Highly Efficient Diastereoselective Reduction of α-Fluoroimines

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Table of Contents:

GENERAL EXPERIMENTAL PROCEDURES **2**

GENERAL PROCEDURE FOR REDUCTION OF α-FLUOROIMINES **2**

^{1}H-NMR, ^{13}C-NMR, ^{19}F-NMR DATA TABLES **4**

N-(2-FLUOROCYCLOHEXYL)-4-METHOXYANILINE (TABLE 3, ENTRY 1) 9
BENZYL-(2-FLUORO-CYCLOHEXYL)-AMINE (TABLE 3, ENTRY 2) 13
CYCLOHEXYL-(2-FLUORO-CYCLOHEXYL)-AMINE (TABLE 3, ENTRY 3) 17
(2-FLUORO-CYCLOHEXYL)-HEXYL-AMINE (TABLE 3, ENTRY 4) 21
(2-FLUORO-INDAN-1-YL)-(4-METHOXY-PHENYL)-AMINE(TABLE 3, ENTRY 7) 25
BENZYL-(2-FLUORO-INDAN-1-YL)-AMINE(TABLE 3, ENTRY 8) 29
(2-FLUORO-INDAN-1-YL)-HEXYL-AMINE(TABLE 3, ENTRY 9) 33
(2-FLUORO-1-PHENYL-PROPYL)-(4-METHOXY-PHENYL)-AMINE (TABLE 3, ENTRY 11) 37
N-BENZYL-2-FLUORO-1-PHENYLPROPAN-1-AMINE (TABLE 3, ENTRY 12) 41

Supporting Information:

General Experimental Procedures

All reactions were performed in an oven-dried apparatus and under an inert atmosphere of nitrogen. Solvents for imine formation were dried by passing through a solvent dry system (MBRAUN MB-SPS). All chemicals were purchased from VWR and were used without further purification. ^{19}F NMR, ^{13}C NMR, ^{1}H NMR spectra were recorded on a 300 MHz (JEOL JNM-ECX-300) multinuclear spectrometer. ^{1}H NMR and ^{13}C NMR spectra were referenced to TMS and ^{19}F NMR using α,α,α-Trifluorotoluene. Gas chromatography-TCD was performed on a Shimadzu GC-2010 with a Restek (RTX®-5MS, 15m x 0.25mmID x 0.25µm) column. Gas chromatography-mass spectrometry data was obtained from a Shimadzu GCMS-QP2010S equipped with a Restek (RTX®-5MS, 15m x 0.25mmID x 0.25µm) column. GC and GC-MS conditions were as follows: initial temp 60 °C hold 3 minutes, ramp 15°C/min, final temperature 300 °C hold 3 minutes. HRMS was conducted at the University of Utah Center for Mass Spectrometry with 2mDa mass accuracy. Reported melting points were conducted using a Mel-Temp apparatus and are uncorrected. Flash chromatography was conducted via a traditional column or utilizing a Biotage Isolera flash chromatography system. Diastereoselectivities were determined from ^{1}H, ^{19}F NMR and/or GC. All α-fluoroketones were prepared via previously reported methods.[1,2]

General Procedure for Reduction of α-fluoroimines

All reactions were conducted on a 50mg scale based upon the starting α-fluoroketone.

To the flame dried reaction vesicle was added α-fluoroketone (1.0 equiv), amine (1.1 equiv), thiourea (0.10 equiv), molecular sieves (0.50 g), and dry toluene (2.0 mL). The reaction was allowed to stir at room temperature (50°C for imines derived from α-fluoropropiophenone) under N_2 monitoring reaction progress by GC, GC-MS, and/or ^{19}F NMR. After imine formation was complete, the solvent was removed under vacuum. The α-fluoroimine was redissolved in anhydrous ethyl acetate (2.0 mL) and cooled to -78°C under N_2. Trichlorosilane (3.0 equiv) was added via syringe and the reaction was allowed to slowly warm to room temperature and stir under N_2 for 12 hours monitoring the reaction by TLC. To the reaction was added aqueous NaF (2.5%, 3 mL), and the resulting solution was allowed to stir for 15 minutes. The organic layer was extracted with EtOAc (3 x 20 mL). After the initial extraction, the aqueous layer pH was adjusted to a pH=10 using aqueous NaOH (10%). The organic layer was again extracted with ethyl acetate (3 x 20 mL) and the combined organic layers were dried over $MgSO_4$. Crude ^{19}F NMR and or GC was conducted to determine diastereoselectivity prior to purification. Products were purified as a mixture of diastereomers using column/flash chromatography or Biotage Flash Chrmoatography (SiO_2) eluting with Petroleum ether/EtOAc/.1% Et_3N. NMR (^{1}H, ^{13}C, and ^{19}F NMR) analysis of the major isomer (*cis/syn-)* is presented below.

Determination of Stereoconfiguration

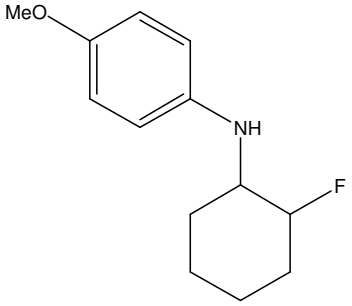
Myers and Flowers have shown in the diastereoselective reduction of α-fluoroketones the ^{19}F NMR signal of the *syn-/cis* diastereomer appears upfield (approx. -200ppm) in comparison to the *anti-/trans* diastereomer (approx. -180 ppm) for the corresponding 2-fluoroalcohols.[3,4] This is consistent with our reduction of α-fluoroimines as the *syn-/cis* diastereomer appears upfield at -200ppm for cyclic and -183-180ppm for the acyclic whereas the *anti-/trans* appears at -180ppm for the cyclic and -180-178ppm for the acyclic. These results are also consistent with previous reports for the stereochemistry analysis of *trans* 2-fluoroamines.[5-9] ^{19}F NMR chemical shift for the *trans*-cyclic 2-fluoroamines was -179ppm supporting our observed stereochemical assignment. Also in the case of Benzyl-(2-fluoro-cyclohexyl)-amine (Table 3, Entry 2)Hou and others assign the ^{19}F NMR for the *trans* diasterosiomer at -179ppm matching our assignement for the minor *trans*- isomer with the major *cis*-isomer having a chemical shift of -200ppm respectiviely.[5-9] ^{1}H, ^{13}C, and ^{19}F NMR for each individual *cis/syn*- is presented below.

1.) Enders, D.; Faure, S.; Potthoff, M.; Rundsink, J. *Synthesis* **2001,** 2307-2319.
2.) Stavber, S.; Jereb, M.; Zupan, M. *Synthesis* **2002,** 2609-2914.
3.) Myers, A.G.; Barbay, J.K.; Zhong, B. *J. Am. Chem. Soc.* **2001,** *123,* 7207-7219.
4.) Mohanta, P.K.; Davis, T.A.; Gooch, J. R.; Flowers, II R.A. *J. Am. Chem. Soc.* **2005,** *127,* 11896-11897.

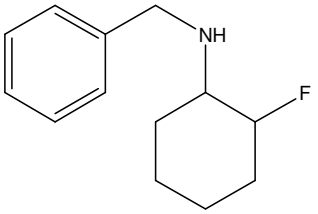
For previous stereochemical assignments of the diastereomers of 2-fluoroamines see:

5.) Fan, R.; Zhou, Y.; Zhang, W.; Hou, X.; Dai, L. *J. Org. Chem.* **2004,** *69,* 335-338.
6.) Alvernhe, G.M.; Ennakoua, C.M.; Lacombe, S. M.; Laurent, A.J. *J. Org. Chem.* **1981,** *46,* 4938-4948.
7.) Wade, T.N. *J. Org. Chem.* **1980,** *45,* 5328-5333.
8.) Avernhe, G.M.; Lacombe, S.M.; Laurent, A. J. *Tetrahedron Lett.* **1980,** *21,* 289.
9.) Toulgui, C.; Chaabouni, M. M.; Baklouti, A.; *J. Fluorine Chem.* **1990,** *46,* 385-391.

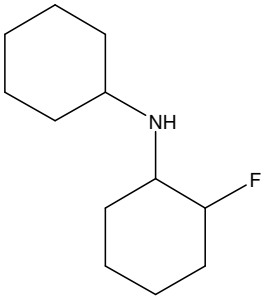
^{1}H-NMR, ^{13}C-NMR, ^{19}F-NMR Data Tables



N-(2-fluorocyclohexyl)-4-methoxyaniline (Table 3, Entry 1)
Red liquid. Yield: 78% (24:1 *cis/trans*)
Cis-diastereomer
^{1}H NMR: ($CDCl_3$, 300 MHz): δ 6.63-6.80 (dd, *J* = 8.9Hz, 40.4Hz, 4.0Hz), 4.78-4.95 (dm, *J* = 49.5Hz, 1H), 3.74 (s, 3H), 3.18-3.34 (qm, *J* = 2.1 Hz, 11.3 Hz, 28.7 Hz, 1H), 2.08-2.14 (m, 1H), 1.75-1.94 (dm, *J* = 35.1 Hz, 2H), 1.29-1.60 (m, 6H)
^{13}C NMR: ($CDCl_3$, 75 MHz): 152.8, 140.1, 116.1, 115.0, 90.0 (d, *J* = 171.2 Hz), 55.8, 55.3 (d, *J* = 19.5 Hz), 30.3 (d, *J* = 20.9 Hz), 27.2, 24.5, 19.7
^{19}F NMR: ($CDCl_3$, 282 MHz): δ -202.3 (m, *cis*), -177.5 (m, *trans*)
HRMS (ESI): *m/z* Calculated: ($M+H^+$) 224.1451 Actual: ($M+H^+$) 224.1441



Benzyl-(2-fluoro-cyclohexyl)-amine (Table 3, Entry 2)
Yellow liquid. Yield: 98% (14:1 *cis/trans*)
Cis-diastereomer
^{1}H NMR: ($CDCl_3$, 300 MHz): δ 7.38-7.21 (m, 5H), 4.79-4.61 (ddd, *J* = 52.3 Hz, 4.8 Hz, 2.5 Hz, 1H), 3.86 (s, 2H), 2.51-2.74 (m, 1H), 2.04-2.16 (m, 1H), 1.18-1.82 (m, 8H)
^{13}C NMR: ($CDCl_3$, 75 MHz): δ 139.5, 128.6, 128.4, 128.3, 127.2, 90.8 (d, 171.9 Hz), 57.1 (d, *J* = 19.5 Hz), 50.1, 29.9 (d, *J* = 20.9 Hz), 27.2, 23.9, 20.2
^{19}F NMR: ($CDCl_3$, 282 MHz): δ -178.7(m, *trans*), -199.7 (m, *cis*)
HRMS (ESI): *m/z* Calculated: ($M+H^+$) 208.1502 Actual: ($M+H^+$) 208.1508



Cyclohexyl-(2-fluoro-cyclohexyl)-amine (Table 3, Entry 3)
Yellow liquid. Yield: 51% (11:1 *cis/trans*)
Cis-diastereomer
^{1}H NMR: ($CDCl_3$, 300 MHz): δ 4.88-4.71 (dd, *J* = 50.2 Hz, 3.4 Hz, 1H), 2.69-2.54 (m, 2H), 2.00-2.17 (m, 1H), 1.73-1.81 (m, 7H), 1.48-1.59 (m, 1H), 1.36-1.54 (m, 2H), 1.02-1.30 (m, 8H)
^{13}C NMR: ($CDCl_3$, 75 MHz): δ 90.9 (d, *J* = 170.5 Hz), 54.2 (d, *J* = 18.8 Hz), 52.8, 33.8, 30.5 (d, *J* = 20.9 Hz), 28.0, 26.2, 25.1, 24.6, 20.0
^{19}F NMR: ($CDCl_3$, 282 MHz): δ -178.44 (m, *trans*), -201.8 (m, *cis*)
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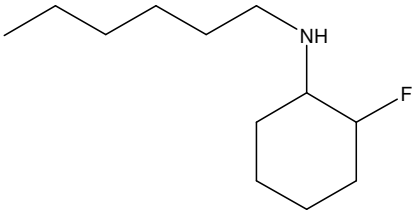
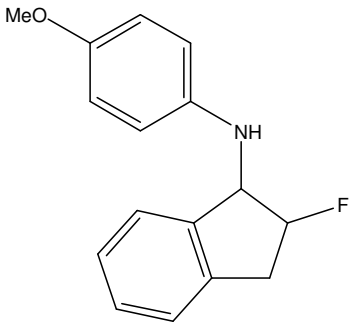
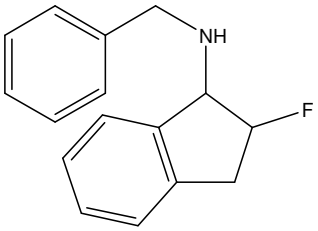


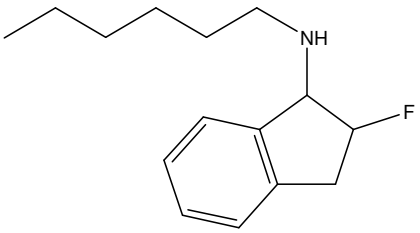
(2-Fluoro-cyclohexyl)-hexyl-amine (Table 3, Entry 4)
Yellow liquid. Yield: 68% (12:1 *cis/trans*)
Cis-diastereomer
^{1}H NMR: ($CDCl_3$, 300 MHz): δ 4.75-4.94 (dt, *J* = 50.0 Hz, 2.4 Hz, 1H), 2.52-2.67 (m, 3H), 2.03-2.12 (m, 1H), 1.72-1.76 (m, 2H), 1.41-1.52 (m, 5H), 1.10-1.90 (m, 8H), 0.85-0.89 (t, *J* = 6.54 Hz, 3H)
^{13}C NMR: ($CDCl_3$, 75 MHz): δ 90.4 (d, *J* = 171.1 Hz), 58.0 (d, *J* = 18.8 Hz), 46.7, 31.9, 30.5, 30.2 (d, *J* = 29.6 Hz), 27.7, 27.2, 24.2, 22.7, 20.2, 14.2
^{19}F NMR: ($CDCl_3$, 282 MHz): δ -178.8 (dm, 49.2 Hz), *trans*), -200.9 (m, *cis*)
HRMS (ESI): *m/z* Calculated: ($M+H^+$) 202.1971 Actual: ($M+H^+$) 202.1970



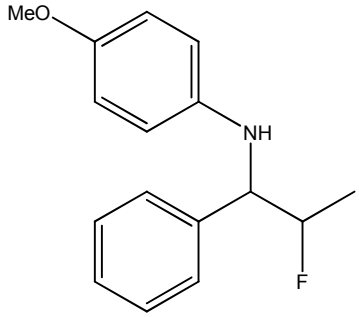
(2-Fluoro-indan-1-yl)-(4-methoxy-phenyl)-amine (Table 3, Entry 7)
Brown liquid Yield: 88% (>100:1 *cis/trans*)
Cis-diastereomer
^{1}H NMR: ($CDCl_3$, 300 MHz): δ 7.28 (s, 1H) 7.26 (s, 4H), 6.83 (s, 4H), 5.33-5.51 (dt, *J* = 53.0 Hz, 4.0 Hz, 1H), 4.96 (dd, *J* = 24.0 Hz, 4.0 Hz, 1H) 3.74 (s, 3H), 3.10-3.25 (m, 2H)
^{13}C NMR: ($CDCl_3$, 75 MHz): δ 152.9, 139.1, 128.3, 127.3, 125.2, 124.5, 115.4, 115.1, 93.1 (d, *J* = 180.0 Hz), 62.5 (d, *J* = 18.6 Hz), 55.9, 37.6 (d, *J* = 22.2 Hz)
^{19}F NMR: ($CDCl_3$, 282 MHz): δ -198.74 (m, *cis*)
HRMS (ESI): *m/z* Calculated: ($M+H^+$) 258.1294 Actual: ($M+H^+$) 258.1302



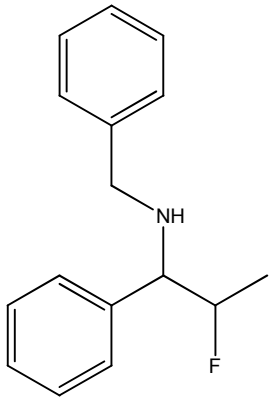
Benzyl-(2-fluoro-indan-1-yl)-amine (Table 3, Entry 8)
Yellow Solid
Yield: 80% (>100:1 *cis/trans*)
Mp= 59.8-60.8°C
Cis-diastereomer
^{1}H NMR: ($CDCl_3$, 300 MHz): δ 7.53-7.28 (m, 9H) 5.33-5.28 (dt, *J* = 53.0 Hz, 4.0 Hz, 1.0 Hz, 1H), 4.11 -3.99(m, *J* = 24.0 Hz, 4.0 Hz, 1.0 Hz, 3H), 3.24 3.15 (m, 2H), 2.18 (s, 1H).
^{13}C NMR: ($CDCl_3$, 75 MHz): δ 142.4, 140.4, 139.0, 128.5, 128.2, 127.2, 125.0, 92.2 (d, *J* = 179.3), 65.2 (d, *J* = 19.4 Hz), 51.6, 37.9 (d, *J* = 22.2 Hz)
^{19}F NMR: ($CDCl_3$, 282 MHz): δ -199.5 (m, *cis*)
HRMS (ESI): *m/z* Calculated: ($M+H^+$) 242.1345 Actual: ($M+H^+$) 242.1342



(2-Fluoro-indan-1-yl)-hexyl-amine (Table 3, Entry 9)
Yellow Liquid
Yield: 57% (78:1 *cis/trans*)
Cis-diastereomer
^{1}H NMR: ($CDCl_3$, 300 MHz):δ 7.50 (m, 1H), 7.26 (s, 3H), 5.17-5.54 (dt, *J* = 54.0 Hz, 3.4Hz 1H) 4.19-4.27 (dd, *J*= 23.7 Hz, 3.1 Hz 1H), 2.92-3.23 (m, 4H), 1.60 (m, 2H), 0.32 (m, 6H),0.89 (t, *J* =6.9Hz 3H)
^{13}C NMR: ($CDCl_3$, 75 MHz): δ 139.1, 128.1, 127.2, 125.0, 124.9, 94.8 (d, *J* = 124.2 Hz), 65.2 (d, 20.1 Hz), 47.9, 37.9 (d, 21.3 Hz), 31.8, 30.3, 27.1, 22.8, 14.2
^{19}F NMR: ($CDCl_3$, 282 MHz): δ -178.6 (m, *trans*), -200.1 (m, *cis*)
HRMS (ESI): *m/z* Calculated: ($M+H^+$) 236.1815 Actual: ($M+H^+$) 236.1819



(2-Fluoro-1-phenyl-propyl)-(4-methoxy-phenyl)-amine (Table 3, Entry 11)
Yellow Liquid. Yield: 51% (19:1 *syn/anti*)
Syn-diastereomer
^{1}H NMR: ($CDCl_3$, 300 MHz): δ 7.22-7.34 (m, 5H), 6.69 (d, *J* = 7.0 Hz, 2H), 6.52 (d, *J* = 7.0 Hz, 2H), 5.15-4.91(ddq, *J* = 47.7 Hz, 5.2 Hz, 3.4 Hz, 1H), 4.5003-4.3796 (dd, *J* = 20.1 Hz, 3.4 Hz, 1H), 1.2882-1.1863 (dd, *J* = 23.0 Hz, 6.0 Hz, 1H)
^{13}C NMR: ($CDCl_3$, 75 MHz): δ 152.4, 141.0, 138.3, 128.6, 128.0, 127.7, 115.3, 114.8, 92.4 (d, *J* = 172.8 Hz), 62.6 (d, *J* = 22.3 Hz), 55.7, 16.7 (d, *J* = 22.2 Hz),
^{19}F NMR: ($CDCl_3$, 282 MHz): δ -183.3 (m, *syn*), -181.3 (m, *anti*)
HRMS (ESI): *m/z* Calculated: ($M+H^+$) 260.1451 Actual: ($M+H^+$) 260.1456



N-benzyl-2-fluoro-1-phenylpropan-1-amine (Table 3, Entry 12)

Yellow liquid. Yield: 68% (4:1 *syn/anti*)

Syn-diastereomer

^{1}H NMR: ($CDCl_3$, 300 MHz): δ 7.39-7.21 (m, 10H), 4.92 (dm, *J* = 47.5 Hz, 1H), 3.89-3.47 (m, 3H), 2.63(bs, 1H), 1.30-1.16 (dd, *J* = 30.1 Hz, 6.5 Hz, 3H)

^{13}C NMR: ($CDCl_3$, 75 MHz): δ 128.7, 128.6, 128.5, 128.4, 127.8, 127.2, 93.0 (d, *J* = 166.1 Hz), 65.6 (d, *J* = 20.2 Hz), 51.0, 16.8 (d, *J* = 22.1 Hz)

^{19}F NMR: ($CDCl_3$, 282 MHz): δ , -180.7557 (m, *syn*), -177.1559 (m, *anti*)

HRMS (ESI): *m/z* Calculated: ($M+H^+$) 244.1502 Actual: ($M+H^+$) 236.1510

N-(2-fluorocyclohexyl)-4-methoxyaniline *(Table 3, entry 1)*

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
759 formula(e) evaluated with 6 results within limits (up to 12 best isotopic matches for each mass)
Elements Used:
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TD #4 16-Dec-2009 15:17:11

