Supporting Information

General Remarks

Most of chemicals were purchased from Sigma-Aldrich, Strem, Acros, TCI or Alfa Aesar and used as such unless stated otherwise. Solvents (Anhydrous and under inert atmosphere) were collected from The Solvent purification system by M BRAUN and used under standard schlenk technique. NMR spectra were recorded on Bruker Avance 300 and Bruker ARX 400 spectrometers. Chemical shifts (ppm) are given relative to solvent: references for $CDCl_3$ were 7.26 ppm (^{1}H NMR) and 77.00 ppm (^{13}C NMR). Multiplets were assigned as s (singlet), d (doublet), t (triplet), q (quartet), p (pentet) dd (doublet of doublet), m (multiplet) and br. s (broad singlet). GC-yields were calculated using hexadecane as internal standard. All measurements were carried out at room temperature unless otherwise stated. Electron impact (EI) mass spectra were recorded on AMD 402 mass spectrometer (70 eV). High resolution mass spectra (HRMS) were recorded on Agilent 6210. The data are given as mass units per charge (m/z). Gas chromatography analysis was performed on an Agilent HP-7890A instrument with a FID detector and HP-5 capillary column (polydimethylsiloxane with 5% phenyl groups, 30 m, 0.32 mm i.d., 0.25 μm film thickness) using argon as carrier gas. The products were isolated from the reaction mixture by column chromatography on silica gel 60, 0.063-0.2 mm, 70-230 mesh (Merck).

General Procedure

A: A 4 mL screw-cap vial was charged with CuBr(Me_2S) (5.1 mg, 5 mol%), 4,4′,4″-tri-*tert*-butyl-2,2′:6′,2″-terpyridine (20 mg, 10 mol%), di(1-adamantyl)-*n*-butylphosphine (8.96 mg, 5mol%), acetonitrile (3 mL) and an oven-dried stirring bar. The vial was closed by Teflon septum and phenolic cap and connected with atmosphere with a needle. After 3-phenyl-1-propanol (0.5 mmol) and DTBP (2 mmol) were injected by syringe, the vial was fixed in an alloy plate and put into Paar 4560 series autoclave (300 mL) under argon atmosphere. At room temperature, the autoclave is flushed with 20 bar of ehtene and 40 bar of carbon monoxide was charged. The autoclave was placed on a heating plate equipped with magnetic stirring and an aluminum block. The reaction is allowed to be heated under 120 ^{o}C for 12 hours. Afterwards, the autoclave is cooled to room temperature and the pressure was carefully released. After removal of solvent under reduced pressure, pure product was obtained by column chromatography on silica gel (eluent: pentane/ethyl acetate = 50-10:1).

B: A 4 mL screw-cap vial was charged with CuBr(Me_2S) (5.1 mg, 5 mol%), 4,4′,4″-tri-*tert*-butyl-2,2′:6′,2″-terpyridine (20 mg, 10 mol%), di(1-adamantyl)-*n*-butylphosphine (8.96 mg, 5mol%), acetonitrile (3 mL) and an oven-dried stirring bar. The vial was closed by Teflon septum and phenolic cap and connected with atmosphere with a needle. After 1-hexene (2 mmol), 3-phenyl-1-propanol (0.5 mmol) and DTBP (2 mmol) were injected by syringe, the vial was fixed in an alloy plate and put into Paar 4560 series autoclave (300 mL) under argon atmosphere. At room temperature, the autoclave is flushed with carbon monoxide for three times and 40 bar of carbon monoxide was charged. The autoclave was placed on a heating plate equipped with magnetic stirring and an aluminum block. The reaction is allowed to be heated under 110 ^{o}C for 12 hours. Afterwards, the autoclave is cooled to room temperature and the pressure was carefully released. After removal of solvent under reduced pressure, pure product was obtained by column chromatography on silica gel (eluent: pentane/ethyl acetate = 50-30:1).

Mechanistic studies

Reaction in the presence of TEMPO

A 4 mL screw-cap vial was charged with $CuBr(Me_2S)$ (5.1 mg, 5 mol%), 4,4′,4″-tri-*tert*-butyl-2,2′:6′,2″-terpyridine (20 mg, 10 mol%), di(1-adamantyl)-*n*-butylphosphine (8.96 mg, 5mol%), Tempo (156 mg, 2 equiv), acetonitrile (3 mL) and an oven-dried stirring bar. The vial was closed by Teflon septum and phenolic cap and connected with atmosphere with a needle. After 3-phenyl-1-propanol (0.5 mmol) and DTBP (2 mmol) were injected by syringe, the vial was fixed in an alloy plate and put into Paar 4560 series autoclave (300 mL) under argon atmosphere. At room temperature, the autoclave is flushed with 20 bar of ethane and 40 bar of carbon monoxide was charged. The autoclave was placed on a heating plate equipped with magnetic stirring and an aluminum block. The reaction is allowed to be heated under 120 ^oC for 12 hours. Afterwards, the autoclave is cooled to room temperature and the pressure was carefully released.

Synthesis of piperidin-2-one[1]

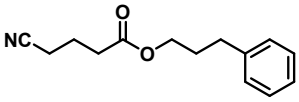
A 4 mL screw-cap vial was charged with PtO_2 (5.6 mg, 10 mol%). The vial was closed by Teflon septum and phenolic cap and connected with atmosphere with a needle. The vial is flushed with carbon monoxide for three times than 3-Phenylpropyl 4-cyanobutanoate (0.25 mmol), MeOH (3 mL) were injected by syringe, the vial was fixed in an alloy plate and put into Paar 4560 series autoclave (300 mL) under argon atmosphere. At room temperature, the autoclave is flushed with H_2 for three times and 5 bar of H_2 was charged. The autoclave was placed on a heating plate equipped with magnetic stirring and an aluminum block. The reaction is allowed to be heated under 25 ^oC for 72 hours. Afterwards, the pressure was carefully released. After removal of solvent under reduced pressure, pure product was obtained by column chromatography on silica gel ($MeOH/CH_2Cl_2$ = 1:10).

Synthesis of estrone derivative

A 4 mL screw-cap vial was charged with $Pd(OAc)_2$ (2.24 mg, 2 mol%), di(1-adamantyl)-*n*-butylphosphine (10.74 mg, 6 mol%), estrone (135 mg, 0.5 mmol), 1-4dioxane (2 mL) and an oven-dried stirring bar. The vial was closed by Teflon septum and phenolic cap and connected with atmosphere with a needle. After 2-bromobenzyl 2-(2-cyanoethyl)octanoate (0.5 mmol), and Et_3N (1 mmol) were injected by syringe, the vial was fixed in an alloy plate and put into Paar 4560 series autoclave (300 mL) under argon atmosphere. At room temperature, the autoclave is flushed with carbon monoxide for three times and 5 bar of carbon monoxide was charged. The autoclave was placed on a heating plate equipped with magnetic stirring and an aluminum block. The reaction is allowed to be heated under 100 ^oC for 16 hours. Afterwards, the autoclave is cooled to room temperature and the pressure was carefully released. After removal of solvent under reduced pressure, pure product was obtained by column chromatography on silica gel (eluent: pentane/ethyl acetate = 5:1).

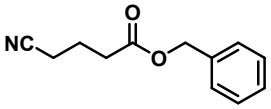
Analytic Data of Products

3-Phenylpropyl 4-cyanobutanoate



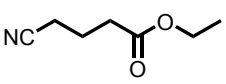
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.28 – 7.05 (m, 5H), 4.05 (t, *J* = 6.5 Hz, 2H), 2.62 (dd, *J* = 8.5, 6.8 Hz, 2H), 2.40 (dt, *J* = 8.2, 7.1 Hz, 2H), 1.98 – 1.85 (m, 4H), 1.45 – 1.31 (m, 2H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.98, 141.02, 128.48, 128.38, 126.08, 118.98, 64.22, 32.34, 32.20, 30.09, 20.75, 16.57.
GC-MS (EI, 70ev): m/z(%) = 231(M+,1), 119(6), 118(85), 117(100), 96(15), 91(59), 78(11), 77(12), 68(15), 65(17), 41(29), 39(13).
HRMS(ESI): calcd. for $[C_{14}H_{17}NO_2+Na]^+$:254.12593, found: 254.11524.

Benzyl 4-cyanobutanoate



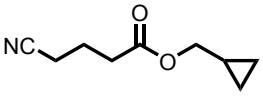
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.43 – 7.30 (m, 5H), 5.14 (s, 2H), 2.54 (t, *J* = 7.1 Hz, 2H), 2.45 (t, *J* = 7.1 Hz, 2H), 2.10 – 1.90 (m, 2H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.79, 135.58, 128.65, 128.43, 128.30, 118.95, 66.65, 32.41, 20.77, 16.54.
GC-MS (EI, 70ev): m/z(%) = 203(M+,10), 109(10), 108(90), 105(14), 96(19), 91(100), 79(24), 77(32), 68(14), 65(32), 63(12), 51(17), 42(11), 41(44), 40(12), 39(28), 29(7).
HRMS(EI): calcd. for $[C_{12}H_{13}NO_2]^+$:203.09452, found: 203.09408.

Ethyl 4-cyanobutanoate[2]



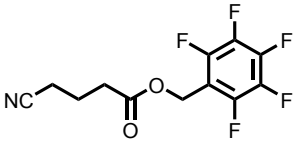
^{1}H NMR (300 MHz, Chloroform-*d*) δ 4.13 (q, *J* = 7.1 Hz, 2H), 2.45 (td, *J* = 7.1, 5.1 Hz, 4H), 2.02 – 1.88 (m, 2H), 1.24 (t, *J* = 7.1 Hz, 3H).
GC-MS (EI, 70ev): m/z(%) = 141(M+, 5), 114(10), 96(100), 68(30), 41(40).

Cyclopropylmethyl 4-cyanobutanoate



^{1}H NMR (300 MHz, Chloroform-*d*) δ 3.92 (d, *J* = 7.3 Hz, 2H), 2.49 (dt, *J* = 12.4, 7.1 Hz, 4H), 2.09 – 1.90 (m, 2H), 1.19 – 1.02 (m, 1H), 0.63 – 0.52 (m, 2H), 0.35 – 0.20 (m, 2H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 172.08, 119.05, 69.64, 32.43, 20.81, 16.56, 9.74, 3.29.
GC-MS (EI, 70ev): m/z(%) = 167(M+,5), 139(10), 114(10), 96(100), 68(40), 55(45), 41(30).

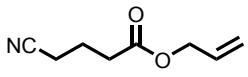
(Perfluorophenyl)methyl 4-cyanobutanoate



^{1}H NMR (300 MHz, Chloroform-*d*) δ 5.23 (t, *J* = 1.6 Hz, 2H), 2.53 (t, *J* = 7.1 Hz, 2H), 2.47 (t, *J* = 7.1 Hz, 2H), 2.11 – 1.90 (m, 2H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.25, 118.77, 53.57, 31.99, 20.58, 16.50.
^{19}F NMR (282 MHz, Chloroform-*d*) δ -141.93 (dddd, *J* = 21.5, 8.0, 3.8, 2.0 Hz), -152.15 (tt, *J* = 20.7, 2.4 Hz), -161.10 – -161.65 (m).

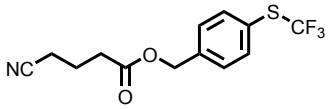
GC-MS (EI, 70ev): m/z(%) = 293(M+,5), 265(10), 211(8), 197(10), 181(100), 161(15), 143(5), 131(8), 117(10), 96(50), 69(15), 41(10).

Allyl 4-cyanobutanoate



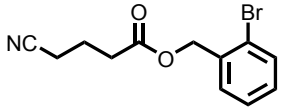
^{1}H NMR (300 MHz, Chloroform-*d*) δ 5.90 (ddt, *J* = 17.2, 10.4, 5.8 Hz, 1H), 5.39 – 5.19 (m, 2H), 4.58 (dt, *J* = 5.8, 1.4 Hz, 2H), 2.49 (dt, *J* = 17.3, 7.1 Hz, 4H), 2.11 – 1.88 (m, 2H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.62, 131.82, 118.64, 65.45, 32.29, 20.73.
GC-MS (EI, 70ev): m/z(%) = 153(M+,5), 138(5), 125(3), 110(5), 96(100), 81(10), 68(40), 55(10), 41(10).

4-((Trifluoromethyl)thio)benzyl 4-cyanobutanoate



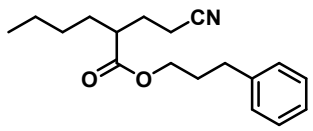
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.72 – 7.58 (m, 2H), 7.45 – 7.33 (m, 2H), 5.16 (s, 2H), 2.57 (t, *J* = 7.1 Hz, 2H), 2.46 (t, *J* = 7.0 Hz, 2H), 2.12 – 1.91 (m, 2H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.64, 138.65, 136.52, 131.54, 128.96, 127.45, 124.40, 118.88, 65.59, 32.27, 20.66, 16.53.

2-Bromobenzyl 4-cyanobutanoate



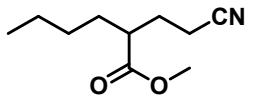
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.59 (ddd, *J* = 8.0, 1.3, 0.4 Hz, 1H), 7.43 – 7.37 (m, 1H), 7.33 (ddd, *J* = 7.3, 1.3 Hz, 1H), 7.25 – 7.17 (m, 1H), 5.22 (s, 2H), 2.58 (t, *J* = 7.1 Hz, 2H), 2.52 – 2.43 (m, 2H), 2.10 – 1.95 (m, 2H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 171.56, 134.88, 132.98, 130.17, 129.99, 127.60, 123.65, 118.92, 66.23, 32.33, 20.77, 16.57.
GC-MS (EI, 70ev): m/z(%) = 281(M+,5), 251(5), 235(5), 239(5), 202(100), 185(10), 168(40), 157(10), 143(3), 131(5), 107(90), 96(20), 89(40), 68(20), 55(15), 41(20).

3-Phenylpropyl 2-(2-cyanoethyl)hexanoate



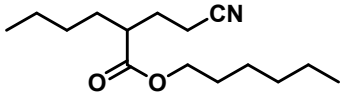
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.28 – 7.03 (m, 5H), 4.04 (td, *J* = 6.5, 1.1 Hz, 2H), 2.62 (dd, *J* = 8.6, 6.7 Hz, 2H), 2.43 (dddd, *J* = 9.5, 8.1, 5.7, 4.7 Hz, 1H), 2.36 – 2.16 (m, 2H), 1.97 – 1.82 (m, 3H), 1.79 – 1.67 (m, 1H), 1.64 – 1.51 (m, 1H), 1.50 – 1.35 (m, 1H), 1.30 – 1.14 (m, 4H), 0.82 (t, *J* = 6.9 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.71, 141.00, 128.50, 128.42, 128.39, 126.11, 119.13, 64.05, 44.20, 32.20, 31.78, 30.22, 29.18, 27.53, 22.52, 15.38, 13.90.
GC-MS (EI, 70ev): m/z(%) = 287(M+,1), 119(10), 118(100), 117(60), 91(54), 79(6), 77(7), 65(9), 55(11), 41(20), 29(8).
HRMS(ESI): calcd. for $[C_{18}H_{25}NO_2+Na]^+$: 310.17775, found: 310.17807; calcd. for $[C_{18}H_{25}NO_2+H]^+$: 288.19581, found: 288.19569.

Methyl 2-(2-cyanoethyl)hexanoate



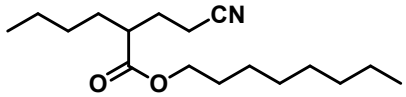
^{1}H NMR (400 MHz, Chloroform-*d*) δ 3.70 (s, 3H), 2.51 (dddd, *J* = 9.7, 8.0, 5.8, 4.6 Hz, 1H), 2.45 – 2.25 (m, 2H), 1.98 (dddd, *J* = 13.7, 9.6, 7.4, 6.2 Hz, 1H), 1.81 (dtd, *J* = 13.8, 7.8, 4.6 Hz, 1H), 1.71 – 1.59 (m, 1H), 1.54 – 1.44 (m, 1H), 1.33 – 1.23 (m, 4H), 0.88 (t, *J* = 7.0 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 175.18, 119.10, 51.81, 44.09, 31.75, 29.15, 27.50, 22.48, 15.38, 13.85.
GC-MS (EI, 70ev): m/z(%) =183(M+,1), 152(100), 113(14), 84(20), 73(10), 69(10), 57(25), 55(62), 53(11), 43(85), 42(17), 41(67), 29(58).
HRMS(ESI): calcd. for [$C_{10}H_{17}NO_2$+H]$^+$: 184.13321, found: 184.1327. calcd. for [$C_{10}H_{17}NO_2$+Na]$^+$: 206.11515, found: 206.11497.

Hexyl 2-(2-cyanoethyl)hexanoate



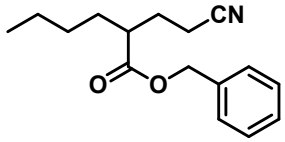
^{1}H NMR (300 MHz, Chloroform-*d*) δ 4.08 (td, *J* = 6.7, 2.2 Hz, 2H), 2.56 – 2.40 (m, 1H), 2.39 – 2.23 (m, 2H), 1.96 (dddd, *J* = 13.6, 9.5, 7.4, 6.2 Hz, 1H), 1.78 (dtd, *J* = 13.7, 7.9, 4.7 Hz, 1H), 1.69 – 1.15 (m, 14H), 0.98 – 0.76 (m, 6H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.74, 119.10, 64.81, 44.21, 31.76, 31.36, 29.13, 28.55, 27.56, 25.56, 22.51, 22.47, 15.34, 13.95, 13.82.
GC-MS (EI, 70ev): m/z(%) =253(M+,1), 152(56), 134(36), 113(11), 85(23), 84(20), 83(15), 73(10), 69(10), 56(31), 55(62), 53(11), 43(100), 42(22), 41(82), 29(69).
HRMS(ESI): calcd. for [$C_{15}H_{27}NO_2$+Na]$^+$: 276.1934, found: 276.19322.

Octyl 2-(2-cyanoethyl)hexanoate



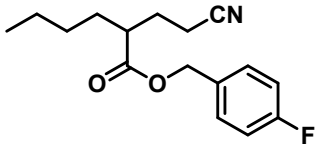
^{1}H NMR (300 MHz, Chloroform-*d*) δ 4.09 (td, *J* = 6.7, 2.4 Hz, 2H), 2.55 – 2.43 (m, 1H), 2.42 – 2.26 (m, 2H), 1.99 (dddd, *J* = 13.7, 9.6, 7.4, 6.2 Hz, 1H), 1.89 – 1.74 (m, 1H), 1.71 – 1.17 (m, 18H), 0.88 (td, *J* = 7.0, 3.3 Hz, 6H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.79, 119.14, 64.86, 44.22, 31.78, 31.76, 29.70, 29.16, 29.14, 28.60, 27.55, 25.91, 22.63, 22.49, 15.37, 14.08, 13.86.
GC-MS (EI, 70ev): m/z(%) = 281(M+,1), 252(5), 238(7), 224(10), 210(4), 166(20), 152(100), 96(16), 84(34), 57(20), 56(31), 55(54), 41(80), 29(40).

Benzyl 2-(2-cyanoethyl)hexanoate



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.33 – 7.22 (m, 5H), 5.08 (d, *J* = 0.7 Hz, 2H), 2.48 (dddd, *J* = 9.5, 8.0, 5.8, 4.7 Hz, 1H), 2.37 – 2.11 (m, 2H), 1.92 (dddd, *J* = 13.7, 9.6, 7.4, 6.2 Hz, 1H), 1.74 (dtd, *J* = 13.8, 7.9, 4.7 Hz, 1H), 1.65 – 1.52 (m, 1H), 1.51 – 1.39 (m, 1H), 1.24 – 1.14 (m, 4H), 0.79 (t, *J* = 7.0 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.52, 135.75, 128.62, 128.41, 128.32, 119.07, 66.52, 44.18, 31.72, 29.08, 27.57, 22.46, 15.30, 13.83.
GC-MS (EI, 70ev): m/z(%) = 259(M+,5), 231(5), 124(10), 108(28), 107(10), 92(10), 91(100), 65(13), 55(10), 41(16), 29(7).
HRMS(ESI): calcd. for [$C_{16}H_{21}NO_2$+Na]$^+$: 282.14645, found: 282.14659.

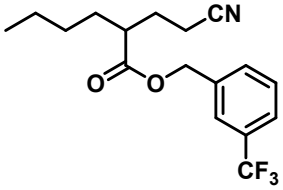
4-Fluorobenzyl 2-(2-cyanoethyl)hexanoate



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.43 – 7.29 (m, 2H), 7.13 – 6.94 (m, 2H), 5.27 – 5.02 (m, 2H), 2.54 (dddd, *J* = 9.5, 8.0, 5.7, 4.7 Hz, 1H), 2.43 – 2.18 (m, 2H), 1.98 (dddd, *J* = 13.6, 9.5, 7.2, 6.2 Hz, 1H), 1.81 (dtd, *J* = 13.8, 7.8, 4.8 Hz, 1H), 1.72 – 1.57 (m, 1H), 1.56 – 1.42 (m, 1H), 1.34 – 1.17 (m, 4H), 0.85 (t, *J* = 7.0 Hz, 3H).
^{13}C NMR (75 MHz, Chloroform-*d*) δ 174.49 , 162.72 (d, *J* = 247.3 Hz), 131.61 (d, *J* = 3.3 Hz), 130.39 (d, *J* = 8.3 Hz), 115.56 (d, *J* = 21.6 Hz), 65.78 , 44.12 , 31.71 , 29.05 , 27.50, 22.44 , 15.31, 13.81.

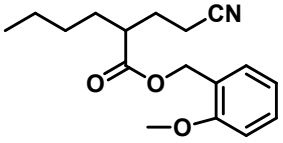
GC-MS (EI, 70ev): m/z(%) = 277(M+,1), 152(5), 109(100), 107(5), 41(13).
HRMS(ESI): calcd. for $[C_{16}H_{20}FNO_2+Na]^+$: 300.13703, found: 300.13645.

3-(Trifluoromethyl)benzyl 2-(2-cyanoethyl)hexanoate



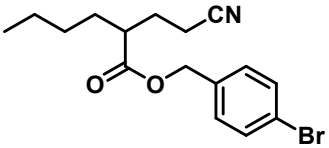
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.67 – 7.44 (m, 4H), 5.28 – 5.10 (m, 5H), 2.59 (dddd, *J* = 9.4, 8.1, 5.7, 4.8 Hz, 1H), 2.47 – 2.22 (m, 2H), 2.01 (dddd, *J* = 13.6, 9.4, 7.1, 6.3 Hz, 1H), 1.83 (dtd, *J* = 13.9, 7.8, 4.8 Hz, 1H), 1.70 – 1.45 (m, 2H), 1.36 – 1.19 (m, 4H), 0.85 (t, *J* = 7.0 Hz, 3H).
^{13}C NMR (75 MHz, Chloroform-*d*) δ 174.39 , 136.77 , 131.47 (d, *J* = 1.6 Hz), 129.17 , 125.02 (dd, *J* = 24.1, 3.8 Hz), 118.95 , 65.57 , 44.09 , 31.74 , 29.06 , 27.45 , 22.43 , 15.32 , 13.75 .
GC-MS (EI, 70ev): m/z(%) = 327(M+,1), 159(100), 152(30), 124(31), 109(20), 82(8), 55(19), 41(27), 39(11), 29(16).
HRMS(ESI): calcd. for $[C_{17}H_{20}F_3NO_2+Na]^+$: 350.13383, found: 350.13328.

2-Methoxybenzyl 2-(2-cyanoethyl)hexanoate



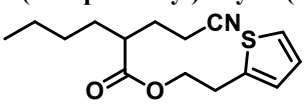
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.33 (td, *J* = 7.5, 1.6 Hz, 2H), 7.02 – 6.84 (m, 2H), 5.18 (s, 2H), 3.85 (s, 3H), 2.64 – 2.47 (m, 1H), 2.45 – 2.20 (m, 2H), 1.99 (dddd, *J* = 13.8, 9.6, 7.7, 6.0 Hz, 1H), 1.89 – 1.76 (m, 1H), 1.74 – 1.61 (m, 1H), 1.56 – 1.43 (m, 1H), 1.35 – 1.23 (m, 4H), 0.92 – 0.82 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.59, 157.67, 130.13, 129.92, 123.91, 120.42, 119.21, 110.47, 62.28, 55.37, 44.31, 31.75, 29.10, 27.75, 22.50, 15.20, 13.85.
GC-MS (EI, 70ev): m/z(%) = 289(M+,7), 138(11), 137(100), 122(11), 121(78), 93(11), 92(11), 91(80),78(15), 65(14),55(14), 41(22), 29(10).
HRMS(ESI): calcd. for $[C_{17}H_{23}NO_3+Na]^+$: 312.15701, found: 312.15707.

4-Bromobenzyl 2-(2-cyanoethyl)hexanoate



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.50 – 7.34 (m, 2H), 7.18 – 7.13 (m, 2H), 5.02 (d, *J* = 1.7 Hz, 2H), 2.49 (dddd, *J* = 9.5, 8.0, 5.8, 4.8 Hz, 1H), 2.38 – 2.16 (m, 2H), 1.92 (dddd, *J* = 13.6, 9.5, 7.2, 6.2 Hz, 1H), 1.82 – 1.69 (m, 1H), 1.66 – 1.53 (m, 1H), 1.49 – 1.36 (m, 1H), 1.18 (ddddd, *J* = 14.6, 10.6, 8.5, 6.7, 2.7 Hz, 4H), 0.79 (t, *J* = 7.0 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.43, 134.72, 131.80, 130.02, 122.50, 118.99, 65.72, 44.09, 31.71, 29.06, 27.46, 22.45, 15.34, 13.82.
GC-MS (EI, 70ev): m/z(%) = 337(M+,5), 311(11), 185(17), 171(100), 170(12), 169(98), 152(15), 124(23), 91(10), 90(55), 89(51), 82(11), 63(19), 55(33), 43(16), 41(47), 39(19), 29(26), 55(10), 41(16), 29(7).
HRMS(ESI): calcd. for $[C_{16}H_{20}BrNO_2+Na]^+$: 360.05696, found: 360.05631, calcd. for $[C_{16}H_{20}BrNO_2+Na]^+$: 362.05507, found: 362.05431.

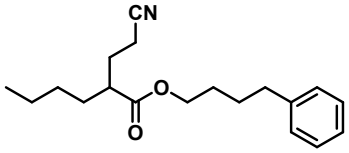
2-(Thiophen-2-yl)ethyl 2-(2-cyanoethyl)hexanoate



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.21 (ddd, *J* = 4.9, 3.0, 0.4 Hz, 1H), 6.97 (ddt, *J* = 3.0, 1.4, 0.9 Hz, 1H), 6.91 (ddt, *J* = 4.9, 1.4, 0.4 Hz, 1H), 4.28 (td, *J* = 6.7, 1.4 Hz, 2H), 3.02 – 2.86 (m, 2H), 2.41 (dddd, *J* = 9.6, 8.1, 5.8, 4.6 Hz, 1H), 2.29 – 2.06 (m, 2H), 1.85 (dddd, *J* = 13.6, 9.6, 7.4, 6.0 Hz, 1H), 1.77 – 1.66 (m, 1H), 1.60 – 1.50 (m, 1H), 1.44 – 1.33 (m, 1H), 1.28 – 1.07 (m, 4H), 0.80 (t, *J* = 7.0 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.59, 137.82, 128.07, 125.82, 121.70, 119.13, 64.36, 44.22, 31.74, 29.59, 29.10, 27.55, 22.49, 15.22, 13.85.

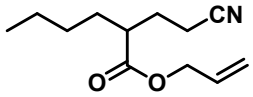
HRMS(ESI): calcd. for [$C_{15}H_{21}NO_2S$+Na]$^+$:302.11852, found: 302.11807.

4-Phenylbutyl 2-(2-cyanoethyl)hexanoate



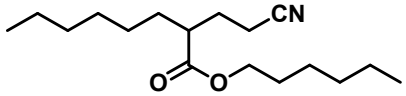
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.24 – 7.17 (m, 2H), 7.15 – 7.05 (m, 3H), 4.04 (tdd, *J* = 6.2, 3.0, 1.8 Hz, 2H), 2.57 (ddt, *J* = 6.5, 4.0, 2.3 Hz, 2H), 2.49 – 2.35 (m, 1H), 2.34 (s, 3H), 1.90 (dddd, *J* = 13.6, 9.5, 7.3, 6.2 Hz, 1H), 1.79 – 1.66 (m, 1H), 1.65 – 1.50 (m, 5H), 1.47 – 1.33 (m, 1H), 1.31 – 1.09 (m, 4H), 0.81 (t, *J* = 6.9 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.75, 141.90, 128.38, 125.90, 119.12, 64.56, 44.21, 35.41, 31.76, 29.16, 28.22, 27.74, 27.54, 22.50, 15.36, 13.87.
GC-MS (EI, 70ev): m/z(%) = 301(M+,1), 152(7), 132(10), 117(15), 107(100), 91(80), 79(10), 65(12), 55(18).
HRMS(ESI): calcd. for [$C_{19}H_{27}NO_2$+Na]$^+$:324.1934, found: 324.19277.

Allyl 2-(2-cyanoethyl)hexanoate



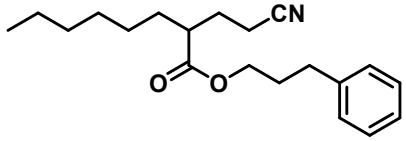
^{1}H NMR (300 MHz, Chloroform-*d*) δ 5.91 (ddt, *J* = 17.2, 10.4, 5.8 Hz, 1H), 5.38 – 5.20 (m, 2H), 4.60 (dt, *J* = 5.8, 1.4 Hz, 2H), 2.53 (dddd, *J* = 9.5, 8.0, 5.9, 4.7 Hz, 1H), 2.43 – 2.26 (m, 2H), 1.99 (dddd, *J* = 13.7, 9.5, 7.4, 6.2 Hz, 1H), 1.82 (dtd, *J* = 13.8, 7.9, 4.7 Hz, 1H), 1.71 – 1.59 (m, 1H), 1.57 – 1.46 (m, 1H), 1.35 – 1.22 (m, 4H), 0.88 (t, *J* = 6.9 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.36, 131.88, 119.10, 118.71, 65.31, 44.14, 31.71, 29.10, 27.51, 22.47, 15.35.
GC-MS (EI, 70ev): m/z(%) = 209(M+,1), 166(5), 124(100), 107(20), 94(10), 81(60), 55(42), 41(60).

Hexyl 2-(2-cyanoethyl)octanoate



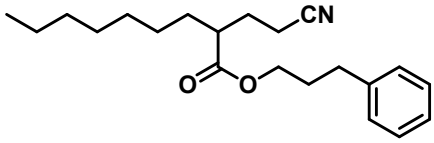
^{1}H NMR (300 MHz, Chloroform-*d*) δ 4.10 (td, *J* = 6.7, 2.5 Hz, 2H), 2.56 – 2.43 (m, 1H), 2.42 – 2.26 (m, 2H), 1.99 (dddd, *J* = 13.7, 9.5, 7.4, 6.2 Hz, 1H), 1.80 (dtd, *J* = 13.9, 7.9, 4.7 Hz, 1H), 1.70 – 1.20 (m, 18H), 0.96 – 0.81 (m, 6H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.80, 119.14, 64.87, 44.27, 32.11, 31.60, 31.39, 29.07, 28.59, 27.58, 26.96, 25.60, 22.55, 22.53, 15.38, 14.03, 13.98.
GC-MS (EI, 70ev): m/z(%) = 281(M+,1), 180(60), 153(5), 152(53), 138(6), 96(16), 94(15), 85(26), 84(34), 73(13), 69(30), 57(20), 56(31), 55(54), 43(100), 41(80), 29(40).
HRMS(ESI): calcd. for [$C_{17}H_{31}NO_2$+Na]$^+$:304.2247, found: 304.22531.

3-Phenylpropyl 2-(2-cyanoethyl)octanoate



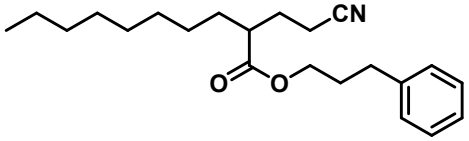
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.26 – 7.17 (m, 2H), 7.16 – 7.06 (m, 3H), 4.05 (td, *J* = 6.5, 1.5 Hz, 2H), 2.62 (dd, *J* = 8.6, 6.7 Hz, 2H), 2.51 – 2.37 (m, 1H), 2.34 – 2.19 (m, 2H), 2.00 – 1.83 (m, 3H), 1.73 (dtd, *J* = 13.8, 7.9, 4.8 Hz, 1H), 1.63 – 1.52 (m, 1H), 1.48 – 1.35 (m, 1H), 1.21 (dd, *J* = 7.7, 3.2 Hz, 8H), 0.90 – 0.76 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.72, 140.98, 128.49, 128.38, 126.11, 119.12, 64.06, 44.23, 32.20, 32.10, 31.62, 30.21, 29.10, 27.53, 27.01, 22.57, 15.39, 14.06.
GC-MS (EI, 70ev): m/z(%) =315(M+,1), 119(12), 118(100), 117(56), 91(58), 78(5), 65(7), 55(11), 41(18), 29(9).
HRMS(ESI): calcd. for [$C_{20}H_{29}NO_2$+Na]$^+$:338.20905, found: 338.20874.

3-Phenylpropyl 2-(2-cyanoethyl)nonanoate



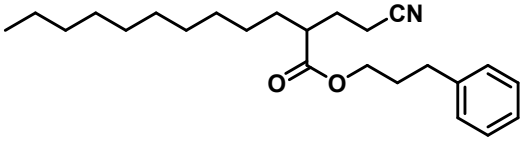
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.30 – 7.02 (m, 5H), 4.05 (td, *J* = 6.6, 1.6 Hz, 2H), 2.62 (dd, *J* = 8.6, 6.7 Hz, 2H), 2.45 (dddd, *J* = 9.5, 8.1, 5.7, 4.7 Hz, 1H), 2.34 – 2.19 (m, 2H), 1.97 – 1.85 (m, 3H), 1.73 (dtd, *J* = 13.8, 7.9, 4.8 Hz, 1H), 1.57 (ddd, *J* = 13.7, 7.8, 5.8 Hz, 1H), 1.47 – 1.34 (m, 1H), 1.20 (ddd, *J* = 7.2, 4.1, 2.2 Hz, 10H), 0.87 – 0.69 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.72, 140.97, 128.49, 128.38, 126.11, 119.11, 64.06, 44.23, 32.20, 32.10, 31.76, 30.21, 29.40, 29.09, 27.52, 27.05, 22.62, 15.39, 14.08.
GC-MS (EI, 70ev): m/z(%) = 329(M+,1), 119(11), 118(100), 117(43), 91(48), 78(10), 65(6), 43(13), 41(20), 29(7).
HRMS(EI): calcd. for $[C_{21}H_{31}NO_2]^+$: 329.23493, found: 329.23511.

3-Phenylpropyl 2-(2-cyanoethyl)decanoate



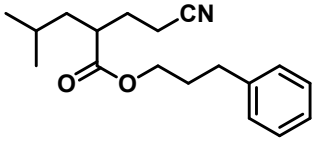
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.28 – 7.07 (m, 5H), 4.06 (td, *J* = 6.6, 1.7 Hz, 2H), 2.63 (dd, *J* = 8.6, 6.8 Hz, 2H), 2.51 – 2.39 (m, 1H), 2.36 – 2.19 (m, 2H), 1.91 (dqd, *J* = 13.0, 6.8, 4.0 Hz, 3H), 1.74 (dtd, *J* = 13.7, 7.8, 4.7 Hz, 1H), 1.57 (p, *J* = 7.2 Hz, 1H), 1.49 – 1.35 (m, 1H), 1.20 (dt, *J* = 6.3, 3.7 Hz, 12H), 0.87 – 0.75 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.73, 140.97, 128.49, 128.38, 126.11, 119.11, 64.07, 44.23, 32.20, 32.11, 31.83, 30.21, 29.44, 29.39, 29.21, 27.52, 27.04, 22.65, 15.40, 14.10.
GC-MS (EI, 70ev): m/z(%) = 343(M+,1), 118(100), 117(35), 103(5), 92(7), 91(49), 43(15), 41(22), 39(6), 29(8).
HRMS(ESI): calcd. for $[C_{22}H_{33}NO_2+Na]^+$:366.24035, found: 366.2402.

3-Phenylpropyl 2-(2-cyanoethyl)dodecanoate



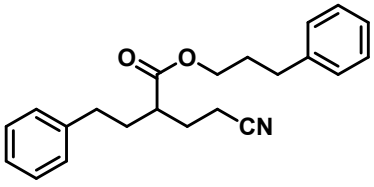
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.29 – 7.03 (m, 5H), 4.05 (td, *J* = 6.5, 1.6 Hz, 2H), 2.63 (dd, *J* = 8.6, 6.8 Hz, 2H), 2.45 (dddd, *J* = 9.6, 8.1, 5.7, 4.7 Hz, 1H), 2.36 – 2.17 (m, 2H), 1.99 – 1.84 (m, 3H), 1.73 (dtd, *J* = 13.9, 7.9, 4.7 Hz, 1H), 1.64 – 1.50 (m, 1H), 1.49 – 1.35 (m, 1H), 1.20 (d, *J* = 10.8 Hz, 16H), 0.87 – 0.70 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.73, 140.97, 128.49, 128.38, 126.11, 119.11, 64.07, 44.23, 32.20, 32.11, 31.90, 30.21, 29.59, 29.56, 29.44, 29.32, 27.52, 27.05, 22.69, 15.39, 14.12.
GC-MS (EI, 70ev): m/z(%) = 371(M+,1), 159(3), 119(14), 118(100), 117(39), 91(45), 79(4), 65(5), 57(6), 43(19), 41(16), 29(7).
HRMS(EI): calcd. for $[C_{24}H_{37}NO_2]^+$: 371.28188, found: 371.28140.

3-Phenylpropyl 2-(2-cyanoethyl)-4-methylpentanoate



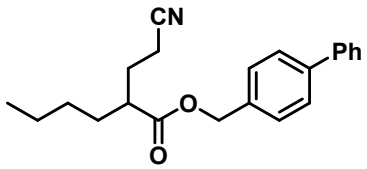
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.32 – 6.97 (m, 5H), 4.05 (td, *J* = 6.6, 1.2 Hz, 2H), 2.62 (dd, *J* = 8.6, 6.8 Hz, 2H), 2.58 – 2.46 (m, 1H), 2.37 – 2.15 (m, 2H), 1.99 – 1.80 (m, 3H), 1.78 – 1.66 (m, 1H), 1.61 – 1.44 (m, 2H), 1.26 – 1.14 (m, 1H), 0.85 (dd, *J* = 8.4, 6.3 Hz, 6H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.95, 140.98, 128.51, 128.43, 128.39, 126.12, 119.06, 64.10, 42.46, 41.31, 32.21, 30.22, 28.07, 26.06, 22.83, 22.10, 15.34.
GC-MS (EI, 70ev): m/z(%) = 310(M+,1), 119(13), 119(12), 118(100), 117(54), 91(60), 55(10), 43(22), 41(25), 39(8).
HRMS(ESI): calcd. for $[C_{18}H_{25}NO_2+Na]^+$:310.17775, found: 310.17803.

3-Phenylpropyl 2-(2-cyanoethyl)-4-methylpentanoate



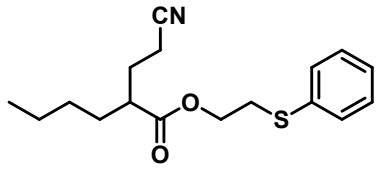
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.24 – 7.16 (m, 4H), 7.14 – 7.06 (m, 6H), 4.05 (t, *J* = 6.6 Hz, 2H), 2.62 (dd, *J* = 8.6, 6.8 Hz, 2H), 2.59 – 2.40 (m, 3H), 2.31 – 2.21 (m, 2H), 1.99 – 1.85 (m, 4H), 1.81 – 1.66 (m, 2H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.37, 140.95, 140.92, 128.64, 128.57, 128.56, 128.53, 128.42, 128.40, 126.27, 126.17, 119.04, 64.29, 43.84, 33.77, 33.36, 32.26, 30.23, 27.66, 15.34.
GC-MS (EI, 70ev): m/z(%) = 335(M+,1), 129(3), 119(12), 118(64), 117(29), 104(10), 103(5), 92(8), 91(100), 77(8), 65(15), 41(5).
HRMS(ESI): calcd. for $[C_{22}H_{25}NO_2+Na]^+$:358.17775, found: 358.17762.

[1,1'-Biphenyl]-4-ylmethyl 2-(2-cyanoethyl)hexanoate



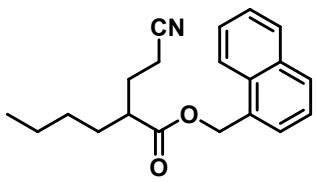
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.61 – 7.19 (m, 9H), 5.10 (d, *J* = 1.3 Hz, 2H), 2.48 (dddd, *J* = 9.5, 8.1, 5.7, 4.7 Hz, 1H), 2.34 – 2.11 (m, 2H), 1.99 – 1.83 (m, 1H), 1.73 (dtd, *J* = 13.8, 7.8, 4.8 Hz, 1H), 1.65 – 1.51 (m, 1H), 1.49 – 1.34 (m, 1H), 1.24 – 1.10 (m, 4H), 0.77 (t, *J* = 6.9 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.57, 141.38, 140.57, 134.76, 128.85, 128.83, 127.53, 127.37, 127.13, 119.12, 66.28, 44.22, 31.75, 29.11, 27.58, 22.50, 15.34, 13.88.
GC-MS (EI, 70ev): m/z(%) = 335(M+,10), 184(10), 167(100), 165(30), 152(15), 124(6), 77(5), 55(9).
HRMS(ESI): calcd. for $[C_{22}H_{25}NO_2+Na]^+$:358.17775, found: 358.17701.

2-(Phenylthio)ethyl 2-(2-cyanoethyl)hexanoate



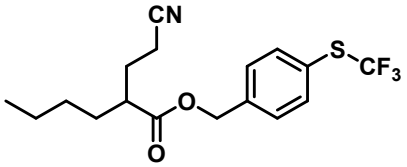
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.34 – 7.28 (m, 2H), 7.27 – 7.20 (m, 2H), 7.18 – 7.11 (m, 1H), 4.20 (t, *J* = 6.7 Hz, 2H), 3.08 (t, *J* = 6.7 Hz, 2H), 2.50 – 2.34 (m, 1H), 2.32 – 2.17 (m, 2H), 1.88 (dddd, *J* = 13.7, 9.4, 7.3, 6.3 Hz, 1H), 1.72 (dtd, *J* = 13.9, 7.9, 4.7 Hz, 1H), 1.61 – 1.48 (m, 1H), 1.46 – 1.34 (m, 1H), 1.31 – 1.10 (m, 4H), 0.90 – 0.74 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.45, 134.97, 129.98, 129.12, 126.72, 119.11, 62.95, 44.15, 32.56, 31.65, 29.12, 27.44, 22.48, 15.37, 13.88.
GC-MS (EI, 70ev): m/z(%) = 305(M+,5), 253(5), 207(7), 152(10), 136(100), 109(20), 91(10), 65(8), 55(9).
HRMS(ESI): calcd. for $[C_{17}H_{23}NO_2+H]^+$:306.15223, found: 306.15276.calcd. for$[C_{17}H_{23}NO_2+Na]^+$:328.13417, found: 328.13381.

Naphthalen-1-ylmethyl 2-(2-cyanoethyl)hexanoate



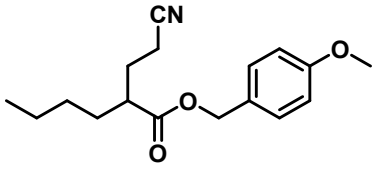
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.06 – 7.97 (m, 1H), 7.93 – 7.83 (m, 2H), 7.63 – 7.41 (m, 4H), 5.70 – 5.53 (m, 2H), 2.55 (dddd, *J* = 9.5, 8.1, 5.7, 4.7 Hz, 1H), 2.38 – 2.15 (m, 2H), 1.98 (dddd, *J* = 13.8, 9.5, 7.3, 6.4 Hz, 1H), 1.78 (dtd, *J* = 13.8, 7.8, 4.7 Hz, 1H), 1.70 – 1.55 (m, 1H), 1.54 – 1.40 (m, 1H), 1.28 – 1.14 (m, 4H), 0.88 – 0.72 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.55, 133.77, 131.58, 131.21, 129.50, 128.81, 127.86, 126.63, 126.04, 125.26, 123.44, 119.06, 64.89, 44.30, 31.74, 29.05, 27.53, 22.44, 15.28, 13.77.
GC-MS (EI, 70ev): m/z(%) = 309(M+,15), 158(20), 141(100), 140(10), 139(12), 115(20), 102(5), 82(8), 55(10).
HRMS(ESI): calcd. for $[C_{20}H_{23}NO_2+Na]^+$:332.1621, found: 332.16163.

