Supplementary Information (SI) for Organic & Biomolecular Chemistry.

Electrophilic Fluorination of Cannabinol (CBN)

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General information:

Unless otherwise noted, all chemicals/reagents and solvents (ACS grade) were purchased from commercial supplier-Sigma Aldrich/Merck and Thermo Fisher Scientific and used without purification. All reactions were performed in a round bottom flask and monitored through thin layer chromatography (TLC silica gel F_{254}), and analyzed using 254 nm UV light and iodine, ninhydrin stains. ^1H NMR, ^{19}F NMR and ^{13}C NMR spectra were recorded with a 300 MHz Bruker Avance NMR spectrometer (^1H = 300; ^{19}F = 282.5 and ^{13}C = 75 MHz). Chemical shift values of ^1H NMR were recorded in parts per million (ppm, δ) relative to tetramethylsilane (TMS, 0.00 ppm) and trichlorofluoromethane ($CFCl_3$, 0.00ppm) in the case of ^{19}F NMR. Multiplicities are indicated as s(singlet), d(doublet), t(triplet), q(quartet), m(multiplet), coupling constants (*J*) were reported in Hertz (Hz) and integration values. Chemical shift values of ^{13}C NMR were recorded in parts per million (ppm, δ) and calibrated to the residual peak as an internal standard ($CDCl_3$: $\delta = 77.0$ ppm and DMSO: $\delta = 39.0$ ppm). UV_{254}- silica gel GF (1500 micron) prepTLC glass plates were used for prepTLC separations. Mass spectra were obtained using the $APCI^+$ method on Advion Expression/Plate Express TLC-mass spectrometer. FTIR spectra were observed on FTIR spectrometer (Thermo Scientific iD7- ATR / Nicolet iS5).

Fluorescence emission spectras were recorded using perkin elmer Enspire 2300 multi-mode microplate luminescence spectrofluorometer, on fluorescence multiwell microplates manufactured from virgin polystyrene (PS) or polypropylene (PP) resin. The emission wavelength (λem) range was 250−550 nm, at the excitation wavelength (λex) of 230 nm and increments of 5 nm were considered for EX and EM sampling intervals.

General procedure for the synthesis of fluorinated cannabinol derivatives (**3a**-**3g**) with FTEDA

To a round bottom flask, were added Selectfluor^{TM} or 1-(Chloromethyl)-4-fluoro-1,4-diazabicyclo[2.2.2]octane bis(tetrafluoroborate) (FTEDA, 1.1 mmol, 2.2 equiv.) in 10ml dry acetonitrile and stirred for 2 minutes to completely dissolve the Selectfluor^{TM} (FTEDA). Cannabinol (CBN, 0.5 mmol, 1.0 equiv.) solution in acetonitrile was added to the flask and continued stirring for 2 hours at room temperature resulting in 94% of the crude yield with the 100% total conversion. After the TLC indicated the total consumption of starting material, the reaction mixture was extracted with ethyl acetate (3X). The combined organic layers were washed with saturated $NaHCO_3$ and dried over Na_2SO_4, followed by concentration under reduced pressure. The resulting residue was purified by flash column chromatography (silica gel, hexane/Et_2O) to give the desired products.

The same reaction was performed on a larger scale of 16.1 mmol (5g) of CBN. A crude yield of 90% was obtained. For larger scale reactions, the overall reaction procedure is as follows: In a 250 ml round bottom flask, FTEDA (12.55 g, 35.4 mmol, 2.2 equiv.) was dissolved in 90 ml of dry acetonitrile. If required, the solution was warmed slightly to dissolve FTEDA completely and cooled to ambient temperature accordingly. CBN (5g, 16.1 mmol, 1.0 equiv.) solution in 10ml dry acetonitrile was added in 2ml portions over a minute, to a round bottom flask containing the FTEDA solution at room temperature and stirring for continued 2hrs at the same temperature. After the completion of the reaction, as monitored by TLC, the reaction mixture was extracted with ethyl acetate three times and washed with a saturated solution of $NaHCO_3$ (60-80ml). The combined organic layers were then dried with Na_2SO_4, filtered and concentrated in vacuo to give the crude product of 90% yield. (Note: the percentage yield has been calculated by taking the monofluorinated product as a sole product for the theoretical yield.) The ^{19}F-NMR yield for FTEDA reaction mixture is as follows: **3a** (spot-1, 4%), **3b** (spot-2, 9%), **3c** (spot-3, 26%), and **3d** (spot-4, 34%) and **3e** +**3f** (spot-5, 9%), **3g** (spot-6, 17%).

Isolation method:

The isolation process proceeded on the large-scale reaction mixture. Using a 3.5cm X 8cm wide TLC plate (silica gel 60 F_{254}) in a 5% diethyl ether: hexane solvent system, the reaction mixture showed a total of six spots on the TLC plates. Spots have the following R_f values (starting from top to bottom): spot-1 (**3a**, 0.68), spot-2 (**3b**, yellow, 0.61), spot-3 (**3c**, 0.55), spot-4 (**3d**, dark yellow, 0.46), spot-5 (**3e** +**3f**, 0.40), and spot-6 (**3g**, 0.34). Purification by flash-silica gel (230-450 mesh size) column chromatography using a 0.2- 1.5 % diethyl ether: hexanes solvent system gave spot 3 (20%) and spot 4 (30%) as a pale yellow solid and yellow oil respectively. Along with these, a mixture of spots 1, 2, 5, and 6 (2.12 g) was obtained.

For the separation of the mixture via preparative thin layer chromatography (prepTLC), the mixture was dissolved in methylene chloride and this solution was streaked out horizontally on 20X 20cm UV_{254}- silica gel GF (1500 micron) prepTLC glass plates using a capillary tube. After loading the solution of 100-125mg mixture on each TLC plate, the plates were developed in a 5% diethyl ether: hexane solvent system, resulting in bands on the TLC plates. These bands were carefully scraped off from the TLC plates with the help of a spatula and collected in separate beakers. The silica was added to methylene chloride and filtered through Whatman® 2 qualitative (12.5 diameter) filter paper. The filtrates were concentrated over vacuo to give pure products for spots 1, 2, 5, and 6. Characterization (^{1}H NMR, ^{19}F NMR and ^{13}C NMR and Mass spectral data) on all pure spots was done to confirm the structures. (Note: the percentage yield has been calculated by taking the monofluorinated product as the sole product for the theoretical yield.)

General procedure for the synthesis of fluorinated cannabinol derivatives (**3a**-**3g**) with NFSI

To a round bottom flask, were added *N*-Fluorobenzenesulfonimide (NFSI, 1.1 mmol, 2.2 equiv.) in 10ml dry acetonitrile and stirred for 2 minutes to completely dissolve the NFSI. Cannabinol (CBN, 0.5 mmol, 1.0 equiv.) was added to the flask and continued stirring for 3 hours at 80ºC resulting in 95% of the crude yield with the 100% total conversion. After the TLC indicated the total consumption of starting material, the reaction mixture was cooled down to ambient temperature. (Note: the percentage yield has been calculated by taking monofluorinated product as a sole product for the theoretical yield).The reaction mixture was extracted with ethyl acetate (3X). The combined organic layers were washed with saturated $NaHCO_3$ and dried over Na_2SO_4, followed by concentration under reduced pressure. ^{19}F-NMR data on NFSI-reaction mixture was compared with the ^{19}F-NMR data of FTEDA reaction mixture and the peaks were closely matching (see page S44). The ^{19}F-NMR yield are as follows: **3a** (spot-1, 4%), **3b** (spot-2, 7%), **3c** (spot-3, 18%), and **3d** (spot-4, 27%), **3e** +**3f** (spot-5, 11%), **3g** (spot-6, 7%). Further, the

TLC of the reaction mixture was analyzed under Advion Plate express TLC Plate reader for the masses of each spot. The Advion Plate Express TLC Plate Reader revealed that the masses of those six NFSI reaction spots were exactly matched to the masses of **3a**–**3g** products.

Characterizations:

2,4,4-trifluoro-6,6,9-trimethyl-3-pentyl-4,6-dihydro-1H-benzo[c]chromen-1-one (**3a** or spot 1, yield = 4%).

^{1}H NMR (CDCl$_3$, 300 MHz): δ = 8.26 (s, 1H), 7.15 (d, *J* = 8.1 Hz, 1H), 7.05 (d, *J* = 7.8 Hz, 1H), 2.47 (t, *J* = 7.8 Hz, 2H), 2.37 (s, 3H), 1.71 (s, 6H), 1.69-1.61 (m, 2H), 1.40-1.35 (m, 4H), 0.93-0.89 (m, 3H) ppm.

^{1}H NMR (CDCl$_3$ +D$_2$O, 300 MHz): δ = 8.26 (s, 1H), 7.17 -7.14 (m, 1H), 7.06-7.03 (m, 1H), 2.47 (t, *J* = 7.8 Hz, 2H), 2.37 (s, 3H), 1.71-1.63 (m, 8H), 1.40-1.36 (m, 4H), 0.93-0.89 (m, 3 H) ppm.

^{19}F-NMR (CDCl$_3$, 282.5 MHz): δ -107.10 (d, *J* = 11.3 Hz), -128.13 (t, *J* = 11.2 Hz,) ppm in 2:1 ratio.

^{13}C-NMR: (CDCl$_3$, 75 MHz) δ = 175.64 (td, *J* = 24.9, 3.75Hz, 1C), 157.48-156.84 (m, 1C), 151.09 (td, *J* = 264.75, 11.25 Hz, 1C), 137.95, 133.25, 129.97, 126.39, 123.30 (d, *J* = 2.25 Hz, 1C), 122.52, 112.60 (dd, *J* = 235.12, 15.75 Hz, 1C), 109.84 (d, *J* = 3.75 Hz, 1C), 83.08, 31.76, 27.79 (d, *J* = 2.25 Hz, 1C), 27.61, 22.71, 22.27, 21.37, 13.90 ppm.

ADVION- Unit resolution (APCI$^+$) calcd. for $C_{21}H_{24}F_3O_2$ $[M + H]^+$: 365.1728; observed : 365.3.

FT-IR (neat) ν$_{max}$: 2962, 2926, 2873, 1672, 1625, 1323, 1256, 1155, 1143, 1113, 1036, 946, 819, 738 cm^{-1}.

2,2,4-trifluoro-6,6,9-trimethyl-3-pentyl-2,6-dihydro-1H-benzo[c]chromen-1-one (**3b** or spot 2, yield = 9%).

^{1}H NMR (CDCl$_3$, 300 MHz): δ = 8.25 (s, 1H), 7.13- 7.10 (m, 1H), 7.02 (d, *J* = 7.8 Hz, 1H), 2.48-2.43 (m, 2H), 2.35 (s, 3H), 1.72 (s, 6H), 1.68-1.58 (m, 2H), 1.39-1.33 (m, 4H), 0.93-0.88 (m, 3H) ppm.

^{1}H NMR (CDCl$_3$ +D$_2$O, 300 MHz): δ = 8.25 (s, 1H), 7.13 -7.10 (m, 1H), 7.03-7.01 (m, 1H), 2.45 (t, *J* = 7.8 Hz, 2H), 2.36 (s, 3H), 1.72 (s, 6H), 1.66-1.60 (m, 2H), 1.39-1.34 (m, 4H), 0.93-0.88 (m, 3 H) ppm.

^{19}F-NMR (CDCl$_3$, 282.5 MHz): -103.73 (d, *J* = 14.1 Hz), -129.22 (tt, *J* = 14.1, 2.8 Hz) ppm in 2:1 ratio.

^{13}C-NMR (CDCl$_3$, 75 MHz): δ = 183.21 (dt, *J* = 24.75, 1.5Hz, 1C), 157.26 (td, *J* = 24, 3.75 Hz, 1C), 150.34 (td, *J* = 261.75, 12.75 Hz, 1C), 138.14, 131.91, 129.46, 125.63, 123.62 (d, *J* = 3 Hz, 1C), 122.45, 106.38 (dd, *J* = 481.12, 15 Hz, 1C), 106.56-106.46 (m, 1C), 106.28, 83.96, 31.71, 28.26, 27.99 (d, *J* = 2.25 Hz, 1C), 23.38, 22.29, 21.37, 13.93 ppm.

ADVION- Unit resolution (APCI$^+$) calcd. for $C_{21}H_{24}F_3O_2$ $[M + H]^+$: 365.1728; observed : 365.3.

FT-IR (neat) ν$_{max}$: 2960, 2930, 2875, 1680, 1589, 1394, 1386, 1366, 1293, 1141, 1121, 1036, 938, 817, 786, 738 cm^{-1}.

4,4-difluoro-6,6,9-trimethyl-3-pentyl-4,6-dihydro-1H-benzo[c]chromen-1-one (**3c** or spot 3, yield = 20%).

^{1}H NMR ($CDCl_3$, 300 MHz): **δ** = 8.25 (s, 1H), 7.14 -7.12 (m, 1H), 7.06-7.03 (m, 1H), 6.11 (t, *J* = 1.5 Hz, 1H), 2.44 (t, *J* = 7.8 Hz, 2H), 2.36 (s, 3H), 1.71 (s, 6H), 1.65-1.60 (m, 2H), 1.41-1.36 (m, 4H), 0.94-0.90 (m, 3 H) ppm.

^{1}H NMR ($CDCl_3$ +D_2O, 300 MHz): **δ** = 8.24 (s, 1H), 7.15 -7.12 (m, 1H), 7.06-7.03 (m, 1H), 6.11 (t, *J* = 1.5 Hz, 1H), 2.44 (t, *J* = 7.8 Hz, 2H), 2.36 (s, 3H), 1.70 (s, 6H), 1.65-1.60 (m, 2H), 1.41-1.36 (m, 4H), 0.94-0.92 (m, 3 H) ppm.

^{19}F-NMR ($CDCl_3$, 282.5 MHz): **δ** = -110.24 (s) ppm.

^{13}C-NMR ($CDCl_3$, 75 MHz): **δ** = 183.29 (t, *J* = 3 Hz, 1C), 156.63 (t, *J* = 22.5 Hz, 1C), 147.36 (t, *J* = 24 Hz, 1C), 137.69, 133.58, 129.62, 128.66 (t, *J* = 6.75 Hz, 1C), 126.62, 123.98, 122.43, 112.05, 111.60 (t, *J* = 3.75 Hz, 1C), 108.92, 105.80, 82.20, 31.35, 22.47, 22.29, 26.36, 22.40, 21.38, 13.95 ppm.

ADVION- Unit resolution (APCI$^+$) calcd for $C_{21}H_{24}F_2O_2$ $[M + H]^+$: 346.1744; observed : 347.3.

FT-IR (neat) *v$_{max}$* : 2960, 2932, 2867, 1678, 1647, 1623, 1368, 1319, 1289, 1179, 1147, 1080, 1036, 934, 817, 738 cm^{-1}.

2,2-difluoro-6,6,9-trimethyl-3-pentyl-2,6-dihydro-1H-benzo[c]chromen-1-one (**3d** or spot 4, yield = 30%).

^{1}H NMR ($CDCl_3$, 300 MHz): **δ** = 8.30 (s, 1H), 7.09 -7.06 (m, 1H), 7.01-6.99 (m, 1H), 6.097-6.093 (m, 1H), 2.46-2.41 (m, 2H), 2.35 (s, 3H), 1.67 (s, 6H), 1.64-1.59 (m, 2H), 1.40-1.36 (m, 4H), 0.94-0.90 (m, 3 H) ppm.

^{1}H NMR ($CDCl_3$+D_2O, 300 MHz) δ = 8.30 (s, 1H), 7.09 -7.06 (m, 1H), 7.01-6.99 (m, 1H), 6.098 (s, 1H), 2.46-2.41 (m, 2H), 2.35 (s, 3H), 1.67 (s, 6H), 1.64-1.59 (m, 2H), 1.40-1.36 (m, 4H), 0.94-0.92 (m, 3 H) ppm.

^{19}F-NMR ($CDCl_3$, 282.5 MHz): **δ** = -108.57 (s) ppm.

^{13}C-NMR ($CDCl_3$, 75 MHz): **δ** = 184.39 (t, *J* = 24 Hz, 1C), 164.18 (t, *J* = 2.25 Hz, 1C), 147.48 (t, *J* = 24 Hz, 1C), 137.85, 131.85, 128.70, 125.35, 124. 32, 123.58 (t, *J* = 7.5 Hz, 1C), 122.33, 107.46, 105.52 (t, *J* = 2.25 Hz, 1C), 104.24, 101.03, 82.76, 31.38, 29.72, 28.61, 28.35, 26.49, 22.41, 21.38, 13.95 ppm.

ADVION- Unit resolution (APCI$^+$) calcd for $C_{21}H_{24}F_2O_2$ $[M + H]^+$: 346.1744; observed : 347.3.

FT-IR (neat) *v$_{max}$* : 2960, 2932, 2867, 1674, 1585, 1566, 1402, 1190, 1141, 1044, 940, 813, 736 cm^{-1}.

2-fluoro-6,6,9-trimethyl-3-pentyl-6H-benzo[c]chromen-1-ol and *4-fluoro-6,6,9-trimethyl-3-pentyl-6H-benzo[c]chromen-1-ol* (**3e+3f** for spot 5, yield = 10%).

^{1}H NMR ($CDCl_3$, 300 MHz) δ = 8.24 (s, 1H), 7.15 -7.07 (m, 2H), 6.35 (d, *J* = 6.6 Hz, 1H), 5.59 (d, *J* = 7.8 Hz, 1H), 2.59 (t, *J* = 7.5 Hz, 2H), 2.39 (s, 3H), 1.64-1.61 (m, 2H), 1.58 (s, 6H), 1.35-1.31 (m, 4H), 0.91-0.87 (m, 3H) ppm.

^{1}H NMR ($CDCl_3$ +D_2O, 300 MHz) δ = 8.24 (s, 1H), 7.15 -7.07 (m, 2H), 6.35 (d, *J* = 6.6 Hz, 1H), 2.60 (t, *J* = 7.2 Hz, 2H), 2.39 (s, 3H), 1.64-1.61 (m, 2H), 1.58 (s, 6H), 1.35-1.33 (m, 4H), 0.91-0.87 (m, 3H) ppm.

^{19}F-NMR ($CDCl_3$, 282.5 MHz): -156.05 and 156.08 (two overlapping doublets appearing as a triplet, *J* = 7.05 and 7.33 Hz) ppm.

^{13}C-NMR ($CDCl_3$, 75 MHz): δ = 149.24 (d, *J* = 2.2 Hz, 1C), 145.10 (d, *J* = 222.7 Hz, 1C), 141.0 (d, *J* = 17.25 Hz, 1C), 136.88, 136.70, 129.28 (d, *J* = 15.75 Hz, 1C), 128.14, 127.18 (d, *J* = 2.2 Hz, 1C), 126.97, 122.48, 109.75, 109.63 (d, *J* = 3.75 Hz, 1C), 77.36, 31.45, 29.41, 28.78 (d, *J* = 1.5 Hz, 1C), 27.12, 22.48, 21.50, 14.01 ppm.

ADVION- Unit resolution (APCI$^+$) calcd. for $C_{21}H_{25}FO_2$ $[M + H]^+$: 329.1917; observed : 329.1.

FT-IR (neat) ν_{max}: 3568, 2954, 2928, 2861, 1635, 1589, 1502, 1447, 1404, 1362, 1283, 1194, 1155, 1054, 946, 815, 738 cm^{-1}.

2,4-difluoro-6,6,9-trimethyl-3-pentyl-6H-benzo[c]chromen-1-ol (**3g** or spot 6, yield = 20%).

^{1}H NMR ($CDCl_3$, 300 MHz): δ = 8.25 (s, 1H), 7.17 -7.10 (m, 2H), 5.38 (d, *J* = 7.2 Hz, 1H), 2.69 (t, *J* = 7.5 Hz, 2H), 2.39 (s, 3H), 1.63 (s, 6H), 1.59-1.58 (m, 2H), 1.36-1.34 (m, 4H), 0.91-0.87 (m, 3H) ppm.

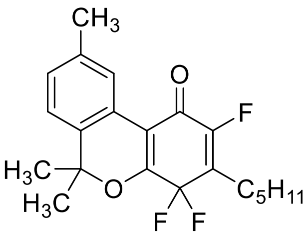
^{1}H NMR ($CDCl_3$ +D_2O, 300 MHz) δ = 8.25 (s, 1H), 7.16 -7.10 (m, 2H), 2.69 (t, *J* = 7.2 Hz, 2H), 2.39 (s, 3H), 1.63 (s, 6H), 1.59-1.58 (m, 2H), 1.36-1.34 (m, 4H), 0.91-0.87 (m, 3H) ppm.

^{19}F-NMR ($CDCl_3$, 282.5 MHz): -150.24 (s), -154.15 (d, *J* = 8.46 Hz) ppm in 1:1 ratio.

^{13}C-NMR ($CDCl_3$, 75 MHz): δ = 144.37 (dd, *J* = 235.5, 9Hz, 1C), 143.72 (dd, *J* = 224.3, 8.25 Hz, 1C), 137.40 (dd, *J* = 12.75, 3Hz, 1C), 137.08, 136.79, 136.75 (dd, *J* = 18, 3.75 Hz, 1C), 128.68, 127.26, 126.54 (t, *J* = 3.75 Hz, 1C), 122.61, 117.84 (t, *J* = 20.25 Hz, 1C), 110.60, 78.11, 31.42, 29.15, 27.04, 22.85, 22.40, 21.48, 13.99 ppm.