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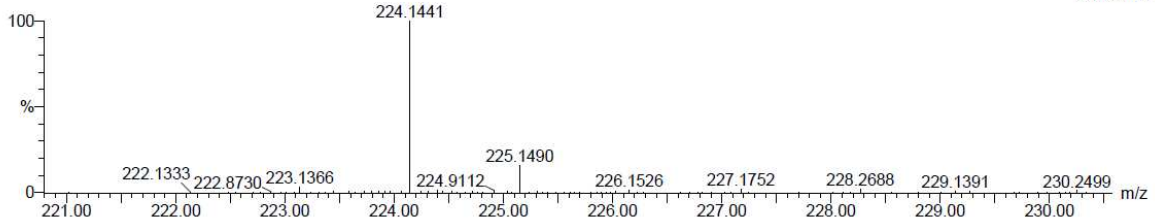

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	224.1444	-0.3	-1.3	1.5	2412.6	C H14 N13 O
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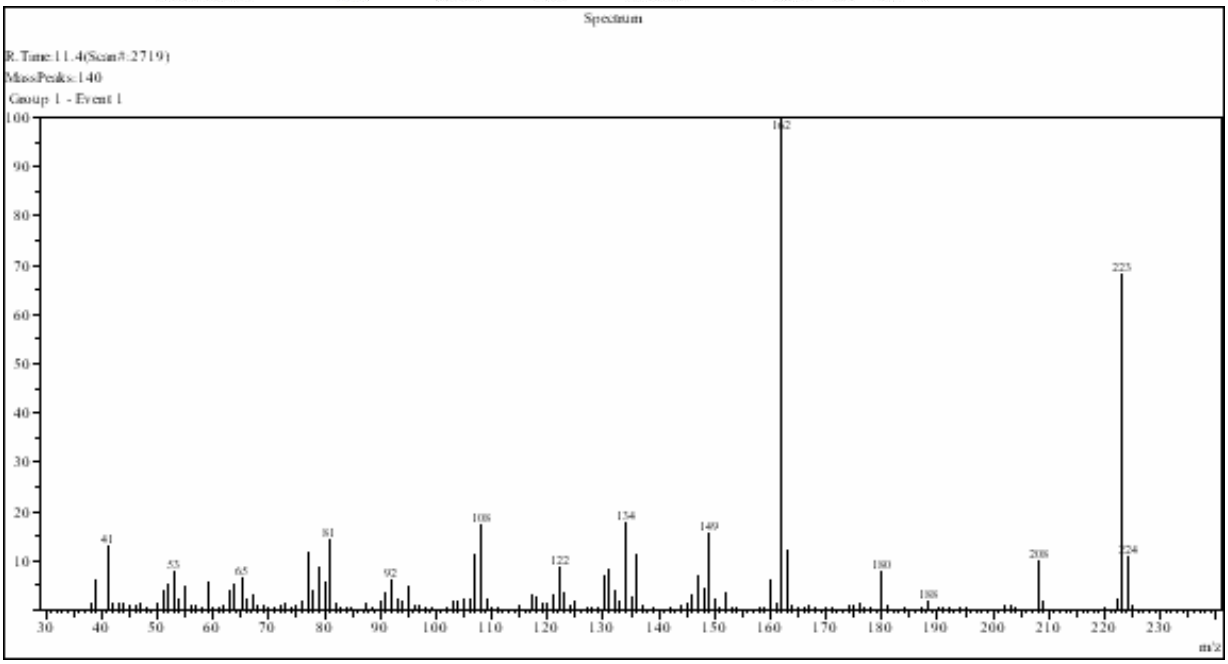
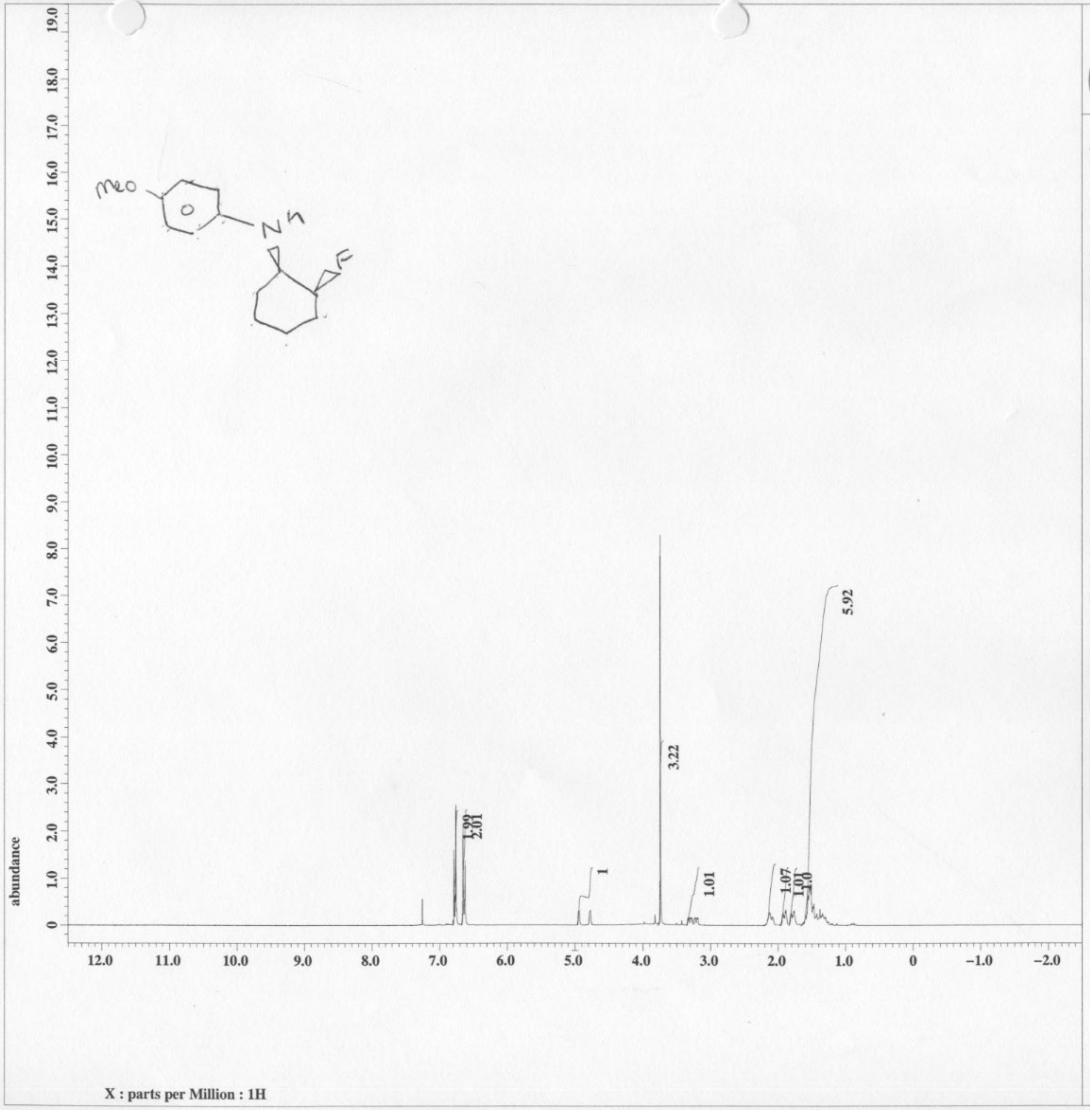


^{1}H NMR:(Table 3, entry 1)



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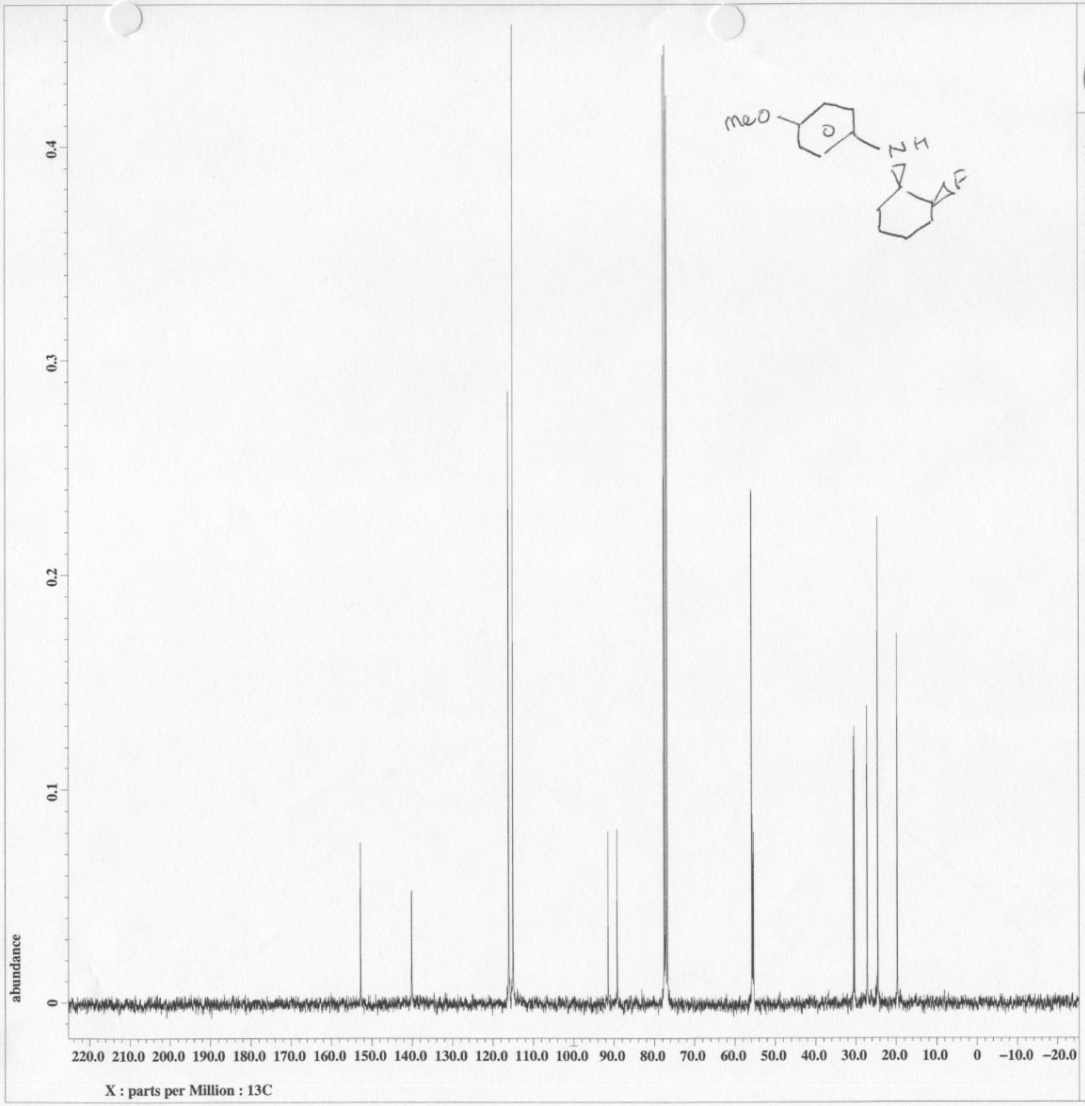
^{13}C NMR:(Table 3, entry 1)

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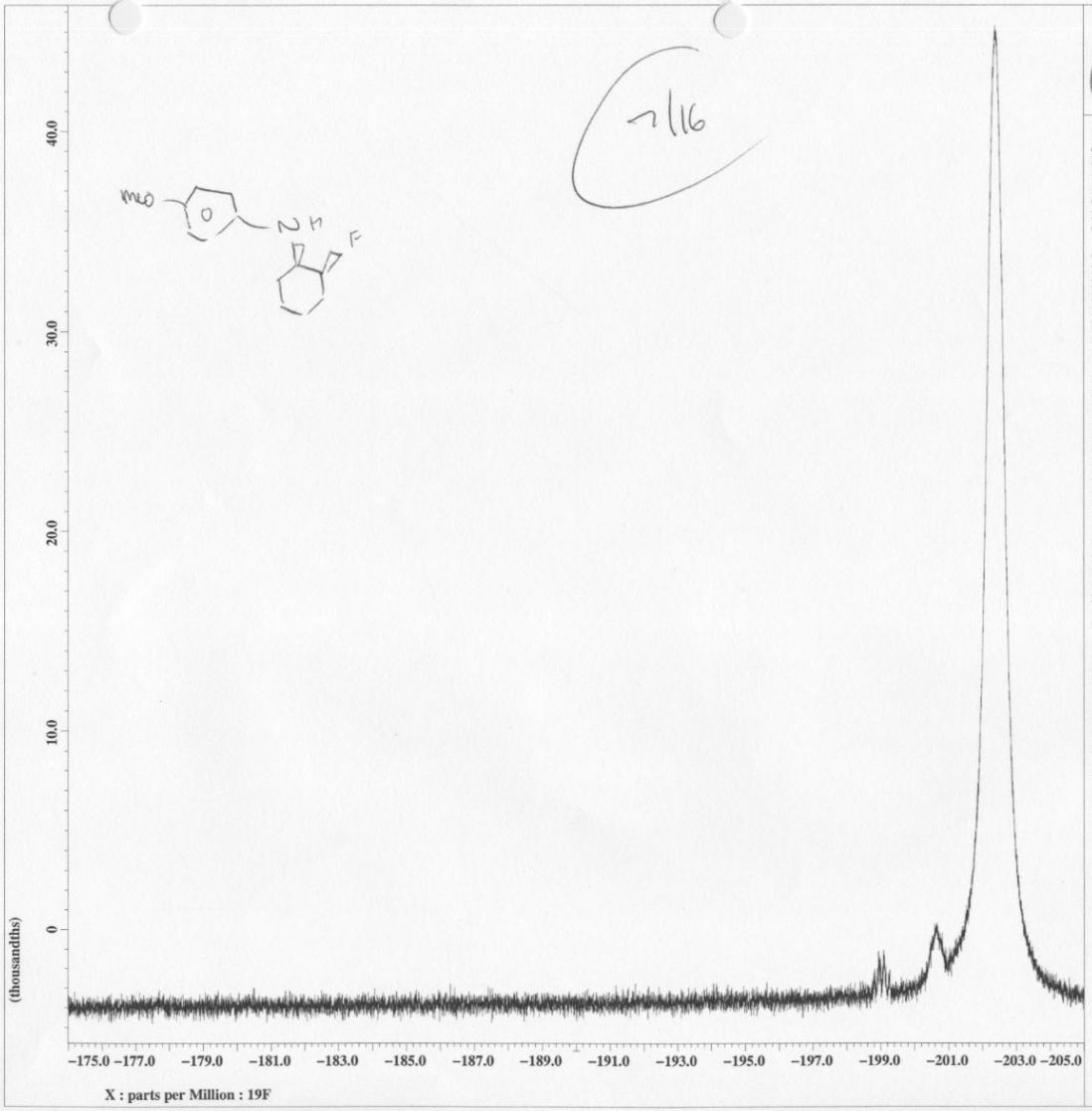
Filename          = RM_20090718_aFCHPMA4_
Author            = Davis
Experiment        = single_pulse_dec
Sample_id         = aFCHPMA4
Solvent           = CHLOROFORM-D
Creation_time     = 18-JUL-2009 20:34:29
Revision_time     = 18-JUL-2009 19:50:06
Current_time      = 18-JUL-2009 19:50:15

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 300
Spectrometer      = JNM-ECX300A

Field_strength    = 7.0586013[T] (300[MHz
X_acq_duration    = 1.38412032[s]
X_domain          = 13C
X_freq            = 75.56823426[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.72248054[Hz]
X_sweep           = 23.67424242[kHz]
Irr_domain        = 1H
Irr_freq          = 300.52965592[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1000
Total_scans       = 1000

X_90_width        = 10.75[us]
X_acq_time        = 1.38412032[s]
X_angle           = 30[deg]
X_atn             = 6[dB]
X_pulse           = 3.58333333[us]
Irr_atn_dec       = 25[dB]
Irr_atn_noe       = 25[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 3.38412032[s]
Temp_get          = 19.1[dC]
```

^{19}F NMR:(Table 3, entry 1)



JEOL

```
Filename          = RM_20090716_aFCHPMA4_
Author            = Davis
Experiment        = single_pulse.ex2
Sample_id         = aFCHPMA4
Solvent           = CHLOROFORM-D
Creation_time     = 16-JUL-2009 14:20:57
Revision_time     = 16-JUL-2009 13:32:46
Current_time      = 16-JUL-2009 13:32:47

Comment           = after Biotage
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 19F
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 300
Spectrometer      = JNM-ECX300A

Field_strength    = 7.0586013[T] (300[MHz
X_acq_duration    = 1.54402816[s]
X_domain          = 19F
X_freq            = 282.78036857[MHz]
X_offset          = -190[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.64765658[Hz]
X_sweep           = 10.61120543[kHz]
Irr_domain        = 19F
Irr_freq          = 282.78036857[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 19F
Tri_freq          = 282.78036857[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 60
Total_scans       = 60