4-((Trifluoromethyl)thio)benzyl 2-(2-cyanoethyl)hexanoate



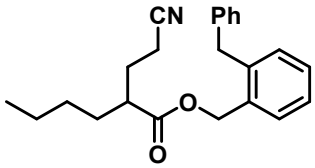
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.74 – 7.53 (m, 2H), 7.47 – 7.34 (m, 2H), 5.17 (d, *J* = 2.4 Hz, 2H), 2.59 (dddd, *J* = 9.4, 8.0, 5.8, 4.8 Hz, 1H), 2.46 – 2.22 (m, 2H), 2.01 (dddd, *J* = 13.6, 9.4, 7.2, 6.4 Hz, 1H), 1.83 (dtd, *J* = 13.9, 7.8, 4.8 Hz, 1H), 1.73 – 1.44 (m, 2H), 1.37 – 1.16 (m, 4H), 0.85 (t, *J* = 7.0 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.39, 138.77, 136.49, 129.02, 118.94, 65.51, 44.08, 31.71, 29.06, 27.43, 22.43, 15.33, 13.78.
GC-MS (EI, 70ev): m/z(%) = 359(M+,10), 331(5), 207(10), 193(8), 192(100), 171(4), 152(20), 124(25), 122(50), 107(10), 82(15), 78(13), 69(10), 55(20).
HRMS(ESI): calcd. for [$C_{17}H_{20}F_3NO_2S$+Na]$^+$:382.10591, found: 382.10582.

4-Methoxybenzyl 2-(2-cyanoethyl)hexanoate



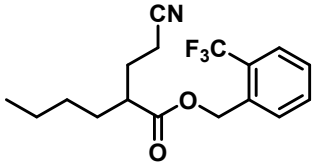
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.29 – 7.14 (m, 2H), 6.87 – 6.72 (m, 2H), 5.00 (s, 2H), 3.73 (s, 3H), 2.50 – 2.36 (m, 1H), 2.33 – 2.10 (m, 2H), 1.89 (dddd, *J* = 13.7, 9.5, 7.4, 6.2 Hz, 1H), 1.72 (dtd, *J* = 13.8, 7.9, 4.7 Hz, 1H), 1.64 – 1.49 (m, 1H), 1.48 – 1.34 (m, 1H), 1.25 – 1.08 (m, 4H), 0.78 (t, *J* = 6.9 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.56, 159.73, 130.16, 127.91, 119.11, 113.98, 66.30, 55.28, 44.20, 31.70, 29.06, 27.59, 22.46, 15.26, 13.82.
GC-MS (EI, 70ev): m/z(%) = 289(M+,10), 138(5), 137(7), 122(10), 121(100), 109(5), 105(4), 91(15), 78(20), 65(10), 55(15).
HRMS(ESI): calcd. for [$C_{17}H_{23}NO_3$+Na]$^+$:312.15701, found: 312.15751.

2-Benzylbenzyl 2-(2-cyanoethyl)hexanoate



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.32 – 7.27 (m, 1H), 7.26 – 7.14 (m, 4H), 7.14 – 7.07 (m, 2H), 7.02 (dddd, *J* = 6.6, 2.1, 1.4, 0.7 Hz, 2H), 5.04 (s, 2H), 4.00 (s, 2H), 2.43 – 2.30 (m, 1H), 2.24 – 2.04 (m, 2H), 1.82 (dddd, *J* = 13.8, 9.3, 7.5, 6.2 Hz, 1H), 1.66 (dtd, *J* = 13.9, 7.9, 4.8 Hz, 1H), 1.57 – 1.45 (m, 1H), 1.43 – 1.33 (m, 1H), 1.23 – 1.09 (m, 4H), 0.77 (t, *J* = 7.0 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.47, 140.20, 139.44, 133.89, 130.79, 130.03, 128.91, 128.68, 128.64, 128.55, 126.80, 126.23, 119.10, 64.57, 44.16, 38.52, 31.64, 29.10, 27.45, 22.50, 15.25, 13.87.
HRMS(ESI): calcd. for[$C_{17}H_{23}NO_2$+Na]$^+$:372.2042, found: 372.259.

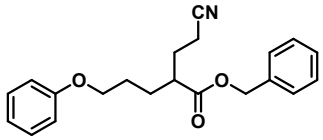
2-(Trifluoromethyl)benzyl 2-(2-cyanoethyl)hexanoate



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.69 (ddt, *J* = 7.7, 1.3, 0.7 Hz, 1H), 7.62 – 7.51 (m, 2H), 7.49 – 7.41 (m, 1H), 5.35 – 5.22 (m, 2H), 2.58 (dddd, *J* = 9.4, 8.0, 5.8, 4.7 Hz, 1H), 2.47 – 2.23 (m, 2H), 2.07 – 1.93 (m, 1H), 1.83 (dtd, *J* = 13.9, 7.8, 4.7 Hz, 1H), 1.73 – 1.60 (m, 1H), 1.58 – 1.43 (m, 1H), 1.35 – 1.20 (m, 4H), 0.86 (t, *J* = 6.9 Hz, 3H).

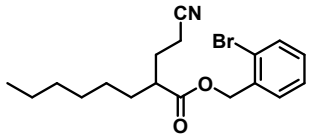
^{13}C NMR (75 MHz, Chloroform-*d*) δ 174.22 , 133.77 (d, *J* = 1.8 Hz), 132.13 (d, *J* = 1.2 Hz), 130.52 , 128.56 , 126.68 – 125.67 (m), 122.30 , 119.02 , 63.06, 44.15 , 31.62 , 29.02 , 27.42 , 22.43 , 15.28 , 13.77 .
GC-MS (EI, 70ev): m/z(%) = 327(M+,1), 307(8), 240(5), 199(8), 176(6), 159(100), 152(30), 140(10), 124(20), 119(10), 110(5), 109(20), 107(5), 98(5), 83(10), 82(12), 55(28).
HRMS(ESI): calcd. for[$C_{17}H_{20}F_3NO_2$+Na]$^+$:350.13383, found: 350.1335.

Benzyl 2-(2-cyanoethyl)-5-phenoxypentanoate



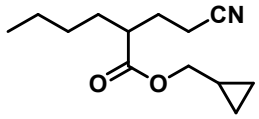
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.34 – 7.09 (m, 7H), 6.91 – 6.83 (m, 1H), 6.82 – 6.74 (m, 2H), 5.08 (s, 2H), 3.91 – 3.81 (m, 2H), 2.62 – 2.52 (m, 1H), 2.36 – 2.15 (m, 2H), 1.96 (dddd, *J* = 13.7, 9.4, 7.3, 6.3 Hz, 1H), 1.87 – 1.64 (m, 5H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.15, 158.79, 135.62, 129.47, 128.67, 128.48, 128.35, 120.77, 118.97, 114.47, 67.03, 66.71, 43.92, 28.63, 27.66, 26.76, 15.27.
GC-MS (EI, 70ev): m/z(%) = 337(M+,5), 224(20), 184(5), 152(8), 99(20), 91(100), 78(10), 65(15), 41(5).

2-Bromobenzyl 2-(2-cyanoethyl)octanoate



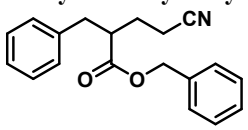
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.58 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.41 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.32 (td, *J* = 7.5, 1.3 Hz, 1H), 7.20 (ddd, *J* = 7.9, 7.4, 1.8 Hz, 1H), 5.21 (s, 2H), 2.58 (dddd, *J* = 9.5, 8.0, 5.7, 4.7 Hz, 1H), 2.46 – 2.23 (m, 2H), 2.01 (dddd, *J* = 13.7, 9.5, 7.4, 6.3 Hz, 1H), 1.82 (dtd, *J* = 13.9, 7.9, 4.7 Hz, 1H), 1.75 – 1.61 (m, 1H), 1.57 – 1.43 (m, 1H), 1.33 – 1.19 (m, 8H), 0.95 – 0.78 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.28, 134.97, 132.97, 130.45, 130.03, 127.58, 123.79, 119.08, 66.20, 44.23, 32.02, 31.57, 29.04, 27.53, 26.91, 22.52, 15.36, 14.04.

Cyclopropylmethyl 2-(2-cyanoethyl)hexanoate



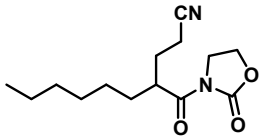
^{1}H NMR (300 MHz, Chloroform-*d*) δ 3.92 (dd, *J* = 7.4, 1.0 Hz, 2H), 2.57 – 2.42 (m, 1H), 2.41 – 2.24 (m, 2H), 1.97 (dddd, *J* = 13.7, 9.6, 7.4, 6.2 Hz, 1H), 1.80 (dtd, *J* = 13.8, 7.9, 4.7 Hz, 1H), 1.63 (dtd, *J* = 9.7, 7.9, 6.2 Hz, 1H), 1.56 – 1.42 (m, 1H), 1.28 (dddd, *J* = 7.1, 6.0, 4.5, 2.7 Hz, 4H), 1.17 – 1.02 (m, 1H), 0.92 – 0.78 (m, 3H), 0.64 – 0.46 (m, 2H), 0.32 – 0.17 (m, 2H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 174.79, 119.14, 69.38, 44.25, 31.76, 29.11, 27.62, 22.46, 15.31, 13.84, 9.88, 3.27.
GC-MS (EI, 70ev): m/z(%) = 223(M+,1), 194(5), 183(10), 167(8), 152(20), 141(10), 127(55), 124(80), 107(10), 95(10), 82(15), 55(100), 54(18), 41(20).

Benzyl 2-benzyl-4-cyanobutanoate



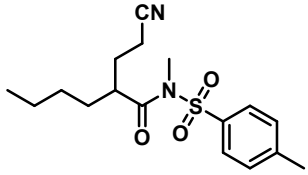
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.28 – 7.22 (m, 3H), 7.19 – 7.12 (m, 5H), 7.06 – 7.01 (m, 2H), 5.00 (s, 2H), 2.94 (dd, *J* = 12.6, 6.7 Hz, 1H), 2.84 – 2.65 (m, 2H), 2.33 – 2.11 (m, 2H), 1.99 – 1.84 (m, 1H), 1.74 (dtd, *J* = 13.9, 7.9, 4.2 Hz, 1H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 173.76, 137.80, 135.48, 128.89, 128.67, 128.63, 128.42, 128.35, 126.84, 118.92, 66.72, 46.05, 38.16, 27.12, 15.30.
GC-MS (EI, 70ev): m/z(%) = 293(M+,20), 248(15), 215(10), 202(21), 180(20), 158(15), 118(30), 107(35), 91(100), 77(11), 65(17).
HRMS(ESI): calcd. for [$C_{19}H_{19}NO_2$+Na]$^+$:316.1308, found: 316.1308.

4-(2-oxooxazolidine-3-carbonyl)decanenitrile



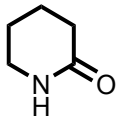
^{1}H NMR (300 MHz, Chloroform-*d*) δ 4.46 – 4.35 (m, 2H), 4.12 – 3.96 (m, 2H), 3.87 (dddd, *J* = 8.8, 7.1, 6.3, 4.5 Hz, 1H), 2.37 (ddd, *J* = 7.5, 7.0, 2.9 Hz, 2H), 2.13 – 2.01 (m, 1H), 1.86 (dddd, *J* = 13.9, 8.0, 6.8, 4.5 Hz, 1H), 1.77 – 1.62 (m, 1H), 1.50 – 1.39 (m, 1H), 1.25 (td, *J* = 5.8, 5.3, 3.4 Hz, 8H), 1.05 – 0.73 (m, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 175.21, 153.25, 119.20, 62.00, 42.75, 41.89, 32.22, 31.57, 29.17, 27.16, 26.83, 22.53, 15.18, 14.02.
GC-MS (EI, 70ev): m/z(%) = 266(M+,1), 226(26), 195(18), 182(15), 170(11), 153(26), 142(80), 140(18), 122(10), 108(20), 100(10), 88(100), 69(20), 55(24), 41(21).

2-(2-cyanoethyl)-N-methyl-N-tosylhexanamide



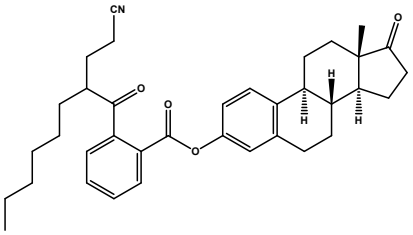
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.84 – 7.70 (m, 2H), 7.40 – 7.30 (m, 2H), 3.36 (s, 3H), 3.31 – 3.16 (m, 1H), 2.44 (dt, *J* = 0.4 Hz, 3H), 2.31 – 2.07 (m, 2H), 1.97 (dddd, *J* = 13.9, 8.4, 7.5, 6.4 Hz, 1H), 1.75 (dddd, *J* = 13.7, 8.0, 7.2, 5.1 Hz, 1H), 1.61 – 1.46 (m, 1H), 1.44 – 1.31 (m, 1H), 1.22 – 1.08 (m, 2H), 1.06 – 0.93 (m, 2H), 0.78 (t, *J* = 7.2 Hz, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 175.52, 145.19, 136.58, 129.97, 127.48, 119.16, 43.88, 33.34, 32.33, 28.90, 27.60, 22.60, 21.62, 14.89, 13.79.
GC-MS (EI, 70ev): m/z(%) = 336(M+,1), 240(5), 216(6), 186(10), 166(15), 165(100), 154(25), 124(20), 122(10), 107(10), 91(50), 82(10), 65(18), 41(10).

2-Piperidinone[3]



^{1}H NMR (300 MHz, Chloroform-*d*) δ 6.37 (s, 1H), 3.30 (dddd, *J* = 6.1, 4.2, 2.2, 0.9 Hz, 2H), 2.39 – 2.31 (m, 2H), 1.86 – 1.70 (m, 4H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 172.46, 42.36, 31.51, 22.28, 20.85.

(8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl 2-(2-(2-cyanoethyl)octanoyl)benzoate



^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.23 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.62 (td, *J* = 7.5, 1.4 Hz, 1H), 7.58 – 7.52 (m, 1H), 7.48 (td, *J* = 7.6, 1.5 Hz, 1H), 7.37 – 7.31 (m, 1H), 7.03 – 6.90 (m, 2H), 5.70 – 5.46 (m, 2H), 2.94 (dd, *J* = 8.3, 3.7 Hz, 2H), 2.65 – 2.22 (m, 6H), 2.20 – 1.92 (m, 5H), 1.81 (dtd, *J* = 13.8, 8.0, 4.6 Hz, 1H), 1.73 – 1.57 (m, 3H), 1.57 – 1.40 (m, 4H), 1.32 – 1.15 (m, 9H), 0.92 (s, 3H), 0.89 – 0.83 (m, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 220.65, 174.12, 165.07, 148.42, 138.06, 137.54, 133.01, 131.36, 129.00, 128.15, 127.99, 126.42, 121.53, 119.07, 118.70, 64.70, 50.30, 47.83, 44.13, 44.05, 37.88, 35.74, 31.93, 31.44, 29.33, 28.93, 27.41, 26.81, 26.22, 25.66, 22.41, 21.48, 15.13, 13.94, 13.72.
LC-MS: calcd. for $[C_{37}H_{45}NO_5+Na]^+$: 606, found $[C_{37}H_{45}NO_5+Na]^+$: 606
HR-MS(EI): calcd. for $[C_{37}H_{45}NO_5]^+$: 583.32922, found: 583.32893

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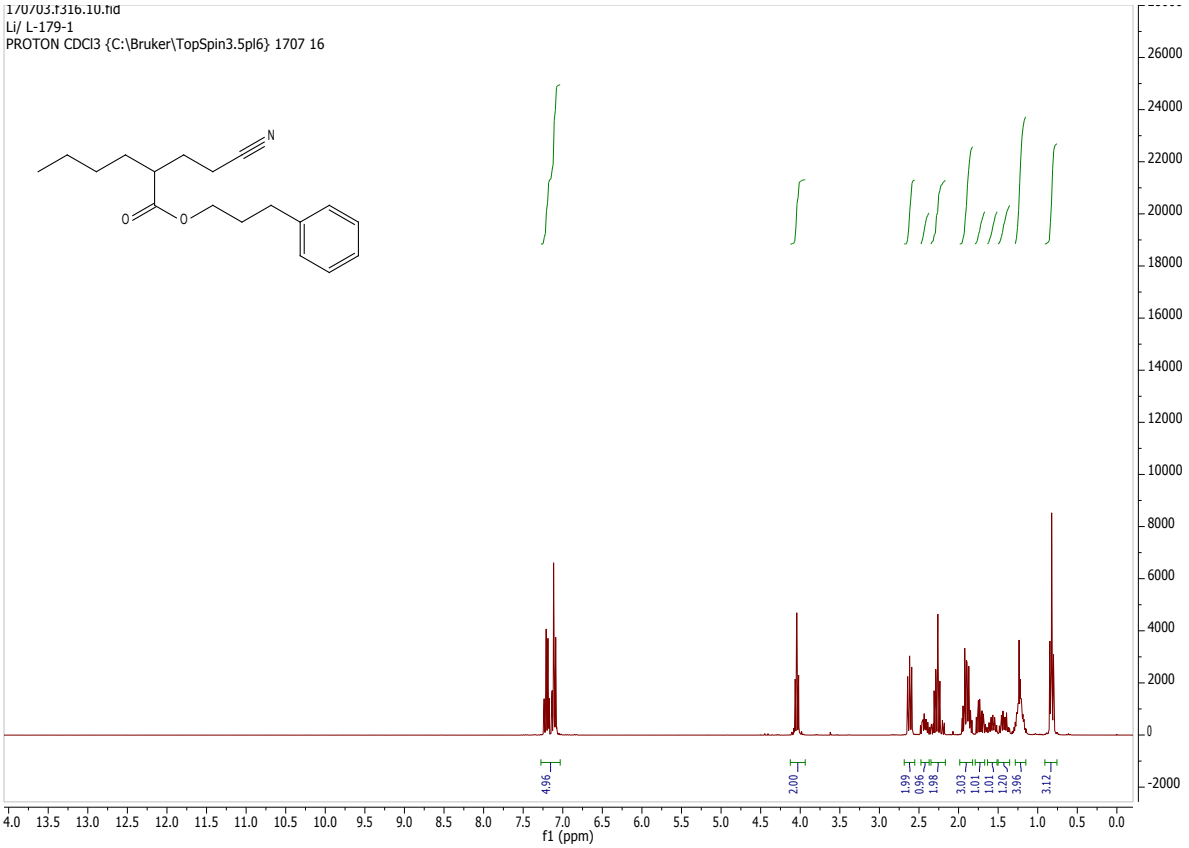
2. M. K. S. Vink, C. A. Schortinghuis, J. Luten, J. H. van Maarseveen, H. E. Schoemaker, H. Hiemstra, F.P. J. T. Rutjes, *J. Org. Chem.* **2002**, *67*, 7869-7871
3. X. Jin, K. Kataoka, T. Yatabe, K. Yamaguchi, N. Mizuno, *Angew.Chem. Int. Ed.* **2016**, *55*,7212 –7217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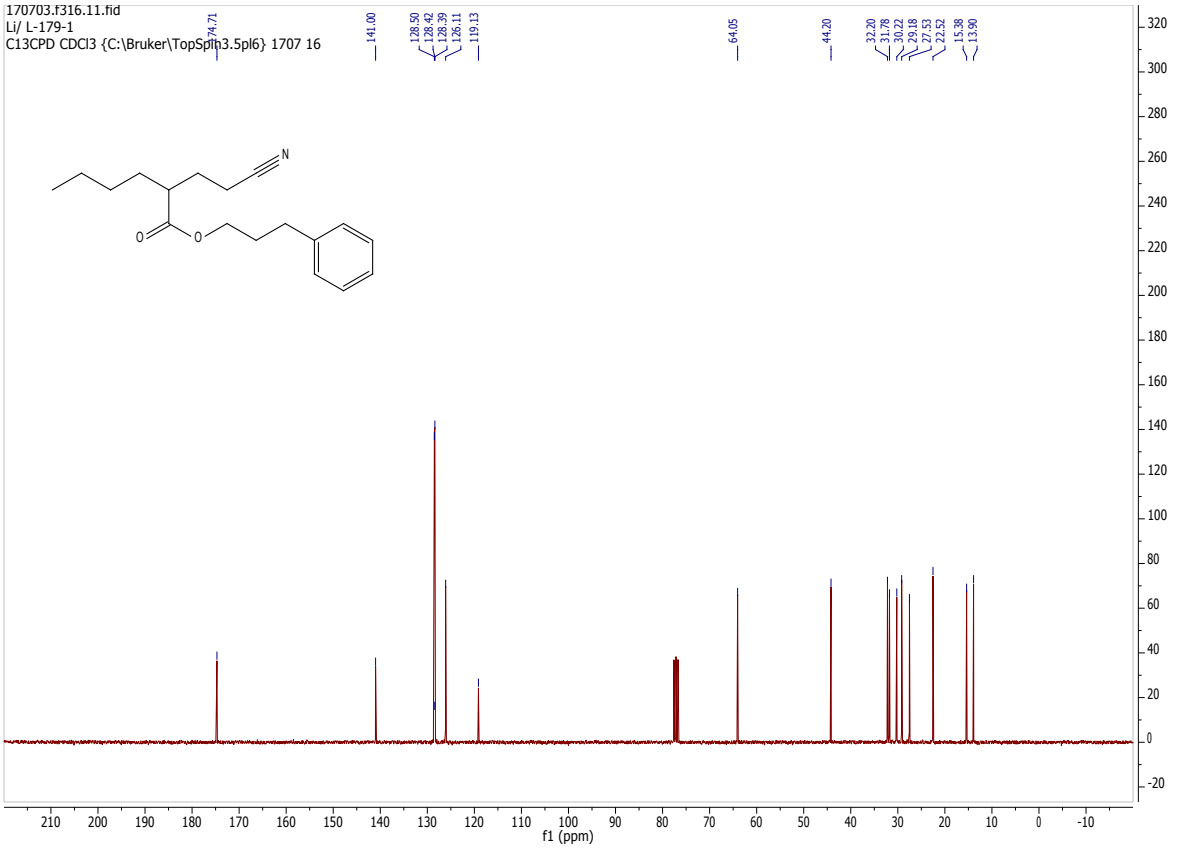
0.96
1.98
3.03
1.01
1.01
1.20
3.96
3.12
f1 (ppm)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O
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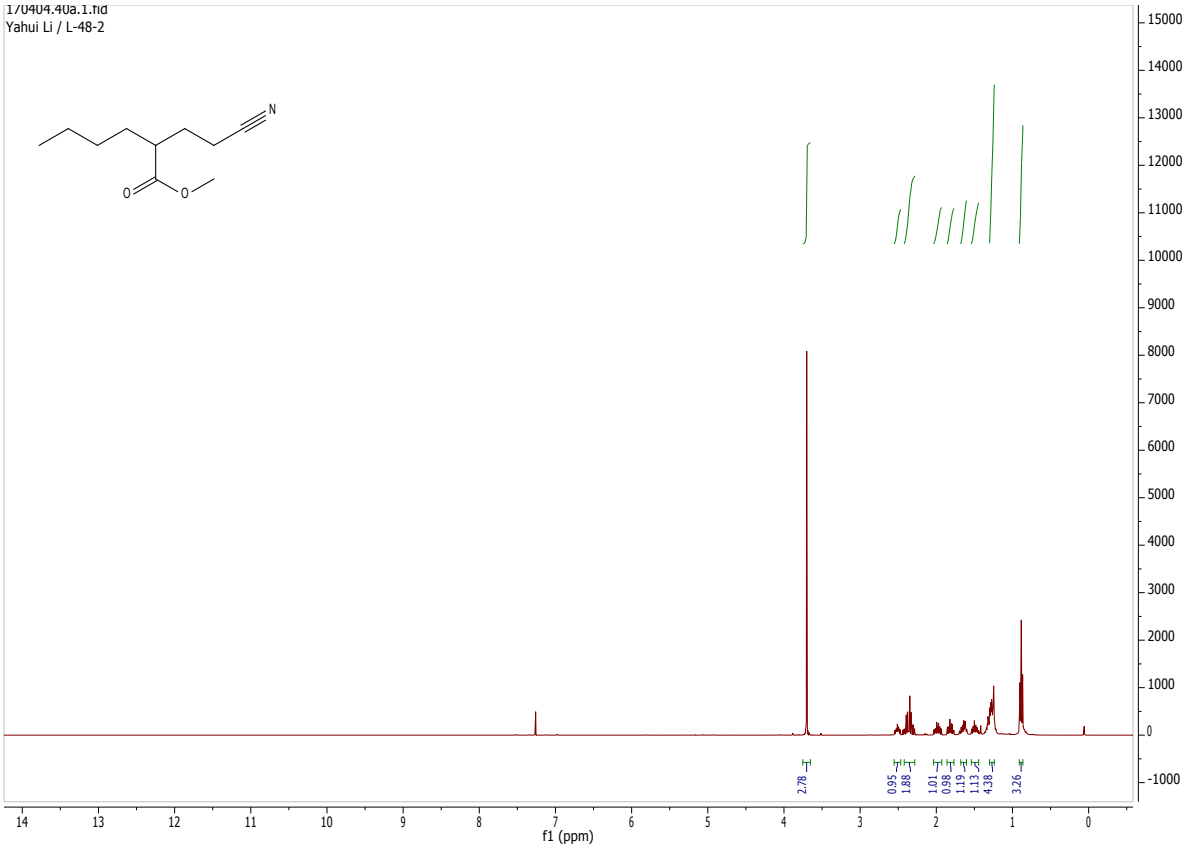
f1 (ppm)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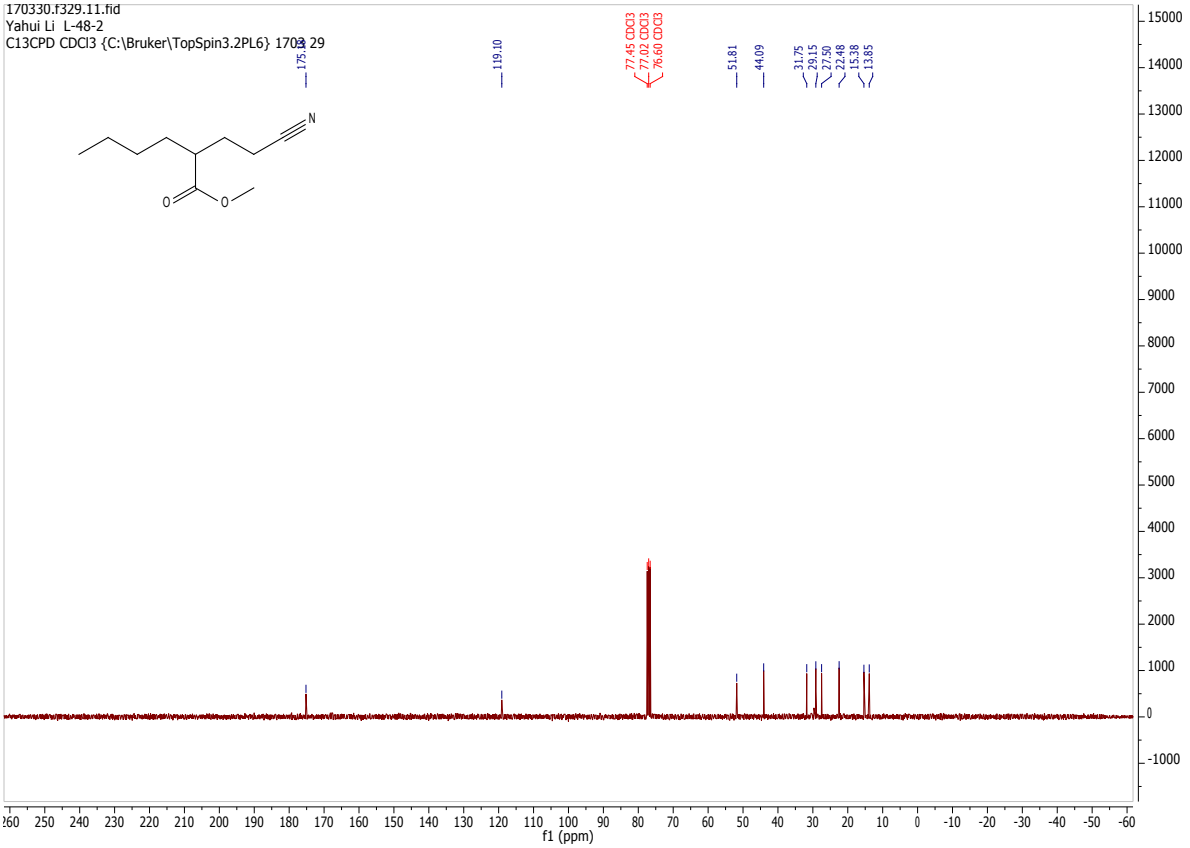
3.26
f1 (ppm)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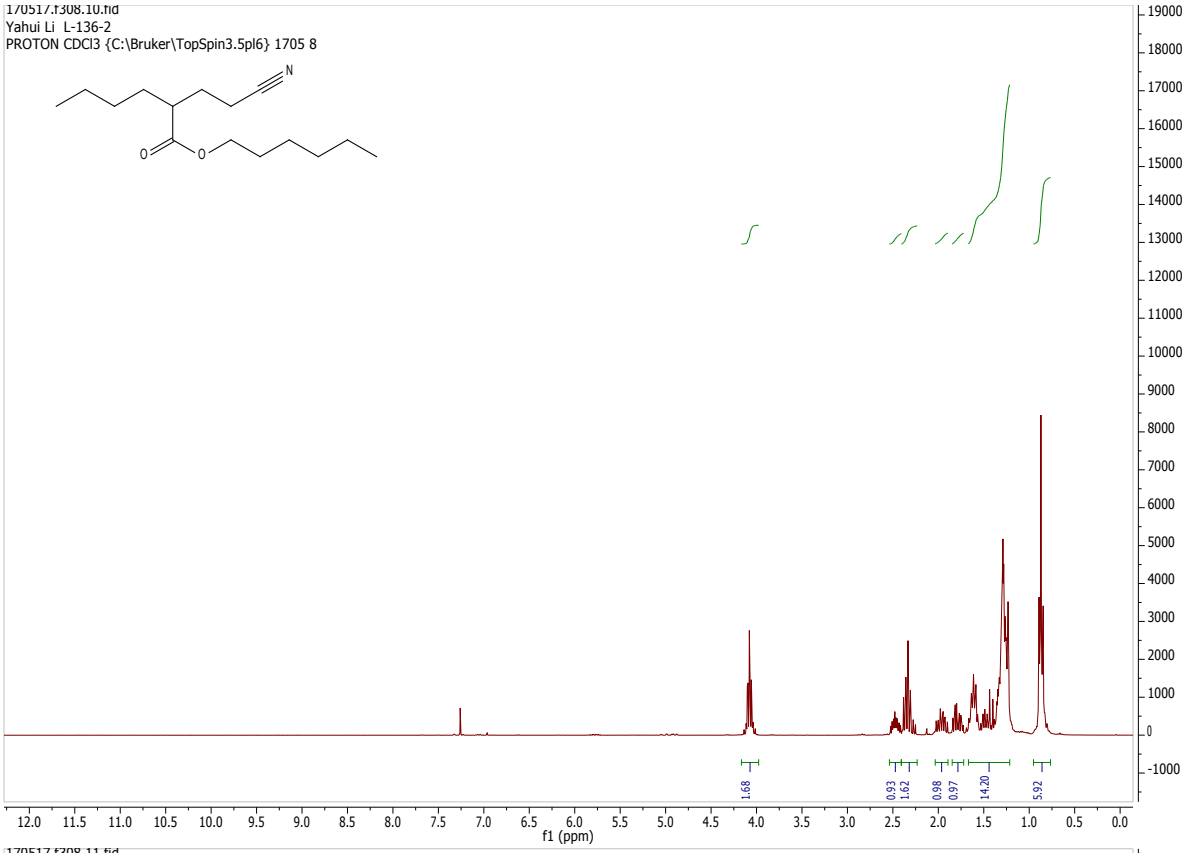
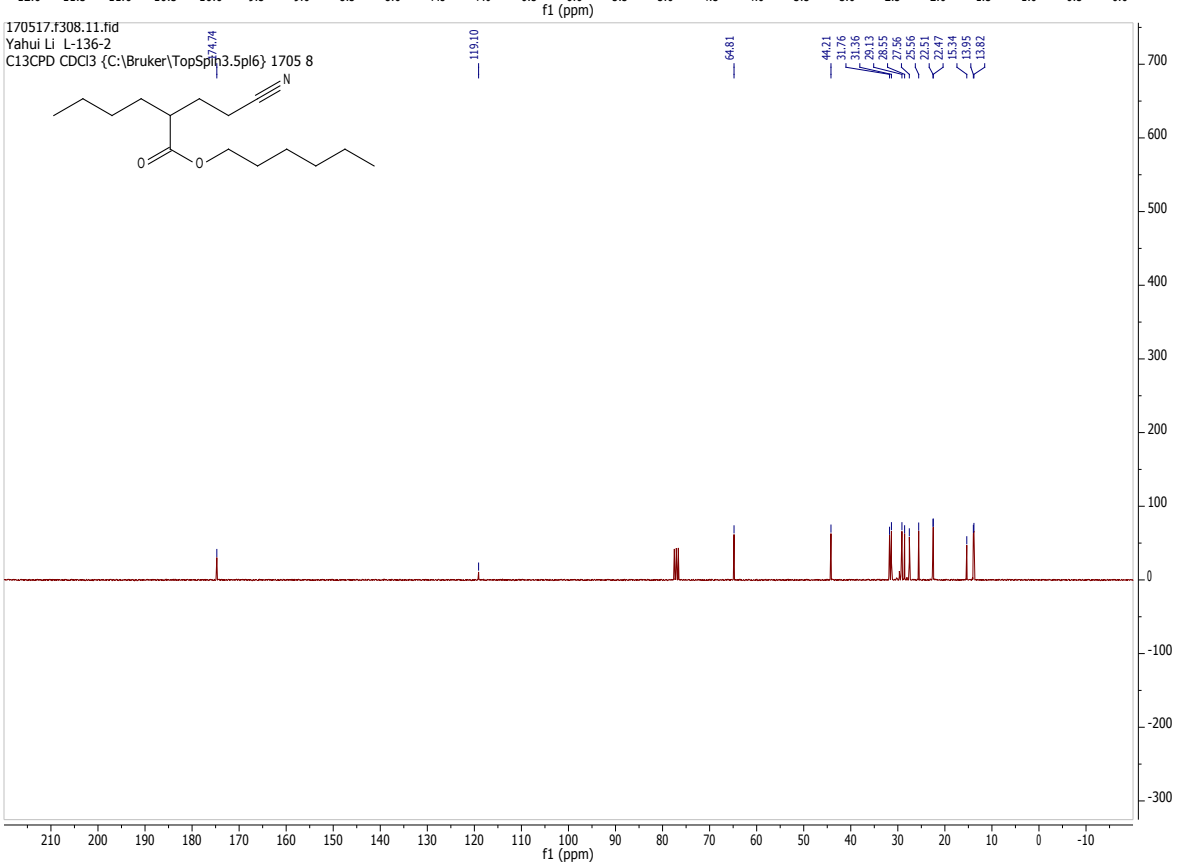
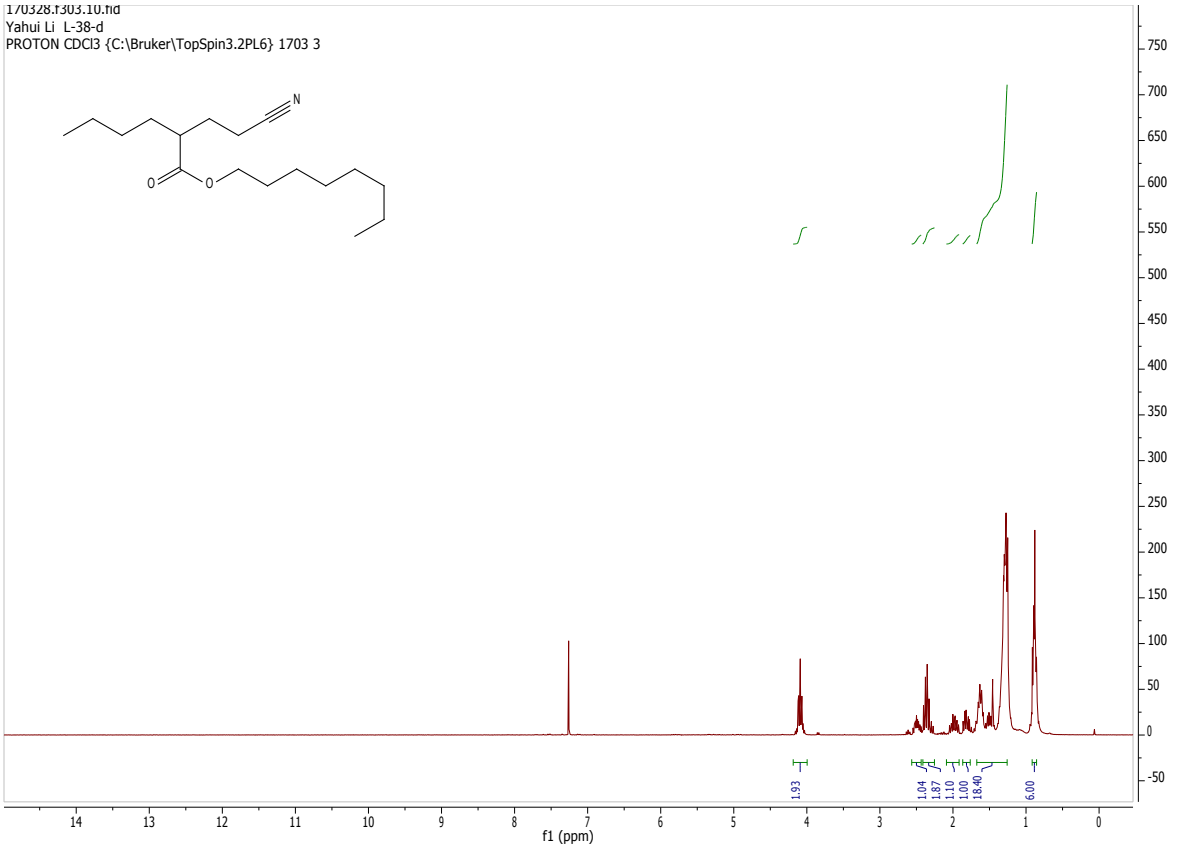
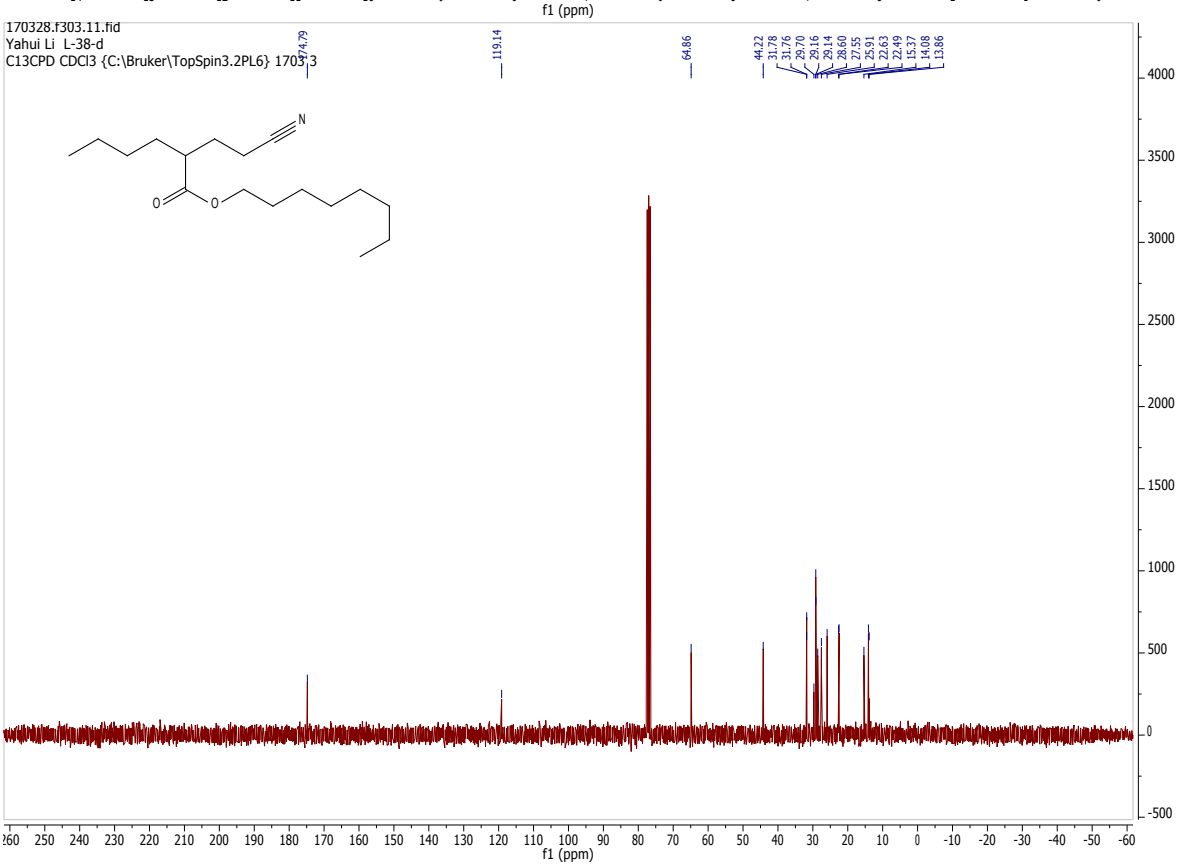
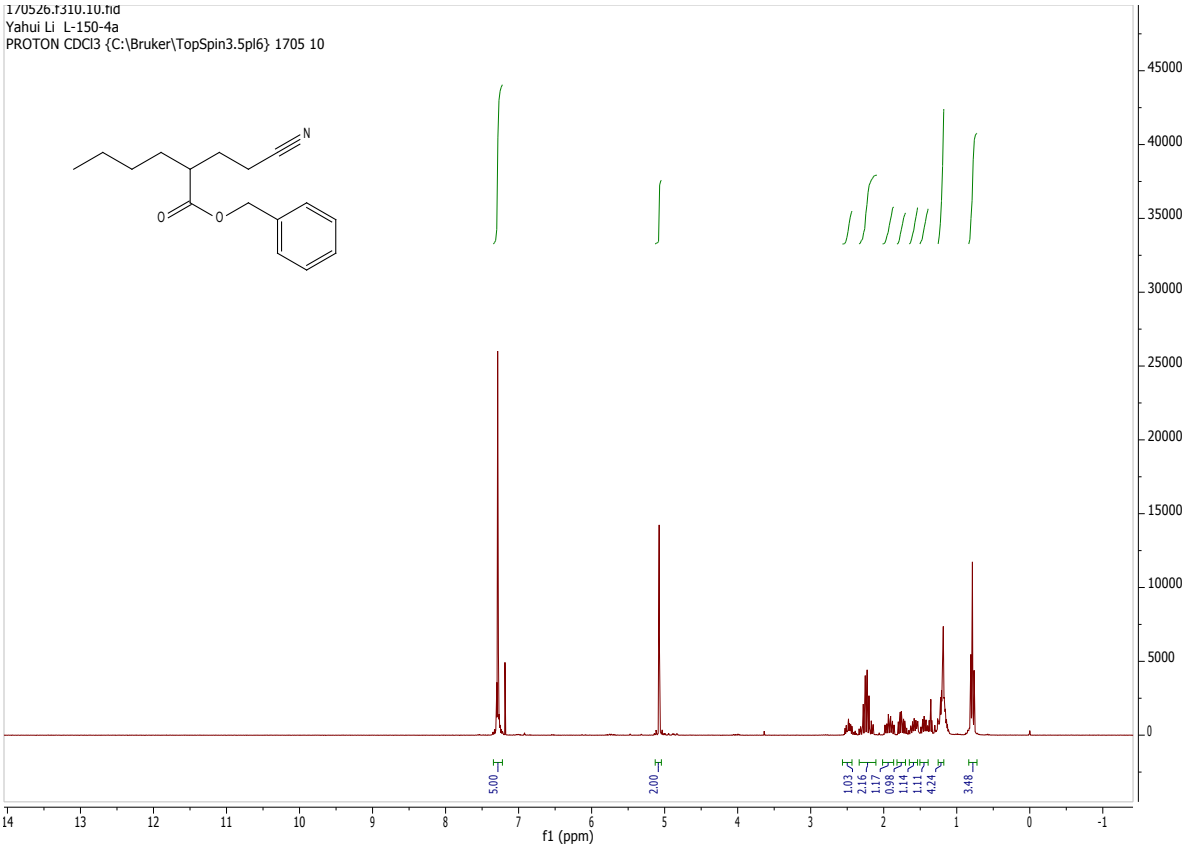
51.81
44.09
31.75
29.15
27.50
22.48
15.38
13.85
N
O
O
f1 (ppm)

