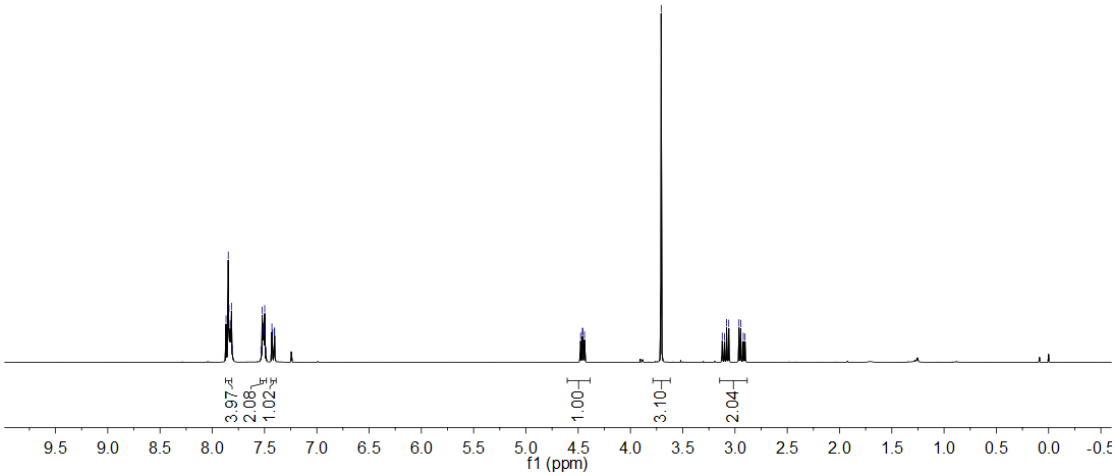

7.55
7.55
7.31
7.31
7.29
7.29
6.91
6.89
4.26
4.24
4.22
3.90
3.72
3.04
3.02
3.00
2.98
2.86
2.84
2.82
2.80
CN
Br
COOMe
MeO
0.97
1.06
1.00
1.00
3.01
3.01
2.02
f1 (ppm)

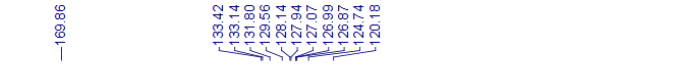

169.66
156.22
132.37
127.86
127.82
119.88
112.42
56.53
52.62
39.85
32.13
CN
Br
COOMe
MeO
f1 (ppm)

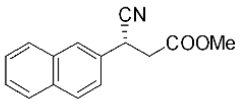

CN
COOMe

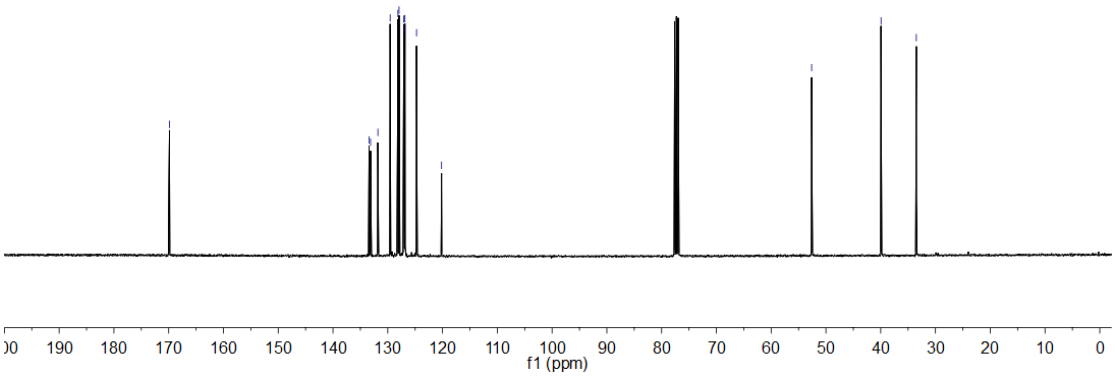

7.87
7.85
7.84
7.83
7.82
7.81
7.53
7.52
7.52
7.51
7.51
7.50
7.50
7.49
7.43
7.42
7.41
7.40
4.48
4.46
4.46
4.44
3.71
3.12
3.10
3.08
3.06
2.96
2.95
2.92
2.90

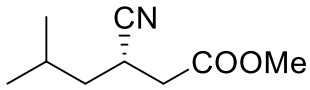

CN
COOMe

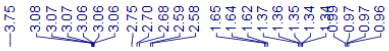

3.97
2.08
1.02
1.00
3.10
2.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

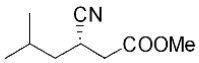

169.86
133.42
133.14
131.80
129.56
128.14
127.94
127.07
126.99
126.87
124.74
120.18
52.61
39.94
33.50

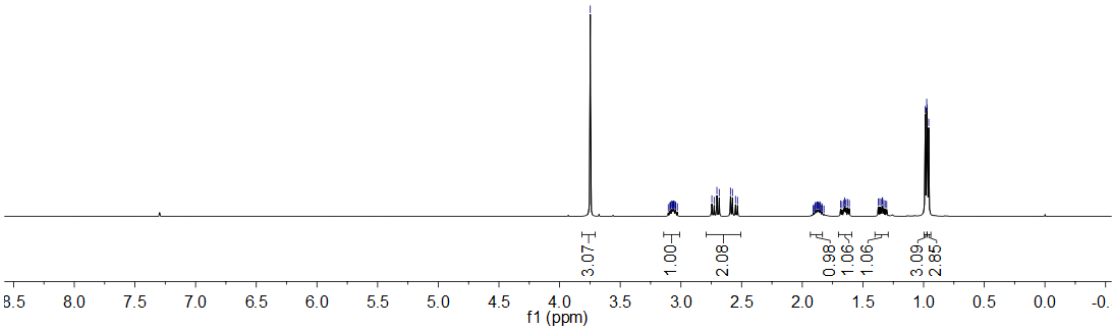

CN
COOMe

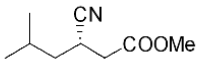

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

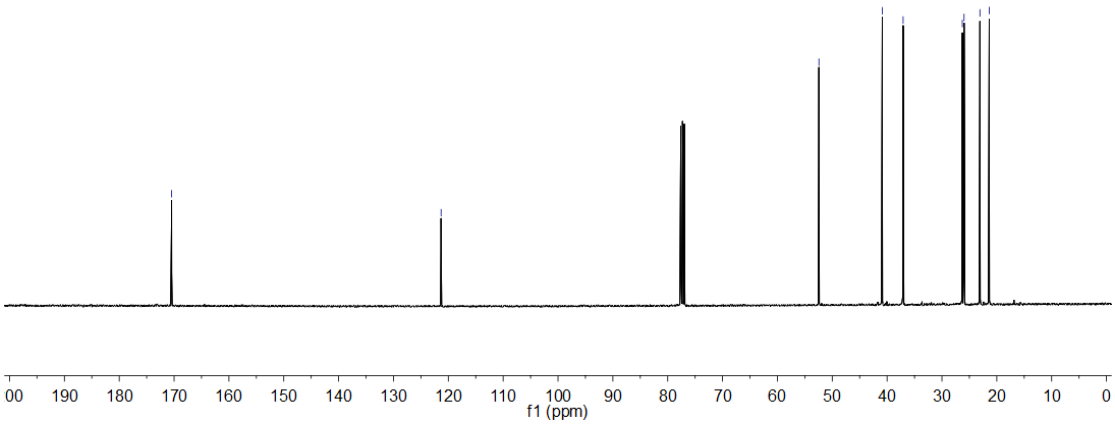




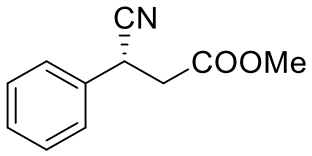






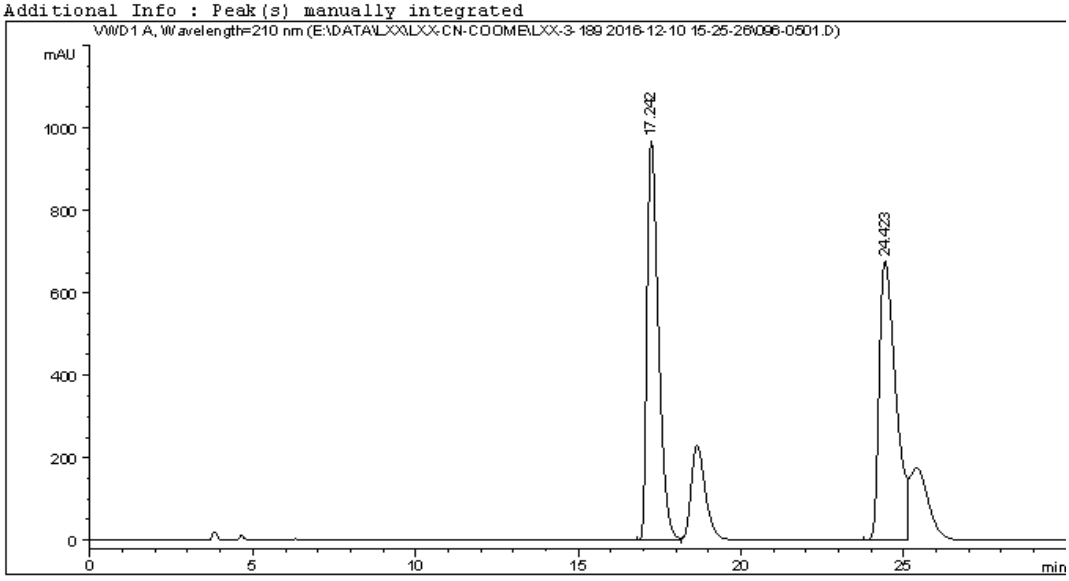


9. HPLC, GC spectra of 2, 3



Data File E:\DATA\LXX\LXX-CN-COOME\LXX-3-189 2016-12-10 15-25-26\096-0501.D
Sample Name: Rac

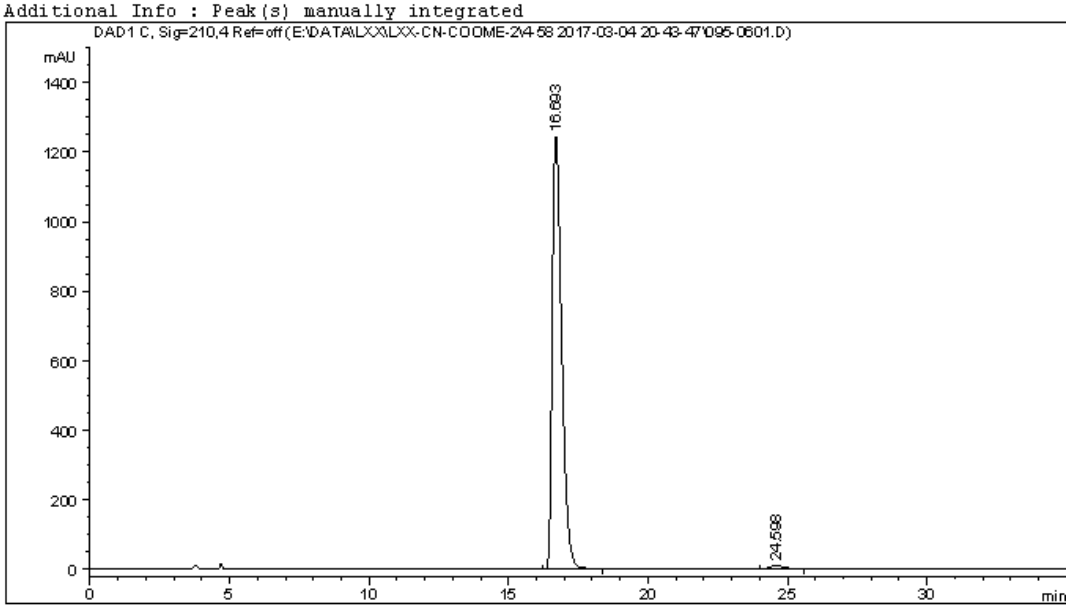
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   5
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 96
    Injection Date  : 12/10/2016 5:39:22 PM             Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME\LXX-3-189 2016-12-10 15-25-26\VWD-OD(1-6)-92-8-
                      0.8ML3UL-210NM-35MIN.M
    Last changed    : 12/10/2016 4:37:01 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME\LXX-3-189 2016-12-10 15-25-26\VWD-OD(1-6)-92-8-
                      0.8ML3UL-210NM-35MIN.M (Sequence Method)
    Last changed    : 12/18/2016 9:28:01 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



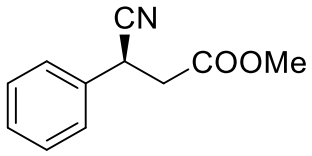

```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  17.242 VV    0.3735 2.36399e4   969.49756  49.6034
       2  24.423 BV    0.5418 2.40179e4   677.18915  50.3966

    Totals :                  4.76578e4  1646.68671

    ======================================================================
                            *** End of Report ***
```

Data File E:\DATA\LXX\LXX-CN-COOME-2\4-58 2017-03-04 20-43-47\095-0601.D
Sample Name: LXX-4-58-6

```
    ==================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   6
    Acq. Instrument : 1260HPLC-DAD                   Location : Vial 95
    Injection Date  : 3/4/2017 11:14:26 PM               Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-58 2017-03-04 20-43-47\DAD-OD(1-2)-92-8-0.
                      8ML-3UL-35MIN.M
    Last changed    : 3/4/2017 8:43:48 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-58 2017-03-04 20-43-47\DAD-OD(1-2)-92-8-0.
                      8ML-3UL-35MIN.M (Sequence Method)
    Last changed    : 3/27/2017 9:35:50 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

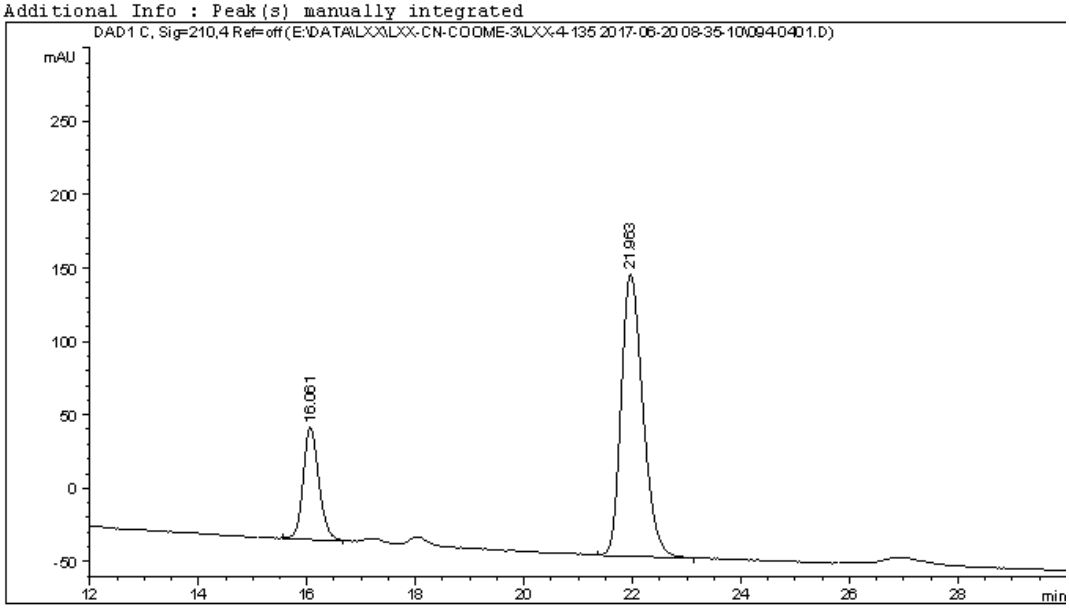



```
    ==================================================================
                            Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 C, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  16.693 BB    0.3589 2.91184e4  1245.00256  98.9993
       2  24.598 BB    0.4578  294.34576    9.38730   1.0007

    Totals :                  2.94127e4  1254.38986


    ==================================================================
                            *** End of Report ***
```

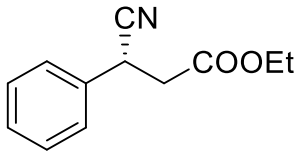


Data File E:\DATA\LXX\LXX-CN-COOME-3\LXX-4-135 2017-06-20 08-35-10\094-0401.D
Sample Name: LXX-4-135

```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   4
    Acq. Instrument : 1260HPLC-DAD                  Location : Vial 94
    Injection Date  : 6/20/2017 10:05:01 AM             Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-3\LXX-4-135 2017-06-20 08-35-10\DAD-OD(1-2)-92-
                      8-0.8ML-3UL-35MIN.M
    Last changed    : 6/20/2017 8:35:11 AM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-3\LXX-4-135 2017-06-20 08-35-10\DAD-OD(1-2)-92-
                      8-0.8ML-3UL-35MIN.M (Sequence Method)
    Last changed    : 11/25/2017 9:22:36 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

