Electronic Supplementary Material (ESI) for Chemical Science.

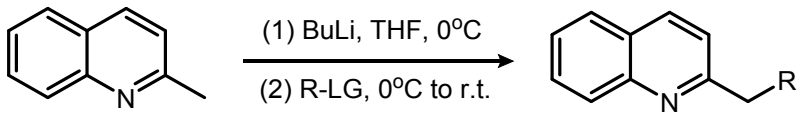
Content

1. General information

All the reactions dealing with air- or moisture- sensitive compounds were carried out in a dry reaction vessel under nitrogen protection or in the nitrogen-filled glove box. Unless otherwise noted, all reagents and solvents were purchased from commercial suppliers without further purification. THF was dried with sodium chips and indicated by benzophenone. Other anhydrous solvents were purchased from Sigma-Aldrich and transferred by syringe. Purification of products was carried out by chromatography using silica gel from ACROS (0.06-0.20mm). Thin layer chromatography was carried out using silica gel plates from Merk (GF254). $[Rh(COD)Cl]_2$ and other metal precursors were purchased from Heraeus.

^{1}H NMR, ^{13}C NMR and ^{31}P NMR spectra were recorded on a Bruker Avance (400 MHz) spectrometer with $CDCl_3$ as the solvent and tetramethylsilane (TMS) as the internal standard. Chemical shifts are reported in parts per million e (ppm, δ scale) downfield from TMS at 0.00 ppm and referenced to the $CDCl_3$ at 7.26 ppm for ^{1}H NMR or 77.0 ppm for ^{13}C NMR. Data is reported as: multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constant in hertz (Hz) and signal area integration in natural numbers. ^{13}C NMR and ^{31}P NMR analyses were ran with decoupling. Enantiomeric excess values were determined with chiral columns on Agilent 7980 Series GC instrument or Agilent 1100 Series HPLC instrument. Optical rotations were measured using a 1 mL cell with a 1 dm path length on a Jasco P–2000 polarimeter at 589 nm and at 20 °C

2. Synthesis of 2-substituted quinolines



2-ethylquinoline[1]**:**

To a solution of 1-methylquinoline (10 mmol) in dry THF (20 ml) at 0°C was added n-butyllithium in THF solution (2.5M) dropwise. The mixture was stirred at room temperature for 1.5h and was cooled back to 0°C. Iodomethane was added dropwise. The mixture was stirred overnight. Water was added carefully to quench the reaction and the mixture was extracted by ethyl acetate (20 ml*3). Organic phases were combined and dried with sodium sulfate. After removing solvent, the crude product was purified by flash chromatography (on silica gel, eluent: hexanes/ethyl acetate). 2-methylquinoline was obtained as yellow oil with 95% yield.

Known compound. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 11.8, 8.5 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.65 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 7.45 (dd, *J* = 11.0, 4.0 Hz, 1H), 7.28 – 7.25 (d, *J* = 8.5 Hz, 1H), 2.99 (q, *J* = 7.6 Hz, 2H), 1.39 (dd, *J* = 7.6 Hz, 3H).

^{13}C NMR (400 MHz, $CDCl_3$): δ 163.97, 147.87, 136.31, 129.30, 128.79, 127.46, 126.37, 125.63, 120.81, 32.28, 13.97.

2-isopropylquinoline[1]

Followed the standard procedure above, using 2-ethylquinoline and iodomethane, 2-isopropylquinoline was abotained as yellow oil with 76% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 8.2, 6.0 Hz, 2H), 7.74 (dd, *J* = 8.1, 1.1 Hz, 1H), 7.65 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H), 7.45 (ddd, *J* = 8.1, 7.0, 1.1 Hz, 1H), 7.30 (t, *J* = 8.6 Hz, 1H), 3.26 (hept, *J* = 6.9 Hz, 1H), 1.38 (d, *J* = 6.9 Hz, 3H).

^{13}C NMR (400 MHz, CDCl3): δ 167.63, 147.79, 136.36, 129.21, 129.04, 127.42, 126.95, 125.62, 119.16, 37.29, 22.52.

2-pentylquinoline[1]

Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (t, *J* = 8.4 Hz, 2H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.66 (t, *J* = 7.7 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.27 (d, *J* = 8.4 Hz, 1H), 2.99 – 2.94 (m, 2H), 1.86 – 1.77 (m, 2H), 1.37 (m, 2H), 0.90 (t, *J* = 6.7 Hz, 3H).

^{13}C NMR (400 MHz, CDCl3): δ 163.10, 147.97, 136.10, 129.25, 128.88, 127.45, 126.72, 125.59, 121.34, 39.35, 31.76, 29.71, 22.56, 14.00.

2-undecylquinoline[1]

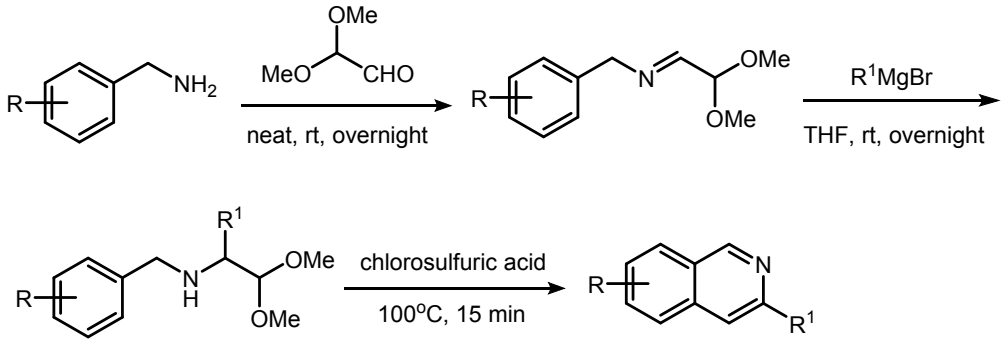
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.67 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 7.46 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 1H), 2.96 (t, *J* = 8.0 Hz, 2H), 1.86 – 1.76 (m, 2H), 1.46 – 1.19 (m, 16H), 0.90 – 0.85 (m, 3H).
^{13}C NMR (400 MHz, CDCl3): δ 163.12, 147.97, 136.09, 129.25, 128.88, 127.44, 126.72, 125.58, 121.34, 39.40, 31.68, 30.03, 29.58, 29.56, 29.52, 29.30, 22.66, 14.09.

2-(3,4-dimethoxyphenethyl)quinoline[1]

Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.4, 1H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.77 (dd, *J* = 8.1, 0.8 Hz, 1H), 7.69 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H), 7.49 (d, *J* = 8.4, 6.9, 1.4 Hz, 1H), 7.22 (d, *J* = 8.4 Hz, 1H), 6.78 (d, *J* = 1.0 Hz, 1H), 6.75 (s, 1H), 3.84 (s, 1H), 3.79 (s, 1H), 3.27 (dd, *J* = 9.6, 6.2 Hz, 1H), 3.10 (dd, *J* = 9.5, 6.4 Hz, 1H).
^{13}C NMR (400 MHz, CDCl3): δ 161.84, 148.83, 148.01, 147.34, 136.16, 134.17, 129.40, 128.86, 127.52, 126.60, 125.79, 121.62, 120.34, 112.01, 111.34, 55.92, 55.77, 41.23, 35.54.

3. Synthesis of 3-substituted isoquinolines

3-substituted isoquinolines were synthesized according to literature with modification:[2]



A round-bottom flask was charged with benzylamine (10 mmol) and glyoxal 1,1-dimethyl acetal (1.1 eq., 60% soluition in water) was added dropwise. The mixture was stirred at

room temperature overnight and two layers were separated. After removal of the aqueous layer, trace water was removed by azeotropic distillation with toluene. The crude imine was used for next step without purification.

To the solution of this imine in dry THF was added Grignard reagent dropwise at 0^{o}C. The mixture was then stirred at room temperature. Once TLC showed the completion of the reaction (usually overnight), saturated aqueous NH_4Cl was added at 0^{o}C. The mixture was extracted with ether and the organic layer was dried with anhydrous sodium sulfate. After removal of solvent, the crude product was obtained as yellow or orange oil. After ^{1}H NMR shows the majority of the desired amine in the crude product, it is used for next step without purification.

A round-bottom flask was filled with nitrogen and charged with chlorosulfuric acid (5ml). The mixture was cooled at 0^{o}C and the crude amine was added dropwise. The mixture was heated at 100^{o}C for 15 min and then cooled to 0^{o}C. The resulting mixture was poured on ice and the neutralized carefully with 40% NaOH solution. After the mixture turned to alkaline, ether was added to extract. The organic phase was dried with sodium sulfate and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (on silica gel, eluent: hexane/ethyl acetate). 3-alkylisoquinoline was obtained as yellow oils.

3-ethylisoquinoline

Yellow oil. 43% yield for 3 steps. ^{1}H NMR (400 MHz, CDCl3): δ 9.06 (s, 1H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.58 (d, *J* = 8.2 Hz, 1H), 7.47 (t, *J* = 6.8 Hz, 1H), 7.35 (t, *J* = 6.8 Hz, 1H), 7.31 (s, 1H), 2.84 (q, *J* = 7.5 Hz, 2H), 1.27 (t, *J* = 7.5 Hz, H).

^{13}C NMR (400 MHz, CDCl3): δ 155.92, 150.95, 135.55, 129.08, 126.37, 126.02, 125.16, 125.02, 115.98, 30.06, 13.02.

m/z (ESI–MS) 158.04 $[M + H]^{+}$.

3-butylisoquinoline

Yellow oil. 38% yield for 3 steps. ^{1}H NMR (400 MHz, CDCl3): δ 9.19 (s, 1H), 7.90 (d, *J* = 8.1 Hz, 1H), 7.72 (d, *J* = 8.2 Hz, 1H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.45 (s, 1H), 2.94 (d, *J* = 8.1 Hz, 2H), 1.80 (m, 2H), 1.43 (m, 2H), 0.96 (t, *J* = 7.3 Hz, 3H).
^{13}C NMR (400 MHz, CDCl3): δ 155.88, 152.04, 136.54, 130.14, 127.46, 127.07, 126.22, 126.06, 117.87, 37.84, 32.14, 22.50, 13.97.
m/z (ESI–MS) 186.06 $[M + H]^{+}$.

3,6-dimethylisoquinoline

White solid. 42% yield for 3 steps. ^{1}H NMR (400 MHz, CDCl3): δ 9.10 (s, 1H), 7.81 (d, *J* = 8.4 Hz, 1H), 7.48 (s, 1H), 7.38 (s, 1H), 7.34 (dd, *J* = 8.4, 1.4 Hz, 1H), 2.38 (s, 3H), 2.52 (s, 3H).
^{13}C NMR (400 MHz, CDCl3): δ 151.67, 151.51, 140.56, 136.92, 128.56, 127.28, 125.37, 124.80, 117.93, 24.18, 22.05.
MP: 76-78^{o}C
m/z (ESI–MS) 158.14 $[M + H]^{+}$.

6-chloro-3-methylisoquinoline

Yellow oil. 56% yield for 3 steps. ^{1}H NMR (400 MHz, CDCl3): δ 9.14 (s, 1H), 7.85 (d, *J* = 8.7 Hz, 1H), 7.69 (d, *J* = 1.8 Hz, 1H), 7.45 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.38 (s, 1H), 2.69 (s, 3H).
^{13}C NMR (400 MHz, CDCl3): δ 152.99, 151.72, 137.26, 129.15, 127.41, 125.04, 124.80, 117.53, 24.25.
m/z (ESI–MS) 178.14 $[M + H]^{+}$.

6-fluoro-3-methylisoquinoline

Yellow oil. 34% yield for 3 steps. ^{1}H NMR (400 MHz, CDCl3): δ 9.12 (s, 1H), 7.91 (dd, *J* = 8.9, 5.6 Hz, 1H), 7.41 (s, 1H), 7.30 (dd, *J* = 10.1, 2.0 Hz, 1H), 7.25 (dd, *J* = 8.7, 2.5 Hz, 1H), 2.68 (s, 3H).

^{13}C NMR (400 MHz, CDCl3): δ 163.28 (d, *J* = 251.9 Hz), 152.66, 151.52, 137.94 (d, *J* = 10.5 Hz), 130.43 (d, *J* = 9.9 Hz), 124.04, 118.01 (d, *J* = 5.3 Hz), 116.81 (d, *J* = 25.8 Hz), 109.14 (d, *J* = 20.9 Hz).
m/z (ESI–MS) 162.04 $[M + H]^+$.

6-trifluoromethyl-3-methylisoquinoline

Yellow oil. 27% yield for 3 steps. ^{1}H NMR (400 MHz, CDCl3): δ 9.26 (s, 1H), 8.05 (s, 1H), 8.03 (s, 2H), 7.68 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.56 (s, 1H), 2.74 (s, 3H).
^{13}C NMR (400 MHz, CDCl3): δ 153.40, 151.92, 144.38, 135.56, 131.90 (q, *J* = 128.4 Hz), 128.69, 127.47, 123.79 (q, *J* = 18.1 Hz), 121.96 (q, *J* = 12.1 Hz), 118.98, 24.20.
m/z (ESI–MS) 211.97 $[M + H]^+$.

8-chloro-3-methylisoquinoline

Yellow oil. 41% yield for 3 steps. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.56 (s, 1H), 7.64 (dd, *J* = 5.5, 3.7 Hz, 1H), 7.54 (s, 1H), 7.53 (d, *J* = 2.3 Hz, 1H), 7.47 (s, 1H), 2.72 (s, 3H).
^{13}C NMR (400 MHz, CDCl3): δ 152.79, 148.94, 137.89, 132.52, 130.19, 126.52, 125.14, 124.01, 118.15, 24.08.
m/z (ESI–MS) 178.16 $[M + H]^+$.

4. General procedure for preparation of quinoline/isoquinoline hydrochlorides

Quinolines or isoquinolines (1mmol) was dissolved in 2 ml dry THF, 1 ml hydrogen chloride solution (2M) in ether (2 eq.) was added dropwse. White precipitate was form. The resulting mixture was filtered and the solid was washed with dry THF (2 ml*2). The white solid was collected and dried under vacuum. Quinolimium/isoquinolinium chloride was obtained as white solid.

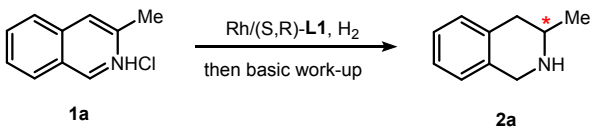
5. General procedure for asymmetric hydrogenation of quinolium/isoquinolinium chlorides

In the nitrogen-filled glovebox, solution of $[Rh(COD)Cl]_2$ (4.9 mg, 0.01 mmol) and ligand (2.1 eq.) in 5.0 ml anhydrous solvent was stirred at room temperature for 30 min. A specified volume of the resulting solution (0.5 ml, 1% Rh catalyst) was transferred) by syringe to a Score-Break ampule charged with substrate solution (0.2 mmol in 0.5 ml). The ampule was placed into an autoclave, which was then charged with 40 atm H_2. The autoclave was stirred at desired temperature for the indicated period of time. After release of H_2, the resulting mixture was concentrated under vacuum. Saturated potassium carbonate solution and dichloromethane was added and the mixture was stirred for 30 min. The organic layer was dried with anhydrous sodium sulfate. After removal of solvent, the crude product was analysed by ^1H NMR to determine the conversion. The enantiomeric excess was determined by GC or HPLC analysis of the crude product or its corresponding trifluoroacetamides. The absolute configurations were assigned according to literature[3,4,5] and their analogues.

6. Counterion effects in asymmetric hydrogenation of isoquinolines

When tetrabutylammonium chloride (TBAC) was added, no significant changes in conversion and enantioselectivity was observed (Table S1, entry 2 vs 1). This suggests the spectator role of tetrabutylammonium cation. The introduction of bromide anion from TBAB does not influence this catalytic reaction (Table S1, entry 3 vs 2). The presence of Iodide anion decreases the conversion, but the it shows trace influence on the enantioselectivity (Table S1, entry 4 vs 2). Fluoride anion, however, inhibits this catalytic reaction dramatically: no product was observed after adding TBAF (Table S1, entry 5). To gain plausible explanation of these observations, further study will be needed in the future.

Table S1, Optimization of condition. [a]



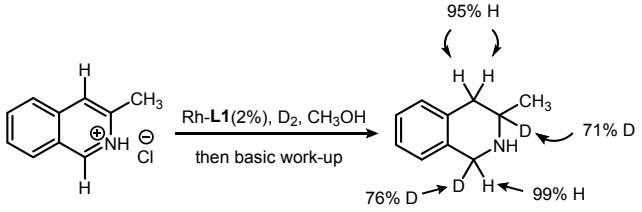
1a 2a

Entry	additive	conversion[b]	ee[c]
1	none	99%	99%
2	TBAC (1.0 eq.)	98%	99%
3	TBAB (1.0 eq.)	99%	99%
4	TBAI (1.0 eq.)	90%	98%
5	TBAF (1.0 eq.)	0	-

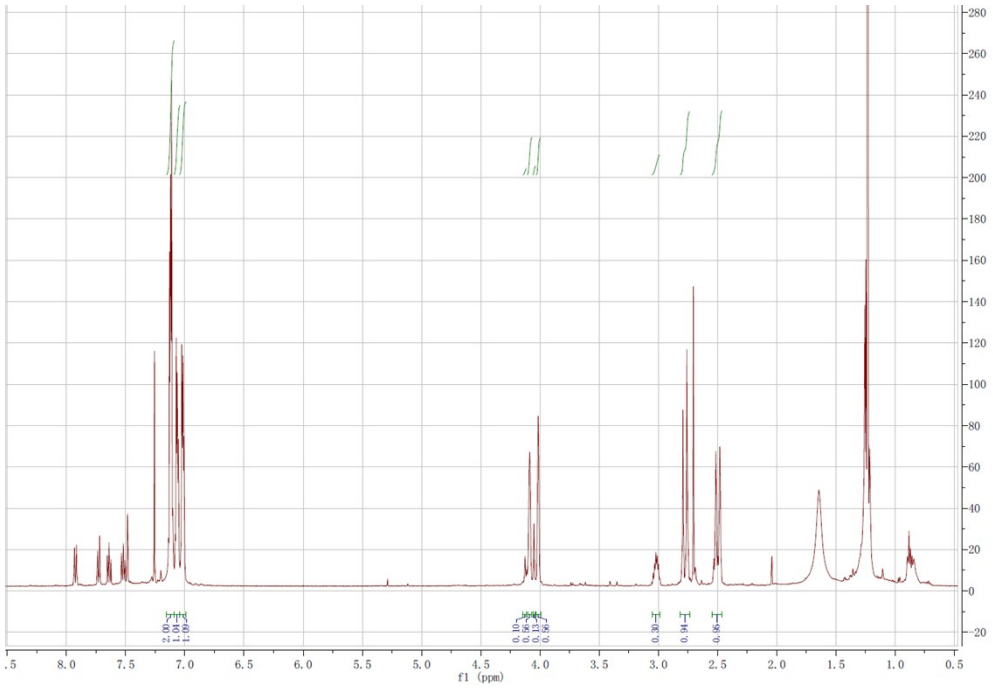
[a]Reaction condition: 1a (0.1 mmol) in 0.6 ml solvent, 1/[Rh(COD)Cl]2/**L1** ratio=100/0.5/1, 40 atm H_2, 25 °C, 48 h; [b]conversion was determined by 1H NMR analysis, no by product was observed; [c]ee was determined by GC with a chiral stationary phase.

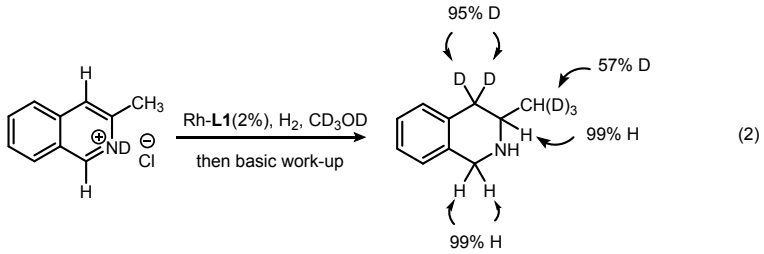
7. Result of deuterium labeling experiments

Following standard hydrogenation procedure, deuterium labeling experiments were conducted with specific modification.

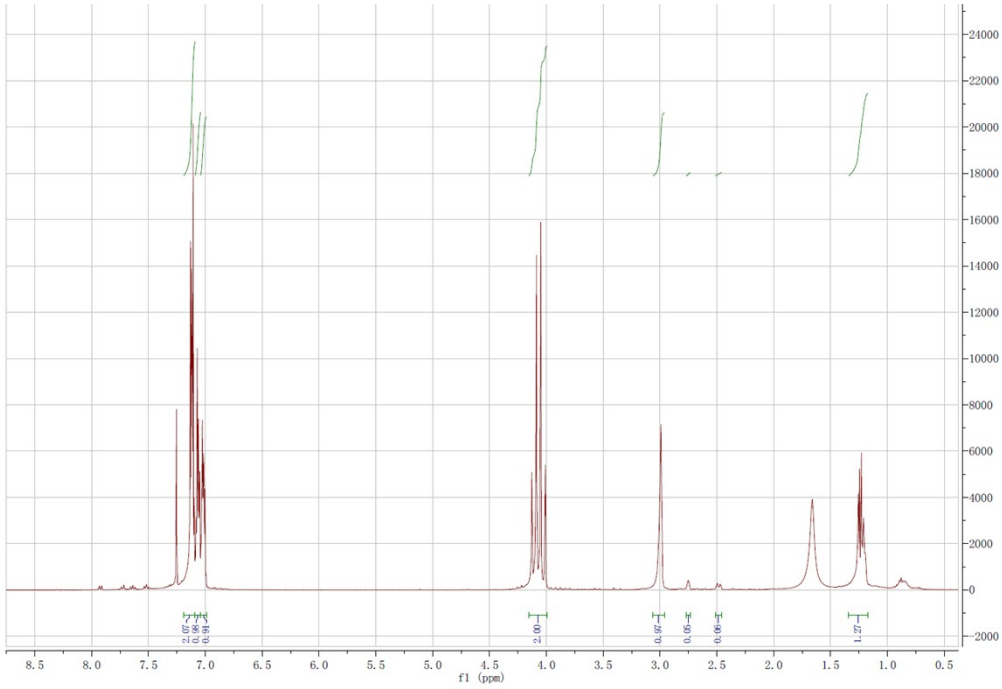


(1)

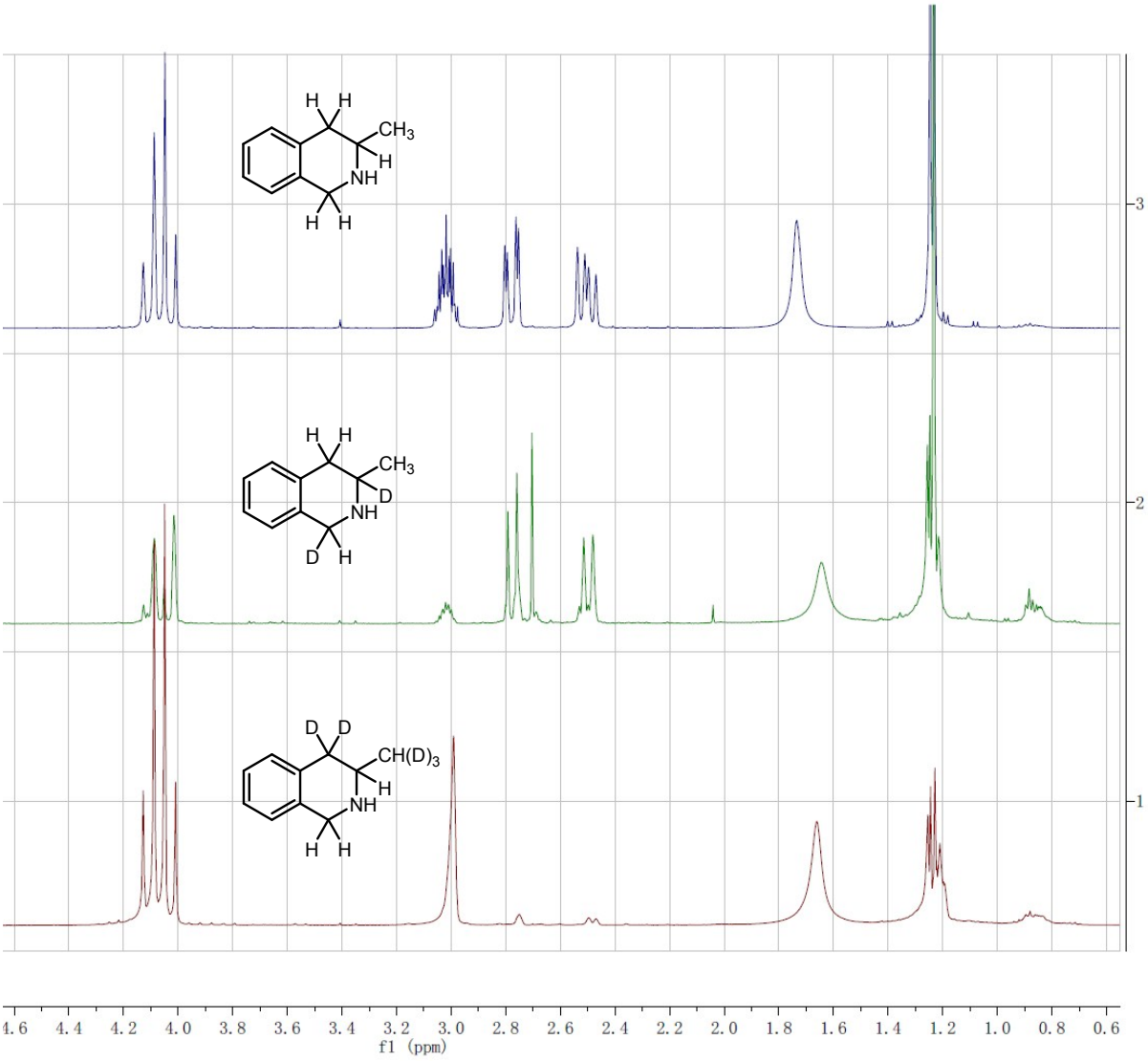

f1 (ppm)


95% D
57% D
99% H
99% H
Rh-L1(2%), H2, CD3OD
then basic work-up
CH(D)3
ND
Cl

(2)


f1 (ppm)

For clarity, combined spectrum for the original 2a and the two deuterated 2a were shown as below:



8. Characterization data of chiral THQs and THIQs

3-methyl-1,2,3,4-tetrahydroisoquinoline (2a)

Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 7.11 (m, 2H), 7.06 (m, 1H), 7.01 (t, 1H), 4.11 (d, *J* =16.0 Hz, 1H), 4.02 (d, *J* =16.0 Hz, 1H), 3.02 (dqd, *J* = 10.3, 6.3, 4.0 Hz, 1H), 2.78

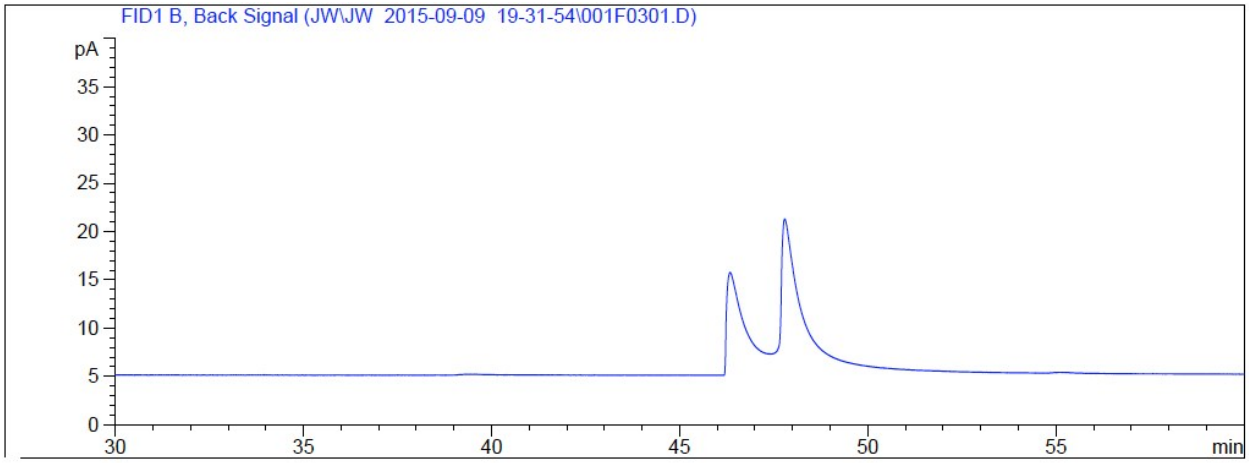
(dd, *J* = 16.4, 3.8 Hz, 1H), 2.51 (dd, *J* = 16.3, 10.7 Hz, 1H), 1.73 (br, 1H), 1.24 (d, *J* = 6.3 Hz, 3H).

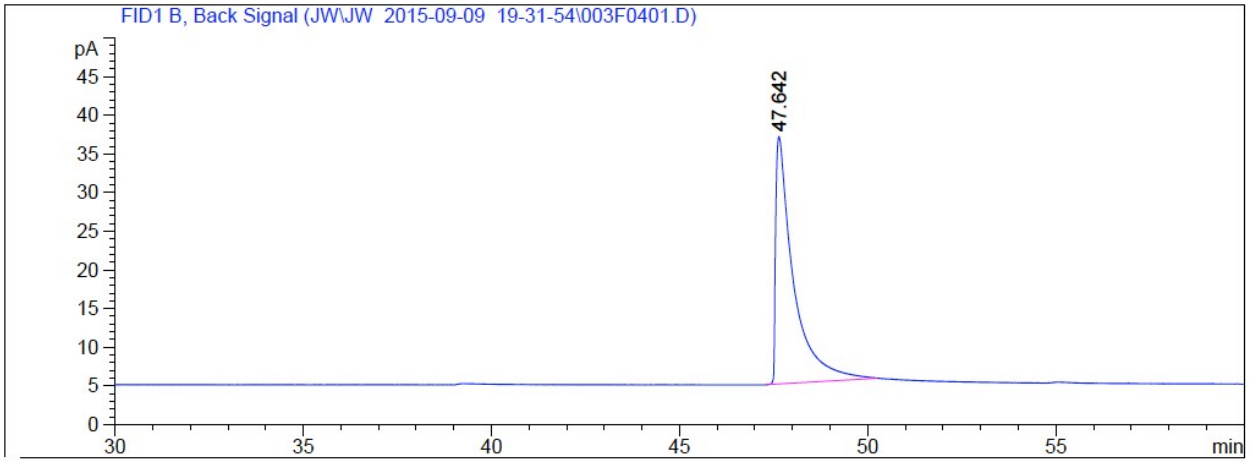
^{13}C NMR (400 MHz, CDCl3): δ 135.39, 134.92, 129.11, 126.01, 126.00, 125.70, 49.25, 48.59, 37.26, 22.50.

$[\alpha]^{22}_{D}$ +103.6 (*c* 0.5, $CHCl_3$).

m/z (ESI–MS) 148.22 $[M + H]^+$.

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 100 °C, t_1 =46.3 min, t_2 =47.7 min.





Signal 1: FID1 B, Back Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	47.642	BB	0.4541	1052.56445	32.00426	1.000e2
Totals :				1052.56445	32.00426	

*** End of Report ***

3-ethyl-1,2,3,4-tetrahydroisoquinoline (2b)

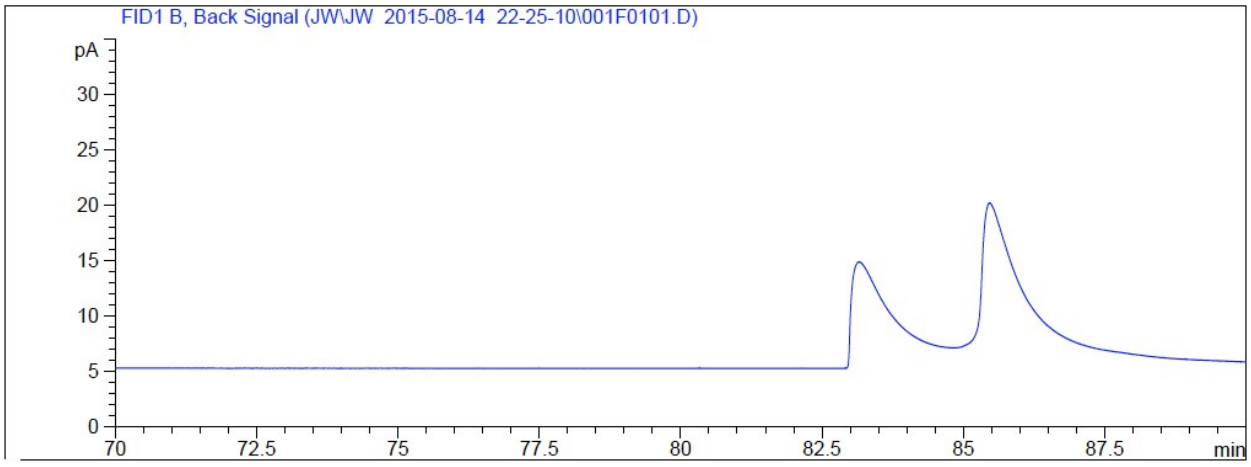
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 7.12 (m, 3H), 7.02 (m, 1H), 4.09 (d, *J* = 12.0 Hz, 1H), 4.03 (d, *J* = 12.0 Hz, 2H), 2.79 (tdd, *J* = 10.4, 6.8, 3.8 Hz, 1H), 2.50 (dd, *J* = 17.0, 11.5 Hz, 1H), 1.74 (br, 1H), 1.64-1.47 (m, 2H), 1.02 (t, 3H).

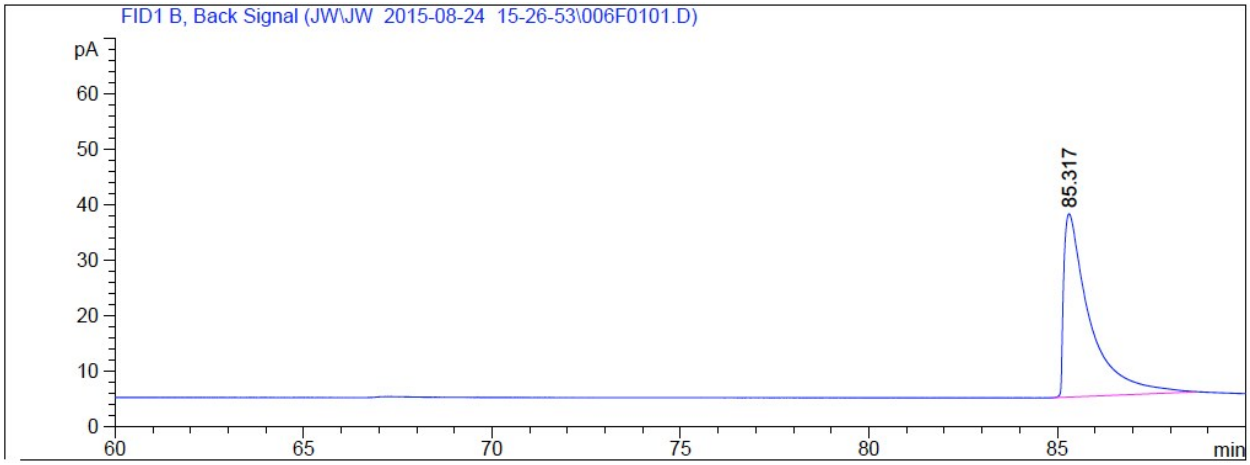
^{13}C NMR (400 MHz, CDCl3): δ 135.76, 134.92, 129.46, 126.01, 125.99, 125.65, 55.25, 48.62, 35.11, 29.61, 10.39.

$[\alpha]^{22}_{D}$ +97.3 (*c* 0.5, $CHCl_3$).

m/z (ESI–MS) 162.09 $[M + H]^+$.

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 100 °C, t_1 =83.2 min, t_2 =85.3 min.





Signal 1: FID1 B, Back Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	85.317	BB	0.6529	1595.54932	33.04603	1.000e2
Totals :				1595.54932	33.04603	

*** End of Report ***

3-butyl-1,2,3,4-tetrahydroisoquinoline (2c)

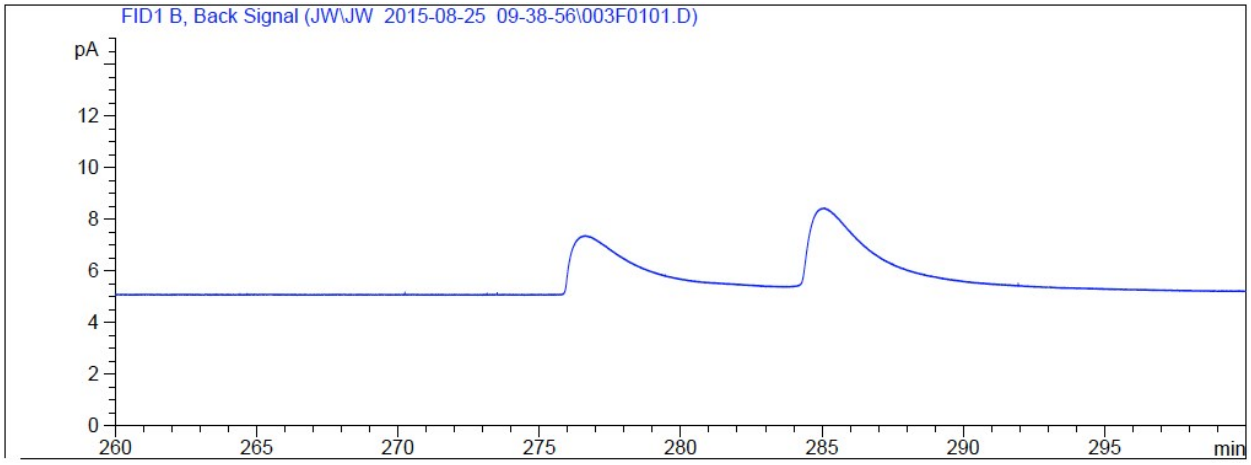
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 7.11 (m, 3H), 7.02 (m, 1H), 4.08 (d, *J* =16.0 Hz, 2H), 4.03 (d, *J* =16.0 Hz, 2H), 2.82 (comp., 2H), 2.50 (dd, *J* = 16.1, 10.4 Hz, 1H), 1.50 (br, 1H), 1.30-1.60 (m, 6H), 1.02 (t, *J* = 3.2 Hz, 3H).

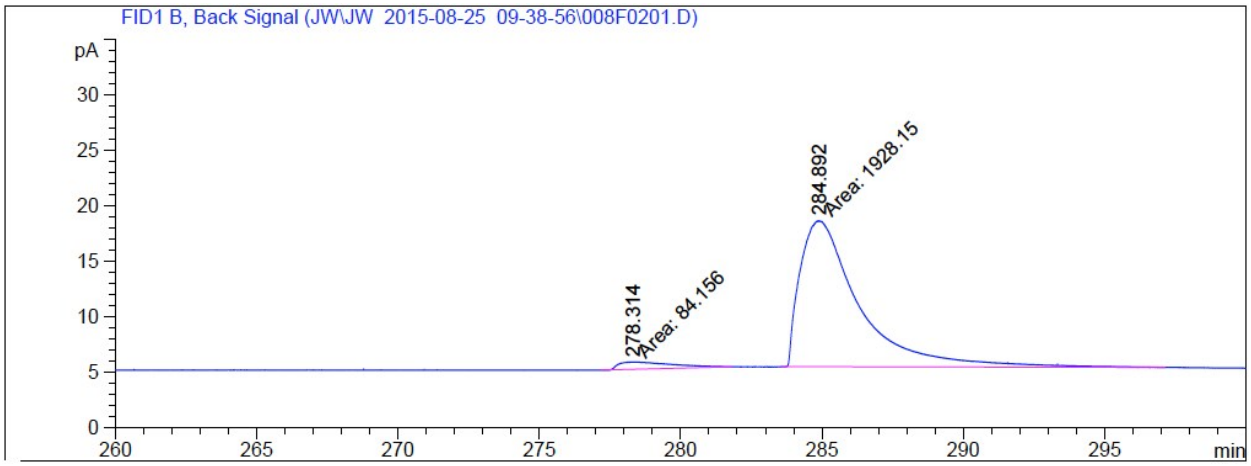
^{13}C NMR (400 MHz, CDCl3): δ 135.78, 134.97, 129.22, 125.99, 125.66, 57.72, 48.60, 36.60, 35.58, 28.19, 22.86, 14.06.

$[\alpha]^{22}_{D}$ +81.8 (*c* 0.5, $CHCl_3$).

m/z (ESI–MS) 190.17 $[M + H]^+$.

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 100 °C, t_1 =278.3 min, t_2 =285.0 min.





Signal 1: FID1 B, Back Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	278.314	MM	2.1398	84.15600	6.55473e-1	4.18207
2	284.892	MM	2.4380	1928.14819	13.18125	95.81793
Totals :				2012.30419	13.83672	

*** End of Report ***

3,6-dimethyl-1,2,3,4-tetrahydroisoquinoline (2d)

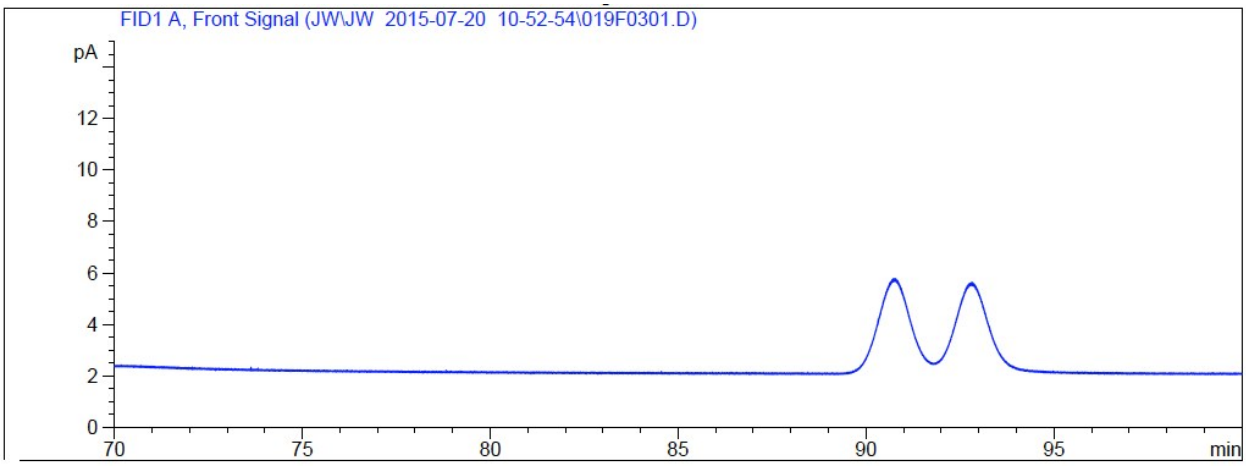
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 7.00 – 6.77 (m, 3H), 4.06 (d, *J* = 15.7 Hz, 1H), 3.99 (d, *J* = 15.8 Hz, 1H), 3.05–2.94 (m, 1H), 2.73 (dd, *J* = 16.3, 3.4 Hz, 1H), 2.46 (dd, *J* = 16.0, 10.8 Hz, 1H), 2.29 (s, 3H), 1.69 (s, 1H), 1.23 (d, *J* = 6.3 Hz, 3H).

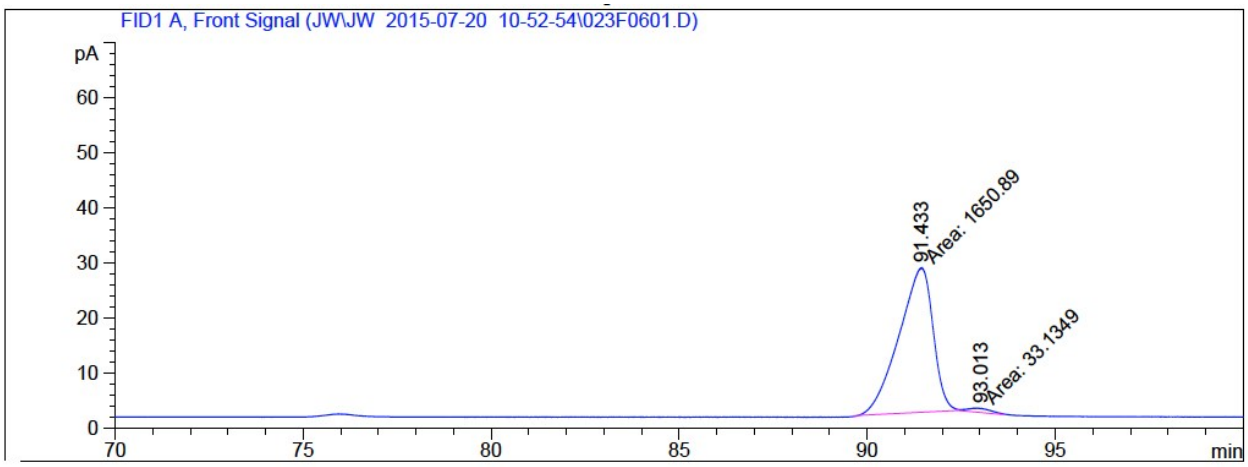
^{13}C NMR (400 MHz, CDCl3): δ 135.45, 134.76, 132.38, 129.60, 126.65, 125.88, 49.28, 48.33, 37.27, 22.49, 20.98.

$[\alpha]^{22}_{D}$ +87.4 (*c* 0.5, $CHCl_3$).

m/z (ESI–MS) 162.08 $[M + H]^+$.

Supelco Chiral Select 1000 column (30 m ×0.25 mm × 0.25 μm) for its corresponding trifluoroacetamide, He 1.0 mL/min, column 120 °C, t_1 =91.4 min, t_2 =93.0 min.