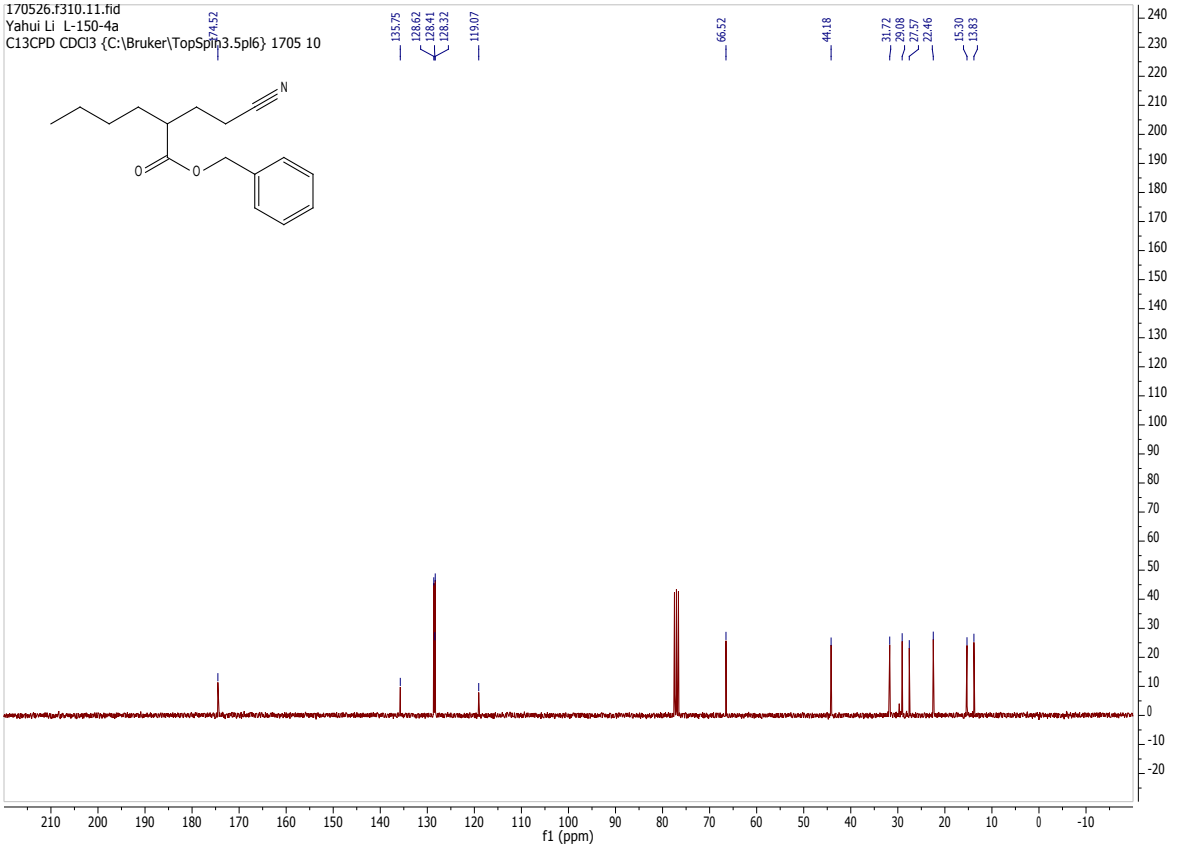

170517.f308.10.fid
Yahui Li L-136-2
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1705 8
N
O
O
1.68
0.93
1.62
0.98
0.97
14.20
5.92
f1 (ppm)

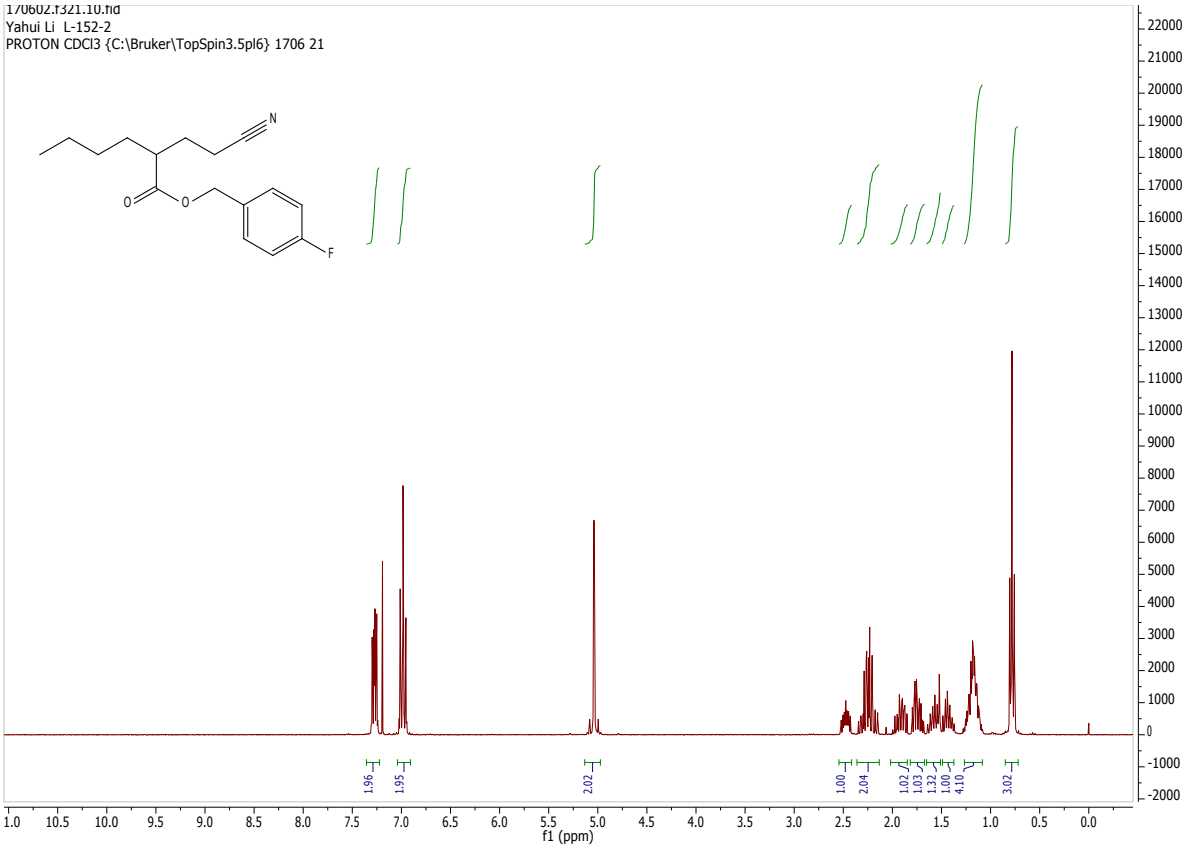

170517.f308.11.fid
Yahui Li L-136-2
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1705 8
N
O
O
174.74
119.10
64.81
44.21
31.76
31.36
29.13
28.55
27.56
25.56
22.51
22.47
15.34
13.95
13.82
f1 (ppm)

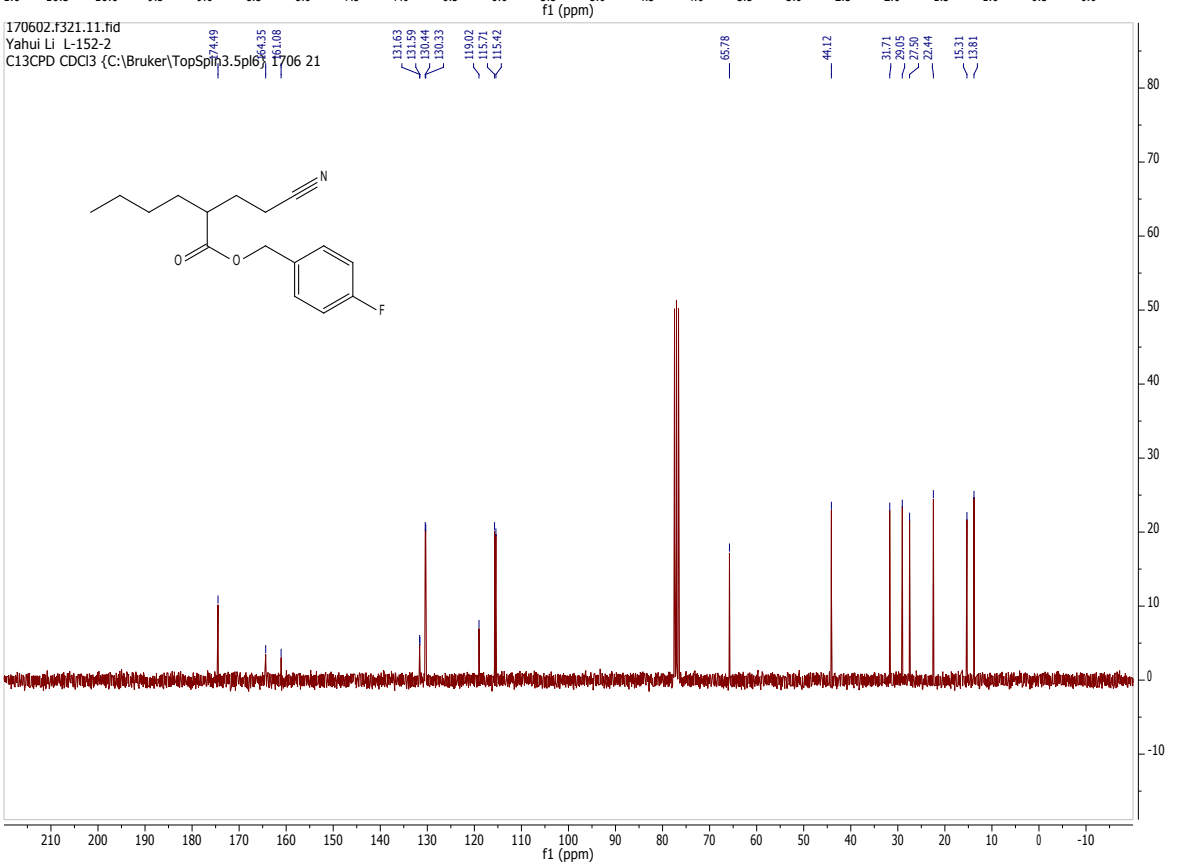

170328.f303.10.fid
Yahui Li L-38-d
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1703 3
N
O
O
1.93
1.04
1.87
1.10
1.00
18.40
6.00
f1 (ppm)

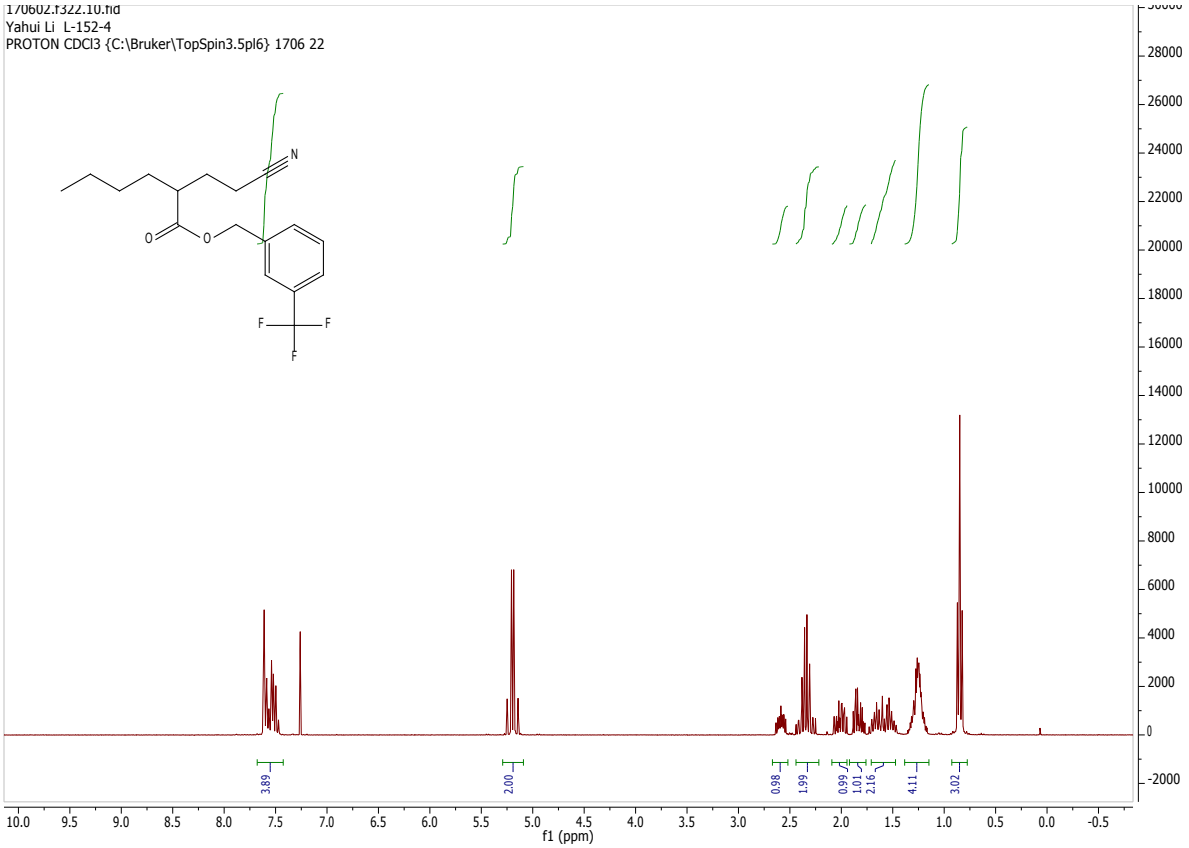

170328.f303.11.fid
Yahui Li L-38-d
C13CPD CDCl3 {C:\Bruker\TopSpin3.2PL6} 1703 3
174.79
119.14
64.86
44.22
31.78
31.76
29.70
29.16
29.14
28.60
27.55
25.91
22.63
22.49
15.37
14.08
13.86
N
O
O
f1 (ppm)

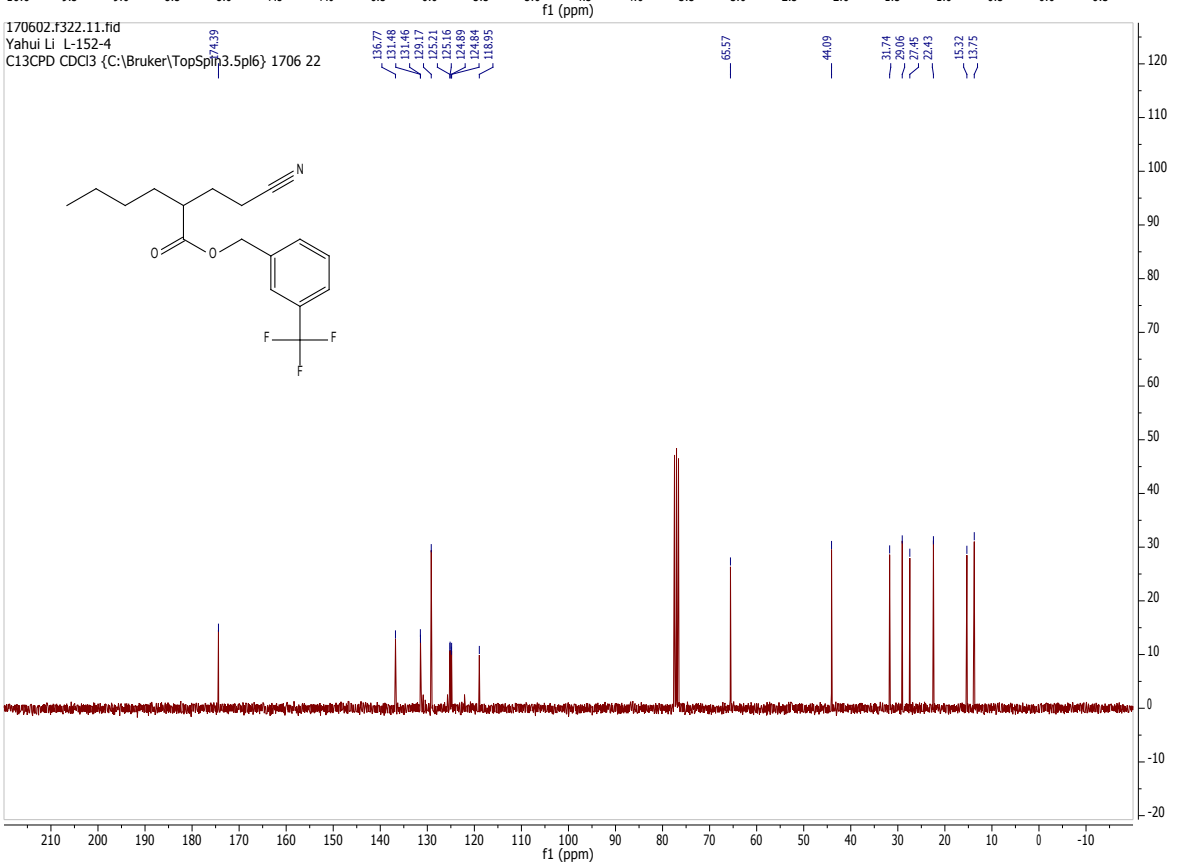

170526.f310.10.fid
Yahui Li L-150-4a
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1705 10
N
O
O
5.00
2.00
1.03
2.16
1.17
0.98
1.14
1.11
4.24
3.48
f1 (ppm)

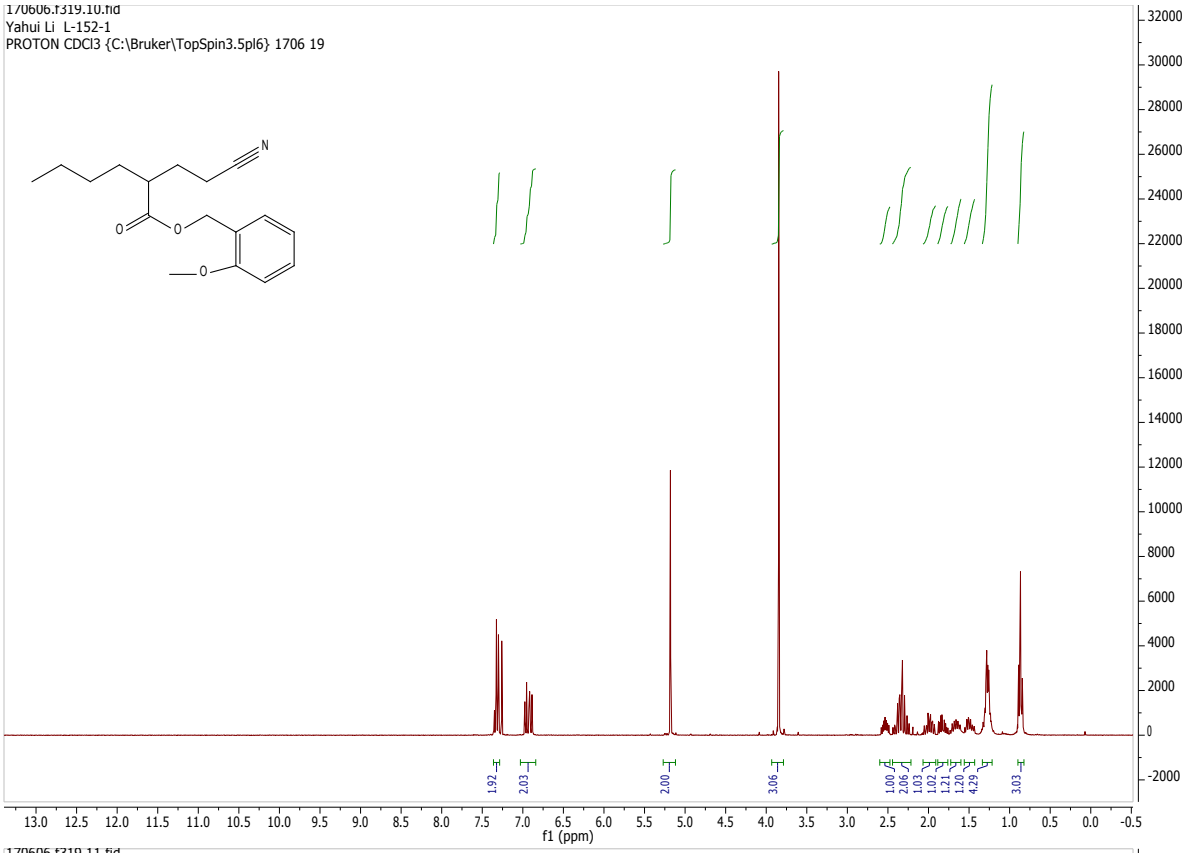

170526.f310.11.fid
Yahui Li L-150-4a
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1705 10
174.52
135.75
128.62
128.41
128.32
119.07
66.52
44.18
31.72
29.08
27.57
22.46
15.30
13.83
N
O
O
f1 (ppm)

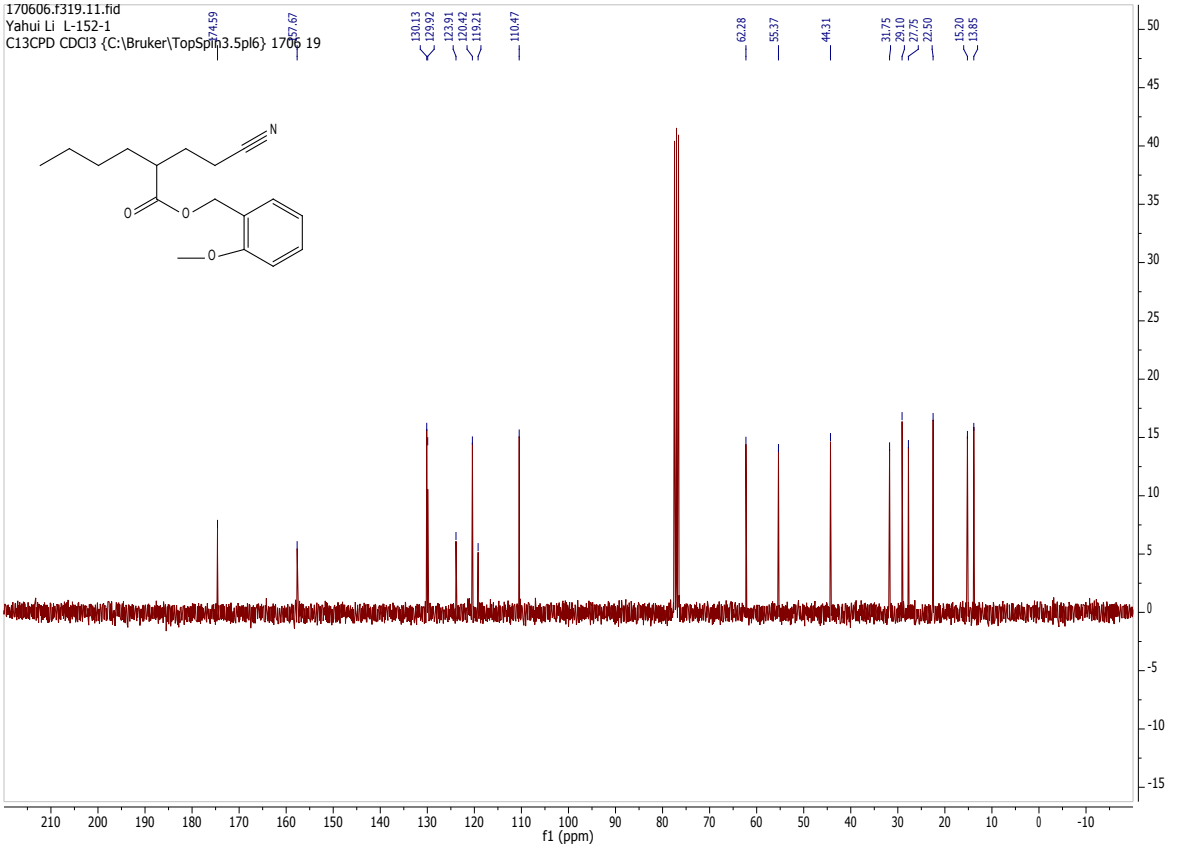

170602.f321.10.fid
Yahui Li L-152-2
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 21
N
O
O
F
1.96
1.95
2.02
1.00
2.04
1.02
1.03
1.32
1.00
4.10
3.02
f1 (ppm)

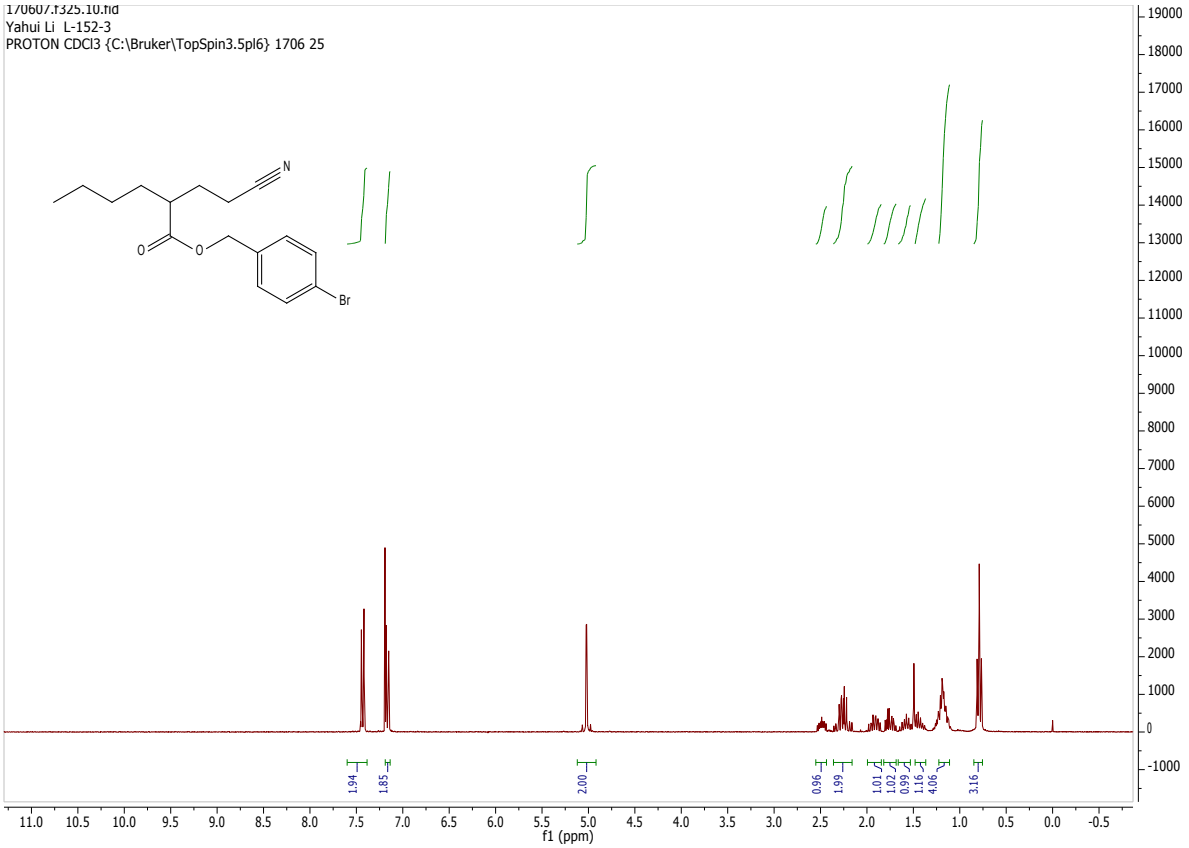

170602.f321.11.fid
Yahui Li L-152-2
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 21
174.49
164.35
161.08
131.63
131.59
130.44
130.33
119.02
115.71
115.42
65.78
44.12
31.71
29.05
27.50
22.44
15.31
13.81
N
O
O
F
f1 (ppm)

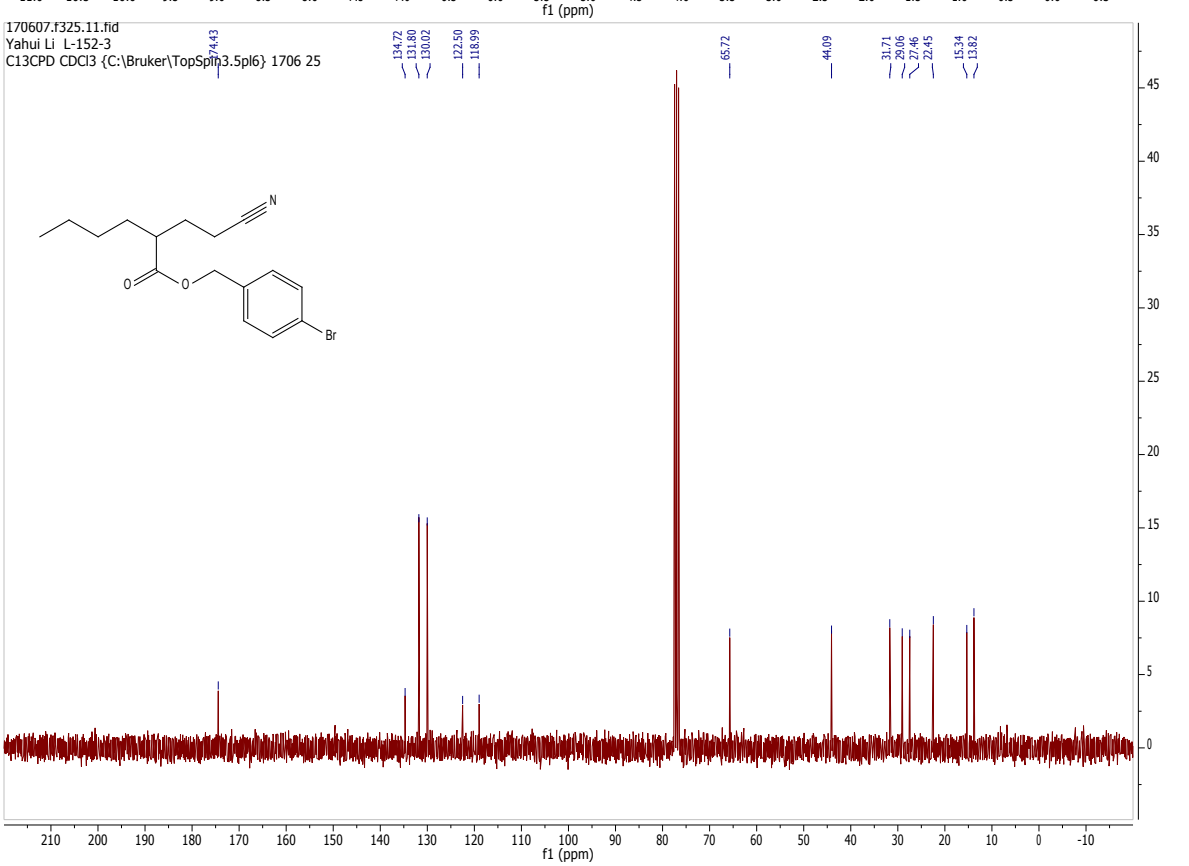

170602.f322.10.fid
Yahui Li L-152-4
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 22
N
O
O
F
F
F
3.89
2.00
0.98
1.99
0.99
1.01
2.16
4.11
3.02
f1 (ppm)

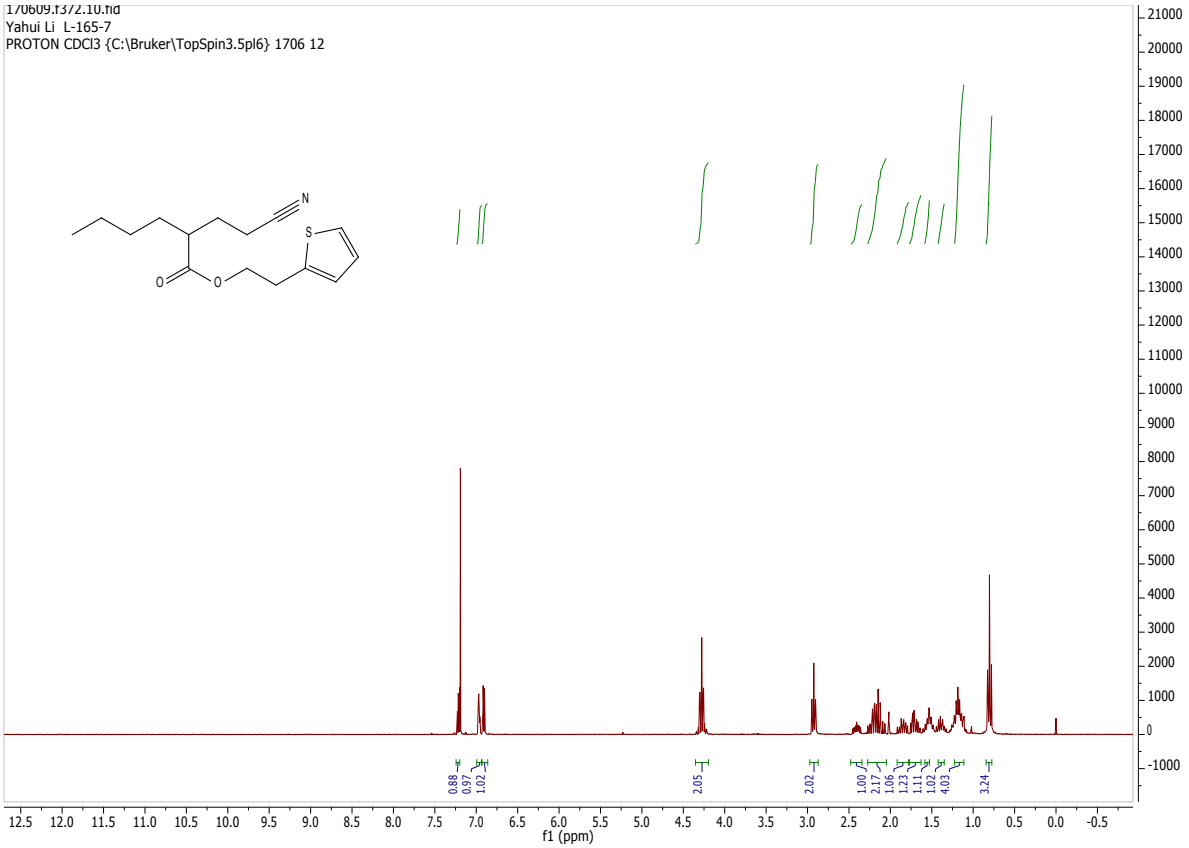

170602.f322.11.fid
Yahui Li L-152-4
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 22
174.39
136.77
131.48
131.46
129.17
125.21
125.16
124.89
124.84
118.95
65.57
44.09
31.74
29.06
27.45
22.43
15.32
13.75
N
O
O
F
F
F
f1 (ppm)

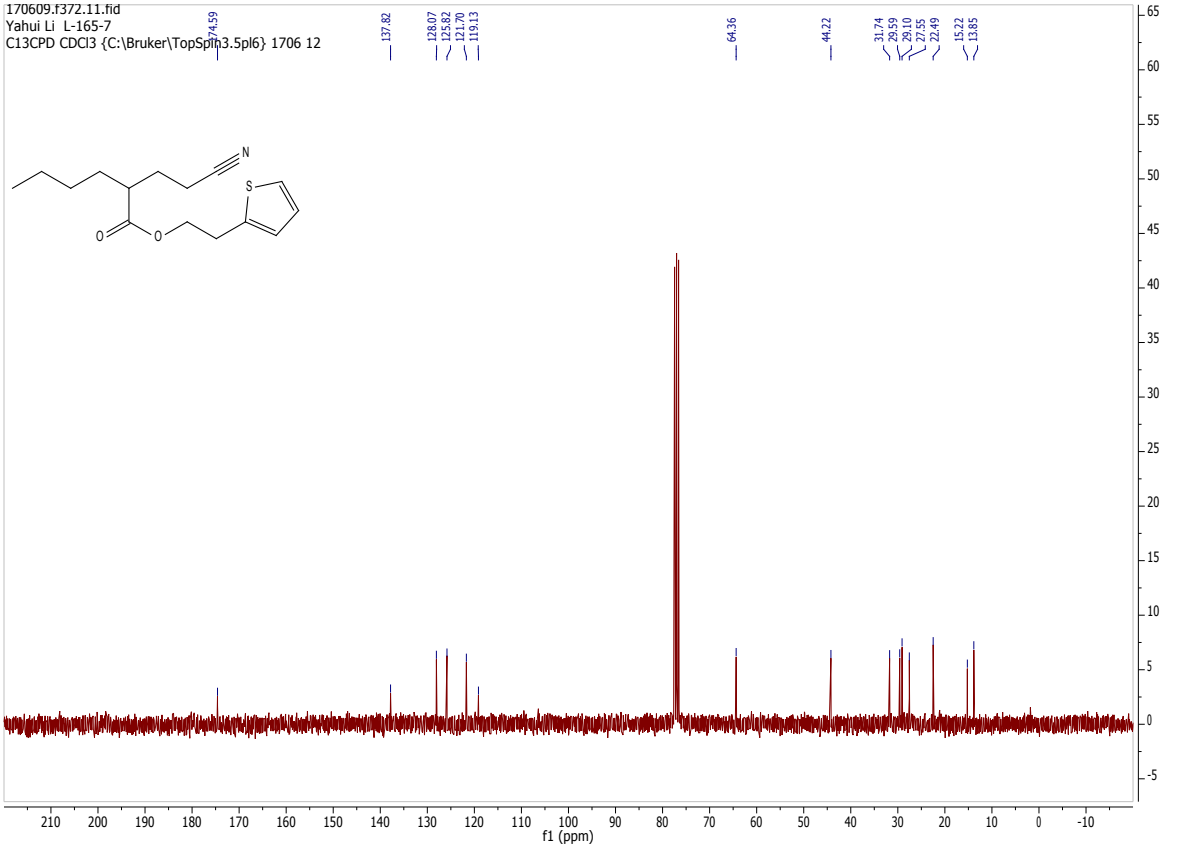

170606.f319.10.fid
Yahui Li L-152-1
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 19
f1 (ppm)

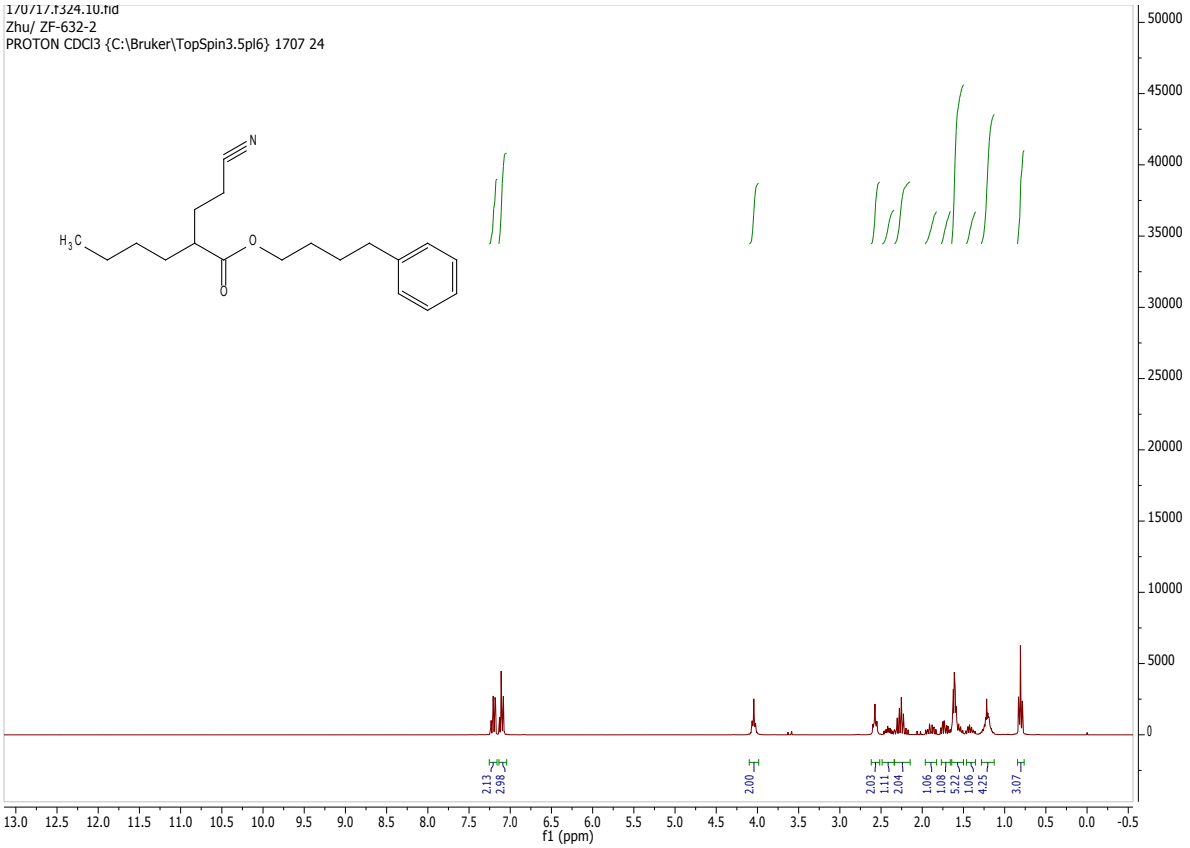

170606.f319.11.fid
Yahui Li L-152-1
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 19
174.59
157.67
130.13
129.92
123.91
120.42
119.21
110.47
62.28
55.37
44.31
31.75
29.10
27.75
22.50
15.20
13.85
f1 (ppm)

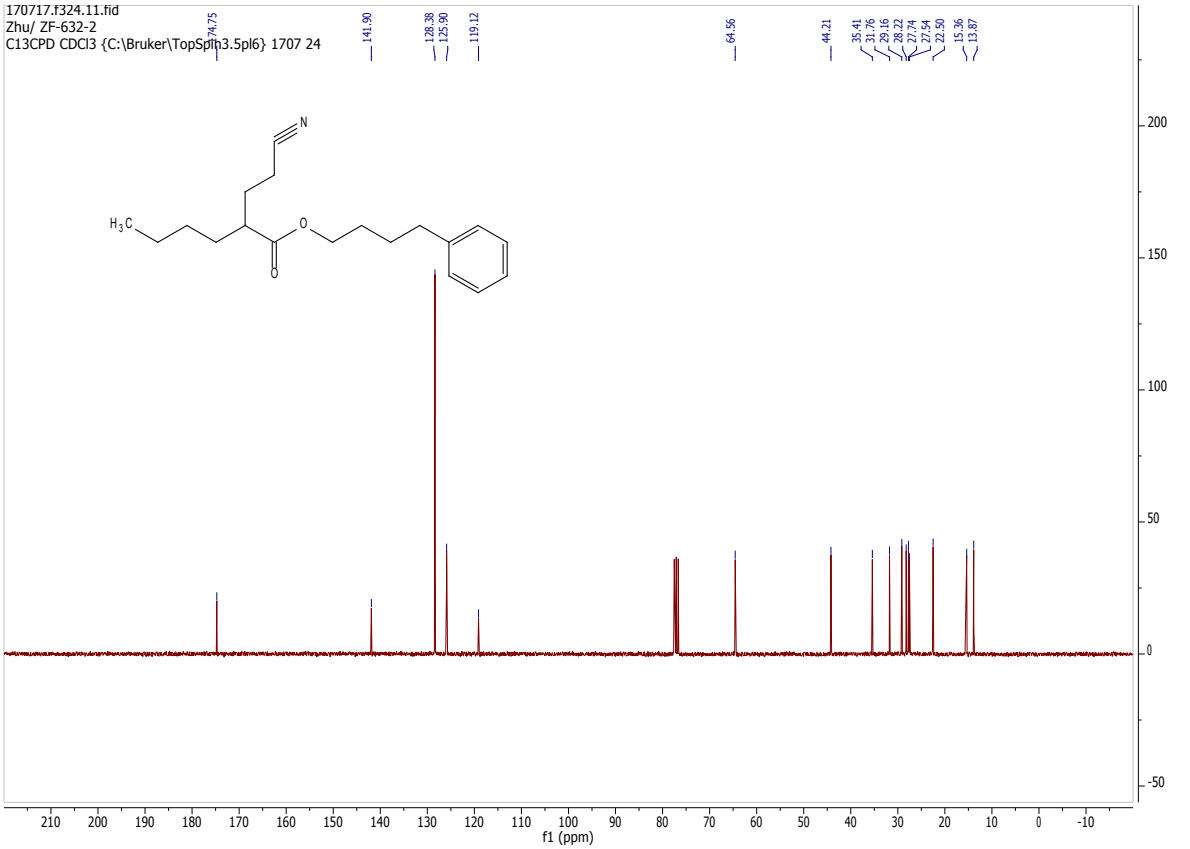

170607.f325.10.fid
Yahui Li L-152-3
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 25
N
O
O
Br
1.94
1.85
2.00
0.96
1.99
1.01
1.02
0.99
1.16
4.06
3.16
f1 (ppm)

