Supporting information

Reusable cobalt catalysts for general and selective α-alkylation of nitriles with alcohols

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S1. Materials and methods

Alcohols and nitriles were obtained commercially from various chemical companies. Cobalt(II) chloride hexahydrate (cat no.255599-100G), zinc(II) chloride (cat no.208086-100G) and silica suspension (Silica LUDOX® AS-40 colloidal silica, cat no. 420840-1L) were purchased from Sigma Aldrich. D-Glucosamine hydrochloride (cat no. A15532-250G) was purchased from Alfa Aesar. Unless otherwise stated all reagents were used directly without purification.

The pyrolysis experiments were carried out in Dekema Austromat 624 oven. All catalytic experiments were carried out in ACS pressure tubes.

GC and GC-MS analysis were recorded on Agilent 6890N instrument. GC conversion and yields were determined by GC-FID, HP6890 chromatograph with FID detector, column HP 530 m x 250 mm x 0.25 μm.

NMR spectra are recorded using Bruker 300 Fourier, Bruker AV 300 and Bruker AV 400 spectrometers. Chemical shifts are reported in ppm relative to the deuterated solvent. Coupling constants are expressed in Hertz (Hz). The following abbreviations are used: s = singlet, bs = broad singlet d = doublet, t = triplet and m = multiple. The residual solvent signals were used as references for ^{1}H and ^{13}C NMR spectra ($CDCl_3$: δH = 7.26 ppm, δC = 77.12 ppm; DMSO-d_6: δH = 2.50 ppm, δC = 39.52 ppm).

XRD powder pattern were recorded on a Panalytical X'Pert diffractometer equipped with a Xcelerator detector using automatic divergence slits and Cu kα1/α2 radiation (40 kV, 40 mA; λ= 0.15406 nm, 0.154443 nm). Cu beta-radiation was excluded using a nickel filter foil. The measurements were performed in 0.0167° steps and 100 s of data collecting time per step. The samples were mounted on silicon zero background holders. The obtained intensities were converted from automatic to fixed divergence slits (0.25°) for further analysis. Peak positions and profile were fitted with Pseudo-Voigt function using the High Score Plus software package (Panalytical). Phase identification was done by using the PDF-2 database of the International Center of Diffraction Data (ICDD).

Scanning transmission electron microscopy (STEM) measurements were performed with a probe aberration-corrected JEM-ARM200F (JEOL, Corrector: CEOS) at 200 kV. The microscope was equipped with an Enfinium ER (GATAN) electron energy-loss spectrometer and a JEOL SDD detector for chemical analysis. High-Angle Annular Dark Field (HAADF) and Annular Bright Field (ABF) detectors were used for general imaging. The solid samples were deposited without any pretreatment on a holey carbon supported Cu-grid (mesh 300) and transferred to the microscope.

The X-ray Photoelectron Spectroscopy (XPS) measurements were performed on an ESCALAB 220iXL (Thermo Fisher Scientific) with monochromated Al Kα radiation (E = 1486.6 eV). Samples are prepared on a stainless-steel holder with conductive double-sided adhesive carbon tape. The electron binding energies were obtained with charge compensation using a flood electron source and referenced to the C 1s core level of adventitious carbon at 284.8 eV (C-C and C-H bonds) for the insolating samples containing Si. For the conductive samples after the removal of SiO_2 no charge referencing was applied, resulting in a C 1s main peak at around 284.7 eV. For quantitative analysis the peaks were deconvoluted with Gaussian-Lorentzian curves using the software Unifit 2021. The peak areas were normalized by the transmission function of the spectrometer and the element specific sensitivity factor of Scofield.

S2. Procedure for the preparation of catalysts

In a 100 mL dried round bottomed flask, 291.1 mg $CoCl_2 \cdot 6H_2O$ (1 mmol), 272.6 mg $ZnCl_2$ (2 mmol), and 2156.4 mg D-glucosamine hydrochloride (DGA; 10 mmol,) were dissolved in 20 mL deionized water by stirring for 30 minutes at room temperature. To this solution, 5 g colloidal silica aqueous solution (Ludox HS-40, 40 wt%,) was added and continued stirring for another 12 hours at room temperature. Then, the reaction mixture was subject to freeze drying to remove the water. The obtained solid material was grounded to a fine powder and transferred to crucible. The crucible was closed with a lid and placed in a pyrosis oven and then heated to the defined temperature (800- 1000 °C) for 3 h at the heating rate of 5 ^{o}C/min under Argon gas. After the completion of pyrolysis, the oven was cooled down to room temperature and the material was removed from the oven (Co@PNC-900-SiO_2). Next, the pyrolyzed materials were etched in 5 M NH_4HF_2 aqueous solution at room temperature for 24 h to remove the SiO_2 template and larger particles. Finally, the resulting catalytic material was filtered and washed subsequently with deionized water and ethanol several times and finally dried under vacuum (Co@PNC-900). Elemental Analysis of optimal catalyst, Co@PNC-900: Co = 1.23 wt% (1.26 wt% was measured by ICP-OES), C = 70 wt%, N = 6.9 wt%, H = 0.68 wt%, Si = 0.34wt%. Other materials such as Co@NC-900 in the absence of $ZnCl_2$, porous N-C material without the addition of cobalt precursors and Co-particles-900 without glucose amine were also prepared using similar procedure.

S3. Characterization of catalysts

XRD patterns

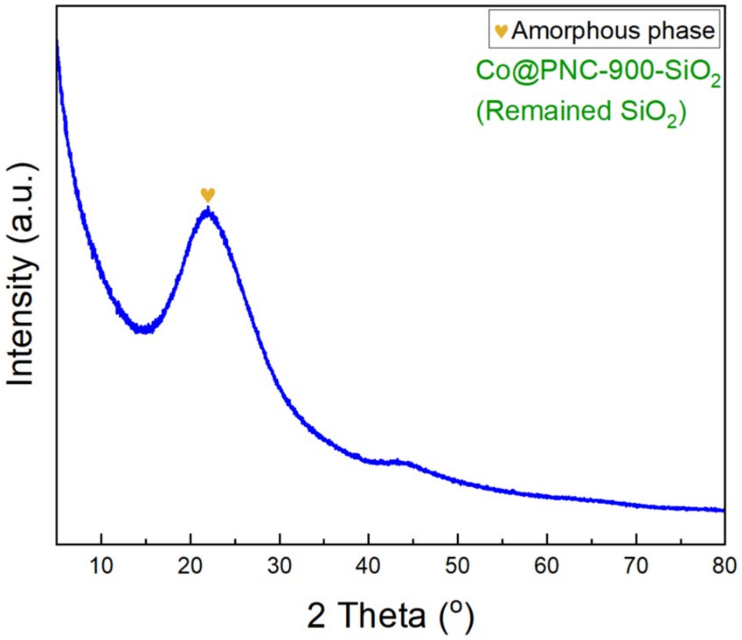


Figure S1. XRD pattern of Co@PNC-900-SiO$_2$ catalyst.

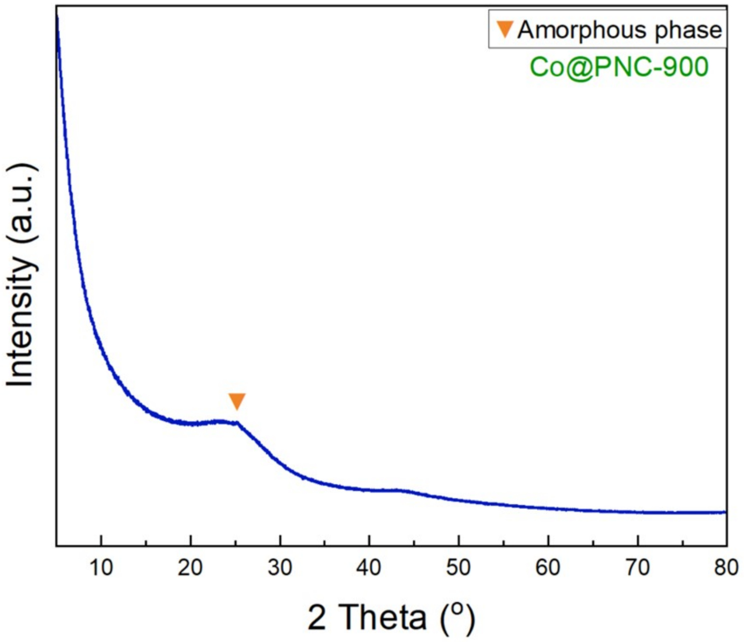


Figure S2. XRD pattern of Co@PNC-900 catalyst.

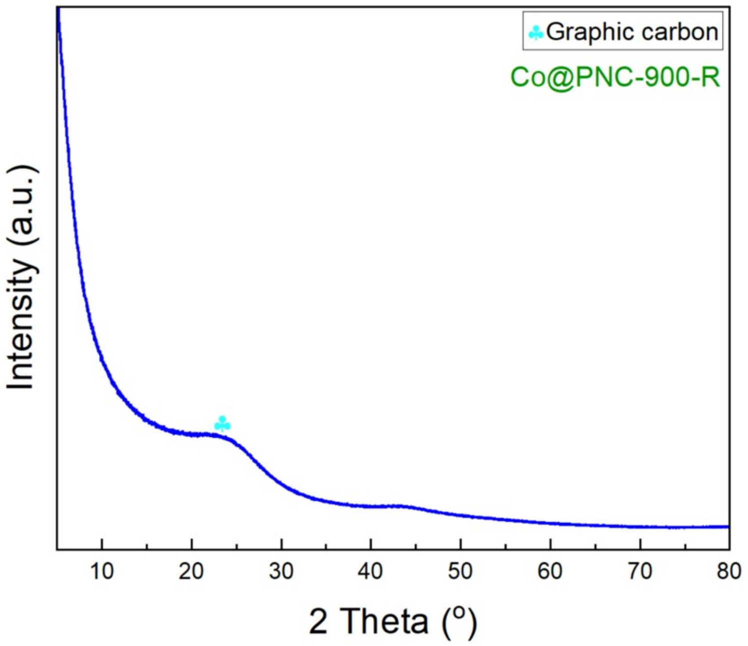


Figure S3. XRD pattern of Co@PNC-900-R (recycled) catalyst.

STEM images

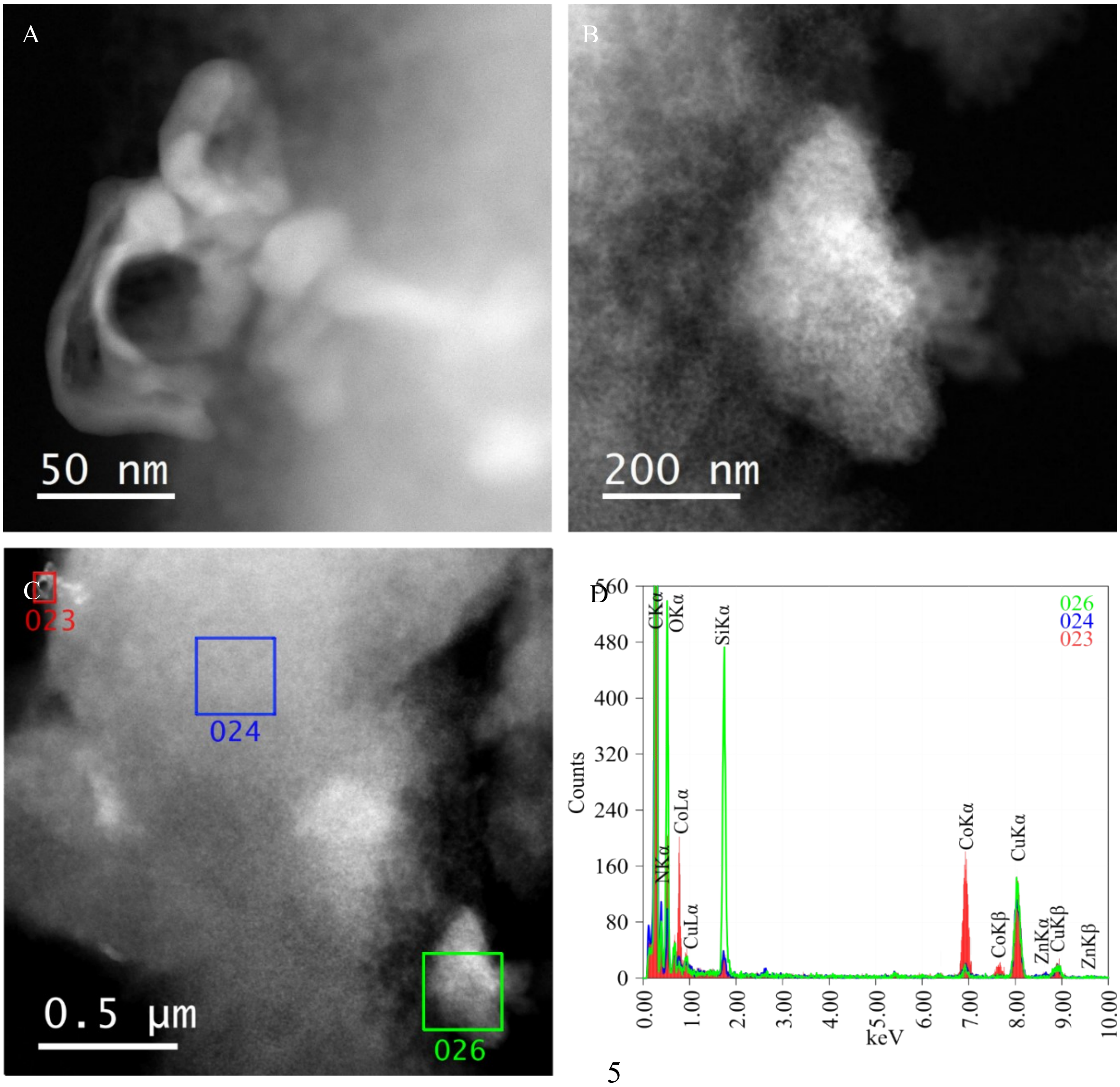


Figure S4. STEM-HAADF images (A-C) of Co@PNC-900 and corresponding EDX spectra (D) of marked regions showing examples of the few Co oxide and SiO_2 particles found in the specimen.

XPS data and spectra

Table S1. Surface composition of different cobalt samples obtained by XPS. All values are given in at.%.

Catalyst	C	O	N	Co	Si	F	Na
CO@PNC-900-SiO_2	43.3	30.7	6.2	0.4	17.9	0.7	0.7
CO@PNC-900	80.9	6.6	11.5	0.4	0.6	-	-
CO@PNC-900-R	82.43	6.03	10.72	0.3	0.5	-	-

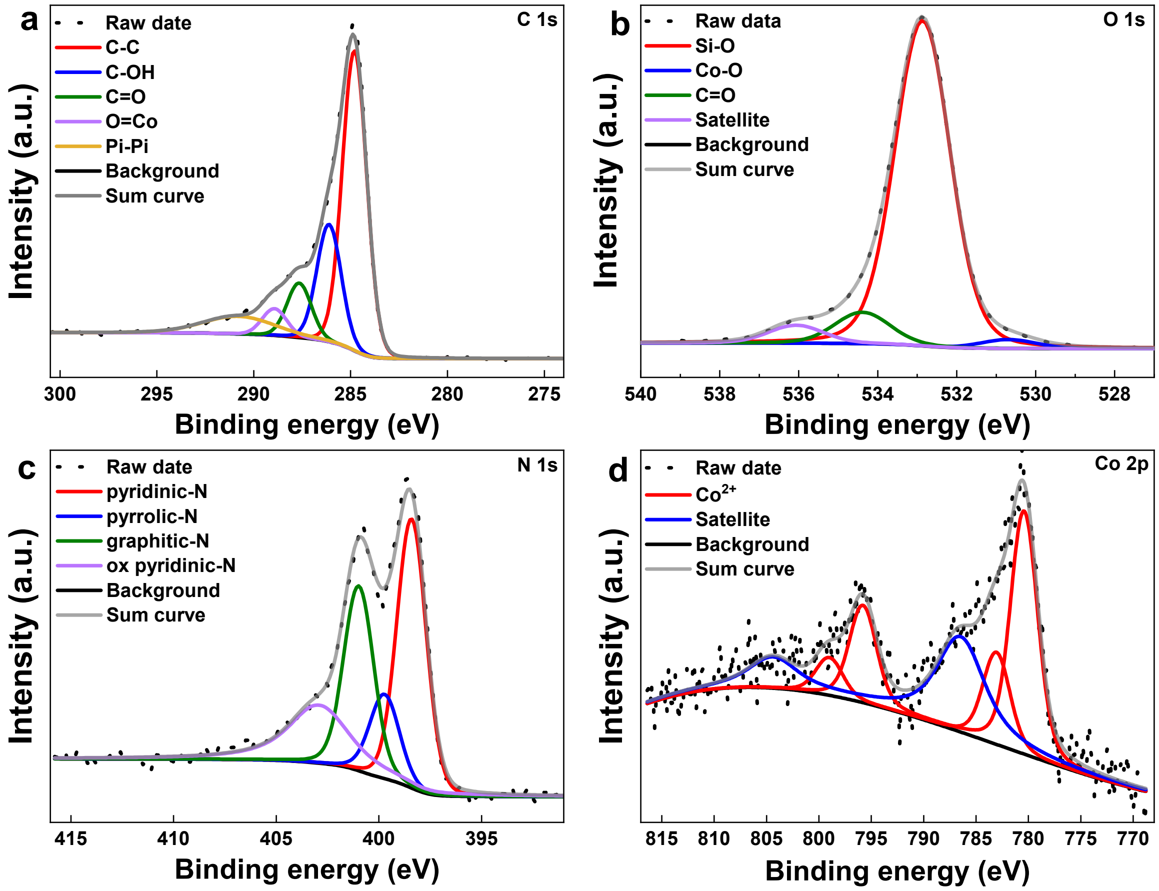


Figure S5. X-ray photoelectron spectra for Co@PNC-900-SiO_2. (a) C 1s, (b) O 1s, (c) N 1s, (d) Co 2p region.

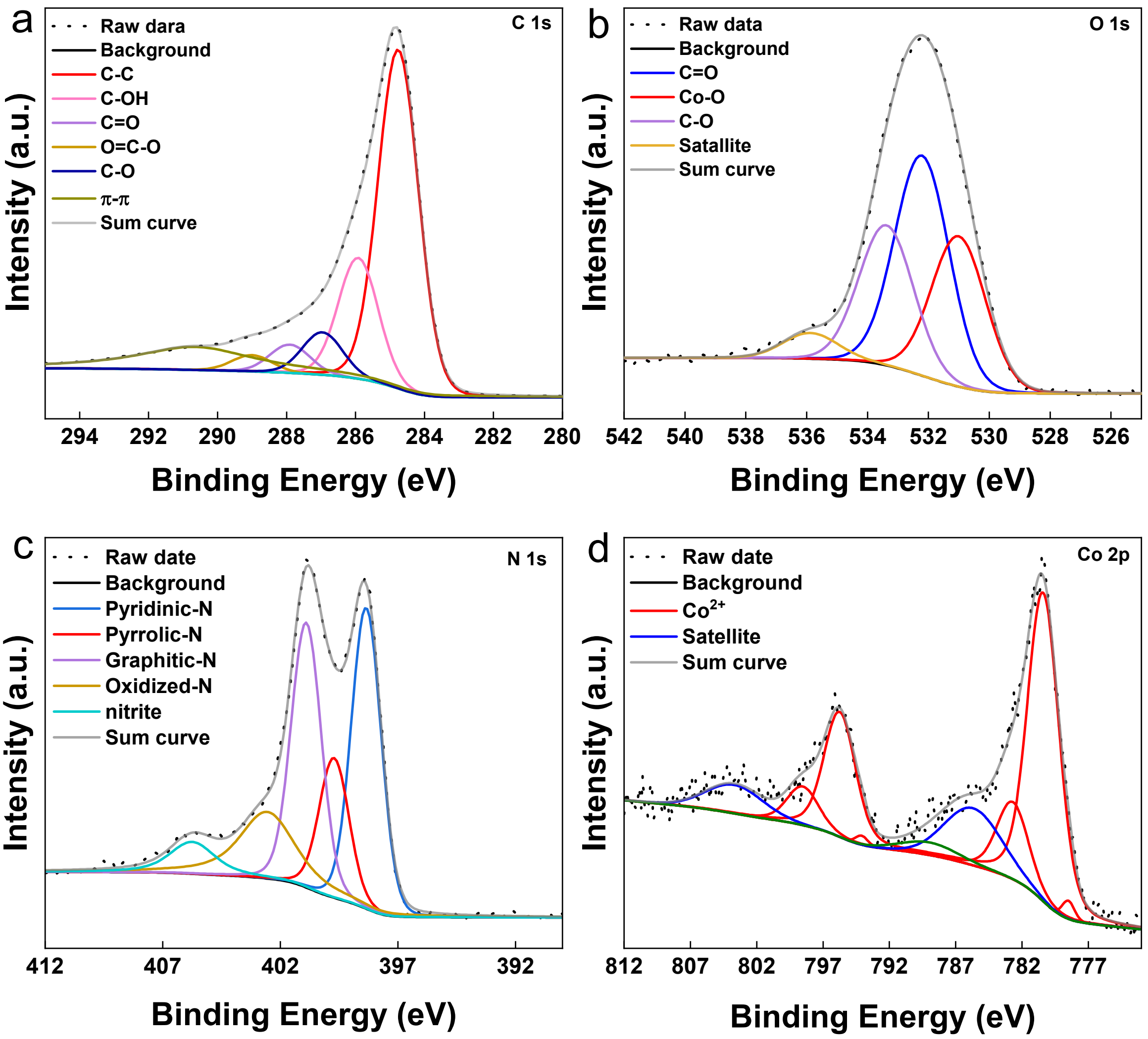
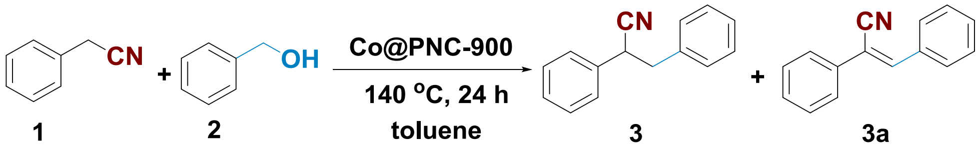


Figure S6. X-ray photoelectron spectra for Co@PNC-900-R. (a) C 1s, (b) O 1s, (c) N 1s, (d) Co 2p region.

S4. General procedure for the α-alkylation of nitriles with alcohols

The magnetic stirring bar, 0.5 mmol nitrile and 1 mmol alcohol, 50 mg catalyst (Co@PNC-900, 2.04 mol% Co) and 0.5 mmol K_3PO_4 (1.0 equiv) were transferred to 20 mL pressure tube. Then, 2 mL dry toluene was added, and the pressure tube was flushed with argon and fitted with screw cap. The pressure tube containing reaction mixture was placed into an aluminum block and reaction was allowed to progress under stirred condition at 140 °C for 24 h. After the completion of the reaction, the pressure tube was cooled to room temperature and the cap was slowly removed. Then, the reaction products were removed from the pressure tube, and the solid catalyst was filtered off and washed thoroughly with ethyl acetate. The reaction products were analyzed by GC-MS. The corresponding products were purified by column chromatography (silica; pentene-ethyl acetate mixture) and characterized by NMR and GCMS spectral analysis. Following procedure is applied for determining the conversion and yields by GC: After completion of the reaction, n-hexadecane (50 µL) as standard was added to the reaction pressure tube and the reaction products were diluted with ethyl acetate followed by filtration using plug of silica. Then the filtrate containing products were analyzed by GC.

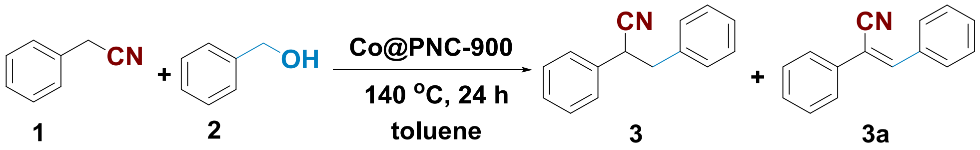
Table S2. Co-catalyzed α-alkylation of phenyl acetonitrile with benzyl alcohol: Testing of different solvents.



Entry	Solvent	Conv. of 1 (%)	Yield of 3 (%)	Yield of 3a (%)
1	THF	70	62	7
2	Toluene	99	95	3
3	1,4-dioxane	67	55	11
4	t-BuOH	85	78	5
5	P-xylene	96	85	10
6	MeCN	54	43	9
7[b]	Toluene	61	50	7
8[c]	Toluene	74	60	10

Reaction conditions: 0.5 mmol phenyl acetonitrile, 1 mmol benzyl alcohol, 50 mg Co@PNC-900 (2.04 mol% Co), 0.5 mmol K_3PO_4, 2 mL solvent, 140 °C, 24 h. [b]: same as “a” with 50 mg Co@PNC-700; [c]: same as “a” with 50 mg Co@PNC-800; conversion and yields are based on phenyl acetonitrile and determined by GC using n-hexadecane as standard.

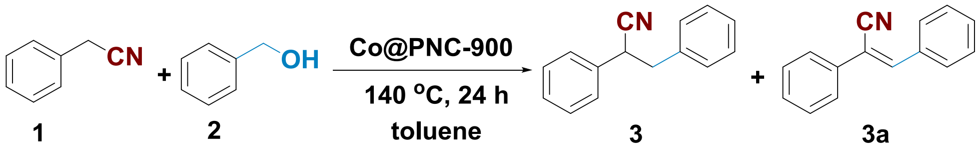
Table S3. Co-catalyzed α-alkylation of phenyl acetonitrile with benzyl alcohol: Testing of different bases.



Entry	Base	Conv. 1 (%)	Yield 3 (%)	Yield 3a (%)
1	KOH	82	78	3
2	K_3PO_4	99	95	3
3	K_2CO_3	20	10	8
4	Cs_2CO_3	76	68	5

Reaction conditions: 0.5 mmol phenyl acetonitrile, 1 mmol benzyl alcohol, 50 mg catalyst (2.04 mol% Co), 0.5 mmol base, 2 mL toluene, 140 °C, 24 h, conversion and yields are based on phenyl acetonitrile and determined by GC using n-hexadecane as standard.

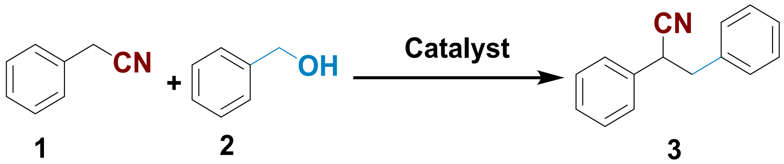
Table S4. Co-catalyzed α-alkylation of phenyl acetonitrile with benzyl alcohol with different amounts of benzyl alcohol[a].



Entry	Benzyl alcohol	Conv. 1 (%)	Yield 3 (%)	Yield 3a (%)
1	0.5 mmol (1 eq)	76	71	3
2	0.7 mmol (1.4 eq)	85	82	--
3	1 mmol (2 eq)	99	95	3
4[b]	1 mmol (2 eq)	90	80	8
5[c]	1 mmol (2 eq)	71	60	10

Reaction conditions[a]: 0.5 mmol phenyl acetonitrile, 0.5-1 mmol benzyl alcohol, 50 mg catalyst (2.04 mol% Co), 0.5 K_3PO_4, 2 mL toluene, 140 °C, 24 h. [b]: 130 °C; [c]: 120 °C. conversion and yields are based on phenyl acetonitrile and determined by GC using n-hexadecane as standard.

Table S5. Comparison of TON value of our Co-catalyst with previously reported heterogeneous catalysts.



Entry	Catalyst	Reaction conditions	Yield. %	Sel. %	TON (TOF h^{-1})	Ref.
1	Cp@PNC-900	140 °C, 24 h	99%	95%	43 (1.8)	This work
2	Ru/HT	180 °C, 20 h	91%	-	121 (6)	(28)
3	Ru/HT	180 °C, 20 h.	77%	-	103 (5.1)	(29)
4	Pd/MgO	180 °C, 24 h	94%	95%	436 (18.1)	(30)

HT: Hydrotalcite; TON: mmol of desired product 3/mmol of catalyst; TOF: TON/time.

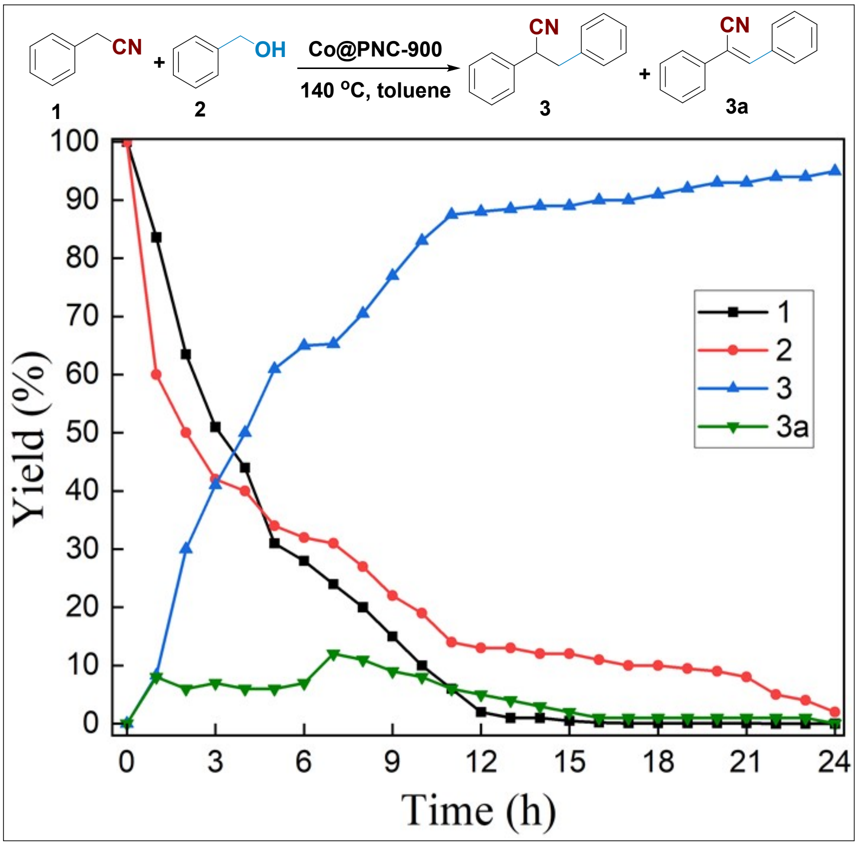
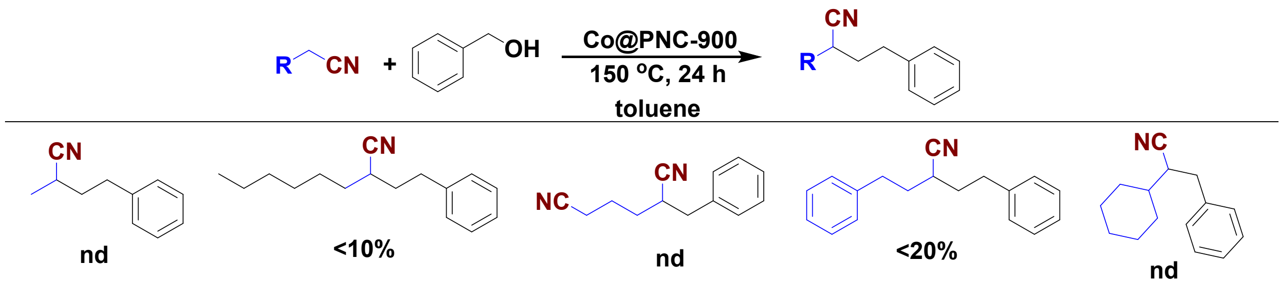


Figure S7. Co-catalyzed α-alkylation of phenyl acetonitrile with benzyl alcohol: Reaction progress with time. **Reaction conditions:** 0.5 mmol phenyl acetonitrile, 1 mmol benzyl alcohol, 50 mg catalyst (2.04 mol% Co), 0.5 mmol K_3PO_4, 2 mL toluene, 140 °C, 1-24 h, conversion and yields are based on phenyl acetonitrile and determined by GC using n-hexadecane as standard.

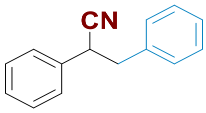


Scheme S1. Failed examples. **Reaction conditions:** 0.5 mmol nitrile, 1.0 mmol alcohol, 70 mg catalyst (2.86 mol% Co), 0.5 K_3PO_4, 2 mL toluene, 150 °C, 24 h. conversion and yields are based on phenyl acetonitrile and determined by GC using n-hexadecane as standard.

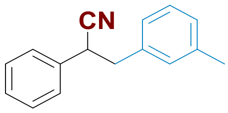
S5. Catalyst recycling

The magnetic stirring bar, 1.5 mmol phenyl acetonitrile and 3 mmol benzyl alcohol, 160 mg Co@PNC-900 and 1.5 mmol K_3PO_4 were transferred to 20 mL pressure tube and 4 mL dry toluene was added. The pressure tube was flushed with argon and closed with screw cap. Then, it was placed into an aluminum block and heated to 140 °C for desired time. After the completion of the reaction, the pressure tube was cooled down to room temperature. To the reaction products, 150 µL n-hexadecane as standard was added. The catalyst was separated by centrifugation and the centrifugate containing reaction products was subjected to GC analysis. The separated catalyst was washed with water, methanol and ethyl acetate and then dried under vacuum. The dried catalyst was used for the next run without further purification or reactivation.

S6. NMR data

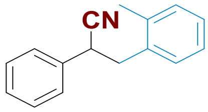


2,3-diphenylpropanenitrile[1]: ^{1}H NMR (300 MHz, CDCl3) δ 7.32 – 7.26 (m, 3H), 7.26 – 7.18 (m, 5H), 7.12 – 7.06 (m, 2H), 3.95 (dd, J = 8.2, 6.5 Hz, 1H), 3.20 – 3.03 (m, 2H).



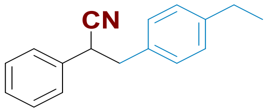
2-phenyl-3-(m-tolyl)propanenitrile[2]: **^{1}H NMR (300 MHz, $CDCl_3$)** δ 7.41 – 7.26 (m, 5H), 7.19 (td, *J* = 7.4, 0.7 Hz, 1H), 7.11 – 7.06 (m, 1H), 7.00 – 6.90 (m, 2H), 3.99 (dd, *J* = 8.4, 6.5 Hz, 1H), 3.20 – 3.05 (m, 2H), 2.32 (d, *J* = 0.7 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 138.33, 136.27, 135.40, 129.95, 129.02, 128.52, 128.19, 128.13, 127.49, 126.20, 112.27, 42.23, 39.90, 21.36.



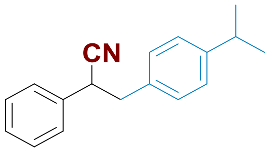
2-phenyl-3-(o-tolyl)propanenitrile[2]: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38 – 7.26 (m, 5H), 7.20 – 7.11 (m, 4H), 3.96 (dd, *J* = 8.7, 6.6 Hz, 1H), 3.30 – 3.08 (m, 2H), 2.23 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 136.29, 135.48, 134.70, 130.61, 130.07, 129.08, 128.25, 127.56, 127.41, 126.30, 120.50, 39.52, 38.78, 19.25.



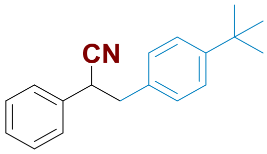
3-(4-ethylphenyl)-2-phenylpropanenitrile[6]: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.31 – 7.14 (m, 5H), 7.07 – 6.95 (m, 4H), 3.94 – 3.81 (m, 1H), 3.10 – 2.95 (m, 2H), 2.53 (q, *J* = 7.6 Hz, 2H), 1.13 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (75 MHz, $CDCl_3$) δ 143.41, 135.46, 133.58, 129.19, 129.05, 128.20, 128.16, 127.53, 120.54, 41.92, 40.00, 28.53, 15.57.



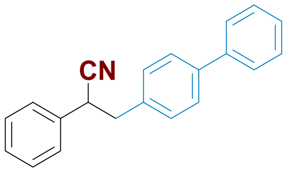
3-(4-isopropylphenyl)-2-phenylpropanenitrile[6]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.32 – 7.13 (m, 5H), 7.11 – 6.97 (m, 4H), 3.94 – 3.84 (m, 1H), 3.13 – 2.97 (m, 2H), 2.87 – 2.77 (m, 1H), 1.16 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 148.05, 135.52, 133.74, 129.15, 129.05, 128.19, 127.51, 126.73, 120.55, 41.94, 40.02, 33.80, 24.01.



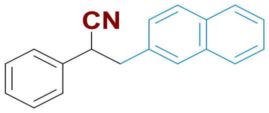
3-(4-(tert-butyl)phenyl)-2-phenylpropanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.32 – 7.15 (m, 7H), 7.06 – 6.99 (m, 2H), 3.94 – 3.82 (m, 1H), 3.12 – 2.96 (m, 2H), 1.23 (s, 9H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 150.33, 135.56, 133.40, 129.06, 128.88, 128.20, 127.49, 125.60, 120.57, 41.84, 40.00, 34.53, 31.38.



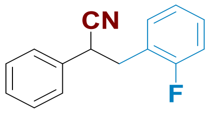
3-([1,1'-biphenyl]-4-yl)-2-phenylpropanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.62 – 7.51 (m, 4H), 7.48 – 7.41 (m, 2H), 7.39 – 7.29 (m, 5H), 7.25 – 7.19 (m, 2H), 4.05 (dd, *J* = 8.2, 6.5 Hz, 1H), 3.30 – 3.15 (m, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 140.63, 140.30, 135.30, 135.21, 129.68, 129.09, 128.81, 128.28, 127.54, 127.38, 127.34, 127.06, 120.40, 41.89, 39.82.



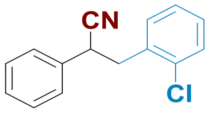
3-(Naphthalen-2-yl)-2-phenylpropanenitrile[1]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.89 – 7.71 (m, 3H), 7.61 (dd, *J* = 1.8, 1.0 Hz, 1H), 7.54 – 7.42 (m, 2H), 7.42 – 7.24 (m, 6H), 4.11 (dd, *J* = 8.1, 6.6 Hz, 1H), 3.47 – 3.23 (m, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 135.22, 133.74, 133.40, 132.61, 129.08, 128.36, 128.27, 128.15, 127.76, 127.68, 127.54, 127.12, 126.25, 125.96, 120.40, 42.39, 39.77.



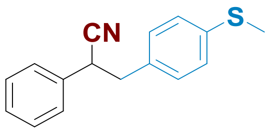
3-(2-fluorophenyl)-2-phenylpropanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.31 – 7.18 (m, 7H), 7.12 – 7.06 (m, 1H), 7.04 – 6.95 (m, 2H), 4.01 (dd, *J* = 8.5, 6.9 Hz, 1H), 3.20 – 3.07 (m, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 162.84, 159.59, 135.19, 131.66, 131.60, 129.52, 129.41, 129.18, 129.12, 128.35, 127.97, 127.40, 124.38, 124.33, 123.65, 123.45, 120.21, 115.65, 115.37, 38.35, 38.32, 35.98, 35.96.



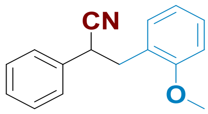
3-(2-chlorophenyl)-2-phenylpropanenitrile: ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.48 – 7.39 (m, 6H), 7.32 – 7.26 (m, 3H), 4.24 (dd, *J* = 9.6, 6.1 Hz, 1H), 3.42 – 3.25 (m, 2H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 135.30, 134.21, 134.05, 131.86, 129.77, 129.17, 129.15, 128.35, 127.34, 127.21, 120.17, 40.48, 37.68.



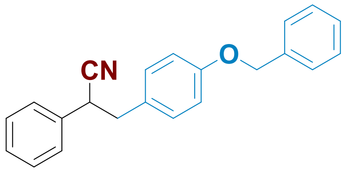
3-(4-(methylthio)phenyl)-2-phenylpropanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.38 (dddd, *J* = 8.5, 4.7, 3.2, 1.6 Hz, 3H), 7.30 – 7.26 (m, 2H), 7.19 (td, *J* = 5.5, 2.2 Hz, 2H), 7.11 – 7.02 (m, 2H), 4.00 (dd, *J* = 8.0, 6.6 Hz, 1H), 3.25 – 3.07 (m, 2H), 2.49 (s, 3H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 137.63, 135.07, 132.97, 129.72, 129.06, 128.25, 127.51, 126.70, 120.31, 41.66, 39.78, 15.79.



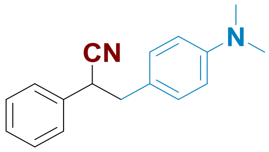
3-(2-Methoxyphenyl)-2-phenylpropanenitrile[1]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.41 – 7.26 (m, 6H), 7.10 (ddd, *J* = 7.5, 1.4, 0.8 Hz, 1H), 6.93 – 6.87 (m, 2H), 4.19 (dd, *J* = 8.9, 6.5 Hz, 1H), 3.86 (s, 3H), 3.24 – 3.11 (m, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 157.46, 136.09, 131.21, 128.93, 128.88, 127.99, 127.41, 124.96, 120.87, 120.65, 110.35, 55.33, 37.79, 37.69.



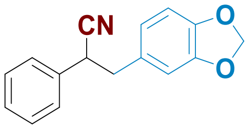
3-(4-(benzyloxy)phenyl)-2-phenylpropanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.49-7.34 (m, 8H), 7.31-7.28 (m, 1H), 7.11-7.03 (m, 3H), 6.98 – 6.90 (m, 2H), 6.79 – 6.72 (m, 1H), 5.07 (s, 2H), 3.99 (dd, *J* = 8.0, 6.6 Hz, 1H), 3.21-3.06 (m, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 158.16, 153.56, 136.97, 135.26, 130.41, 130.07, 129.73, 129.07, 128.66, 128.23, 128.07, 127.58, 120.57, 115.19, 115.03, 70.09, 41.43, 40.07, 20.54.



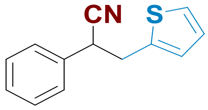
3-(4-(dimethylamino)phenyl)-2-phenylpropanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.42 – 7.27 (m, 5H), 7.06 – 7.00 (m, 2H), 6.72 – 6.65 (m, 2H), 3.95 (dd, *J* = 8.2, 6.5 Hz, 1H), 3.19 – 3.03 (m, 2H), 2.95 (s, 6H). ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.42 – 7.27 (m, 5H), 7.06 – 7.00 (m, 2H), 6.72 – 6.65 (m, 2H), 3.95 (dd, *J* = 8.2, 6.5 Hz, 1H), 3.19 – 3.03 (m, 2H), 2.95 (s, 6H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 149.88, 135.68, 129.95, 128.97, 128.05, 127.58, 124.09, 120.79, 112.66, 41.52, 40.63, 40.33.



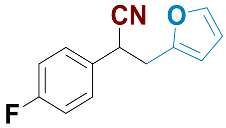
3-(benzodioxol-5-yl)-2-phenylpropanenitrile[1]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.28 – 7.25 (m, 2H), 7.21 – 7.16 (m, 2H), 6.66 – 6.60 (m, 1H), 6.55 – 6.48 (m, 2H), 5.84 (s, 2H), 3.91 – 3.84 (m, 1H), 3.02 – 2.93 (m, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 147.77, 146.90, 135.16, 129.97, 129.07, 128.26, 127.50, 122.53, 120.40, 109.51, 108.38, 101.09, 41.95, 40.04.



2-phenyl-3-(thiophen-2-yl)propanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.39 – 7.33 (m, 3H), 7.32 – 7.28 (m, 2H), 7.18 (dd, *J* = 5.1, 1.2 Hz, 1H), 6.93 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.88 – 6.82 (m, 1H), 4.09 – 4.01 (m, 1H), 3.49 – 3.31 (m, 2H).

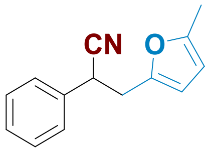
^{13}C NMR (75 MHz, CDCl$_3$) δ 137.92, 134.74, 129.12, 128.44, 127.48, 127.00, 124.94, 120.13, 40.11, 36.21.



2-(4-fluorophenyl)-3-(furan-2-yl)propanenitrile[4]: ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.35 (dd, *J* = 1.9, 0.8 Hz, 1H), 7.28 – 7.21 (m, 2H), 7.10 – 7.01 (m, 2H), 6.29 (dd, *J* = 3.2, 1.9 Hz, 1H), 6.10 (dq, *J* = 3.2, 0.8 Hz, 1H), 4.14 (dd, *J* = 8.0, 6.8 Hz, 1H), 3.31 – 3.08 (m, 2H).

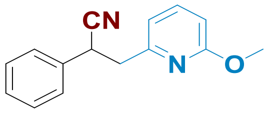
^{13}C NMR (101 MHz, CDCl$_3$) δ 163.76, 161.30, 149.64, 142.27, 130.66, 130.62, 129.11, 129.02, 119.97, 116.20, 115.98, 110.56, 108.43, 36.33, 34.65.

^{19}F NMR (282 MHz, CDCl$_3$) δ -113.31.



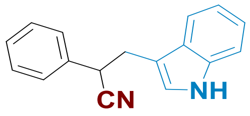
3-(5-methylfuran-2-yl)-2-phenylpropanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.38 – 7.22 (m, 5H), 5.94 (dq, *J* = 3.2, 0.6 Hz, 1H), 5.82 (dq, *J* = 3.2, 1.0 Hz, 1H), 4.08 (dd, *J* = 8.7, 6.4 Hz, 1H), 3.20 – 2.99 (m, 2H), 2.23 – 2.20 (m, 3H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 151.78, 148.14, 135.10, 129.08, 128.29, 127.32, 120.24, 108.92, 106.35, 37.31, 34.85, 13.54.



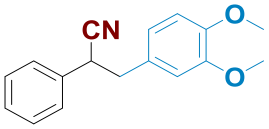
3-(6-methoxypyridin-2-yl)-2-phenylpropanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.38 (dd, *J* = 8.3, 7.2 Hz, 1H), 7.29 – 7.24 (m, 5H), 6.60 – 6.51 (m, 2H), 4.42 (dd, *J* = 8.8, 6.5 Hz, 1H), 3.87 (s, 3H), 3.26 – 3.06 (m, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 163.89, 153.64, 139.13, 135.69, 129.06, 128.11, 127.45, 120.89, 116.24, 109.28, 53.47, 43.42, 36.71.



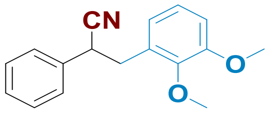
3-(1H-indol-3-yl)-2-phenylpropanenitrile[4]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 8.01 (s, 1H), 7.38 (ddt, *J* = 7.8, 1.4, 0.8 Hz, 1H), 7.32 – 7.20 (m, 6H), 7.16 – 7.10 (m, 1H), 7.07 – 7.01 (m, 1H), 6.95 – 6.91 (m, 1H), 4.03 (dd, *J* = 8.5, 6.2 Hz, 1H), 3.35 – 3.17 (m, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 136.16, 135.91, 129.08, 128.18, 127.48, 126.89, 123.34, 122.30, 121.18, 119.73, 118.18, 111.48, 110.89, 39.21, 32.49.



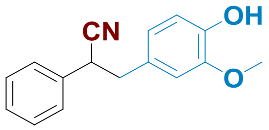
3-(3,4-dimethoxyphenyl)-2-phenylpropanenitrile[5]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.41 – 7.31 (m, 3H), 7.27 – 7.22 (m, 2H), 6.79 (d, *J* = 8.2 Hz, 1H), 6.73 – 6.67 (m, 1H), 6.52 (d, *J* = 2.0 Hz, 1H), 3.99 – 3.94 (m, 1H), 3.86 (s, 3H), 3.76 (s, 3H), 3.21 – 3.04 (m, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 148.74, 148.31, 135.21, 129.00, 128.64, 128.16, 127.61, 121.45, 120.50, 112.45, 111.16, 55.87, 55.78, 41.82, 39.95.



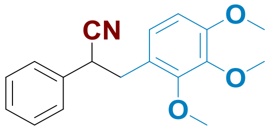
3-(2,3-dimethoxyphenyl)-2-phenylpropanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.36 – 7.28 (m, 5H), 6.98 (dd, *J* = 8.3, 7.5 Hz, 1H), 6.88 – 6.85 (m, 1H), 6.74 (s, 1H), 4.17 – 4.10 (m, 1H), 3.88 (m, 3H), 3.86 (m, 3H), 3.18 – 3.13 (m, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 152.65, 147.29, 135.94, 130.34, 129.02, 128.09, 127.38, 123.97, 122.74, 120.77, 112.01, 77.47, 77.05, 76.63, 60.69, 55.75, 38.47, 37.49.



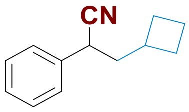
3-(4-hydroxy-3-methoxyphenyl)-2-phenylpropanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.41 – 7.23 (m, 5H), 6.81 – 6.70 (m, 2H), 6.68 – 6.63 (m, 1H), 5.66 (s, 1H), 3.96 (dd, *J* = 8.3, 6.6 Hz, 1H), 3.86 (s, 3H), 3.16 – 2.99 (m, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 145.93, 145.63, 135.36, 129.55, 129.04, 128.19, 127.49, 120.90, 120.52, 115.25, 110.70, 55.96, 41.71, 39.99.



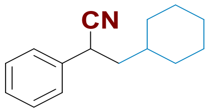
2-phenyl-3-(2,3,4-trimethoxyphenyl)propanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.41 – 7.22 (m, 5H), 6.82 (d, *J* = 8.4 Hz, 1H), 6.59 (d, *J* = 8.5 Hz, 1H), 4.08 (dd, *J* = 9.0, 6.4 Hz, 1H), 3.90 (s, 3H), 3.85 (d, *J* = 6.8 Hz, 6H), 3.15 – 2.99 (m, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 153.43, 151.90, 142.03, 135.94, 129.00, 128.04, 127.37, 125.07, 122.34, 120.84, 106.97, 60.92, 60.76, 55.96, 38.80, 37.33.



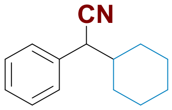
3-cyclobutyl-2-phenylpropanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.40 – 7.28 (m, 5H), 3.67 (dd, *J* = 8.6, 6.5 Hz, 1H), 2.52 – 2.36 (m, 1H), 2.18 – 1.71 (m, 6H), 1.70 – 1.54 (m, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 136.03, 129.04, 127.25, 125.64, 121.00, 42.84, 35.49, 33.59, 28.01, 18.44.



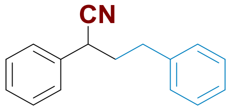
3-Cyclohexyl-2-phenylpropanenitrile[1]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.57 – 7.22 (m, 5H), 3.89 – 3.82 (m, 1H), 1.97 – 1.78 (m, 2H), 1.78 – 1.07 (m, 11H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 136.52, 129.10, 127.96, 127.22, 121.15, 43.71, 35.31, 34.82, 33.29, 32.36, 26.34, 25.96, 25.87.



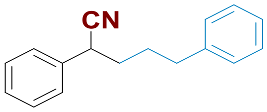
2-cyclohexyl-2-phenylacetonitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.30 – 7.15 (m, 5H), 3.52 (d, *J* = 6.6 Hz, 1H), 1.79 – 1.53 (m, 6H), 1.06 (tq, *J* = 12.3, 3.4 Hz, 5H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 134.70, 128.80, 127.99, 127.91, 120.15, 44.36, 42.78, 31.24, 29.58, 25.95, 25.85, 25.80.



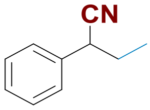
2,4-Diphenylbutanenitrile[1]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.25 – 7.06 (m, 10H), 6.60 – 6.11 (m, 1H), 3.45 (d, *J* = 6.3 Hz, 1H), 2.58 – 2.52 (m, 2H), 1.92 – 1.82 (m, 1H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 142.32, 131.10, 129.26, 128.71, 128.48, 128.34, 127.14, 126.16, 125.77, 39.38, 35.47, 32.99.



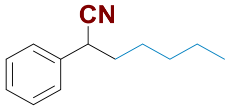
2,5-Diphenylpentanenitrile[3]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.60 – 7.19 (m, 10H), 3.90 – 3.72 (m, 1H), 2.72 (q, *J* = 8.2 Hz, 2H), 1.96 (dp, *J* = 21.1, 8.6 Hz, 4H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 141.25, 135.87, 129.17, 128.56, 128.46, 128.15, 127.33, 126.17, 120.87, 37.32, 35.29, 35.18, 28.64.



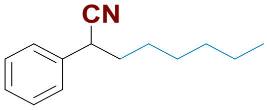
2-Phenylbutanenitrile[1]: ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.44 – 7.32 (m, 5H), 3.77 (t, *J* = 7.2 Hz, 1H), 2.03 – 1.94 (m, 2H), 1.10 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 135.78, 129.04, 128.03, 127.32, 120.79, 38.92, 29.24, 11.50.



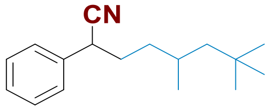
2-Phenylheptanenitrile[3]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.29 – 7.15 (m, 5H), 3.65 (dd, *J* = 8.4, 6.4 Hz, 1H), 1.83 – 1.64 (m, 2H), 1.43 – 1.28 (m, 2H), 1.22 – 1.15 (m, 4H), 0.79 – 0.74 (m, 3H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 136.13, 129.05, 127.99, 127.25, 120.97, 37.42, 35.91, 31.12, 26.73, 22.37, 13.96.



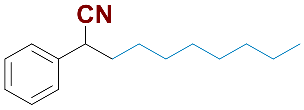
2-Phenyloctanenitrile[3]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.36 – 7.21 (m, 5H), 3.72 (dd, *J* = 8.4, 6.4 Hz, 1H), 1.91 – 1.75 (m, 2H), 1.50 – 1.36 (m, 2H), 1.28 – 1.20 (m, 6H), 0.85 – 0.80 (m, 3H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 136.13, 129.05, 127.98, 127.25, 120.97, 37.43, 35.95, 31.50, 28.64, 27.02, 22.54, 14.03.



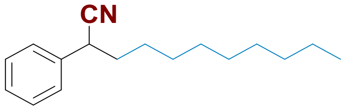
5,7,7-trimethyl-2-phenyloctanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.99 – 7.92 (m, 1H), 3.00 – 2.92 (m, 1H), 1.64 – 1.51 (m, 2H), 1.33 – 1.28 (m, 1H), 1.25 (d, *J* = 1.4 Hz, 1H), 0.98 (d, *J* = 6.4 Hz, 2H), 0.93 – 0.92 (m, 2H), 0.90 (s, 9H), 0.87 (d, *J* = 1.7 Hz, 3H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 200.78, 132.85, 129.05, 128.56, 128.05, 127.23, 77.47, 77.04, 76.62, 51.04, 36.52, 33.69, 31.09, 30.07, 30.00, 29.04, 22.53.



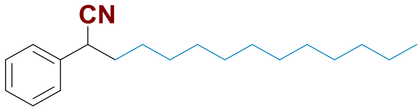
2-phenyldecanenitrile[3]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.49 – 7.21 (m, 5H), 3.80 – 3.73 (m, 1H), 2.14 – 1.67 (m, 2H), 1.31 – 1.24 (m, 12H), 0.88 (td, *J* = 3.6, 2.2 Hz, 3H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 136.11, 129.04, 127.97, 127.24, 120.96, 37.41, 35.93, 31.80, 29.27, 29.17, 28.97, 27.05, 22.63, 14.09.



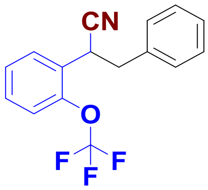
2-phenylundecanenitrile[1]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.25 – 7.13 (m, 5H), 3.70 – 3.59 (m, 1H), 1.86 – 1.64 (m, 2H), 1.16 – 1.09 (m, 14H), 0.75 (q, *J* = 2.5 Hz, 3H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 136.13, 129.04, 127.97, 127.24, 120.95, 37.42, 35.95, 31.86, 29.47, 29.32, 29.26, 28.97, 27.06, 22.68, 14.12.



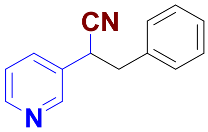
2-Phenyltetradecanenitrile[3]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.34 – 7.16 (m, 5H), 3.68 (dd, *J* = 8.4, 6.4 Hz, 1H), 1.87 – 1.71 (m, 2H), 1.19 – 1.16 (m, 20H), 0.80 (s, 3H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 136.14, 129.03, 127.96, 127.24, 120.92, 37.42, 35.96, 31.94, 29.65, 29.61, 29.52, 29.38, 29.32, 28.98, 27.07, 22.72, 14.14.



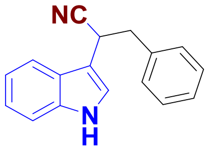
3-phenyl-2-(2-(trifluoromethoxy)phenyl)propanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.49 (dd, *J* = 7.9, 1.9 Hz, 1H), 7.41 – 7.37 (m, 1H), 7.31 (dddd, *J* = 6.8, 4.8, 2.6, 1.4 Hz, 5H), 7.22 – 7.18 (m, 2H), 4.39 (dd, *J* = 8.8, 5.5 Hz, 1H), 3.20 – 3.08 (m, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 146.31, 135.95, 129.93, 129.53, 129.18, 128.76, 128.52, 128.33, 127.60, 127.52, 127.21, 120.00, 119.59, 40.60, 34.30.



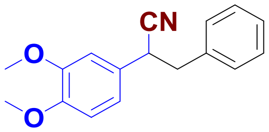
3-phenyl-2-(pyridin-3-yl)propanenitrile[4]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 8.57 – 8.30 (m, 2H), 7.50 (dt, *J* = 7.9, 1.8 Hz, 1H), 7.27 – 7.15 (m, 4H), 7.07 – 6.98 (m, 2H), 4.05 – 3.95 (m, 1H), 3.11 (qd, *J* = 13.6, 7.3 Hz, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 149.67, 148.85, 135.34, 135.09, 131.04, 129.26, 128.82, 127.73, 123.74, 119.45, 41.78, 37.24.



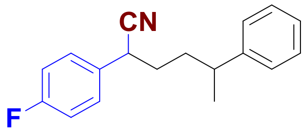
2-(1H-indol-3-yl)-3-phenylpropanenitrile[4]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 8.37 (s, 1H), 7.72 (ddt, *J* = 7.6, 1.5, 0.8 Hz, 1H), 7.42 (s, 2H), 7.37 – 7.32 (m, 3H), 7.26 (ddt, *J* = 7.0, 3.7, 1.7 Hz, 3H), 7.09 (dd, *J* = 2.6, 0.8 Hz, 1H), 4.75 (s, 1H), 4.35 (ddd, *J* = 8.4, 6.0, 0.8 Hz, 1H), 3.42 – 3.29 (m, 2H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 137.02, 136.49, 129.27, 128.65, 127.73, 127.34, 127.09, 125.20, 122.79, 120.23, 118.34, 111.84, 109.90, 65.34, 40.22, 31.53.



2-(3,4-dimethoxyphenyl)-3-phenylpropanenitrile[6]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.37 – 7.28 (m, 3H), 7.16 – 7.08 (m, 2H), 6.84 – 6.79 (m, 2H), 6.64 (d, *J* = 1.7 Hz, 1H), 3.98 – 3.93 (m, 1H), 3.88 (s, 3H), 3.81 (s, 3H), 3.16 (qd, *J* = 13.5, 7.3 Hz, 2H).

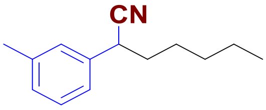
^{13}C NMR (75 MHz, CDCl$_3$) δ 149.13, 148.87, 136.33, 129.34, 128.61, 127.48, 127.35, 120.63, 119.80, 111.31, 110.61, 55.96, 55.92, 42.24, 39.27.



2-(4-fluorophenyl)-5-phenylhexanenitrile: **^{1}H NMR (400 MHz, CDCl$_3$)** δ 7.37 – 7.30 (m, 2H), 7.28 – 7.21 (m, 3H), 7.20 – 7.15 (m, 2H), 7.10 – 7.03 (m, 2H), 3.79 – 3.63 (m, 1H), 2.84 – 2.65 (m, 1H), 1.95 – 1.67 (m, 4H), 1.29 (d, *J* = 7.0 Hz, 3H).

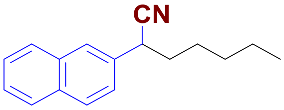
^{13}C NMR (101 MHz, CDCl$_3$) δ 198.71, 166.90, 164.37, 146.45, 133.40, 133.37, 130.67, 130.58, 128.55, 127.09, 126.27, 115.68, 115.47, 39.53, 36.61, 32.46, 29.73, 22.62.

^{19}F NMR (282 MHz, CDCl$_3$) δ -113.88.



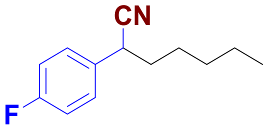
2-(m-tolyl)heptanenitrile: **^{1}H NMR (300 MHz, CDCl$_3$)** δ 7.29 – 7.23 (m, 1H), 7.16 – 7.08 (m, 3H), 3.73 (dd, *J* = 8.5, 6.3 Hz, 1H), 2.37 (t, *J* = 0.7 Hz, 3H), 1.99 – 1.76 (m, 2H), 1.56 – 1.42 (m, 2H), 1.36 – 1.28 (m, 4H), 0.91 – 0.85 (m, 3H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 138.87, 136.03, 128.90, 128.71, 127.90, 124.30, 121.10, 37.36, 35.92, 31.13, 26.78, 22.37, 21.39, 13.96.