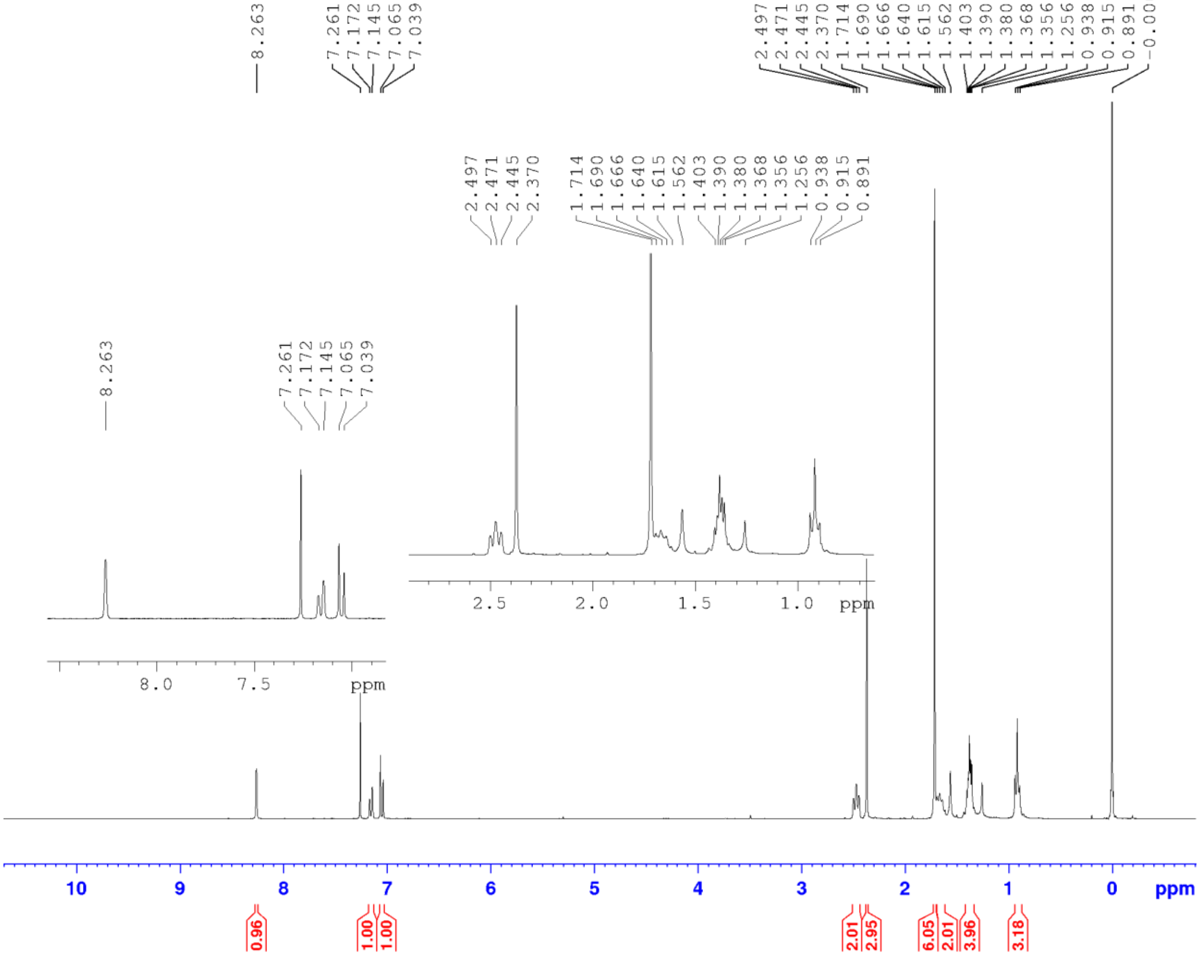
ADVION- Unit resolution (APCI$^+$) calcd. for $C_{21}H_{22}F_2O_2$ $[M + H]^+$: 347.1823; observed : 347.1.

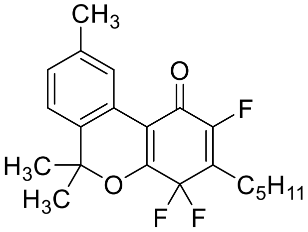
FT-IR (neat) ν_{max}: 3554, 2960, 2930, 2863, 1510, 1461, 1408, 1386, 1273, 1149, 1111, 993, 944, 815, 744 cm^{-1}.



^{1}H-NMR

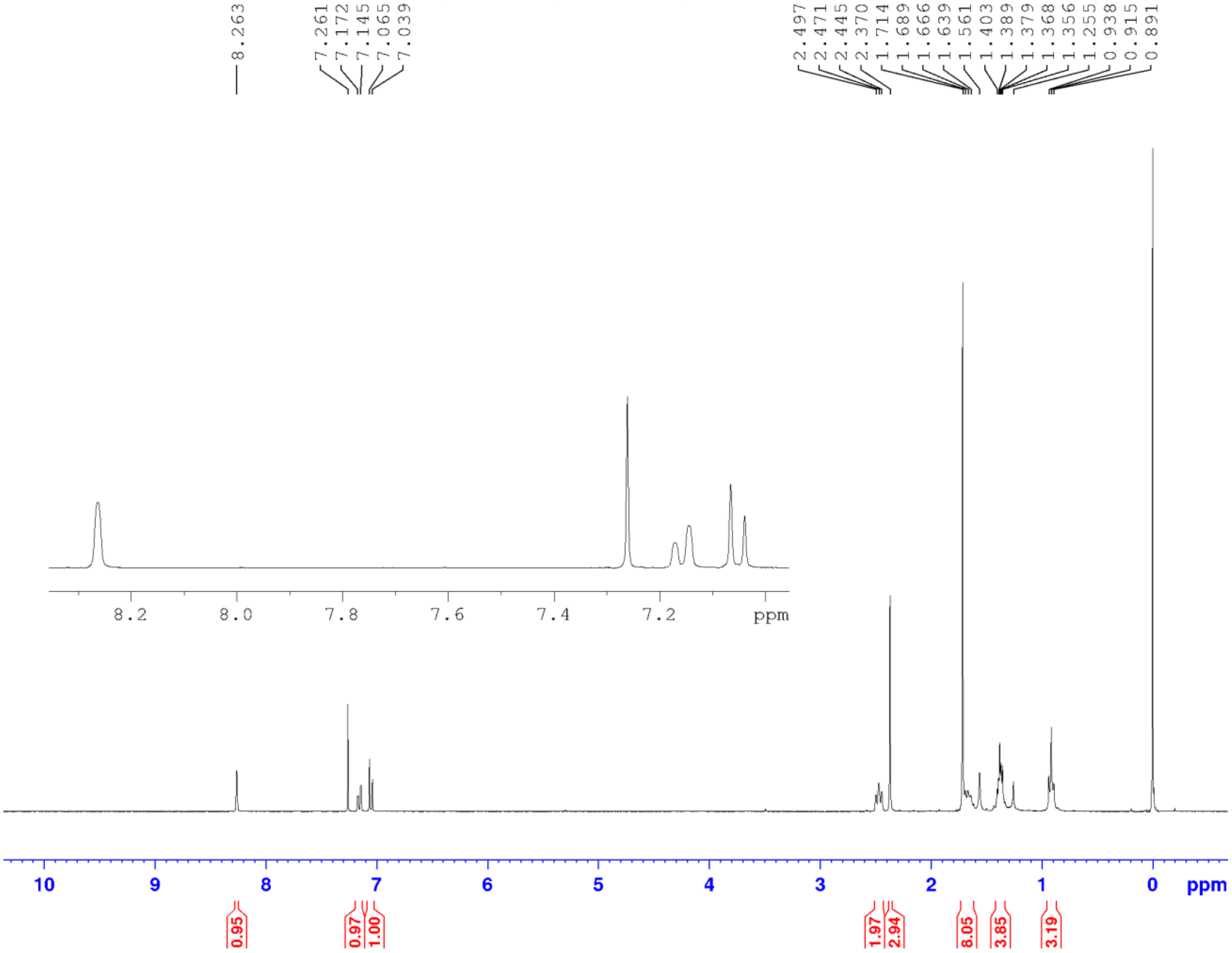
2,4,4-trifluoro-6,6,9-trimethyl-3-pentyl-4,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3a**

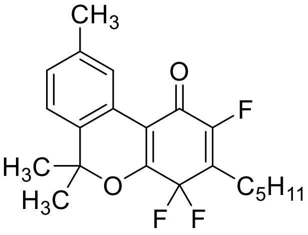




^{1}H-NMR- D_2O exchange

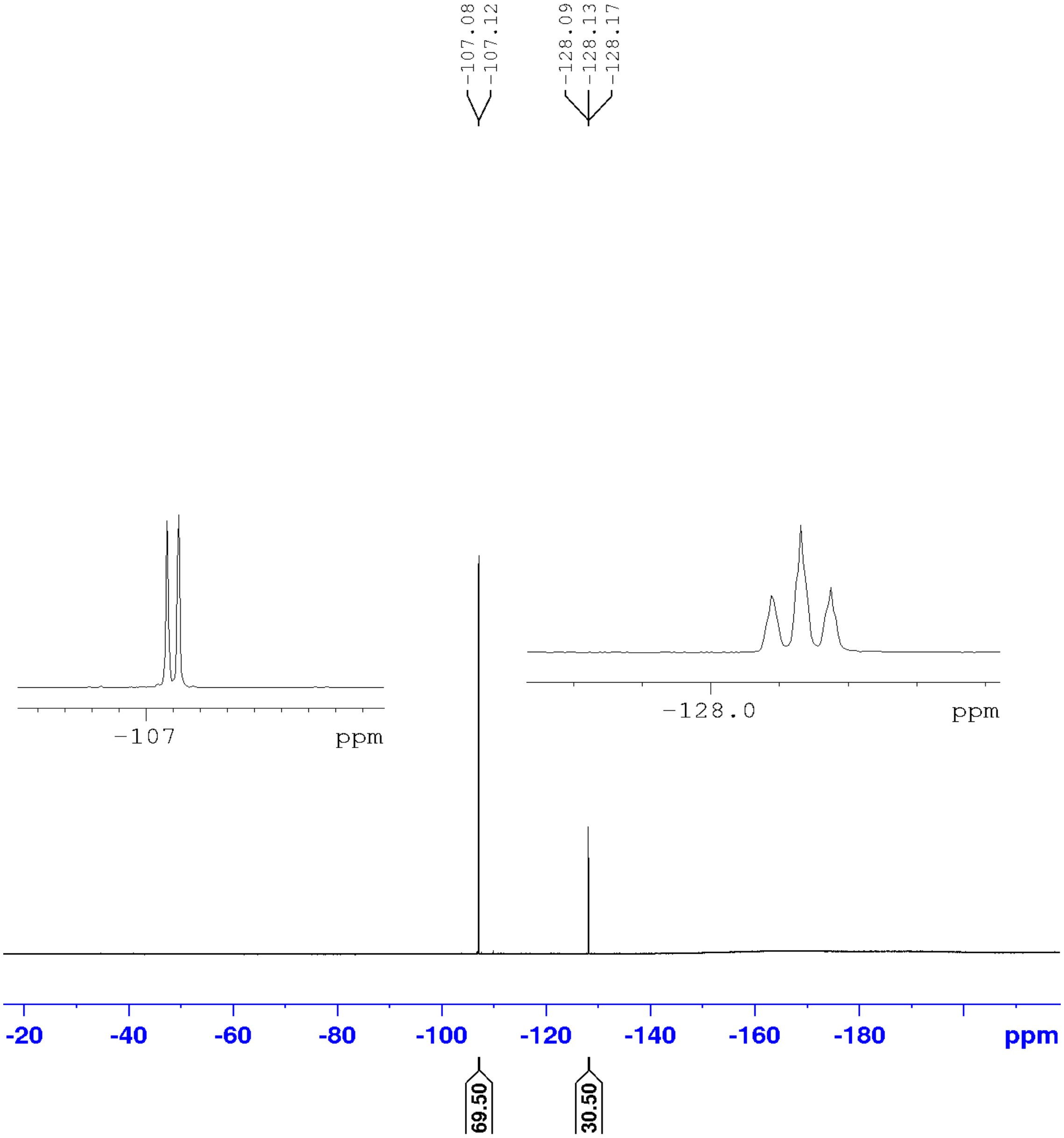
2,4,4-trifluoro-6,6,9-trimethyl-3-pentyl-4,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3a**

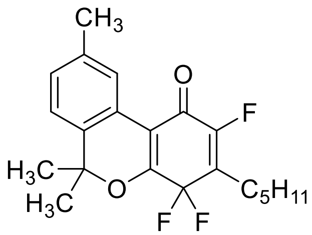




^{19}F-NMR

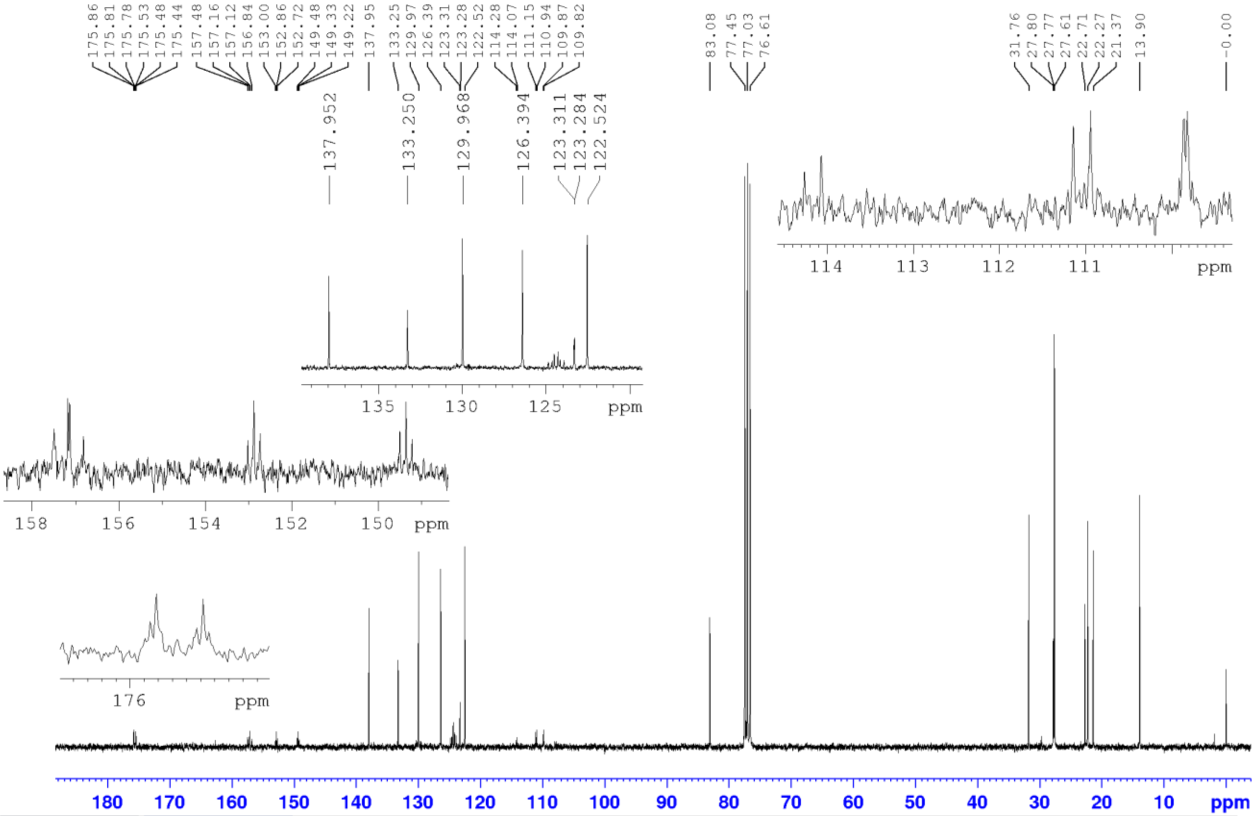
2,4,4-trifluoro-6,6,9-trimethyl-3-pentyl-4,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3a**

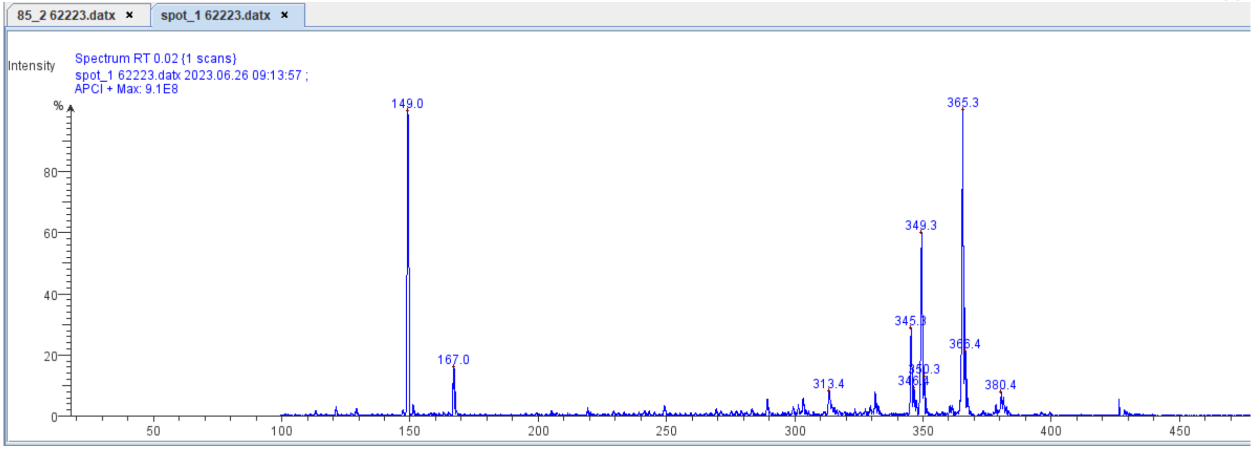


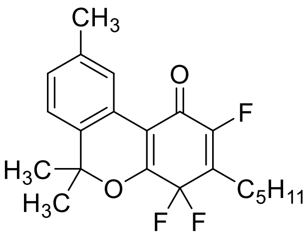


^{13}C-NMR and Mass spectrum

2,4,4-trifluoro-6,6,9-trimethyl-3-pentyl-4,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3a**