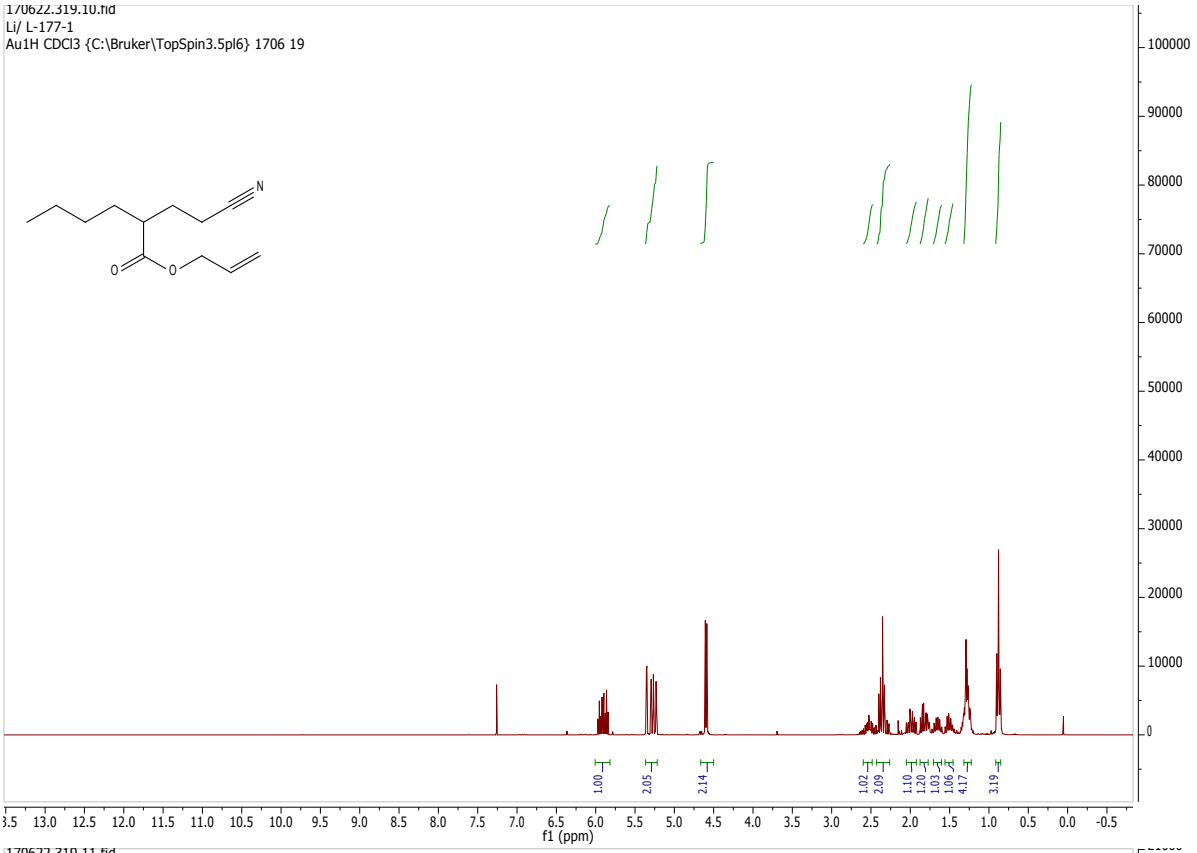

170607.f325.11.fid
Yahui Li L-152-3
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 25
174.43
134.72
131.80
130.02
122.50
118.99
65.72
44.09
31.71
29.06
27.46
22.45
15.34
13.82
N
O
O
Br
f1 (ppm)

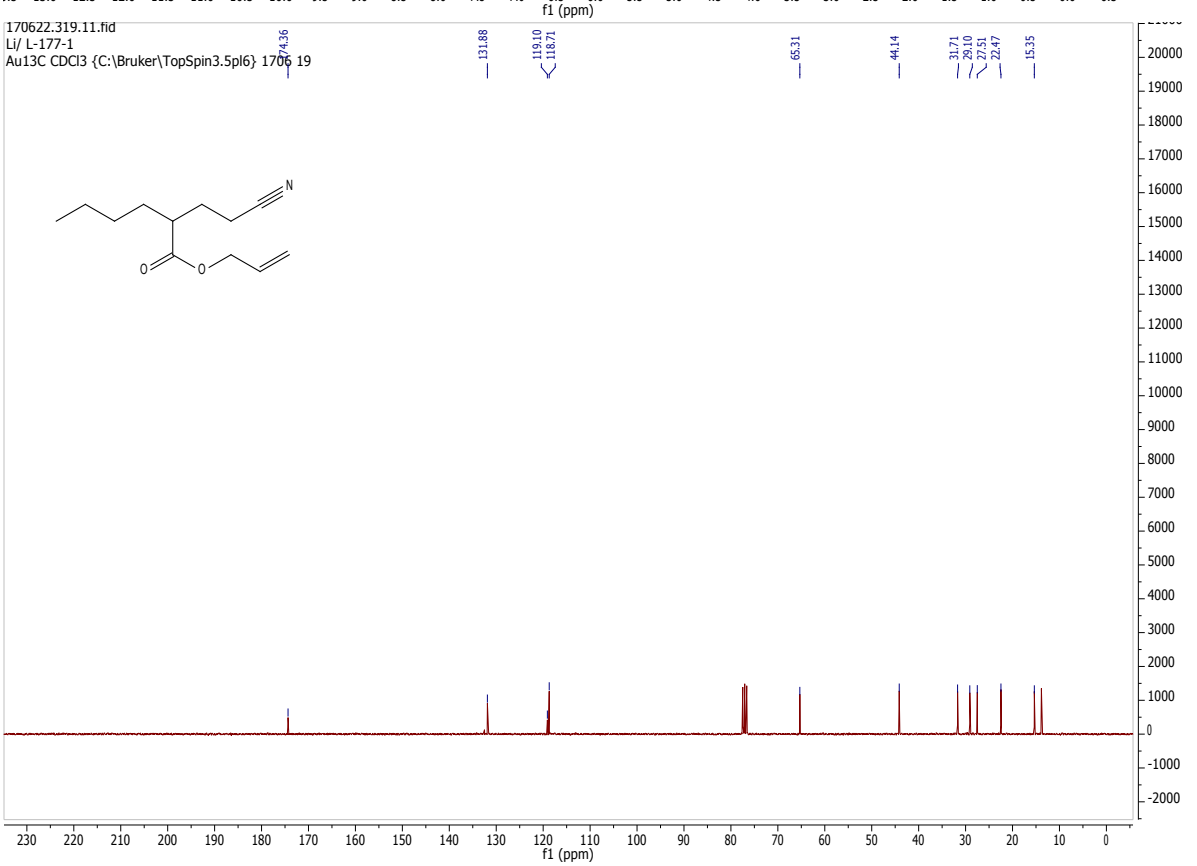

170609.f372.10.fid
Yahui Li L-165-7
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 12
f1 (ppm)

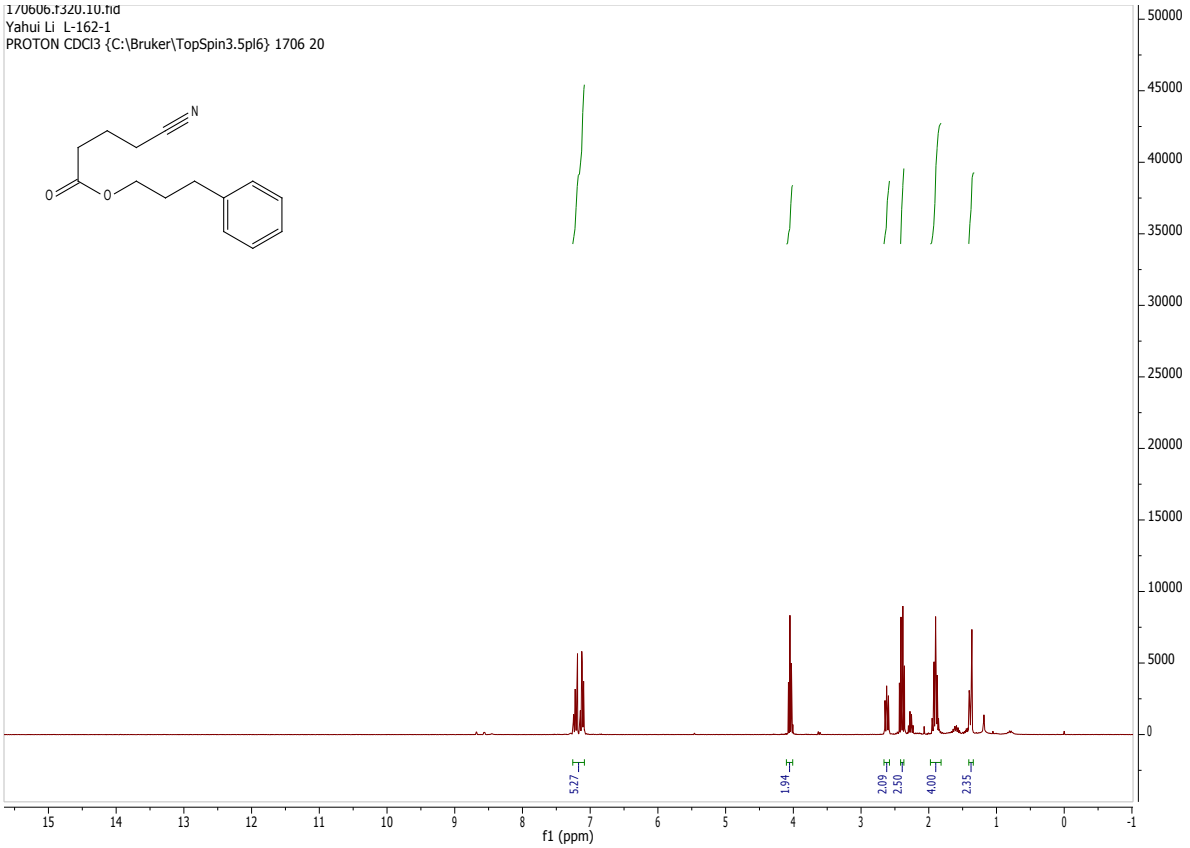

170609.f372.11.fid
Yahui Li L-165-7
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 12
f1 (ppm)

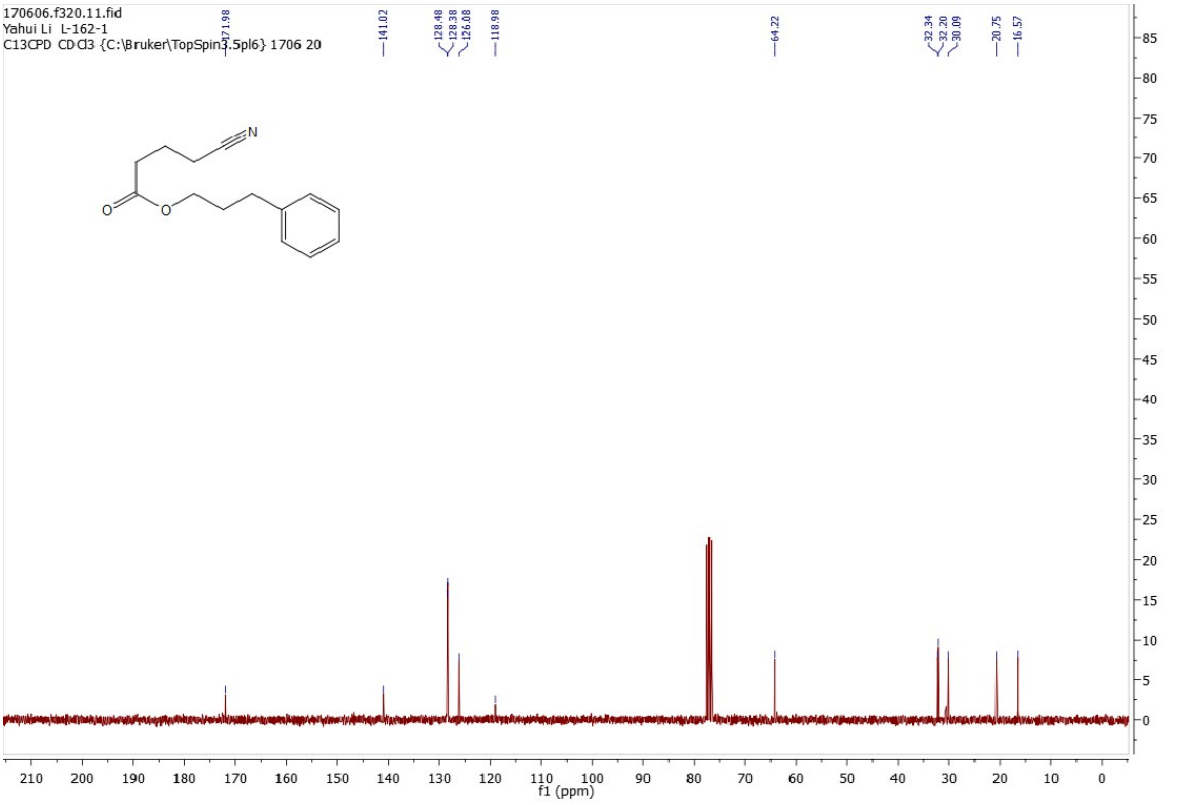

170717.f324.10.fid
Zhu/ ZF-632-2
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 24
N
H3C
O
O
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
2.13
2.98
2.00
2.03
1.11
2.04
1.06
1.08
5.22
1.06
4.25
3.07
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

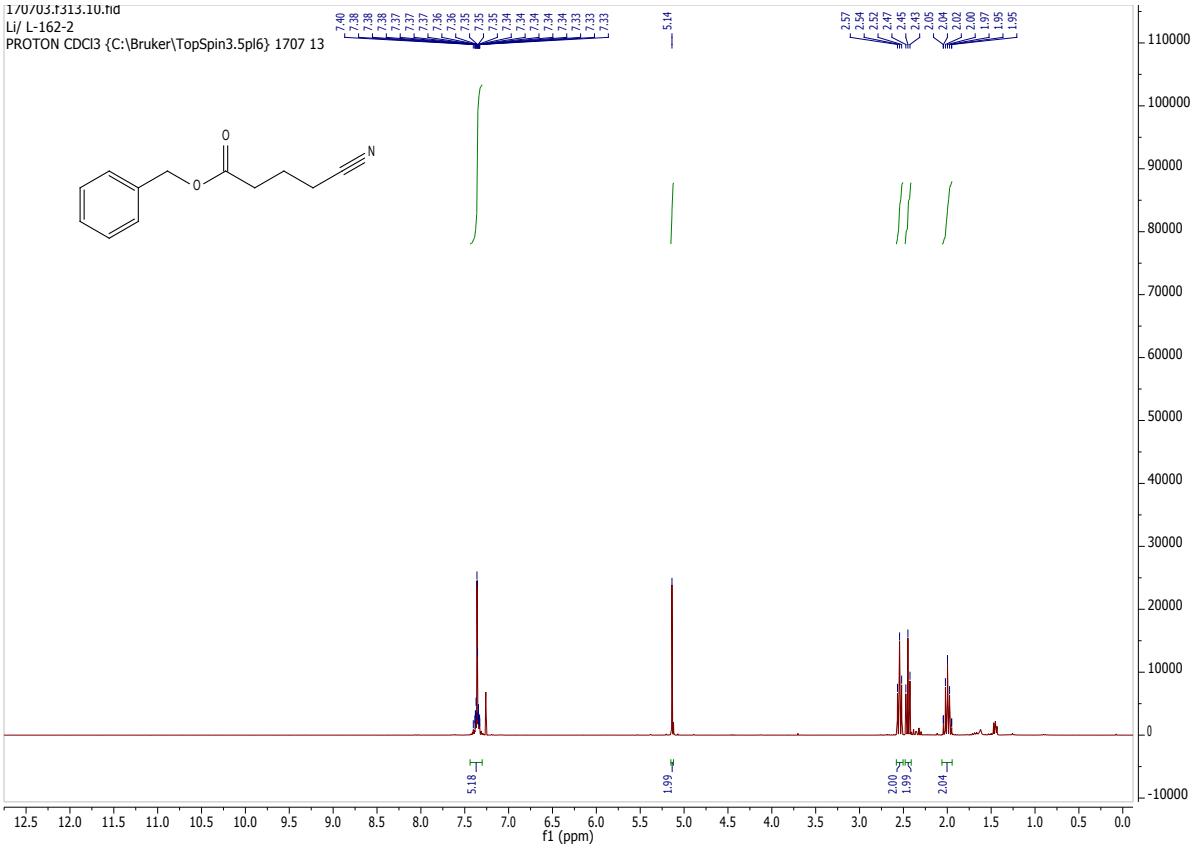

170717.f324.11.fid
Zhu/ ZF-632-2
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 24
74.75
141.90
128.38
125.90
119.12
64.56
44.21
35.41
31.76
29.16
28.22
27.74
27.54
22.50
15.36
13.87
N
H3C
O
O
200
150
100
50
0
-50
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

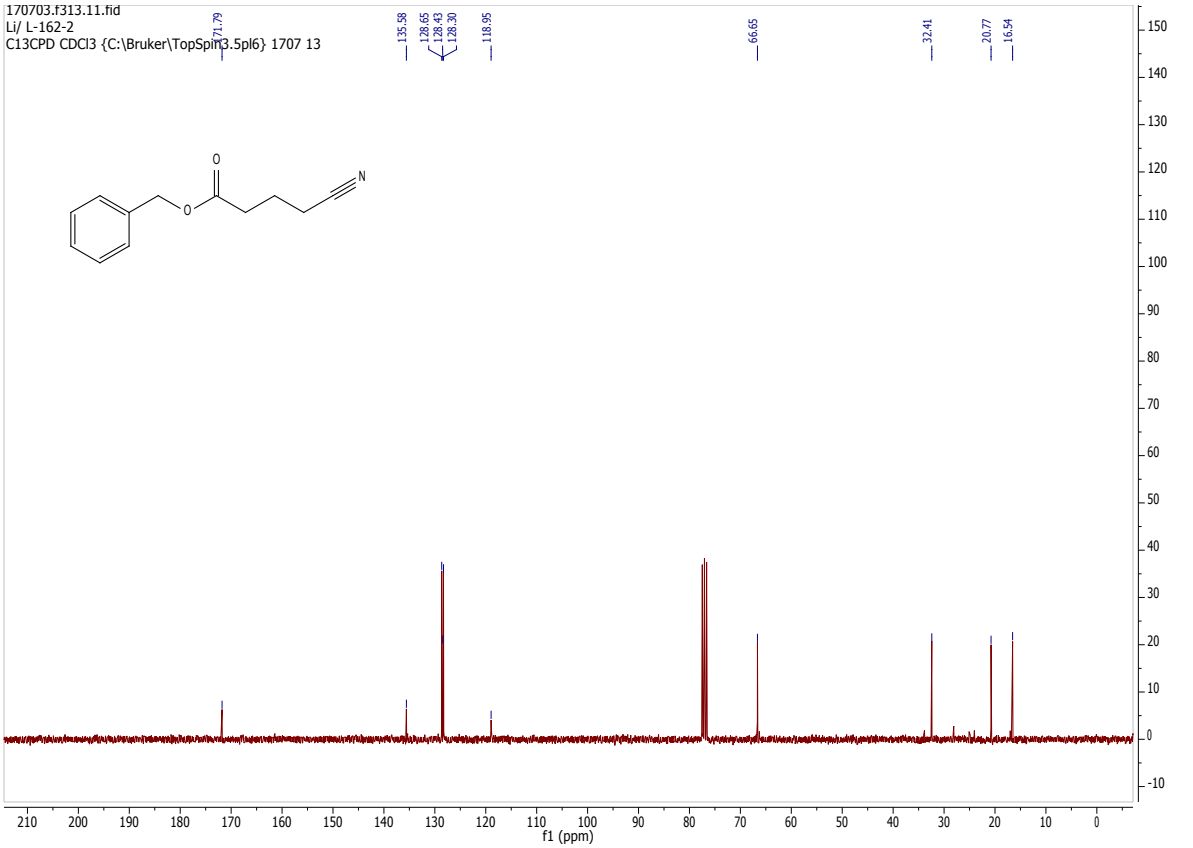

170622.319.10.fid
Li/ L-177-1
Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 19
N
O
O
1.00
2.05
2.14
1.02
2.09
1.10
1.20
1.03
1.06
4.17
3.19
f1 (ppm)

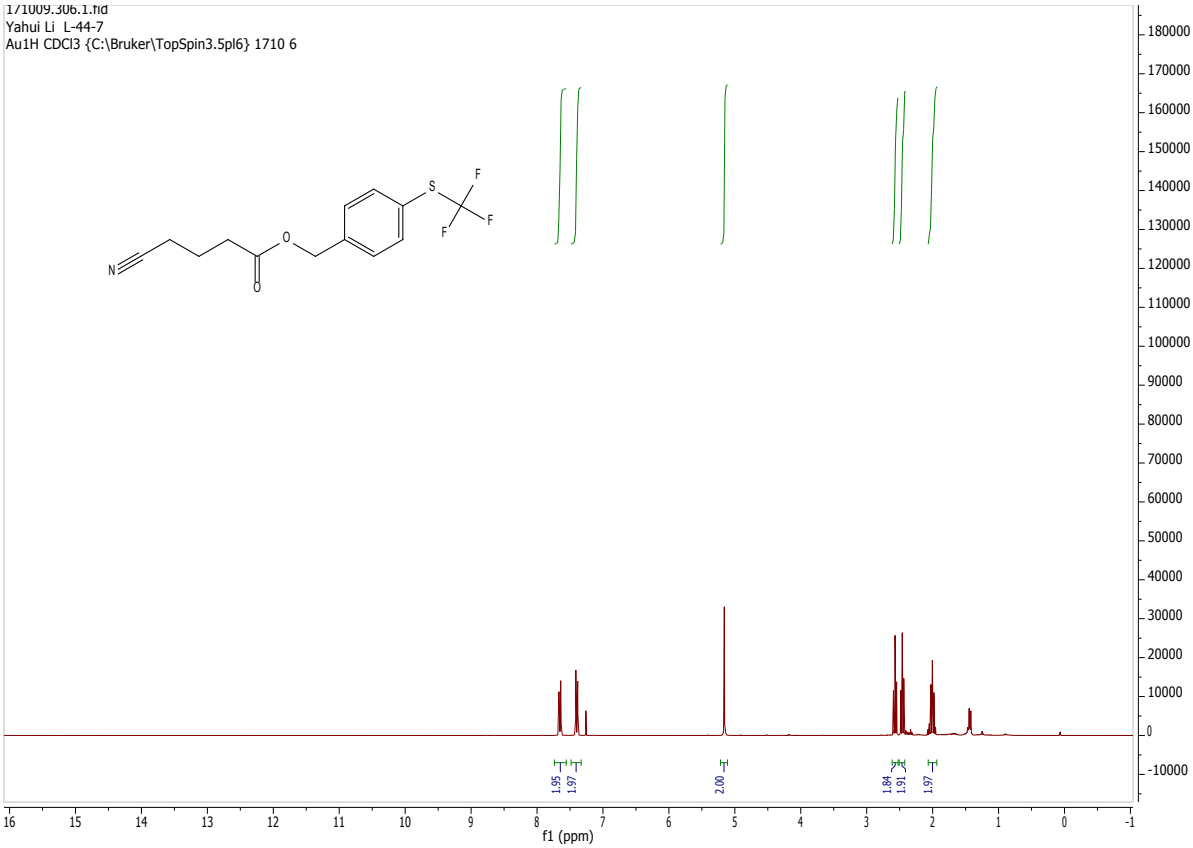

170622.319.11.fid
Li/ L-177-1
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 19
174.36
131.88
119.10
118.71
65.31
44.14
31.71
29.10
27.51
22.47
15.35
N
O
O
f1 (ppm)

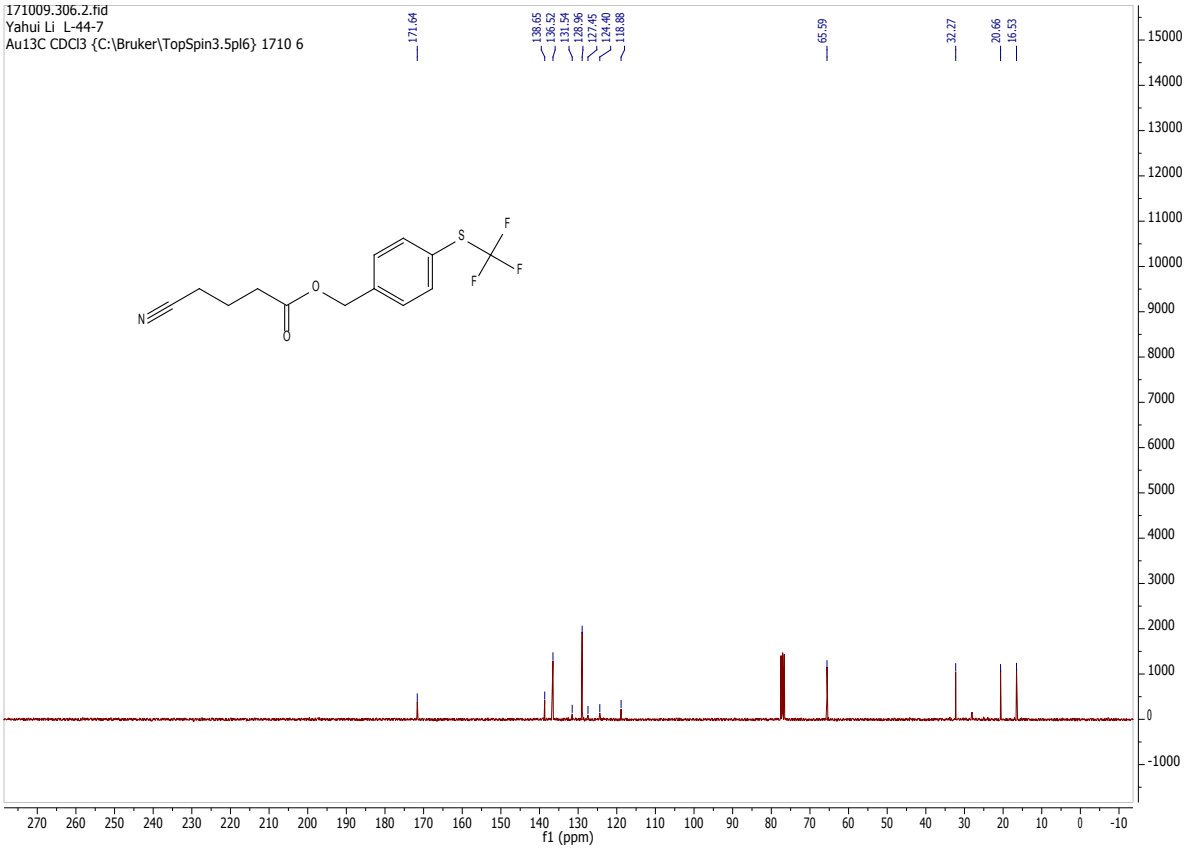

170606.f320.10.fid
Yahui Li L-162-1
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 20
N
O
O
5.27
1.94
2.09
2.50
4.00
2.35
f1 (ppm)

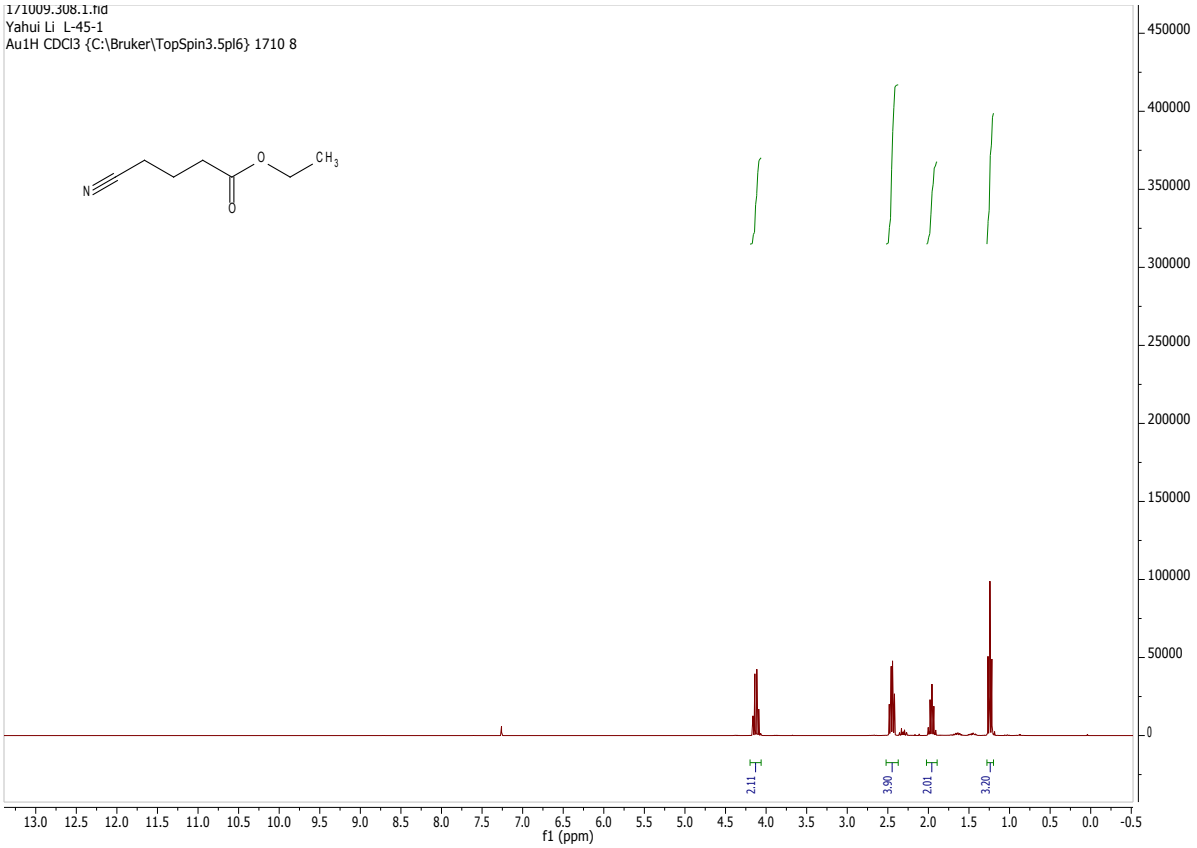

170606.f320.11.fid
Yahui Li L-162-1
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 20
171.98
141.02
128.48
128.38
126.08
118.98
64.22
32.34
32.20
30.09
20.75
16.57
N
O
O
f1 (ppm)

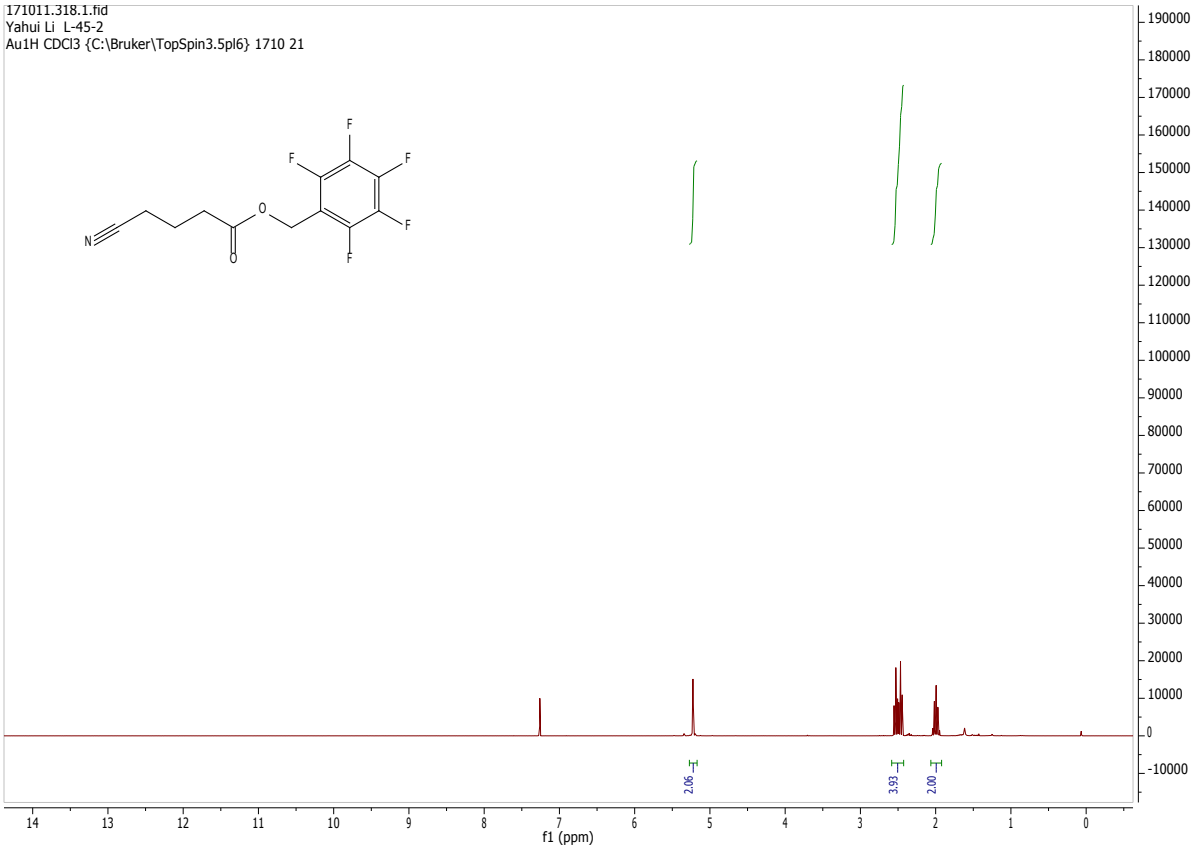

170703.f313.10.fid
Li/ L-162-2
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 13
7.40 7.38 7.38 7.38 7.37 7.37 7.37 7.36 7.36 7.35 7.35 7.35 7.34 7.34 7.34 7.34 7.34 7.33 7.33 7.33
5.14
2.57 2.54 2.52 2.47 2.45 2.43 2.05 2.04 2.02 2.00 1.97 1.95 1.95
O
O
N
5.18
1.99
2.00
1.99
2.04
f1 (ppm)

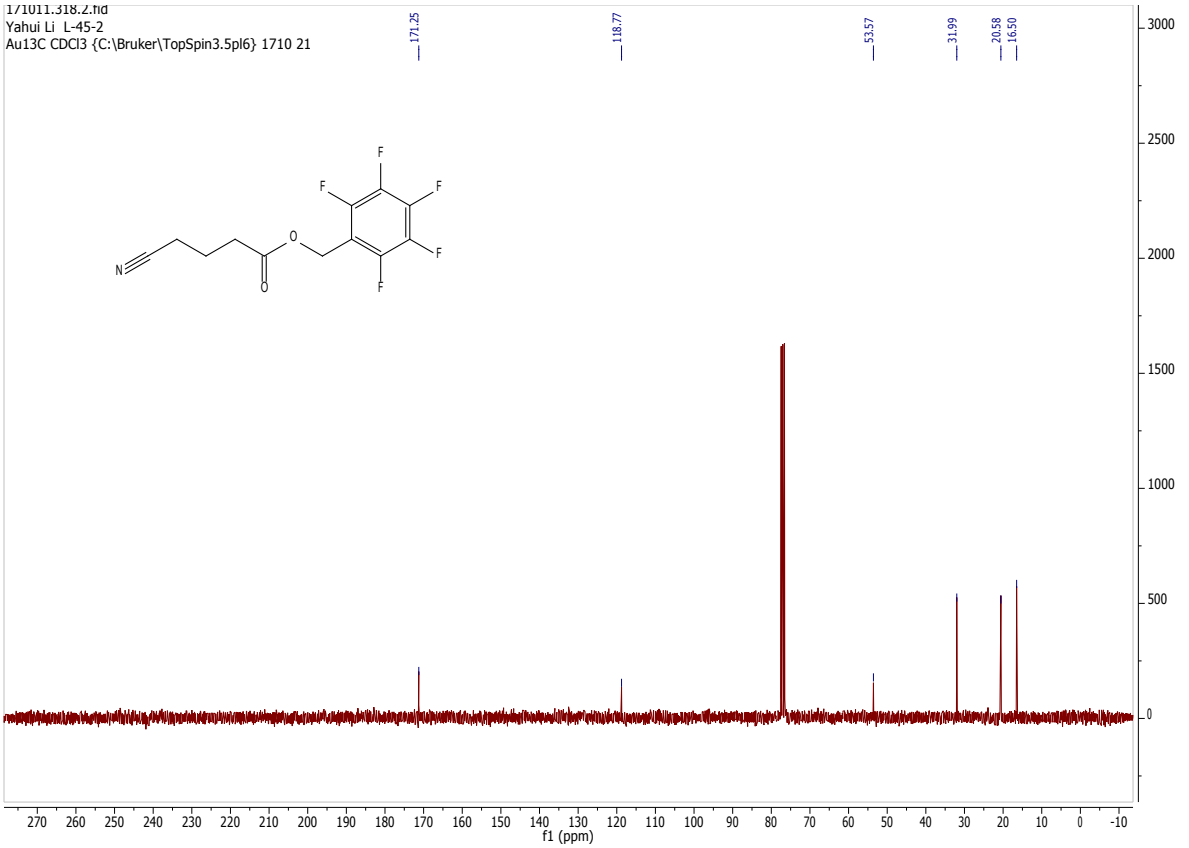

170703.f313.11.fid
Li/ L-162-2
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 13
171.79
135.58
128.65
128.43
128.30
118.95
66.65
32.41
20.77
16.54
O
O
N
f1 (ppm)

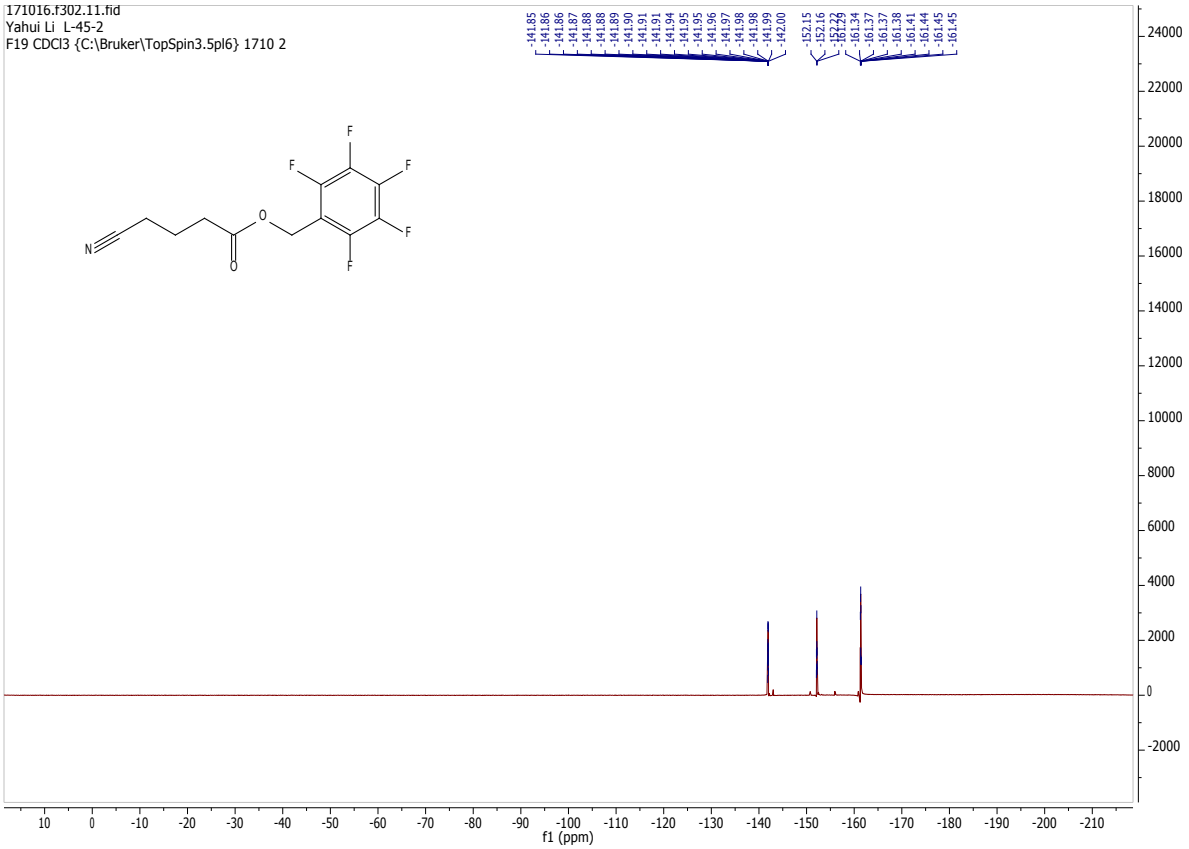

171009.306.1.fid
Yahui Li L-44-7
Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 1710 6
1.95
1.97
2.00
1.84
1.91
1.97
f1 (ppm)

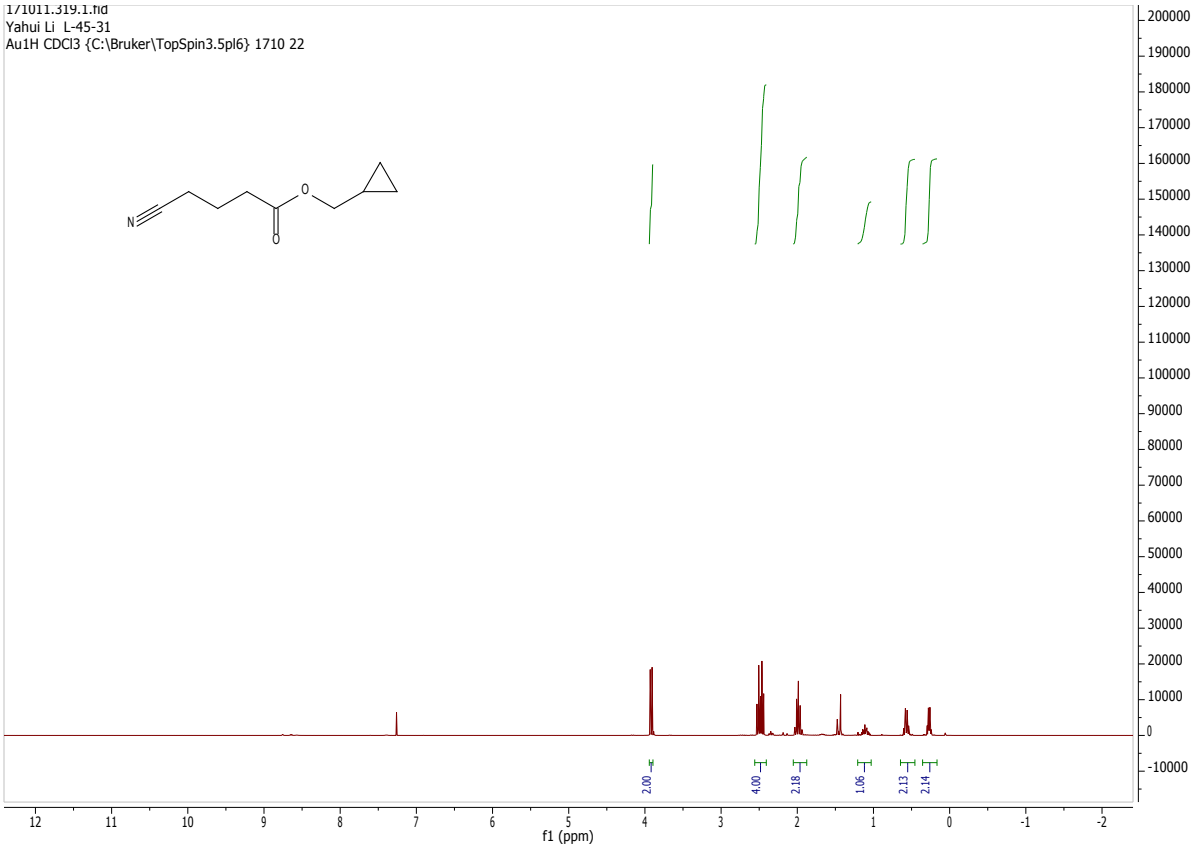

171009.306.2.fid
Yahui Li L-44-7
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 1710 6
171.64
138.65
136.52
131.54
128.96
127.45
124.40
118.88
65.59
32.27
20.66
16.53
f1 (ppm)