Signal 1: FID1 A, Front Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	91.433	MM	1.0499	1650.89038	26.20647	98.03240
2	93.013	MM	0.7184	33.13491	7.68718e-1	1.96760
Totals :				1684.02529	26.97519	

*** End of Report ***

6-trifluoromethyl-3-methyl-1,2,3,4-tetrahydroisoquinoline (2e)

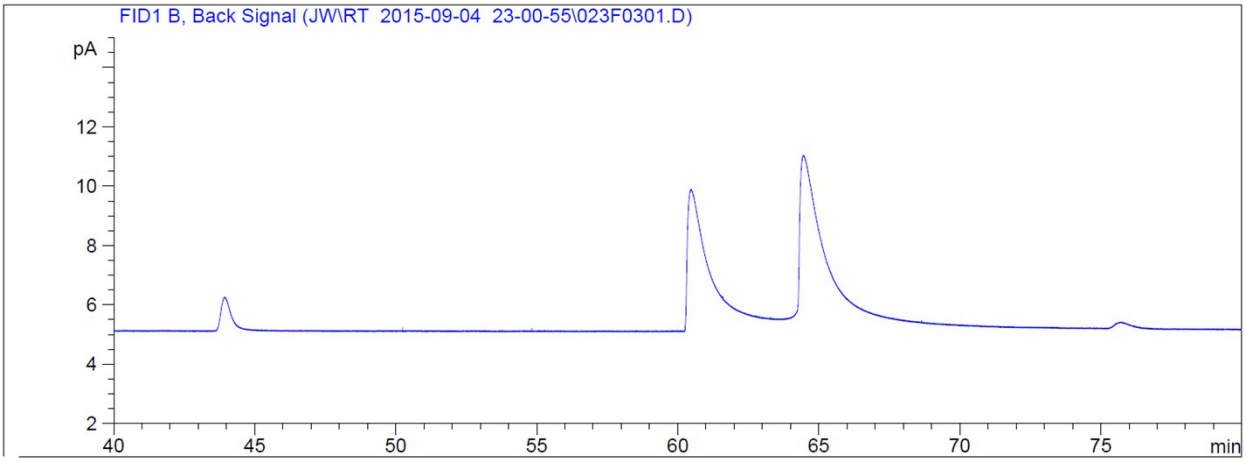
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 7.36 (d, *J* = 8.1 Hz, 1H), 7.32 (s, 1H), 7.12 (d, *J* = 8.0 Hz, 1H), 3.14 (d, *J* = 16.4 Hz, 1H), 3.09 (d, *J* = 16.4 Hz, 1H), 2.83 (dd, *J* = 16.5, 3.7 Hz, 1H), 2.54 (dd, *J* = 16.4, 10.6 Hz, 1H), 1.26 (d, *J* = 6.3 Hz, 3H).

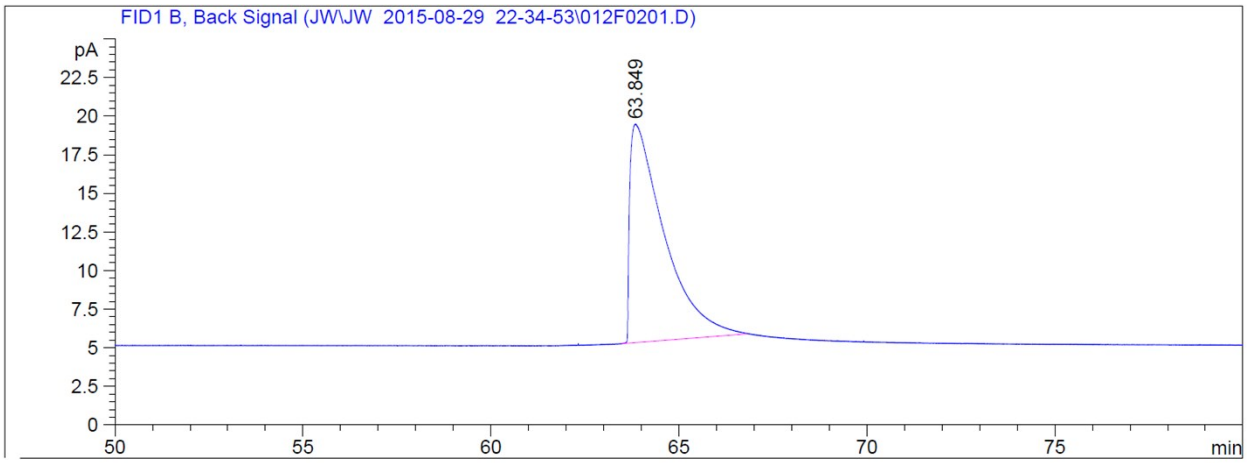
^{13}C NMR (400 MHz, CDCl3): δ 139.32, 135.72, 128.46 (q, *J* = 127.6 Hz), 126.46, 125.96 (q, *J* = 15.2 Hz), 122.97, 122.48 (q, *J* = 7.0 Hz), 49.03, 48.44, 37.13, 22.27.

$[\alpha]^{22}_{D}$ +80.2 (*c* 0.5, $CHCl_3$).

m/z (ESI–MS) 216.01 $[M + H]^+$.

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 100 °C, t_1 =60.8 min, t_2 =64.7 min.





Signal 1: FID1 B, Back Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	63.849	BB	0.8115	897.82019	14.13314	1.000e2
Totals :				897.82019	14.13314	

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*** End of Report ***

6-chloro-3-methyl-1,2,3,4-tetrahydroisoquinoline (2f)

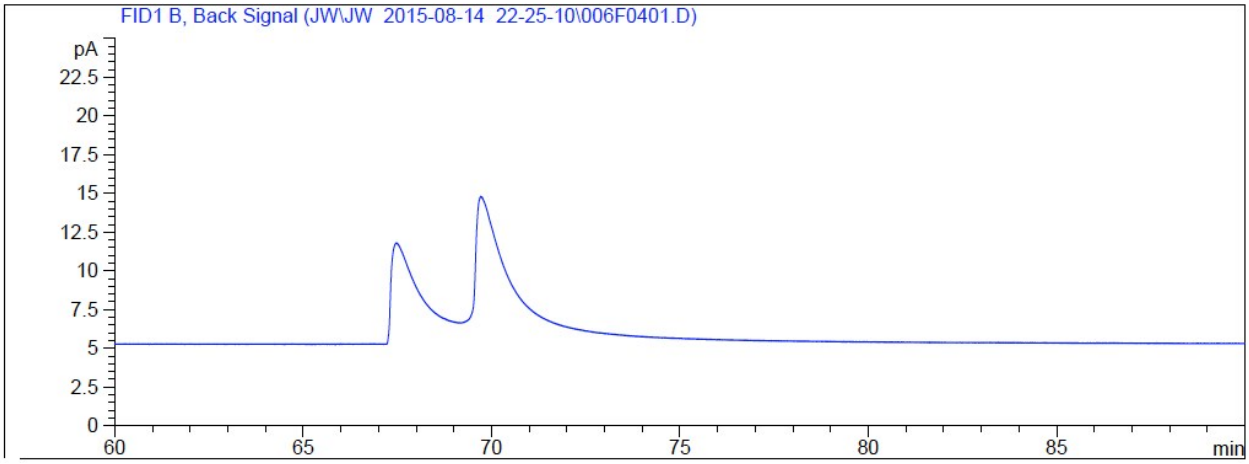
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 7.07 (t, 2H), 6.94 (d, *J* = 8.1 Hz, 1H), 4.05 (d, *J* = 16.0 Hz, 1H), 3.99 (d, *J* = 16.0 Hz, 1H), 2.99 (dqd, *J* = 12.6, 6.3, 4.0 Hz, 1H), 2.74 (dd, *J* = 16.5, 3.7 Hz, 1H), 2.48 (dd, *J* = 16.5, 10.6 Hz, 1H), 1.71 (br, 1H), 1.24 (d, *J* = 6.3 Hz, 3H).

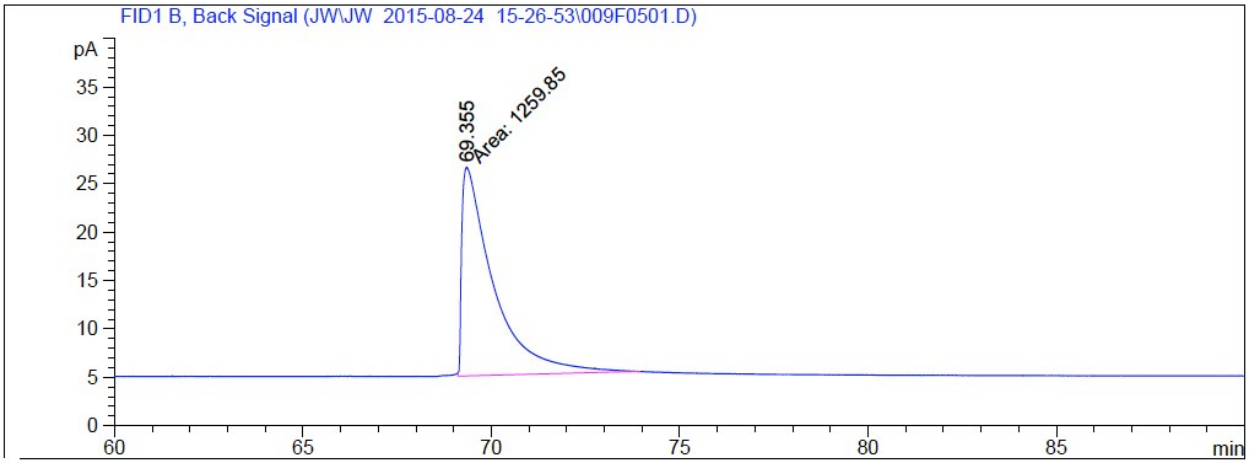
^{13}C NMR (400 MHz, CDCl3): δ 136.86, 133.77, 131.48, 128.83, 127.33, 125.87, 48.92, 48.09, 37.04, 29.29.

$[\alpha]^{22}_{D}$ +72.1 (*c* 0.5, $CHCl_3$).

m/z (ESI–MS) 182.15, 184.02 $[M + H]^+$.

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 120 °C, t_1 =67.5 min, t_2 =69.4 min.





Signal 1: FID1 B, Back Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	69.355	MM	0.9725	1259.84631	21.59215	1.000e2
Totals :				1259.84631	21.59215	

*** End of Report ***

6-fluoro-3-methyl-1,2,3,4-tetrahydroisoquinoline (2g)

Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 6.96 (dd, *J* = 8.3, 5.8 Hz, 1H), 6.81 (td, *J* = 8.5, 2.6 Hz, 1H), 6.76 (dd, *J* = 9.6, 2.5 Hz, 1H), 4.05 (d, *J* = 15.6 Hz, 2H), 4.00 (d, *J* = 15.6 Hz, 2H), 2.99 (dqd, *J* = 10.3, 6.3, 4.0 Hz, 1H), 2.75 (dd, *J* = 16.5, 3.8 Hz, 1H), 2.49 (dd, *J* = 16.5, 10.7 Hz, 1H), 1.24 (d, *J* = 6.3 Hz, 3H).

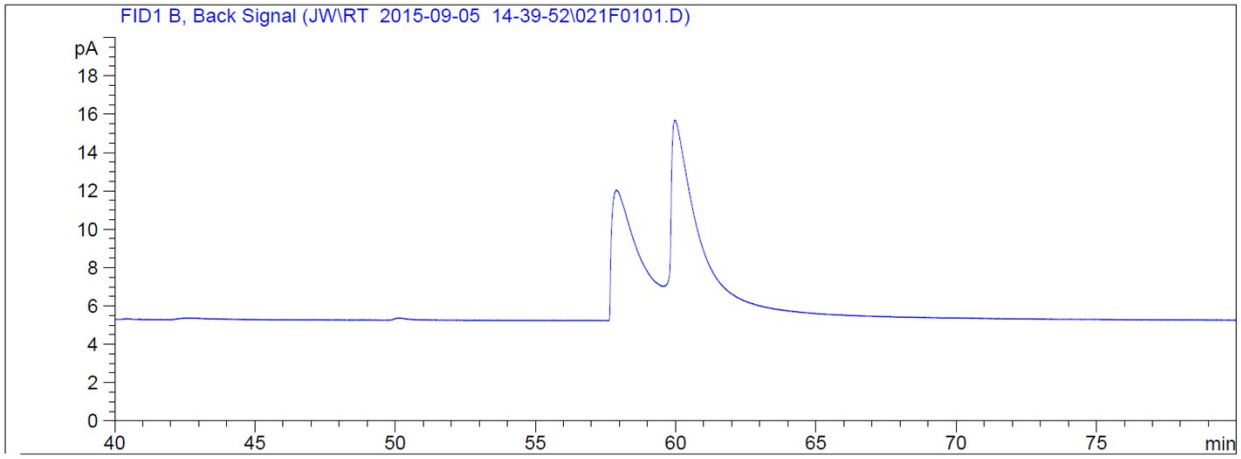
^{13}C NMR (400 MHz, CDCl3): δ 161.18 (d, *J* = 964.4 Hz), 137.00 (d *J* = 29.4 Hz), 130.90 (d, *J* = 11.6 Hz), 127.35 (d, *J* = 32.4 Hz), 115.34 (d, *J* = 81.2 Hz), 112.79 (d, *J* = 86.0 Hz), 48.93, 48.05, 37.32, 22.30.

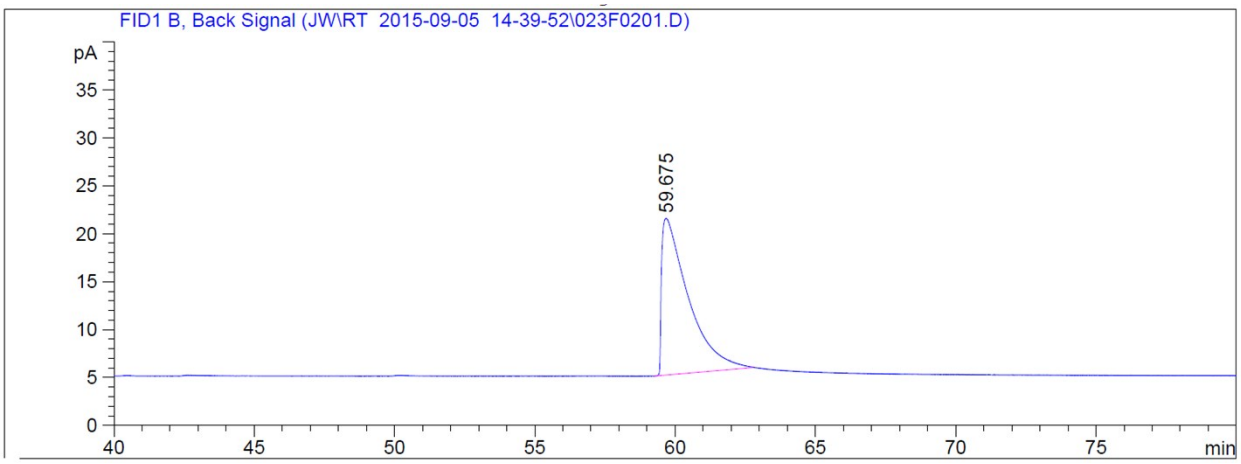
^{19}F NMR (500 MHz, CDCl3): δ -117.42.

$[\alpha]^{22}_{D}$ +82.1 (*c* 0.5, $CHCl_3$).

m/z (ESI–MS) 166.24 $[M + H]^+$.

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 100 °C, t_1 =58.0 min, t_2 =60.0 min.





Signal 1: FID1 B, Back Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	59.675	BB	0.8510	1079.47339	16.33518	1.000e2
Totals :				1079.47339	16.33518	

*** End of Report ***

8-chloro-3-methyl-1,2,3,4-tetrahydroisoquinoline (2h)

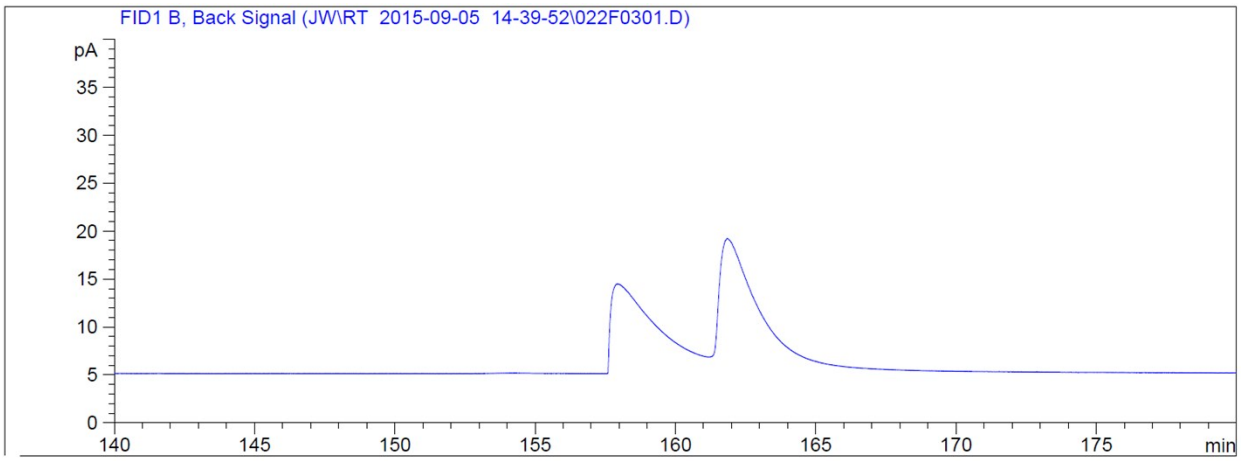
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 7.16 (d, *J* = 7.8 Hz, 1H), 7.06 (t, *J* = 7.7 Hz, 1H), 6.97 (d, *J* = 7.5 Hz, 1H), 4.20 (d, *J* = 16.9 Hz, 1H), 3.94 (d, *J* = 16.9 Hz, 1H), 2.97 (dqd, *J* = 10.1, 6.3, 3.8 Hz, 1H), 2.77 (dd, *J* = 16.3, 3.5 Hz, 1H), 2.50 (dd, *J* = 16.3, 10.6 Hz, 1H), 1.67 (s, 1H), 1.24 (d, *J* = 6.3 Hz, 3H).

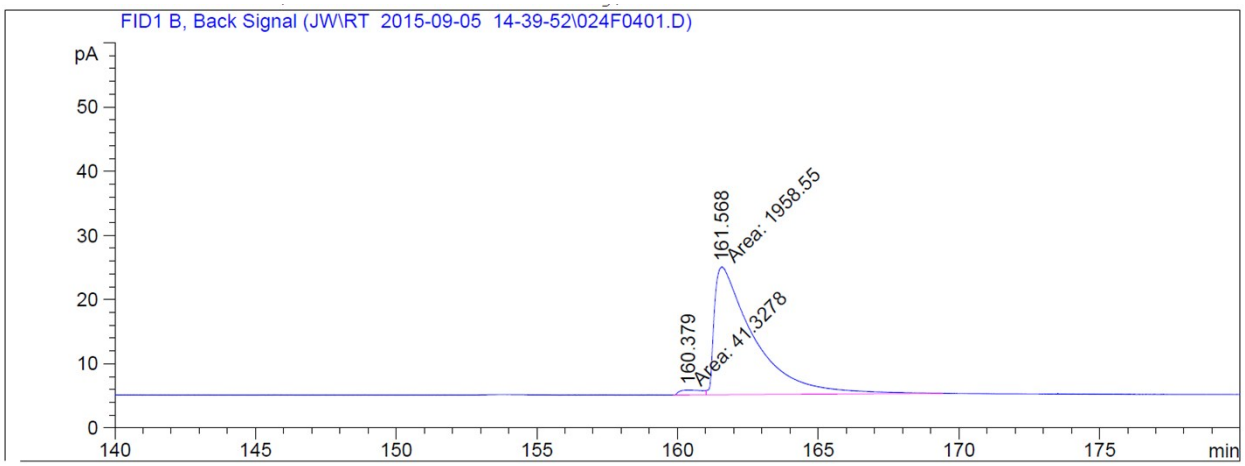
^{13}C NMR (400 MHz, CDCl3): δ 137.42, 133.23, 132.21, 127.52, 126.84, 126.52, 48.57, 46.79, 37.36, 22.19.

$[\alpha]^{22}_{D}$ +117.7 (*c* 0.5, $CHCl_3$).

m/z (ESI–MS) 182.09, 184.01 $[M + H]^+$.

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 100 °C, t_1 =158.2 min, t_2 =160.4 min.





Signal 1: FID1 B, Back Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	160.379	MF	0.9163	41.32780	7.51749e-1	2.06652
2	161.568	FM	1.6383	1958.54700	19.92477	97.93348
Totals :				1999.87479	20.67652	

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*** End of Report ***

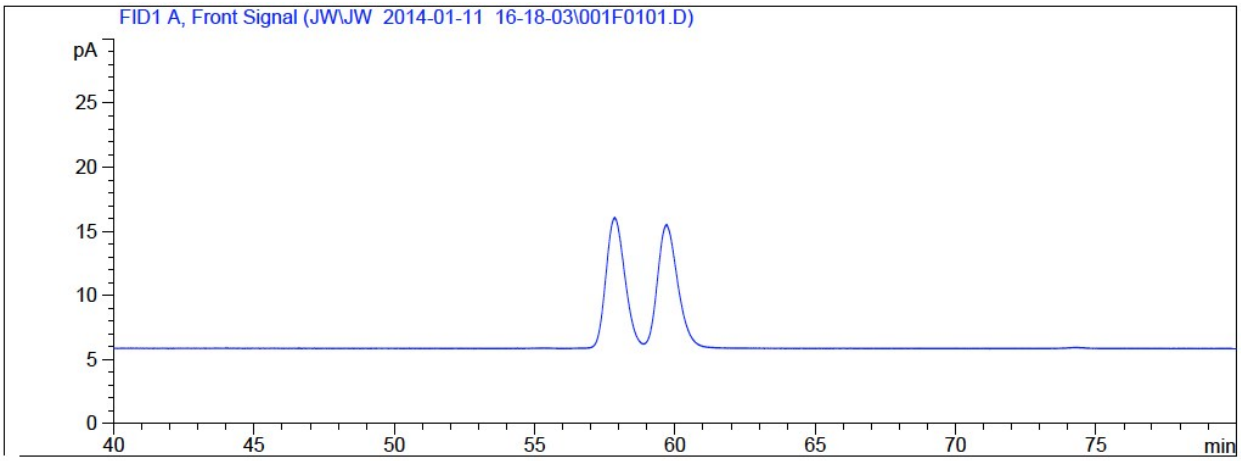
1-methyl-1,2,3,4-tetrahydroisoquinoline (2i)

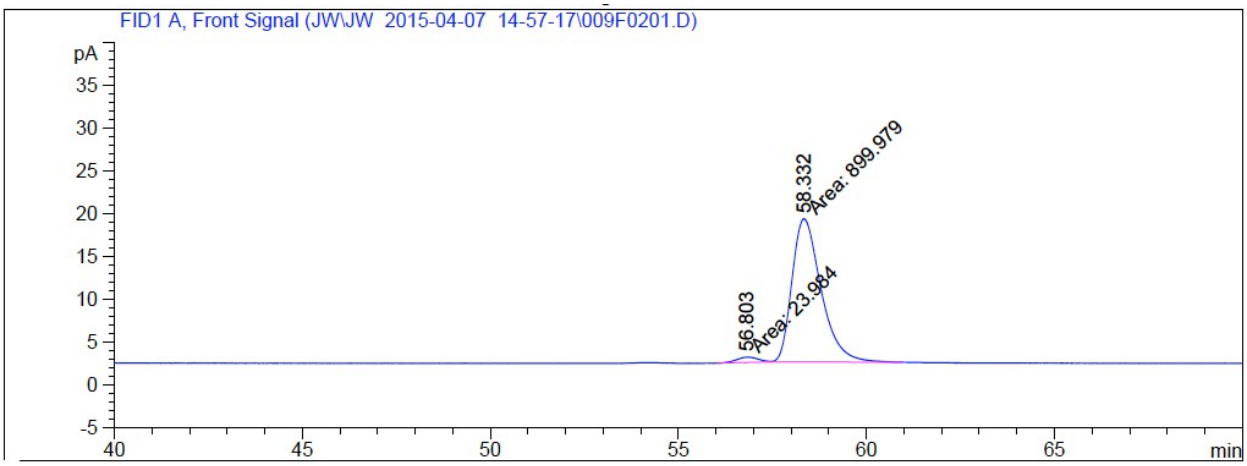
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ7.22 – 7.03 (m, 4H), 4.14 (d, *J* = 6.8 Hz, 1H), 3.31 (M, 1H), 3.03 (m, 1H), 2.92 (m, 1H), 2.82 – 2.60 (m, 1H), 2.25 (br, 1H), 1.47 (d, *J* = 5.6 Hz, 3H).

^{13}C NMR (400 MHz, CDCl3): δ 140.32, 134.68, 129.20, 125.99, 129.90 (overlap), 51.57, 41.71, 29.91, 22.63.

$[\alpha]^{22}_{D}$ -77.0 (*c* 0.5, $CHCl_3$).

Supelco Chiral Select 1000 column (30 m ×0.25 mm × 0.25 μm) for its corresponding trifluoroacetamide, He 1.0 mL/min, column 120 °C, t_1 =56.8 min, t_2 =58.3 min.





Signal 1: FID1 A, Front Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	56.803	MM	0.6386	23.98396	6.25927e-1	2.59577
2	58.332	MM	0.8972	899.97919	16.71776	97.40423
Totals :				923.96314	17.34369	

*** End of Report ***

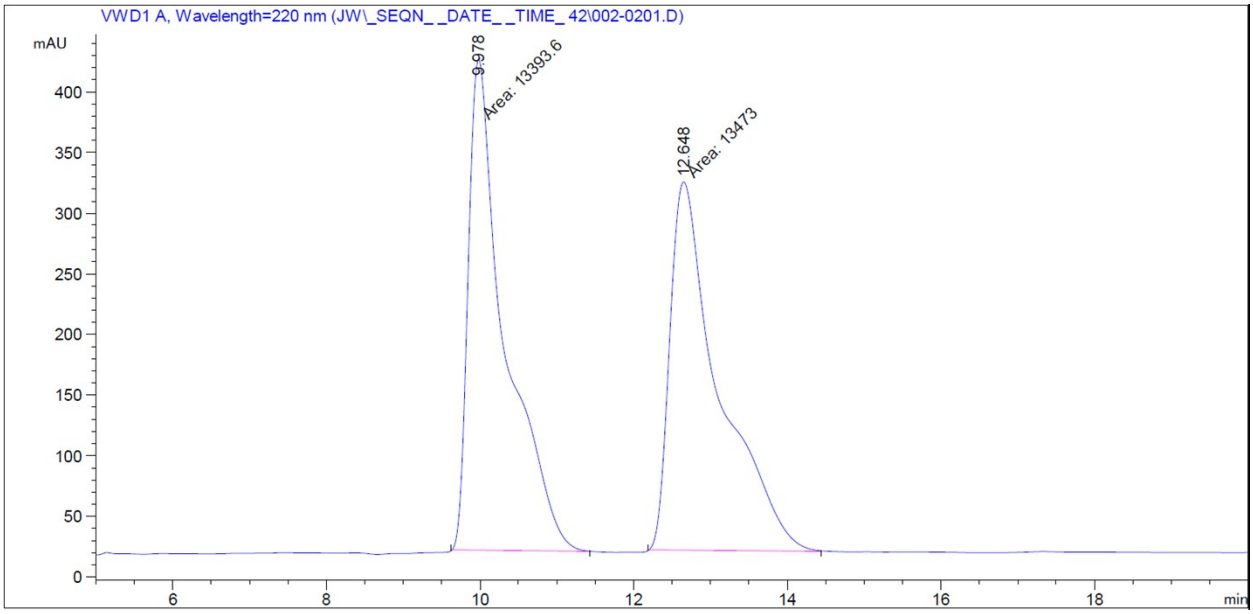
3-phenyl-1,2,3,4-tetrahydroisoquinoline (2j)

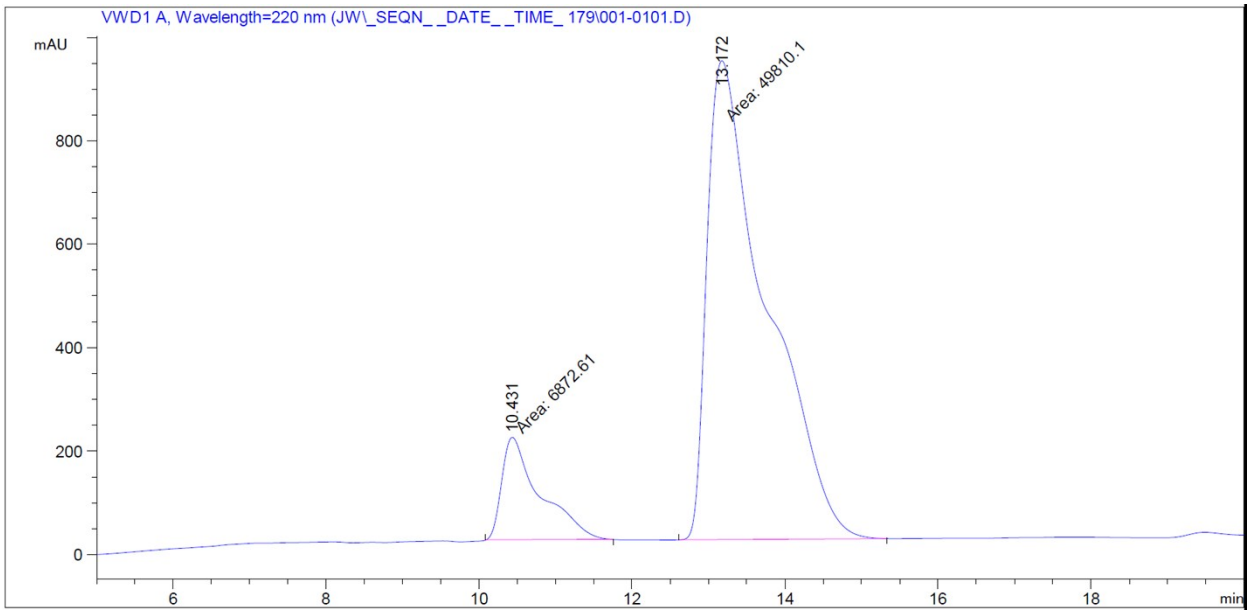
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 7.9 Hz, 2H), 7.36 (dd, *J* = 8.0, 6.5 Hz, 2H), 7.28 (t, *J* = 7.2 Hz, 1H), 7.18-7.05 (m, 4H), 4.26 (d, *J* = 15.6 Hz, 1H), 4.16 (d, *J* = 15.6 Hz, 1H), 4.00 (t, *J* = 7.5 Hz, 1H), 2.97 (d, *J* = 7.3 Hz, 2H), 1.93 (br, 1H).

^{13}C NMR (400 MHz, CDCl3): δ 144.33, 135.04, 134.92, 129.10, 128.63, 127.39, 126.55, 126.26, 126.18, 125.90, 58.61, 49.27, 37.73.

Daicel Chiralpak OD-H for its corresponding trifluoroacetamide, hexanes/i-PrOH = 98/2, Flow rate = 1.0 ml/min, UV = 220 nm, t_1 = 10.4 min, t_2 = 13.1 min.

$[\alpha]^{22}_{D}$ +100.3 (*c* 0.5, $CHCl_3$) for (R) isomer[7].





Signal 1: VWD1 A, Wavelength=220 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	10.431	MM	0.5781	6872.61035	198.15254	12.1247
2	13.172	MM	0.8965	4.98101e4	925.97284	87.8753
Totals :				5.66827e4	1124.12538	

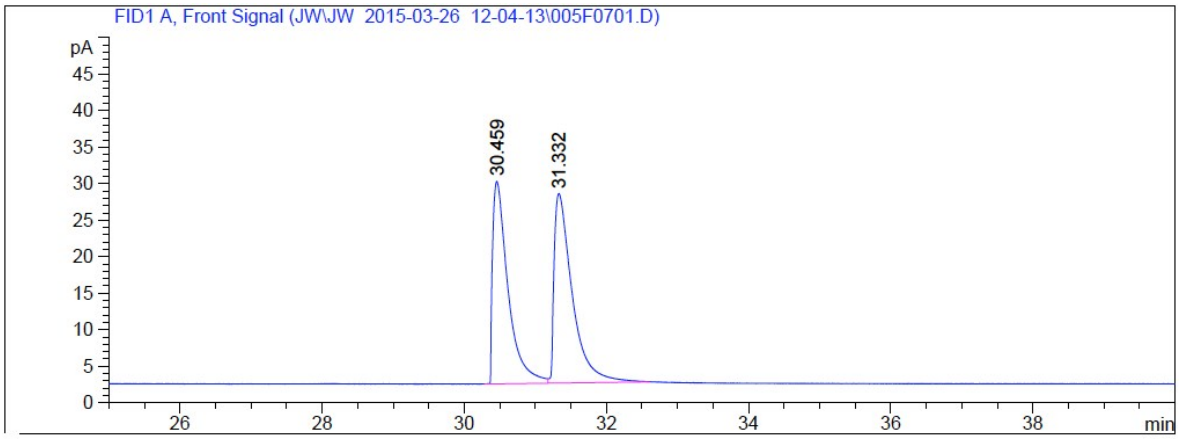
2-methyl-1,2,3,4-tetrahydroquinoline (4a)

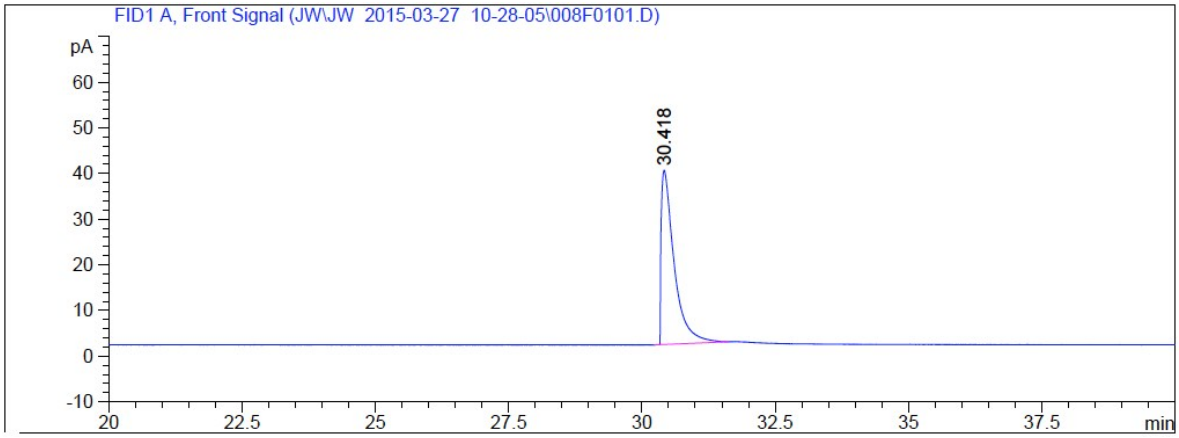
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 6.98 – 6.92 (m, 2H), 6.59 (td, *J* = 7.4, 1.1 Hz, 1H), 6.45 (dd, *J* = 5.2, 3.2 Hz, 1H), 3.67 (b, 1H), 3.43 – 3.35 (m, 1H), 2.83 (ddd, *J* = 16.9, 11.5, 5.6 Hz, 1H), 2.75 – 2.68 (m, 1H), 1.95 – 1.88 (m, 1H), 1.58 (dddd, *J* = 12.8, 11.6, 10.0, 5.4 Hz, 1H), 1.20 (d, *J* = 6.3 Hz, 3H).

^{13}C NMR (400 MHz, CDCl3): δ 143.73, 128.22, 125.65, 120.09, 115.97, 112.98, 46.15, 29.12, 25.55, 21.56.

$[\alpha]^{22}_{D}$ -44.3 (*c* 0.5, $CHCl_3$).

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 120 °C, t_1 =30.5 min, t_2 =31.3 min.





Signal 1: FID1 A, Front Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	30.418	BB	0.2479	643.22015	38.15113	1.000e2
Totals :				643.22015	38.15113	

*** End of Report ***

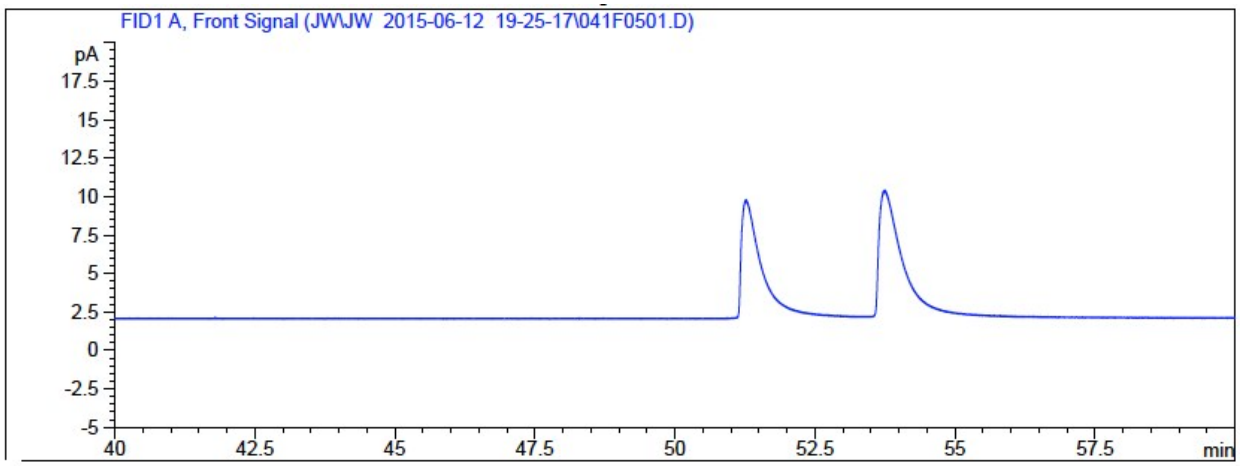
2-ethyl-1,2,3,4-tetrahydroquinoline (4b)

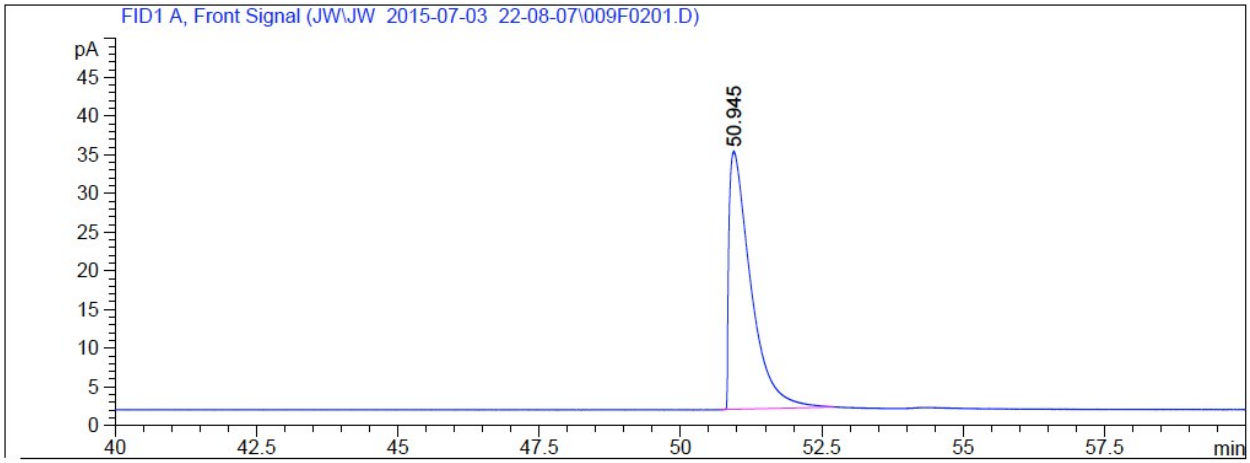
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 6.95 (t, *J* = 7.2 Hz, 2H), 6.59 (t, *J* = 7.3 Hz, 1H), 6.47 (d, *J* = 8.1 Hz, 1H), 3.76 (br, 1H), 3.20 – 3.12 (m, 1H), 2.81 (ddd, *J* = 16.4, 11.0, 5.5 Hz, 1H), 2.76 – 2.68 (m, 1H), 2.00 – 1.92 (m, 1H), 1.65 – 1.55 (m, 1H), 1.51 (dd, *J* = 14.3, 7.2 Hz, 2H), 0.98 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (400 MHz, CDCl3): δ 143.72, 128.18, 125.66, 120.36, 115.84, 112.96, 52.03, 28.73, 26.57, 25.38, 8.98.

$[\alpha]^{22}_{D}$ -74.4 (*c* 0.5, $CHCl_3$).

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 120 °C, t_1 =51.3 min, t_2 =53.7 min.





Signal 1: FID1 A, Front Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	50.945	BB	0.3928	892.10315	33.27738	1.000e2
Totals :				892.10315	33.27738	

*** End of Report ***

2-isopropyl-1,2,3,4-tetrahydroquinoline (4c)

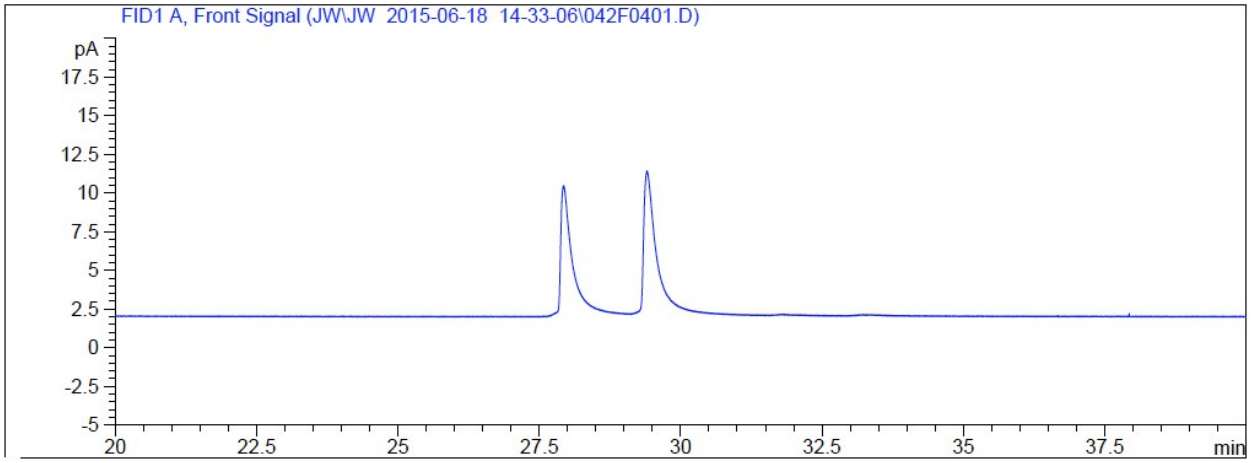
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 6.95 (t, *J* = 7.7 Hz, 2H), 6.58 (t, *J* = 7.3 Hz, 1H), 6.47 (d, *J* = 8.0 Hz, 1H), 3.75 (s, 1H), 3.05 – 3.00 (m, 1H), 2.80 (ddd, *J* = 14.0, 9.9,

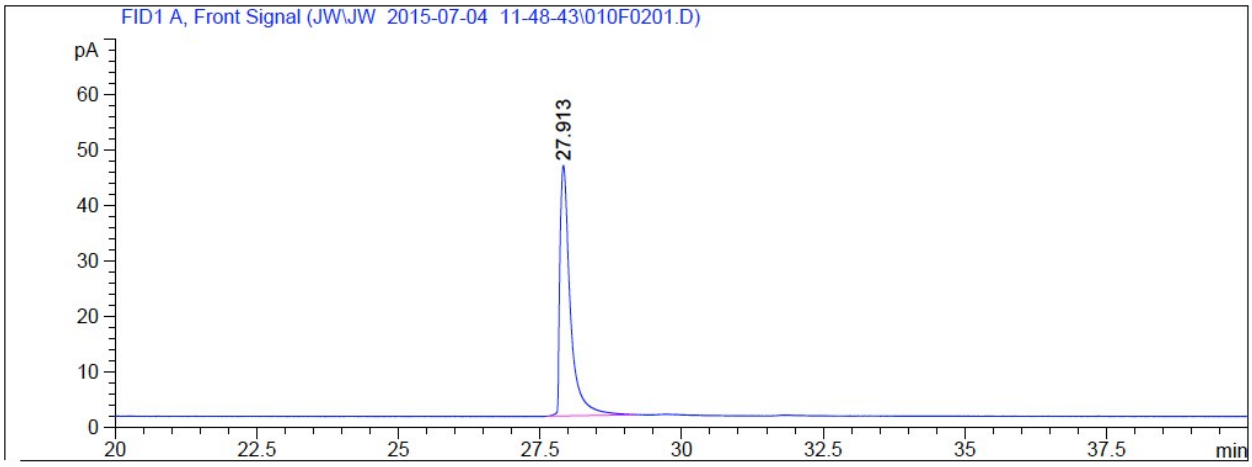
4.2 Hz, 1H), 2.76 – 2.68 (m, 1H), 1.91 (ddt, *J* = 5.9, 4.5, 3.2 Hz, 1H), 1.76 – 1.58 (m, 2iH), 0.98 (dd, *J* = 10.2, 6.8 Hz, 6H).δ 6.95 (t, 2H), 6.58 (t, 1H), 6.47 (d, 1H), 3.03 (m, 1H), 2.75 (m, 2H), 1.91 (m, 1H), 1.69 (m, 2H), 0.98 (dd, 6H).

^{13}C NMR (400 MHz, CDCl3): δ 144.00, 128.08, 125.66, 120.40, 115.70, 112.93, 56.29, 31.51, 25.61, 23.53, 17.38 (d).

$[\alpha]^{22}_{D}$ -44.0 (*c* 0.5, $CHCl_3$).

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 140 °C, t_1 =27.9 min, t_2 =29.4 min.





