

Supporting Information

Synthesis of Fluorinated Polycyclic Dehydroaltenusin Analogs through Hypervalent Iodine-Catalyzed Dearomatization

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1. Experimental Section

General Information. ^1H - and ^{13}C -NMR spectra were recorded in CDCl_3 solution on a Bruker Avance 500 spectrometer at 20~25 °C. ^1H NMR spectra were reported in parts per million using tetramethylsilane TMS ($\delta = 0.00$ ppm) as an internal standard. The data of ^1H NMR were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (J , Hz), and integration. ^{13}C NMR spectra were reported in parts per million using solvent CDCl_3 ($\delta = 77.2$ ppm) as an internal standard. The data of ^{13}C NMR were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), and coupling constants (J , Hz). High resolution mass spectra (HRMS) were obtained with a Q-TOF MS spectrometer. Thin layer chromatography (TLC) was performed on a glass plate coated with GF254 silica gel and observed under 254nm UV light, while column chromatography was performed using silica gel HG/T2354-2010. All reagents were analytically pure, purchased from commercial suppliers and used directly unless further purification is indicated otherwise. All reactions were performed at atmospheric pressure and all reagent weighing was performed at room temperature in air.

Typical Procedure for Synthesis of 1.

For starting materials: **1a, 1b, 1c, 1d, 1e, 1f, 1g, 1h, 1i, 1j and 1k.**

(i) To a solution of bromobenzoate (10 mmol), 2 N Na_2CO_3 (10 mL, 2 equivalents) and (3-hydroxyphenyl) boronic acid (10 mmol, 1 equivalent) in toluene (50 mL) was added $\text{Pd}(\text{dppf})\text{Cl}_2$ (0.5 mmol, 5 mol %) under argon. After stirring for 14 h, the solvent was removed by vacuum and the mixture was purified by silica-gel column chromatography (10 : 1 petroleum ether : EtOAc) to give colourless oil liquid biphenyl-carboxylate (90% yield). (ii) To a solution of biphenyl-carboxylate (9 mmol) in THF (25.0 mL) and MeOH (25.0 mL) was added 2 N NaOH (25.0 mL, 5.6 equivalents) and stirred overnight at room temperature. The reaction mixture was cooled to 0 °C, quenched with 1 N HCl until pH reached to 2, and extracted with EtOAc (30 mL \times 3). The organic layers were dried over anhydrous MgSO_4 and the solvents were removed in vacuo to give pure solid biphenyl-carboxylic acid with quantitative yield.

For starting materials: **1l, 1m, 1n, 1o and 1p.**

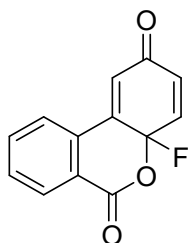
(i) To a solution of 3-bromophenol (10 mmol), 2 N Na_2CO_3 (10 mL, 2 equivalents) and (2-(methoxycarbonyl)phenyl) boronic acid (10 mmol, 1 equivalent) in DMF (50 mL) was added $\text{Pd}(\text{PPh}_3)_4$ (0.5 mmol, 5 mol %) under argon. After stirring for 14 h, the solvent was removed by vacuum and the mixture was purified by silica-gel column chromatography (10 : 1 petroleum ether : EtOAc) to give colourless oil liquid biphenyl-carboxylate (80% yield). (ii) To a solution of biphenyl-carboxylate (9 mmol) in THF (25.0 mL) and MeOH (25.0 mL) was added 2 N NaOH (25.0 mL, 5.6 equivalents) and stirred overnight at room temperature. The reaction mixture was cooled to 0 °C, quenched with 1 N HCl until pH reached to 2, and extracted with EtOAc (30 mL \times 3). The organic layers were dried over anhydrous MgSO_4 and the solvents were removed in vacuo to give pure solid biphenyl-carboxylic acid with quantitative yield.

General Procedure for Synthesis of 2.

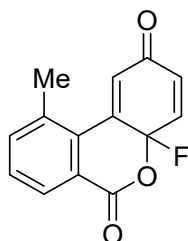
To a round-bottom flask was charged with **1** (0.3 mmol), 20 wt% HFIP, *m*-CPBA (1.2 mmol), PhI (0.15 mmol) and pyr-HF (1.8 mmol) in DCM (1 mL) at 35 °C for 10 h. The reaction was quenched with saturated solution of $\text{Na}_2\text{S}_2\text{O}_3$ (1 mL). The organic phase was separated, and the aqueous layer was extracted with DCM (5 mL \times 3). The combined

organic solution was dried with Mg_2SO_4 and concentrated in vacuo. The resulting residue was purified by a column chromatography to give **2**.

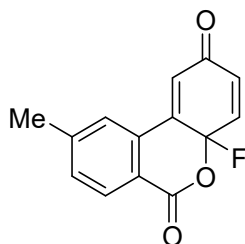
2. ¹H-NMR, ¹³C-NMR, ¹⁹F-NMR and HRMS Analytical Data



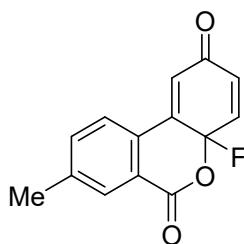
4a-fluoro-6H-benzo[c]chromene-2,6(4aH)-dione (**2a**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 63.5 mg (92%) of **2a**. yellowish solid. mp 140-141 °C. ¹H NMR (500 MHz, CDCl₃) δ 8.23 (d, *J* = 8 Hz, 1H), 7.80 (t, *J* = 8 Hz, 1H), 7.75 (d, *J* = 8 Hz, 1H), 7.69 (t, *J* = 8 Hz, 1H), 6.98 (dd, *J* = 10, 3 Hz, 1H), 6.70 (s, 1H), 6.44 (d, *J* = 10 Hz, 1H). ¹³C {H} NMR (126 MHz, CDCl₃) δ 184.0 (d, *J* = 4 Hz), 160.2, 141.2 (d, *J* = 10 Hz), 138.3 (d, *J* = 10 Hz), 135.6, 132.2, 132.1, 131.2, 131.1, 124.8, 124.4 (d, *J* = 4 Hz), 122.8, 102.6 (d, *J* = 214 Hz). HRMS (ESI-TOF) *m/z* calcd for C₁₃H₇FO₃ (M-H)⁻ 229.0306, found 229.0302. ¹⁹F NMR(376 MHz, CDCl₃): -90.6 ppm.



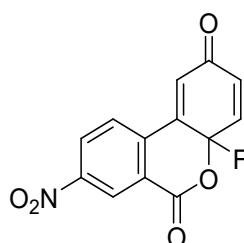
4a-fluoro-10-methyl-6H-benzo[c]chromene-2,6(4aH)-dione (**2b**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 69.1 mg (94%) of **2b**. yellowish solid. mp 146-147 °C. ¹H NMR (500 MHz, CDCl₃) δ 8.10 (d, *J* = 7.5 Hz, 1H), 7.63 (d, *J* = 7.5 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 6.97 (dd, *J* = 10, 5 Hz, 1H), 6.59 (s, 1H), 6.45 (d, *J* = 10 Hz, 1H), 2.59 (s, 3H). ¹³C {H} NMR (126 MHz, CDCl₃) δ 184.1 (d, *J* = 4 Hz), 160.7, 140.6 (d, *J* = 25 Hz), 138.6 (d, *J* = 25 Hz), 138.3, 137.1, 130.9, 130.6, 130.3 (d, *J* = 8 Hz), 129.3, 128.2 (d, *J* = 5 Hz), 123.9, 102.3 (d, *J* = 215 Hz), 21.3. HRMS (ESI-TOF) *m/z* calcd for C₁₄H₉FO₃ (M+Na)⁺ 267.0427, found 267.0429. ¹⁹F NMR(376 MHz, CDCl₃): -96.6 ppm.



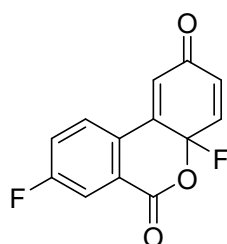
4a-fluoro-9-methyl-6H-benzo[c]chromene-2,6(4aH)-dione (**2c**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 66.1 mg (90%) of **2c**. yellowish solid. mp 145-147 °C. ¹H NMR (500 MHz, CDCl₃) δ 8.12 (d, *J* = 8 Hz, 1H), 7.54 (s, 1H), 7.48 (d, *J* = 8 Hz, 1H), 6.97 (dd, *J* = 10, 4 Hz, 1H), 6.69 (s, 1H), 6.44 (d, *J* = 10 Hz, 1H), 2.52 (s, 3H). ¹³C {H} NMR (126 MHz, CDCl₃) δ 184.2 (d, *J* = 4 Hz), 160.3, 147.0, 141.5 (d, *J* = 25 Hz), 138.4 (d, *J* = 25 Hz), 133.2, 132.0, 131.2, 131.0 (d, *J* = 8 Hz), 125.1, 124.1 (d, *J* = 4 Hz), 120.3, 102.7 (d, *J* = 212 Hz), 22.2. HRMS (ESI-TOF) *m/z* calcd for C₁₄H₉FO₃ (M-H)⁻ 243.0463, found 243.0464. ¹⁹F NMR(376 MHz, CDCl₃): -90.8 ppm.



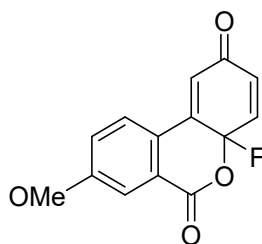
4a-fluoro-8-methyl-6H-benzo[c]chromene-2,6(4aH)-dione (**2d**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 67.6 mg (92%) of **2d**. yellowish solid. mp 144-145 °C. ^1H NMR (500 MHz, CDCl_3) δ 8.10 (d, J = 8 Hz, 1H), 7.54 (s, 1H), 7.48 (d, J = 8 Hz, 1H), 6.97 (dd, J = 10, 5 Hz, 1H), 6.69 (s, 1H), 6.44 (d, J = 10 Hz, 1H), 2.53 (s, 3H). ^{13}C {H} NMR (126 MHz, CDCl_3) δ 184.1 (d, J = 5 Hz), 160.3, 147.0, 141.4 (d, J = 25 Hz), 138.4 (d, J = 25 Hz), 133.2, 132.0, 131.1, 131.0 (d, J = 8 Hz), 125.2, 124.1 (d, J = 4 Hz), 120.2, 102.7 (d, J = 212 Hz), 22.2. HRMS (ESI-TOF) m/z calcd for $\text{C}_{14}\text{H}_9\text{FO}_3$ (M-H) $^-$ 243.0463, found 243.0462. ^{19}F NMR(376 MHz, CDCl_3): -90.8 ppm.