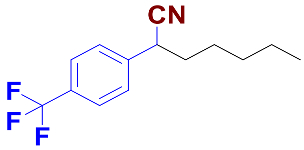
2-(naphthalen-2-yl)heptanenitrile: **^{1}H NMR (300 MHz, CDCl$_3$)** δ 7.84 – 7.80 (m, 2H), 7.77 – 7.73 (m, 1H), 7.60 (dd, *J* = 7.1, 1.3 Hz, 1H), 7.51 – 7.40 (m, 3H), 4.45 (t, *J* = 7.2 Hz, 1H), 1.95 (td, *J* = 8.0, 7.0 Hz, 2H), 1.59 – 0.94 (m, 6H), 0.82 (q, *J* = 2.7 Hz, 3H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 136.72, 134.05, 131.77, 129.98, 129.35, 128.87, 126.87, 126.08, 125.49, 122.09, 121.21, 34.81, 34.47, 31.16, 27.21, 22.44, 13.97.



2-(4-fluorophenyl)heptanenitrile: **^{1}H NMR (300 MHz, CDCl$_3$)** δ 7.34 – 7.25 (m, 2H), 7.11 – 7.02 (m, 2H), 3.75 (dd, *J* = 8.5, 6.4 Hz, 1H), 1.97 – 1.76 (m, 2H), 1.53 – 1.39 (m, 2H), 1.35 – 1.27 (m, 4H), 0.91 – 0.86 (m, 3H).

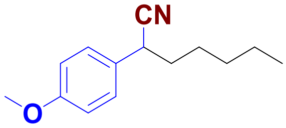
^{13}C NMR (75 MHz, CDCl$_3$) δ 163.97, 160.70, 131.89, 131.85, 128.98, 128.87, 120.77, 116.16, 115.87, 36.70, 35.90, 31.06, 26.63, 22.34, 13.92.



2-(4-(trifluoromethyl)phenyl)heptanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.61 – 7.53 (m, 2H), 7.43 – 7.34 (m, 2H), 3.78 (dd, *J* = 8.4, 6.3 Hz, 1H), 1.89 – 1.72 (m, 2H), 1.46 – 1.35 (m, 2H), 1.24 (tq, *J* = 4.0, 2.9 Hz, 4H), 0.84 – 0.79 (m, 3H).

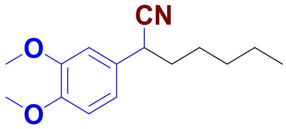
^{13}C NMR (75 MHz, CDCl$_3$) δ 140.03, 128.37, 127.71, 126.16, 126.11, 126.06, 126.01, 125.67, 125.62, 122.03, 120.12, 37.28, 35.73, 31.03, 26.65, 22.31, 13.89.

^{19}F NMR (282 MHz, CDCl$_3$) δ -62.71, -63.10.



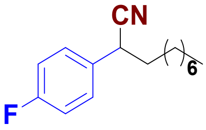
2-(4-methoxyphenyl)heptanenitrile[7]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.25 – 7.12 (m, 2H), 6.93 – 6.83 (m, 2H), 3.78 (s, 3H), 3.70 (dd, *J* = 8.4, 6.4 Hz, 1H), 1.96 – 1.70 (m, 2H), 1.36 – 1.23 (m, 6H), 0.89 – 0.84 (m, 3H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 159.26, 128.33, 128.07, 121.24, 114.38, 55.30, 36.55, 35.89, 31.10, 26.65, 22.36, 13.92.



2-(3,4-dimethoxyphenyl)heptanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 6.83 – 6.80 (m, 2H), 6.78 (dd, *J* = 2.0, 0.8 Hz, 1H), 3.85 (s, 3H), 3.83 (s, 3H), 3.68 (dd, *J* = 8.5, 6.5 Hz, 1H), 1.93 – 1.72 (m, 2H), 1.32 – 1.22 (m, 6H), 0.84 (q, *J* = 4.0 Hz, 3H).

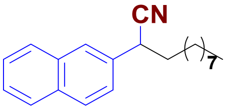
^{13}C NMR (75 MHz, CDCl$_3$) δ 149.32, 148.74, 128.49, 121.15, 119.54, 111.41, 110.26, 55.97, 55.92, 36.93, 35.85, 31.08, 26.68, 22.34, 13.90.



2-(4-fluorophenyl)undecanenitrile: ^{1}**H NMR (300 MHz, CDCl$_3$)** δ 7.34 – 7.26 (m, 2H), 7.12 – 7.02 (m, 2H), 3.80 – 3.69 (m, 1H), 1.97 – 1.75 (m, 2H), 1.32 – 1.23 (m, 12H), 0.89 – 0.85 (m, 3H).

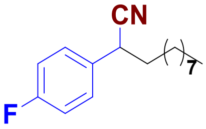
^{13}**C NMR (75 MHz, CDCl$_3$)** δ 163.97, 160.69, 131.89, 131.85, 130.73, 128.98, 128.87, 120.77, 116.15, 115.87, 115.76, 36.70, 35.94, 31.78, 29.25, 29.14, 28.92, 26.96, 22.62, 14.08.

^{19}**F NMR (282 MHz, CDCl$_3$)** δ -114.00.



2-(naphthalen-2-yl)dodecanenitrile: ^{1}**H NMR (300 MHz, CDCl$_3$)** δ 7.93 – 7.88 (m, 2H), 7.84 (dt, *J* = 8.4, 1.0 Hz, 1H), 7.69 (dd, *J* = 7.2, 1.3 Hz, 1H), 7.61 – 7.48 (m, 3H), 4.62 – 4.47 (m, 1H), 2.08 (d, *J* = 8.3 Hz, 2H), 1.27 (t, *J* = 3.8 Hz, 14H), 0.89 (d, *J* = 2.5 Hz, 3H).

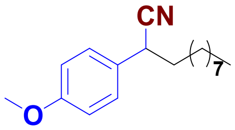
^{13}**C NMR (75 MHz, CDCl$_3$)** δ 134.05, 131.78, 129.99, 129.34, 128.86, 128.84, 126.86, 126.07, 125.49, 122.10, 121.20, 34.84, 34.47, 31.86, 29.48, 29.37, 29.27, 29.02, 27.52, 22.68, 14.13.



2-(4-fluorophenyl)dodecanenitrile: ^{1}**H NMR (300 MHz, CDCl$_3$)** δ 7.26 – 7.19 (m, 2H), 7.02 – 6.95 (m, 2H), 3.68 (dd, *J* = 8.4, 6.4 Hz, 1H), 1.90 – 1.71 (m, 2H), 1.19 (t, *J* = 3.8 Hz, 14H), 0.80 (d, *J* = 2.7 Hz, 3H).

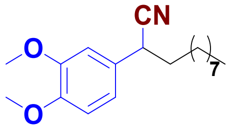
^{13}**C NMR (75 MHz, CDCl$_3$)** δ 198.95, 167.31, 163.96, 160.69, 133.54, 131.91, 131.86, 130.72, 130.60, 128.97, 128.86, 120.76, 116.18, 116.14, 115.90, 115.85, 115.74, 115.45, 36.69, 35.94, 31.83, 29.44, 29.29, 29.23, 28.92, 26.96, 22.66, 14.09.

^{19}**F NMR (282 MHz, CDCl$_3$)** δ -113.99.



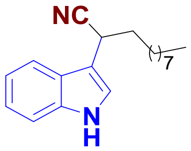
2-(4-methoxyphenyl)dodecanenitrile[7]: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.25 – 7.18 (m, 2H), 6.92 – 6.85 (m, 2H), 3.79 (s, 3H), 3.70 (dd, *J* = 8.4, 6.5 Hz, 1H), 1.94 – 1.72 (m, 2H), 1.29 – 1.24 (m, 14H), 0.88 (d, *J* = 4.3 Hz, 3H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 159.25, 128.34, 128.08, 121.24, 114.37, 55.30, 36.57, 35.96, 31.85, 29.46, 29.32, 29.25, 28.97, 26.99, 22.67, 14.11.



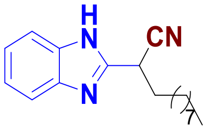
2-(3,4-dimethoxyphenyl)dodecanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 6.84 – 6.81 (m, 2H), 6.80 (dt, *J* = 2.1, 0.7 Hz, 1H), 3.91 (d, *J* = 2.1 Hz, 1H), 3.86 (d, *J* = 6.9 Hz, 6H), 1.92 – 1.76 (m, 2H), 1.24 (d, *J* = 4.1 Hz, 14H), 0.86 (d, *J* = 1.2 Hz, 3H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 149.32, 148.72, 128.49, 121.16, 119.54, 111.36, 110.20, 55.96, 55.92, 36.97, 35.94, 31.83, 29.44, 29.31, 29.23, 28.96, 27.04, 22.65, 14.09.



2-(1H-indol-3-yl)octadecanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 8.44 (s, 1H), 7.55 (ddt, *J* = 7.7, 1.5, 0.7 Hz, 1H), 7.31 (t, *J* = 2.3 Hz, 1H), 7.17 – 7.13 (m, 1H), 7.12 – 7.09 (m, 1H), 7.05 – 7.03 (m, 1H), 3.96 (ddd, *J* = 7.5, 6.8, 0.7 Hz, 1H), 1.98 – 1.88 (m, 2H), 1.21 – 1.18 (m, 14H), 0.81 (d, *J* = 1.6 Hz, 3H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 136.54, 125.32, 122.60, 122.38, 121.44, 119.98, 118.39, 111.76, 110.56, 33.98, 31.90, 29.54, 29.43, 29.31, 29.05, 28.93, 27.27, 22.71, 14.16.



2-(1H-benzo[d]imidazol-2-yl)octadecanenitrile: ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.91 (d, *J* = 8.0 Hz, 1H), 7.56 (d, *J* = 7.7 Hz, 1H), 7.44 – 7.33 (m, 2H), 3.31 (dd, *J* = 7.8, 7.1 Hz, 2H), 1.88 – 1.75 (m, 2H), 1.37 – 1.20 (m, 14H), 0.89 – 0.85 (m, 3H).

^{13}C NMR (75 MHz, CDCl$_3$) δ 147.61, 143.42, 126.44, 123.79, 121.89, 38.35, 31.88, 29.46, 29.43, 29.29, 29.22, 24.01, 22.67, 14.11.

S7. References

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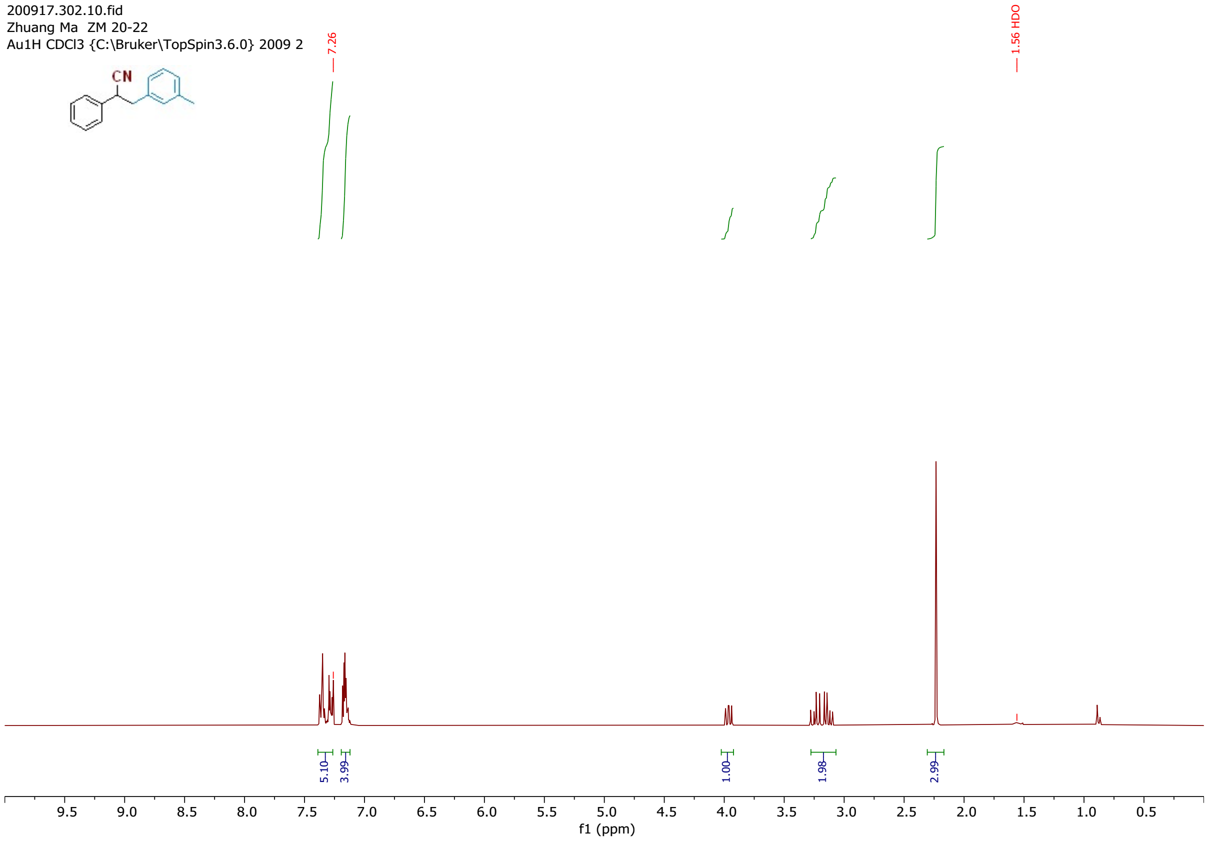
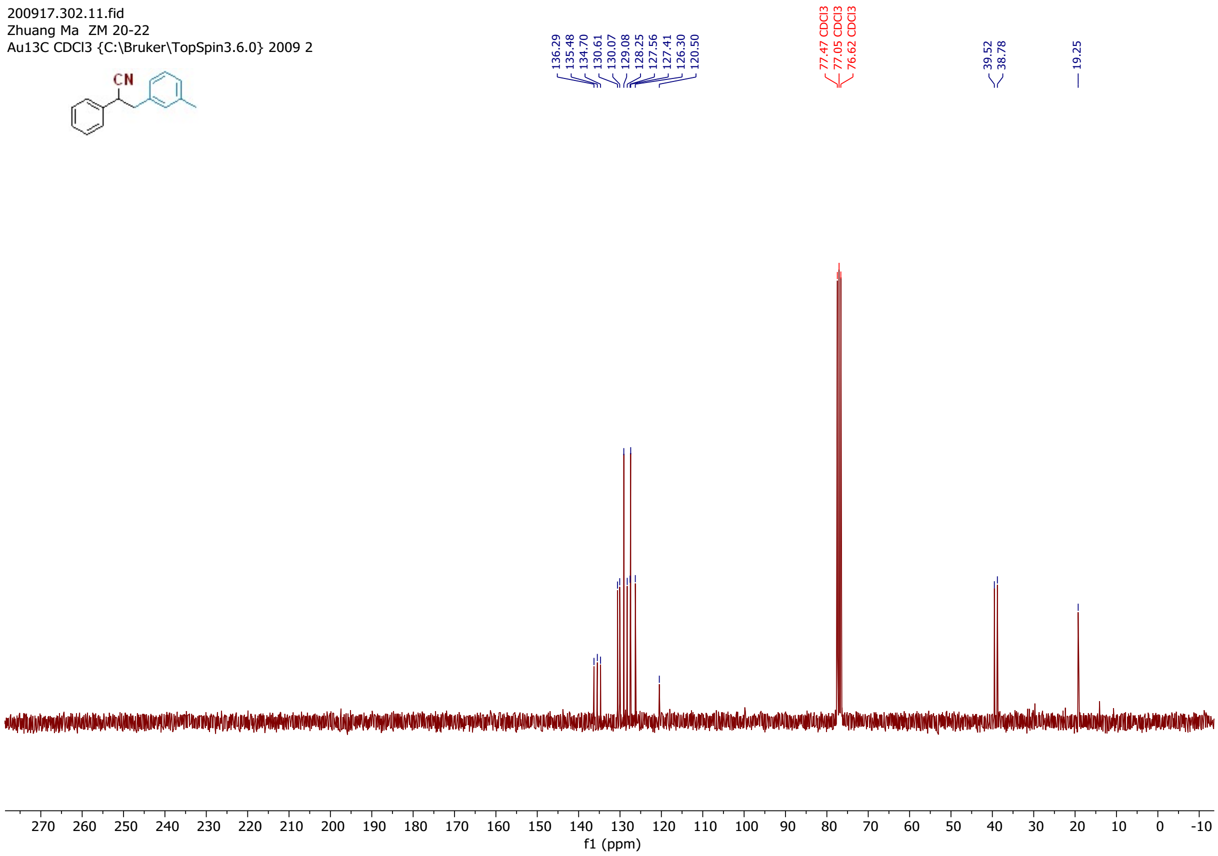
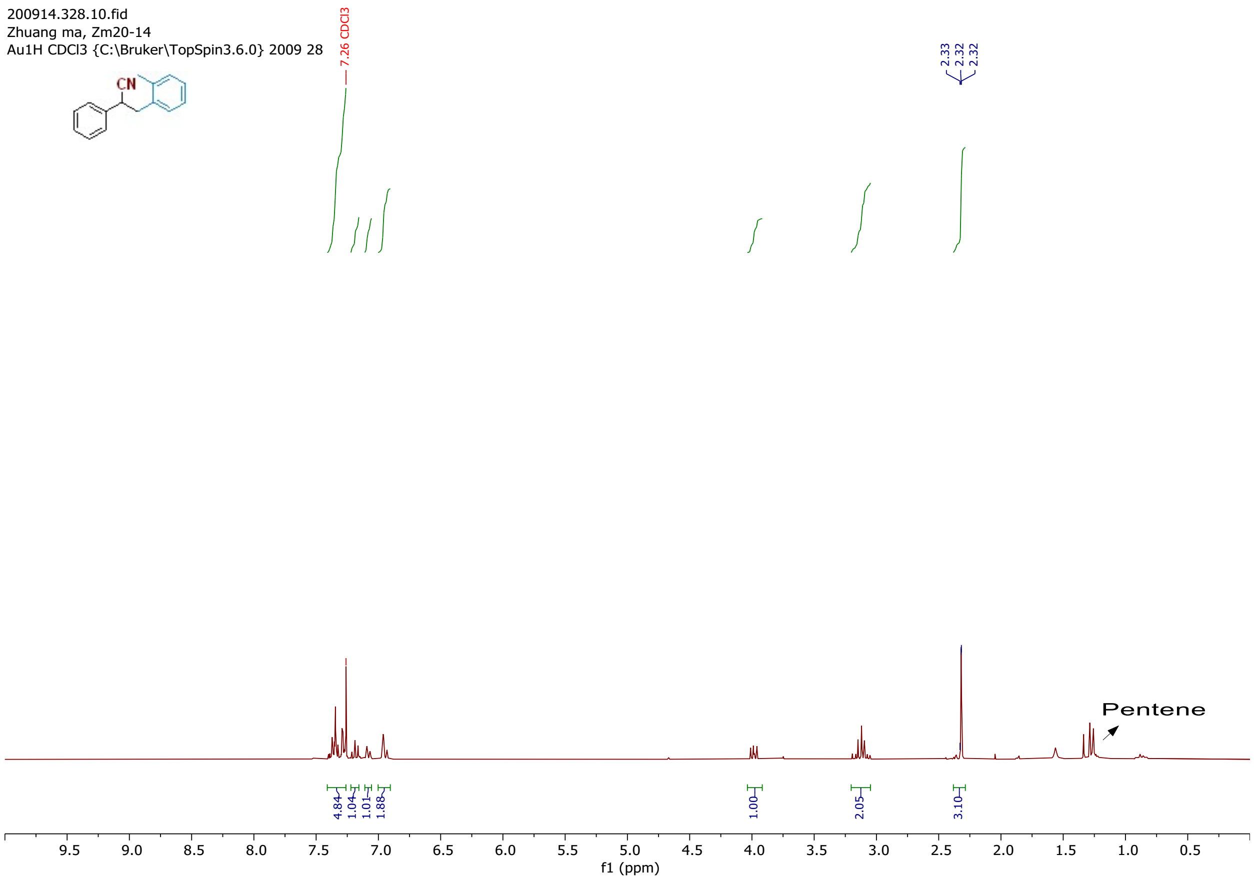
S8. NMR Spectra



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2.32
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1.88
1.00
2.05
3.10
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6.0
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4.0
3.5
3.0
2.5
2.0
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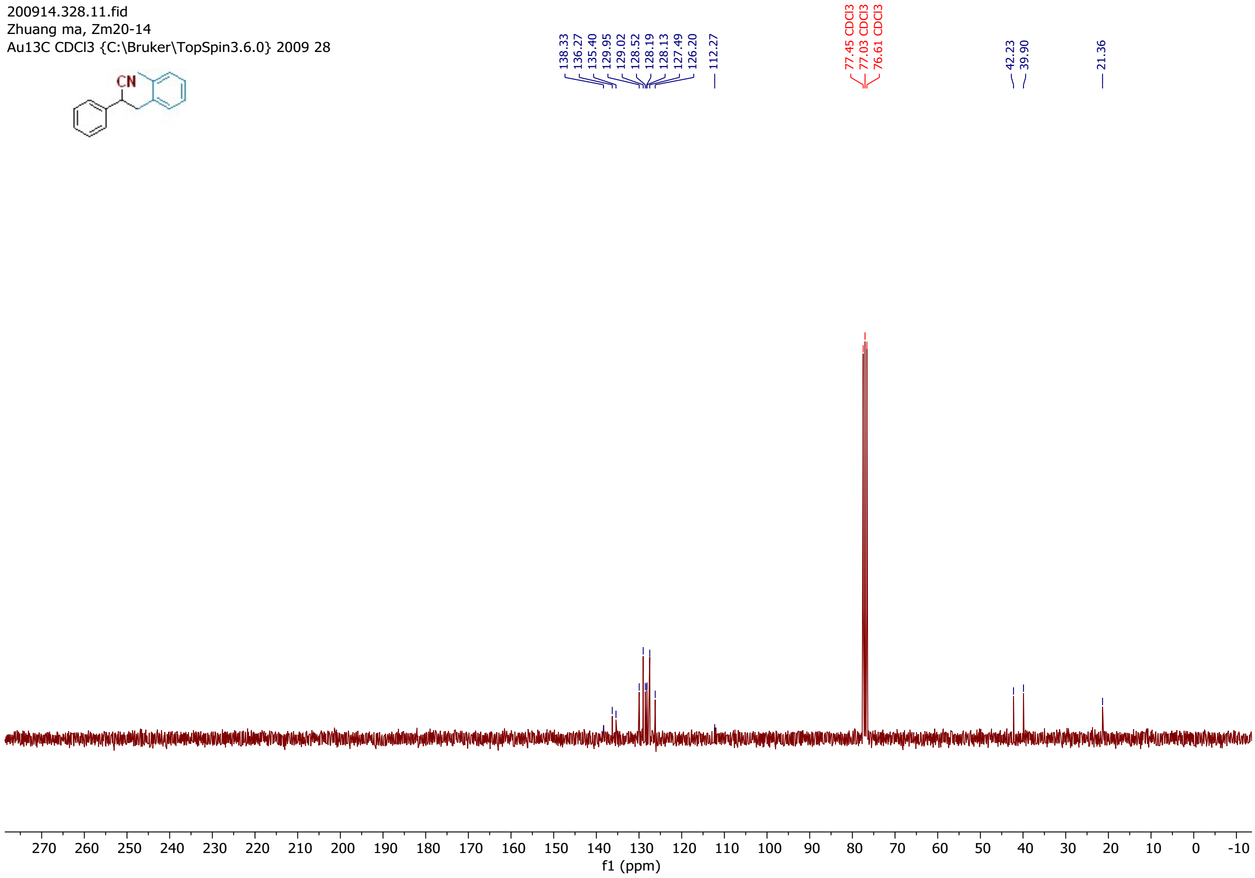
1.0
0.5
f1 (ppm)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76.61 CDCl3
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39.90
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260
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240
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220
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200
190
180
170
160
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140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
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f1 (ppm)

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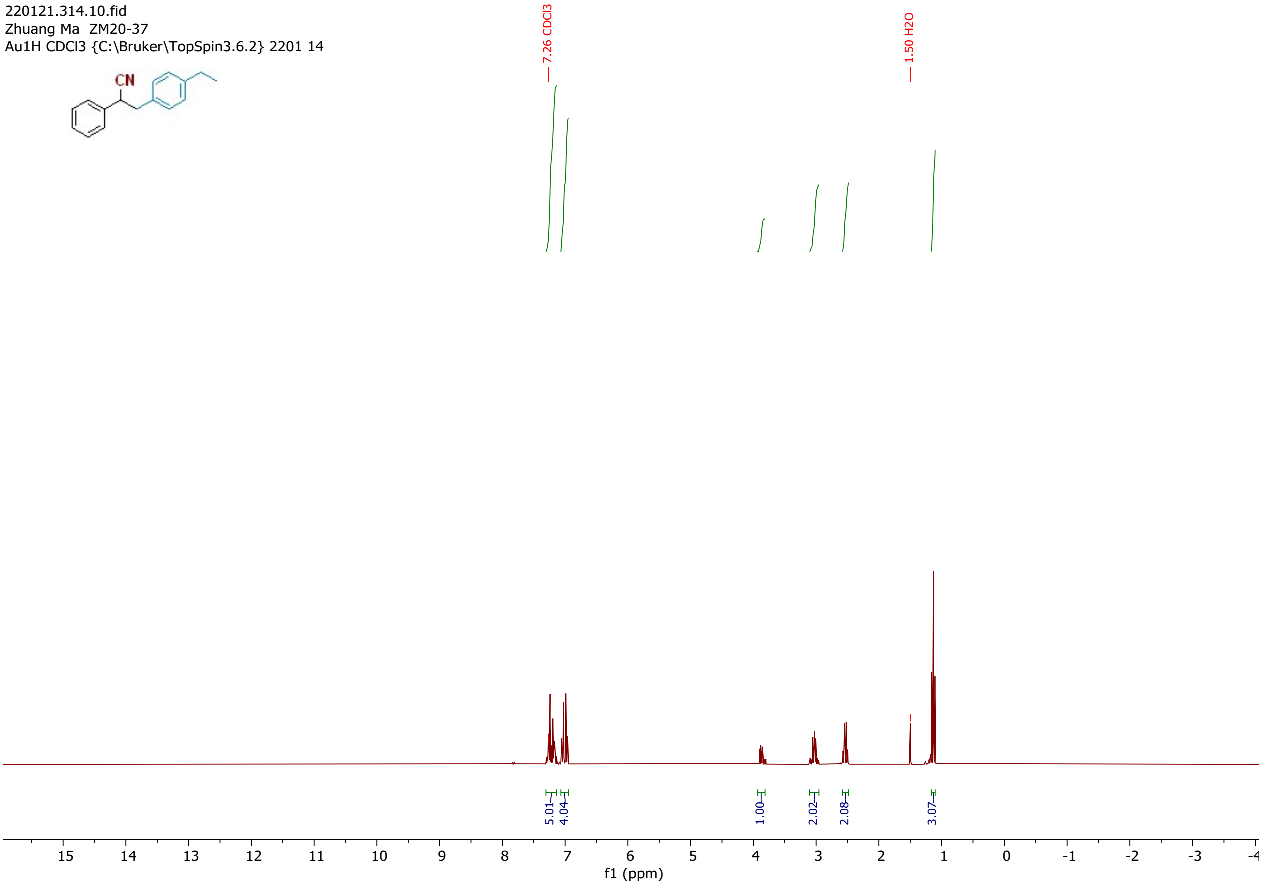

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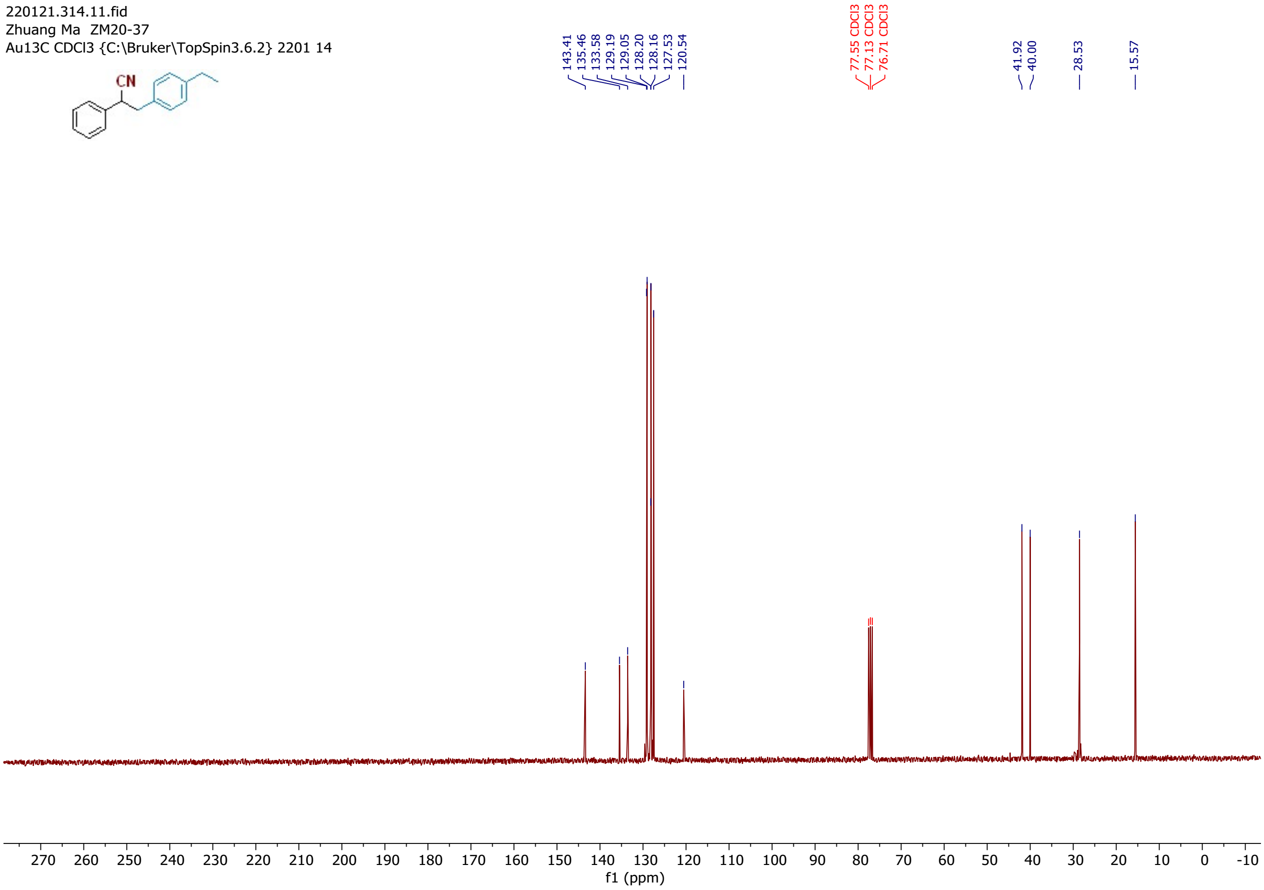

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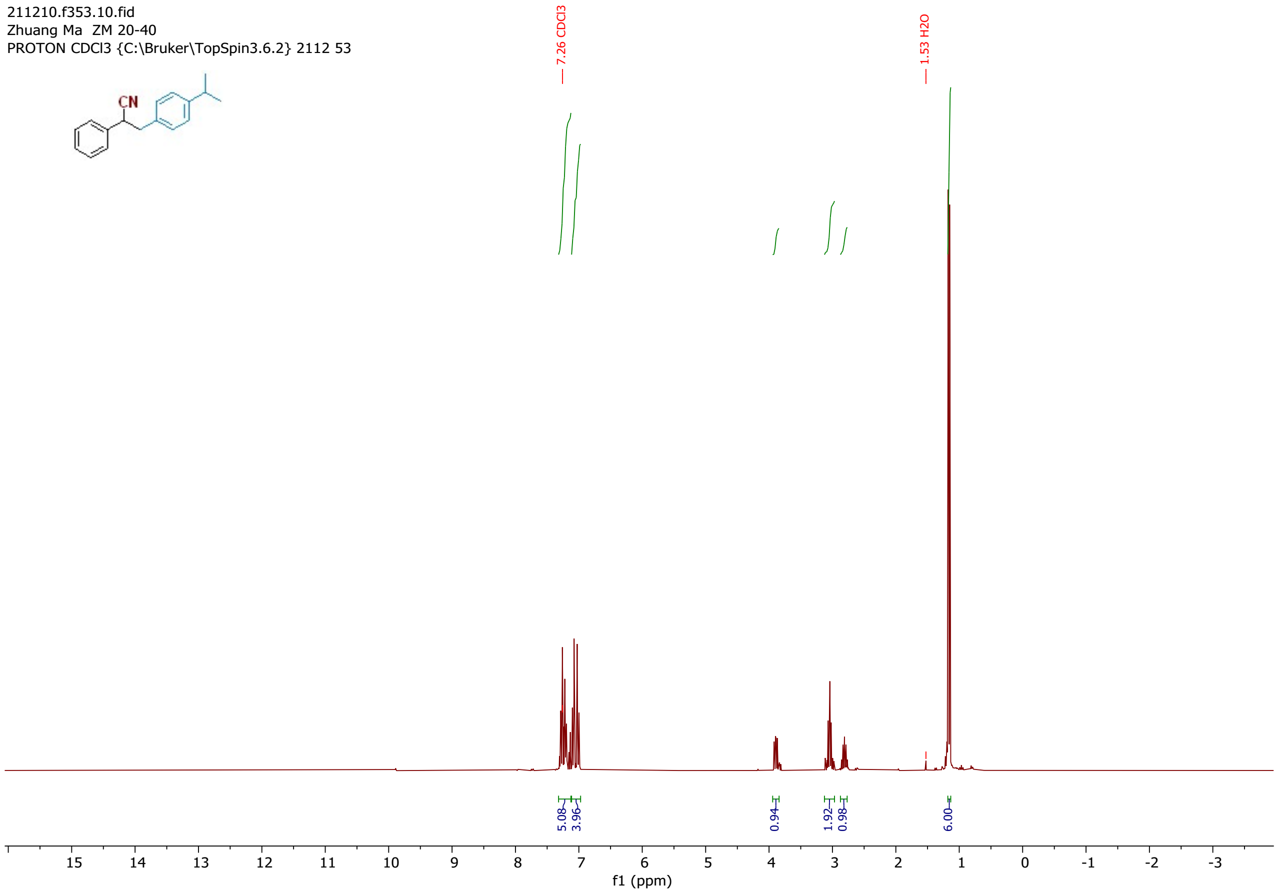

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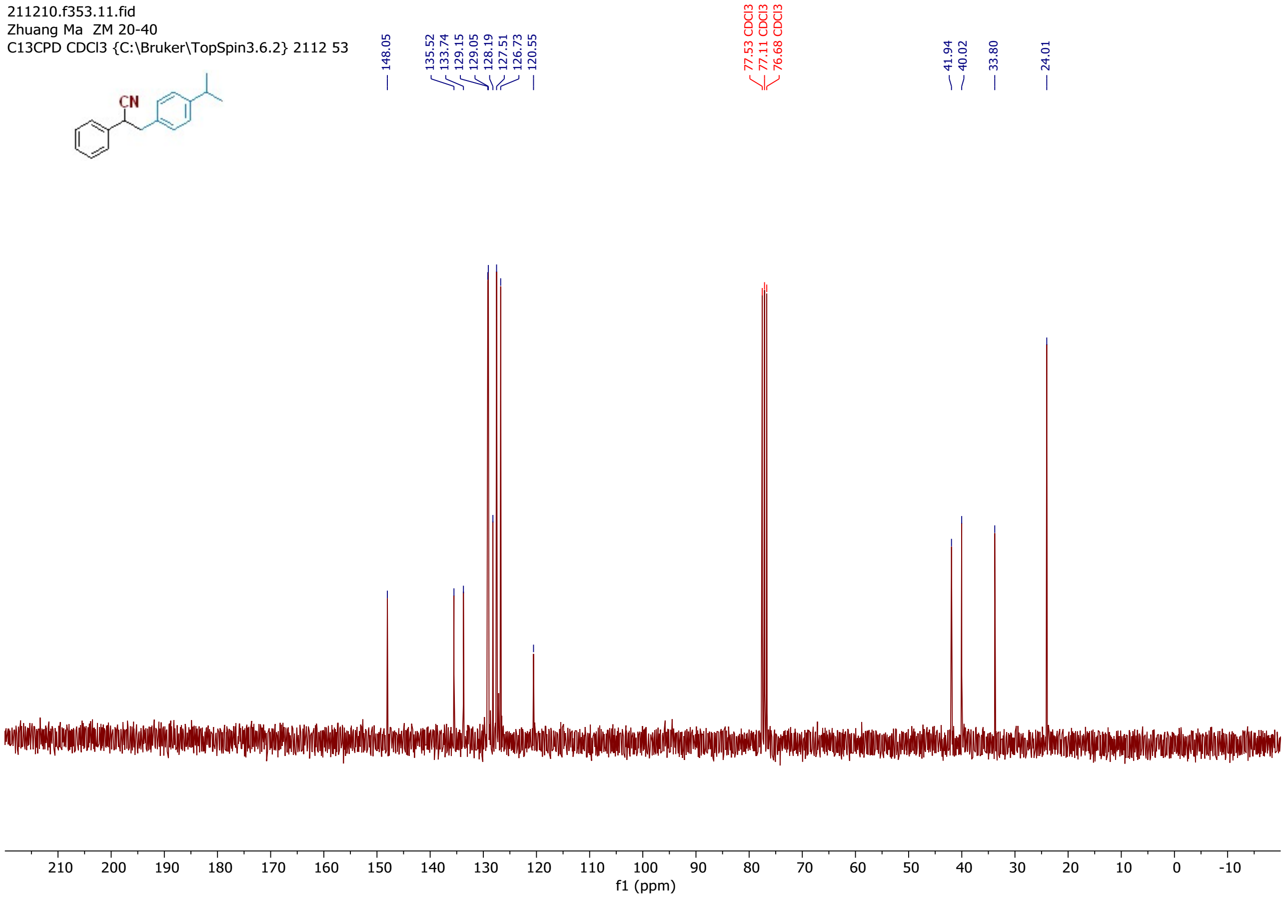

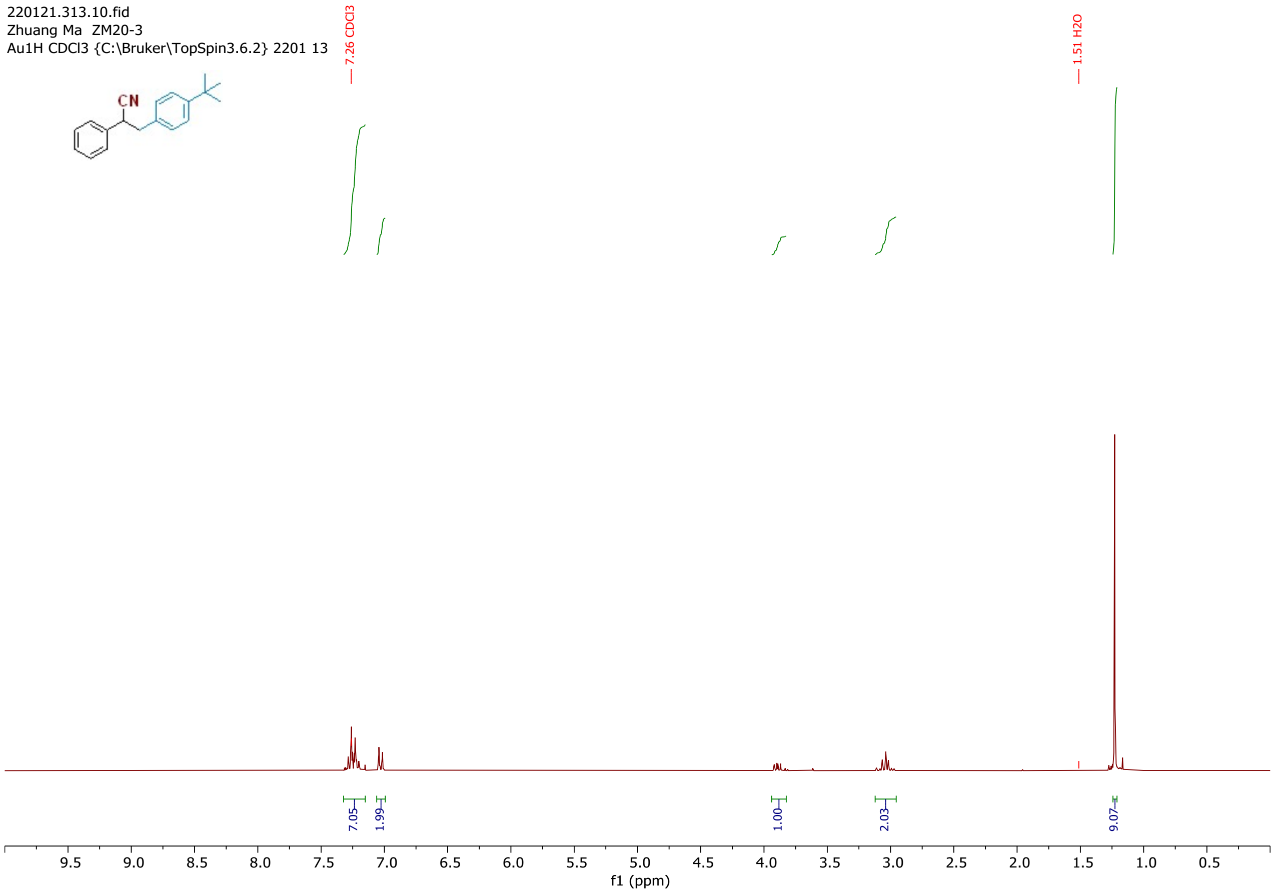
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2.5
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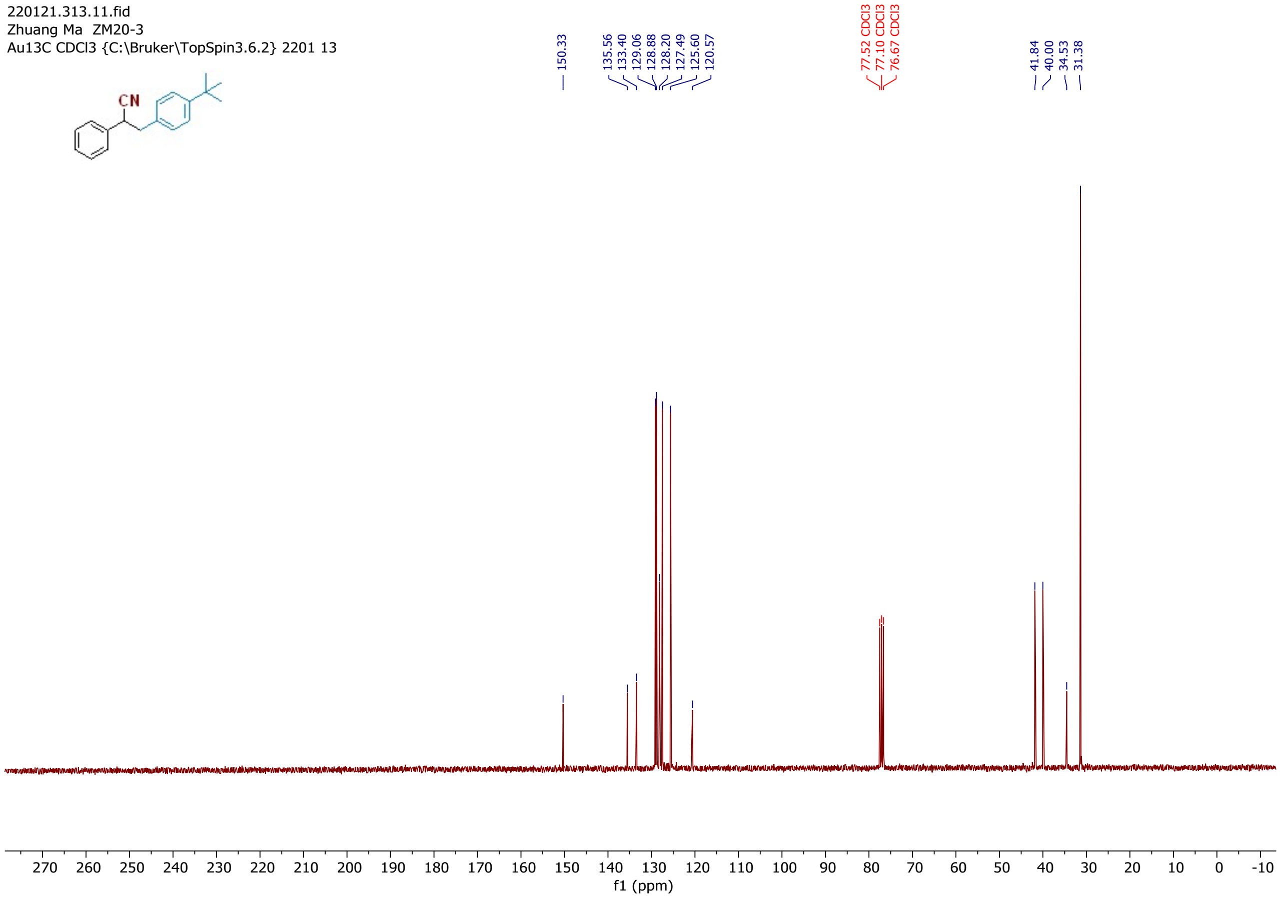
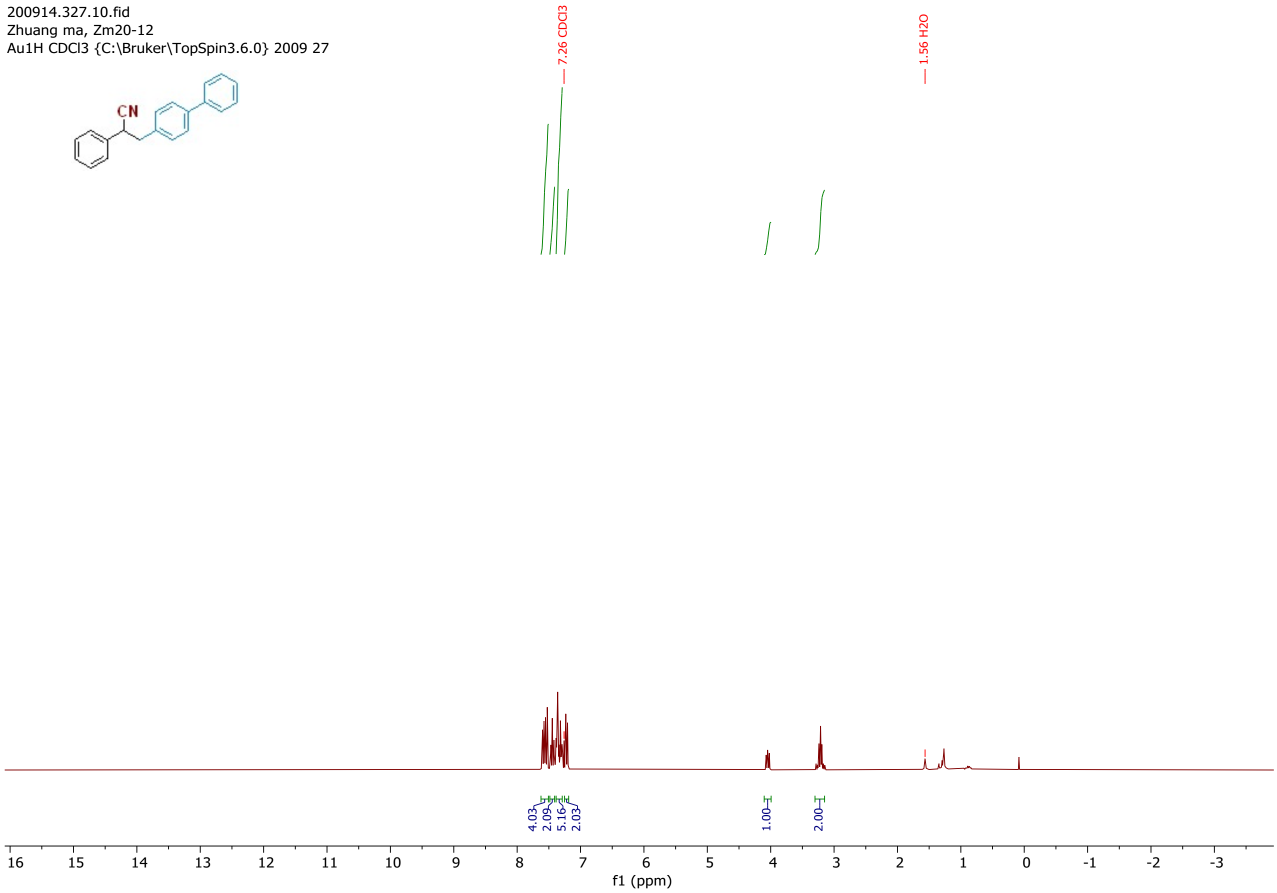
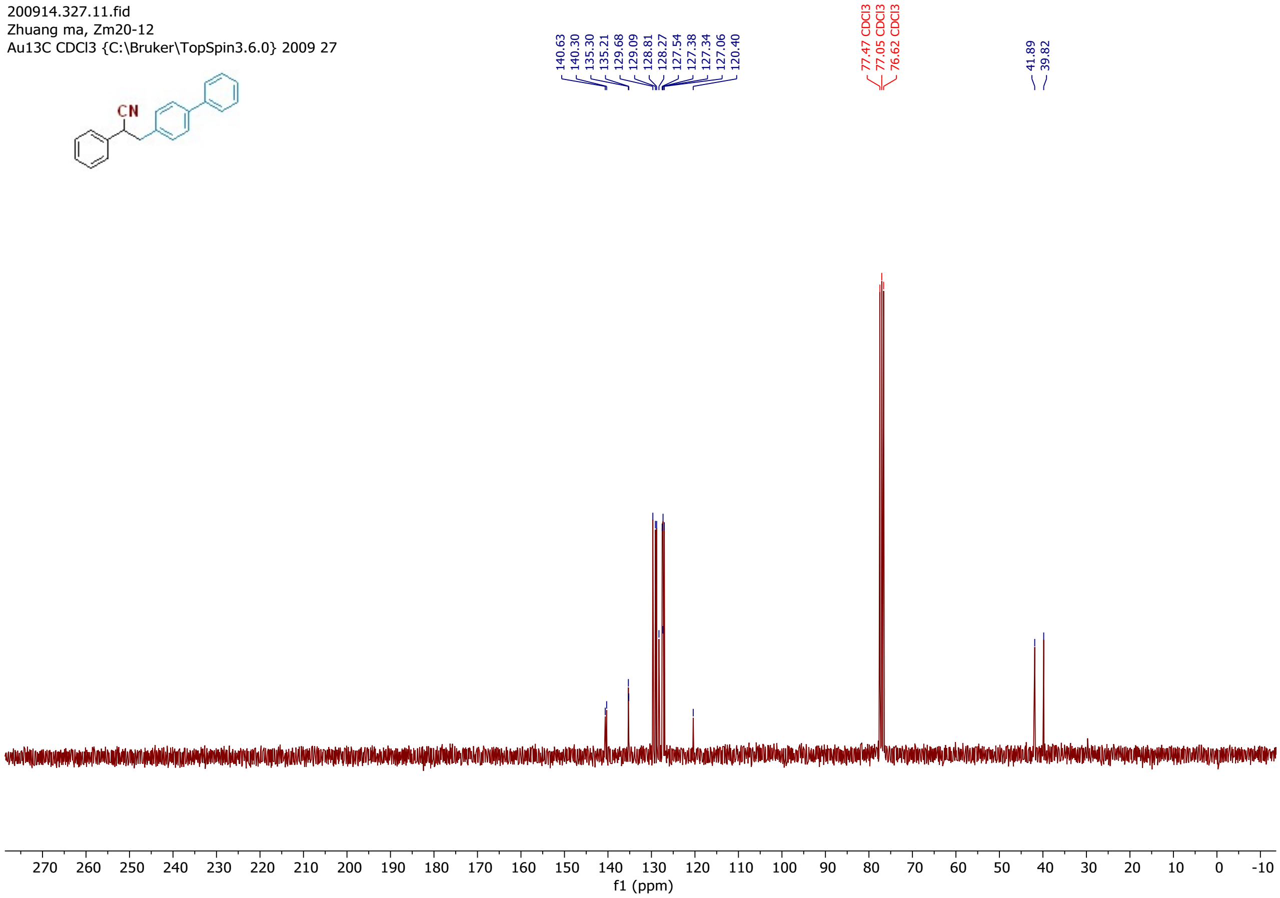
1.0
0.5
f1 (ppm)


220121.313.11.fid
Zhuang Ma ZM20-3
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 13
CN
150.33
135.56
133.40
129.06
128.88
128.20
127.49
125.60
120.57
77.52 CDCl3
77.10 CDCl3
76.67 CDCl3
41.84
40.00
34.53
31.38
270
260
250
240
230
220
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)

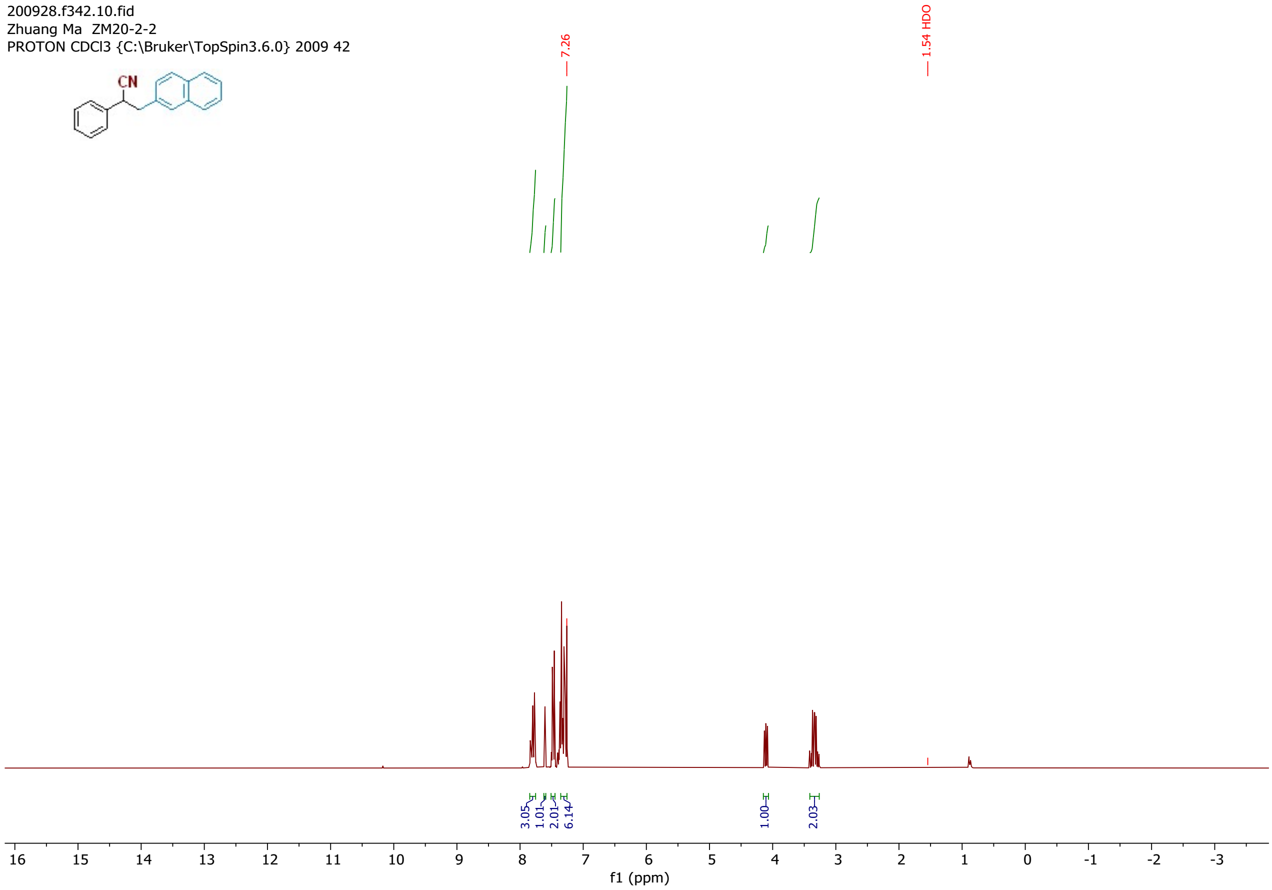
200914.327.10.fid
Zhuang ma, Zm20-12
Au1H CDCl3 {C:\Bruker\TopSpin3.6.0} 2009 27



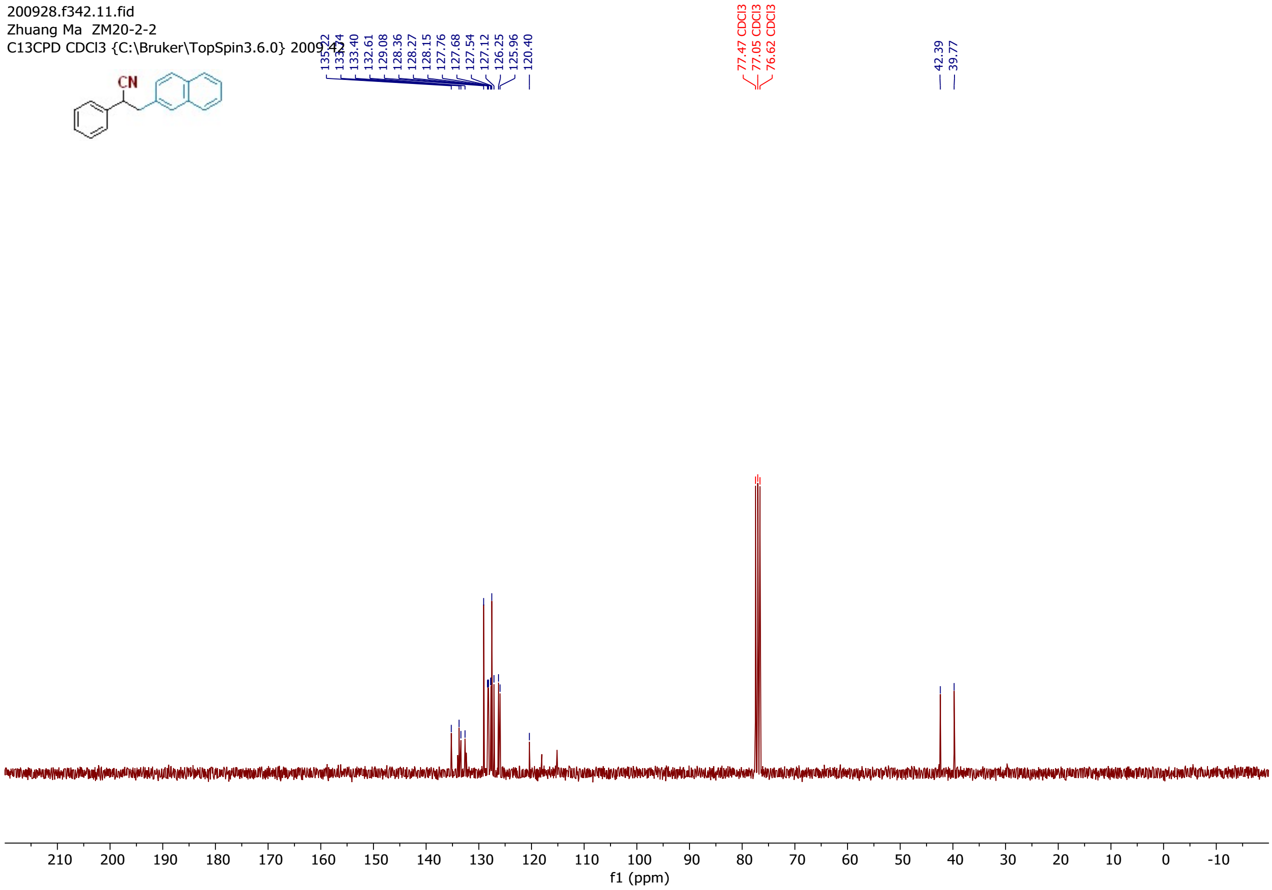
200914.327.11.fid
Zhuang ma, Zm20-12
Au13C CDCl3 {C:\Bruker\TopSpin3.6.0} 2009 27