X_90_width        = 10.2[us]
X_acq_time        = 1.54402816[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 5.1[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 40
Relaxation_delay  = 5[s]
Repetition_time   = 6.54402816[s]
Temp_get          = 19.4[dC]
```

Benzyl-(2-fluoro-cyclohexyl)-amine *(Table 3, entry 2)*

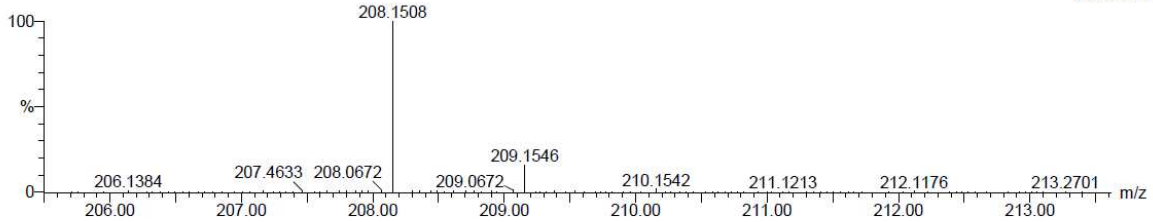
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

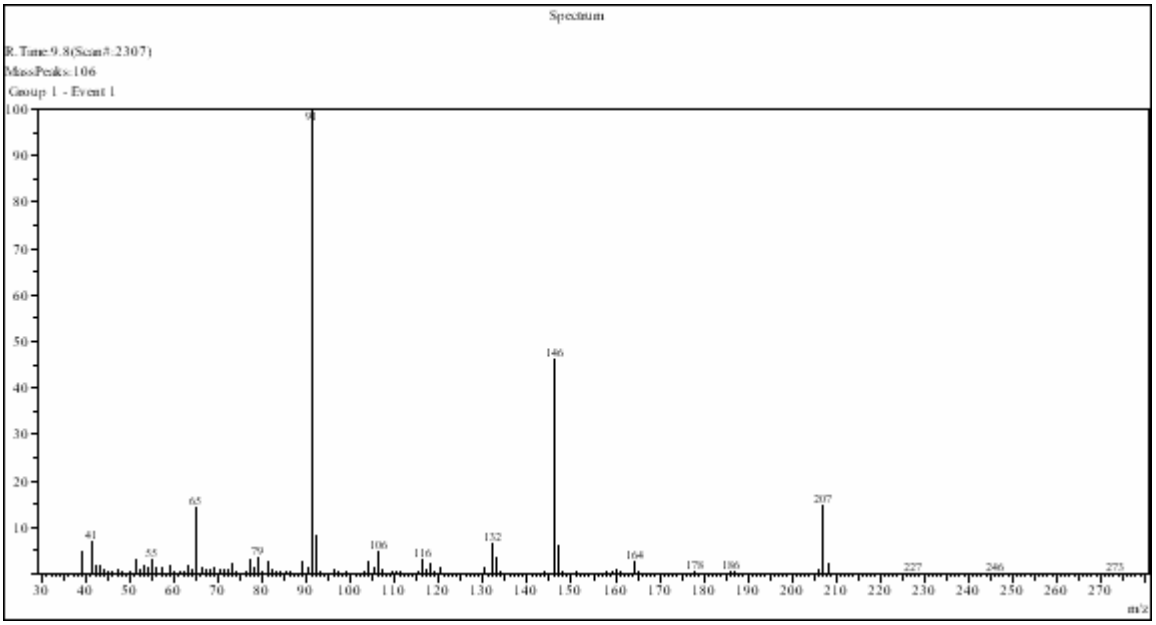
Monoisotopic Mass, Even Electron Ions
637 formula(e) evaluated with 7 results within limits (up to 12 best isotopic matches for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-50 O: 0-50 F: 0-1

TD #7 16-Dec-2009 14:33:42

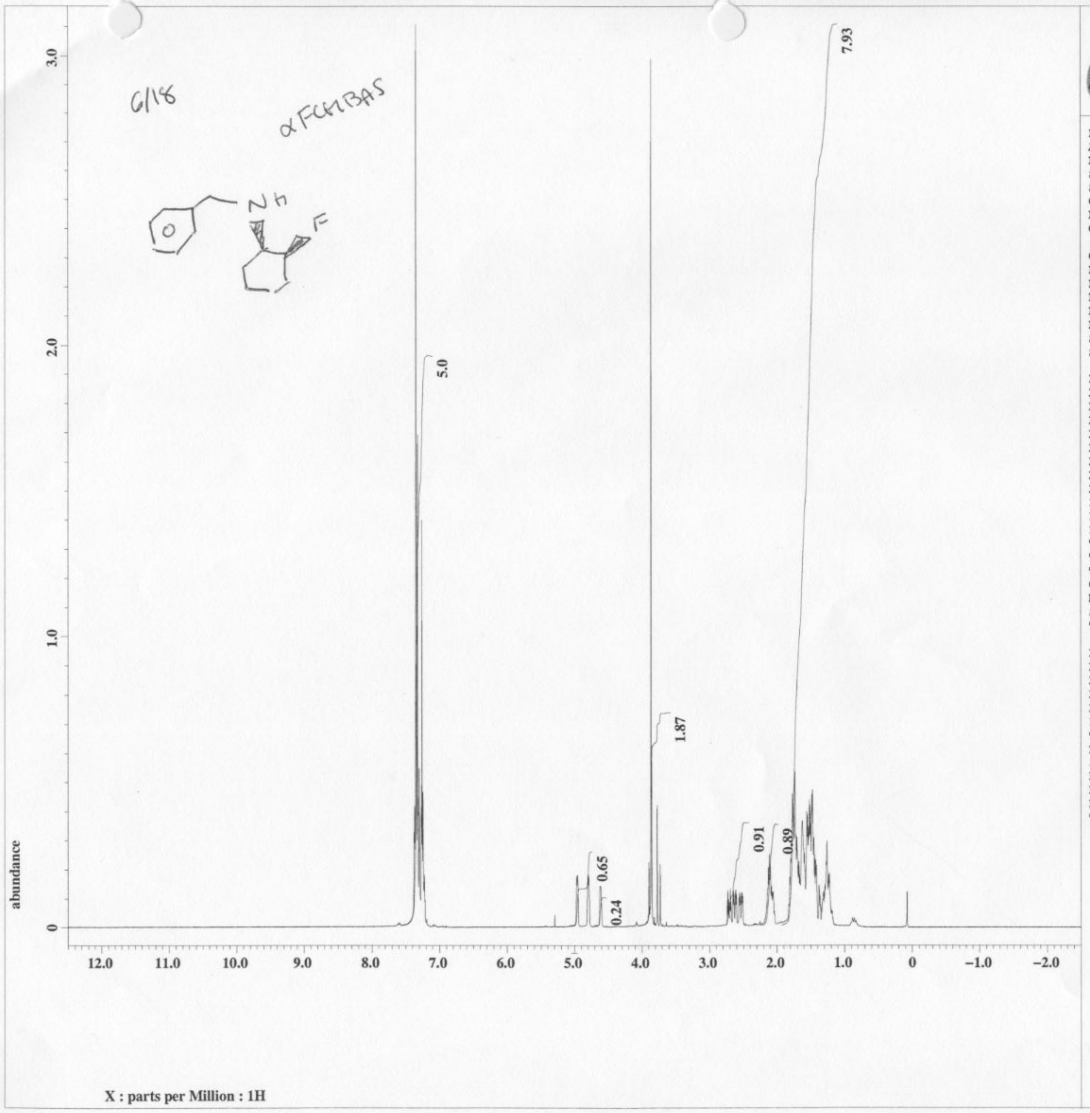
09MSL1216_LCT_2 247 (4.556) AM (Cen,4, 80.00, Ar,6500.0,556.28,0.70,LS 25); Sm (SG, 2x3.00); Sb (3,40.00); Cm (241:273) 1: TOF MS ES+ 3.24e+004



Minimum:				-10.0		
Maximum:		3.0	100.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
208.1508	208.1502	0.6	2.9	4.5	32.0	C13 H19 N F
	208.1522	-1.4	-6.7	0.5	585.0	C5 H18 N7 O2
	208.1509	-0.1	-0.5	-4.5	924.6	C4 H22 N3 O6
	208.1495	1.3	6.2	1.5	1146.0	C H14 N13
	208.1533	-2.5	-12.0	-3.5	1199.3	C2 H19 N7 O3 F
	208.1482	2.6	12.5	-3.5	1545.8	H18 N9 O4
	208.1520	-1.2	-5.8	-8.5	1700.0	C H23 N3 O7 F



^{1}H NMR: **(Table 3, entry 2)**



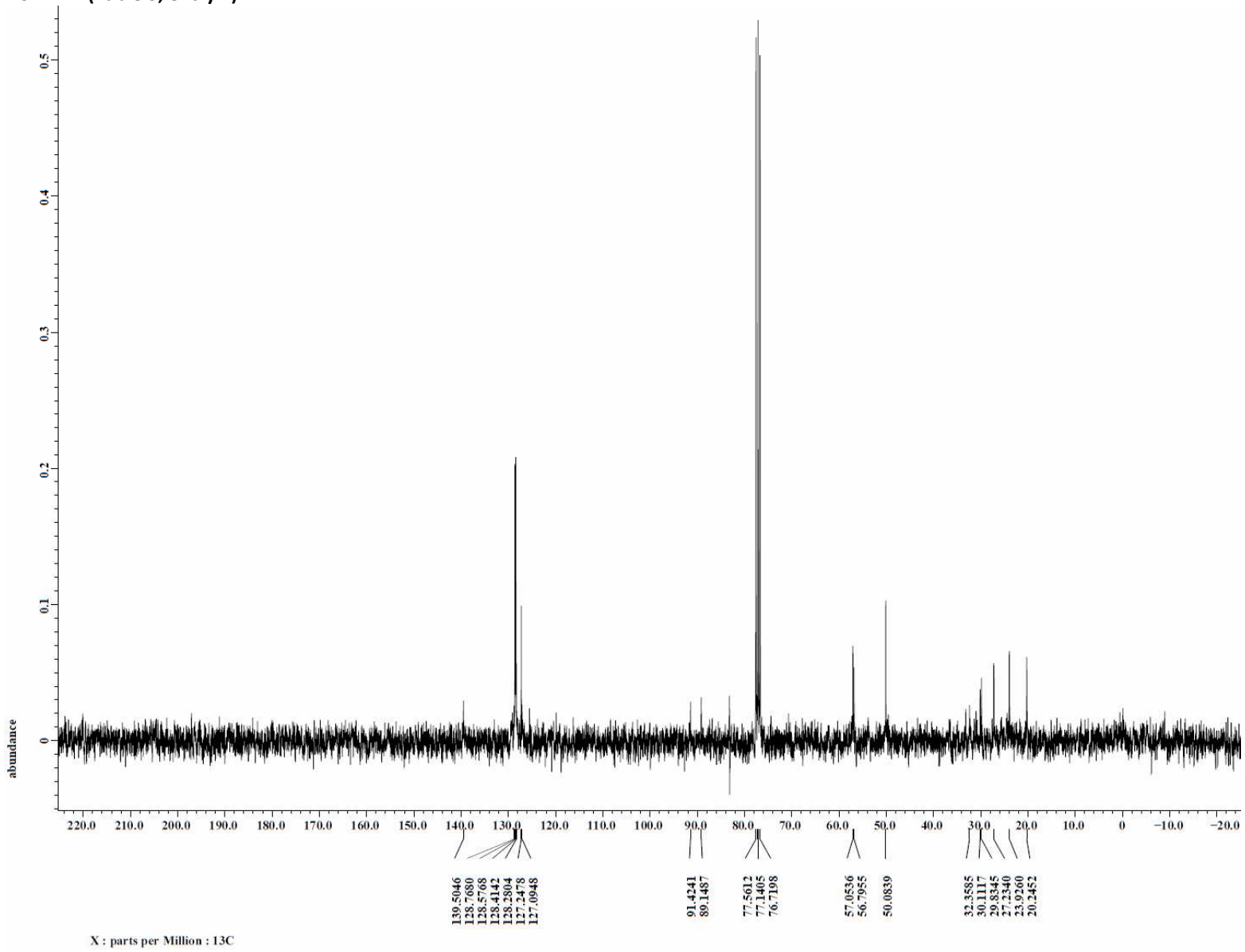

```
Filename          = RM_20090618_aFCHBA5_1
Author            = Davis
Experiment        = single_pulse.ex2
Sample_id         = aFCHBA5
Solvent           = CHLOROFORM-D
Creation_time     = 18-JUN-2009 12:01:13
Revision_time     = 18-JUN-2009 11:15:36
Current_time      = 18-JUN-2009 11:16:34

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 300
Spectrometer      = JNM-ECX300A

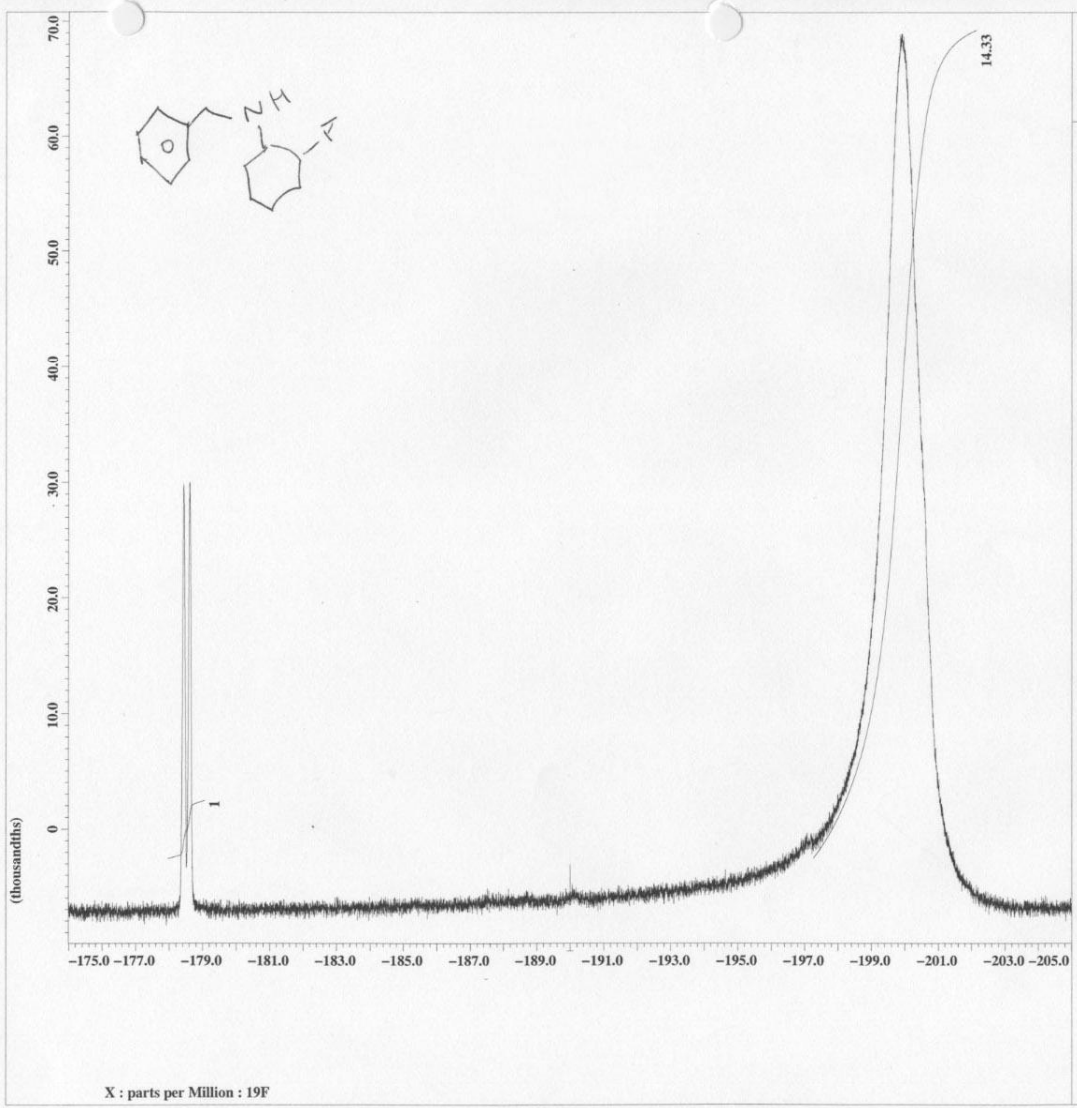
Field_strength    = 7.0586013[T] (300[MHz
X_acq_duration    = 2.90717696[s]
X_domain          = 1H
X_freq            = 300.52965592[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.34397631[Hz]
X_sweep           = 5.63570784[kHz]
Irr_domain        = 1H
Irr_freq          = 300.52965592[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 300.52965592[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 10.33[us]
X_acq_time        = 2.90717696[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 5.165[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 38
Relaxation_delay  = 5[s]
Repetition_time   = 7.90717696[s]
Temp_get          = 20.1[dC]
```

^{13}C NMR: **(Table 3, entry 2)**



^{19}F NMR: **(Table 3, entry 2)**



JEOL

```
Filename          = RM_20090618_I89_aFCHB
Author            = Davis
Experiment        = single_pulse.ex2
Sample_id         = aFCHBA5
Solvent           = CHLOROFORM-D
Creation_time     =  4-MAY-2009 14:31:41
Revision_time     =  4-MAY-2009 13:36:57
Current_time      =  4-MAY-2009 13:37:12

Comment           = 2nd crude NMR
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 19F
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 300
Spectrometer      = JNM-ECX300A

Field_strength    = 7.0586013[T] (300[MHz
X_acq_duration    = 1.54402816[s]
X_domain          = 19F
X_freq            = 282.78036857[MHz]
X_offset          = -190[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.64765658[Hz]
X_sweep           = 10.61120543[kHz]
Irr_domain        = 19F
Irr_freq          = 282.78036857[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 19F
Tri_freq          = 282.78036857[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 128
Total_scans       = 128

X_90_width        = 10.2[us]
X_acq_time        = 1.54402816[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 5.1[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 44
Relaxation_delay  = 5[s]
Repetition_time   = 6.54402816[s]
Temp_get          = 19[dC]
```

Cyclohexyl-(2-fluoro-cyclohexyl)-amine *(Table 3, entry 3)*

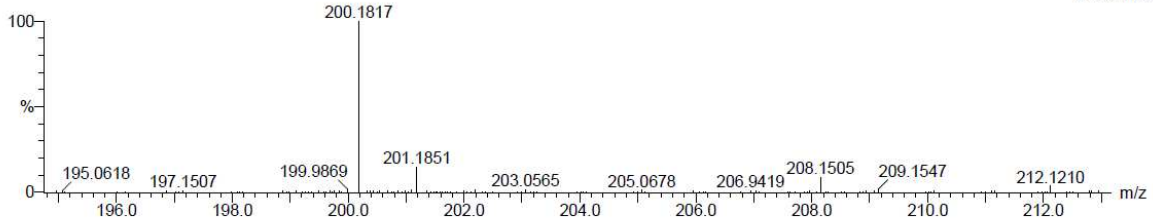
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

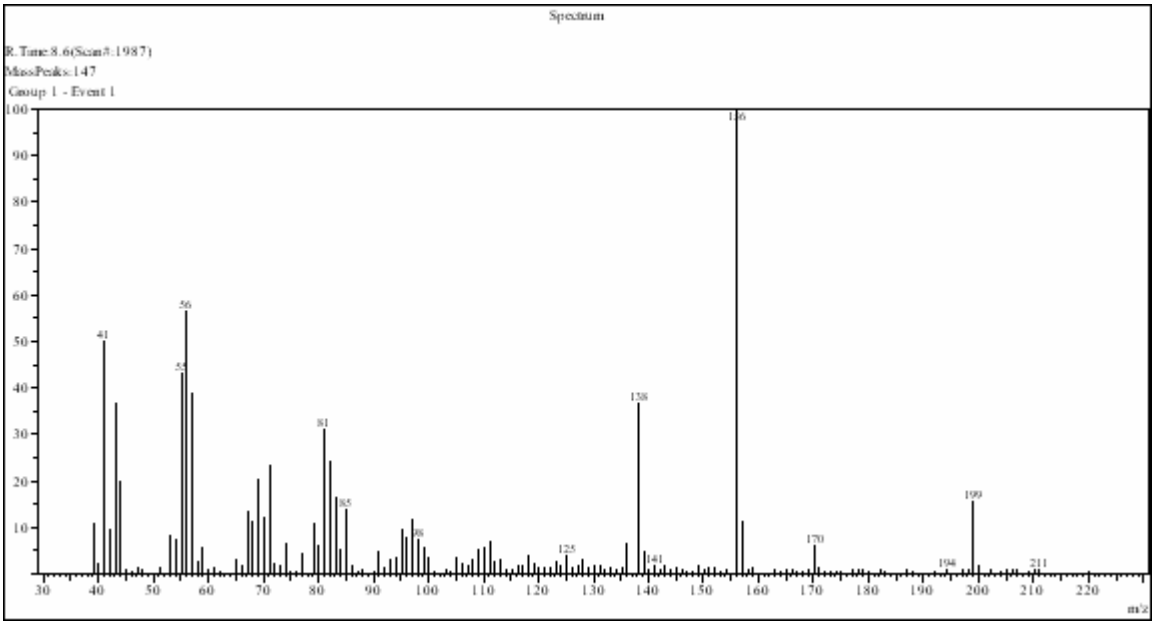
Monoisotopic Mass, Even Electron Ions
576 formula(e) evaluated with 5 results within limits (up to 12 best isotopic matches for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-50 O: 0-50 F: 0-1

TD #5 16-Dec-2009 14:47:12

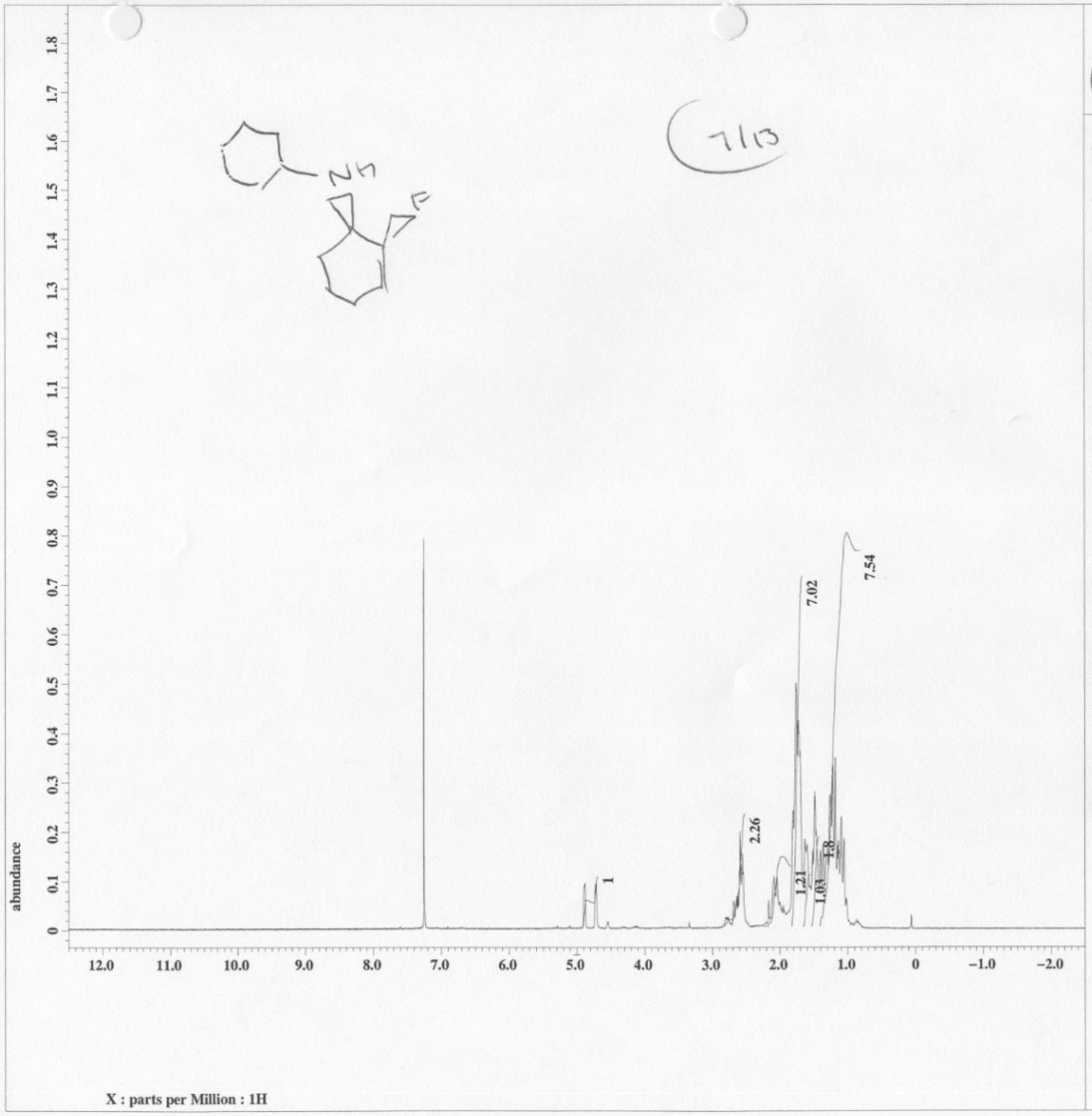
09MSL1216_LCT_3 218 (4.021) AM (Cen,4, 80.00, Ar,6500.0,556.28,0.70,LS 10); Sm (SG, 2x3.00); Sb (3,40.00); Cm (75:262) 1: TOF MS ES+ 2.12e+005



Minimum:				-10.0		
Maximum:		3.0	100.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
200.1817	200.1815	0.2	1.0	1.5	86.3	C12 H23 N F
	200.1835	-1.8	-9.0	-2.5	3660.4	C4 H22 N7 O2
	200.1822	-0.5	-2.5	-7.5	6211.4	C3 H26 N3 O6
	200.1808	0.9	4.5	-1.5	7398.5	H18 N13
	200.1846	-2.9	-14.5	-6.5	7892.0	C H23 N7 O3 F



^{1}H NMR: **(Table 3, entry 3)**



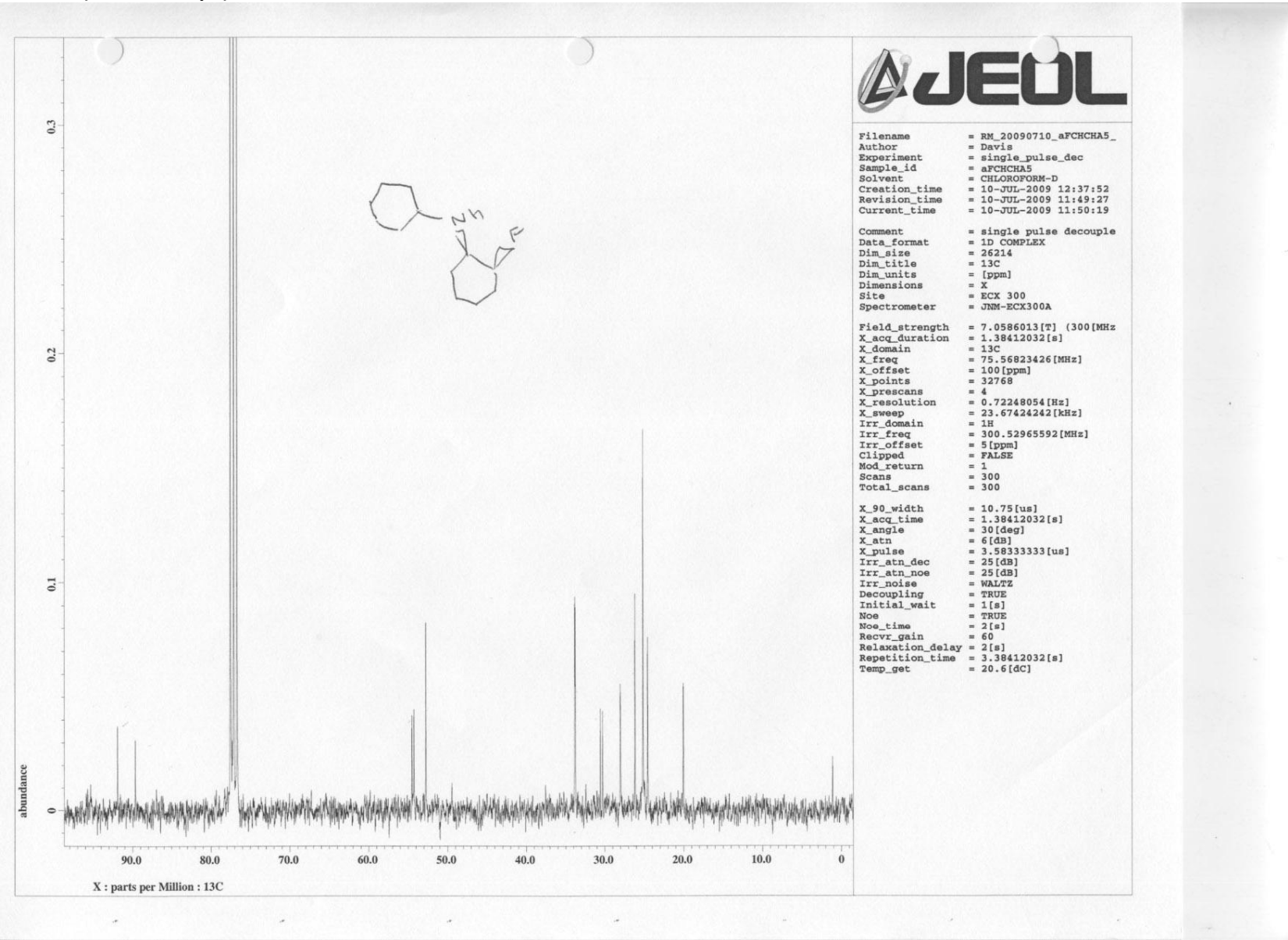