Signal 1: FID1 A, Front Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	27.913	BB	0.1944	578.82666	45.13346	1.000e2
Totals :				578.82666	45.13346	

*** End of Report ***

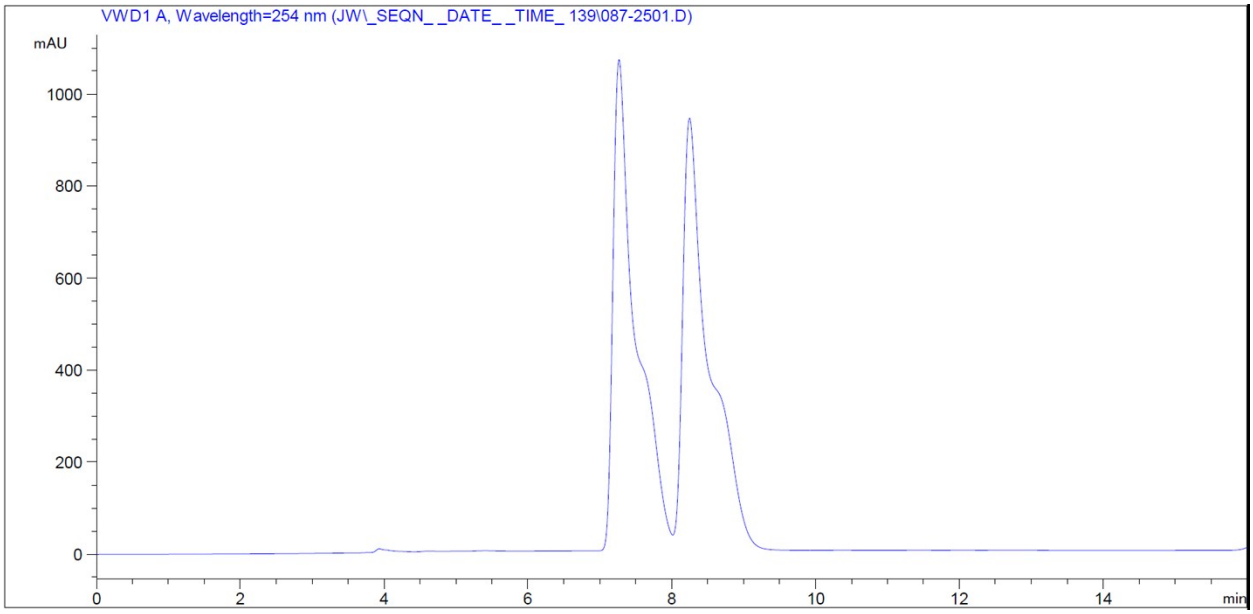
2-pentyl-1,2,3,4-tetrahydroquinoline (4d)

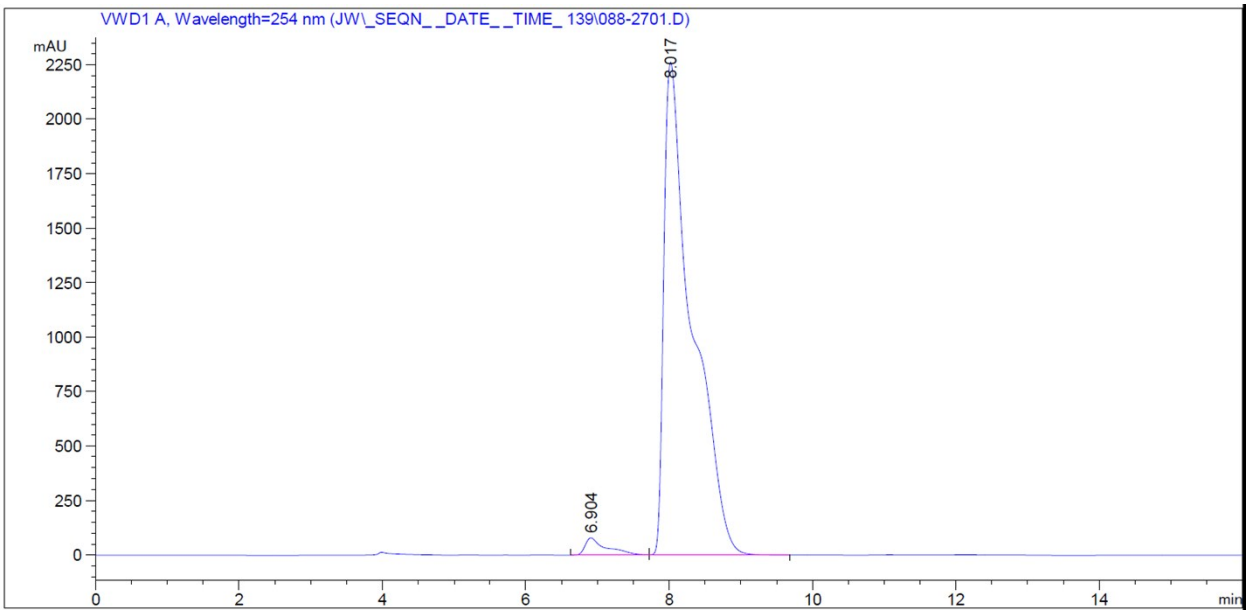
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 6.95 (t, *J* = 7.2 Hz, 2H), 6.58 (t, *J* = 7.4, 1H), 6.46 (d, *J* = 7.5 Hz, 1H), 3.75 (br, 1H), 3.22 (dtd, *J* = 9.4, 6.3, 2.9 Hz, 1H), 2.86 – 2.75 (m, 1H), 2.71 (dt, *J* = 16.3, 4.8 Hz, 1H), 1.99 – 1.91 (m, 1H), 1.64 – 1.53 (m, 1H), 1.47 (t, *J* = 6.7 Hz, 2H), 1.42 – 1.27 (m, 6H), 0.90 (t, *J* = 6.9 Hz, 3H).

^{13}C NMR (400 MHz, CDCl3): δ 143.71, 128.19, 125.65, 120.36, 115.84, 112.99, 50.58, 35.66, 30.93, 27.11, 25.40, 24.36, 21.59, 12.98 (d).

$[\alpha]^{22}_{D}$ -78.2 (*c* 0.5, $CHCl_3$).

Daicel Chiralpak OD-H, hexanes/i-PrOH = 99/1, Flow rate = 1.0 ml/min, UV = 254 nm, t_1 = 6.9 min, t_2 = 8.0 min.





Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	6.904	VV	0.2857	1660.45337	79.54791	2.6200
2	8.017	VB	0.3809	6.17146e4	2262.38330	97.3800
Totals :				6.33750e4	2341.93121	

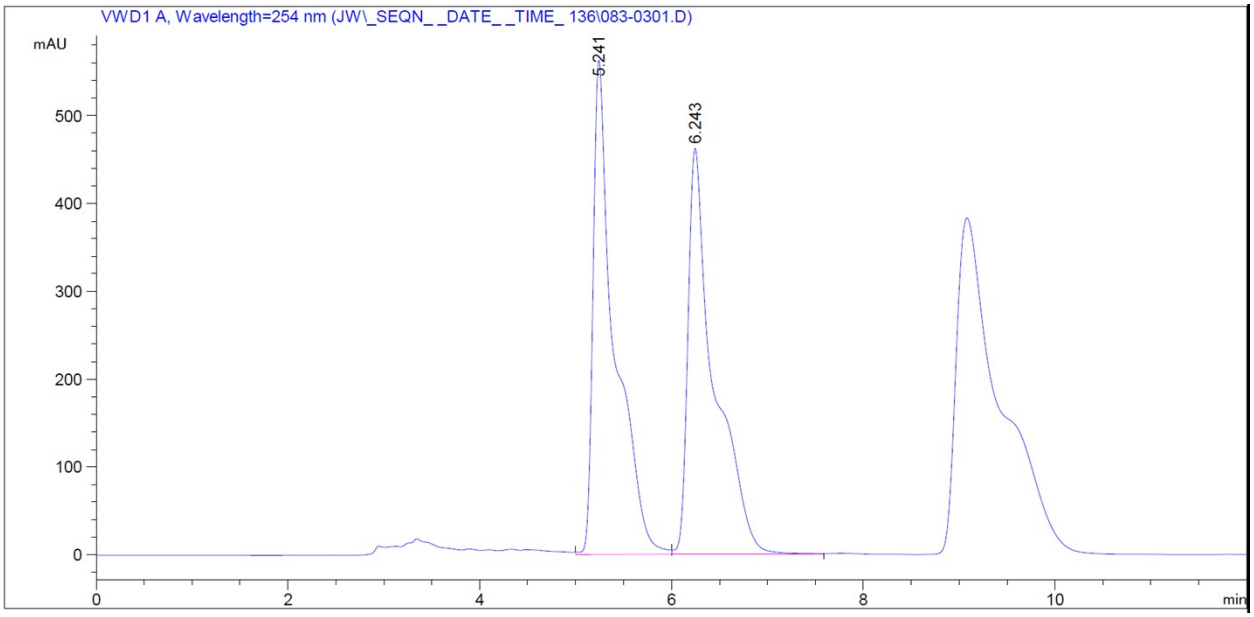
2-undecyl-1,2,3,4-tetrahydroquinoline (4e0

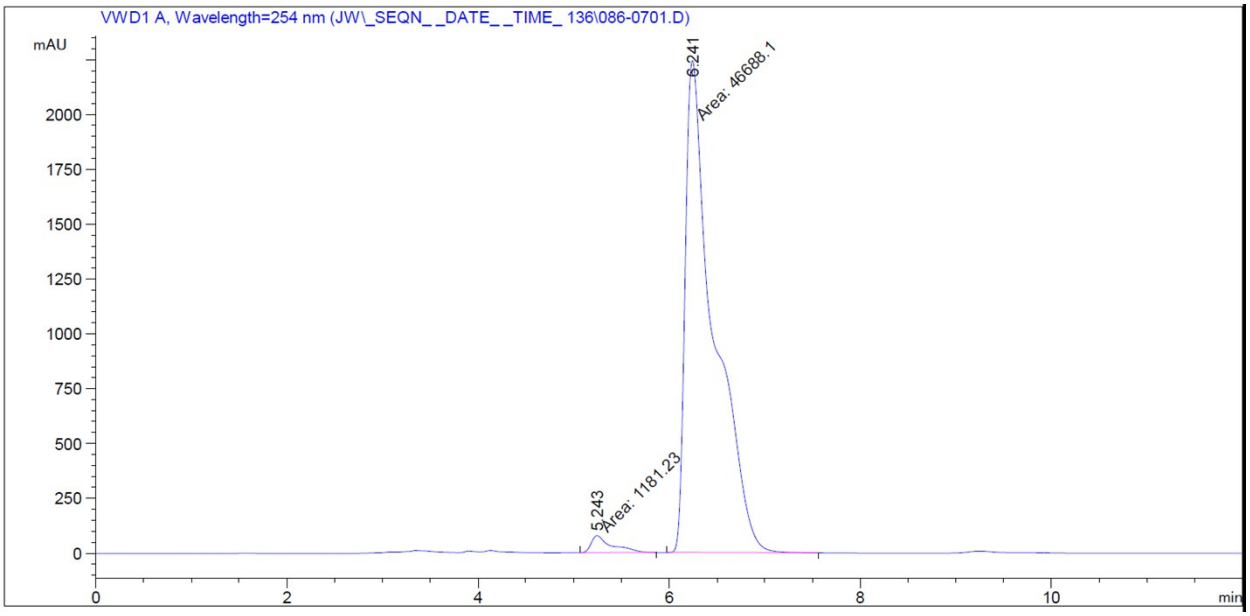
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 6.95 (t, *J* = 7.5 Hz, 2H), 6.58 (td, *J* = 7.4, 1.1 Hz, 1H), 6.47 (dd, *J* = 9.0, 8.2 Hz, 1H), 3.74 (br, 1H), 3.27 – 3.18 (m, 1H), 2.80 (ddd, *J* = 16.4, 10.9, 5.5 Hz, 1H), 2.71 (dt, *J* = 16.3, 4.7 Hz, 1H), 1.95 (ddt, *J* = 6.9, 5.5, 4.0 Hz, 1H), 1.65 – 1.53 (m, 1H), 1.43 – 1.51 (m, 2H), 1.34 (dd, *J* = 45.4, 7.5 Hz, 18H), 0.88 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (400 MHz, CDCl3): δ 143.71, 128.19, 125.65, 120.35, 115.84, 112.99, 50.59, 35.71, 30.88, 28.74, 28.59, 28.30, 27.12, 25.41, 24.70, 21.65, 13.05 (d).

Daicel Chiralpak OD-H, hexanes/i-PrOH = 98/2, Flow rate = 1.0 ml/min, UV = 254 nm, t_1 = 5.2 min, t_2 = 6.2 min.

$[\alpha]^{22}_{D}$ -55.1 (*c* 0.5, $CHCl_3$).





Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	5.243	MM	0.2518	1181.22571	78.17448	2.4676
2	6.241	MM	0.3466	4.66881e4	2244.74536	97.5324
Totals :				4.78693e4	2322.91985	

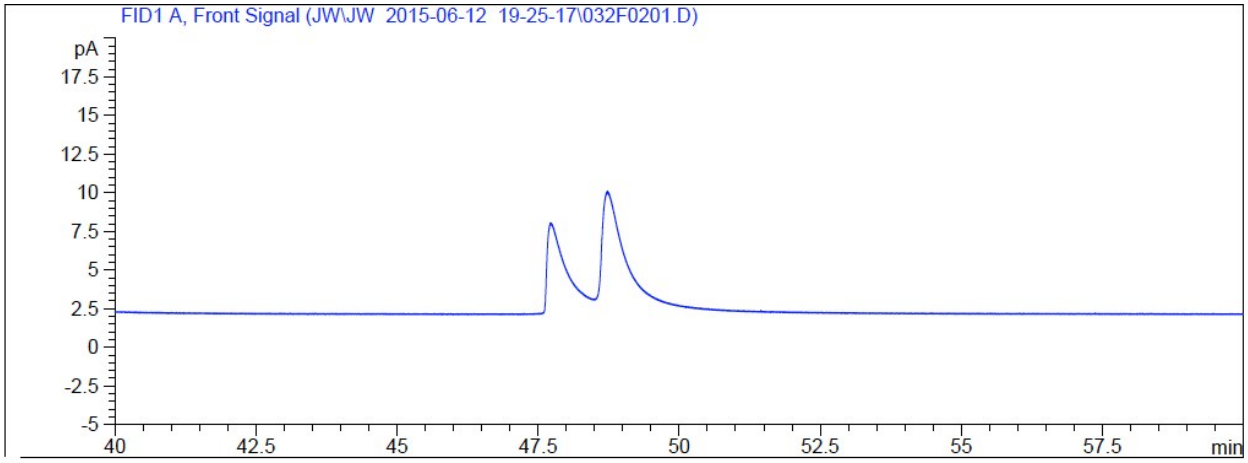
2,6-dimethyl-1,2,3,4-tetrahydroquinoline (4f)

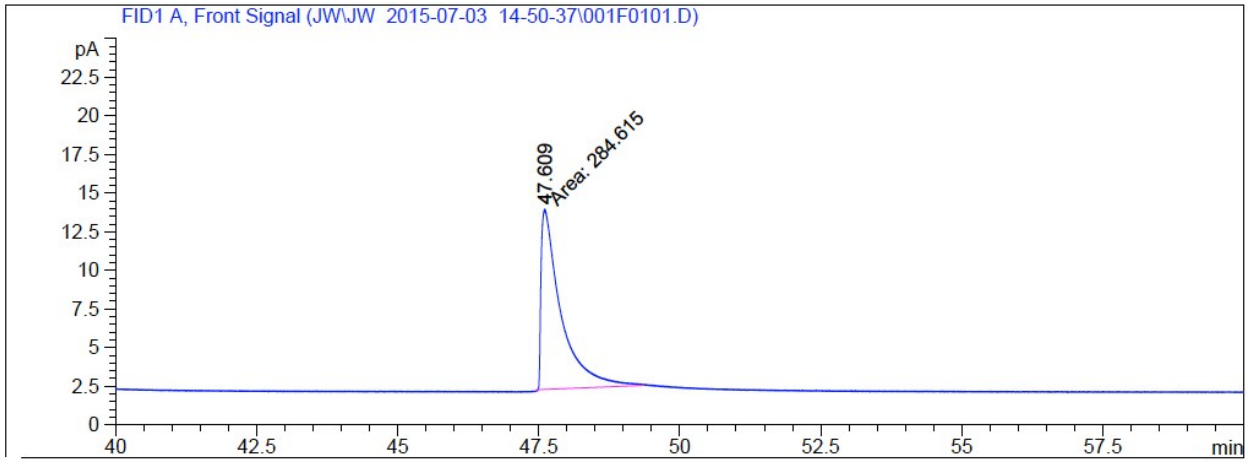
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): 6.77 (d, *J* = 8.4 Hz, 2H), 6.39 (d, *J* = 8.4 Hz, 1H), 3.35 (dqd, *J* = 12.5, 6.3, 2.8 Hz, 1H), 2.80 (ddd, *J* = 17.1, 11.5, 5.8 Hz, 1H), 2.68 (ddd, *J* = 16.4, 5.3, 3.5 Hz, 1H), 2.19 (s, 3H), 1.94 – 1.86 (m, 1H), 1.56 (dddd, *J* = 12.8, 11.5, 10.0, 5.4 Hz, 1H), 1.18 (d, *J* = 6.3 Hz, 3H).

^{13}C NMR (400 MHz, CDCl3): δ 142.46, 129.83, 127.23, 126.26, 121.24, 114.27, 47.35, 30.39, 26.59, 22.59, 20.40.

$[\alpha]^{22}_{D}$ -44.8 (*c* 0.5, $CHCl_3$).

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 120 °C, t_1 =47.8 min, t_2 =48.8 min.





Signal 1: FID1 A, Front Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	47.609	MM	0.4073	284.61505	11.64730	1.000e2
Totals :				284.61505	11.64730	

*** End of Report ***

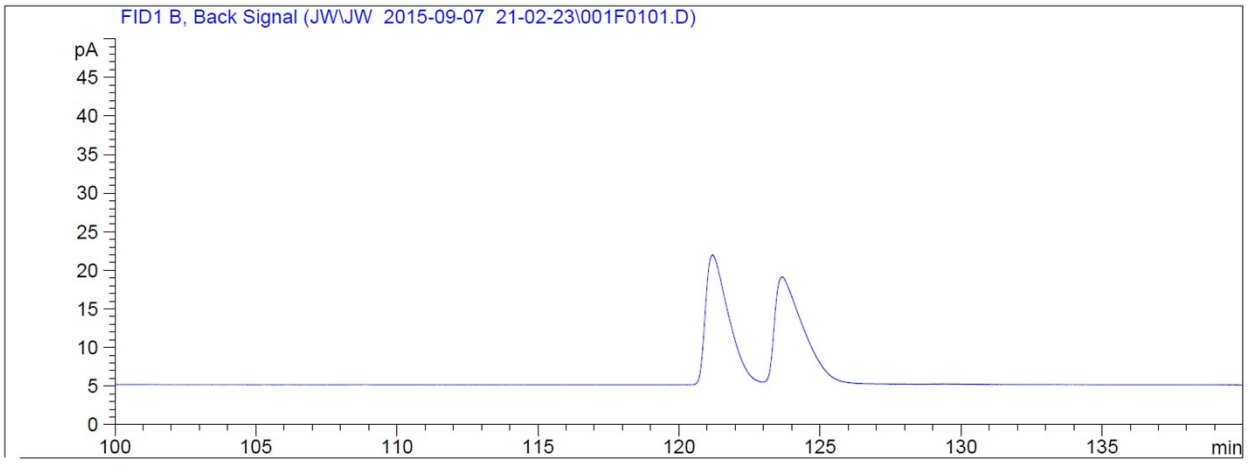
6-methoxy-2-methyl-1,2,3,4-tetrahydroquinoline (4g)

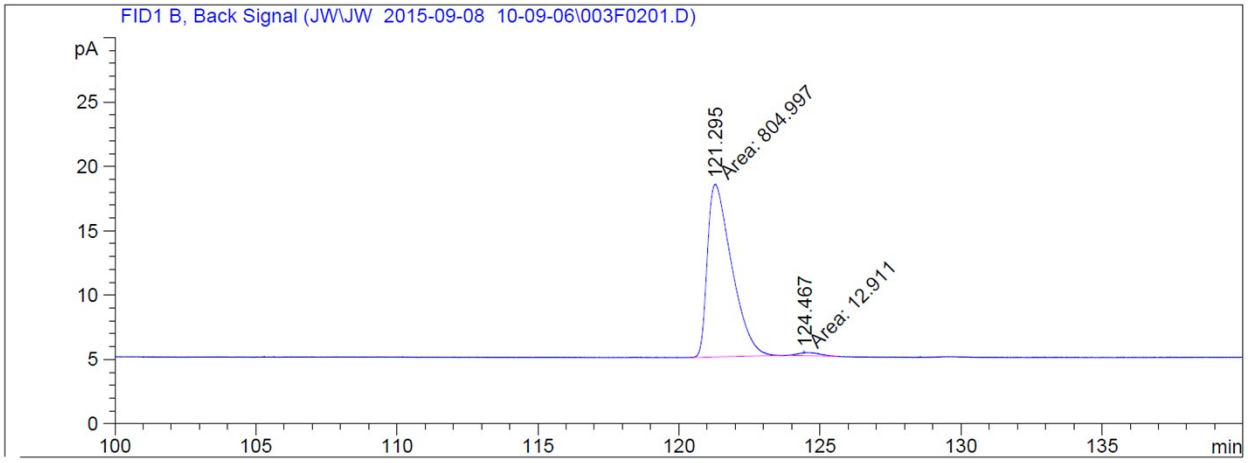
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 6.58 (m, 2H), 6.44 (d, *J* = 8.3 Hz, 1H), 3.72 (s, 3H), 3.37 – 3.27 (m, 1H), 3.17 (br, 1H), 2.83 (ddd, *J* = 17.3, 11.6, 5.9 Hz, 1H), 2.70 (ddd, *J* = 16.6, 5.4, 3.2 Hz, 1H), 1.90 (ddt, *J* = 12.6, 5.9, 2.9 Hz, 1H), 1.56 (dddd, *J* = 12.8, 11.6, 10.2, 5.5 Hz, 1H), 1.19 (d, *J* = 6.3 Hz, 3H).

^{13}C NMR (400 MHz, CDCl3): δ 151.92, 138.93, 122.53, 115.33, 114.72, 112.91, 55.83, 47.50, 30.34, 26.91, 22.54.

$[\alpha]^{22}_{D}$ -34.7 (*c* 0.5, $CHCl_3$).

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 120 °C, t_1 =121.3 min, t_2 =124.5 min.





Signal 1: FID1 B, Back Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	121.295	MM	0.9984	804.99701	13.43821	98.42146
2	124.467	MM	0.7978	12.91097	2.69705e-1	1.57854
Totals :				817.90798	13.70791	

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*** End of Report ***

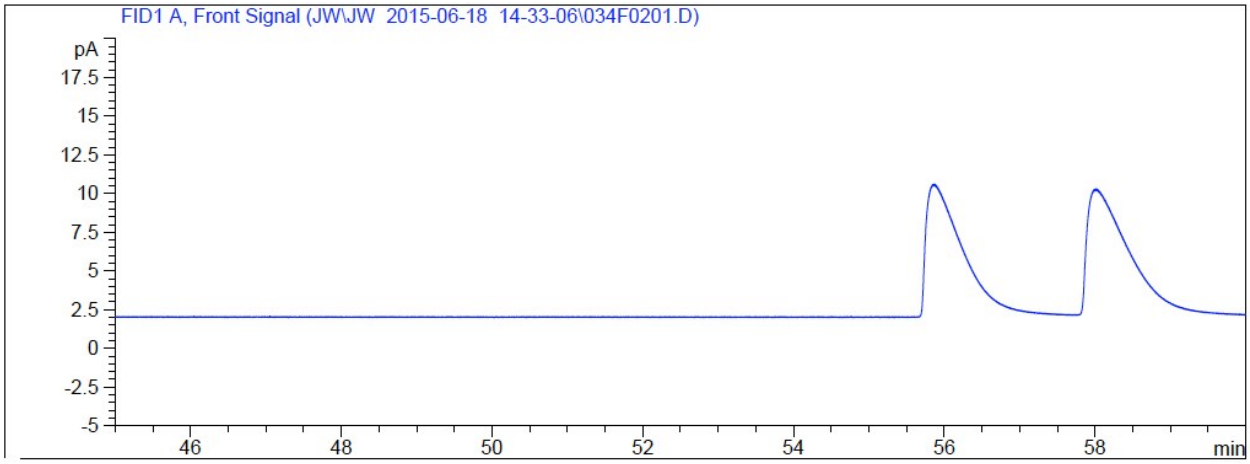
6-chloro-2-methyl-1,2,3,4-tetrahydroquinoline (4h)

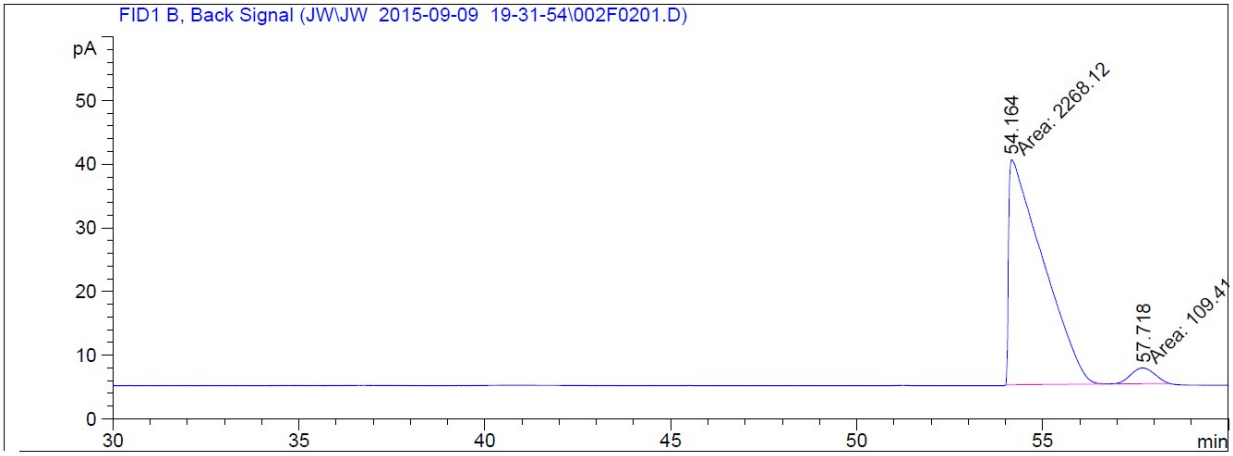
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 6.93 – 6.86 (m, 2H), 6.37 (d, *J* = 8.4 Hz, 1H), 3.68 (br, 1H), 3.41 – 3.32 (m, 1H), 2.84 – 2.72 (m, 1H), 2.72 – 2.63 (m, 1H), 1.95 – 1.87 (m, 1H), 1.54 (dddd, *J* = 12.9, 11.4, 9.9, 5.4 Hz, 1H), 1.20 (t, *J* = 5.2 Hz, 3H).

^{13}C NMR (400 MHz, CDCl3): δ 142.29, 127.78, 125.45, 121.56, 120.25, 113.90, 46.12, 28.67, 25.41, 21.41.

$[\alpha]^{22}_{D}$ -81.4 (*c* 0.5, $CHCl_3$).

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 140 °C, t_1 =55.9 min, t_2 =58.0 min.





Signal 1: FID1 B, Back Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	54.164	MM	1.0692	2268.11865	35.35589	95.39800
2	57.718	MM	0.7403	109.41407	2.46312	4.60200
Totals :				2377.53272	37.81902	

*** End of Report ***

6-fluoro-2-methyl-1,2,3,4-tetrahydroquinoline (4i)

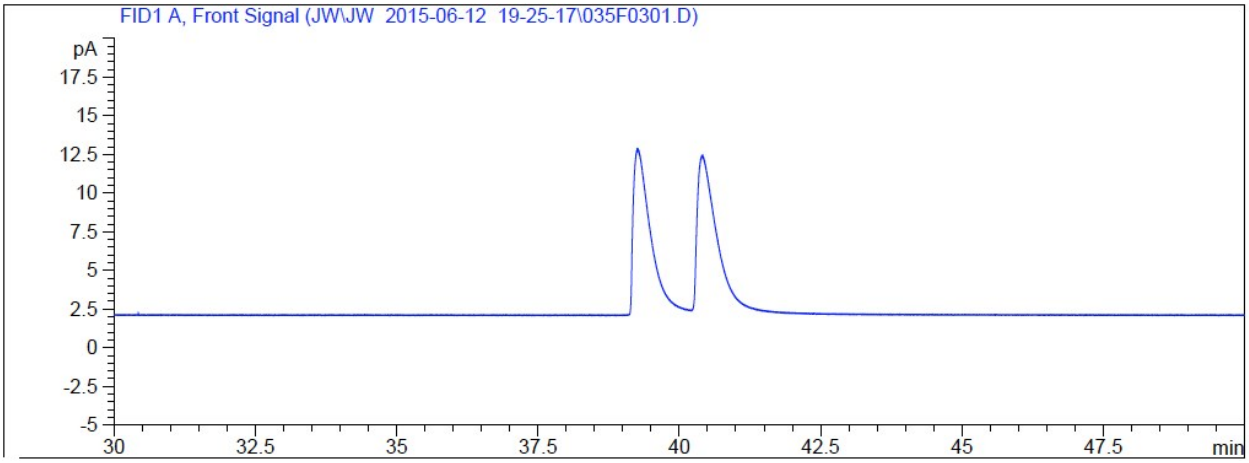
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 6.64 – 6.70 (m, 5.8 Hz, 2H), 6.42 – 6.35 (m, 1H), 3.57 (br, 1H), 3.34 (dqd, *J* = 12.6, 6.2, 2.7 Hz, 1H), 2.81 (ddd, *J* = 11.6, 8.7, 5.6 Hz,

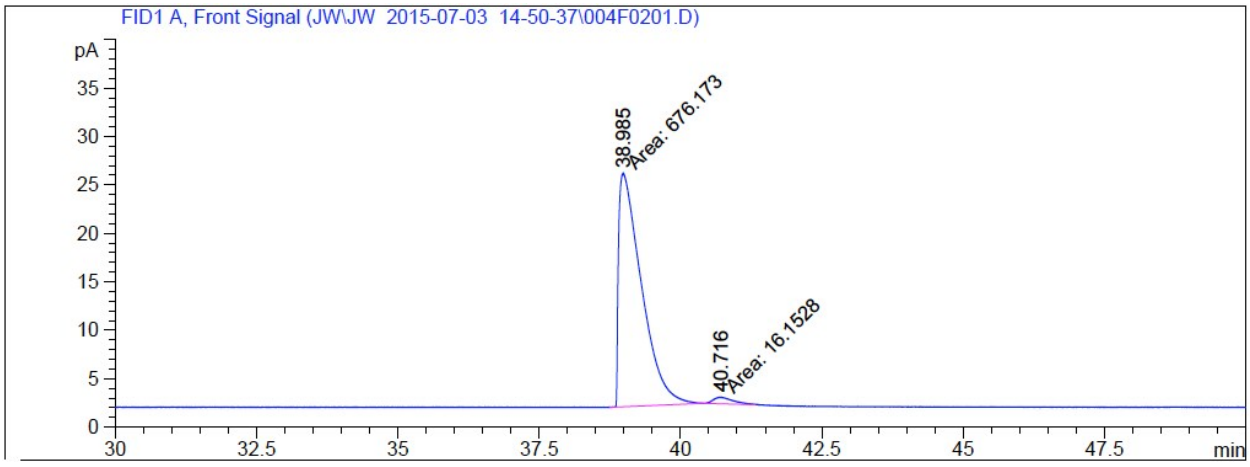
1H), 2.69 (ddd, *J* = 16.6, 5.3, 3.4 Hz, 1H), 1.91 (dtd, *J* = 8.8, 5.9, 3.0 Hz, 1H), 1.55 (dddd, *J* = 12.9, 11.6, 10.1, 5.5 Hz, 1H), 1.20 (d, *J* = 6.3 Hz, 3H).

^{13}C NMR (400 MHz, CDCl3): δ 154.51 (d, *J* = 938.4 Hz), 139.95, 121.44 (d, *J* = 26.4 Hz), 114.34 (d, *J* = 86.4 Hz), 113.68 (d, *J* = 30.4 Hz), 112.12 (d, *J* = 89.6 Hz), 46.29, 28.87, 25.67, 21.44.

$[\alpha]^{22}_{D}$ –63.84 (*c* 0.5, $CHCl_3$).

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 120 °C, t_1 =39.0 min, t_2 =40.7 min.





Signal 1: FID1 A, Front Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	38.985	MM	0.4684	676.17346	24.05771	97.66689
2	40.716	MM	0.4012	16.15275	6.71097e-1	2.33311
Totals :				692.32621	24.72881	

*** End of Report ***

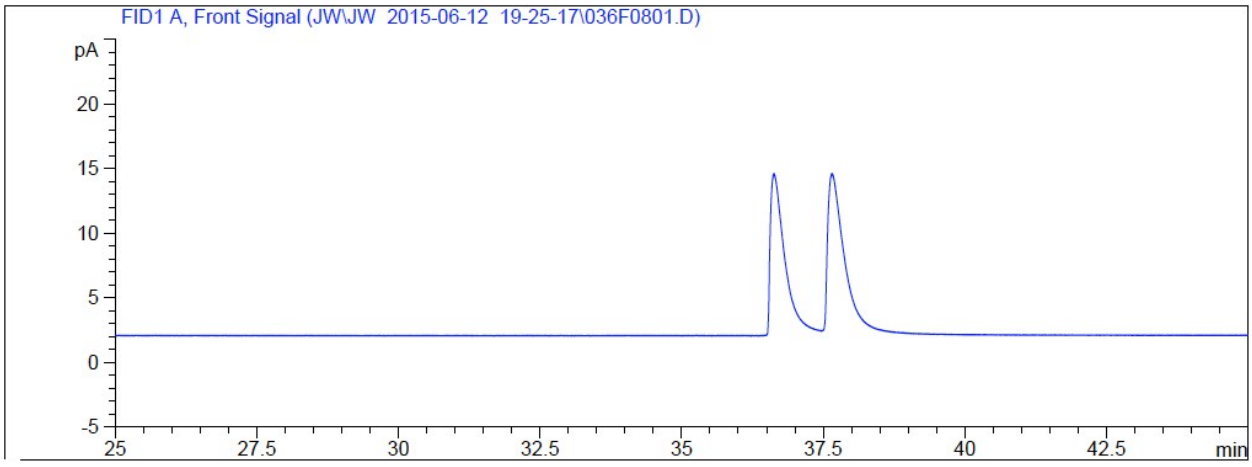
6-bromo-2-methyl-1,2,3,4-tetrahydroquinoline (4j)

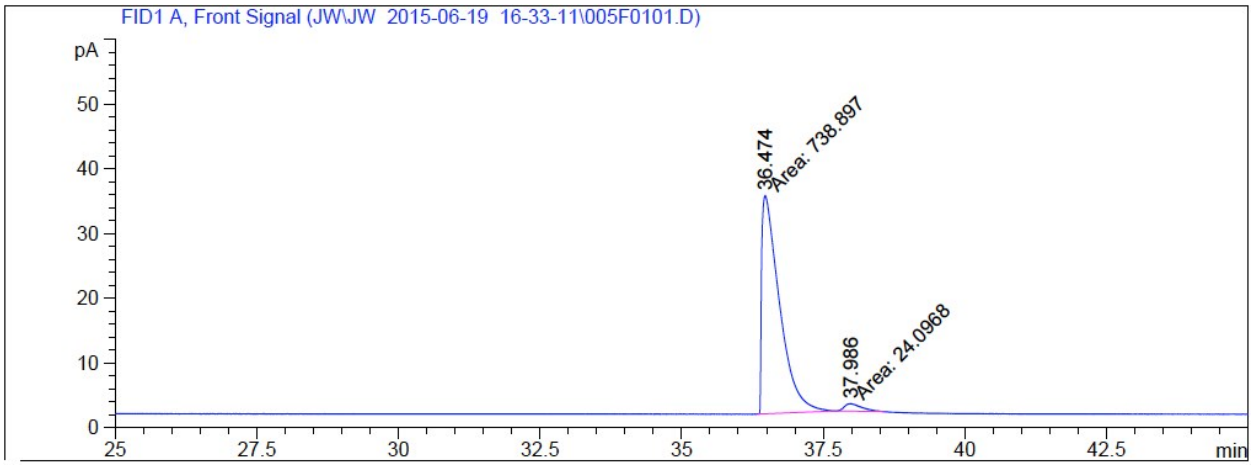
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 7.05 (d, *J* = 1.0 Hz, 1H), 7.02 (d, *J* = 8.4 Hz, 1H), 6.32 (d, *J* = 8.4 Hz, 1H), 3.69 (s, 1H), 3.41 – 3.31 (m, 1H), 2.84 – 2.73 (m, 1H), 2.72 – 2.64 (m, 1H), 1.90 (dtd, *J* = 8.4, 5.6, 2.8 Hz, 1H), 1.53 (dtd, *J* = 11.8, 10.7, 5.3 Hz, 2H), 1.19 (d, *J* = 6.4 Hz, 3H).

^{13}C NMR (400 MHz, CDCl3): δ 142.73, 130.62, 128.30, 122.08, 114.33, 107.25, 46.06, 28.60, 25.35, 21.40.

$[\alpha]^{22}_{D}$ –66.7 (*c* 0.5, $CHCl_3$).

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 160 °C, t_1 =36.6 min, t_2 =37.6 min.





Signal 1: FID1 A, Front Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	36.474	MM	0.3649	738.89734	33.75223	96.84181
2	37.986	MM	0.3442	24.09677	1.16684	3.15819
Totals :				762.99411	34.91906	

*** End of Report ***

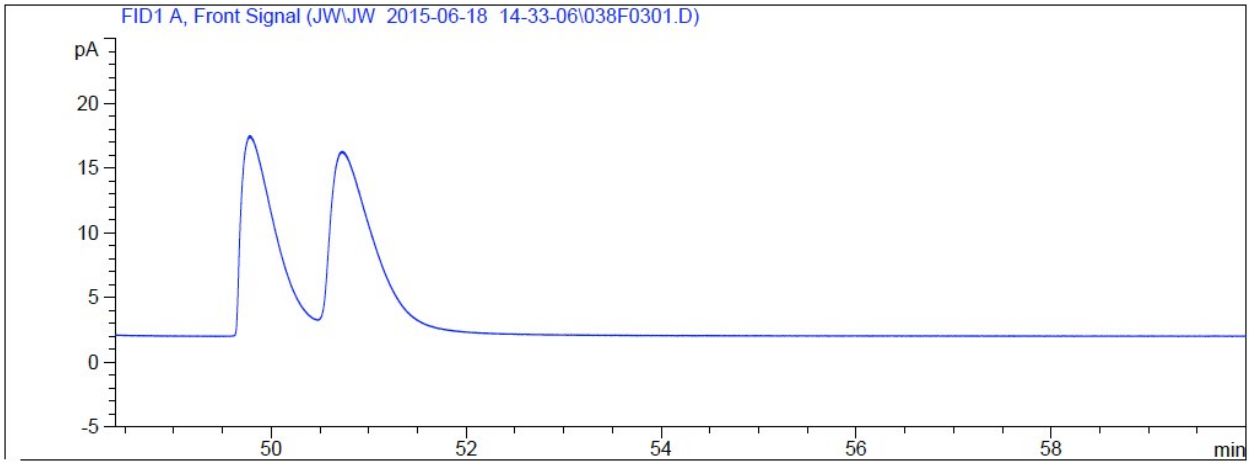
7-chloro-2-methyl-1,2,3,4-tetrahydroquinoline (4k)

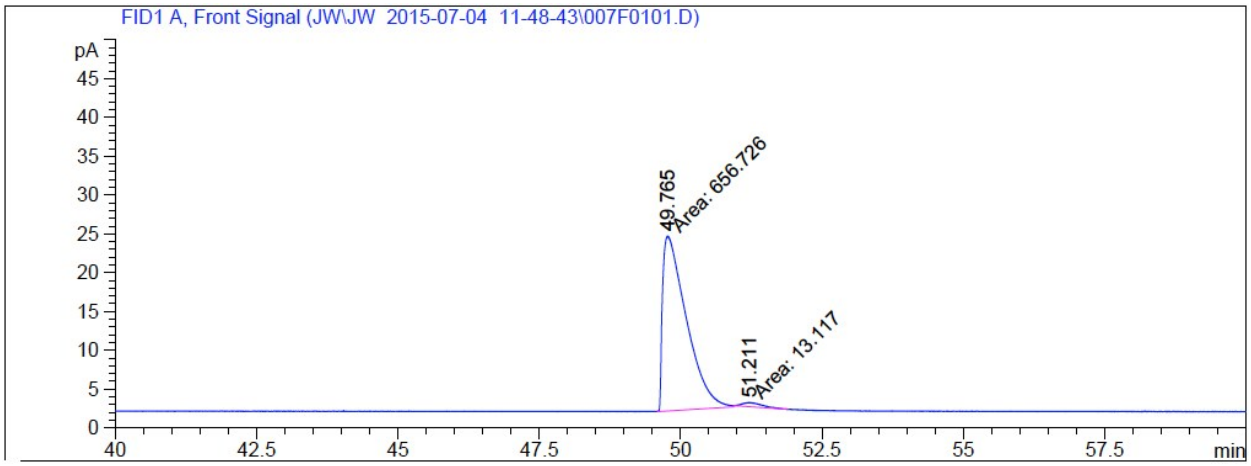
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 6.84 (d, *J* = 8.0 Hz, 1H), 6.53 (dd, *J* = 8.0, 2.0 Hz, 1H), 6.42 (d, *J* = 2.0 Hz, 1H), 3.72 (br, 1H), 3.38 (dqd, *J* = 9.3, 6.3, 3.0 Hz, 1H), 2.81 – 2.61 (m, 1H), 1.97 – 1.82 (m, 1H), 1.54 (dddd, *J* = 12.9, 11.1, 9.8, 5.5 Hz, 1H), 1.18 (t, *J* = 10.1 Hz, 3H).

^{13}C NMR (400 MHz, CDCl3): δ 144.89, 130.89, 129.11, 118.28, 115.55, 112.24, 45.96, 28.75, 25.01, 21.41.

$[\alpha]^{22}_{D}$ -73.3 (*c* 0.5, $CHCl_3$).

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 140 °C, t_1 =49.8 min, t_2 =50.7 min.





Signal 1: FID1 A, Front Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	49.765	MM	0.4851	656.72589	22.56477	98.04178
2	51.211	MM	0.4062	13.11703	5.38164e-1	1.95822
Totals :				669.84292	23.10293	

*** End of Report ***

8-chloro-2-methyl-1,2,3,4-tetrahydroquinoline (4l)

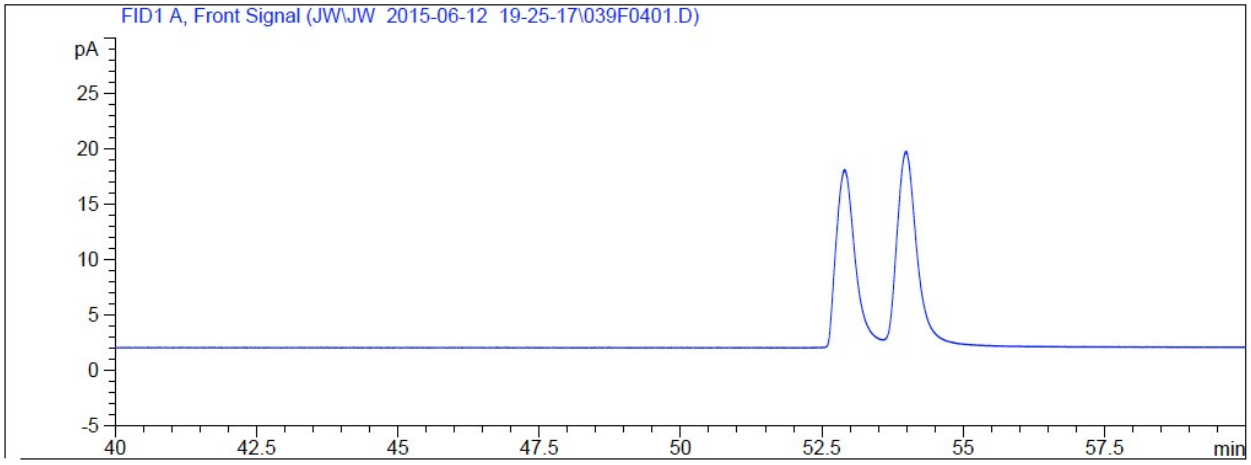
Yellow oil. ^{1}H NMR (400 MHz, CDCl3): δ 7.05 (d, *J* = 7.9 Hz, 1H), 6.86 (dd, *J* = 7.4, 0.9 Hz, 1H), 6.50 (t, *J* = 7.7 Hz, 1H), 4.25 (br, 1H), 3.46 (dqd, *J* = 9.4, 6.3, 3.1 Hz, 1H), 2.83

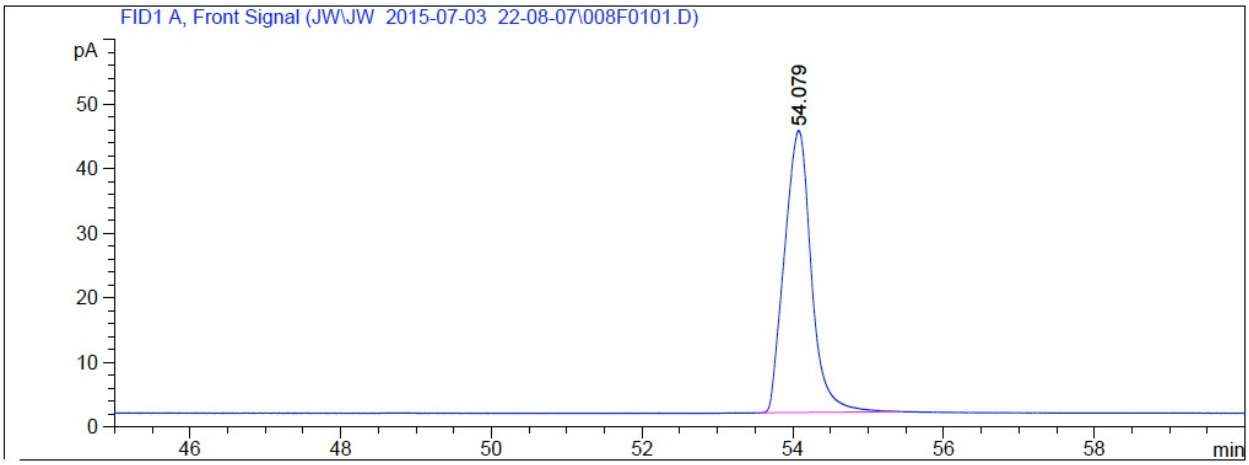
(ddd, *J* = 16.6, 11.2, 5.4 Hz, 1H), 2.78 – 2.70 (m, 1H), 1.98 – 1.90 (m, 1H), 1.58 (dddd, *J* = 12.9, 11.2, 9.8, 5.3 Hz, 1H), 1.27 (d, *J* = 6.3 Hz, 3H).

^{13}C NMR (400 MHz, CDCl3): δ 140.74, 127.43, 126.74, 122.39, 117.84, 116.35, 47.18, 29.64, 26.74, 22.52.

$[\alpha]^{22}_{D}$ -68.7 (*c* 0.5, $CHCl_3$).

Supelco gama Dex 225 column (30 m ×0.25 mm × 0.25 μm), He 1.0 mL/min, column 120 °C, t_1 =52.9 min, t_2 =54.0 min.