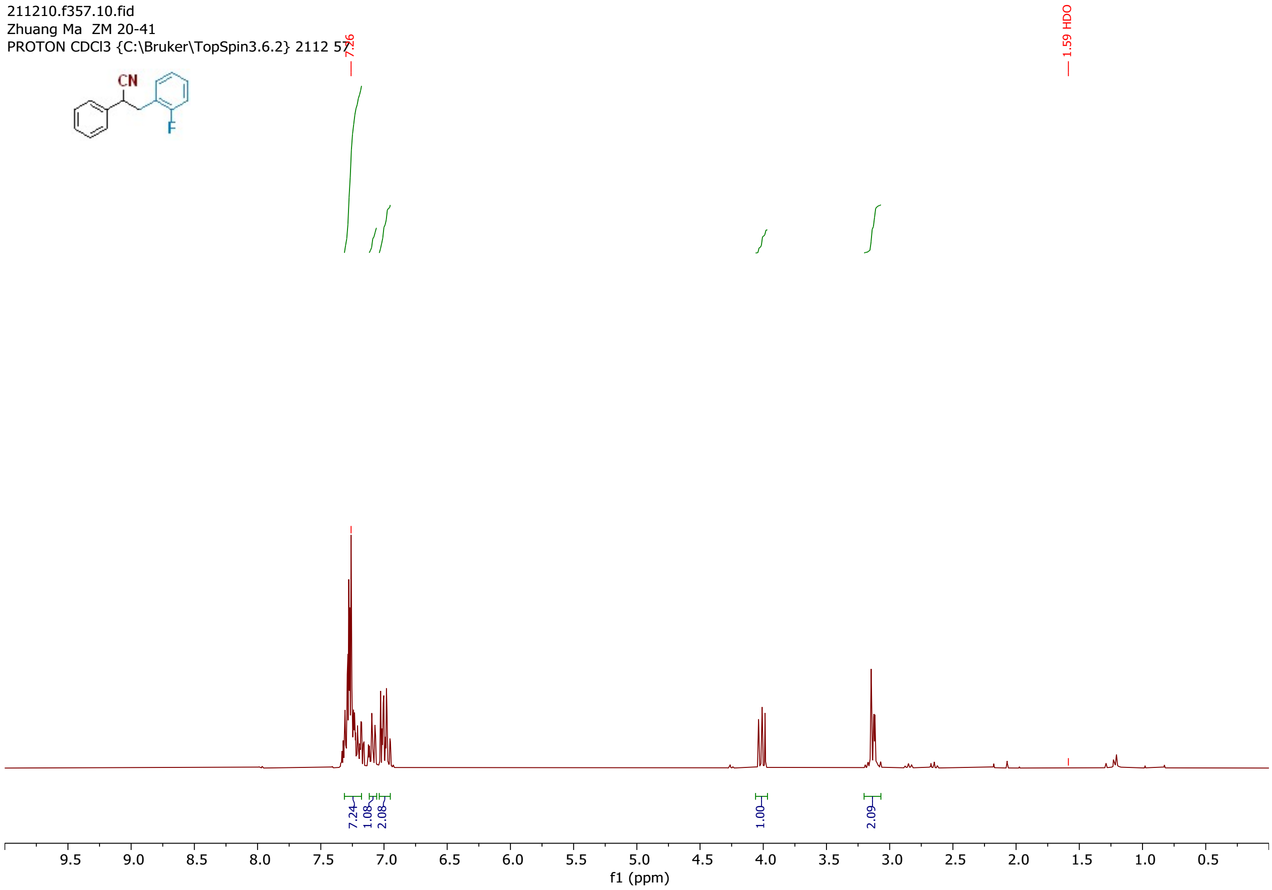


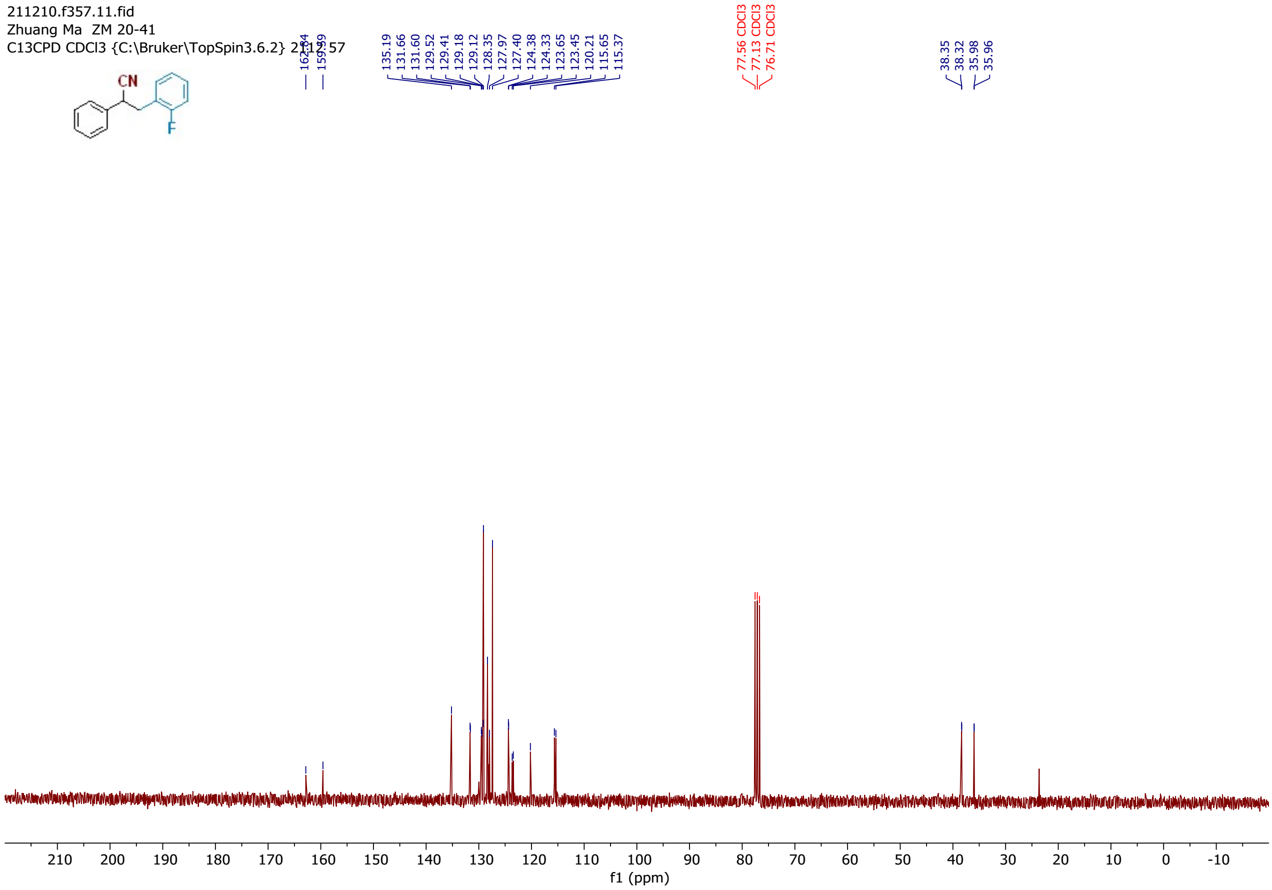
200928.f342.10.fid
Zhuang Ma ZM20-2-2
PROTON CDCl3 {C:\Bruker\TopSpin3.6.0} 2009 42

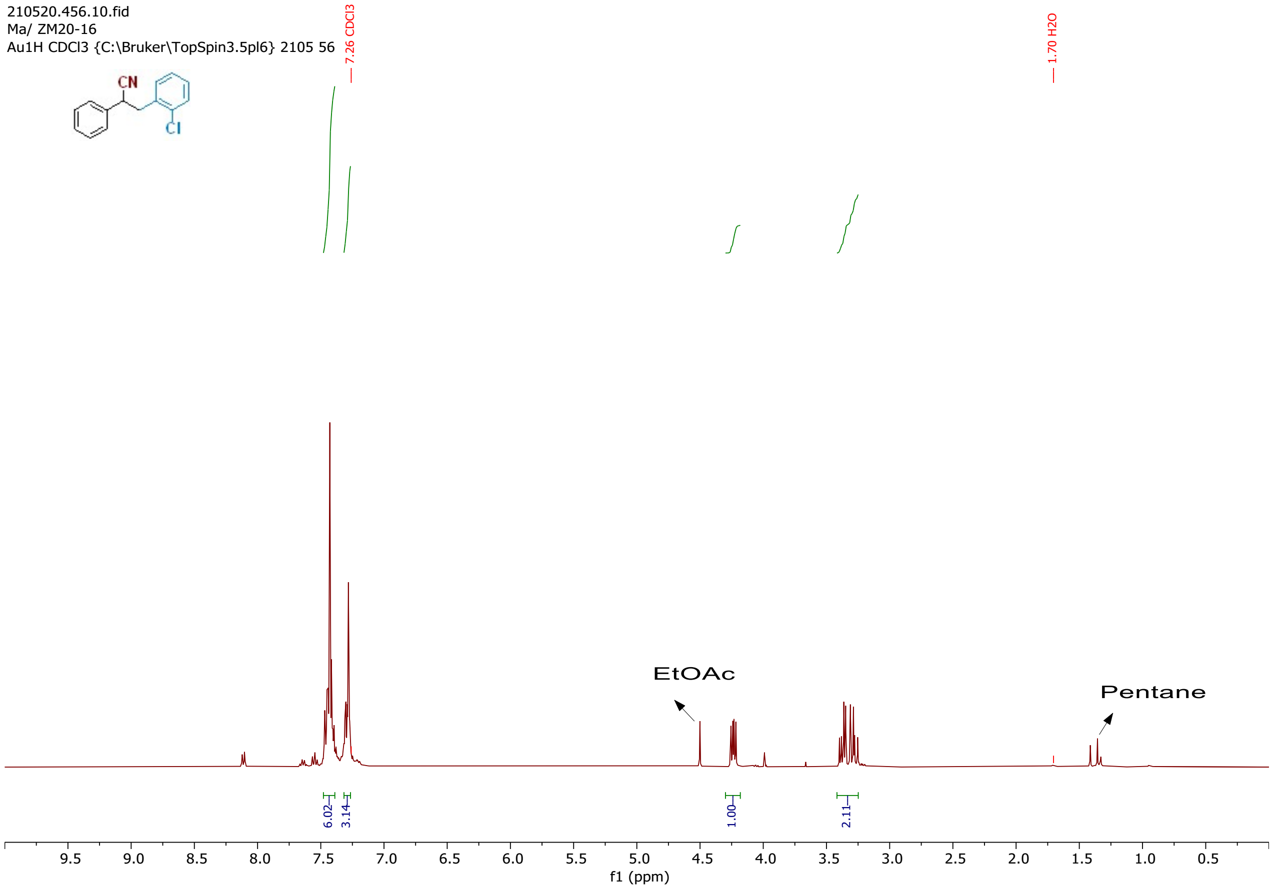


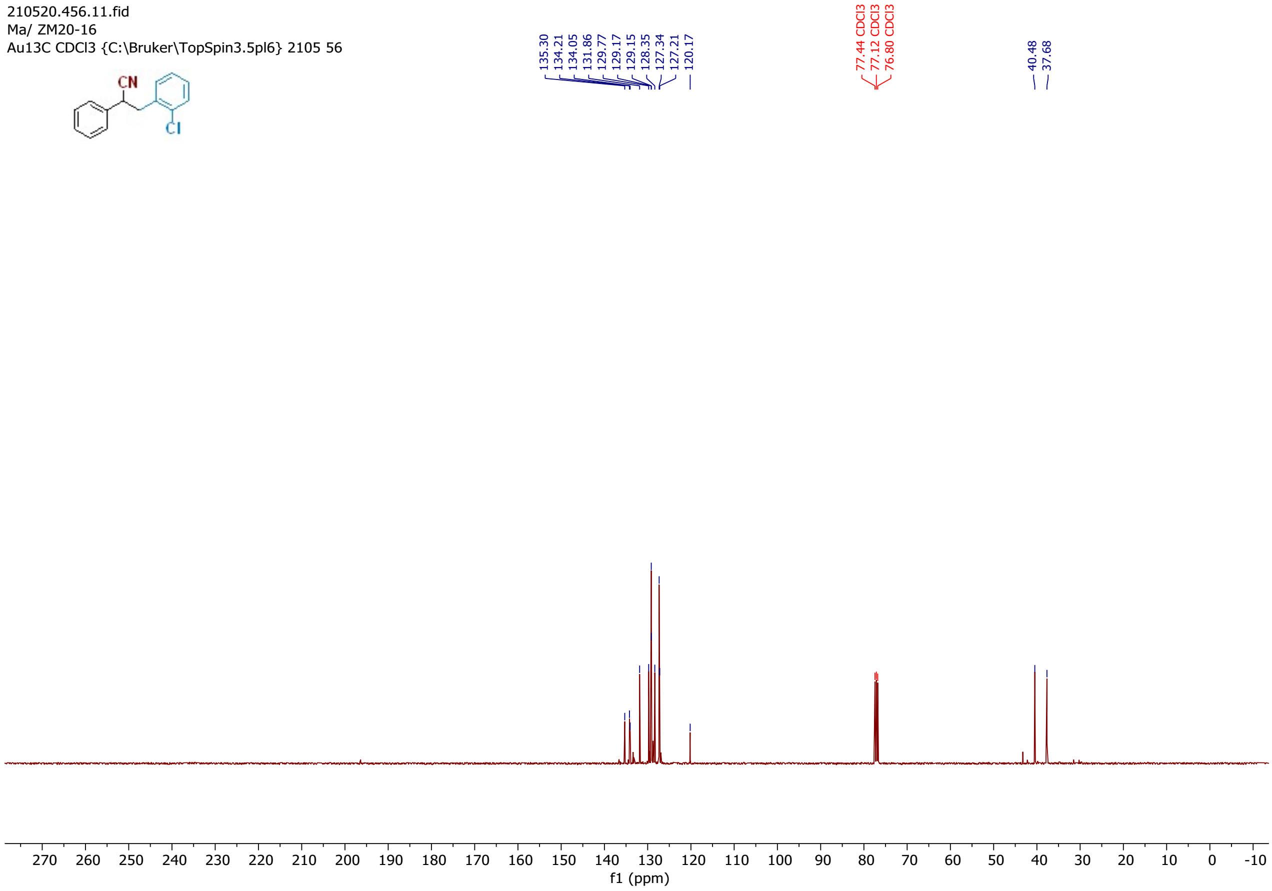
200928.f342.11.fid
Zhuang Ma ZM20-2-2
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2009 42

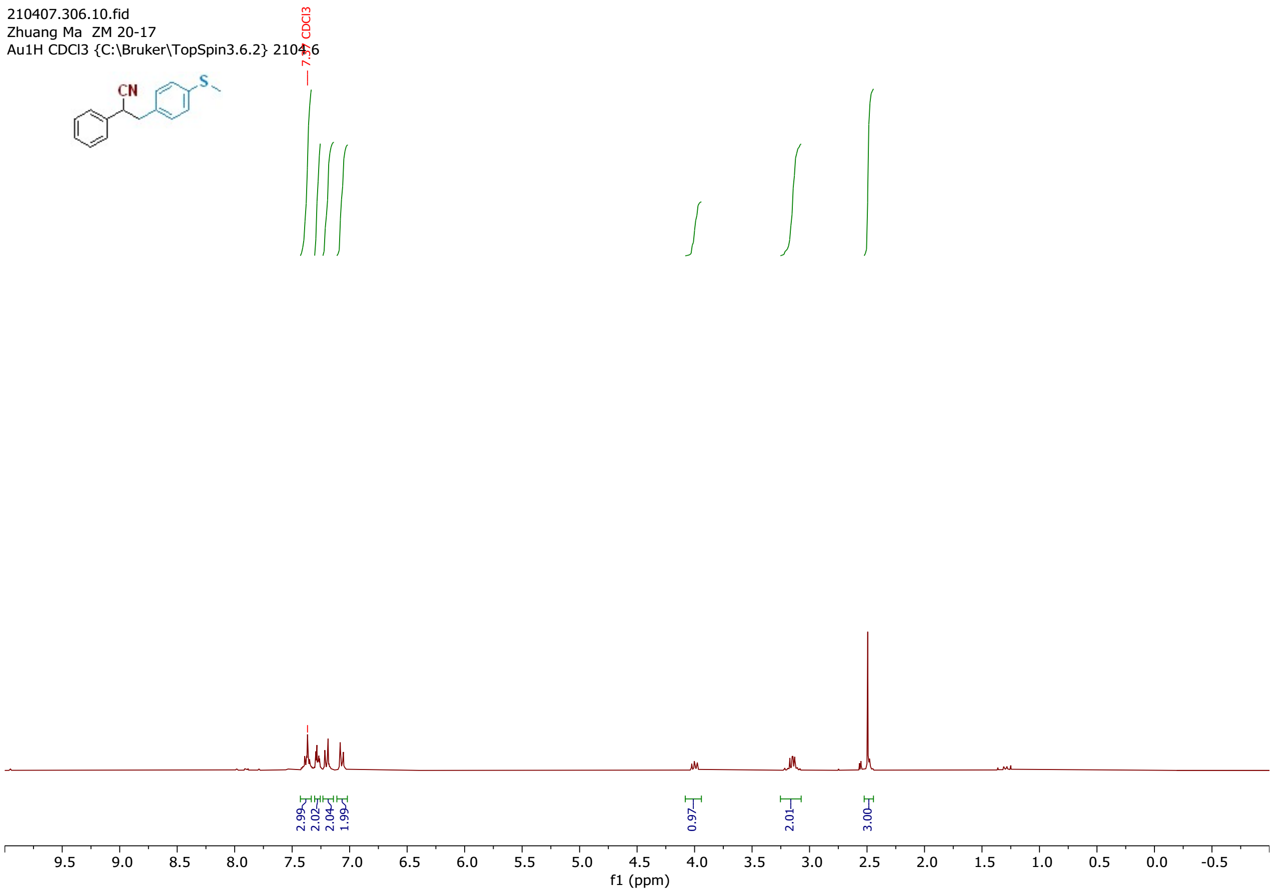


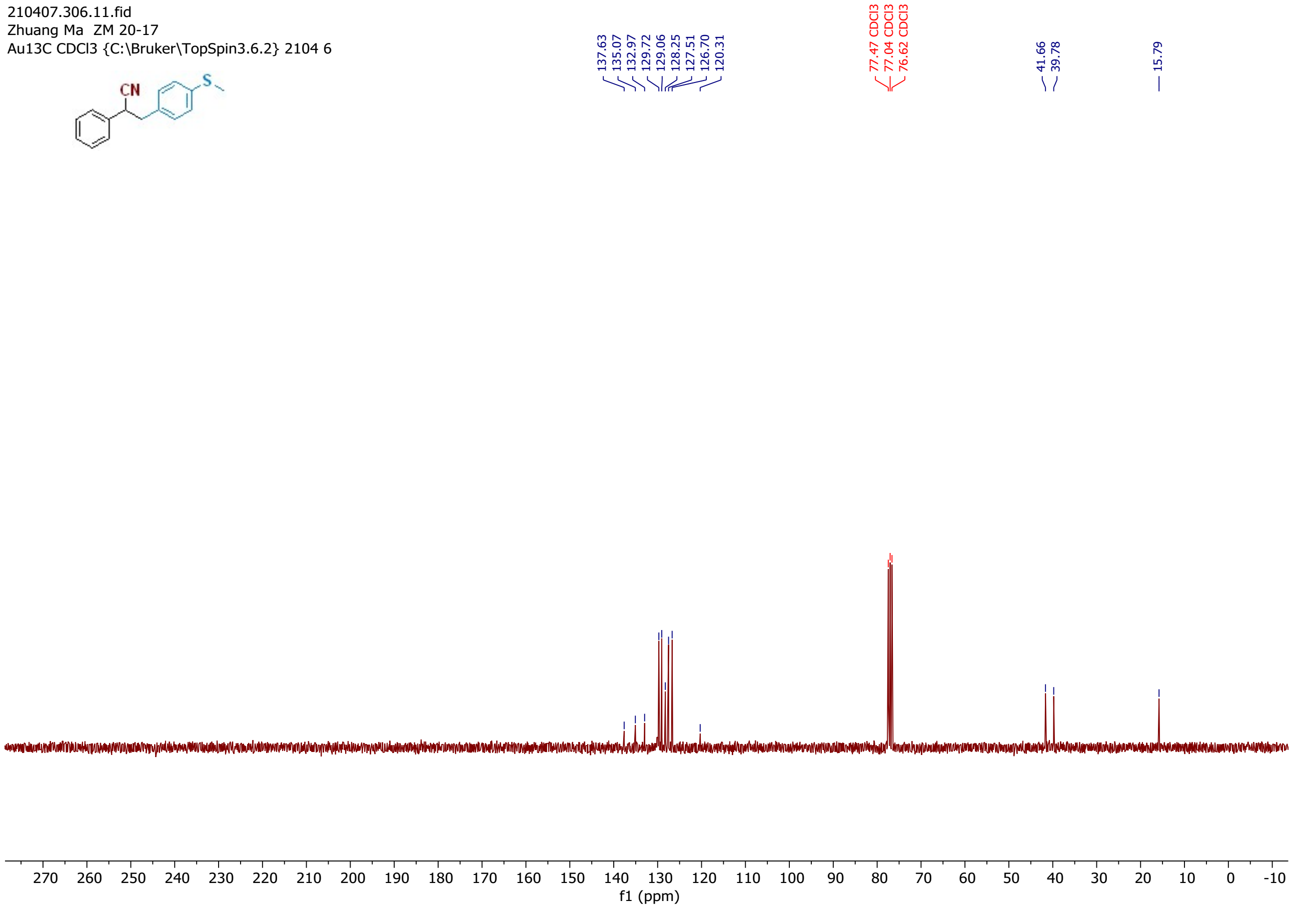

211210.f357.10.fid
Zhuang Ma ZM 20-41
PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2112 57
CN
F
7.26
1.59 HDO
7.24
1.08
2.08
1.00
2.09
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


211210.f357.11.fid
Zhuang Ma ZM 20-41
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2112 57
CN
F
162.84
159.99
135.19
131.66
131.60
129.52
129.41
129.18
129.12
128.35
127.97
127.40
124.38
124.33
123.65
123.45
120.21
115.65
115.37
77.56 CDCl3
77.13 CDCl3
76.71 CDCl3
38.35
38.32
35.98
35.96
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)

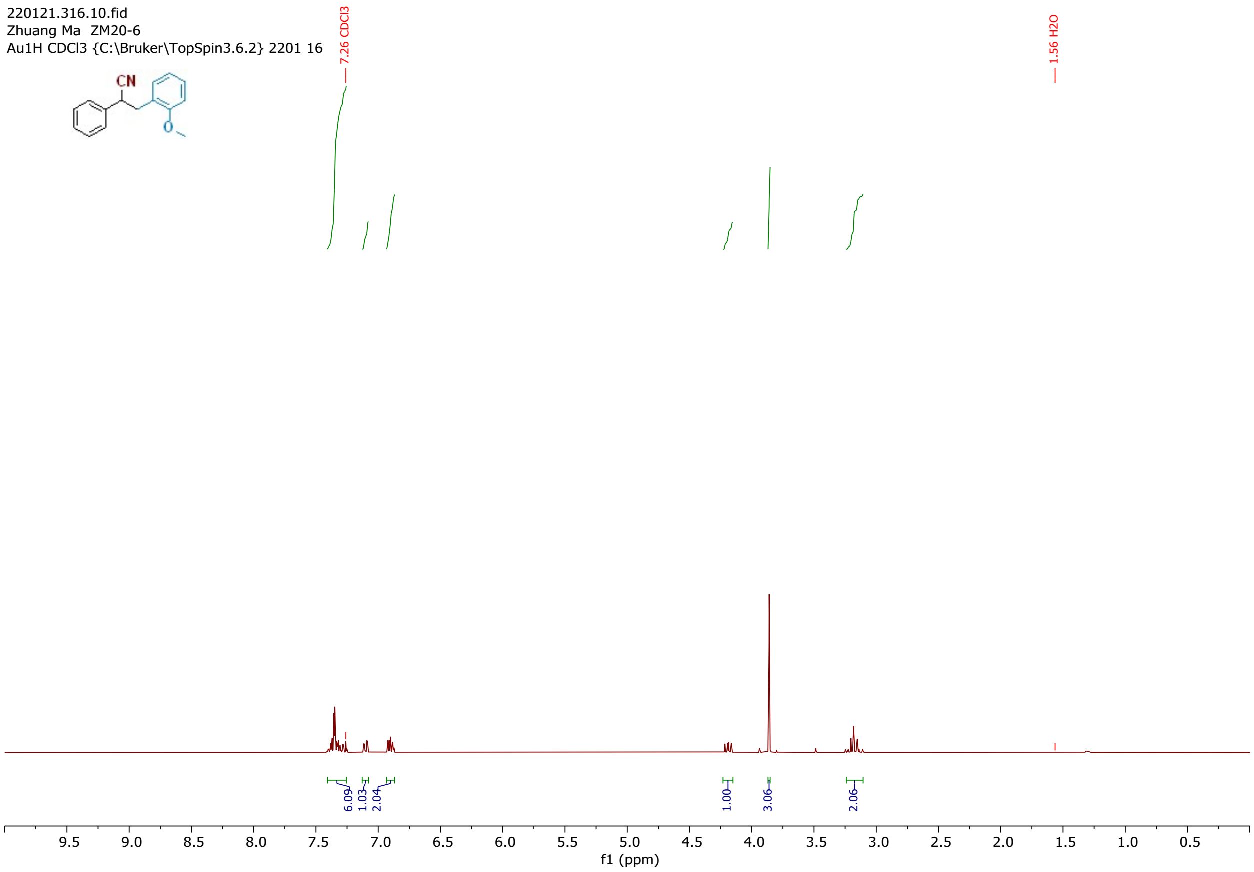

210520.456.10.fid
Ma/ ZM20-16
Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 2105 56
CN
Cl
7.26 CDCl3
1.70 H2O
EtOAc
Pentane
6.02
3.14
1.00
2.11
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


210520.456.11.fid
Ma/ ZM20-16
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2105 56
CN
Cl
135.30
134.21
134.05
131.86
129.77
129.17
129.15
128.35
127.34
127.21
120.17
77.44 CDCl3
77.12 CDCl3
76.80 CDCl3
40.48
37.68
270
260
250
240
230
220
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)

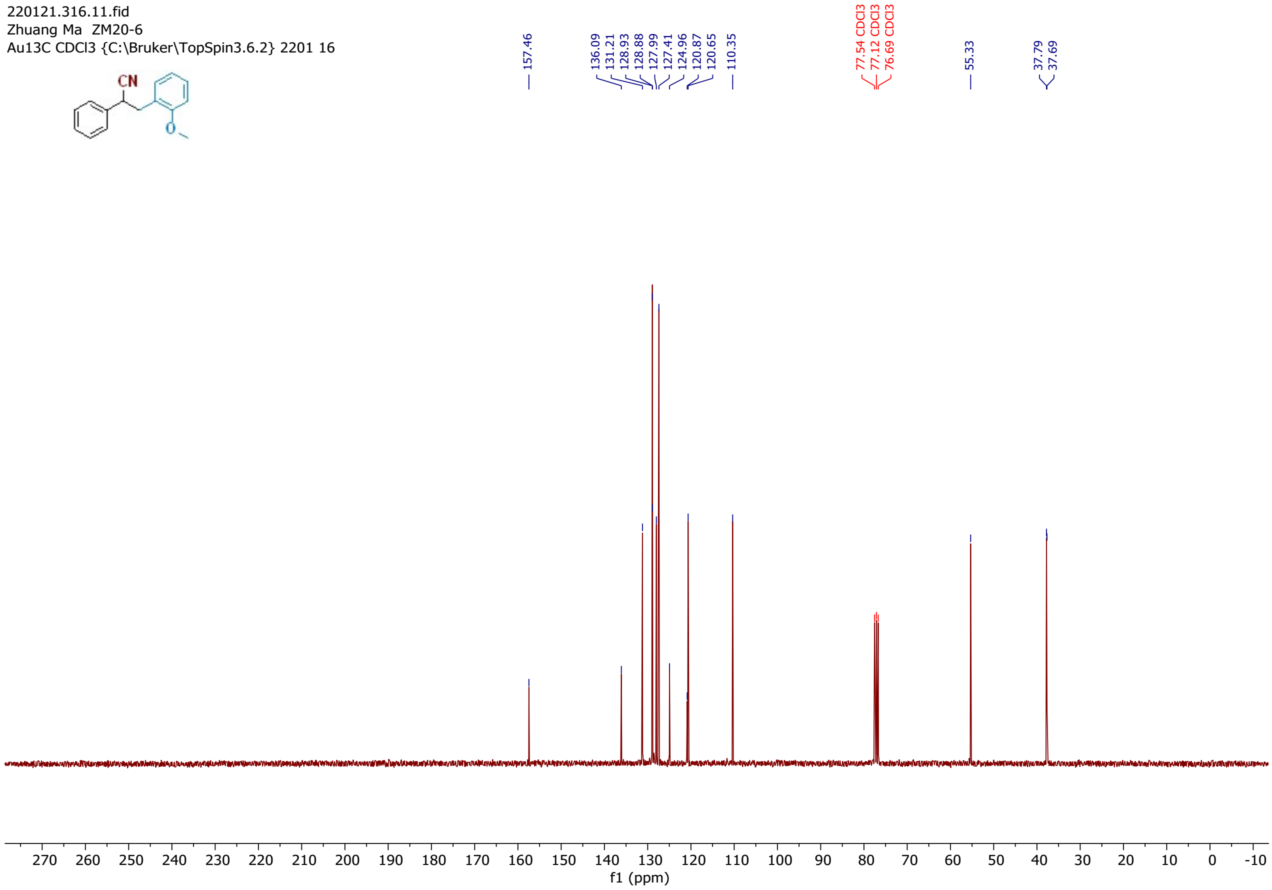

210407.306.10.fid
Zhuang Ma ZM 20-17
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2104 6
CN
S
7.37 CDCl3
2.99
2.02
2.04
1.99
0.97
2.01
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

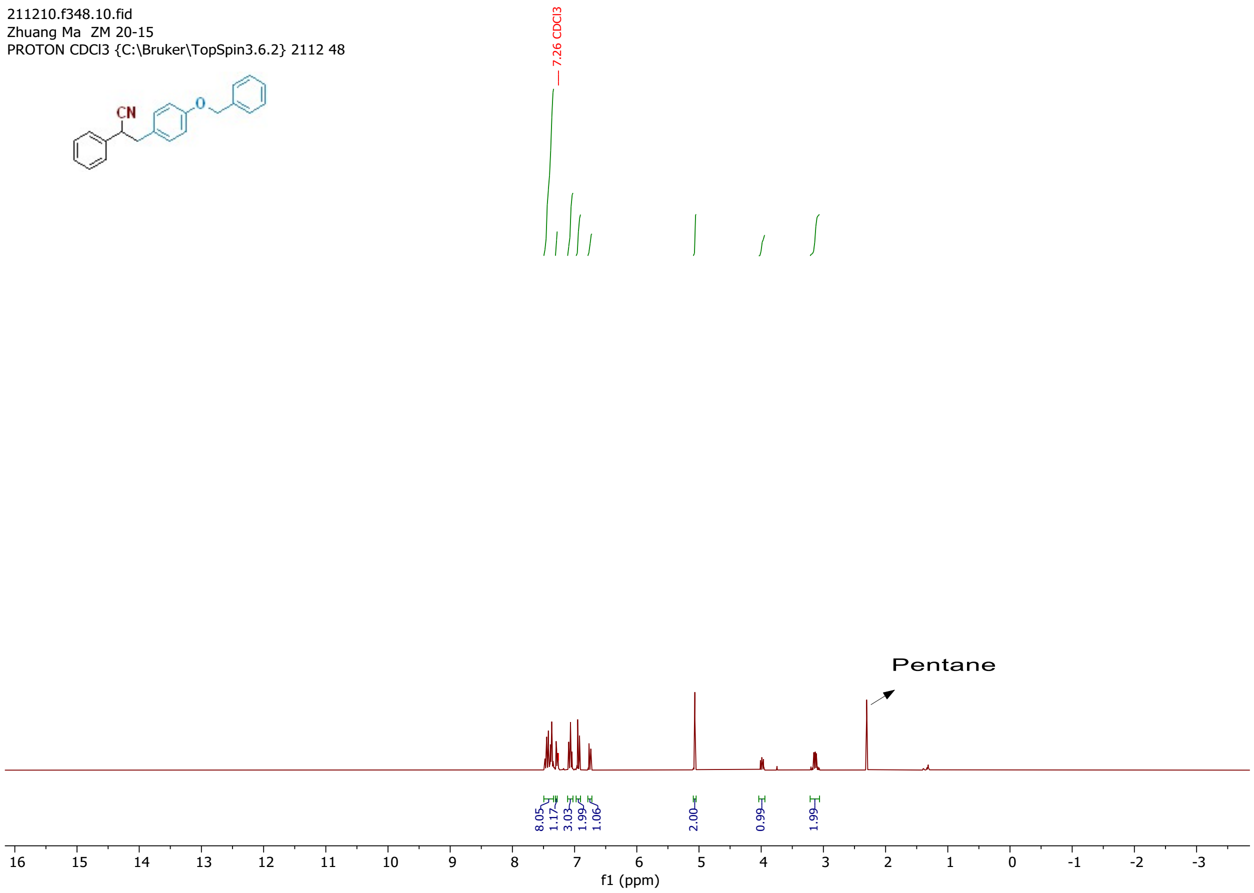

210407.306.11.fid
Zhuang Ma ZM 20-17
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2104 6
CN
S
137.63
135.07
132.97
129.72
129.06
128.25
127.51
126.70
120.31
77.47 CDCl3
77.04 CDCl3
76.62 CDCl3
41.66
39.78
15.79
270
260
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

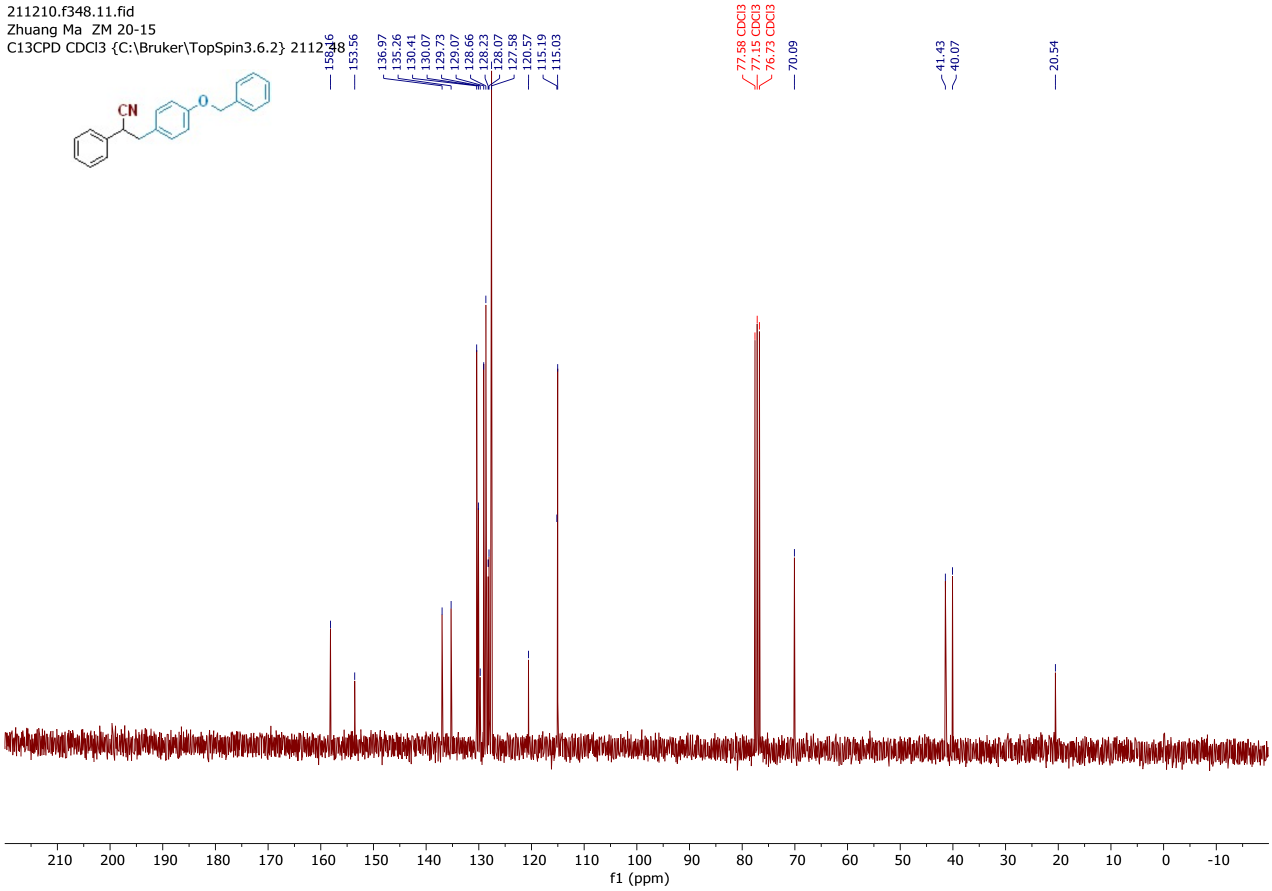
220121.316.10.fid
Zhuang Ma ZM20-6
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 16

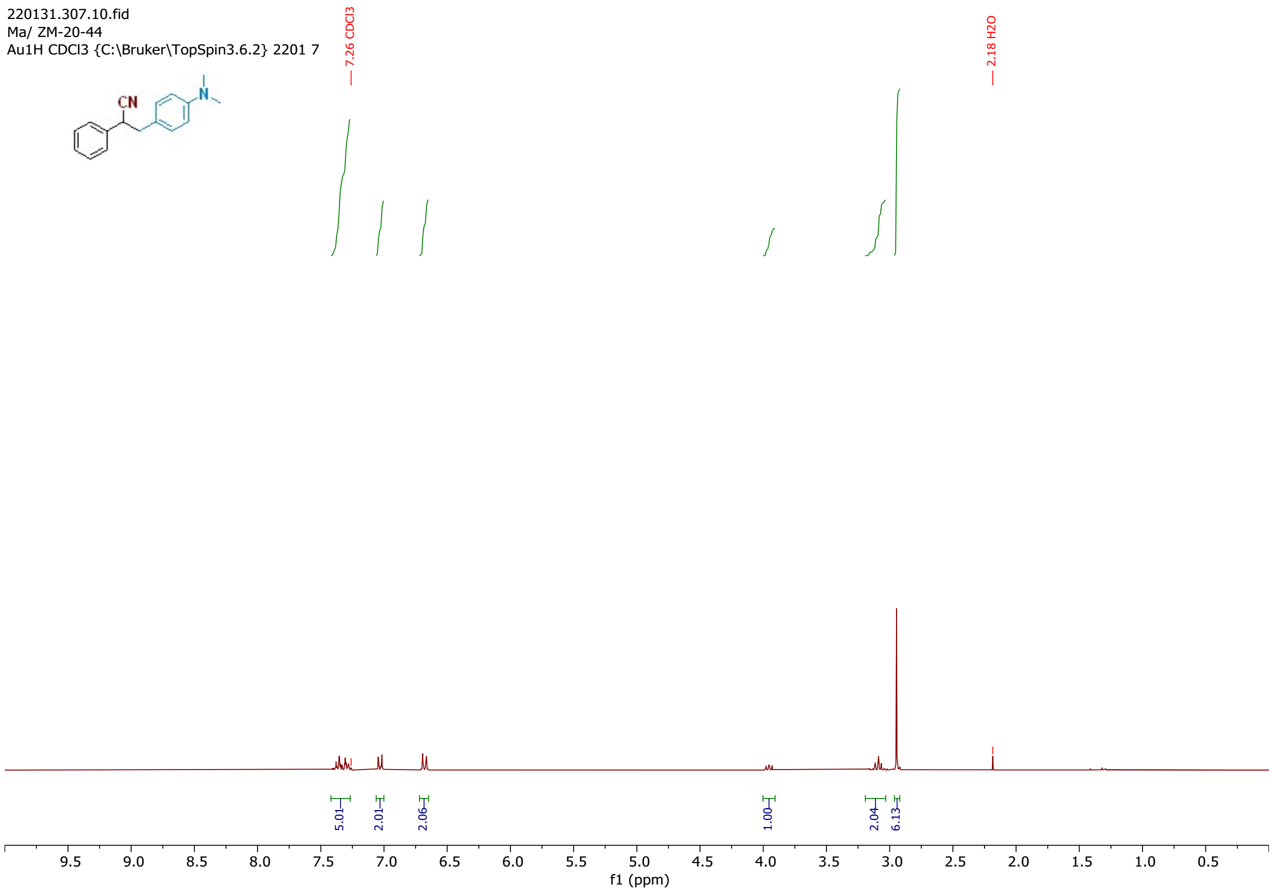


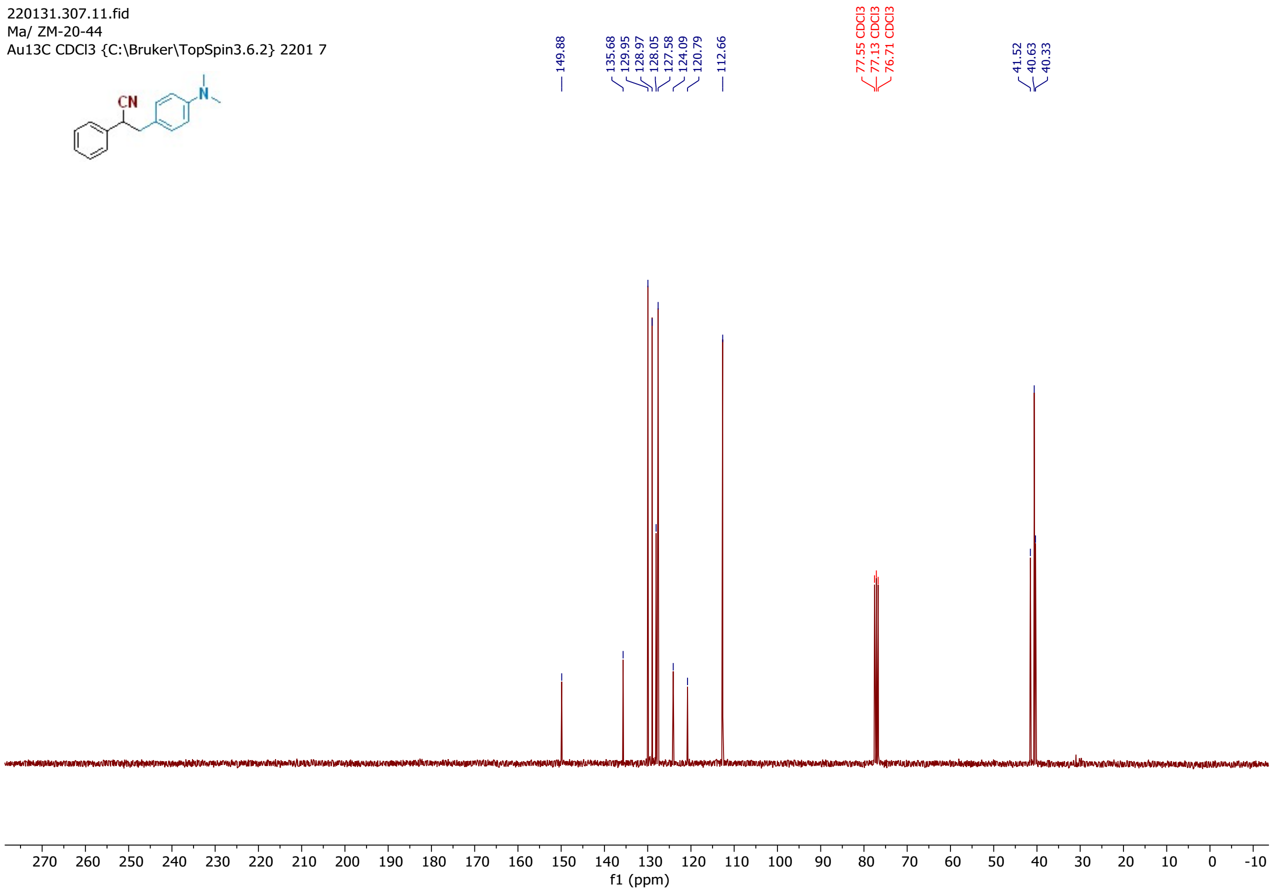
220121.316.11.fid
Zhuang Ma ZM20-6
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 16

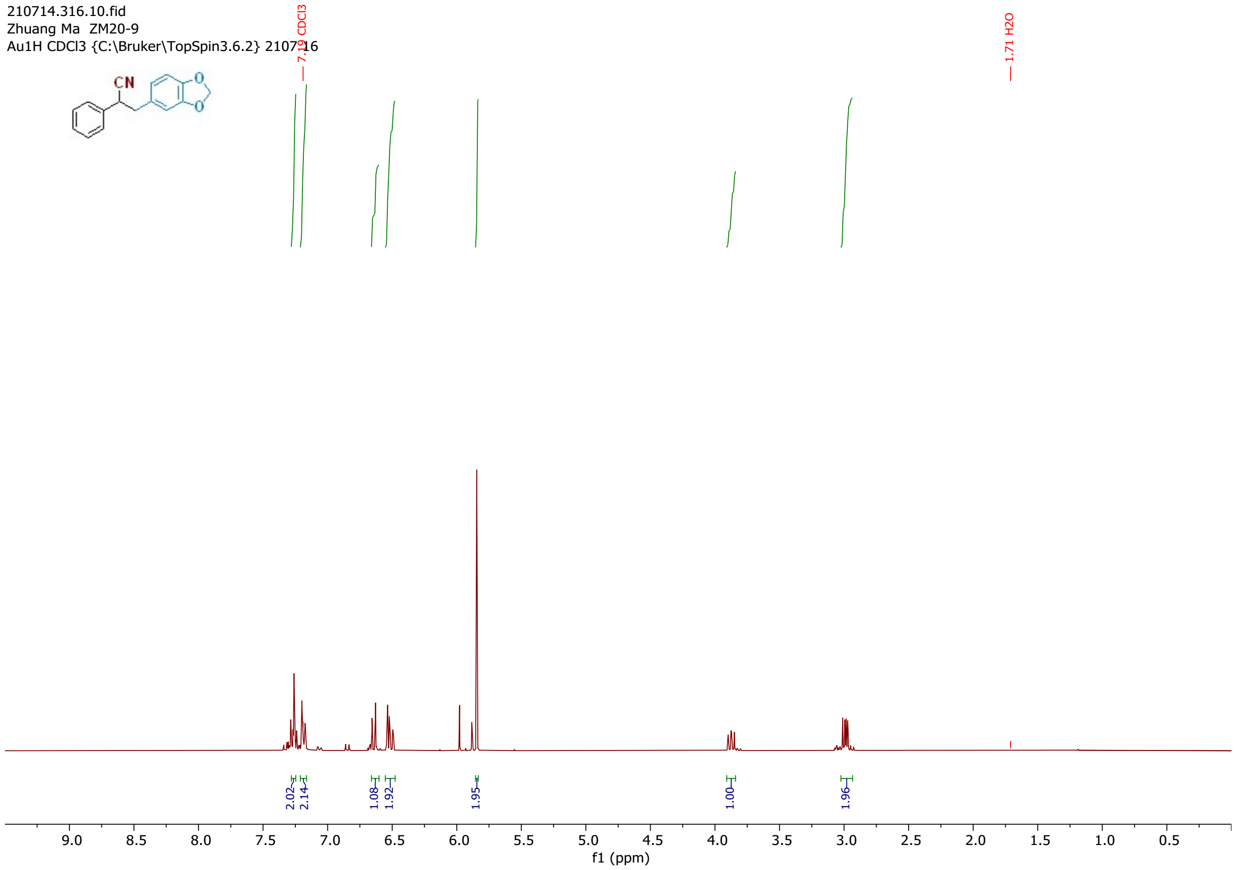


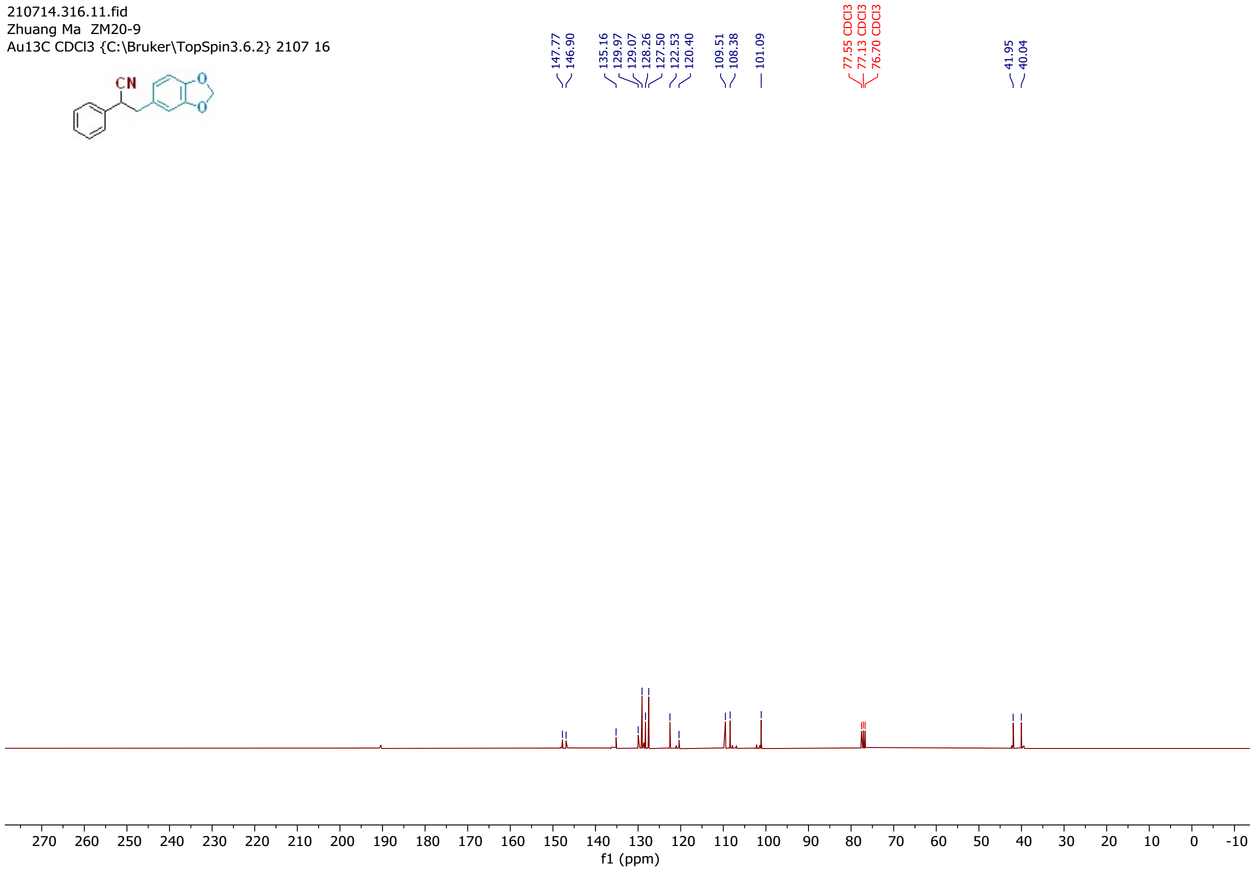

211210.f348.10.fid
Zhuang Ma ZM 20-15
PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2112 48
CN
O
7.26 CDCl3
Pentane
8.05
1.17
3.03
1.99
1.06
2.00
0.99
1.99
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

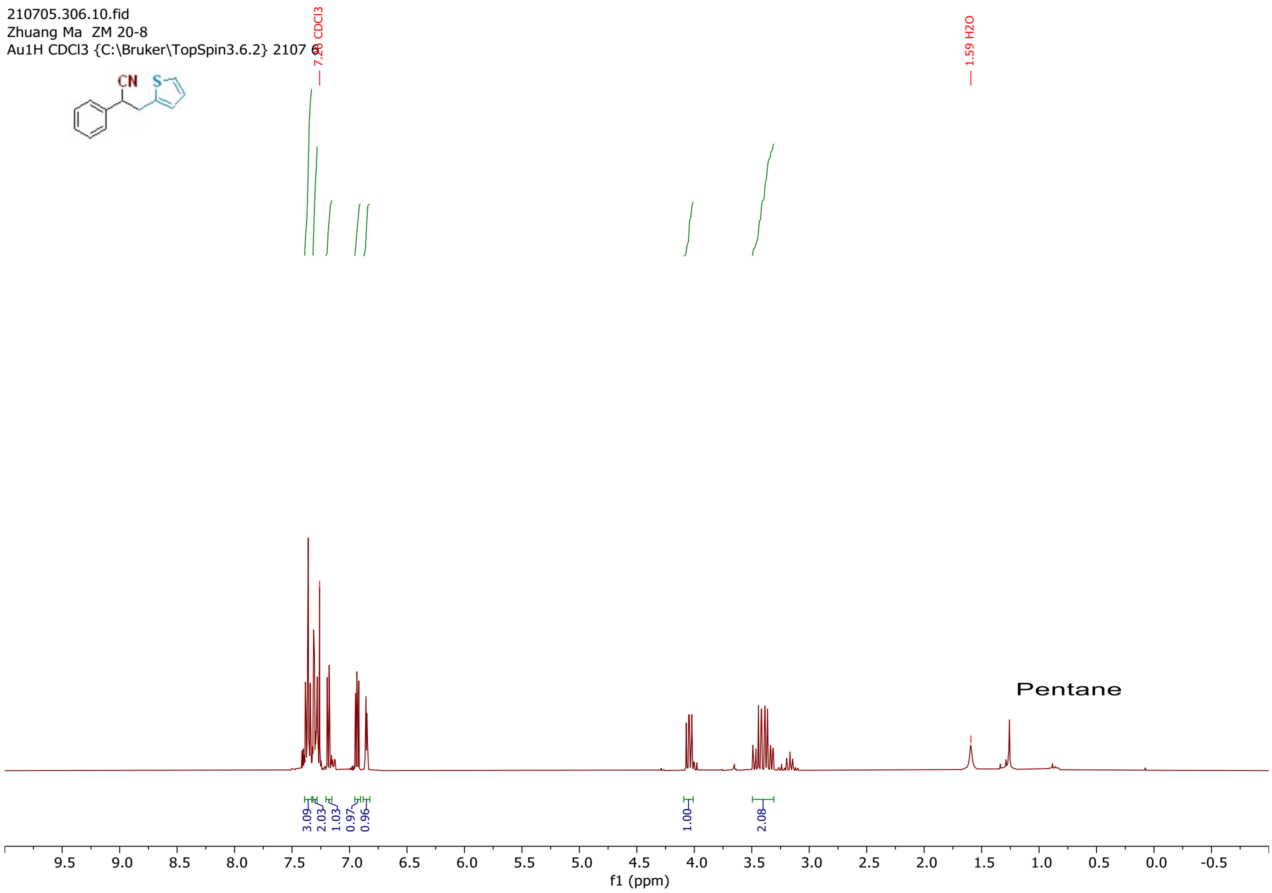

211210.f348.11.fid
Zhuang Ma ZM 20-15
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2112 48
CN
O
158.16
153.56
136.97
135.26
130.41
130.07
129.73
129.07
128.66
128.23
128.07
127.58
120.57
115.19
115.03
77.58 CDCl3
77.15 CDCl3
76.73 CDCl3
70.09
41.43
40.07
20.54
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

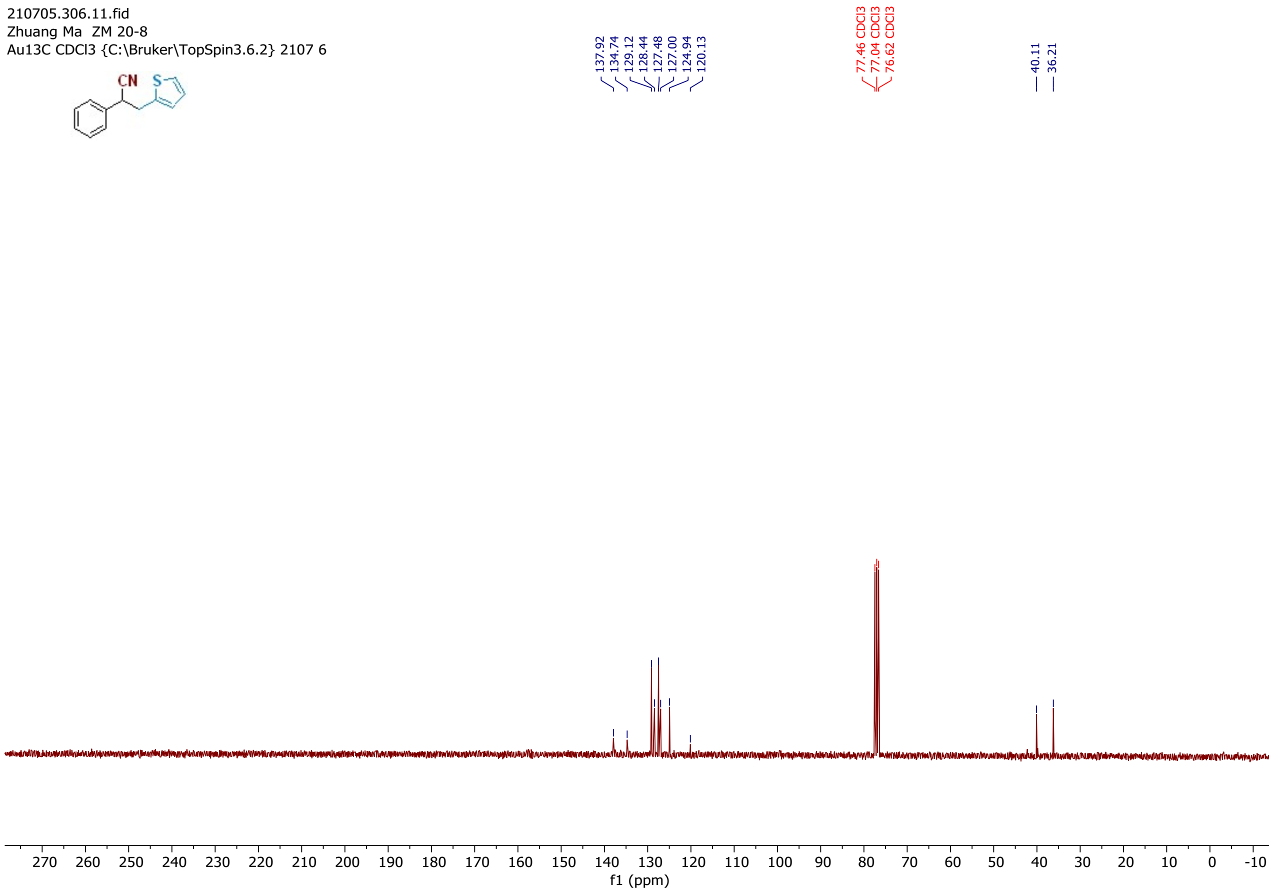

220131.307.10.fid
Ma/ ZM-20-44
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 7
CN
N
7.26 CDCl3
2.18 H2O
5.01
2.01
2.06
1.00
2.04
6.13
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

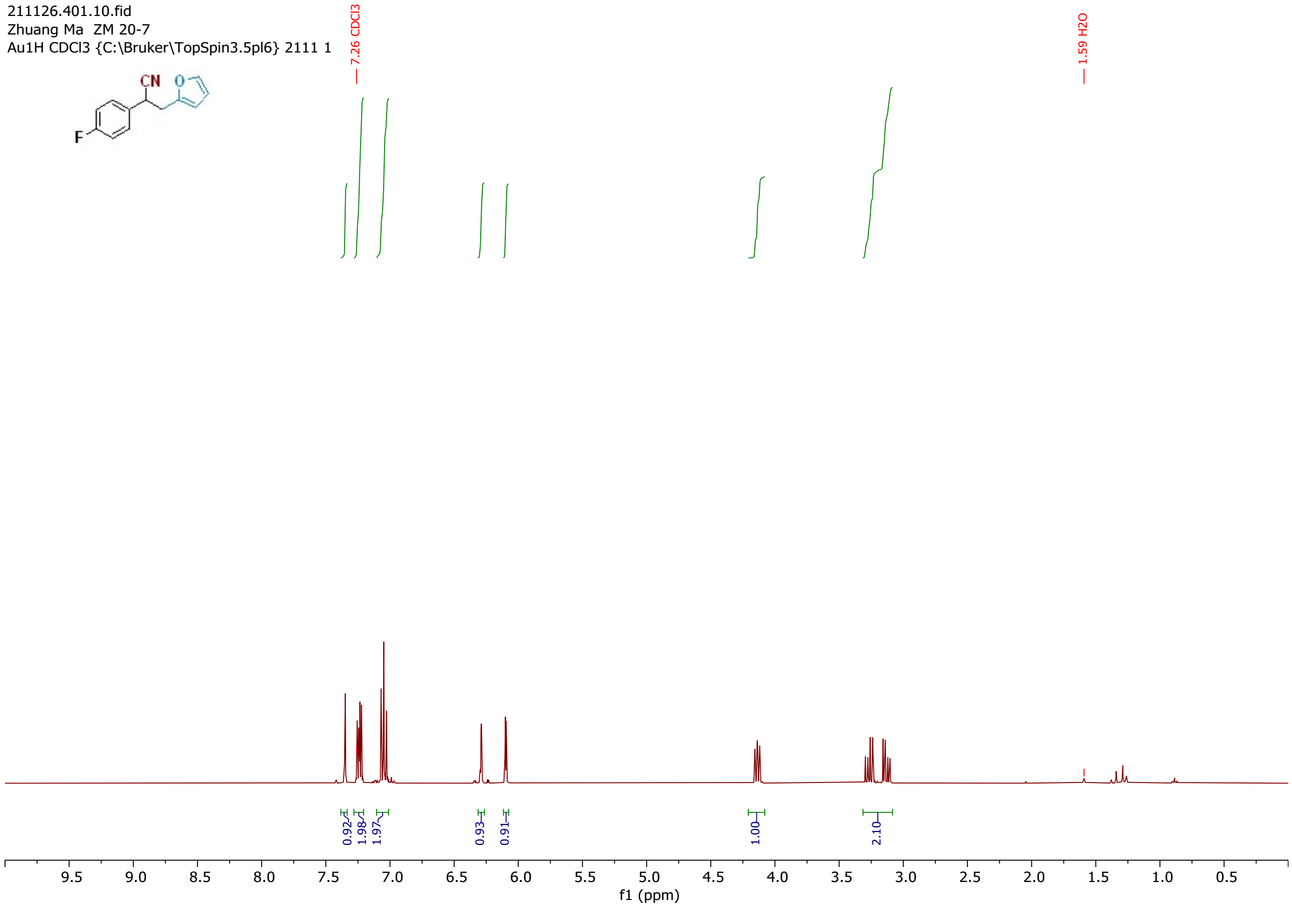

220131.307.11.fid
Ma/ ZM-20-44
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 7
CN
N
149.88
135.68
129.95
128.97
128.05
127.58
124.09
120.79
112.66
77.55 CDCl3
77.13 CDCl3
76.71 CDCl3
41.52
40.63
40.33
270
260
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