```
Filename          = RM_20090713_aFCHCHA5_
Author            = Davis
Experiment        = single_pulse.ex2
Sample_id         = aFCHCHA5
Solvent           = CHLOROFORM-D
Creation_time     = 13-JUL-2009 13:30:01
Revision_time     = 13-JUL-2009 12:47:32
Current_time      = 13-JUL-2009 12:48:16

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 300
Spectrometer      = JNM-ECX300A

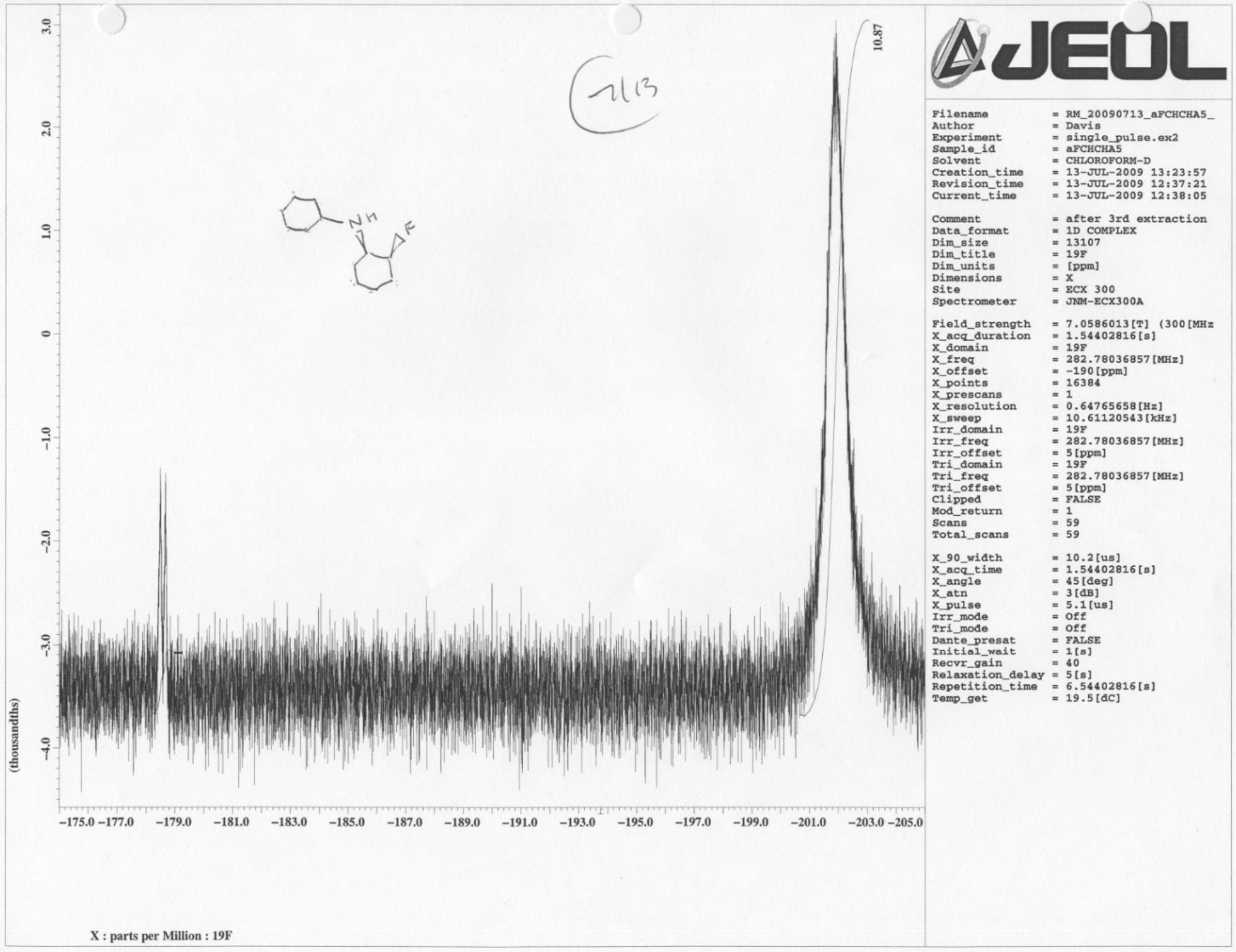
Field_strength    = 7.0586013[T] (300[MHz
X_acq_duration    = 2.90717696[s]
X_domain          = 1H
X_freq            = 300.52965592[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.34397631[Hz]
X_sweep           = 5.63570784[kHz]
Irr_domain        = 1H
Irr_freq          = 300.52965592[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 300.52965592[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 10.33[us]
X_acq_time        = 2.90717696[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 5.165[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 42
Relaxation_delay  = 5[s]
Repetition_time   = 7.90717696[s]
Temp_get          = 20.2[dC]
```

^{13}C NMR: **(Table 3, entry 3)**



^{19}F NMR: **(Table 3, entry 3)**



(2-Fluoro-cyclohexyl)-hexyl-amine *(Table 3, entry 4)*

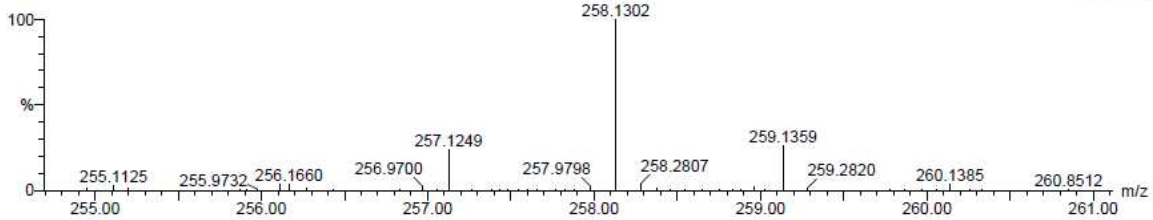
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

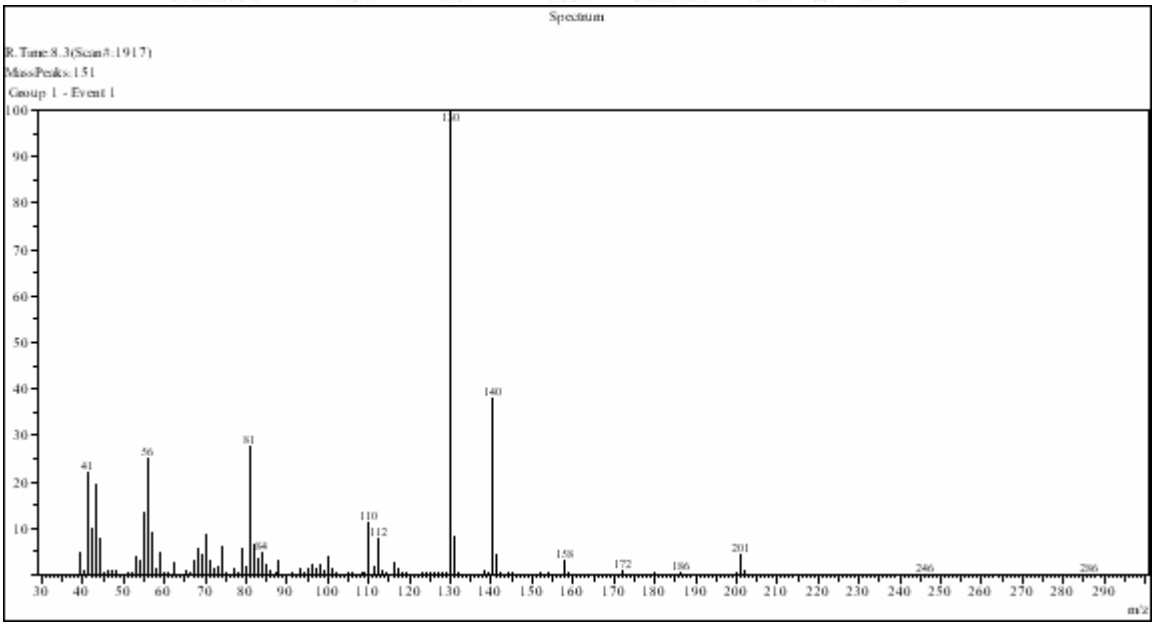
Monoisotopic Mass, Even Electron Ions
486 formula(e) evaluated with 5 results within limits (up to 12 best isotopic matches for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-50 O: 0-50 F: 1-1

TD #3 16-Dec-2009 15:33:30

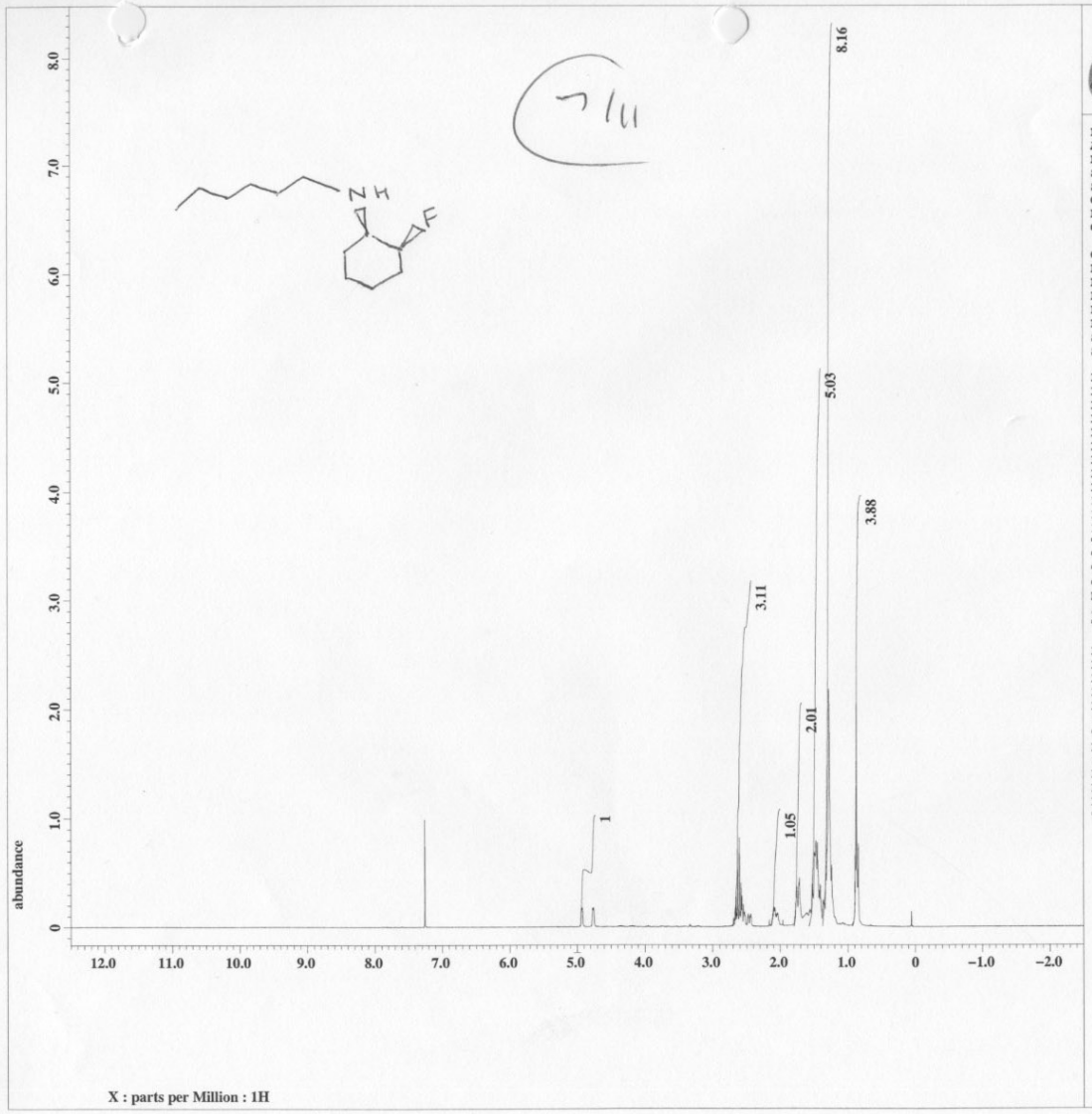
09MSL1216_LCT_6 379 (6.995) AM (Cen,4, 80.00, Ar,6500.0,556.28,0.70,LS 25); Sm (SG, 2x3.00); Sb (3,40.00); Cm (312:395) 1: TOF MS ES+ 9.49e+004



Minimum:				-10.0		
Maximum:		3.0	100.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
258.1302	258.1294	0.8	3.1	8.5	949.5	C16 H17 N O F
	258.1326	-2.4	-9.3	0.5	5474.4	C5 H17 N7 O4 F
	258.1313	-1.1	-4.3	-4.5	7121.2	C4 H21 N3 O8 F
	258.1299	0.3	1.2	1.5	7176.6	C H13 N13 O2 F
	258.1286	1.6	6.2	-3.5	9091.2	H17 N9 O6 F



^{1}H NMR: **(Table 3, entry 4)**



JEOL

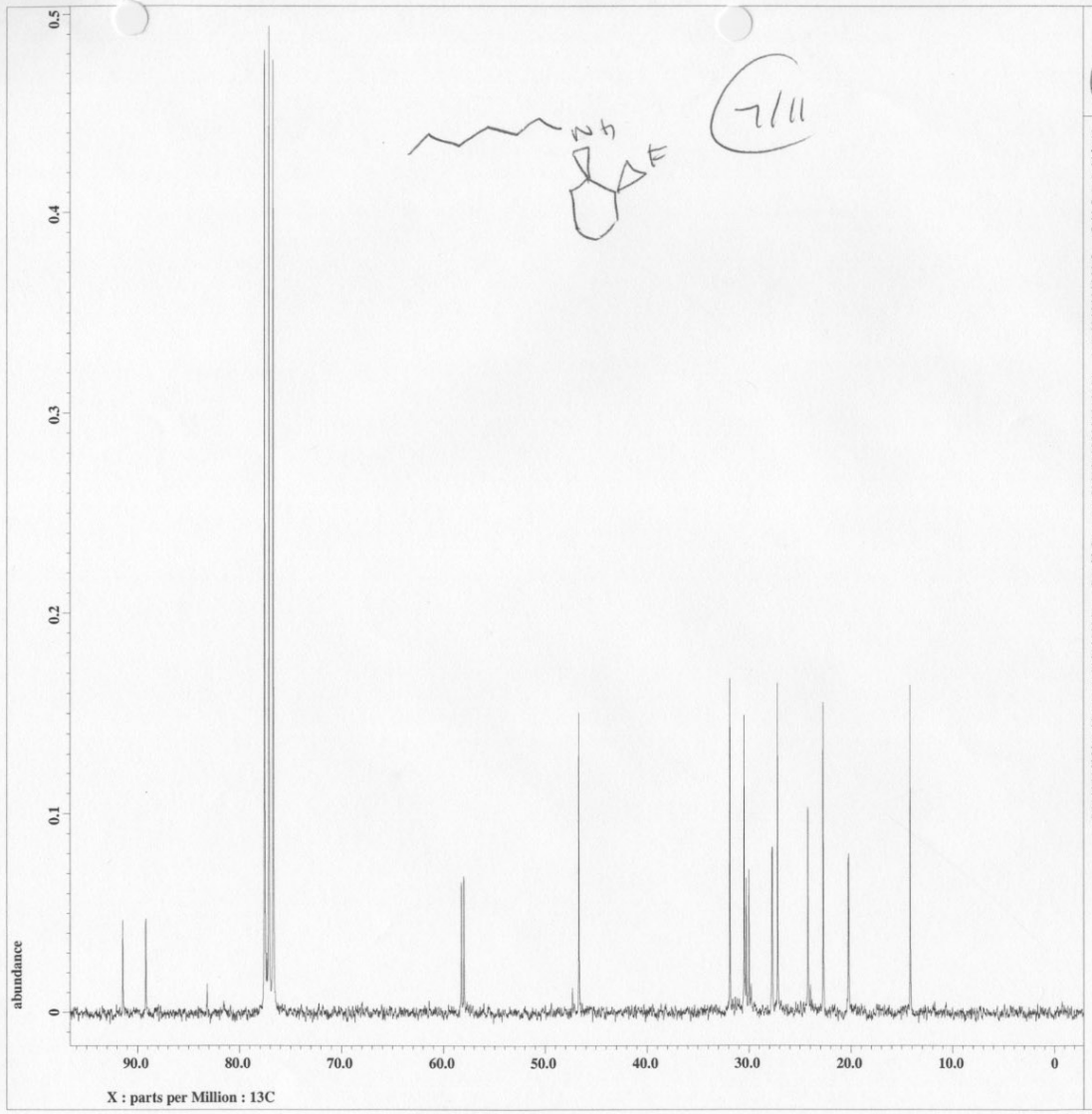
```
Filename          = RM_20090711_aFCHHA3_1
Author            = Davis
Experiment        = single_pulse.ex2
Sample_id         = aFCHHA3
Solvent           = CHLOROFORM-D
Creation_time     = 11-JUL-2009 17:20:19
Revision_time     = 11-JUL-2009 16:39:57
Current_time      = 11-JUL-2009 16:41:28