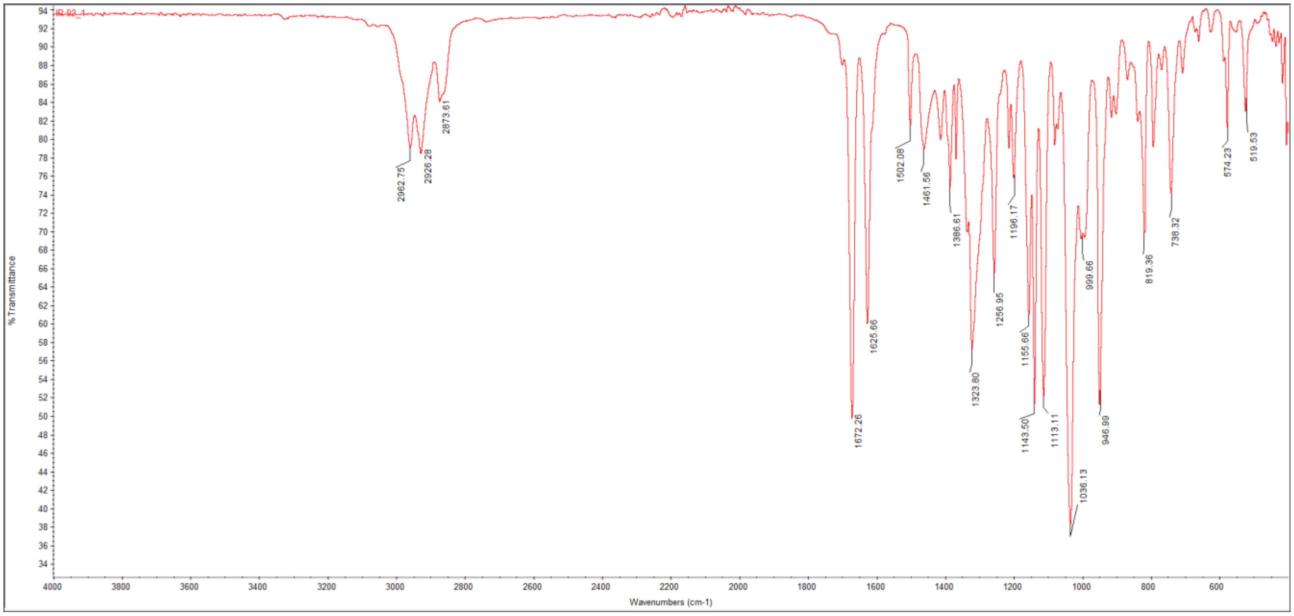


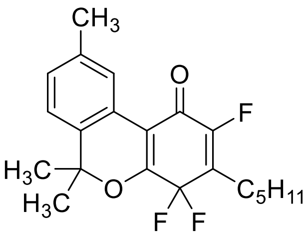




IR data

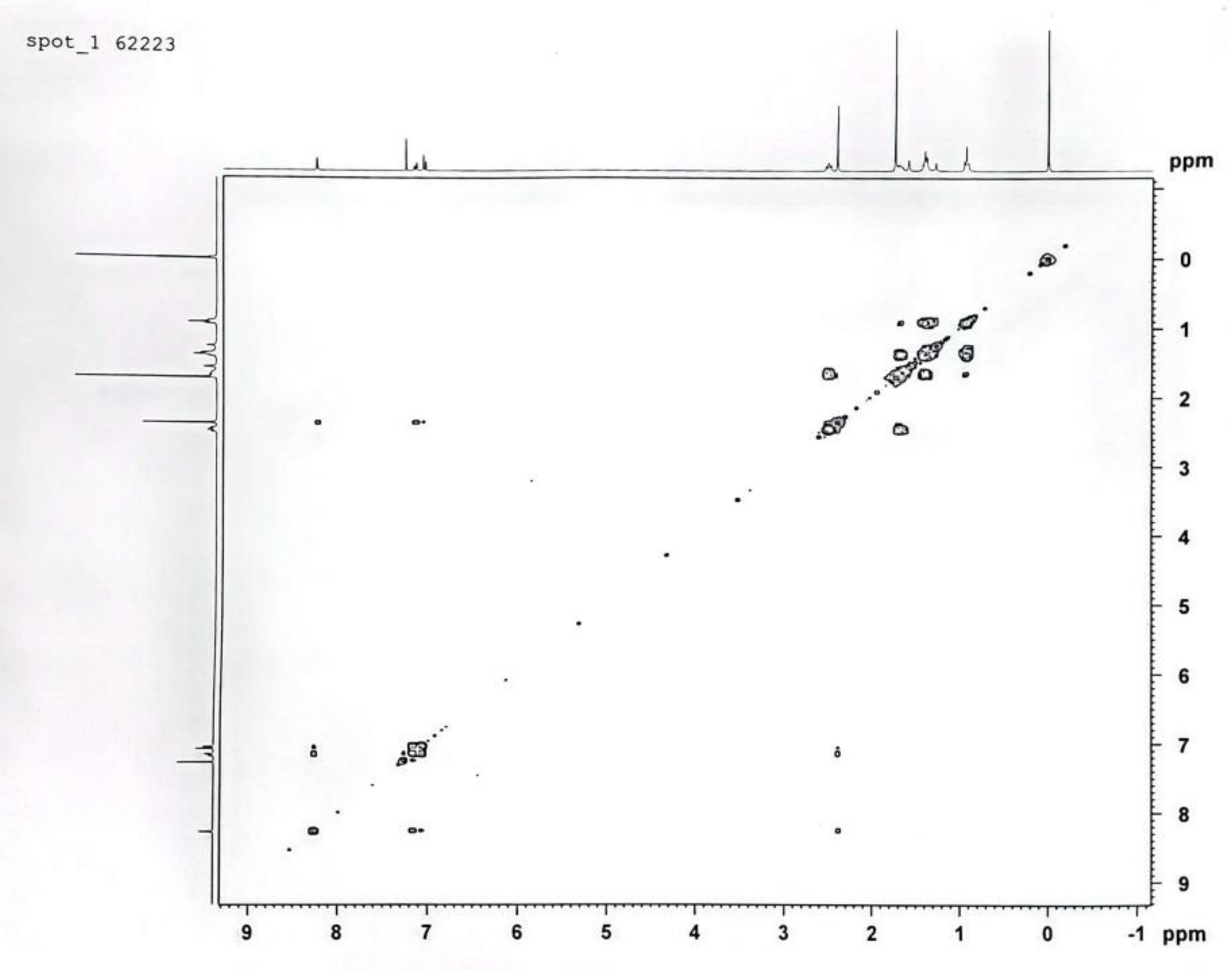
2,4,4-trifluoro-6,6,9-trimethyl-3-pentyl-4,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3a**

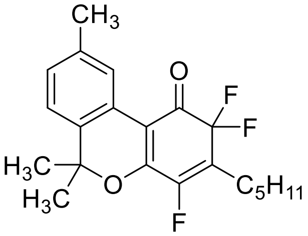




2D-NMR

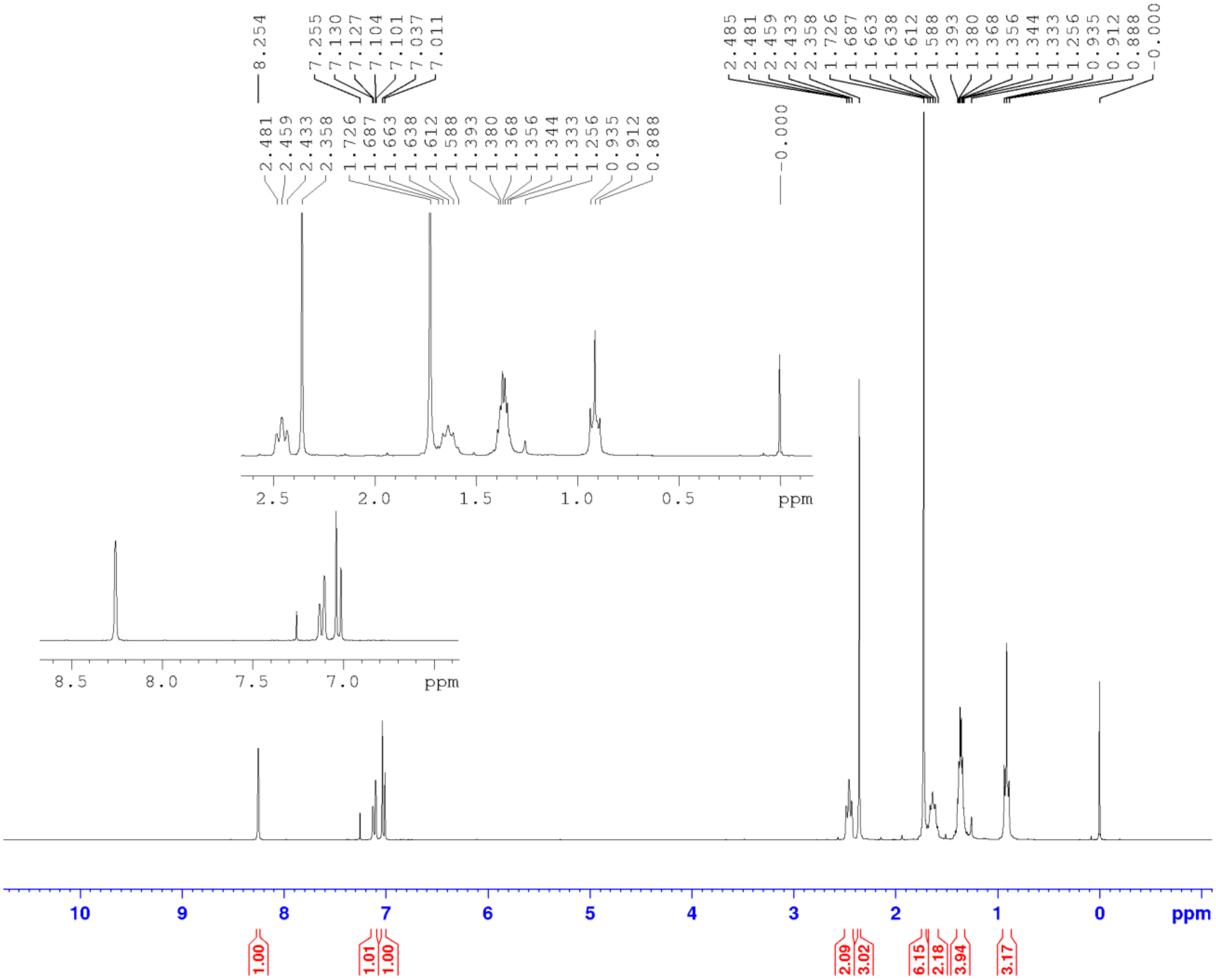
2,4,4-trifluoro-6,6,9-trimethyl-3-pentyl-4,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3a**

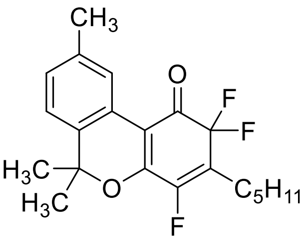




^{1}H-NMR

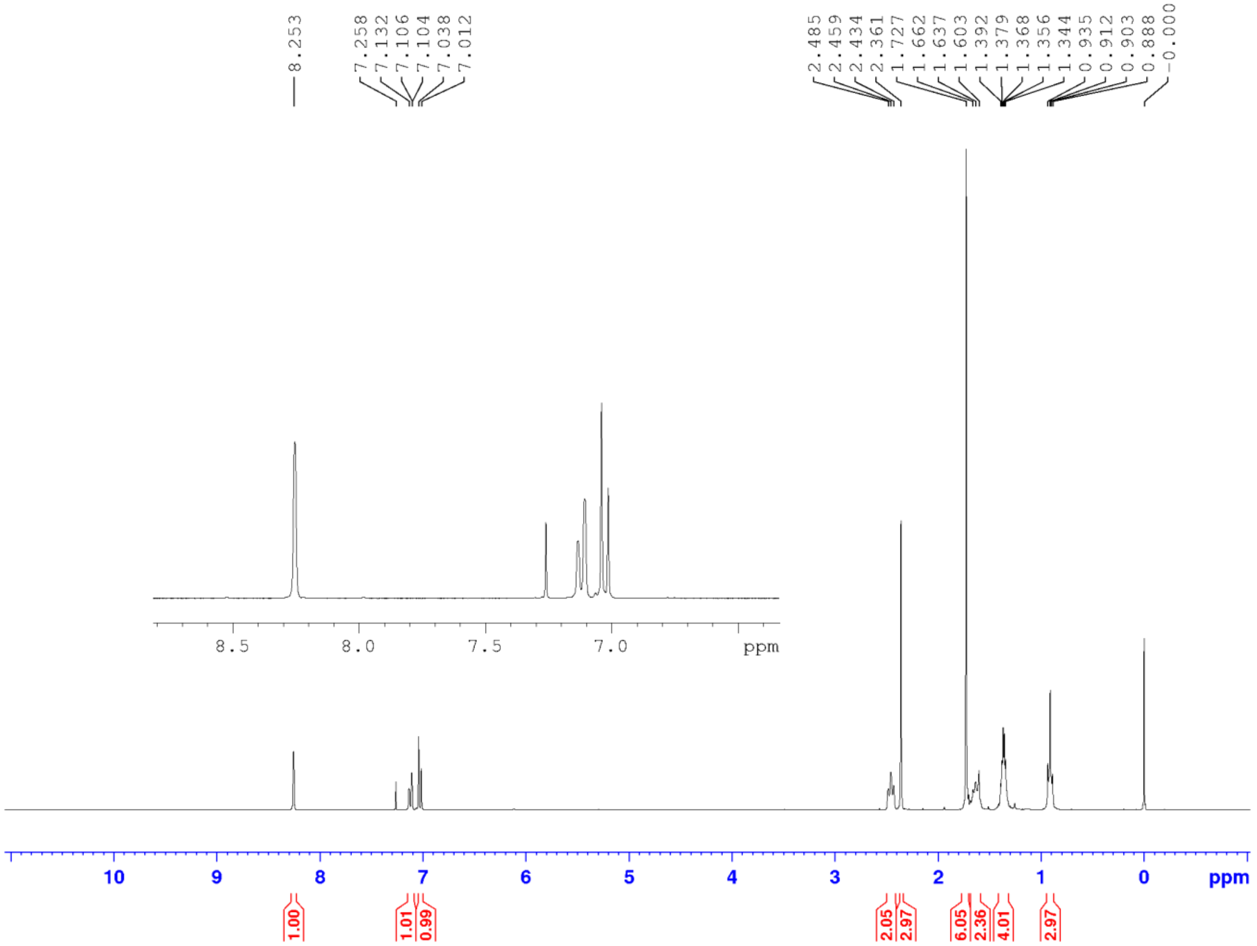
2,2,4-trifluoro-6,6,9-trimethyl-3-pentyl-2,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3b**

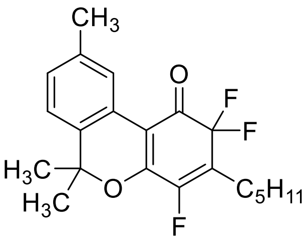




^{1}H-NMR- D_2O exchange

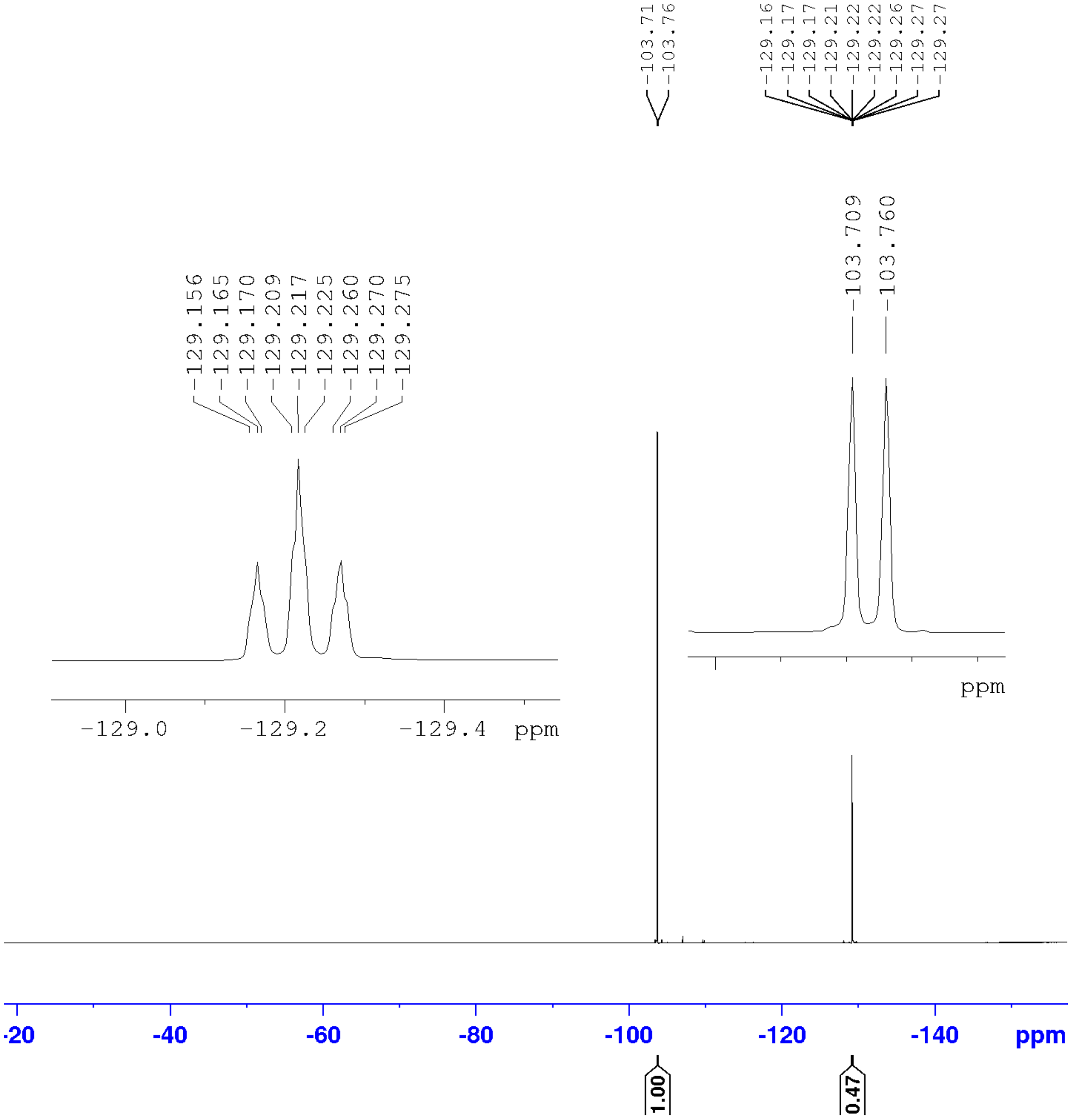
2,2,4-trifluoro-6,6,9-trimethyl-3-pentyl-2,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3b**

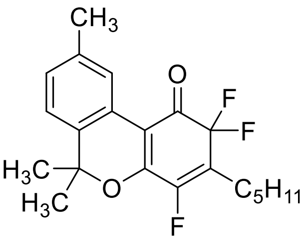




^{19}F-NMR

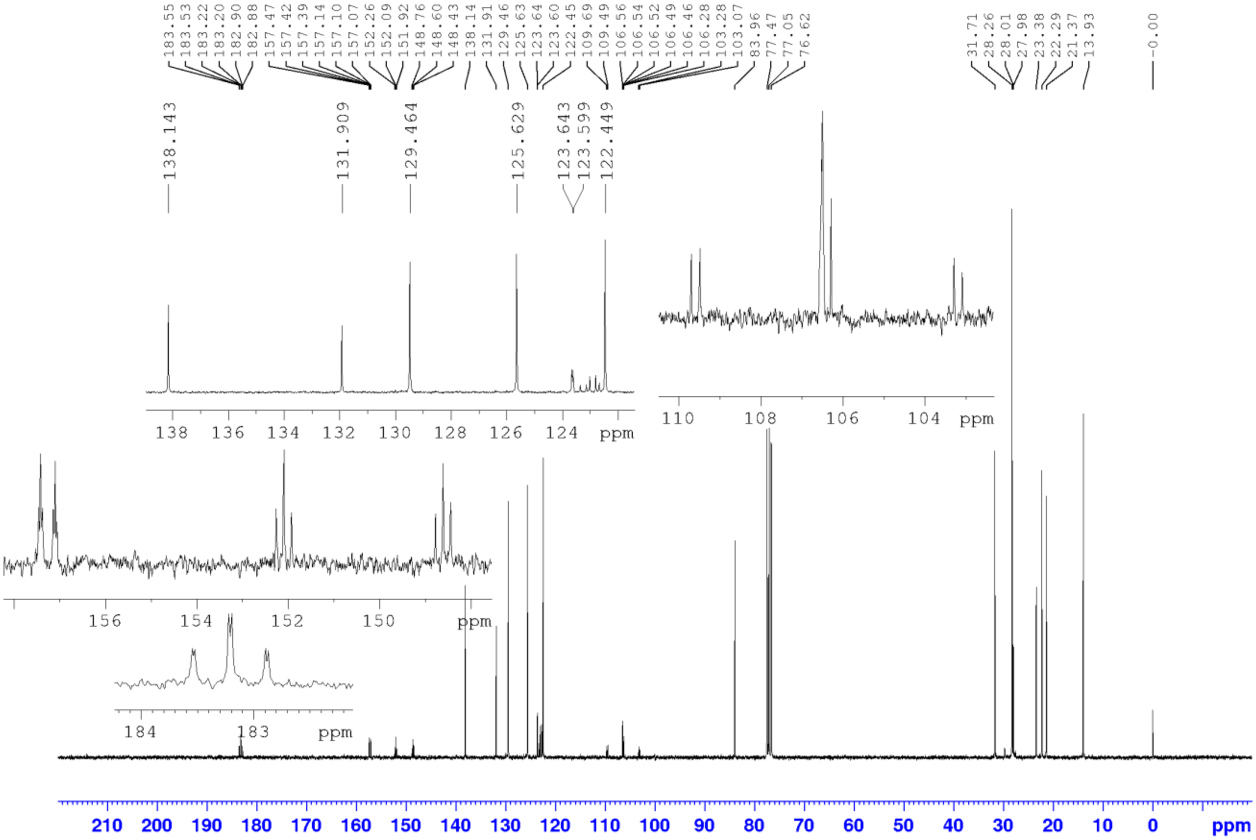
2,2,4-trifluoro-6,6,9-trimethyl-3-pentyl-2,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3b**

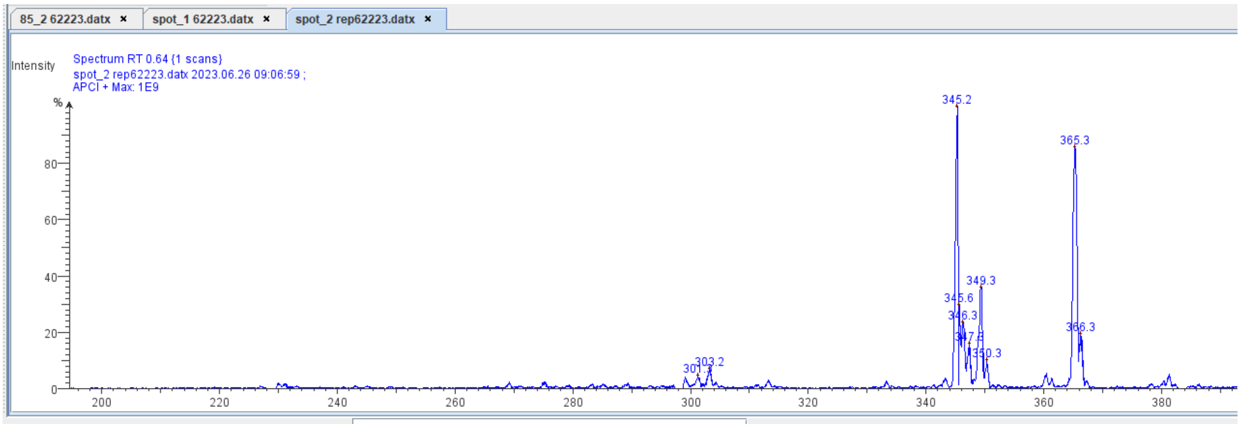




^{13}C-NMR and Mass spectrum

2,2,4-trifluoro-6,6,9-trimethyl-3-pentyl-2,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3b**