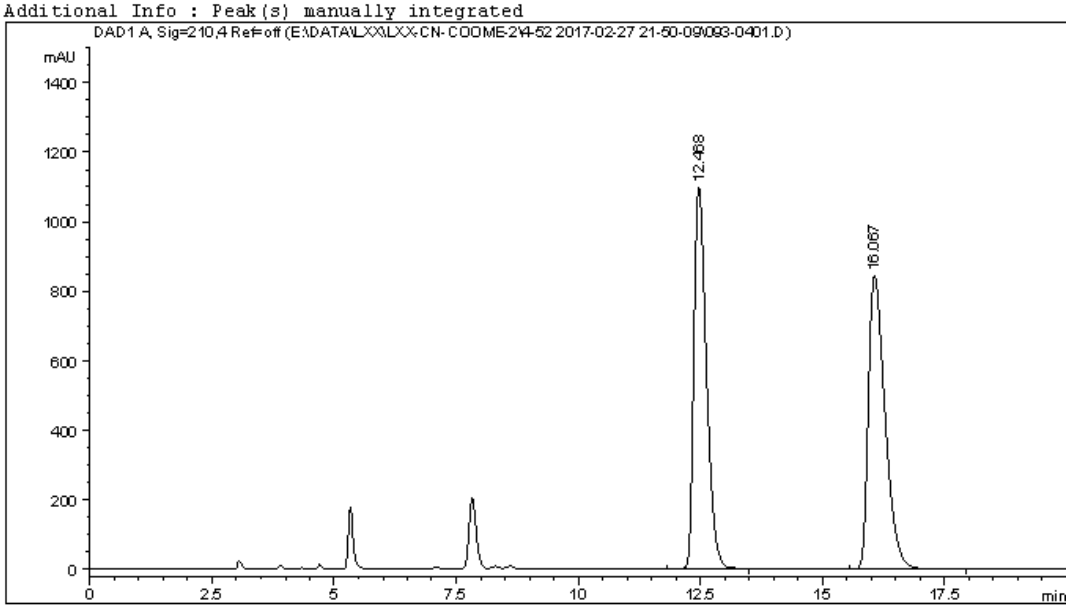



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 C, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  16.061 VV    0.2868 1541.32751   76.57160  22.3837
       2  21.963 VV    0.4167 5344.62061  192.05255  77.6163

    Totals :                  6885.94812  268.62415


    ======================================================================
                              *** End of Report ***
```



Data File E:\DATA\LXX\LXX-CN-COOME-2\4-52 2017-02-27 21-50-09\093-0401.D
Sample Name: CN-COOEt-Rac

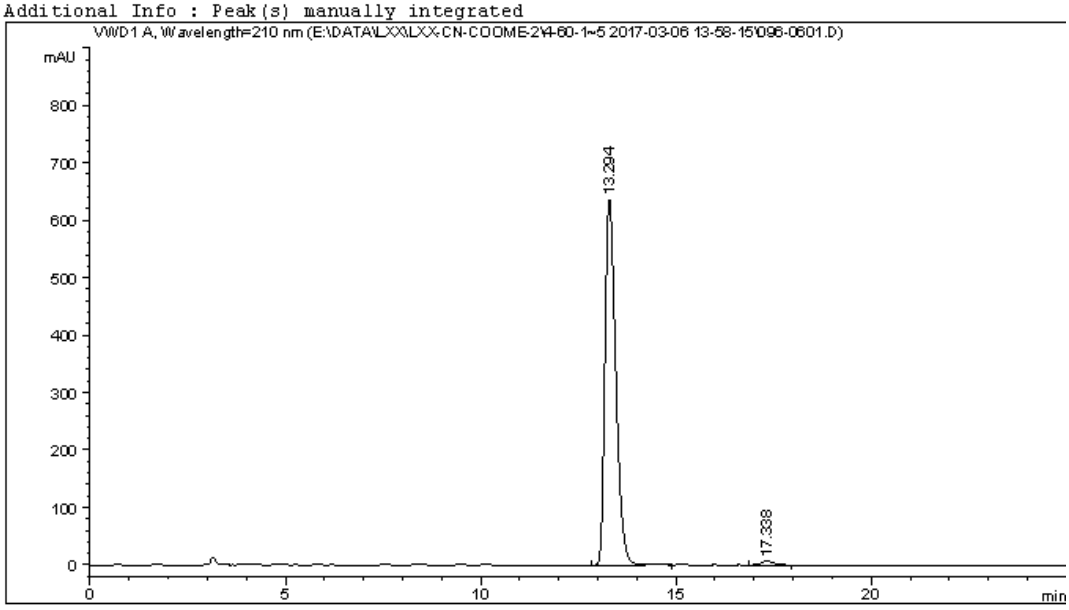
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   4
    Acq. Instrument : 1260HPLC-DAD                   Location : Vial 93
    Injection Date  : 2/27/2017 11:23:55 PM               Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-52 2017-02-27 21-50-09\DAD-OD(1-2)-95-5-1ML
                      -3UL-45MIN.M
    Last changed    : 2/27/2017 9:50:09 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-52 2017-02-27 21-50-09\DAD-OD(1-2)-95-5-1ML
                      -3UL-45MIN.M (Sequence Method)
    Last changed    : 3/27/2017 9:24:03 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



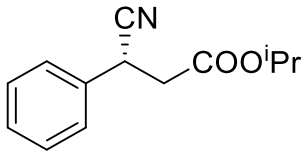

```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  12.468 BB    0.2751 1.96991e4  1099.05493  49.4948
       2  16.067 BB    0.3637 2.01012e4   844.36353  50.5052

    Totals :                  3.98003e4  1943.41846


    ======================================================================
                              *** End of Report ***
```

Data File E:\DATA\LXX\LXX-CN-COOME-2\4-60-1~5 2017-03-06 13-58-15\096-0601.D
Sample Name: LXX-4-60-5

```
    ==================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   6
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 96
    Injection Date  : 3/6/2017 5:32:43 PM                 Inj :   1
                                                  Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-60-1~5 2017-03-06 13-58-15\VWD-OD(1-2)-95-5
                      -1ML-3UL-210NM-40MIN.M
    Last changed    : 3/6/2017 5:12:56 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-60-1~5 2017-03-06 13-58-15\VWD-OD(1-2)-95-5
                      -1ML-3UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 3/27/2017 10:01:48 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

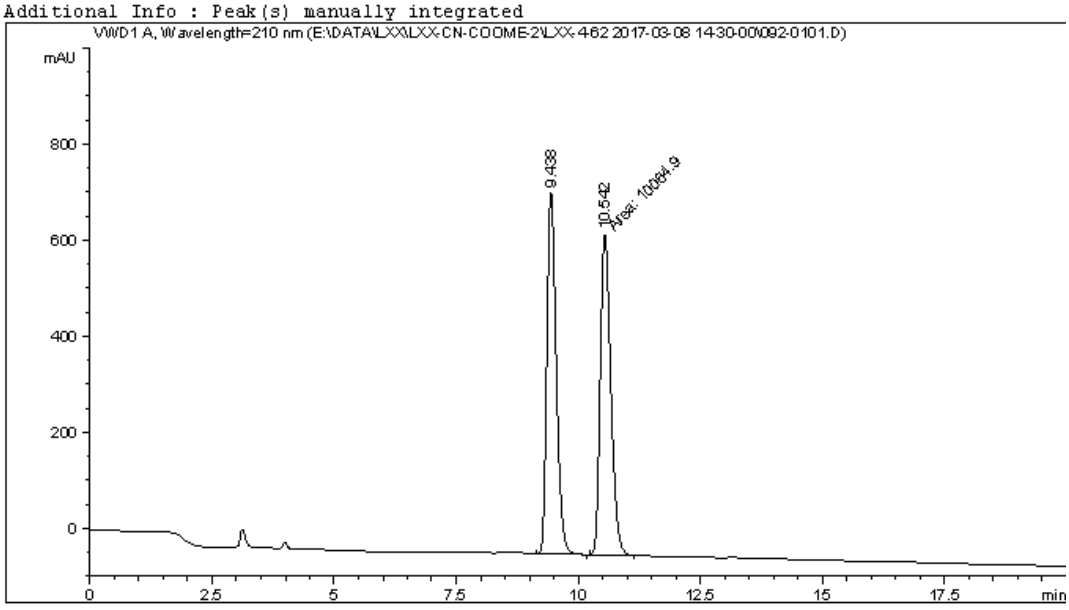



```
    ==================================================================
                          Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  13.294 BB    0.2957 1.22191e4   637.21674  98.7722
       2  17.338 BB    0.3583  151.88567    6.53176   1.2278

    Totals :                  1.23710e4   643.74849


    ==================================================================
                          *** End of Report ***
```



Data File E:\DATA\LXX\LXX-CN-COOME-2\LXX-4-62 2017-03-08 14-30-00\092-0101.D
Sample Name: iPr-Rac

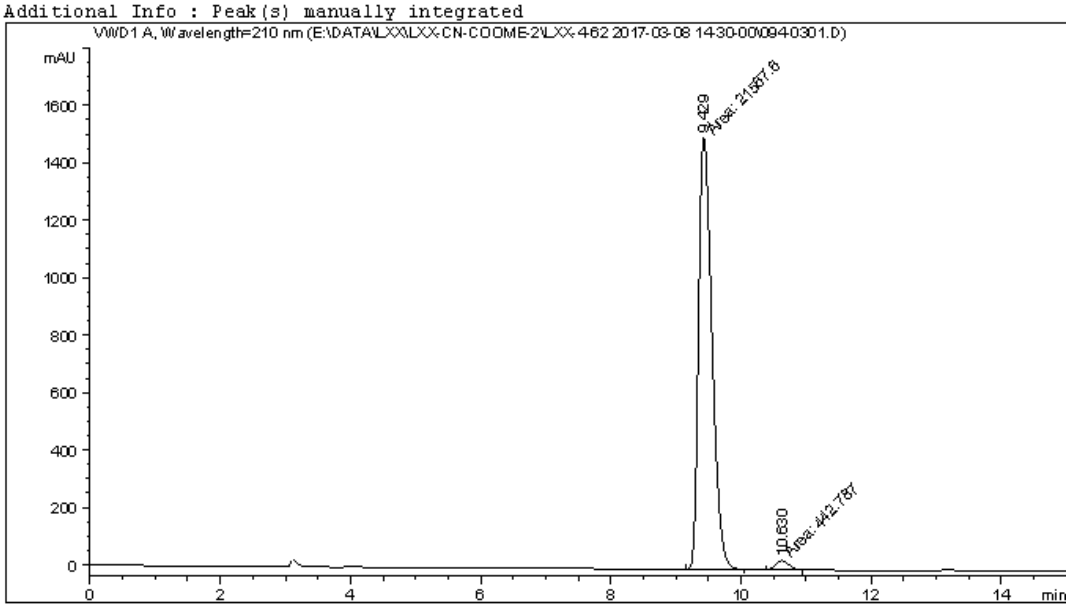
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   1
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 92
    Injection Date  : 3/8/2017 2:30:45 PM                 Inj :   1
                                                  Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\LXX-4-62 2017-03-08 14-30-00\VWD-OD(1-2)-95-5
                      -1ML-3UL-210NM-40MIN.M
    Last changed    : 3/8/2017 2:53:57 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\LXX-4-62 2017-03-08 14-30-00\VWD-OD(1-2)-95-5
                      -1ML-3UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 3/27/2017 9:29:33 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



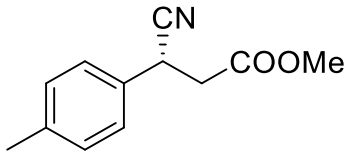

```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   9.438 BB    0.2055 1.00395e4   753.30194  49.9368
       2  10.542 MM    0.2510 1.00649e4   668.42224  50.0632

    Totals :                  2.01044e4  1421.72418


    ======================================================================
```

Data File E:\DATA\LXX\LXX-CN-COOME-2\LXX-4-62 2017-03-08 14-30-00\094-0301.D
Sample Name: LXX-4-62-2

```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   3
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 94
    Injection Date  : 3/8/2017 3:15:29 PM                Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\LXX-4-62 2017-03-08 14-30-00\VWD-OD(1-2)-95-5
                      -1ML-3UL-210NM-40MIN.M
    Last changed    : 3/8/2017 3:21:31 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\LXX-4-62 2017-03-08 14-30-00\VWD-OD(1-2)-95-5
                      -1ML-3UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 3/27/2017 9:30:55 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

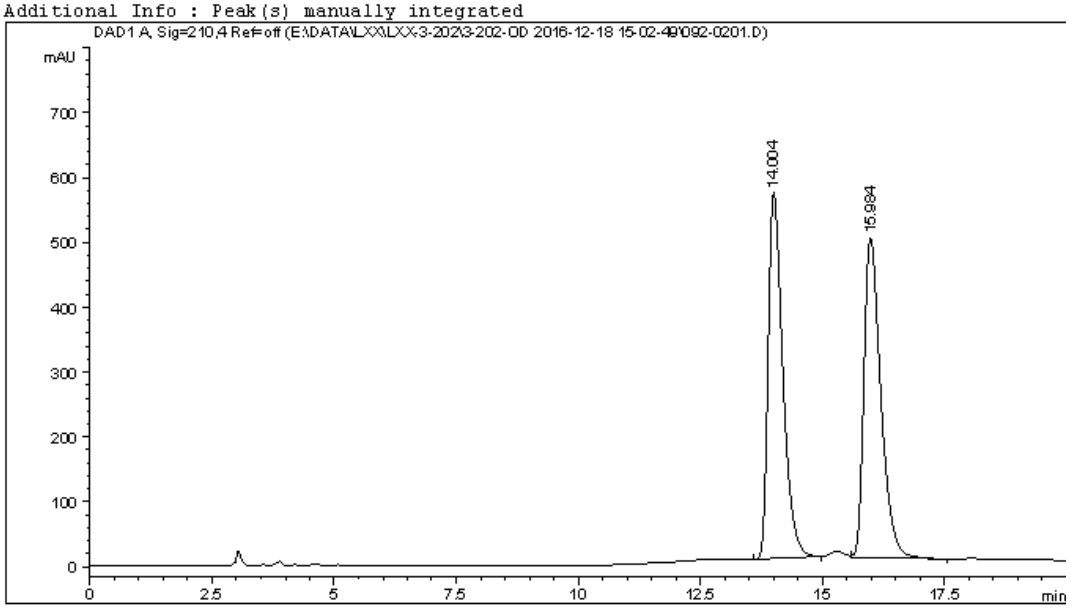



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   9.429 MM    0.2392 2.15676e4  1502.63293  97.9883
       2  10.630 MM    0.2343  442.78708   31.49628   2.0117

    Totals :                  2.20104e4  1534.12922


    ======================================================================
```



Data File E:\DATA\LXX\LXX-3-202\3-202-OD 2016-12-18 15-02-49\092-0201.D
Sample Name: p-Me-Rac

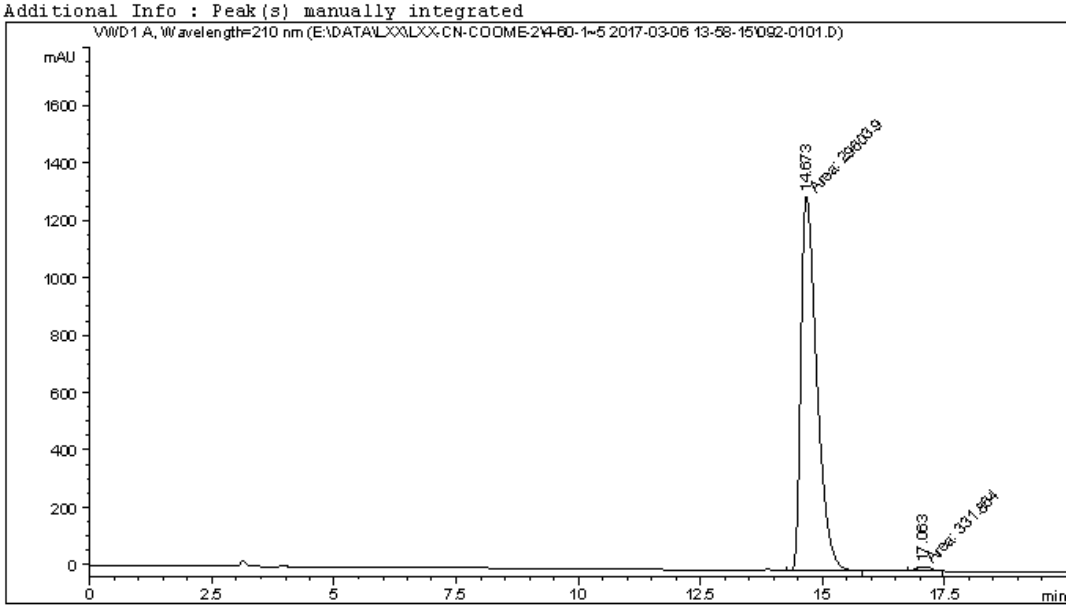
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   2
    Acq. Instrument : 1260HPLC-DAD                   Location : Vial 92
    Injection Date  : 12/18/2016 3:19:57 PM              Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-3-202\3-202-OD 2016-12-18 15-02-49\DAD-OD(1-2)-95-5-1ML-
                      3UL-45MIN.M
    Last changed    : 12/18/2016 3:02:50 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-3-202\3-202-OD 2016-12-18 15-02-49\DAD-OD(1-2)-95-5-1ML-
                      3UL-45MIN.M (Sequence Method)
    Last changed    : 12/18/2016 6:46:23 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



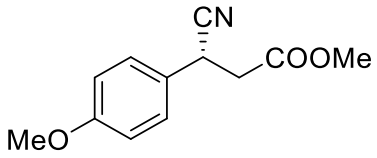

```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  14.004 BB    0.3181 1.17888e4   563.41455  49.8813
       2  15.984 VB    0.3686 1.18449e4   492.45203  50.1187

    Totals :                  2.36337e4  1055.86658


    ======================================================================
                              *** End of Report ***
```