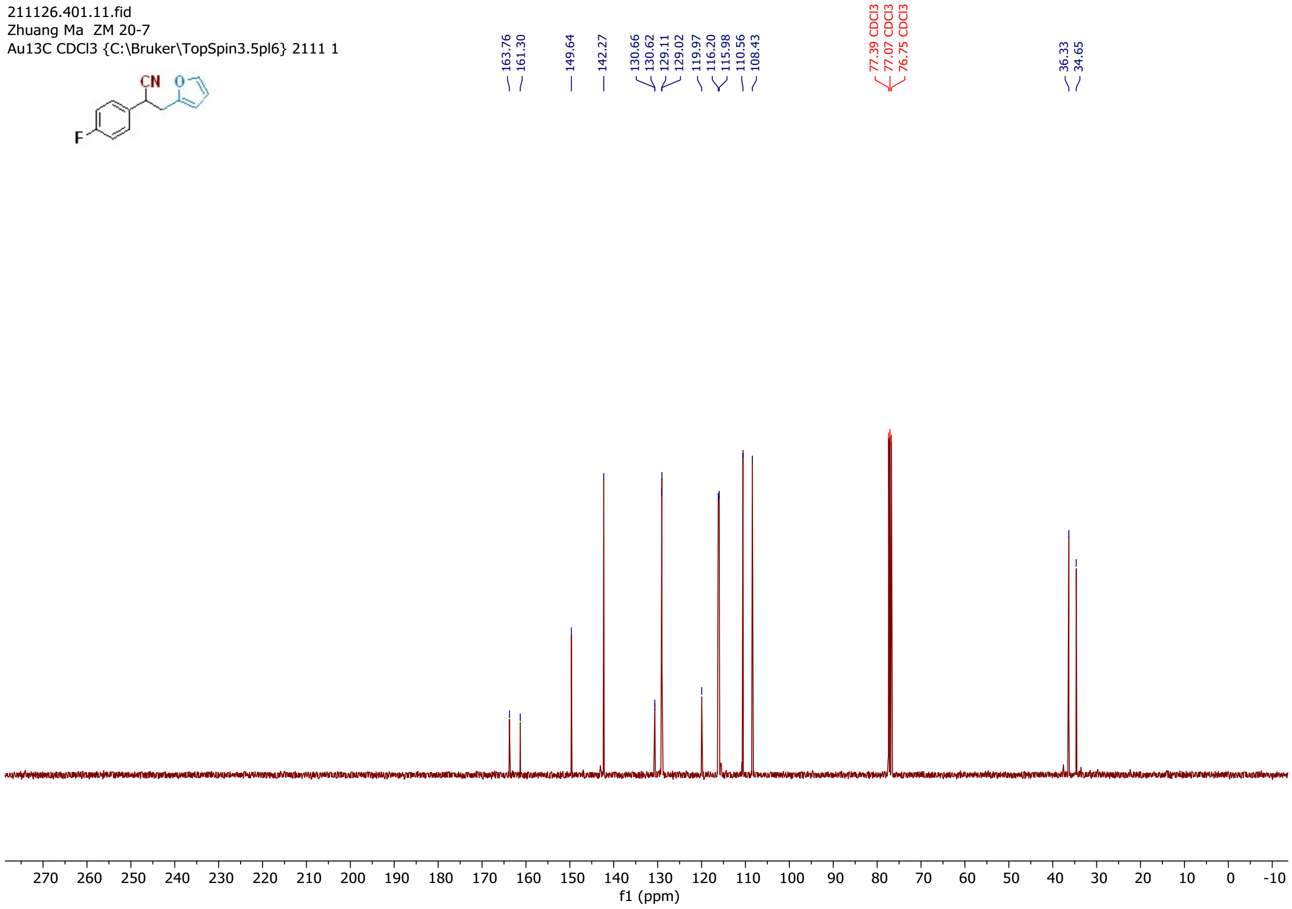

210714.316.10.fid
Zhuang Ma ZM20-9
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 210716
CN
O
O
7.19 CDCl3
1.71 H2O
2.02
2.14
1.08
1.92
1.95
1.00
1.96
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

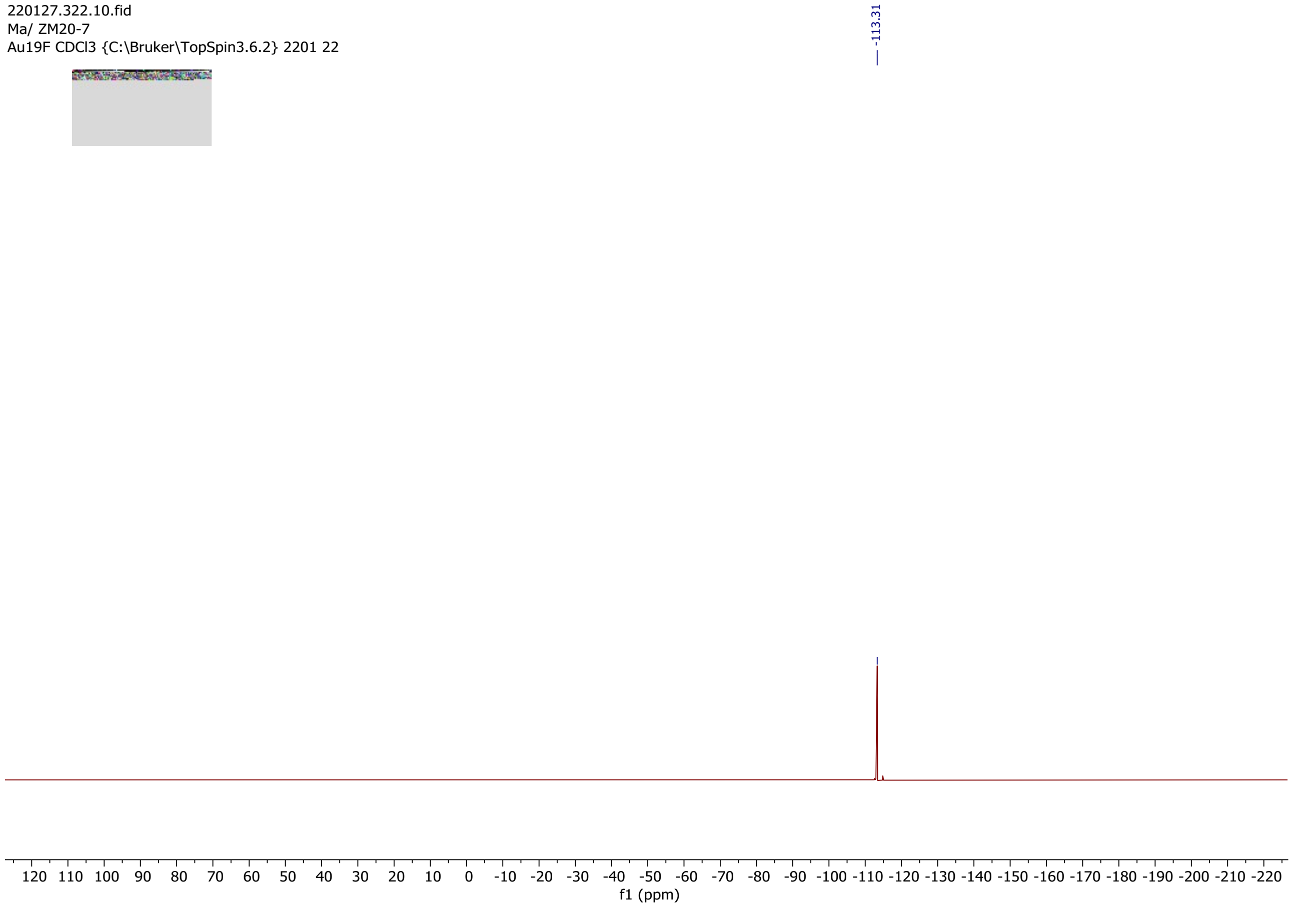

210714.316.11.fid
Zhuang Ma ZM20-9
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2107 16
CN
O
O
147.77
146.90
135.16
129.97
129.07
128.26
127.50
122.53
120.40
109.51
108.38
101.09
77.55 CDCl3
77.13 CDCl3
76.70 CDCl3
41.95
40.04
270
260
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

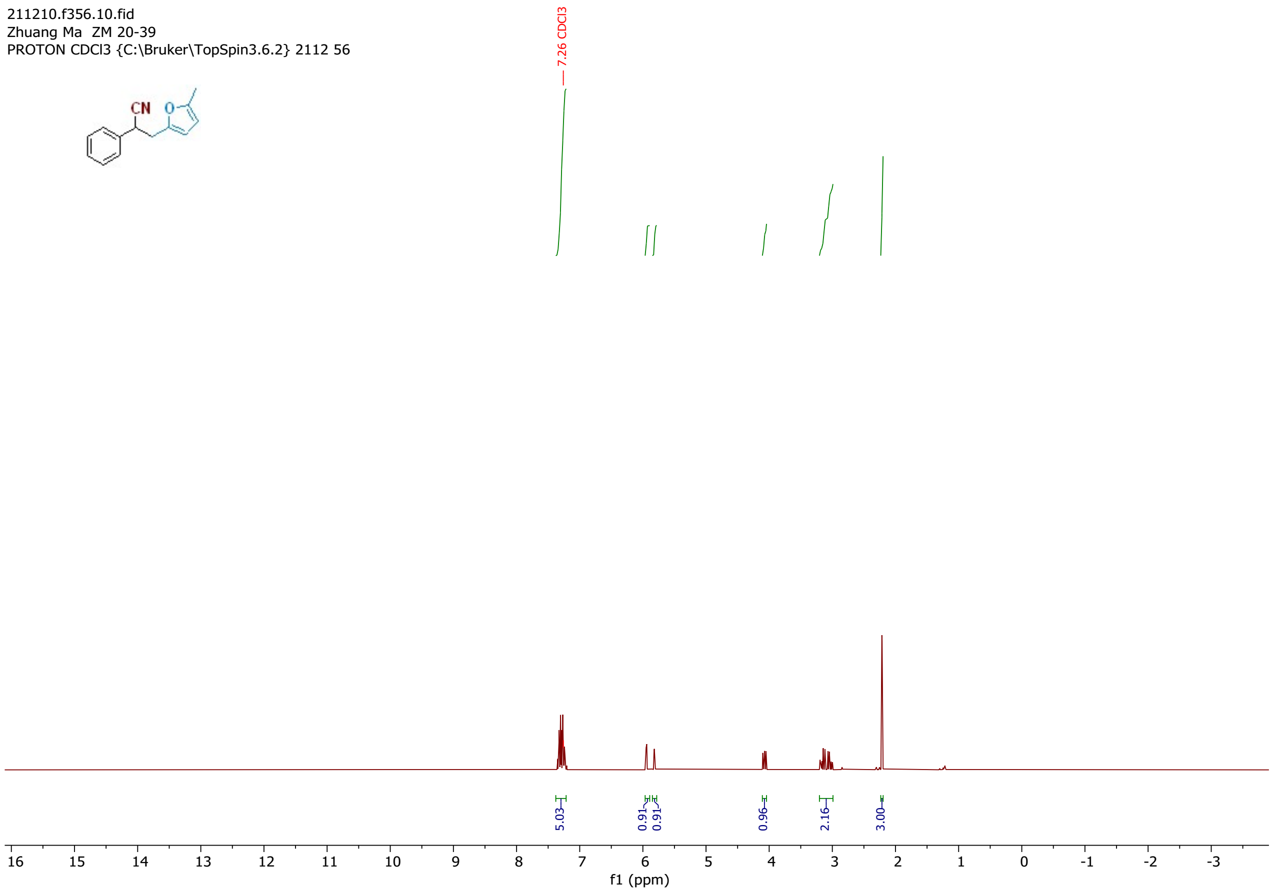

210705.306.10.fid
Zhuang Ma ZM 20-8
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2107 6
CN
S
7.26 CDCl3
1.59 H2O
Pentane
3.09
2.03
1.03
0.97
0.96
1.00
2.08
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

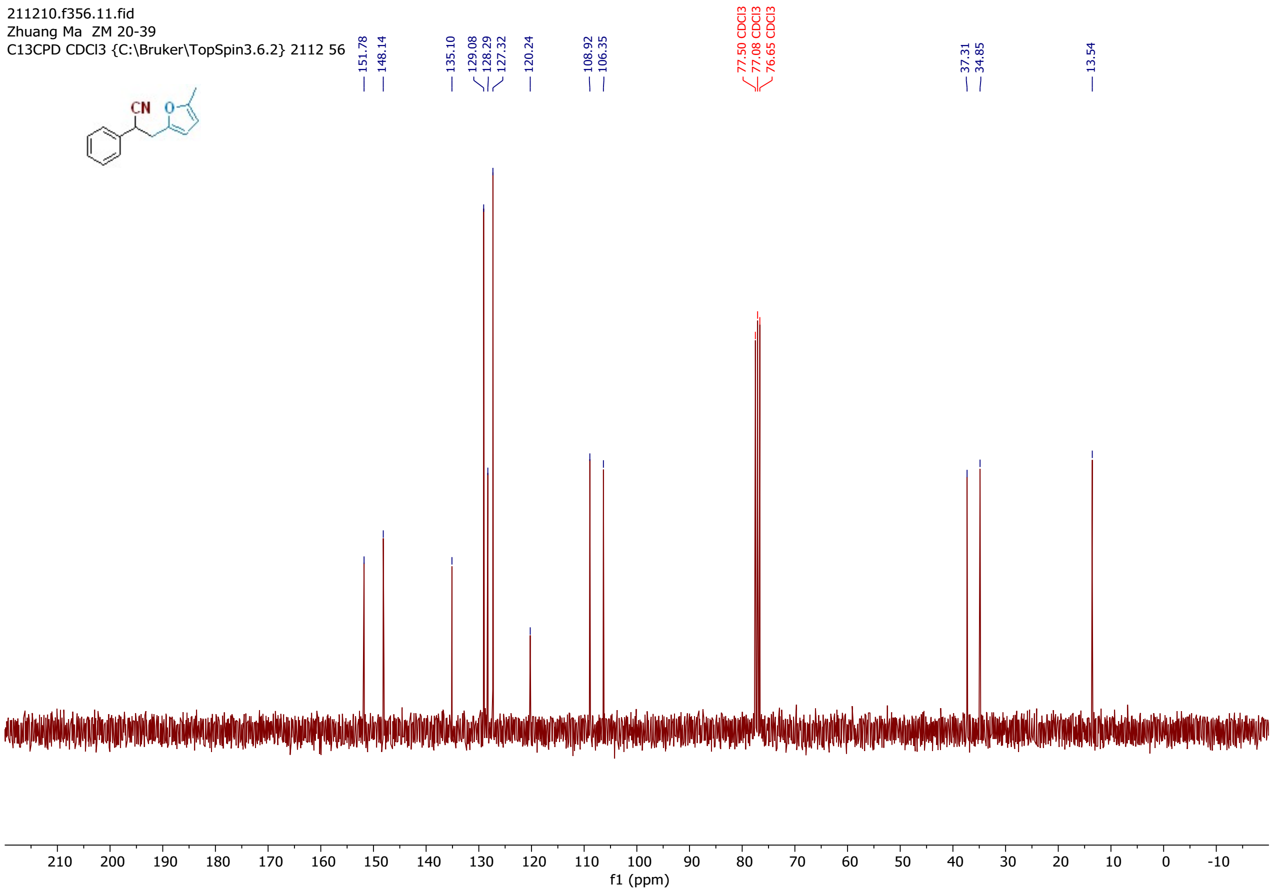

210705.306.11.fid
Zhuang Ma ZM 20-8
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2107 6
CN
S
137.92
134.74
129.12
128.44
127.48
127.00
124.94
120.13
77.46 CDCl3
77.04 CDCl3
76.62 CDCl3
40.11
36.21
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

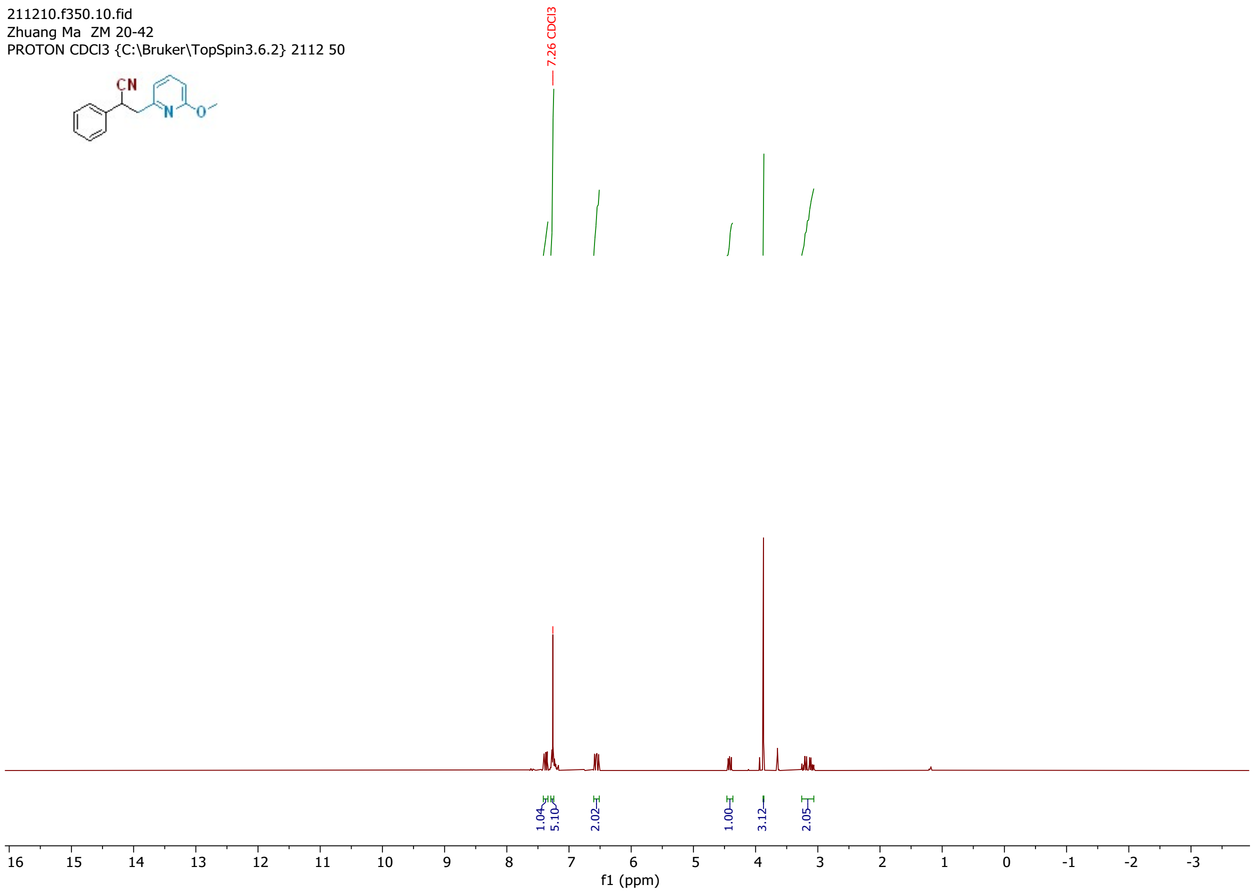

211126.401.10.fid
Zhuang Ma ZM 20-7
Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 2111 1
CN
O
F
7.26 CDCl3
1.59 H2O
0.92
1.98
1.97
0.93
0.91
1.00
2.10
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

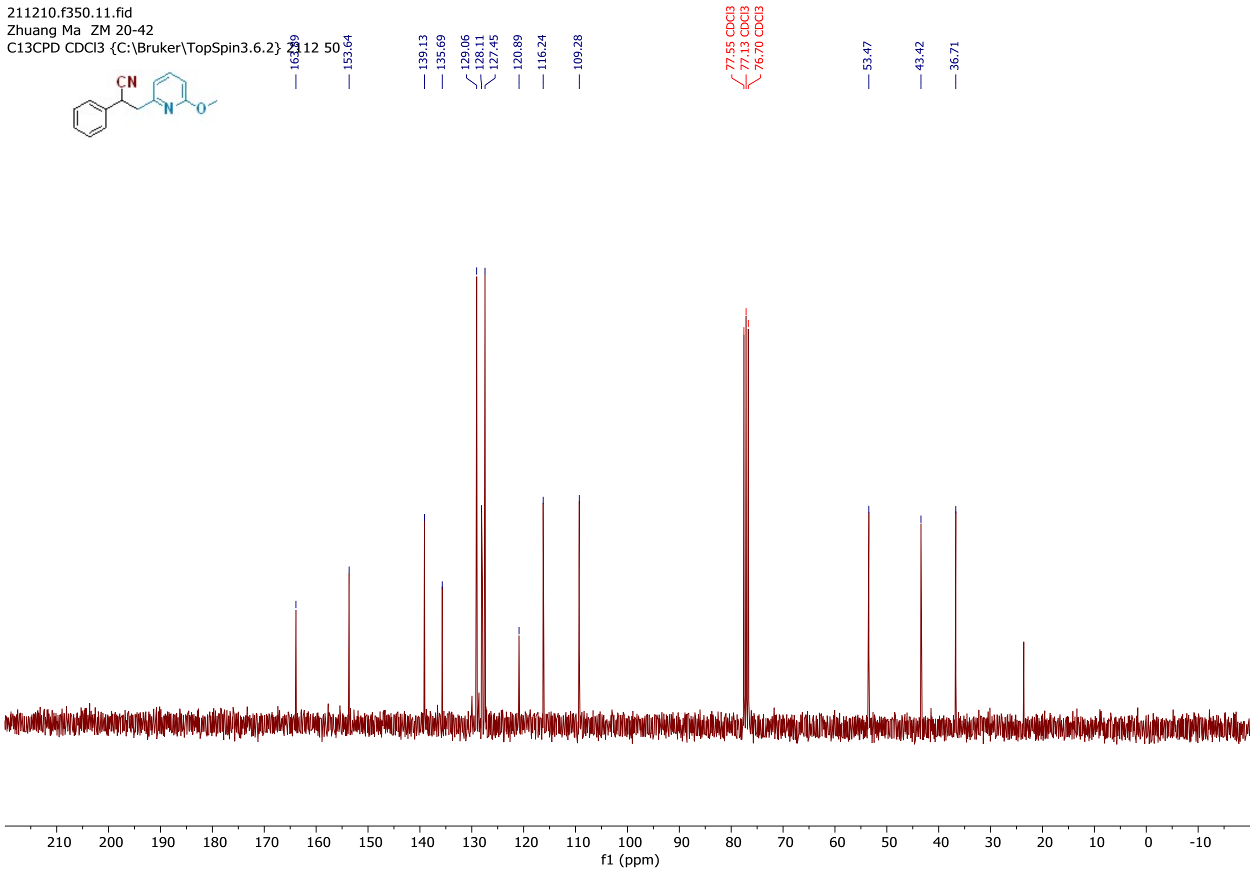

211126.401.11.fid
Zhuang Ma ZM 20-7
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2111 1
CN
O
F
163.76
161.30
149.64
142.27
130.66
130.62
129.11
129.02
119.97
116.20
115.98
110.56
108.43
77.39 CDCl3
77.07 CDCl3
76.75 CDCl3
36.33
34.65
270
260
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

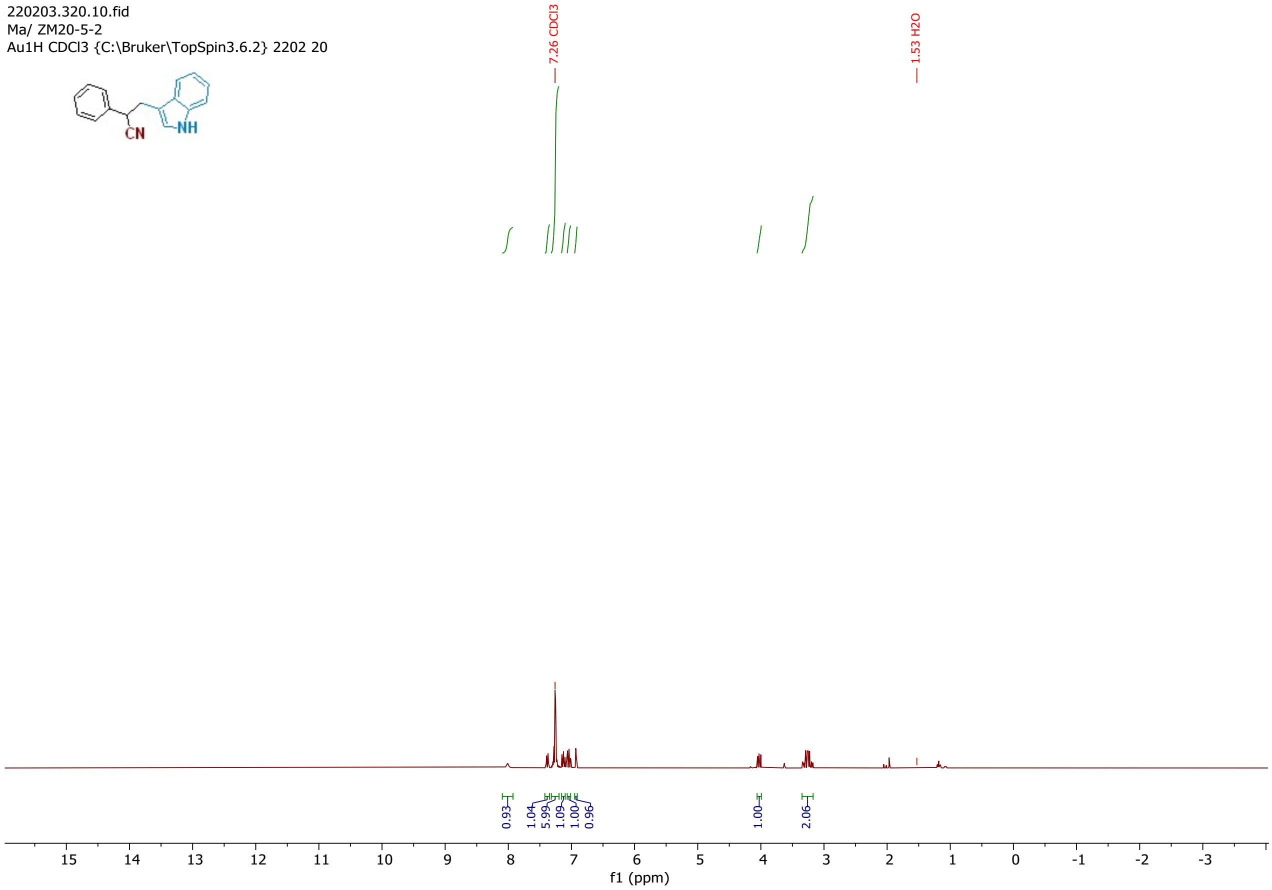

220127.322.10.fid
Ma/ ZM20-7
Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 22
-113.31
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

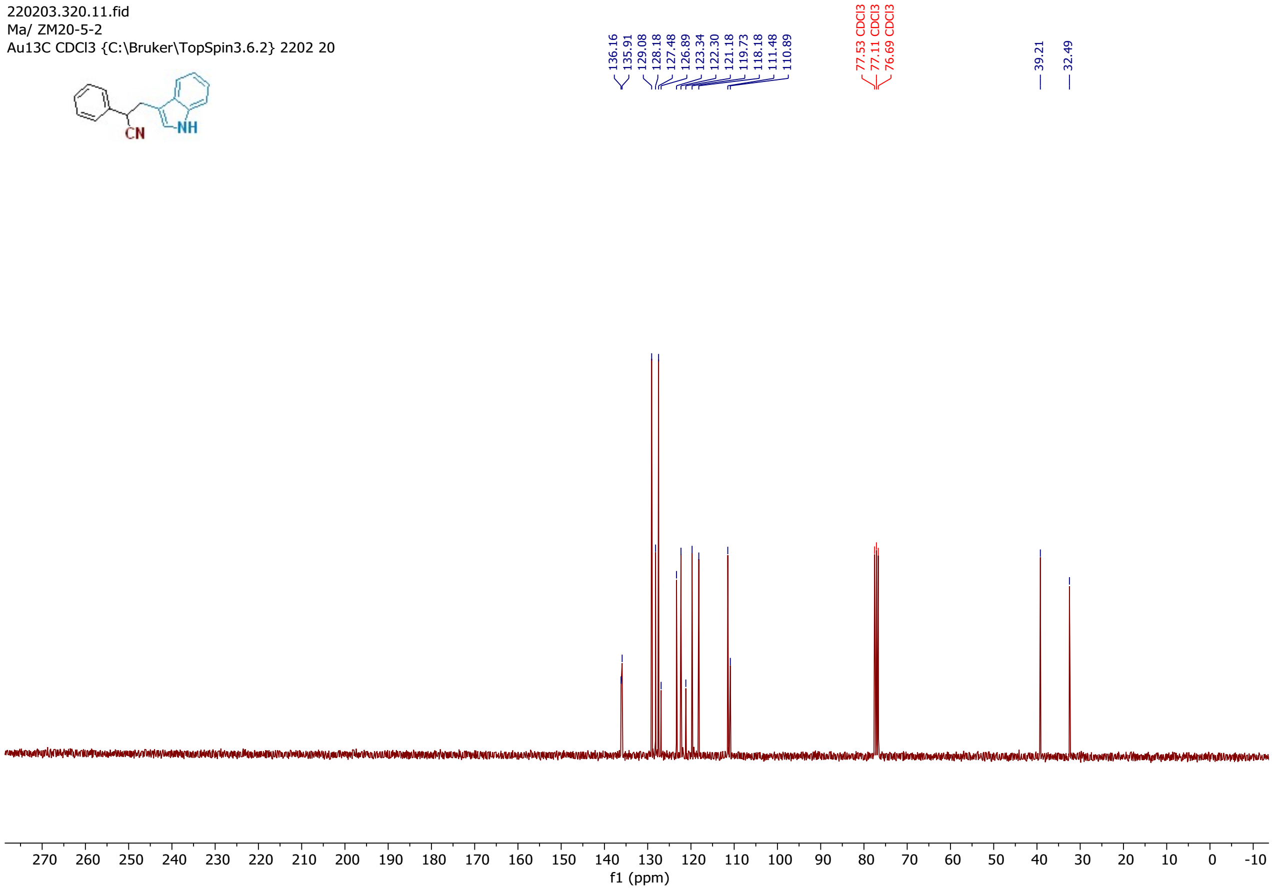

211210.f356.10.fid
Zhuang Ma ZM 20-39
PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2112 56

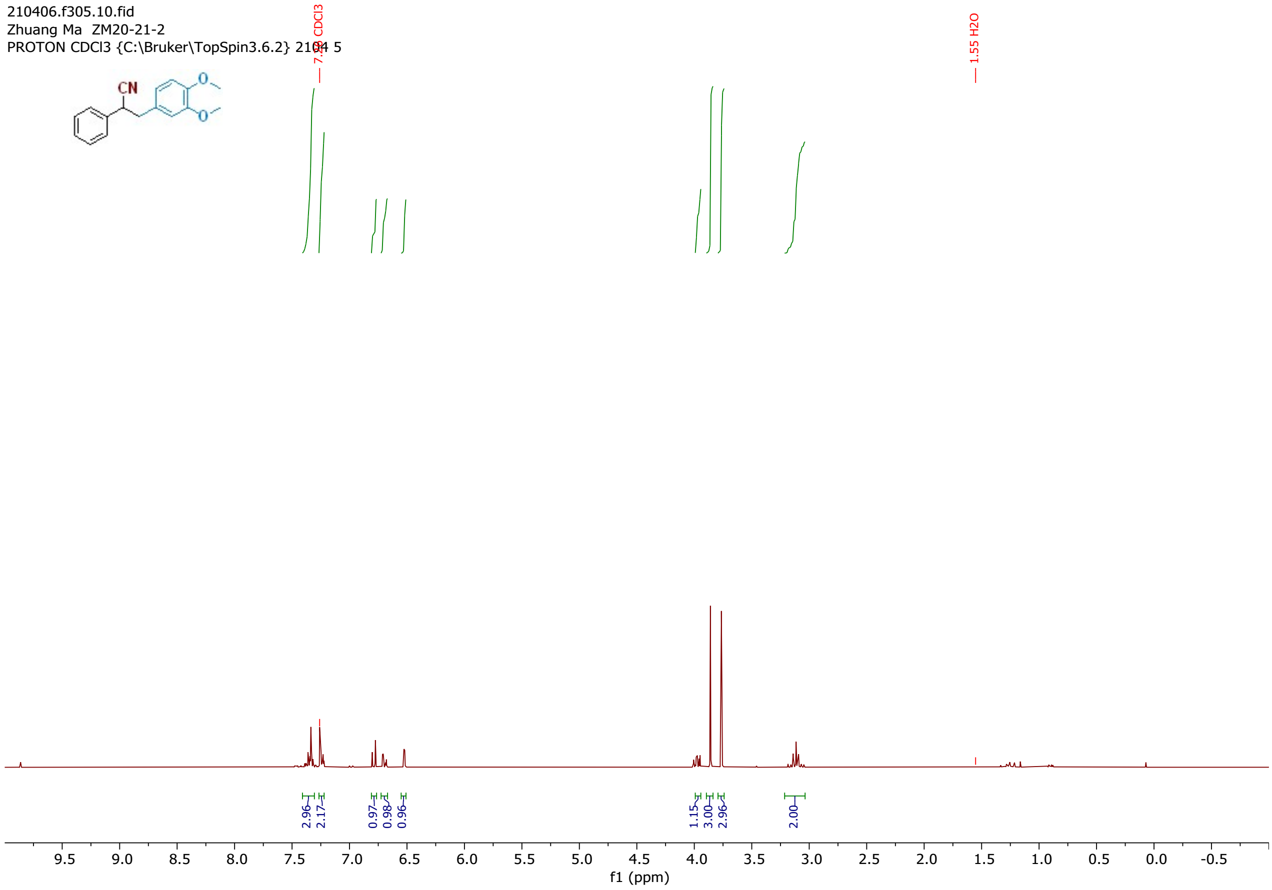

211210.f356.11.fid
Zhuang Ma ZM 20-39
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2112 56

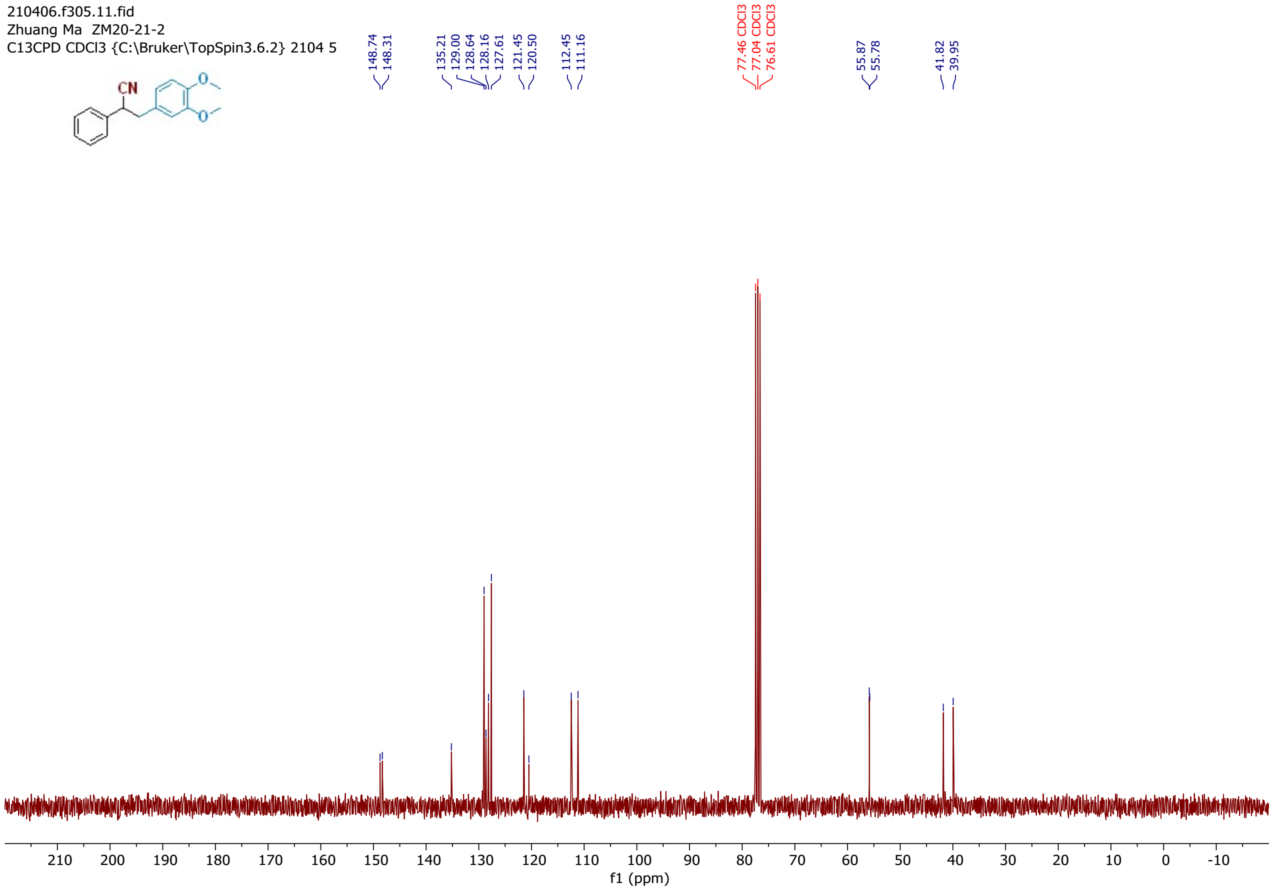

211210.f350.10.fid
Zhuang Ma ZM 20-42
PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2112 50
CN
N
O
7.26 CDCl3
1.04
5.10
2.02
1.00
3.12
2.05
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

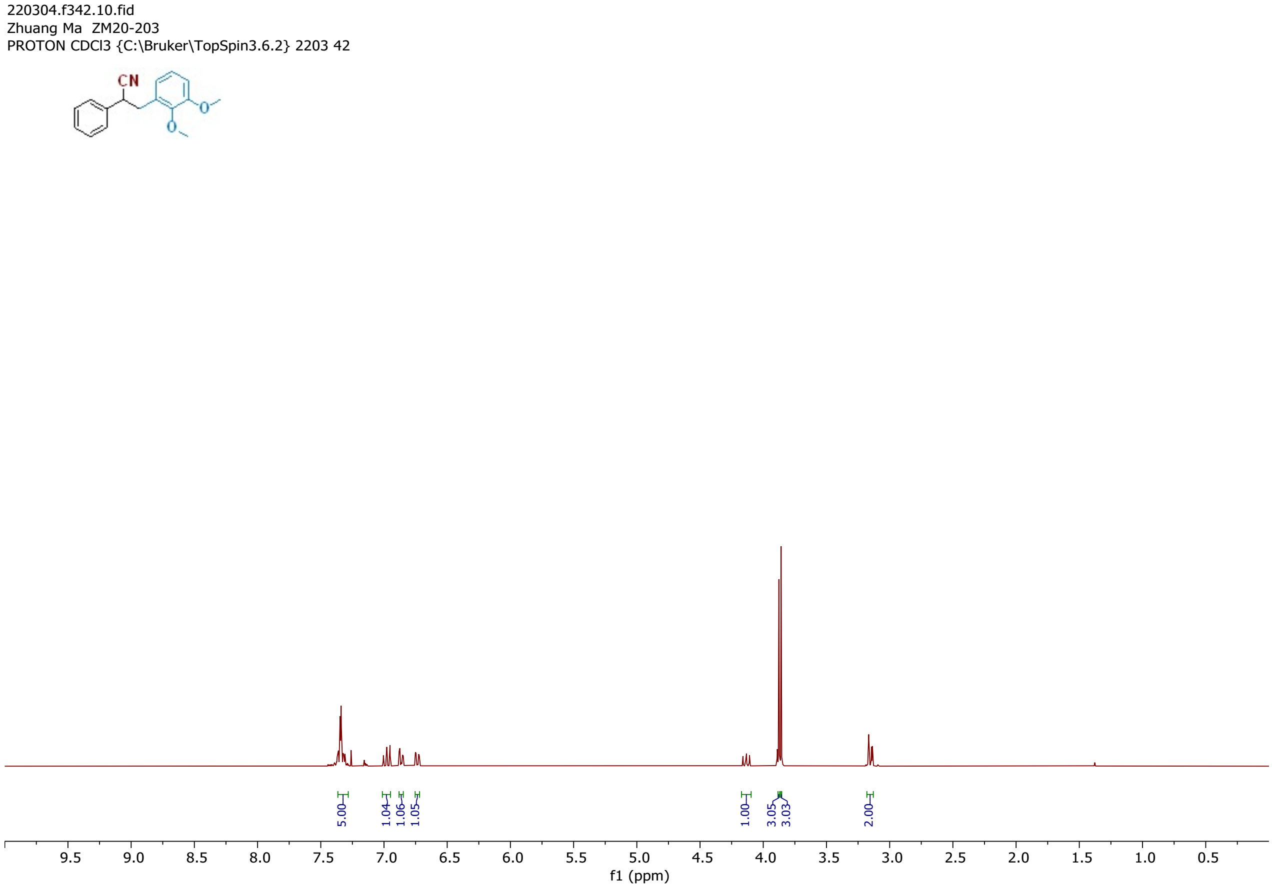

211210.f350.11.fid
Zhuang Ma ZM 20-42
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2112 50
CN
N
O
163.89
153.64
139.13
135.69
129.06
128.11
127.45
120.89
116.24
109.28
77.55 CDCl3
77.13 CDCl3
76.70 CDCl3
53.47
43.42
36.71
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

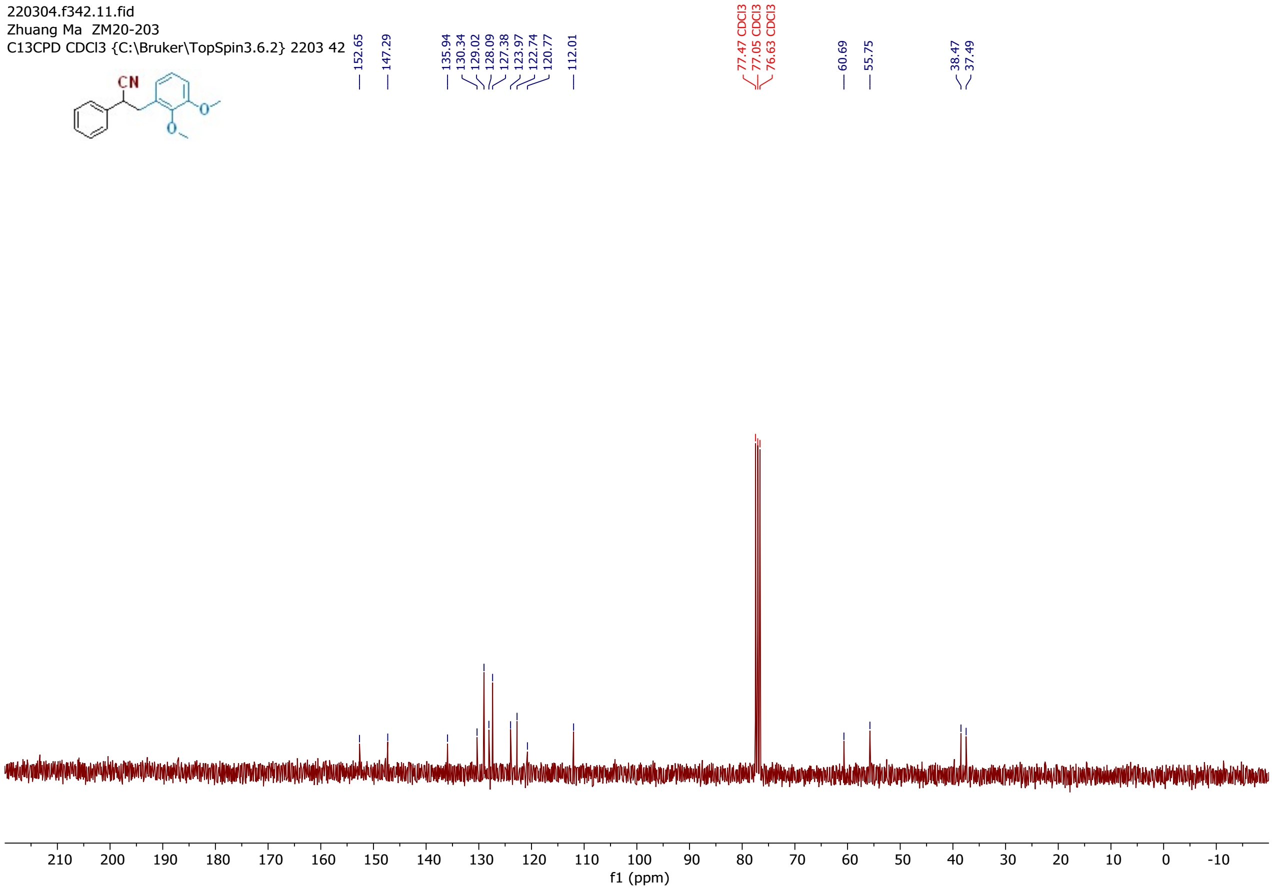

220203.320.10.fid
Ma/ ZM20-5-2
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2202 20
CN
NH
7.26 CDCl3
1.53 H2O
0.93
1.04
5.99
1.09
1.00
0.96
1.00
2.06
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


220203.320.11.fid
Ma/ ZM20-5-2
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2202 20
CN
NH
136.16
135.91
129.08
128.18
127.48
126.89
123.34
122.30
121.18
119.73
118.18
111.48
110.89
77.53 CDCl3
77.11 CDCl3
76.69 CDCl3
39.21
32.49
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

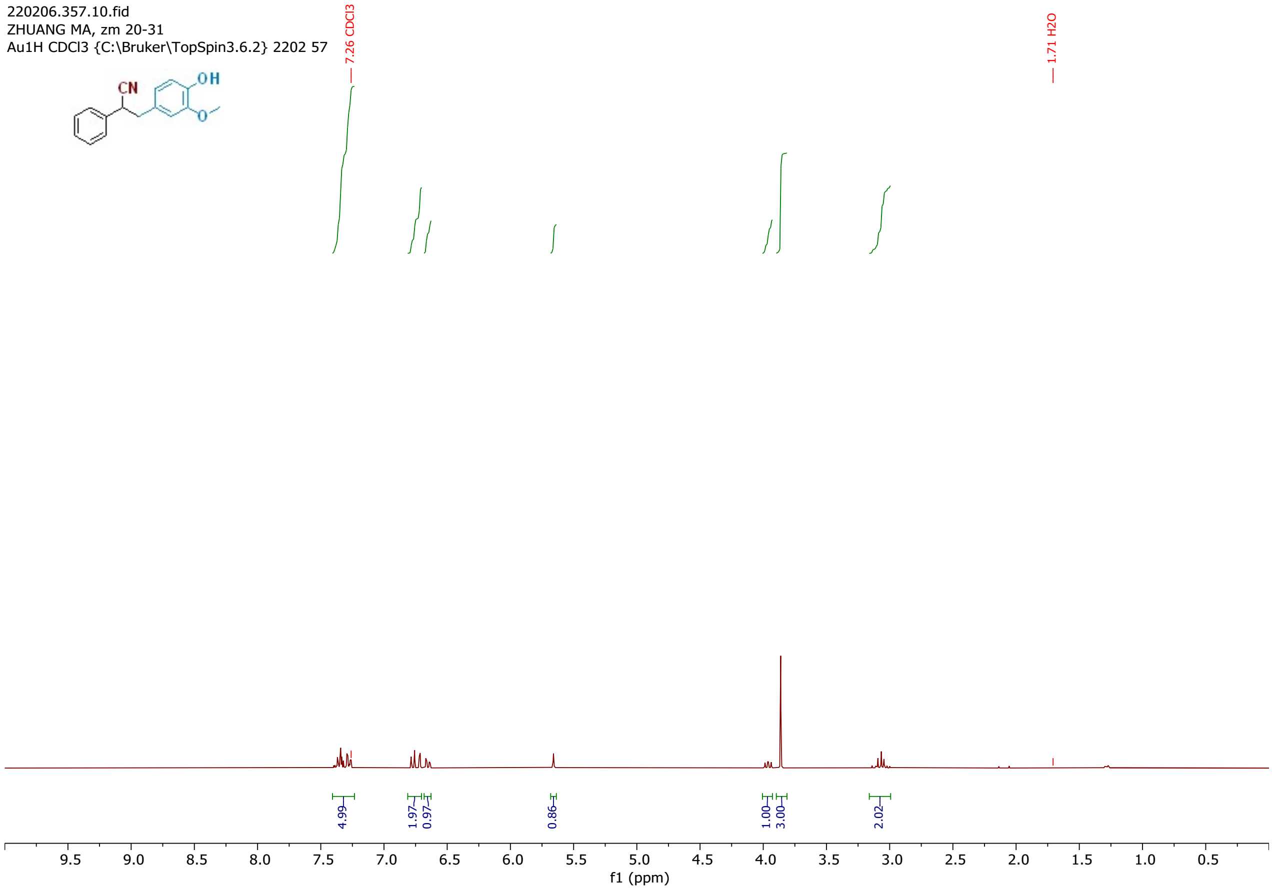

210406.f305.10.fid
Zhuang Ma ZM20-21-2
PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2104 5
CN
O
O
7.26 CDCl3
1.55 H2O
2.96
2.17
0.97
0.98
0.96
1.15
3.00
2.96
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


210406.f305.11.fid
Zhuang Ma ZM20-21-2
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2104 5
CN
O
O
148.74
148.31
135.21
129.00
128.64
128.16
127.61
121.45
120.50
112.45
111.16
77.46 CDCl3
77.04 CDCl3
76.61 CDCl3
55.87
55.78
41.82
39.95
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)

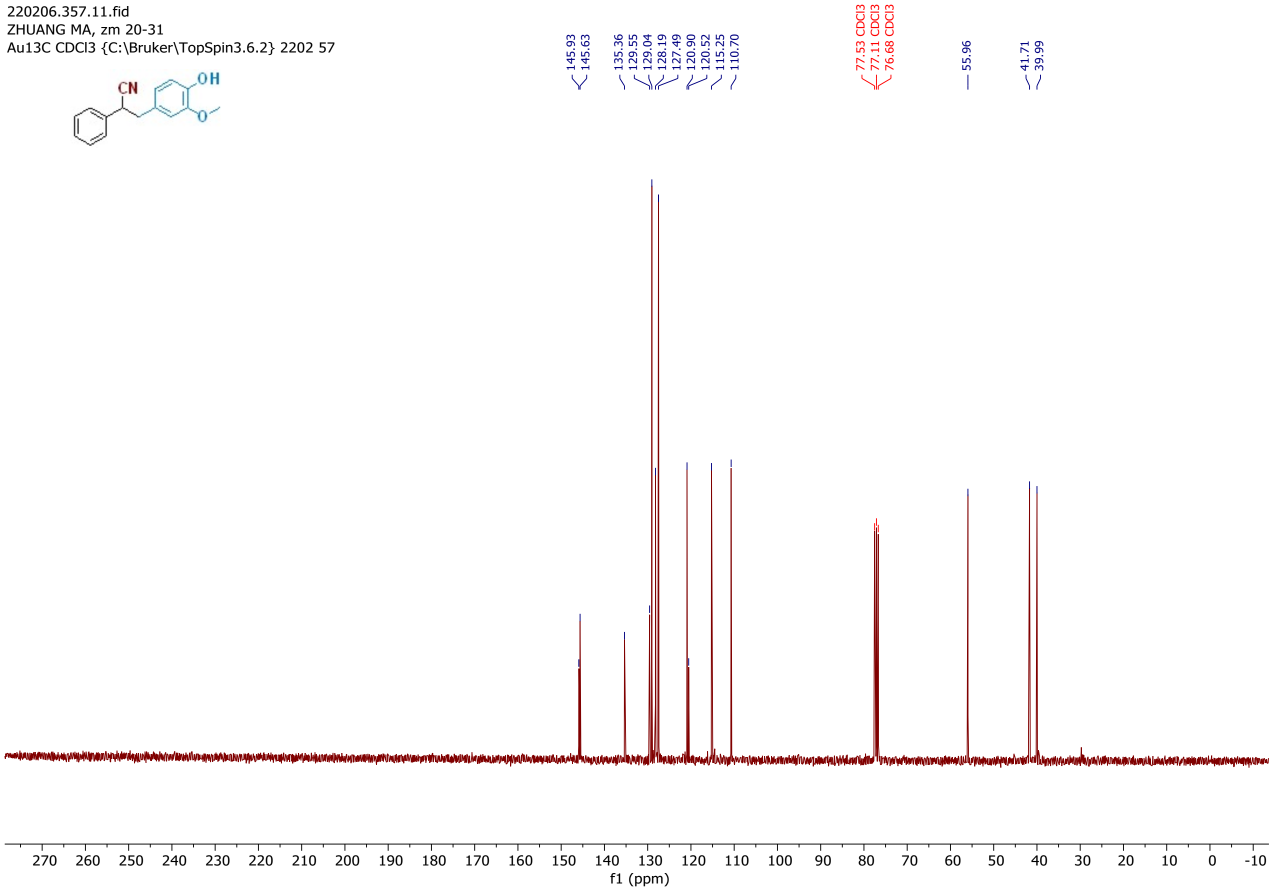

220304.f342.10.fid
Zhuang Ma ZM20-203
PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2203 42
CN
O
O
5.00
1.04
1.06
1.05
1.00
3.05
3.03
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

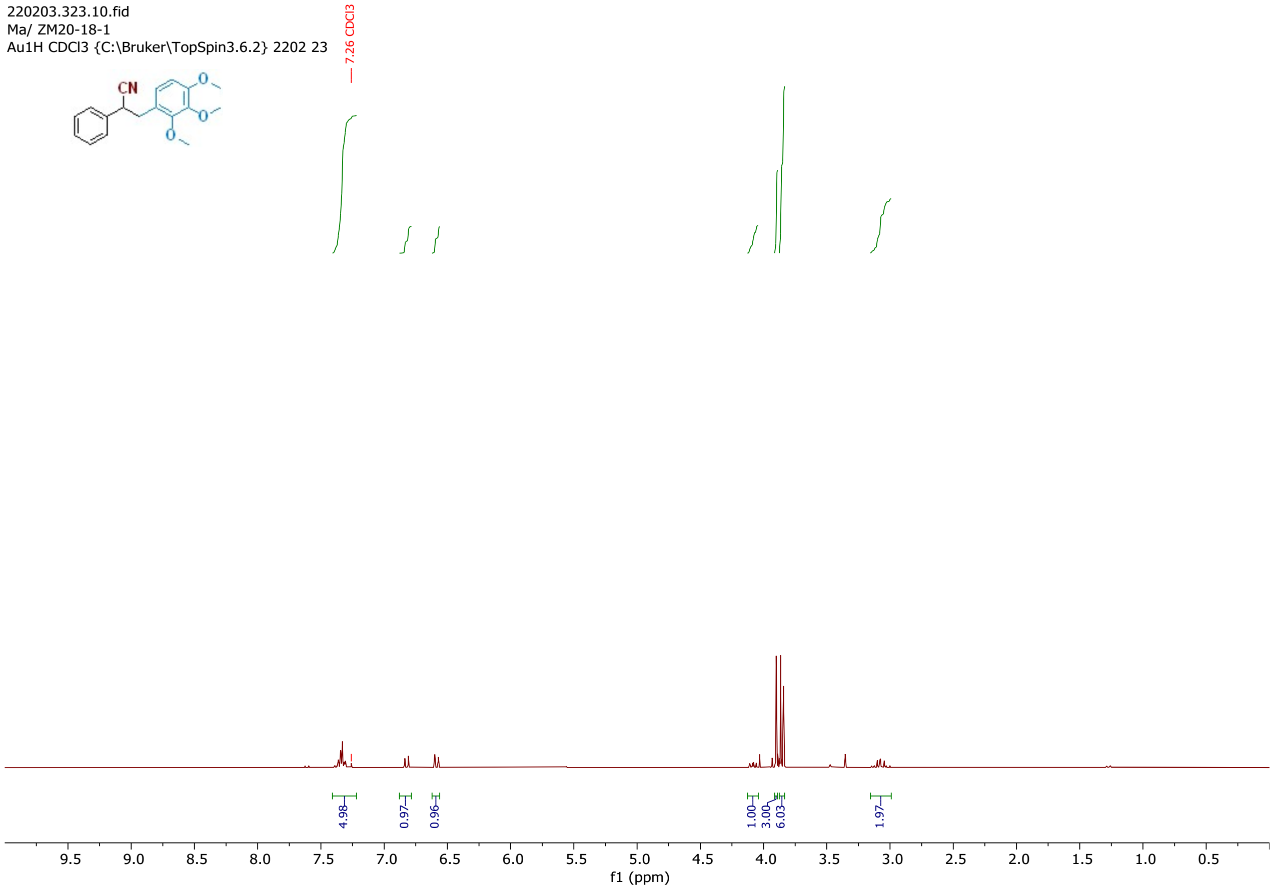

220304.f342.11.fid
Zhuang Ma ZM20-203
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2203 42
CN
O
O
152.65
147.29
135.94
130.34
129.02
128.09
127.38
123.97
122.74
120.77
112.01
77.47 CDCl3
77.05 CDCl3
76.63 CDCl3
60.69
55.75
38.47
37.49
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

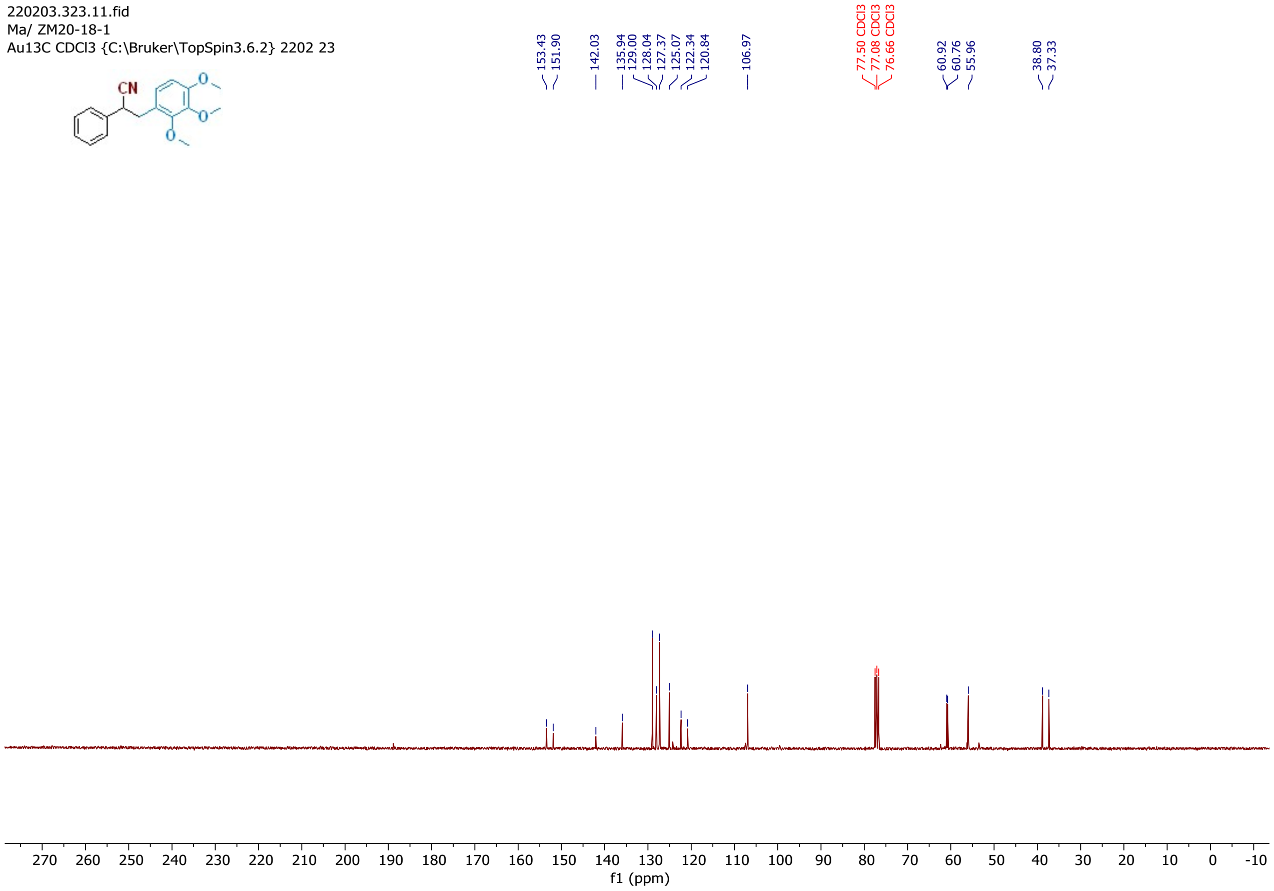
220206.357.10.fid
ZHUANG MA, zm 20-31
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2202 57