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 300
Spectrometer      = JNM-ECX300A

Field_strength    = 7.0586013[T] (300[MHz
X_acq_duration    = 2.90717696[s]
X_domain          = 1H
X_freq            = 300.52965592[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.34397631[Hz]
X_sweep           = 5.63570784[kHz]
Irr_domain        = 1H
Irr_freq          = 300.52965592[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 300.52965592[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 10.33[us]
X_acq_time        = 2.90717696[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 5.165[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 38
Relaxation_delay  = 5[s]
Repetition_time   = 7.90717696[s]
Temp_get          = 19.6[dC]
```

^{13}C NMR: **(Table 3, entry 4)**

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Filename          = RM_20090711_aFCHHA3_1
Author            = Davis
Experiment        = single_pulse_dec
Sample_id         = aFCHHA3
Solvent           = CHLOROFORM-D
Creation_time     = 11-JUL-2009 18:42:41
Revision_time     = 11-JUL-2009 17:53:39
Current_time      = 11-JUL-2009 17:55:56

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 300
Spectrometer      = JNM-ECX300A

Field_strength    = 7.0586013[T] (300[MHz
X_acq_duration    = 1.38412032[s]
X_domain          = 13C
X_freq            = 75.56823426[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.72248054[Hz]
X_sweep           = 23.67424242[kHz]
Irr_domain        = 1H
Irr_freq          = 300.52965592[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 1000
Total_scans       = 1000

X_90_width        = 10.75[us]
X_acq_time        = 1.38412032[s]
X_angle           = 30[deg]
X_atn             = 6[dB]
X_pulse           = 3.58333333[us]
Irr_atn_dec       = 25[dB]
Irr_atn_noe       = 25[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 3.38412032[s]
Temp_get          = 19.8[dC]
```
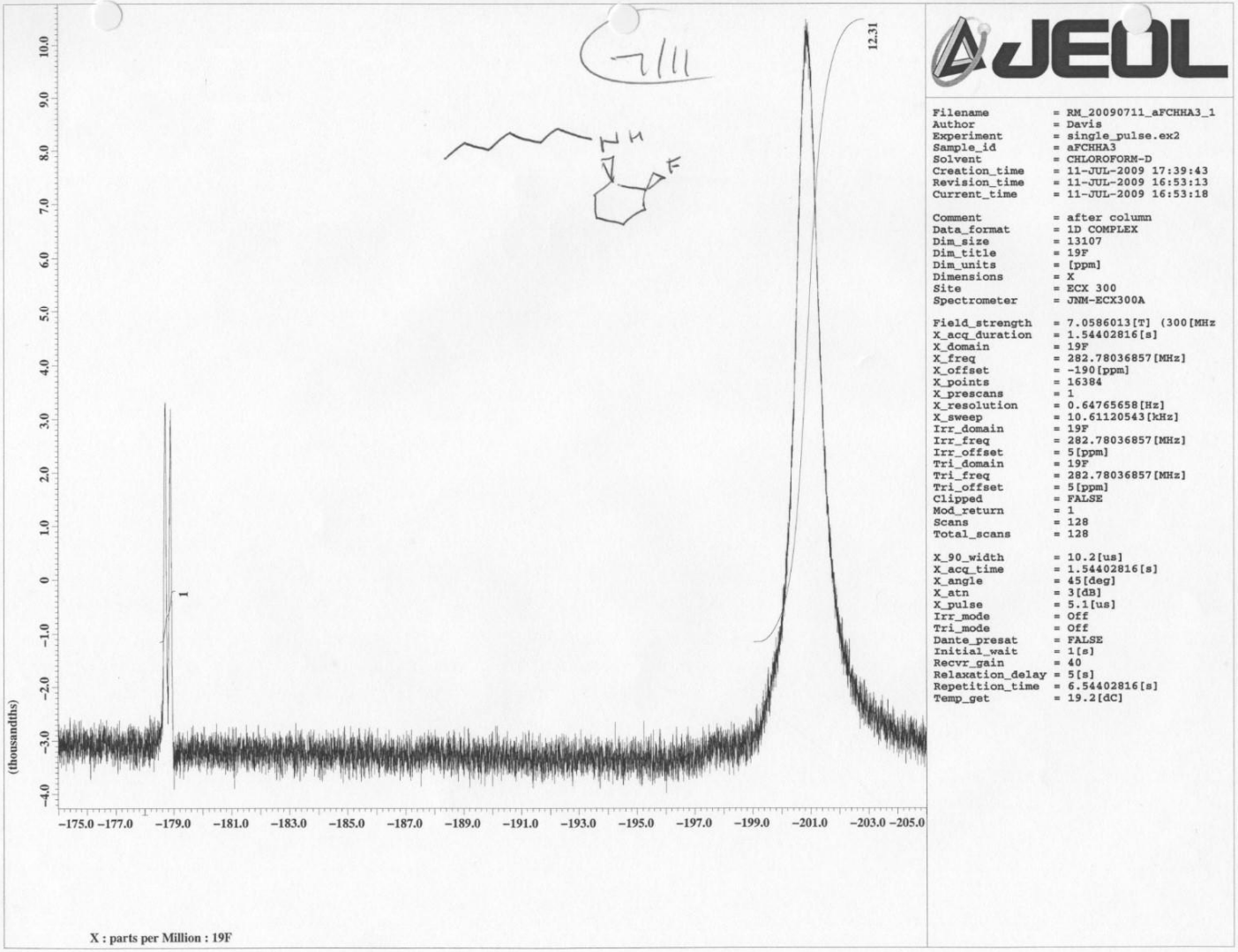

^{19}F NMR: **(Table 3, entry 4)**



(2-Fluoro-indan-1-yl)-(4-methoxy-phenyl)-amine(*Table 3, entry 7)*

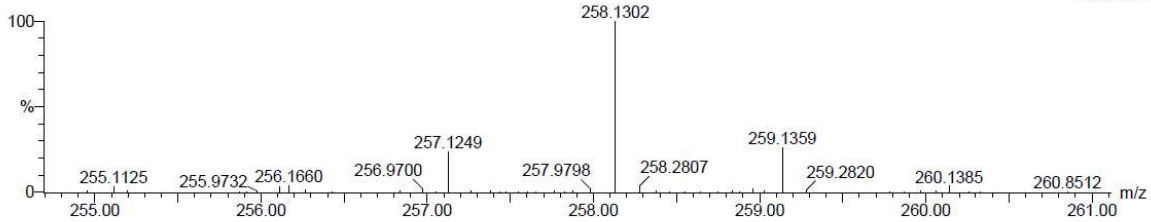
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

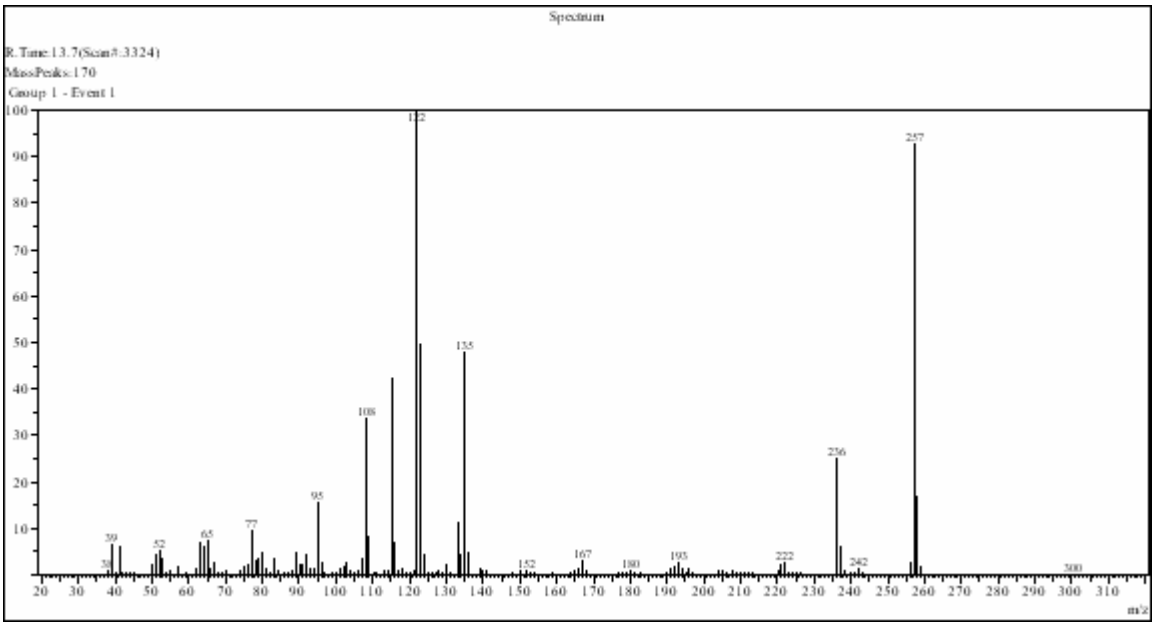
Monoisotopic Mass, Even Electron Ions
486 formula(e) evaluated with 5 results within limits (up to 12 best isotopic matches for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-50 O: 0-50 F: 1-1

TD #3 16-Dec-2009 15:33:30

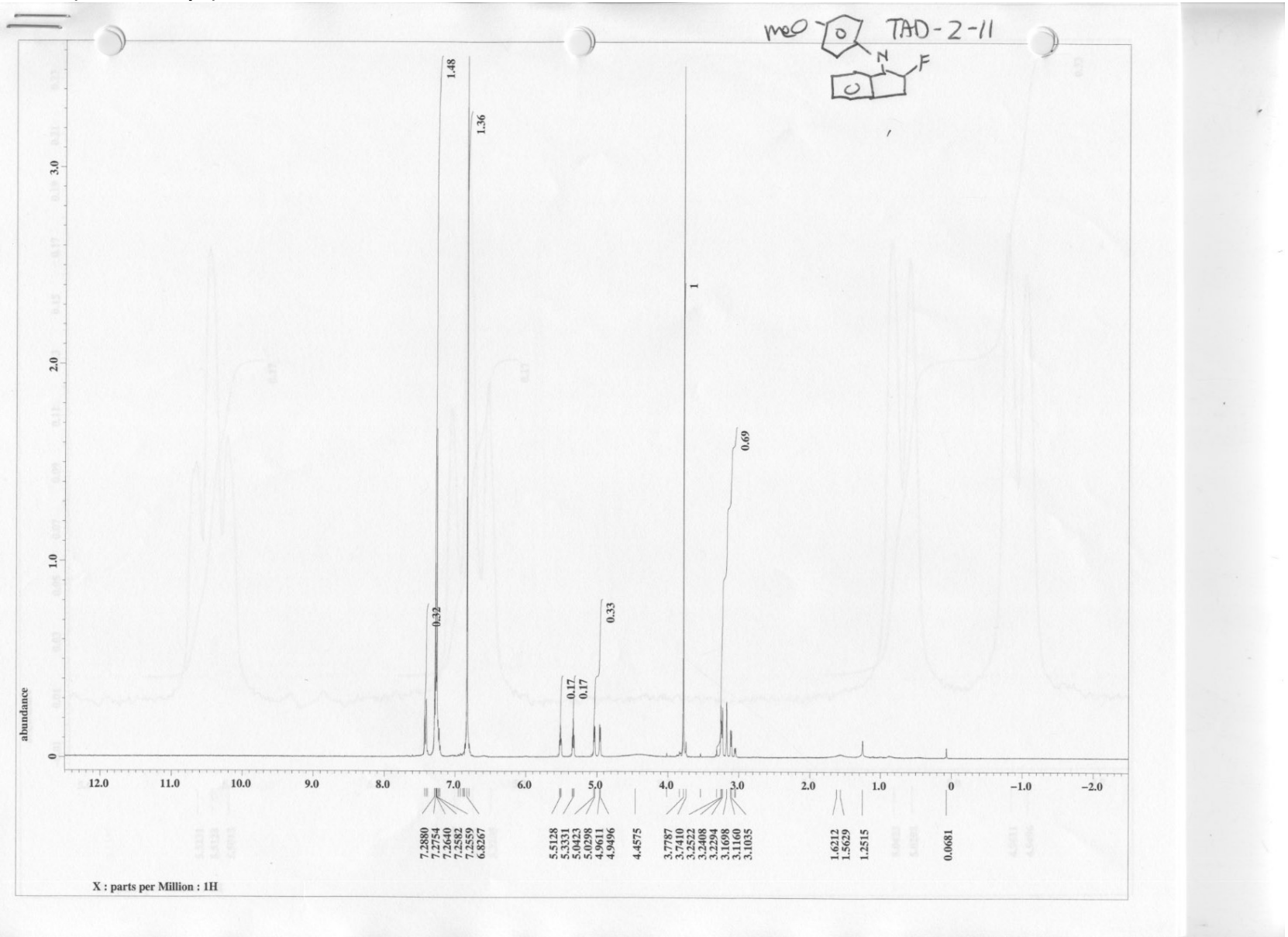
09MSL1216_LCT_6 379 (6.995) AM (Cen,4, 80.00, Ar,6500.0,556.28,0.70,LS 25); Sm (SG, 2x3.00); Sb (3,40.00); Cm (312:395) 1: TOF MS ES+ 9.49e+004



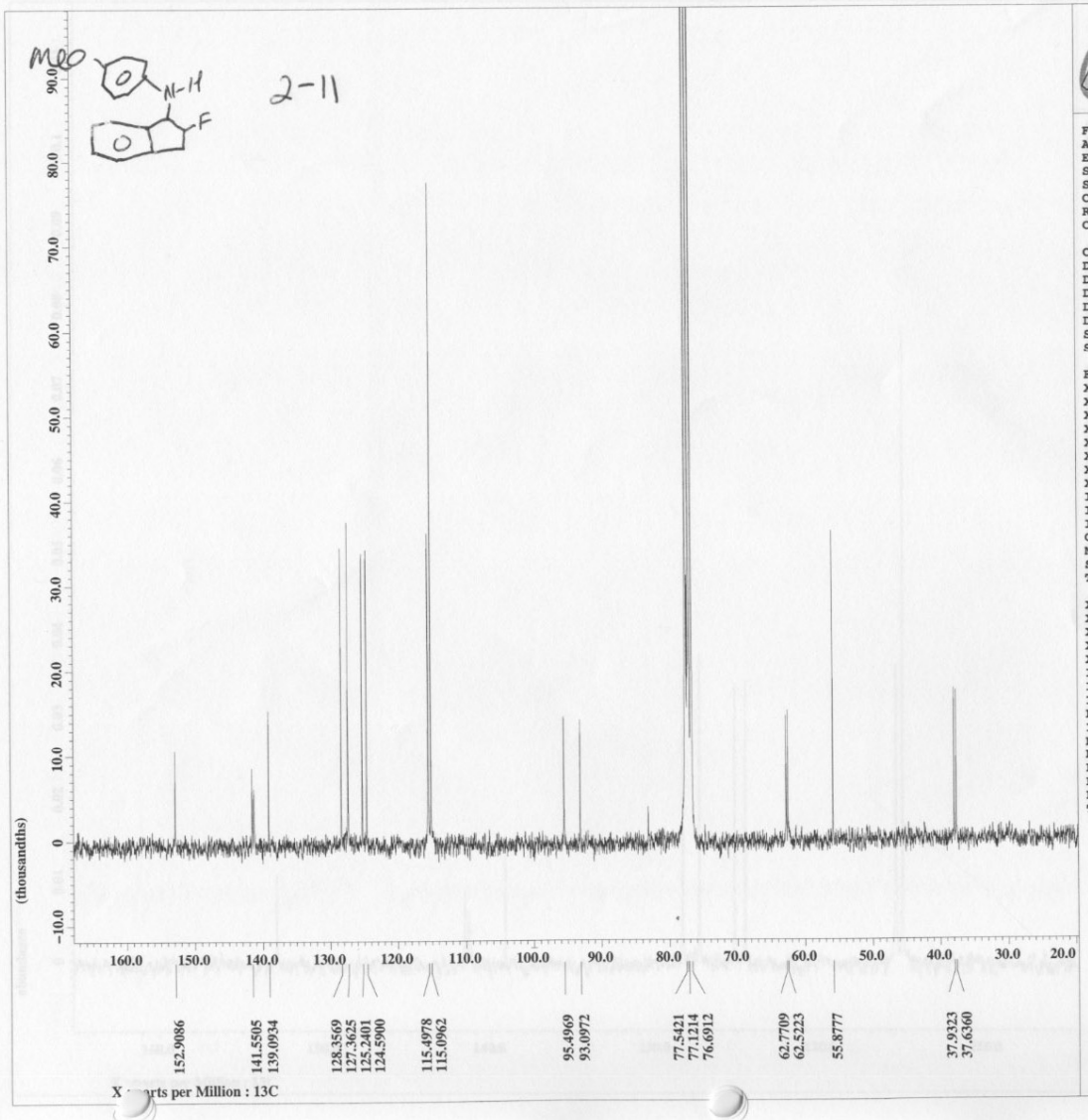
Minimum:				-10.0		
Maximum:		3.0	100.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
258.1302	258.1294	0.8	3.1	8.5	949.5	C16 H17 N O F
	258.1326	-2.4	-9.3	0.5	5474.4	C5 H17 N7 O4 F
	258.1313	-1.1	-4.3	-4.5	7121.2	C4 H21 N3 O8 F
	258.1299	0.3	1.2	1.5	7176.6	C H13 N13 O2 F
	258.1286	1.6	6.2	-3.5	9091.2	H17 N9 O6 F



^{1}HNMR: **(Table 3, entry 7)**



^{13}C NMR: **(Table 3, entry 7)**



JEOL

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Author              = Davis
Experiment          = single_pulse_dec
Sample_id           = indanoneanisidine13C
Solvent             = CHLOROFORM-D
Creation_time       = 10-JUN-2009 01:40:42
Revision_time       = 10-JUN-2009 07:57:34
Current_time        = 10-JUN-2009 07:57:38

Comment             = single pulse decouple
Data_format         = 1D COMPLEX
Dim_size            = 26214
Dim_title           = 13C
Dim_units           = [ppm]
Dimensions          = X
Site                = ECX 300
Spectrometer        = JNM-ECX300A

Field_strength      = 7.0586013[T] (300[MHz
X_acq_duration      = 1.38412032[s]
X_domain            = 13C
X_freq              = 75.56823426[MHz]
X_offset            = 100[ppm]
X_points            = 32768
X_prescans          = 4
X_resolution        = 0.72248054[Hz]
X_sweep             = 23.67424242[kHz]
Irr_domain          = 1H
Irr_freq            = 300.52965592[MHz]
Irr_offset          = 5[ppm]
Clipped             = FALSE
Mod_return          = 1
Scans               = 8000
Total_scans         = 8000

X_90_width          = 10.75[us]
X_acq_time          = 1.38412032[s]
X_angle             = 30[deg]
X_atn               = 6[dB]
X_pulse             = 3.58333333[us]
Irr_atn_dec         = 25[dB]
Irr_atn_noe         = 25[dB]
Irr_noise           = WALTZ
Decoupling          = TRUE
Initial_wait        = 1[s]
Noe                 = TRUE
Noe_time            = 2[s]
Recvr_gain          = 60
Relaxation_delay    = 2[s]
Repetition_time     = 3.38412032[s]
Temp_get            = 19.9[dC]
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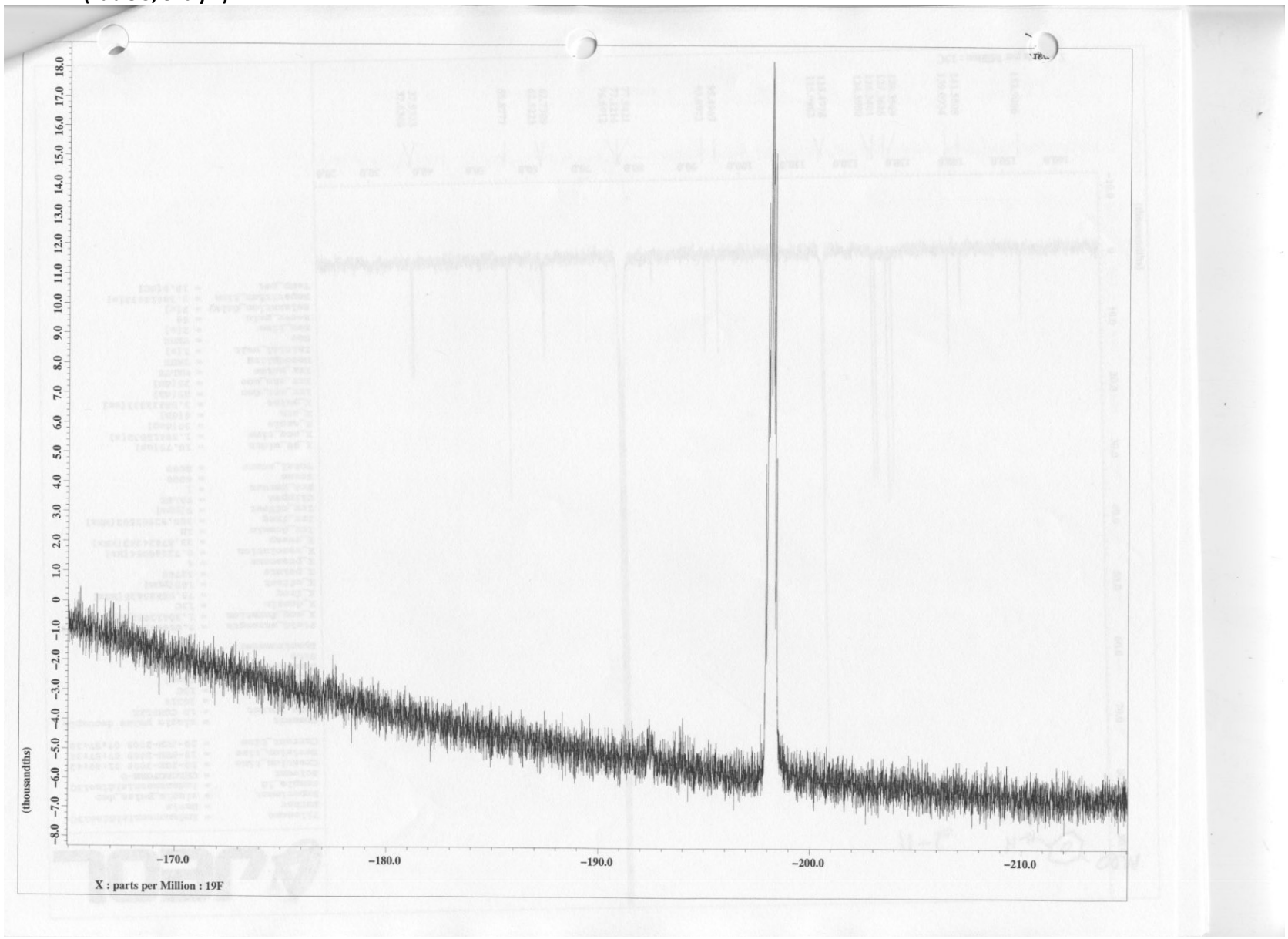
^{19}F NMR: **(Table 3, entry 7)**