Data File E:\DATA\LXX\LXX-CN-COOME-2\4-60-1~5 2017-03-06 13-58-15\092-0101.D
Sample Name: LXX-4-60-1

```
    ==================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   1
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 92
    Injection Date  : 3/6/2017 1:59:00 PM                 Inj :   1
                                                  Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-60-1~5 2017-03-06 13-58-15\VWD-OD(1-2)-95-5
                      -1ML-3UL-210NM-40MIN.M
    Last changed    : 3/6/2017 1:58:15 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-60-1~5 2017-03-06 13-58-15\VWD-OD(1-2)-95-5
                      -1ML-3UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 3/27/2017 9:55:57 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

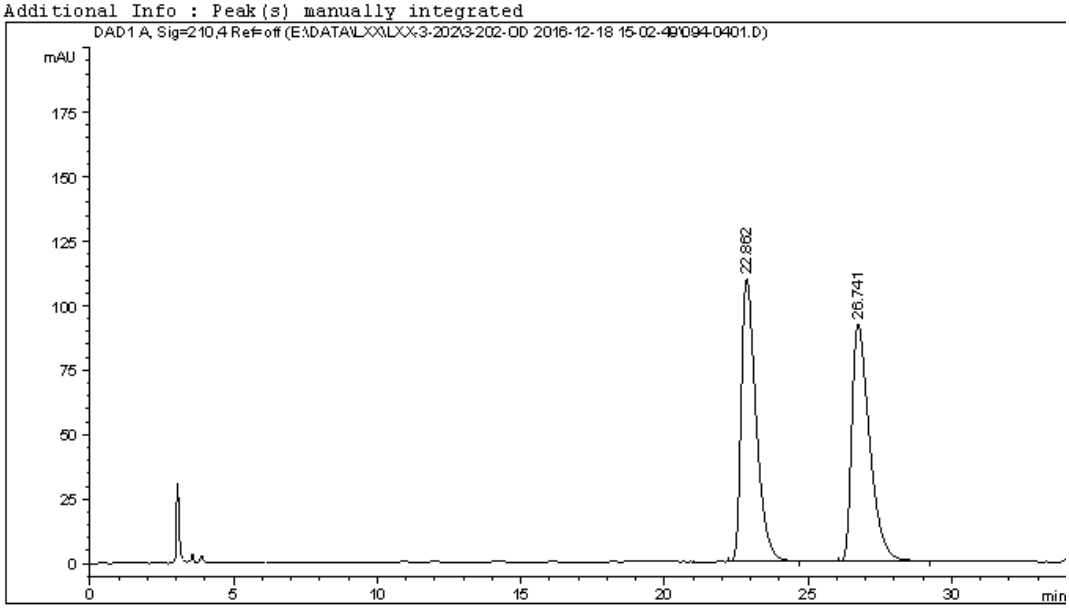



```
    ==================================================================
                          Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  14.673 MM    0.3781 2.96039e4  1304.99109  98.8914
       2  17.063 MM    0.3620  331.86447   15.27958   1.1086

    Totals :                  2.99358e4  1320.27067


    ==================================================================
                          *** End of Report ***
```



Data File E:\DATA\LXX\LXX-3-202\3-202-OD 2016-12-18 15-02-49\094-0401.D
Sample Name: p-OMe-Rac

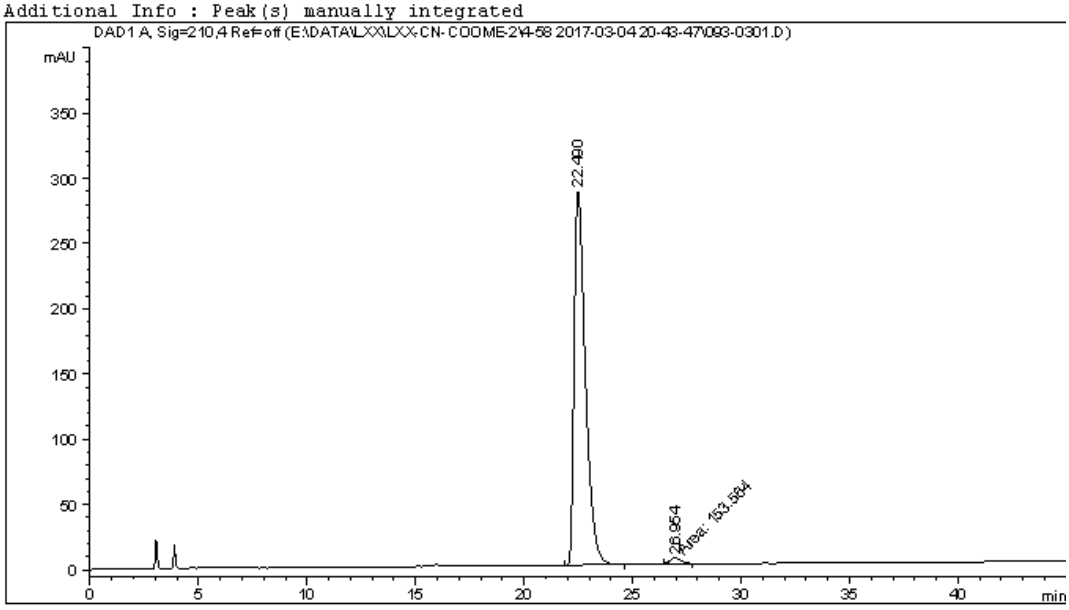
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   4
    Acq. Instrument : 1260HPLC-DAD                   Location : Vial 94
    Injection Date  : 12/18/2016 4:51:49 PM              Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-3-202\3-202-OD 2016-12-18 15-02-49\DAD-OD(1-2)-95-5-1ML-
                      3UL-45MIN.M
    Last changed    : 12/18/2016 3:02:50 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-3-202\3-202-OD 2016-12-18 15-02-49\DAD-OD(1-2)-95-5-1ML-
                      3UL-45MIN.M (Sequence Method)
    Last changed    : 12/18/2016 6:53:52 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



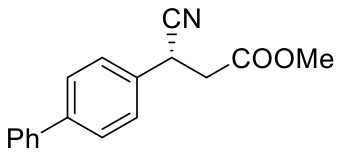

```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1  22.862 BB    0.5416 3928.15894  109.74193  49.8420
       2  26.741 BB    0.6425 3953.06689   92.14471  50.1580

    Totals :                  7881.22583  201.88663


    ======================================================================
                              *** End of Report ***
```

Data File E:\DATA\LXX\LXX-CN-COOME-2\4-58 2017-03-04 20-43-47\093-0301.D
Sample Name: LXX-4-58-4

```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   3
    Acq. Instrument : 1260HPLC-DAD                     Location : Vial 93
    Injection Date  : 3/4/2017 9:36:33 PM                  Inj :   1
                                                     Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-58 2017-03-04 20-43-47\DAD-OD(1-2)-95-5-1ML
                      -3UL-45MIN.M
    Last changed    : 3/4/2017 8:43:47 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-58 2017-03-04 20-43-47\DAD-OD(1-2)-95-5-1ML
                      -3UL-45MIN.M (Sequence Method)
    Last changed    : 3/27/2017 9:47:43 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

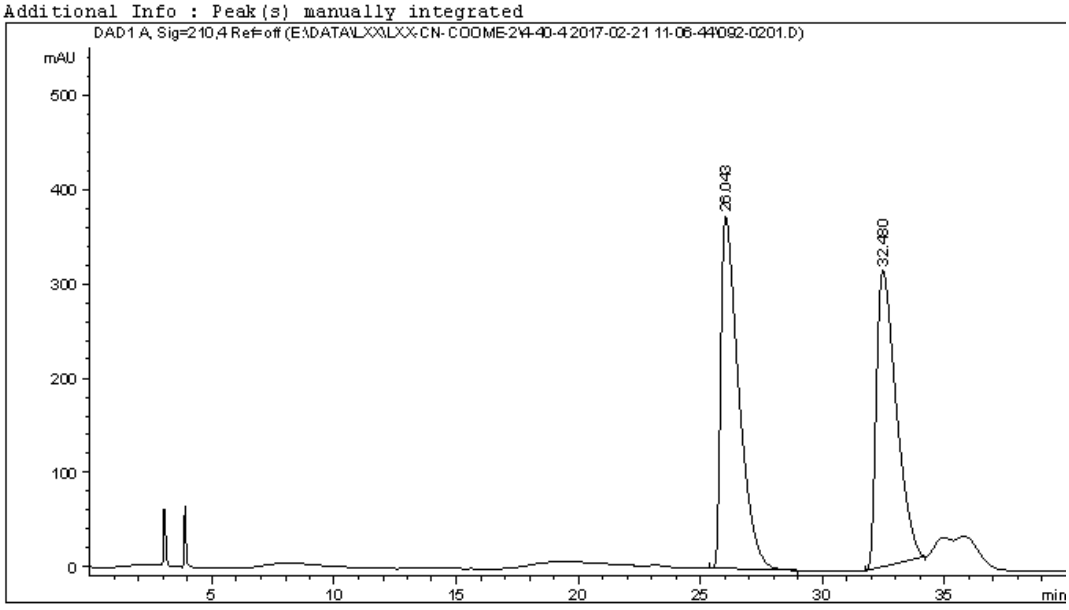



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  22.490 BB    0.5450 1.03288e4   286.25229  98.5350
       2  26.954 MM    0.5963  153.56422    4.29245   1.4650

    Totals :                  1.04824e4   290.54474


    ======================================================================
                              *** End of Report ***
```



Data File E:\DATA\LXX\LXX-CN-COOME-2\4-40-4 2017-02-21 11-06-44\092-0201.D
Sample Name: p-Ph-Rac

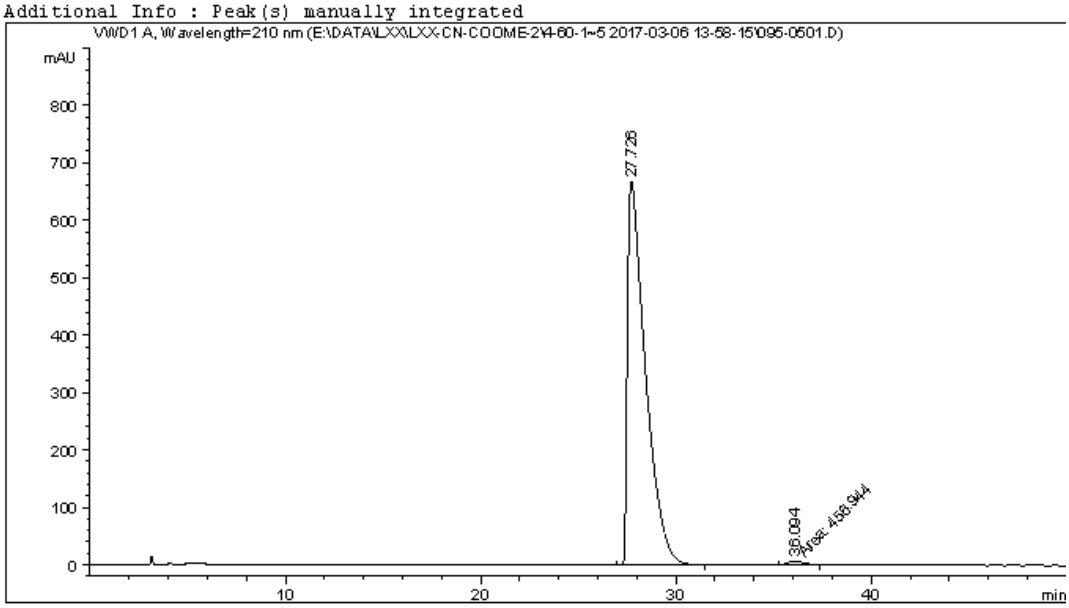
```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   2
    Acq. Instrument : 1260HPLC-DAD                     Location : Vial 92
    Injection Date  : 2/21/2017 11:23:36 AM                 Inj :   1
                                                    Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-40-4 2017-02-21 11-06-44\DAD-OD(1-2)-95-5-
                      1ML-3UL-45MIN.M
    Last changed    : 2/21/2017 11:51:17 AM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-40-4 2017-02-21 11-06-44\DAD-OD(1-2)-95-5-
                      1ML-3UL-45MIN.M (Sequence Method)
    Last changed    : 3/27/2017 9:20:06 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



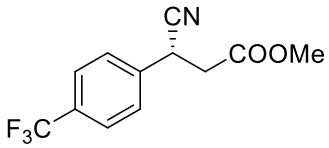

```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  26.043 BB    0.7576 1.9021le4   372.57068  51.7127
       2  32.480 BB    0.8508 1.77612e4   313.57501  48.2873

    Totals :                  3.67823e4   686.14569


    ======================================================================
```

Data File E:\DATA\LXX\LXX-CN-COOME-2\4-60-1~5 2017-03-06 13-58-15\095-0501.D
Sample Name: LXX-4-60-4

```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   5
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 95
    Injection Date  : 3/6/2017 4:41:58 PM                  Inj :   1
                                                     Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-60-1~5 2017-03-06 13-58-15\VWD-OD(1-2)-95-5
                      -1ML-3UL-210NM-40MIN.M
    Last changed    : 3/6/2017 5:12:56 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-60-1~5 2017-03-06 13-58-15\VWD-OD(1-2)-95-5
                      -1ML-3UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 3/27/2017 10:00:23 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

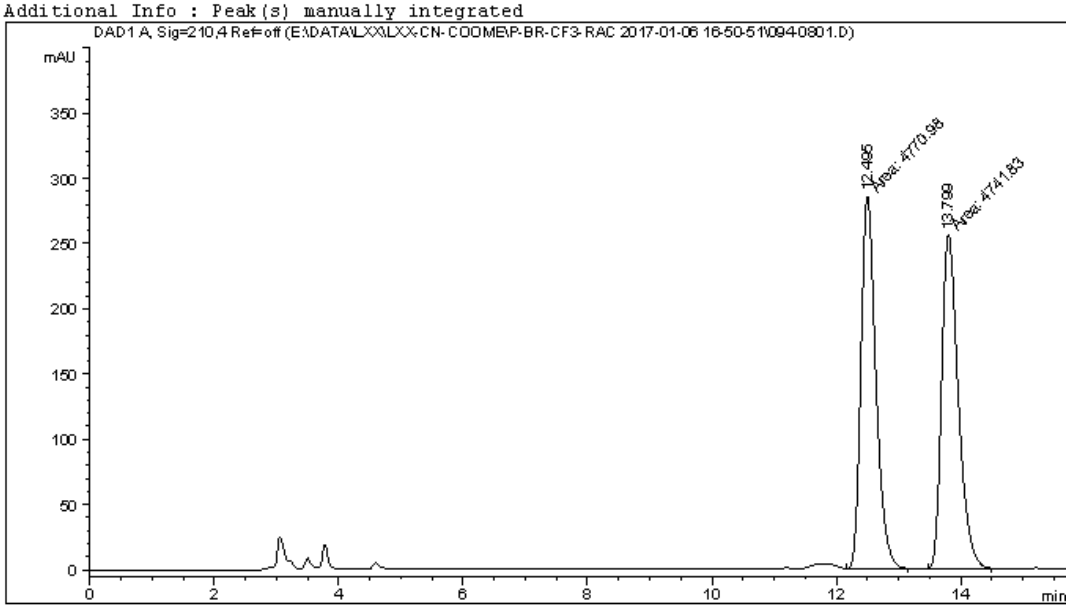



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  27.726 BB    0.9335 4.27655e4   667.50934  98.9428
       2  36.094 MM    1.0060  456.94446    7.57046   1.0572

    Totals :                  4.32225e4   675.07980


    ======================================================================
```



Data File E:\DATA\LXX\LXX-CN-COOME\P-BR-CF3-RAC 2017-01-06 16-50-51\094-0801.D
Sample Name: p-CF3-Rac

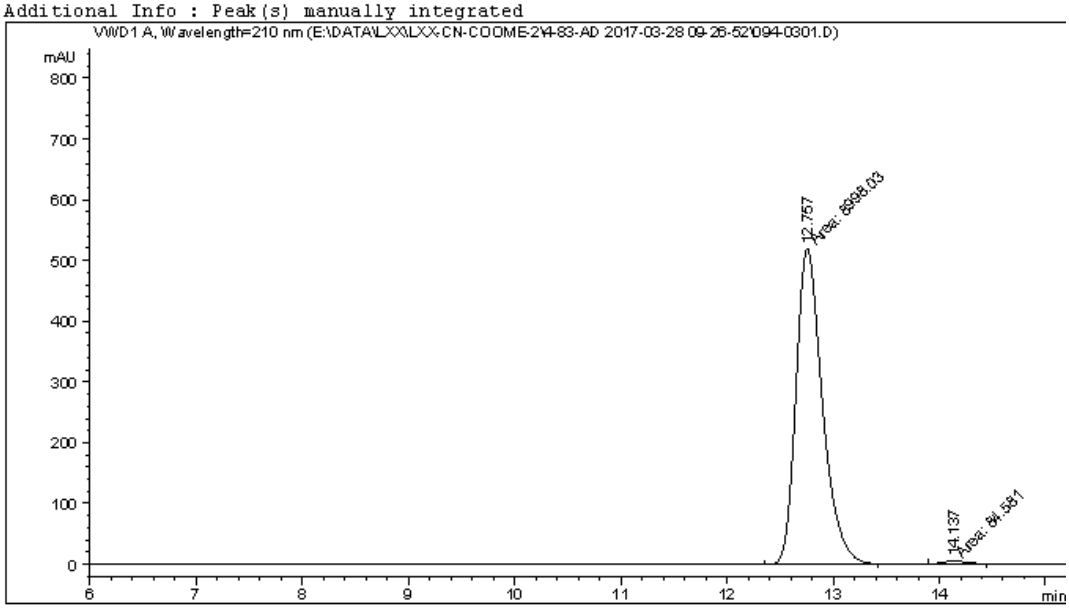
```
    ==================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   8
    Acq. Instrument : 1260HPLC-DAD                   Location : Vial 94
    Injection Date  : 1/6/2017 9:05:56 PM                 Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME\P-BR-CF3-RAC 2017-01-06 16-50-51\DAD-AD(1-6)-95
                      -5-1ML-3UL-45MIN.M
    Last changed    : 1/6/2017 4:50:51 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME\P-BR-CF3-RAC 2017-01-06 16-50-51\DAD-AD(1-6)-95
                      -5-1ML-3UL-45MIN.M (Sequence Method)
    Last changed    : 3/27/2017 8:55:05 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



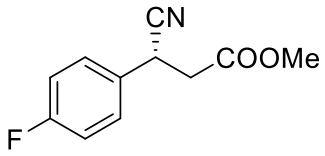