Signal 1: FID1 A, Front Signal

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	54.079	BB	0.3756	1081.64124	43.63175	1.000e2
Totals :				1081.64124	43.63175	

*** End of Report ***

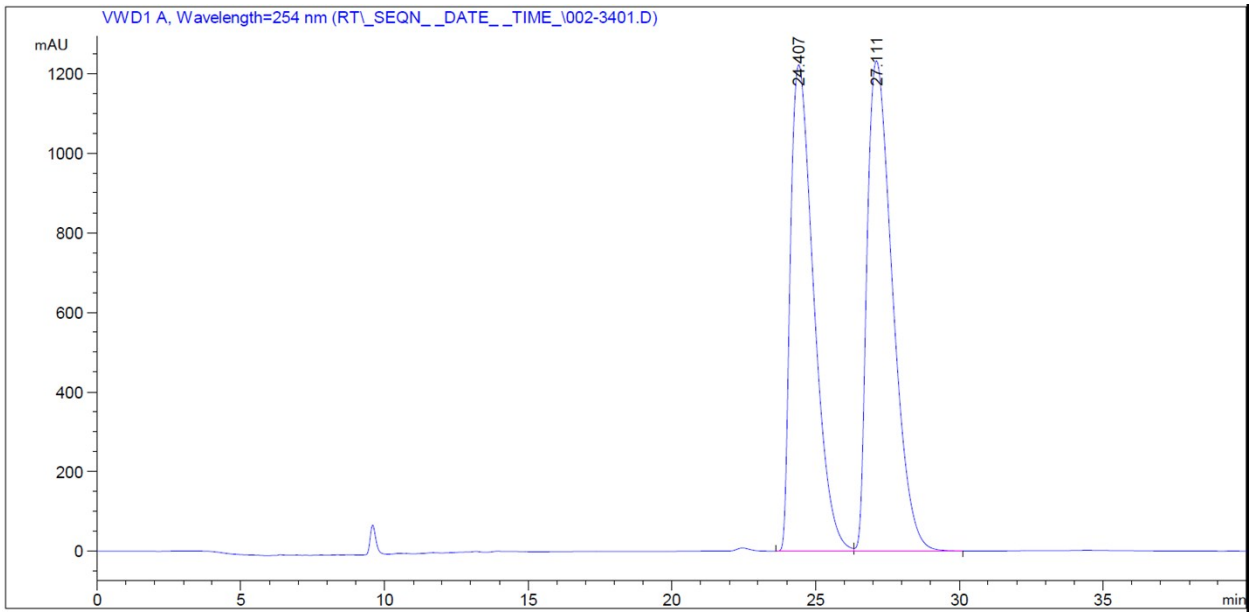
2-(3,4-dimethoxyphenethyl)-1,2,3,4-tetrahydroquinoline (4m)

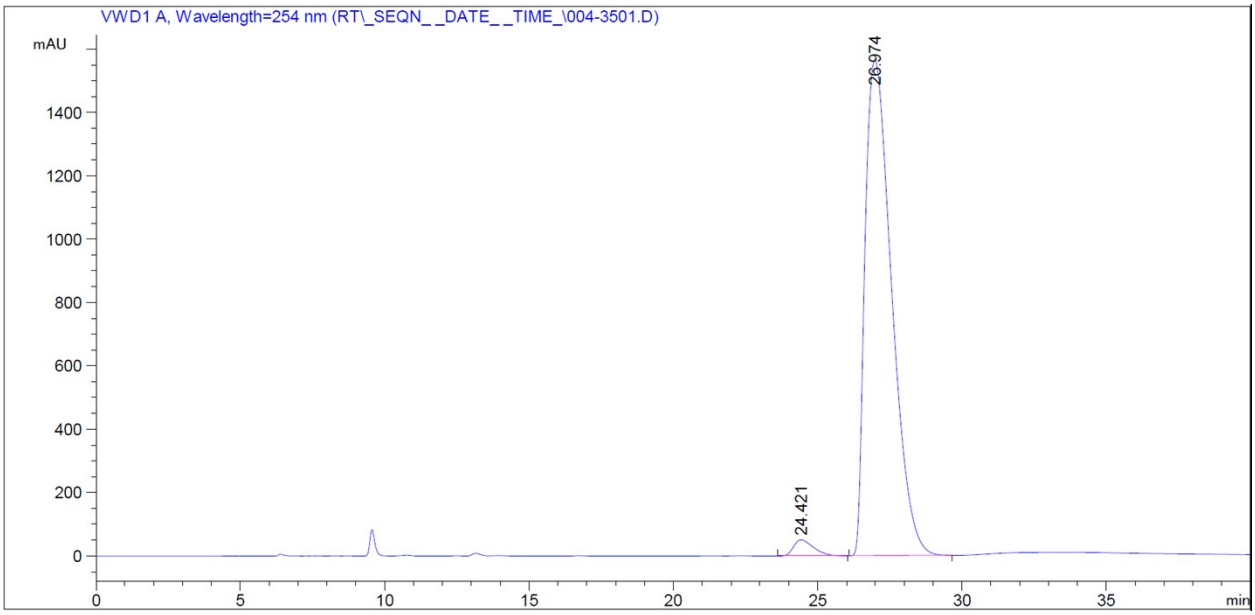
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (t, *J* = 7.1 Hz, 2H), 6.83–6.77 (m, 1H), 6.77–6.71 (m, 2H), 6.60 (td, *J* = 7.4, 0.9 Hz, 1H), 6.44 (dd, *J* = 8.4, 0.9 Hz, 1H), 3.87 (s, 3H), 3.85 (s, 3H), 3.77 (br, 1H), 3.30 (dtd, *J* = 9.3, 6.3, 3.0 Hz, 1H), 2.81 (ddd, *J* = 13.1, 9.0, 4.1 Hz, 1H), 2.73–2.64 (m, 2H), 2.03 – 1.95 (m, 1H), 1.81 (ddd, *J* = 10.2, 7.2, 1.2 Hz, 2H), 1.72–1.61 (m, 1H).

^{13}C NMR (400 MHz, CDCl3): δ 149.02, 147.37, 144.54, 134.52, 129.27, 126.76, 121.30, 120.17, 117.05, 114.16, 111.74, 111.43, 56.00, 55.90, 51.25, 38.44, 31.86, 28.05, 26.23.

$[\alpha]^{22}_{D}$ -60.8 (*c* 0.5, $CHCl_3$).

Daicel Chiralpak AS-H, hexanes/i-PrOH = 95/5, Flow rate = 0.5 ml/min, UV = 254 nm, t_1 = 24.4 min, t_2 = 27.0 min.





Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	24.421	BB	0.7352	2461.57397	51.10365	2.3987
2	26.974	BB	1.0158	1.00159e5	1565.46924	97.6013
Totals :				1.02621e5	1616.57289	

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[2] M. Fakhfakha, X. Francka, A. Fourneta, R. Hocquemillera, B. Figadère, *Tetrah. Lett.* **2001**, *42*, 3847.

[3] K. Kido and Y. Watanabe, *Chem. Pharm. Bull.* **1987**, *35*, 4964-4966.

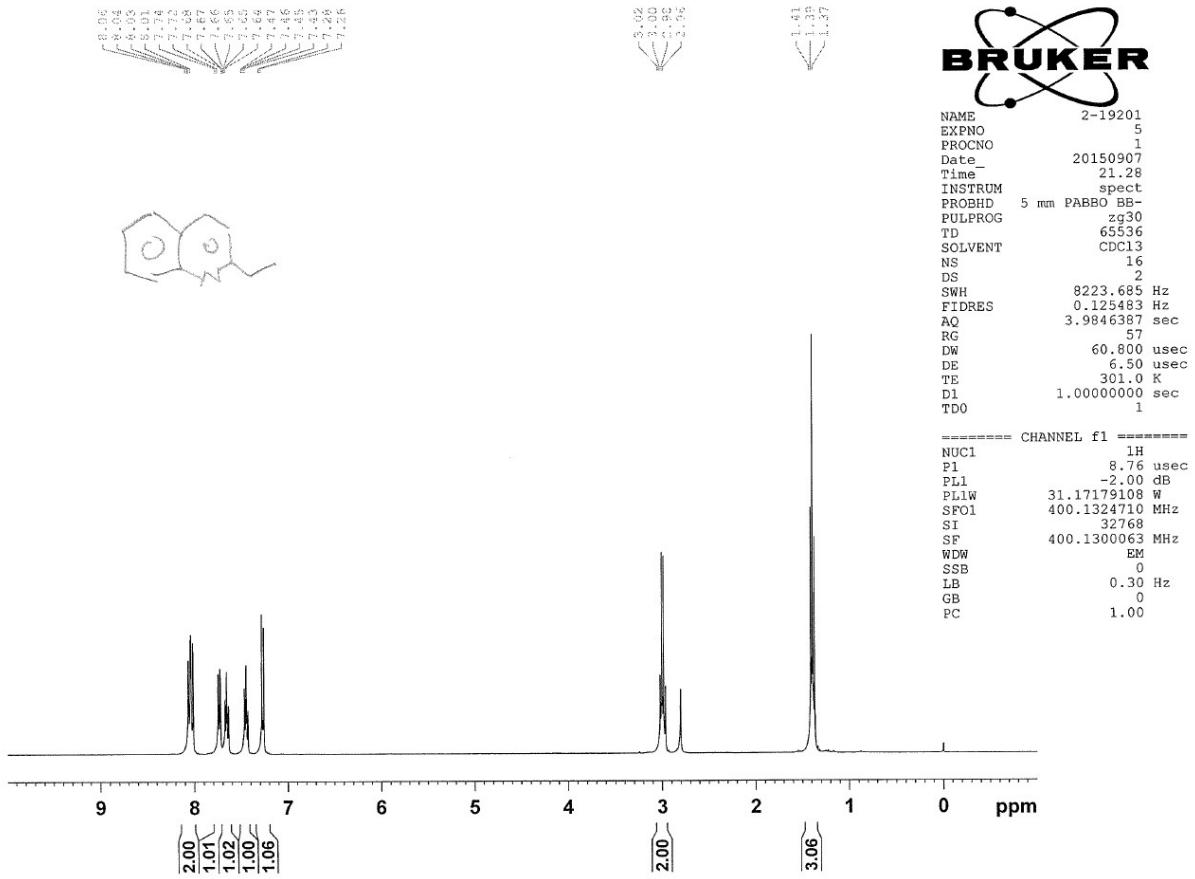
[4] J. Mangas-Sanchez, E. Busto, V. Gotor-Fernandez and V. Gotor, *Catal. Sci. Technol.* **2012**, *2*, 1590.

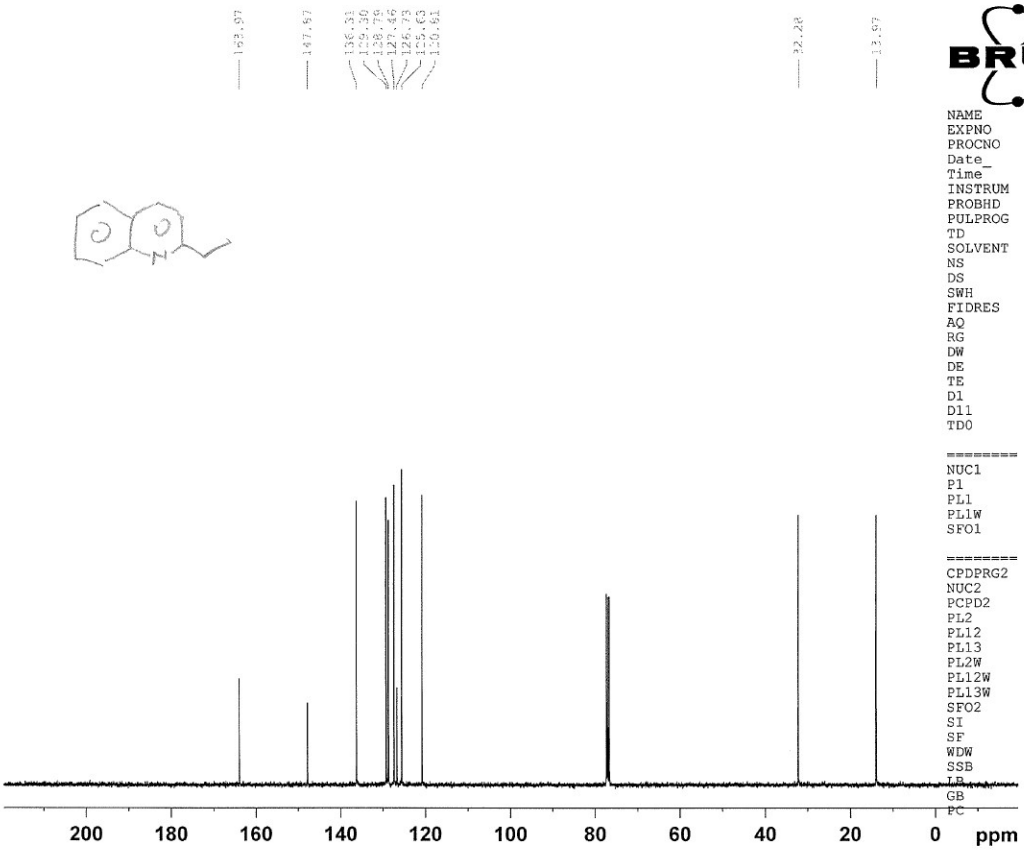
[5] F. Gou, W. Li, X. Zhang and Y. Liang, *Adv. Synth. Catal.* **2010**, *352*, 2441.

[6] J. Xie, P. Yan, Q. Zhang, K. Yuan and Q. Zhou, *ACS Catal.* **2012**, *2*, 561.

[7] D. García, B. Moreno, T. Soler, F. Foubelo, M. Yus, *Tetrahedron Lett.* **2009**, 50, 4710.

9. NMR spectroscopy





BRUKER

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PROCNO	1
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RG	2050
DW	20.800 usec
DE	6.50 usec
TE	302.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
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P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
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NUC2	1H
PCPD2	90.00 usec
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PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
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SSB	0
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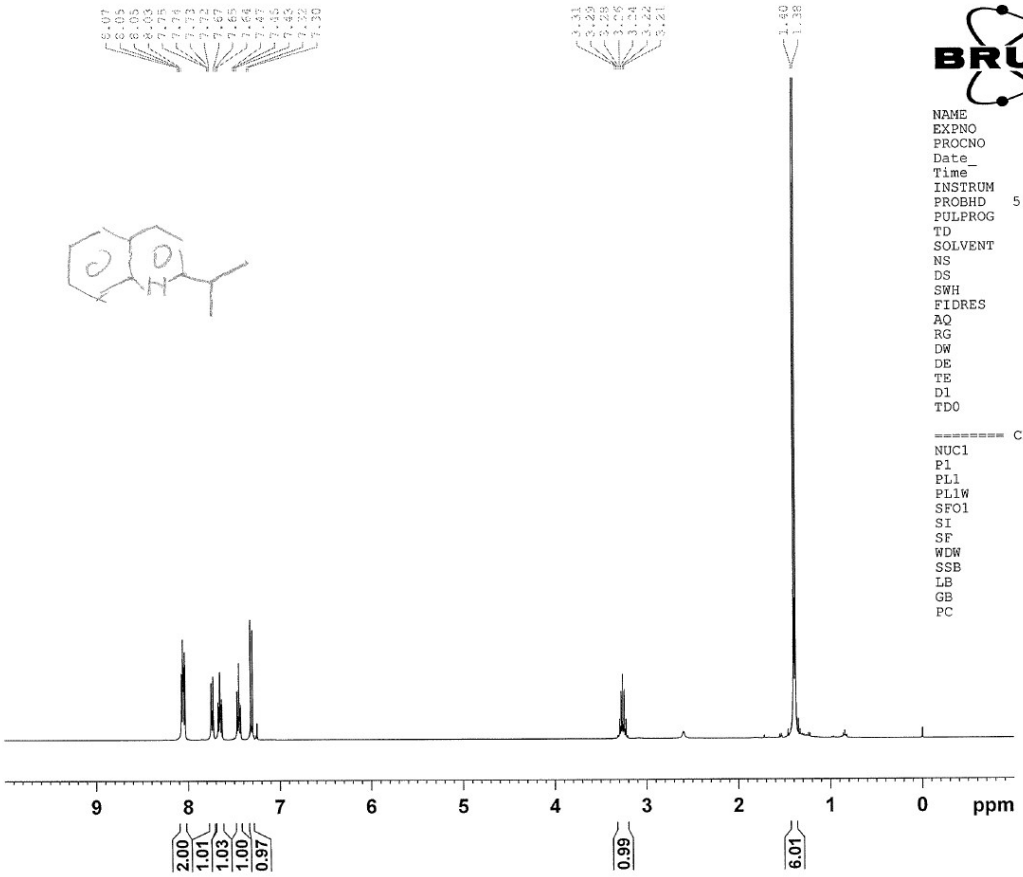
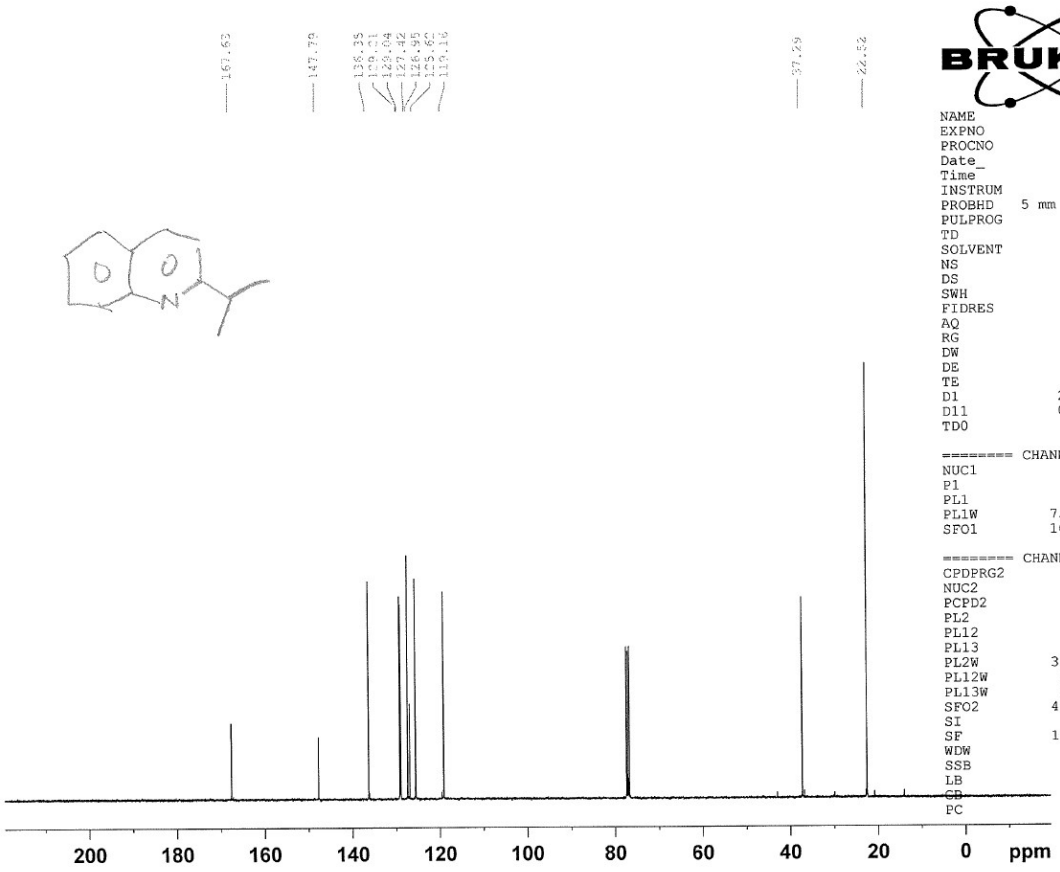
GB	0
PC	1.40



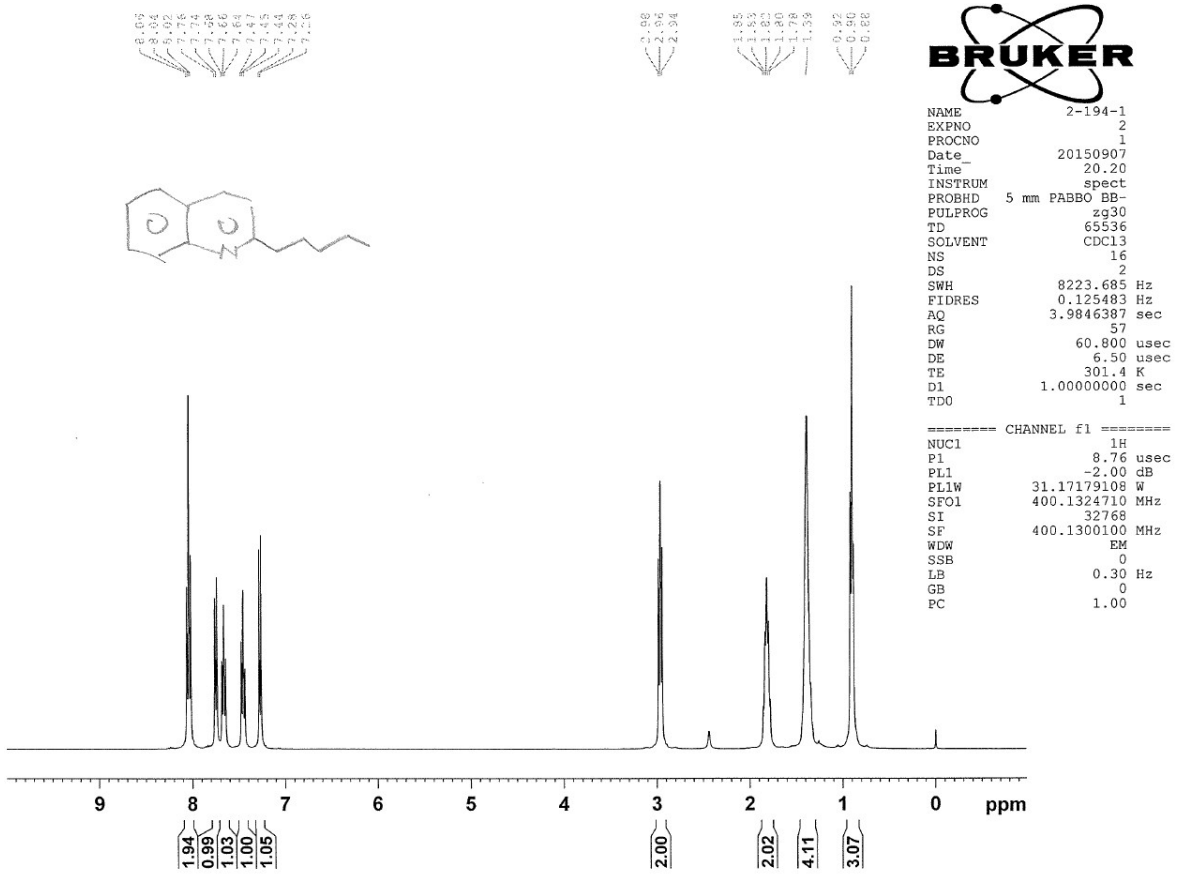
BRUKER

NAME	2-192-2
EXPNO	3
PROCNO	1
Date_	20150907
Time	19.42
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	50.8
DW	60.800 usec
DE	6.50 usec
TE	301.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300140 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



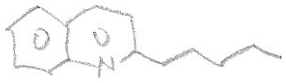
BRUKER

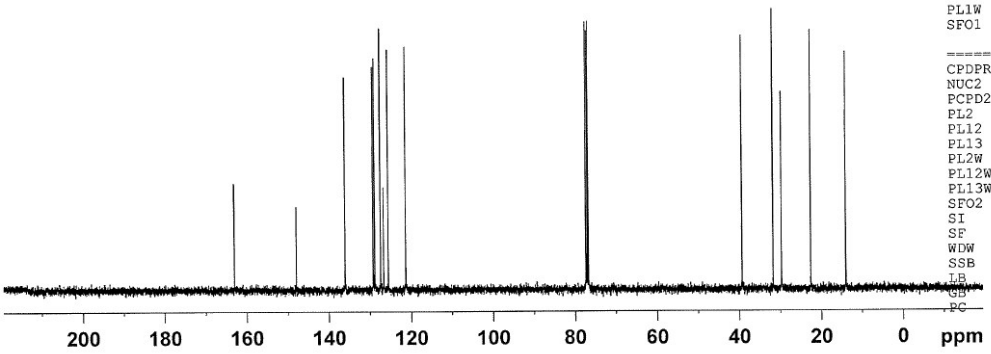
NAME	2-192-2
EXPNO	4
PROCNO	1
Date_	20150907
Time	20.13
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	302.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



BRUKER

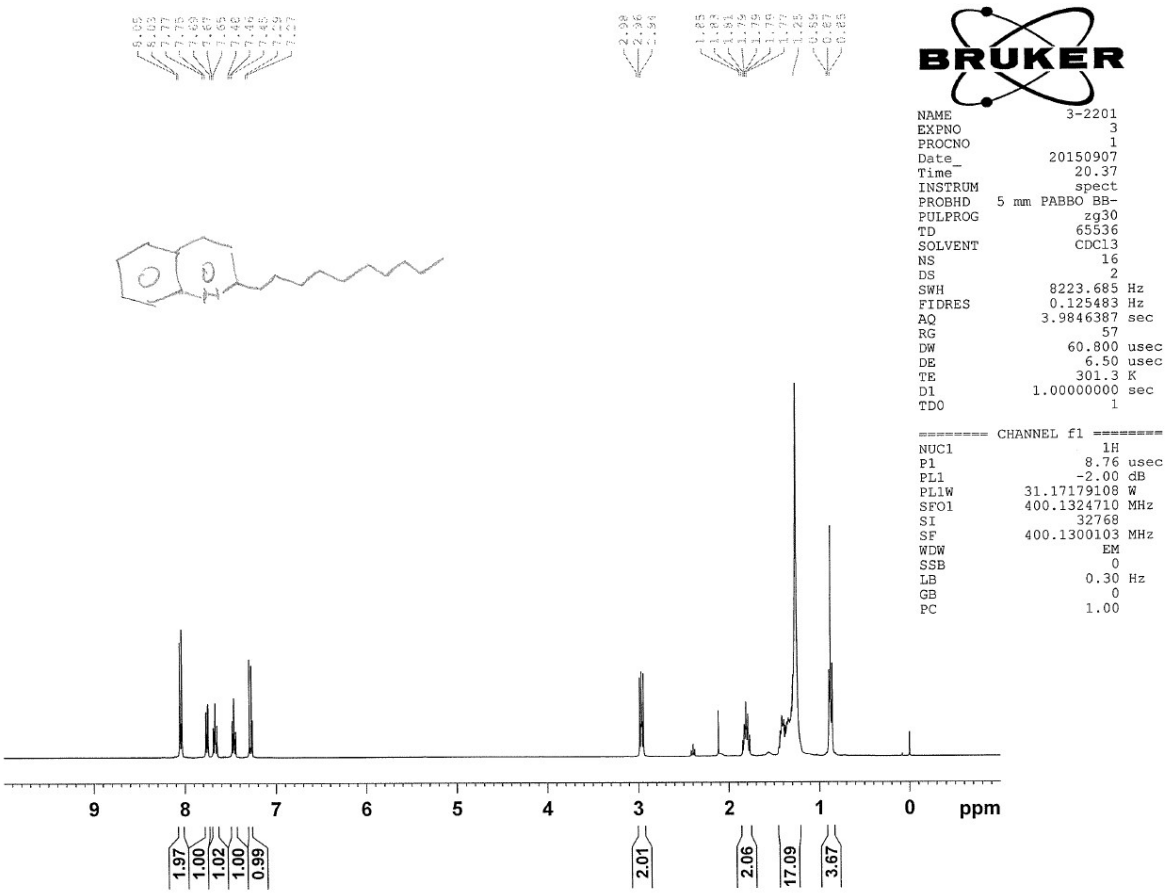
NAME	2-194-1
EXPNO	2
PROCNO	1
Date_	20150907
Time	20.20
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	57
DW	60.800 usec
DE	6.50 usec
TE	301.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300100 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

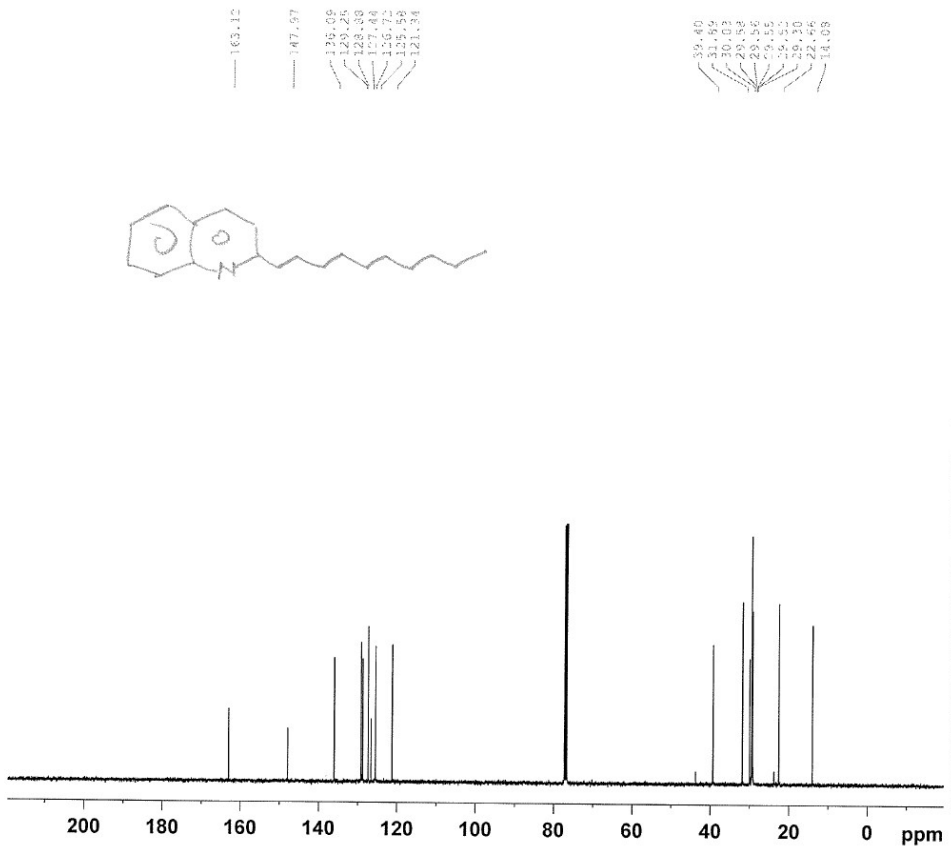




BRUKER

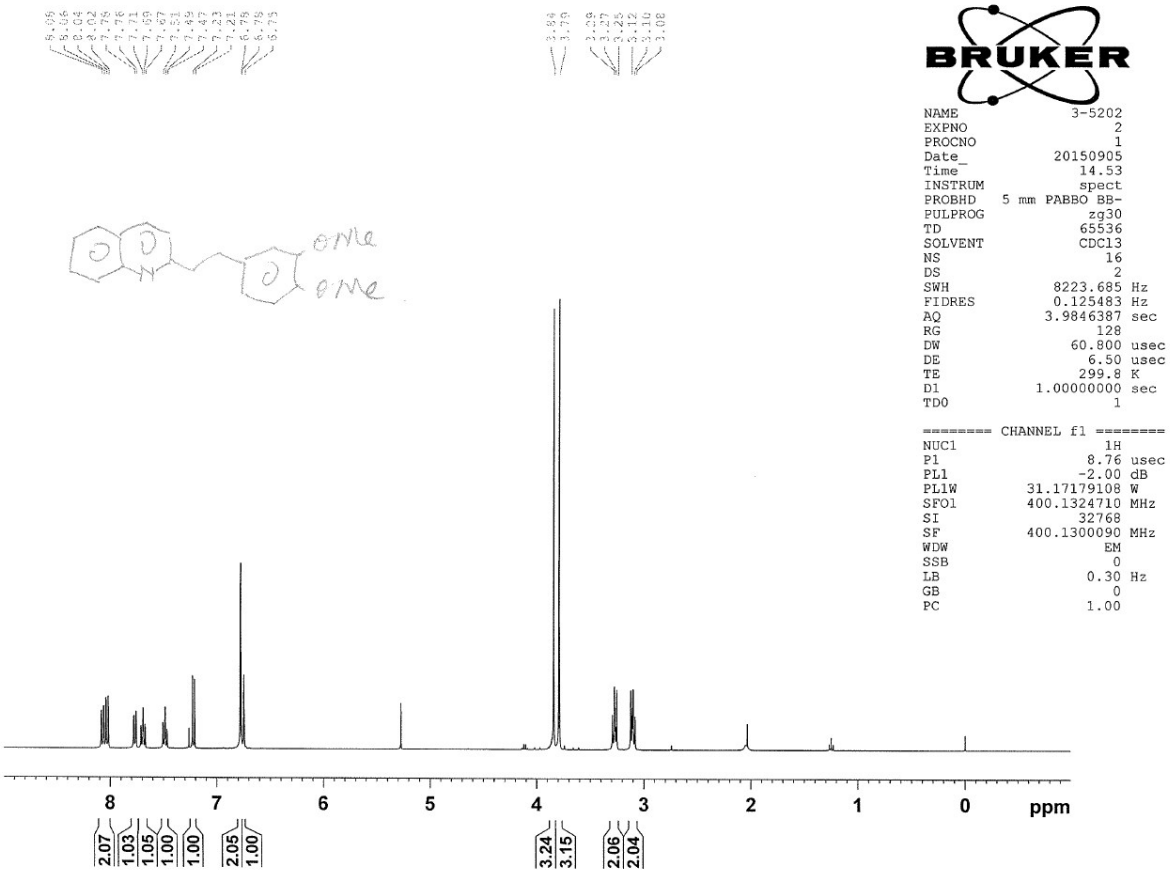
NAME	2-194-1
EXPNO	3
PROCNO	1
Date_	20150907
Time	20.28
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	154
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	302.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

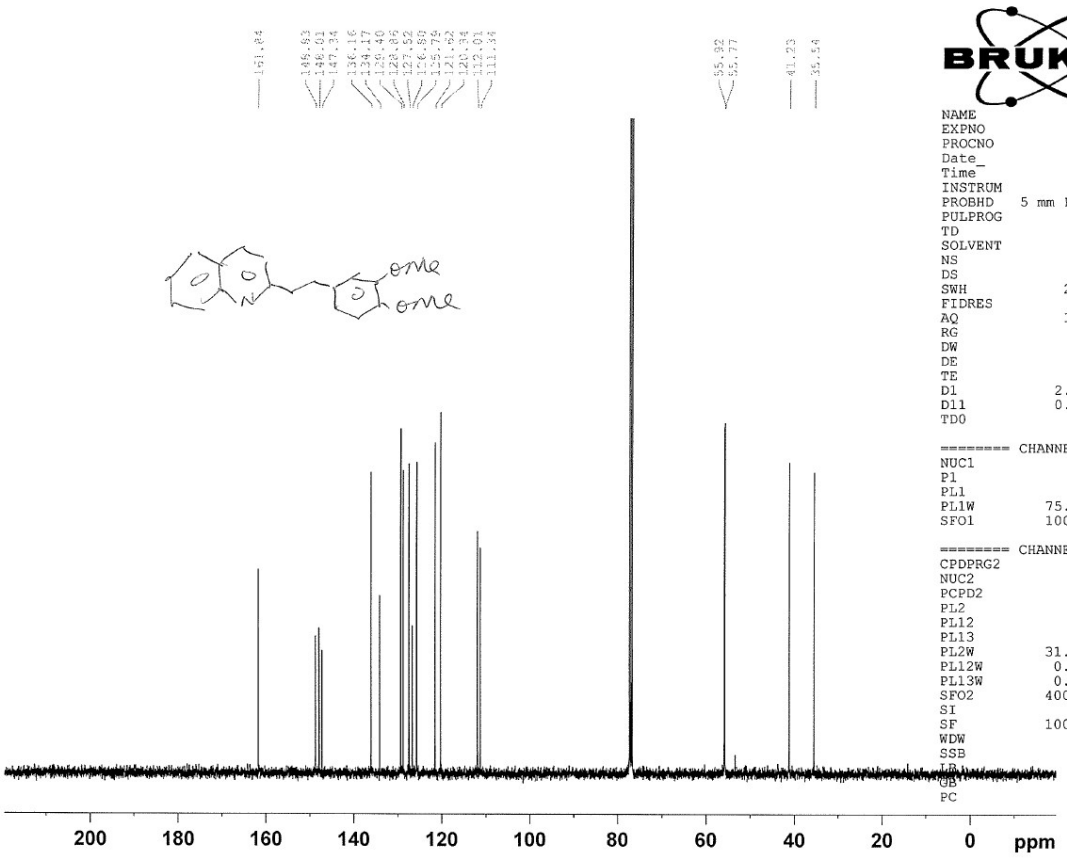

8.05
8.03
7.77
7.75
7.63
7.61
7.48
7.46
7.45
7.43
7.27
2.98
2.96
2.94
1.85
1.83
1.81
1.79
1.75
1.73
1.27
0.85
0.83
0.81
BRUKER
NAME 3-2201
EXPNO 3
PROCNO 1
Date_ 20150907
Time 20.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 57
DW 60.800 usec
DE 6.50 usec
TE 301.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
1.97
1.00
1.02
1.00
0.99
2.01
2.06
17.09
3.67



BRUKER

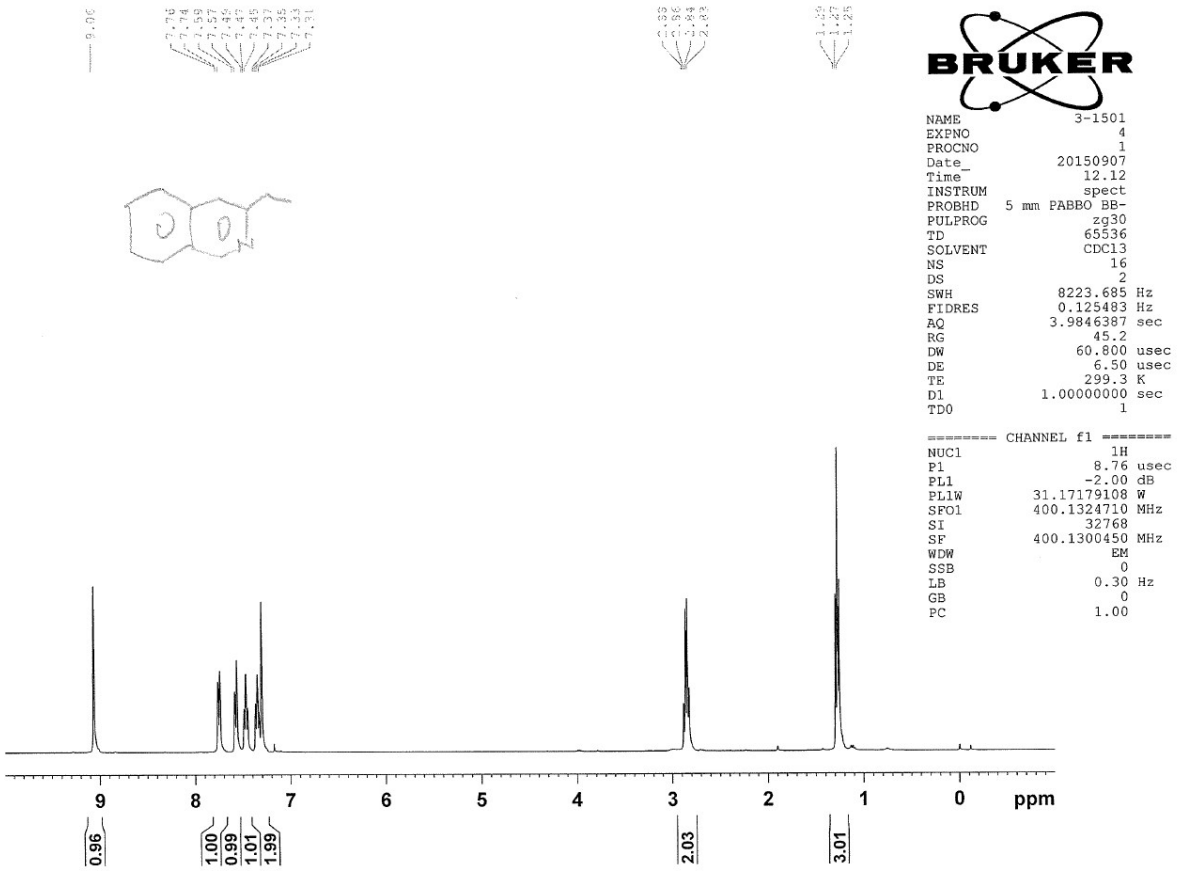
NAME	3-2201
EXPNO	4
PROCNO	1
Date_	20150907
Time	20.45
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	302.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

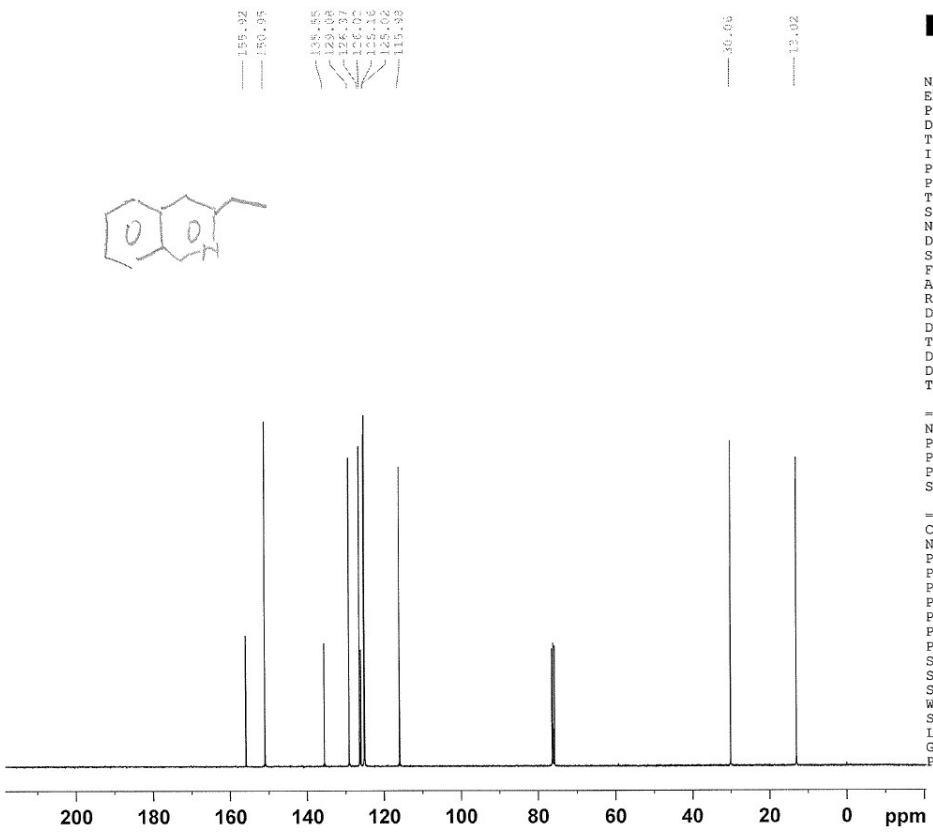

8.05
8.04
8.02
7.76
7.71
7.69
7.67
7.51
7.49
7.47
7.23
7.21
6.79
6.75
3.84
3.79
3.29
3.27
3.25
3.12
3.10
3.08
OMe
OMe
BRUKER
NAME 3-5202
EXPNO 2
PROCNO 1
Date_ 20150905
Time 14.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.50 usec
TE 299.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8
7
6
5
4
3
2
1
0
ppm
2.07
1.03
1.05
1.00
1.00
2.05
1.00
3.24
3.15
2.06
2.04



BRUKER

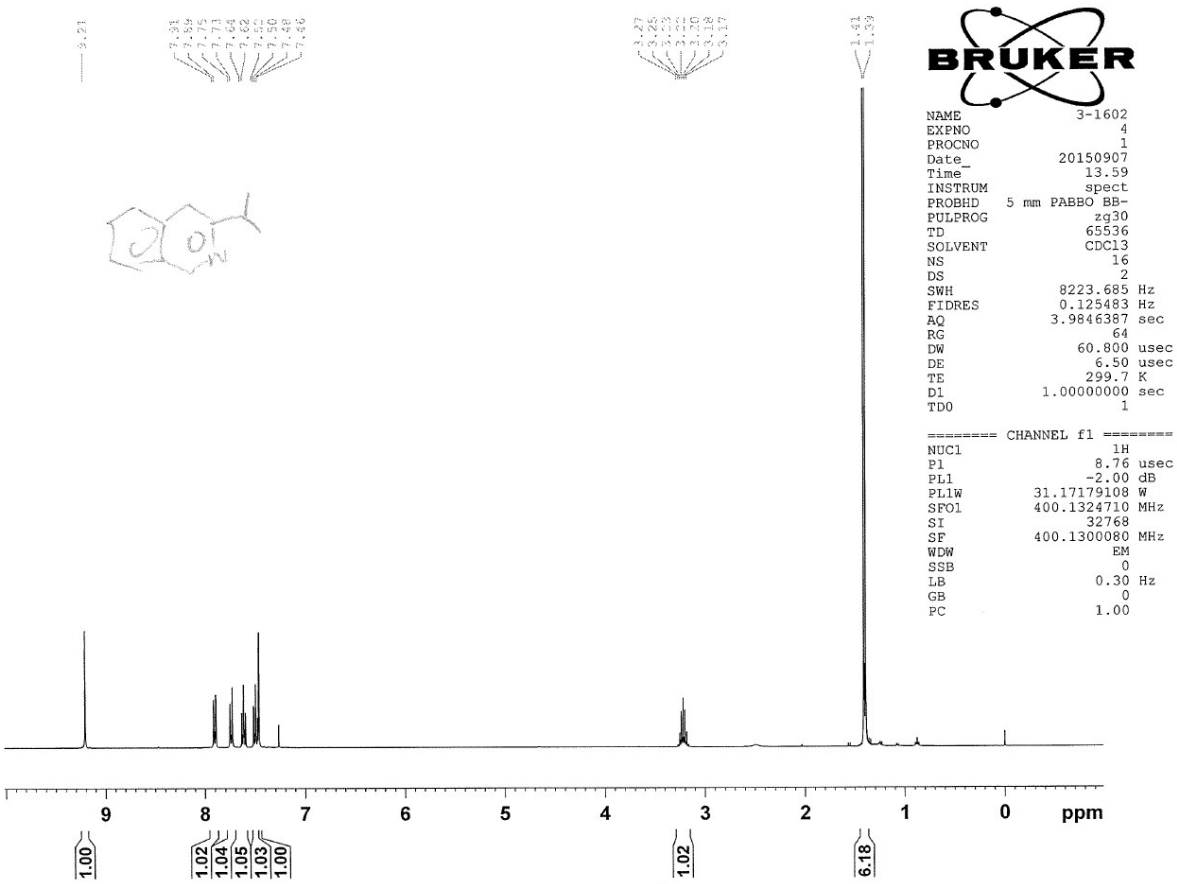
NAME	3-5202
EXPNO	3
PROCNO	1
Date_	20150905
Time	18.56
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	497
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	302.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