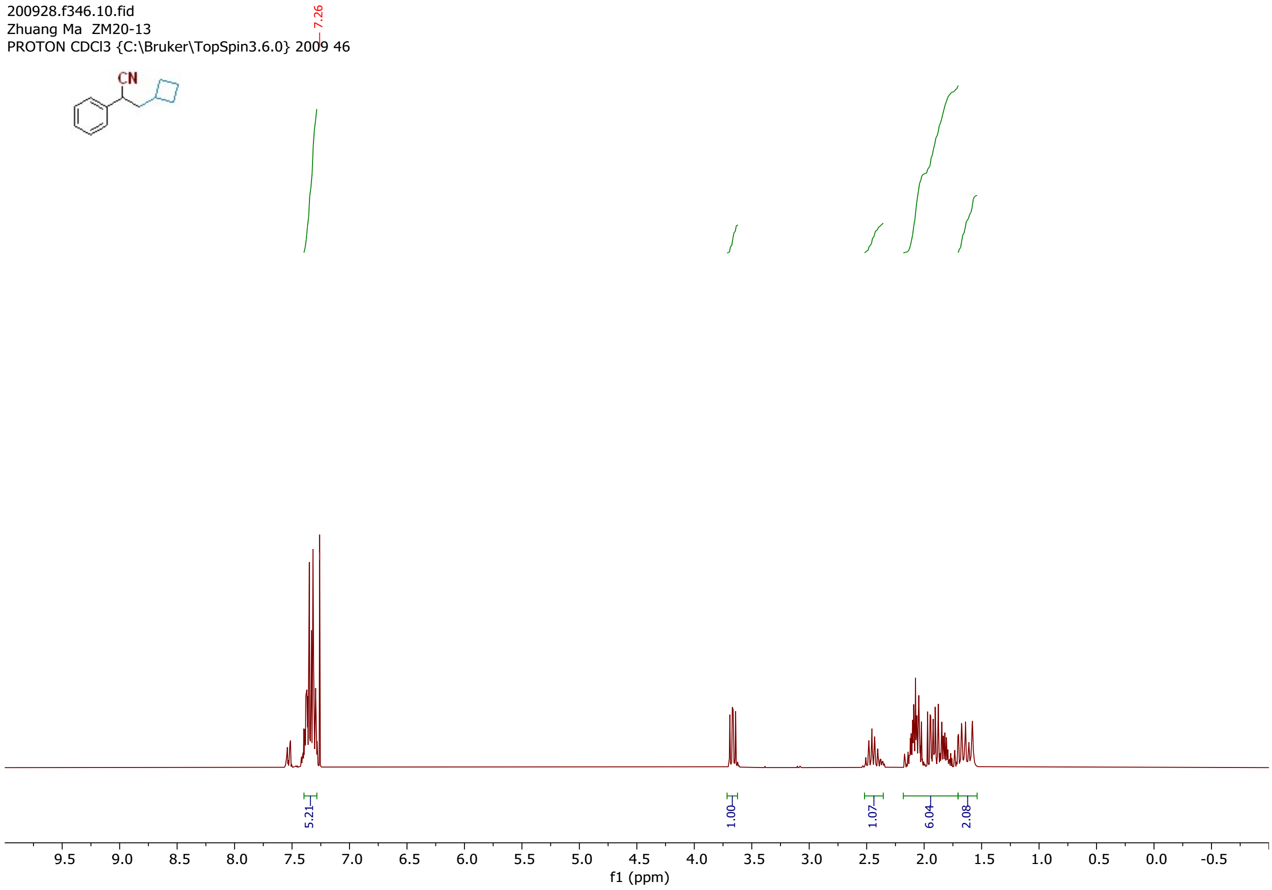


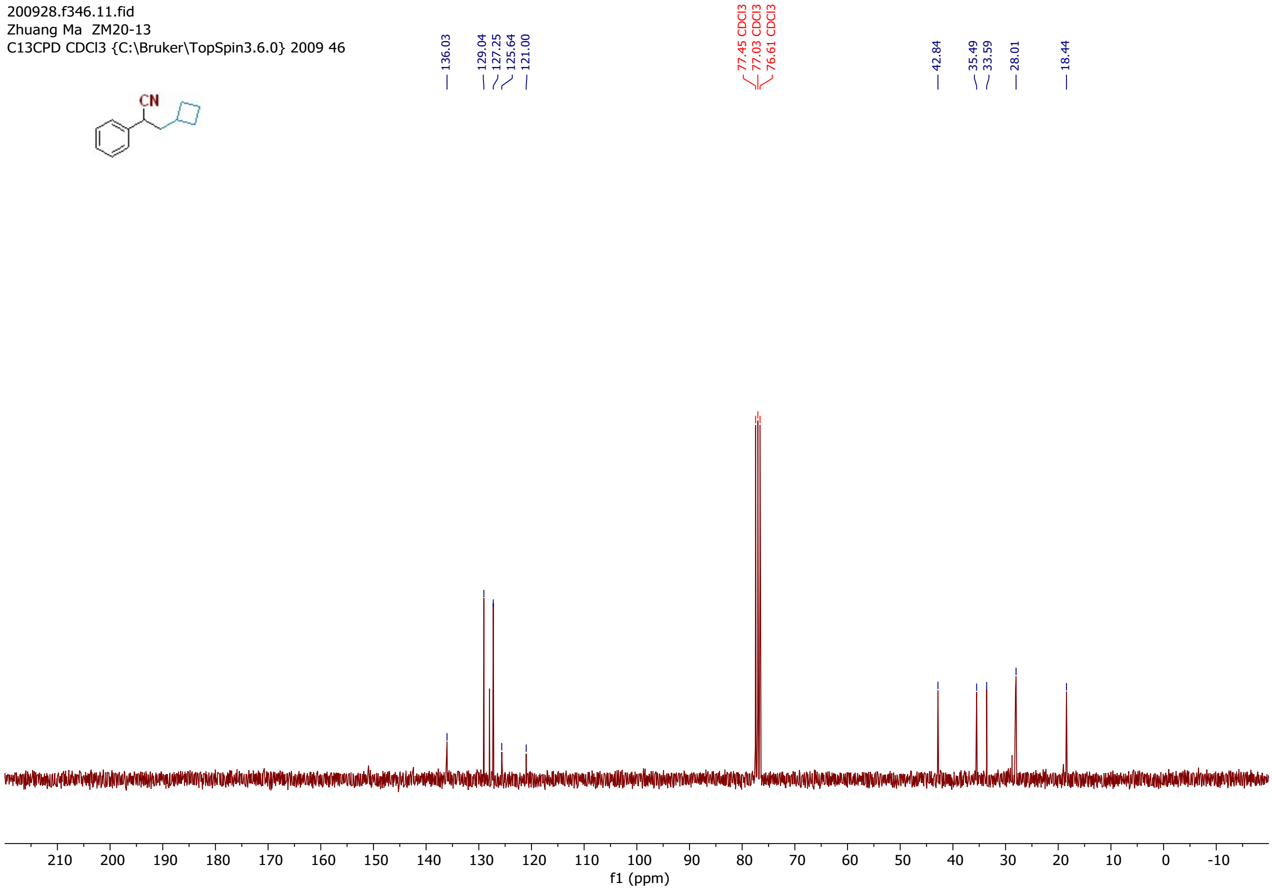
220206.357.11.fid
ZHUANG MA, zm 20-31
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2202 57

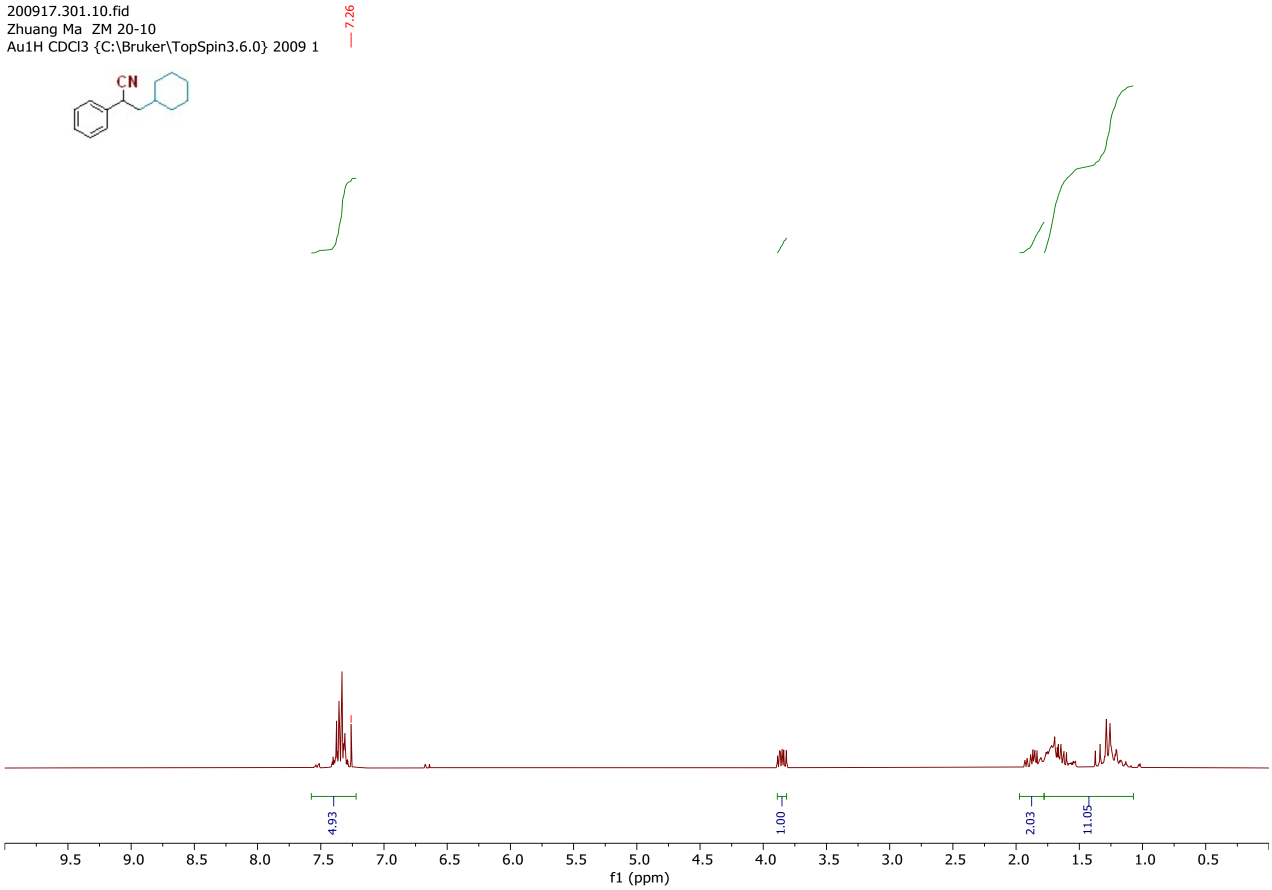


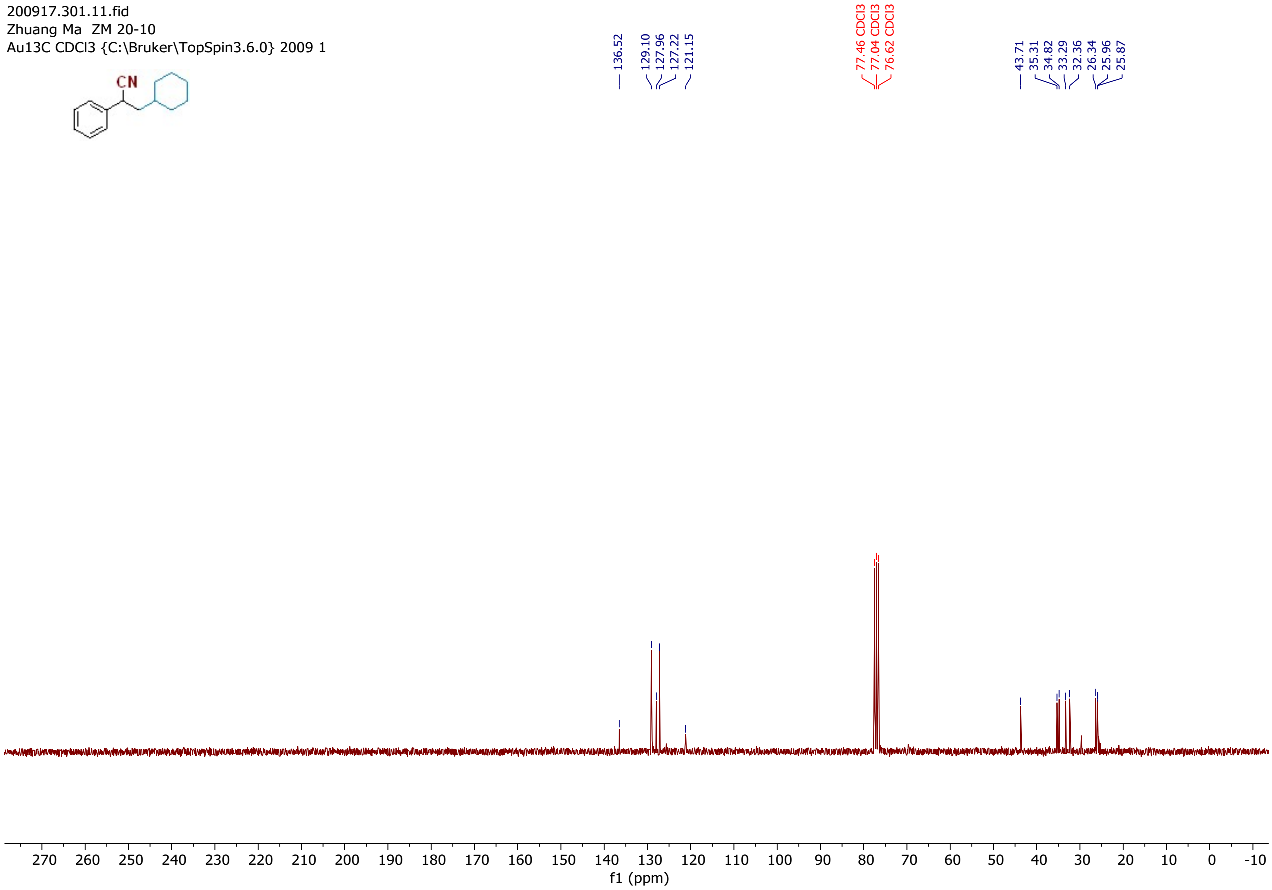

220203.323.10.fid
Ma/ ZM20-18-1
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2202 23
CN
O
O
O
7.26 CDCl3
4.98
0.97
0.96
1.00
3.00
6.03
1.97
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

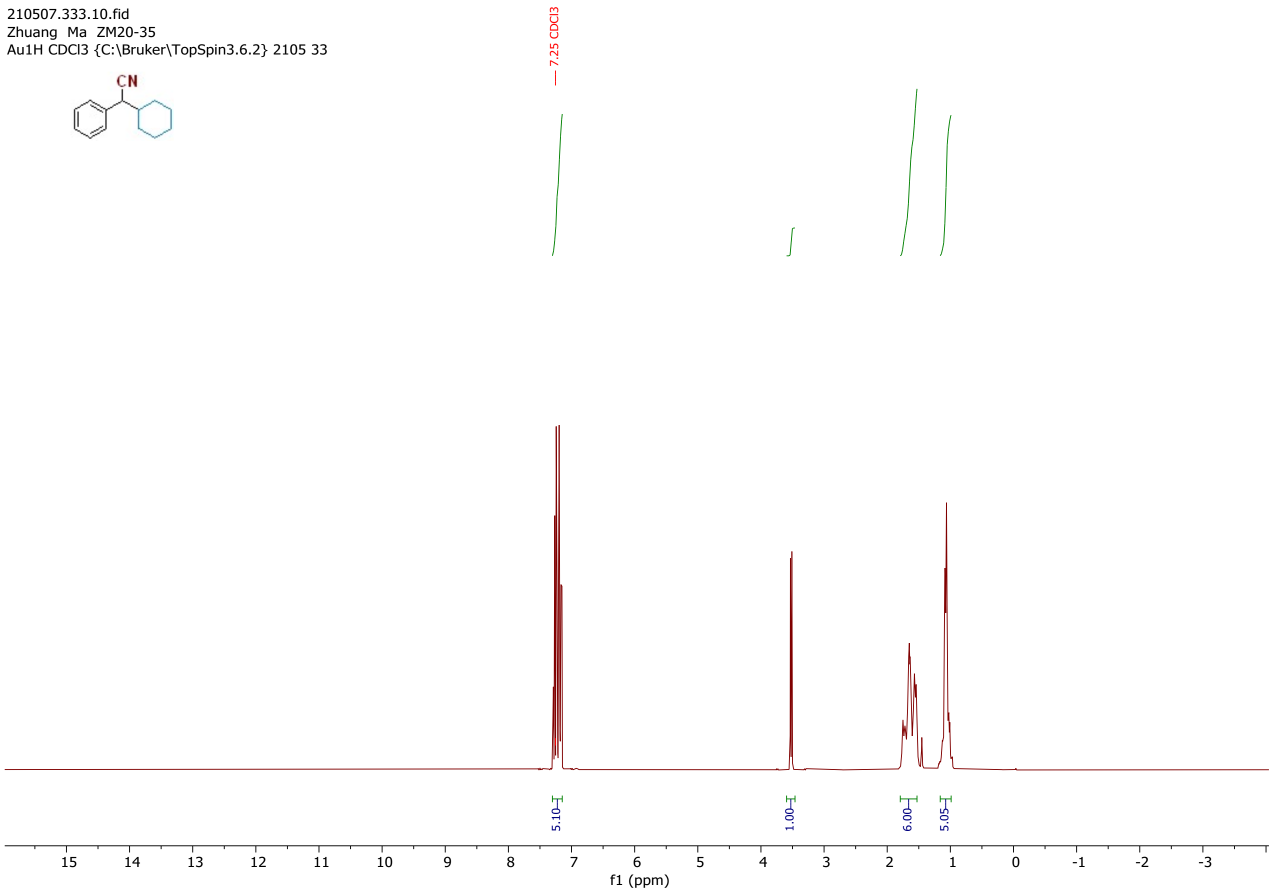

220203.323.11.fid
Ma/ ZM20-18-1
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2202 23
CN
O
O
O
153.43
151.90
142.03
135.94
129.00
128.04
127.37
125.07
122.34
120.84
106.97
77.50 CDCl3
77.08 CDCl3
76.66 CDCl3
60.92
60.76
55.96
38.80
37.33
270
260
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

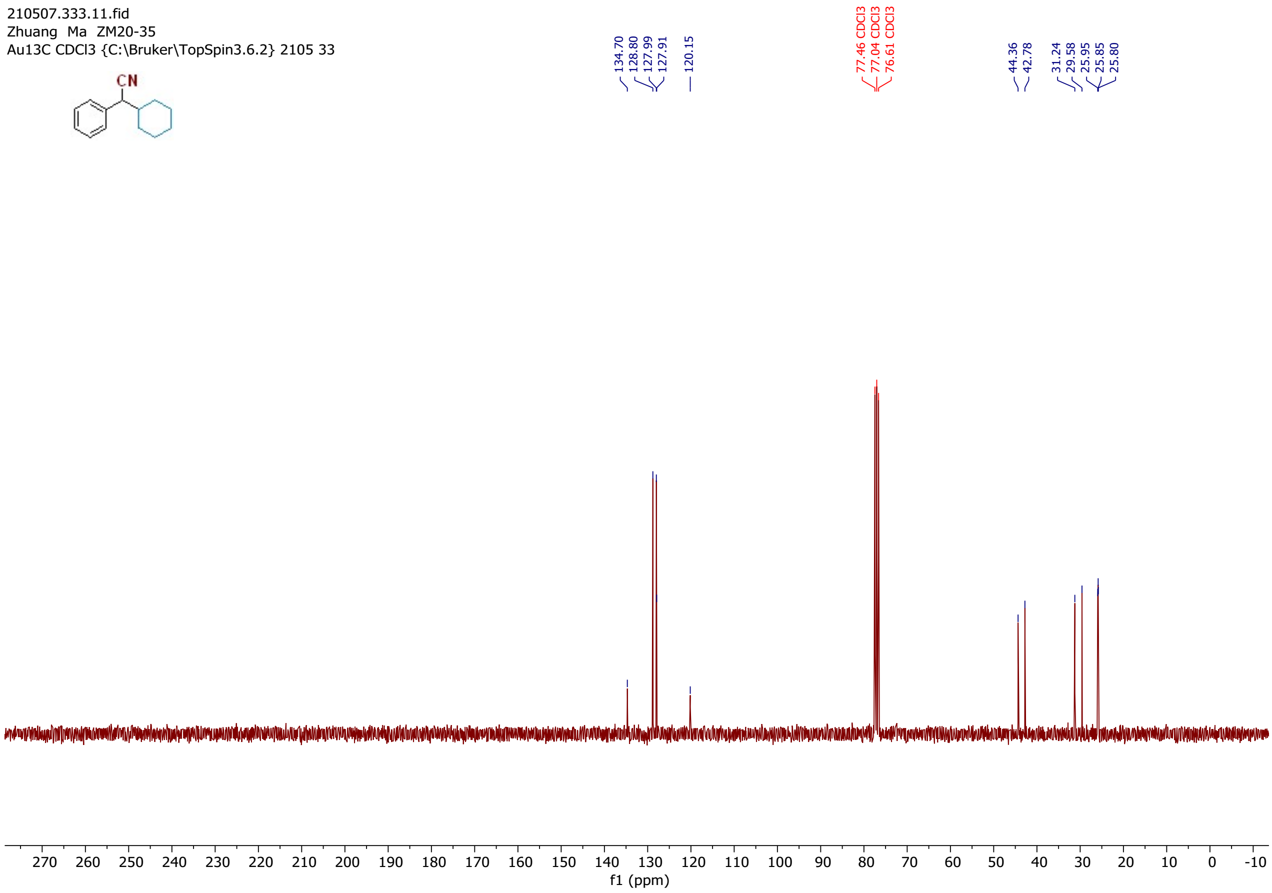

200928.f346.10.fid
Zhuang Ma ZM20-13
PROTON CDCl3 {C:\Bruker\TopSpin3.6.0} 2009 46
CN
7.26
5.21
1.00
1.07
6.04
2.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

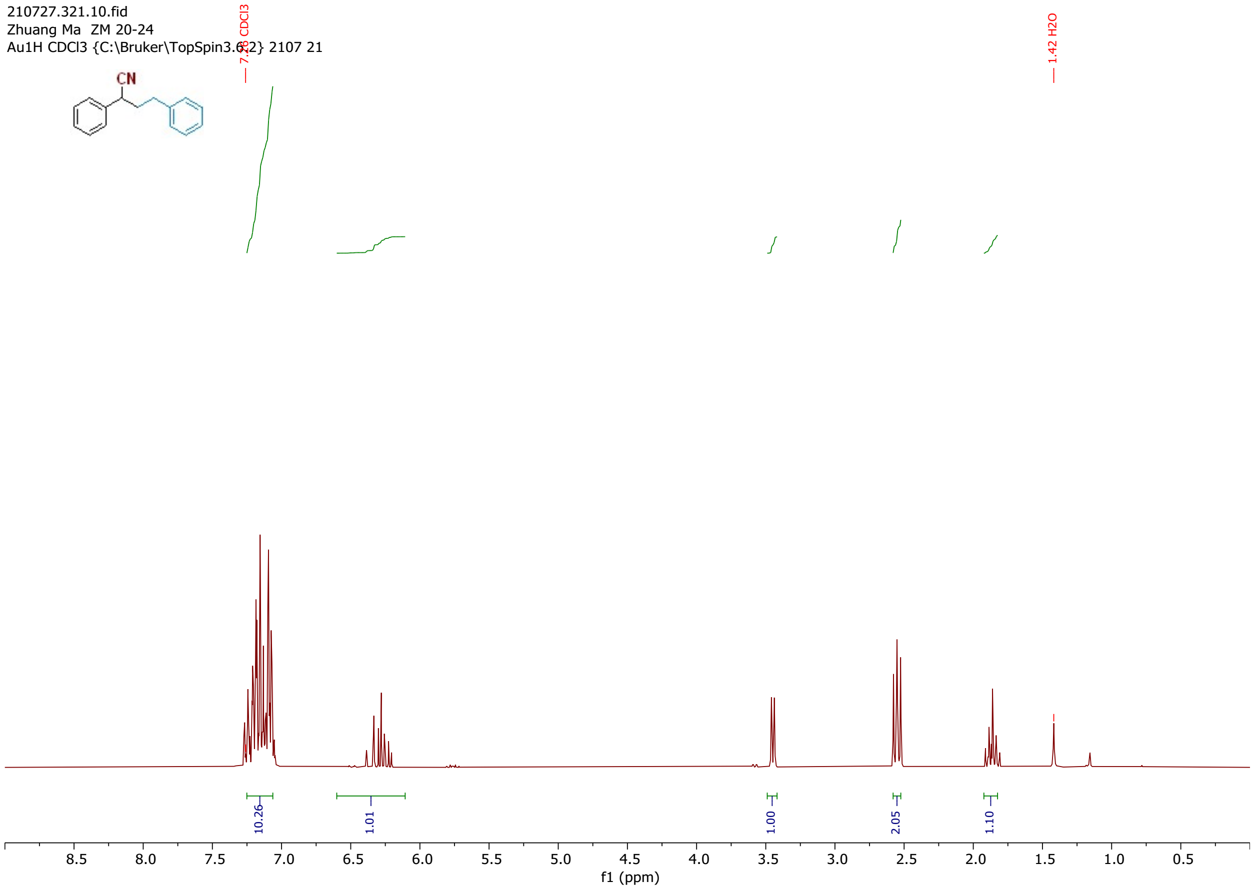

200928.f346.11.fid
Zhuang Ma ZM20-13
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 2009 46
CN
136.03
129.04
127.25
125.64
121.00
77.45 CDCl3
77.03 CDCl3
76.61 CDCl3
42.84
35.49
33.59
28.01
18.44
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

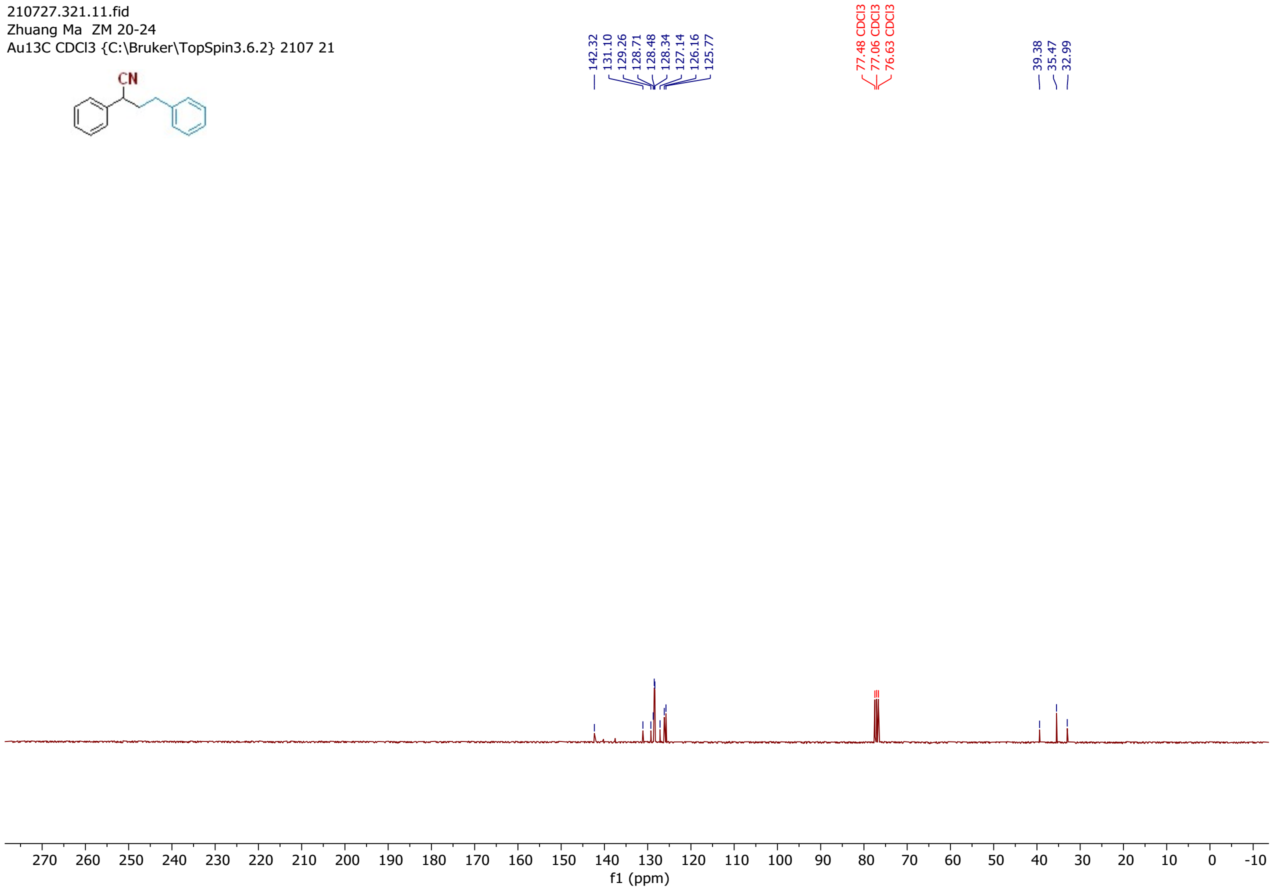

200917.301.10.fid
Zhuang Ma ZM 20-10
Au1H CDCl3 {C:\Bruker\TopSpin3.6.0} 2009 1
CN
7.26
4.93
1.00
2.03
11.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


200917.301.11.fid
Zhuang Ma ZM 20-10
Au13C CDCl3 {C:\Bruker\TopSpin3.6.0} 2009 1
CN
136.52
129.10
127.96
127.22
121.15
77.46 CDCl3
77.04 CDCl3
76.62 CDCl3
43.71
35.31
34.82
33.29
32.36
26.34
25.96
25.87
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

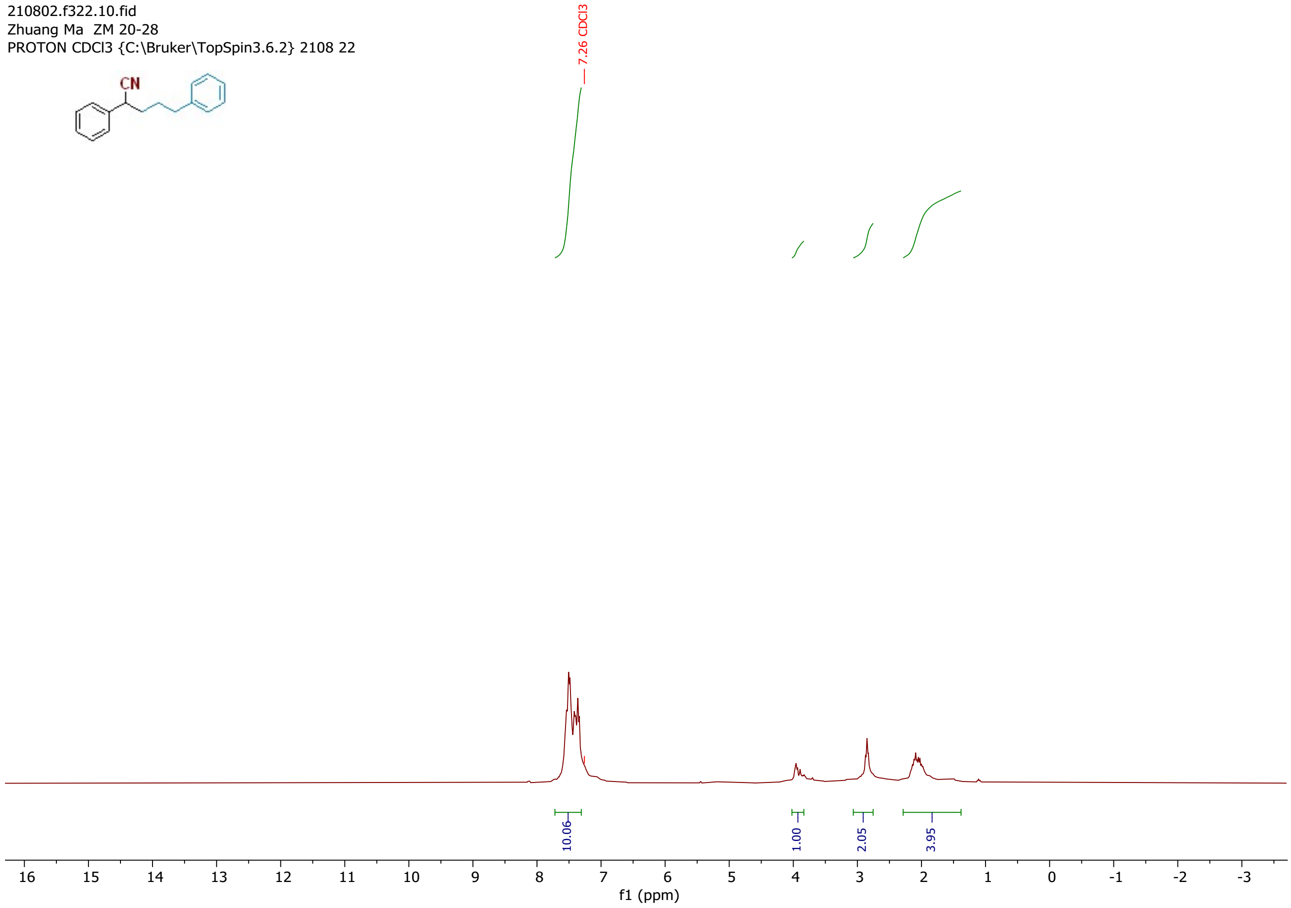

210507.333.10.fid
Zhuang Ma ZM20-35
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2105 33
CN
7.25 CDCl3
5.10
1.00
6.00
5.05
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


210507.333.11.fid
Zhuang Ma ZM20-35
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2105 33
CN
134.70
128.80
127.99
127.91
120.15
77.46 CDCl3
77.04 CDCl3
76.61 CDCl3
44.36
42.78
31.24
29.58
25.95
25.85
25.80
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

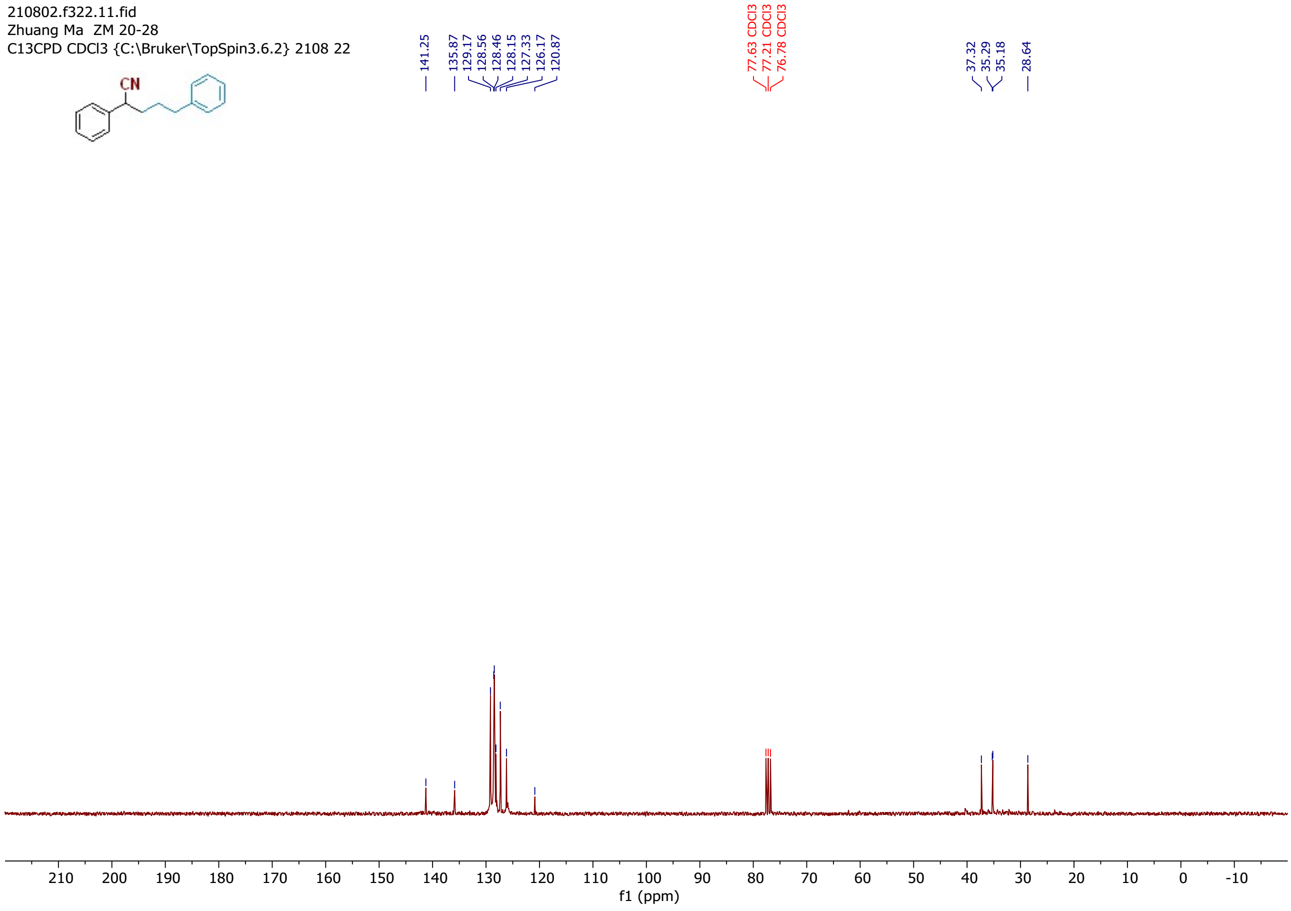

210727.321.10.fid
Zhuang Ma ZM 20-24
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2107 21
CN
7.26 CDCl3
1.42 H2O
10.26
1.01
1.00
2.05
1.10
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

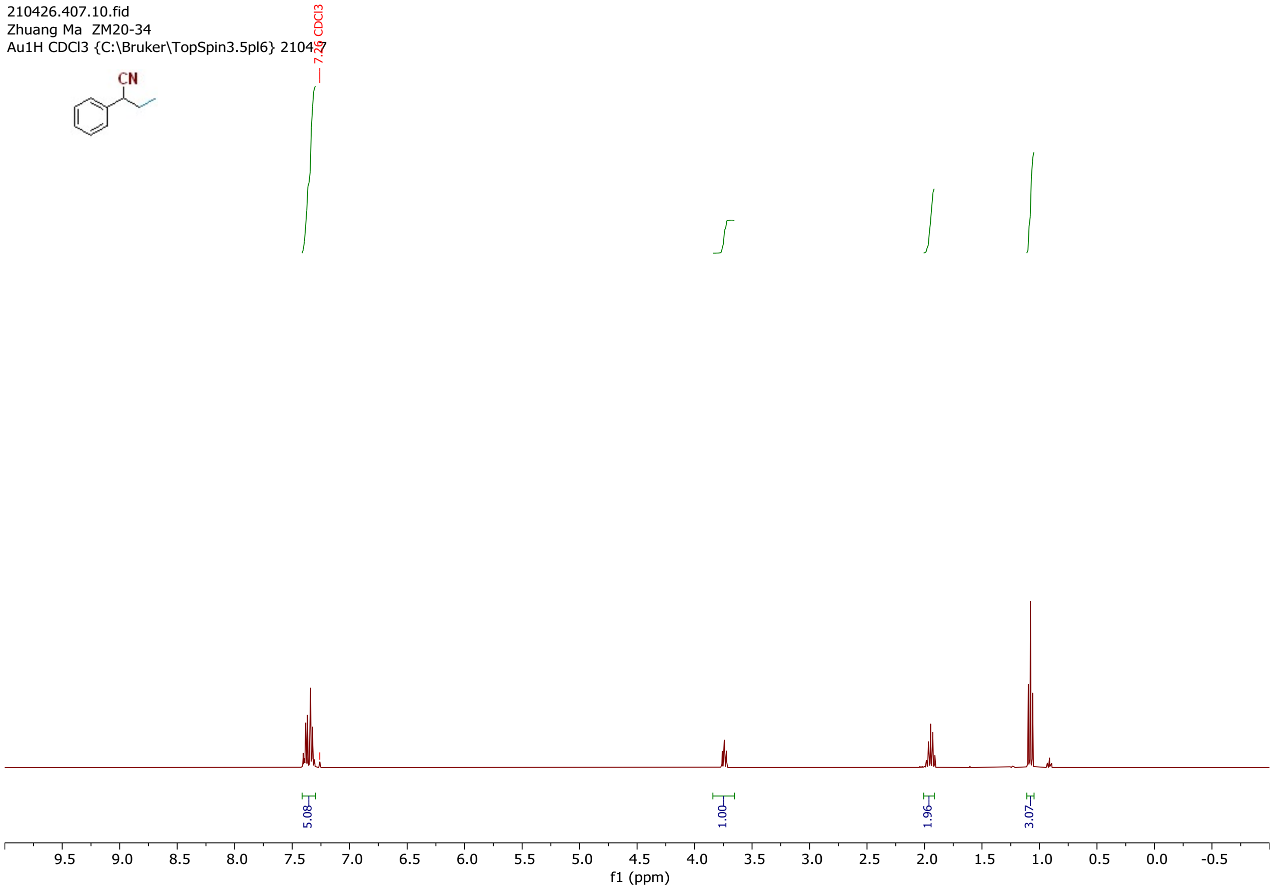

210727.321.11.fid
Zhuang Ma ZM 20-24
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2107 21
CN
142.32
131.10
129.26
128.71
128.48
128.34
127.14
126.16
125.77
77.48 CDCl3
77.06 CDCl3
76.63 CDCl3
39.38
35.47
32.99
270
260
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

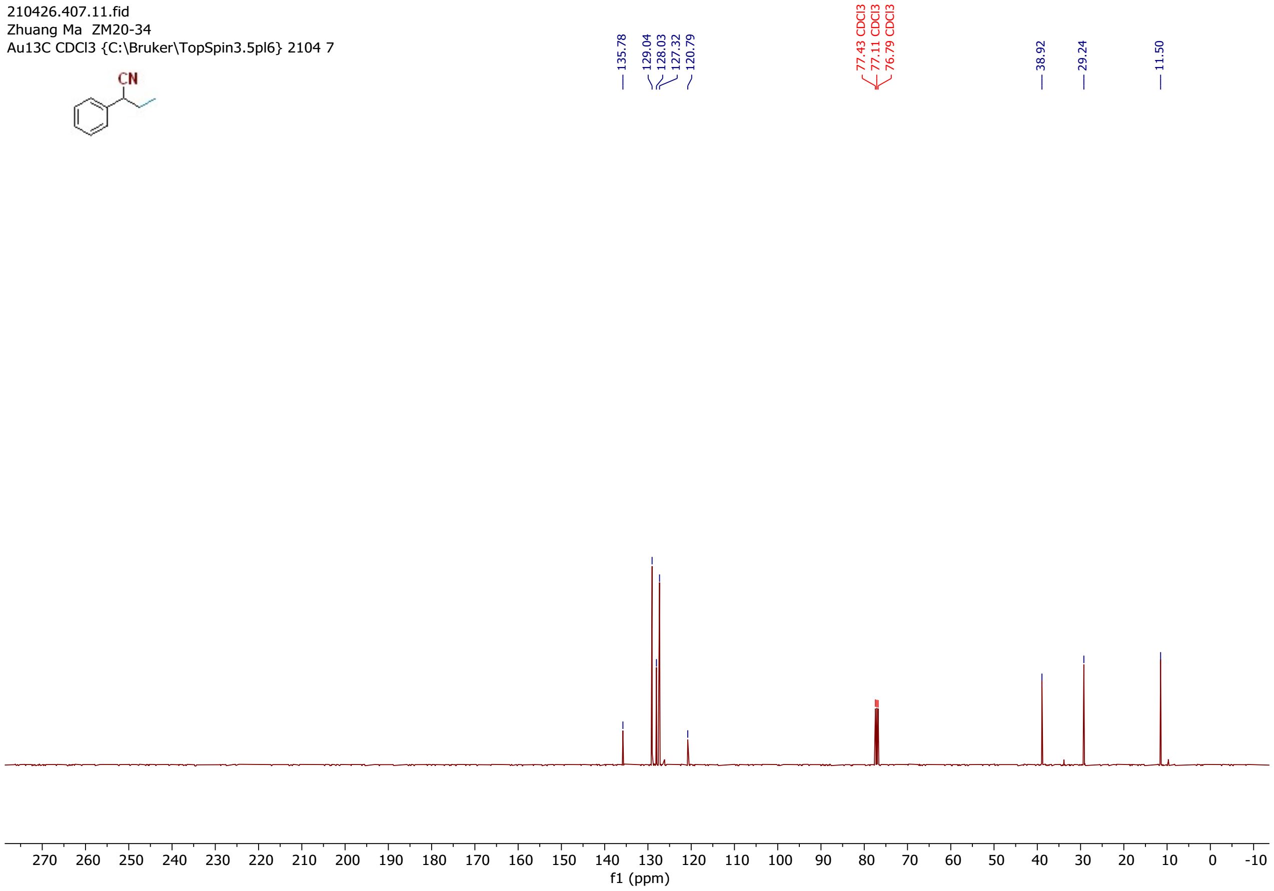
210802.f322.10.fid
Zhuang Ma ZM 20-28
PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 22

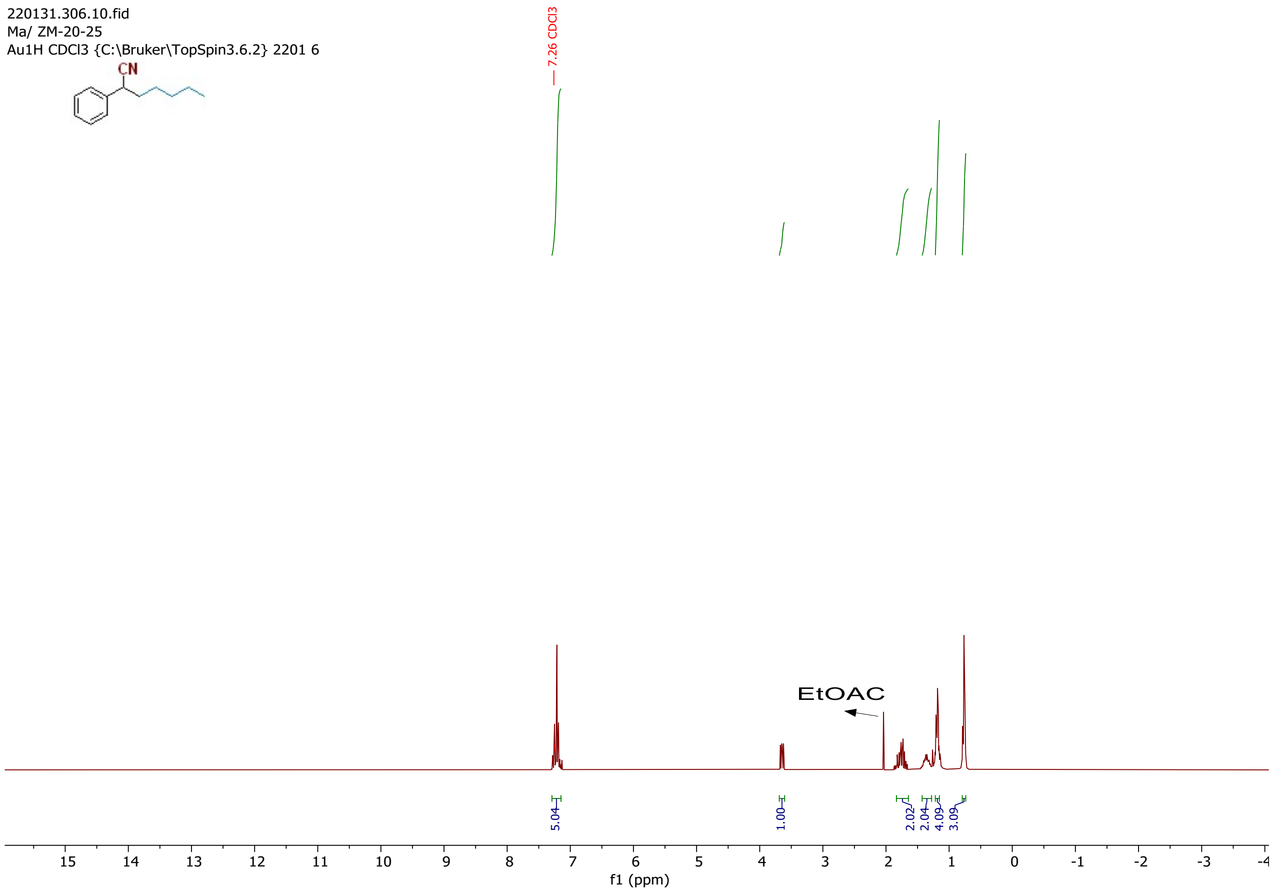


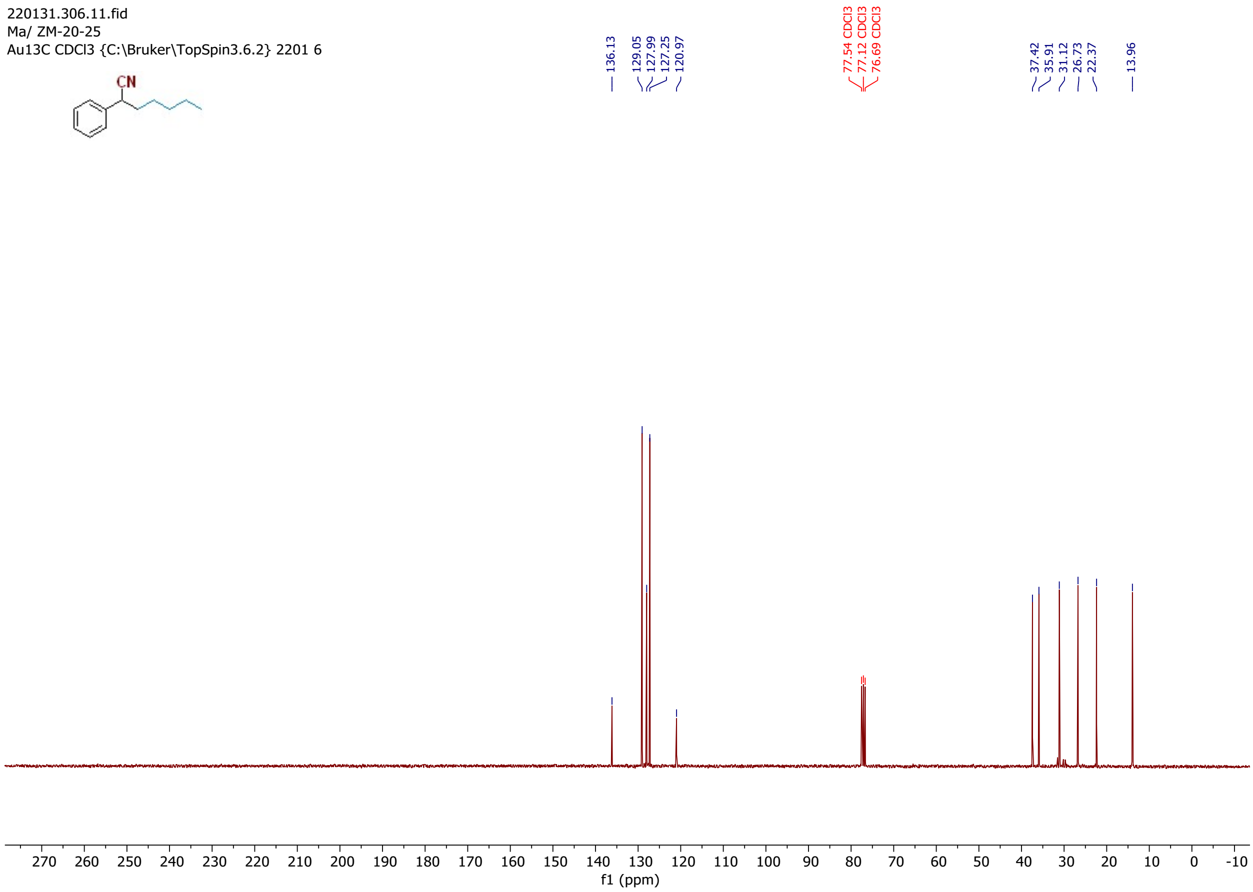
210802.f322.11.fid
Zhuang Ma ZM 20-28
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 22

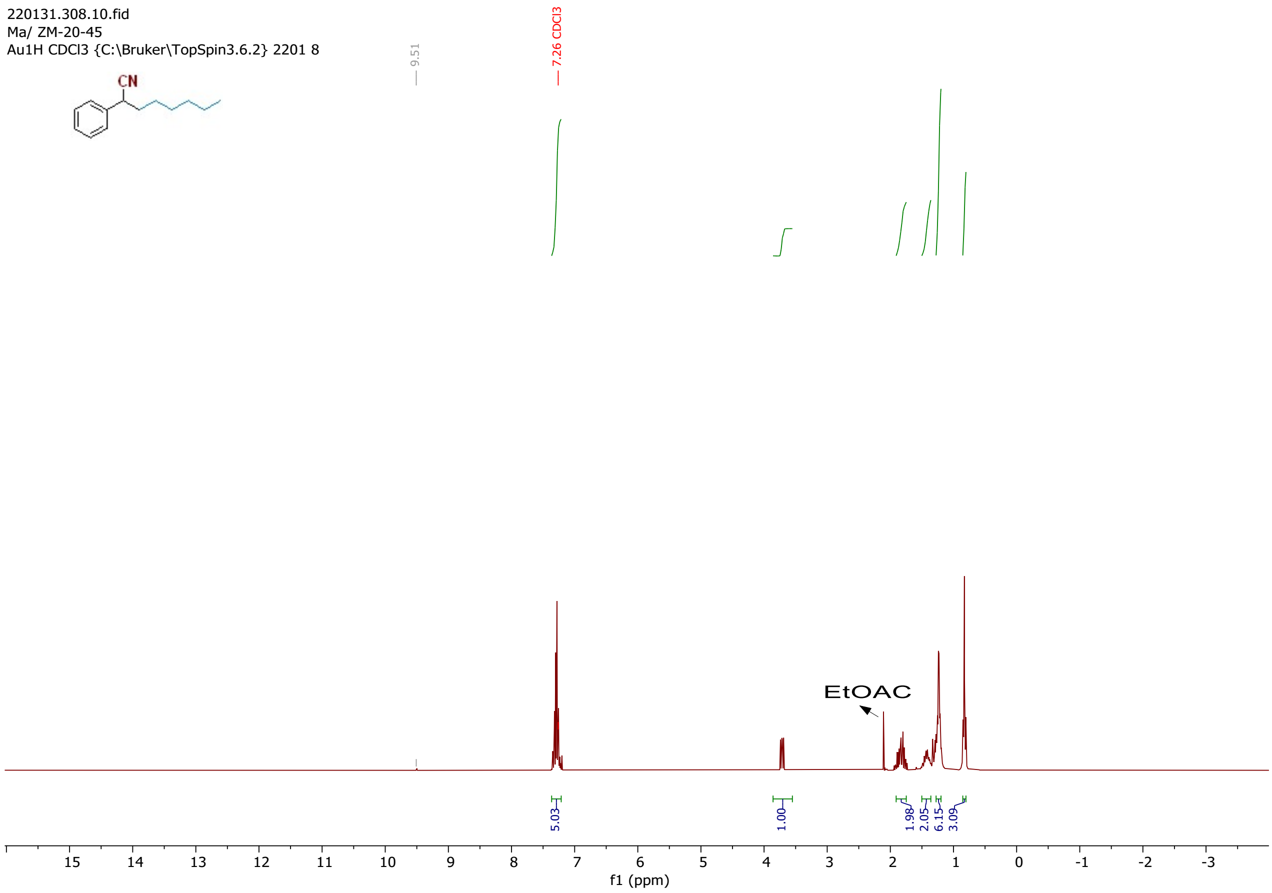


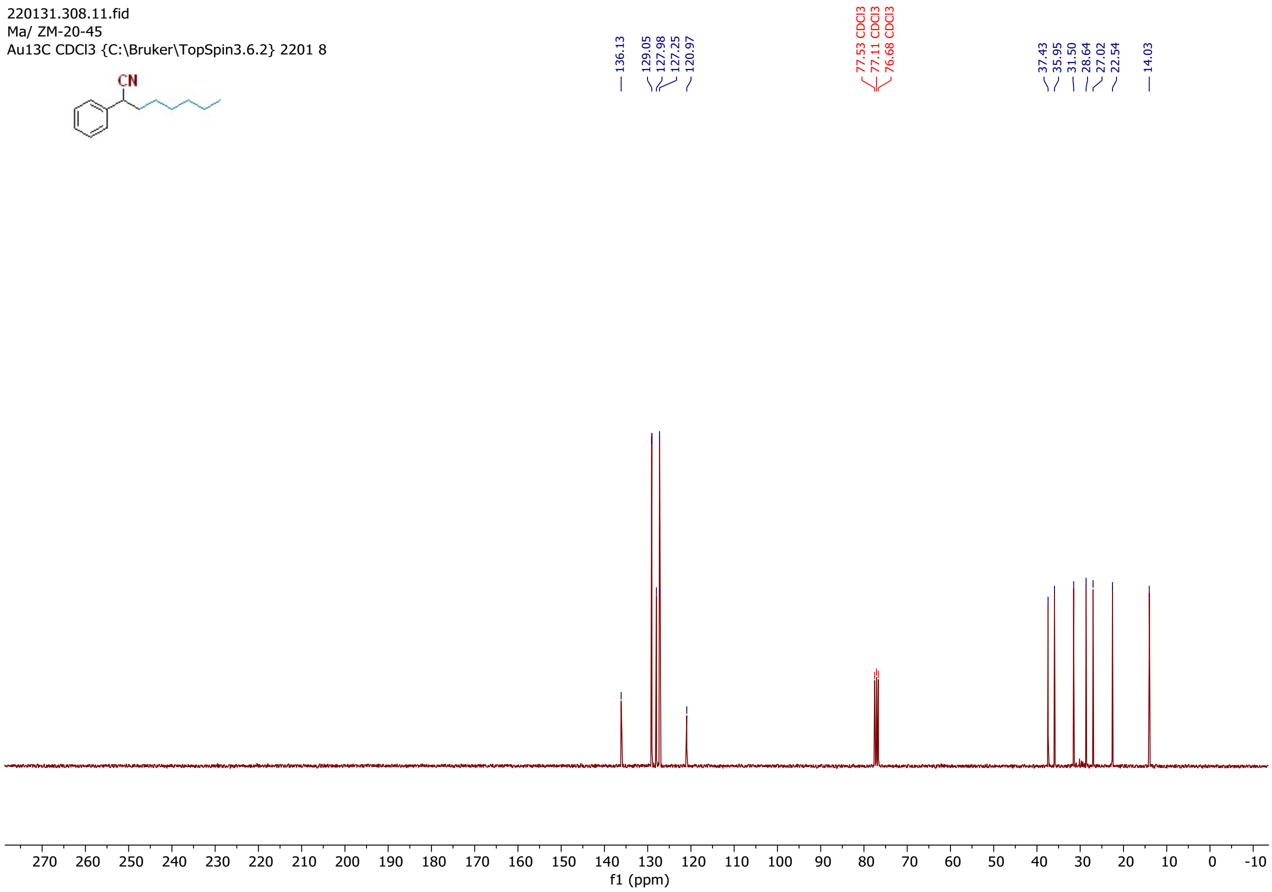

210426.407.10.fid
Zhuang Ma ZM20-34
Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 2104 7
CN
7.26 CDCl3
5.08
1.00
1.96
3.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

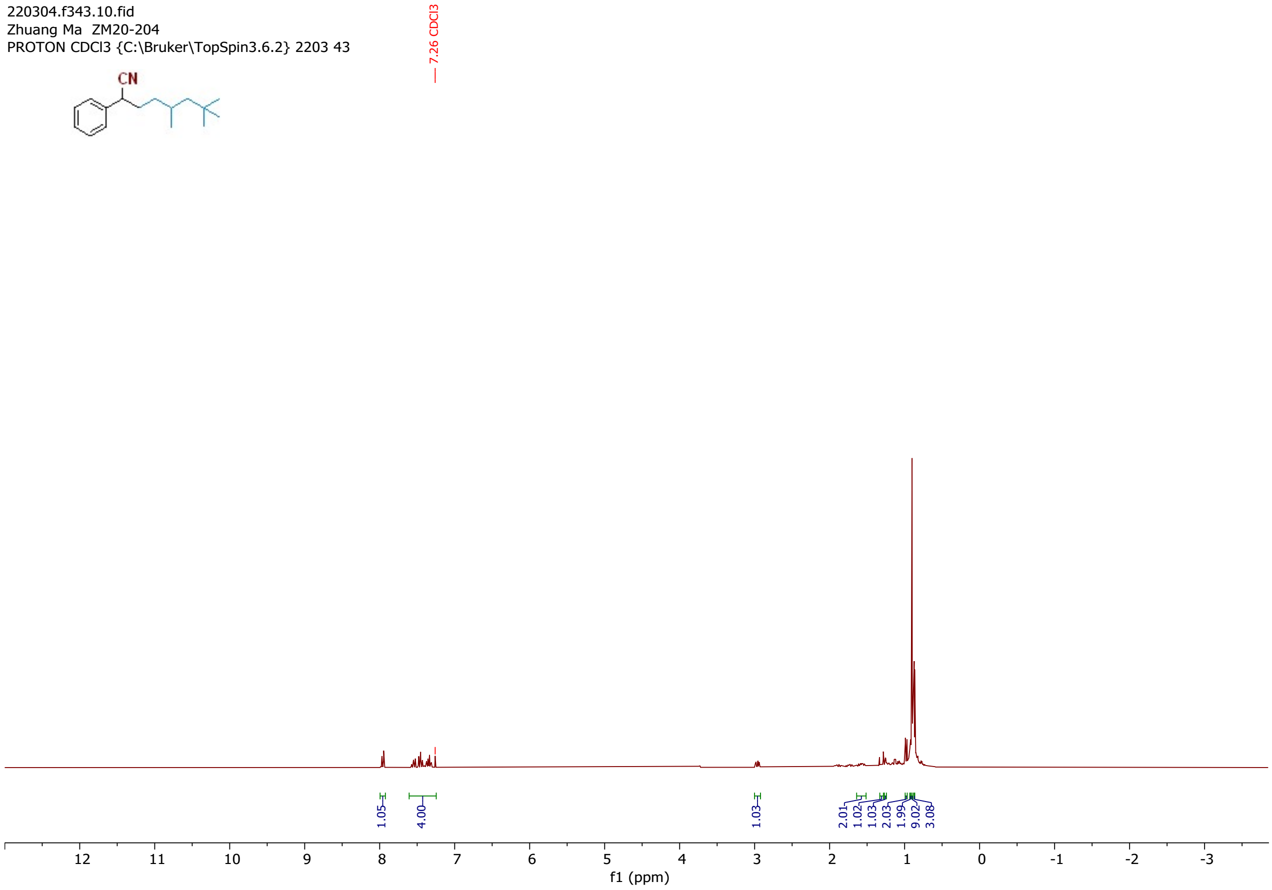

210426.407.11.fid
Zhuang Ma ZM20-34
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2104 7
CN
135.78
129.04
128.03
127.32
120.79
77.43 CDCl3
77.11 CDCl3
76.79 CDCl3
38.92
29.24
11.50
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