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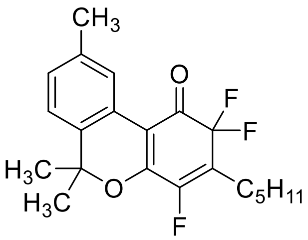
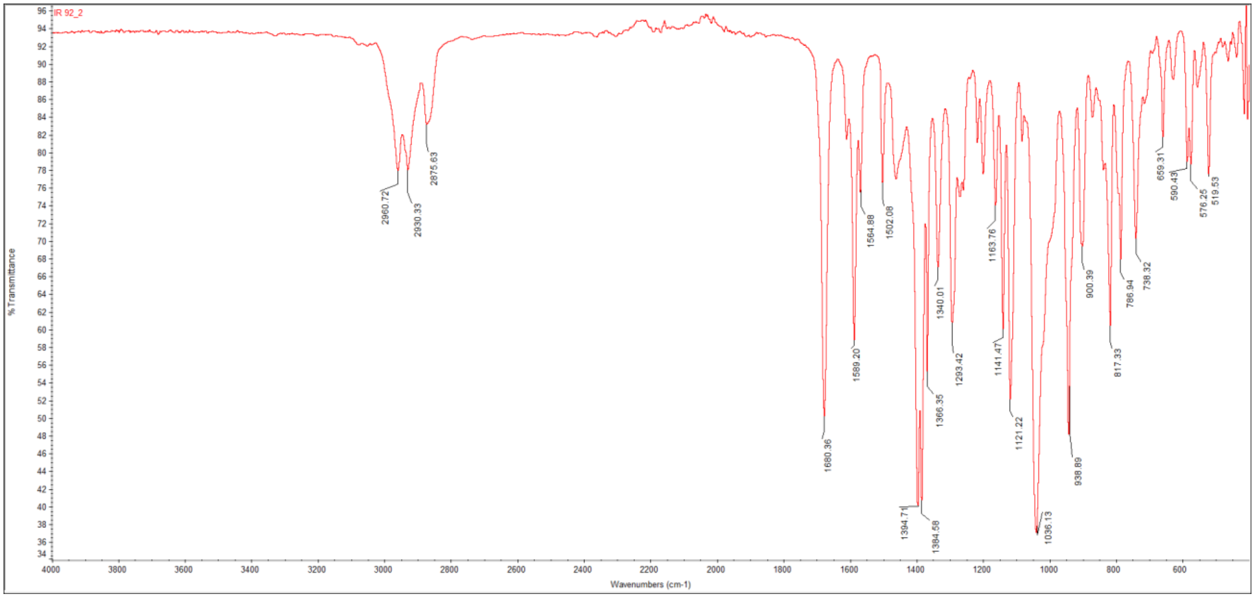
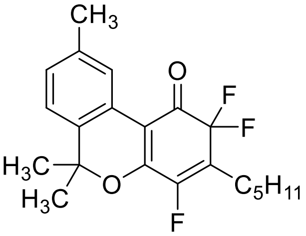


IR data

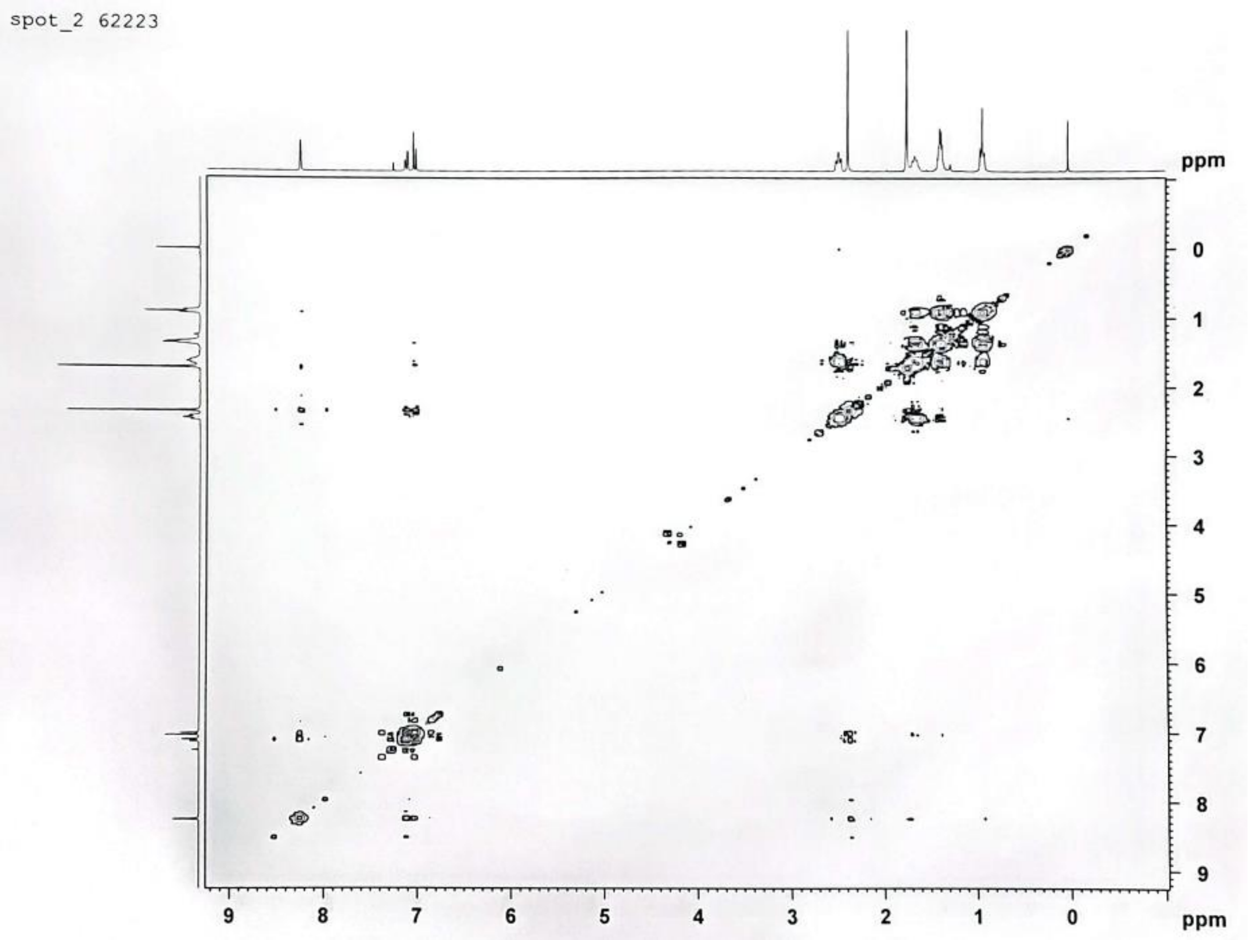
2,2,4-trifluoro-6,6,9-trimethyl-3-pentyl-2,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3b**

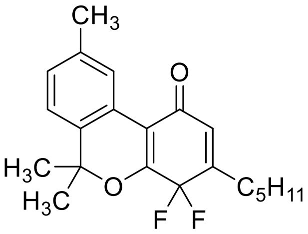




2D-NMR

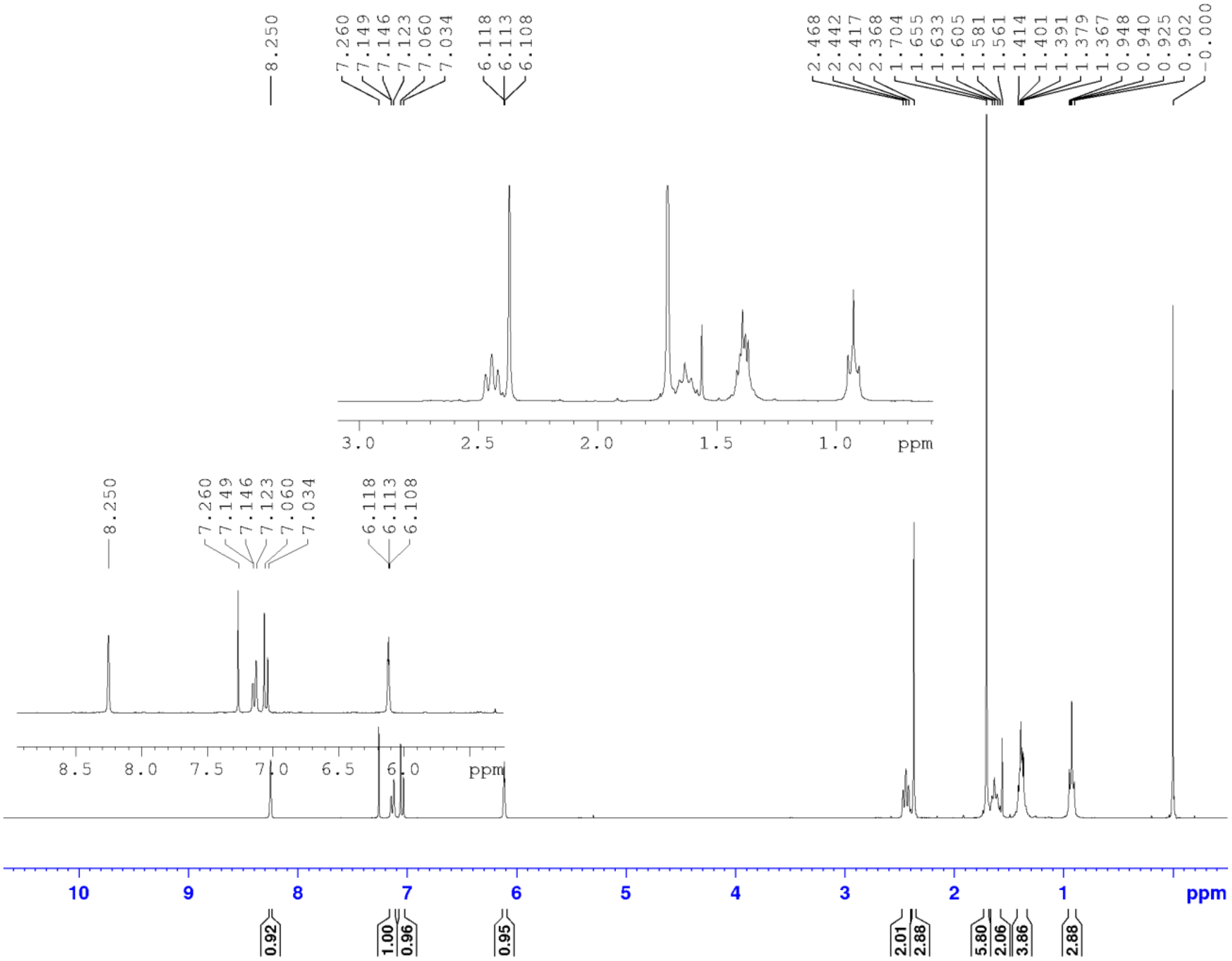
2,2,4-trifluoro-6,6,9-trimethyl-3-pentyl-2,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3b**

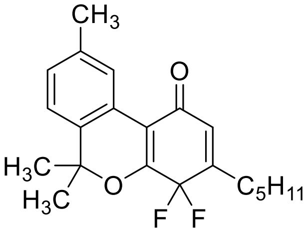




^{1}H-NMR

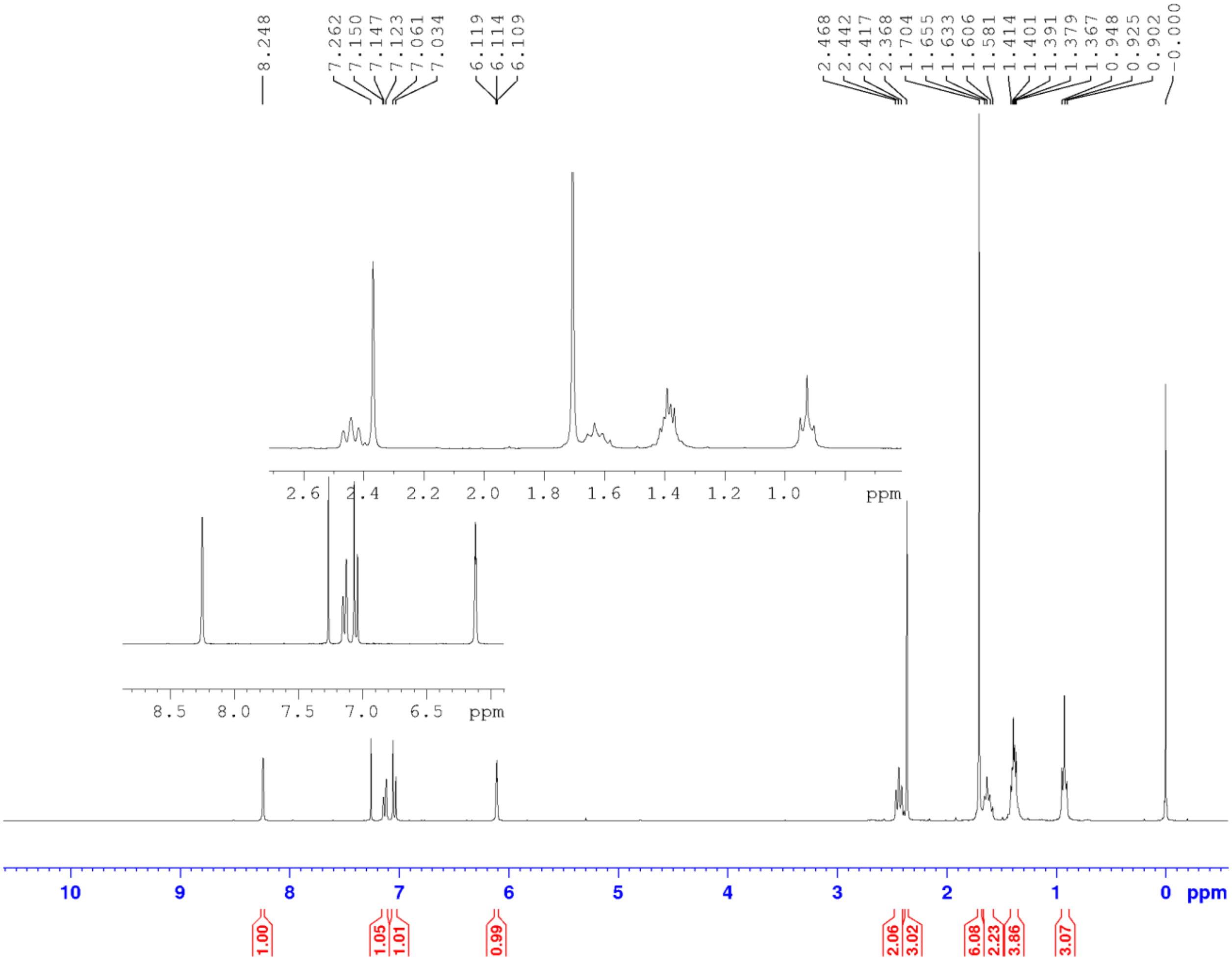
4,4-difluoro-6,6,9-trimethyl-3-pentyl-4,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3c**

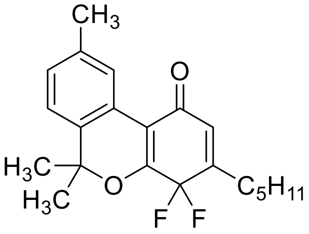




^{1}H-NMR-D_2O exchange

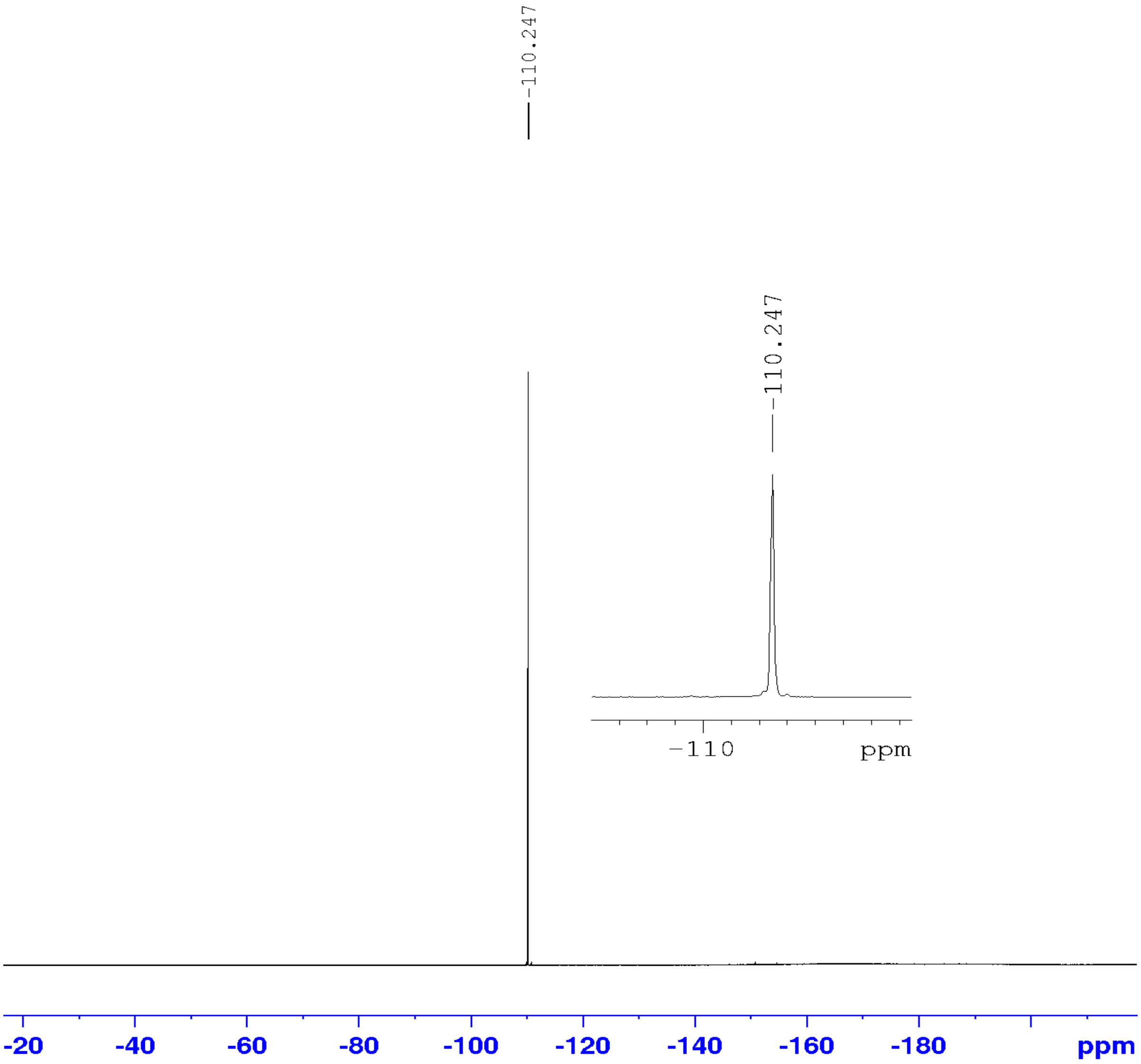
4,4-difluoro-6,6,9-trimethyl-3-pentyl-4,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3c**