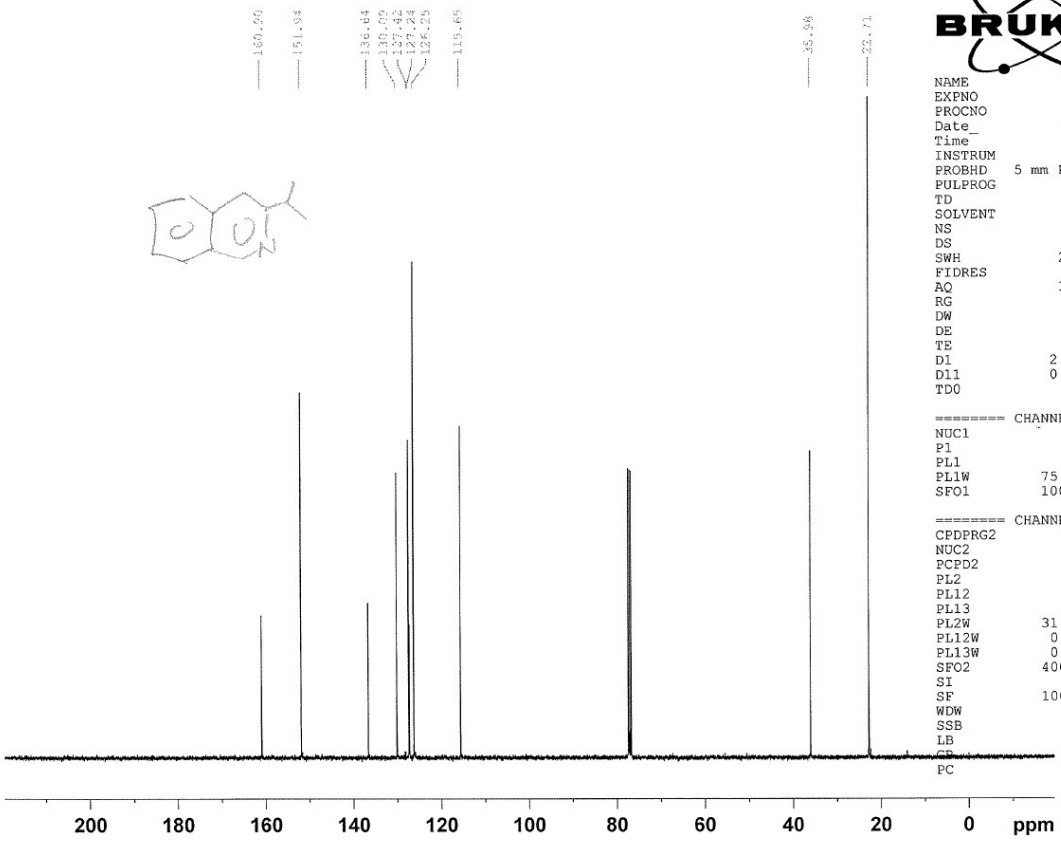

9.06
7.76
7.74
7.59
7.57
7.45
7.43
7.45
7.37
7.35
7.33
7.31
2.93
2.86
2.84
2.82
1.29
1.27
1.25
BRUKER
NAME 3-1501
EXPNO 4
PROCNO 1
Date_ 20150907
Time 12.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 45.2
DW 60.800 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300450 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
0.96
1.00
0.99
1.01
1.99
2.03
3.01



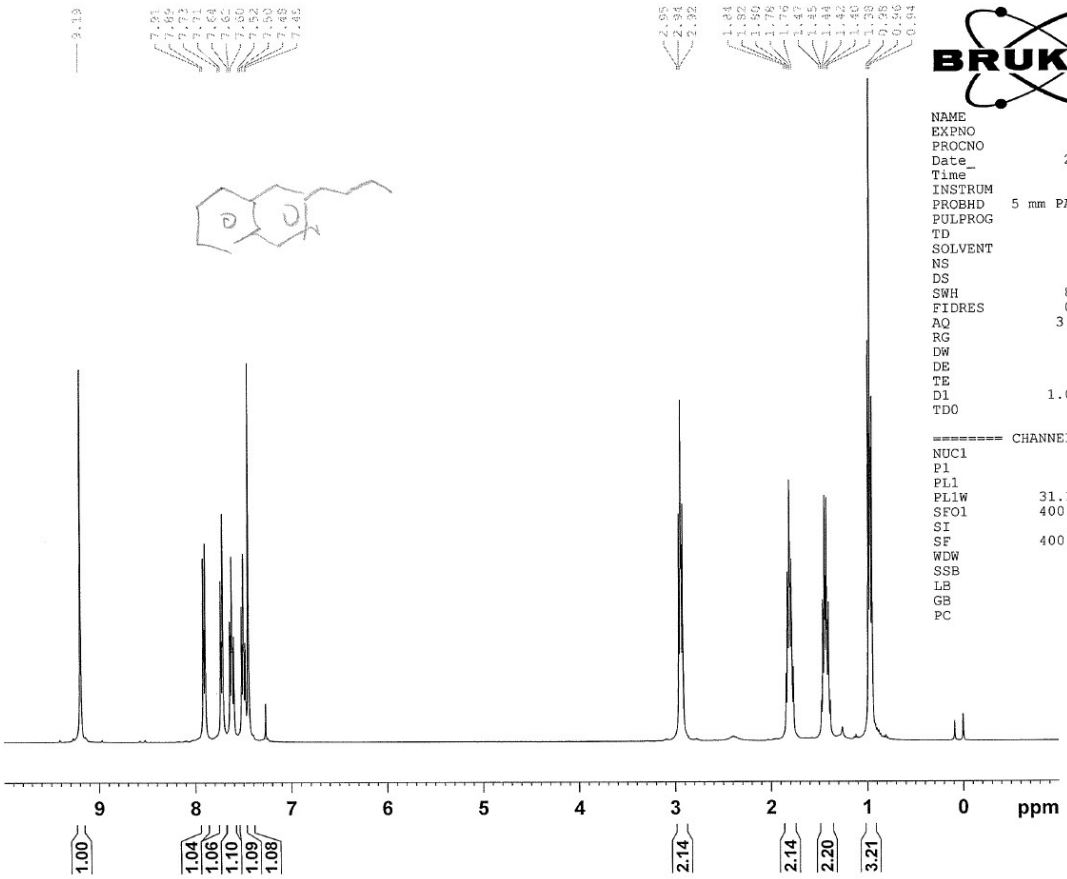
BRUKER

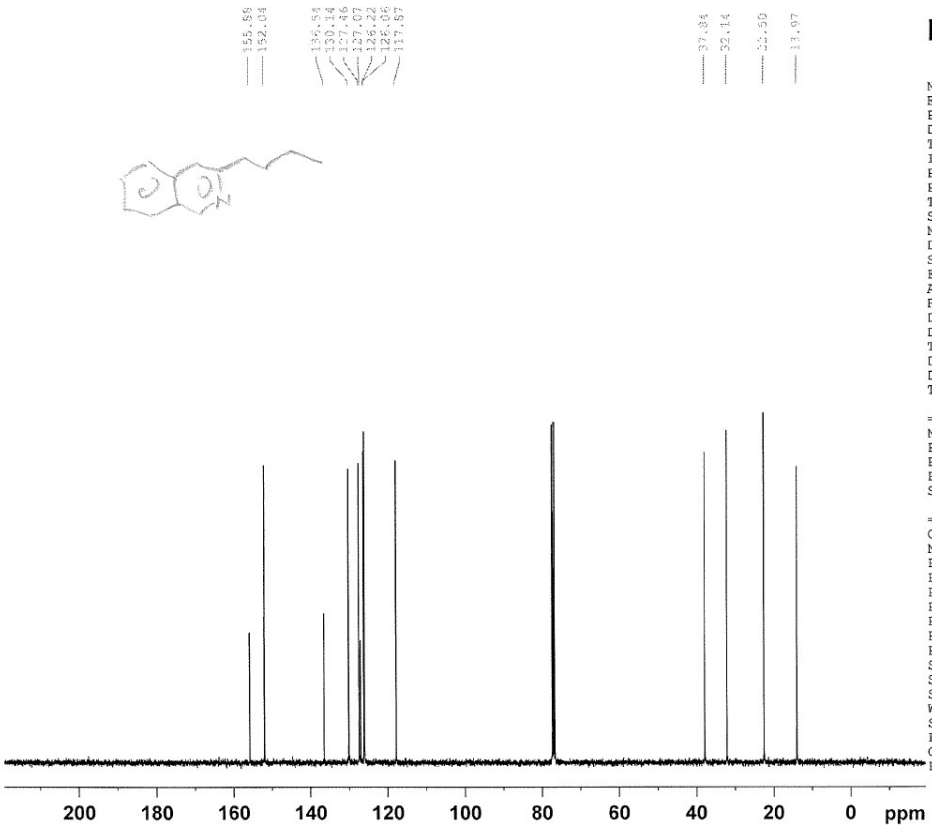
NAME	3-1501
EXPNO	5
PROCNO	1
Date_	20150907
Time	13.11
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	301.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128737 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


9.21
7.81
7.79
7.75
7.73
7.64
7.62
7.52
7.50
7.48
7.46
3.27
3.25
3.23
3.21
3.20
3.18
3.17
1.41
1.39
BRUKER
NAME 3-1602
EXPNO 4
PROCNO 1
Date_ 20150907
Time 13.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 64
DW 60.800 usec
DE 6.50 usec
TE 299.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300080 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.02
1.04
1.05
1.03
1.00
1.02
6.18



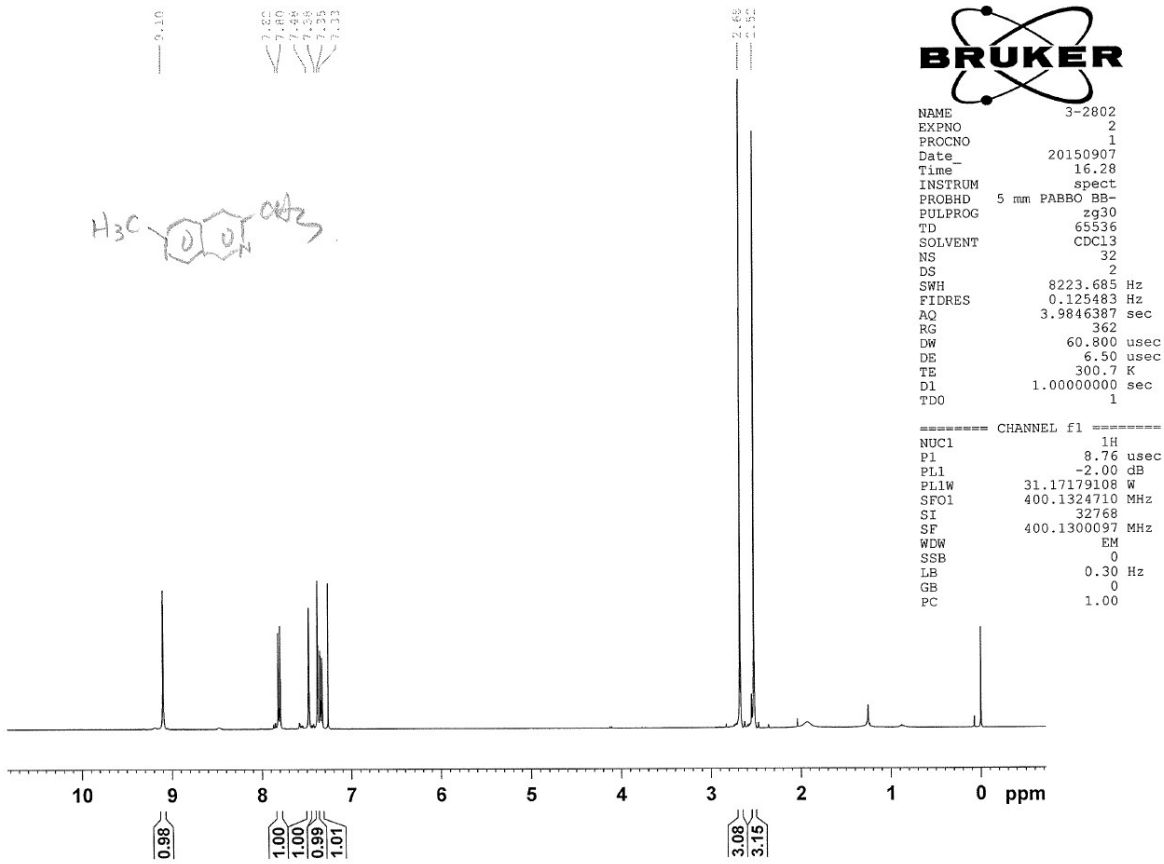
NAME	3-1602
EXPNO	5
PROCNO	1
Date_	20150907
Time	14.19
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	301.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


9.19
7.91
7.84
7.72
7.71
7.64
7.62
7.60
7.52
7.50
7.48
7.45
2.95
2.94
2.92
1.84
1.82
1.80
1.78
1.76
1.47
1.45
1.44
1.42
1.40
1.38
0.96
0.94
BRUKER
NAME 3-1902
EXPNO 1
PROCNO 1
Date_ 20150907
Time 14.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 64
DW 60.800 usec
DE 6.50 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300076 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.04
1.06
1.10
1.09
1.08
2.14
2.14
2.20
3.21



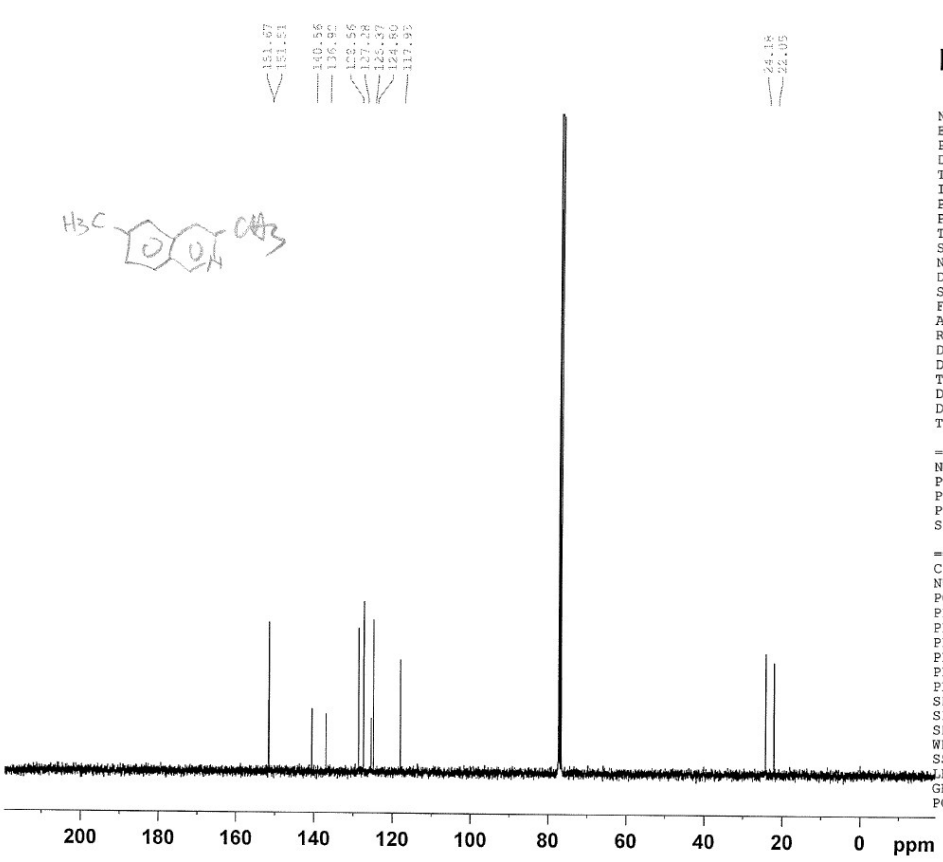
BRUKER

NAME	3-1902
EXPNO	2
PROCNO	1
Date_	20150907
Time	15.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	301.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



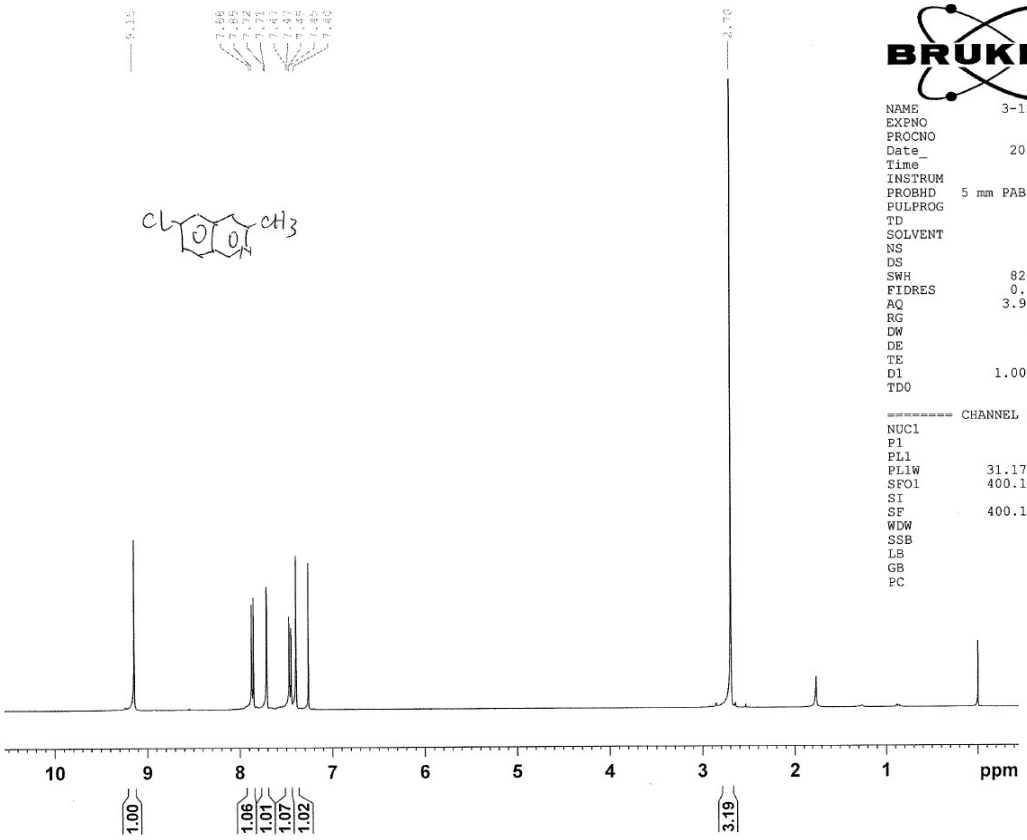
BRUKER

NAME	3-2802
EXPNO	2
PROCNO	1
Date_	20150907
Time	16.28
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	362
DW	60.800 usec
DE	6.50 usec
TE	300.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300097 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



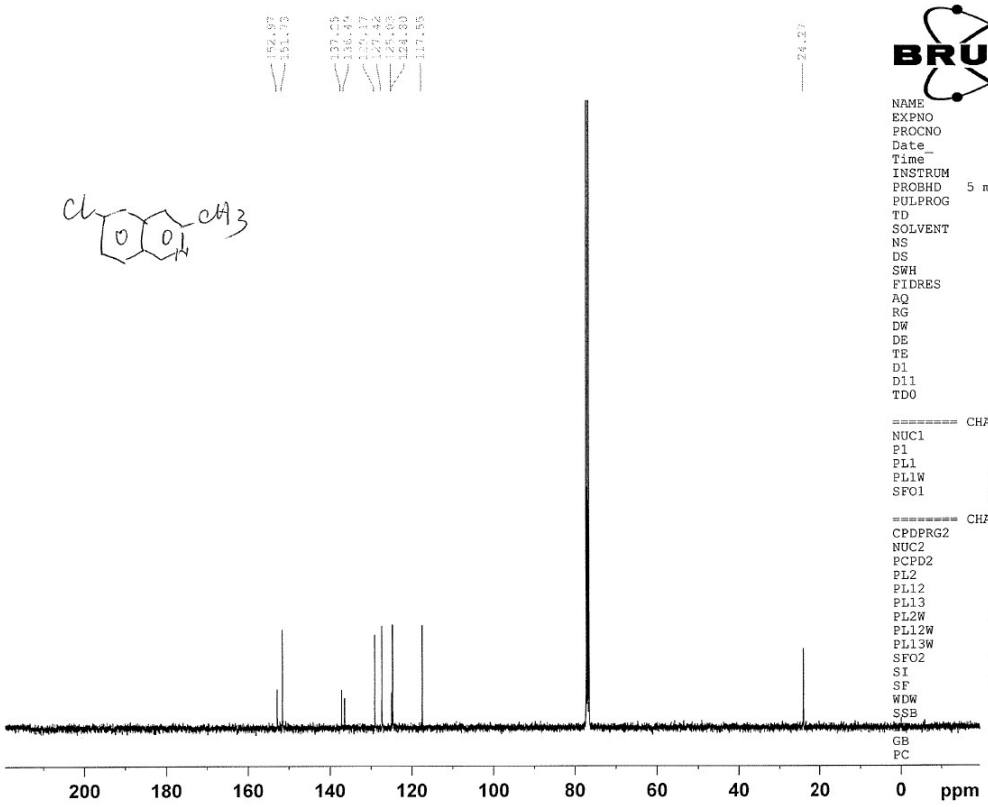
BRUKER

NAME	3-2802
EXPNO	3
PROCNO	1
Date_	20150907
Time	16.53
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	594
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	302.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



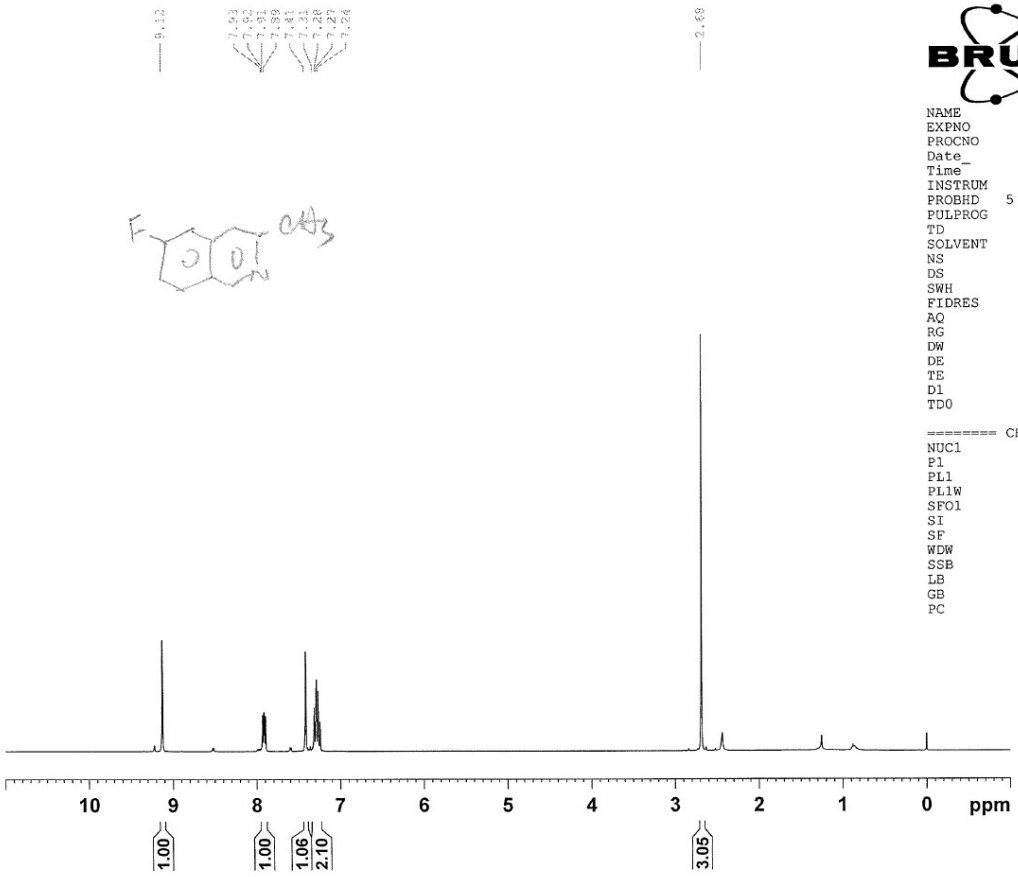
BRUKER

NAME	3-12402-5
EXPNO	7
PROCNO	1
Date_	20160115
Time	13.22
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	456
DW	60.800 usec
DE	6.50 usec
TE	295.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300083 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



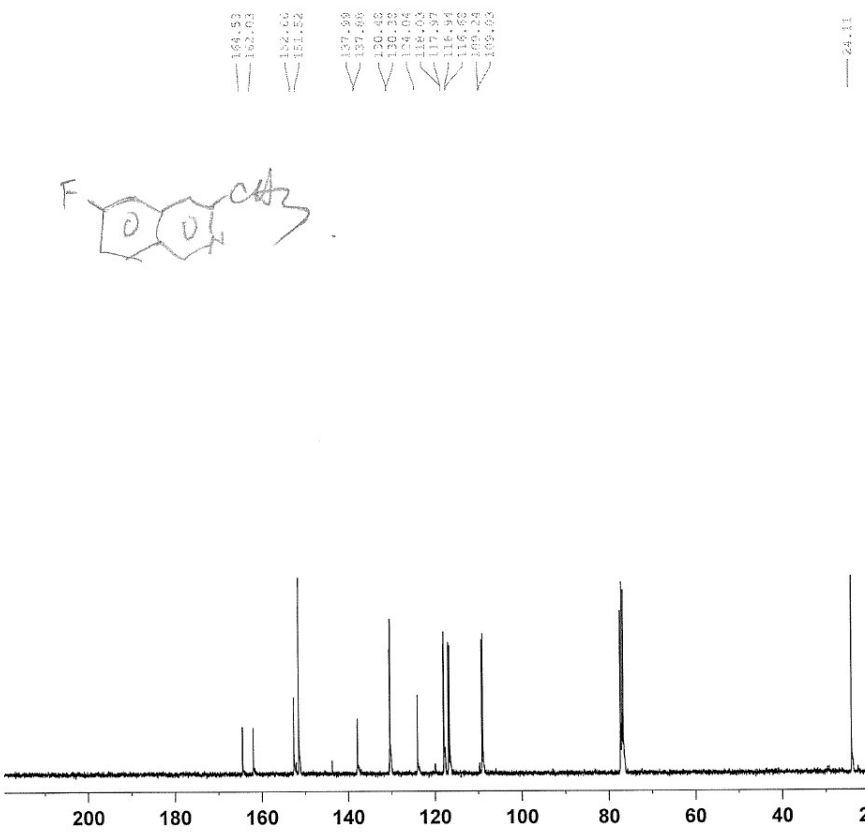
BRUKER

NAME	3-12402-5
EXPNO	4
PROCNO	1
Date_	20160114
Time	1.01
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2048
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	297.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



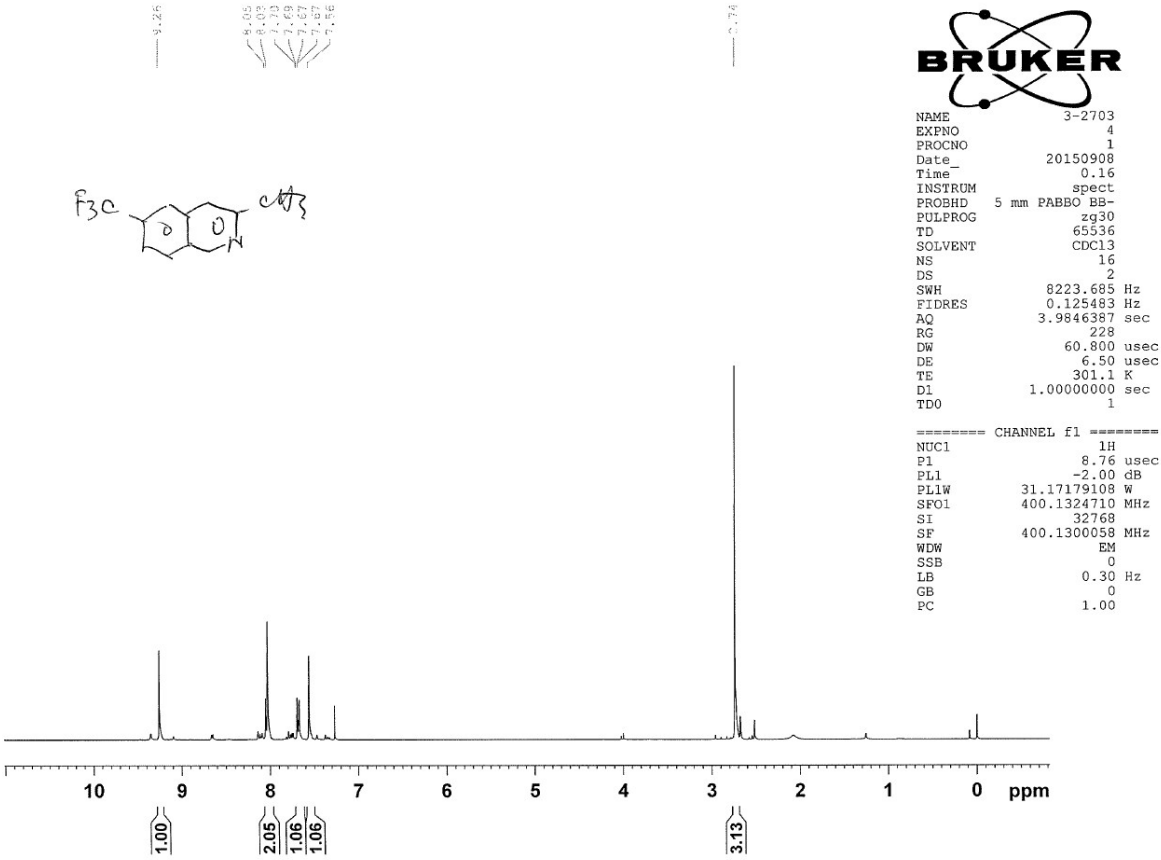
BRUKER

NAME	3-4802
EXPNO	4
PROCNO	1
Date_	20150907
Time	21.45
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	144
DW	60.800 usec
DE	6.50 usec
TE	300.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300005 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



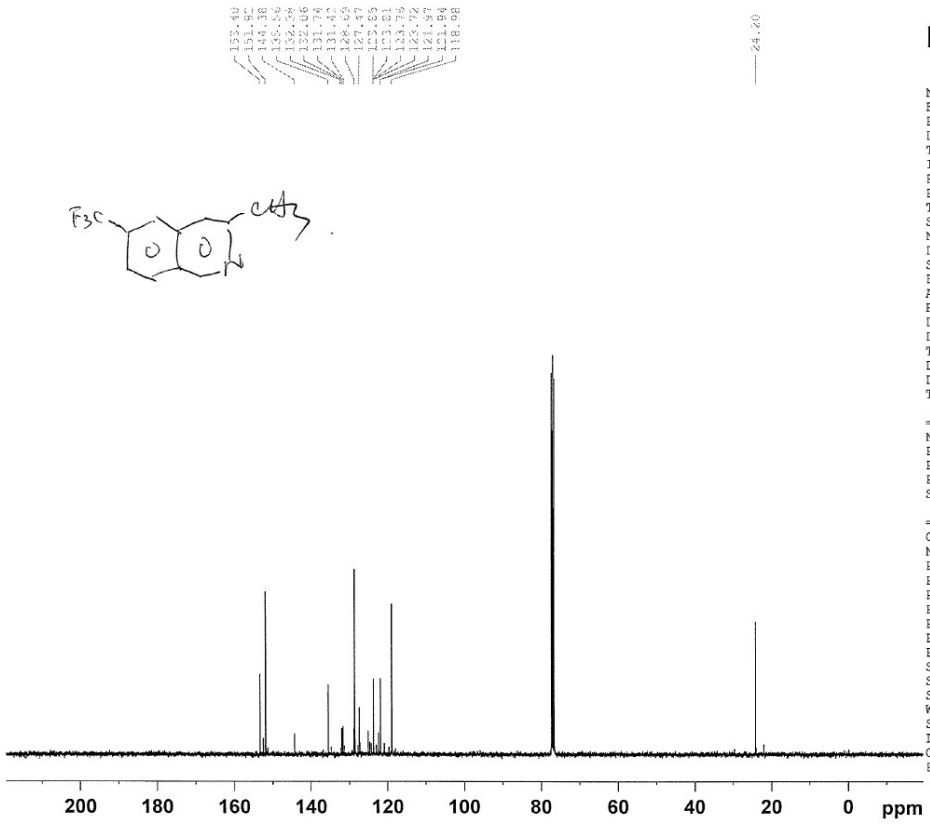
BRUKER

NAME	3-4802
EXPNO	2
PROCNO	1
Date_	20150831
Time	9.04
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	302.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



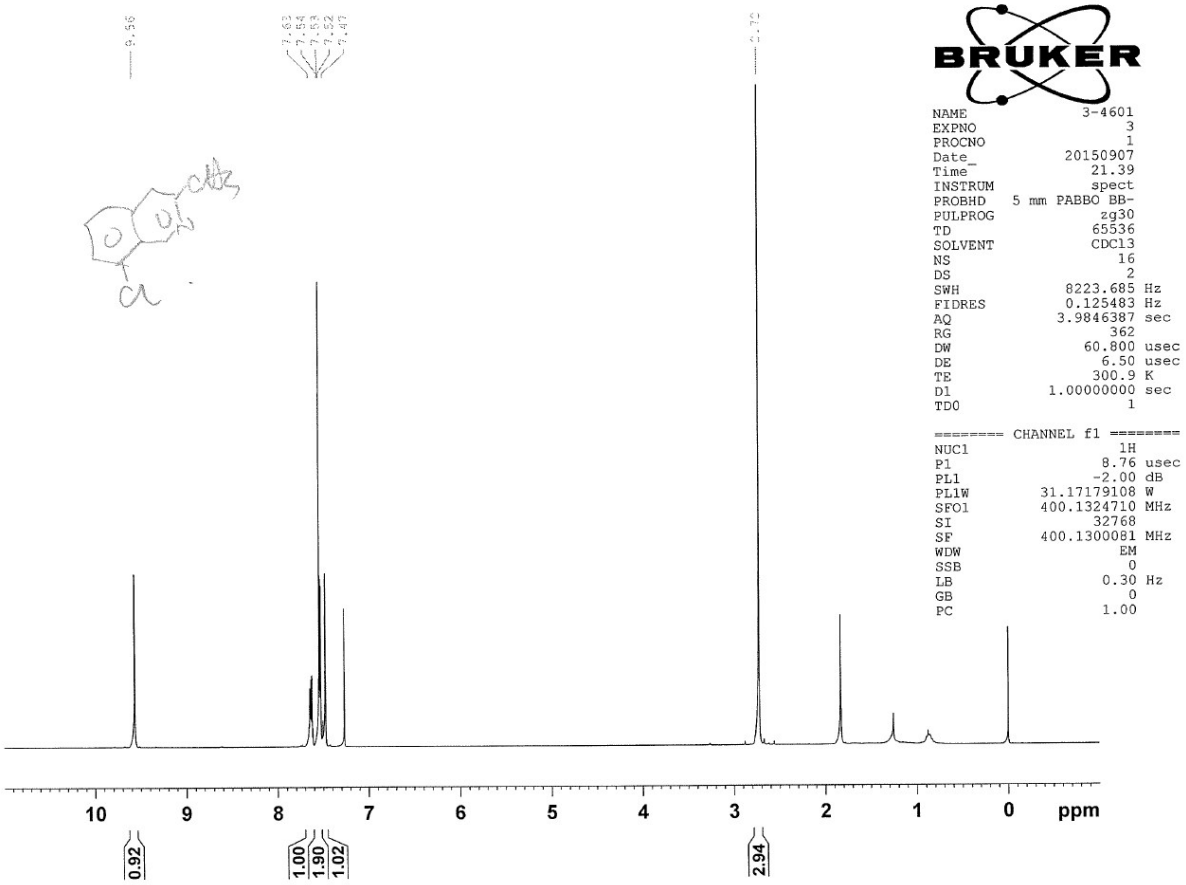
BRUKER

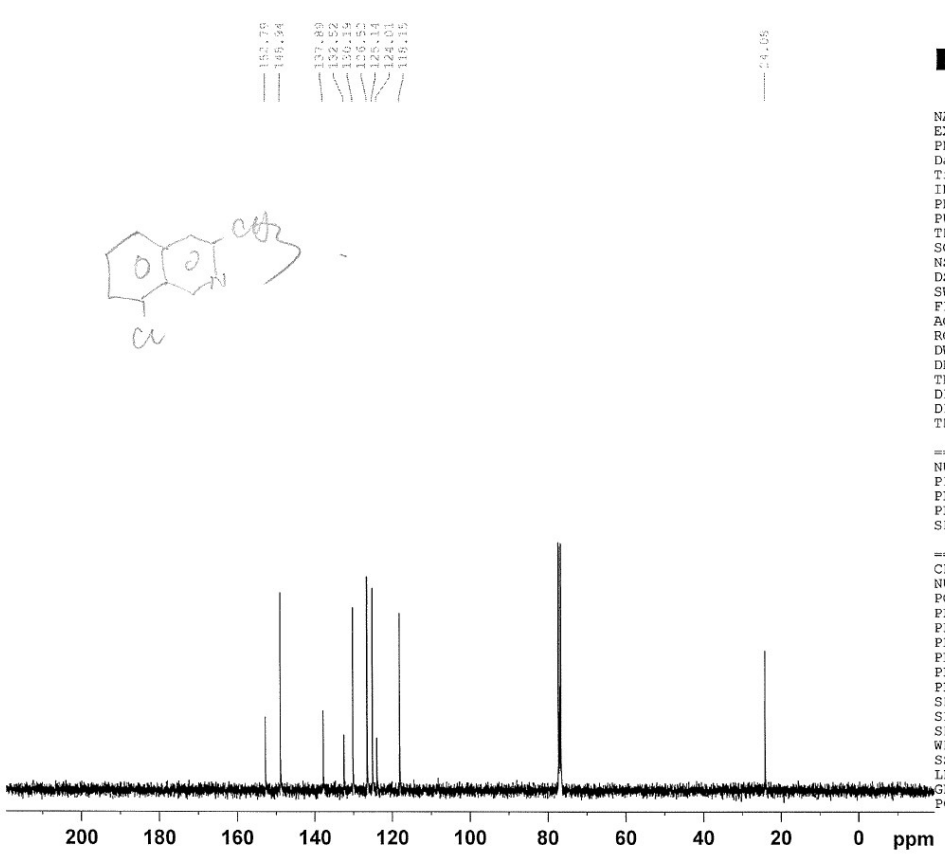
NAME	3-2703
EXPNO	4
PROCNO	1
Date_	20150908
Time	0.16
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	228
DW	60.800 usec
DE	6.50 usec
TE	301.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300058 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



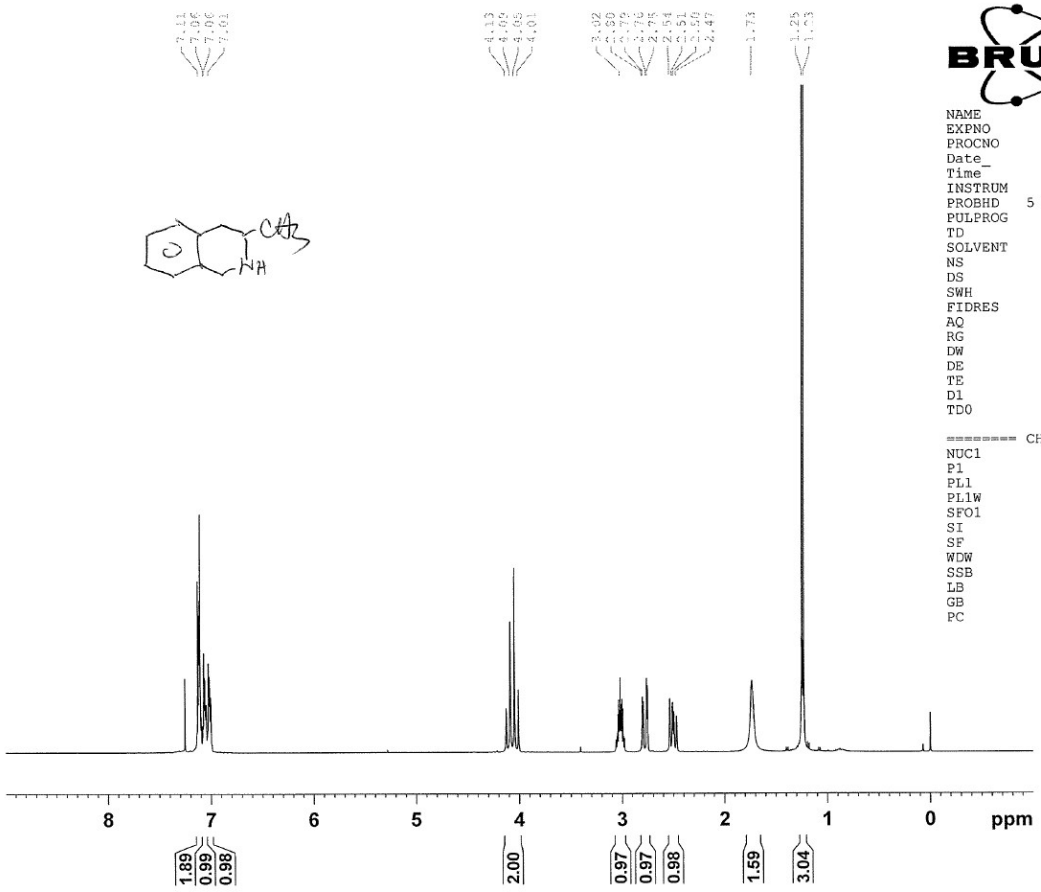
BRUKER

NAME	3-2703
EXPNO	5
PROCNO	1
Date_	20150908
Time	1.15
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	302.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


9.56
7.63
7.54
7.53
7.52
7.43
2.79
BRUKER
NAME 3-4601
EXPNO 3
PROCNO 1
Date_ 20150907
Time 21.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 362
DW 60.800 usec
DE 6.50 usec
TE 300.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
0.92
1.00
1.90
1.02
2.94

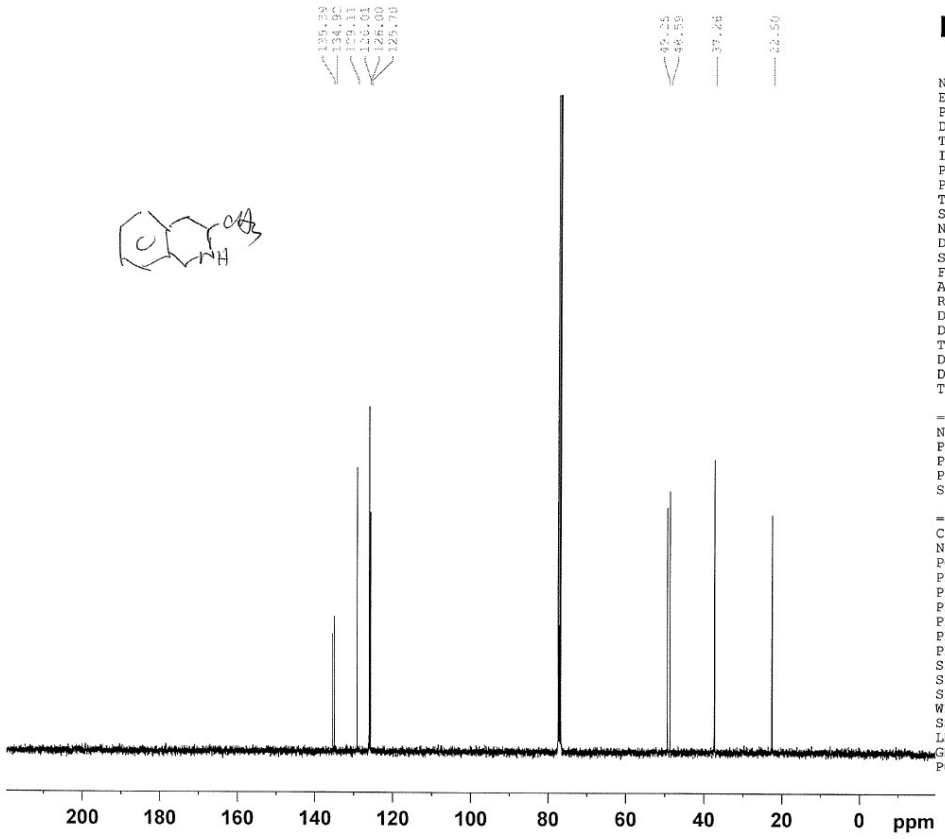


NAME	3-4601
EXPNO	2
PROCNO	1
Date_	20150831
Time	22.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	129
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	302.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