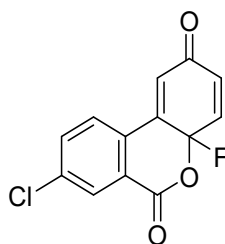
4a-fluoro-8-nitro-6H-benzo[c]chromene-2,6(4aH)-dione (**2e**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 60.4 mg (73%) of **2e**. yellowish solid. mp 157-159 °C. ^1H NMR (500 MHz, CDCl_3) δ 9.05 (s, 1H), 8.63 (d, J = 8 Hz, 1H), 7.99 (d, J = 8 Hz, 1H), 7.04 (dd, J = 10, 4 Hz, 1H), 6.85 (s, 1H), 6.52 (d, J = 10 Hz, 1H). ^{13}C {H} NMR (126 MHz, CDCl_3) δ 183.2 (d, J = 4 Hz), 158.4, 149.8, 139.0 (d, J = 25 Hz), 137.9 (d, J = 25 Hz), 137.2, 131.4 (d, J = 8 Hz), 129.7, 126.9 (d, J = 5 Hz), 126.6, 126.3, 124.4, 102.6 (d, J = 215 Hz). HRMS (ESI-TOF) m/z calcd for $\text{C}_{13}\text{H}_6\text{FNO}_5$ (M-H) $^-$ 274.0157, found 274.0152. ^{19}F NMR(376 MHz, CDCl_3): -91.1 ppm.



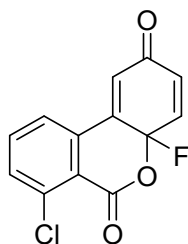
4a,8-difluoro-6H-benzo[c]chromene-2,6(4aH)-dione (**2f**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 50.8 mg (68%) of **2f**. yellowish solid. mp 151-152 °C. ^1H NMR (500 MHz, CDCl_3) δ 7.91 (dd, J = 8, 2.5 Hz, 1H), 7.78 (dd, J = 8, 5 Hz, 1H), 7.51 (dt, J = 8, 2.5 Hz, 1H), 6.98 (dd, J = 10, 4 Hz, 1H), 6.67 (d, J = 1 Hz, 1H), 6.46 (d, J = 10 Hz, 1H). ^{13}C {H} NMR (126 MHz, CDCl_3) δ 183.8 (d, J = 5 Hz), 164.6 (d, J = 250 Hz), 159.3 (d, J = 3 Hz), 140.2 (d, J = 25 Hz), 137.9 (d, J = 25 Hz), 131.3 (d, J = 8 Hz), 128.3 (d, J = 3 Hz), 127.4 (d, J = 8 Hz), 125.1 (d, J = 8 Hz), 124.3 (d, J = 3 Hz), 123.4 (d, J = 25 Hz), 117.8 (d, J = 25 Hz), 102.7 (d, J = 213 Hz). HRMS (ESI-TOF) m/z calcd for $\text{C}_{13}\text{H}_6\text{F}_2\text{O}_3$ (M-H) $^-$ 247.0212, found 247.0212. ^{19}F NMR(376 MHz, CDCl_3): -90.8, -99.3 ppm.



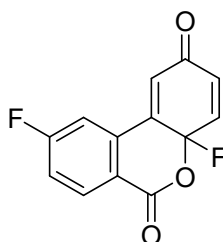
4a-fluoro-8-methoxy-6H-benzo[c]chromene-2,6(4aH)-dione (**2g**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 63.4 mg (81%) of **2g**. yellowish solid. mp 143-144 °C. ¹H NMR (500 MHz, CDCl₃) δ 7.66-7.68 (m, 2H), 7.30 (dd, *J* = 10, 3 Hz, 1H), 6.95 (dd, *J* = 10, 4 Hz, 1H), 6.60 (d, *J* = 2 Hz, 1H), 6.42 (d, *J* = 10 Hz, 1H), 3.93 (s, 3H). ¹³C {¹H} NMR (126 MHz, CDCl₃) δ 184.1 (d, *J* = 5 Hz), 162.7, 160.4, 141.2 (d, *J* = 25 Hz), 137.9 (d, *J* = 25 Hz), 131.3 (d, *J* = 6 Hz), 126.6, 124.6, 124.3, 123.3, 122.6 (d, *J* = 4 Hz), 113.8, 102.8 (d, *J* = 212 Hz), 56.2. HRMS (ESI-TOF) *m/z* calcd for C₁₄H₉FO₄ (M-H)⁻ 259.0412, found 259.0410. ¹⁹F NMR(376 MHz, CDCl₃): -88.6 ppm.



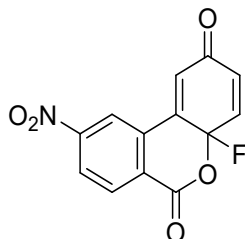
8-chloro-4a-fluoro-6H-benzo[c]chromene-2,6(4aH)-dione (**2h**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 60.4 mg (76%) of **2h**. yellowish solid. mp 145-146 °C. ¹H NMR (500 MHz, CDCl₃) δ 8.20 (s, 1H), 7.76 (d, *J* = 8 Hz, 1H), 7.70 (d, *J* = 8 Hz, 1H), 6.98 (dd, *J* = 10, 4 Hz, 1H), 6.70 (s, 1H), 6.46 (d, *J* = 10 Hz, 1H). ¹³C {¹H} NMR (126 MHz, CDCl₃) δ 183.7 (d, *J* = 5 Hz), 159.2, 140.1 (d, *J* = 25 Hz), 138.7, 138.0 (d, *J* = 25 Hz), 135.7, 131.2 (d, *J* = 8 Hz), 130.9, 130.4, 126.4, 124.6 (d, *J* = 4 Hz), 124.2, 102.6 (d, *J* = 213 Hz). HRMS (ESI-TOF) *m/z* calcd for C₁₃H₆ClFO₃ (M-H)⁻ 262.9916, found 262.9920. ¹⁹F NMR(376 MHz, CDCl₃): -90.3 ppm.



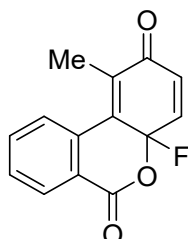
7-chloro-4a-fluoro-6H-benzo[c]chromene-2,6(4aH)-dione (**2i**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 57.2 mg (72%) of **2i**. yellowish solid. mp 147-148 °C. ¹H NMR (500 MHz, CDCl₃) δ 7.64-7.73 (m, 3H), 6.98 (dd, *J* = 10, 5 Hz, 1H), 6.69 (s, 1H), 6.46 (d, *J* = 10 Hz, 1H). ¹³C {¹H} NMR (126 MHz, CDCl₃) δ 183.8 (d, *J* = 4 Hz), 156.6, 141.9 (d, *J* = 25 Hz), 138.4, 138.0 (d, *J* = 25 Hz), 135.2 (d, *J* = 8 Hz), 134.6, 131.0 (d, *J* = 8 Hz), 124.9 (d, *J* = 4 Hz), 123.9, 120.3, 102.1 (d, *J* = 213 Hz). HRMS (ESI-TOF) *m/z* calcd for C₁₃H₆ClFO₃ (M-H)⁻ 262.9916, found 262.9913. ¹⁹F NMR(376 MHz, CDCl₃): -94.2 ppm.



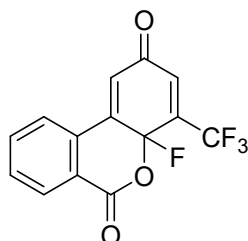
4a,9-difluoro-6*H*-benzo[*c*]chromene-2,6(4*aH*)-dione (**2j**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 50.8 mg (68%) of **2j**. yellowish solid. mp 141-143 °C. ¹H NMR (500 MHz, CDCl₃) δ 8.27 (dd, *J* = 8, 5 Hz, 1H), 7.42 (d, *J* = 8 Hz, 1H), 7.36 (t, *J* = 8 Hz, 1H), 6.99 (dd, *J* = 10, 4 Hz, 1H), 6.69 (s, 1H), 6.46 (d, *J* = 10 Hz, 1H). ¹³C {¹H} NMR (126 MHz, CDCl₃) δ 183.7 (d, *J* = 5 Hz), 166.9 (d, *J* = 256 Hz), 159.3, 140.2 (d, *J* = 25 Hz), 138.2 (d, *J* = 25 Hz), 134.8 (d, *J* = 10 Hz), 134.3 (d, *J* = 10 Hz), 131.1 (d, *J* = 6 Hz), 125.2 (d, *J* = 5 Hz), 119.8 (d, *J* = 25 Hz), 119.2 (d, *J* = 4 Hz), 111.8 (d, *J* = 25 Hz), 102.6 (d, *J* = 218 Hz). HRMS (ESI-TOF) *m/z* calcd for C₁₃H₆F₂O₃ (M-H)⁻ 247.0212, found 247.0211. ¹⁹F NMR(376 MHz, CDCl₃): -90.6, -104.4 ppm.



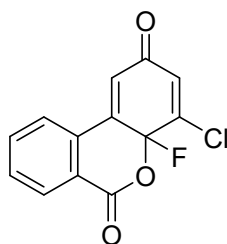
4a-fluoro-9-nitro-6*H*-benzo[*c*]chromene-2,6(4*aH*)-dione (**2k**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 62.9 mg (76%) of **2k**. yellowish solid. mp 167-168 °C. ¹H NMR (500 MHz, CDCl₃) δ 8.60 (d, *J* = 2 Hz, 1H), 8.45-8.50 (m, 2H), 7.03 (dd, *J* = 10, 4 Hz, 1H), 6.87 (d, *J* = 2 Hz, 1H), 6.53 (d, *J* = 10 Hz, 1H). ¹³C {¹H} NMR (126 MHz, CDCl₃) δ 183.2 (d, *J* = 4 Hz), 158.6, 152.0, 139.0 (d, *J* = 25 Hz), 137.7 (d, *J* = 25 Hz), 133.7, 132.9, 131.5 (d, *J* = 8 Hz), 127.4, 126.3 (d, *J* = 5 Hz), 126.2, 120.2, 102.7 (d, *J* = 213 Hz). HRMS (ESI-TOF) *m/z* calcd for C₁₃H₆FNO₅ (M-H)⁻ 274.0157, found 274.0155. ¹⁹F NMR(376 MHz, CDCl₃): -91.1 ppm.