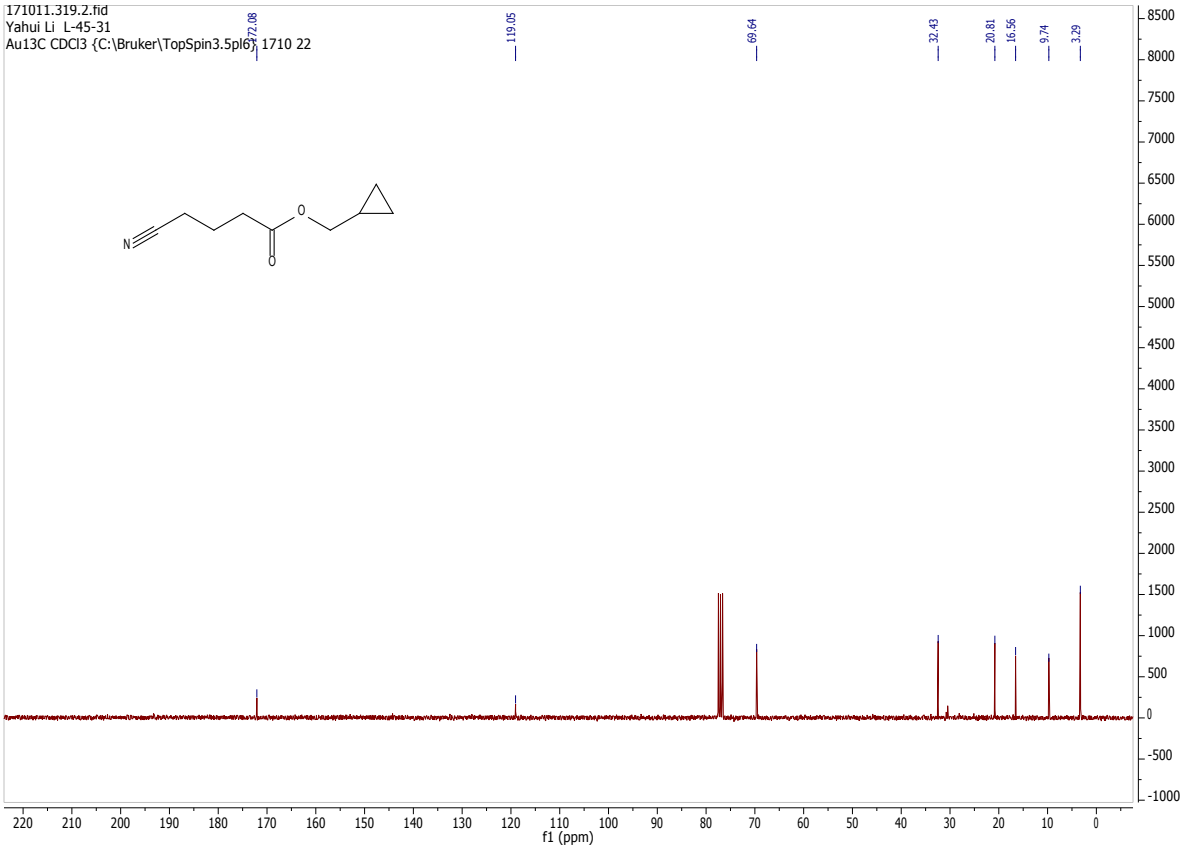

171009.308.1.fid
Yahui Li L-45-1
Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 1710 8
N
O
O
CH3
2.11
3.90
2.01
3.20
f1 (ppm)

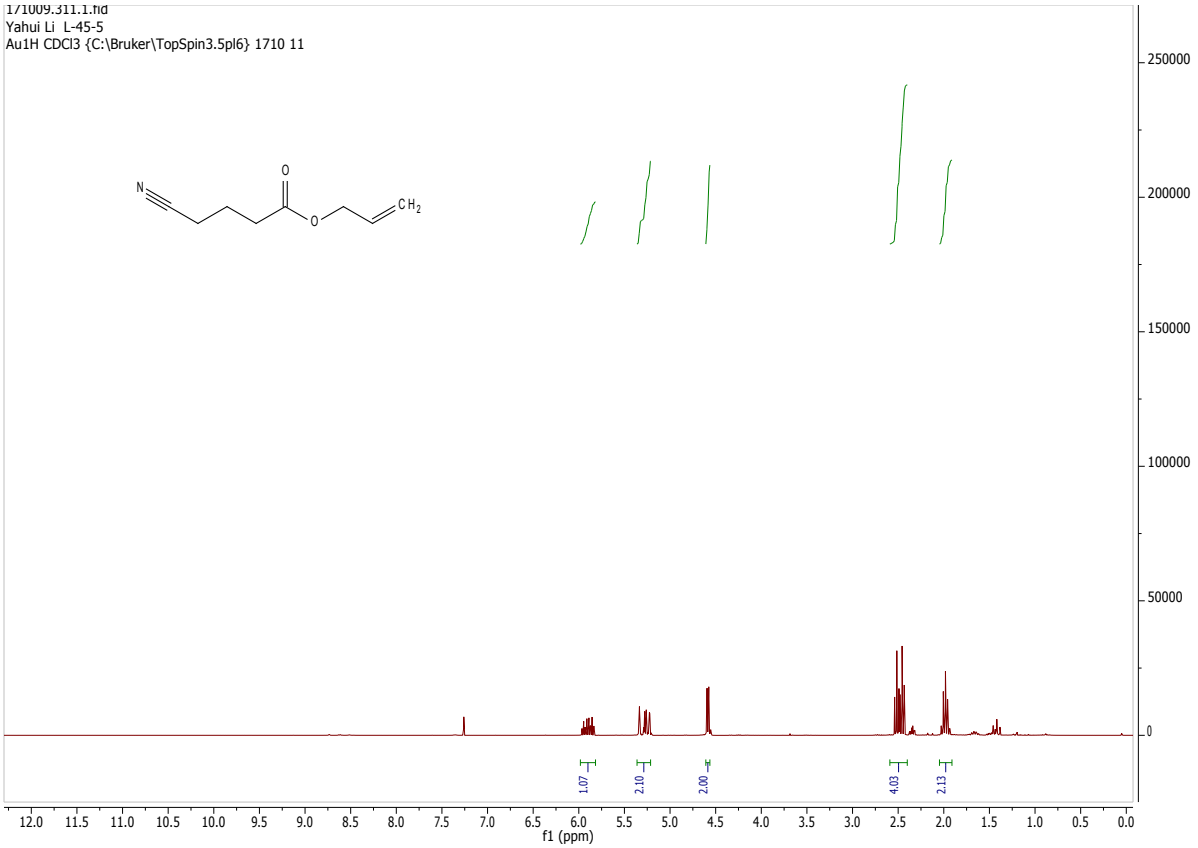

171011.318.1.fid
Yahui Li L-45-2
Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 1710 21
N
O
O
F
F
F
F
F
2.06
3.93
2.00
f1 (ppm)

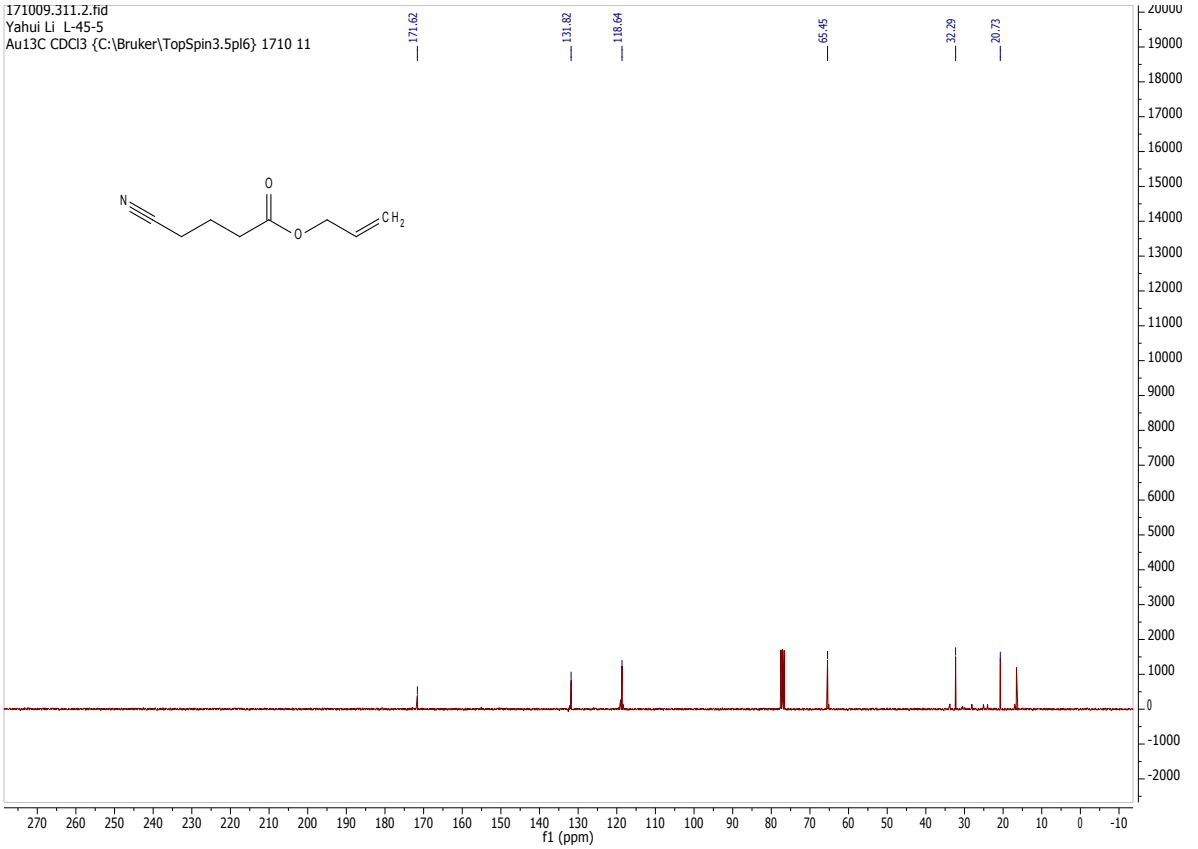

171011.318.2.fid
Yahui Li L-45-2
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 1710 21
171.25
118.77
53.57
31.99
20.58
16.50
f1 (ppm)

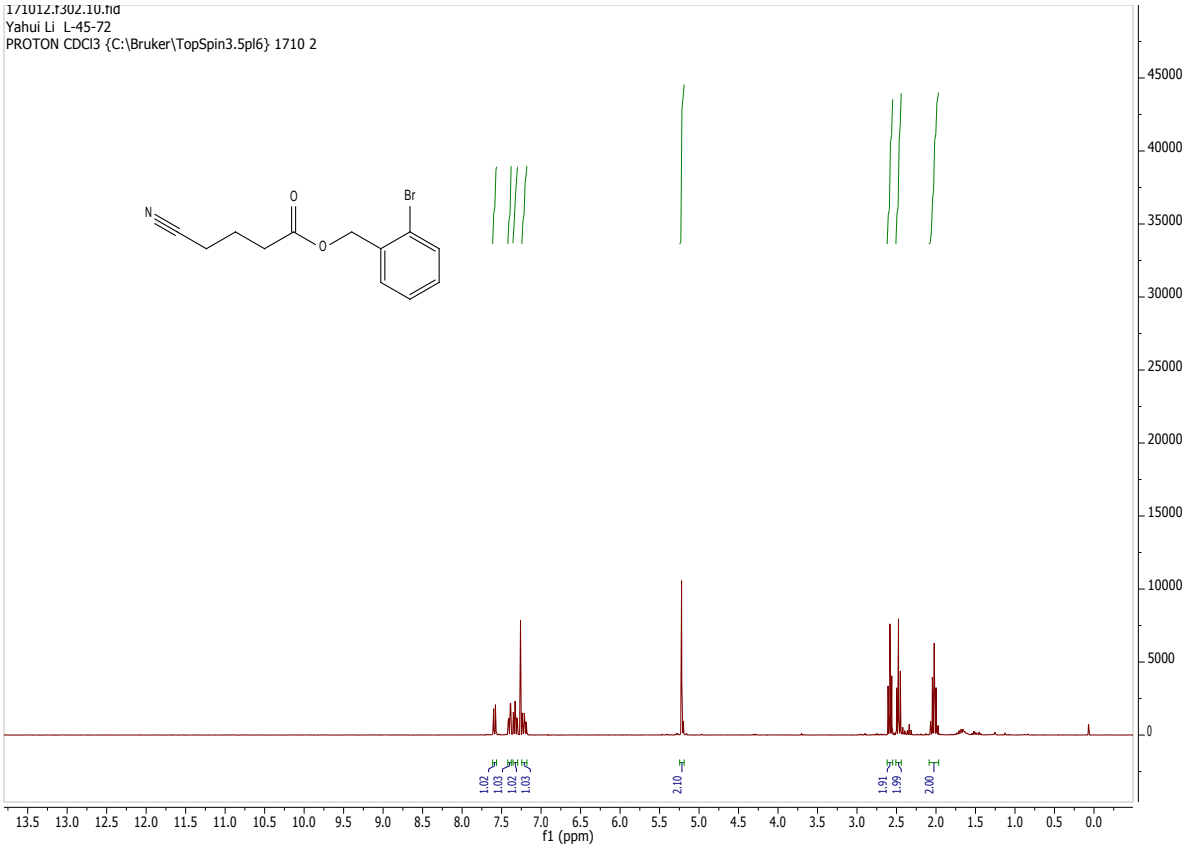

171016.f302.11.fid
Yahui Li L-45-2
F19 CDCl3 {C:\Bruker\TopSpin3.5pl6} 1710 2
f1 (ppm)

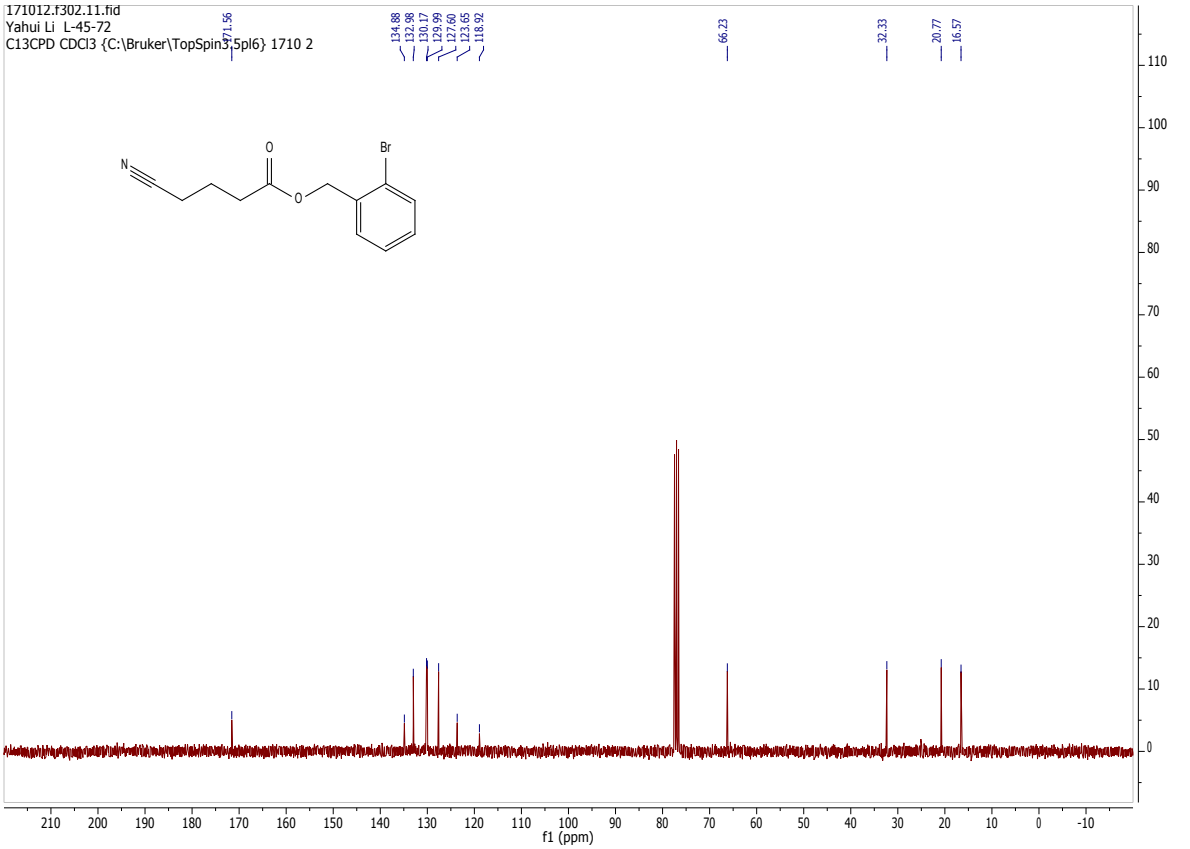

171011.319.1.fid
Yahui Li L-45-31
Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 1710 22
2.00
4.00
2.18
1.06
2.13
2.14
f1 (ppm)

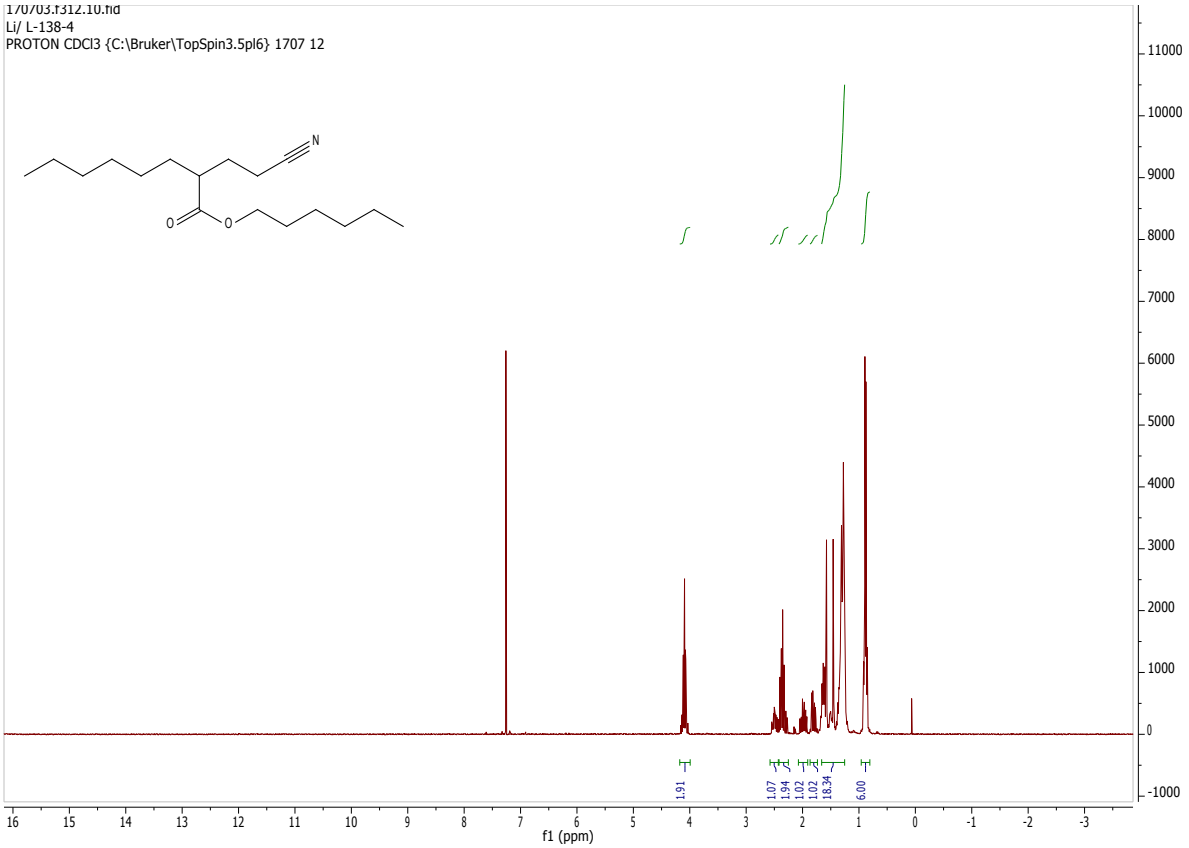

171011.319.2.fid
Yahui Li L-45-31
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 1710 22
172.08
119.05
69.64
32.43
20.81
16.56
9.74
3.29
f1 (ppm)

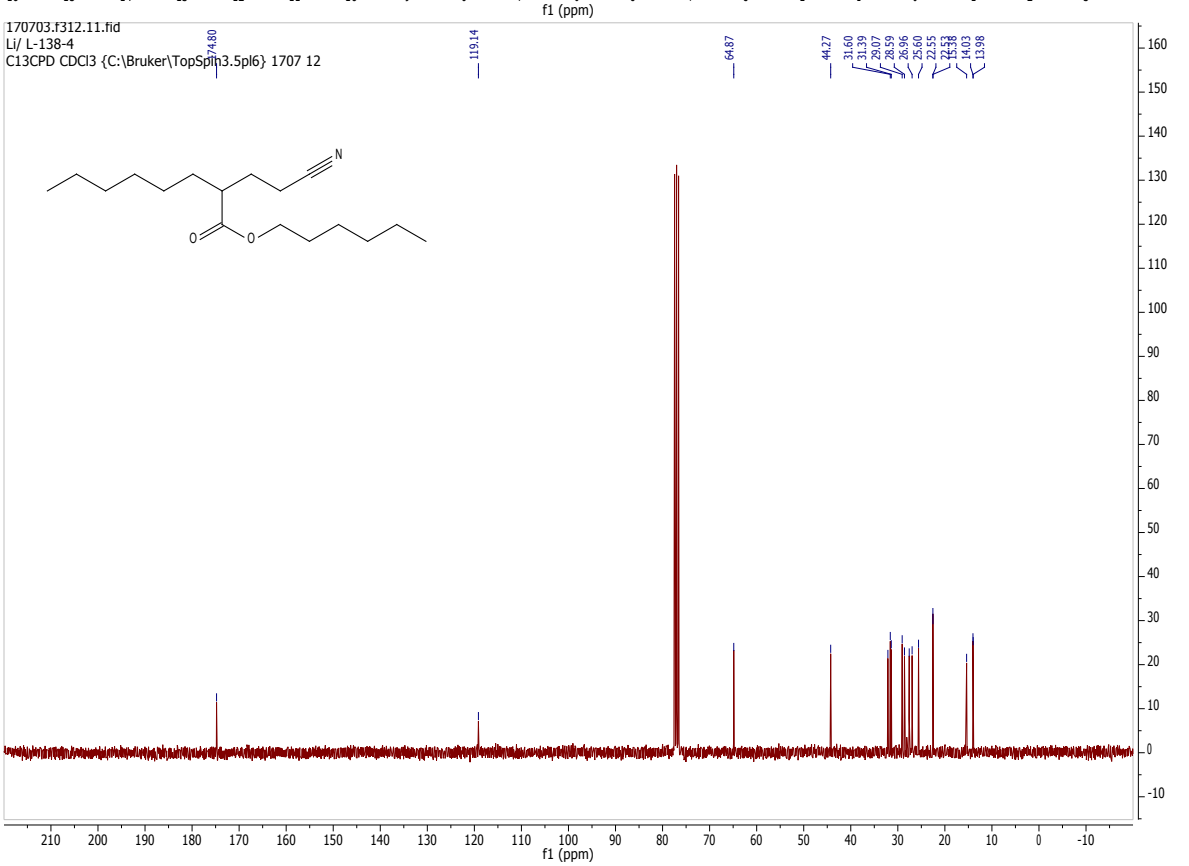

171009.311.1.fid
Yahui Li L-45-5
Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 1710 11
1.07
2.10
2.00
4.03
2.13
f1 (ppm)

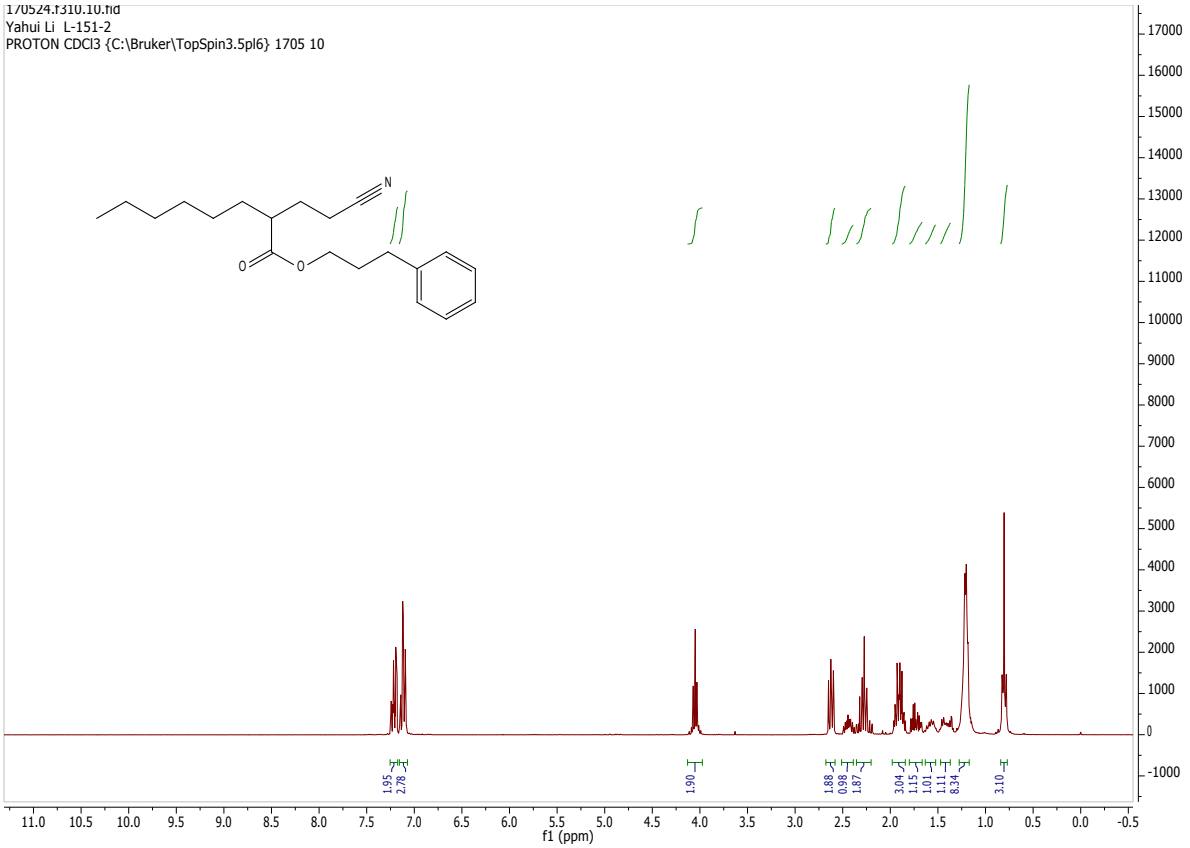

171009.311.2.fid
Yahui Li L-45-5
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 1710 11
171.62
131.82
118.64
65.45
32.29
20.73
f1 (ppm)

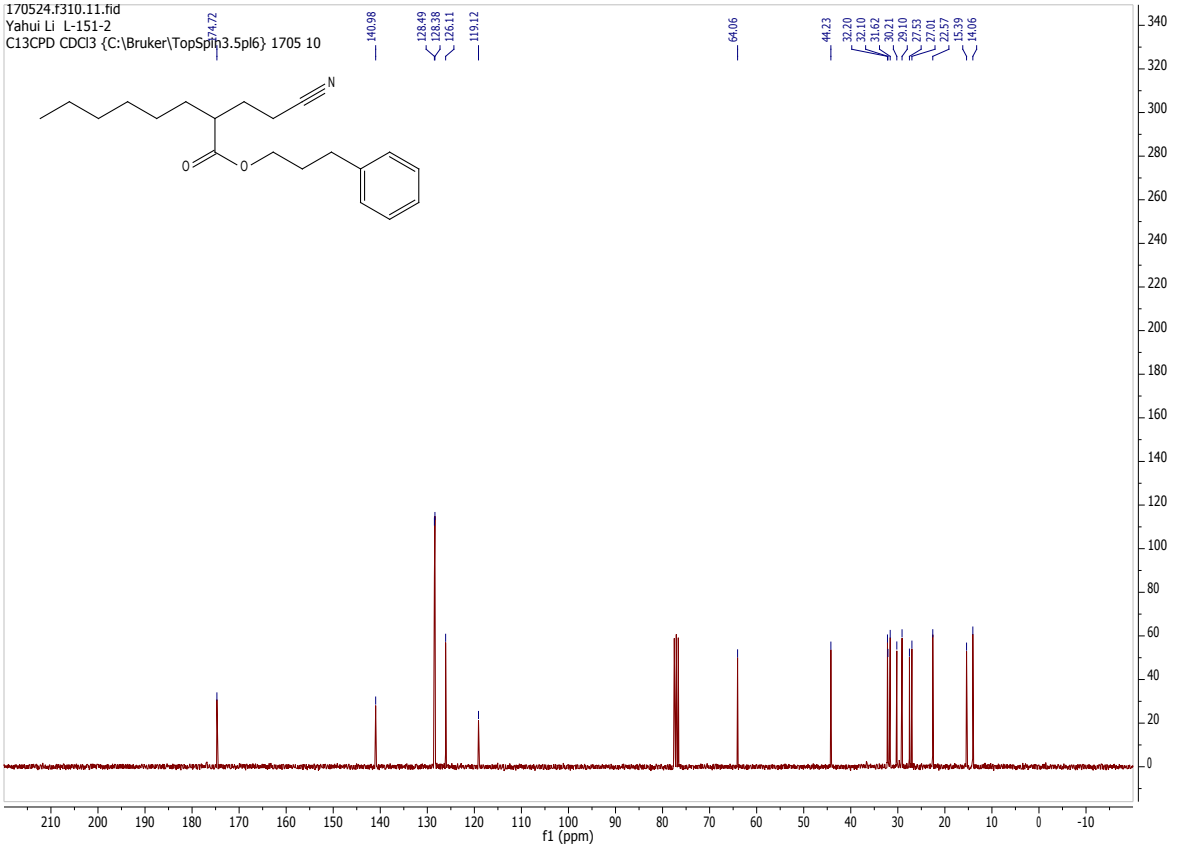

171012.f302.10.fid
Yahui Li L-45-72
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1710 2
N
O
O
Br
1.02
1.03
1.02
1.03
2.10
1.91
1.99
2.00
f1 (ppm)

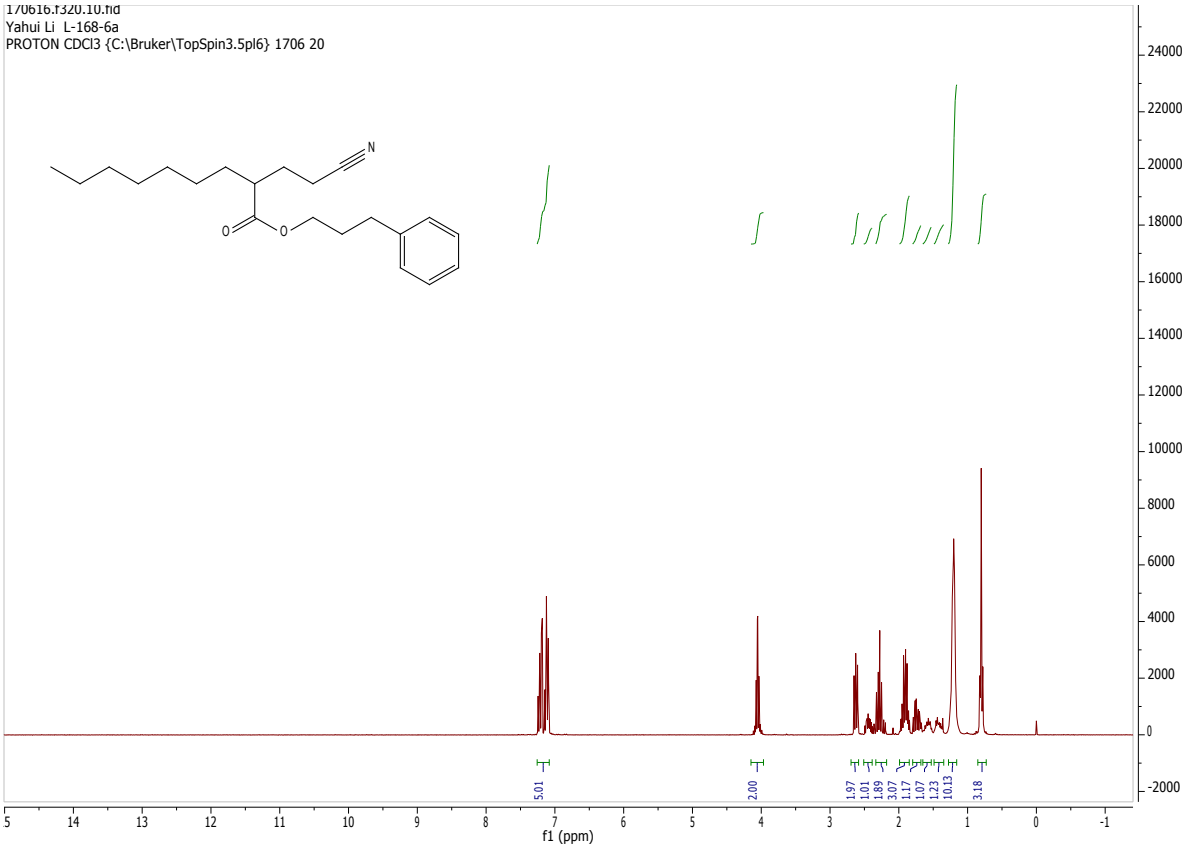

171012.f302.11.fid
Yahui Li L-45-72
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1710 2
171.56
134.88
132.98
130.17
129.99
127.60
123.65
118.92
66.23
32.33
20.77
16.57
N
O
O
Br
f1 (ppm)

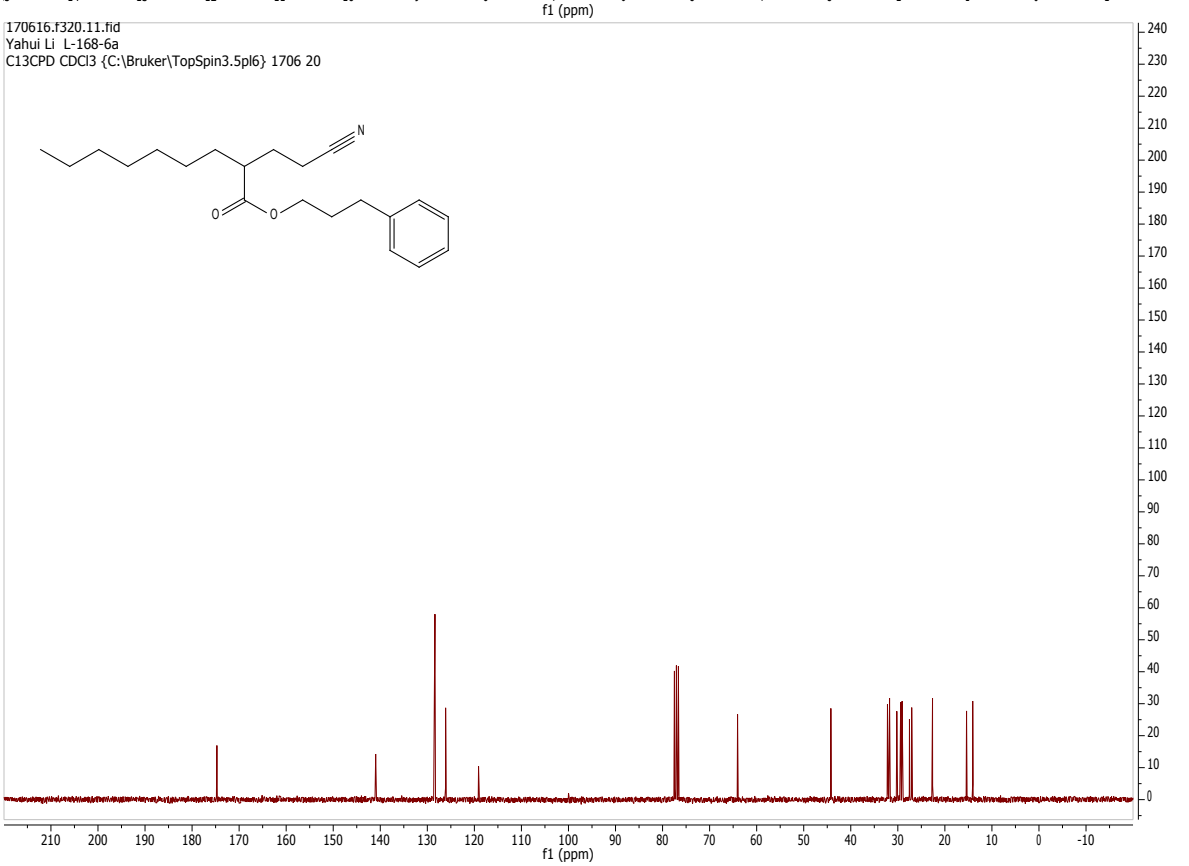

170703.f312.10.fid
Li/ L-138-4
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 12
N
O
O
1.91
1.07
1.94
1.02
1.02
18.34
6.00
f1 (ppm)

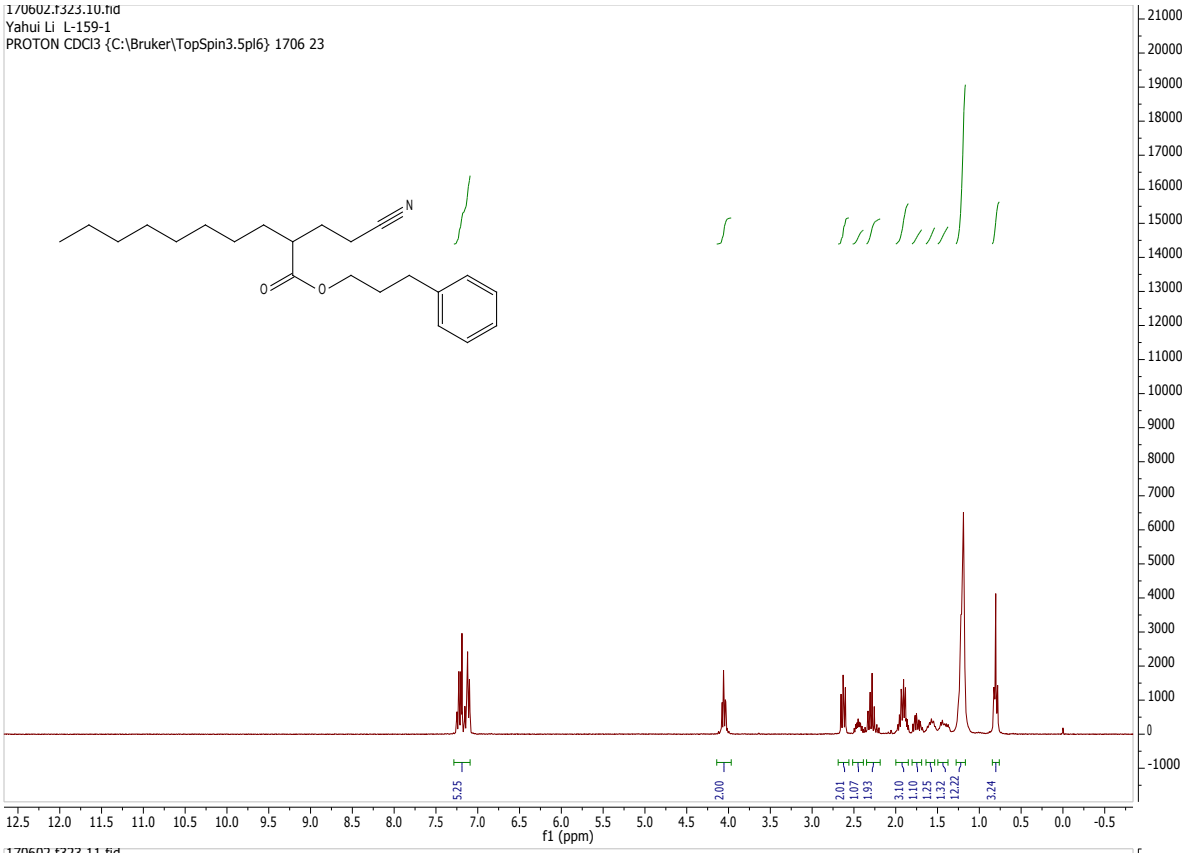

170703.f312.11.fid
Li/ L-138-4
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 12
174.80
119.14
64.87
44.27
31.60
31.39
29.07
28.59
26.96
25.60
22.55
22.53
15.38
14.03
13.98
N
O
O
f1 (ppm)

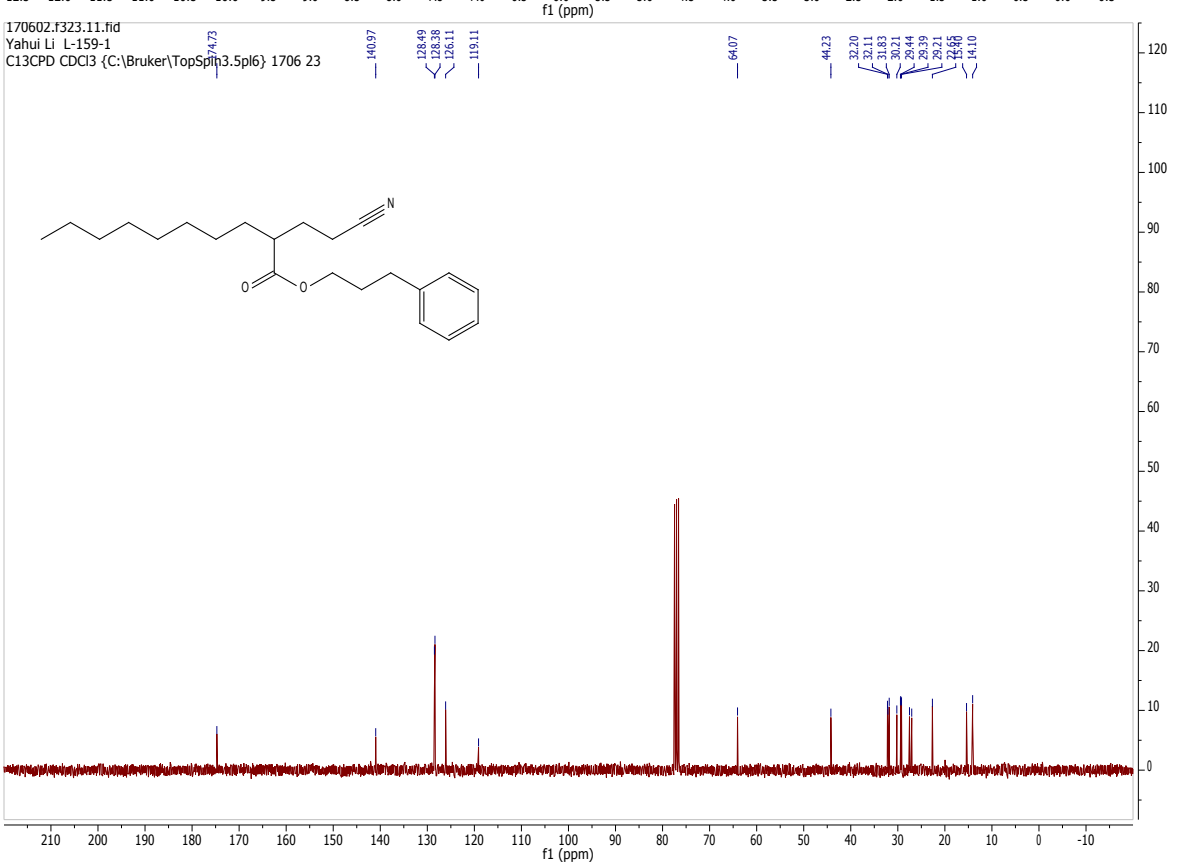

170524.f310.10.fid
Yahui Li L-151-2
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1705 10
N
O
O
1.95
2.78
1.90
1.88
0.98
1.87
3.04
1.15
1.01
1.11
8.34
3.10
f1 (ppm)

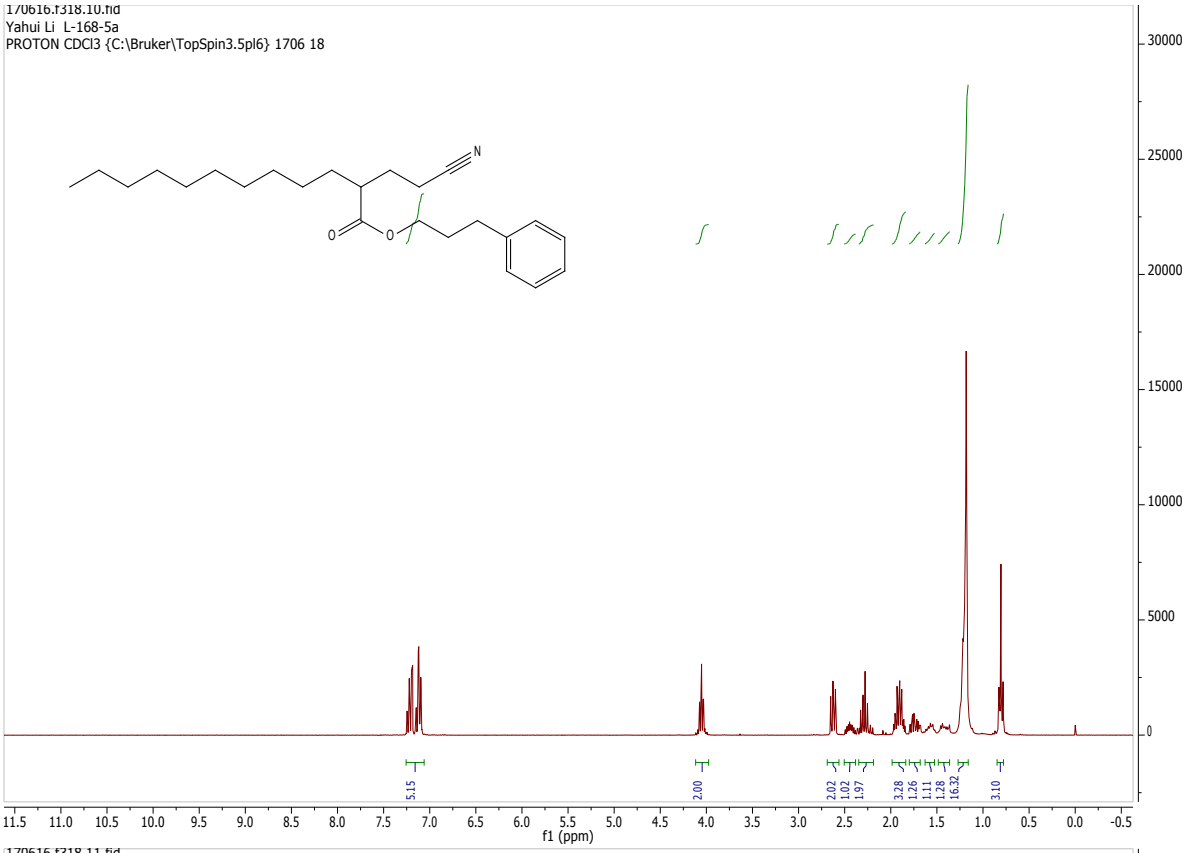

170524.f310.11.fid
Yahui Li L-151-2
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1705 10
174.72
140.98
128.49
128.38
126.11
119.12
64.06
44.23
32.20
32.10
31.62
30.21
29.10
27.53
27.01
22.57
15.39
14.06
N
O
O
f1 (ppm)