```
    ==================================================================
                            Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  12.495 MM    0.2778 4770.98340  286.21664  50.1532
       2  13.799 MM    0.3089 4741.83301  255.87935  49.8468

    Totals :                  9512.81641  542.09599


    ==================================================================
                            *** End of Report ***
```

Data File E:\DATA\LXX\LXX-CN-COOME-2\4-83-AD 2017-03-28 09-26-52\094-0301.D
Sample Name: 4-84-6

```
    ==================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   3
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 94
    Injection Date  : 3/28/2017 10:46:55 AM              Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-83-AD 2017-03-28 09-26-52\VWD-AD(1-2)-95-5-
                      1ML-3UL-210NM-50MIN.M
    Last changed    : 3/28/2017 10:15:28 AM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-83-AD 2017-03-28 09-26-52\VWD-AD(1-2)-95-5-
                      1ML-3UL-210NM-50MIN.M (Sequence Method)
    Last changed    : 4/28/2017 5:12:20 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

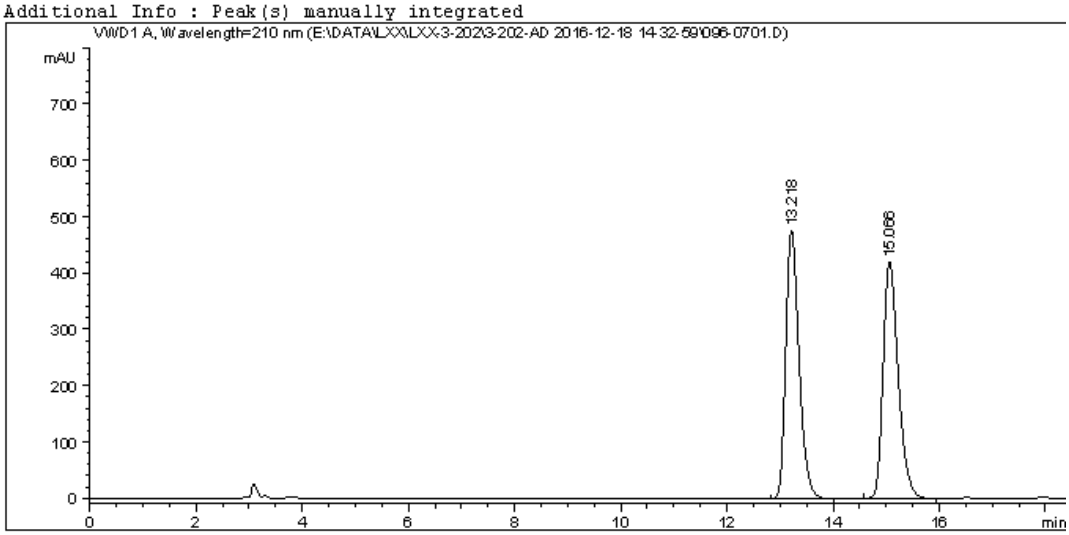



```
    ==================================================================
                          Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  12.757 MM    0.2883 8998.02734  520.14764  99.0688
       2  14.137 MM    0.2819   84.58096    5.00100   0.9312

    Totals :                  9082.60831  525.14864


    ==================================================================
                          *** End of Report ***
```



Data File E:\DATA\LXX\LXX-3-202\3-202-AD 2016-12-18 14-32-59\096-0701.D
Sample Name: p-F-Rac

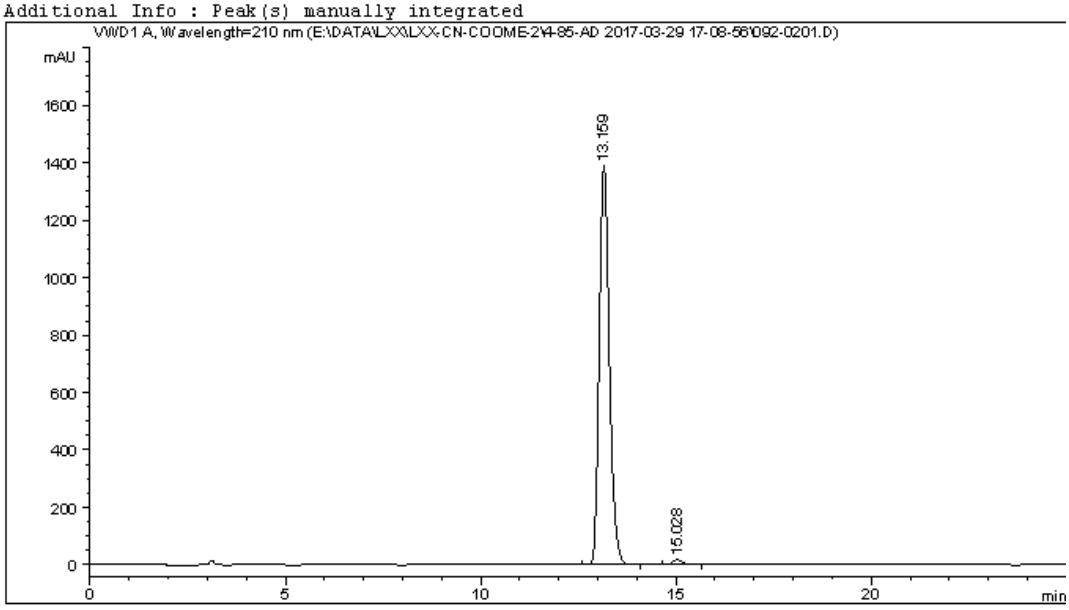
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   7
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 96
    Injection Date  : 12/18/2016 6:19:14 PM               Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-3-202\3-202-AD 2016-12-18 14-32-59\VWD-AD(1-6)-95-5-1ML-
                      3UL-210NM-45MIN.M
    Last changed    : 12/18/2016 6:54:42 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\LXX\LXX-3-202\3-202-AD 2016-12-18 14-32-59\VWD-AD(1-6)-95-5-1ML-
                      3UL-210NM-45MIN.M (Sequence Method)
    Last changed    : 12/18/2016 9:03:21 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



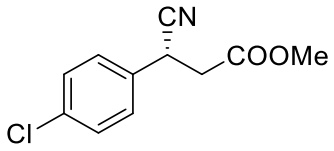

```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  13.218 VB    0.2654 8254.85254  475.73526  49.9811
       2  15.066 BB    0.3007 8261.09277  419.56238  50.0189

    Totals :                  1.65159e4   895.29764

    ======================================================================
                            *** End of Report ***
```

Data File E:\DATA\LXX\LXX-CN-COOME-2\4-85-AD 2017-03-29 17-08-56\092-0201.D
Sample Name: 4-85-1

```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   2
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 92
    Injection Date  : 3/29/2017 5:25:29 PM                 Inj :   1
                                                     Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-85-AD 2017-03-29 17-08-56\VWD-AD(1-2)-95-5-
                      1ML-3UL-210NM-35MIN.M
    Last changed    : 3/29/2017 5:08:56 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-85-AD 2017-03-29 17-08-56\VWD-AD(1-2)-95-5-
                      1ML-3UL-210NM-35MIN.M (Sequence Method)
    Last changed    : 4/28/2017 5:27:28 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

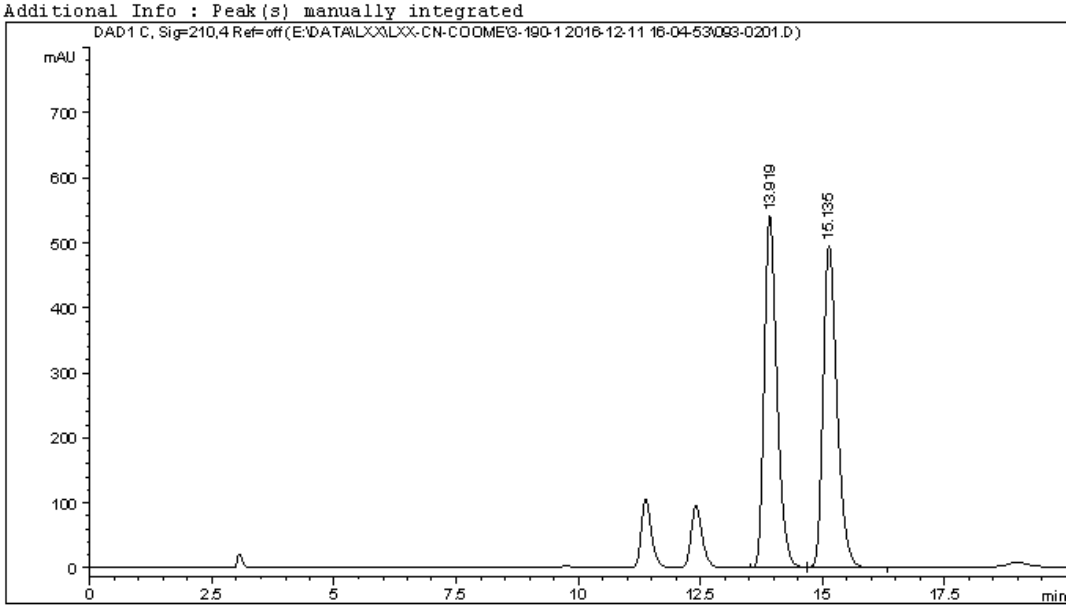



```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  13.159 BB    0.2790 2.50885e4  1387.14917  98.7776
       2  15.028 BB    0.2908  310.46652   16.25759   1.2224

    Totals :                  2.53990e4  1403.40676


    ======================================================================
                              *** End of Report ***
```



Data File E:\DATA\LXX\LXX-CN-COOME\3-190-1 2016-12-11 16-04-53\093-0201.D
Sample Name: LXX-3-190-1-Rac

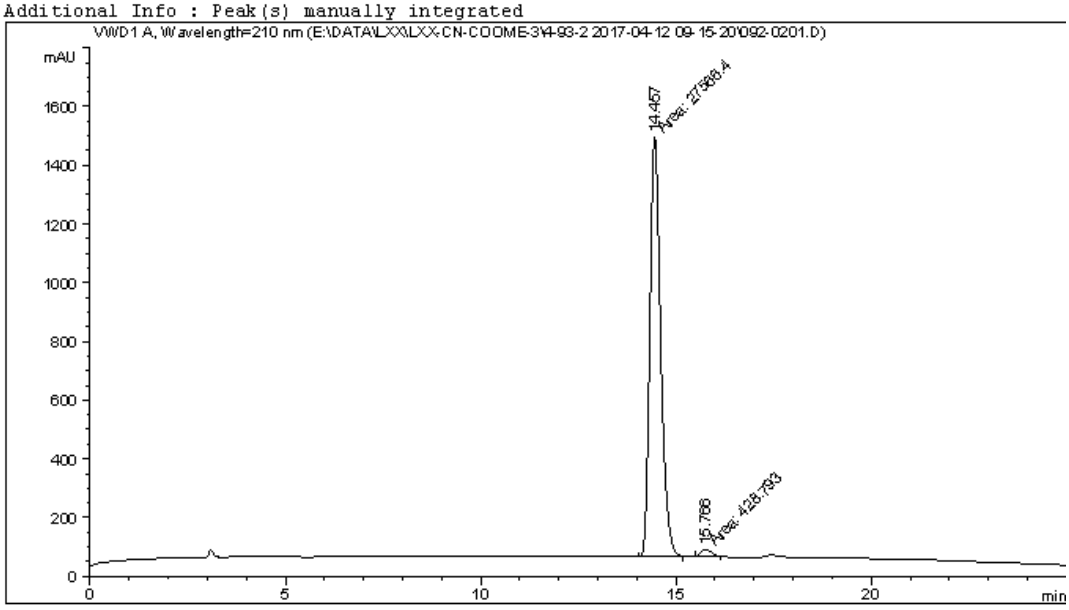
```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   2
    Acq. Instrument : 1260HPLC-DAD                     Location : Vial 93
    Injection Date  : 12/11/2016 4:46:41 PM                 Inj :   1
                                                     Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME\3-190-1 2016-12-11 16-04-53\DAD-AD(1-2)-95-5-1.
                      0ML-3UL-40MIN.M
    Last changed    : 12/11/2016 4:04:53 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME\3-190-1 2016-12-11 16-04-53\DAD-AD(1-2)-95-5-1.
                      0ML-3UL-40MIN.M (Sequence Method)
    Last changed    : 12/18/2016 9:05:43 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



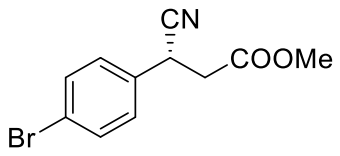

```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 C, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  13.919 BB    0.2744 9738.87109  540.04681  49.9304
       2  15.135 BB    0.3001 9766.01758  495.26901  50.0696

    Totals :                  1.95049e4  1035.31583


    ======================================================================
                              *** End of Report ***
```

Data File E:\DATA\LXX\LXX-CN-COOME-3\4-93-2 2017-04-12 09-15-20\092-0201.D
Sample Name: 4-93-2

```
    ==================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   2
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 92
    Injection Date  : 4/12/2017 9:31:52 AM               Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-3\4-93-2 2017-04-12 09-15-20\VWD-AD(1-2)-95-5-
                      1ML-3UL-210NM-35MIN.M
    Last changed    : 4/12/2017 9:15:21 AM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-3\4-93-2 2017-04-12 09-15-20\VWD-AD(1-2)-95-5-
                      1ML-3UL-210NM-35MIN.M (Sequence Method)
    Last changed    : 4/28/2017 5:20:38 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

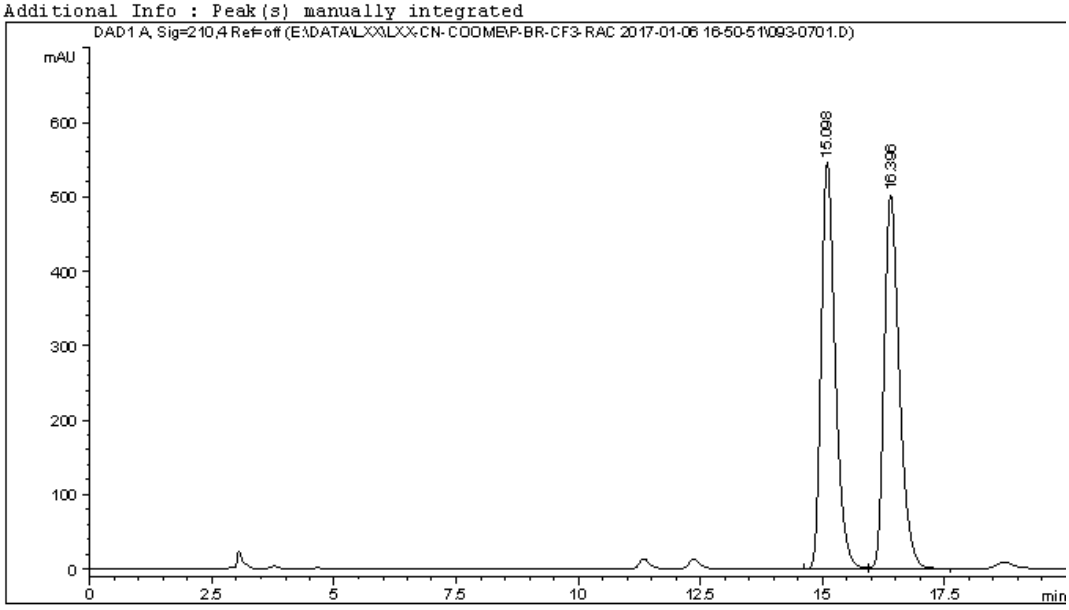



```
    ==================================================================
                            Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  14.457 MM    0.3216 2.75664e4  1428.63757  98.4683
       2  15.766 MM    0.3045  428.79294   23.47210   1.5317

    Totals :                  2.79952e4  1452.10968


    ==================================================================
                            *** End of Report ***
```



Data File E:\DATA\LXX\LXX-CN-COOME\P-BR-CF3-RAC 2017-01-06 16-50-51\093-0701.D
Sample Name: p-Br-Rac

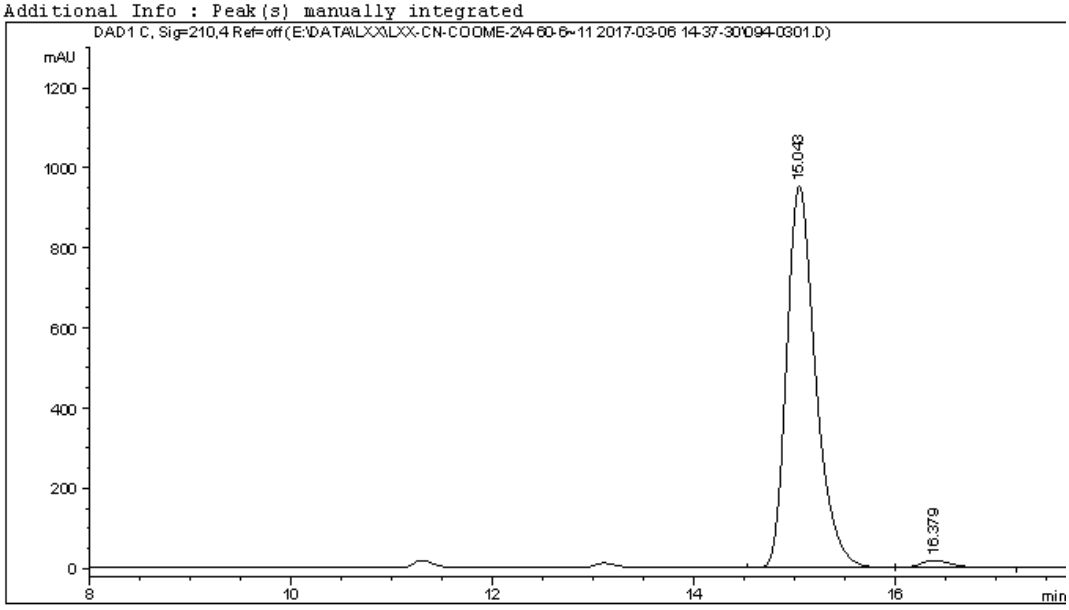
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   7
    Acq. Instrument : 1260HPLC-DAD                   Location : Vial 93
    Injection Date  : 1/6/2017 8:20:01 PM                 Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME\P-BR-CF3-RAC 2017-01-06 16-50-51\DAD-AD(1-6)-95
                      -5-1ML-3UL-45MIN.M
    Last changed    : 1/6/2017 4:50:51 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME\P-BR-CF3-RAC 2017-01-06 16-50-51\DAD-AD(1-6)-95
                      -5-1ML-3UL-45MIN.M (Sequence Method)
    Last changed    : 3/27/2017 8:49:55 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



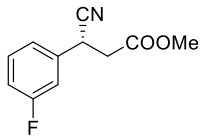