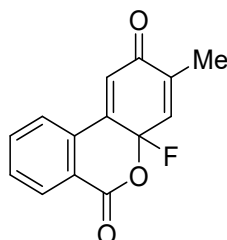
4a-fluoro-1-methyl-6*H*-benzo[*c*]chromene-2,6(4*aH*)-dione (**2l**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 38.1 mg (52%) of **2l**. yellowish solid. mp 161-162 °C. ¹H NMR (500 MHz, CDCl₃) δ 8.22 (d, *J* = 8 Hz, 1H), 8.64-8.80 (m, 3H), 6.93 (dd, *J* = 10, 4 Hz, 1H), 6.46 (d, *J* = 8 Hz, 1H), 2.24 (s, 3H). ¹³C {¹H} NMR (126 MHz, CDCl₃) δ 184.6 (d, *J* = 4 Hz), 160.8, 137.9 (d, *J* = 25 Hz), 135.8 (d, *J* = 25 Hz), 134.4, 134.1, 132.9, 130.8 (d, *J* = 8 Hz), 130.6 (d, *J* = 5 Hz), 128.9, 124.4, 103.4 (d, *J* = 213 Hz), 12.8. HRMS (ESI-TOF) *m/z* calcd for C₁₄H₉FO₃ (M+H)⁺ 267.0427, found 267.0430. ¹⁹F NMR(376 MHz, CDCl₃): -95.9 ppm.



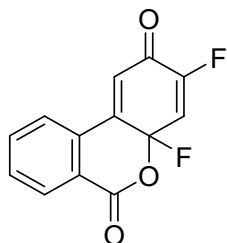
4a-fluoro-4-(trifluoromethyl)-6*H*-benzo[*c*]chromene-2,6(4*aH*)-dione (**2m**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 33.9 mg (38%) of **2m**. yellowish solid. mp 164-165 °C. ¹H NMR (500 MHz, CDCl₃) δ 8.26 (d, *J* = 8 Hz, 1H), 7.74-7.84 (m, 3H), 6.86 (s, 4 Hz, 1H), 6.80 (s, 1H). ¹³C {¹H} NMR (126 MHz, CDCl₃) δ 182.2 (d, *J* = 4 Hz), 158.5, 142.0 (d, *J* = 25 Hz), 137.8 (dt, *J* = 25, 10 Hz), 135.8, 132.9, 132.2 (t, *J* = 6 Hz), 131.3, 131.2, 125.3, 123.5 (d, *J* = 5 Hz), 122.7, 120.9 (d, *J* = 275 Hz), 102.2 (d, *J* = 213 Hz). HRMS (ESI-TOF) *m/z* calcd for C₁₄H₆F₄O₃ (M-H)⁻ 297.0180, found 297.0178. ¹⁹F NMR(376 MHz, CDCl₃): -63.1, -90.9 ppm.



4-chloro-4a-fluoro-6H-benzo[c]chromene-2,6(4aH)-dione (**2n**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 24.4 mg (31%) of **2n**. yellowish solid. mp 164-165 °C. ^1H NMR (500 MHz, CDCl_3) δ 8.25 (d, J = 8 Hz, 1H), 7.72-7.83 (m, 3H), 6.72 (s, 4 Hz, 1H), 6.66 (s, 1H). ^{13}C {H} NMR (126 MHz, CDCl_3) δ 181.7 (d, J = 4 Hz), 159.1, 146.1 (d, J = 25 Hz), 141.6 (d, J = 25 Hz), 135.8, 132.5, 131.8, 131.2, 130.2 (d, J = 4 Hz), 124.9, 124.2, 122.8, 101.2 (d, J = 221 Hz). HRMS (ESI-TOF) m/z calcd for $\text{C}_{13}\text{H}_6\text{ClFO}_3$ (M-H) $^-$ 262.9916, found 262.9914. ^{19}F NMR(376 MHz, CDCl_3): -93.8 ppm.



4a-fluoro-3-methyl-6H-benzo[c]chromene-2,6(4aH)-dione (**2o**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 19.7 mg (27%) of **2o**. yellowish solid. mp 164-165 °C. ^1H NMR (500 MHz, CDCl_3) δ 8.23 (d, J = 8 Hz, 1H), 7.67-7.79 (m, 3H), 6.76 (d, J = 1.5 Hz, 1H), 6.69 (s, 1H), 2.03 (t, J = 2.5 Hz, 3H). ^{13}C {H} NMR (126 MHz, CDCl_3) δ 184.9 (d, J = 4 Hz), 160.6, 141.1 (d, J = 10 Hz), 139.0 (d, J = 10 Hz), 135.4, 133.9, 133.6, 132.4 (d, J = 4 Hz), 131.0, 124.8, 124.4 (d, J = 4 Hz), 122.9, 102.3 (d, J = 208 Hz), 15.4. HRMS (ESI-TOF) m/z calcd for $\text{C}_{14}\text{H}_9\text{FO}_3$ (M+Na) $^+$ 267.0427, found 267.0431. ^{19}F NMR(376 MHz, CDCl_3): -90.3 ppm.

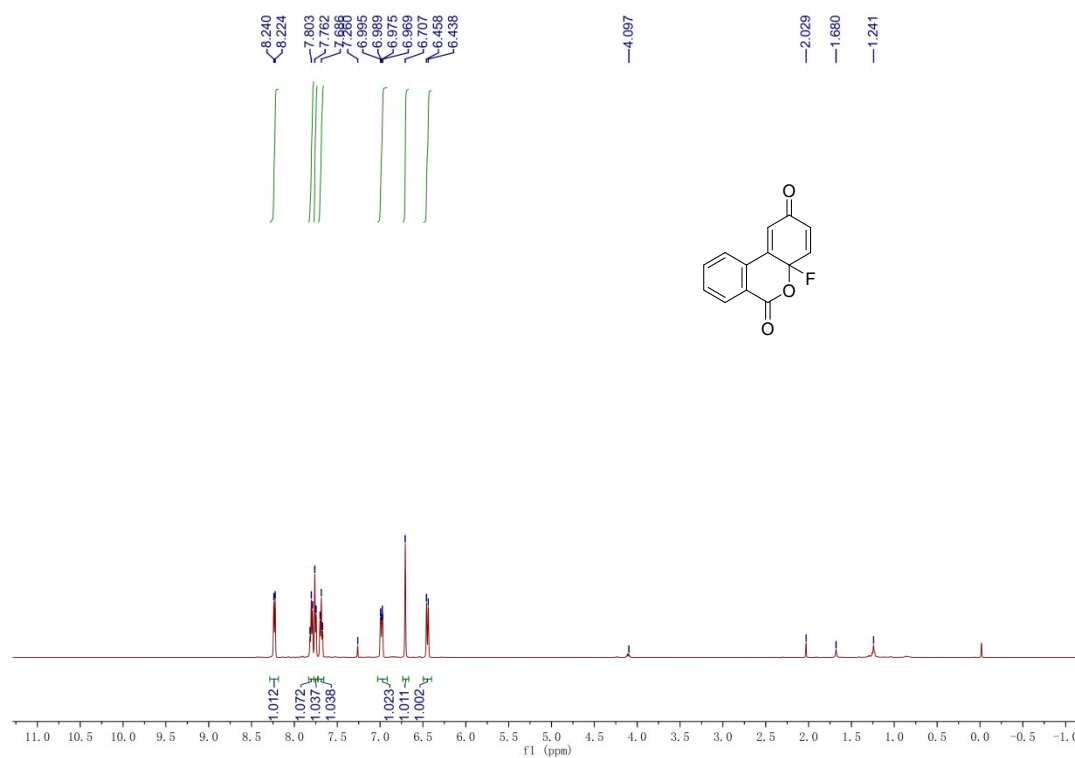


3,4a-difluoro-6H-benzo[c]chromene-2,6(4aH)-dione (**2p**). Purification was performed by column chromatography (petroleum ether / ethyl acetate = 10 / 1) to afford 11.6 mg (29%) of **2p**. yellowish solid. mp 164-165 °C. ^1H NMR (500 MHz, CDCl_3) δ 8.25 (d, J = 8 Hz, 1H), 7.73-7.83 (m, 3H), 6.70 (d, J = 6 Hz, 1H), 6.60 (dd, J = 3.5, 5 Hz, 1H). ^{13}C {H} NMR (126 MHz, CDCl_3) δ 177.1 (dd, J = 4, 20 Hz), 159.7, 155.6 (dd, J = 10, 275 Hz), 142,5 (d, J = 30 Hz), 135.7, 132.8, 131.4, 131.3, 125.1, 122.8, 122.5 (d, J = 4 Hz), 115.6 (d, J = 4 Hz), 105.7 (dd, J = 15, 213 Hz). HRMS (ESI-TOF) m/z calcd for $\text{C}_{13}\text{H}_6\text{F}_2\text{O}_3$ (M-H) $^-$ 247.0212, found 247.0210. ^{19}F NMR(376 MHz, CDCl_3): -87.3, -123.7 ppm.