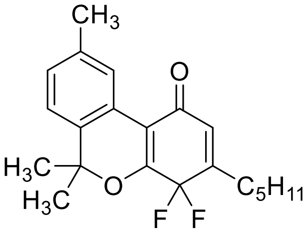




^{19}F-NMR

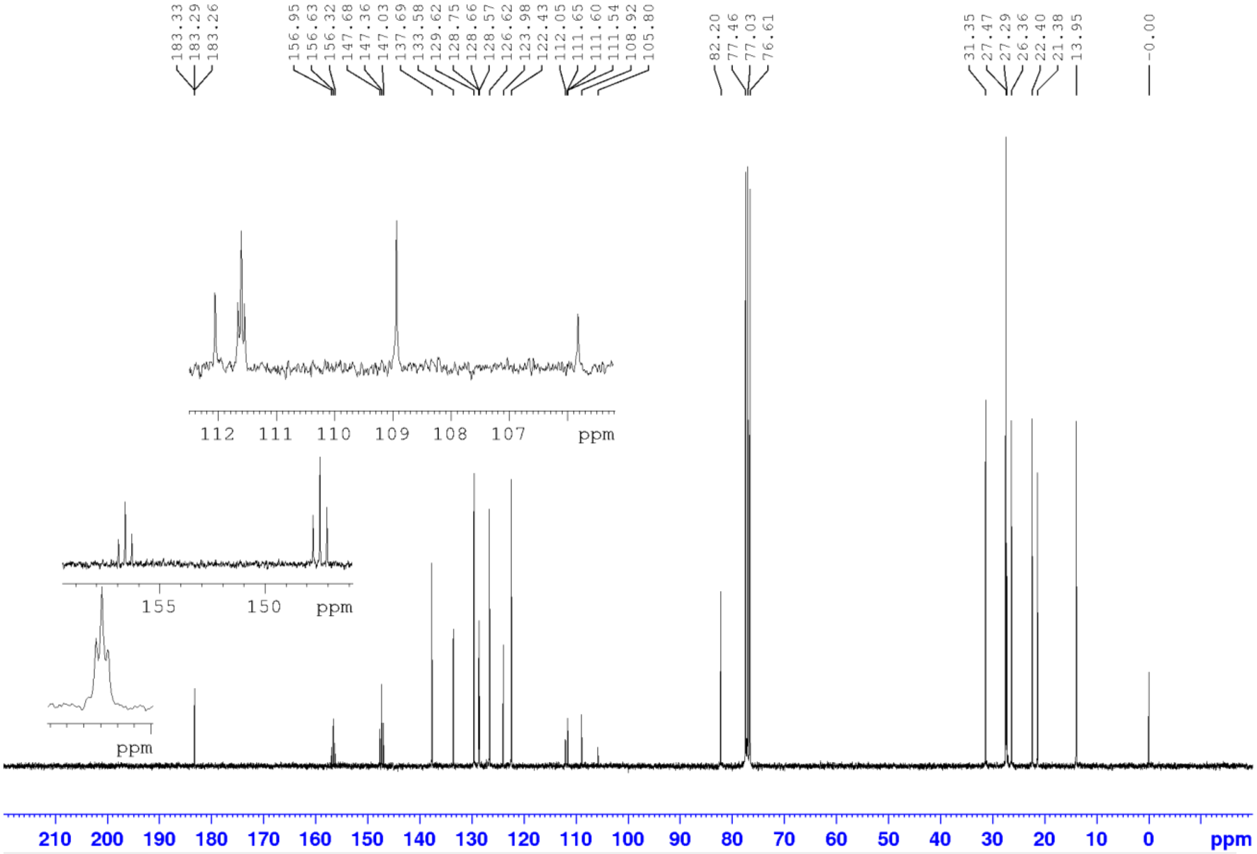
4,4-difluoro-6,6,9-trimethyl-3-pentyl-4,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3c**

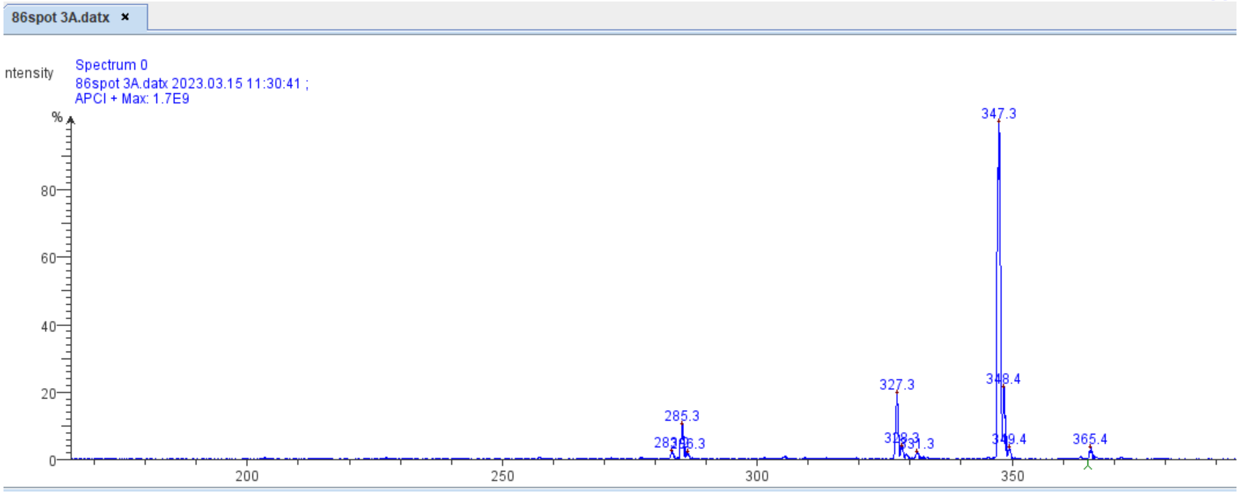


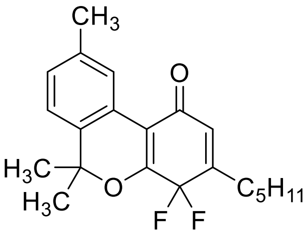


^{13}C-NMR and Mass spectrum

4,4-difluoro-6,6,9-trimethyl-3-pentyl-4,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3c**

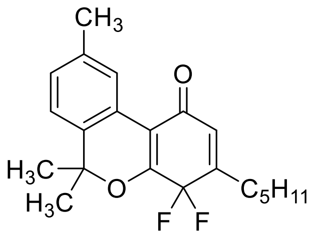




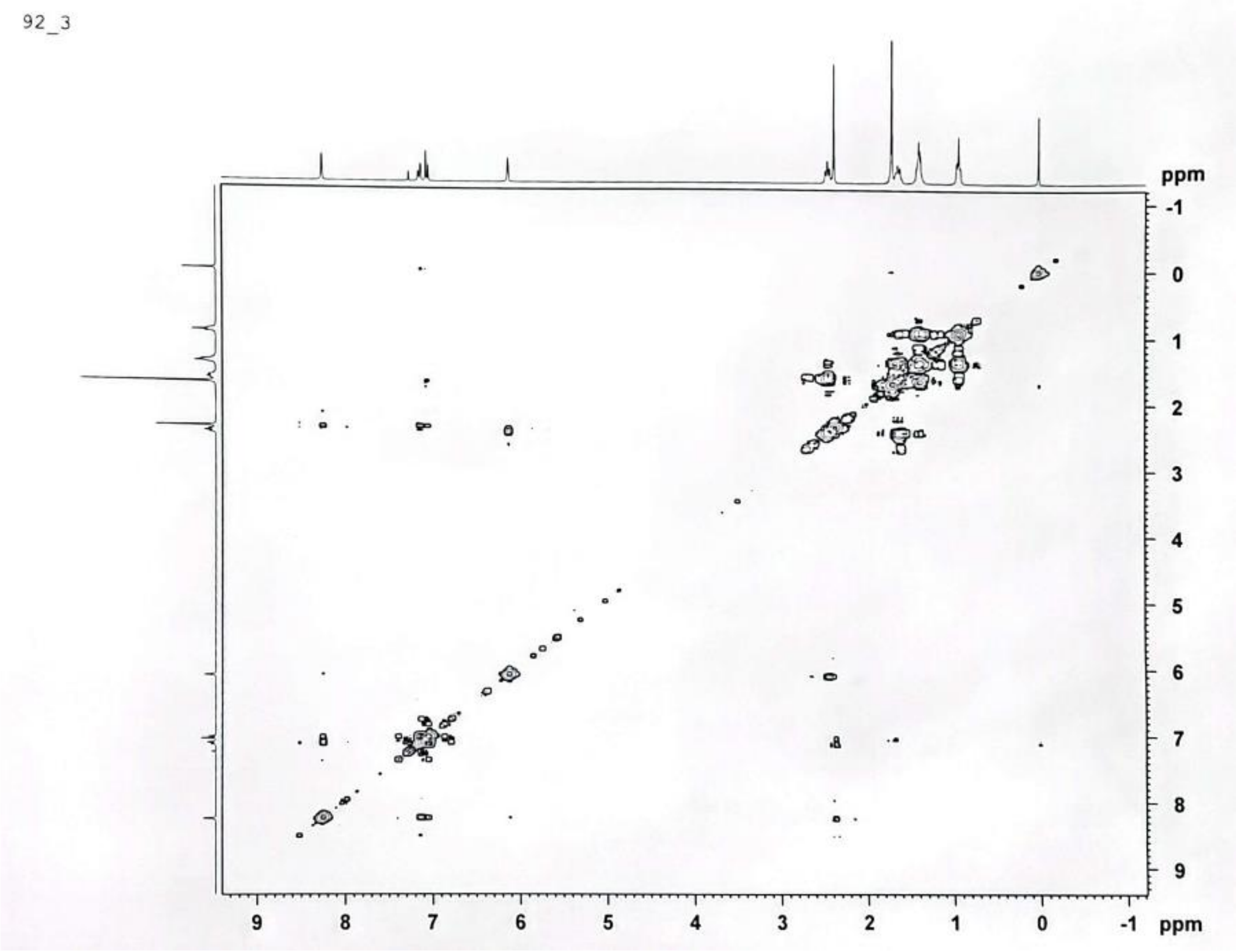


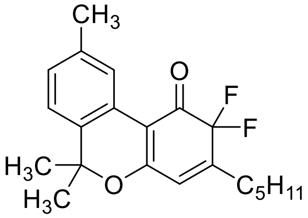
IR data

4,4-difluoro-6,6,9-trimethyl-3-pentyl-4,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3c**



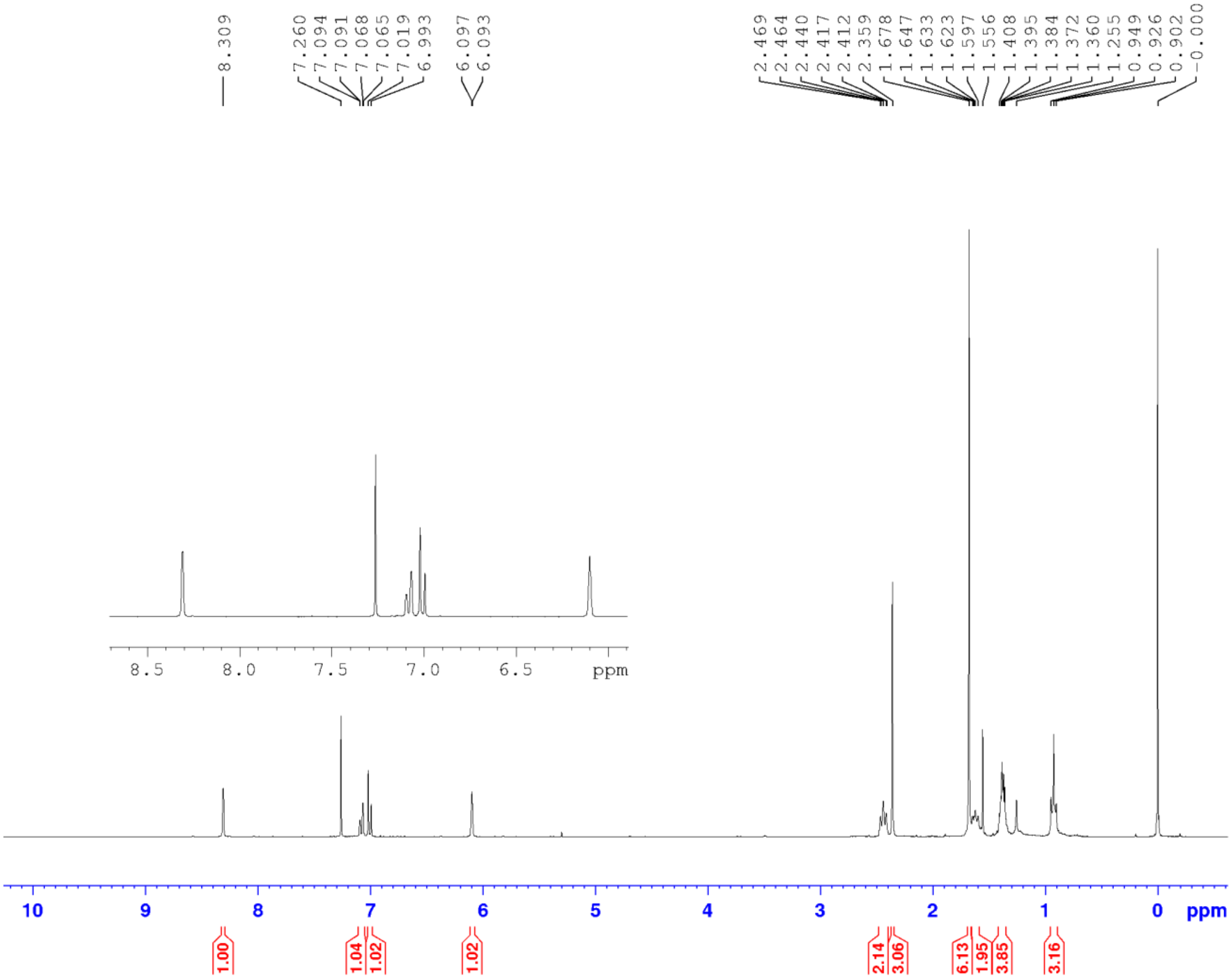
2D-NMR
4,4-difluoro-6,6,9-trimethyl-3-pentyl-4,6-dihydro-1*H*-benzo[*c*]chromen-1-one, **3c**

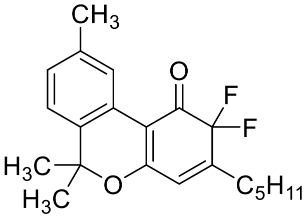




^{1}H-NMR

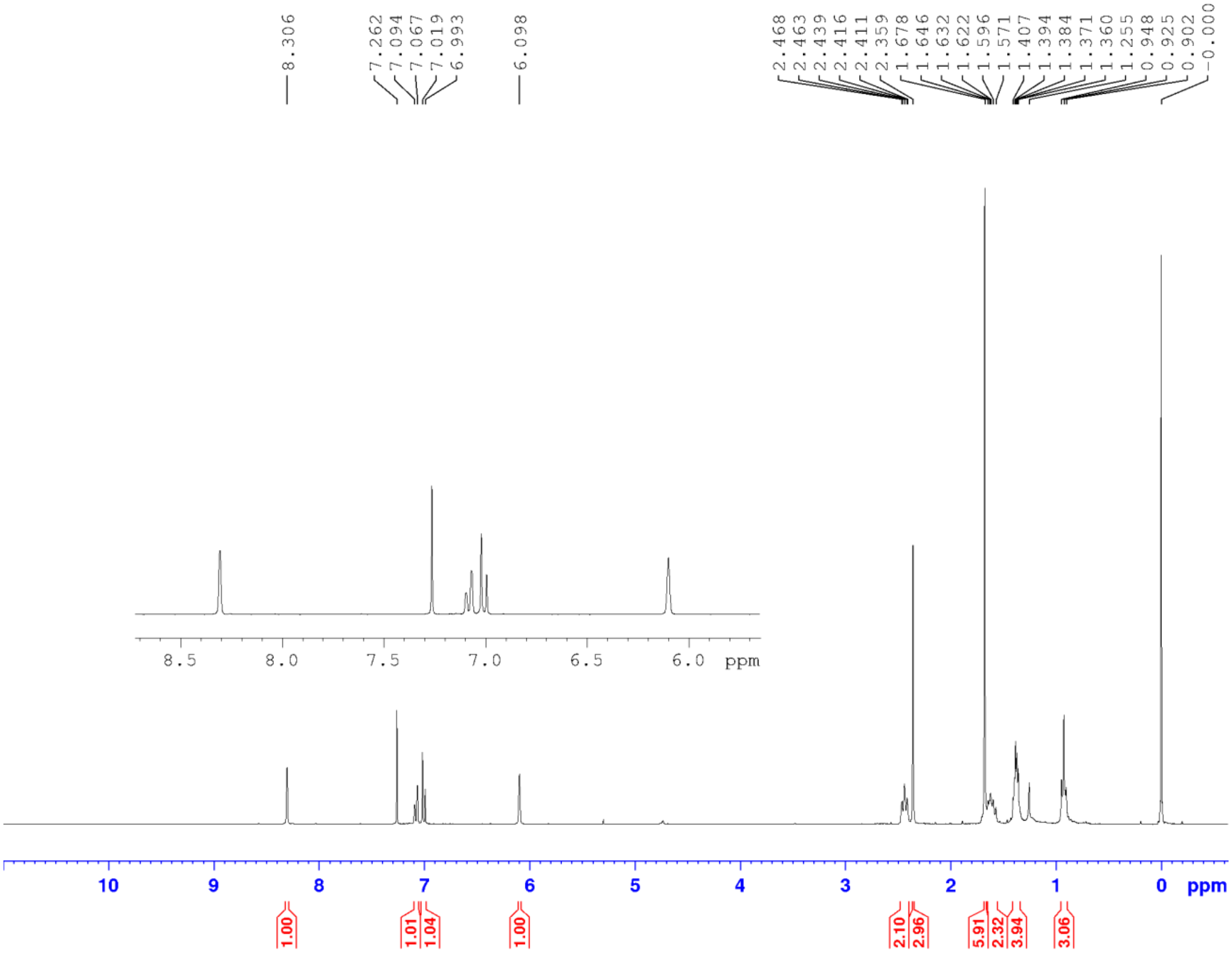
2,2-difluoro-6,6,9-trimethyl-3-pentyl-2,6-dihydro-1*H*-benzo[*c*]chromen-1-one , **3d**

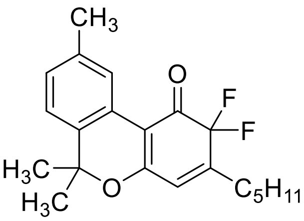




^{1}H-NMR-D_2O exchange

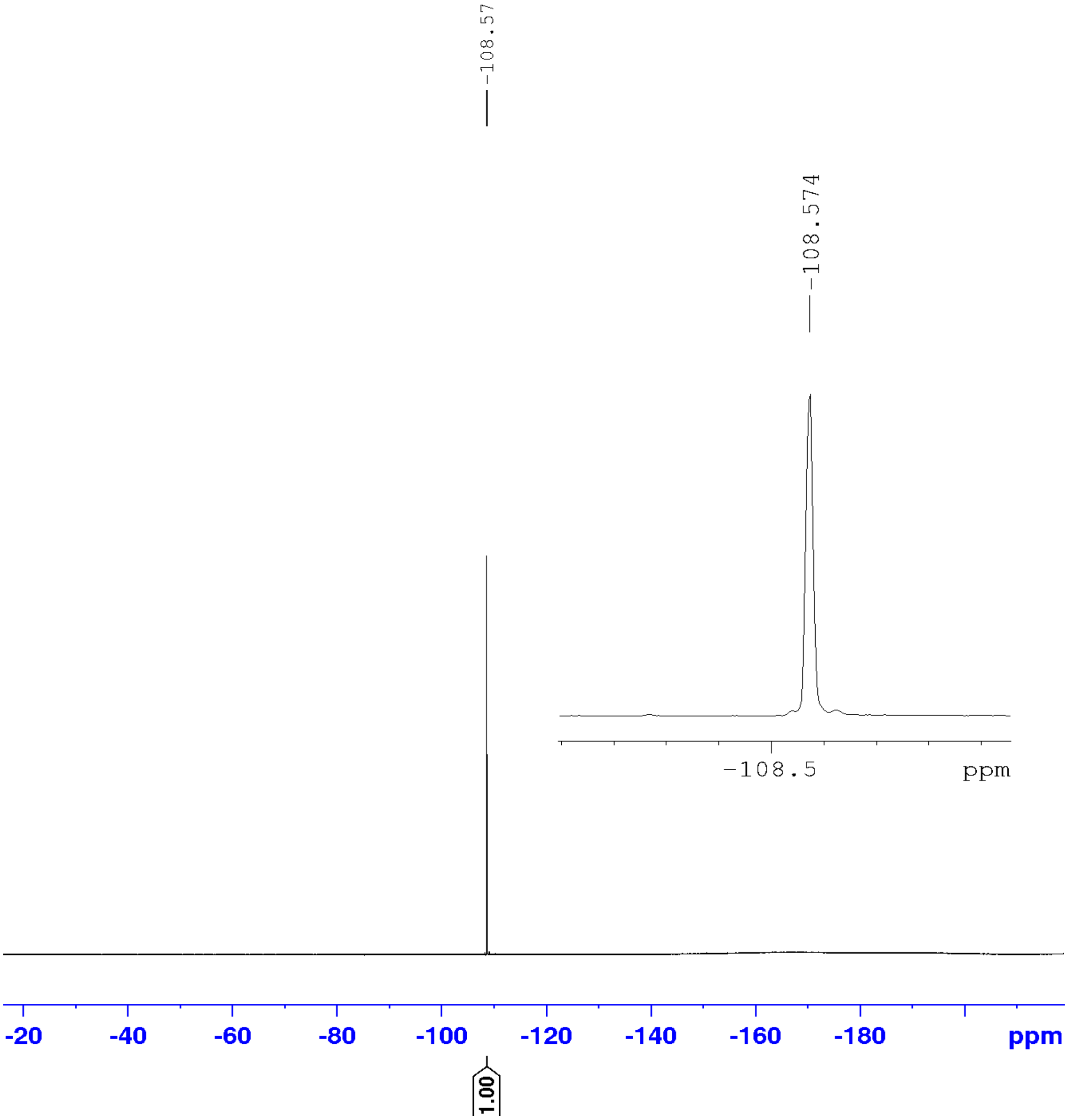
2,2-difluoro-6,6,9-trimethyl-3-pentyl-2,6-dihydro-1*H*-benzo[*c*]chromen-1-one , **3d**