```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  15.098 BB    0.3030 1.0794le4   545.14502  49.9782
       2  16.396 BB    0.3277 1.08035e4   500.80716  50.0218

    Totals :                  2.15976e4  1045.95218


    ======================================================================
                              *** End of Report ***
```

Data File E:\DATA\LXX\LXX-CN-COOME-2\4-60-6~11 2017-03-06 14-37-30\094-0301.D
Sample Name: LXX-4-60-8

```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   3
    Acq. Instrument : 1260HPLC-DAD                   Location : Vial 94
    Injection Date  : 3/6/2017 3:40:12 PM                 Inj :   1
                                                  Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-60-6~11 2017-03-06 14-37-30\DAD-AD(1-2)-95-
                      5-1ML-35MIN.M
    Last changed    : 3/6/2017 3:27:34 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-60-6~11 2017-03-06 14-37-30\DAD-AD(1-2)-95-
                      5-1ML-35MIN.M (Sequence Method)
    Last changed    : 4/28/2017 5:06:22 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

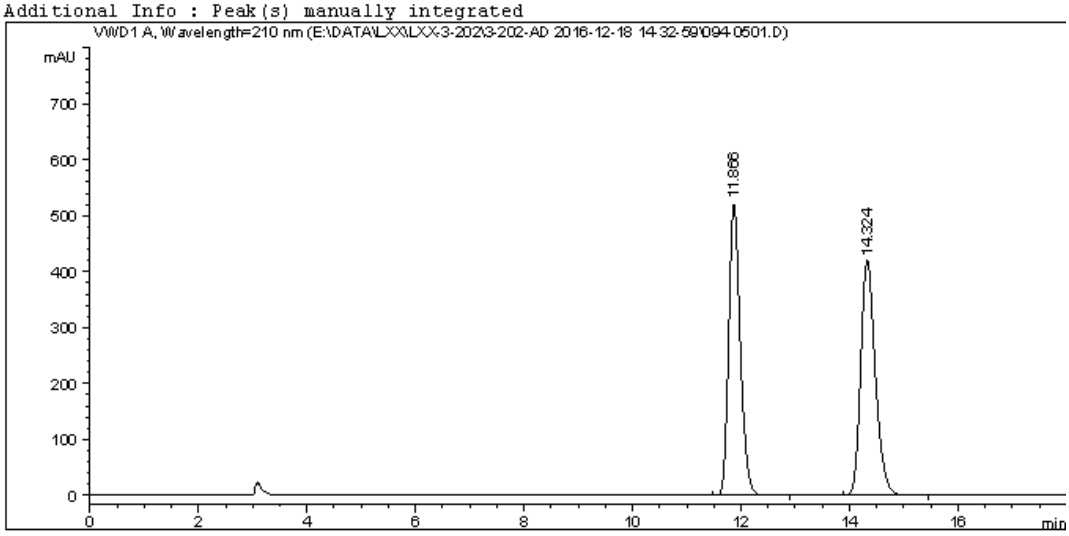



```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 C, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  15.043 BB    0.3022 1.89833e4   953.59711  97.9781
       2  16.379 BB    0.3176  391.74384   18.61033   2.0219

    Totals :                  1.9375le4   972.20744


    ======================================================================
                               *** End of Report ***
```



Data File E:\DATA\LXX\LXX-3-202\3-202-AD 2016-12-18 14-32-59\094-0501.D
Sample Name: m-F-Rac

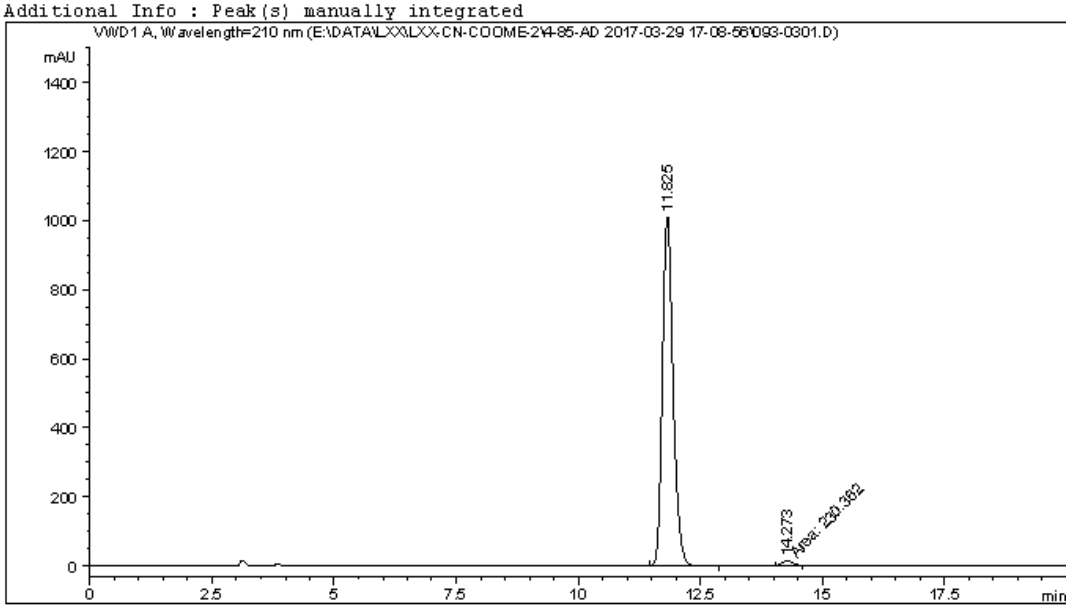
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   5
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 94
    Injection Date  : 12/18/2016 4:57:45 PM               Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-3-202\3-202-AD 2016-12-18 14-32-59\VWD-AD(1-6)-95-5-1ML-
                      3UL-210NM-45MIN.M
    Last changed    : 12/18/2016 4:09:58 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-3-202\3-202-AD 2016-12-18 14-32-59\VWD-AD(1-6)-95-5-1ML-
                      3UL-210NM-45MIN.M (Sequence Method)
    Last changed    : 12/18/2016 6:35:11 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



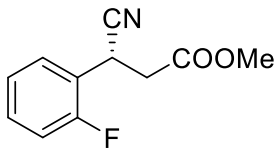

```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  11.866 BB    0.2277 7770.65430  521.81769  49.7058
       2  14.324 VB    0.2856 7862.64990  419.66696  50.2942

    Totals :                  1.56333e4   941.48465

    ======================================================================
                            *** End of Report ***
```

Data File E:\DATA\LXX\LXX-CN-COOME-2\4-85-AD 2017-03-29 17-08-56\093-0301.D
Sample Name: 4-85-2

```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   3
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 93
    Injection Date  : 3/29/2017 6:01:13 PM                 Inj :   1
                                                     Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-85-AD 2017-03-29 17-08-56\VWD-AD(1-2)-95-5-
                      1ML-3UL-210NM-35MIN.M
    Last changed    : 3/29/2017 5:08:56 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-85-AD 2017-03-29 17-08-56\VWD-AD(1-2)-95-5-
                      1ML-3UL-210NM-35MIN.M (Sequence Method)
    Last changed    : 4/28/2017 4:51:47 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

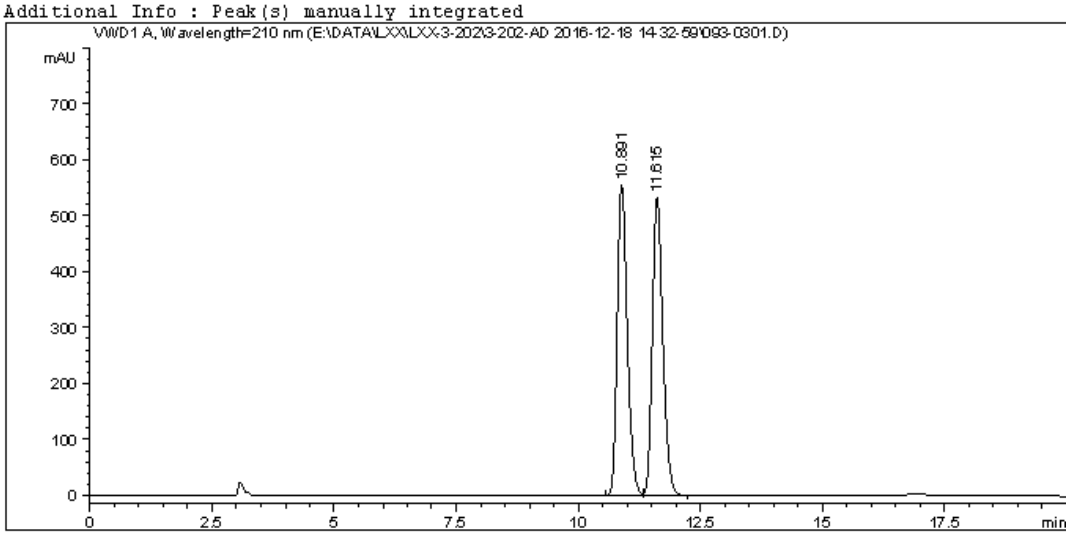



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  11.825 VB    0.2327 1.54134e4  1011.81360  98.5275
       2  14.273 MM    0.2803  230.36197   13.69639   1.4725

    Totals :                  1.56438e4  1025.50999


    ======================================================================
                              *** End of Report ***
```



Data File E:\DATA\LXX\LXX-3-202\3-202-AD 2016-12-18 14-32-59\093-0301.D
Sample Name: o-F-Rac

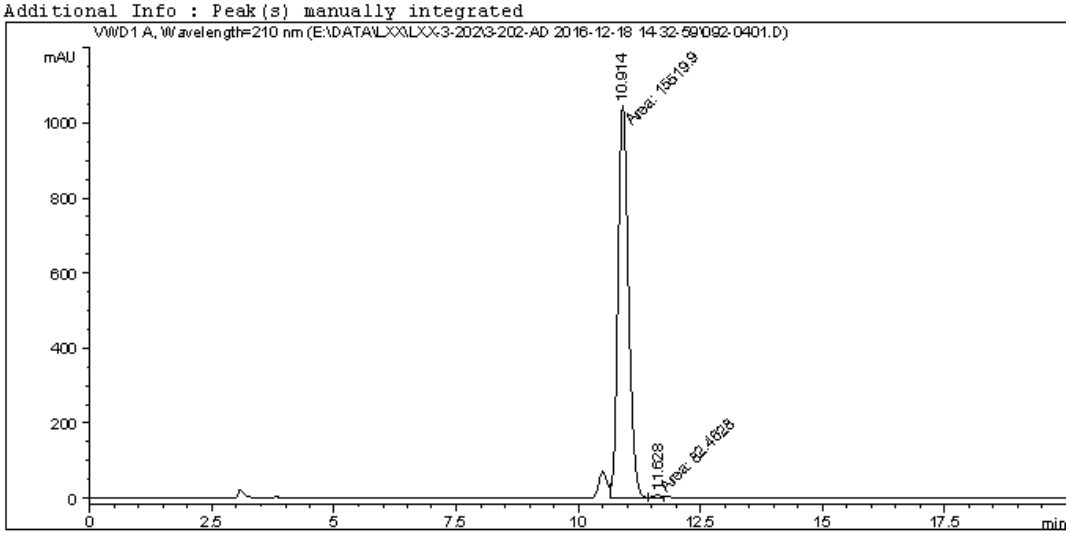
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   3
    Acq. Instrument : 1260HPLC-VWD                  Location : Vial 93
    Injection Date  : 12/18/2016 3:36:15 PM              Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-3-202\3-202-AD 2016-12-18 14-32-59\VWD-AD(1-6)-95-5-1ML-
                      3UL-210NM-45MIN.M
    Last changed    : 12/18/2016 4:09:58 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\LXX\LXX-3-202\3-202-AD 2016-12-18 14-32-59\VWD-AD(1-6)-95-5-1ML-
                      3UL-210NM-45MIN.M (Sequence Method)
    Last changed    : 12/18/2016 6:30:53 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



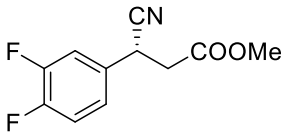

```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  10.891 BV    0.2197 7932.28271  555.18420  49.7909
       2  11.615 VB    0.2301 7998.89844  532.94104  50.2091

    Totals :                  1.59312e4  1088.12524

    ======================================================================
                            *** End of Report ***
```

Data File E:\DATA\LXX\LXX-3-202\3-202-AD 2016-12-18 14-32-59\092-0401.D
Sample Name: lxx-3-202-4

```
=====================================================================
Acq. Operator   : SYSTEM                          Seq. Line :   4
Acq. Instrument : 1260HPLC-VWD                     Location : Vial 92
Injection Date  : 12/18/2016 4:16:59 PM                 Inj :   1
                                                  Inj Volume : 3.000 µl
Acq. Method     : E:\DATA\LXX\LXX-3-202\3-202-AD 2016-12-18 14-32-59\VWD-AD(1-6)-95-5-1ML-
                  3UL-210NM-45MIN.M
Last changed    : 12/18/2016 4:09:58 PM by SYSTEM
Analysis Method : E:\DATA\LXX\LXX-3-202\3-202-AD 2016-12-18 14-32-59\VWD-AD(1-6)-95-5-1ML-
                  3UL-210NM-45MIN.M (Sequence Method)
Last changed    : 12/18/2016 6:28:51 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```

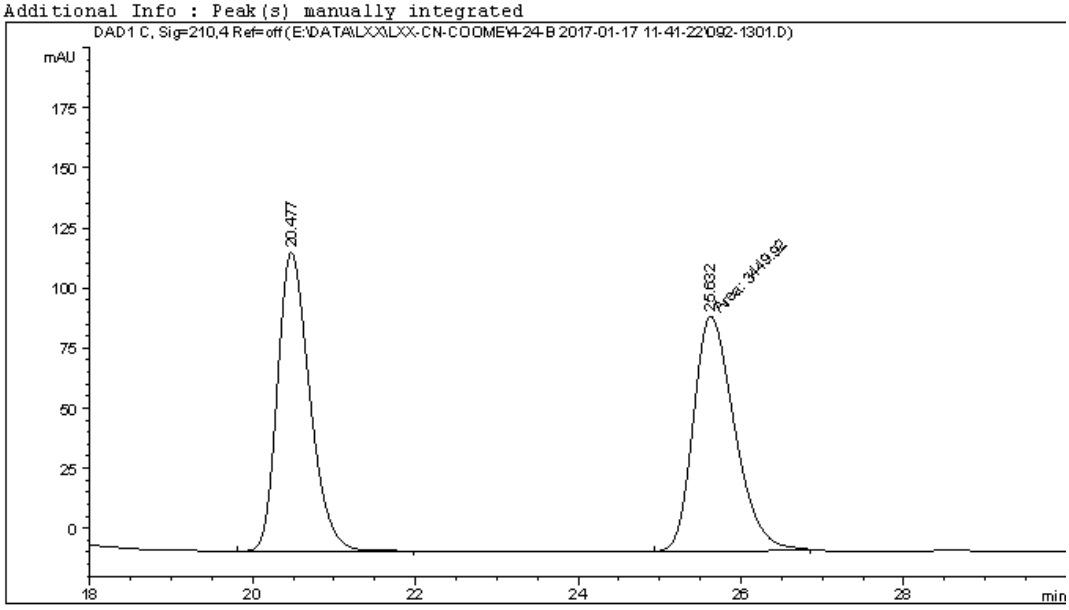



```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=210 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.914 FM    0.2479 1.55199e4  1043.61145  99.4715
   2  11.628 FM    0.2137   82.46284    6.43165   0.5285