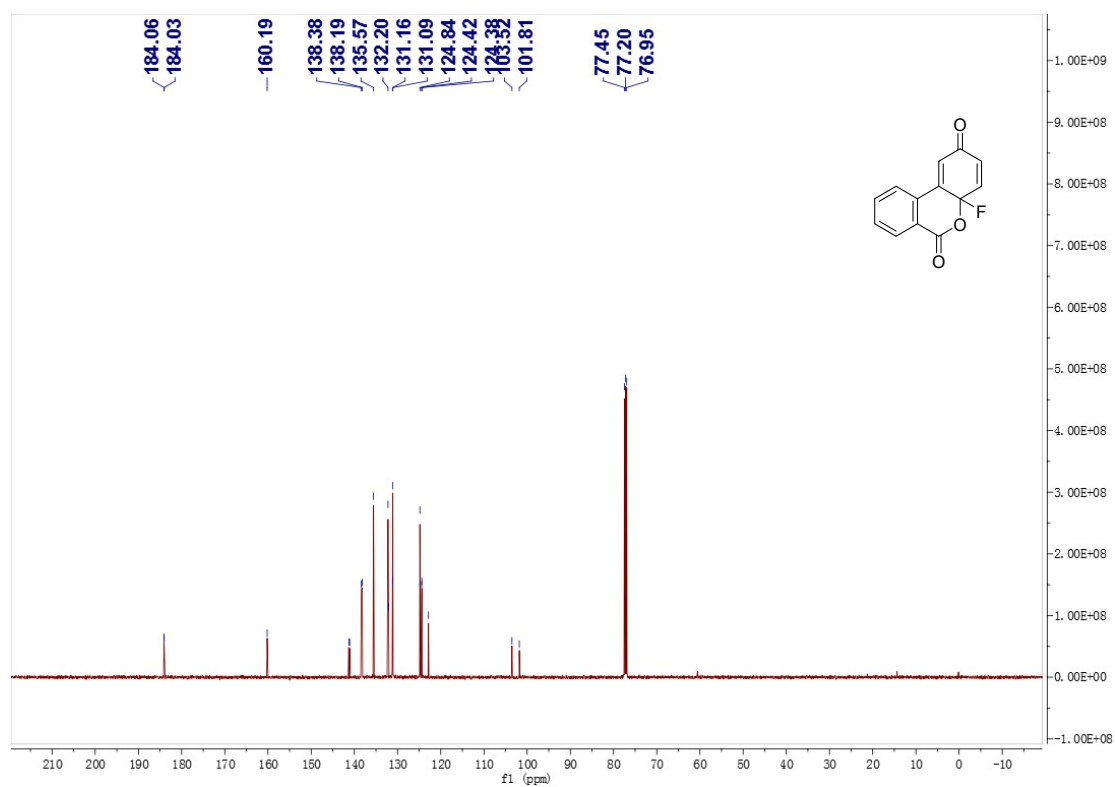
3. Copies of ^1H -NMR, ^{13}C -NMR, ^{19}F -NMR and HRMS spectra of products

4a-fluoro-6*H*-benzo[*c*]chromene-2,6(4*aH*)-dione (**2a**)

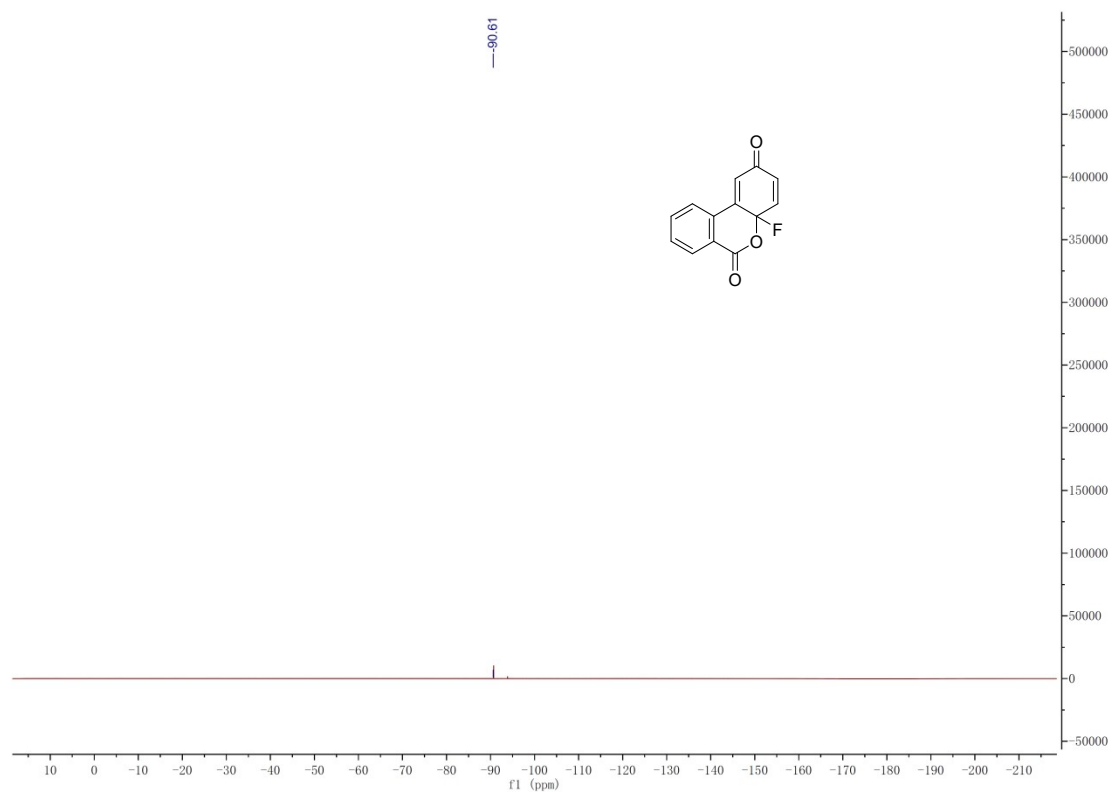
^1H NMR (500 MHz, CDCl_3)



^{13}C { ^1H } NMR (126 MHz, CDCl_3)



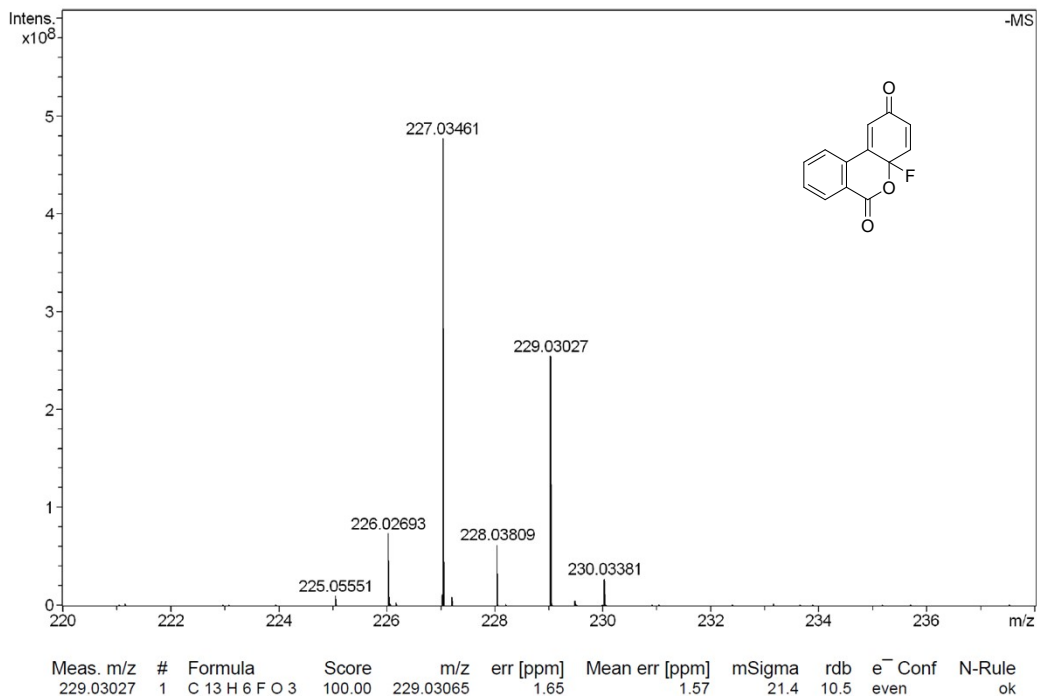
^{19}F NMR(376 MHz, CDCl_3)



HRMS (ESI-TOF) m/z calcd for $\text{C}_{13}\text{H}_7\text{FO}_3$ ($\text{M}-\text{H}$) $^-$ 229.0307, found 229.0303.

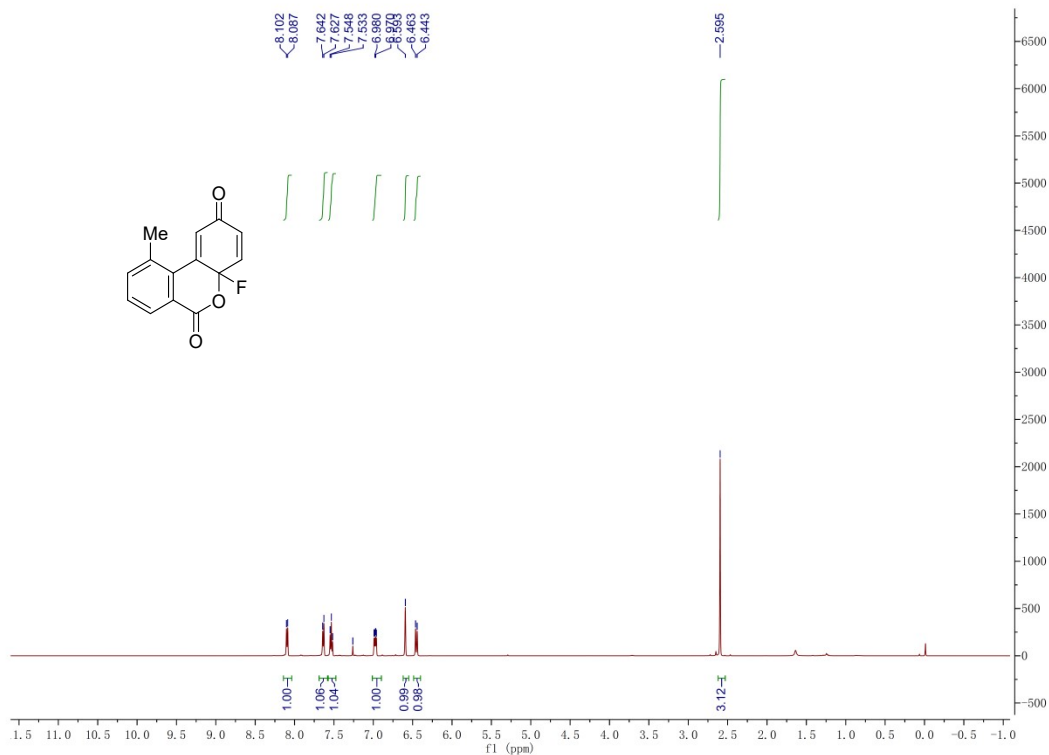
Acquisition Parameter

Polarity	Negative	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	200.7 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Wed Jun 17 02:41:42
Pulse Program	basic	n/a	n/a	Data Acquisition Size	1020576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.200 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec				