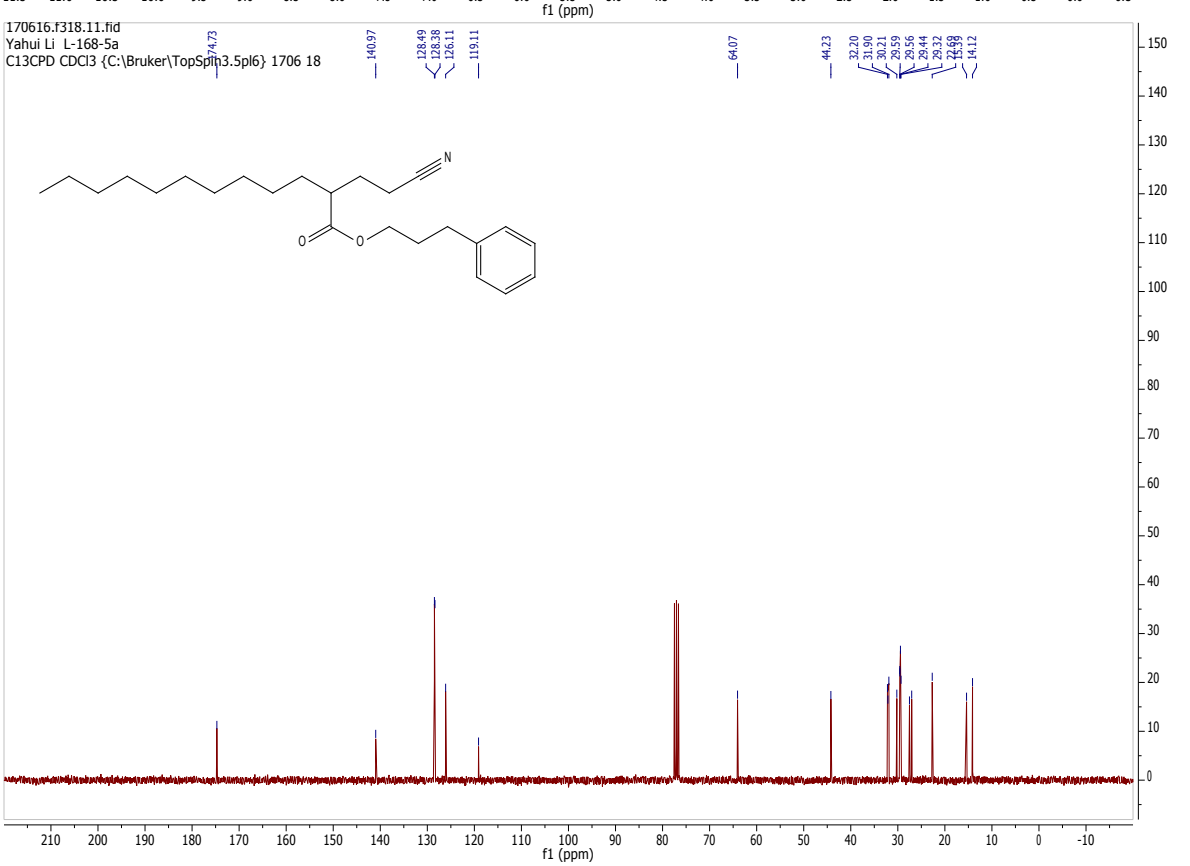

170616.f320.10.fid
Yahui Li L-168-6a
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 20
N
O
O
5.01
2.00
1.97
1.01
1.89
3.07
1.17
1.07
1.23
10.13
3.18
f1 (ppm)

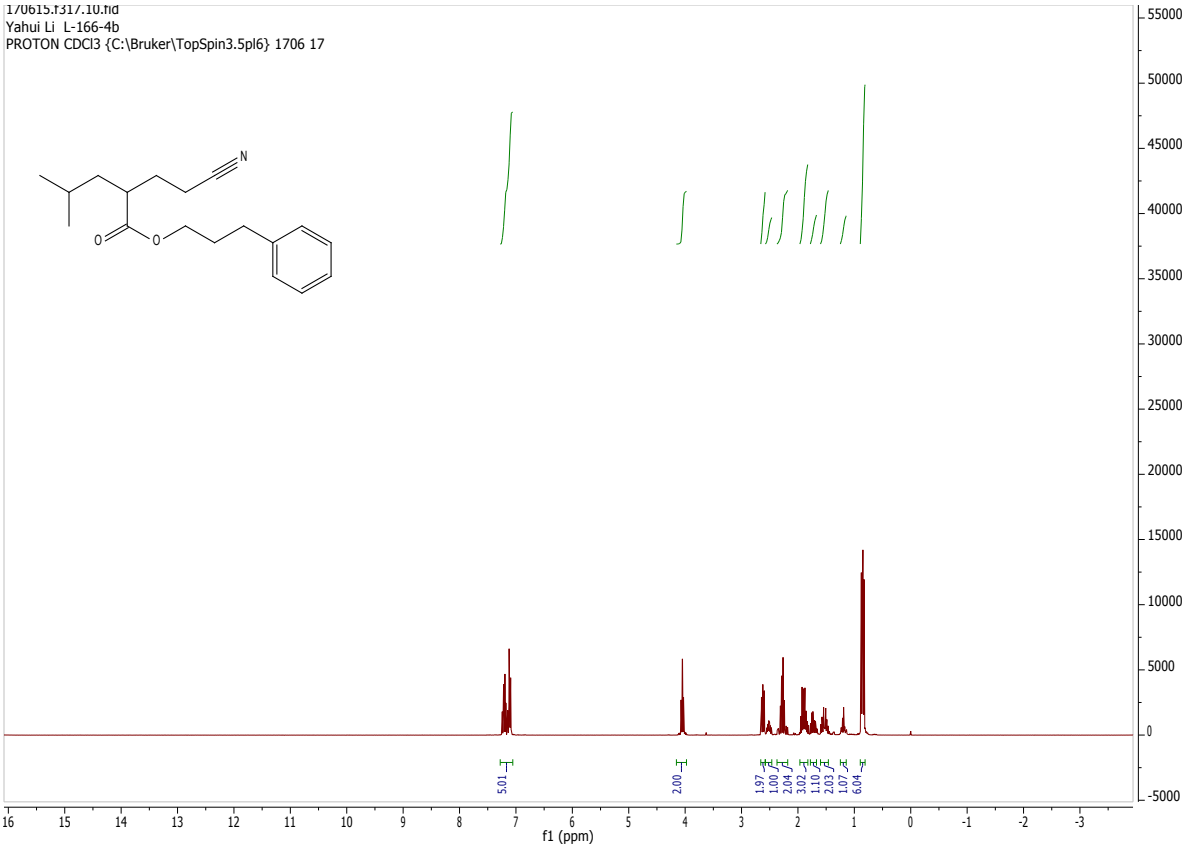

170616.f320.11.fid
Yahui Li L-168-6a
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 20
N
O
O
f1 (ppm)

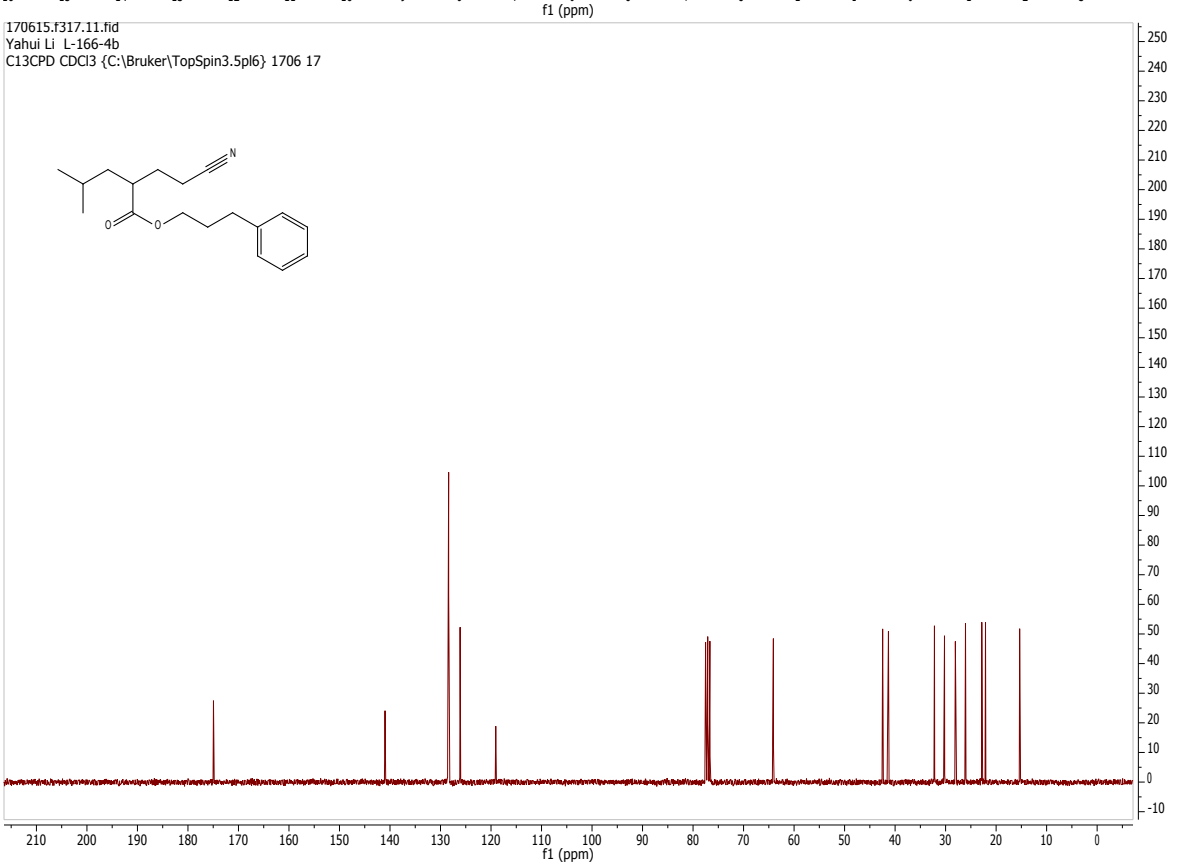

170602.f323.10.fid
Yahui Li L-159-1
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 23
N
O
O
5.25
2.00
2.01
1.07
1.93
3.10
1.10
1.25
1.32
12.22
3.24
f1 (ppm)

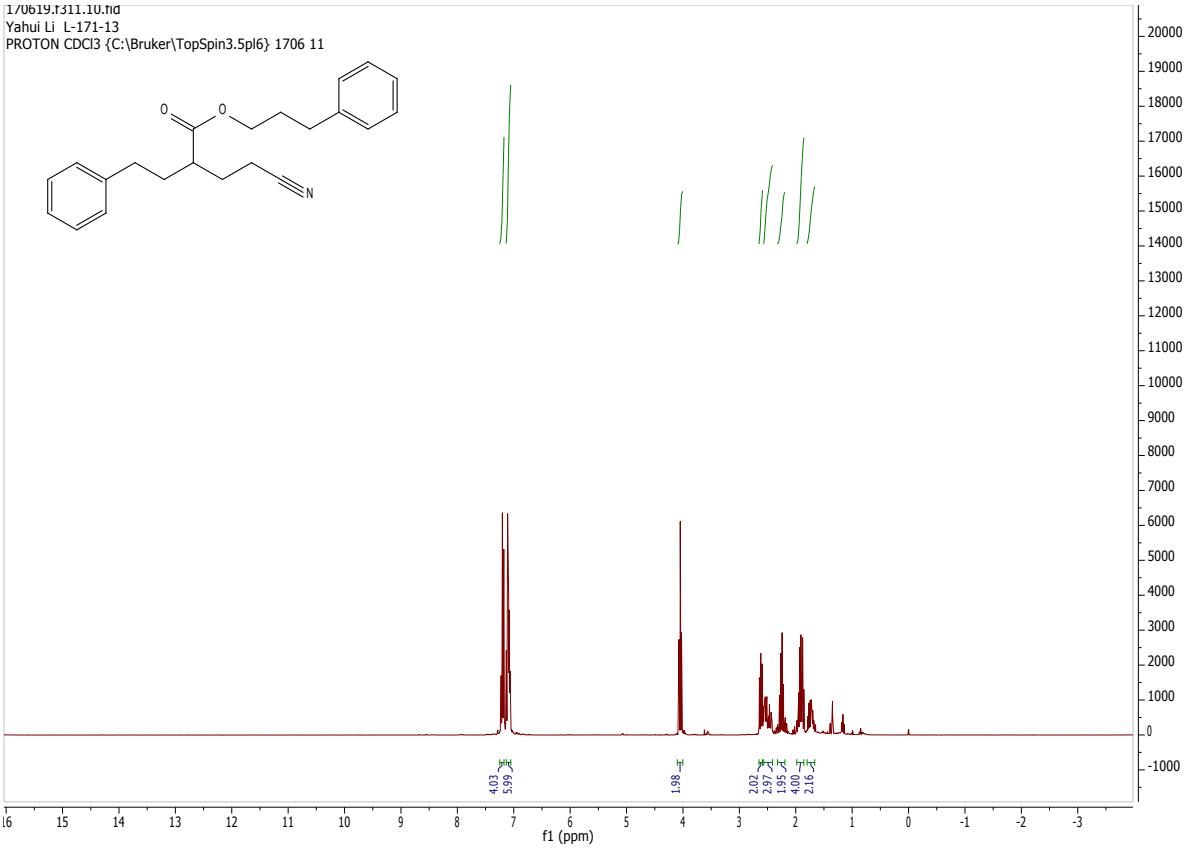

170602.f323.11.fid
Yahui Li L-159-1
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 23
174.73
140.97
128.49
128.38
126.11
119.11
64.07
44.23
32.20
32.11
31.83
30.21
29.44
29.39
29.21
25.85
14.10
N
O
O
f1 (ppm)

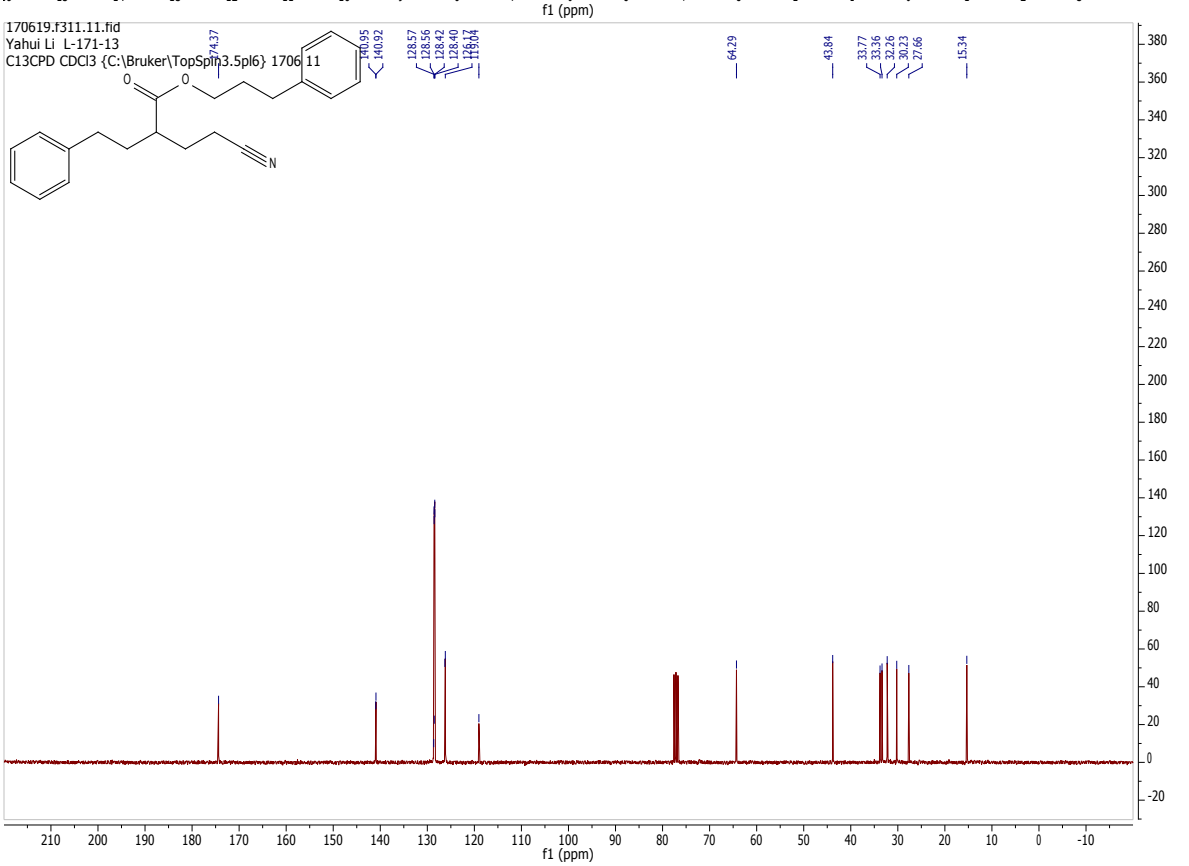

170616.f318.10.fid
Yahui Li L-168-5a
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 18
N
O
O
5.15
2.00
2.02
1.02
1.97
3.28
1.26
1.11
1.28
16.32
3.10
f1 (ppm)

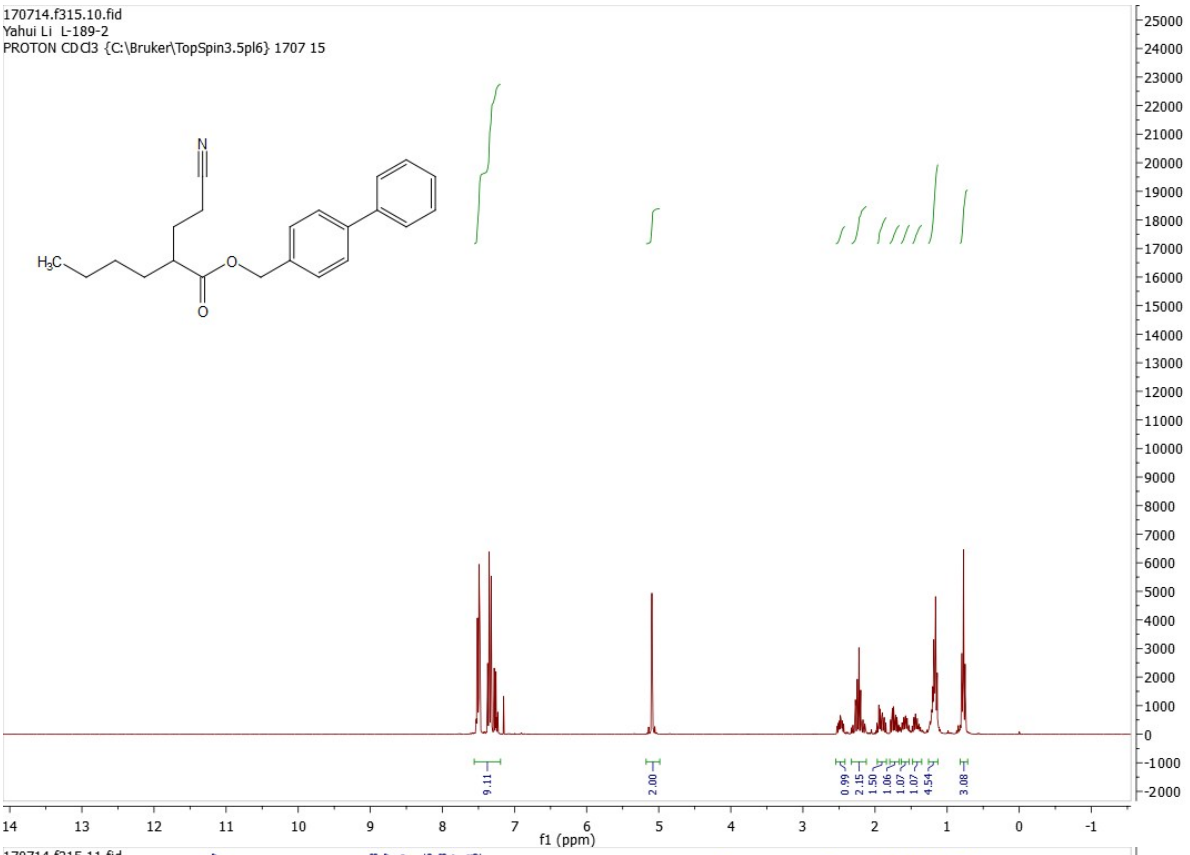

170616.f318.11.fid
Yahui Li L-168-5a
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 18
174.73
140.97
128.49
128.38
126.11
119.11
64.07
44.23
32.20
31.90
30.21
29.59
29.56
29.44
29.32
14.12
N
O
O
f1 (ppm)

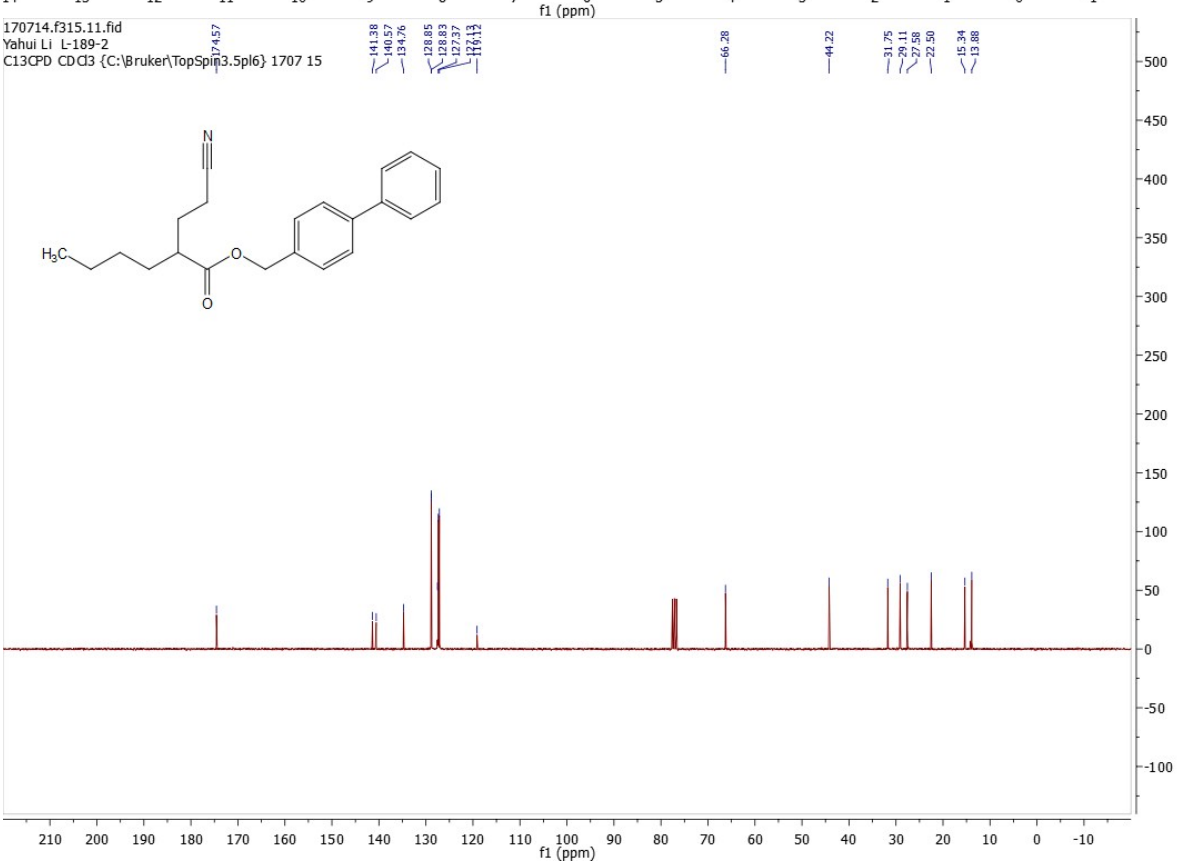

170615.f317.10.fid
Yahui Li L-166-4b
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 17
N
O
O
5.01
2.00
1.97
1.00
2.04
3.02
1.10
2.03
1.07
6.04
f1 (ppm)

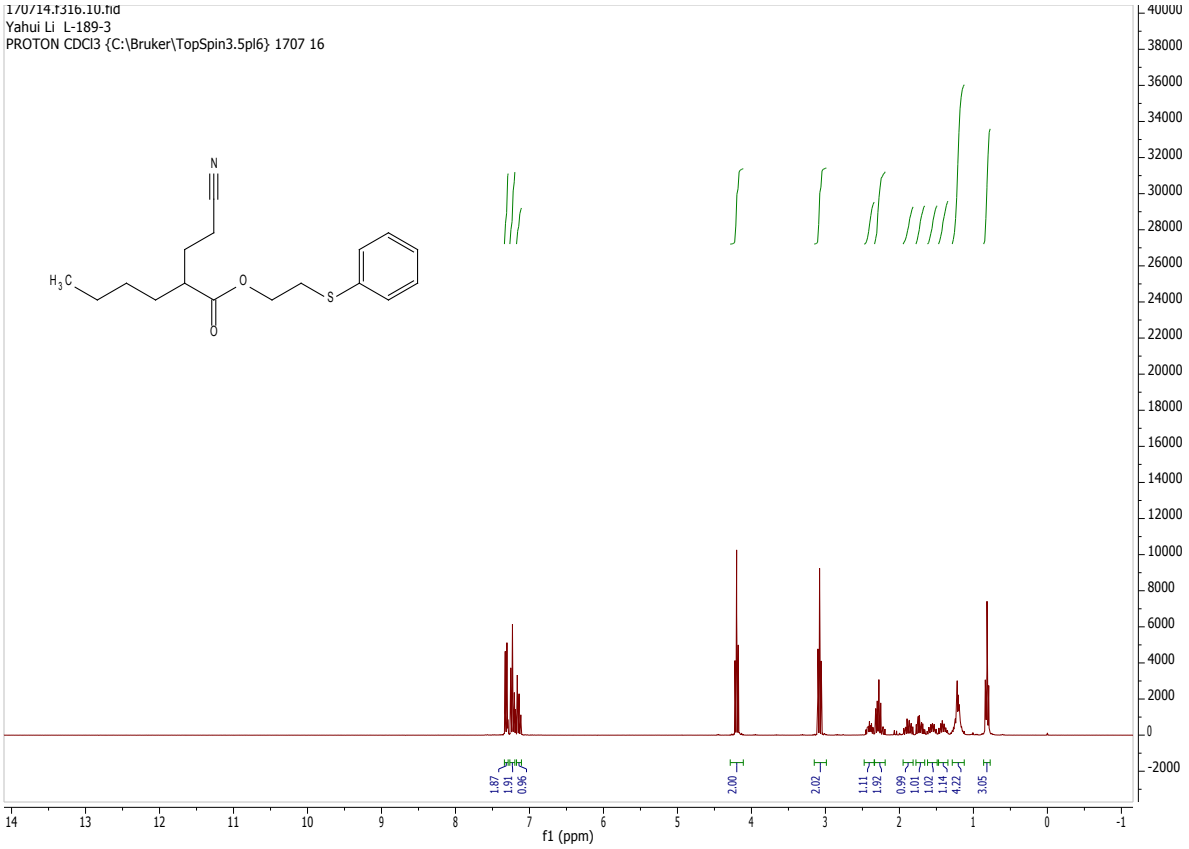

170615.f317.11.fid
Yahui Li L-166-4b
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 17
N
O
O
f1 (ppm)

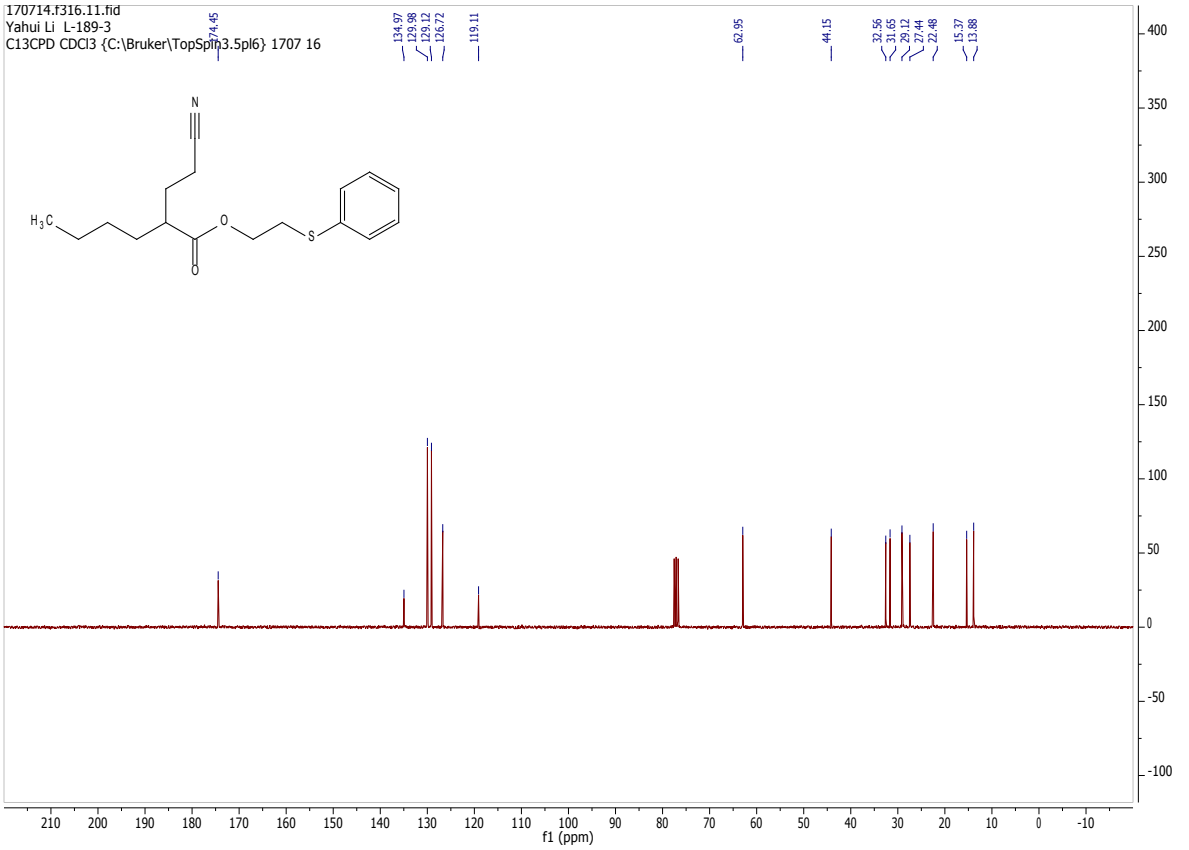

170619.f311.10.fid
Yahui Li L-171-13
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 11
O
O
N
4.03
5.99
1.98
2.02
2.97
1.95
4.00
2.16
f1 (ppm)

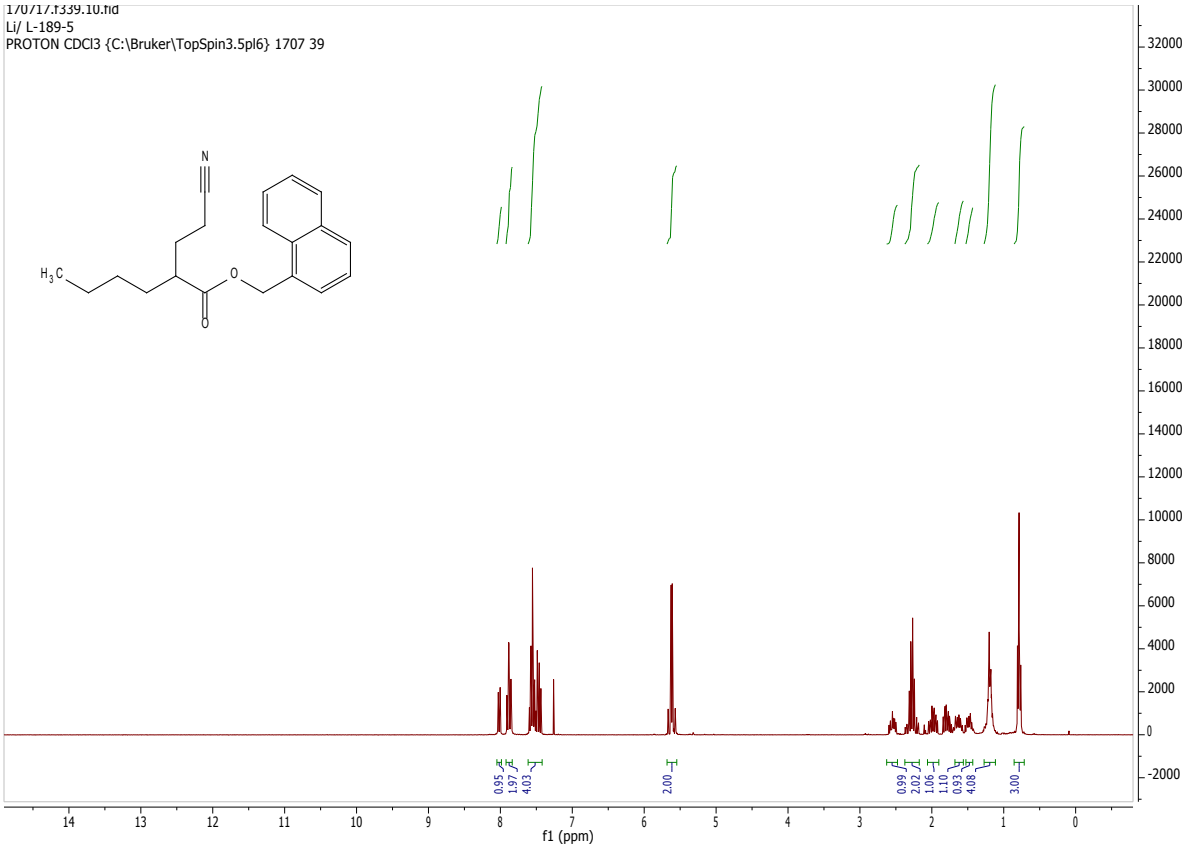

170619.f311.11.fid
Yahui Li L-171-13
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1706 11
O
O
N
174.37
140.95
140.92
128.57
128.56
128.42
128.40
126.17
119.04
64.29
43.84
33.77
33.36
32.26
30.23
27.66
15.34
f1 (ppm)

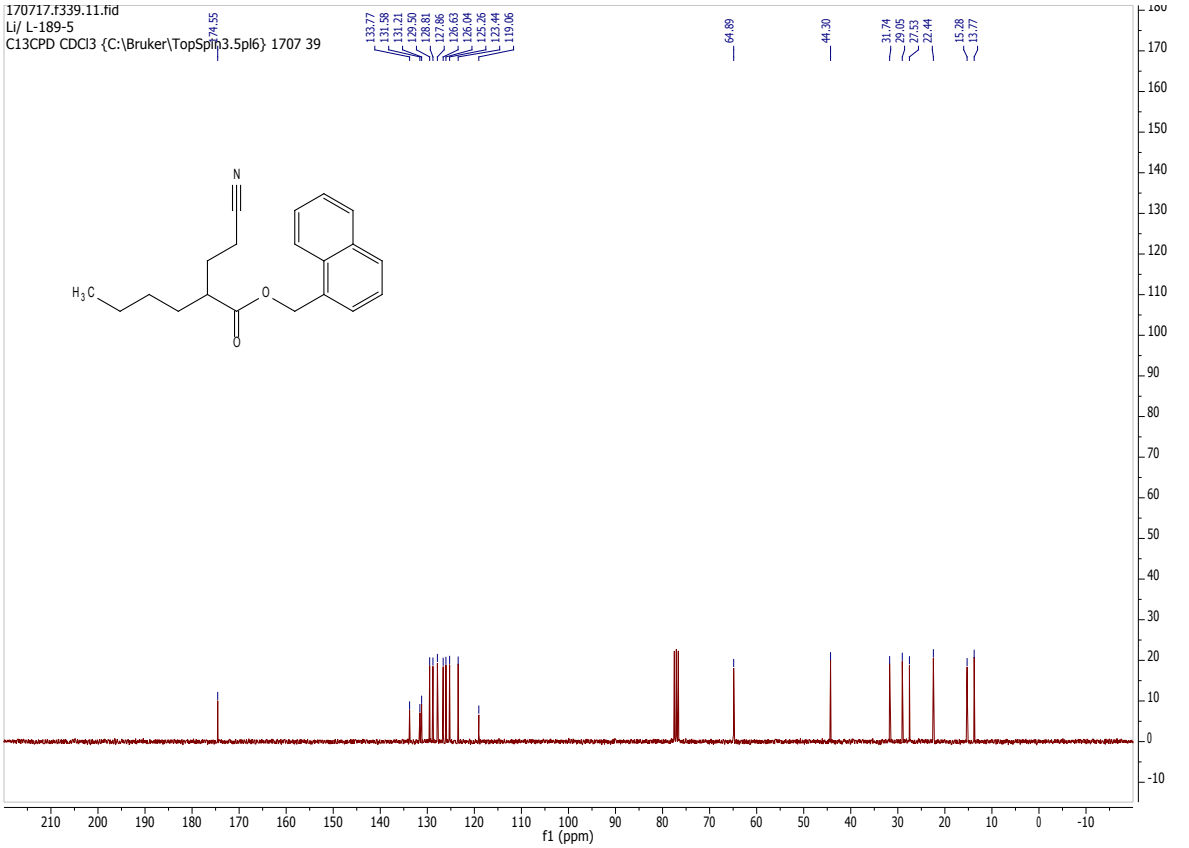

170714.f315.10.fid
Yahui Li L-189-2
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 15
N
H3C
O
O
9.11
2.00
0.99
2.15
1.50
1.06
1.07
1.07
4.54
3.08
f1 (ppm)

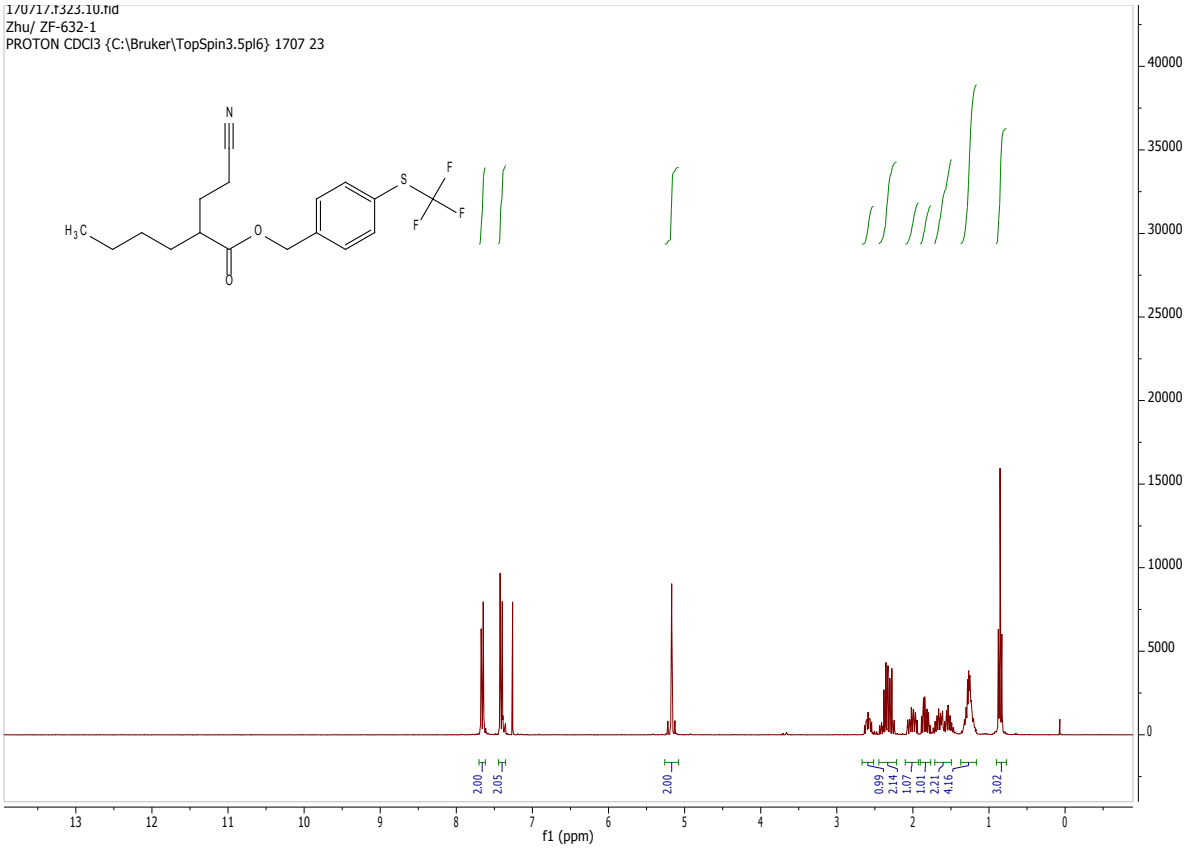

170714.f315.11.fid
Yahui Li L-189-2
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 15
174.57
141.38
140.57
134.76
128.85
128.83
127.37
127.13
119.12
66.28
44.22
31.75
29.11
27.58
22.50
15.34
13.88
N
H3C
O
O
f1 (ppm)

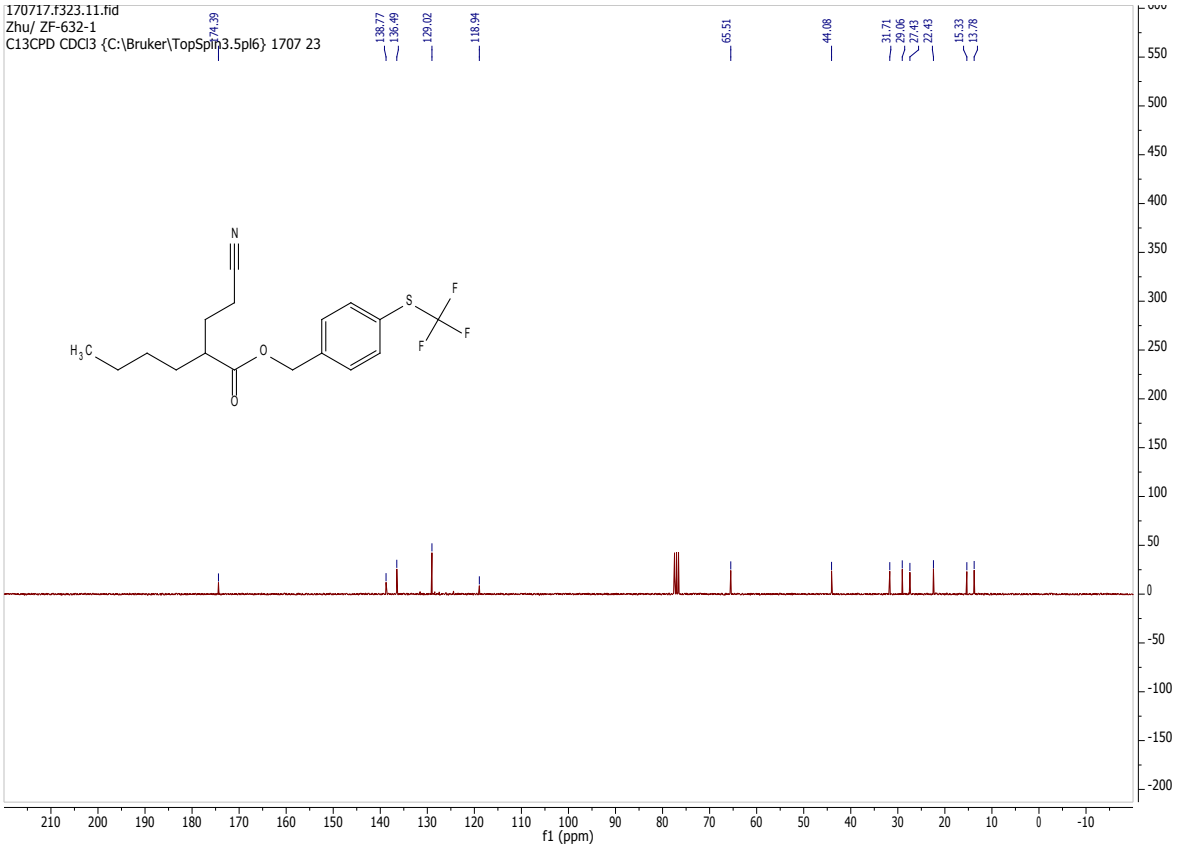

170714.f316.10.fid
Yahui Li L-189-3
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 16
N
H3C
O
S
O
1.87
1.91
0.96
2.00
2.02
1.11
1.92
0.99
1.01
1.02
1.14
4.22
3.05
f1 (ppm)