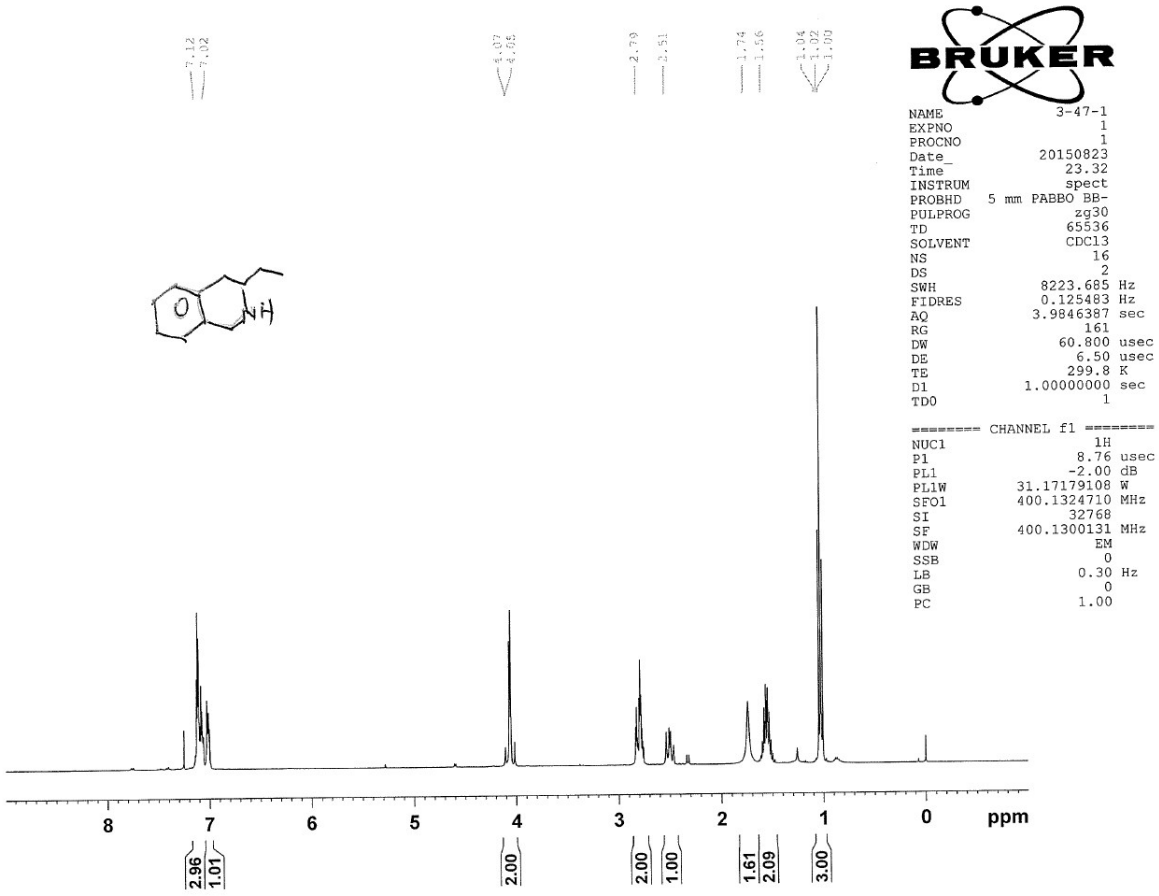
BRUKER

NAME	3-51-4
EXPNO	1
PROCNO	1
Date_	20150904
Time	21.53
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	181
DW	60.800 usec
DE	6.50 usec
TE	301.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300128 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	3-51-4
EXPNO	2
PROCNO	1
Date_	20150905
Time	17.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	743
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	301.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

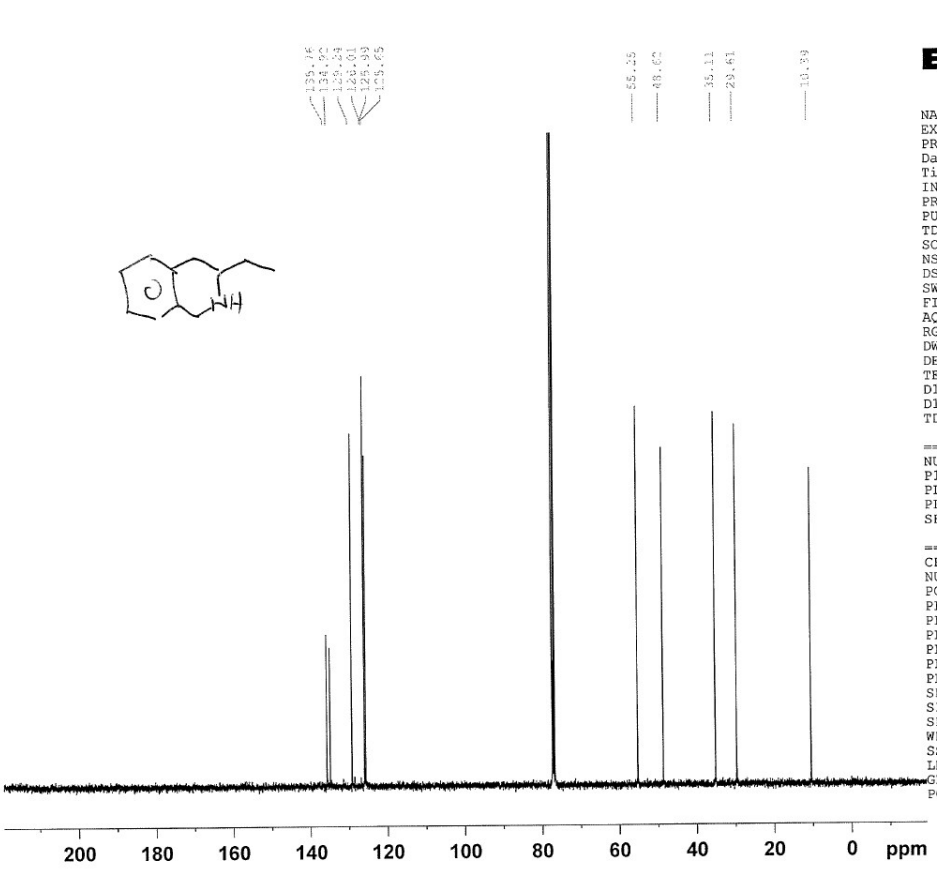


BRUKER

NAME	3-47-1
EXPNO	1
PROCNO	1
Date_	20150823
Time	23.32
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	161
DW	60.800 usec
DE	6.50 usec
TE	299.8 K
D1	1.00000000 sec
TD0	1

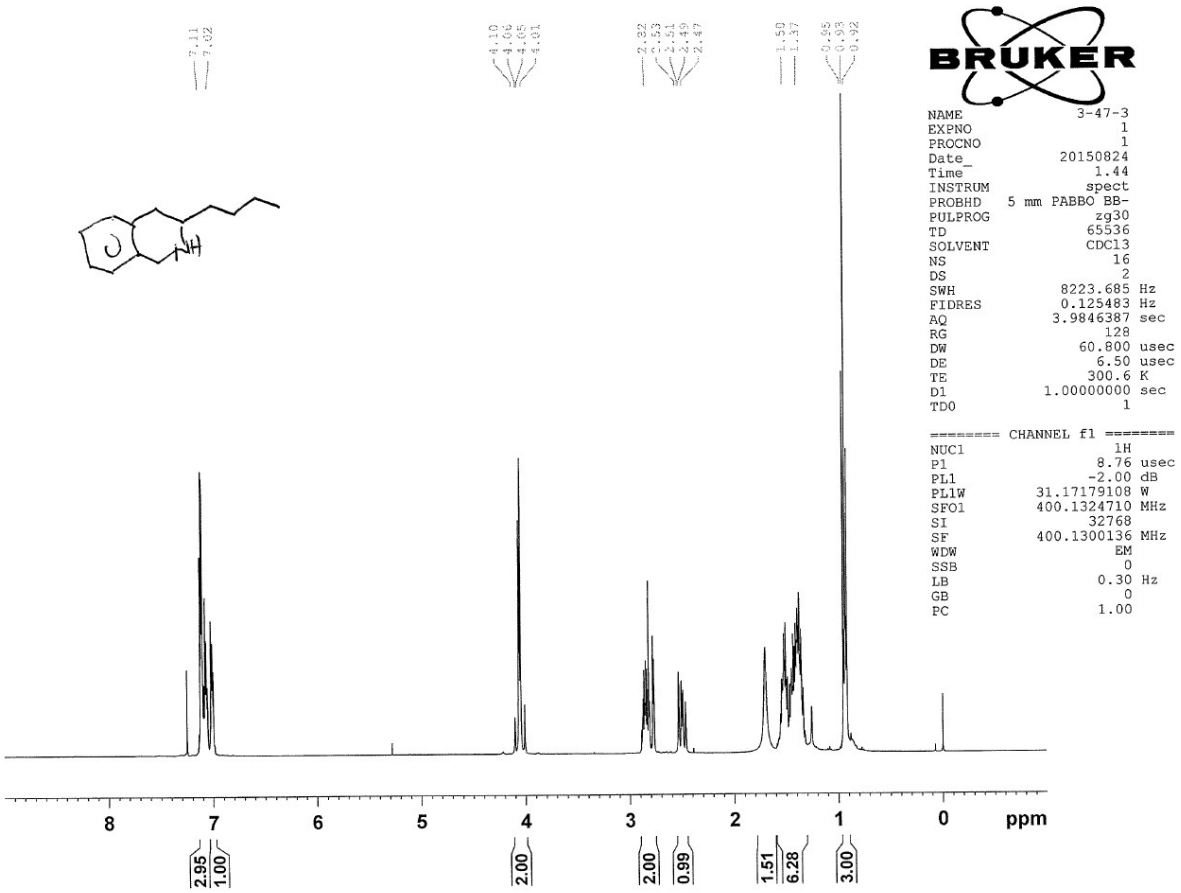
======== CHANNEL f1 ========

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300131 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



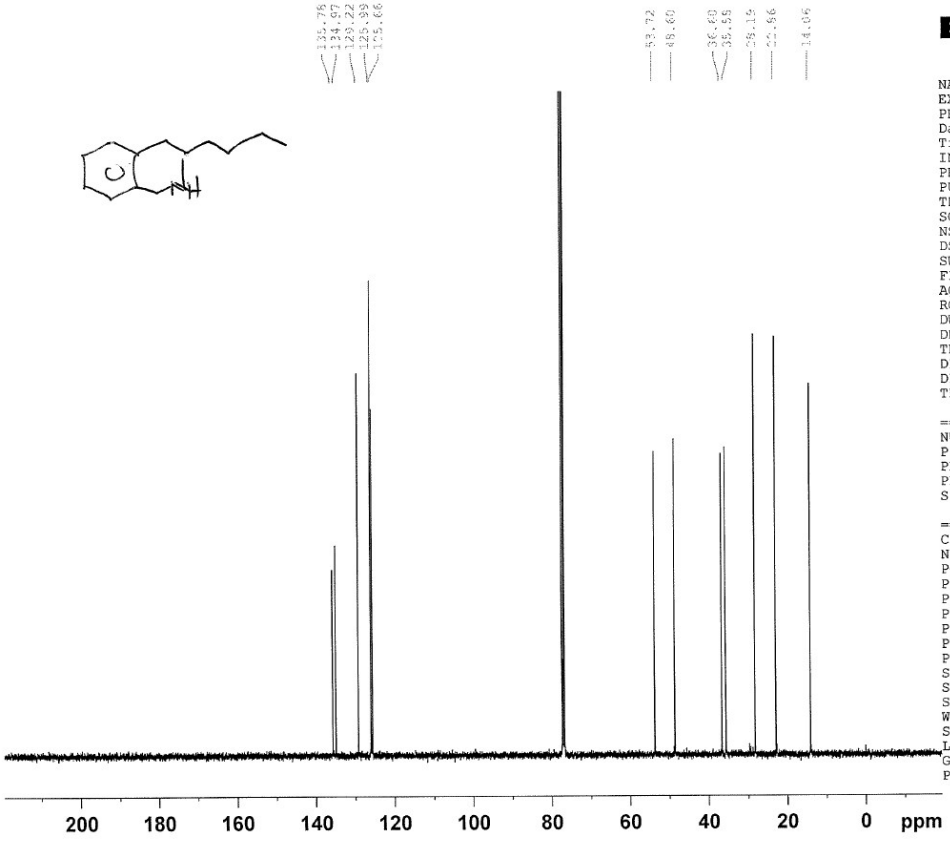
BRUKER

NAME	3-47-1
EXPNO	2
PROCNO	1
Date_	20150824
Time	0.33
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	301.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



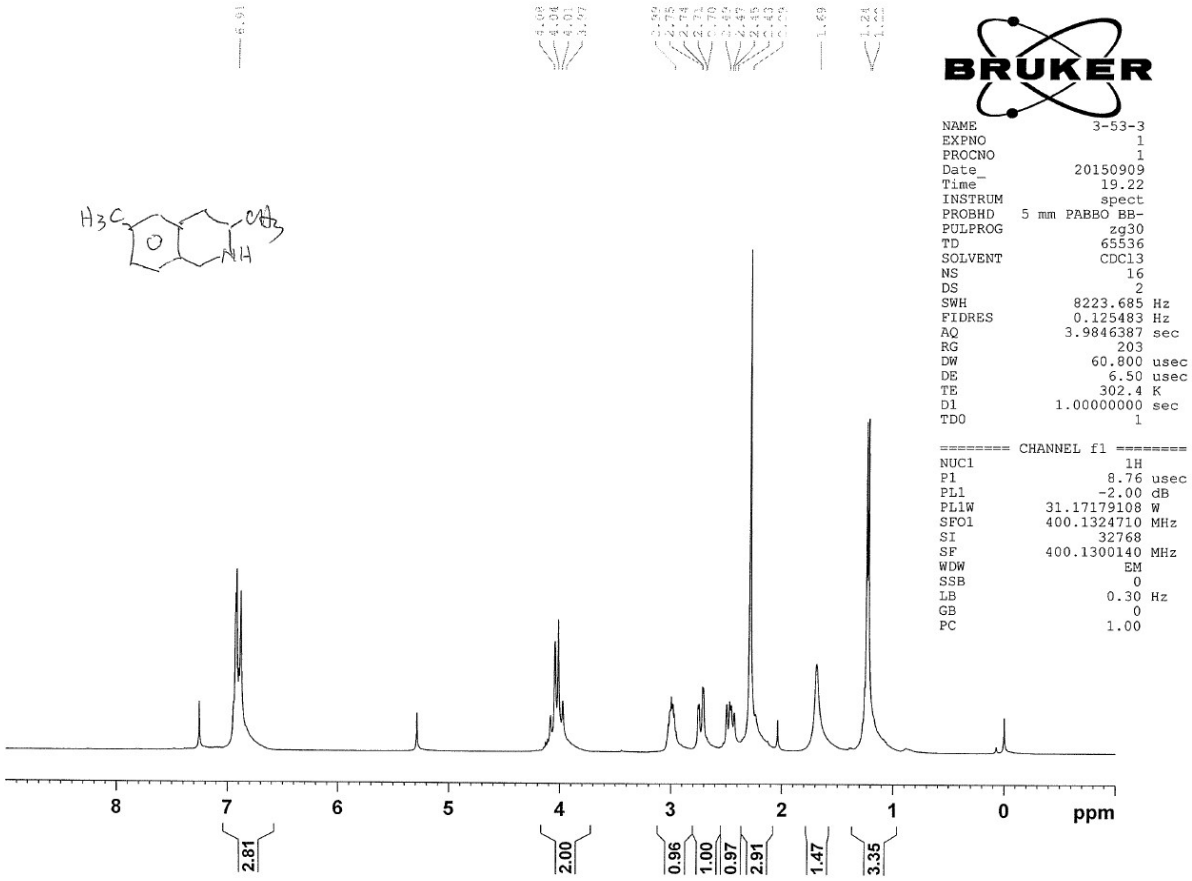
BRUKER

NAME	3-47-3
EXPNO	1
PROCNO	1
Date_	20150824
Time	1.44
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	128
DW	60.800 usec
DE	6.50 usec
TE	300.6 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300136 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



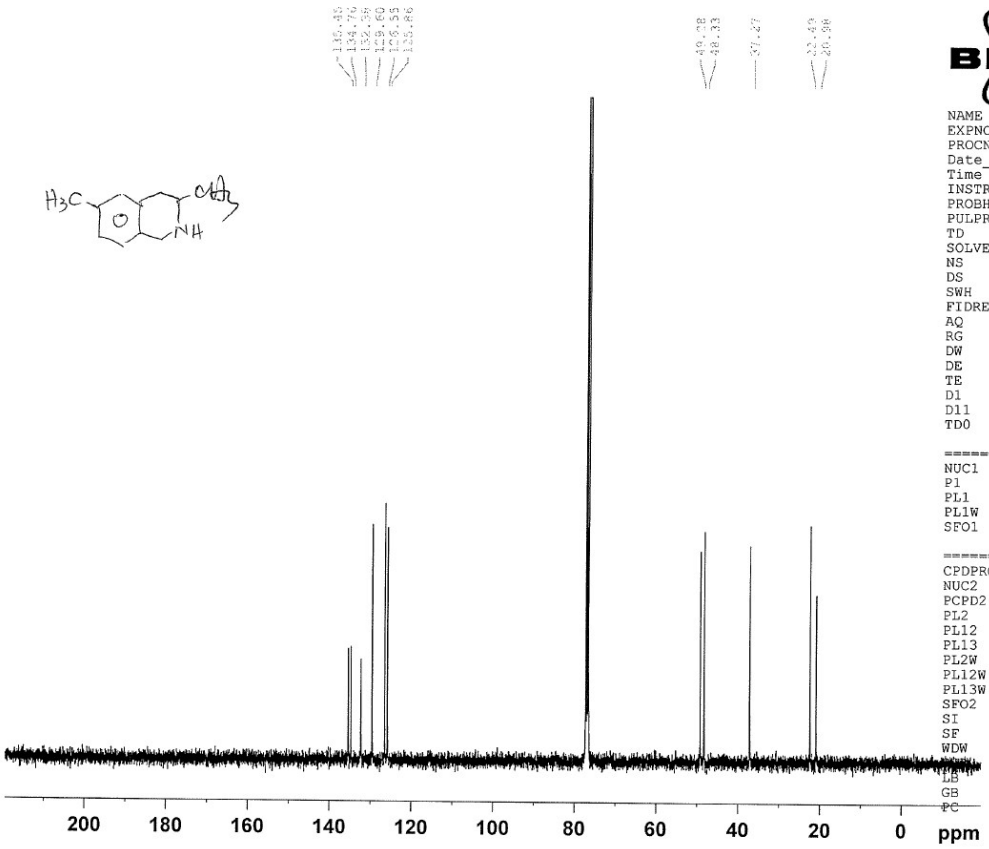
BRUKER

NAME	3-47-3
EXPNO	2
PROCNO	1
Date_	20150824
Time	2.45
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	301.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



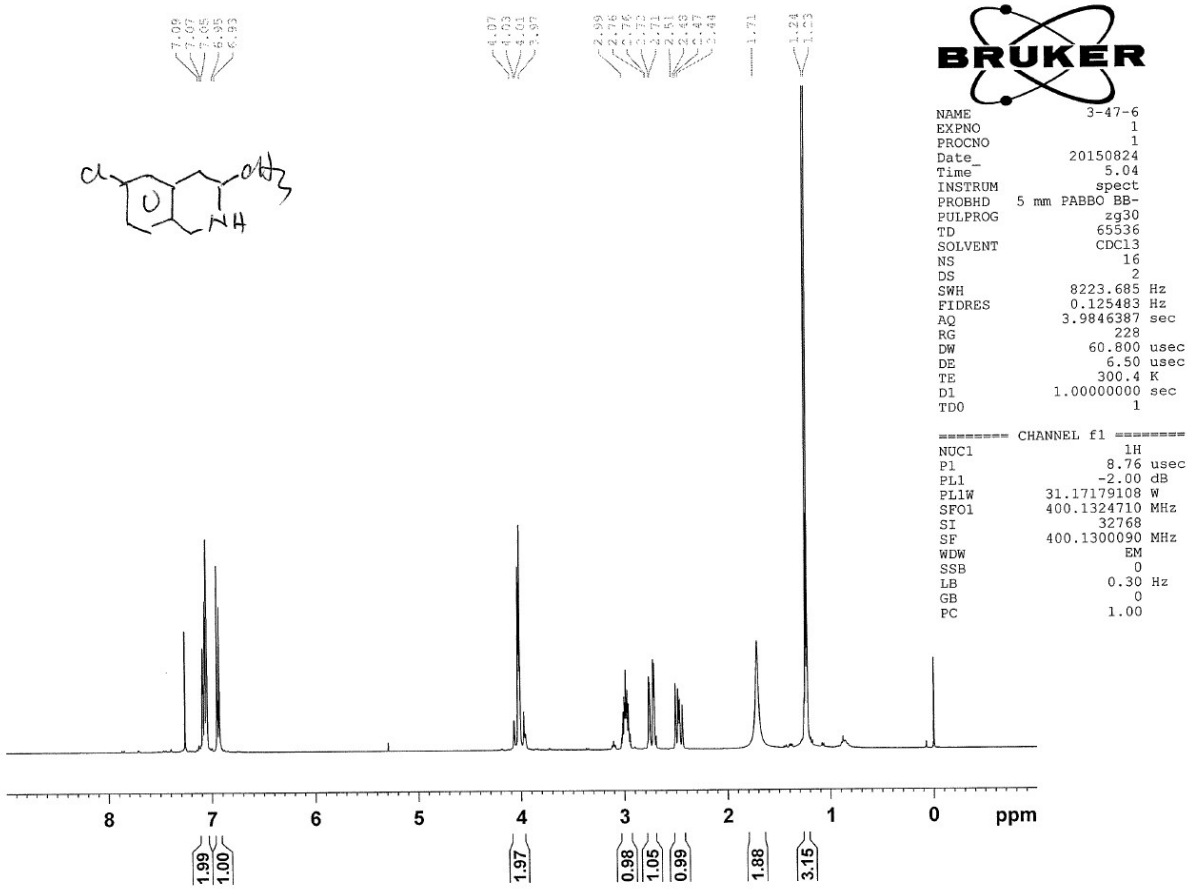
BRUKER

NAME	3-53-3
EXPNO	1
PROCNO	1
Date_	20150909
Time	19.22
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	302.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300140 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



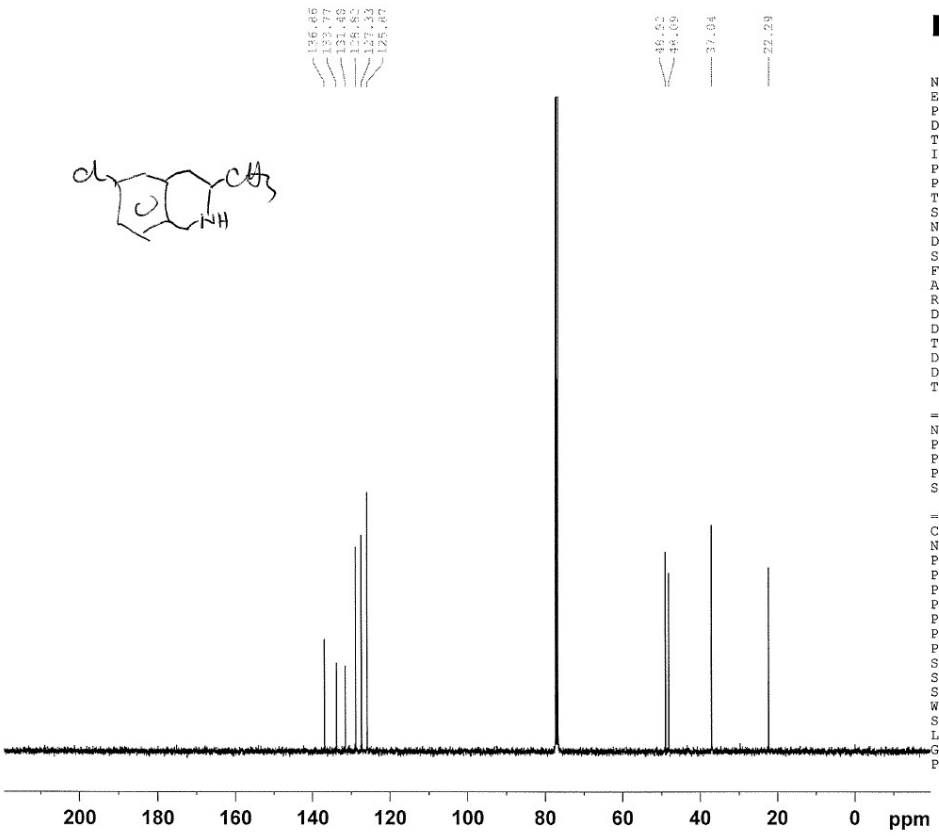
BRUKER

NAME	3-53-3
EXPNO	2
PROCNO	1
Date_	20150909
Time	21.39
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	304.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



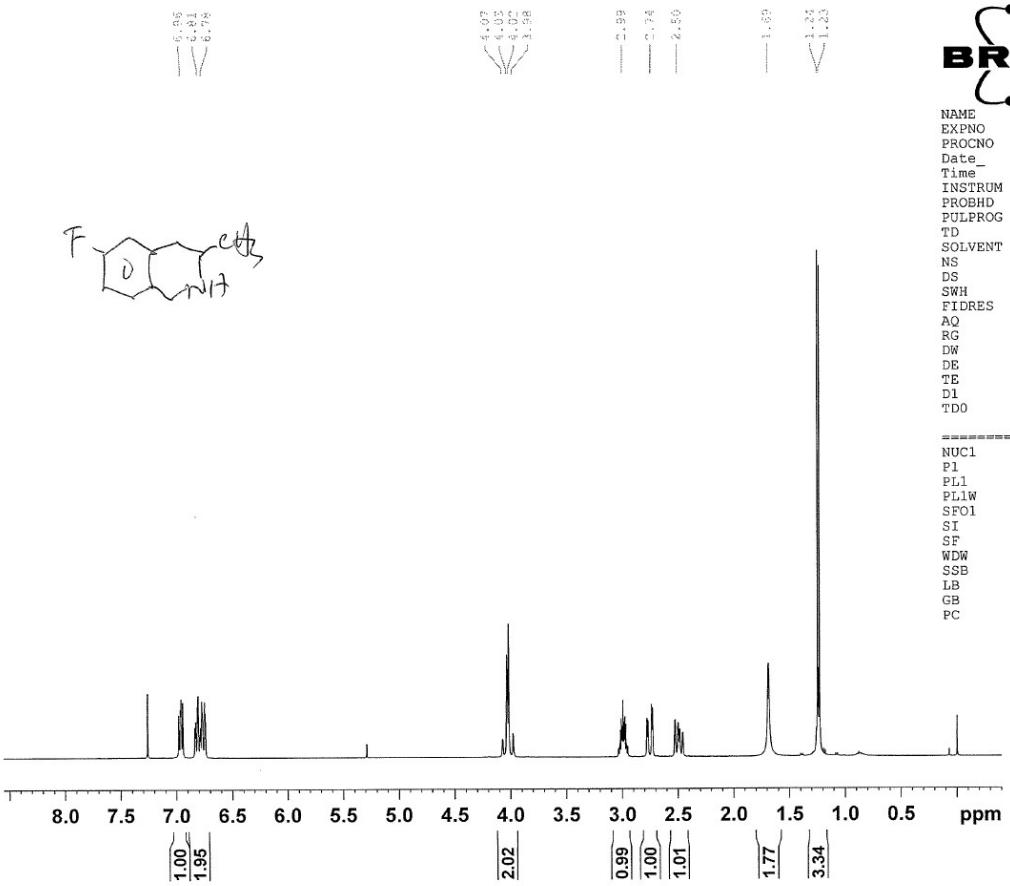
BRUKER

NAME	3-47-6
EXPNO	1
PROCNO	1
Date_	20150824
Time	5.04
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	228
DW	60.800 usec
DE	6.50 usec
TE	300.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



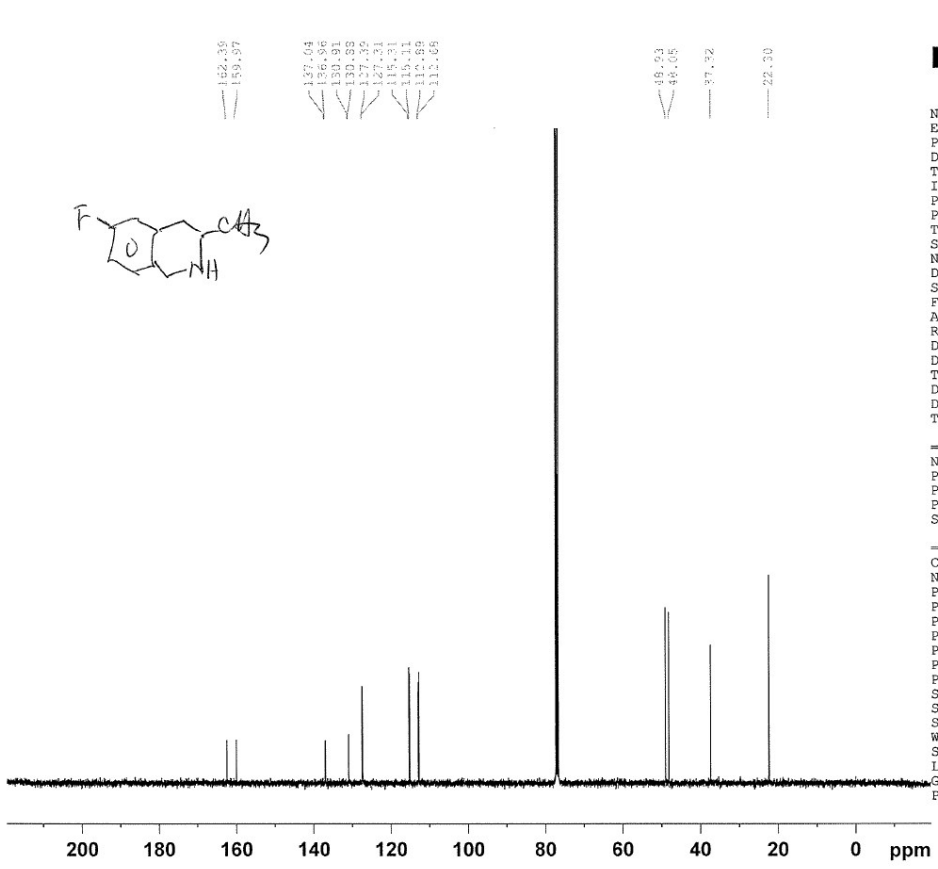
BRUKER

NAME	3-47-6
EXPNO	2
PROCNO	1
Date_	20150824
Time	6.04
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	301.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



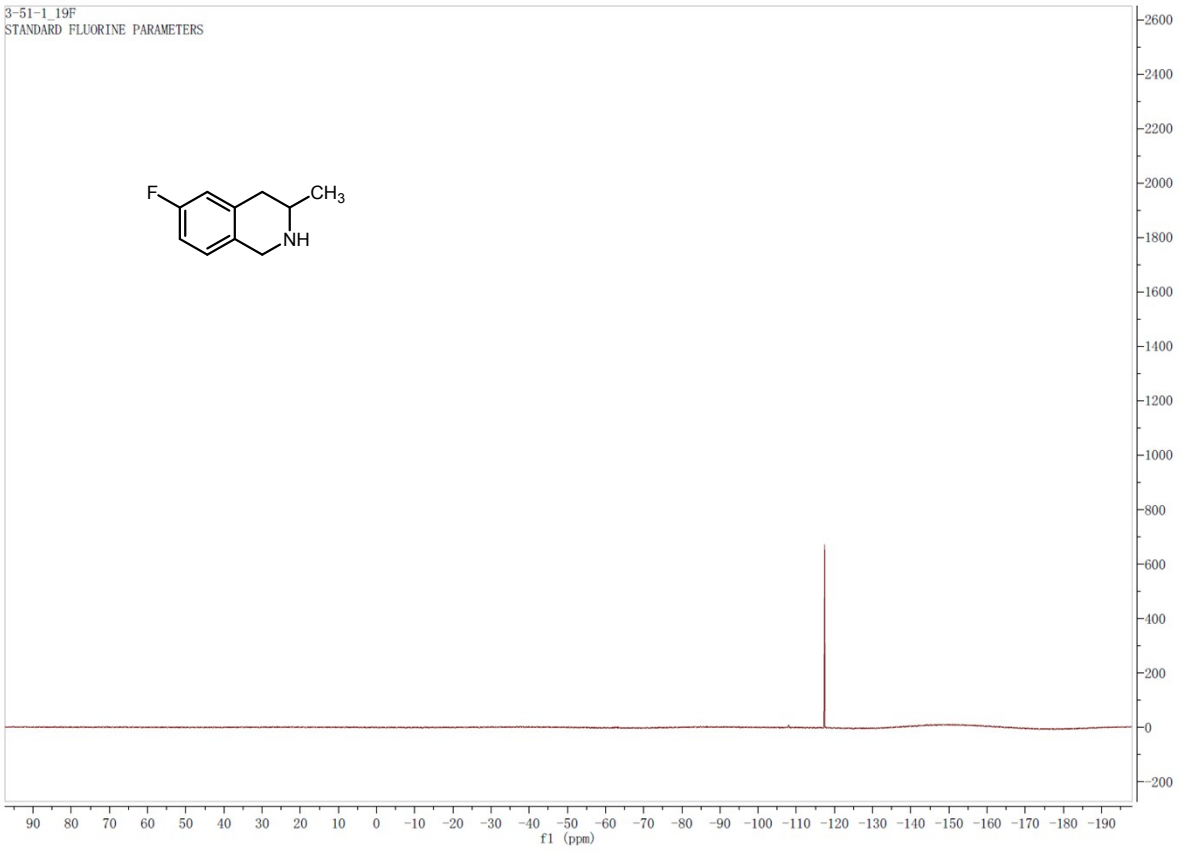
BRUKER

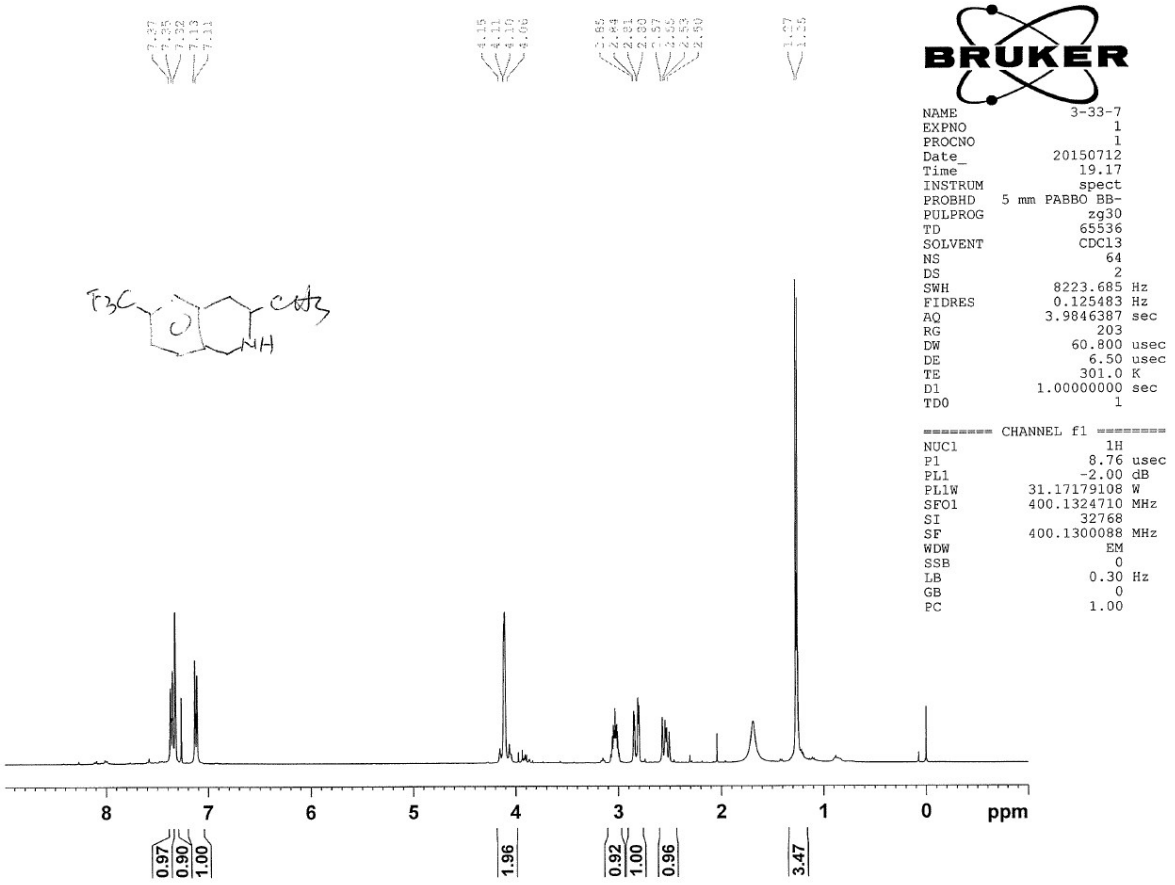
NAME	3-51-5
EXPNO	1
PROCNO	1
Date_	20150904
Time	21.59
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	228
DW	60.800 usec
DE	6.50 usec
TE	301.6 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300092 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	3-51-5
EXPNO	3
PROCNO	1
Date_	20150905
Time	18.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	301.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

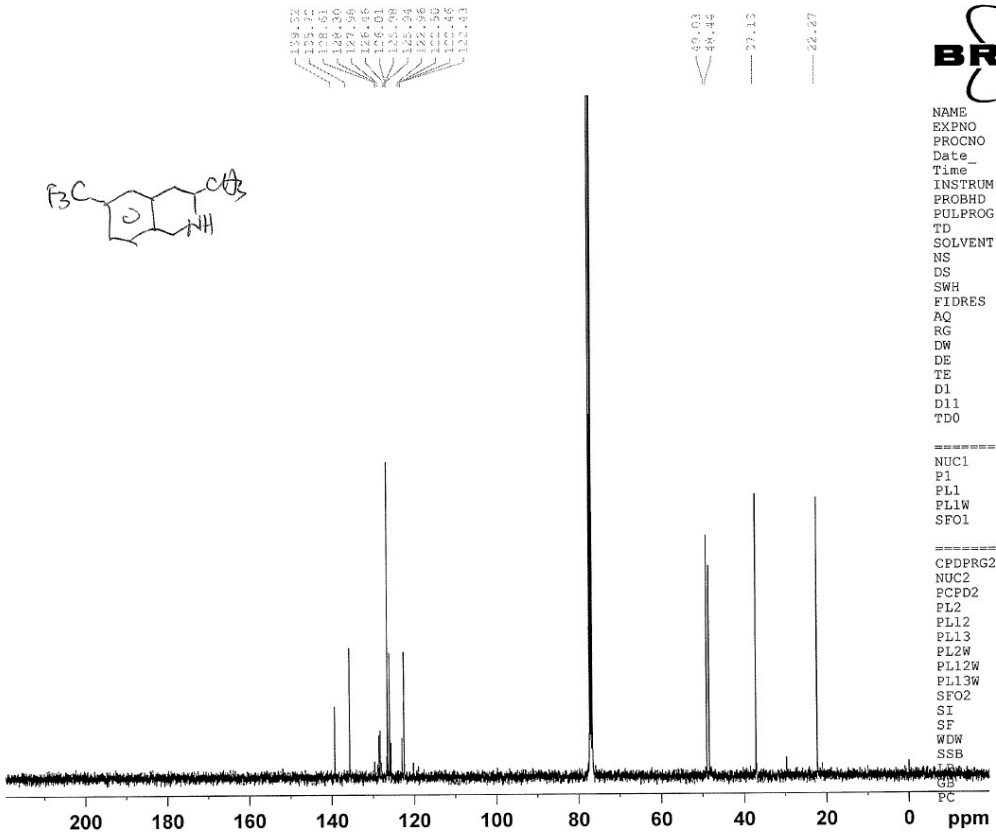

3-51-1_19F
STANDARD FLUORINE PARAMETERS
F
CH3
NH
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)



NAME	3-33-7
EXPNO	1
PROCNO	1
Date_	20150712
Time	19.17
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	301.0 K
D1	1.00000000 sec
TD0	1

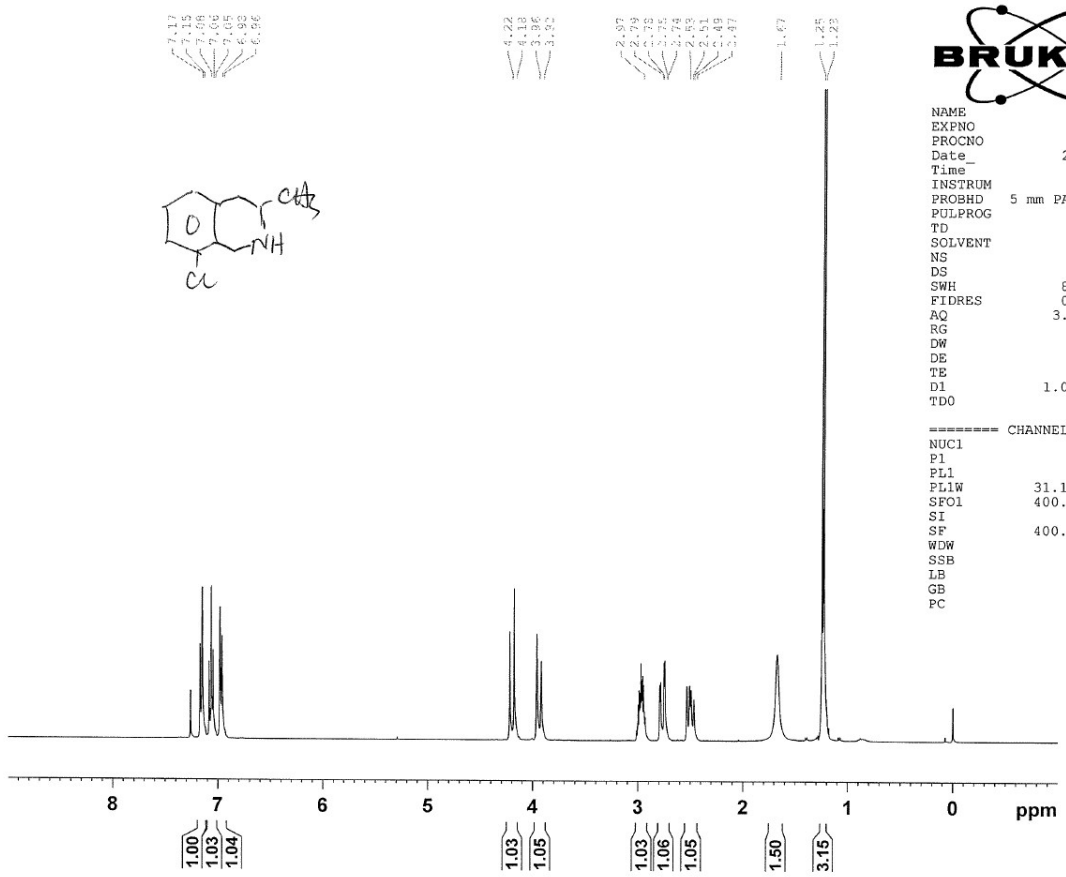
======== CHANNEL f1 ========

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300088 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	3-51-3
EXPNO	5
PROCNO	1
Date_	20150905
Time	23.53
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	5000
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	301.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127662 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

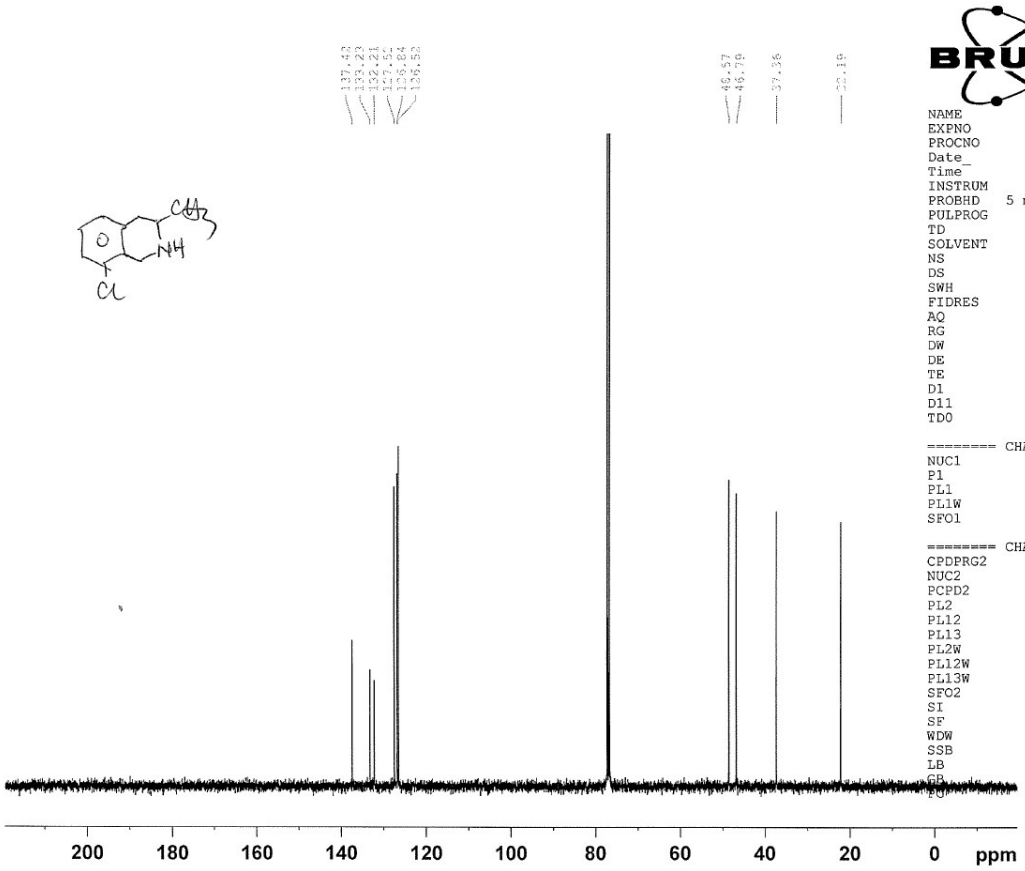


BRUKER

NAME	3-51-2
EXPNO	1
PROCNO	1
Date_	20150904
Time	21.41
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	301.8 K
D1	1.00000000 sec
TD0	1