Totals :                  1.56024e4  1050.04311


=====================================================================
                        *** End of Report ***
```



Data File E:\DATA\LXX\LXX-CN-COOME\4-24-B 2017-01-17 11-41-22\092-1301.D
Sample Name: 3,4-F-Rac

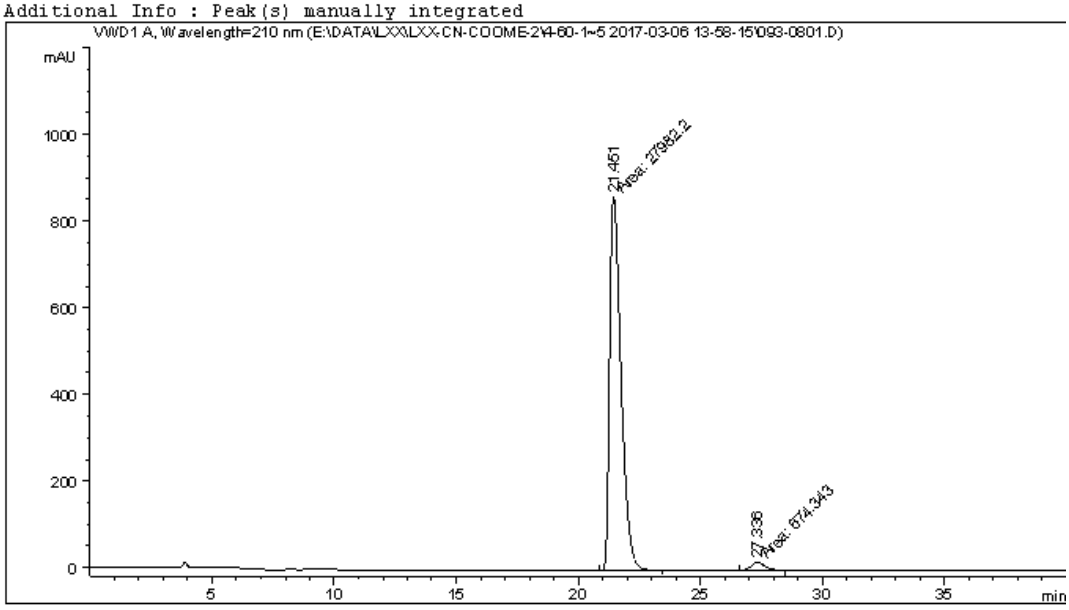
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :  13
    Acq. Instrument : 1260HPLC-DAD                   Location : Vial 92
    Injection Date  : 1/17/2017 5:32:49 PM                Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME\4-24-B 2017-01-17 11-41-22\DAD-OD(1-2)-92-8-0.
                      8ML-3UL-35MIN.M
    Last changed    : 1/17/2017 11:41:23 AM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME\4-24-B 2017-01-17 11-41-22\DAD-OD(1-2)-92-8-0.
                      8ML-3UL-35MIN.M (Sequence Method)
    Last changed    : 3/27/2017 9:08:25 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



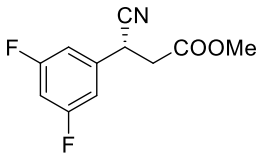

```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 C, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1  20.477 BB    0.4227 3418.46045  124.35276  49.7710
       2  25.632 MM    0.5868 3449.91821   97.98963  50.2290

    Totals :                  6868.37866  222.34239


    ======================================================================
                              *** End of Report ***
```

Data File E:\DATA\LXX\LXX-CN-COOME-2\4-60-1~5 2017-03-06 13-58-15\093-0801.D
Sample Name: LXX-4-60-2

```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   8
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 93
    Injection Date  : 3/6/2017 6:34:18 PM                  Inj :   1
                                                    Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-60-1~5 2017-03-06 13-58-15\VWD-OD(1-2)-92-8
                      -0.8ML-3UL-210NM-40MIN.M
    Last changed    : 3/6/2017 3:54:21 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-60-1~5 2017-03-06 13-58-15\VWD-OD(1-2)-92-8
                      -0.8ML-3UL-210NM-40MIN.M (Sequence Method)
    Last changed    : 3/27/2017 9:57:45 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

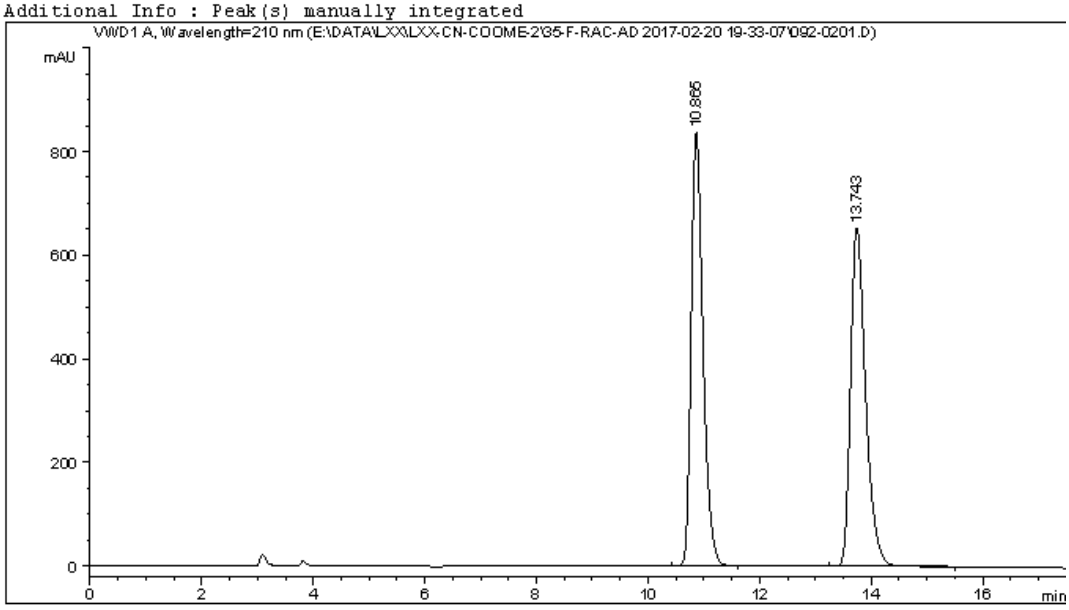



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  21.451 MM    0.5413 2.79822e4   861.54102  97.6468
       2  27.336 MM    0.6367  674.34253   17.65099   2.3532

    Totals :                  2.86565e4   879.19201


    ======================================================================
                              *** End of Report ***
```



Data File E:\DATA\LXX\LXX-CN-COOME-2\35-F-RAC-AD 2017-02-20 19-33-07\092-0201.D
Sample Name: 3,5-F-Rac

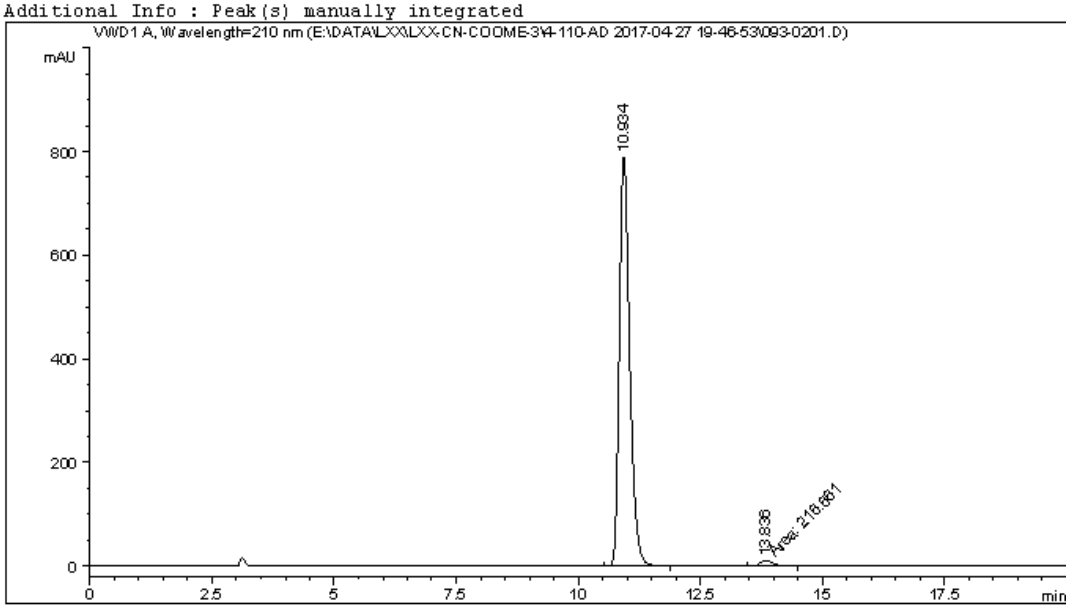
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   2
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 92
    Injection Date  : 2/20/2017 7:49:38 PM               Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\35-F-RAC-AD 2017-02-20 19-33-07\VWD-AD(1-2)-
                      95-5-1ML-3UL-210NM-35MIN.M
    Last changed    : 2/20/2017 7:33:07 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\35-F-RAC-AD 2017-02-20 19-33-07\VWD-AD(1-2)-
                      95-5-1ML-3UL-210NM-35MIN.M (Sequence Method)
    Last changed    : 3/27/2017 9:14:58 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



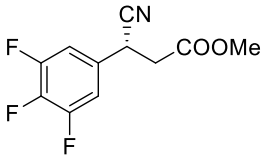

```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  10.865 BB    0.2236 1.23030e4   836.48236  50.1968
       2  13.743 BB    0.2839 1.22065e4   653.42096  49.8032

    Totals :                  2.45094e4  1489.90332


    ======================================================================
                              *** End of Report ***
```

Data File E:\DATA\LXX\LXX-CN-COOME-3\4-110-AD 2017-04-27 19-46-53\093-0201.D
Sample Name: 4-110-2

```
    ====================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   2
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 93
    Injection Date  : 4/27/2017 8:13:20 PM               Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-3\4-110-AD 2017-04-27 19-46-53\VWD-AD(1-2)-95-5
                      -1ML-3UL-210NM-35MIN.M
    Last changed    : 4/27/2017 7:47:56 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-3\4-110-AD 2017-04-27 19-46-53\VWD-AD(1-2)-95-5
                      -1ML-3UL-210NM-35MIN.M (Sequence Method)
    Last changed    : 4/28/2017 4:45:36 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

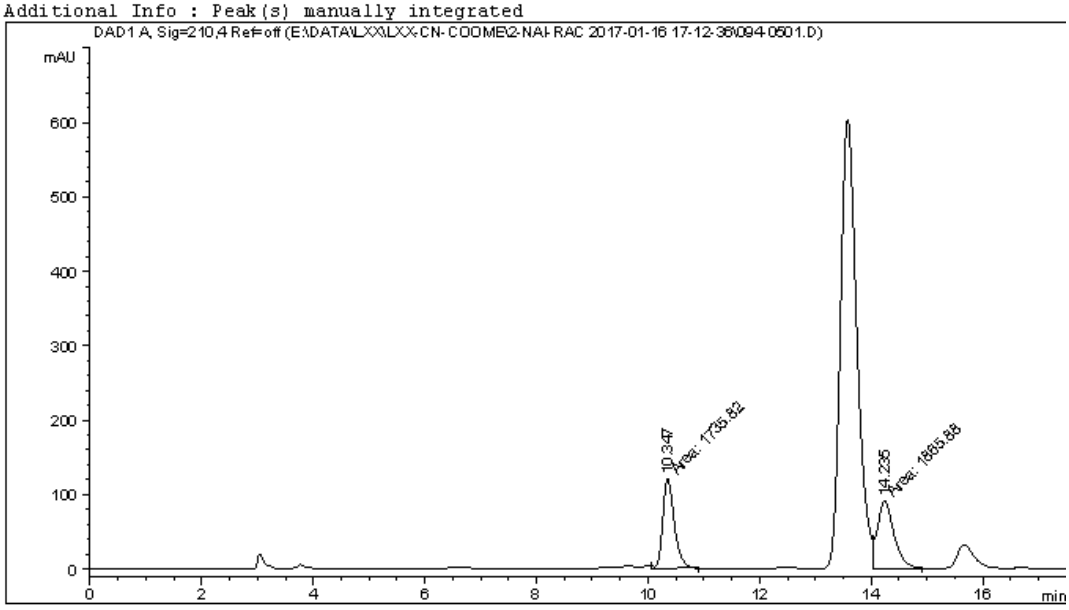



```
    ====================================================================
                            Area Percent Report
    ====================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  10.934 BB    0.2235 1.16123e4   789.93463  98.1684
       2  13.836 MM    0.3223  216.66106   11.20491   1.8316

    Totals :                  1.18290e4   801.13954


    ====================================================================
                            *** End of Report ***
```



Data File E:\DATA\LXX\LXX-CN-COOME\2-NAI-RAC 2017-01-16 17-12-36\094-0501.D
Sample Name: 3,4,5-F-Rac

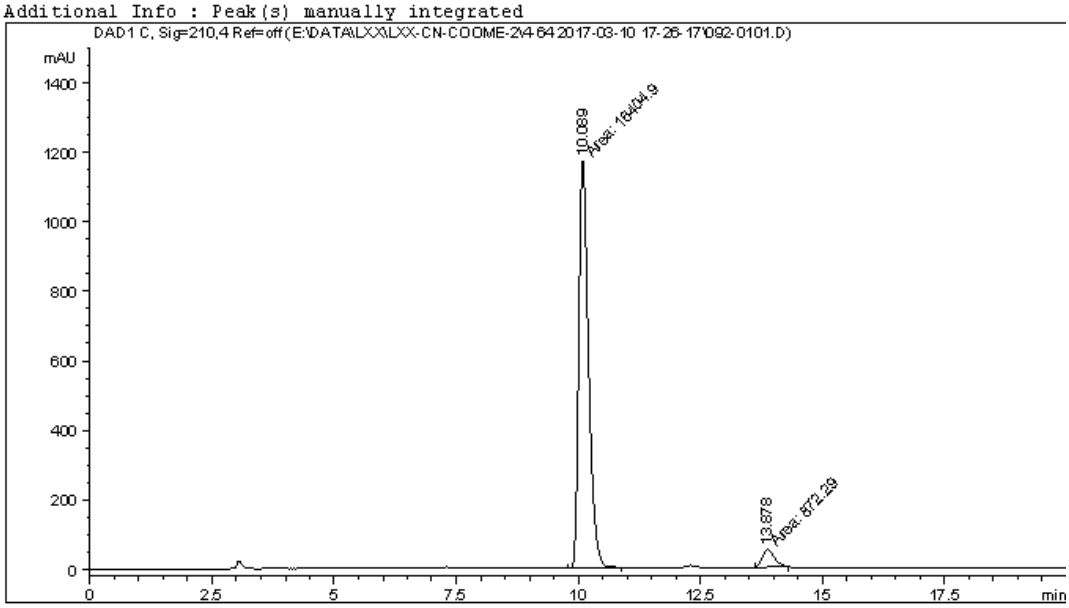
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   5
    Acq. Instrument : 1260HPLC-DAD                  Location : Vial 94
    Injection Date  : 1/16/2017 7:12:27 PM               Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME\2-NAI-RAC 2017-01-16 17-12-36\DAD-AD(1-6)-95-5-
                      1ML-3UL-45MIN.M
    Last changed    : 1/16/2017 7:02:04 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME\2-NAI-RAC 2017-01-16 17-12-36\DAD-AD(1-6)-95-5-
                      1ML-3UL-45MIN.M (Sequence Method)
    Last changed    : 3/27/2017 9:01:15 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



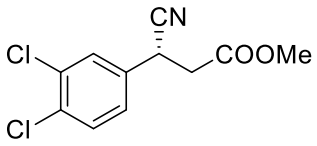

```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1  10.347 MM    0.2397 1735.81763  120.67649  48.1944
       2  14.235 FM    0.3401 1865.87903   91.44936  51.8056

    Totals :                  3601.69666  212.12585


    ======================================================================
                              *** End of Report ***
```

Data File E:\DATA\LXX\LXX-CN-COOME-2\4-64 2017-03-10 17-26-17\092-0101.D
Sample Name: 4-64-3

```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   1
    Acq. Instrument : 1260HPLC-DAD                     Location : Vial 92
    Injection Date  : 3/10/2017 5:27:15 PM                  Inj :   1
                                                     Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-64 2017-03-10 17-26-17\DAD-AD(1-2)-95-5-1ML
                      -35MIN.M
    Last changed    : 3/10/2017 5:51:04 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-64 2017-03-10 17-26-17\DAD-AD(1-2)-95-5-1ML
                      -35MIN.M (Sequence Method)
    Last changed    : 4/28/2017 4:42:31 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

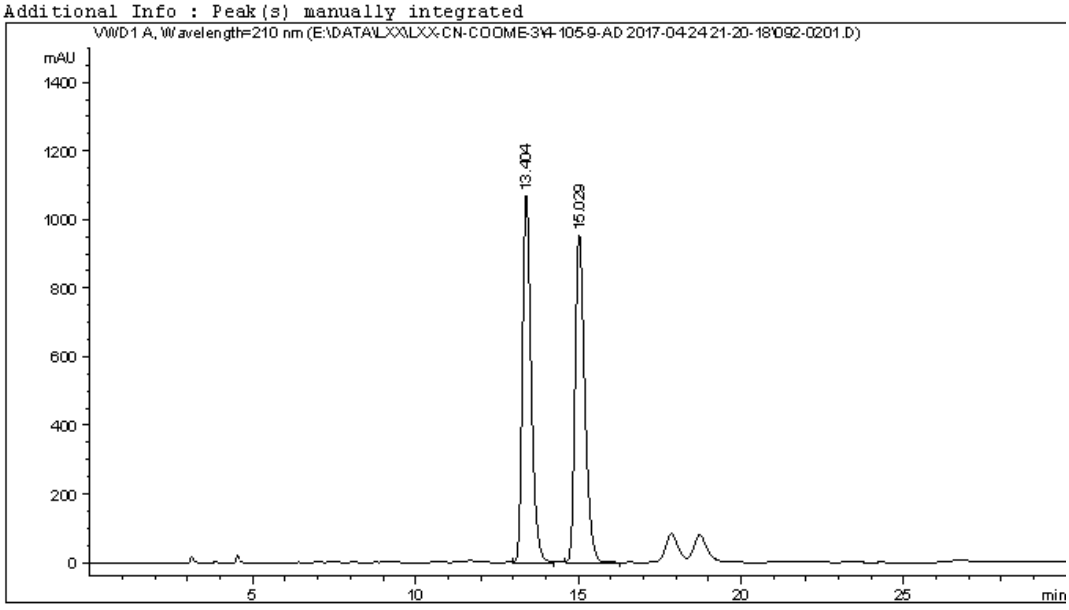



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 C, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  10.089 MM    0.2333 1.64049e4  1171.97876  94.9512
       2  13.878 MM    0.2873  872.29022   50.60963   5.0488

    Totals :                  1.72772e4  1222.58839


    ======================================================================
```