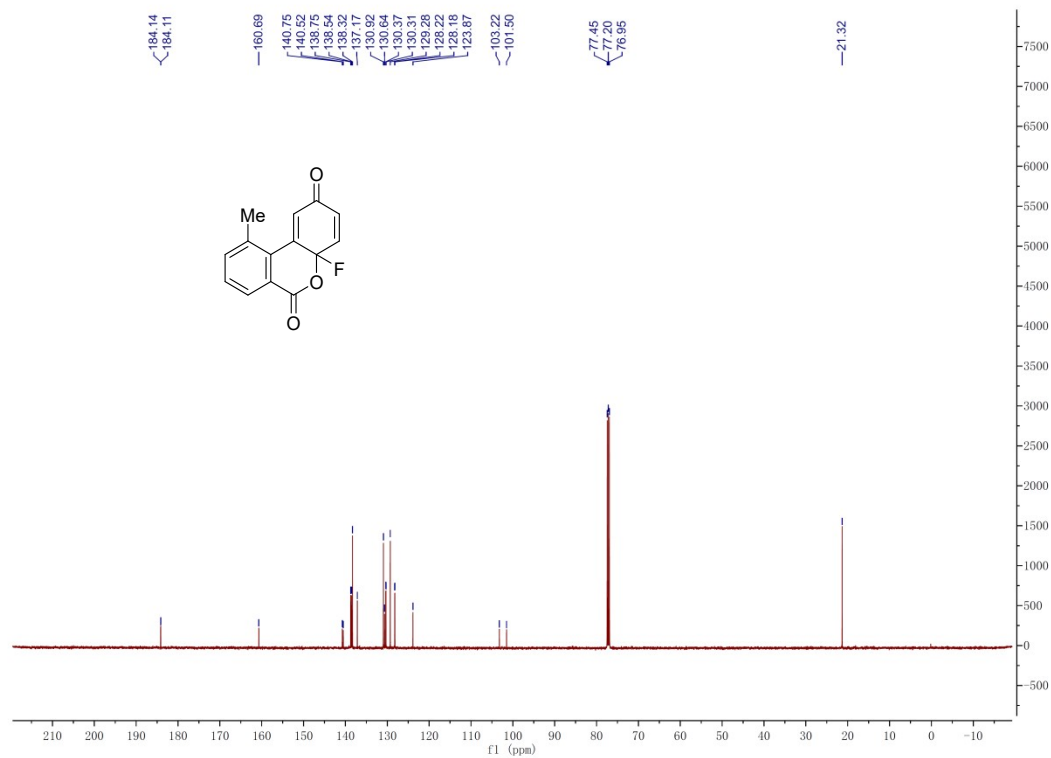


4a-fluoro-10-methyl-6H-benzo[c]chromene-2,6(4aH)-dione (**2b**)

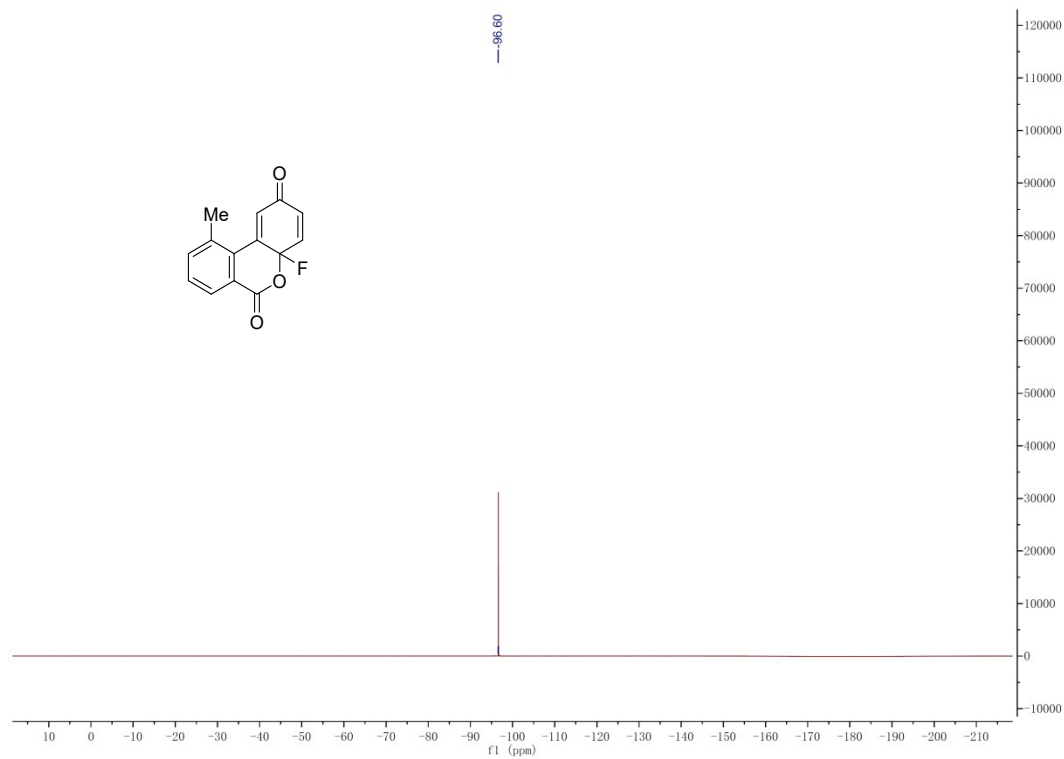
¹H NMR (500 MHz, CDCl₃)



^{13}C { ^1H } NMR (126 MHz, CDCl_3)



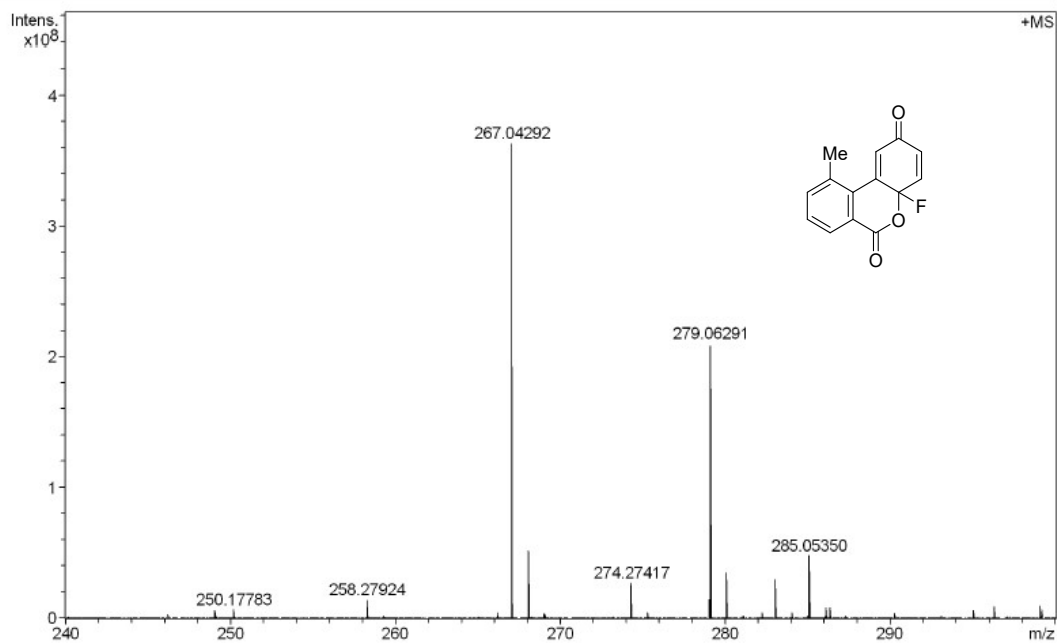
^{19}F NMR(376 MHz, CDCl_3)



HRMS (ESI-TOF) m/z calcd for $\text{C}_{14}\text{H}_9\text{FO}_3$ ($\text{M}+\text{Na}$) $^+$ 267.0428, found 267.0429.

Acquisition Parameter

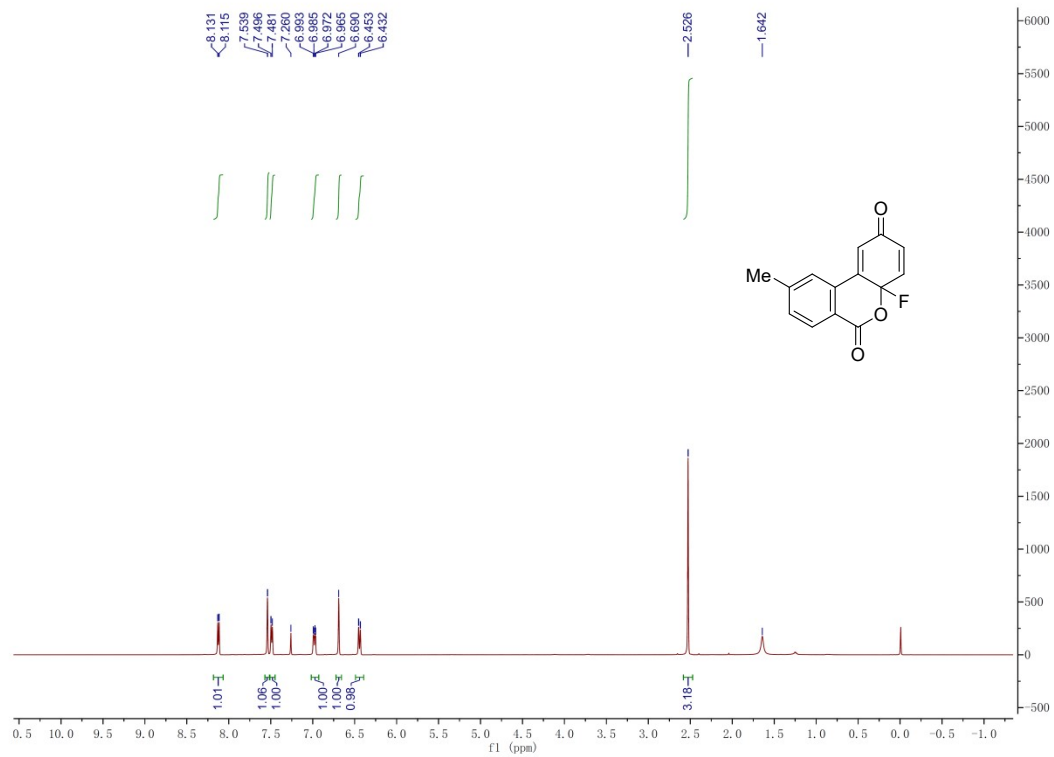
Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	100.4 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Wed Jun 17 02:41:42
Pulse Program	basic	n/a	n/a	Data Acquisition Size	2028576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.200 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec				