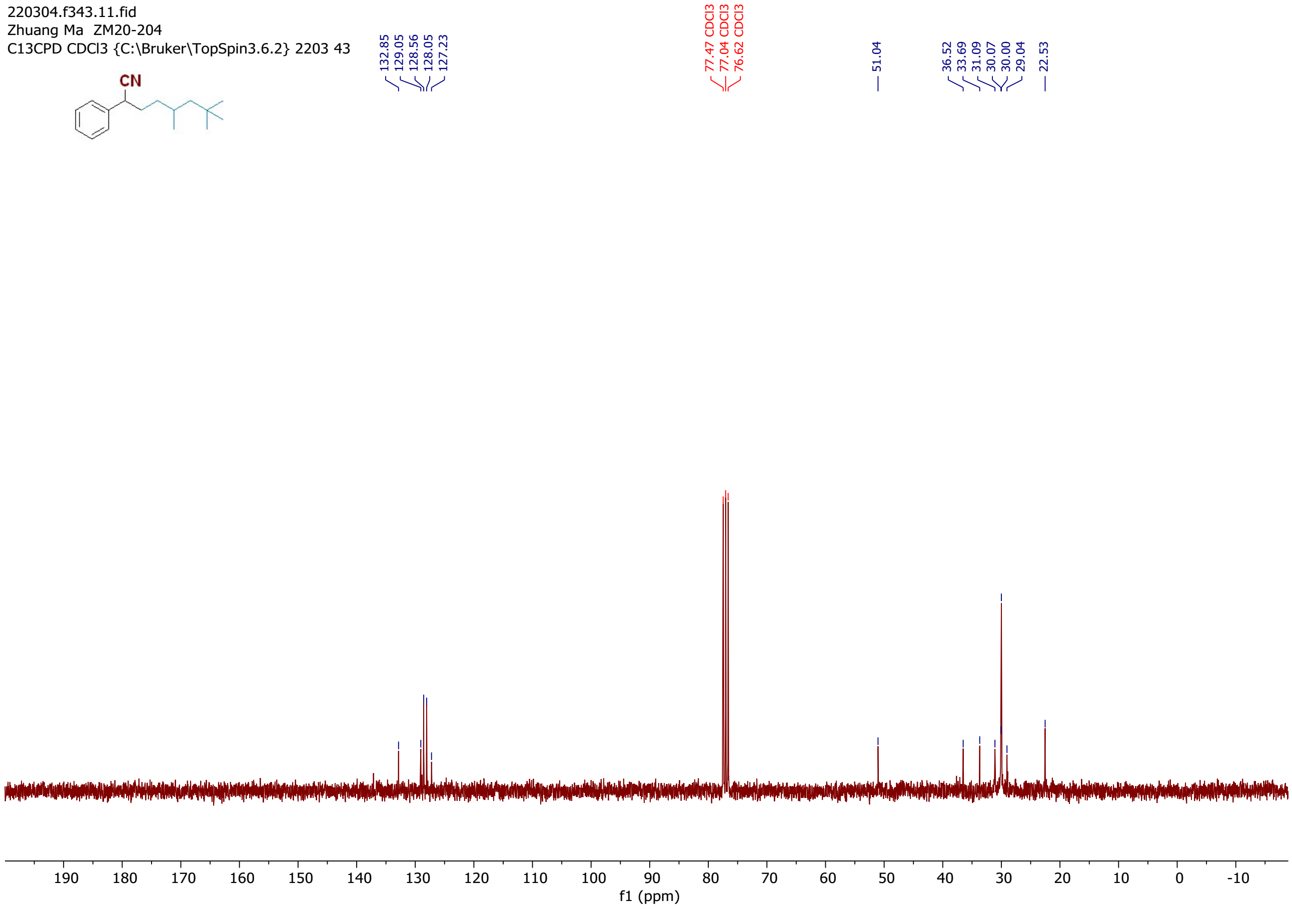

220131.306.10.fid
Ma/ ZM-20-25
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 6
CN
7.26 CDCl3
EtOAC
5.04
1.00
2.02
2.04
4.09
3.09
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

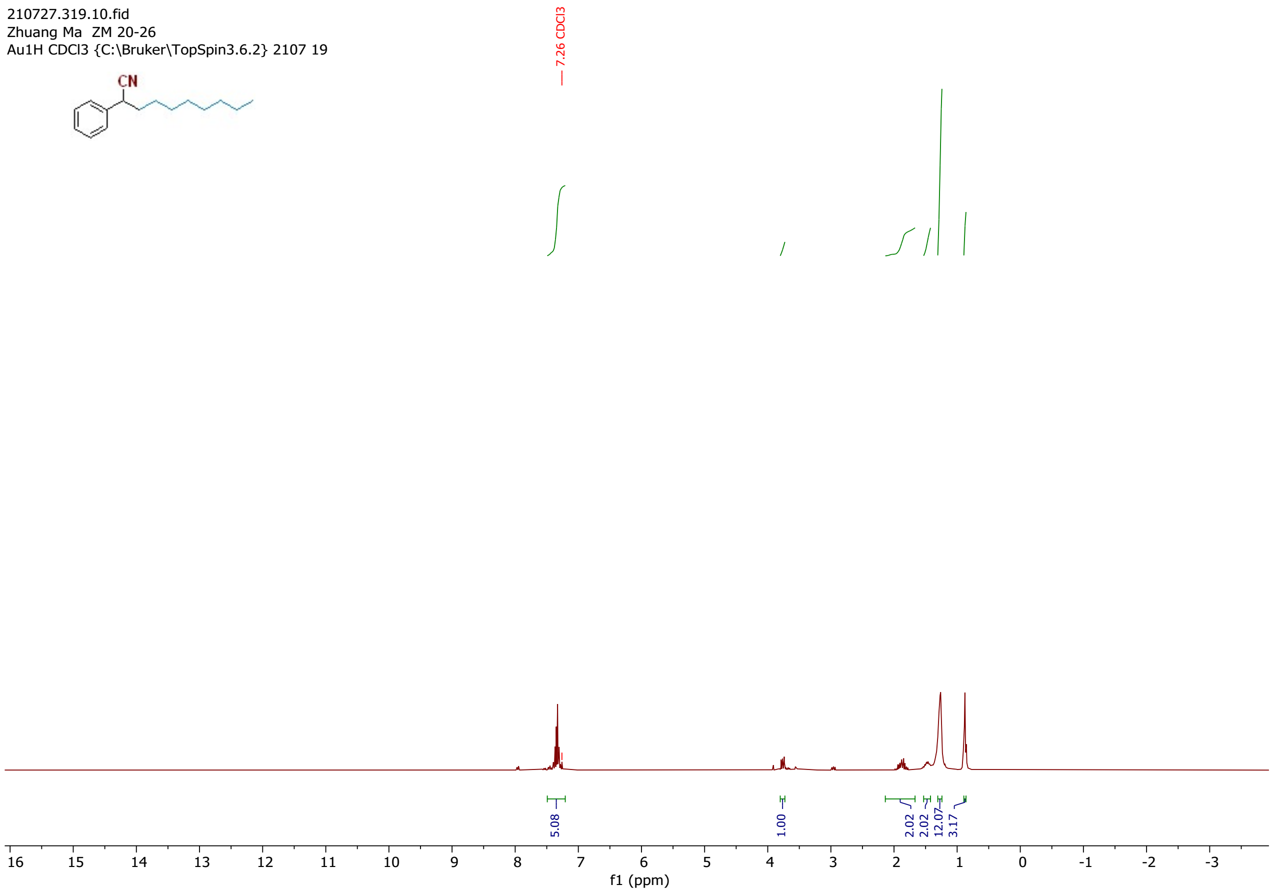

220131.306.11.fid
Ma/ ZM-20-25
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 6
CN
136.13
129.05
127.99
127.25
120.97
77.54 CDCl3
77.12 CDCl3
76.69 CDCl3
37.42
35.91
31.12
26.73
22.37
13.96
270
260
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

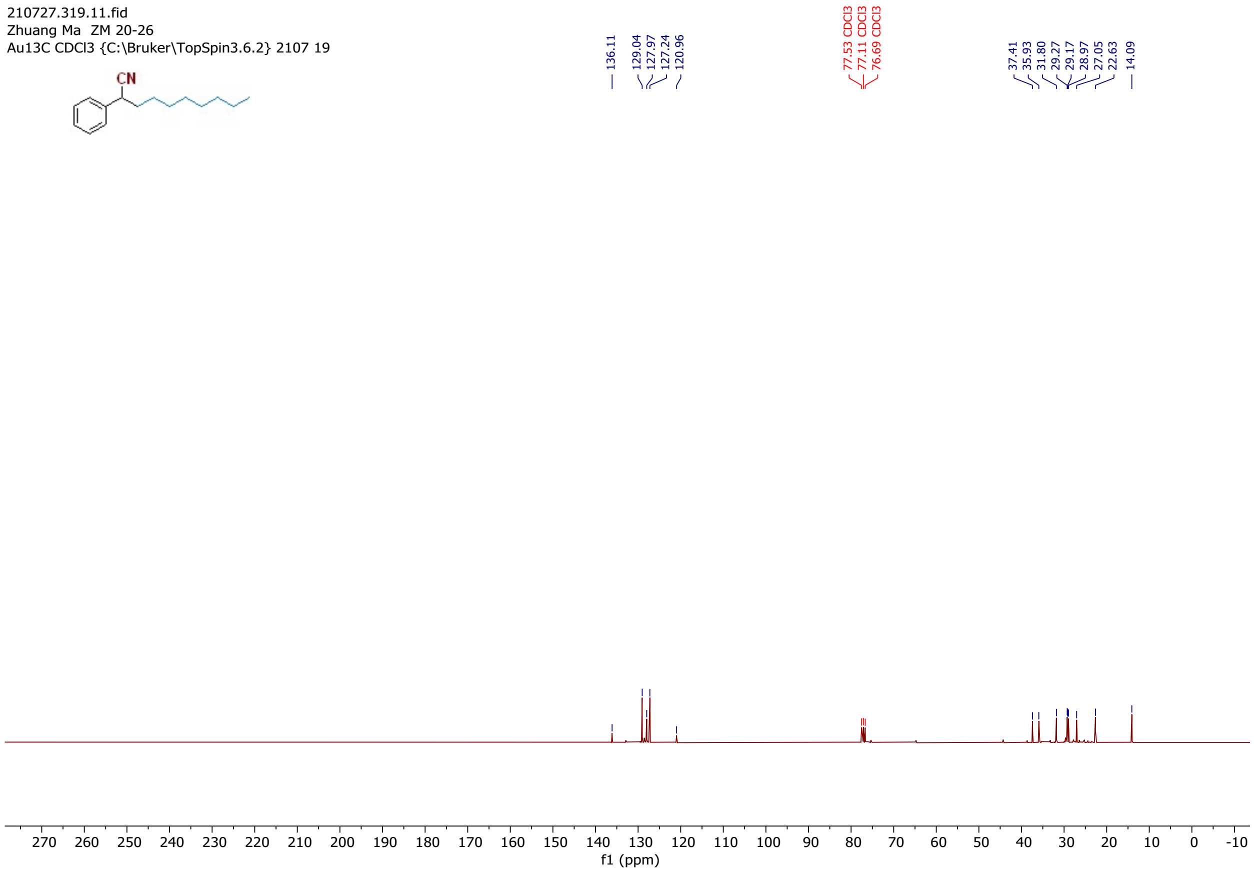

220131.308.10.fid
Ma/ ZM-20-45
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 8
CN
9.51
7.26 CDCl3
EtOAC
5.03
1.00
1.98
2.05
6.15
3.09
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

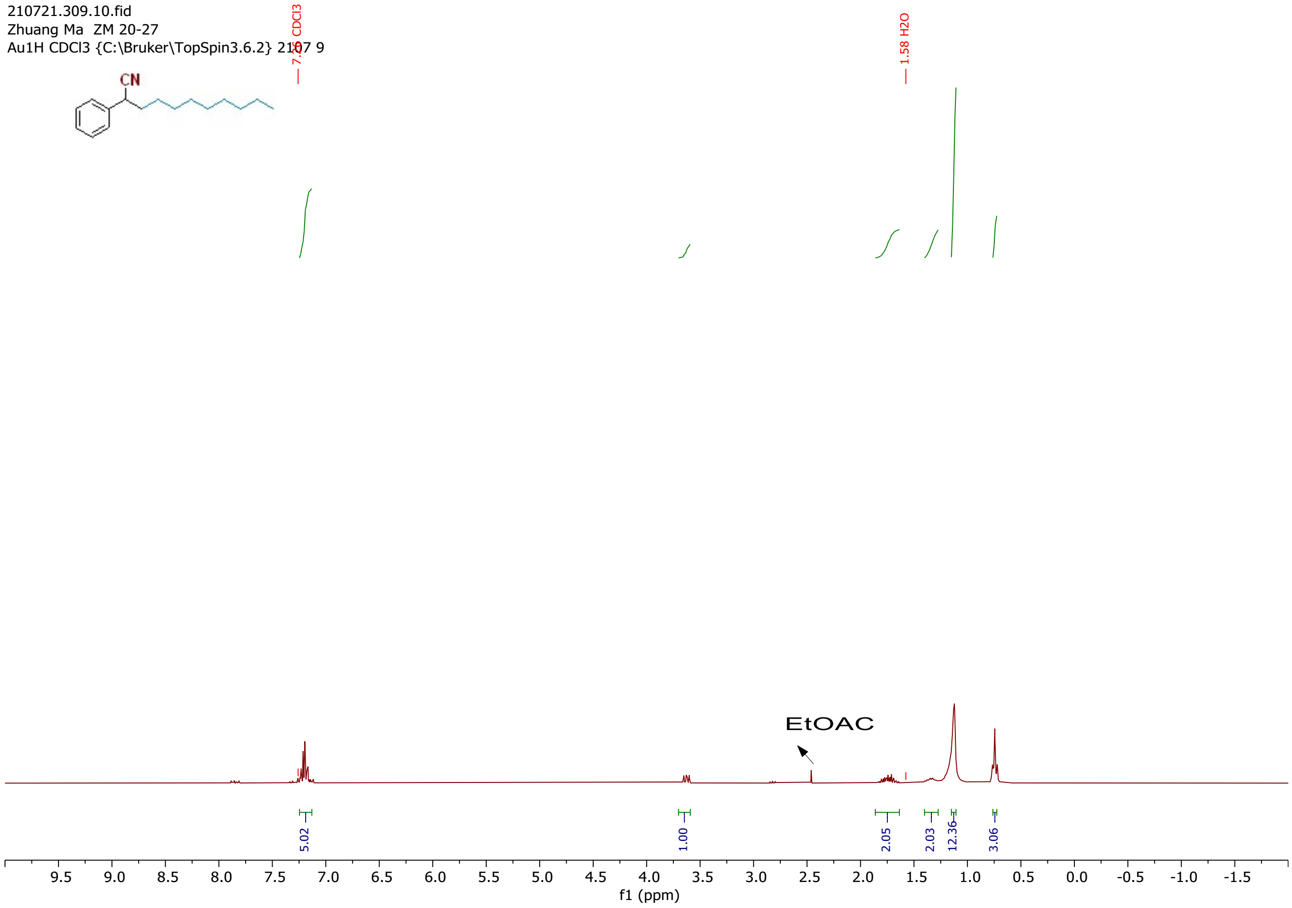

220131.308.11.fid
Ma/ ZM-20-45
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 8
CN
136.13
129.05
127.98
127.25
120.97
77.53 CDCl3
77.11 CDCl3
76.68 CDCl3
37.43
35.95
31.50
28.64
27.02
22.54
14.03
270
260
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

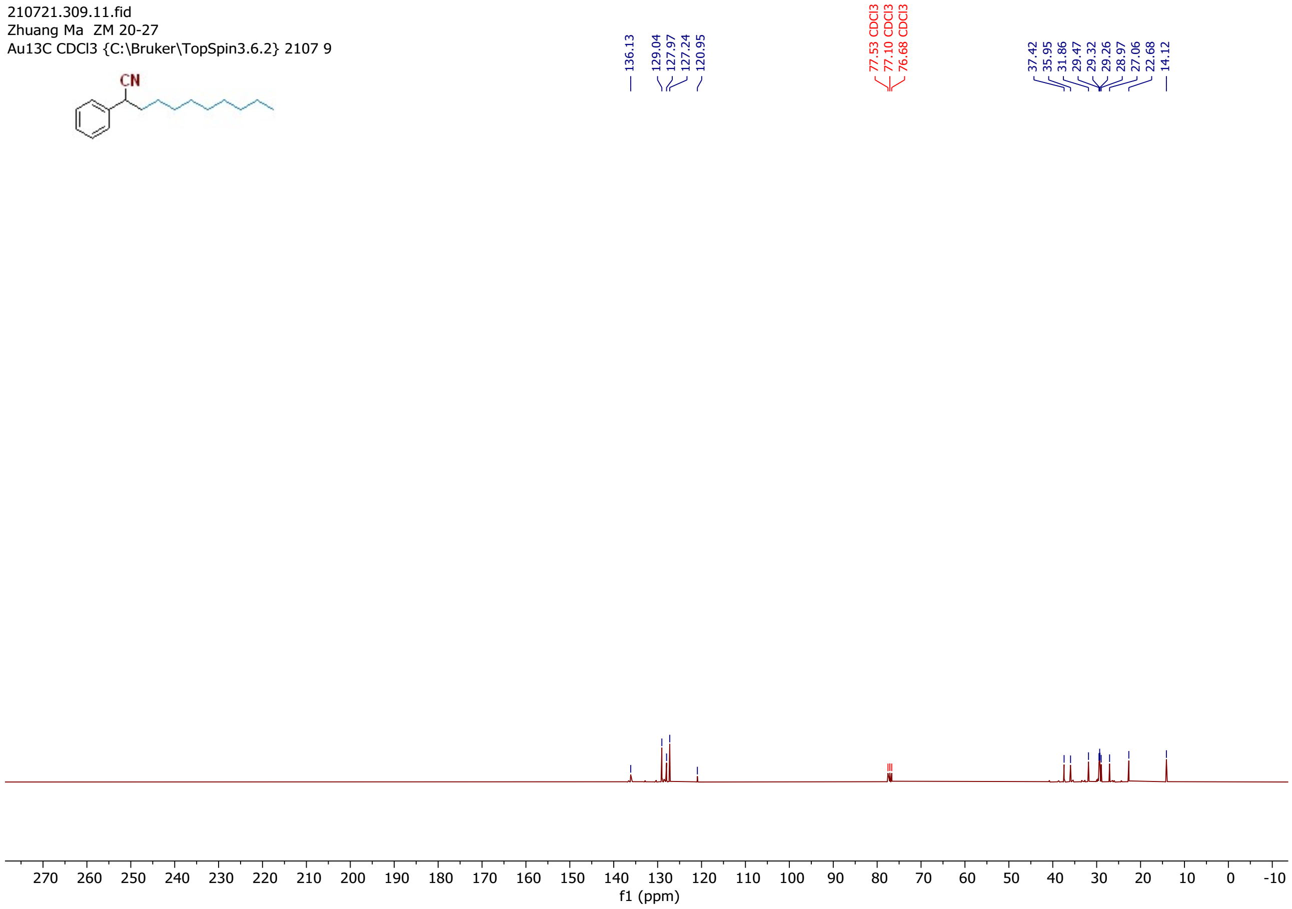

220304.f343.10.fid
Zhuang Ma ZM20-204
PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2203 43
CN
7.26 CDCl3
1.05
4.00
1.03
2.01
1.02
1.03
2.03
1.99
9.02
3.08
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


220304.f343.11.fid
Zhuang Ma ZM20-204
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2203 43
CN
132.85
129.05
128.56
128.05
127.23
77.47 CDCl3
77.04 CDCl3
76.62 CDCl3
51.04
36.52
33.69
31.09
30.07
30.00
29.04
22.53
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

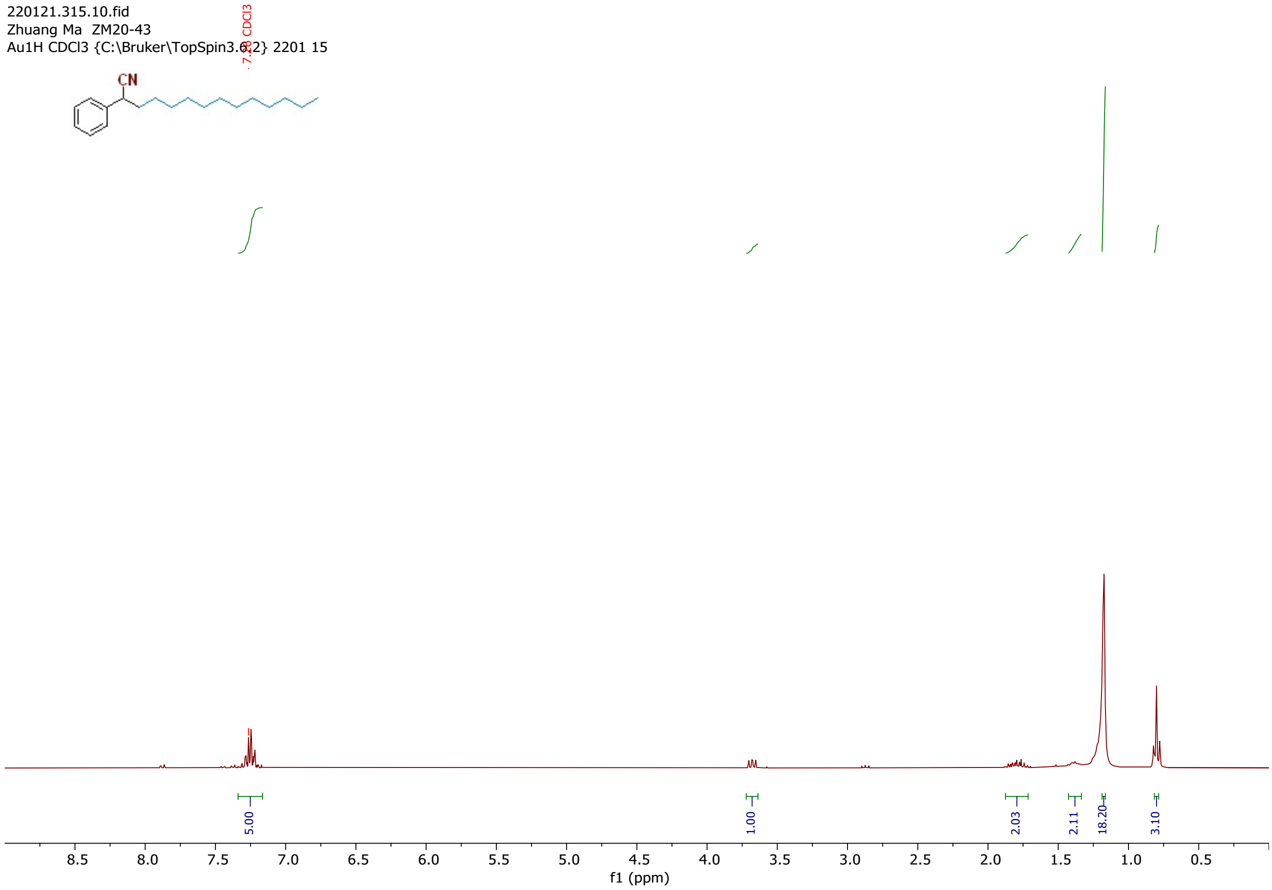

210727.319.10.fid
Zhuang Ma ZM 20-26
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2107 19
CN
7.26 CDCl3
5.08
1.00
2.02
2.02
12.07
3.17
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


210727.319.11.fid
Zhuang Ma ZM 20-26
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2107 19
CN
136.11
129.04
127.97
127.24
120.96
77.53 CDCl3
77.11 CDCl3
76.69 CDCl3
37.41
35.93
31.80
29.27
29.17
28.97
27.05
22.63
14.09
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

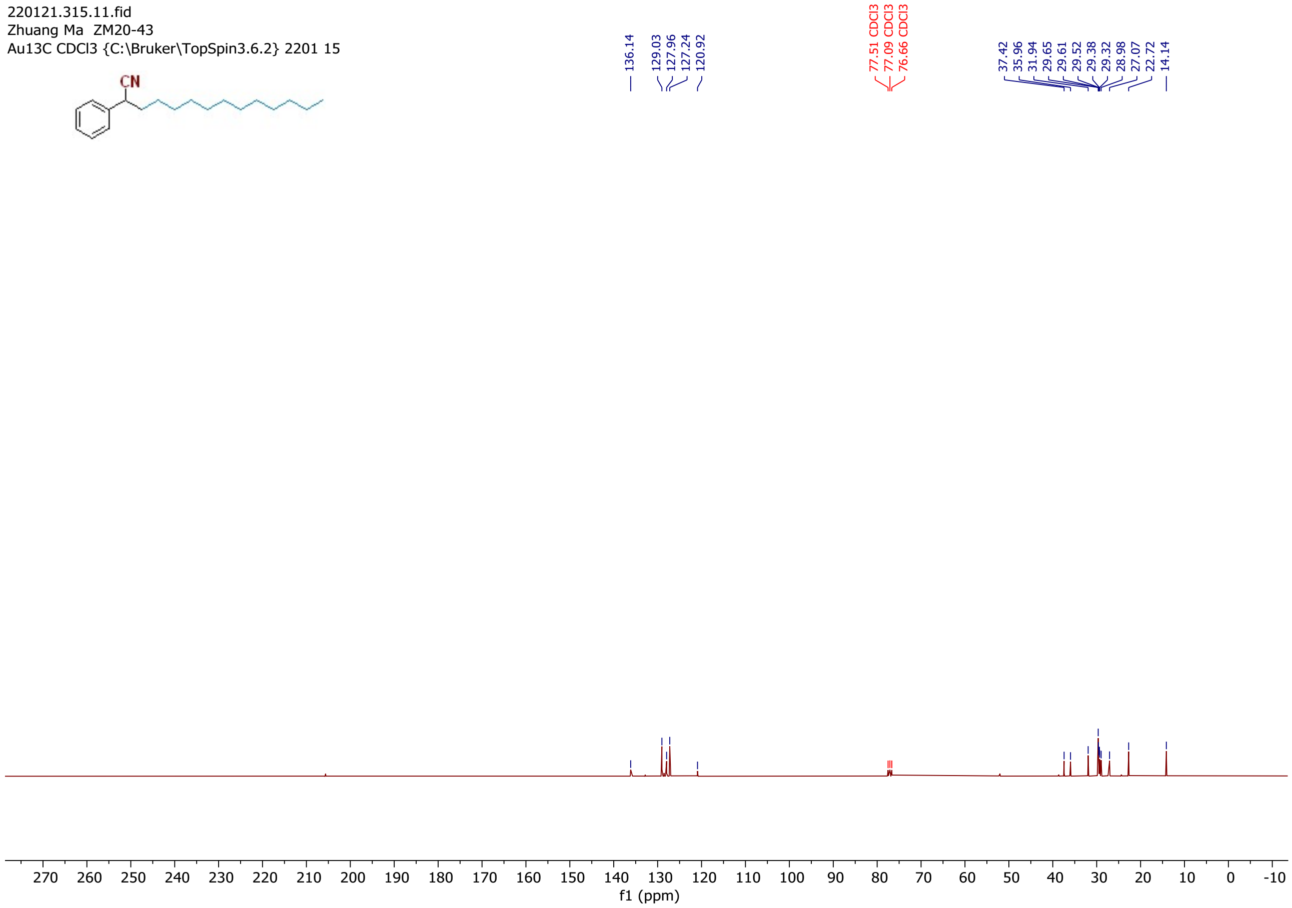

210721.309.10.fid
Zhuang Ma ZM 20-27
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2107 9
CN
7.26 CDCl3
1.58 H2O
EtOAC
5.02
1.00
2.05
2.03
12.36
3.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

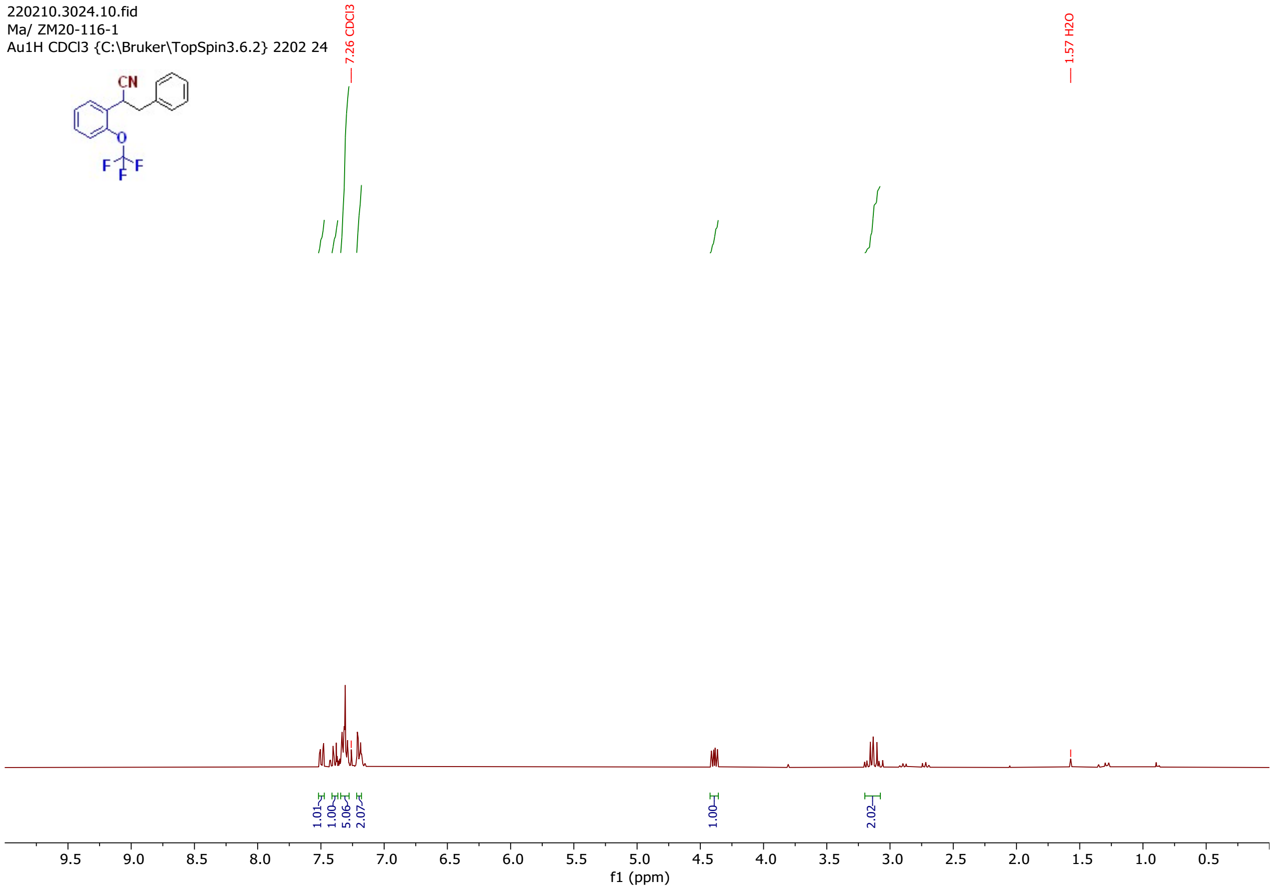

210721.309.11.fid
Zhuang Ma ZM 20-27
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2107 9
CN
136.13
129.04
127.97
127.24
120.95
77.53 CDCl3
77.10 CDCl3
76.68 CDCl3
37.42
35.95
31.86
29.47
29.32
29.26
28.97
27.06
22.68
14.12
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

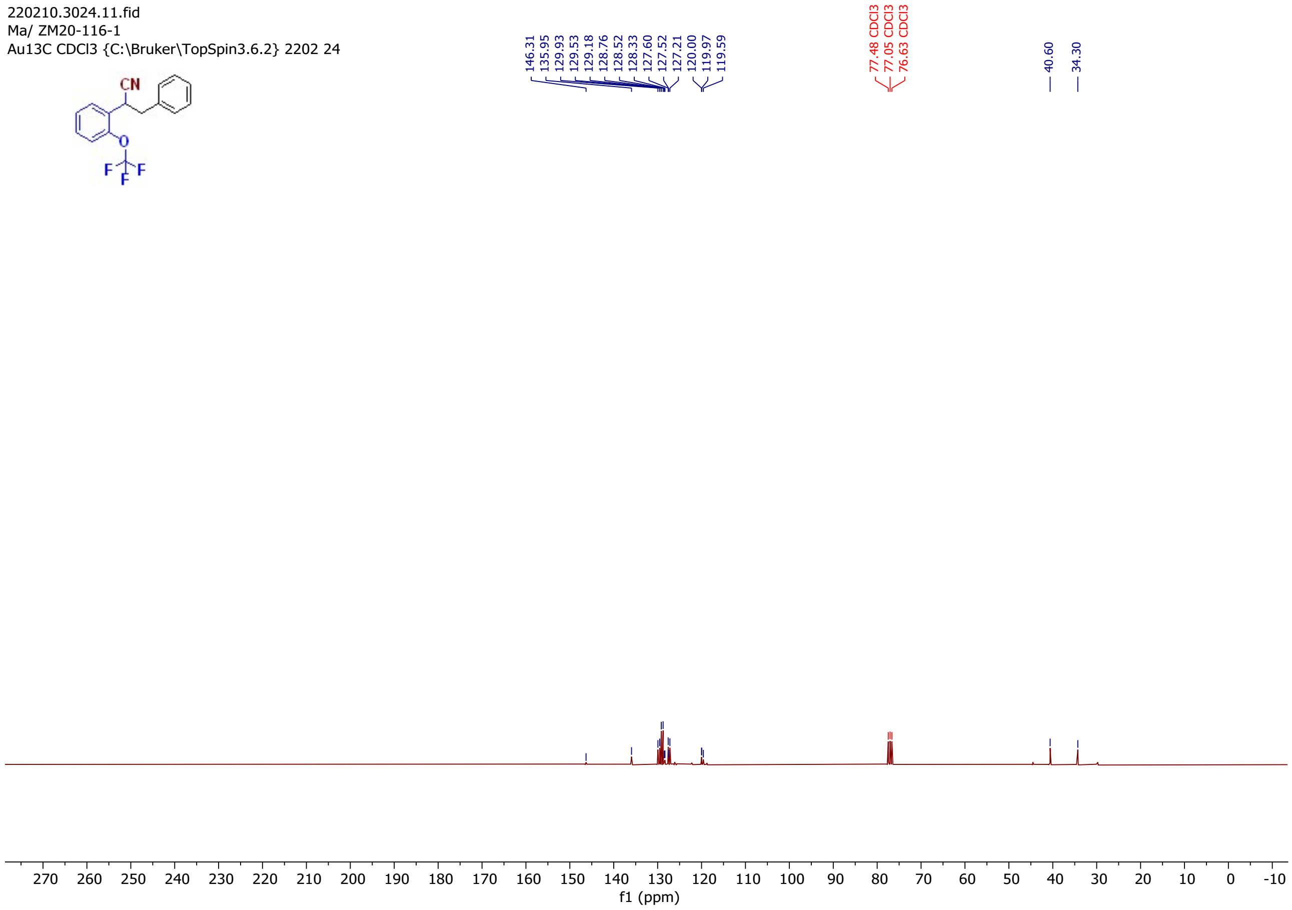
220121.315.10.fid
Zhuang Ma ZM20-43
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 15



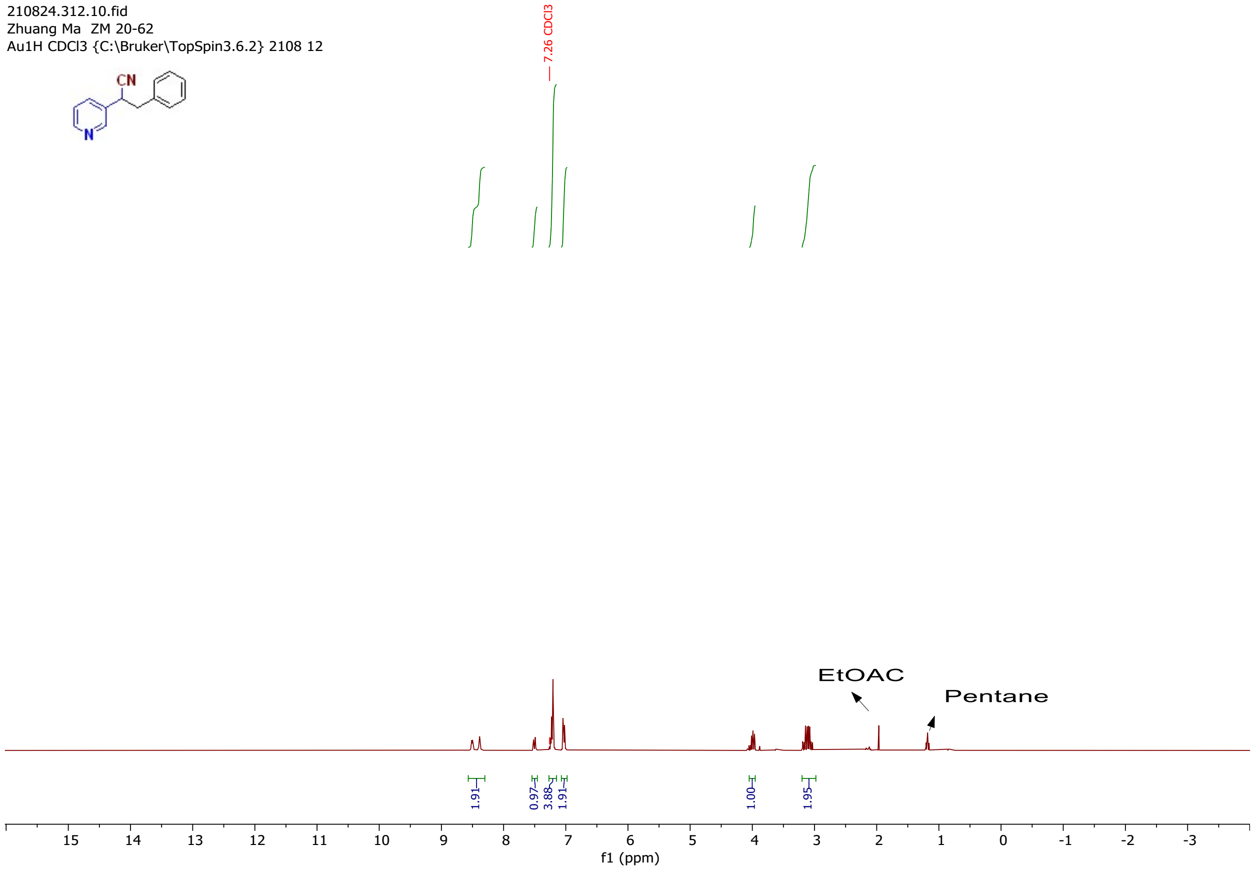
220121.315.11.fid
Zhuang Ma ZM20-43
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 15



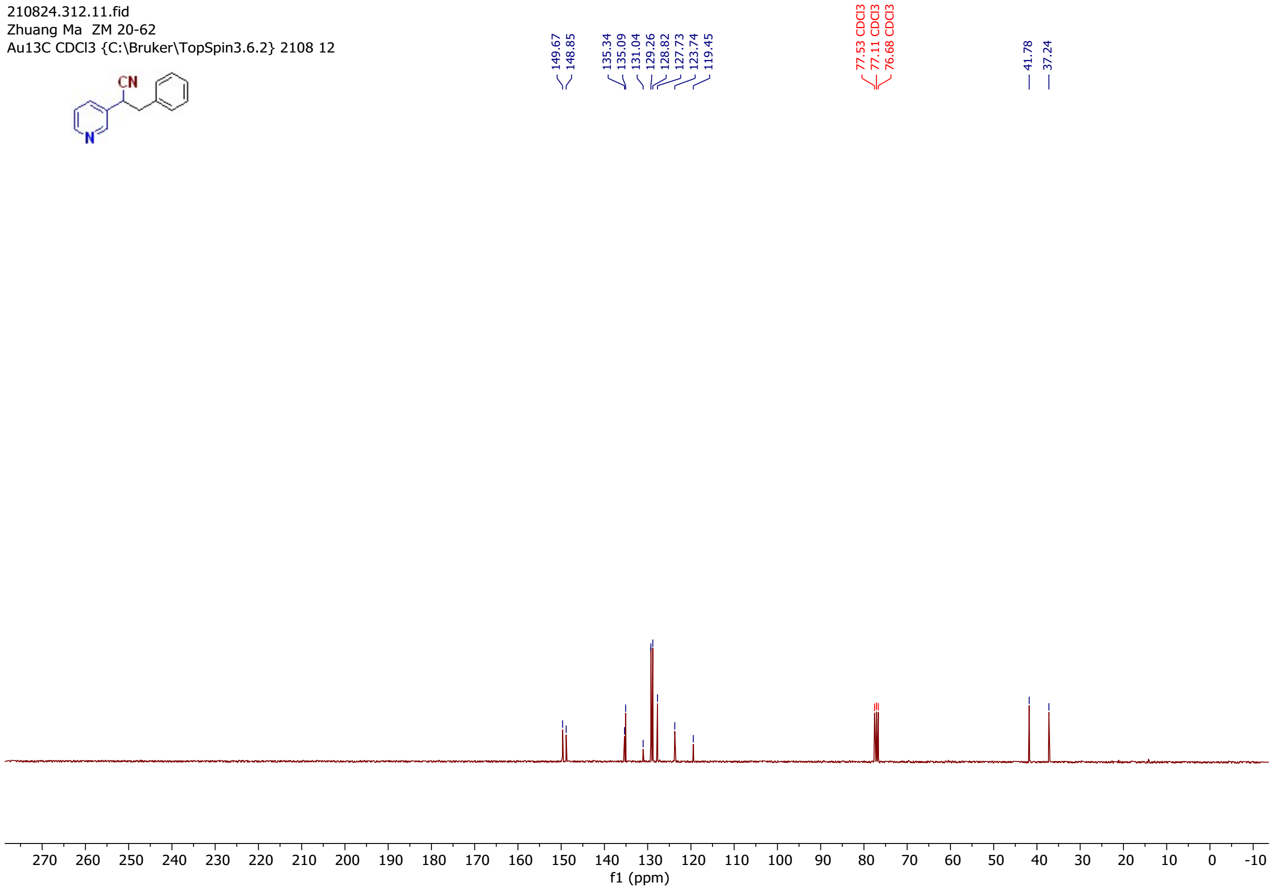

220210.3024.10.fid
Ma/ ZM20-116-1
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2202 24
CN
O
F
F
F
7.26 CDCl3
1.57 H2O
1.01
1.00
5.06
2.07
1.00
2.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

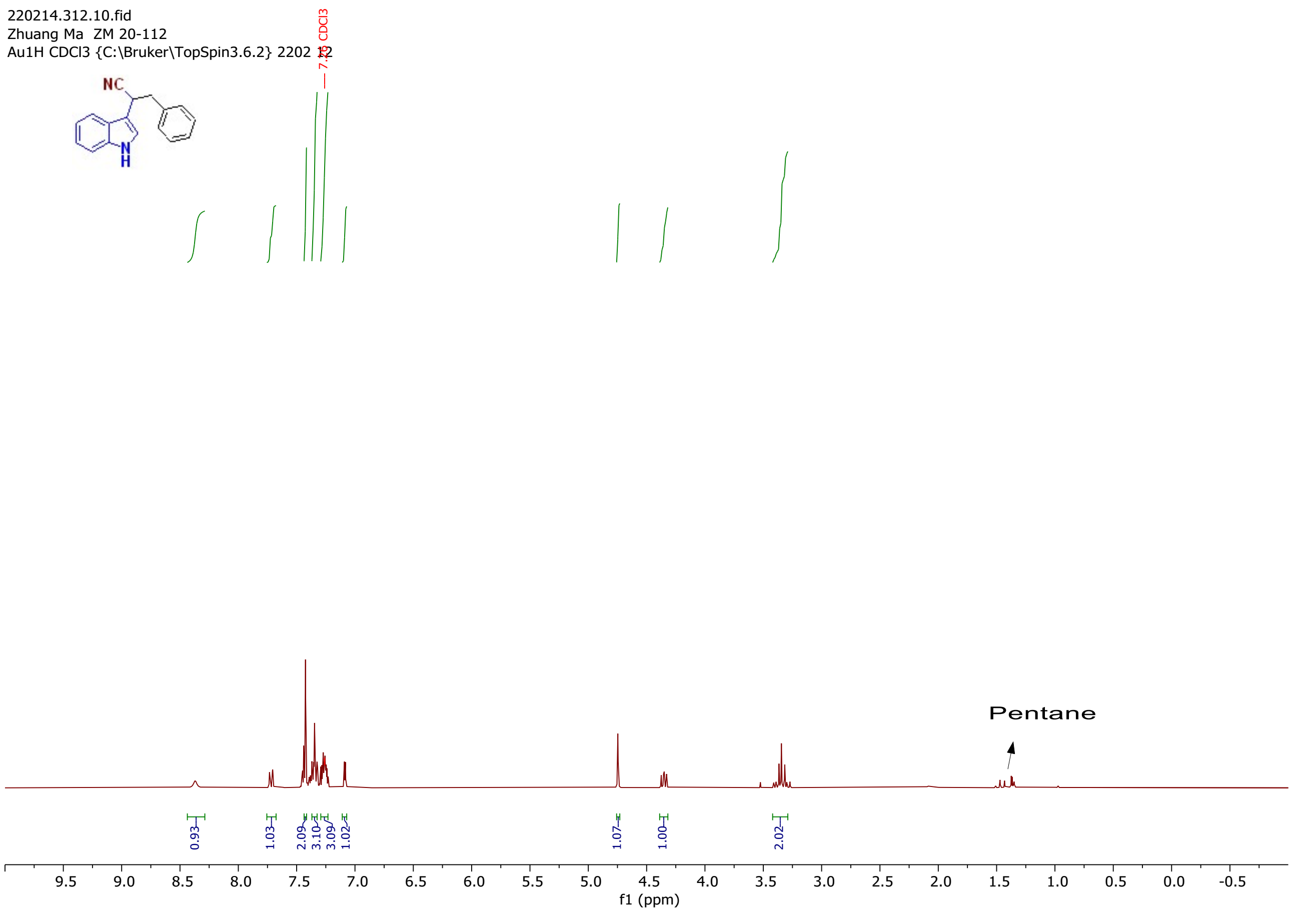

220210.3024.11.fid
Ma/ ZM20-116-1
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2202 24
CN
O
F
F
F
146.31
135.95
129.93
129.53
129.18
128.76
128.52
128.33
127.60
127.52
127.21
120.00
119.97
119.59
77.48 CDCl3
77.05 CDCl3
76.63 CDCl3
40.60
34.30
270
260
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

210824.312.10.fid
Zhuang Ma ZM 20-62
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 12

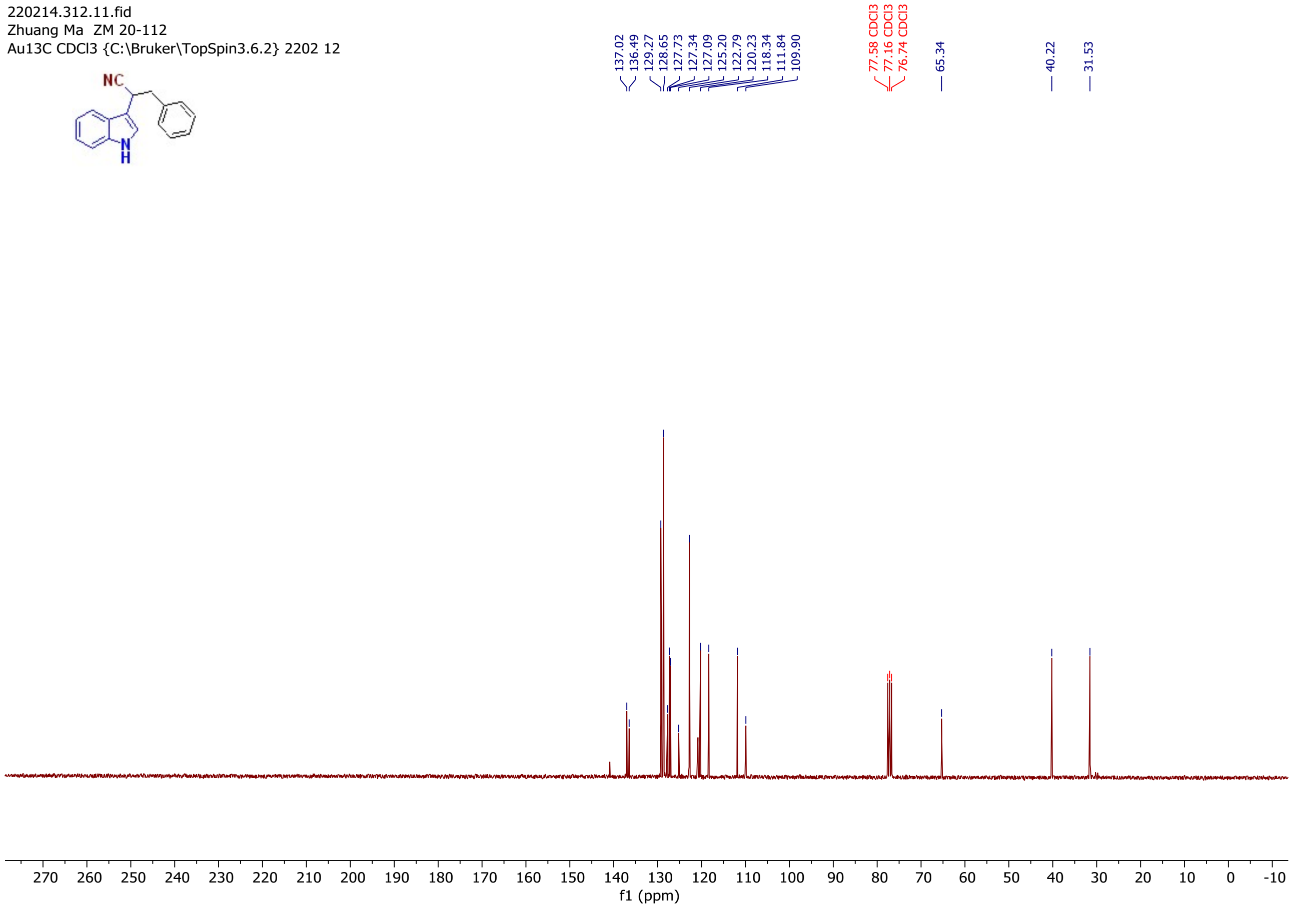


210824.312.11.fid
Zhuang Ma ZM 20-62
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 12

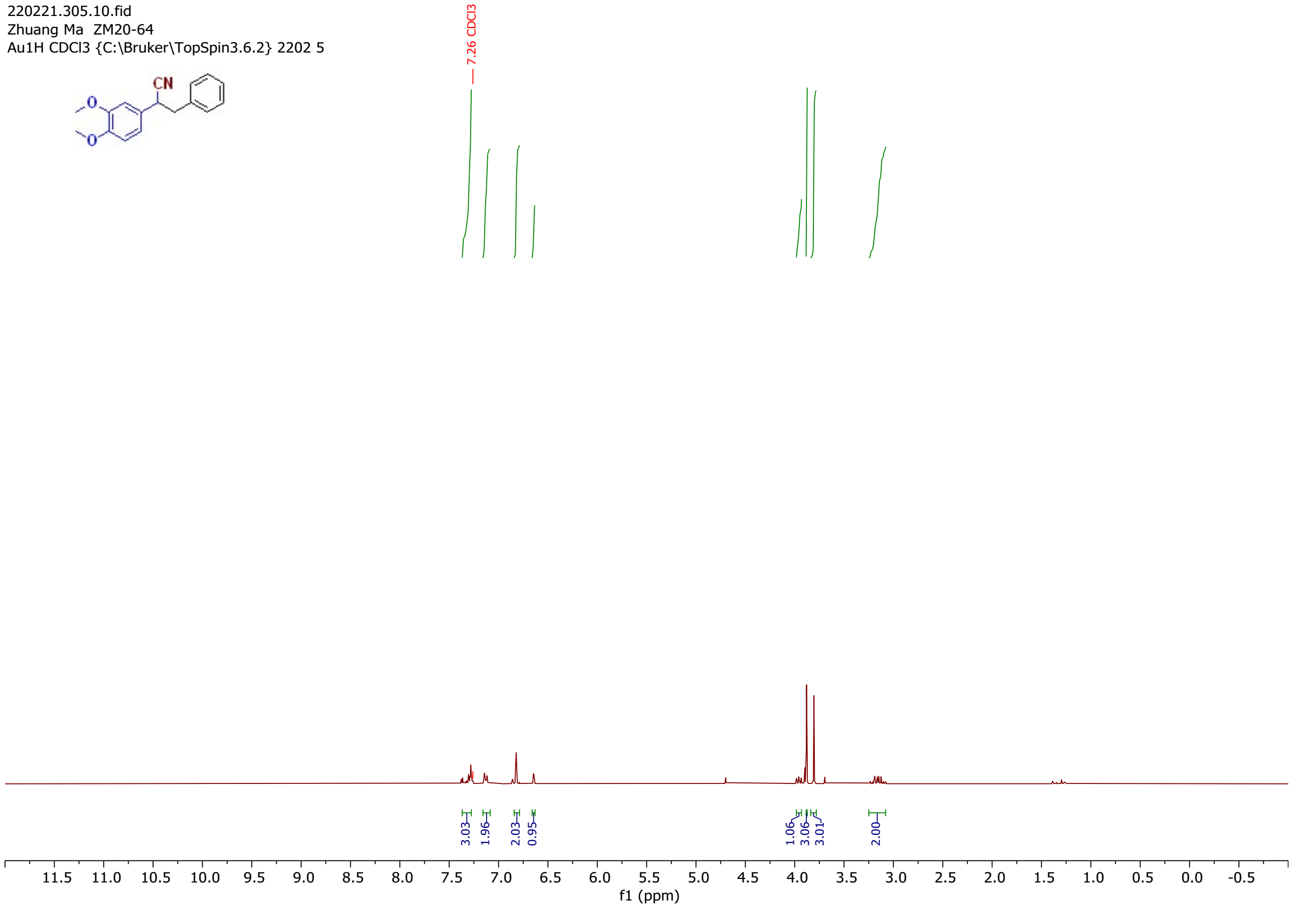


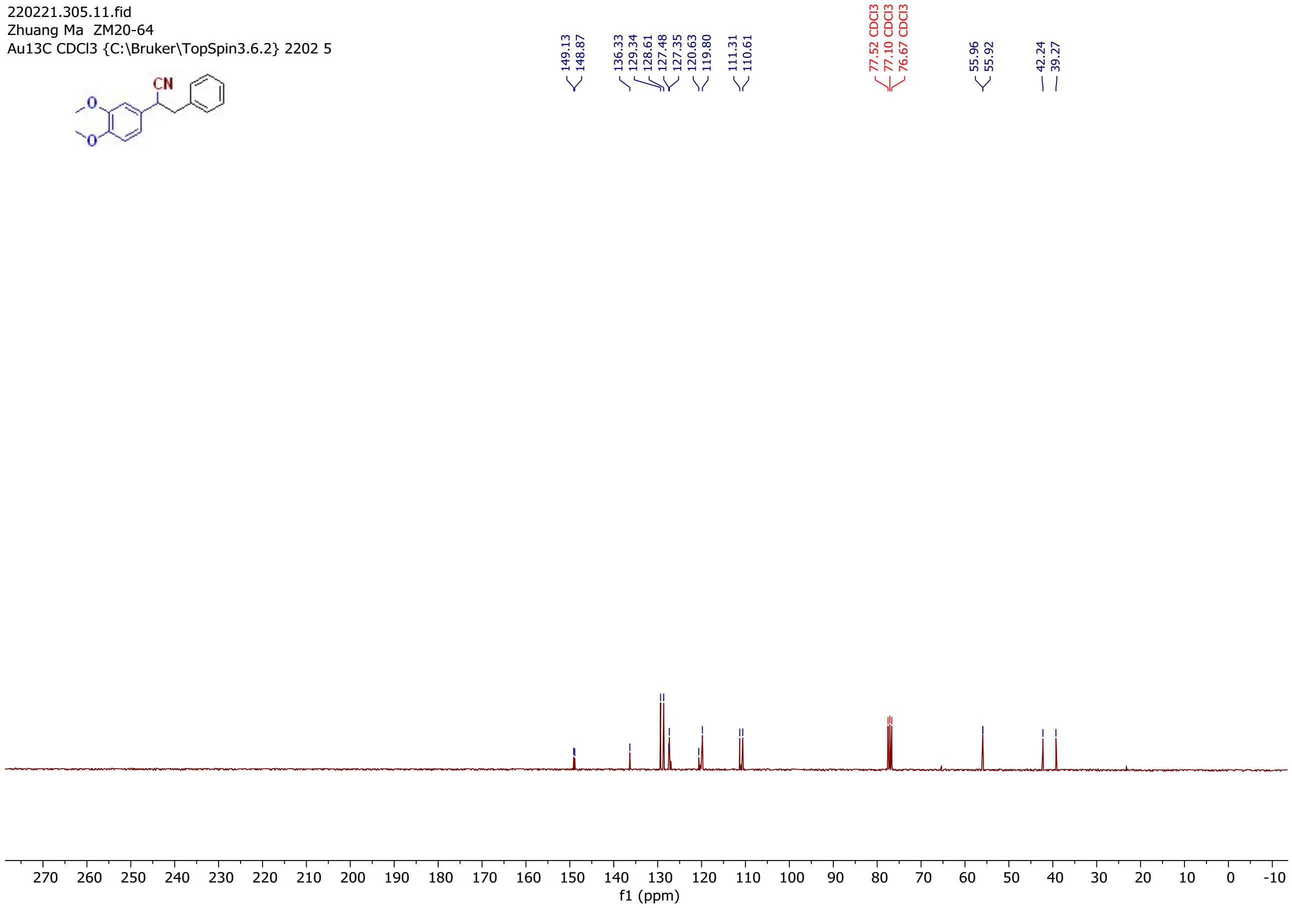


220214.312.10.fid
Zhuang Ma ZM 20-112
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2202 12

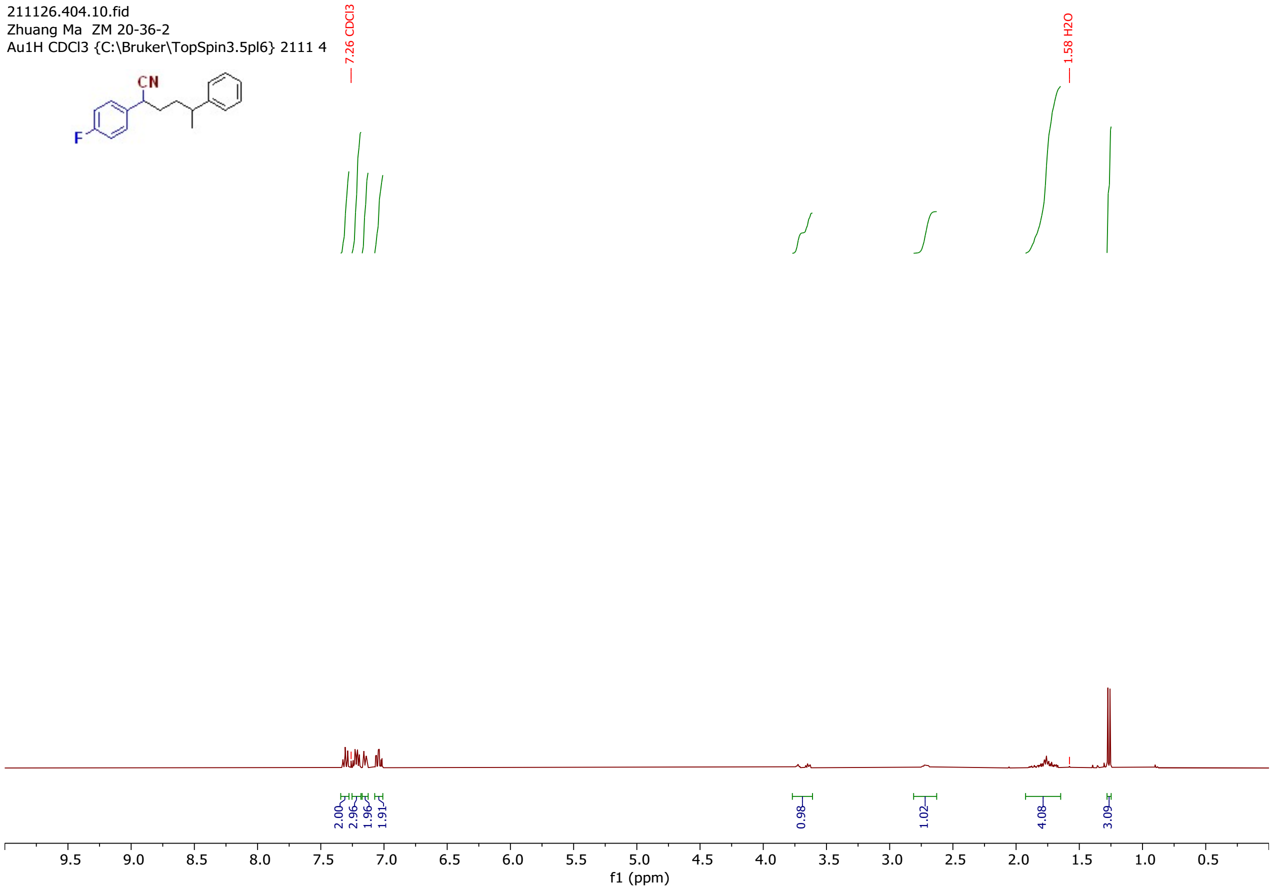


220214.312.11.fid
Zhuang Ma ZM 20-112
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2202 12