Data File E:\DATA\LXX\LXX-CN-COOME-3\4-105-9-AD 2017-04-24 21-20-18\092-0201.D
Sample Name: 3,4-Cl-Rac

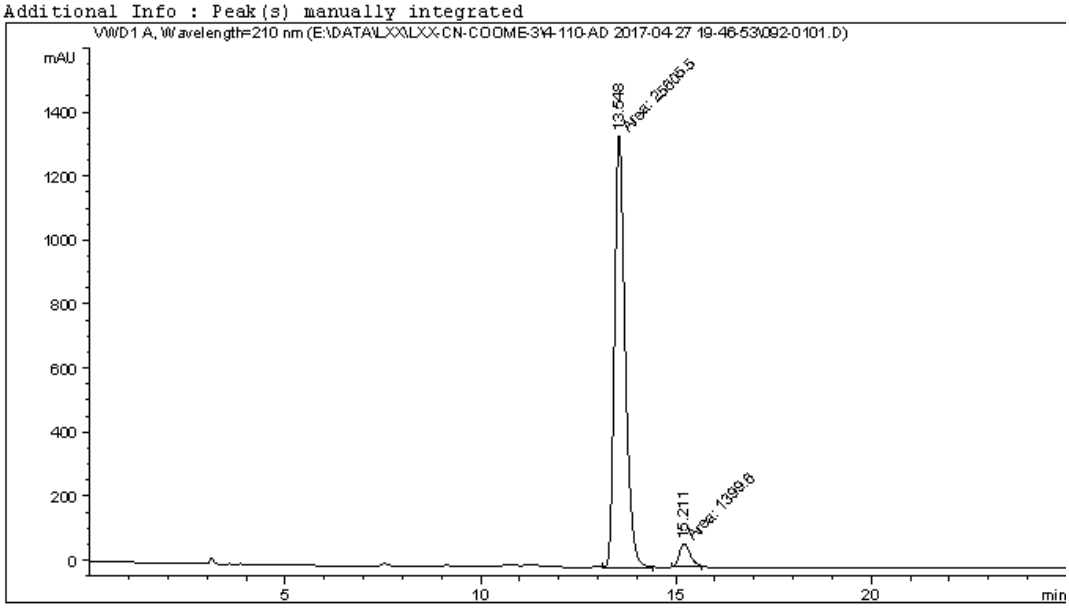
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   2
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 92
    Injection Date  : 4/24/2017 9:36:49 PM               Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-3\4-105-9-AD 2017-04-24 21-20-18\VWD-AD(1-2)-95
                      -5-1ML-3UL-210NM-35MIN.M
    Last changed    : 4/24/2017 10:06:40 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-3\4-105-9-AD 2017-04-24 21-20-18\VWD-AD(1-2)-95
                      -5-1ML-3UL-210NM-35MIN.M (Sequence Method)
    Last changed    : 4/27/2017 8:23:02 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



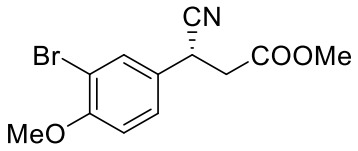

```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  13.404 VV    0.2837 1.99516e4  1069.18677  50.1119
       2  15.029 VB    0.3171 1.98625e4   953.22827  49.8881

    Totals :                  3.98140e4  2022.41504


    ======================================================================
```

Data File E:\DATA\LXX\LXX-CN-COOME-3\4-110-AD 2017-04-27 19-46-53\092-0101.D
Sample Name: 4-110-3

```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   1
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 92
    Injection Date  : 4/27/2017 7:47:36 PM                  Inj :   1
                                                     Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-3\4-110-AD 2017-04-27 19-46-53\VWD-AD(1-2)-95-5
                      -1ML-3UL-210NM-35MIN.M
    Last changed    : 4/27/2017 7:47:56 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-3\4-110-AD 2017-04-27 19-46-53\VWD-AD(1-2)-95-5
                      -1ML-3UL-210NM-35MIN.M (Sequence Method)
    Last changed    : 4/27/2017 8:21:29 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

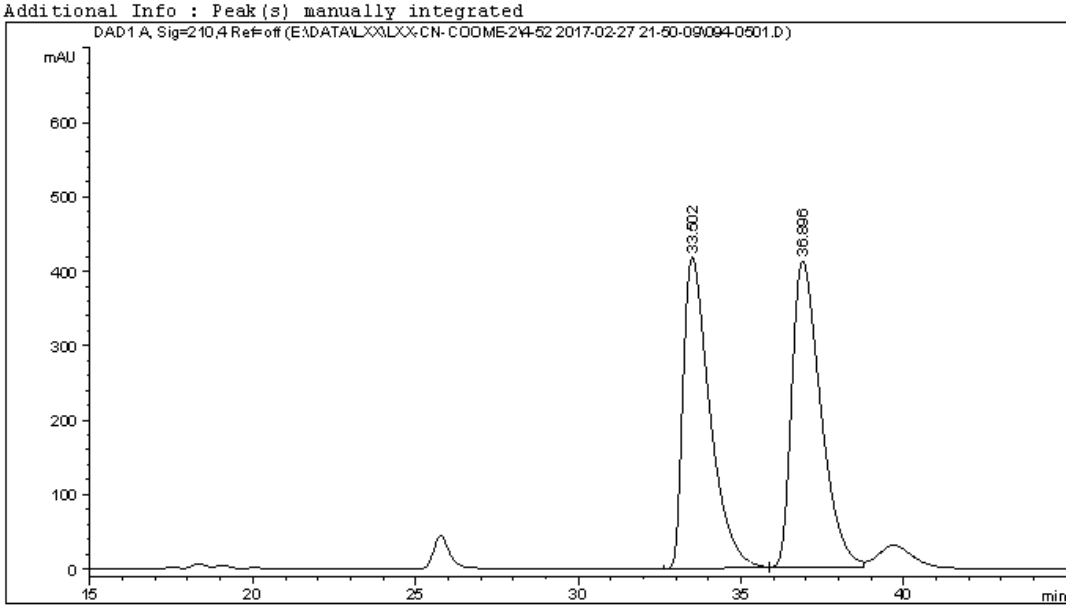



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  13.548 MM    0.3163 2.56055e4  1349.18579  94.8173
       2  15.211 MM    0.3253 1399.59705   71.69808   5.1827

    Totals :                  2.70051e4  1420.88387


    ======================================================================
```



Data File E:\DATA\LXX\LXX-CN-COOME-2\4-52 2017-02-27 21-50-09\094-0501.D
Sample Name: 3-Br-4-OMe-Rac

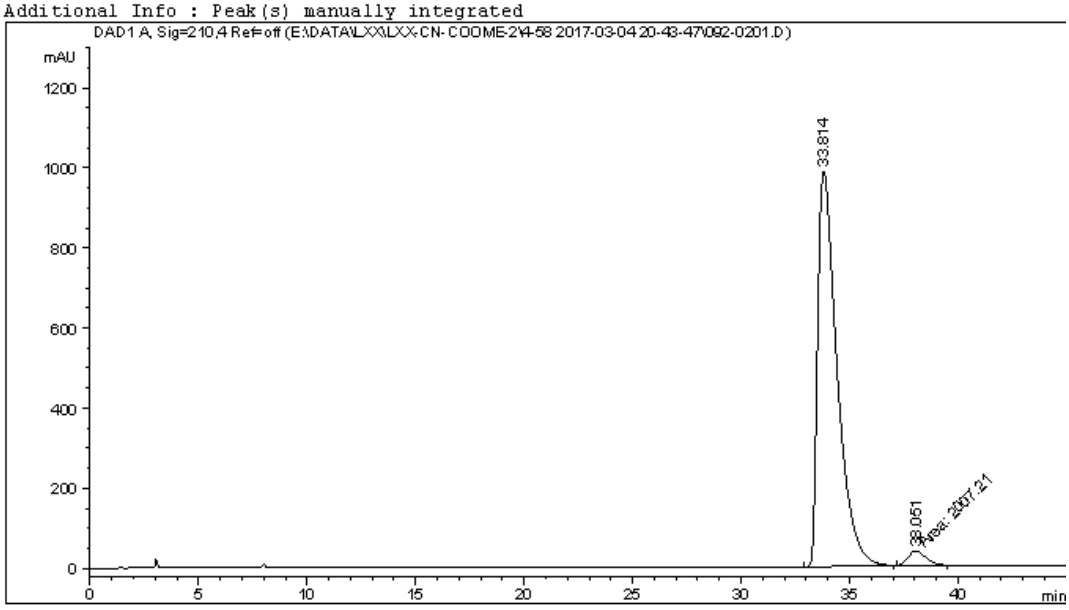
```
    ==================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   5
    Acq. Instrument : 1260HPLC-DAD                   Location : Vial 94
    Injection Date  : 2/28/2017 12:09:50 AM               Inj :   1
                                                  Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-52 2017-02-27 21-50-09\DAD-OD(1-2)-95-5-1ML
                      -3UL-45MIN.M
    Last changed    : 2/27/2017 9:50:09 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-52 2017-02-27 21-50-09\DAD-OD(1-2)-95-5-1ML
                      -3UL-45MIN.M (Sequence Method)
    Last changed    : 3/27/2017 9:25:41 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



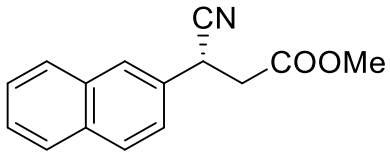

```
    ==================================================================
                            Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  33.502 BB    0.8624 2.38600e4   417.74380  48.3934
       2  36.896 BV    0.9324 2.54443e4   412.04178  51.6066

    Totals :                  4.93043e4   829.78558


    ==================================================================
                            *** End of Report ***
```

Data File E:\DATA\LXX\LXX-CN-COOME-2\4-58 2017-03-04 20-43-47\092-0201.D
Sample Name: LXX-4-58-2

```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   2
    Acq. Instrument : 1260HPLC-DAD                   Location : Vial 92
    Injection Date  : 3/4/2017 8:50:39 PM                 Inj :   1
                                                  Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-58 2017-03-04 20-43-47\DAD-OD(1-2)-95-5-1ML
                      -3UL-45MIN.M
    Last changed    : 3/4/2017 8:43:47 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-58 2017-03-04 20-43-47\DAD-OD(1-2)-95-5-1ML
                      -3UL-45MIN.M (Sequence Method)
    Last changed    : 3/27/2017 9:38:19 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

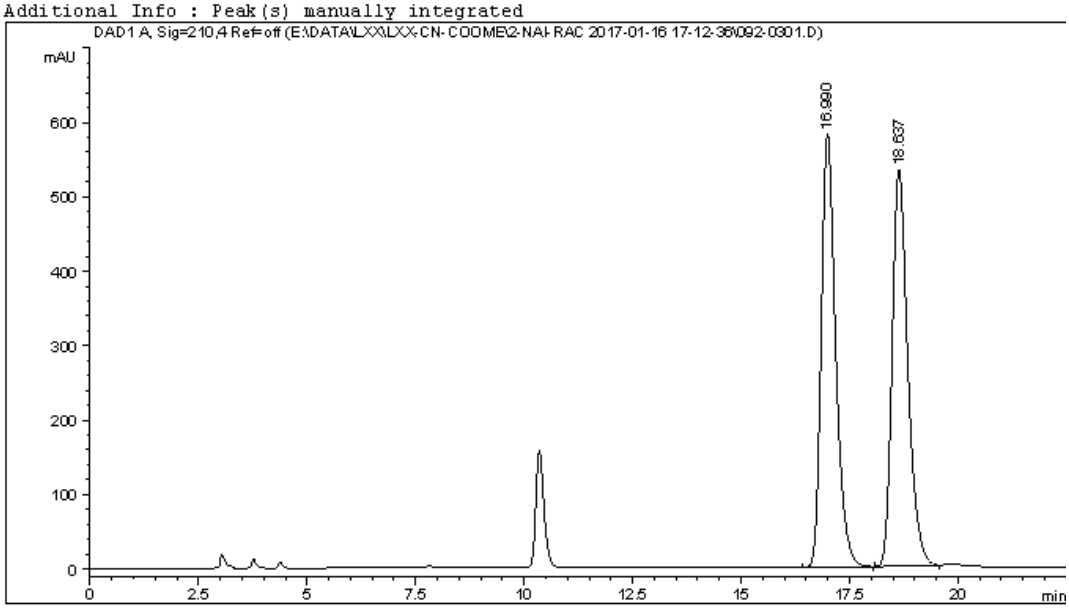



```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  33.814 BB    0.9195 6.12764e4   988.05878  96.8282
       2  38.051 MM    0.9592 2007.20947   34.87535   3.1718

    Totals :                  6.32836e4  1022.93413


    ======================================================================
                              *** End of Report ***
```



Data File E:\DATA\LXX\LXX-CN-COOME\2-NAI-RAC 2017-01-16 17-12-36\092-0301.D
Sample Name: 2-NAI-Rac

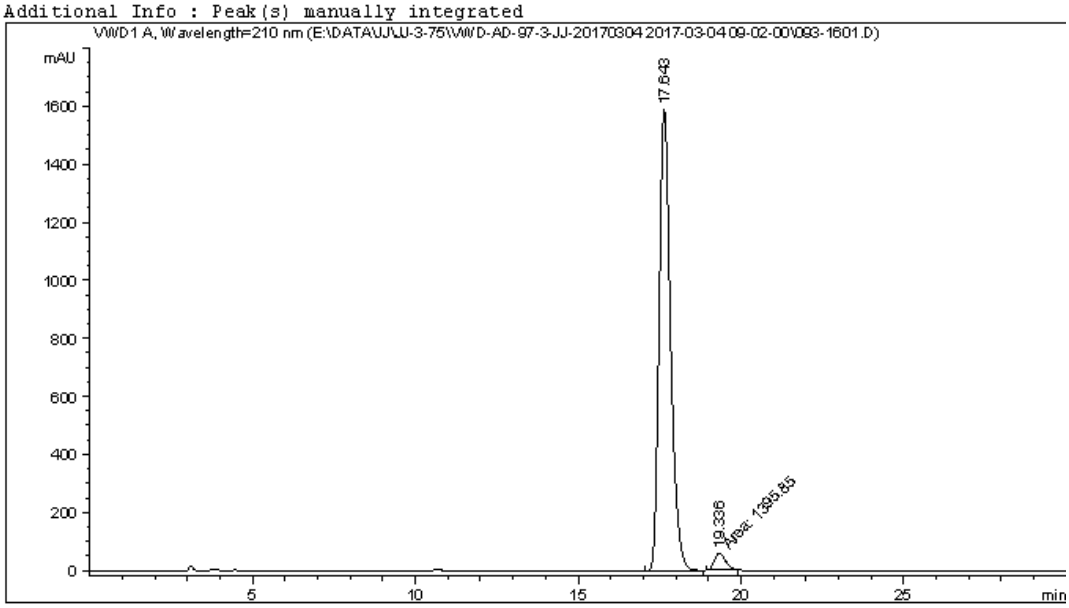
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   3
    Acq. Instrument : 1260HPLC-DAD                   Location : Vial 92
    Injection Date  : 1/16/2017 5:50:35 PM                Inj :   1
                                                  Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME\2-NAI-RAC 2017-01-16 17-12-36\DAD-AD(1-6)-95-5-
                      1ML-3UL-45MIN.M
    Last changed    : 1/16/2017 5:12:37 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME\2-NAI-RAC 2017-01-16 17-12-36\DAD-AD(1-6)-95-5-
                      1ML-3UL-45MIN.M (Sequence Method)
    Last changed    : 3/27/2017 8:59:46 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  16.990 BB    0.3488 1.33809e4   580.82922  50.1713
       2  18.637 BB    0.3792 1.32895e4   532.36285  49.8287

    Totals :                  2.66705e4  1113.19208


    ======================================================================
                              *** End of Report ***
```

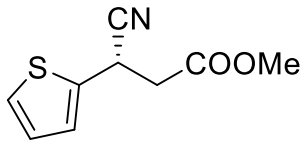
Data File E:\DATA\JJ\JJ-3-75\VWD-AD-97-3-JJ-20170304 2017-03-04 09-02-00\093-1601.D
Sample Name: LXX-4-58-4

```
    ==================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :  16
    Acq. Instrument : 1260HPLC-VWD                   Location : Vial 93
    Injection Date  : 3/4/2017 9:00:58 PM                 Inj :  1
                                                  Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\JJ\JJ-3-75\VWD-AD-97-3-JJ-20170304 2017-03-04 09-02-00\VWD-AD(1-
                      2)-95-5-1ML-3UL-210NM-35MIN.M
    Last changed    : 3/4/2017 9:10:30 PM by SYSTEM
                      (modified after loading)
    Analysis Method : E:\DATA\JJ\JJ-3-75\VWD-AD-97-3-JJ-20170304 2017-03-04 09-02-00\VWD-AD(1-
                      2)-95-5-1ML-3UL-210NM-35MIN.M (Sequence Method)
    Last changed    : 3/27/2017 9:44:01 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