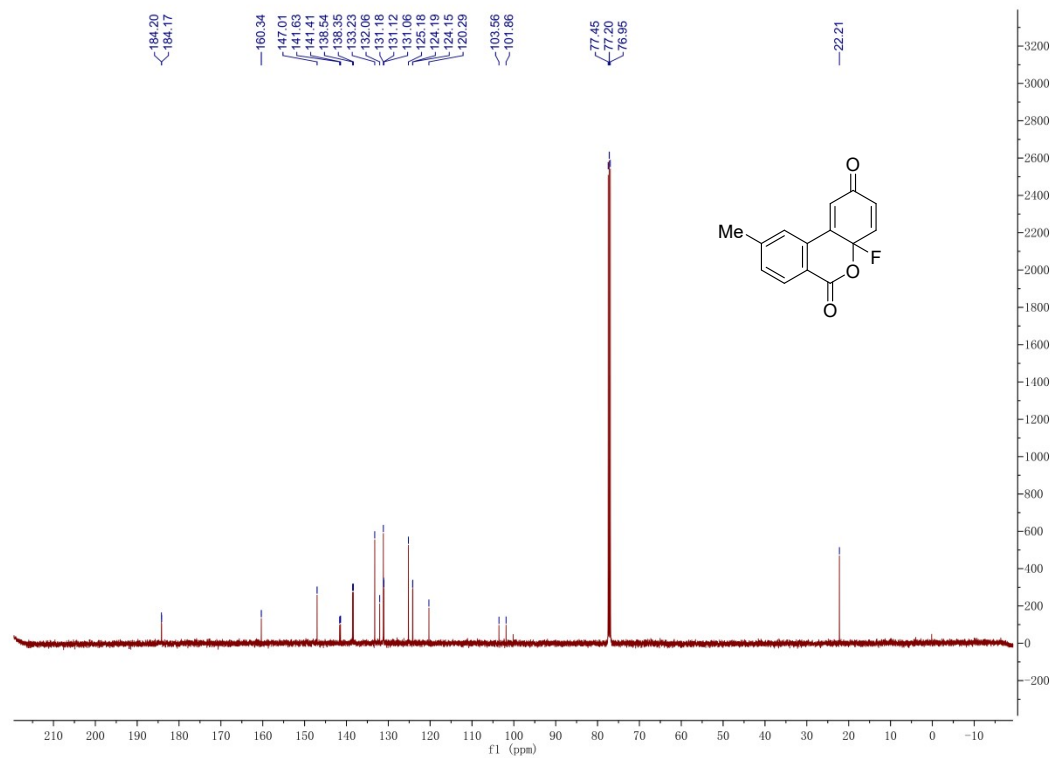
Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSig ma	rdb	e ⁻ Conf	N-R ule
267.04292	1	C ₁₄ H ₉ FNaO ₃	100.00	267.04279	-0.46	-0.45	6.5	9.5	even	ok

4a-fluoro-9-methyl-6H-benzo[c]chromene-2,6(4aH)-dione (**2c**)

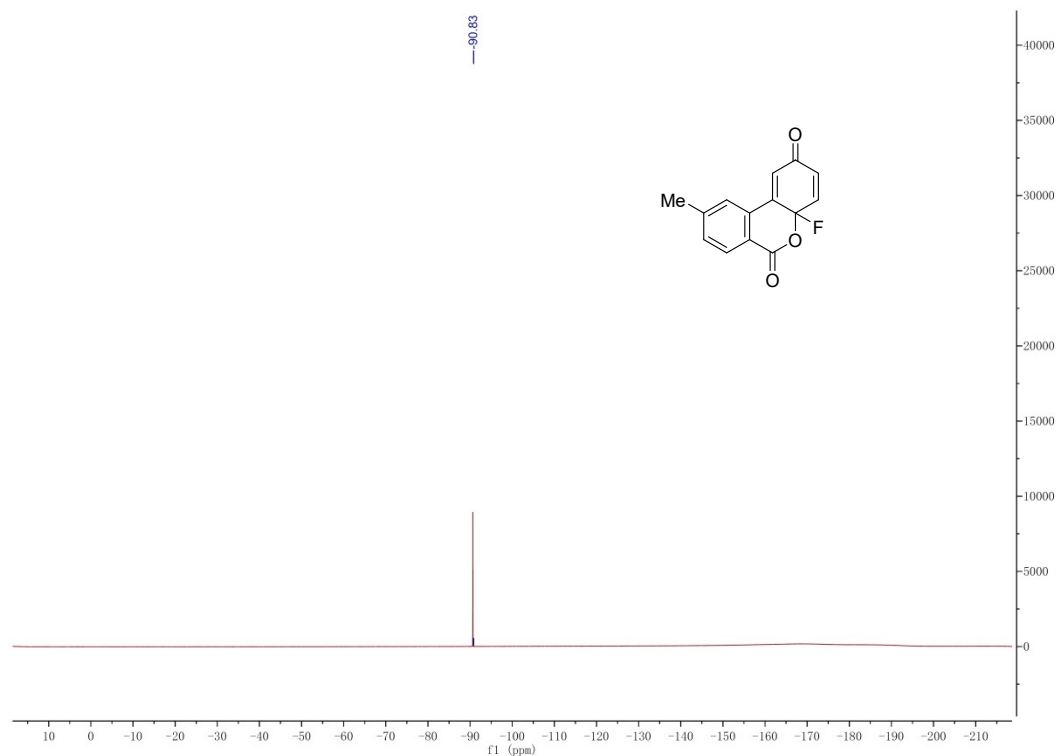
¹H NMR (500 MHz, CDCl₃)



¹³C {¹H} NMR (126 MHz, CDCl₃)



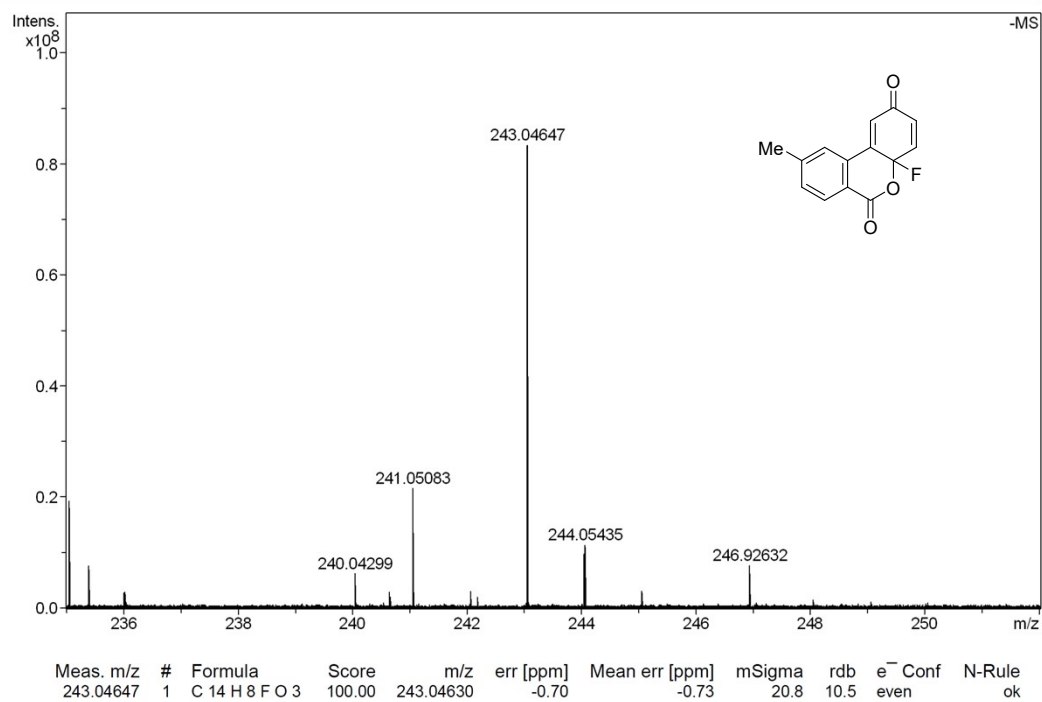
¹⁹F NMR (376 MHz, CDCl₃)



HRMS (ESI-TOF) m/z calcd for $C_{14}H_9FO_3$ (M-H)⁻ 243.0463, found 243.0465.