Benzyl-(2-fluoro-indan-1-yl)-amine(Table 3, entry 8)

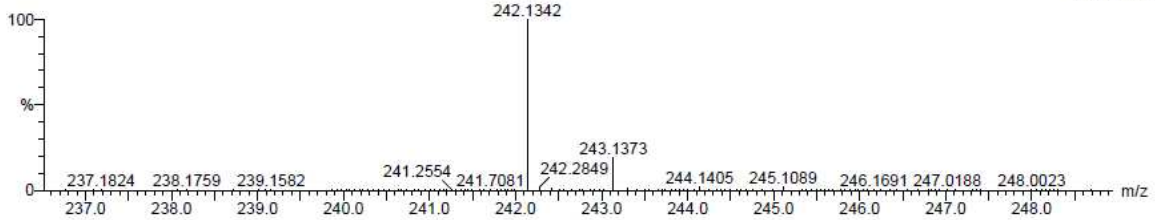
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

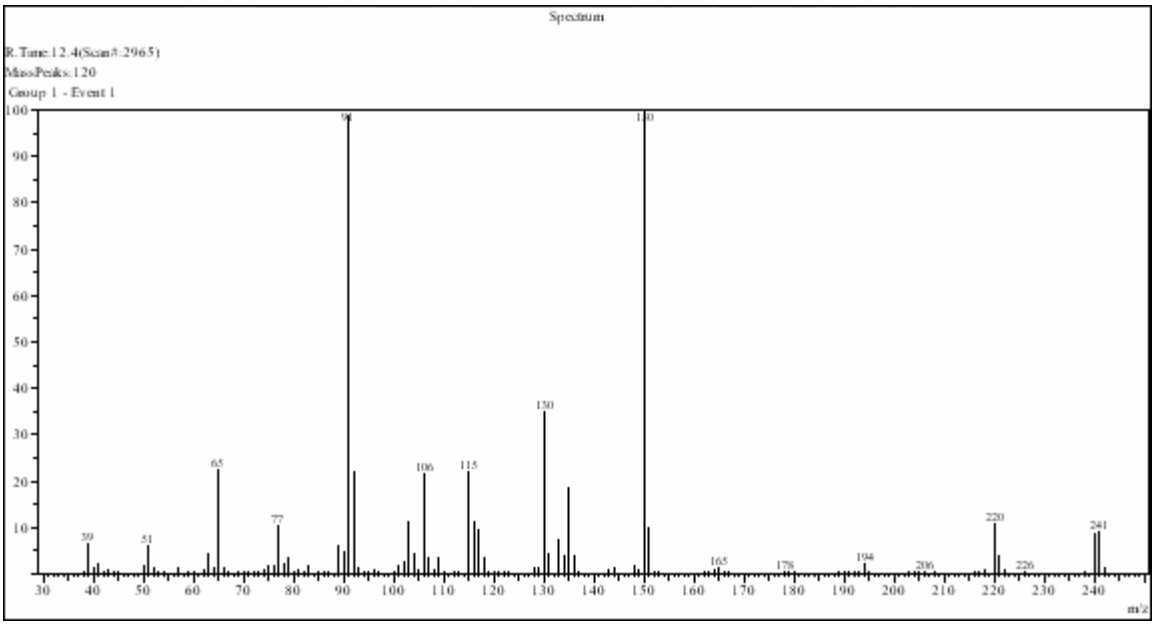
Monoisotopic Mass, Even Electron Ions
415 formula(e) evaluated with 4 results within limits (up to 12 best isotopic matches for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-50 O: 0-50 F: 1-1

TD #2 16-Dec-2009 15:48:58

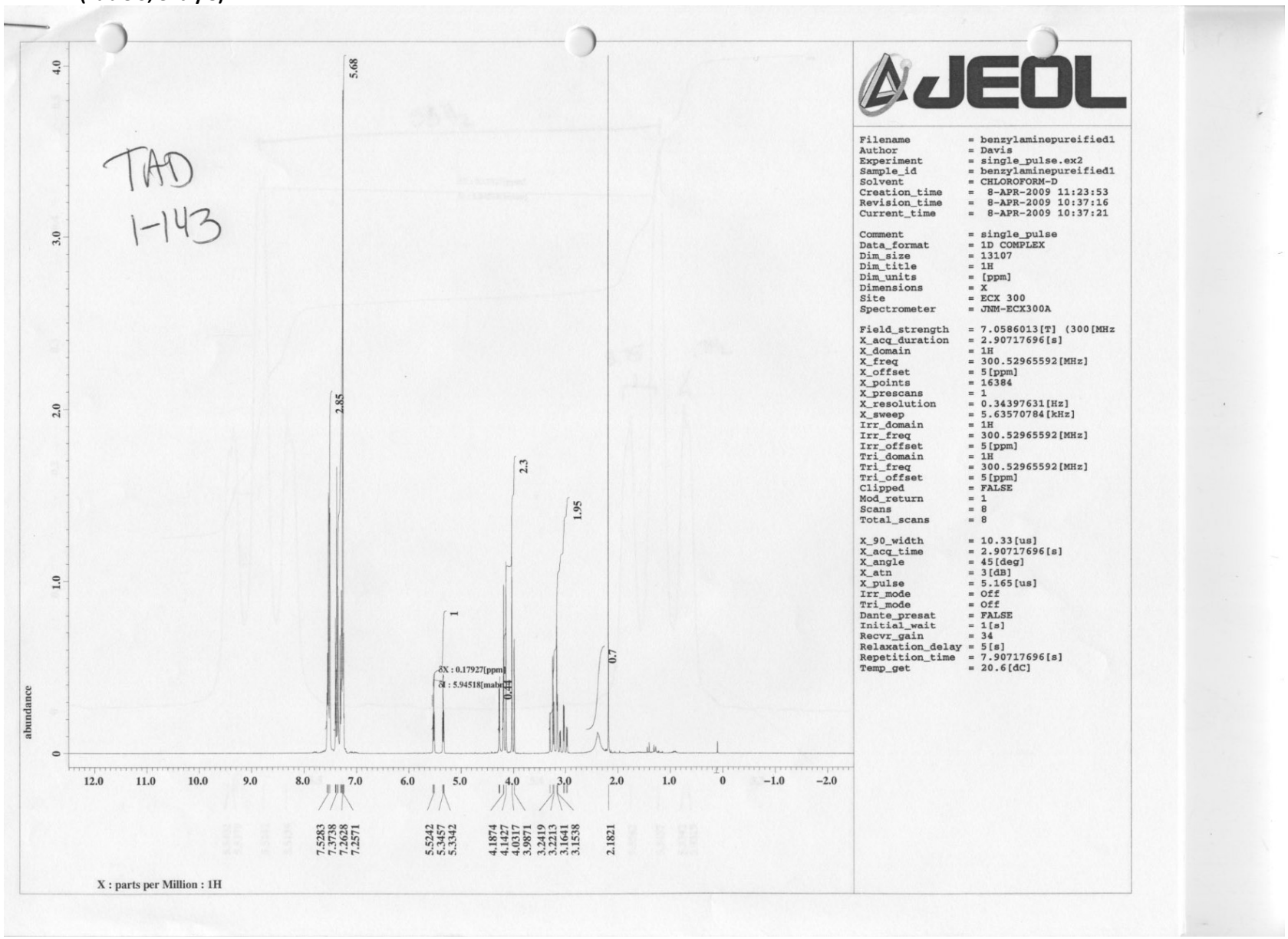
09MSL1216_LCT_8 287 (5.302) AM (Cen,4, 80.00, Ar,6500.0,556.28,0.70,LS 25); Sm (SG, 2x3.00); Sb (3,40.00); Cm (244:395) 1: TOF MS ES+ 1.77e+005



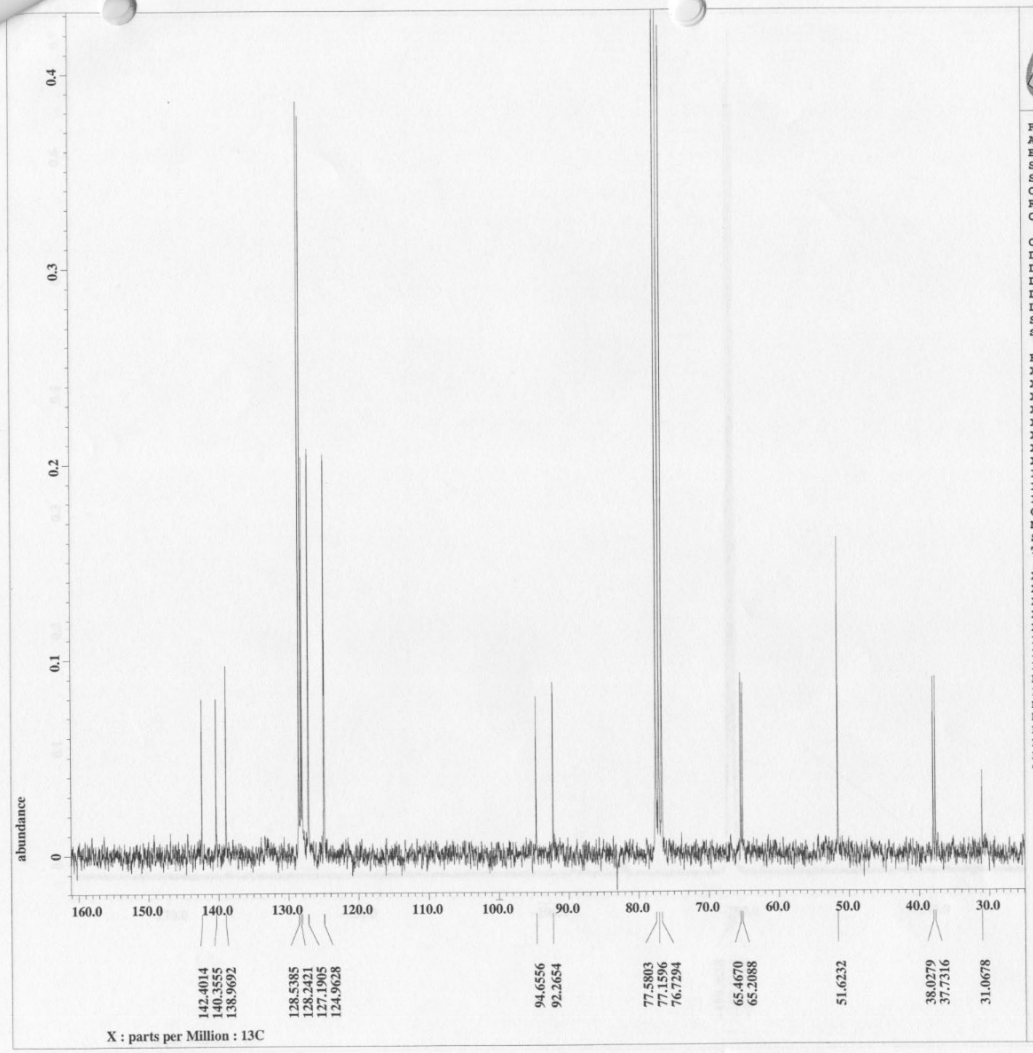
Minimum:				-10.0		
Maximum:		3.0	100.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
242.1342	242.1345	-0.3	-1.2	8.5	8.7	C16 H17 N F
	242.1350	-0.8	-3.3	1.5	7493.4	C H13 N13 O F
	242.1364	-2.2	-9.1	-4.5	7495.4	C4 H21 N3 O7 F
	242.1337	0.5	2.1	-3.5	10679.7	H17 N9 O5 F



^{1}H NMR: **(Table 3, entry 8)**



^{13}C NMR: **(Table 3, entry 8)**

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Author            = Davis
Experiment        = single_pulse_dec
Sample_id         = tadpurifiedreductionp
Solvent           = CHLOROFORM-D
Creation_time     =  8-APR-2009 11:50:15
Revision_time     =  8-APR-2009 10:52:41
Current_time      =  8-APR-2009 10:52:54

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 300
Spectrometer      = JNM-ECX300A

Field_strength    = 7.0586013[T] (300[MHz
X_acq_duration    = 1.38412032[s]
X_domain          = 13C
X_freq            = 75.56823426[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.72248054[Hz]
X_sweep           = 23.67424242[kHz]
Irr_domain        = 1H
Irr_freq          = 300.52965592[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 237
Total_scans       = 237

X_90_width        = 10.75[us]
X_acq_time        = 1.38412032[s]
X_angle           = 30[deg]
X_atn             = 6[dB]
X_pulse           = 3.58333333[us]
Irr_atn_dec       = 25[dB]
Irr_atn_noe       = 25[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 3.38412032[s]
Temp_get          = 20.6[dC]
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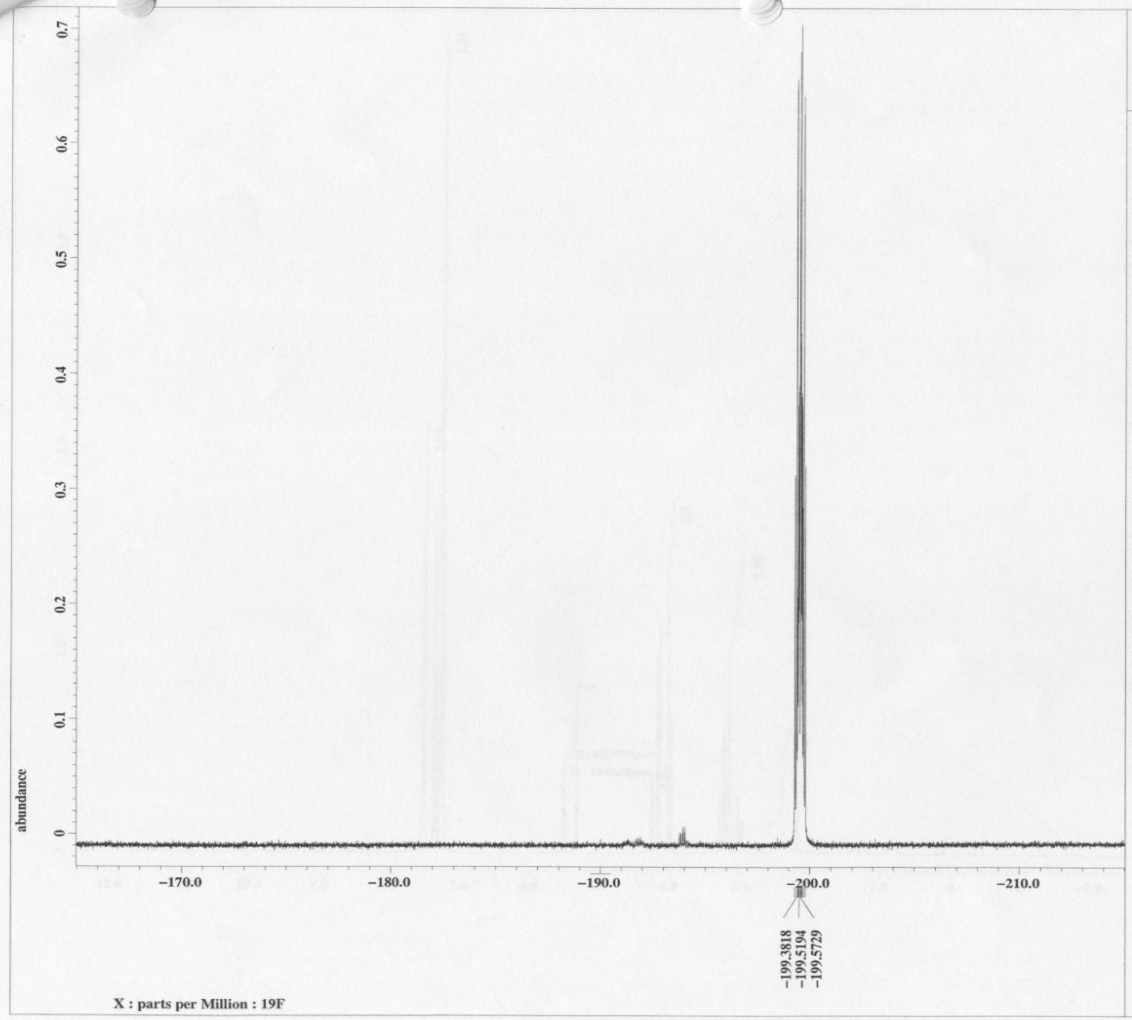
^{19}F NMR: **(Table 3, entry 8)**

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Filename          = tadpurifiedreductionp
Author            = Davis
Experiment        = single_pulse.ex2
Sample_id         = tadpurifiedreductionp
Solvent           = CHLOROFORM-D
Creation_time     =  8-APR-2009 11:54:02
Revision_time     =  8-APR-2009 10:56:42
Current_time      =  8-APR-2009 10:56:49

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 19F
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 300
Spectrometer      = JNM-ECX300A

Field_strength    = 7.0586013[T] (300[MHz
X_acq_duration    = 0.92536832[s]
X_domain          = 19F
X_freq            = 282.78036857[MHz]
X_offset          = -190[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 1.08065078[Hz]
X_sweep           = 17.70538244[kHz]
Irr_domain        = 19F
Irr_freq          = 282.78036857[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 19F
Tri_freq          = 282.78036857[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 12
Total_scans       = 12