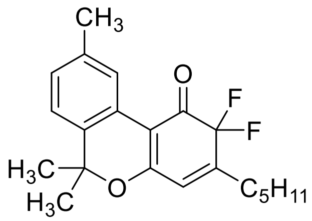




^{19}F-NMR

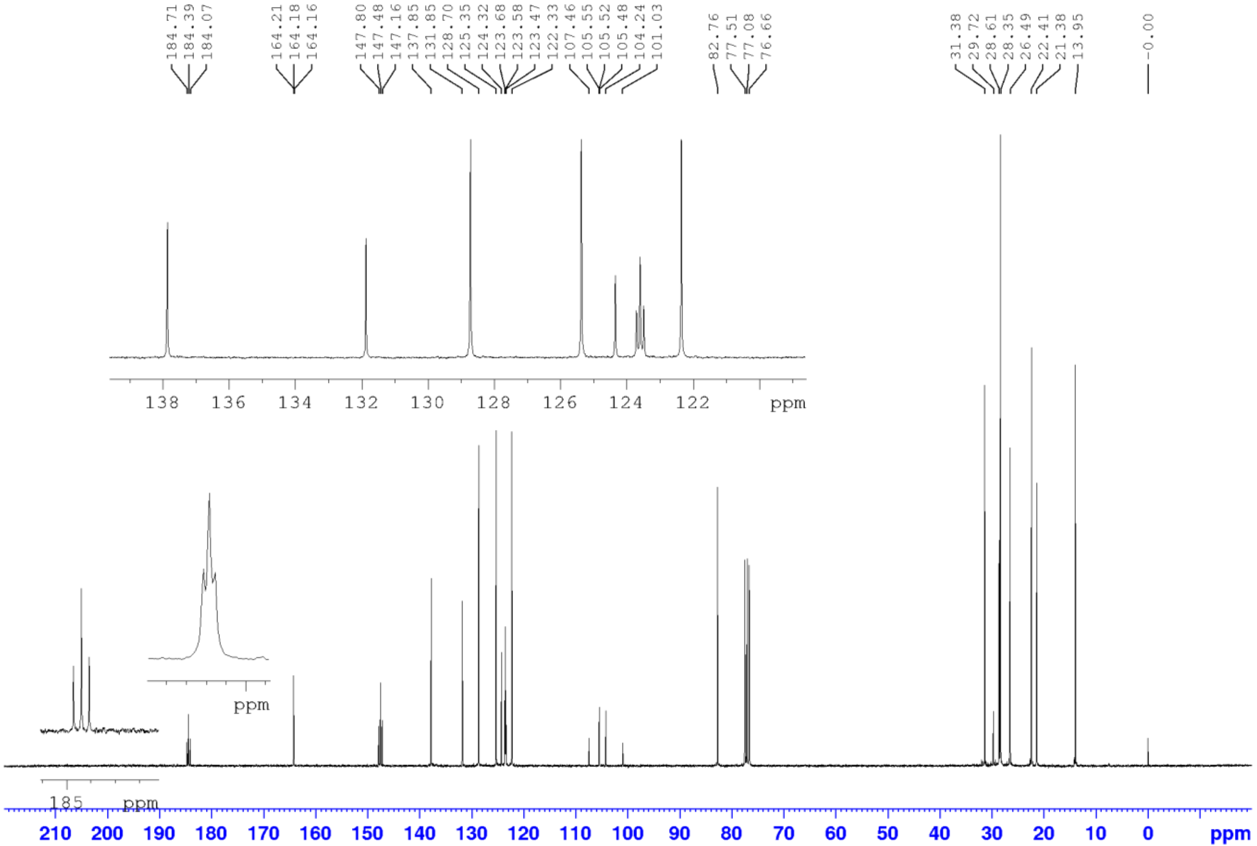
2,2-difluoro-6,6,9-trimethyl-3-pentyl-2,6-dihydro-1*H*-benzo[*c*]chromen-1-one , **3d**

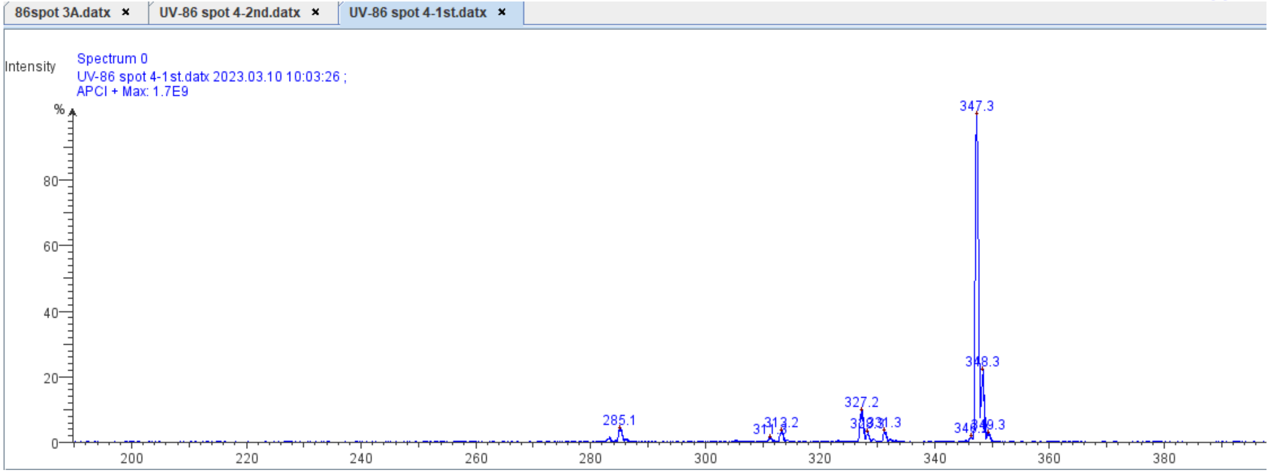


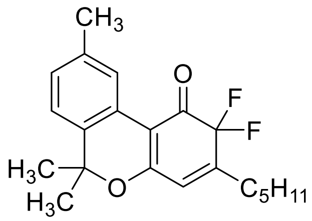


^{13}C-NMR and Mass spectrum

2,2-difluoro-6,6,9-trimethyl-3-pentyl-2,6-dihydro-1*H*-benzo[*c*]chromen-1-one , **3d**

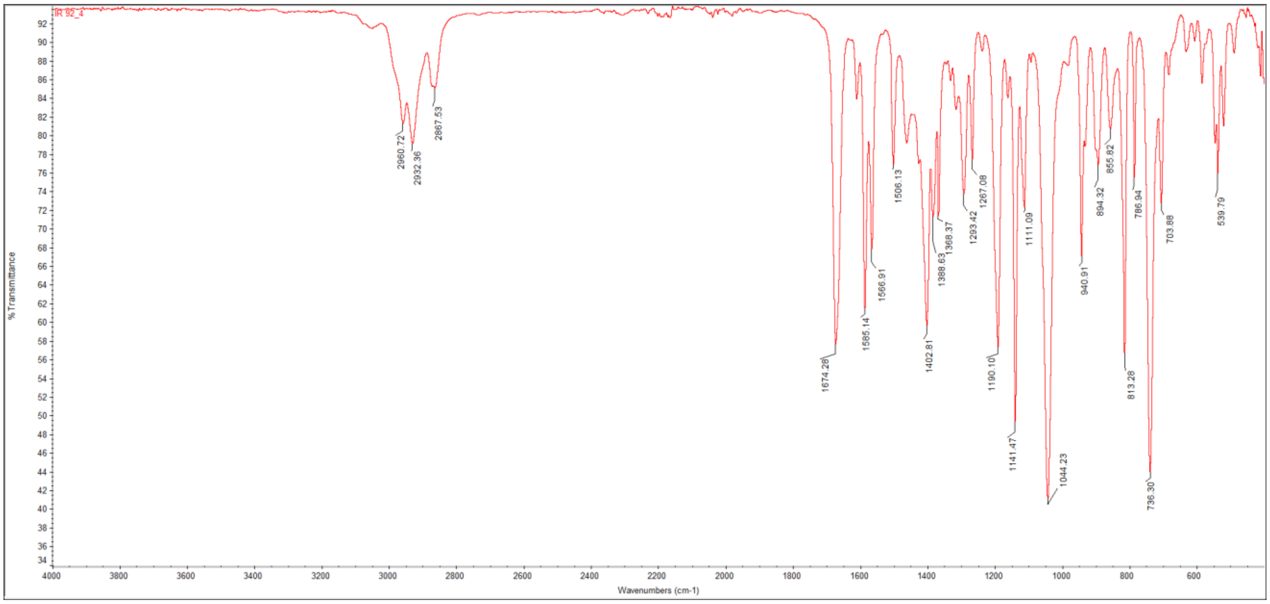


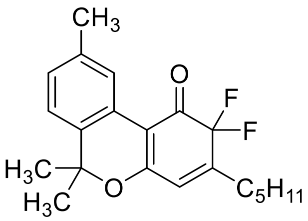




IR data

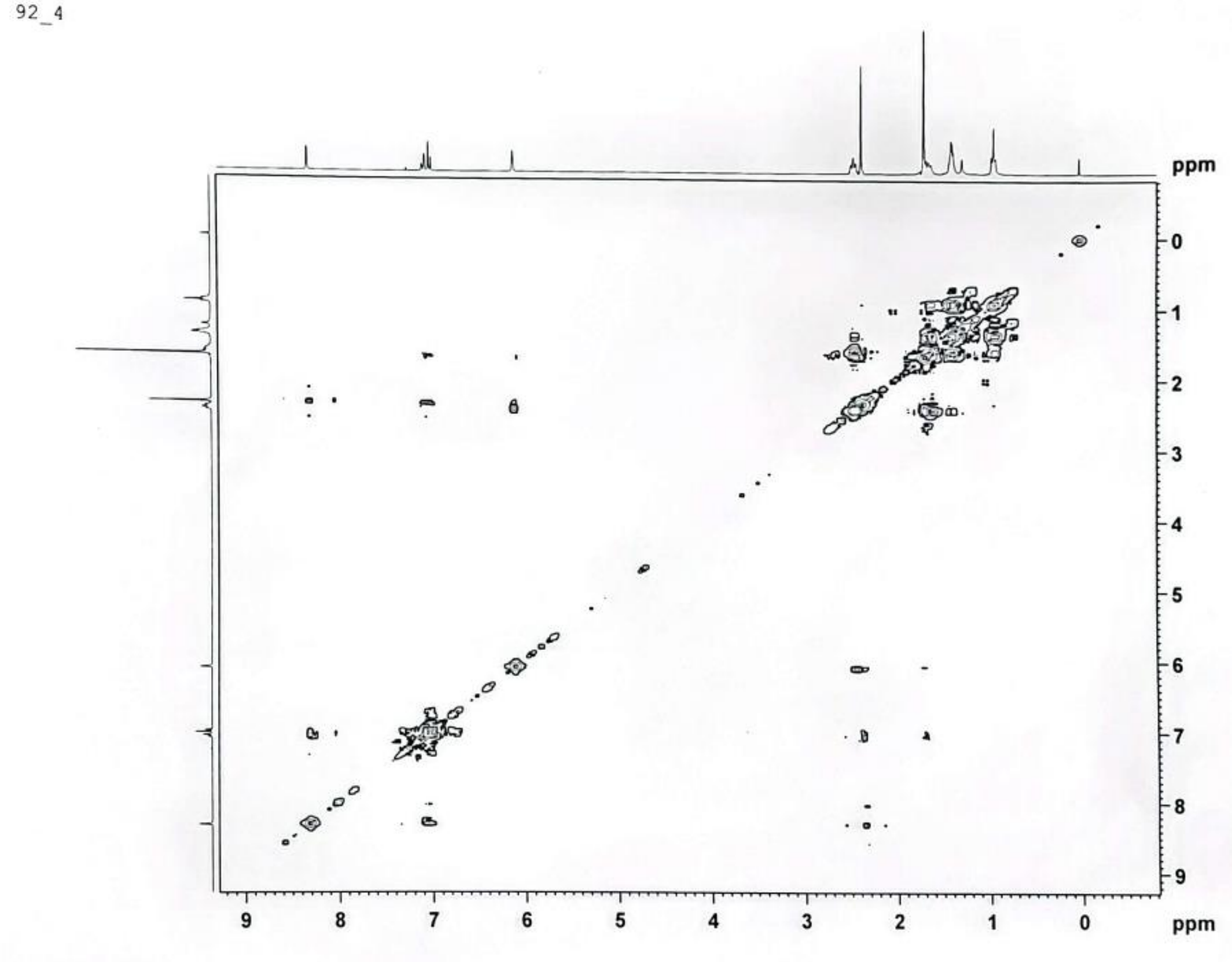
2,2-difluoro-6,6,9-trimethyl-3-pentyl-2,6-dihydro-1*H*-benzo[*c*]chromen-1-one , **3d**

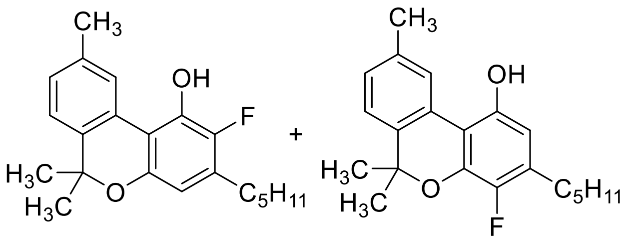




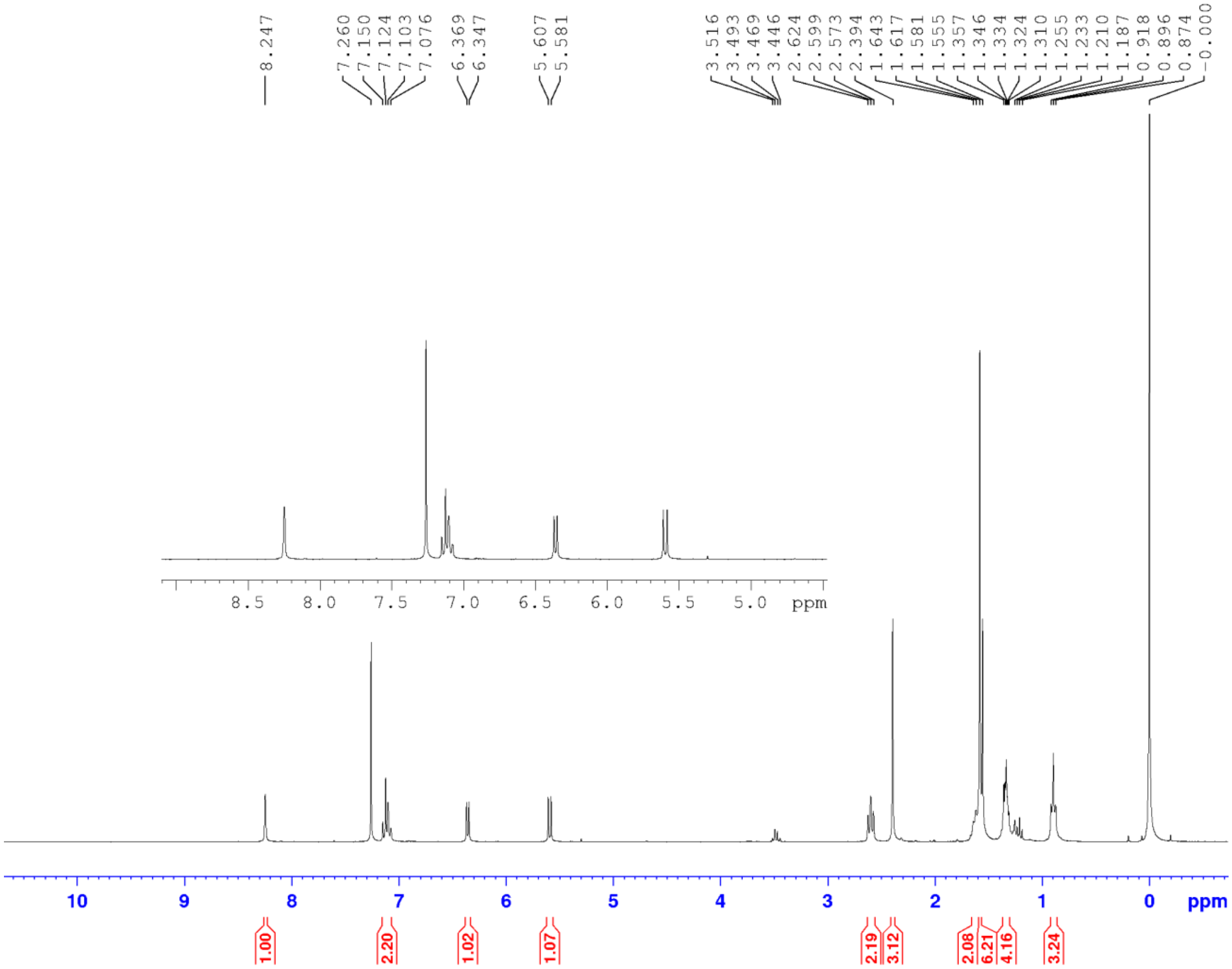
2D-NMR

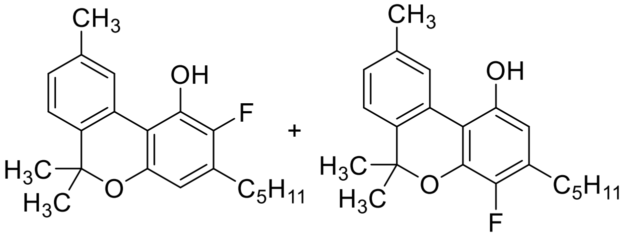
2,2-difluoro-6,6,9-trimethyl-3-pentyl-2,6-dihydro-1*H*-benzo[*c*]chromen-1-one , **3d**





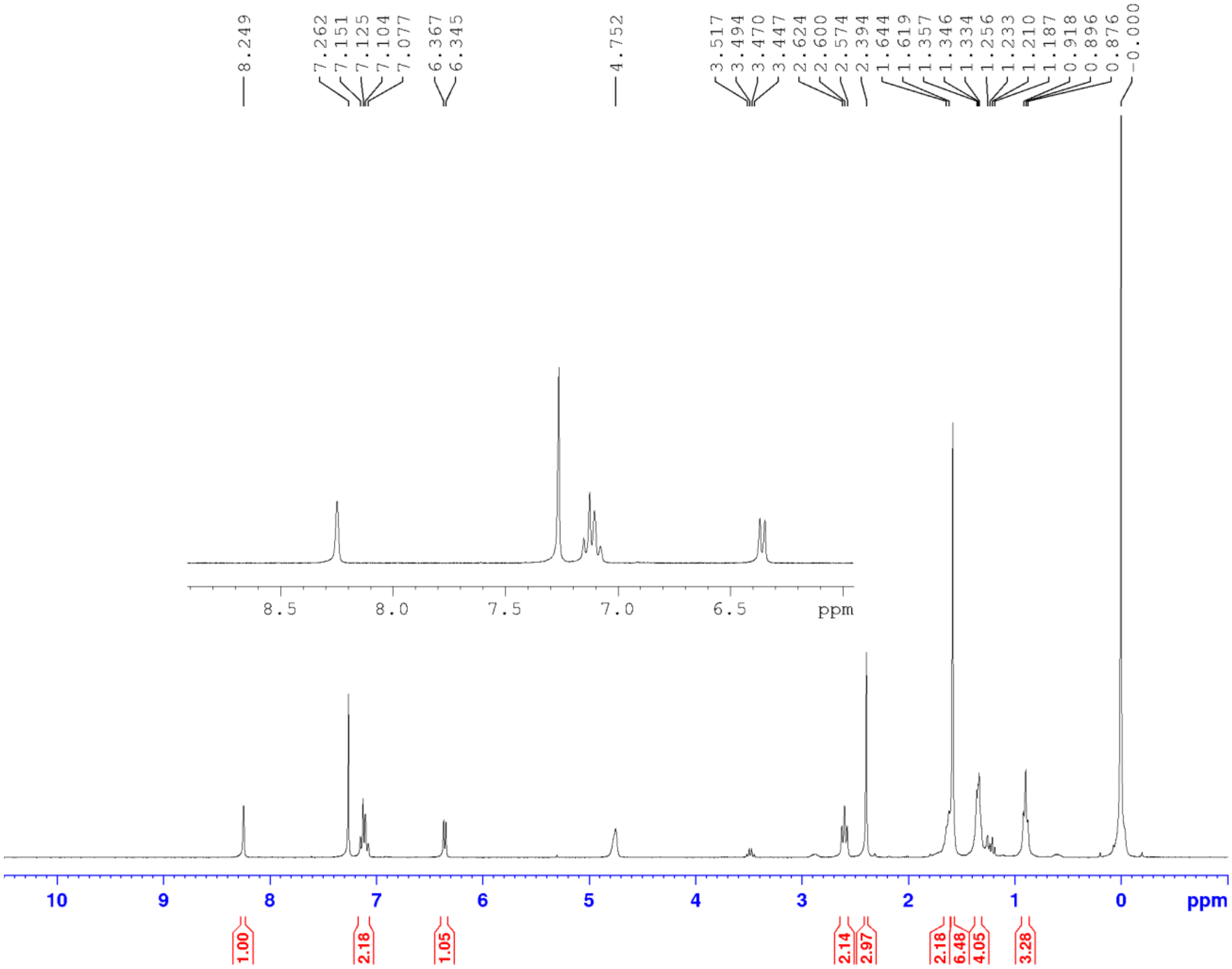
^{1}H-NMR
2-fluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol and 4-fluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol, (**3e**+**3f**)