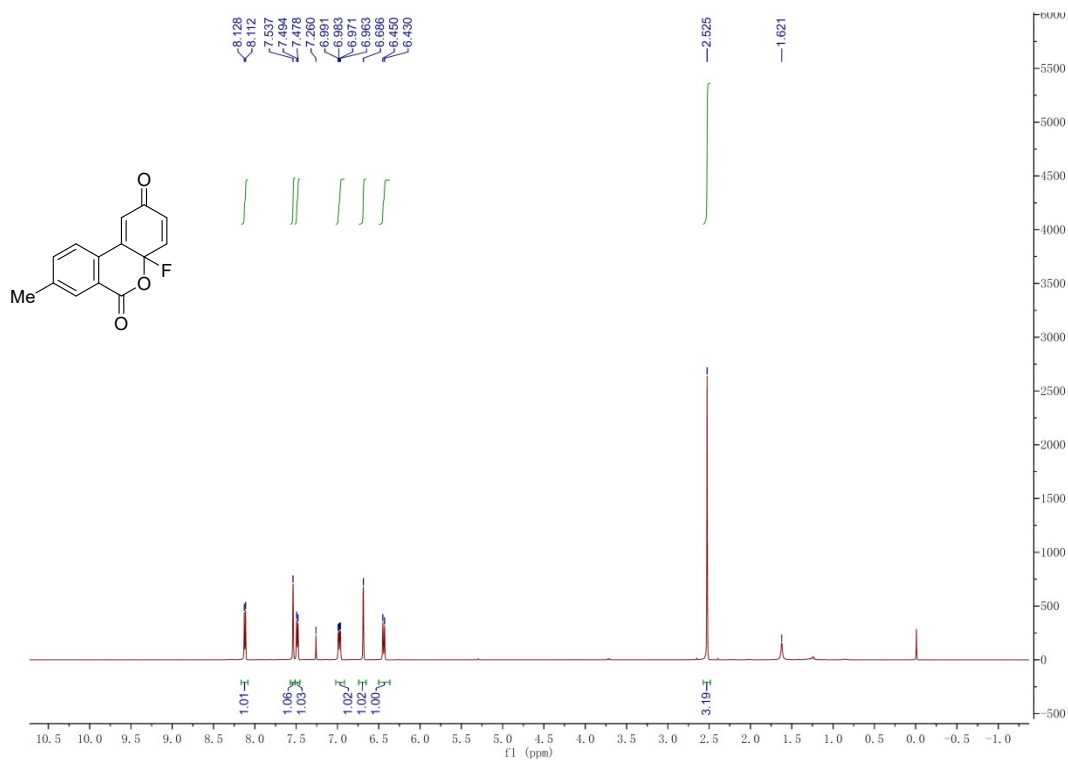
Acquisition Parameter

Polarity	Negative	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	200.7 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Wed Jun 17 02:41:42
Pulse Program	basic	n/a	n/a	Data Acquisition Size	2028576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.100 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec				

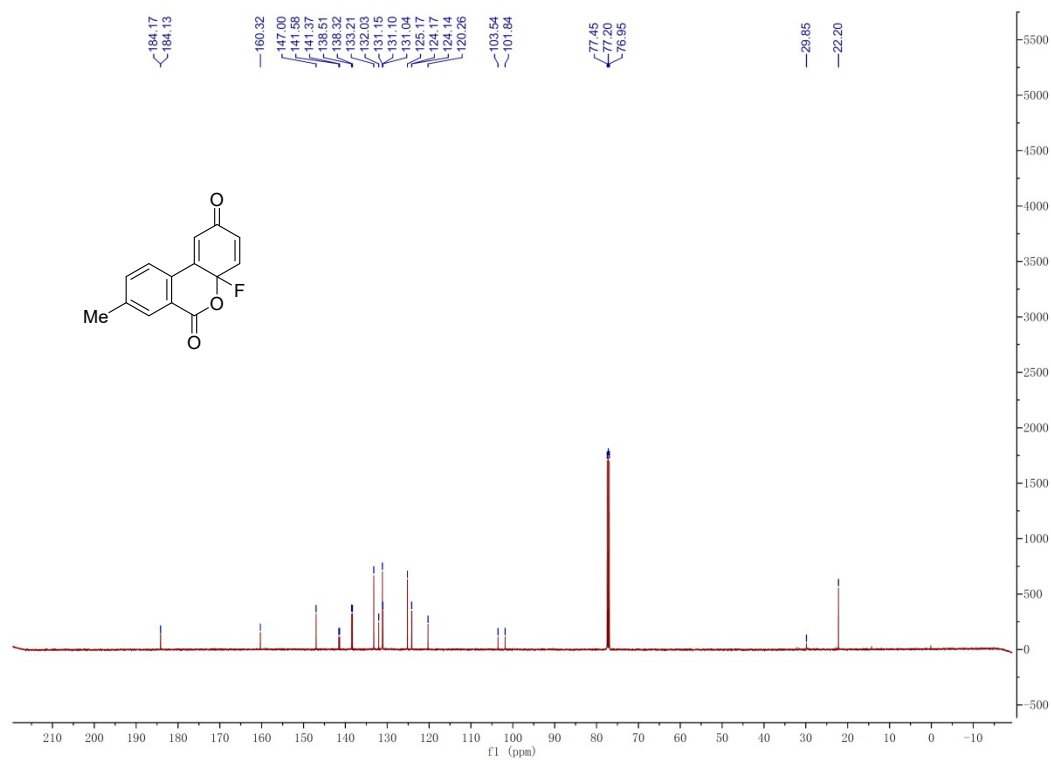


4a-fluoro-8-methyl-6H-benzo[c]chromene-2,6(4aH)-dione (**2d**)

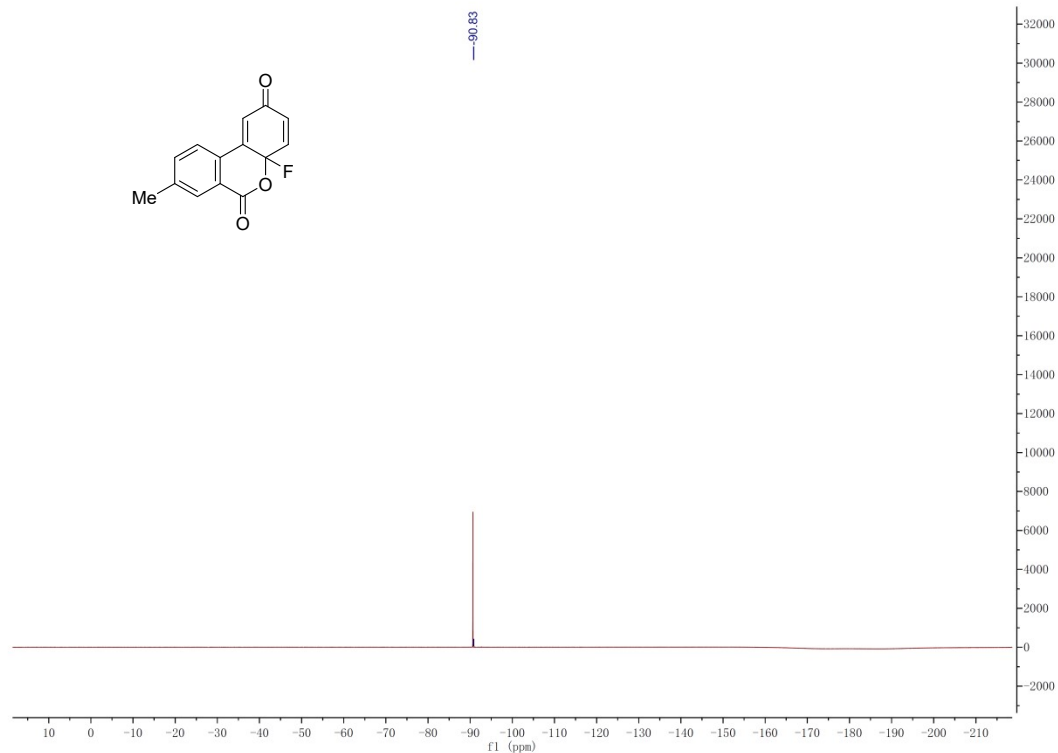
¹H NMR (500 MHz, CDCl₃)



¹³C {¹H} NMR (126 MHz, CDCl₃)



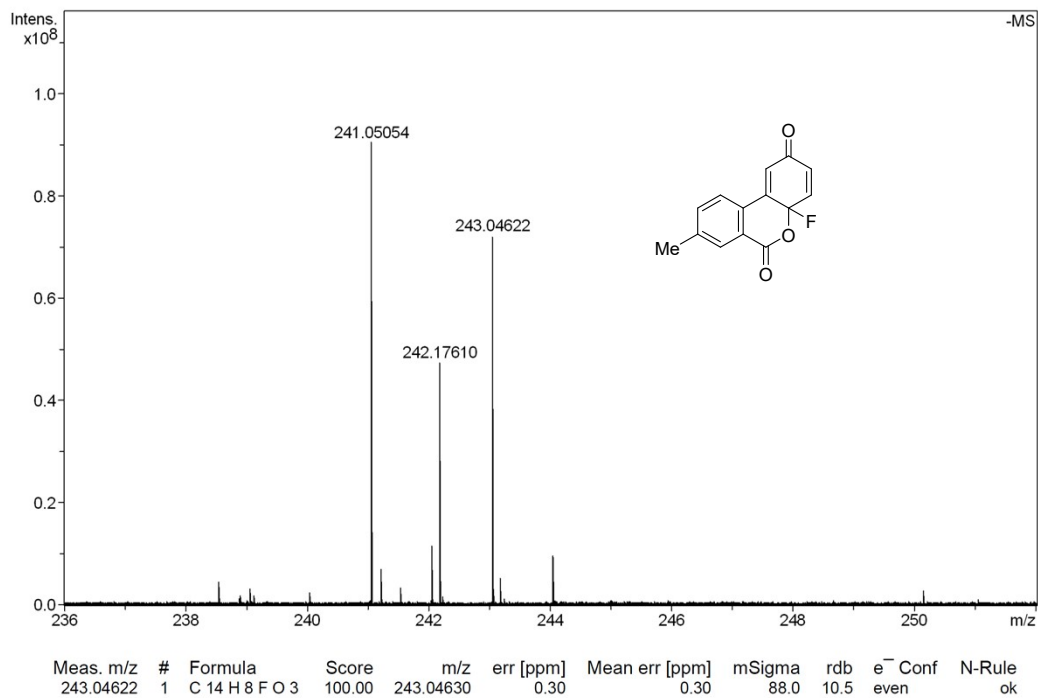
¹⁹F NMR (376 MHz, CDCl₃)



HRMS (ESI-TOF) m/z calcd for $C_{14}H_9FO_3$ (M-H)⁻ 243.0463, found 243.0462.