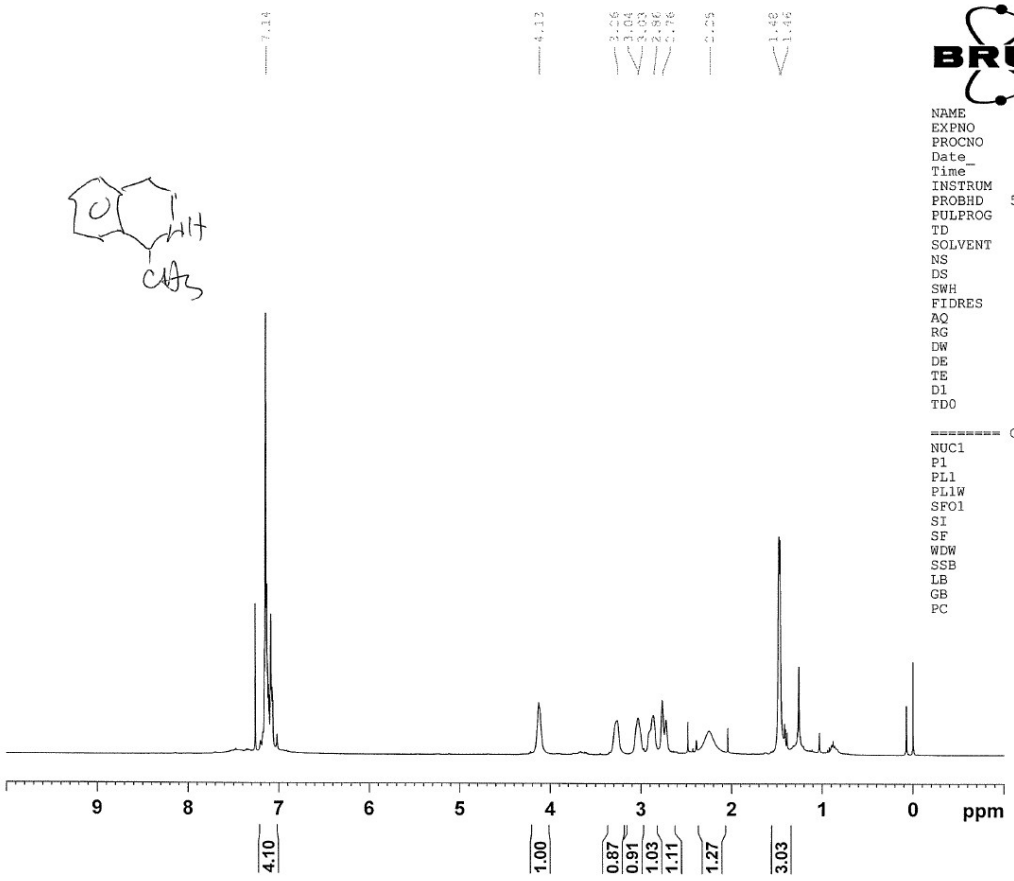
======== CHANNEL f1 ========

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300100 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



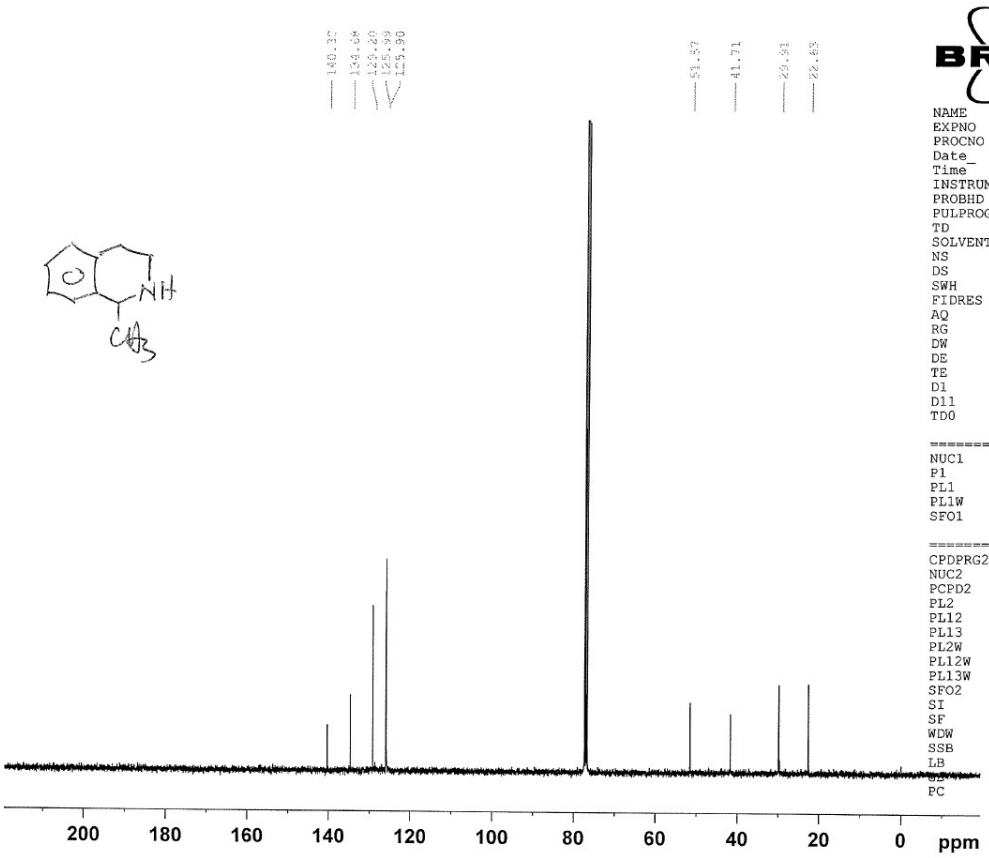
BRUKER

NAME	3-51-6
EXPNO	2
PROCNO	1
Date_	20150905
Time	16.18
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	381
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	301.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



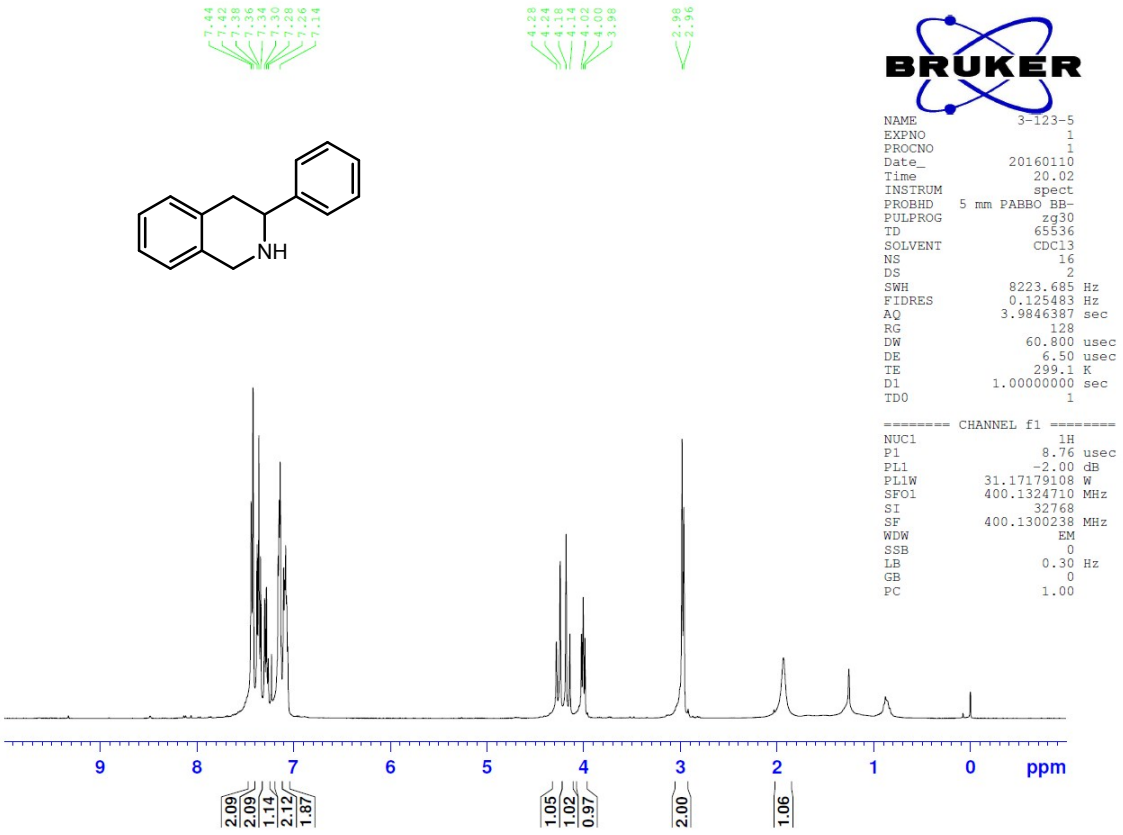
BRUKER

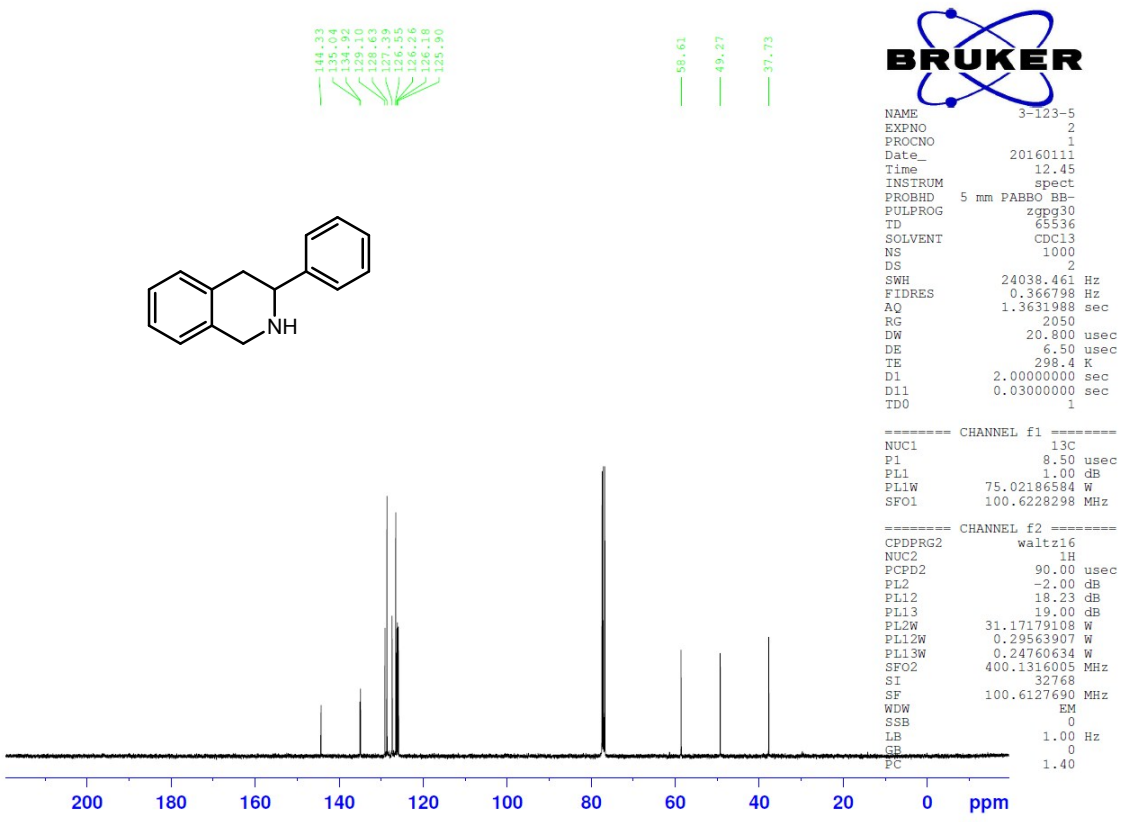
NAME	3-56-1
EXPNO	1
PROCNO	1
Date_	20150918
Time	5.29
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	299.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300117 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

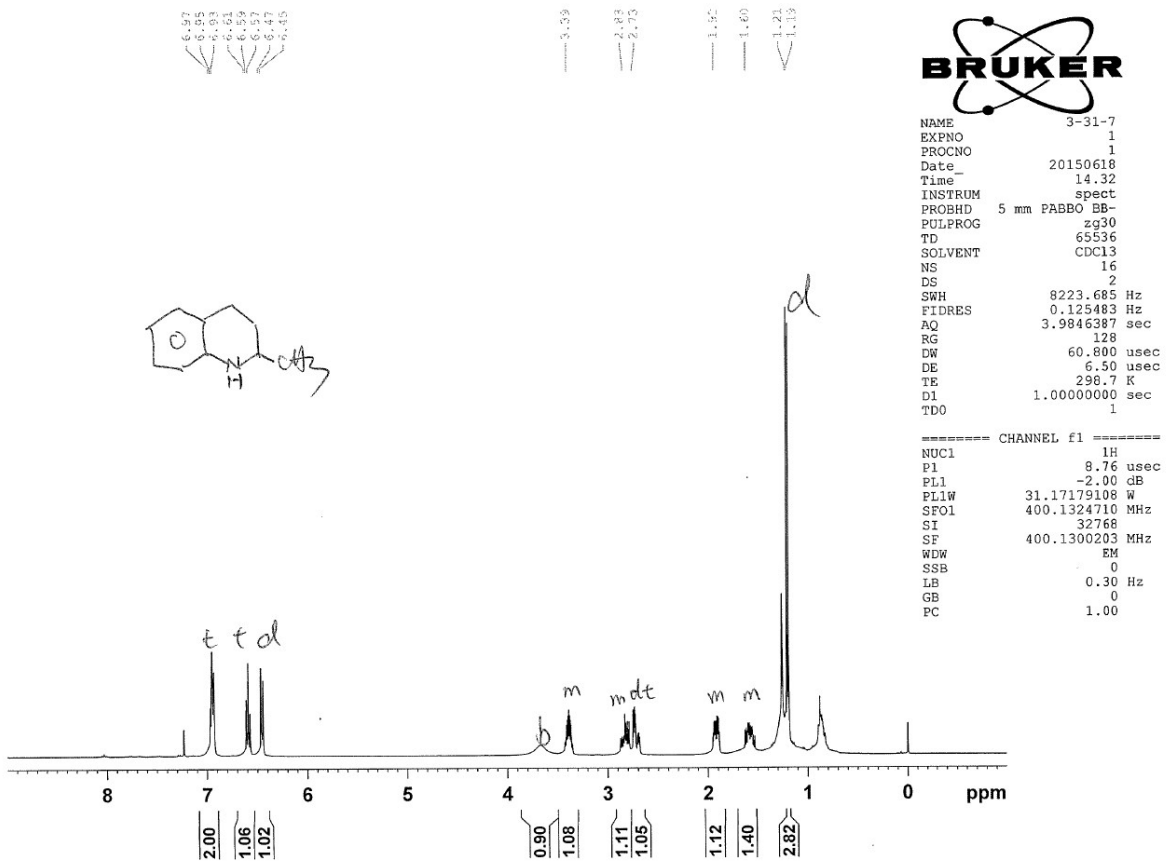
NAME	3-56-1
EXPNO	2
PROCNO	1
Date_	20150918
Time	6.28
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	300.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

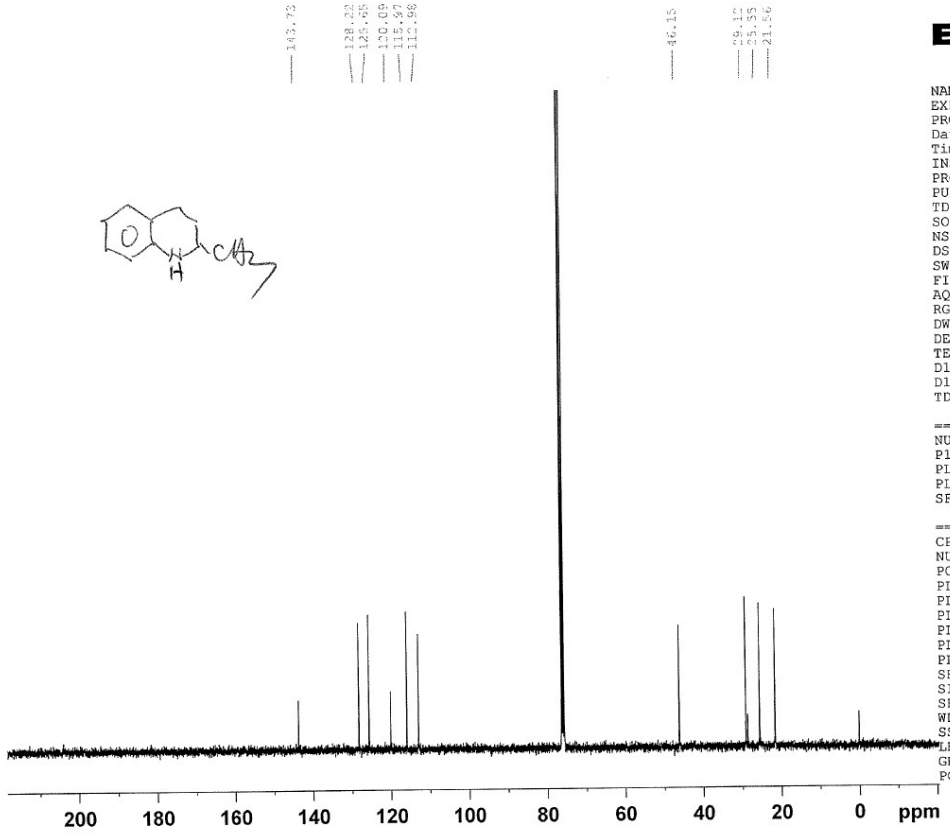

7.44
7.42
7.38
7.36
7.34
7.30
7.28
7.26
7.14
4.28
4.24
4.18
4.14
4.10
4.02
4.00
3.98
2.98
2.96
NH
BRUKER
NAME 3-123-5
EXPNO 1
PROCNO 1
Date_ 20160110
Time 20.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.50 usec
TE 299.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300238 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
2.09
2.09
1.14
2.12
1.87
1.05
1.02
0.97
2.00
1.06



BRUKER

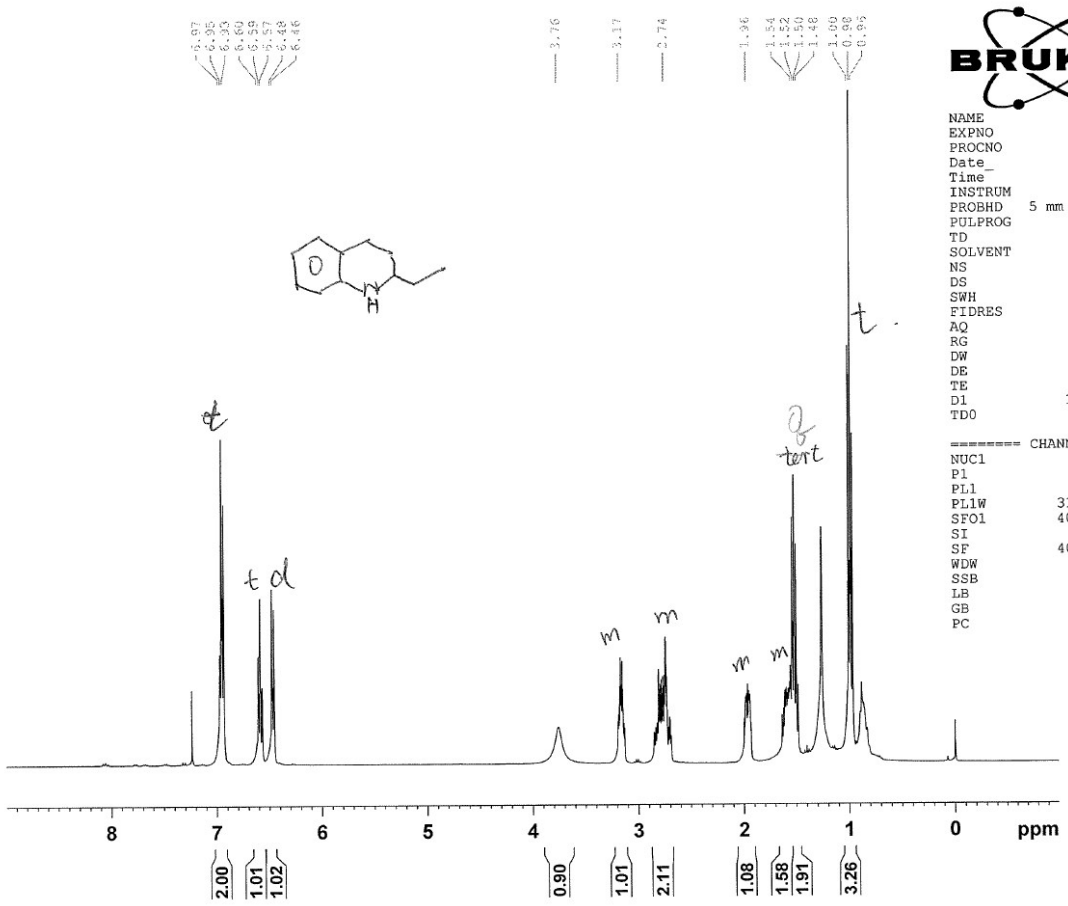
NAME	3-123-5
EXPNO	2
PROCNO	1
Date_	20160111
Time	12.45
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	298.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


6.97
6.95
6.93
6.61
6.59
6.57
6.47
6.45
3.39
2.83
2.73
1.95
1.60
1.21
1.13
BRUKER
NAME 3-31-7
EXPNO 1
PROCNO 1
Date_ 20150618
Time 14.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300203 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
t
t
d
m
m
dt
m
m
d
8
7
6
5
4
3
2
1
0
ppm
2.00
1.06
1.02
0.90
1.08
1.11
1.05
1.12
1.40
2.82



BRUKER

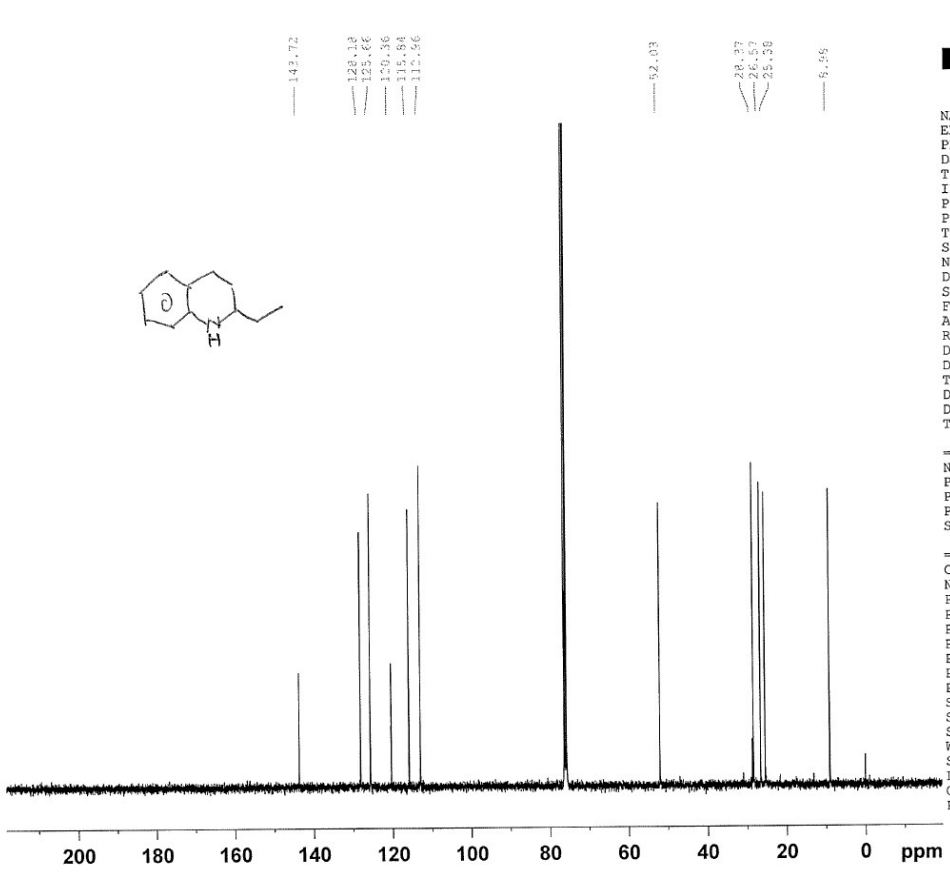
NAME	3-31-7
EXPNO	3
PROCNO	1
Date_	20150822
Time	1.48
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	303.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128727 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



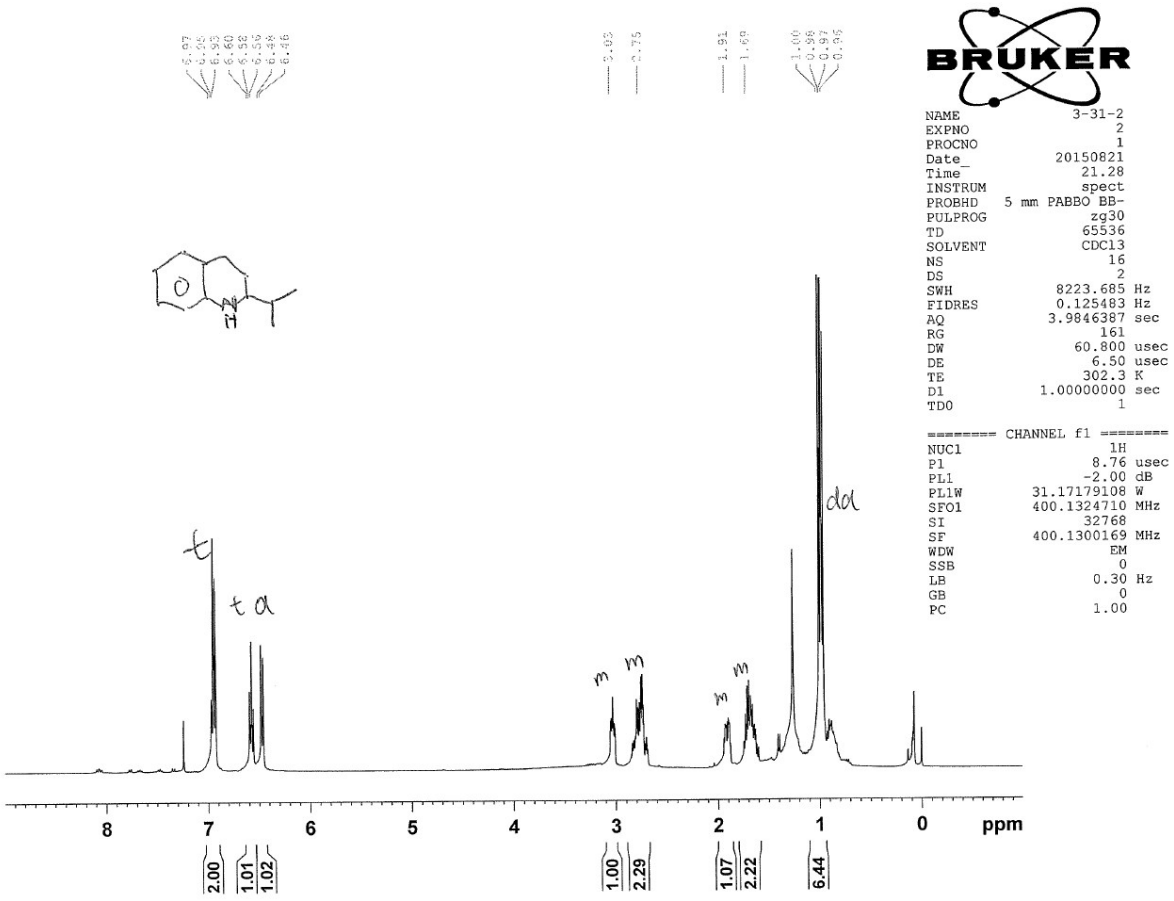
NAME	3-31-1
EXPNO	1
PROCNO	1
Date_	20150618
Time	13.50
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	128
DW	60.800 usec
DE	6.50 usec
TE	299.1 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300197 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

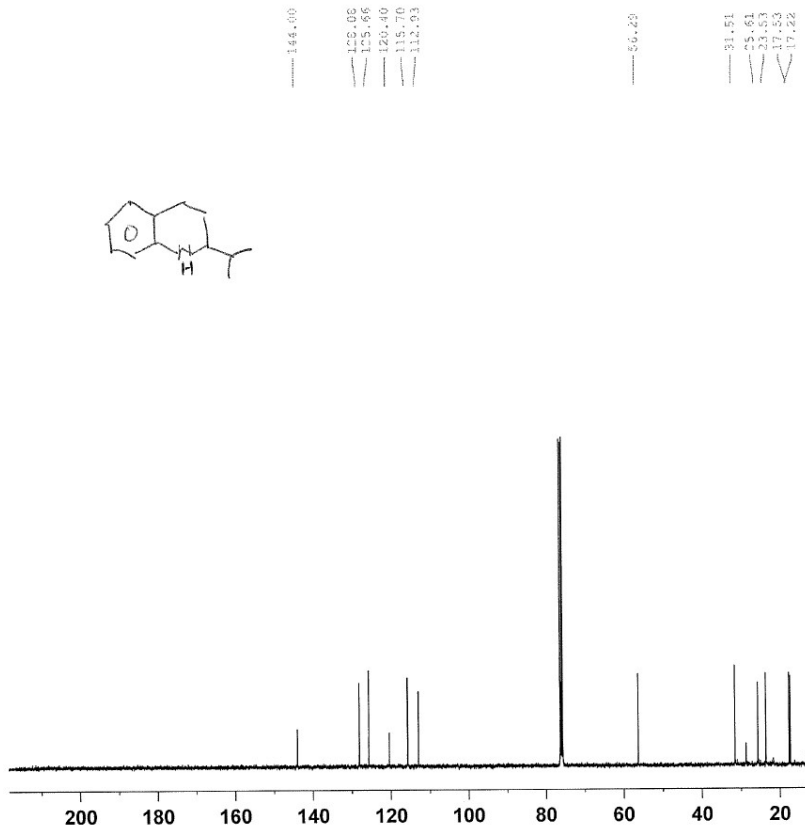


NAME	3-31-1
EXPNO	3
PROCNO	1
Date_	20150821
Time	21.22
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	303.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128738 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



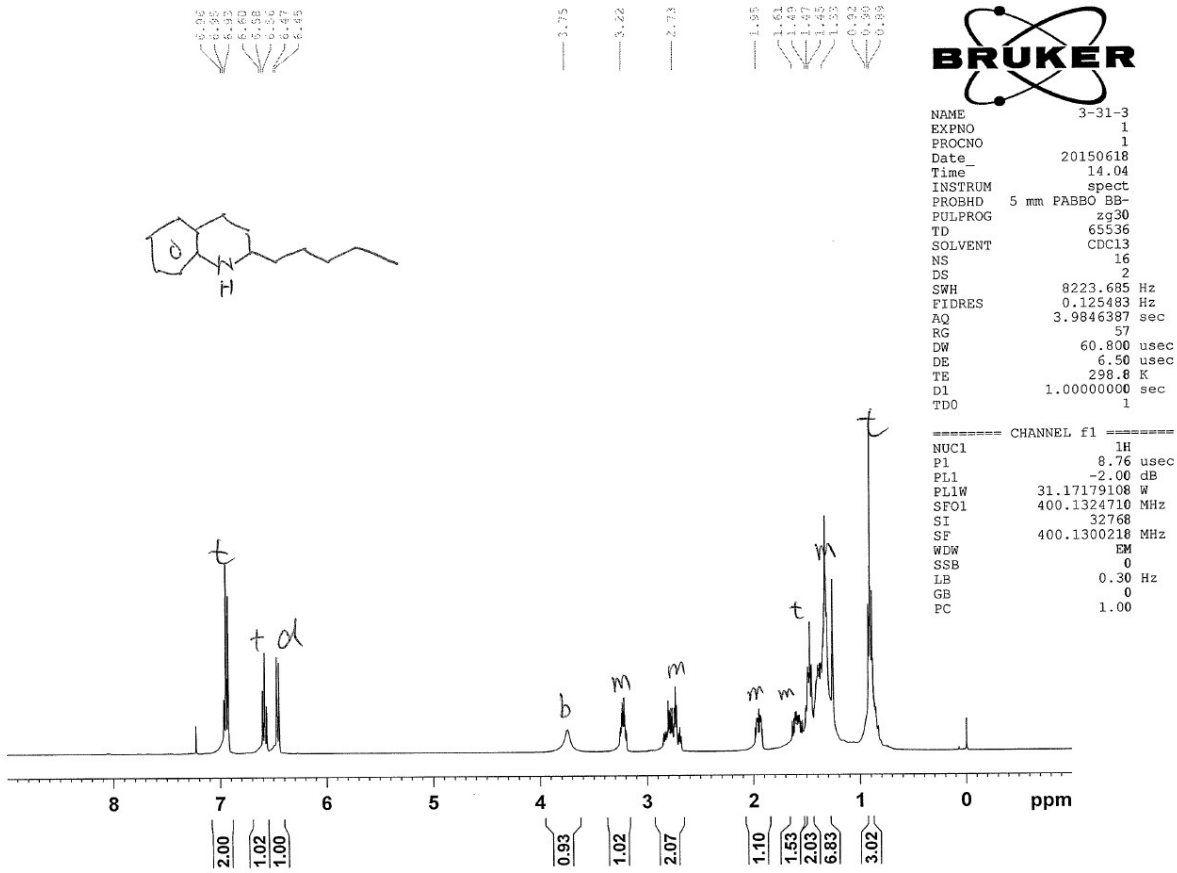
BRUKER

NAME	3-31-2
EXPNO	2
PROCNO	1
Date_	20150821
Time	21.28
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	161
DW	60.800 usec
DE	6.50 usec
TE	302.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300169 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	3-31-2
EXPNO	3
PROCNO	1
Date_	20150821
Time	22.29
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	303.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128734 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


6.98
6.95
6.93
6.60
6.58
6.56
6.47
6.45
3.75
3.22
2.73
1.95
1.61
1.49
1.47
1.45
1.33
0.92
0.90
0.89
BRUKER
NAME 3-31-3
EXPNO 1
PROCNO 1
Date_ 20150618
Time 14.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 57
DW 60.800 usec
DE 6.50 usec
TE 298.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300218 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
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7
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5
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3
2
1
0
ppm
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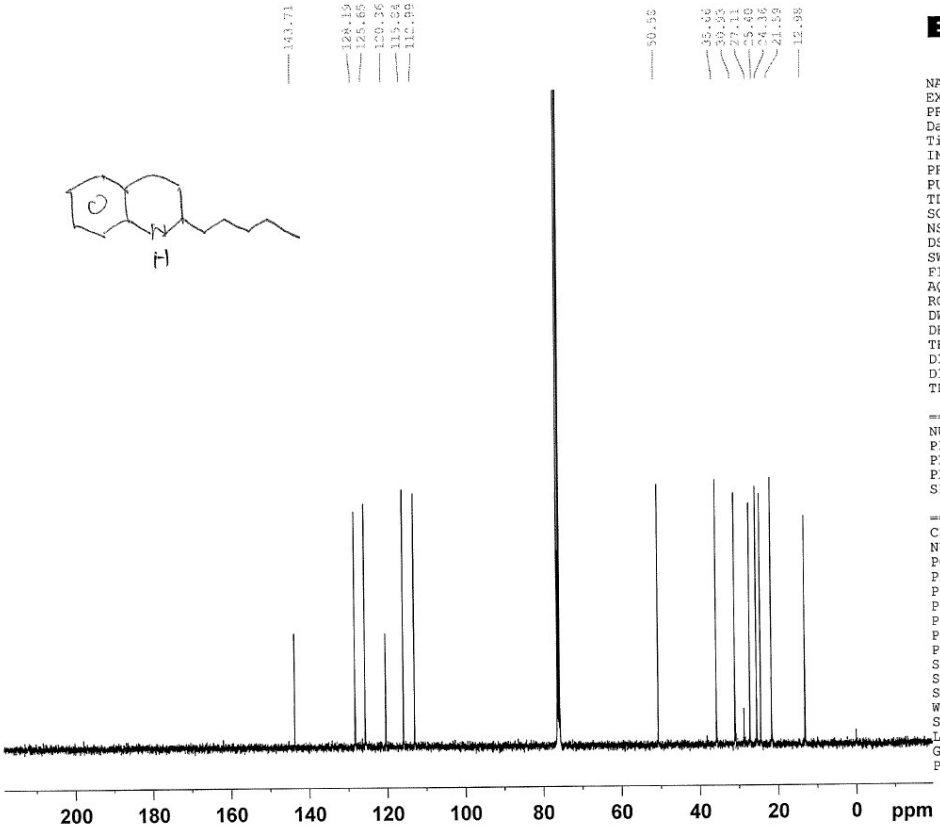
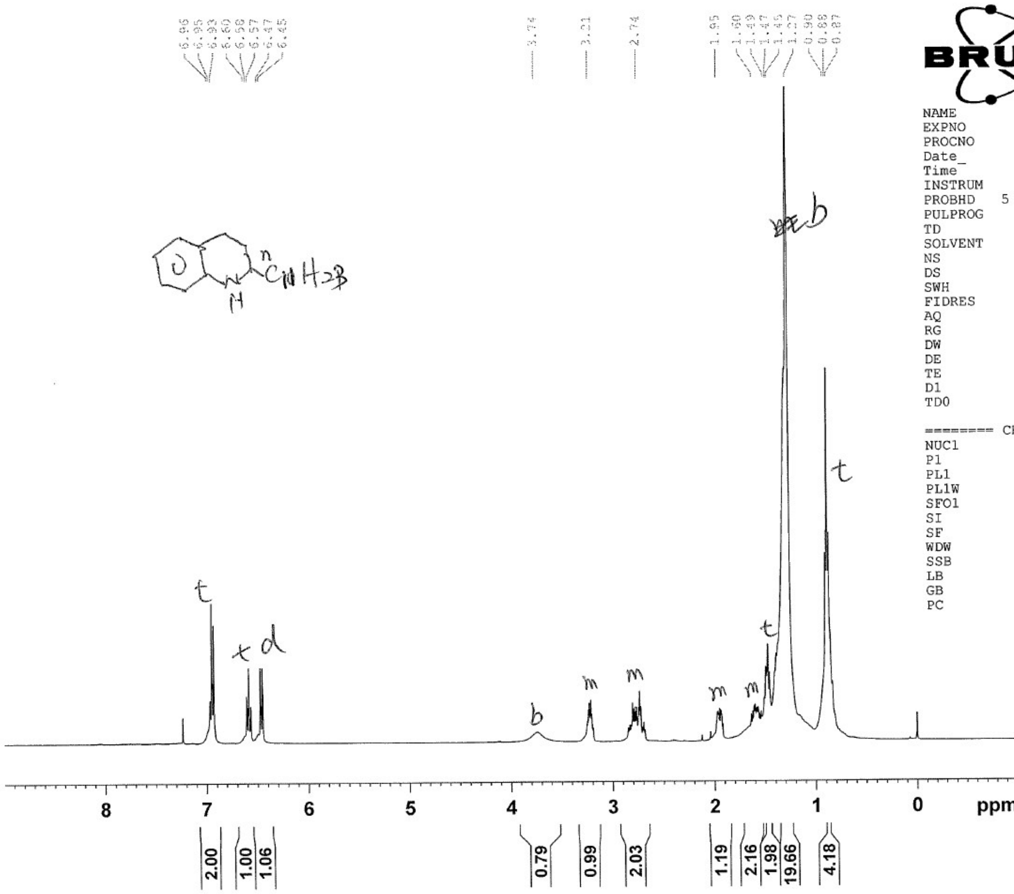
1.02
1.00
0.93
1.02
2.07
1.10
1.53
2.03
6.83
3.02



BRUKER

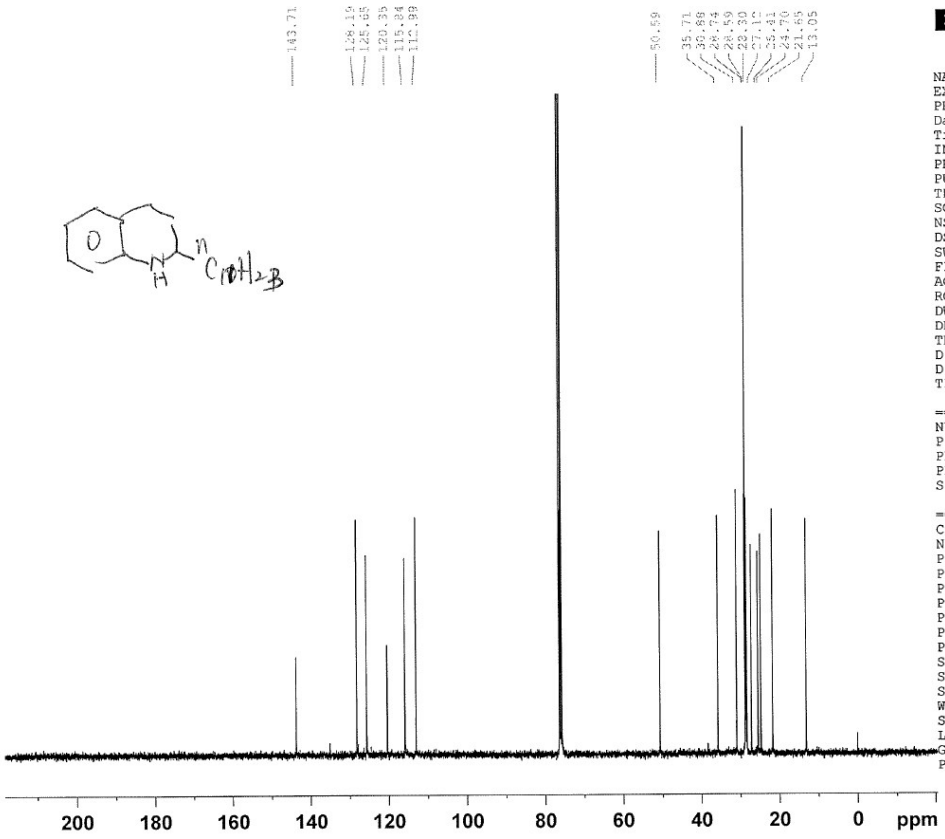
NAME	3-31-3
EXPNO	3
PROCNO	1
Date_	20150821
Time	23.37
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	303.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128741 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



NAME	3-31-5
EXPNO	1
PROCNO	1
Date_	20150618
Time	14.19
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	45.2
DW	60.800 usec
DE	6.50 usec
TE	298.7 K
D1	1.00000000 sec
TD0	1

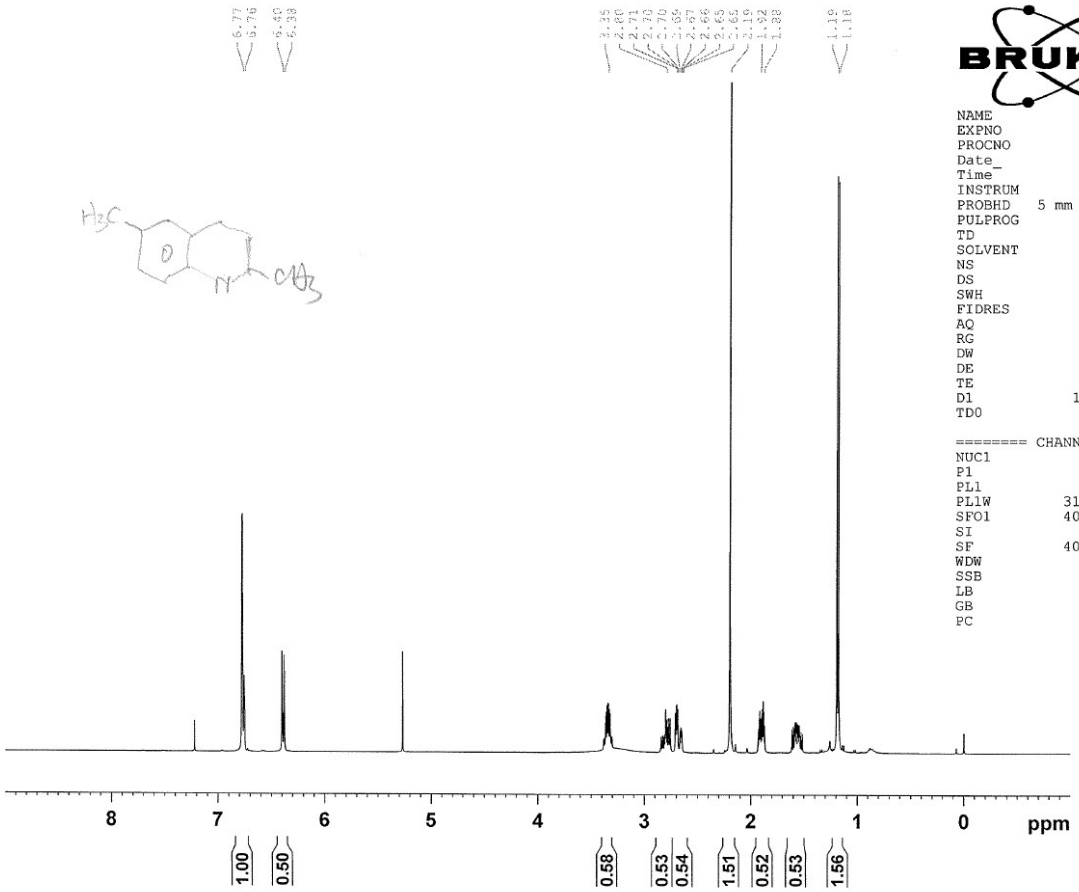
======== CHANNEL f1 ========

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300205 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



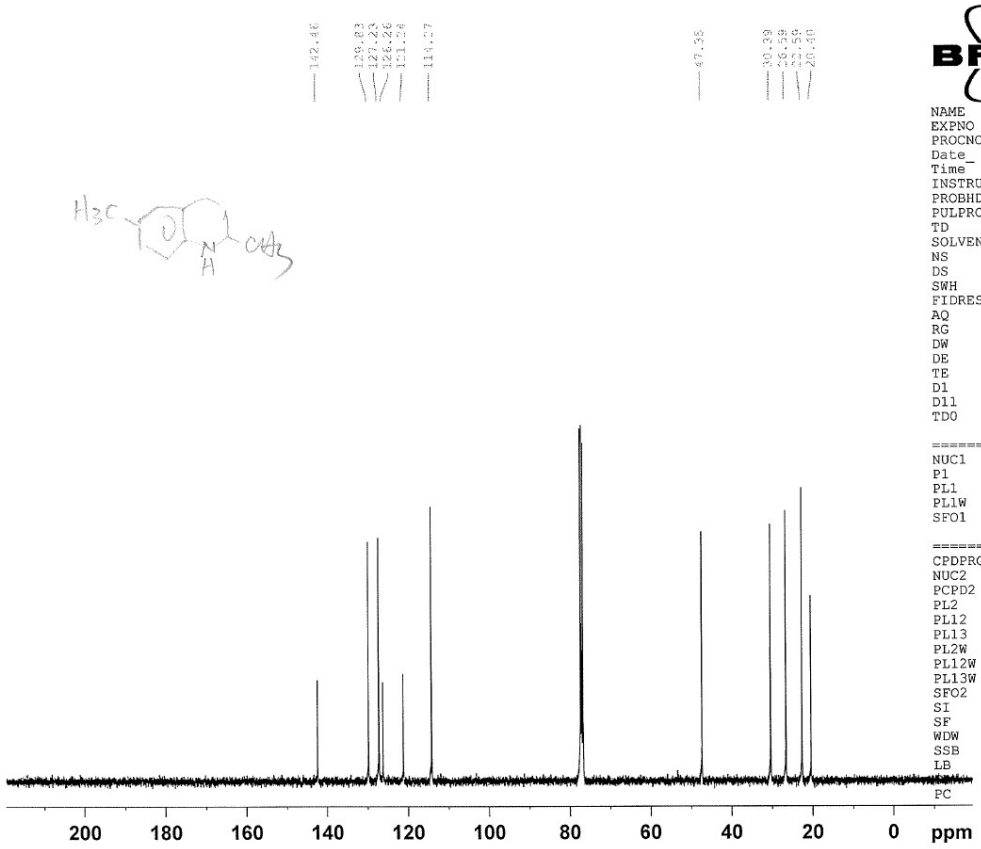
BRUKER

NAME	3-31-5
EXPNO	3
PROCNO	1
Date_	20150822
Time	0.43
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	303.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128738 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