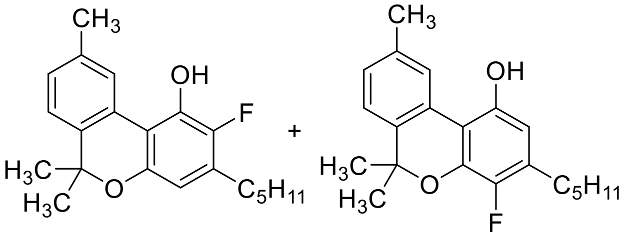




^{1}H-NMR-D_2O exchange

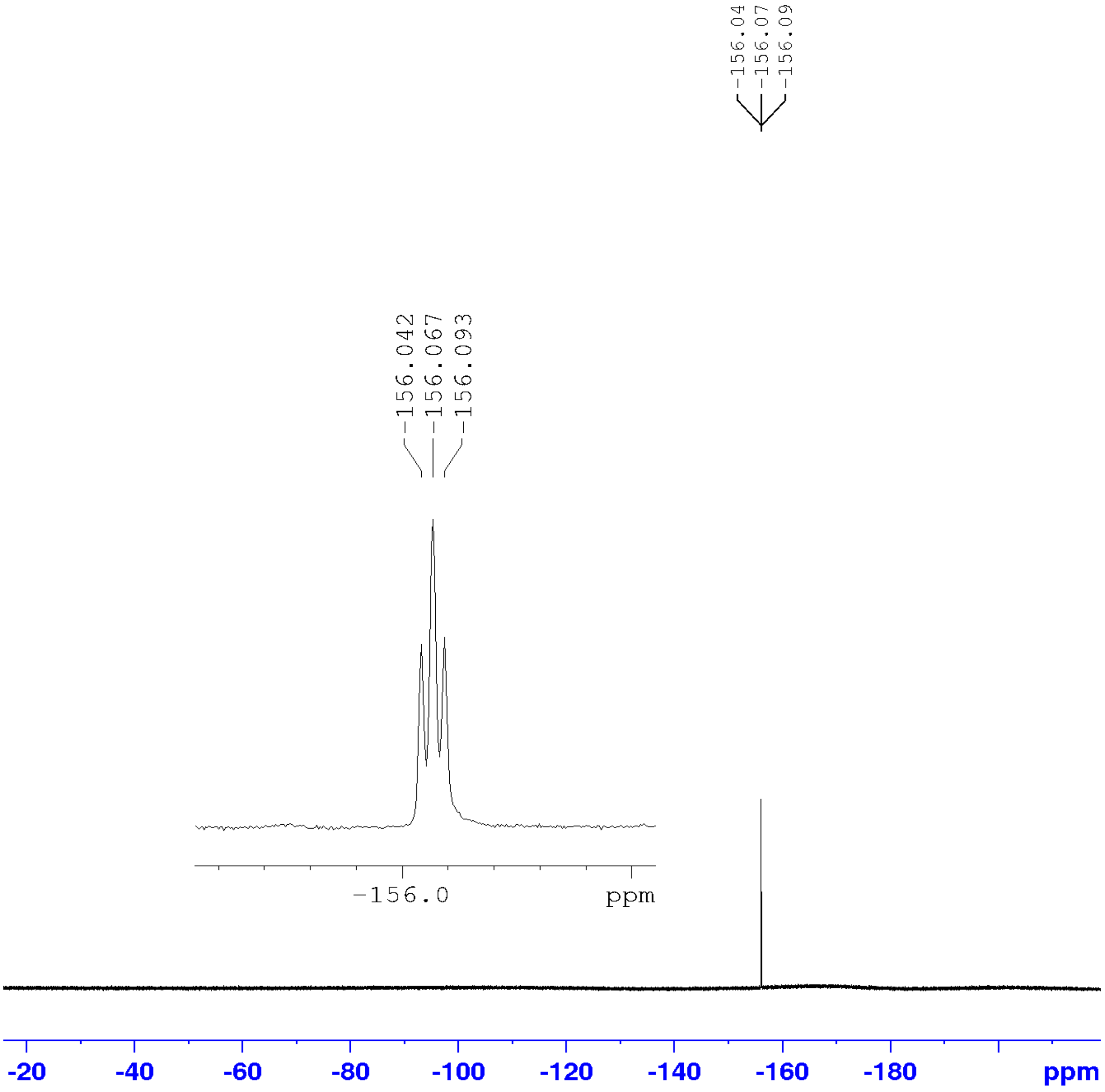
2-fluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol and 4-fluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol, (**3e**+**3f**)

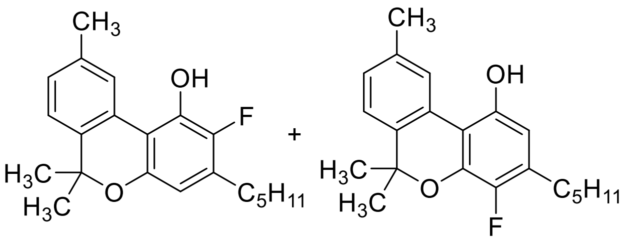




^{19}F-NMR

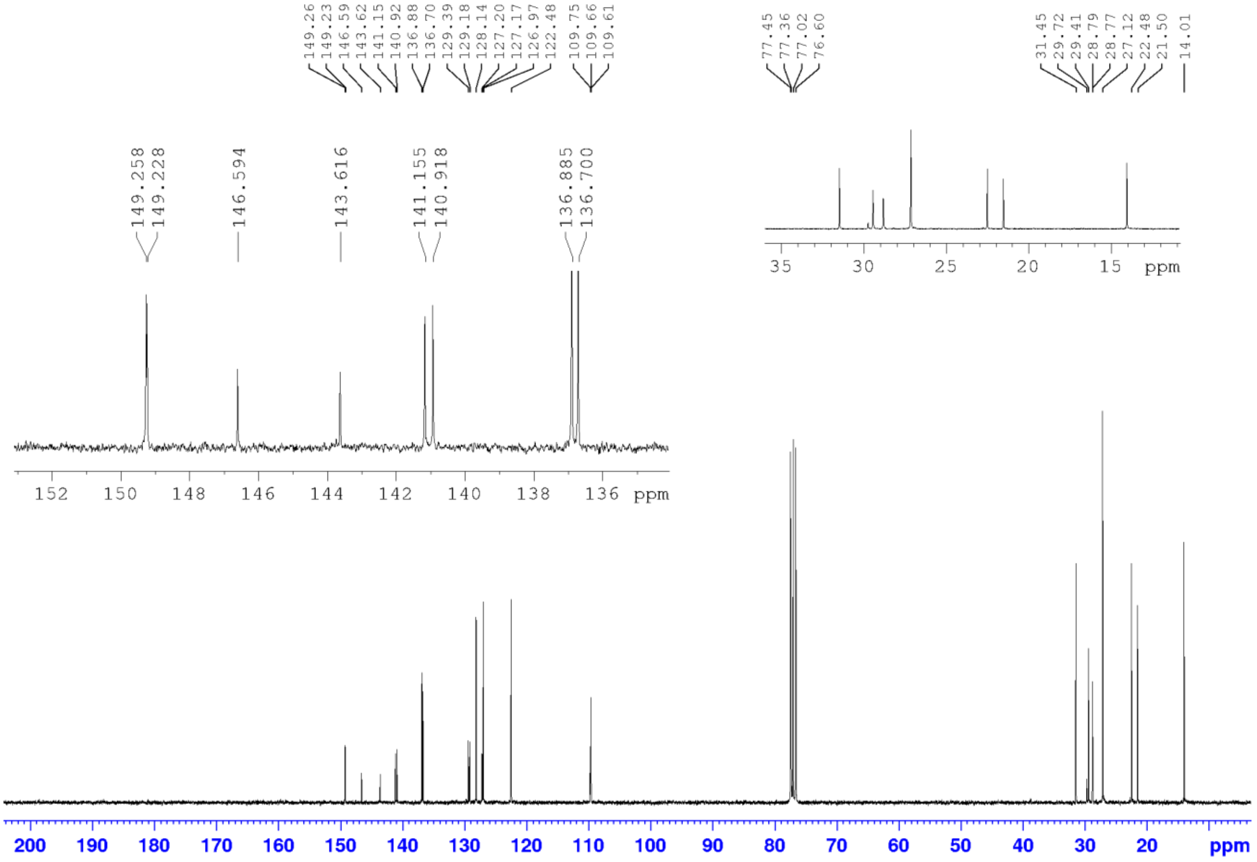
2-fluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol and 4-fluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol, (**3e**+**3f**)

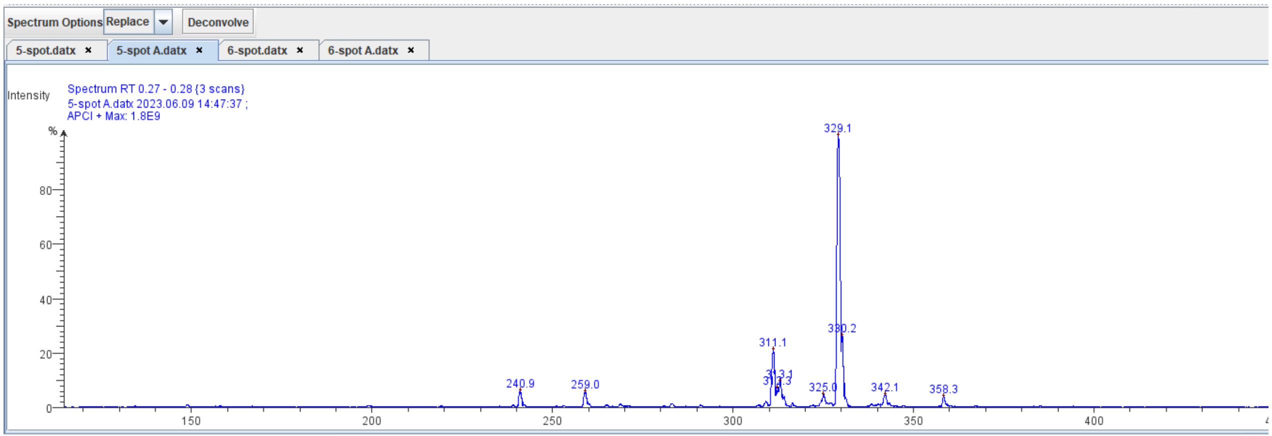




^{13}C-NMR and Mass spectrum

2-fluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol and 4-fluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol, (**3e**+**3f**)





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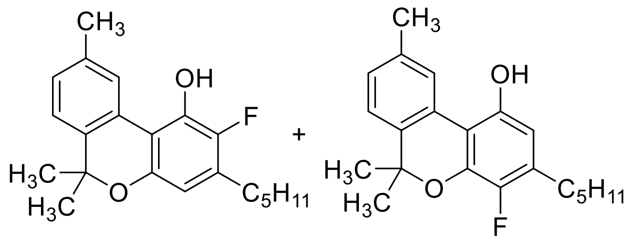
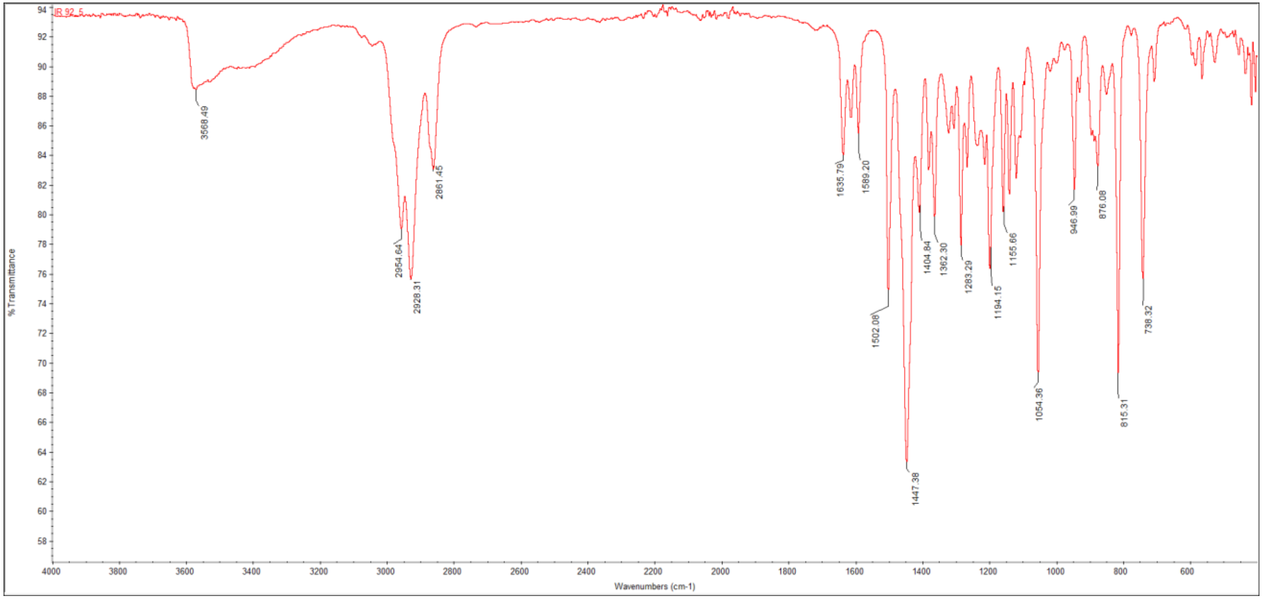
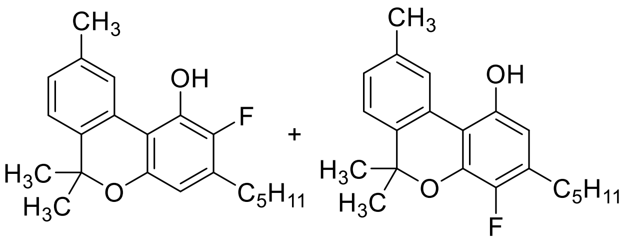


IR data

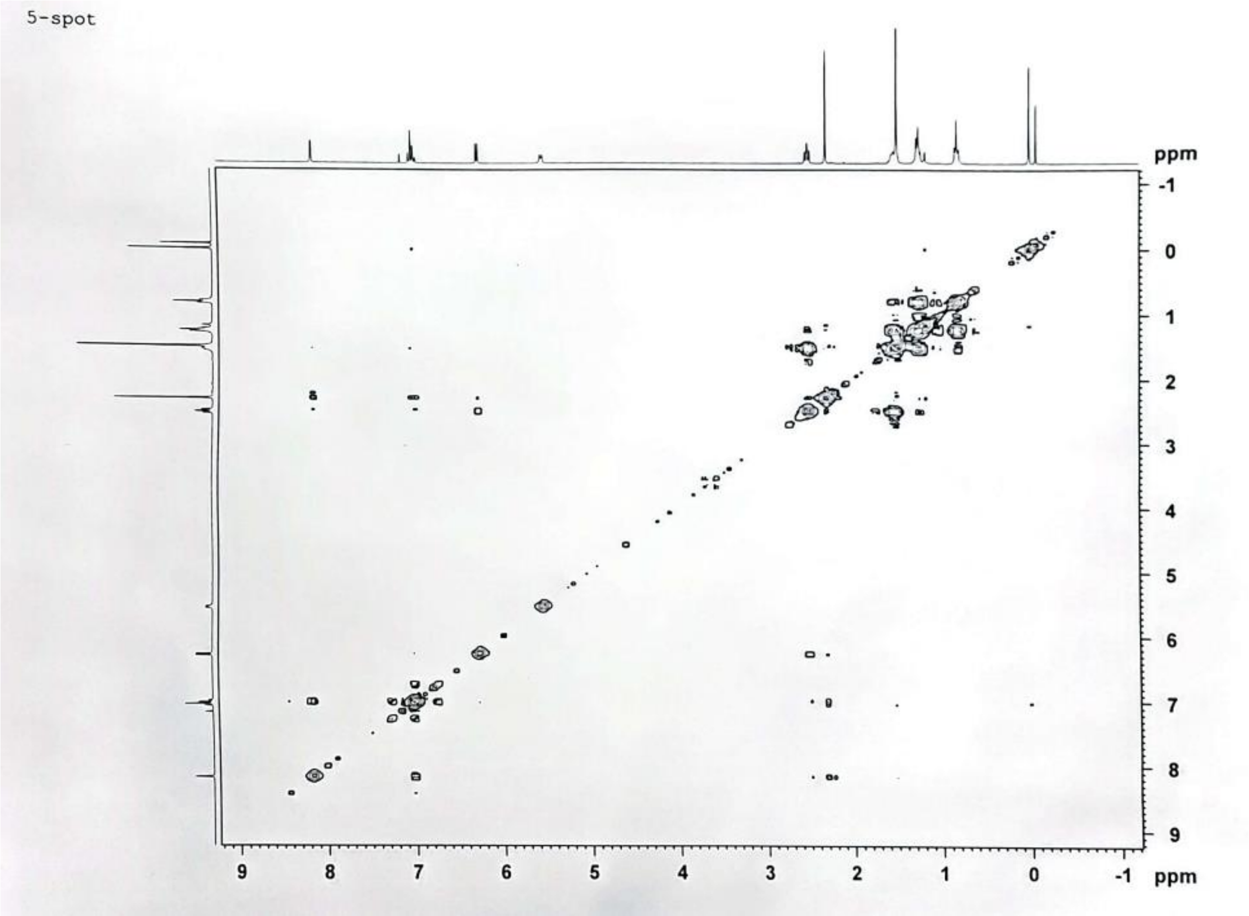
2-fluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol and 4-fluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol, (**3e**+**3f**)

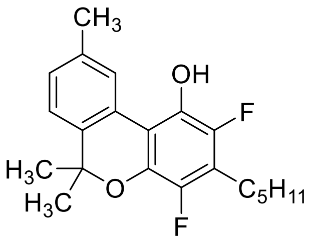




2D-NMR

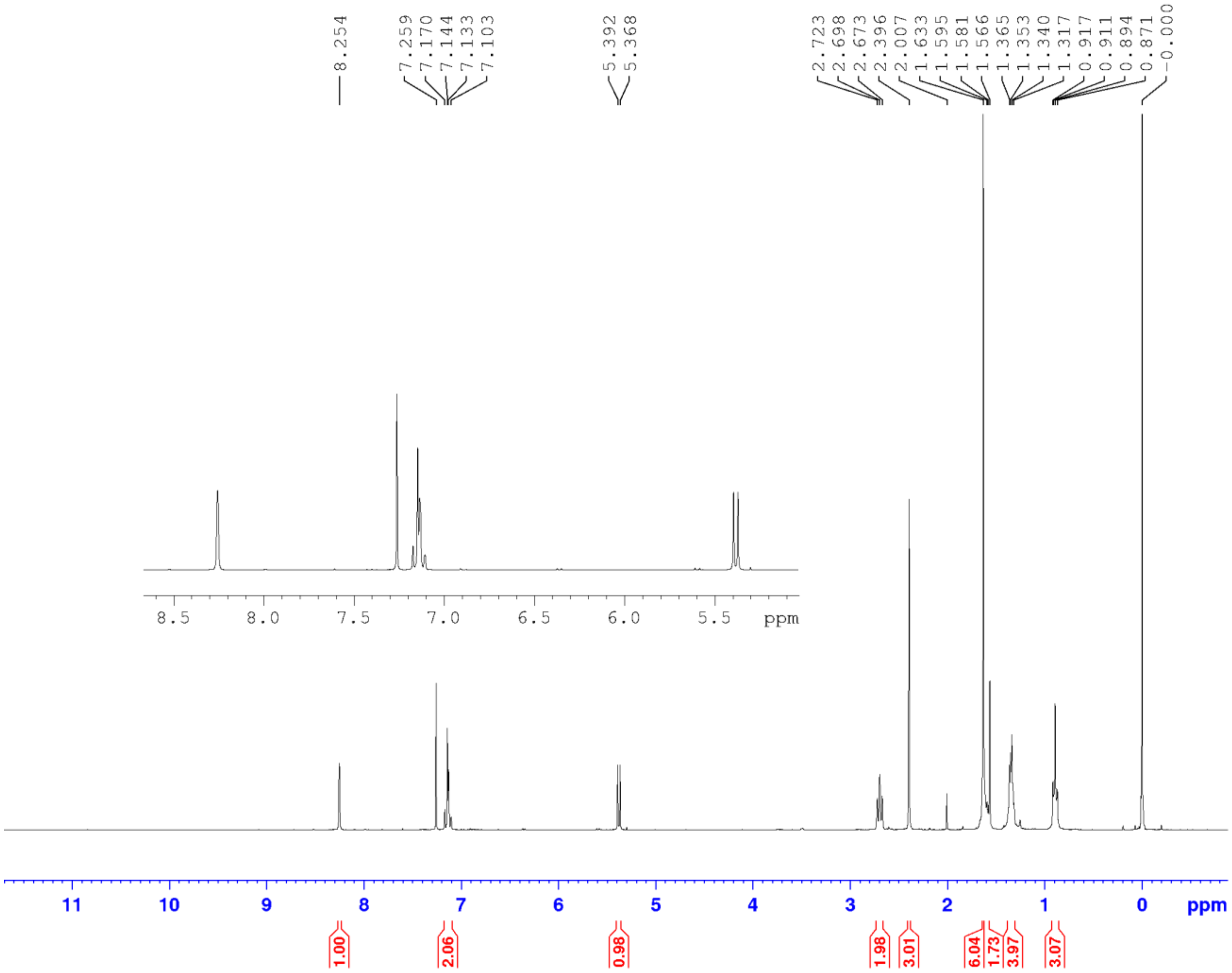
2-fluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol and 4-fluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol, (**3e**+**3f**)