X_90_width        = 10.2[us]
X_acq_time        = 0.92536832[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 5.1[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 42
Relaxation_delay  = 5[s]
Repetition_time   = 5.92536832[s]
Temp_get          = 21[dC]
```

(2-Fluoro-indan-1-yl)-hexyl-amine(*Table 3, entry 9*)

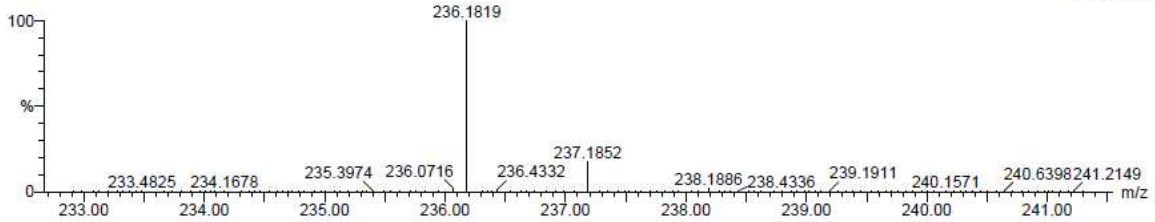
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 3.0 mDa / DBE: min = -10.0, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
853 formula(e) evaluated with 8 results within limits (up to 12 best isotopic matches for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-50 O: 0-50 F: 0-1

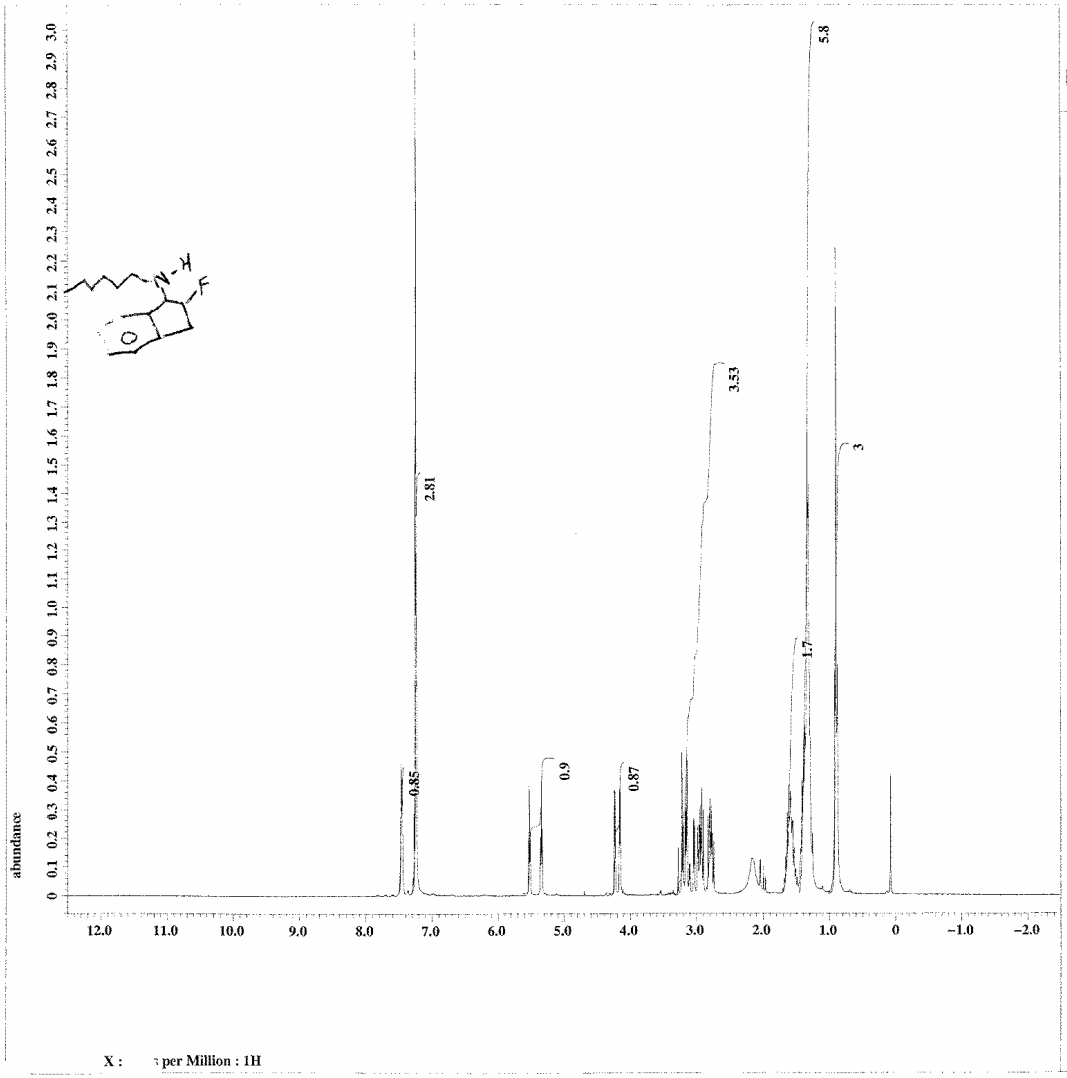
TD #1 16-Dec-2009 12:15:46

09MSL1216_LCT_1 309 (5.716) AM (Cen,4, 80.00, Ar,6500.0,556.28,0.70,LS 25); Sm (SG, 2x3.00); Sb (3,40.00); Cm (265:350) 1: TOF MS ES+ 1.03e+005



Minimum:				-10.0						
Maximum:		3.0	100.0	100.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula				
236.1819	236.1815	0.4	1.7	4.5	9.6	C15	H23	N	F	
	236.1835	-1.6	-6.8	0.5	1382.2	C7	H22	N7	O2	
	236.1822	-0.3	-1.3	-4.5	2338.4	C6	H26	N3	O6	
	236.1808	1.1	4.7	1.5	2876.6	C3	H18	N13		
	236.1846	-2.7	-11.4	-3.5	3047.9	C4	H23	N7	O3	F
	236.1795	2.4	10.2	-3.5	3962.5	C2	H22	N9	O4	
	236.1833	-1.4	-5.9	-8.5	4448.3	C3	H27	N3	O7	F
	236.1820	-0.1	-0.4	-2.5	4984.0	H19	N13	O	F	

^{1}H NMR: **(Table 3, entry 9)**

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Author            = Davis
Experiment        = single_pulse.ex2
Sample_id         = hexylimineindanonered
Solvent           = CHLOROFORM-D
Creation_time     = 30-NOV-2009 12:55:37
Revision_time     = 30-NOV-2009 12:19:22
Current_time      = 30-NOV-2009 12:19:35

Comment           = single_pulse
Data_format       = 1D COMPLEX
Dim_size          = 13107
Dim_title         = 1H
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 300
Spectrometer      = JNM-ECX300A

Field_strength    = 7.0586013[T] (300[MHz
X_acq_duration    = 2.90717696[s]
X_domain          = 1H
X_freq            = 300.52965592[MHz]
X_offset          = 5[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 0.34397631[Hz]
X_sweep           = 5.63570784[kHz]
Irr_domain        = 1H
Irr_freq          = 300.52965592[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 1H
Tri_freq          = 300.52965592[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 8
Total_scans       = 8

X_90_width        = 10.33[us]
X_acq_time        = 2.90717696[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 5.165[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 38
Relaxation_delay  = 5[s]
Repetition_time   = 7.90717696[s]
Temp_get          = 19.9[dC]
```
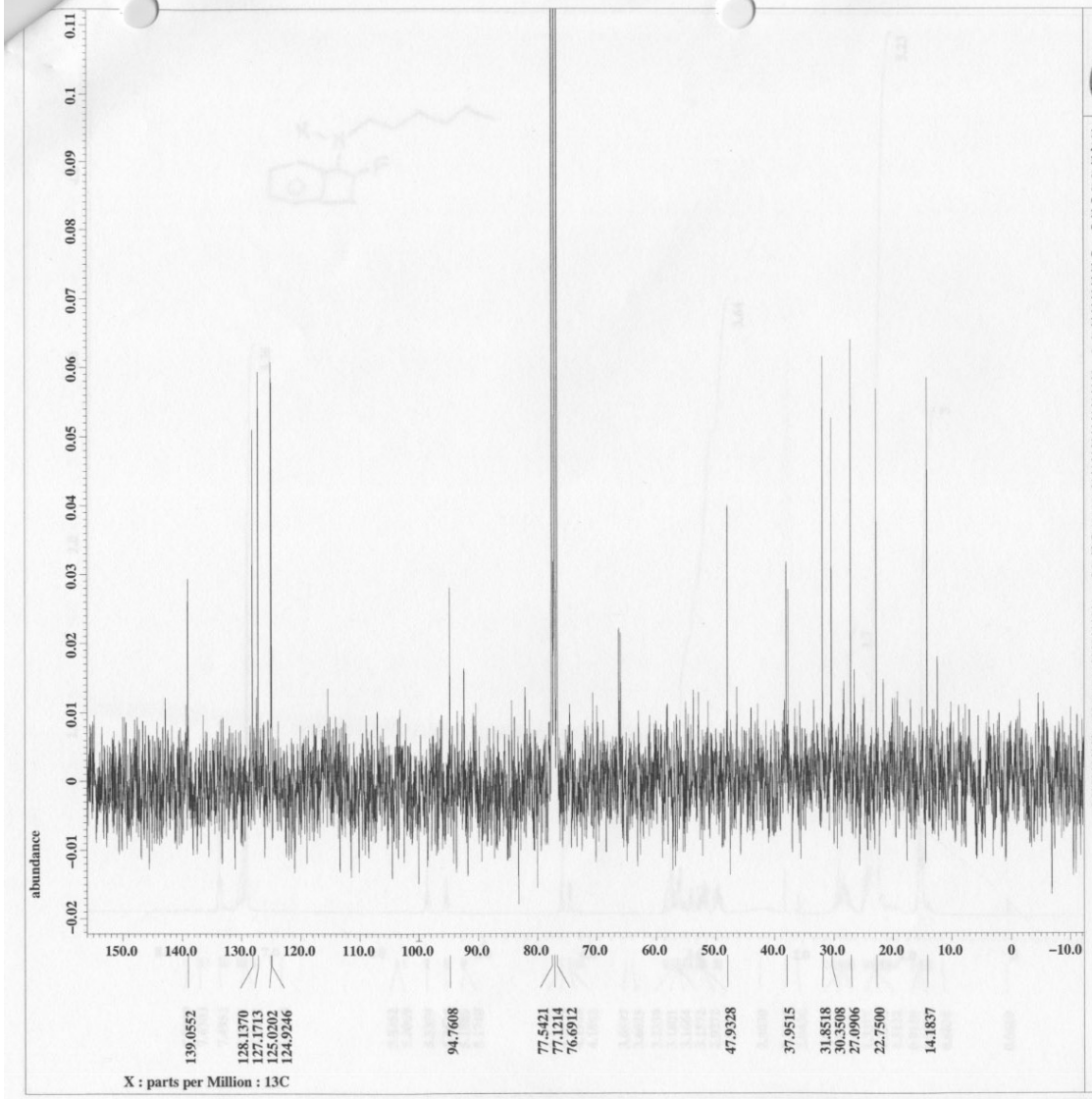

^{13}C NMR: **(Table 3, entry 9)**



JEOL

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Experiment        = single_pulse_dec
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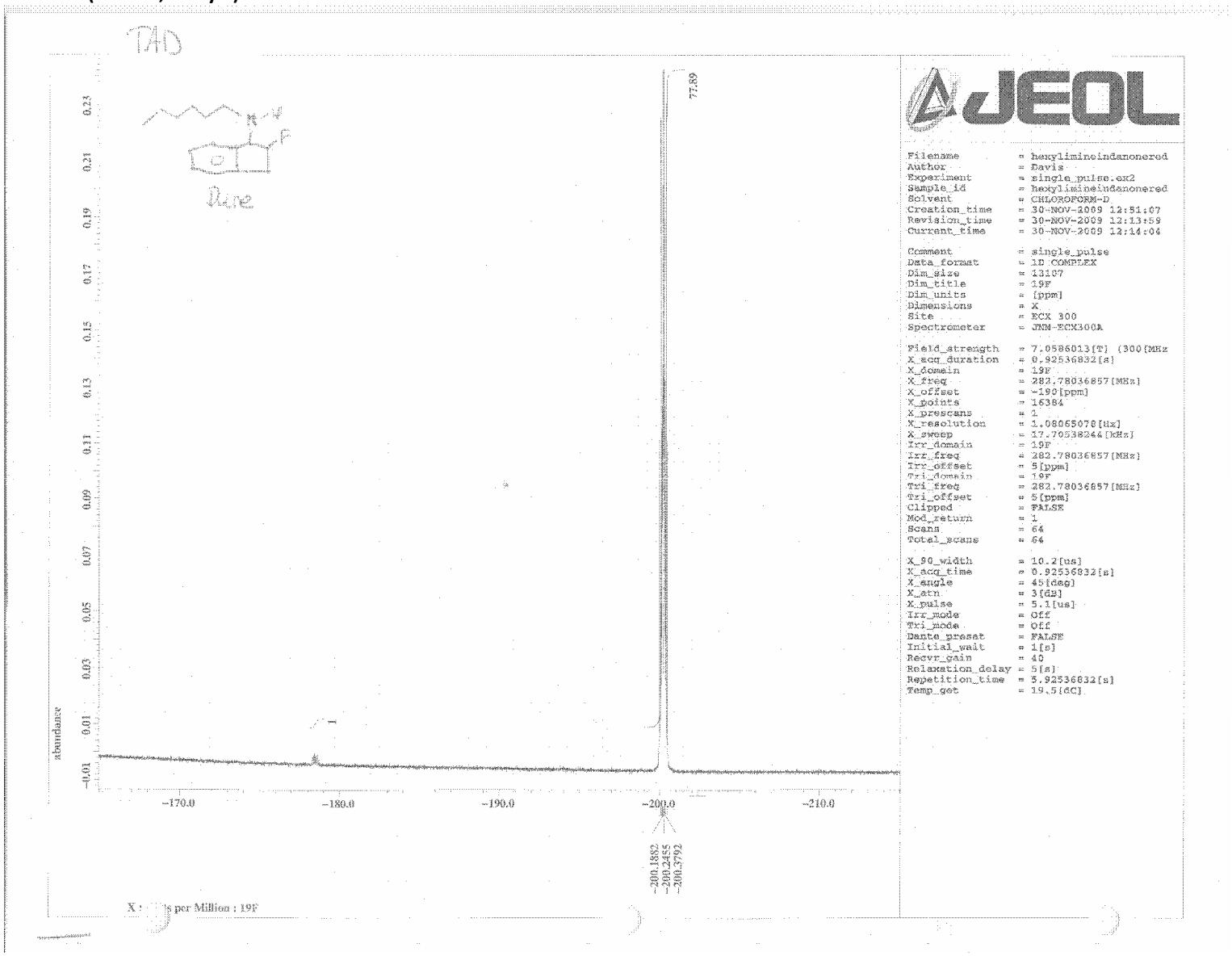
Revision_time     = 27-JUL-2009 10:57:14
Current_time      = 27-JUL-2009 10:57:30

Comment           = single pulse decouple
Data_format       = 1D COMPLEX
Dim_size          = 26214
Dim_title         = 13C
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 300
Spectrometer      = JNM-ECX300A

Field_strength    = 7.0586013[T] (300[MHz
X_acq_duration    = 1.38412032[s]
X_domain          = 13C
X_freq            = 75.56823426[MHz]
X_offset          = 100[ppm]
X_points          = 32768
X_prescans        = 4
X_resolution      = 0.72248054[Hz]
X_sweep           = 23.67424242[kHz]
Irr_domain        = 1H
Irr_freq          = 300.52965592[MHz]
Irr_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 152
Total_scans       = 152