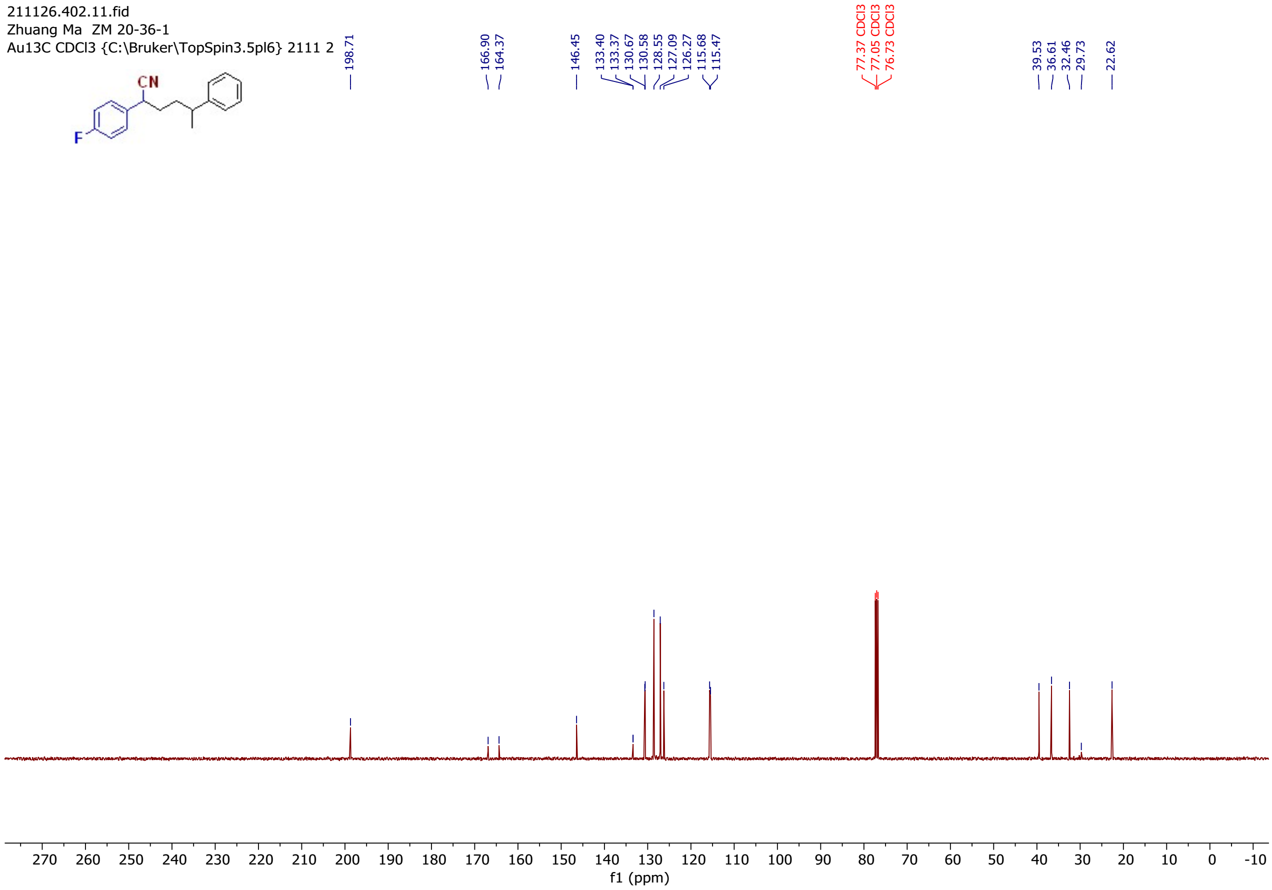

220221.305.10.fid
Zhuang Ma ZM20-64
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2202 5
CN
O
O
7.26 CDCl3
3.03
1.96
2.03
0.95
1.06
3.06
3.01
2.00
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

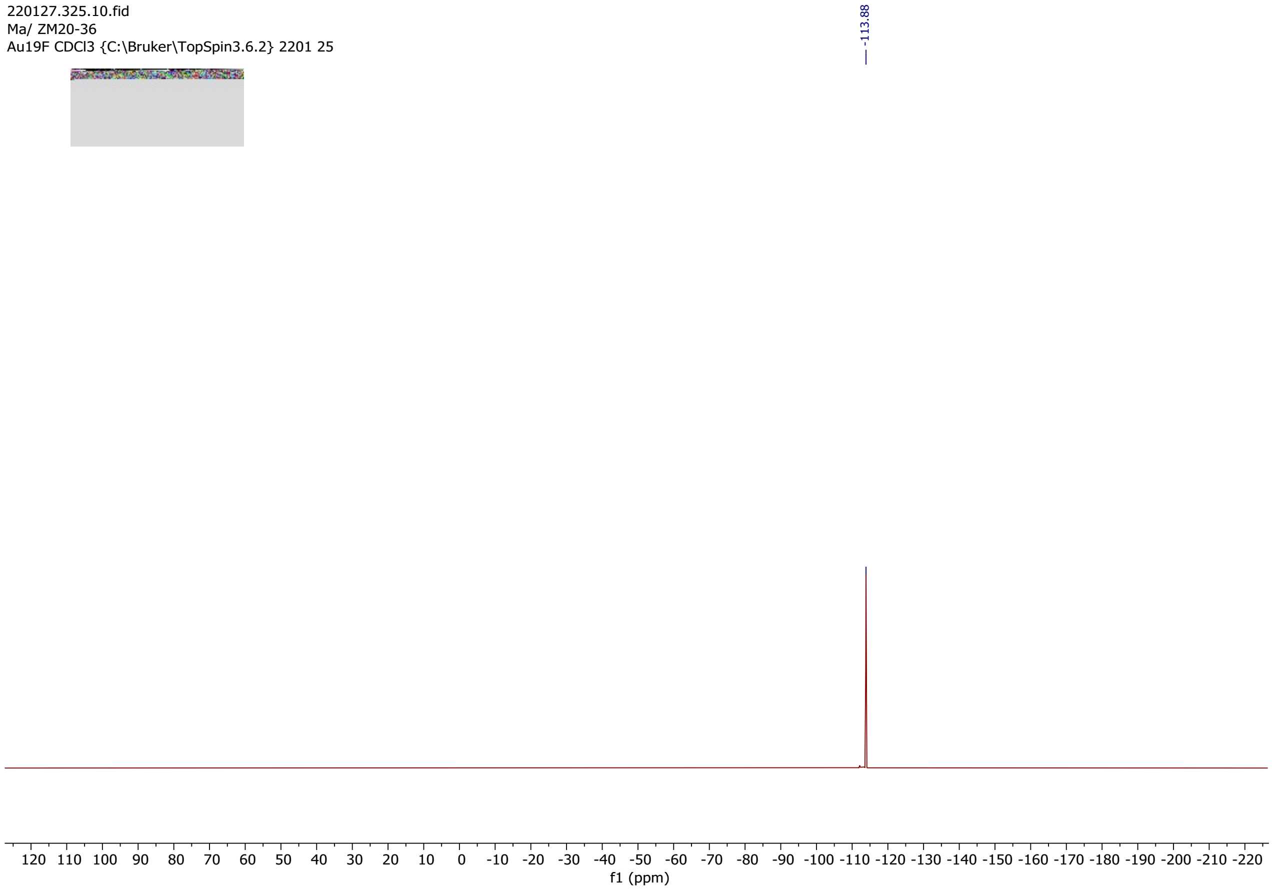

220221.305.11.fid
Zhuang Ma ZM20-64
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2202 5
CN
O
O
149.13
148.87
136.33
129.34
128.61
127.48
127.35
120.63
119.80
111.31
110.61
77.52 CDCl3
77.10 CDCl3
76.67 CDCl3
55.96
55.92
42.24
39.27
270
260
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

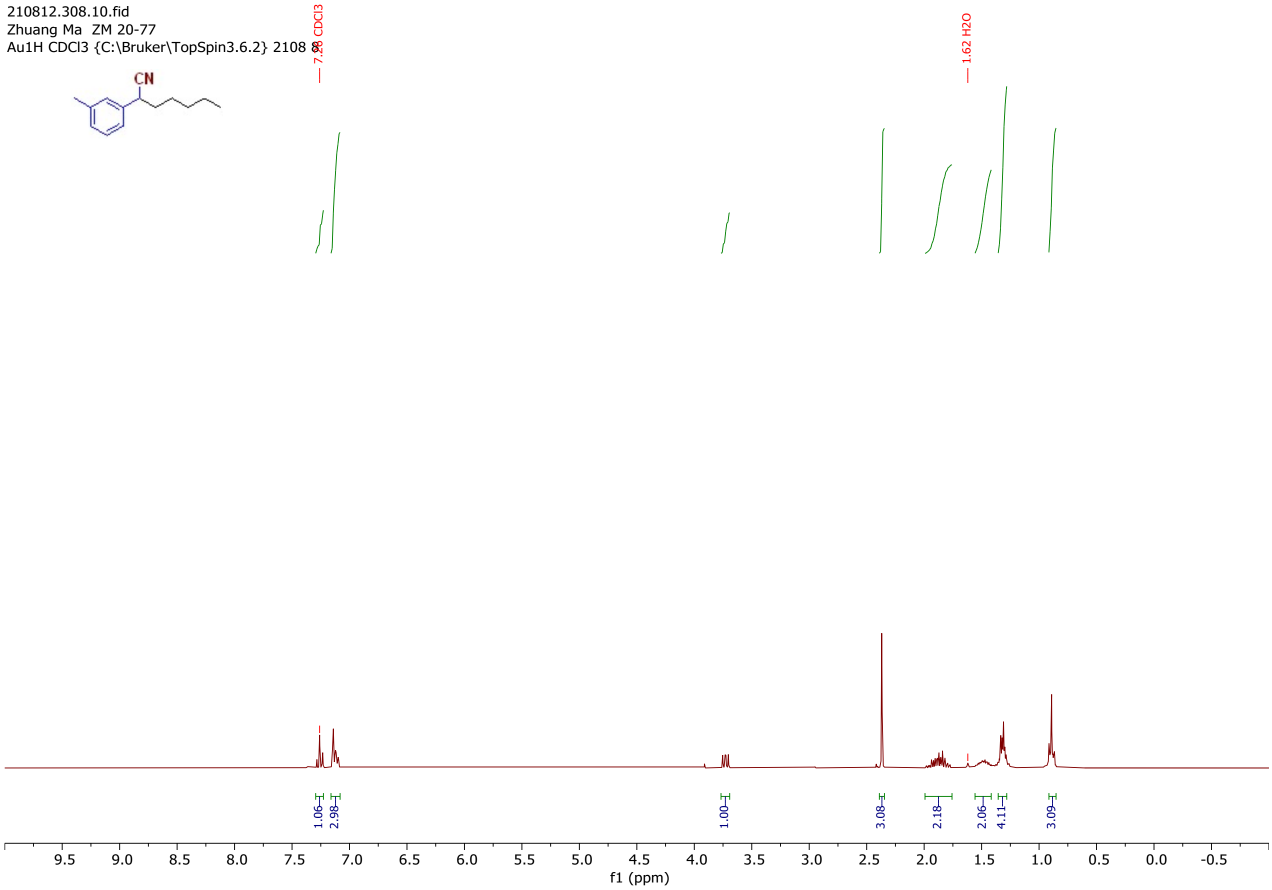
211126.404.10.fid
Zhuang Ma ZM 20-36-2
Au1H CDCl3 {C:\Bruker\TopSpin3.5pl6} 2111 4

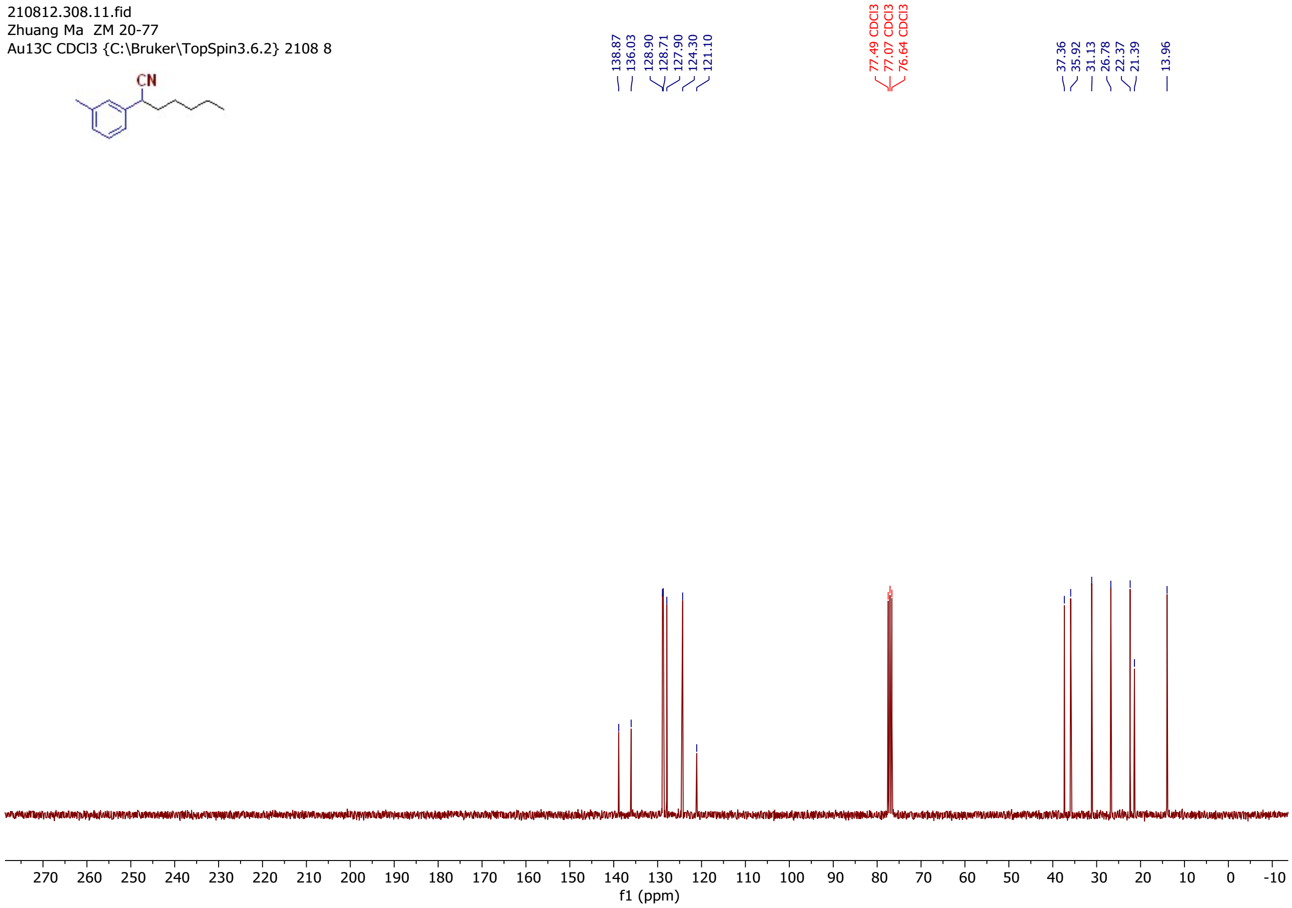


211126.402.11.fid
Zhuang Ma ZM 20-36-1
Au13C CDCl3 {C:\Bruker\TopSpin3.5pl6} 2111 2

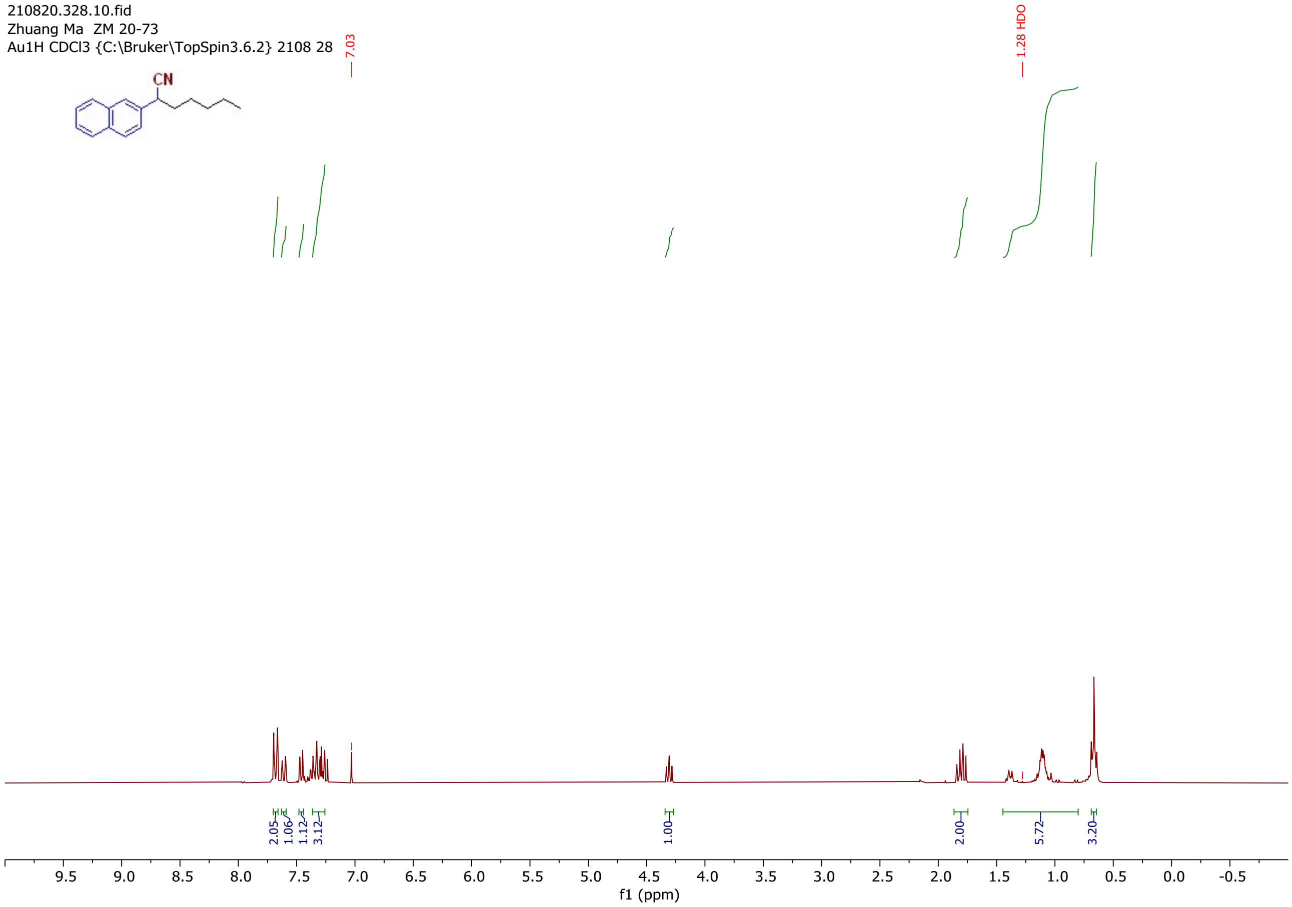



220127.325.10.fid
Ma/ ZM20-36
Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 25
-113.88
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

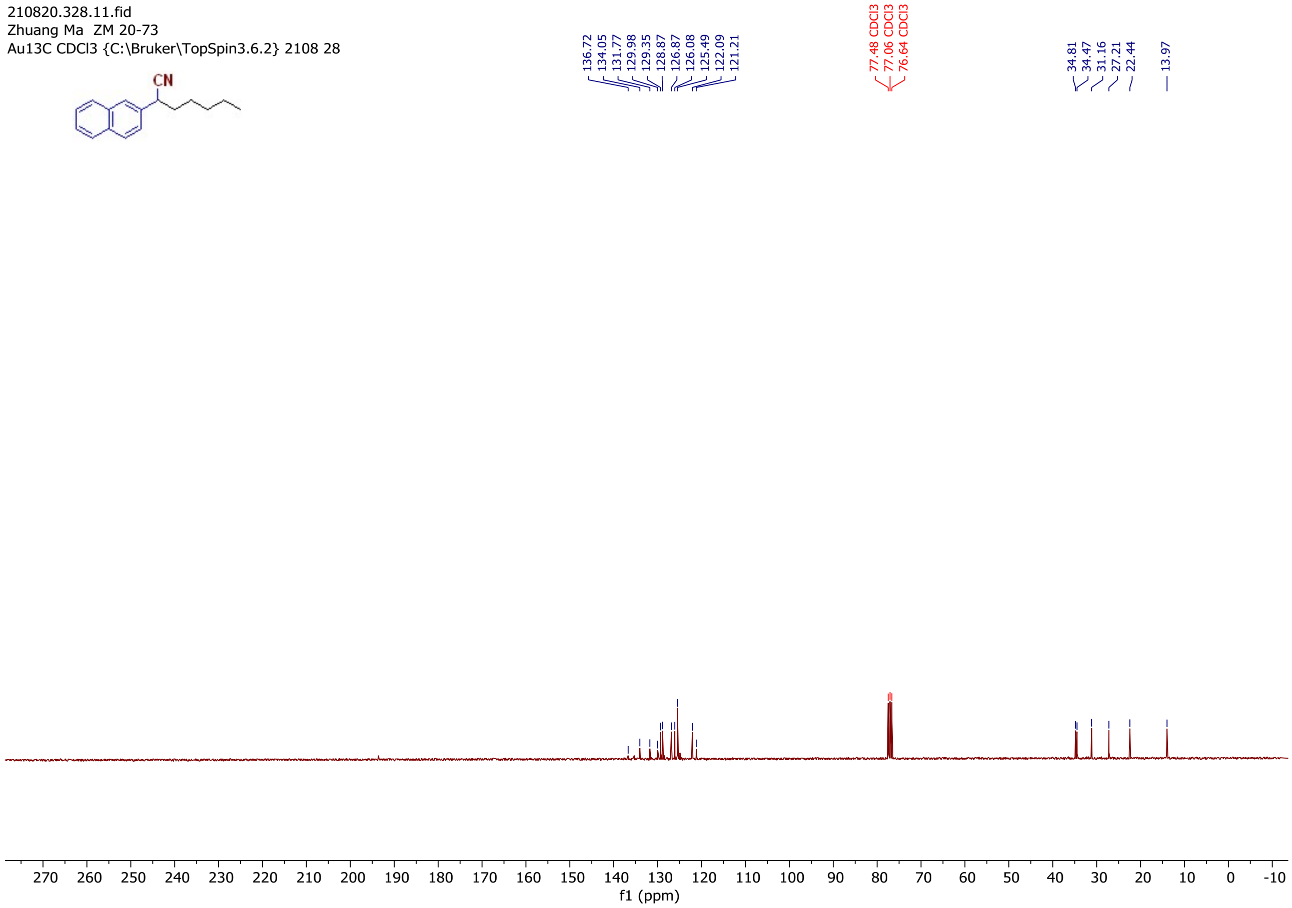

210812.308.10.fid
Zhuang Ma ZM 20-77
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 8
CN
7.26 CDCl3
1.62 H2O
1.06
2.98
1.00
3.08
2.18
2.06
4.11
3.09
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

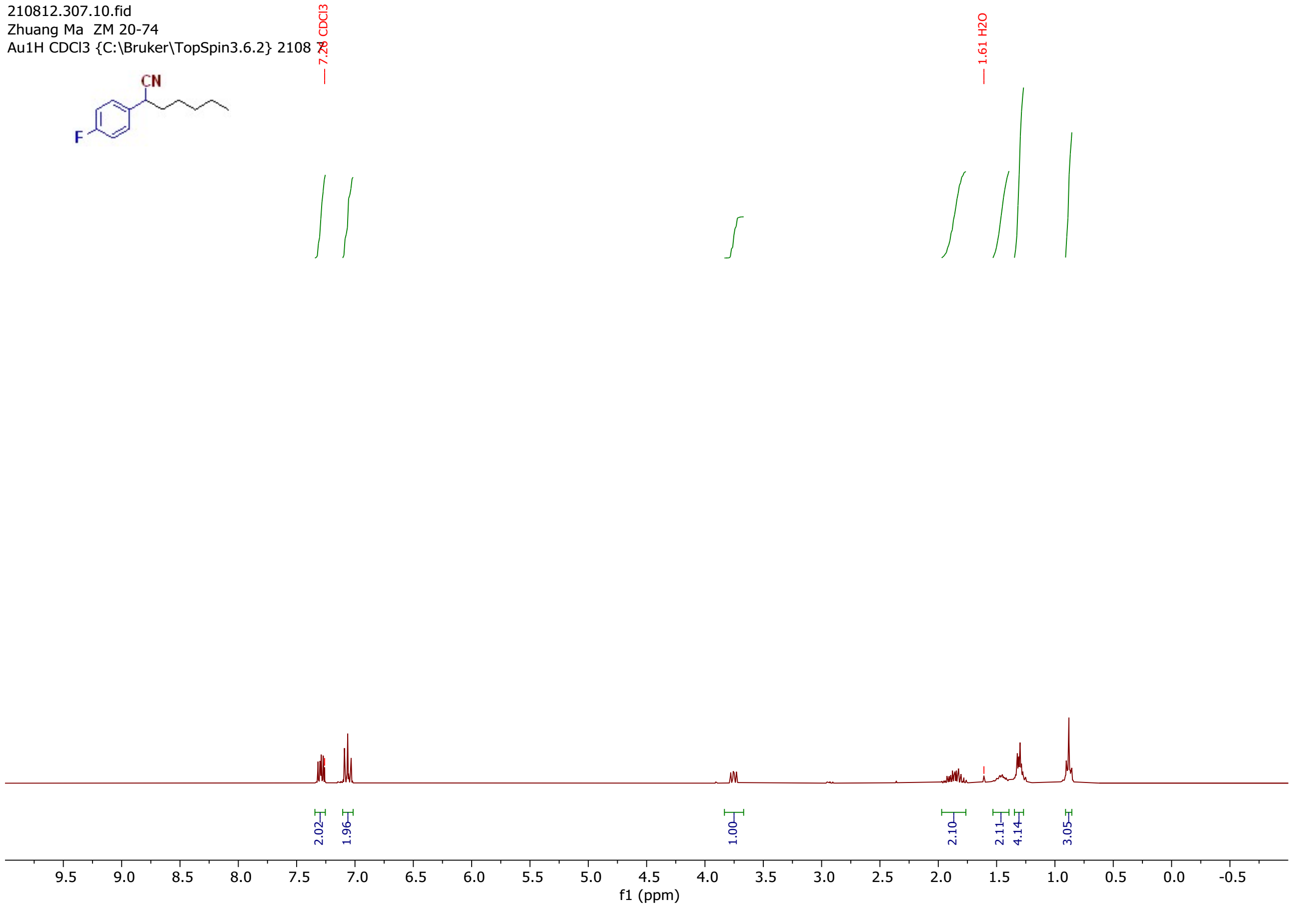

210812.308.11.fid
Zhuang Ma ZM 20-77
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 8
CN
138.87
136.03
128.90
128.71
127.90
124.30
121.10
77.49 CDCl3
77.07 CDCl3
76.64 CDCl3
37.36
35.92
31.13
26.78
22.37
21.39
13.96
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

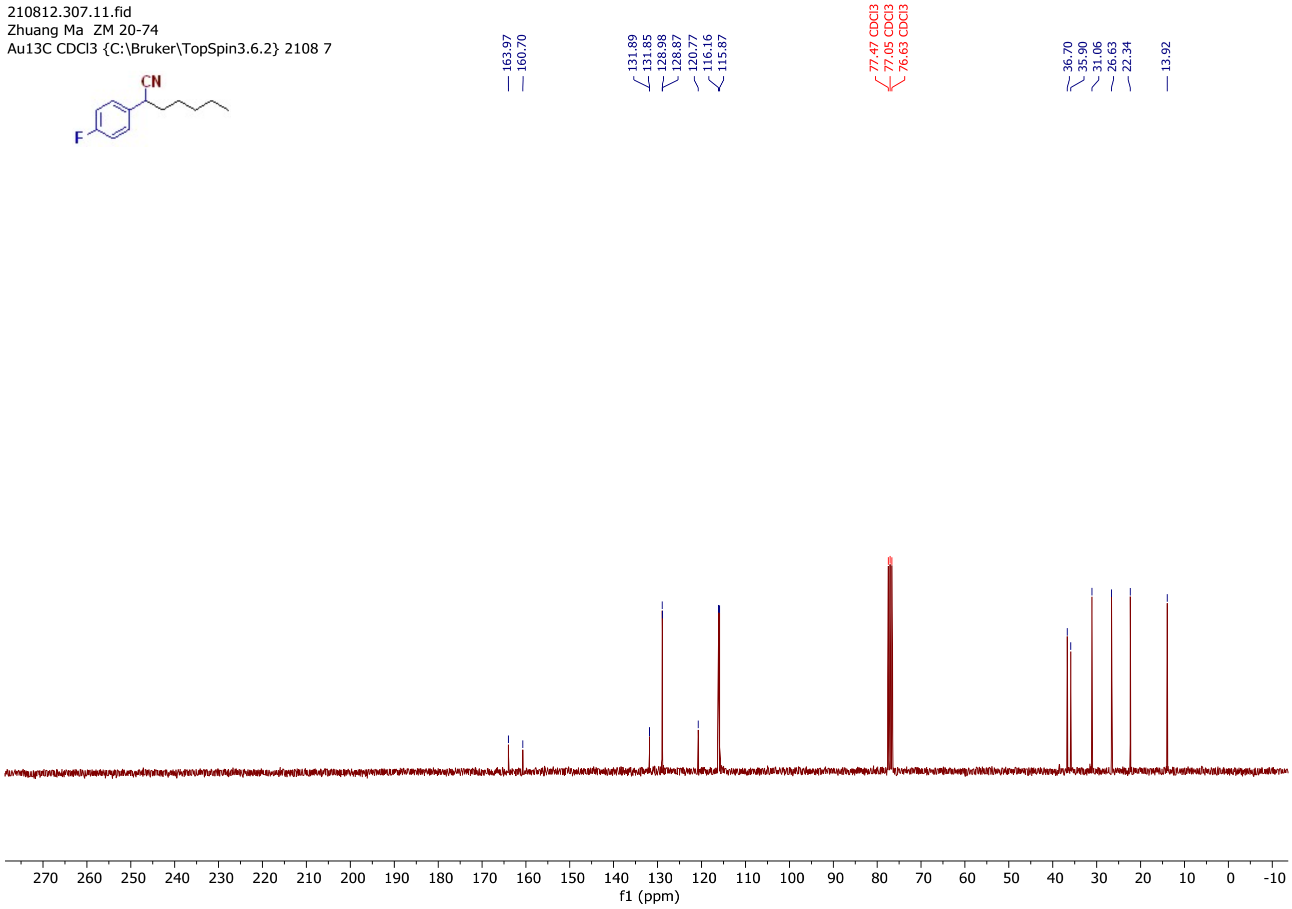
210820.328.10.fid
Zhuang Ma ZM 20-73
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 28

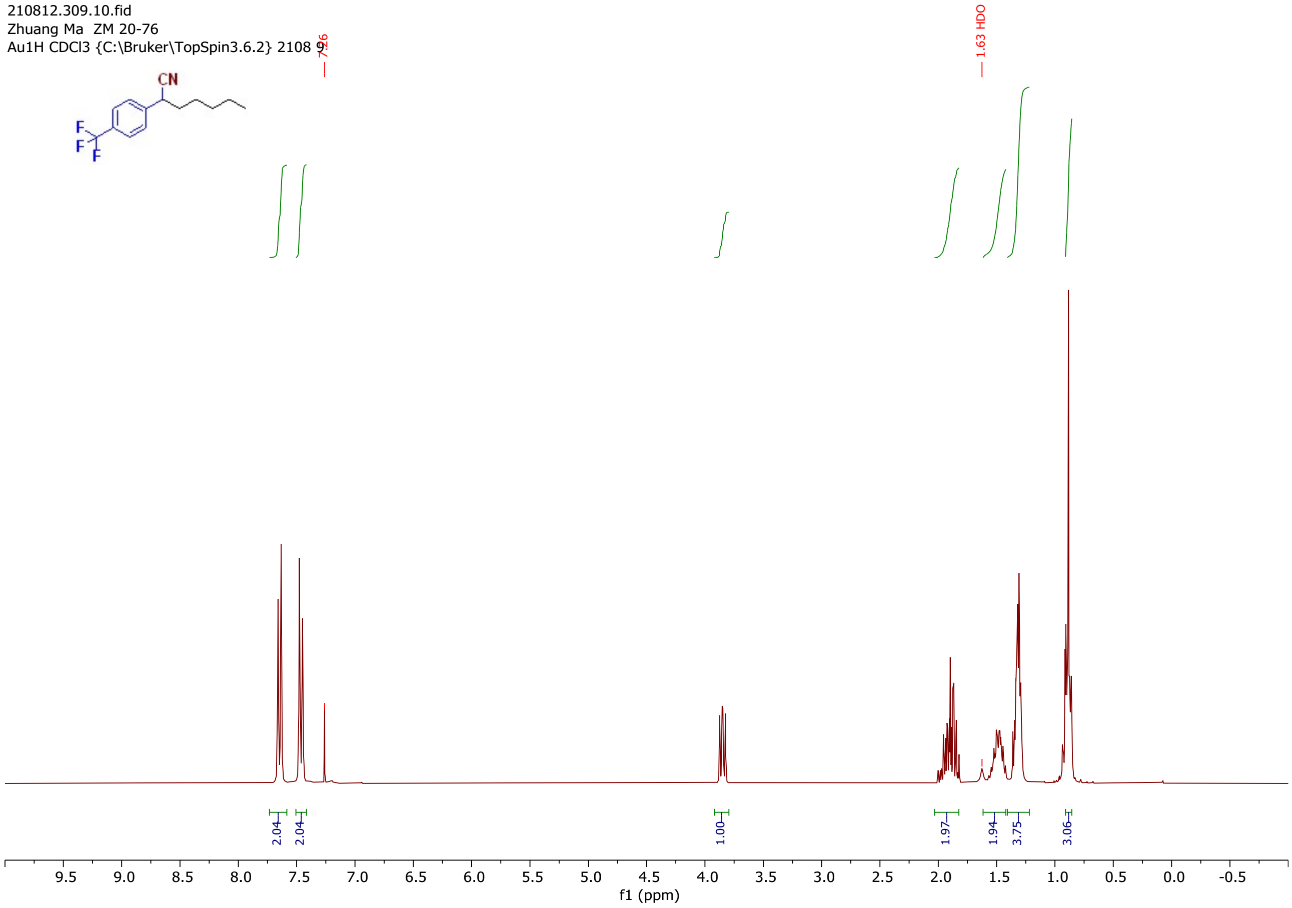


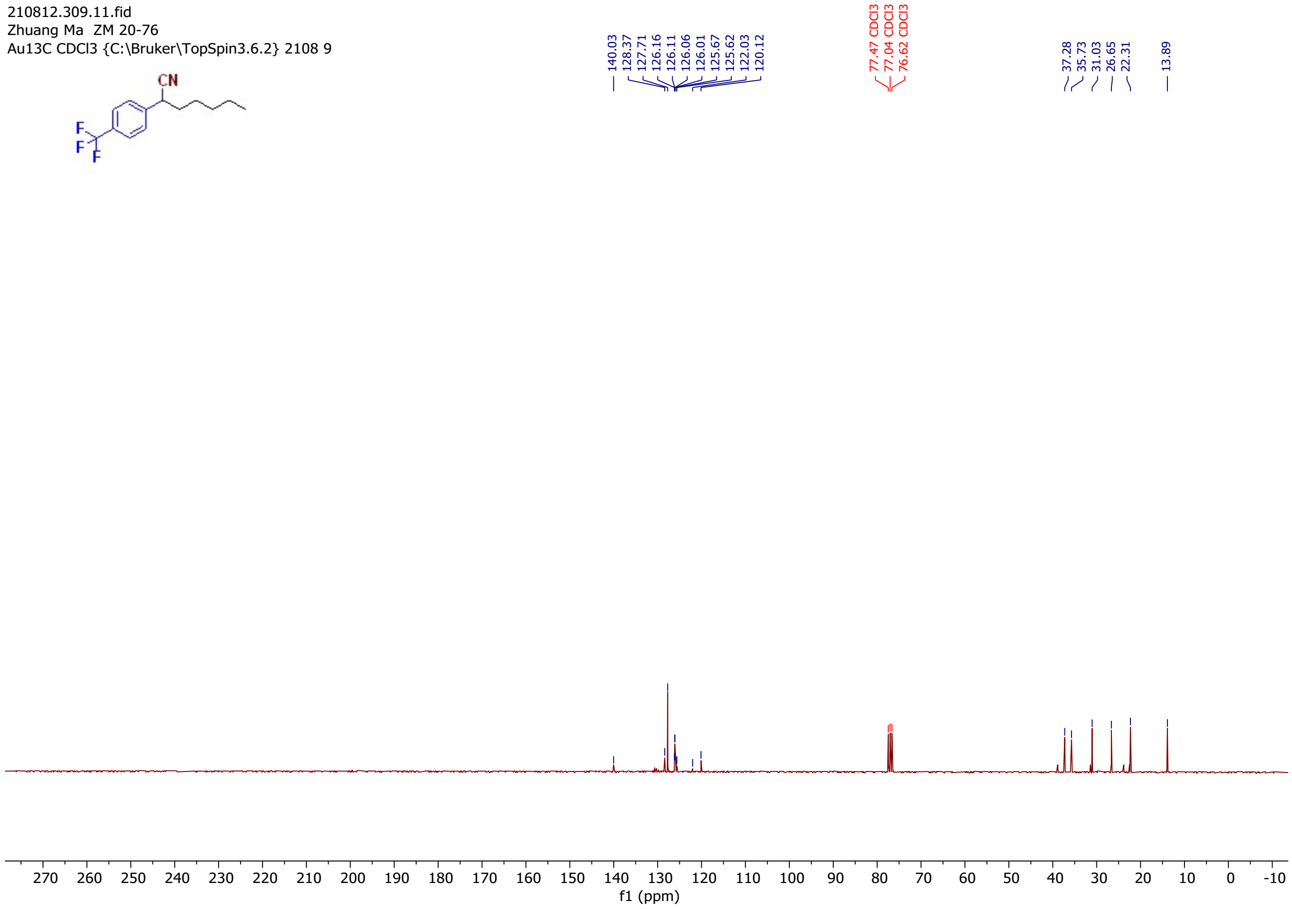
210820.328.11.fid
Zhuang Ma ZM 20-73
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 28

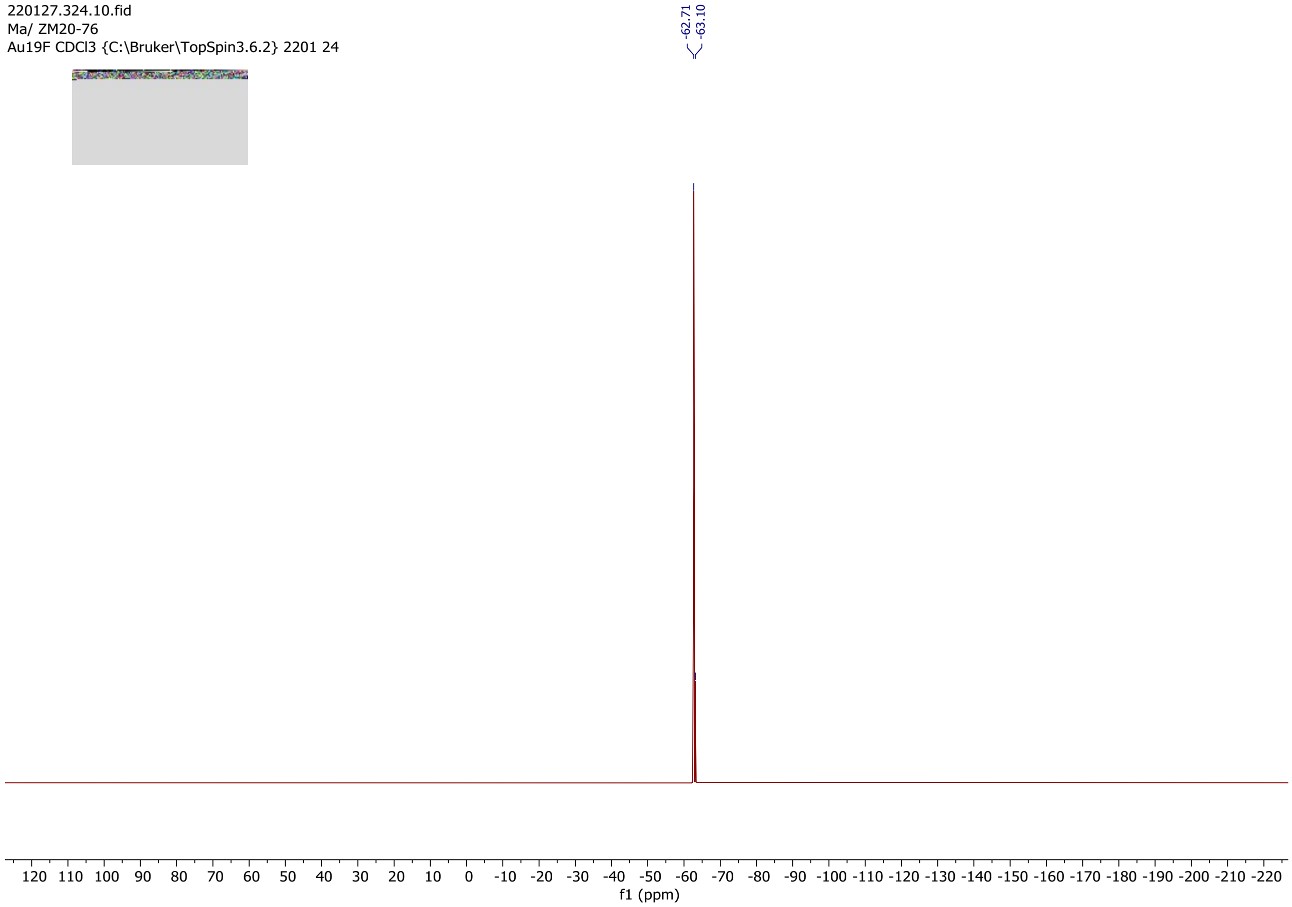


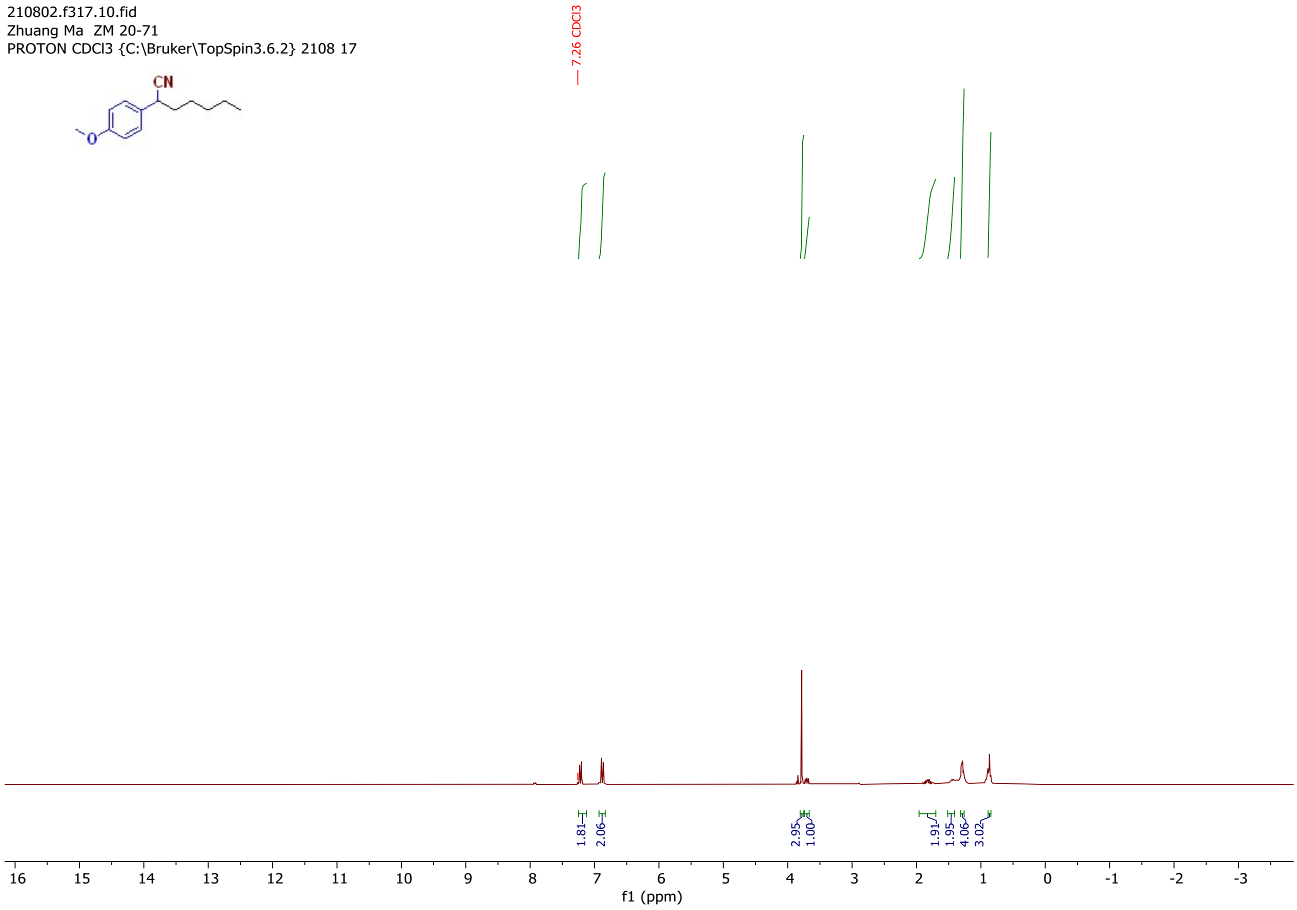

210812.307.10.fid
Zhuang Ma ZM 20-74
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 7
CN
F
7.26 CDCl3
1.61 H2O
2.02
1.96
1.00
2.10
2.11
4.14
3.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


210812.307.11.fid
Zhuang Ma ZM 20-74
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 7
CN
F
163.97
160.70
131.89
131.85
128.98
128.87
120.77
116.16
115.87
77.47 CDCl3
77.05 CDCl3
76.63 CDCl3
36.70
35.90
31.06
26.63
22.34
13.92
270
260
250
240
230
220
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)

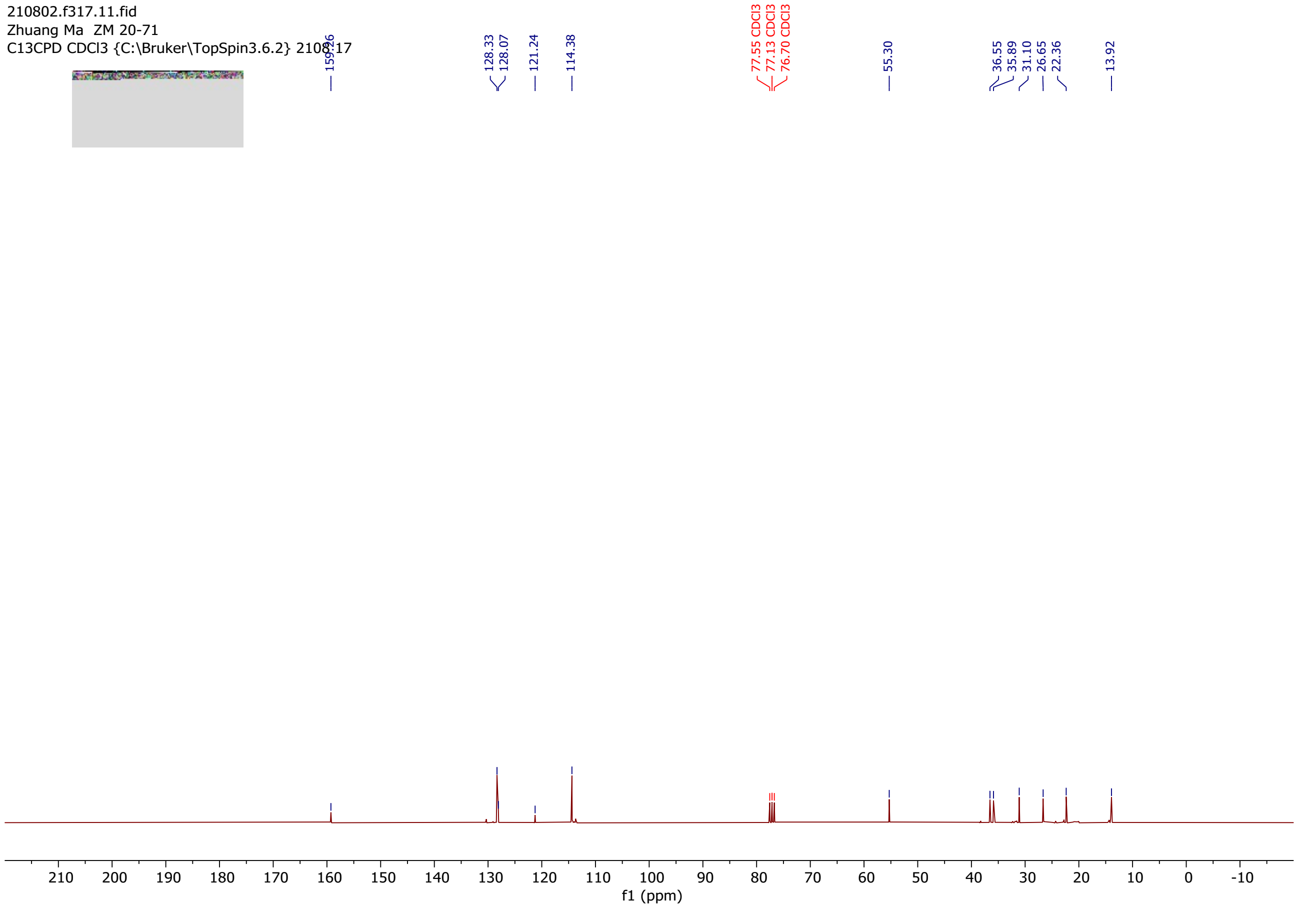

210812.309.10.fid
Zhuang Ma ZM 20-76
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 9
CN
F
F
F
7.26
1.63 HDO
2.04
2.04
1.00
1.97
1.94
3.75
3.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


210812.309.11.fid
Zhuang Ma ZM 20-76
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 9
CN
F
F
F
140.03
128.37
127.71
126.16
126.11
126.06
126.01
125.67
125.62
122.03
120.12
77.47 CDCl3
77.04 CDCl3
76.62 CDCl3
37.28
35.73
31.03
26.65
22.31
13.89
270
260
250
240
230
220
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)

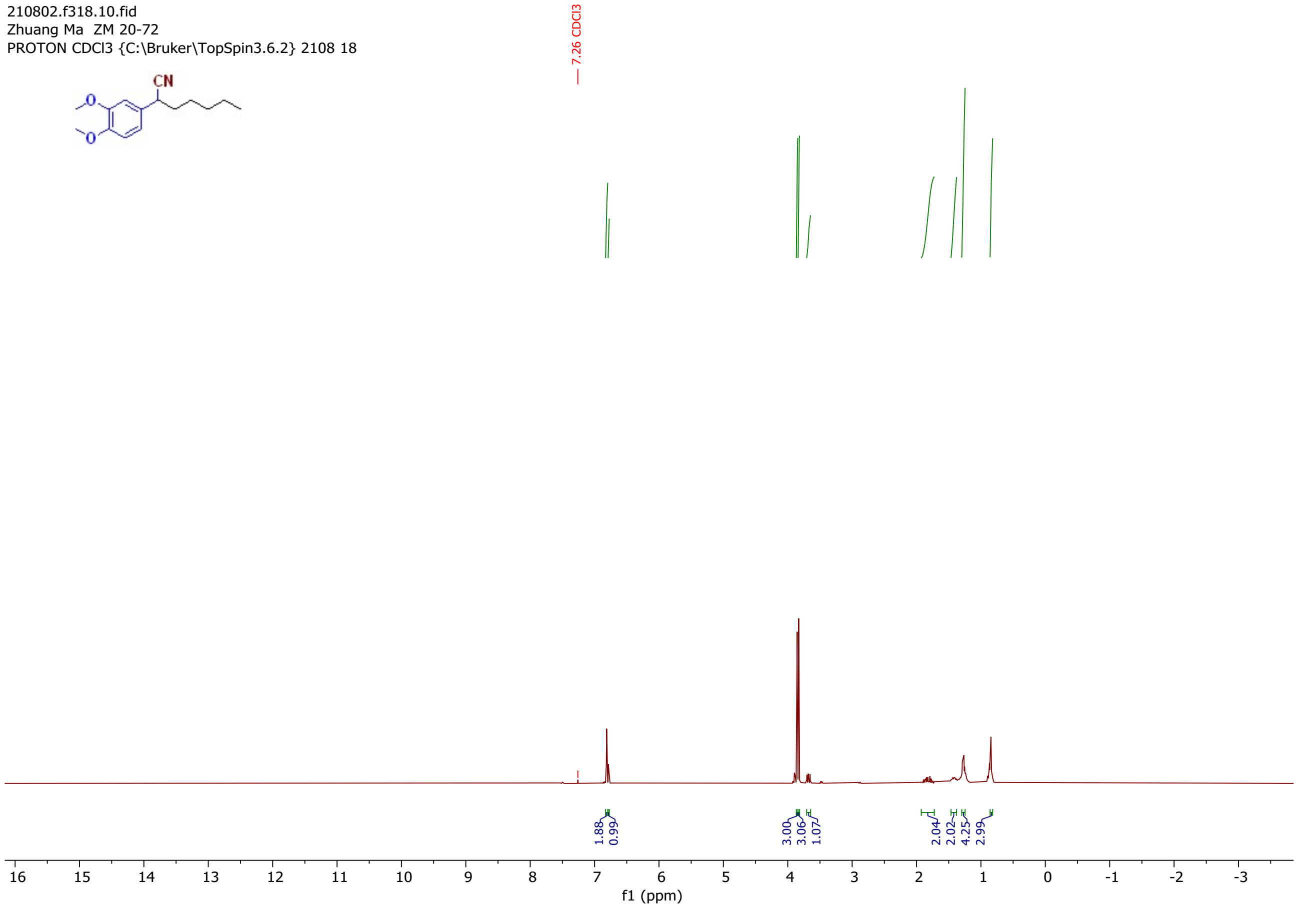

220127.324.10.fid
Ma/ ZM20-76
Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 24
-62.71
-63.10
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)

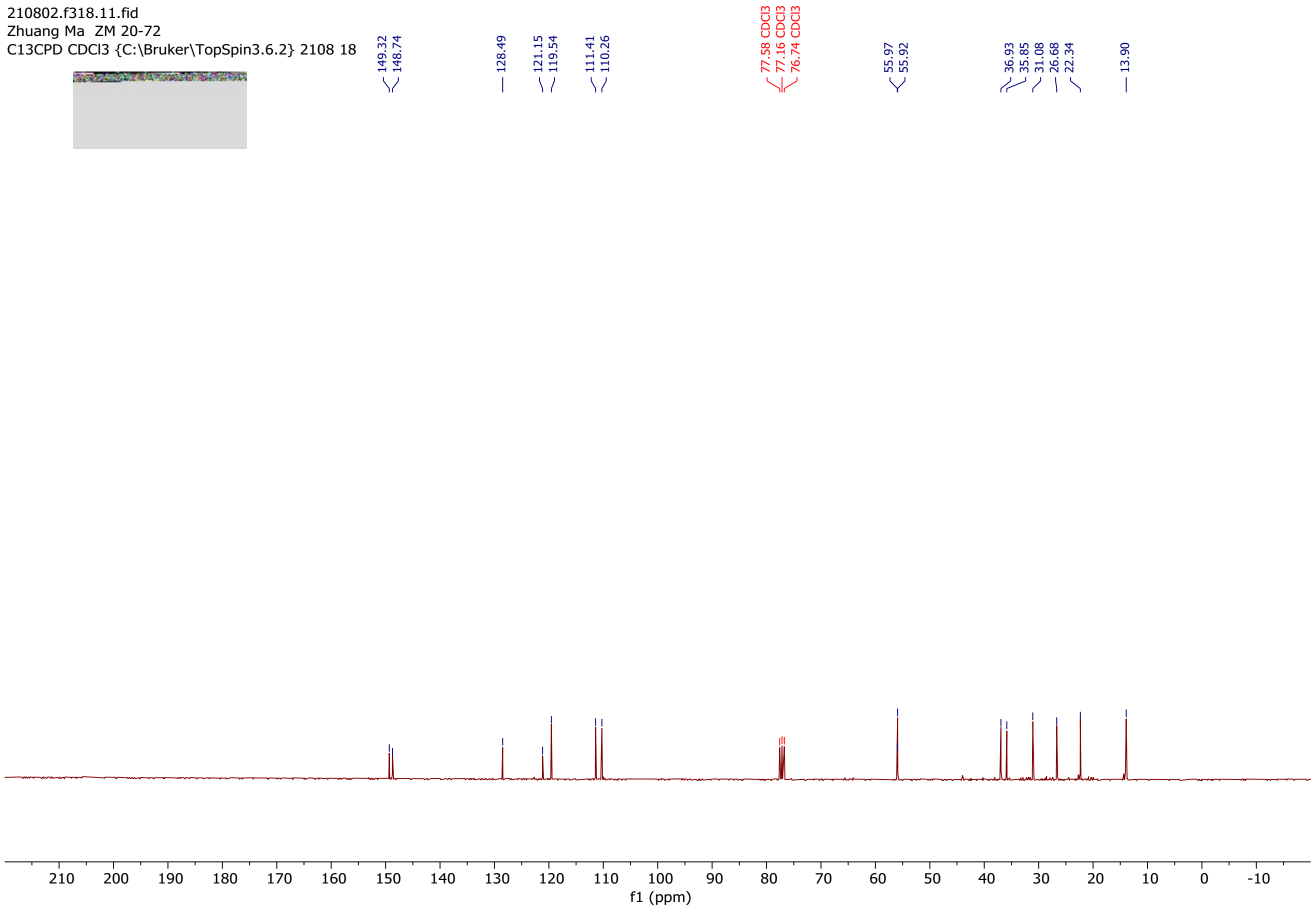

210802.f317.10.fid
Zhuang Ma ZM 20-71
PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 17
CN
O
7.26 CDCl3
1.81
2.06
2.95
1.00
1.91
1.95
4.06
3.02
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