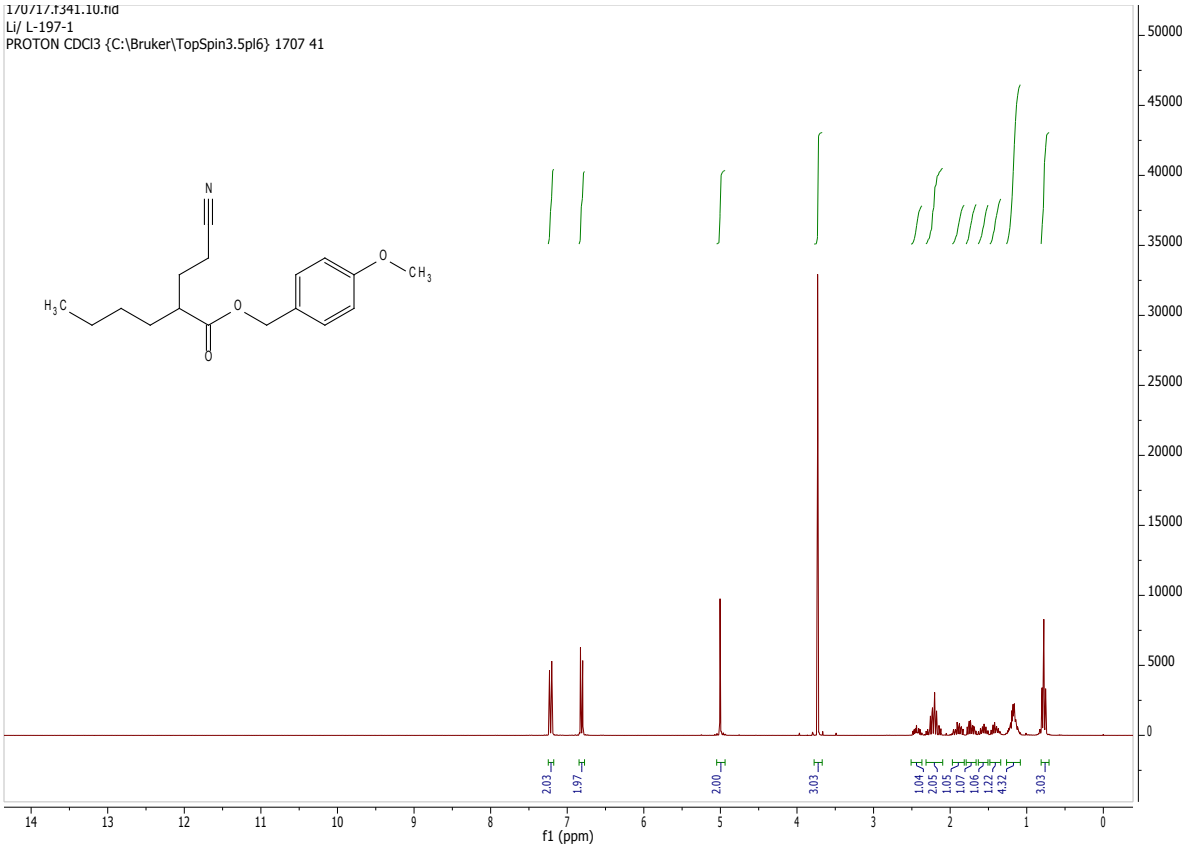

170714.f316.11.fid
Yahui Li L-189-3
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 16
174.45
134.97
129.98
129.12
126.72
119.11
62.95
44.15
32.56
31.65
29.12
27.44
22.48
15.37
13.88
N
H3C
O
S
O
f1 (ppm)

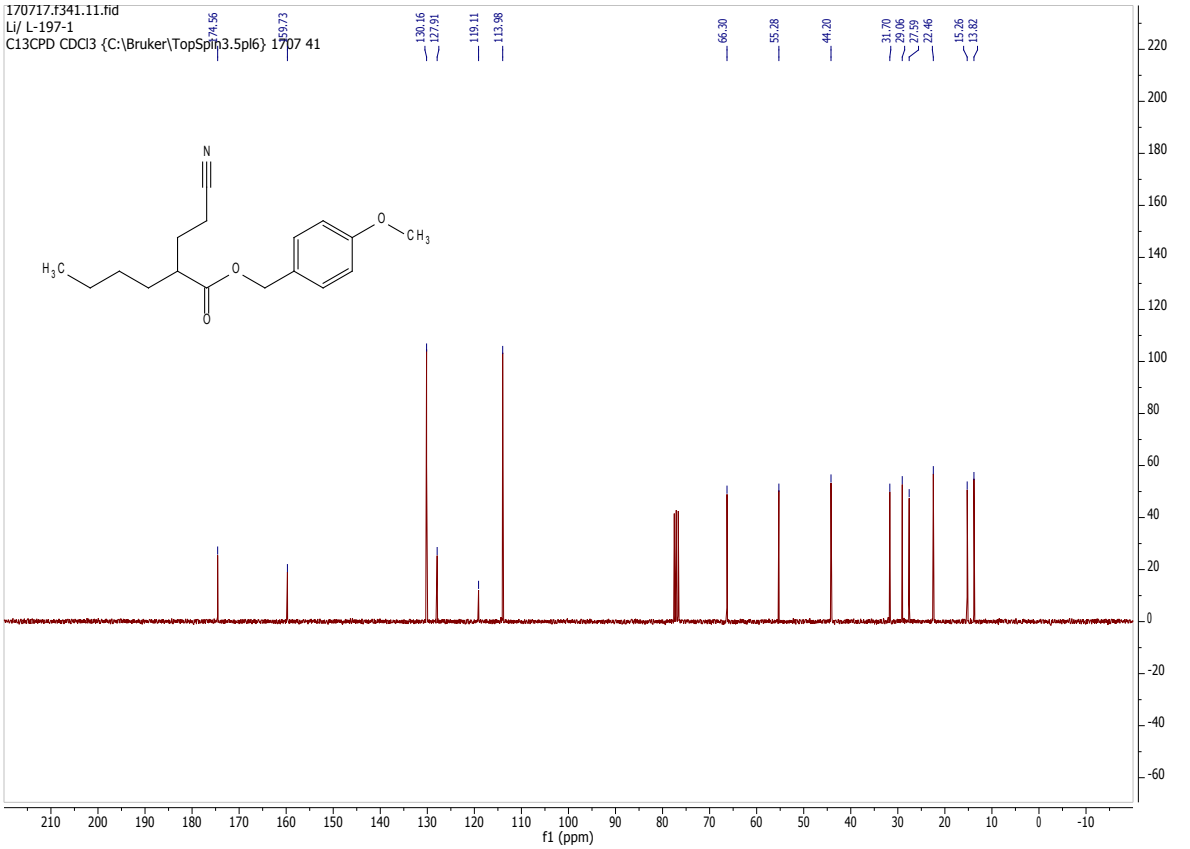

170717.f339.10.fid
Li/ L-189-5
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 39
N
H3C
O
O
0.95
1.97
4.03
2.00
0.99
2.02
1.06
1.10
0.93
4.08
3.00
f1 (ppm)

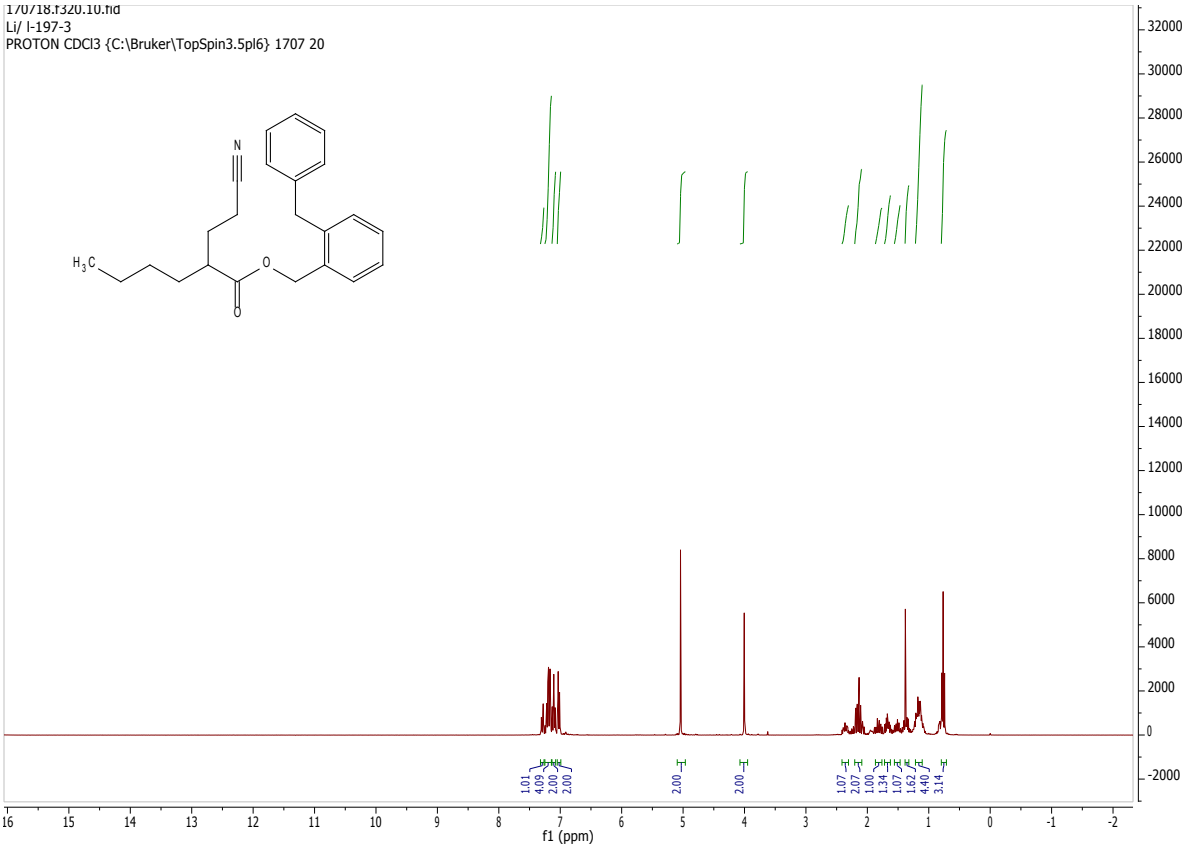

170717.f339.11.fid
Li/ L-189-5
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 39
174.55
133.77
131.58
131.21
129.50
128.81
127.86
126.63
126.04
125.26
123.44
119.06
64.89
44.30
31.74
29.05
27.53
22.44
15.28
13.77
N
H3C
O
O
f1 (ppm)

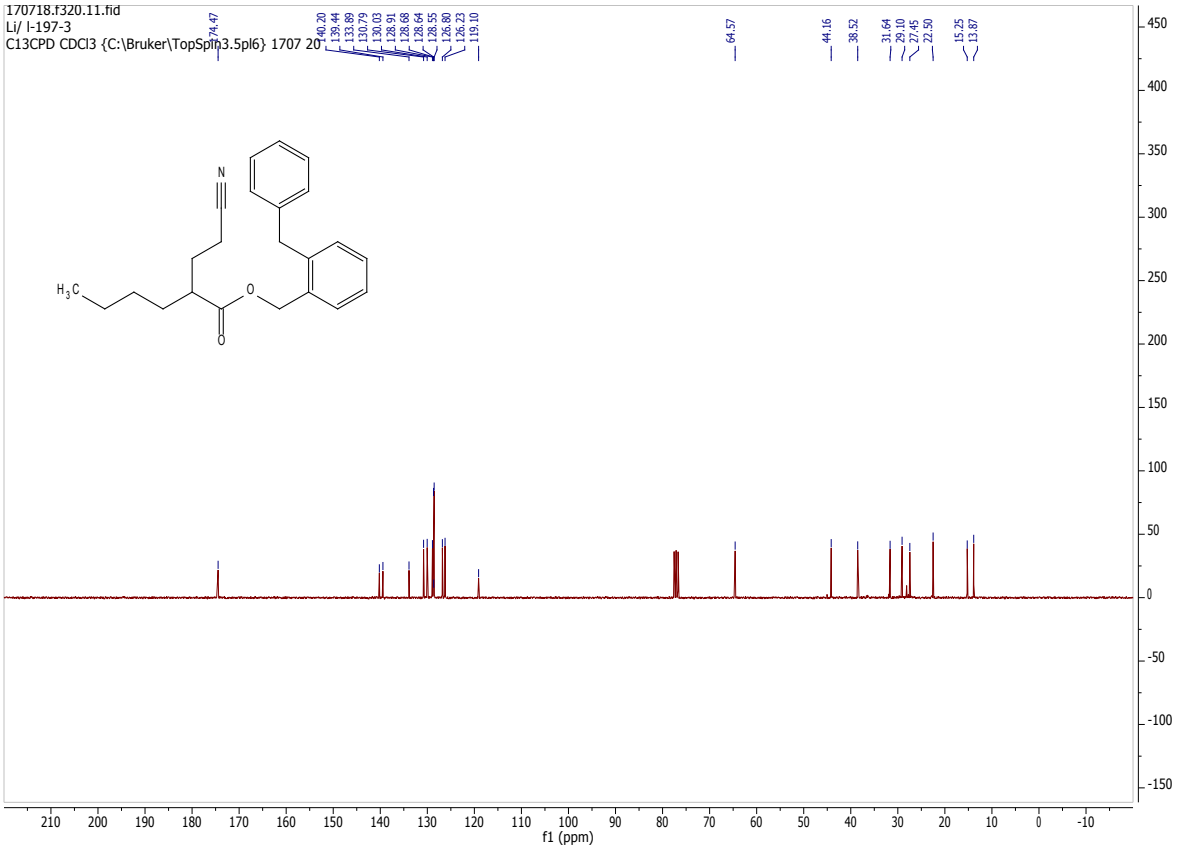

170717.f323.10.fid
Zhu/ ZF-632-1
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 23
N
S
F
F
F
H3C
O
O
40000
35000
30000
25000
20000
15000
10000
5000
0
2.00
2.05
2.00
0.99
2.14
1.07
1.01
2.21
4.16
3.02
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

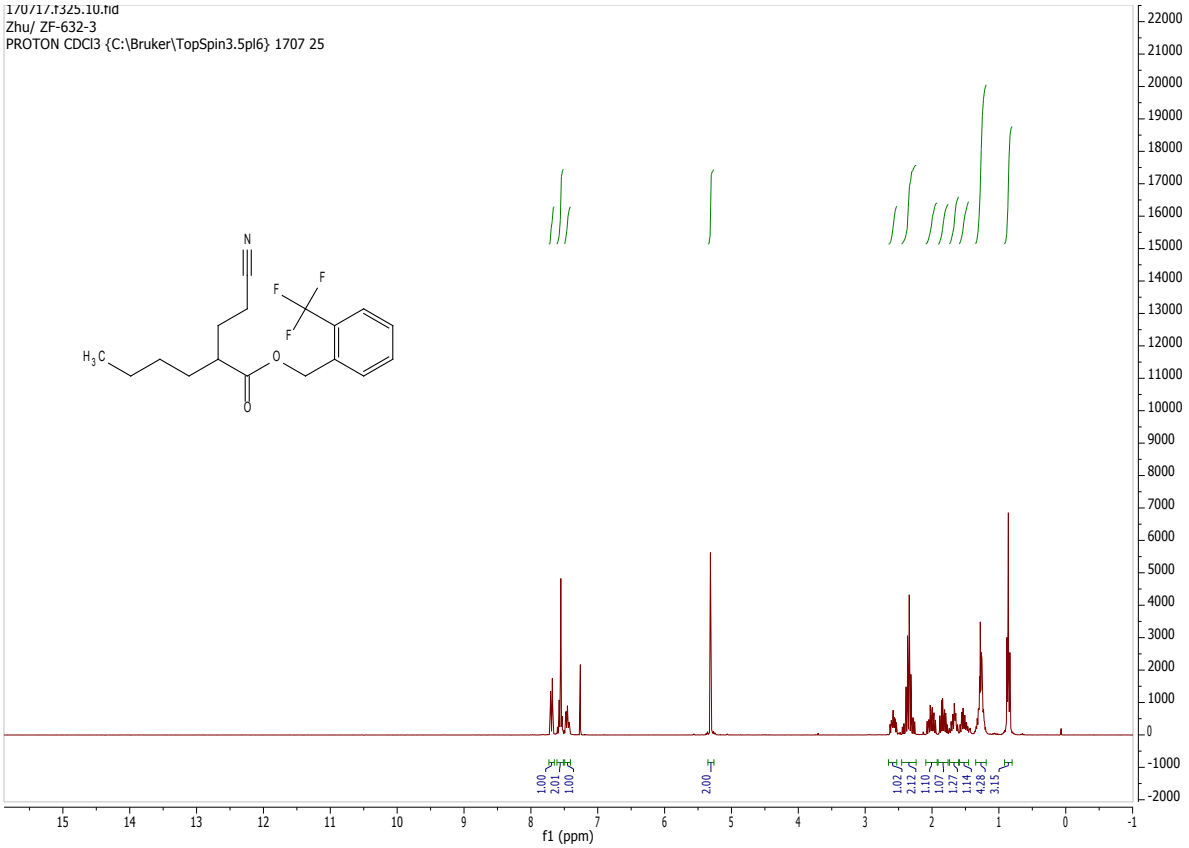

170717.f323.11.fid
Zhu/ ZF-632-1
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 23
174.39
138.77
136.49
129.02
118.94
65.51
44.08
31.71
29.06
27.43
22.43
15.33
13.78
N
S
F
F
F
H3C
O
O
550
500
450
400
350
300
250
200
150
100
50
0
-50
-100
-150
-200
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

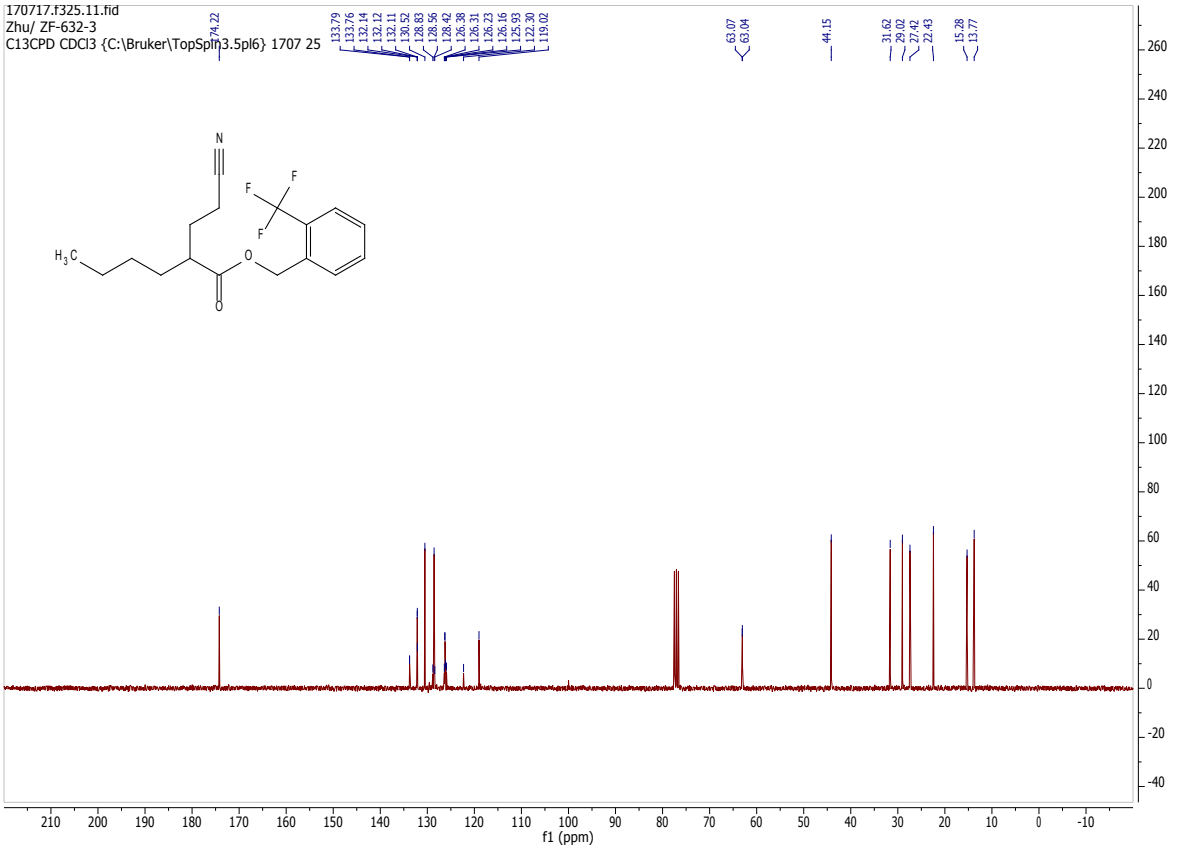

170717.f341.10.fid
Li/ L-197-1
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 41
N
O
CH3
H3C
O
O
2.03
1.97
2.00
3.03
1.04
2.05
1.05
1.07
1.06
1.22
4.32
3.03
f1 (ppm)

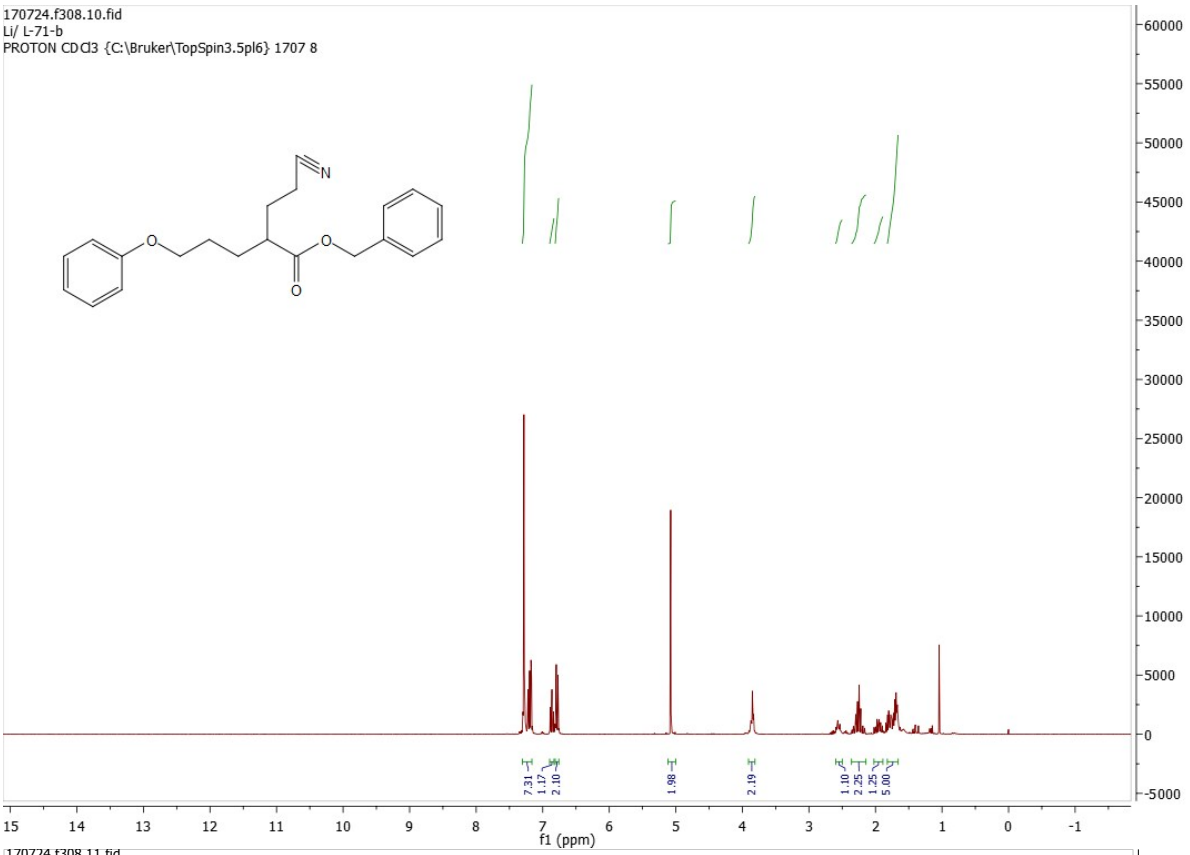

170717.f341.11.fid
Li/ L-197-1
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 41
174.56
159.73
130.16
127.91
119.11
113.98
66.30
55.28
44.20
31.70
29.06
27.59
22.46
15.26
13.82
N
O
CH3
H3C
O
O
f1 (ppm)

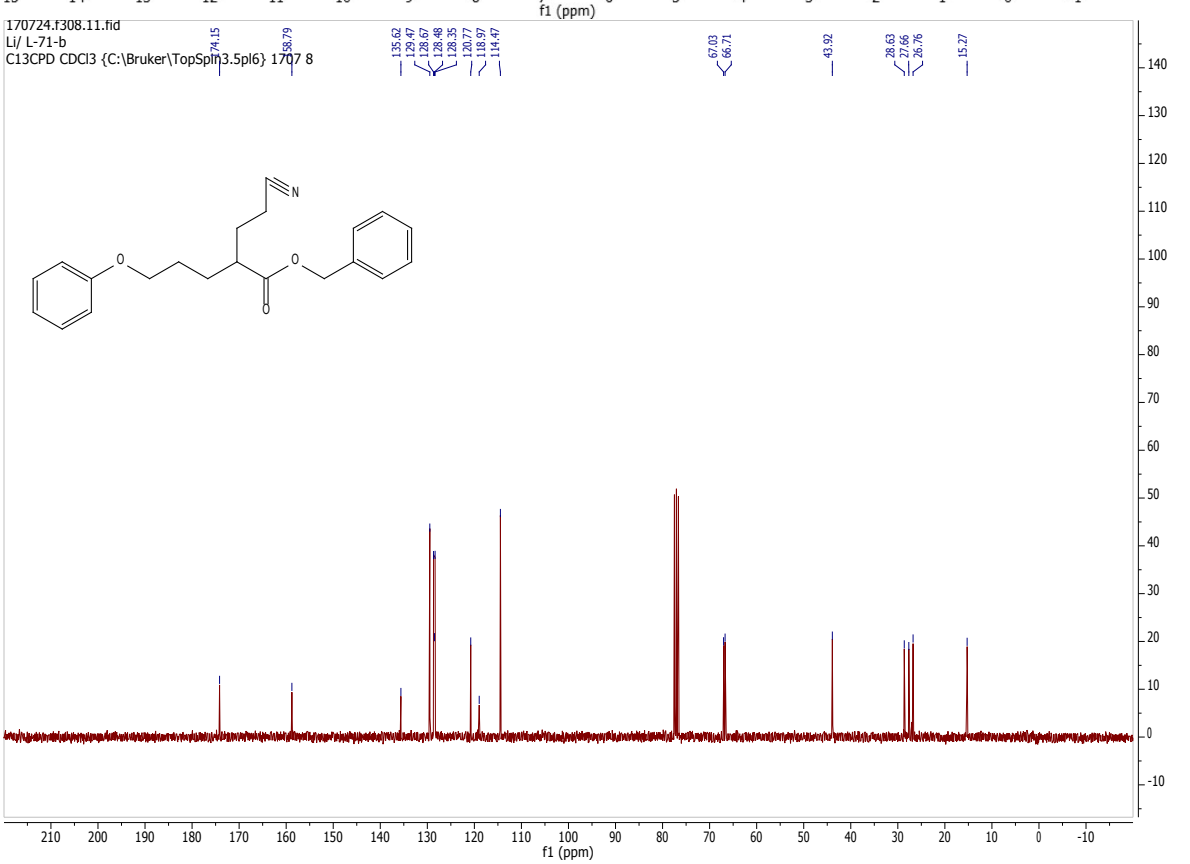

170718.f320.10.fid
Li/ l-197-3
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 20
N
H3C
O
O
1.01
4.09
2.00
2.00
2.00
2.00
1.07
2.07
1.00
1.34
1.07
1.62
4.40
3.14
f1 (ppm)

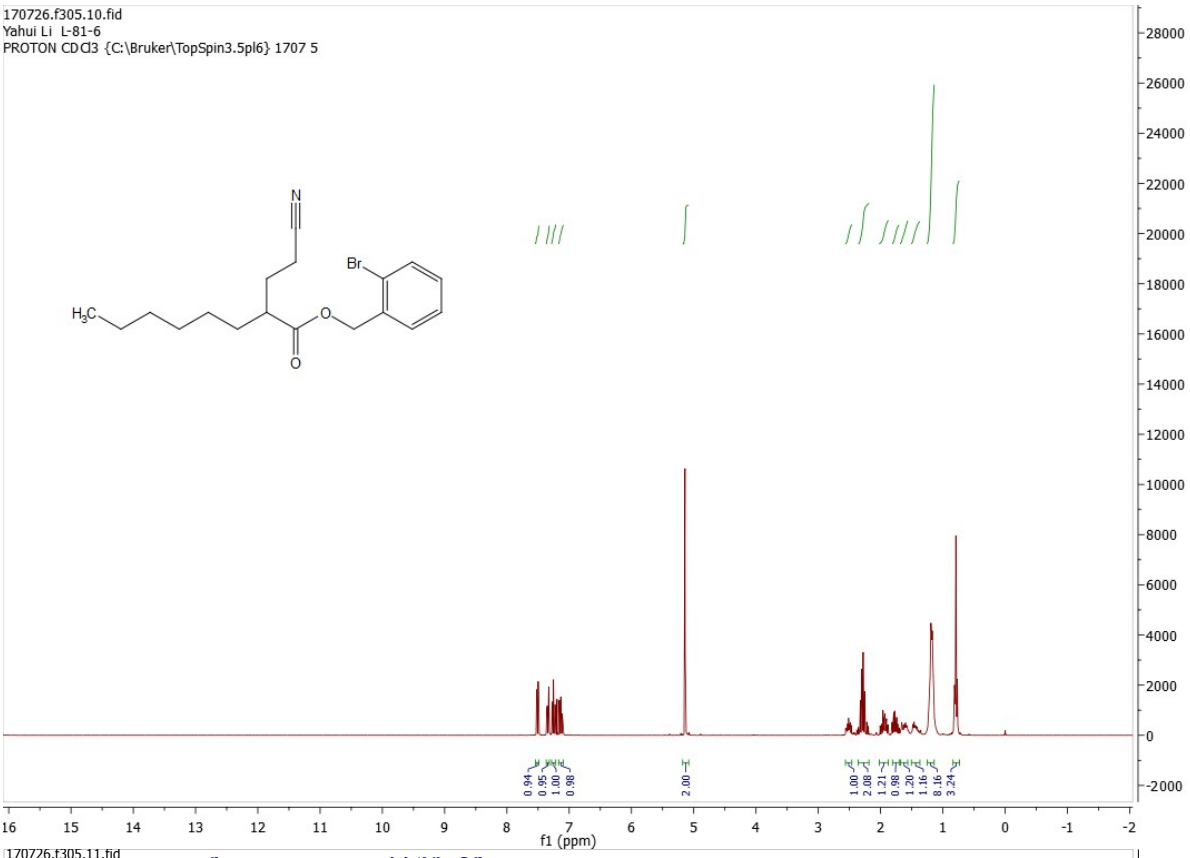

170718.f320.11.fid
Li/ l-197-3
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 20
174.47
140.20
139.44
133.89
130.79
130.03
128.91
128.68
128.64
128.55
126.80
126.23
119.10
64.57
44.16
38.52
31.64
29.10
27.45
22.50
15.25
13.87
N
H3C
O
O
f1 (ppm)

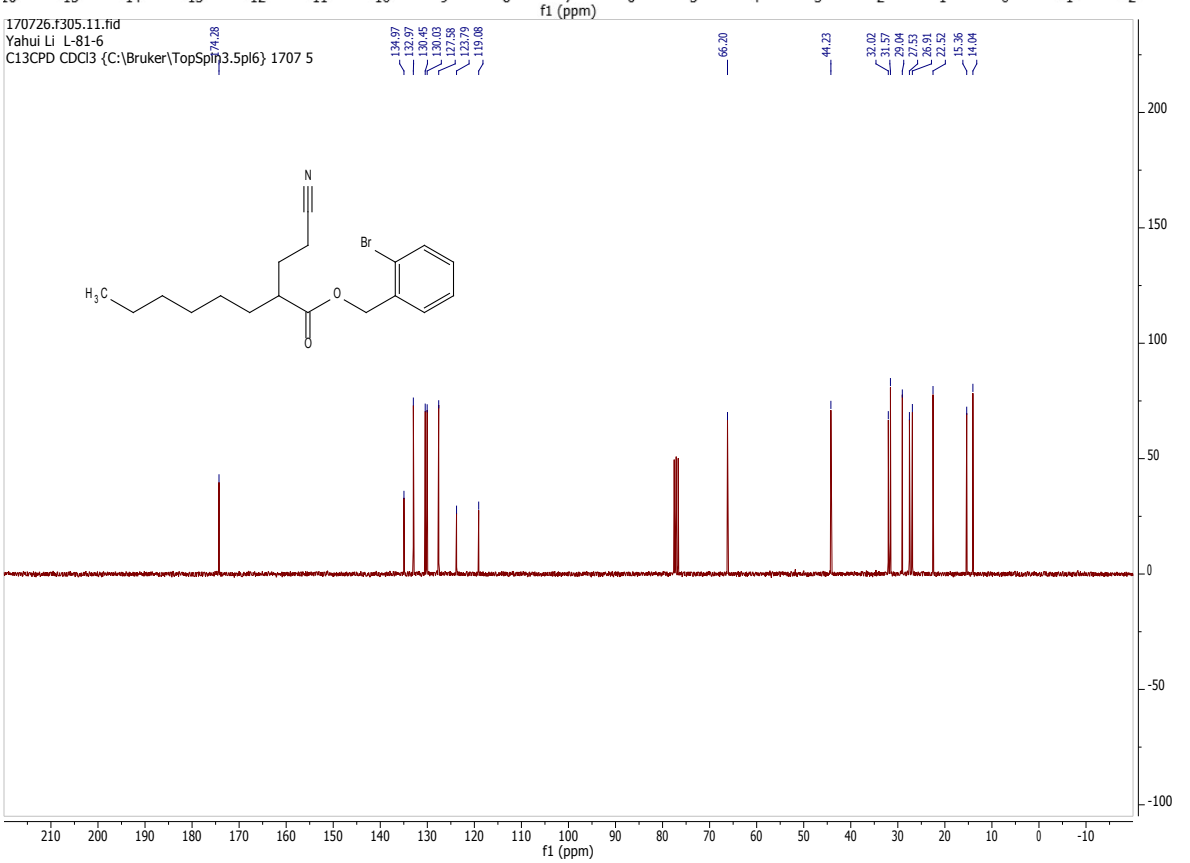

170717.f325.10.fid
Zhu/ ZF-632-3
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 25
f1 (ppm)

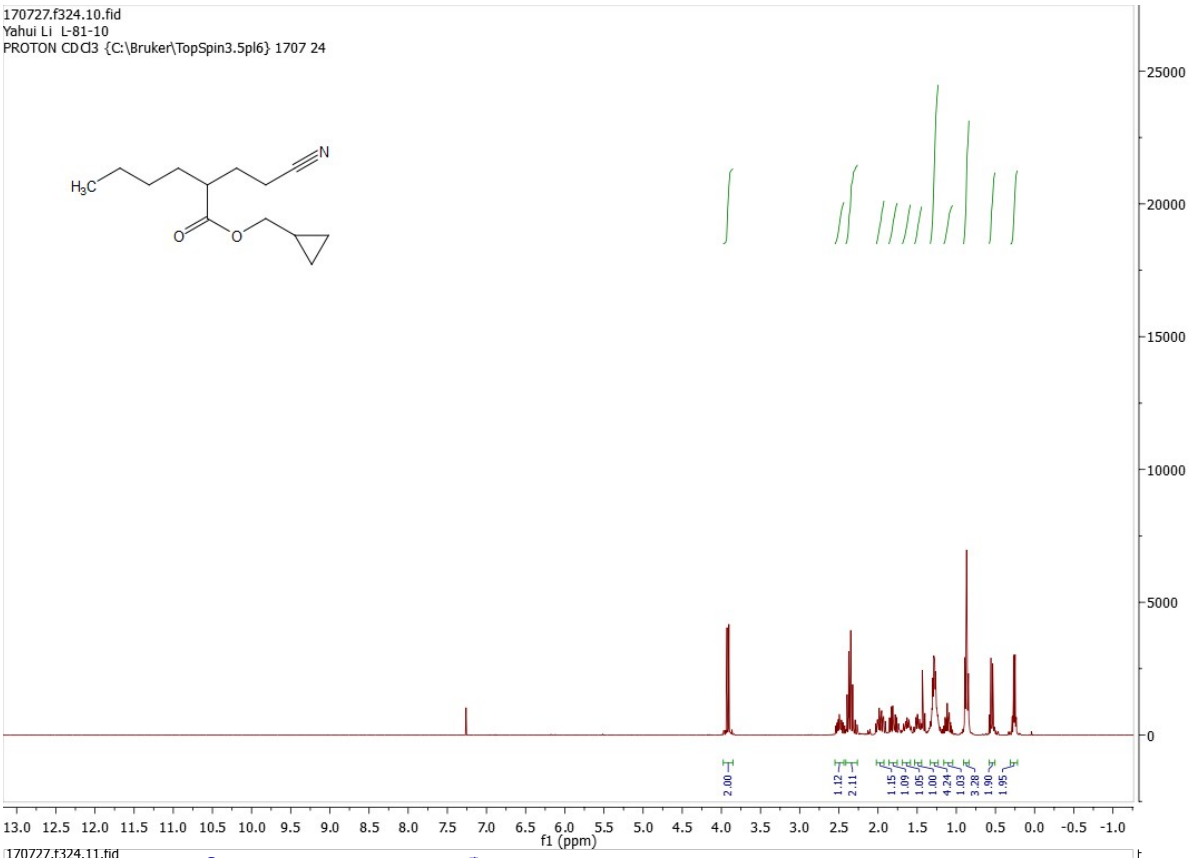

170717.f325.11.fid
Zhu/ ZF-632-3
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 25
f1 (ppm)

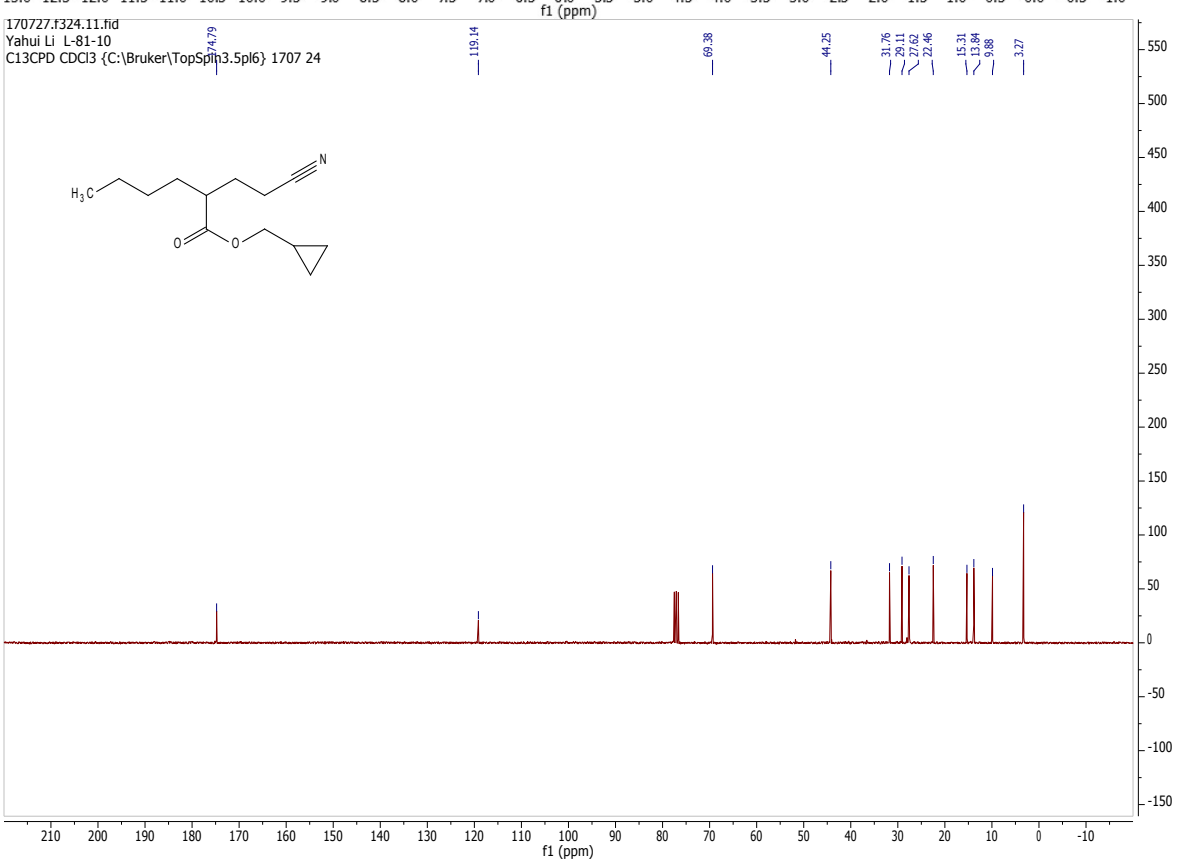

170724.f308.10.fid
Li/ L-71-b
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 8
7.31
1.17
2.10
1.98
2.19
1.10
2.25
1.25
5.00
f1 (ppm)

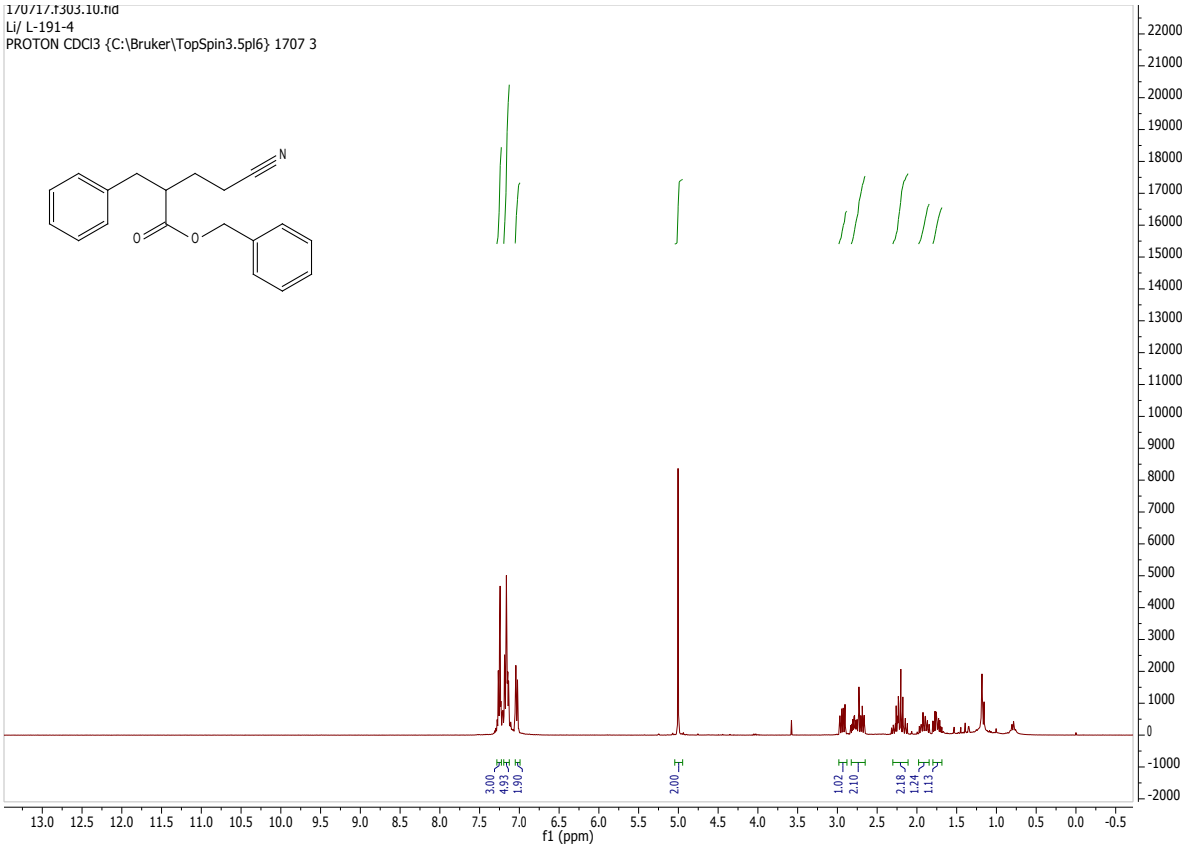

170724.f308.11.fid
Li/ L-71-b
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 8
174.15
158.79
135.62
129.47
128.67
128.48
128.35
120.77
118.97
114.47
67.03
66.71
43.92
28.63
27.66
26.76
15.27
f1 (ppm)