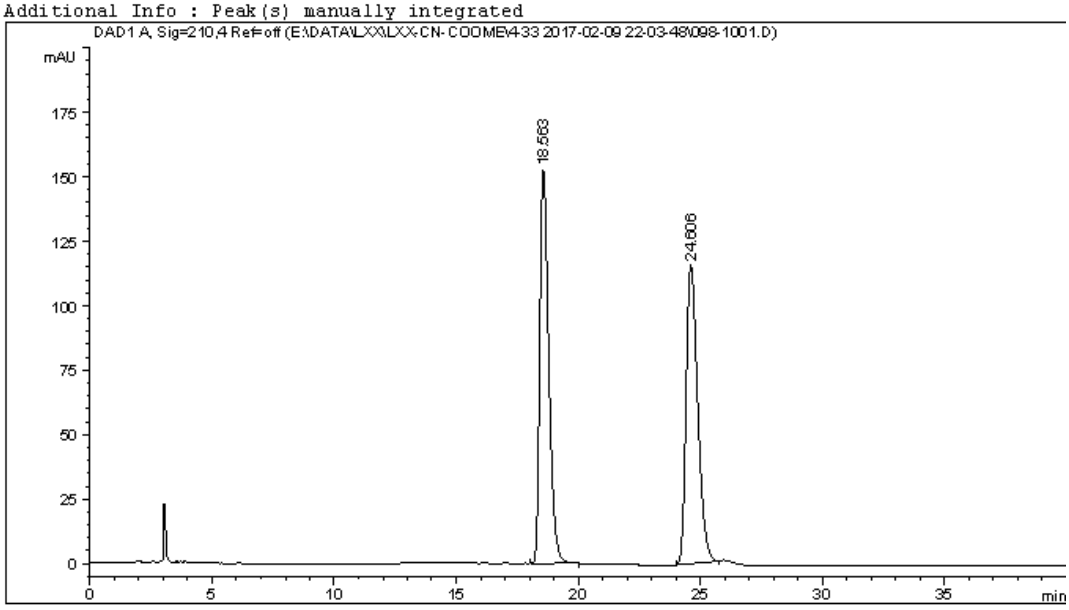

```
    ==================================================================
                          Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  17.643 BV    0.3724 3.88649e4  1588.46228  96.5330
       2  19.336 MM    0.4000 1395.85303   58.16449   3.4670

    Totals :                  4.02607e4  1646.62677


    ==================================================================
```

1260HPLC-VWD 3/27/2017 9:44:05 PM SYSTEM Page 1 of 1



Data File E:\DATA\LXX\LXX-CN-COOME\4-33 2017-02-09 22-03-48\098-1001.D
Sample Name: Saifen-Rac

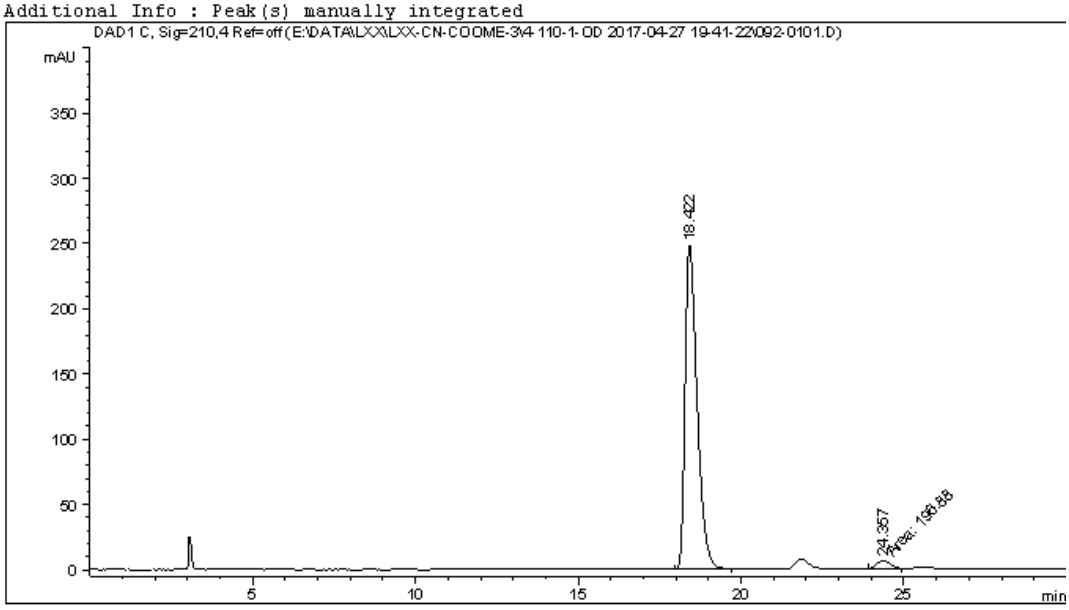
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :  10
    Acq. Instrument : 1260HPLC-DAD                   Location : Vial 98
    Injection Date  : 2/10/2017 2:34:05 AM                Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME\4-33 2017-02-09 22-03-48\DAD-OD(1-2)-95-5-1ML-
                      3UL-45MIN.M
    Last changed    : 2/9/2017 10:03:49 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME\4-33 2017-02-09 22-03-48\DAD-OD(1-2)-95-5-1ML-
                      3UL-45MIN.M (Sequence Method)
    Last changed    : 3/27/2017 9:12:06 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



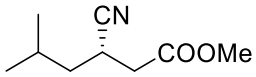

```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]        %
    ----|-------|----|-------|----------|----------|--------|
       1  18.563 BB    0.3877 3889.81250  152.46037  50.4629
       2  24.606 BB    0.5089 3818.44995  115.73651  49.5371

    Totals :                  7708.26245  268.19688


    ======================================================================
                              *** End of Report ***
```

Data File E:\DATA\LXX\LXX-CN-COOME-3\4-110-1-OD 2017-04-27 19-41-22\092-0101.D
Sample Name: LXX-4-110-1

```
    ====================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   1
    Acq. Instrument : 1260HPLC-DAD                   Location : Vial 92
    Injection Date  : 4/27/2017 7:42:15 PM               Inj :   1
                                                   Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-3\4-110-1-OD 2017-04-27 19-41-22\DAD-OD(1-2)-95
                      -5-1ML-3UL-30MIN.M
    Last changed    : 4/27/2017 7:41:22 PM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-3\4-110-1-OD 2017-04-27 19-41-22\DAD-OD(1-2)-95
                      -5-1ML-3UL-30MIN.M (Sequence Method)
    Last changed    : 4/28/2017 5:33:48 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ====================================================================
                            Area Percent Report
    ====================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 C, Sig=210,4 Ref=off

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  18.422 BB    0.3934 6365.65039  248.07104  96.9999
       2  24.357 MM    0.4950  196.88002    6.62878   3.0001

    Totals :                  6562.53041  254.69982


    ====================================================================
                            *** End of Report ***
```

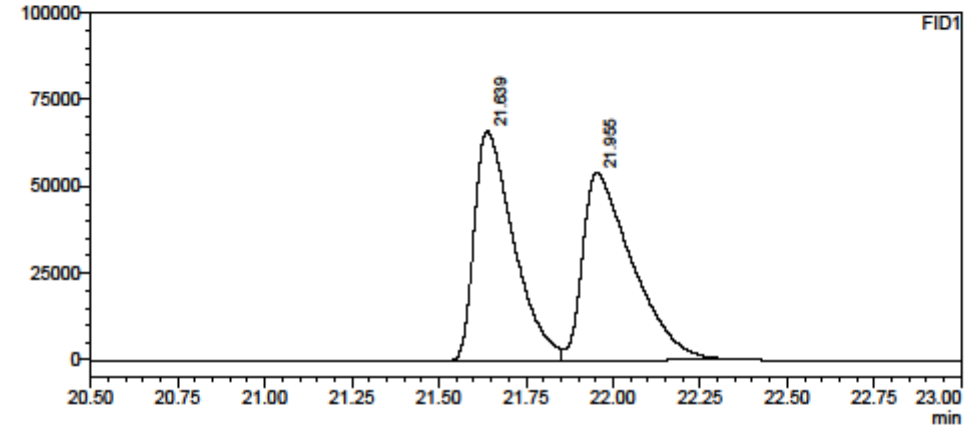


LabSolutions Analysis Report

<Sample Information>

Sample Name	: lxx-4-99-rac-2		
Sample ID	: RhRu,1h1k,1ml,140,i-Pr/DCM/TFE		
Data Filename	: lxx-4-99-rac-2.gcd		
Method Filename	: bdex225-250-100(5)-2-140(0)-260-25min.gcm		
Batch Filename	: lxx-4-99.gcb		
Vial #	: 1	Sample Type	: Unknown
Injection Volume	: 1 uL		
Date Acquired	: 2017-4-18 14:37:25	Acquired by	: System Administrator
Date Processed	: 2017-4-18 22:55:21	Processed by	: System Administrator

<Chromatogram>



<Peak Table>

FID1

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	21.639	519379	66165	49.025		M	
2	21.955	540048	54094	50.975		V M	
Total		1059427	120259				

D:\DATA FILE\lxx\Data\lxx-4-99\lxx-4-99-rac-2.gcd

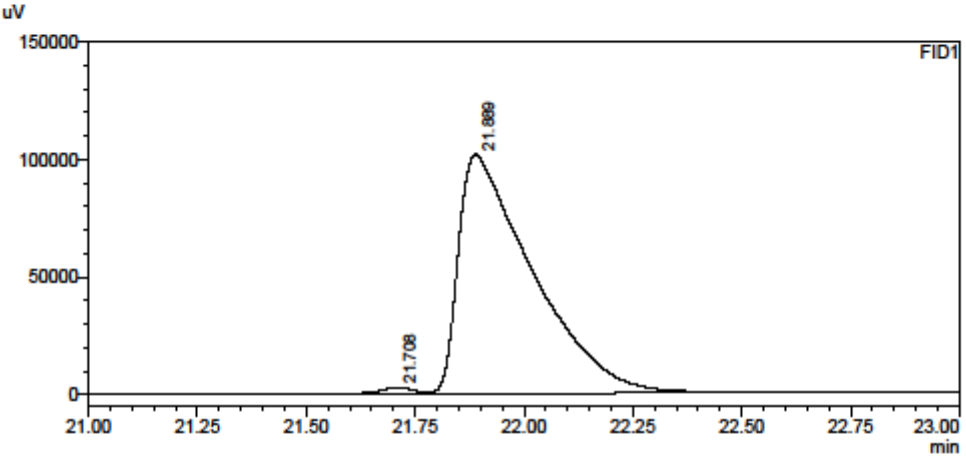
SHIMADZU LabSolutions

Analysis Report

<Sample Information>

Sample Name	: lxx-4-99-2		
Sample ID	: RhRu,1h1k,1ml,140,i-Pr/DCM/TFE0		
Data Filename	: lxx-4-99-2.gcd		
Method Filename	: bdex225-250-100(5)-2-140(0)-260-25min.gcm		
Batch Filename	: lxx-4-99.gcb		
Vial #	: 2	Sample Type	: Unknown
Injection Volume	: 1 uL		
Date Acquired	: 2017-4-18 15:35:47	Acquired by	: System Administrator
Date Processed	: 2017-4-27 19:45:31	Processed by	: System Administrator

<Chromatogram>

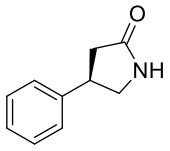


<Peak Table>

FID1

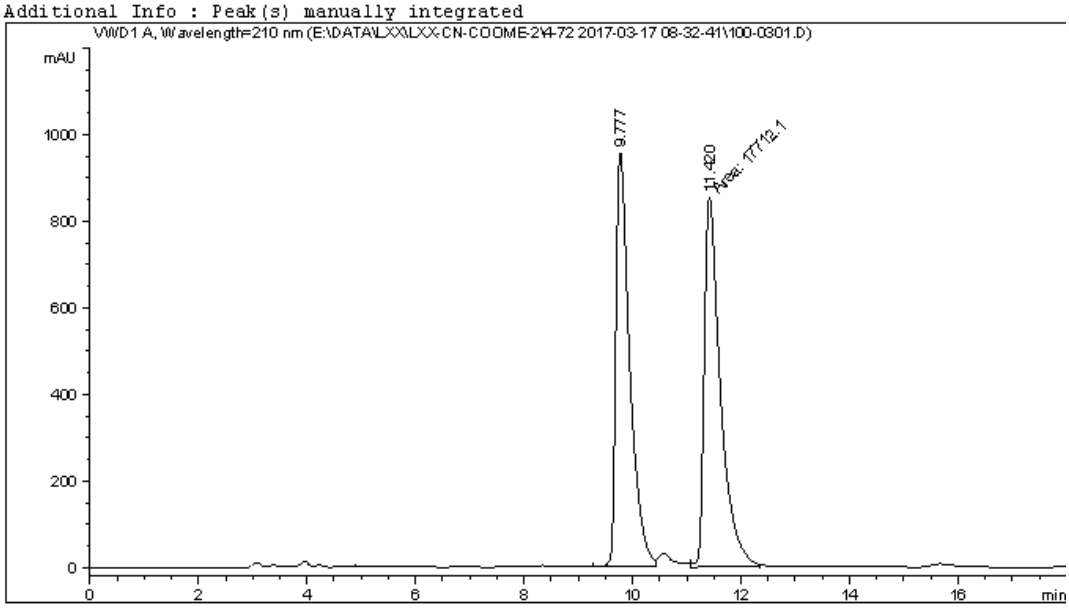
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	21.708	11697	2488	0.963		M	
2	21.889	1202673	101478	99.037		V M	
Total		1214370	103965				

D:\DATA FILE\lxx\Data\lxx-4-99\lxx-4-99-2.gcd



Data File E:\DATA\LXX\LXX-CN-COOME-2\4-72 2017-03-17 08-32-41\100-0301.D
Sample Name: LXX-4-48-Rac

Acq. Operator	: SYSTEM
Acq. Instrument	: 1260HPLC-VWD
Injection Date	: 3/17/2017 9:40:01 AM
Acq. Method	: E:\DATA\LXX\LXX-CN-COOME-2\4-72 2017-03-17 08-32-41\VWD-AD(1-2)-90-10-1ML-3UL-210NM-50MIN.M
Last changed	: 3/17/2017 9:53:05 AM by SYSTEM (modified after loading)
Analysis Method	: E:\DATA\LXX\LXX-CN-COOME-2\4-72 2017-03-17 08-32-41\VWD-AD(1-2)-90-10-1ML-3UL-210NM-50MIN.M (Sequence Method)
Last changed	: 5/3/2017 3:01:32 PM by SYSTEM (modified after loading)
Additional Info	: Peak(s) manually integrated
Seq. Line	: 3
Location	: Vial 100
Inj	: 1
Inj Volume	: 3.000 µl



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

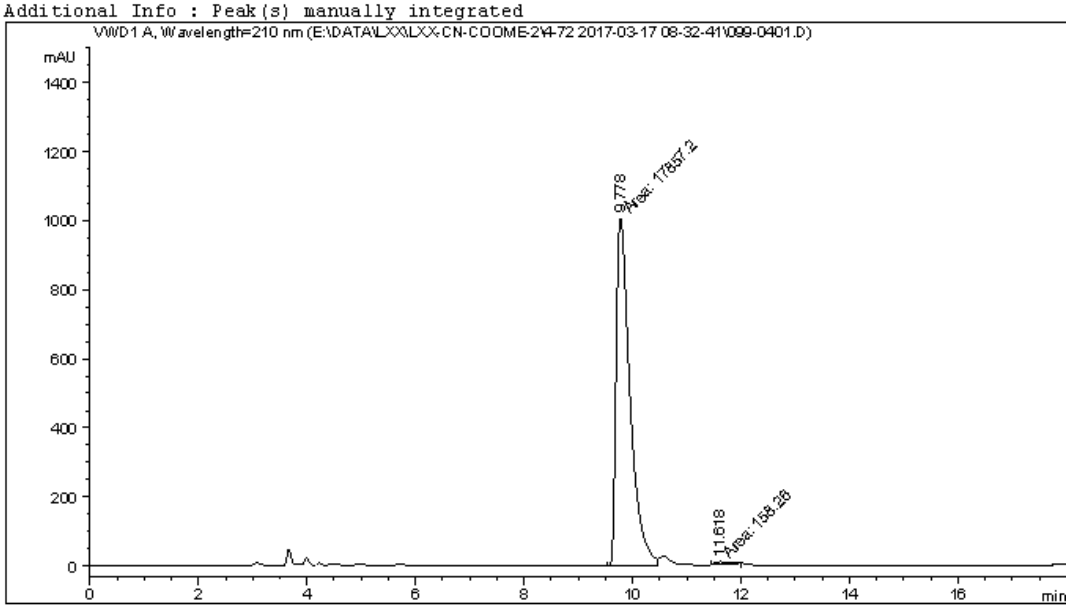
Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.777	BV	0.2646	1.70299e4	957.14807	49.0183
2	11.420	MM	0.3459	1.77121e4	853.42456	50.9817

Totals : 3.47420e4 1810.57263

Data File E:\DATA\LXX\LXX-CN-COOME-2\4-72 2017-03-17 08-32-41\099-0401.D
Sample Name: LXX-4-72

```
    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :   4
    Acq. Instrument : 1260HPLC-VWD                     Location : Vial 99
    Injection Date  : 3/17/2017 10:15:49 AM                Inj :   1
                                                     Inj Volume : 3.000 µl
    Acq. Method     : E:\DATA\LXX\LXX-CN-COOME-2\4-72 2017-03-17 08-32-41\VWD-AD(1-2)-90-10-
                      1ML-3UL-210NM-50MIN.M
    Last changed    : 3/17/2017 9:53:05 AM by SYSTEM
    Analysis Method : E:\DATA\LXX\LXX-CN-COOME-2\4-72 2017-03-17 08-32-41\VWD-AD(1-2)-90-10-
                      1ML-3UL-210NM-50MIN.M (Sequence Method)
    Last changed    : 5/3/2017 2:57:56 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```




```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Do not use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=210 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   9.778 MF    0.2953 1.78572e4  1007.69324  99.1215
       2  11.618 MM    0.3341  158.25952    7.89511   0.8785

    Totals :                  1.80155e4  1015.58835


    ======================================================================
                              *** End of Report ***
```