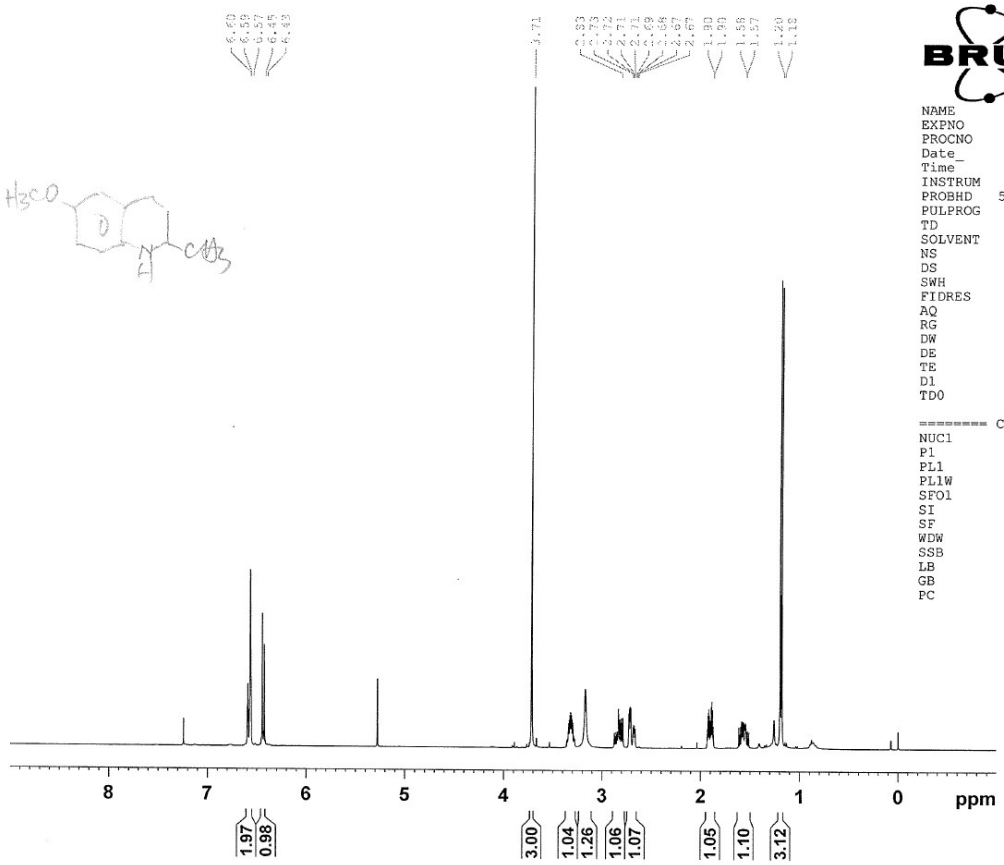
BRUKER

NAME	3-49-1(2)
EXPNO	3
PROCNO	1
Date_	20150904
Time	13.45
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	71.8
DW	60.800 usec
DE	6.50 usec
TE	301.8 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300260 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



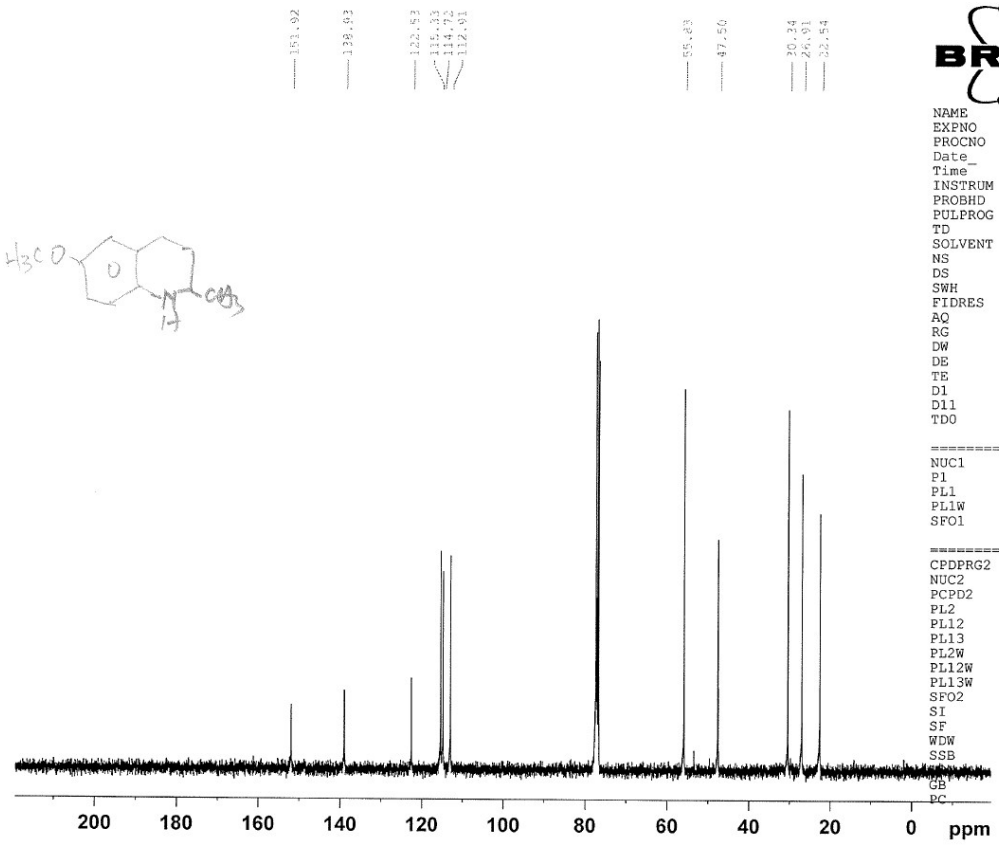
BRUKER

NAME	3-49-1(2)
EXPNO	2
PROCNO	1
Date_	20150903
Time	19.55
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	303.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



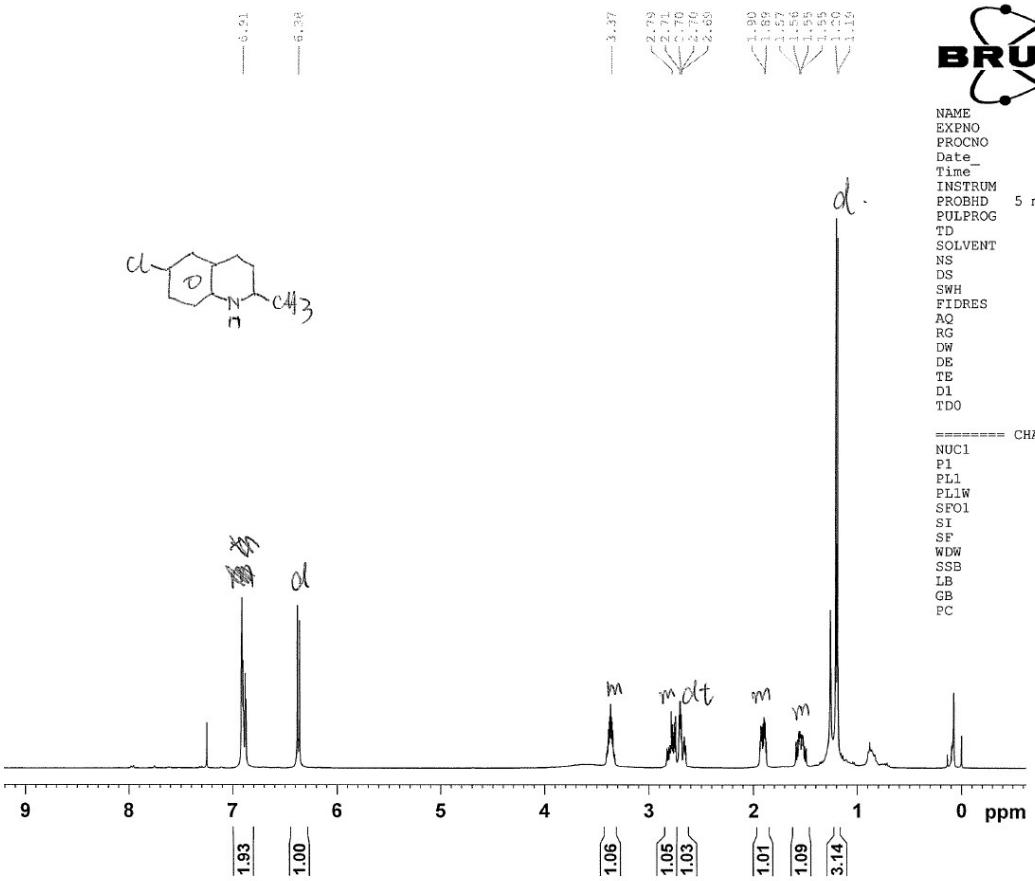
BRUKER

NAME	3-49-2(2)
EXPNO	3
PROCNO	1
Date_	20150904
Time	13.52
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	80.6
DW	60.800 usec
DE	6.50 usec
TE	301.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300171 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



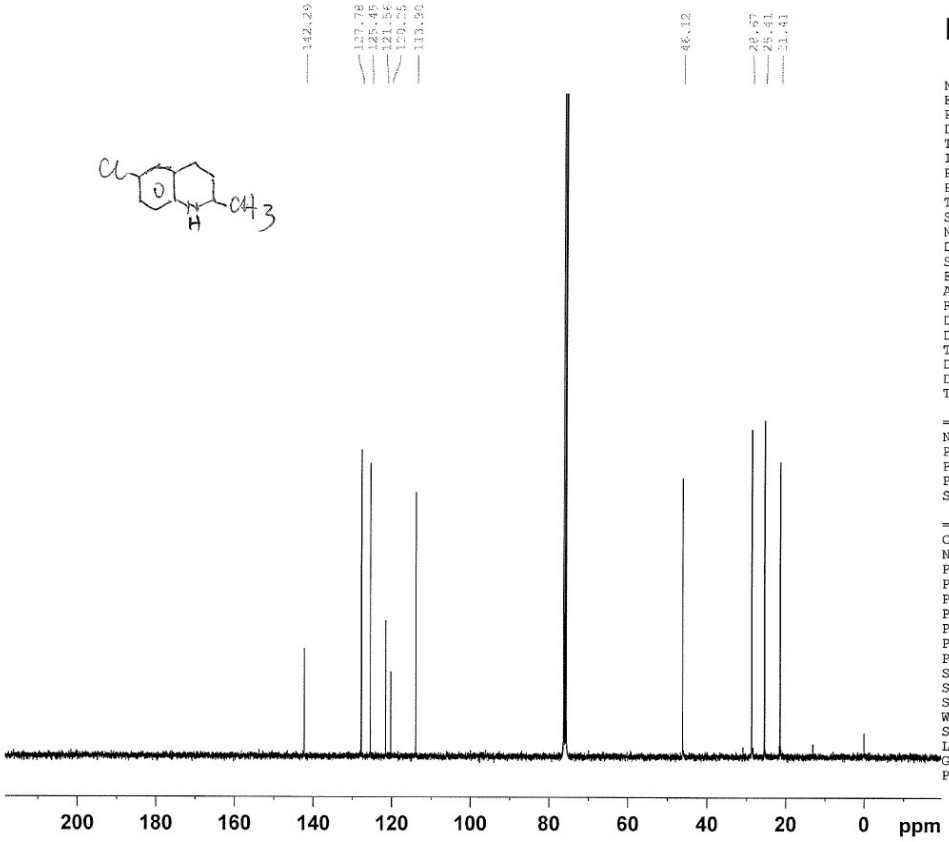
BRUKER

NAME	3-49-2(2)
EXPNO	2
PROCNO	1
Date_	20150903
Time	20.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	303.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



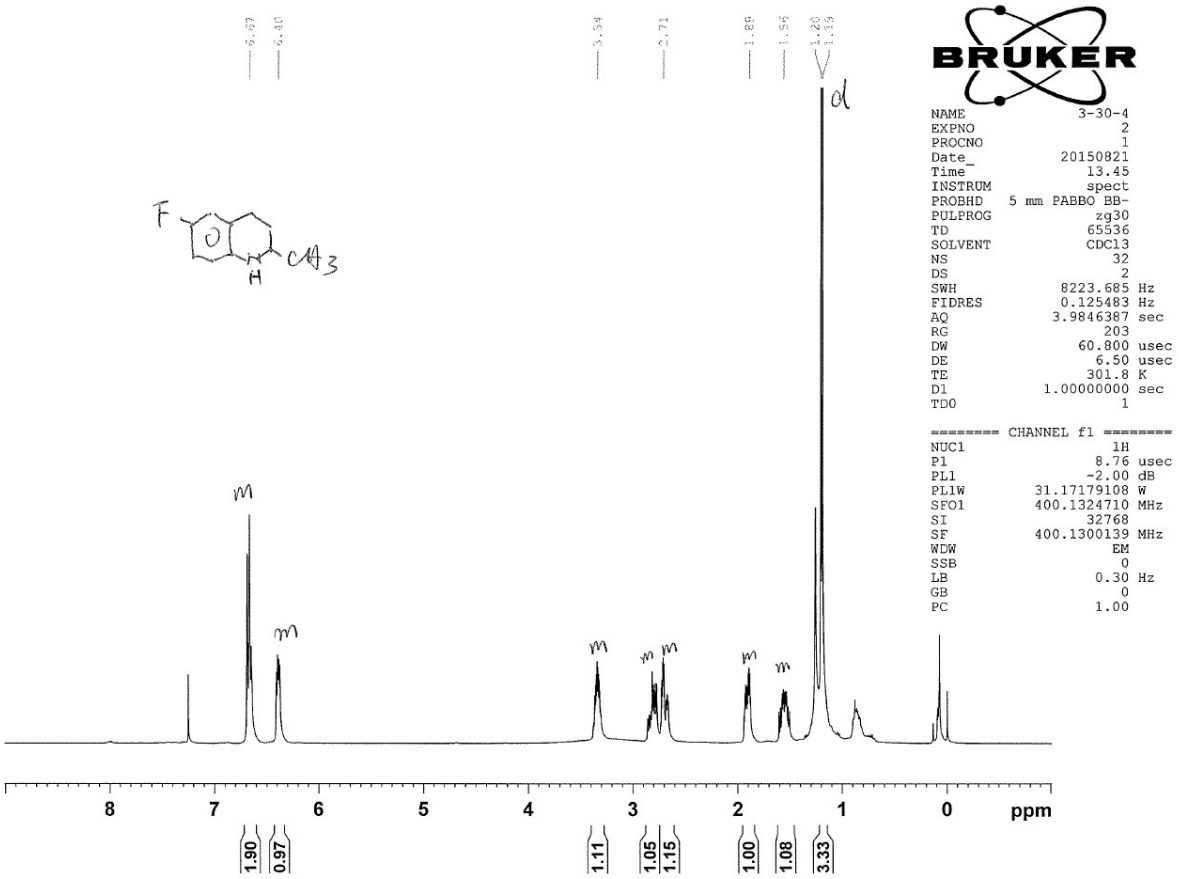
BRUKER

NAME	3-30-3
EXPNO	2
PROCNO	1
Date_	20150821
Time	12.37
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	161
DW	60.800 usec
DE	6.50 usec
TE	301.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300144 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



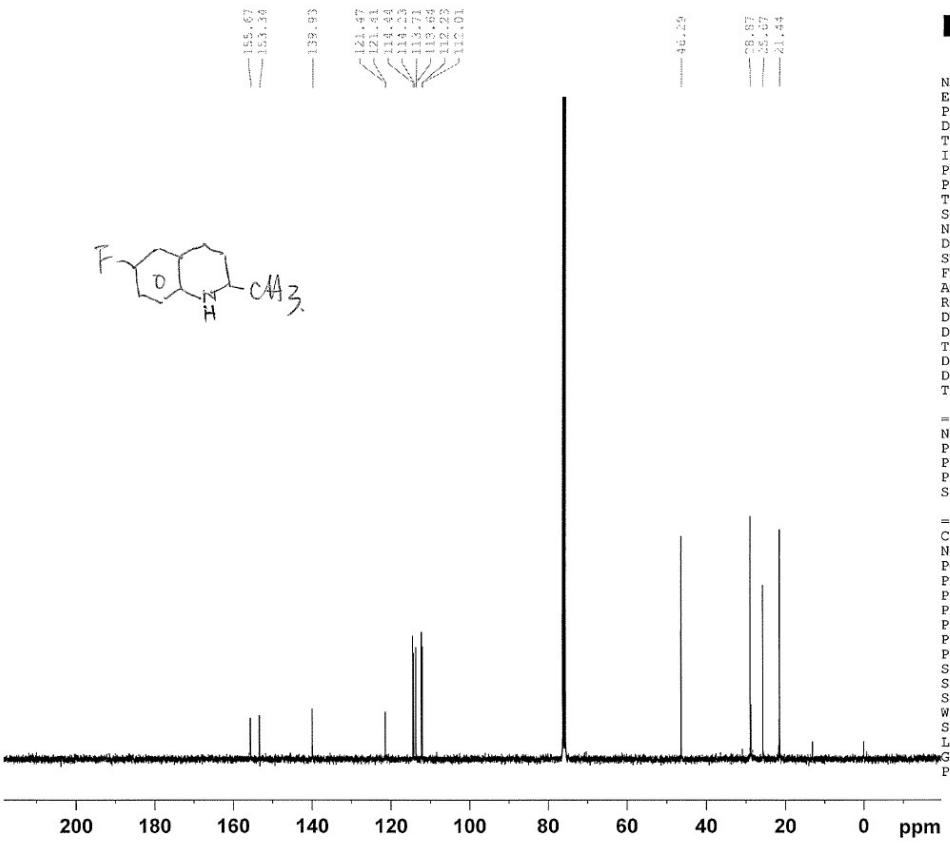
BRUKER

NAME	3-30-3
EXPNO	3
PROCNO	1
Date_	20150821
Time	13.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	303.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128729 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



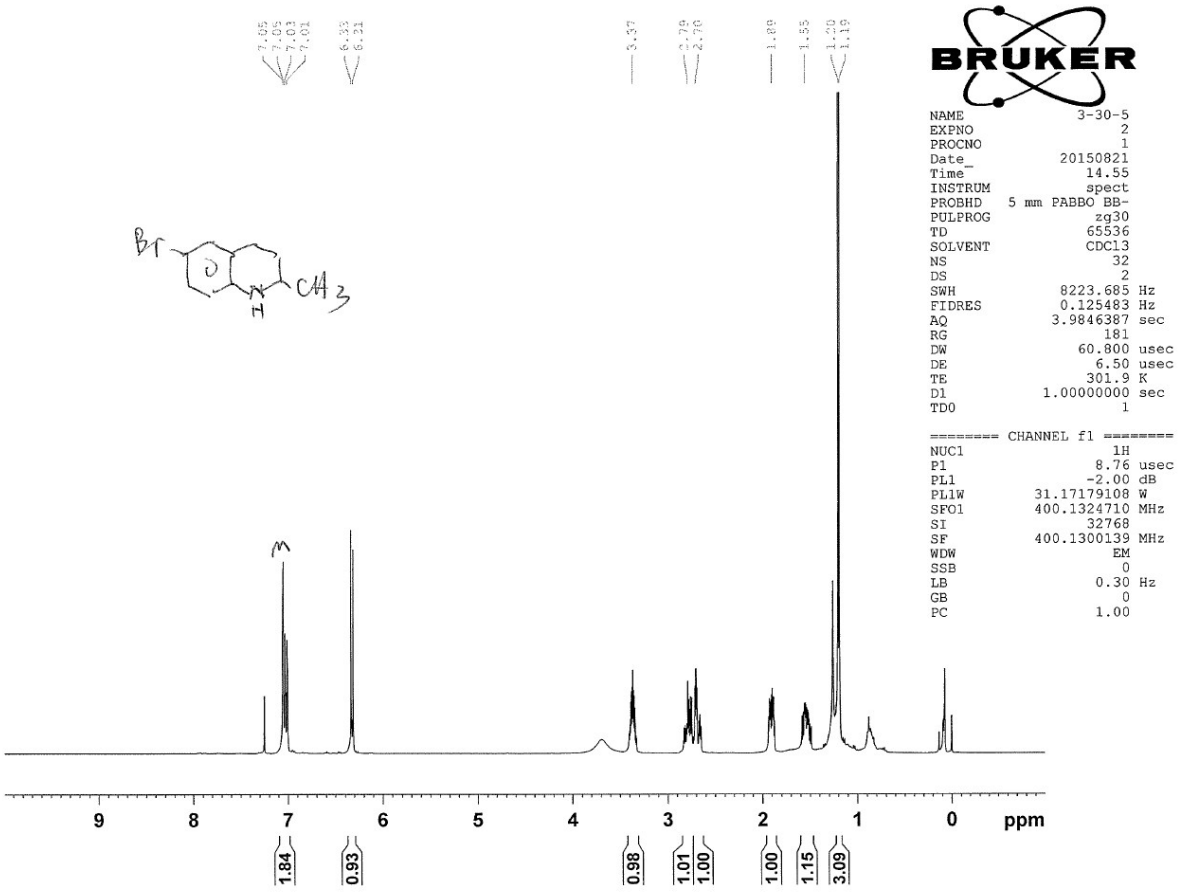
BRUKER

NAME	3-30-4
EXPNO	2
PROCNO	1
Date_	20150821
Time	13.45
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	301.8 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300139 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



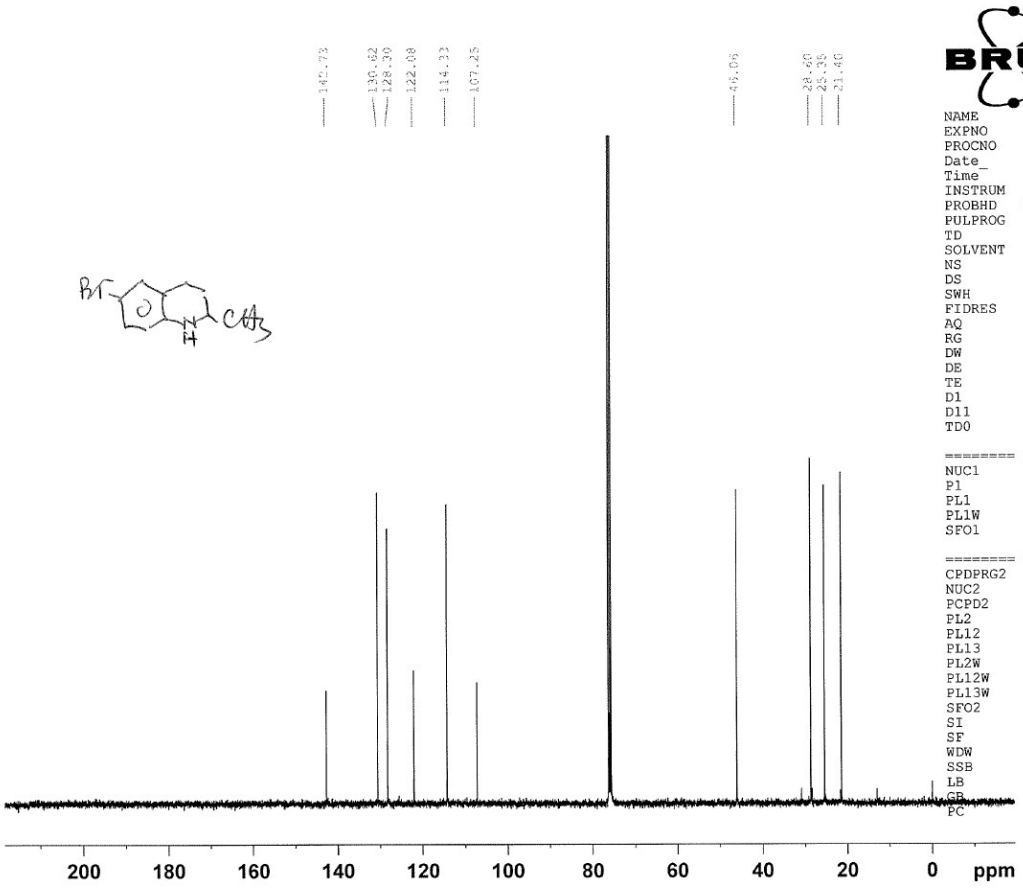
BRUKER

NAME	3-30-4
EXPNO	3
PROCNO	1
Date_	20150821
Time	13.49
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	302.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128722 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



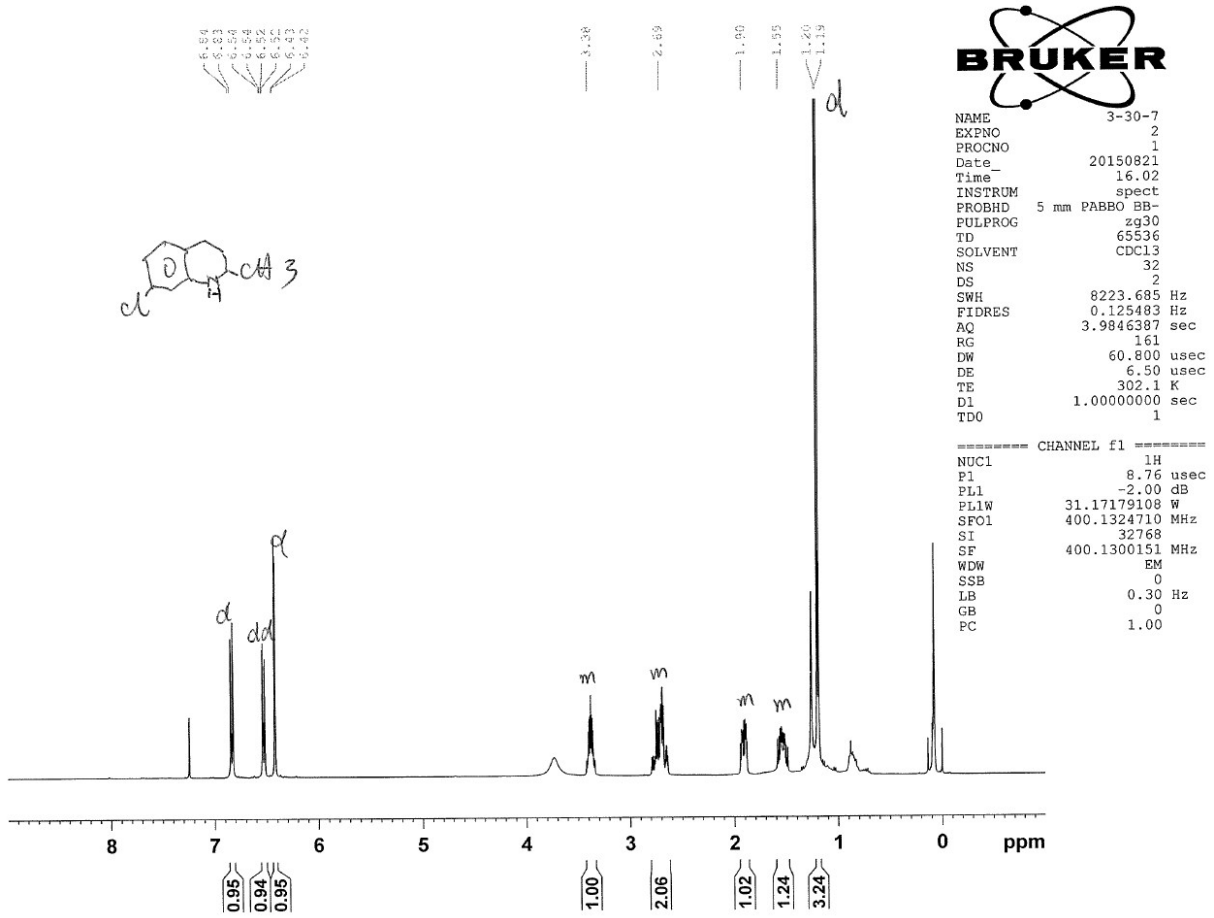
BRUKER

NAME	3-30-5
EXPNO	2
PROCNO	1
Date_	20150821
Time	14.55
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	181
DW	60.800 usec
DE	6.50 usec
TE	301.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300139 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	3-30-5
EXPNO	3
PROCNO	1
Date_	20150821
Time	15.31
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	303.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
========	CHANNEL f1 ========
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
========	CHANNEL f2 ========
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128733 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

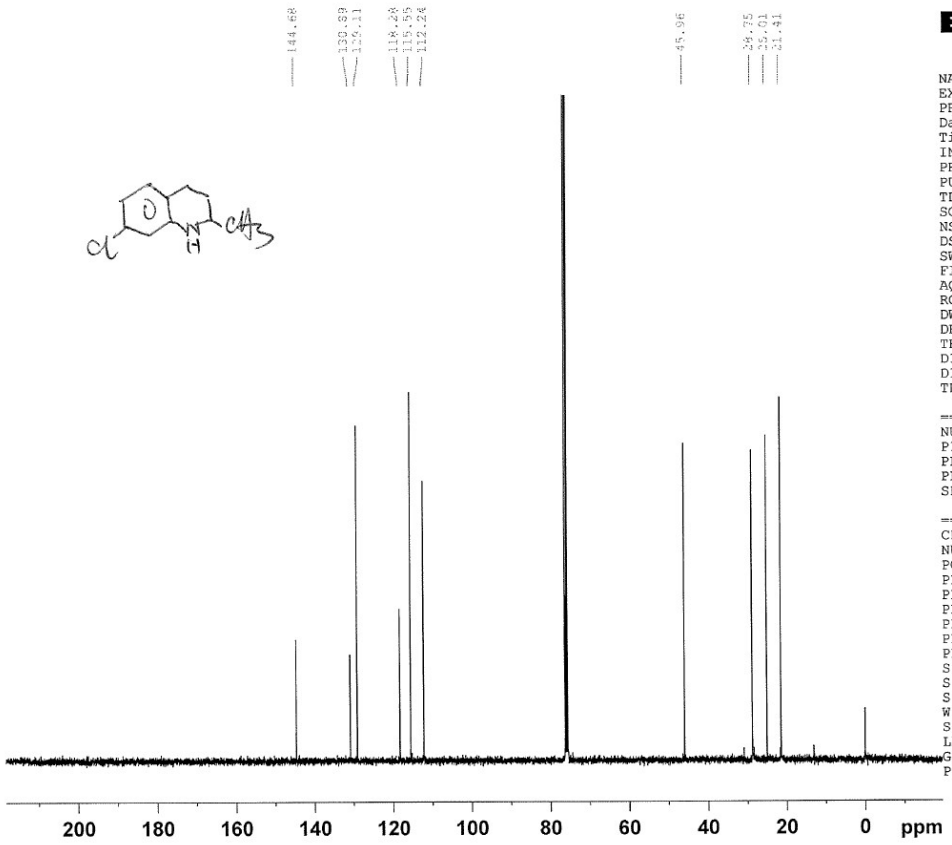


BRUKER

NAME	3-30-7
EXPNO	2
PROCNO	1
Date_	20150821
Time	16.02
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	161
DW	60.800 usec
DE	6.50 usec
TE	302.1 K
D1	1.00000000 sec
TD0	1

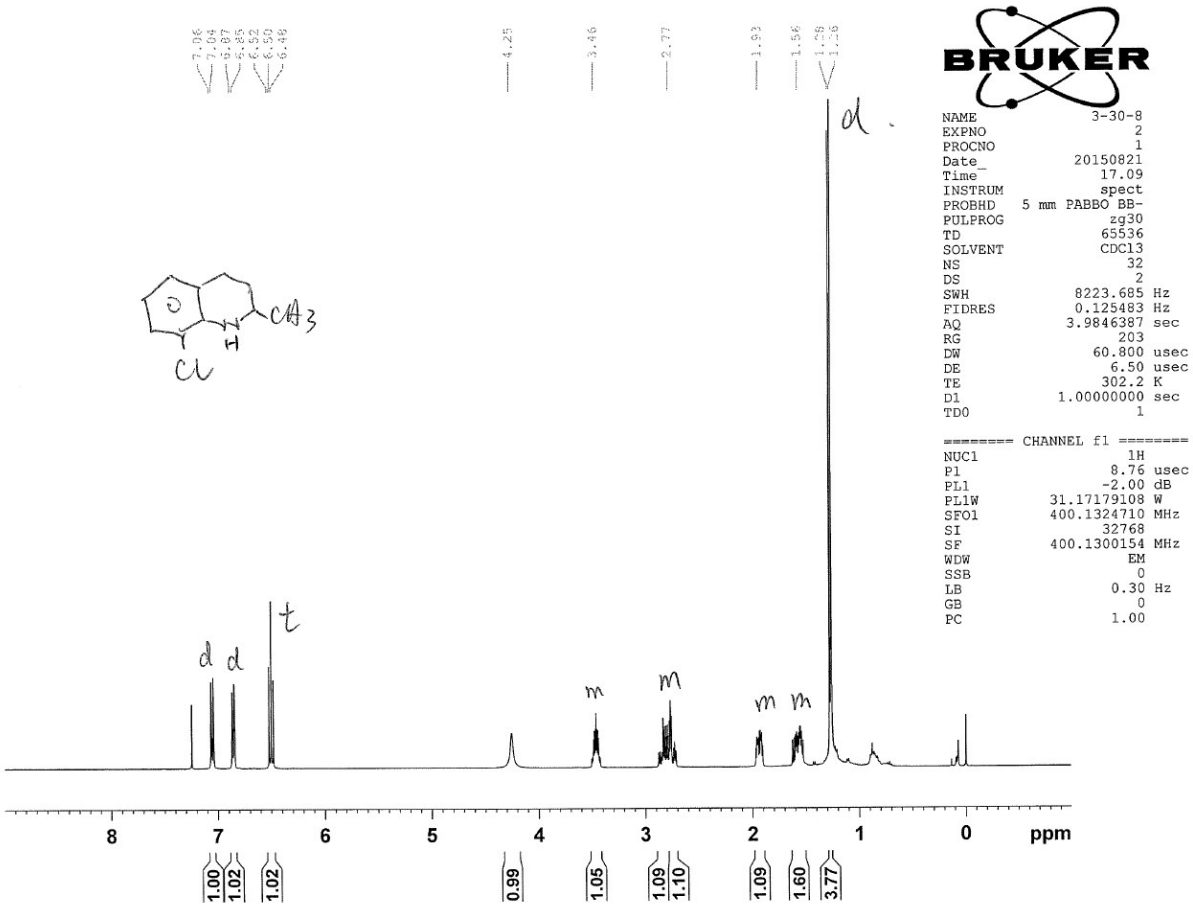
======== CHANNEL f1 ========

NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300151 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	3-30-7
EXPNO	3
PROCNO	1
Date_	20150821
Time	17.01
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	303.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128730 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

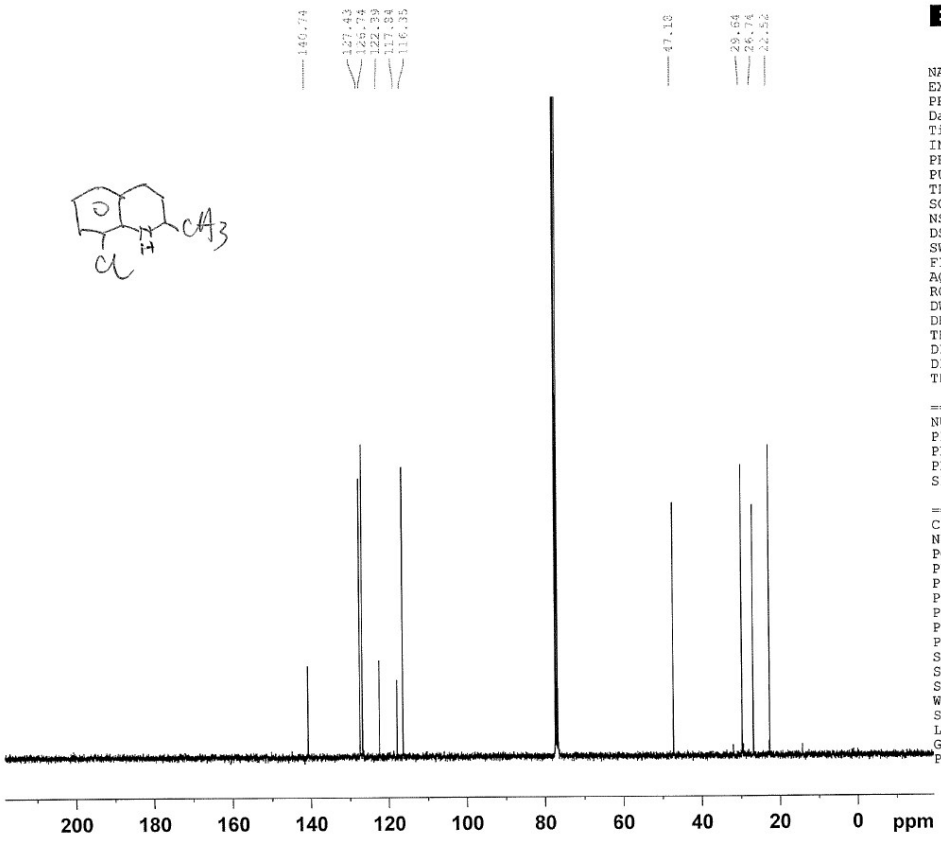


BRUKER

NAME	3-30-8
EXPNO	2
PROCNO	1
Date_	20150821
Time	17.09
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	302.2 K
D1	1.00000000 sec
TD0	1

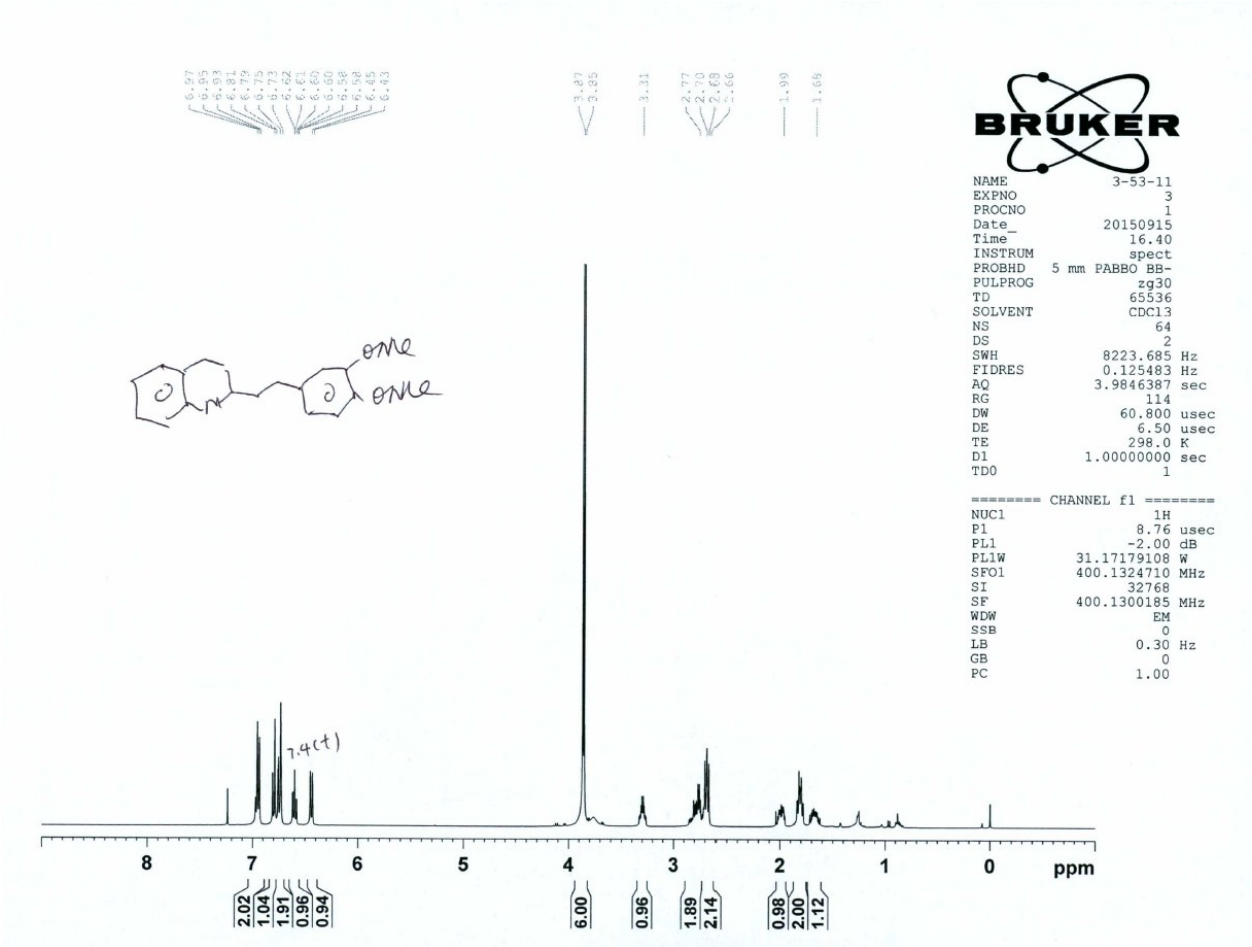
======== CHANNEL f1 ========

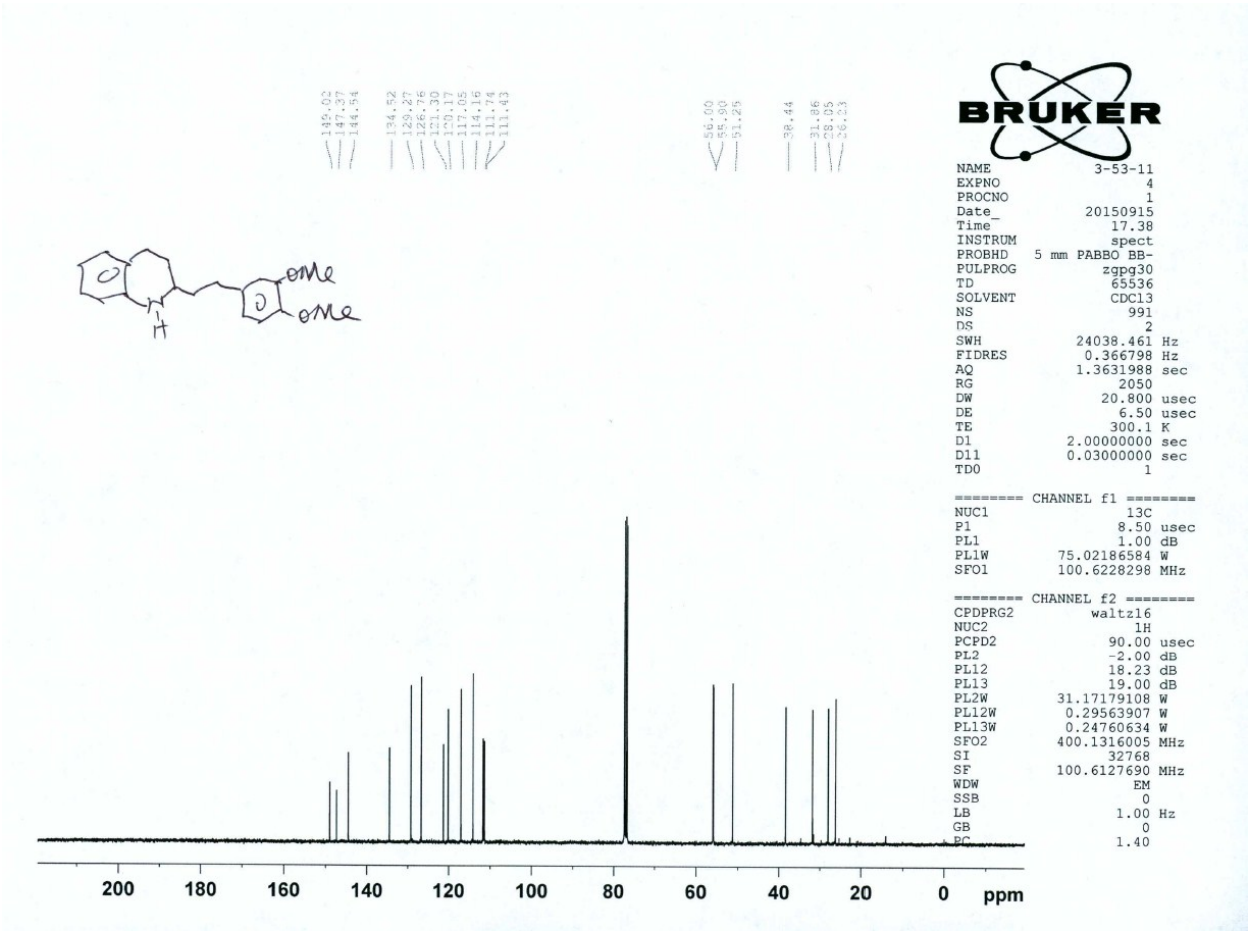
NUC1	1H
P1	8.76 usec
PL1	-2.00 dB
PL1W	31.17179108 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300154 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	3-30-8
EXPNO	3
PROCNO	1
Date_	20150821
Time	18.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1000
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	303.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


6.97
6.95
6.93
6.81
6.79
6.75
6.73
6.62
6.61
6.60
6.60
6.58
6.58
6.45
6.43
3.87
3.85
3.31
2.77
2.70
2.68
2.66
1.99
1.66
BRUKER
NAME 3-53-11
EXPNO 3
PROCNO 1
Date_ 20150915
Time 16.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 114
DW 60.800 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 8.76 usec
PL1 -2.00 dB
PL1W 31.17179108 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300185 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OMe
OMe
7.4(t)
8
7
6
5
4
3
2
1
0
ppm
2.02
1.04
1.91
0.96
0.94
6.00
0.96
1.89
2.14
0.98
2.00
1.12



BRUKER

NAME	3-53-11
EXPNO	4
PROCNO	1
Date_	20150915
Time	17.38
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	991
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	300.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	1.00 dB
PL1W	75.02186584 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.00 dB
PL12	18.23 dB
PL13	19.00 dB
PL2W	31.17179108 W
PL12W	0.29563907 W
PL13W	0.24760634 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40