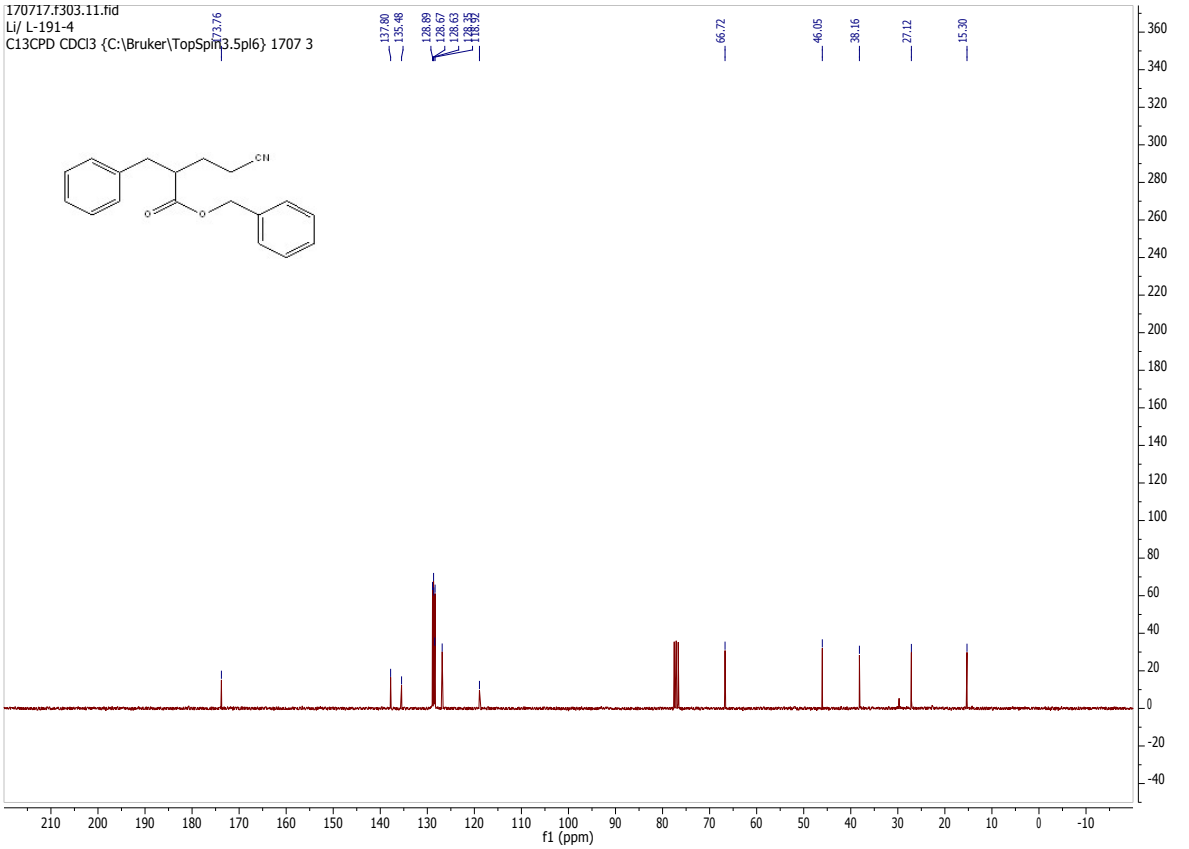

170726.f305.10.fid
Yahui Li L-81-6
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 5
N
Br
H3C
O
O
0.94
0.95
1.00
0.98
2.00
1.00
2.08
1.21
0.98
1.20
1.16
8.16
3.24
f1 (ppm)

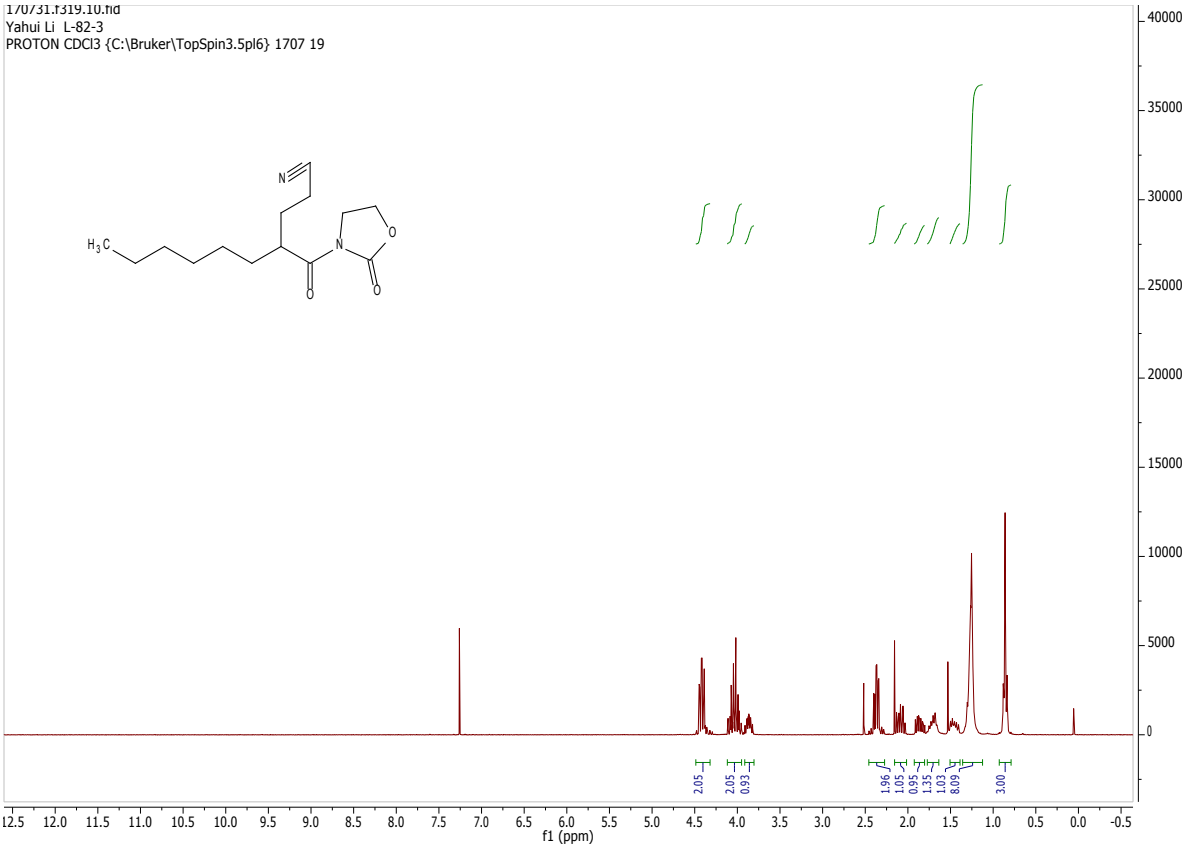

170726.f305.11.fid
Yahui Li L-81-6
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 5
174.28
134.97
132.97
130.45
130.03
127.58
123.79
119.08
66.20
44.23
32.02
31.57
29.04
27.53
26.91
22.52
15.36
14.04
N
Br
H3C
O
O
f1 (ppm)

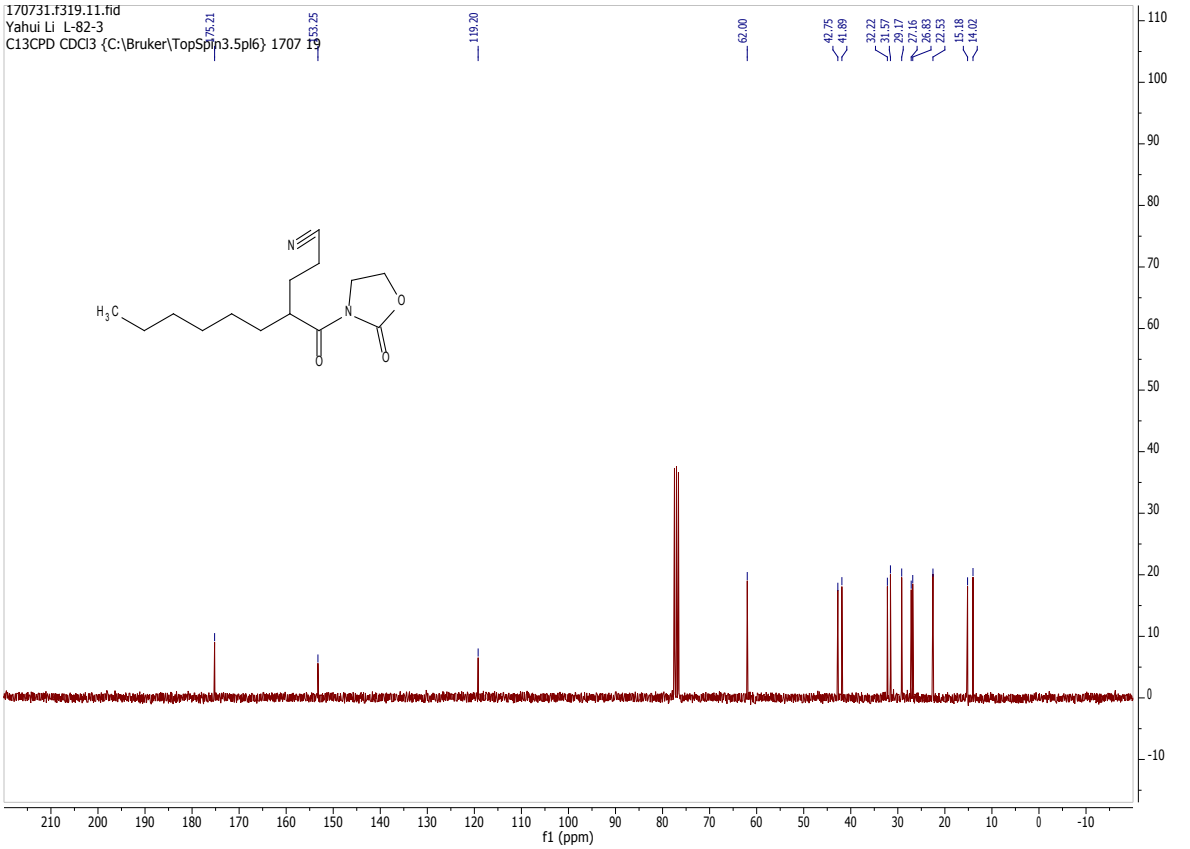

170727.f324.10.fid
Yahui Li L-81-10
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 24
H3C
N
O
O
25000
20000
15000
10000
5000
0
2.00
1.12
2.11
1.15
1.09
1.05
1.00
4.24
1.03
3.28
1.90
1.95
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

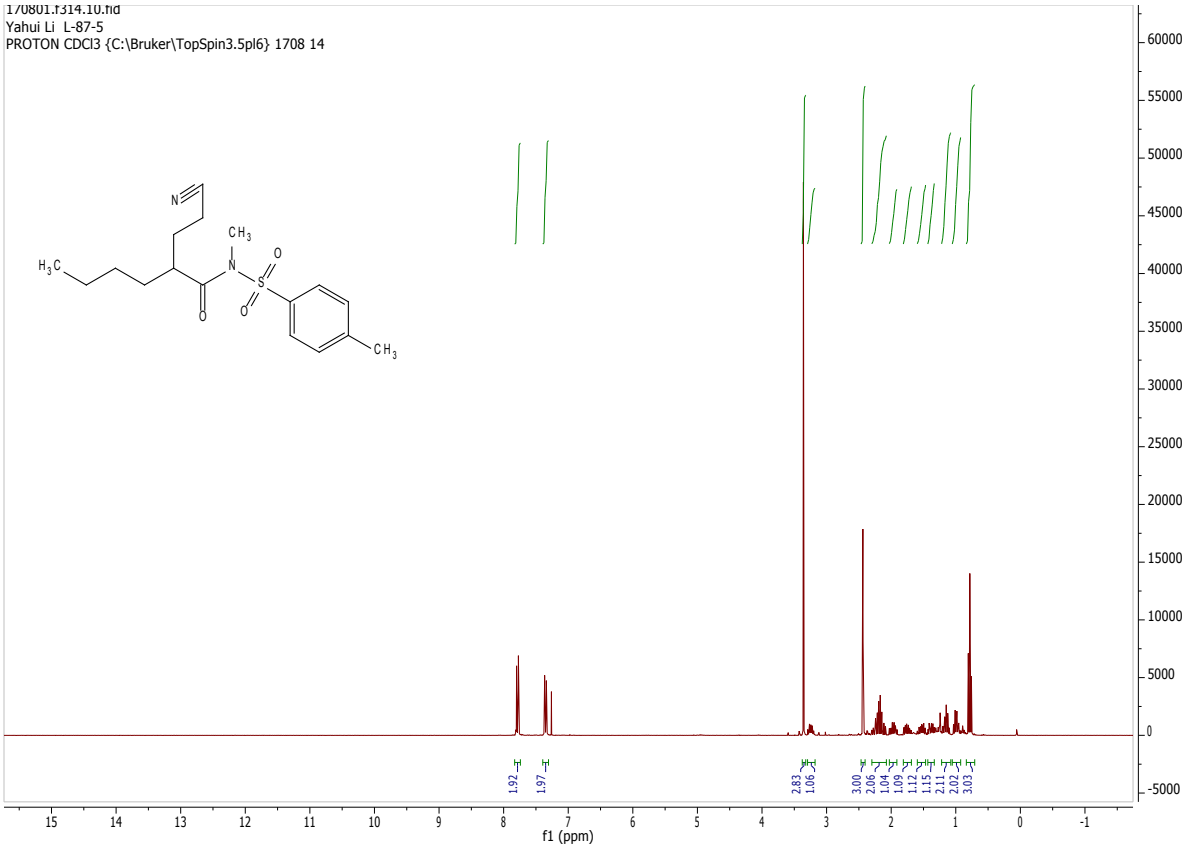

170727.f324.11.fid
Yahui Li L-81-10
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 24
174.79
119.14
69.38
44.25
31.76
29.11
27.62
22.46
15.31
13.84
9.88
3.27
H3C
N
O
O
550
500
450
400
350
300
250
200
150
100
50
0
-50
-100
-150
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

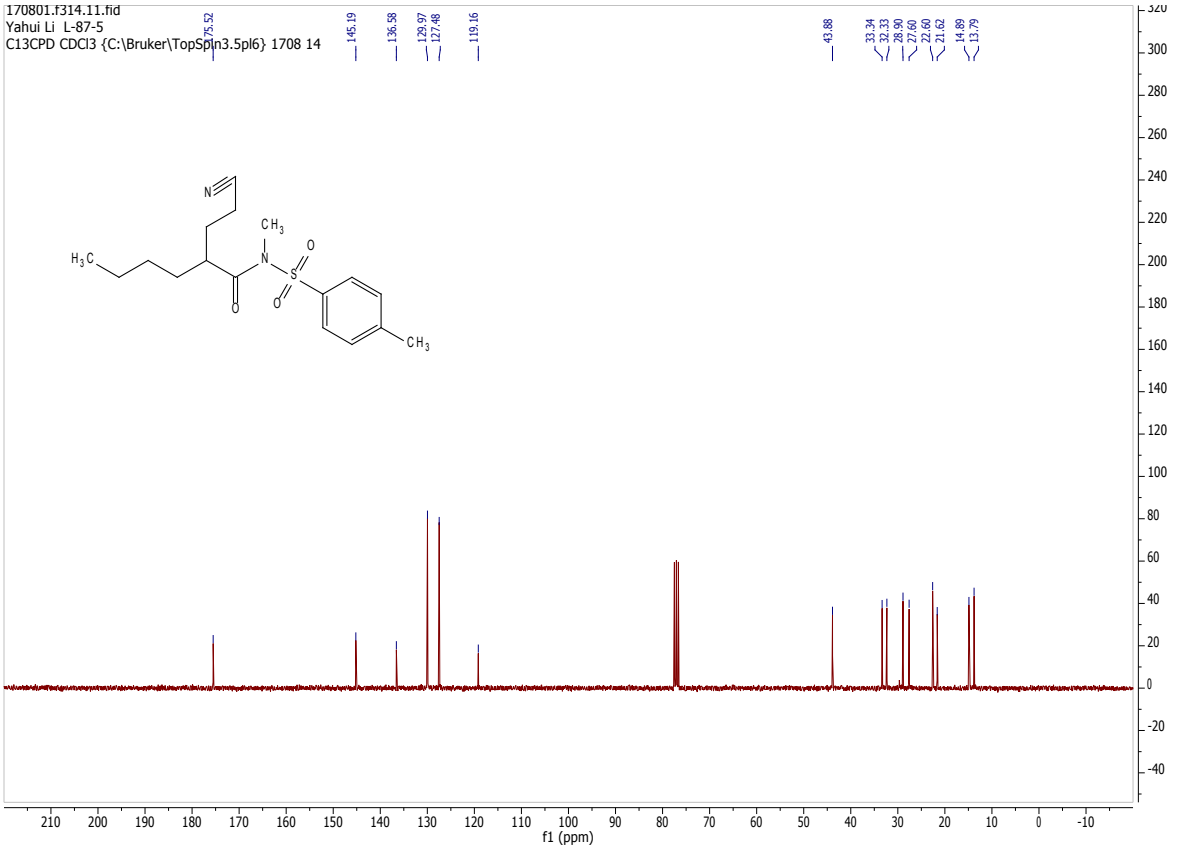

170717.f303.10.fid
Li/ L-191-4
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 3
N
O
O
3.00
4.93
1.90
2.00
1.02
2.10
2.18
1.24
1.13
f1 (ppm)

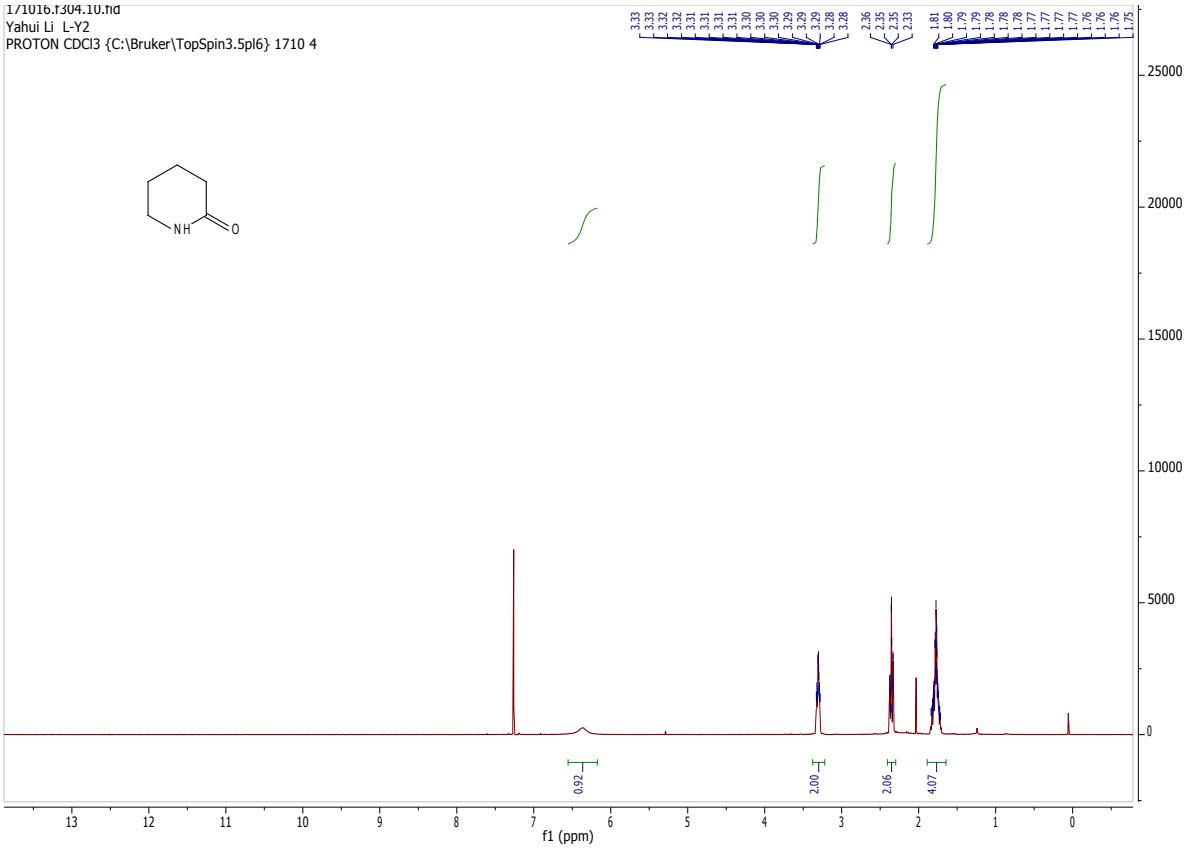

170717.f303.11.fid
Li/ L-191-4
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 3
173.76
137.80
135.48
128.89
128.67
128.63
66.72
46.05
38.16
27.12
15.30
CN
O
O
f1 (ppm)

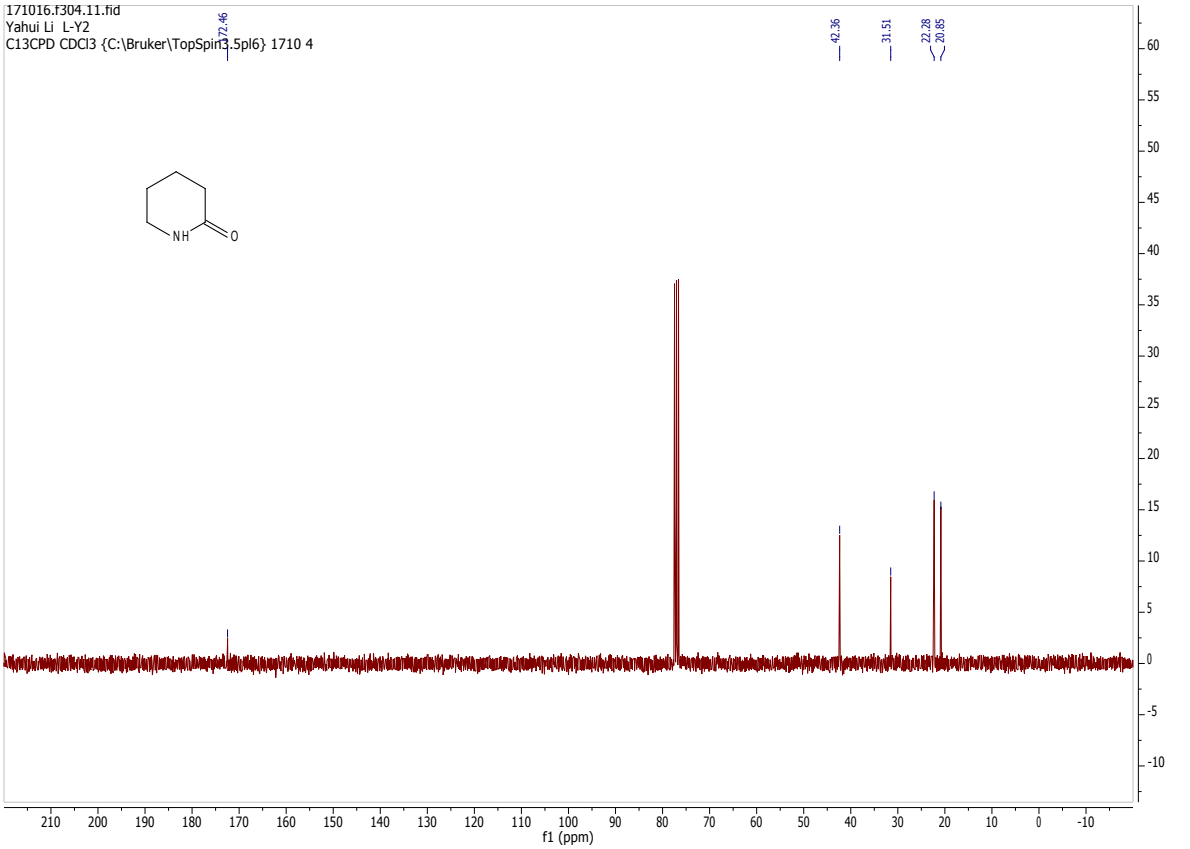

170731.f319.10.fid
Yahui Li L-82-3
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 19
f1 (ppm)

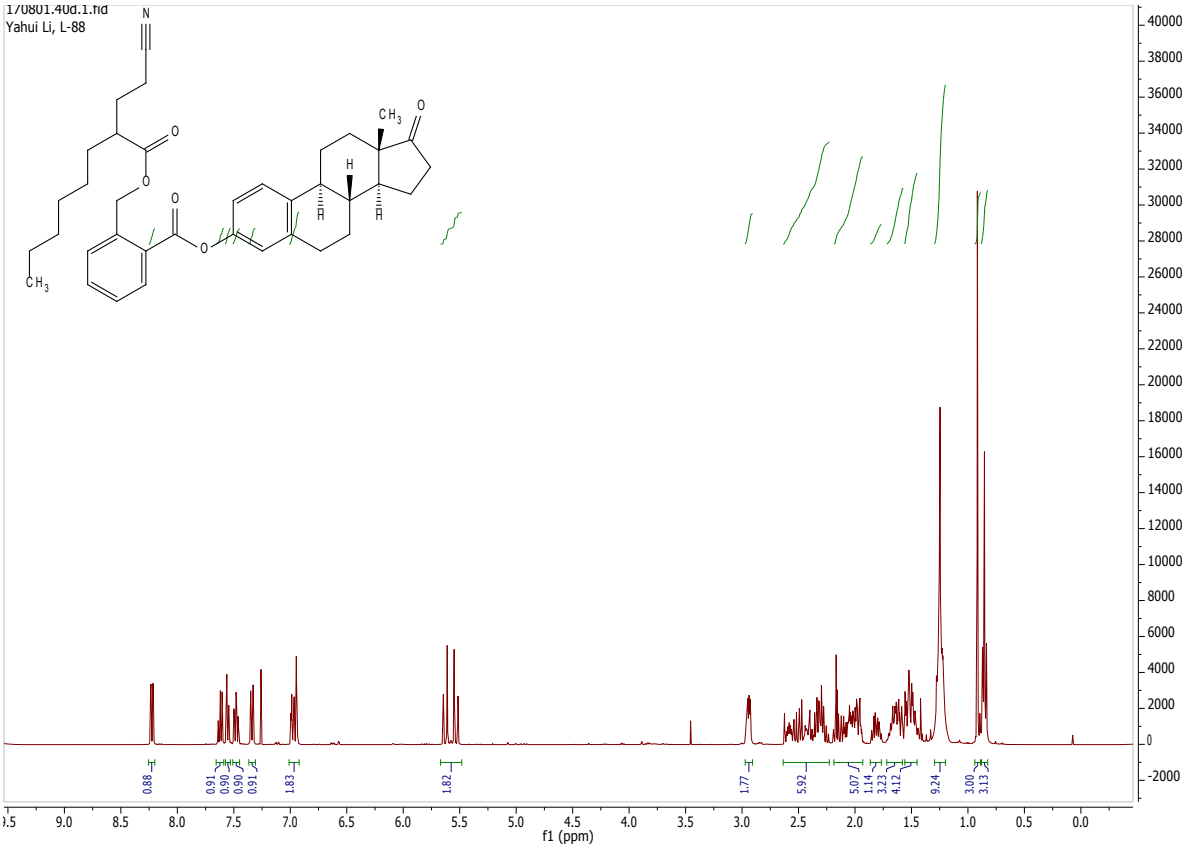

170731.f319.11.fid
Yahui Li L-82-3
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1707 19
175.21
153.25
119.20
62.00
42.75
41.89
32.22
31.57
29.17
27.16
26.83
22.53
15.18
14.02
f1 (ppm)

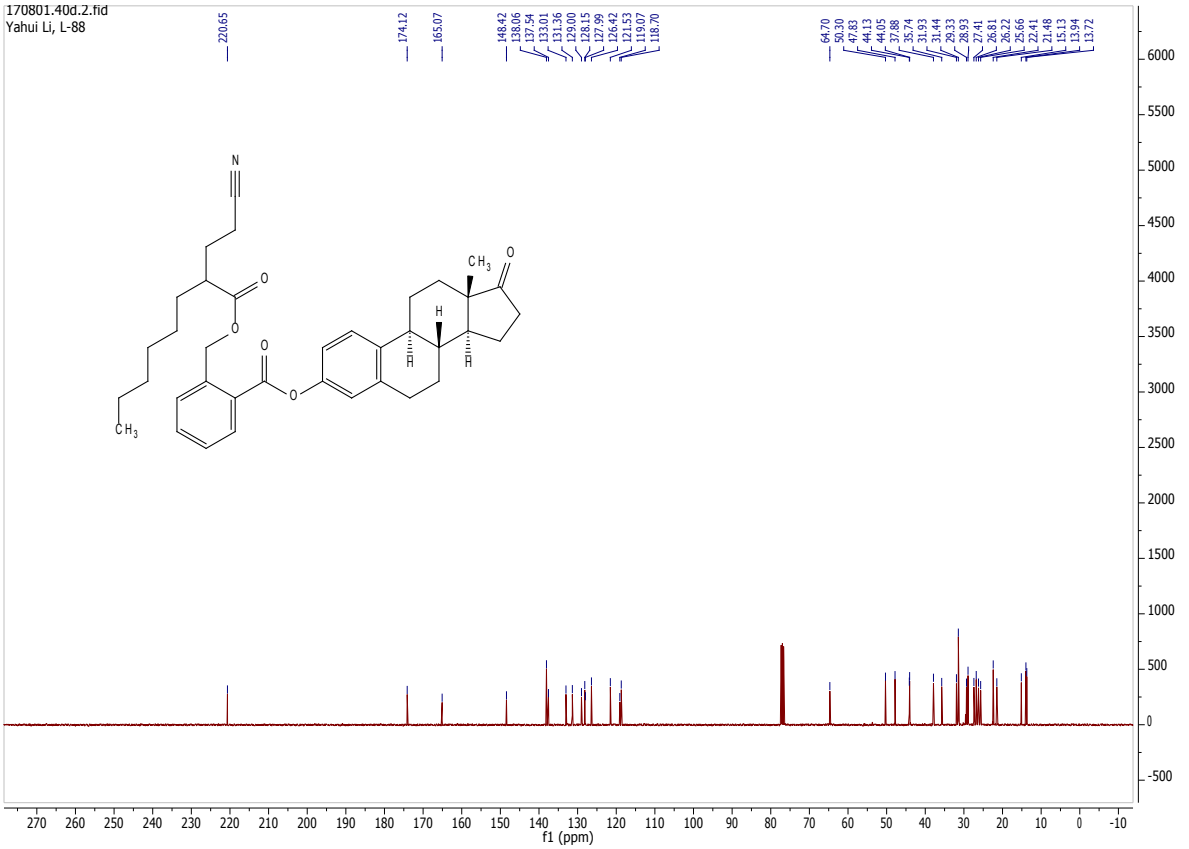

170801.f314.10.fid
Yahui Li L-87-5
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 14
f1 (ppm)

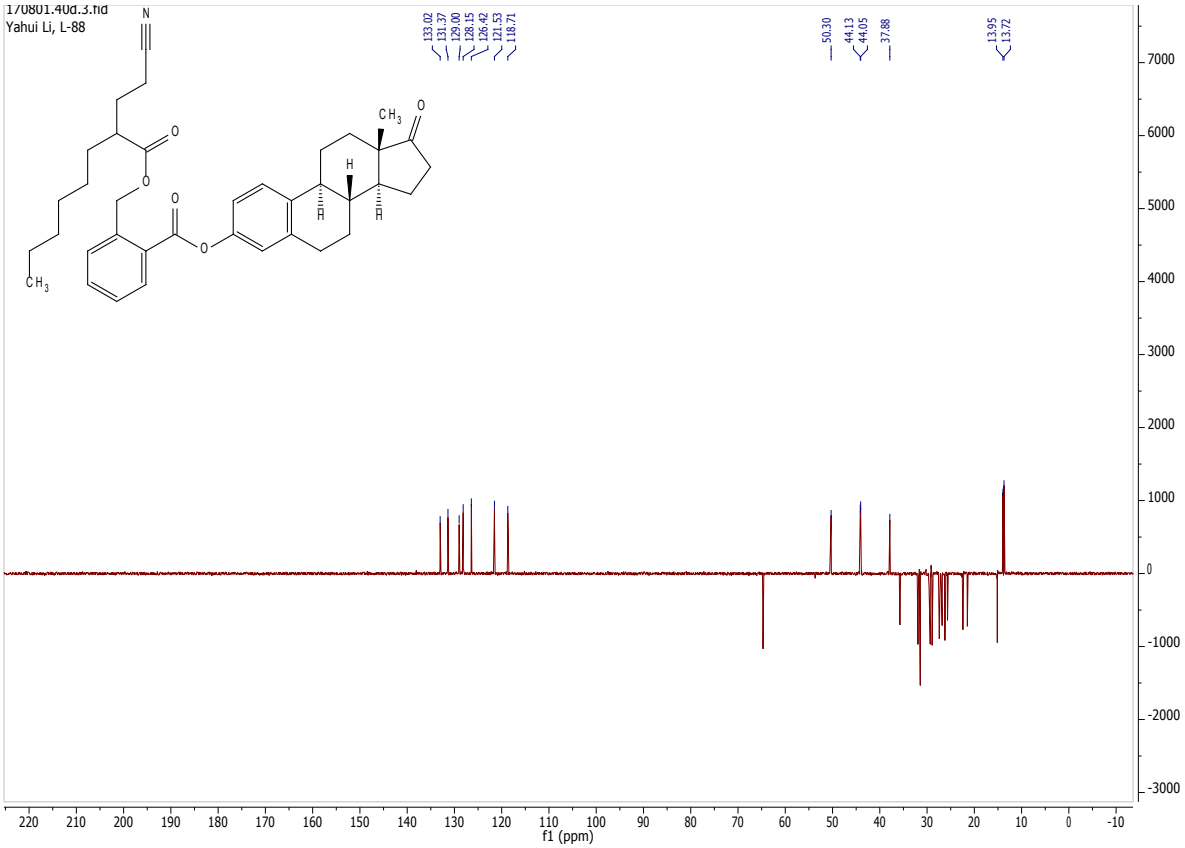

170801.f314.11.fid
Yahui Li L-87-5
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 14
f1 (ppm)


171016.f304.10.fid
Yahui Li L-Y2
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1710 4
NH
O
0.92
2.00
2.06
4.07
f1 (ppm)

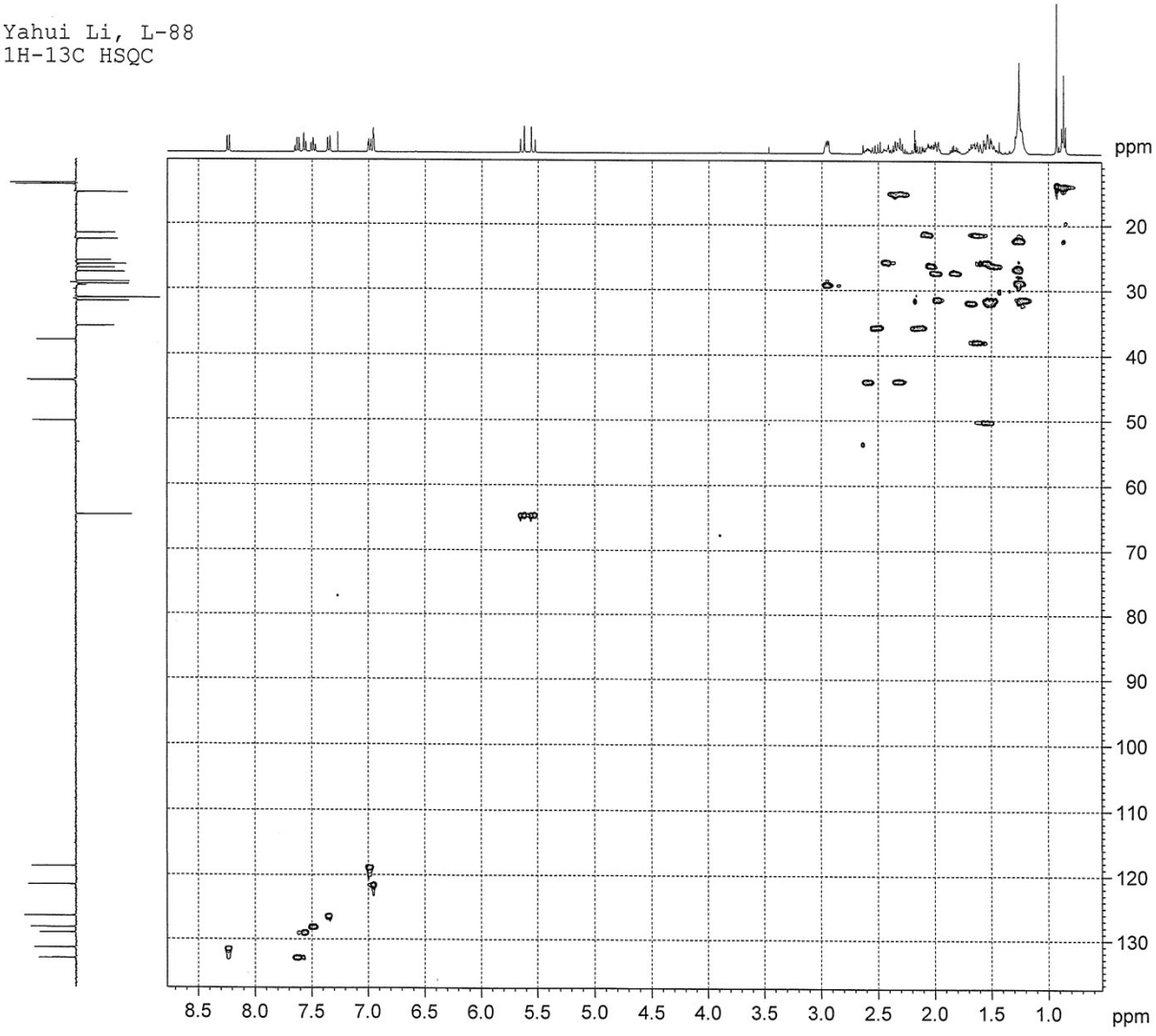

171016.f304.11.fid
Yahui Li L-Y2
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1710 4
172.46
42.36
31.51
22.28
20.85
NH
O
f1 (ppm)


170801.40d.1.fid
Yahui Li, L-88
f1 (ppm)


170801.40d.2.fid
Yahui Li, L-88
f1 (ppm)


170801.40d.3.fid
Yahui Li, L-88
133.02
131.37
129.00
128.15
126.42
121.53
118.71
50.30
44.13
44.05
37.88
13.95
13.72
f1 (ppm)

Yahui Li, L-88
1H-13C HSQC

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Current Data Parameters
NAME          170801.40d
EXPNO                  5
PROCNO                 1

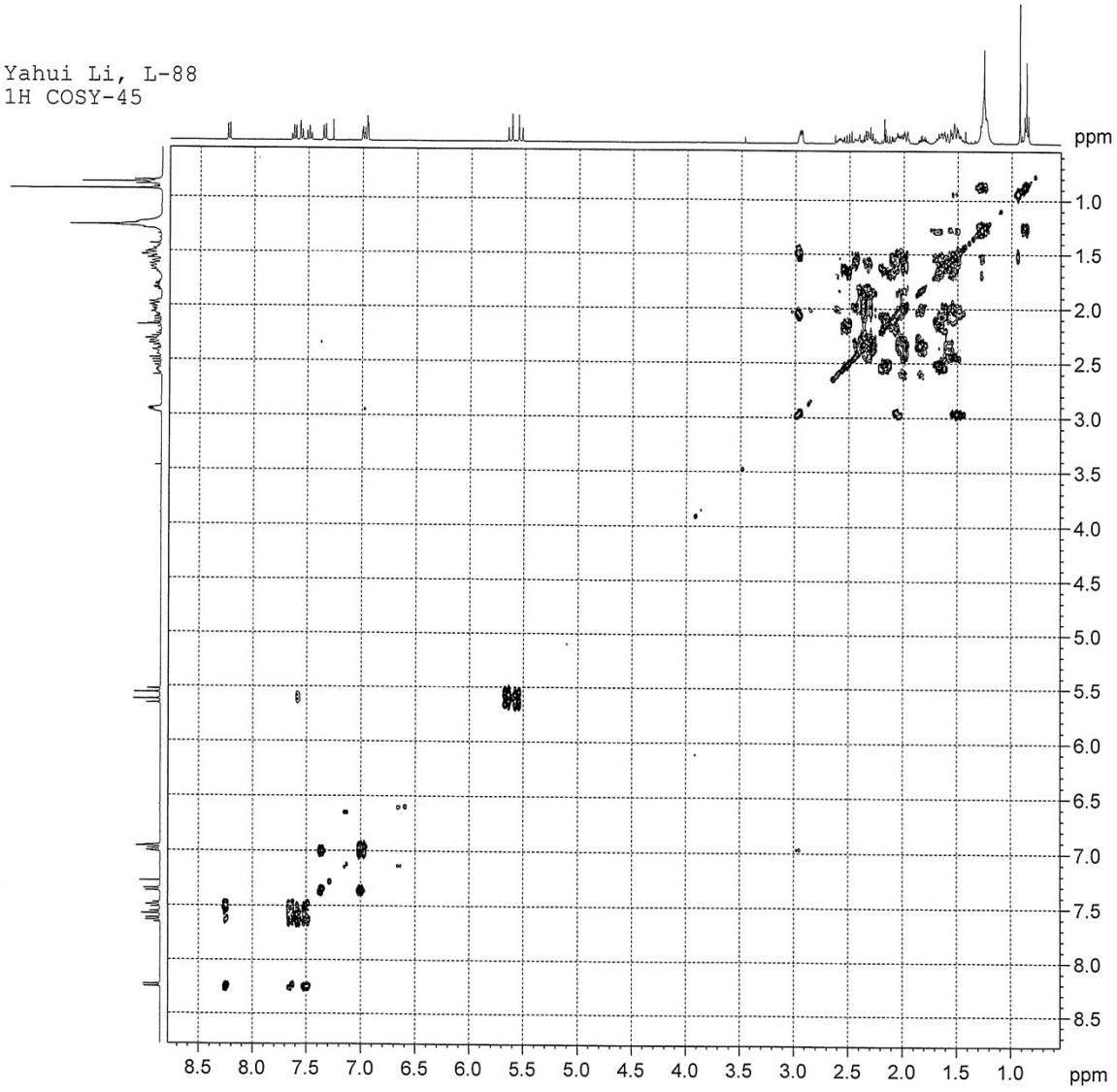
F2 - Acquisition Parameters
Date_          20170801
Time              18.59 h
INSTRUM           spect
PROBHD   Z824801_0180 (
PULPROG        hsqcetgp
TD                1024
SOLVENT           CDCl3
NS                   4
DS                  16
SWH            3301.056 Hz
FIDRES         6.447376 Hz
AQ            0.1551019 sec
RG                209.7
DW              151.467 usec
DE                8.00 usec
TE               297.1 K
CNST2        145.0000000
D0            0.00000300 sec
D1            2.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
IN0           0.00003890 sec
TDav                   1
ZGOPTNS
SFO1         400.1318650 MHz
NUC1                1H
P1                10.05 usec
P2                20.10 usec
P28             1000.00 usec
PLW1         18.00000000 W
SFO2         100.6202065 MHz
NUC2                13C
CPDPRG[2           garp
P3                12.10 usec
P4                24.20 usec
PCPD2             80.00 usec
PLW2         30.00000000 W
PLW12         0.68629998 W
GPNAM[1]     SMSQ10.100
GPZ1              80.00 %
GPNAM[2]     SMSQ10.100
GPZ2              20.10 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                 256
SFO1          100.6202 MHz
FIDRES        100.417740 Hz
SW            127.742 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                1024
SF          400.1300059 MHz
WDW               QSINE
SSB                   2
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
SI                1024
MC2       echo-antiecho
SF          100.6127820 MHz
WDW               QSINE
SSB                   2
LB        0 Hz
GB        0
```

Yahui Li, L-88
1H COSY-45




```
Current Data Parameters
NAME          170801.40d
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170801
Time              18.29 h
INSTRUM             spect
PROBHD   Z824801_0180 (
PULPROG       cosygpppqf
TD                  2048
SOLVENT             CDCl3
NS                     2
DS                    16
SWH             3301.056 Hz
FIDRES          3.223688 Hz
AQ              0.3102037 sec
RG                 83.22
DW               151.467 usec
DE                 8.00 usec
TE                297.0 K
D0            0.00000300 sec
D1            3.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00030300 sec
TDav                   1
SFO1         400.1318650 MHz
NUC1                  1H
P0                 5.10 usec
P1                10.05 usec
P17             2500.00 usec
PLW1         18.00000000 W
PLW10         2.02010012 W
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                   256
SFO1           400.1319 MHz
FIDRES         25.783829 Hz
SW                 8.248 ppm
FnMODE                QF

F2 - Processing parameters
SI                  1024
SF           400.1300000 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           400.1300000 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
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