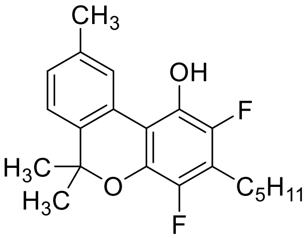




^{1}H-NMR

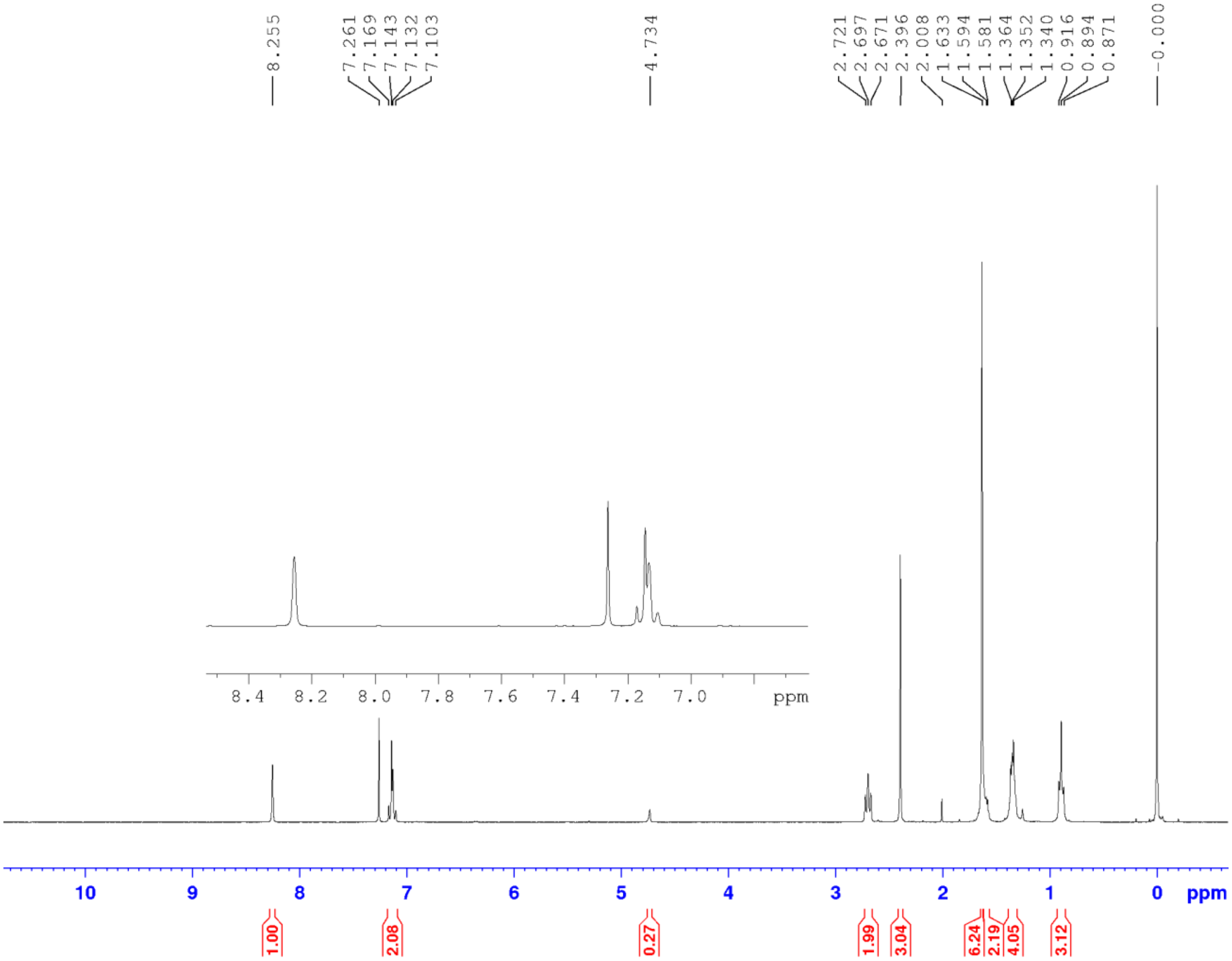
2,4-difluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol, **3g**

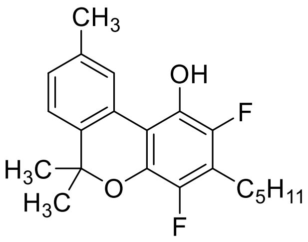




^{1}H-NMR-D_2O exchange

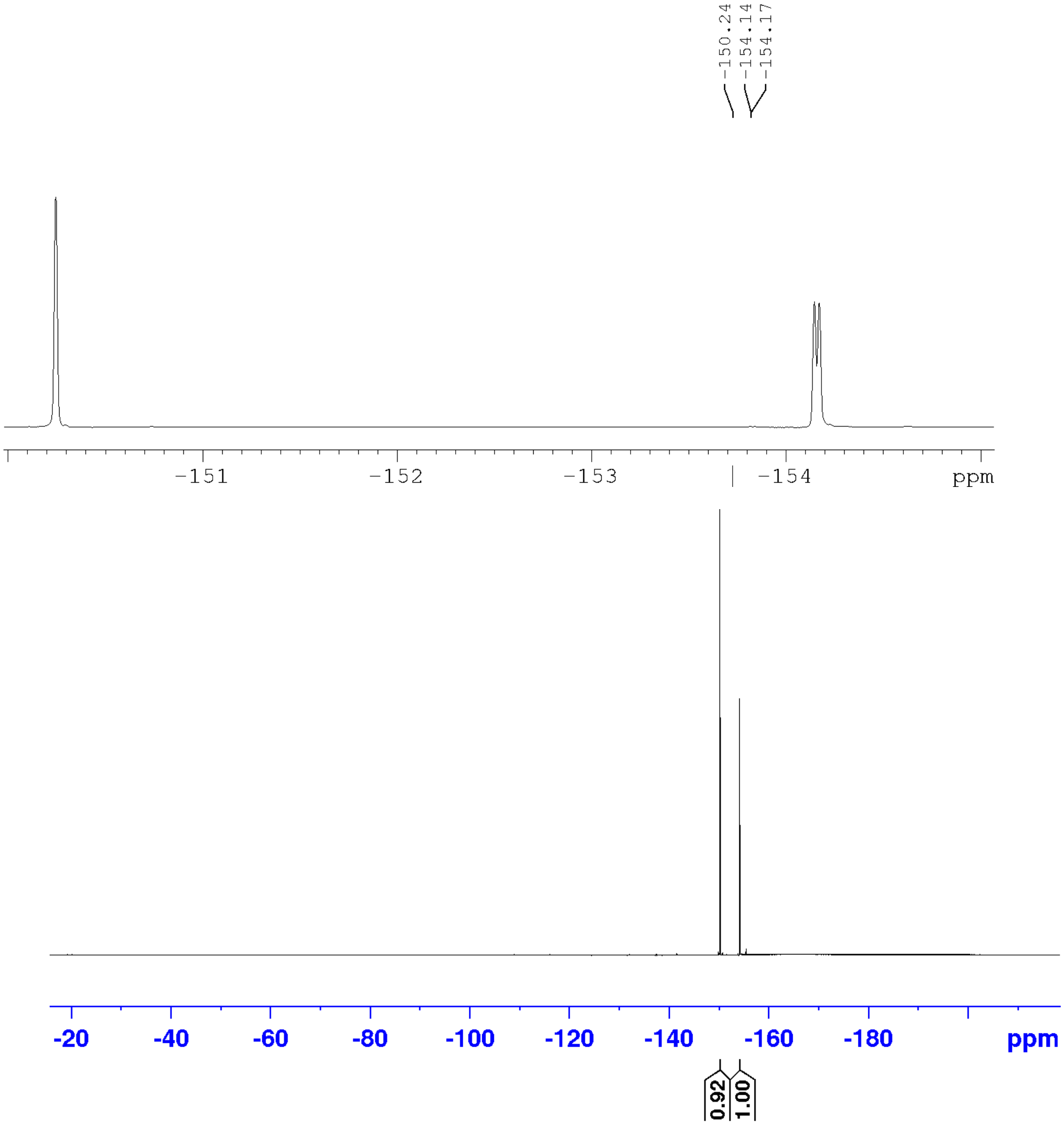
2,4-difluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol, **3g**

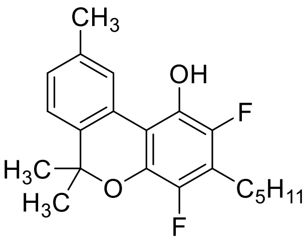




^{19}F-NMR

2,4-difluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol, **3g**

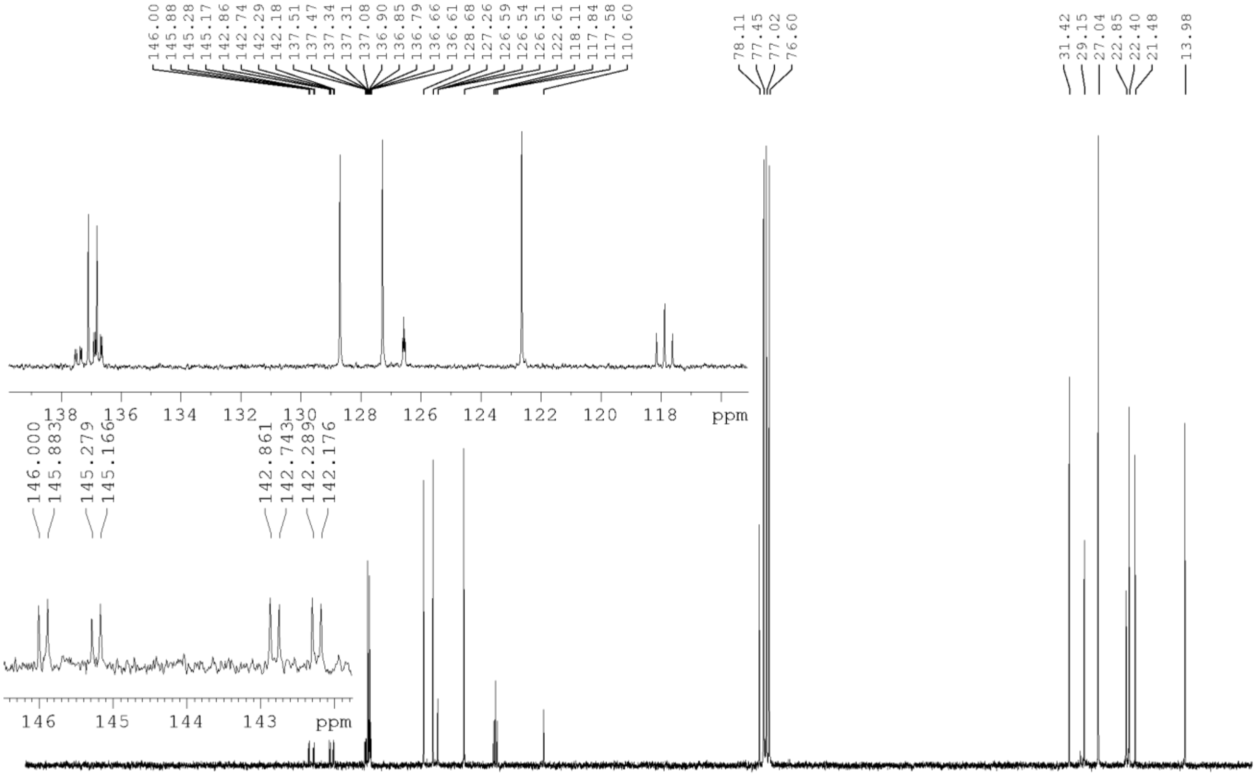


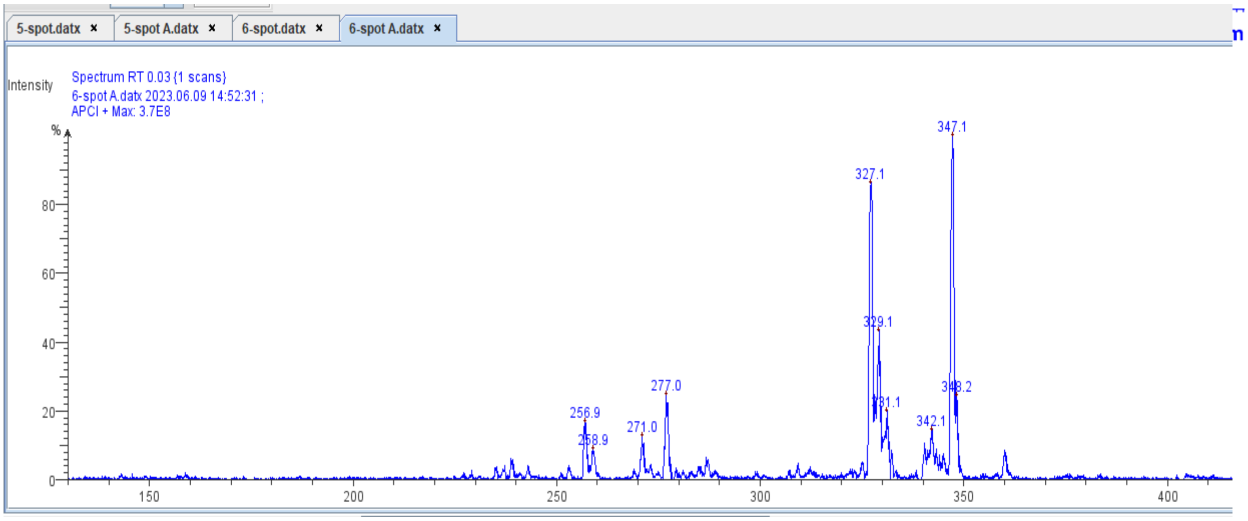


^{13}C-NMR and Mass spectrum

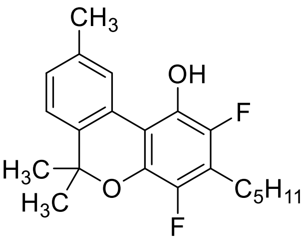
2,4-difluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol,

3g



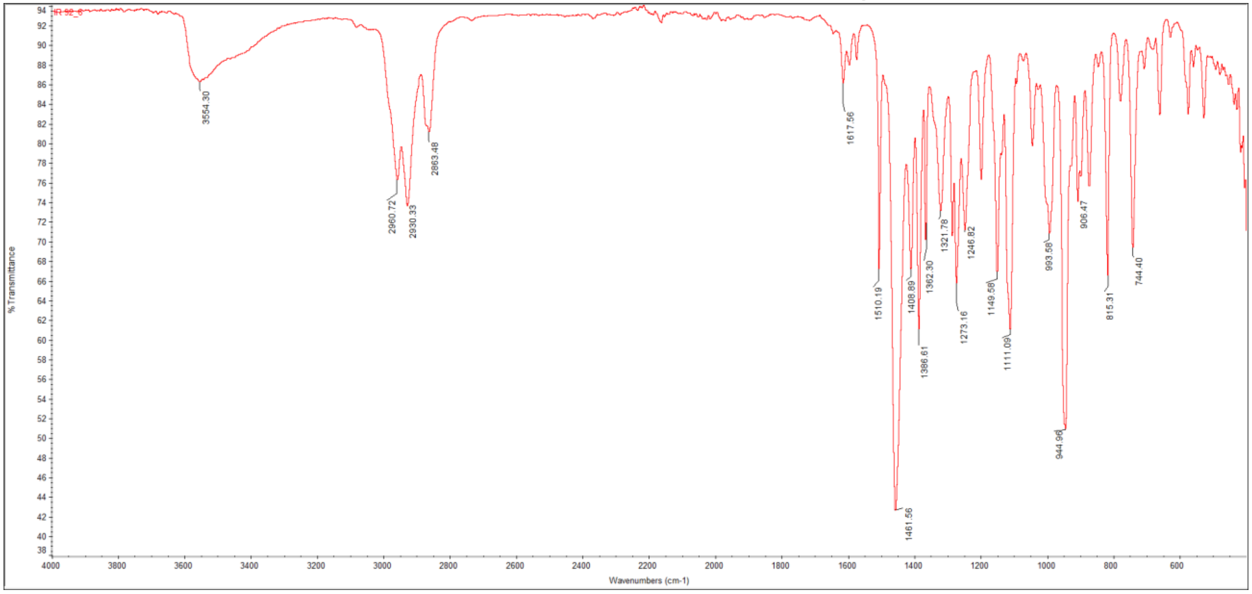


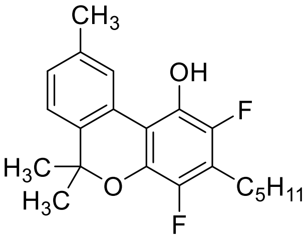
Spectrum RT 0.03 (1 scans)
6-spot A.datx 2023.06.09 14:52:31 ;
APCI + Max: 3.7E8



IR data

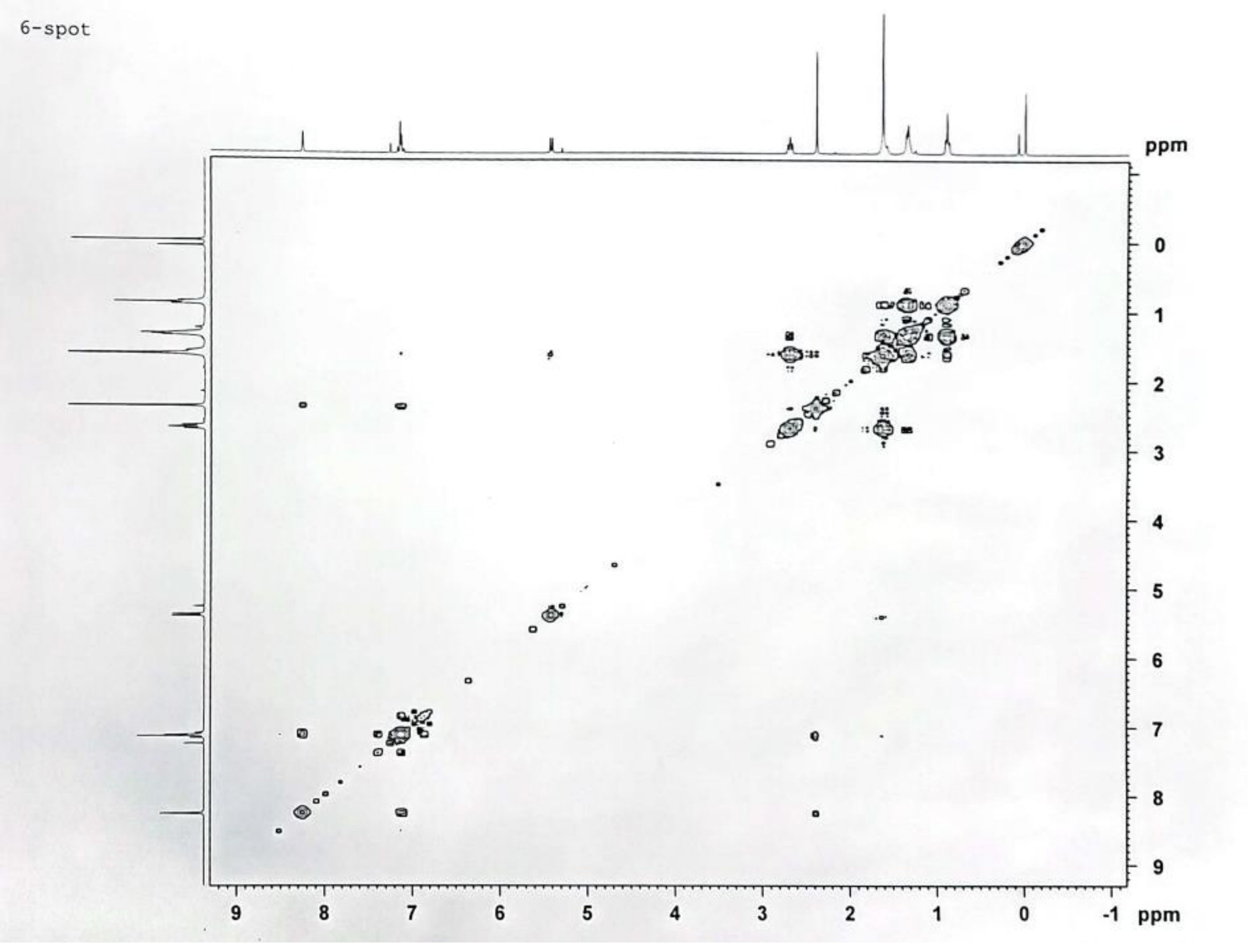
2,4-difluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol, **3g**





2D- NMR

2,4-difluoro-6,6,9-trimethyl-3-pentyl-6*H*-benzo[*c*]chromen-1-ol, **3g**



^{19}F-NMR comparison for FTEDA reaction mixture and NFSI reaction mixture