X_90_width        = 10.75[us]
X_acq_time        = 1.38412032[s]
X_angle           = 30[deg]
X_atn             = 6[dB]
X_pulse           = 3.58333333[us]
Irr_atn_dec       = 25[dB]
Irr_atn_noe       = 25[dB]
Irr_noise         = WALTZ
Decoupling        = TRUE
Initial_wait      = 1[s]
Noe               = TRUE
Noe_time          = 2[s]
Recvr_gain        = 60
Relaxation_delay  = 2[s]
Repetition_time   = 3.38412032[s]
Temp_get          = 20[dC]
```

^{19}F NMR: **(Table 3, entry 9)**

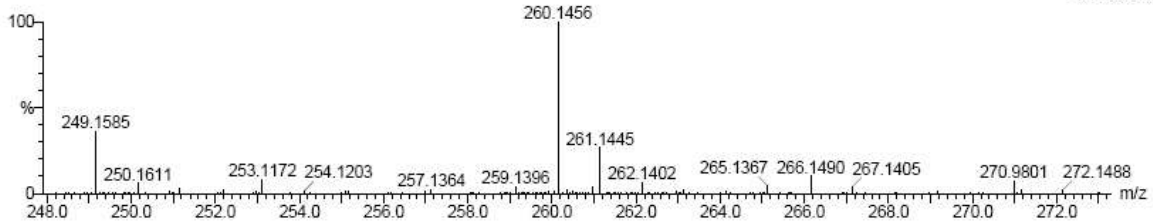


(2-Fluoro-1-phenyl-propyl)-(4-methoxy-phenyl)-amine *(Table 3, entry 11)*

Elemental Composition Report **Page 1**

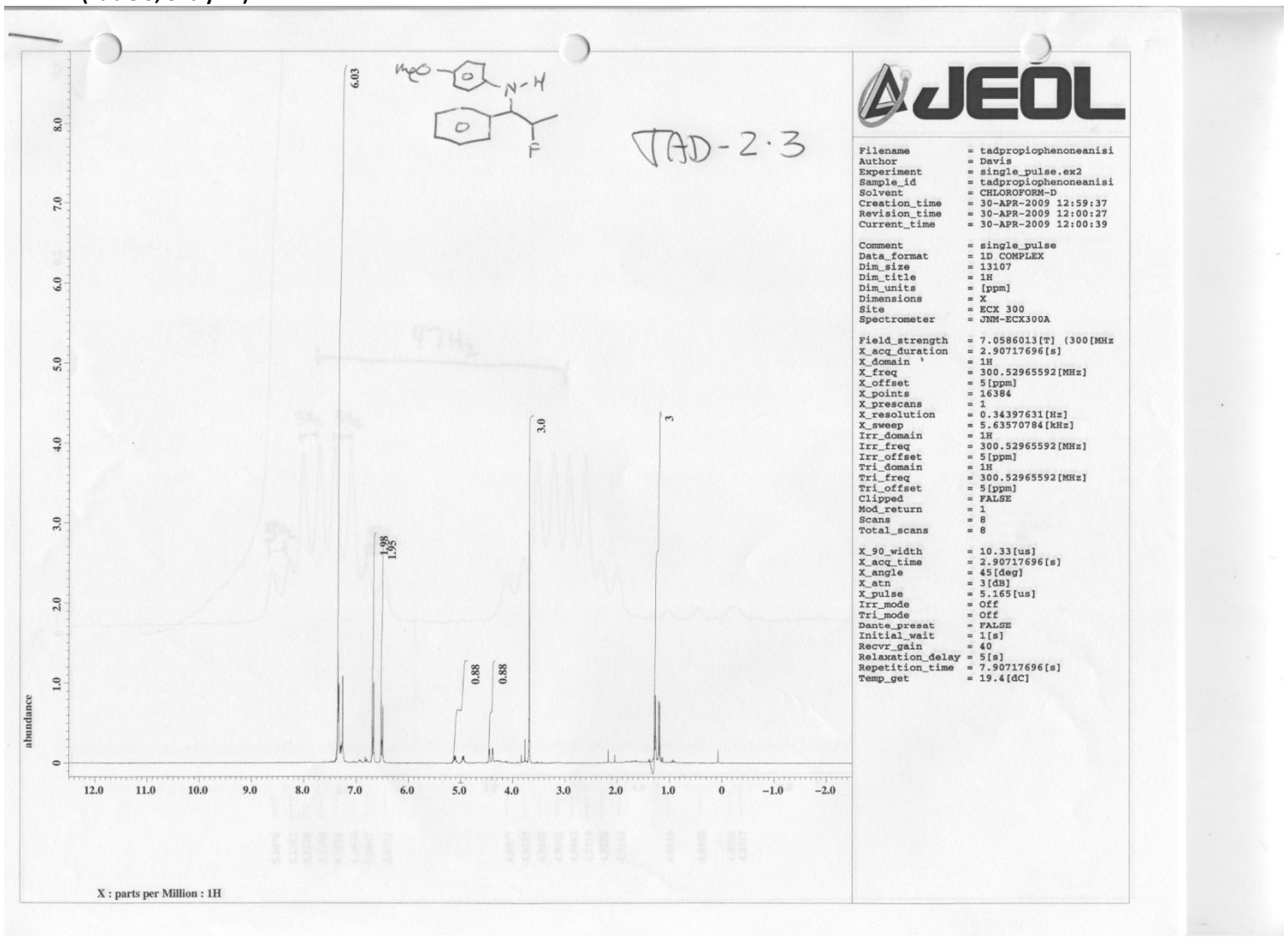
Single Mass Analysis
Tolerance = 3.0 mDa / DBE: min = -100.0, max = 400.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
539 formula(e) evaluated with 2 results within limits (up to 12 best isotopic matches for each mass)
Elements Used:
C: 5-100 H: 1-125 N: 0-50 O: 0-50 F: 1-1
(2-F-1-Ph-propyl)-(4-MeO-Ph)-amine KE319
LCT XE
10TD0302_LCT_1 93 (1.709) AM (Cen,4, 80.00, Ar,6500.0,556.28,0.70,LS 10); Sm (SG, 2x3.00); Sb (3,40.00); Cm (56:95) 1: TOF MS ES+
3.11e+004

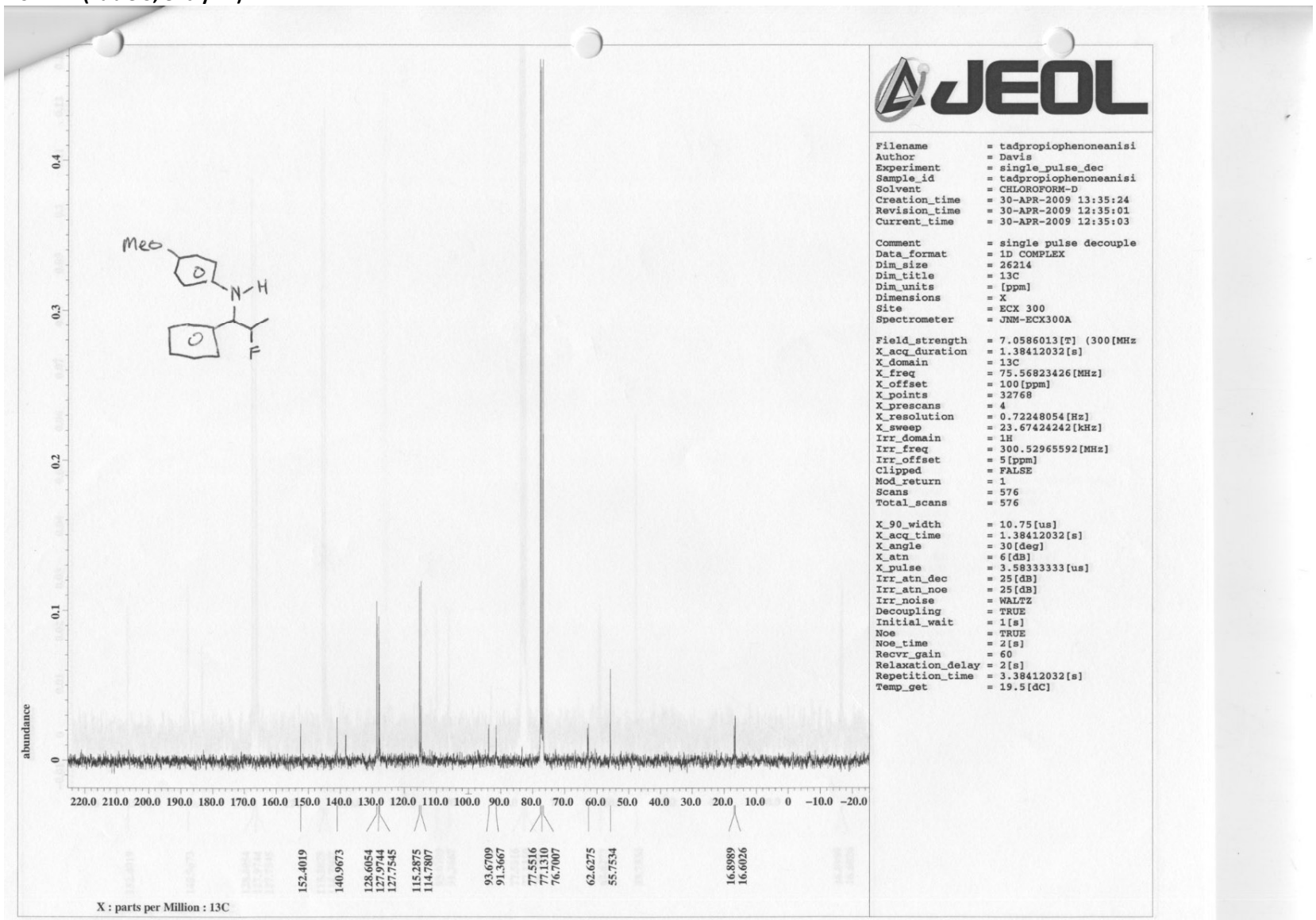


Minimum:				-100.0			
Maximum:		3.0	5.0	400.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
260.1456	260.1451	0.5	1.9	7.5	288.9	0.2	C16 H19 N O F
	260.1483	-2.7	-10.4	-0.5	290.4	1.7	C5 H19 N7 O4 F

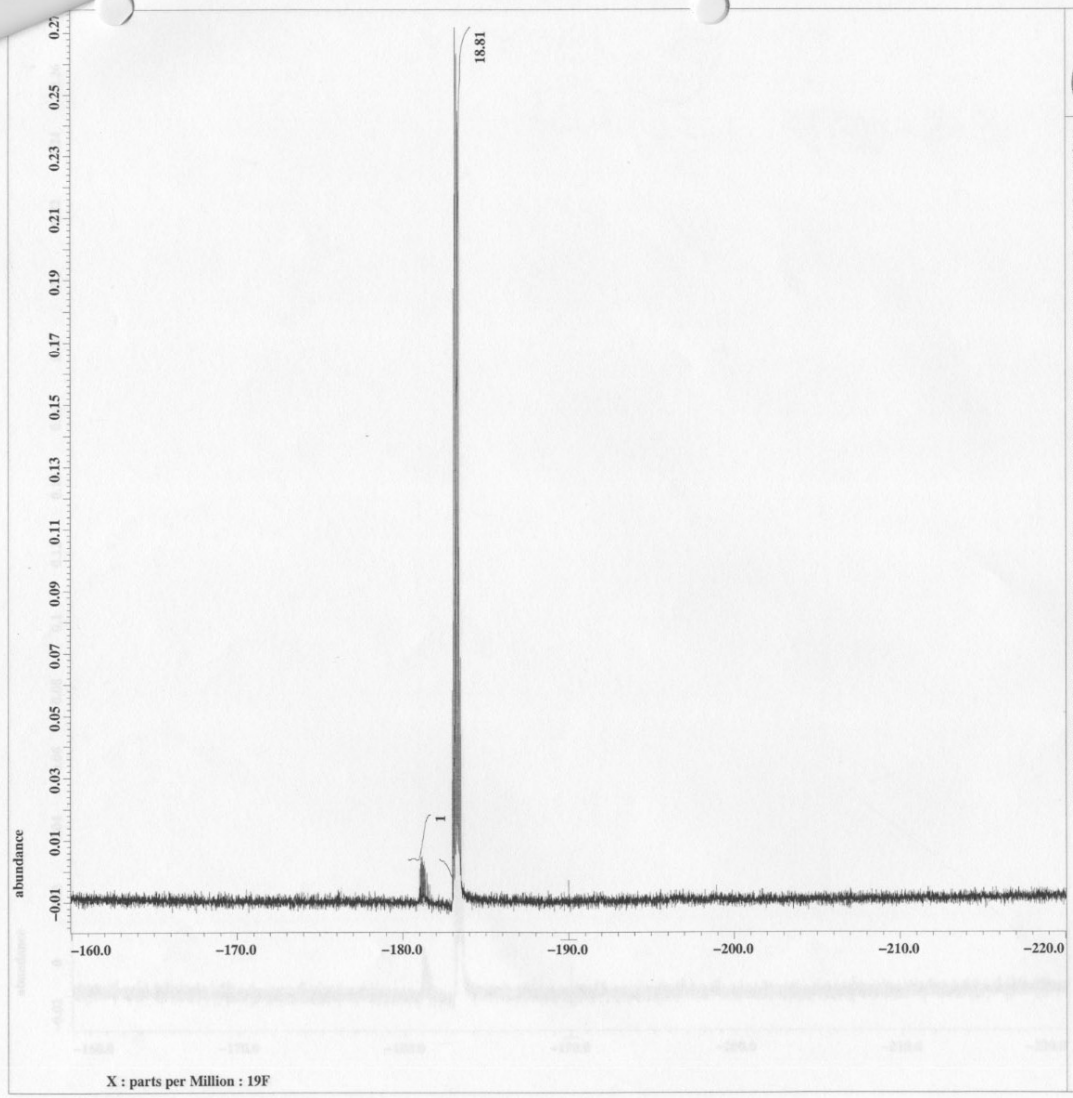
^{1}H NMR:**(Table 3, entry 11)**



^{13}C NMR:**(Table 3, entry 11)**



^{19}F NMR:**(Table 3, entry 11)**



JEOL

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Experiment        = single_pulse.ex2
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Revision_time     = 30-APR-2009 12:40:29
Current_time      = 30-APR-2009 12:40:34

Comment           = single_pulse
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Dim_size          = 13107
Dim_title         = 19F
Dim_units         = [ppm]
Dimensions        = X
Site              = ECX 300
Spectrometer      = JNM-ECX300A

Field_strength    = 7.0586013[T] (300[MHz
X_acq_duration    = 0.77070336[s]
X_domain          = 19F
X_freq            = 282.78036857[MHz]
X_offset          = -190[ppm]
X_points          = 16384
X_prescans        = 1
X_resolution      = 1.29751608[Hz]
X_sweep           = 21.2585034[kHz]
Irr_domain        = 19F
Irr_freq          = 282.78036857[MHz]
Irr_offset        = 5[ppm]
Tri_domain        = 19F
Tri_freq          = 282.78036857[MHz]
Tri_offset        = 5[ppm]
Clipped           = FALSE
Mod_return        = 1
Scans             = 22
Total_scans       = 22

X_90_width        = 10.2[us]
X_acq_time        = 0.77070336[s]
X_angle           = 45[deg]
X_atn             = 3[dB]
X_pulse           = 5.1[us]
Irr_mode          = Off
Tri_mode          = Off
Dante_presat      = FALSE
Initial_wait      = 1[s]
Recvr_gain        = 42
Relaxation_delay  = 5[s]
Repetition_time   = 5.77070336[s]
Temp_get          = 19.3[dC]
```

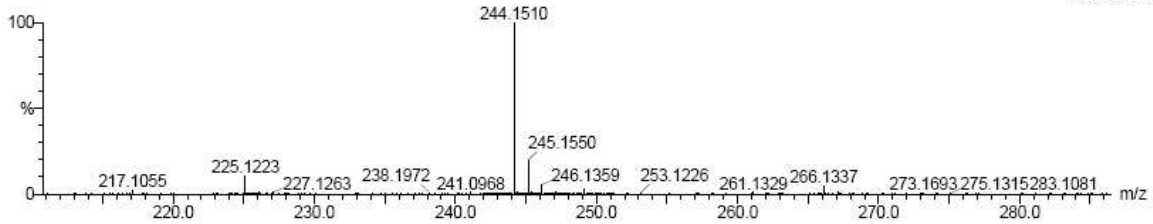
N-benzyl-2-fluoro-1-phenylpropan-1-amine (Table 3, Entry 12)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 3.0 mDa / DBE: min = -100.0, max = 400.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

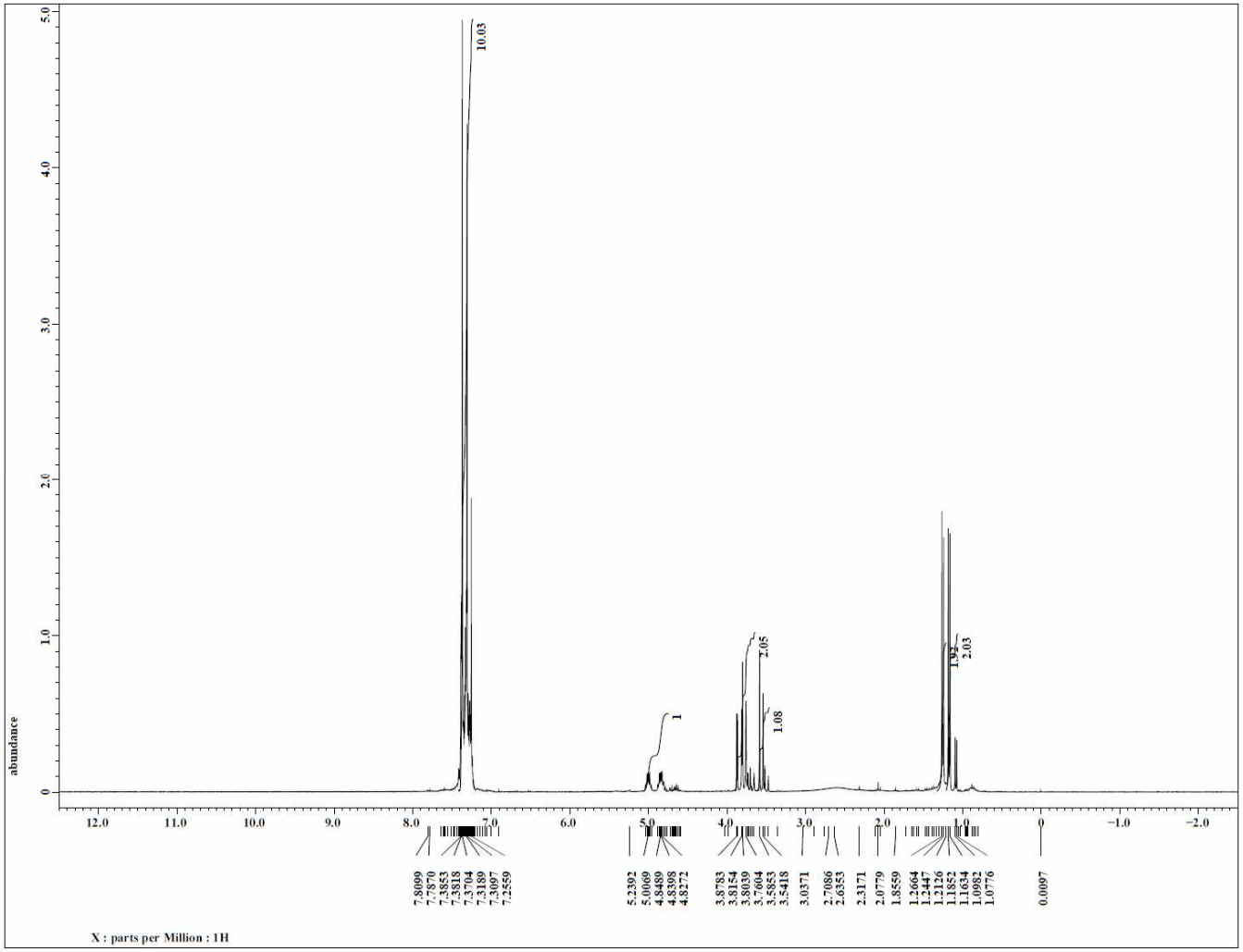
Monoisotopic Mass, Even Electron Ions
437 formula(e) evaluated with 2 results within limits (up to 12 best isotopic matches for each mass)
Elements Used:
C: 5-100 H: 1-125 N: 0-50 O: 0-50 F: 1-1

Benyl-(2-F-1-Ph-propyl)-amine KE319
LCT XE
10TD0302_LCT_2 44 (0.813) AM (Cen,4, 80.00, Ar,6500.0,556.28,0.70,LS 3); Sm (SG, 2x3.00); Sb (3,40.00); Cm (44:101) 1: TOF MS ES+
4.82e+004

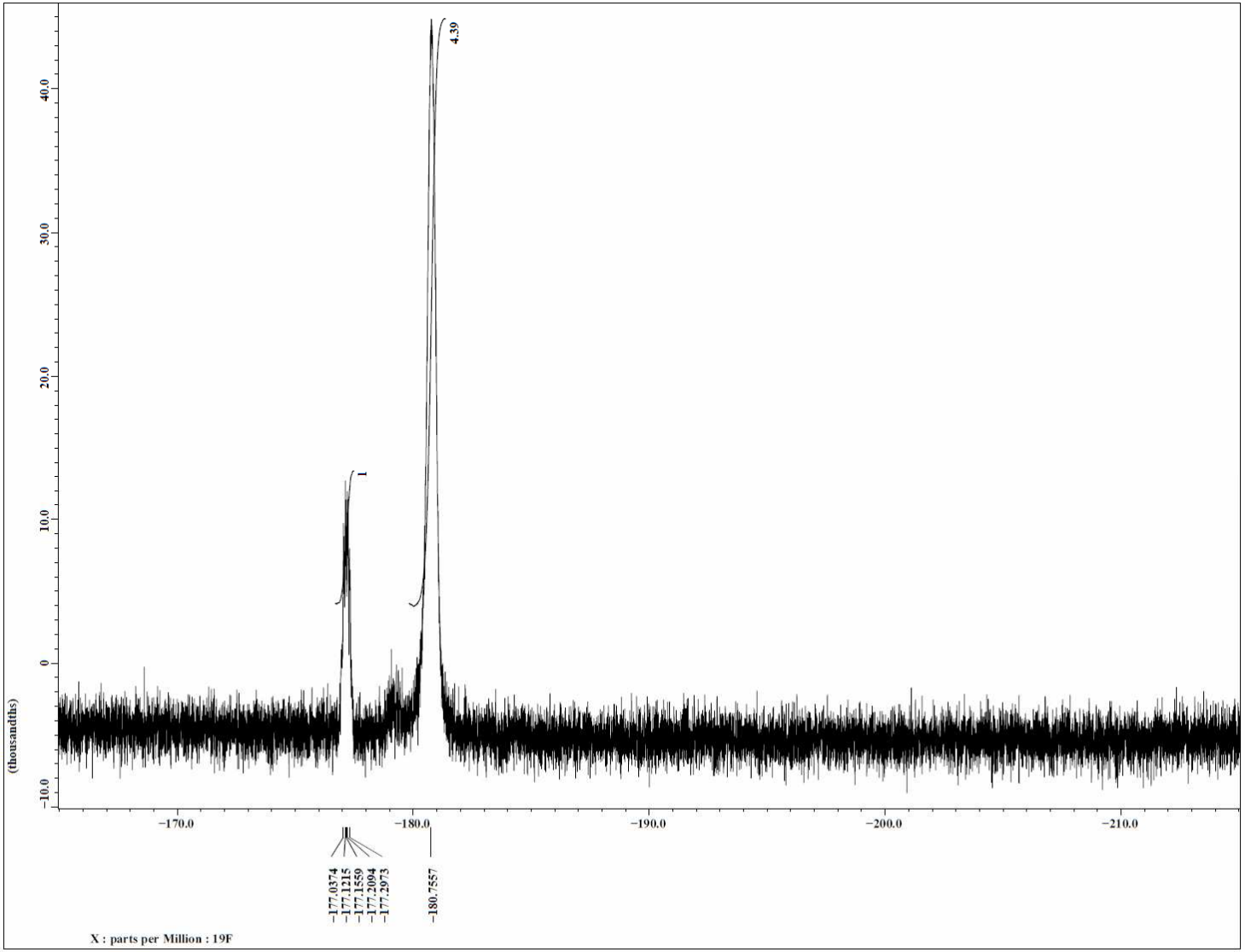
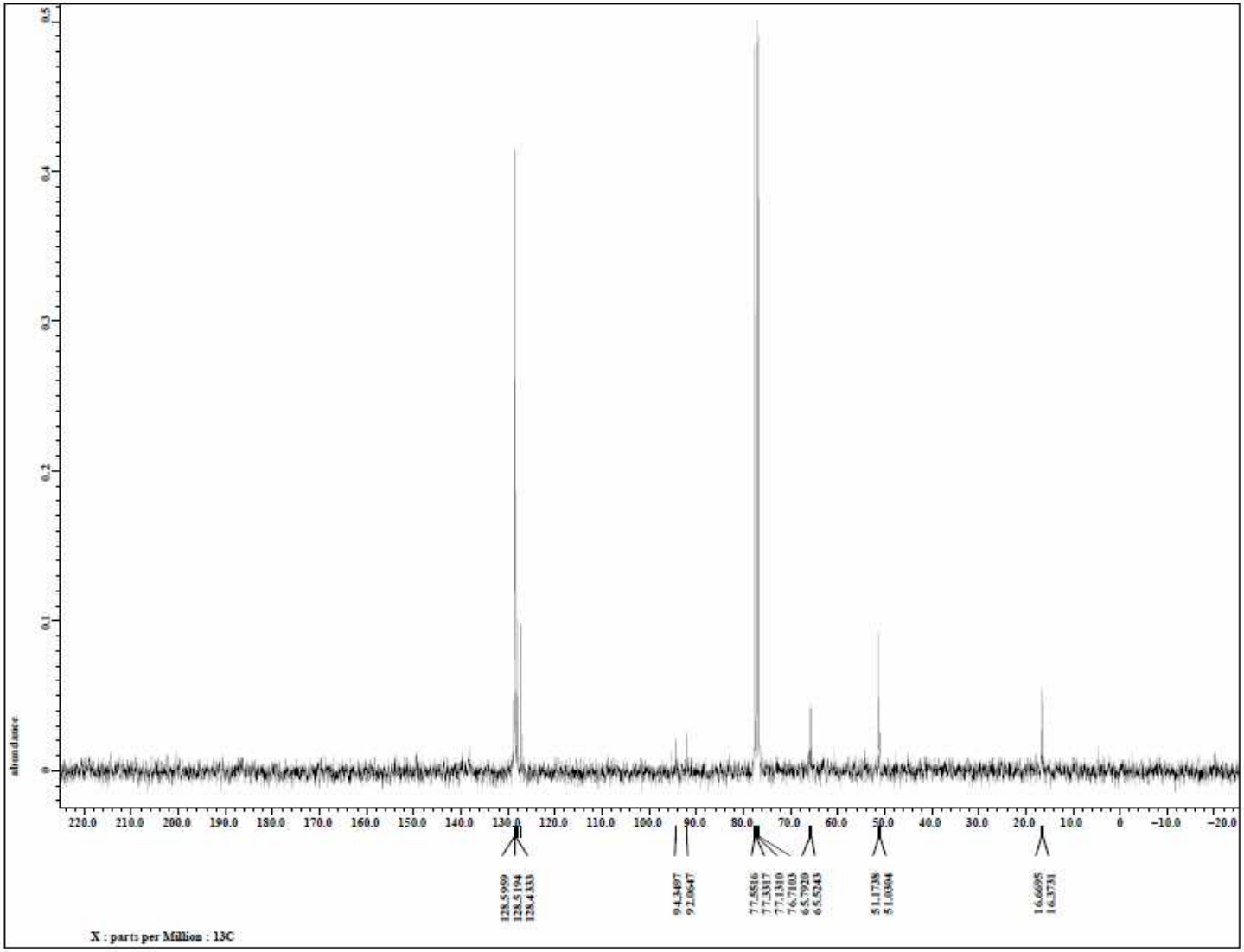


Minimum:				-100.0			
Maximum:		3.0	5.0	400.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
244.1510	244.1502	0.8	3.3	7.5	305.8	0.1	C16 H19 N F
	244.1533	-2.3	-9.4	-0.5	308.1	2.4	C5 H19 N7 O3 F

^{1}H NMR: **(Table 3, Entry 12)**



^{19}F NMR: **(Table 3, Entry 12)**



^{13}C NMR: **(Table 3, Entry 12)**