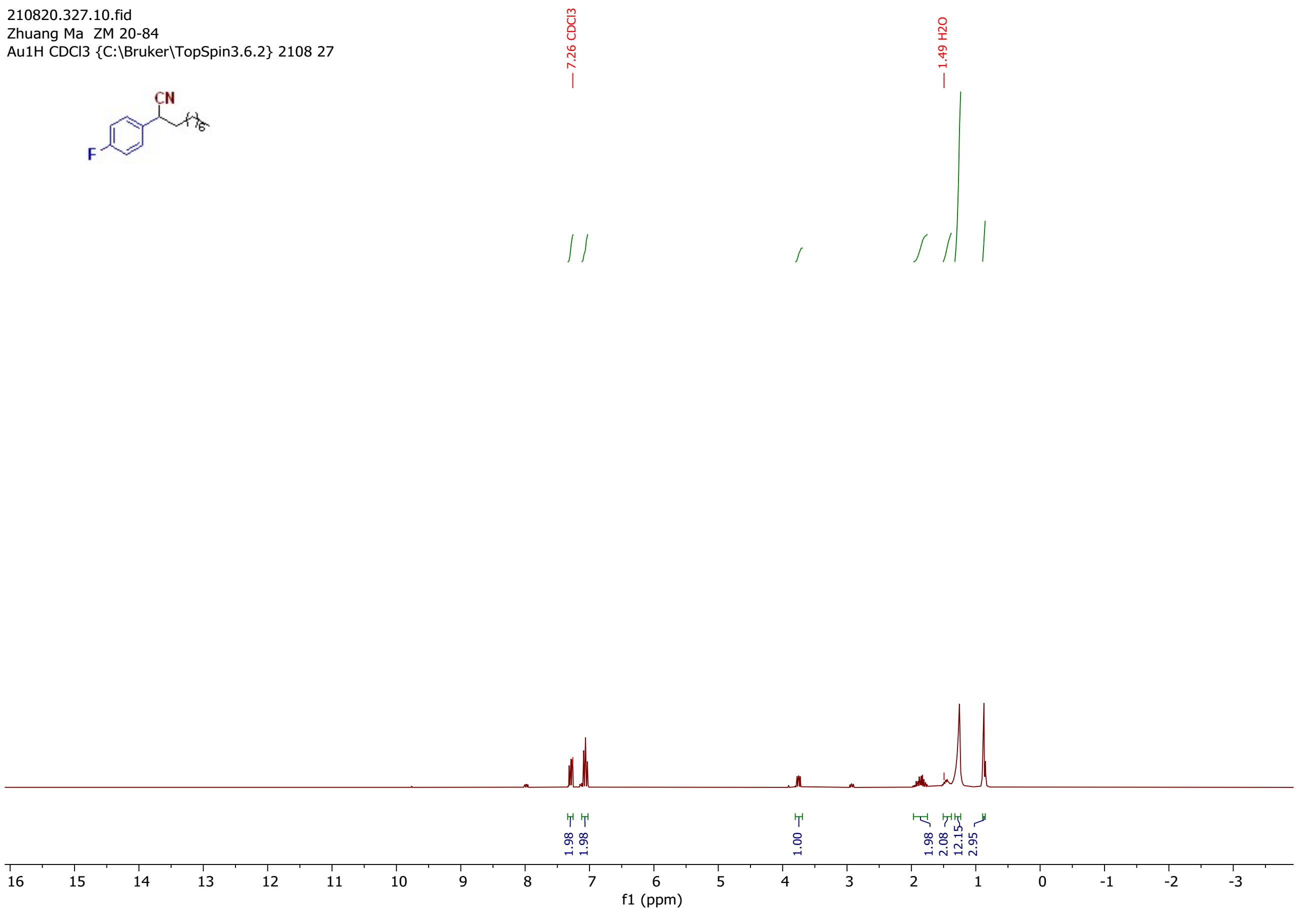
210802.f317.11.fid
Zhuang Ma ZM 20-71
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 17



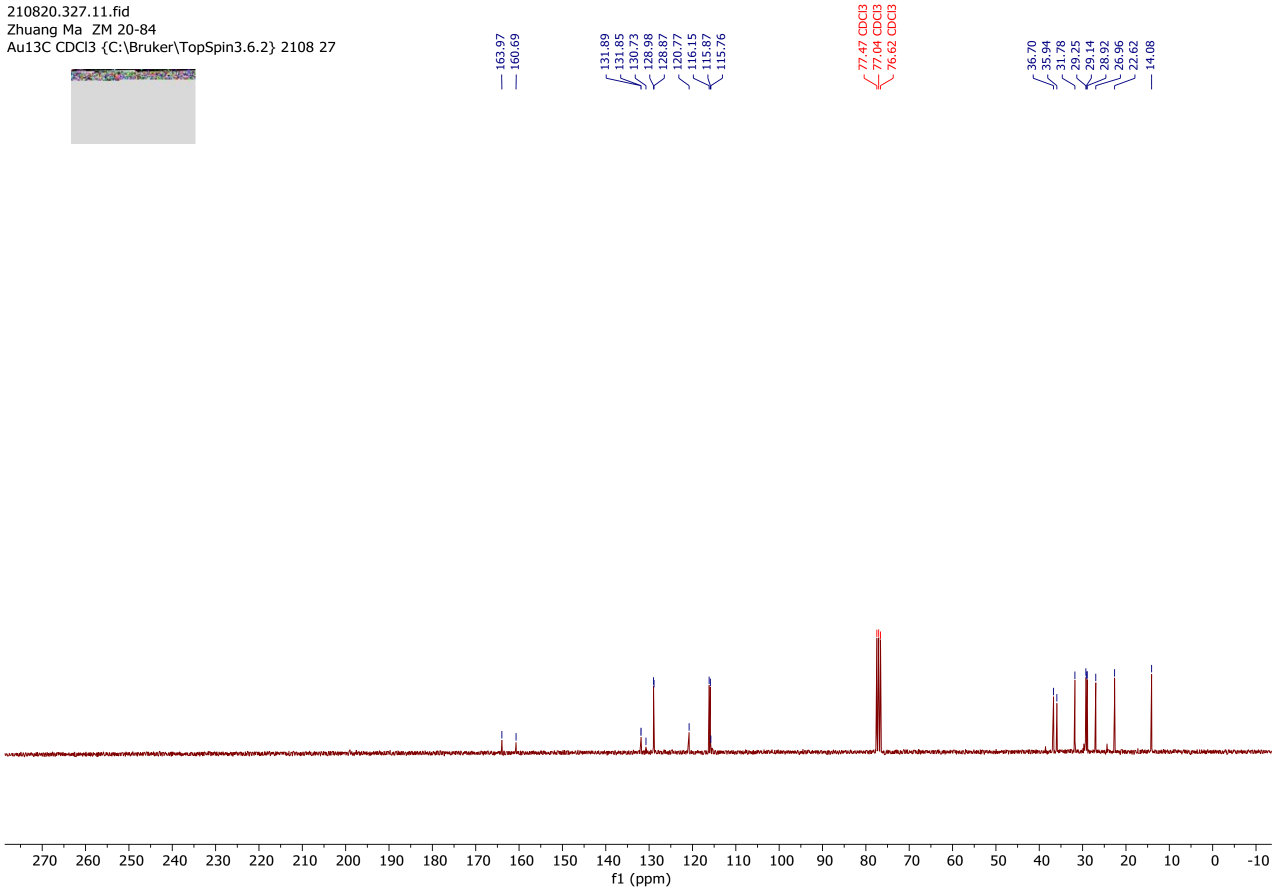
210802.f318.10.fid
Zhuang Ma ZM 20-72
PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 18

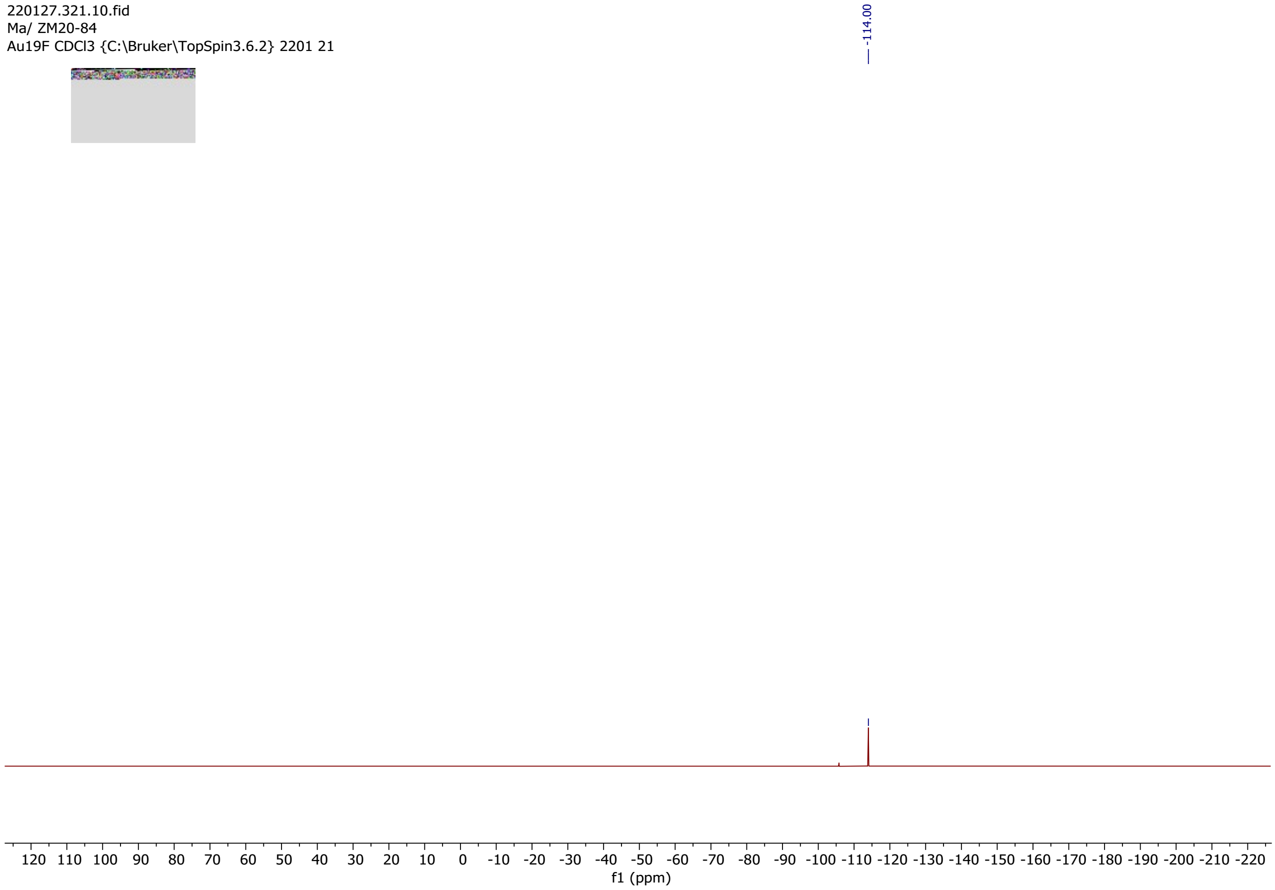


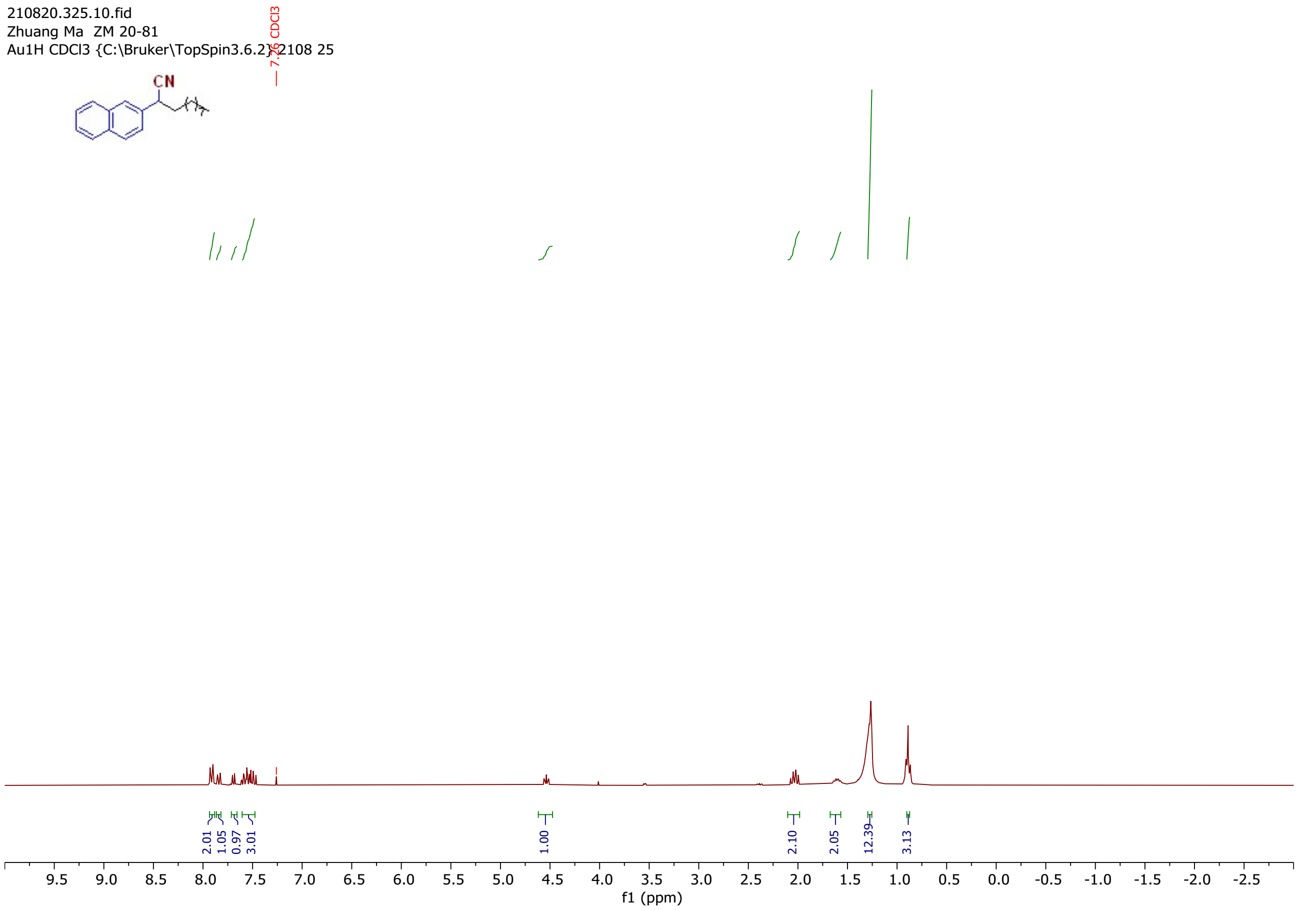

210802.f318.11.fid
Zhuang Ma ZM 20-72
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 18
149.32
148.74
128.49
121.15
119.54
111.41
110.26
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
55.97
55.92
36.93
35.85
31.08
26.68
22.34
13.90
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

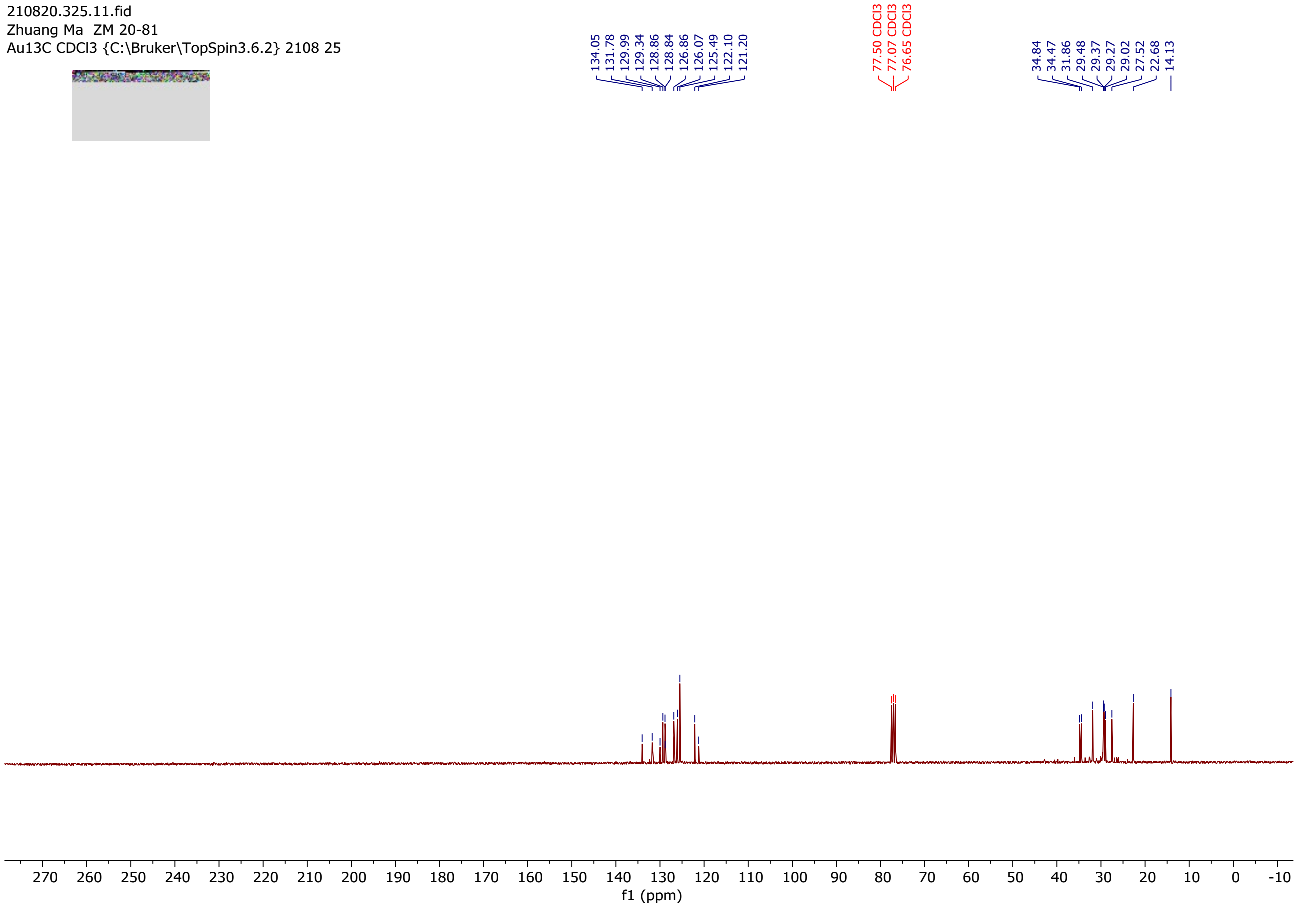


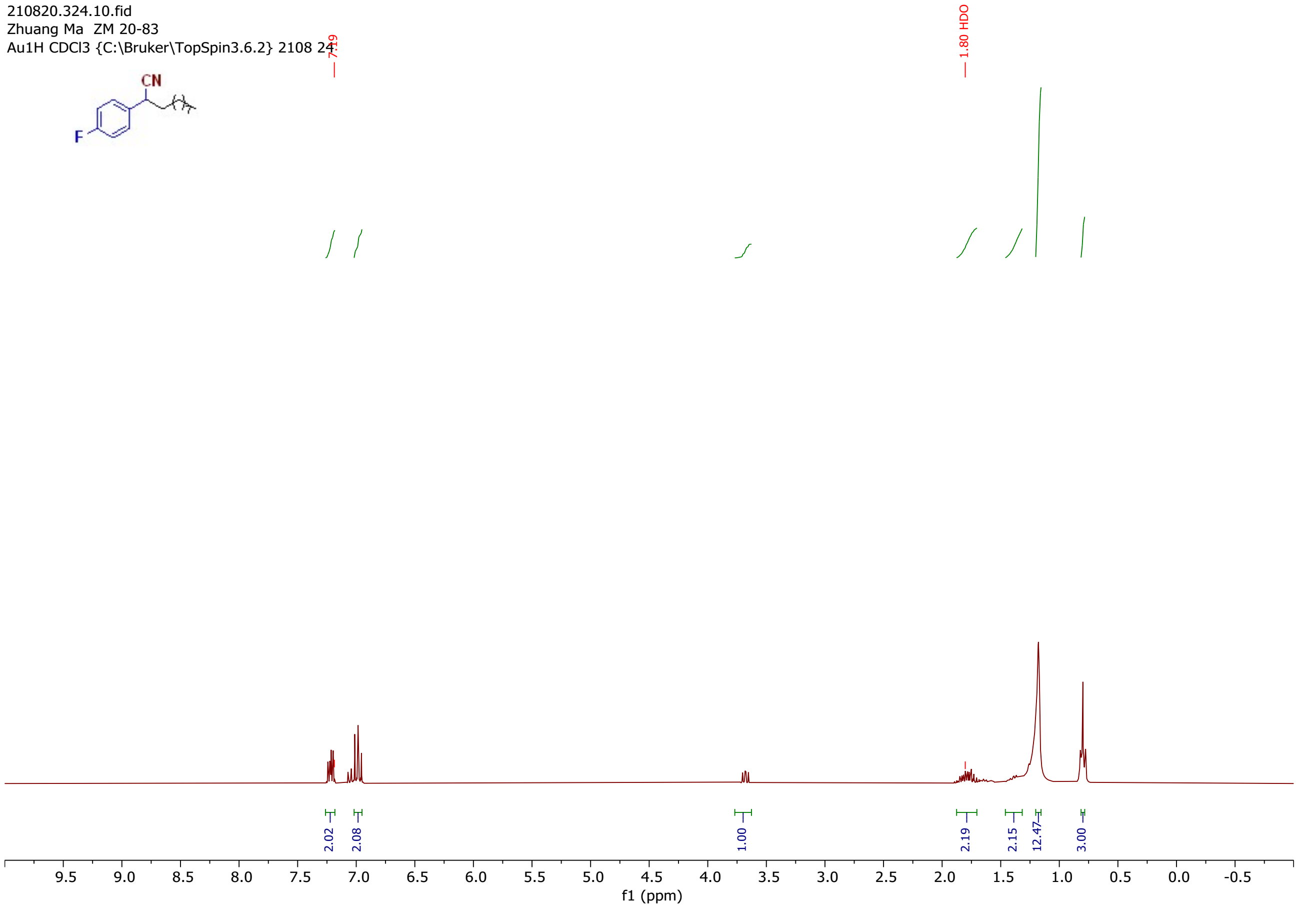
210820.327.10.fid
Zhuang Ma ZM 20-84
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 27

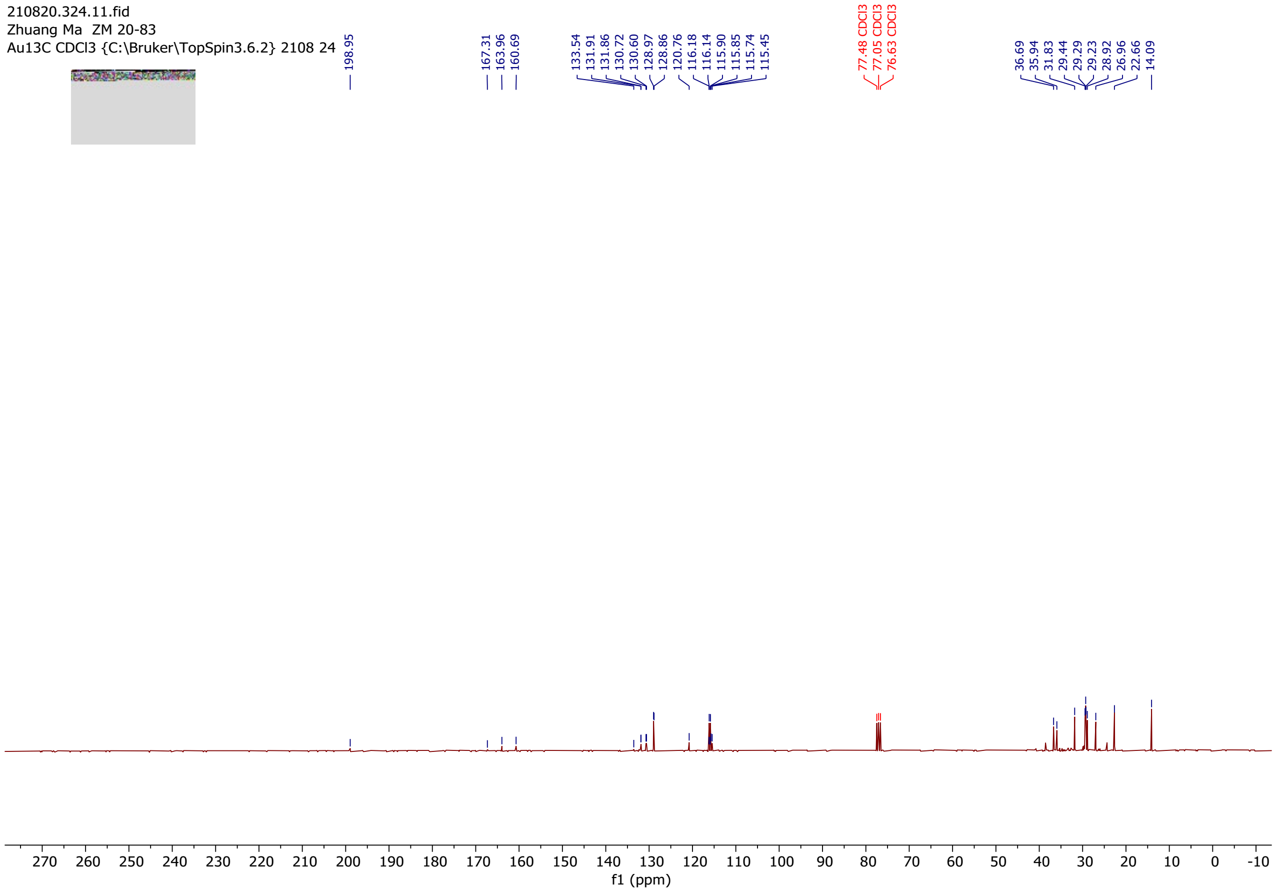

210820.327.11.fid
Zhuang Ma ZM 20-84
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 27
163.97
160.69
131.89
131.85
130.73
128.98
128.87
120.77
116.15
115.87
115.76
77.47 CDCl3
77.04 CDCl3
76.62 CDCl3
36.70
35.94
31.78
29.25
29.14
28.92
26.96
22.62
14.08
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

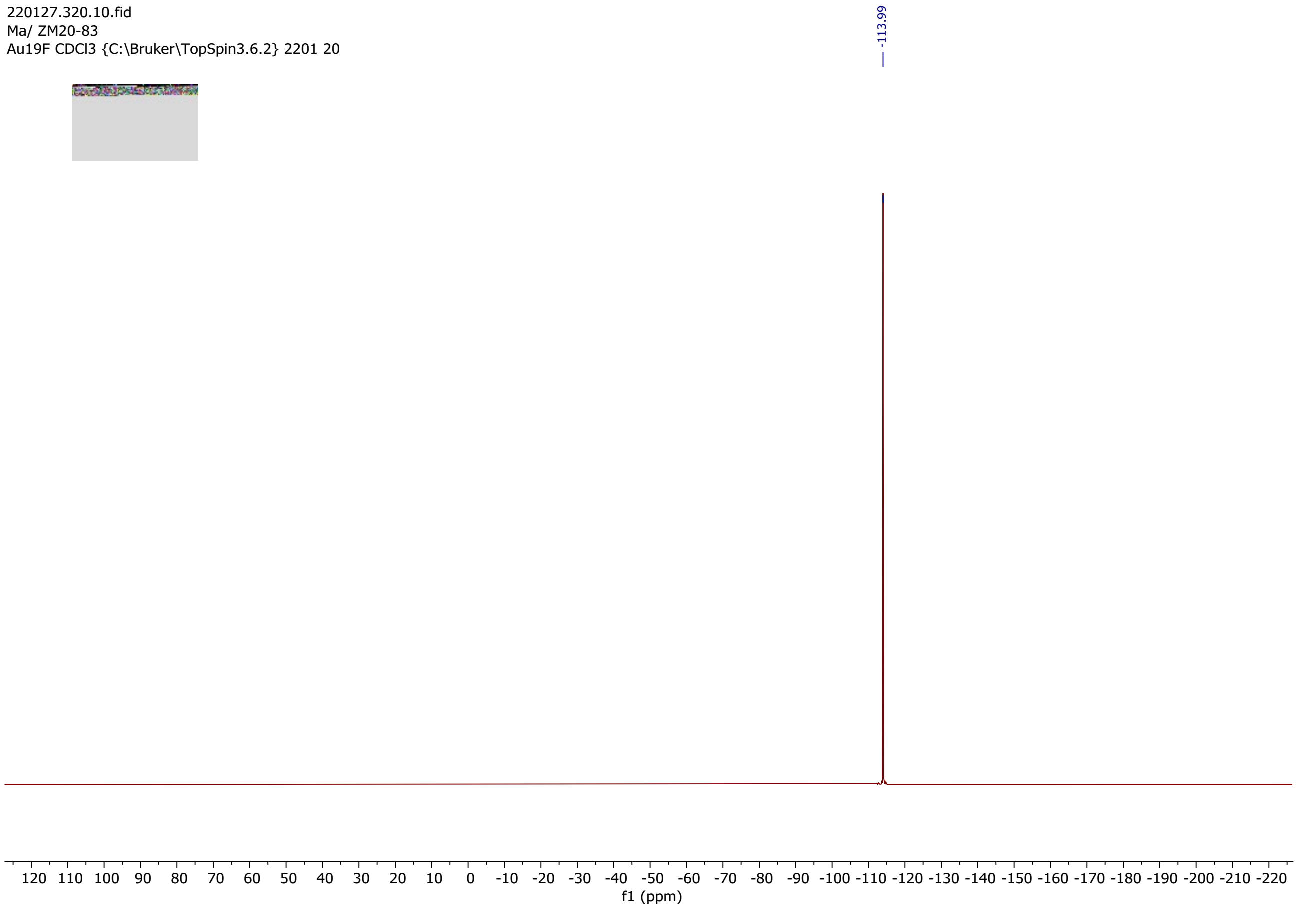

220127.321.10.fid
Ma/ ZM20-84
Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 21
-114.00
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220
f1 (ppm)


210820.325.10.fid
Zhuang Ma ZM 20-81
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 25
7.26 CDCl3
CN
7
2.01
1.05
0.97
3.01
1.00
2.10
2.05
12.39
3.13
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
-1.5
-2.0
-2.5
f1 (ppm)

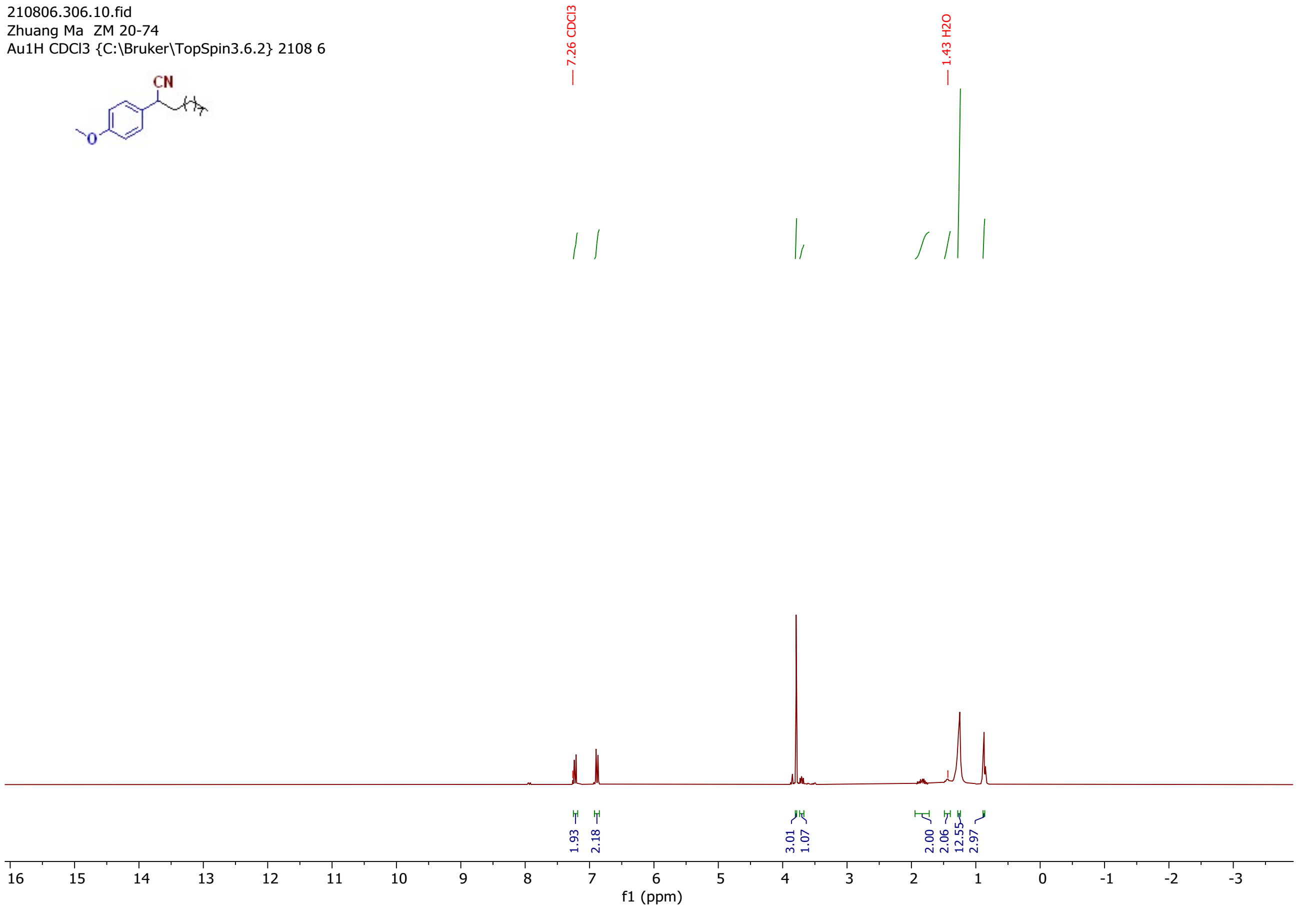

210820.325.11.fid
Zhuang Ma ZM 20-81
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 25
134.05
131.78
129.99
129.34
128.86
128.84
126.86
126.07
125.49
122.10
121.20
77.50 CDCl3
77.07 CDCl3
76.65 CDCl3
34.84
34.47
31.86
29.48
29.37
29.27
29.02
27.52
22.68
14.13
270
260
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

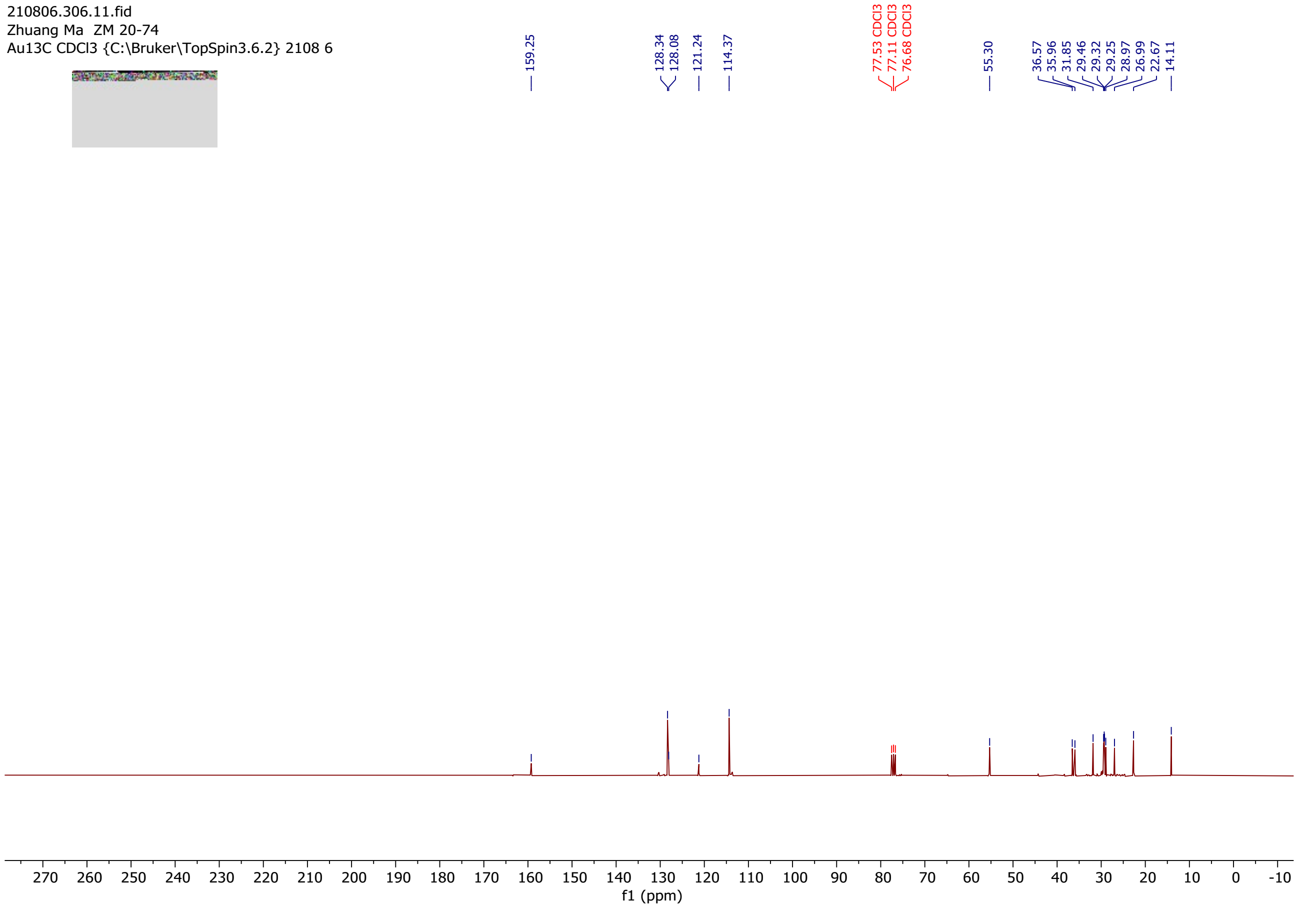

210820.324.10.fid
Zhuang Ma ZM 20-83
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 24
7.19
1.80 HDO
CN
F
2.02
2.08
1.00
2.19
2.15
12.47
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

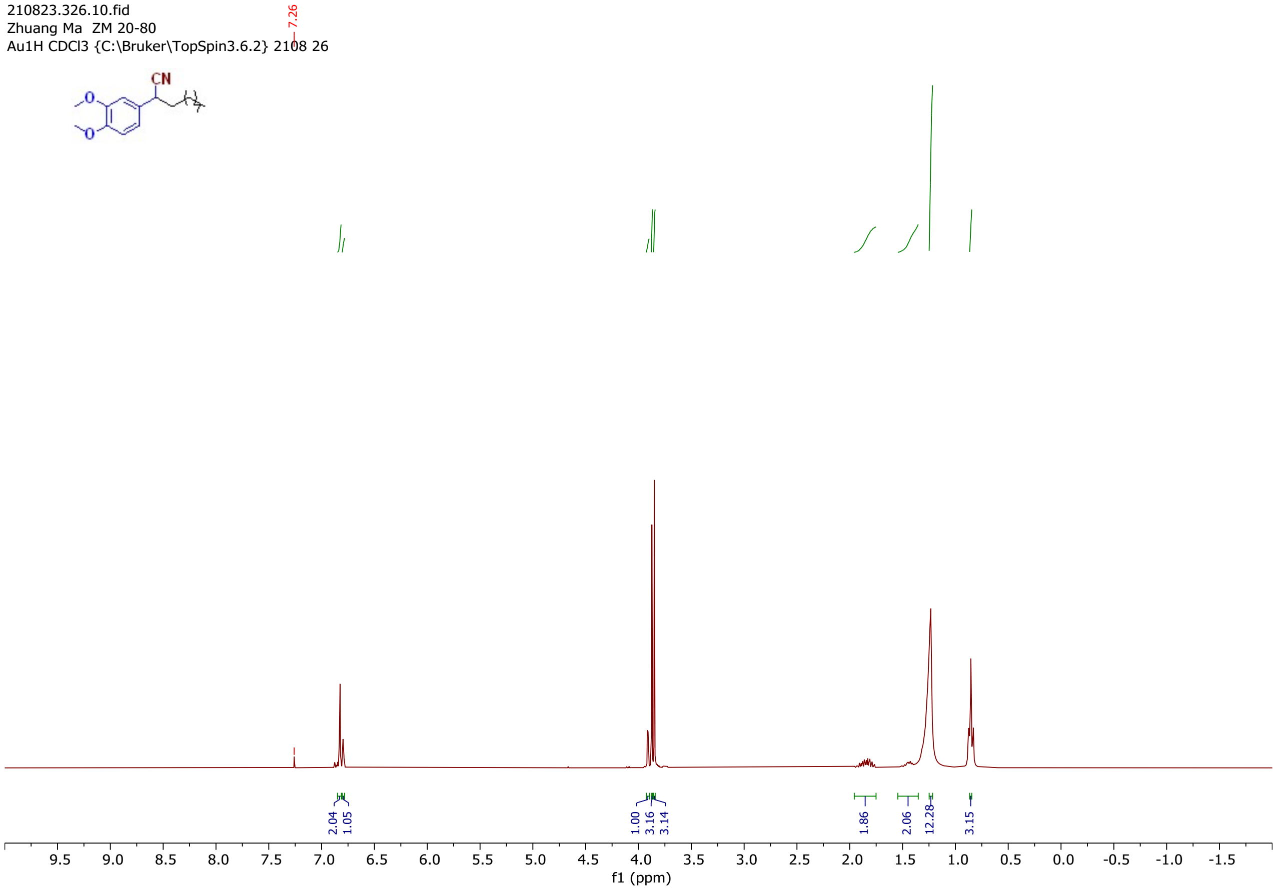

210820.324.11.fid
Zhuang Ma ZM 20-83
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 24
198.95
167.31
163.96
160.69
133.54
131.91
131.86
130.72
130.60
128.97
128.86
120.76
116.18
116.14
115.90
115.85
115.74
115.45
77.48 CDCl3
77.05 CDCl3
76.63 CDCl3
36.69
35.94
31.83
29.44
29.29
29.23
28.92
26.96
22.66
14.09
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

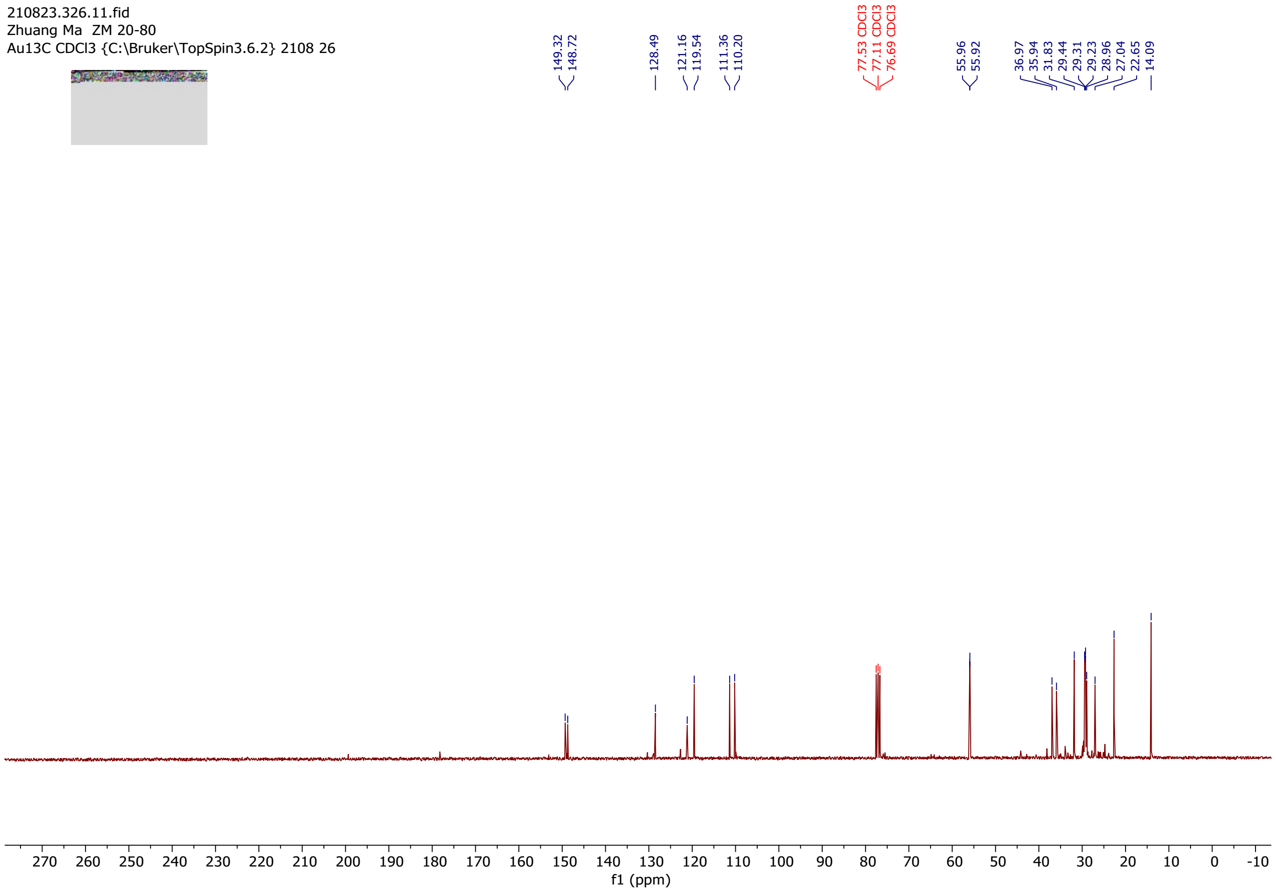


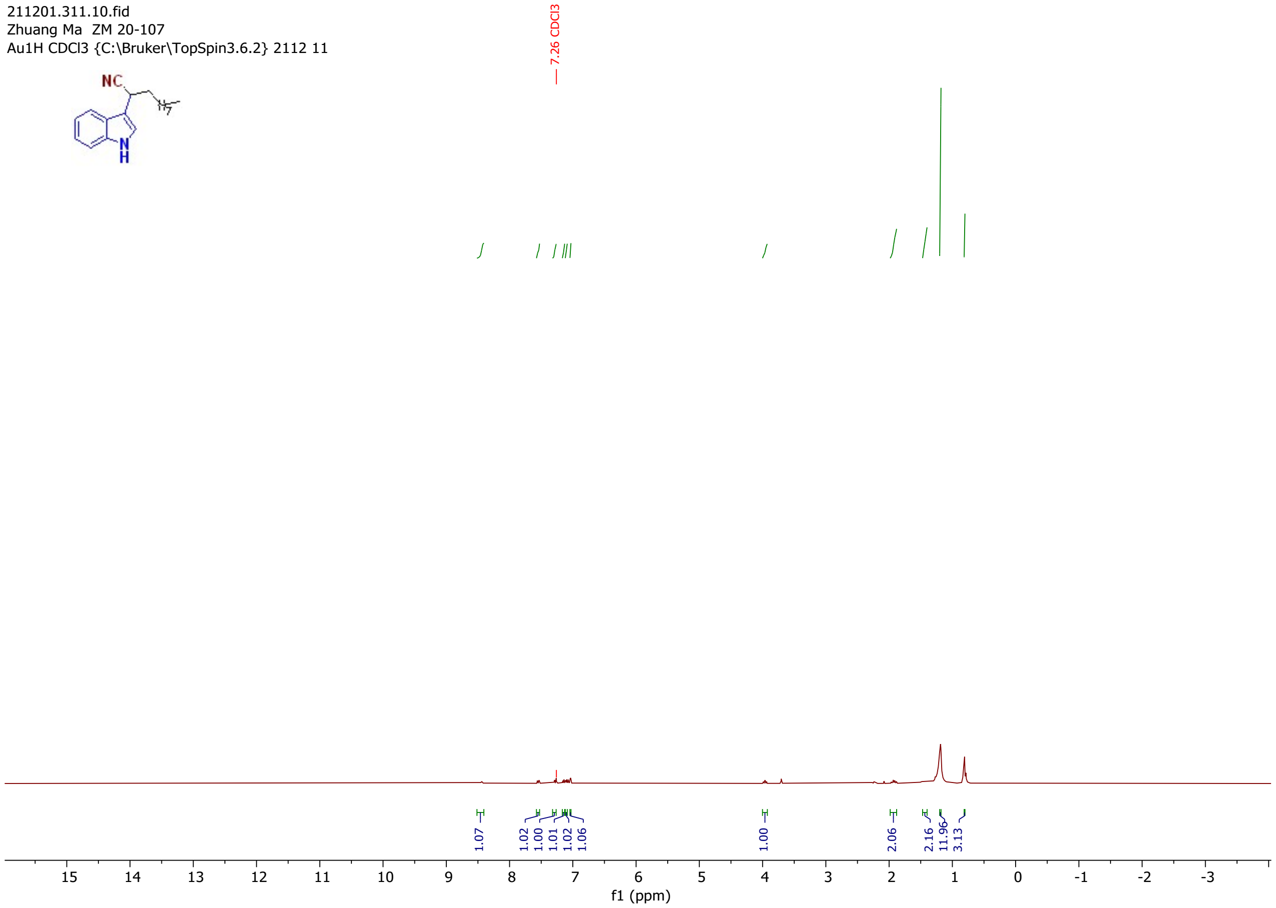
220127.320.10.fid
Ma/ ZM20-83
Au19F CDCl3 {C:\Bruker\TopSpin3.6.2} 2201 20

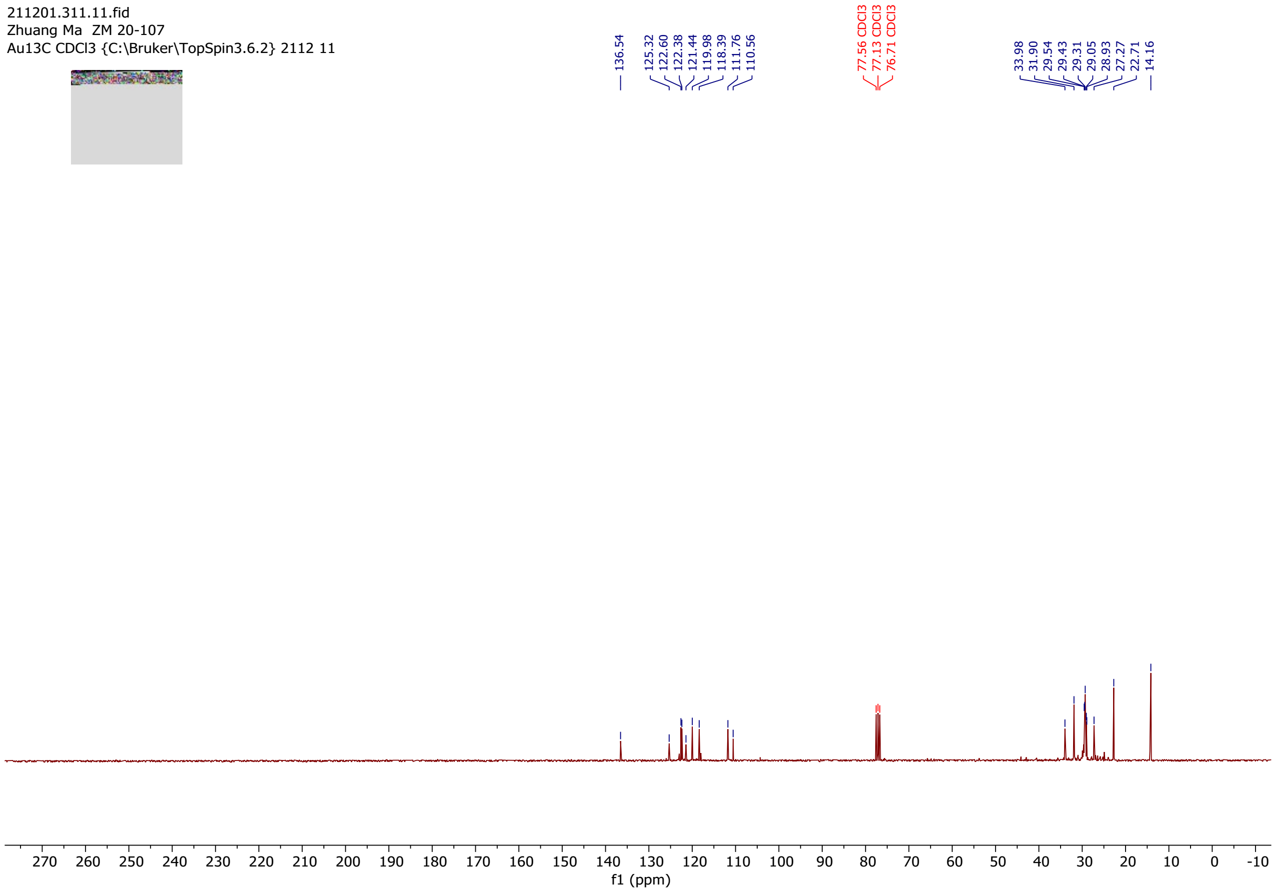

210806.306.10.fid
Zhuang Ma ZM 20-74
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 6
CN
O
7
7.26 CDCl3
1.43 H2O
1.93
2.18
3.01
1.07
2.00
2.06
12.55
2.97
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

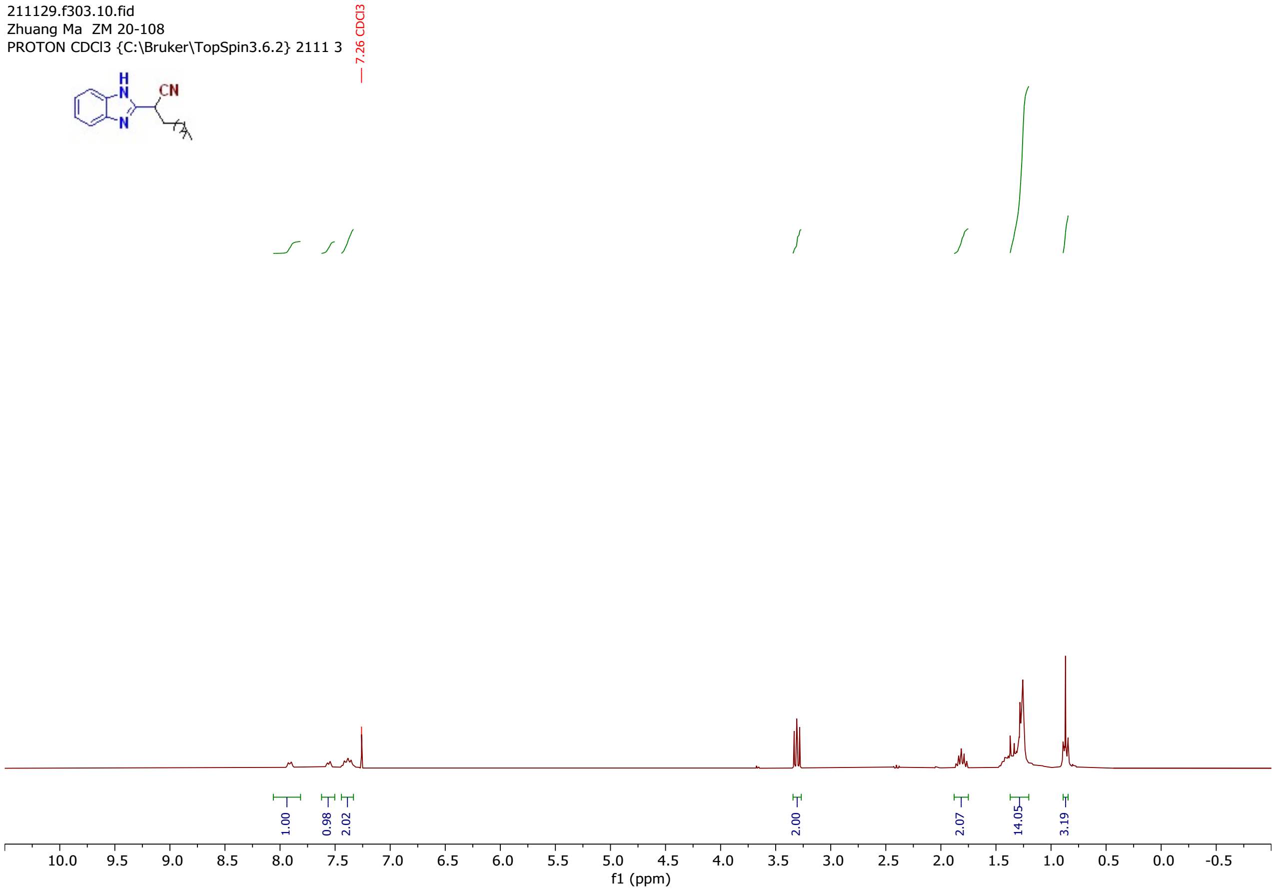

210806.306.11.fid
Zhuang Ma ZM 20-74
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 6
159.25
128.34
128.08
121.24
114.37
77.53 CDCl3
77.11 CDCl3
76.68 CDCl3
55.30
36.57
35.96
31.85
29.46
29.32
29.25
28.97
26.99
22.67
14.11
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

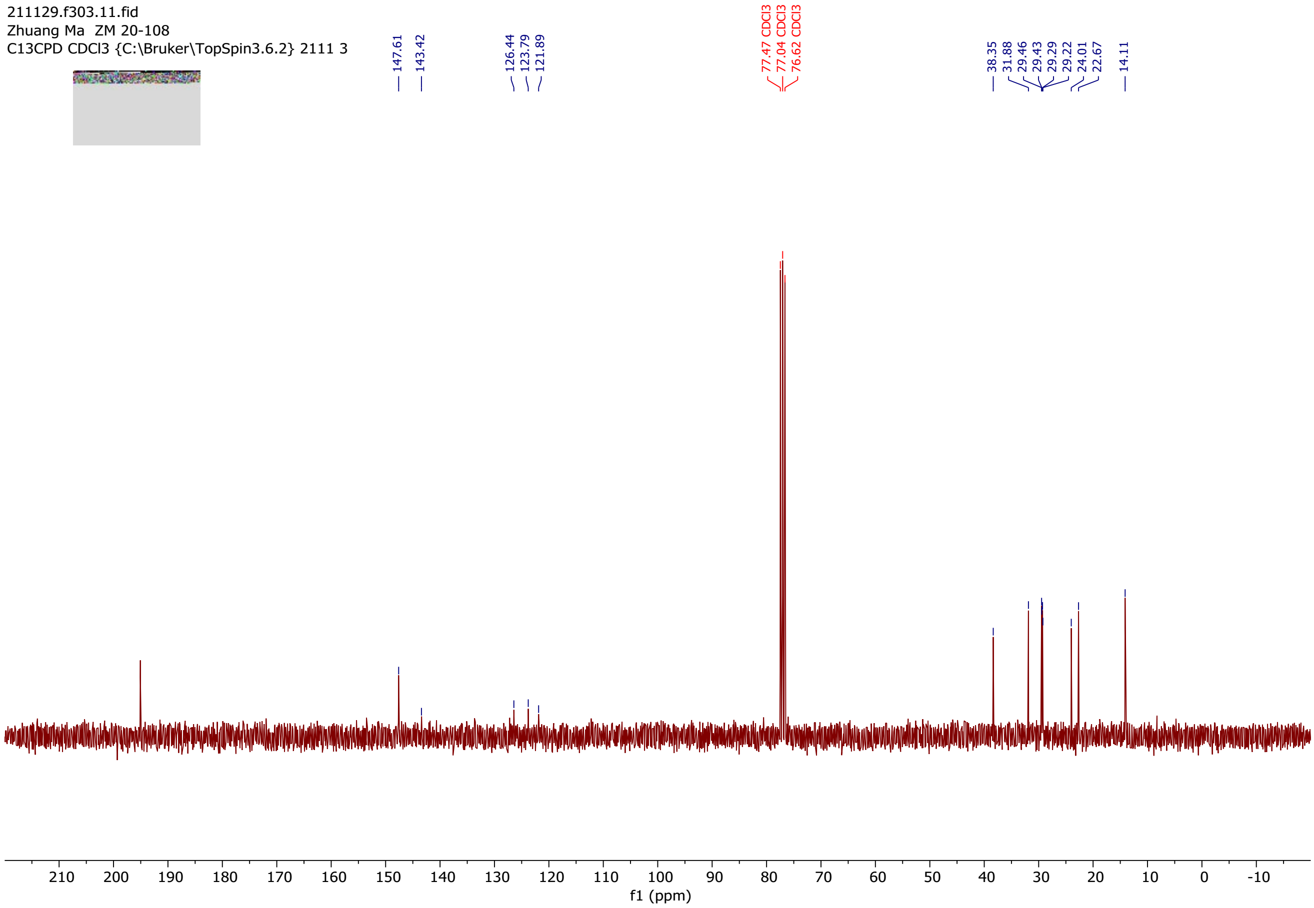

210823.326.10.fid
Zhuang Ma ZM 20-80
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 26
7.26
CN
O
O
7
2.04
1.05
1.00
3.16
3.14
1.86
2.06
12.28
3.15
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)


210823.326.11.fid
Zhuang Ma ZM 20-80
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2108 26
149.32
148.72
128.49
121.16
119.54
111.36
110.20
77.53 CDCl3
77.11 CDCl3
76.69 CDCl3
55.96
55.92
36.97
35.94
31.83
29.44
29.31
29.23
28.96
27.04
22.65
14.09
270
260
250
240
230
220
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)


211201.311.10.fid
Zhuang Ma ZM 20-107
Au1H CDCl3 {C:\Bruker\TopSpin3.6.2} 2112 11
NC
7
N
H
7.26 CDCl3
1.07
1.02
1.00
1.01
1.02
1.06
1.00
2.06
2.16
11.96
3.13
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


211201.311.11.fid
Zhuang Ma ZM 20-107
Au13C CDCl3 {C:\Bruker\TopSpin3.6.2} 2112 11
136.54
125.32
122.60
122.38
121.44
119.98
118.39
111.76
110.56
77.56 CDCl3
77.13 CDCl3
76.71 CDCl3
33.98
31.90
29.54
29.43
29.31
29.05
28.93
27.27
22.71
14.16
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


211129.f303.10.fid
Zhuang Ma ZM 20-108
PROTON CDCl3 {C:\Bruker\TopSpin3.6.2} 2111 3
7.26 CDCl3
H
N
N
CN
1.00
0.98
2.02
2.00
2.07
14.05
3.19
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)


211129.f303.11.fid
Zhuang Ma ZM 20-108
C13CPD CDCl3 {C:\Bruker\TopSpin3.6.2} 2111 3
147.61
143.42
126.44
123.79
121.89
77.47 CDCl3
77.04 CDCl3
76.62 CDCl3
38.35
31.88
29.46
29.43
29.29
29.22
24.01
22.67
14.11
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)