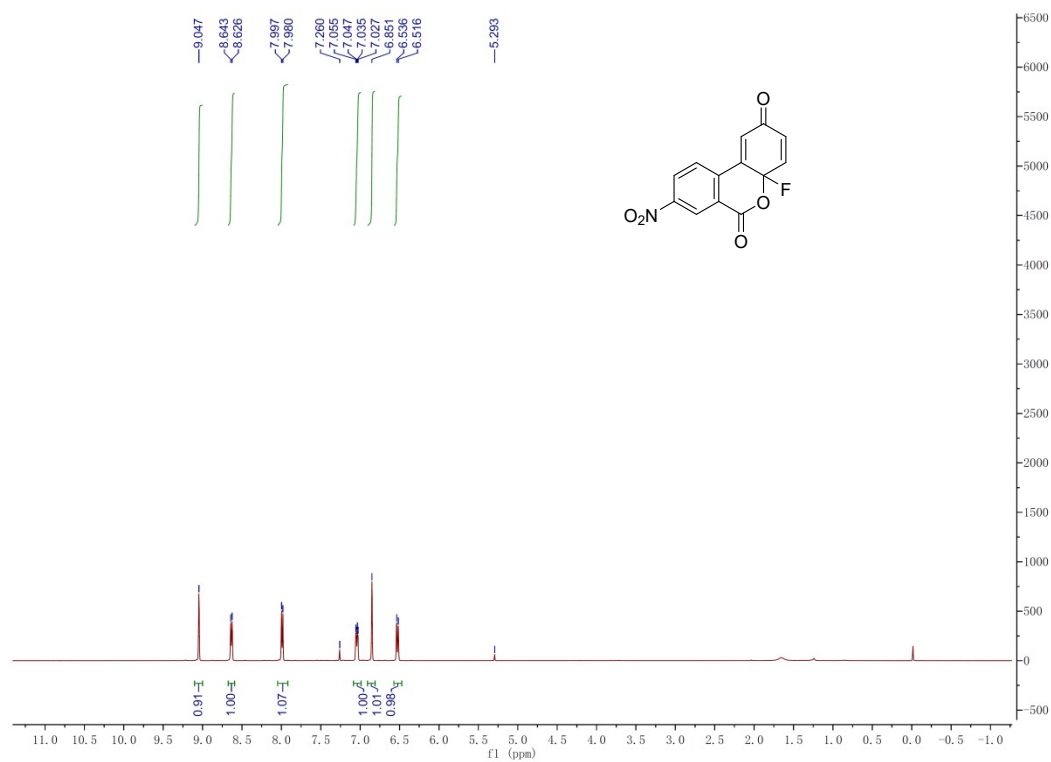
Acquisition Parameter

Polarity	Negative	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 Ip
Broadband Low Mass	200.7 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Wed Jun 17 02:41:42
Pulse Program	basic	n/a	n/a	Data Acquisition Size	2020576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.200 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec	n/a	n/a		

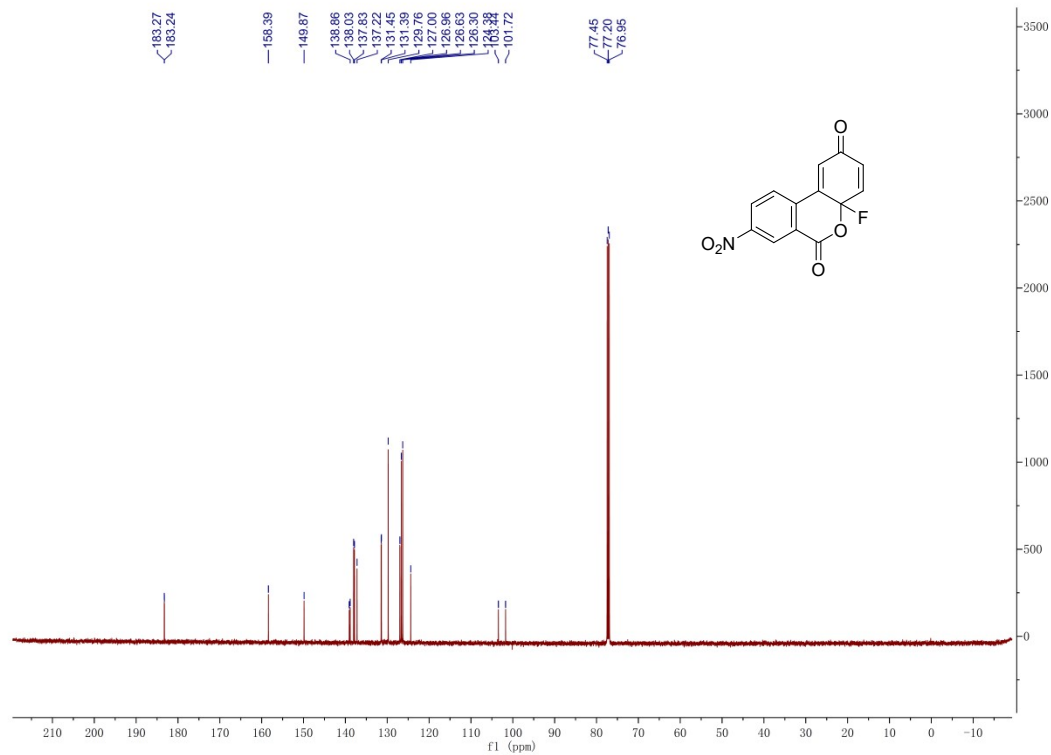


4a-fluoro-8-nitro-6H-benzo[c]chromene-2,6(4aH)-dione (**2e**)

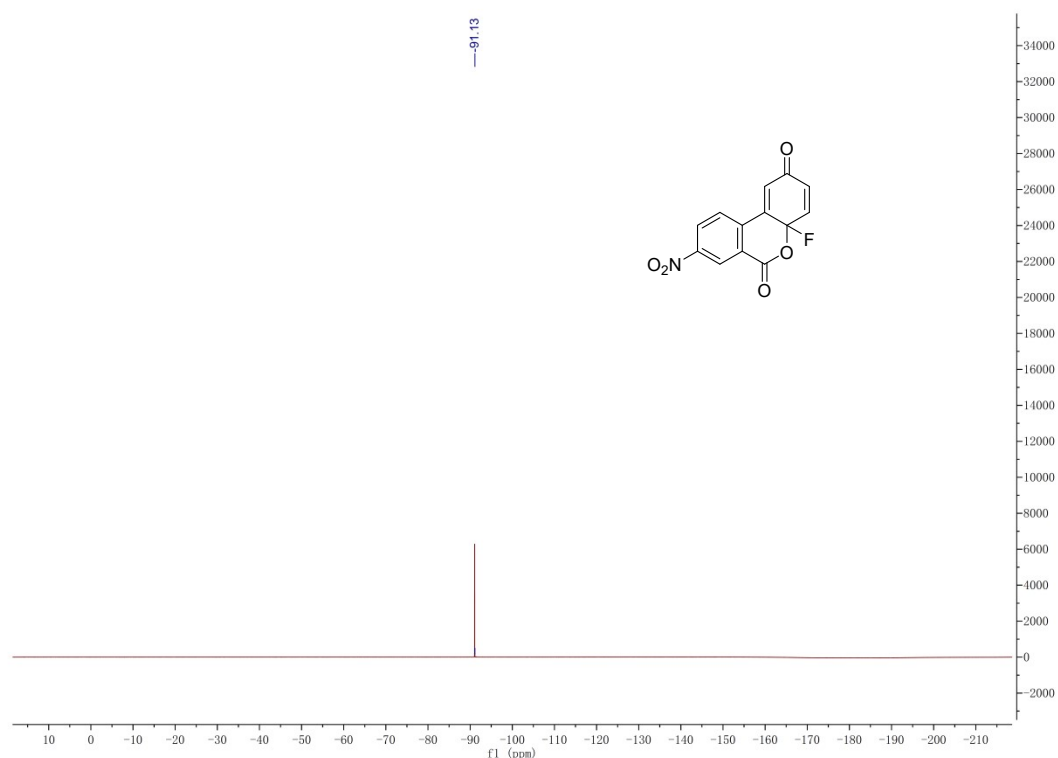
^1H NMR (500 MHz, CDCl_3)



^{13}C { ^1H } NMR (126 MHz, CDCl_3)



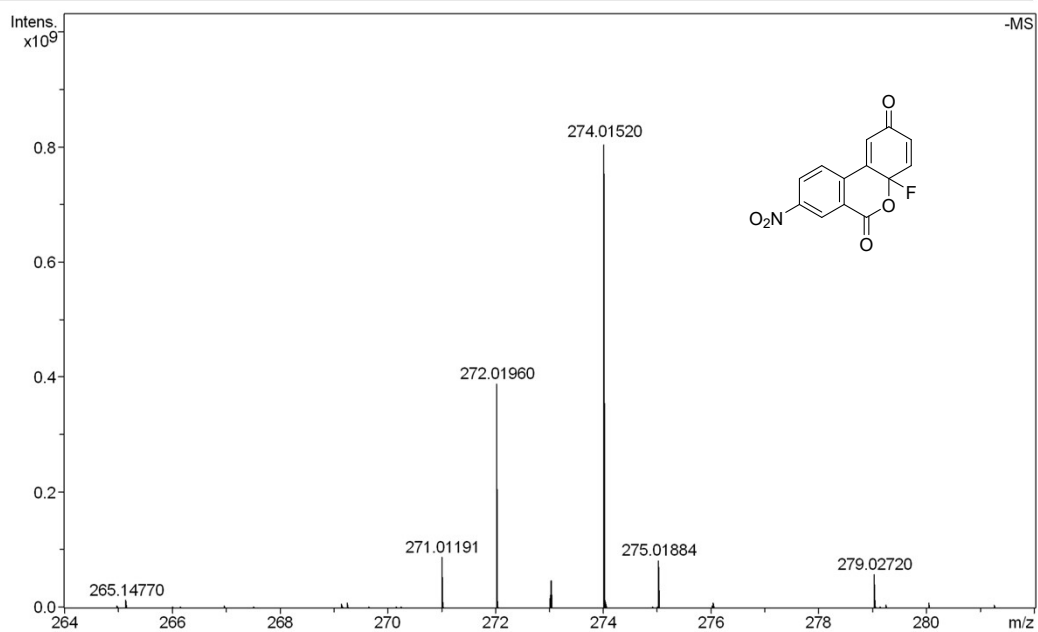
¹⁹F NMR(376 MHz, CDCl₃)



HRMS (ESI-TOF) m/z calcd for C₁₃H₆FNO₅ (M-H)⁻ 274.0157, found 274.0152.

Acquisition Parameter

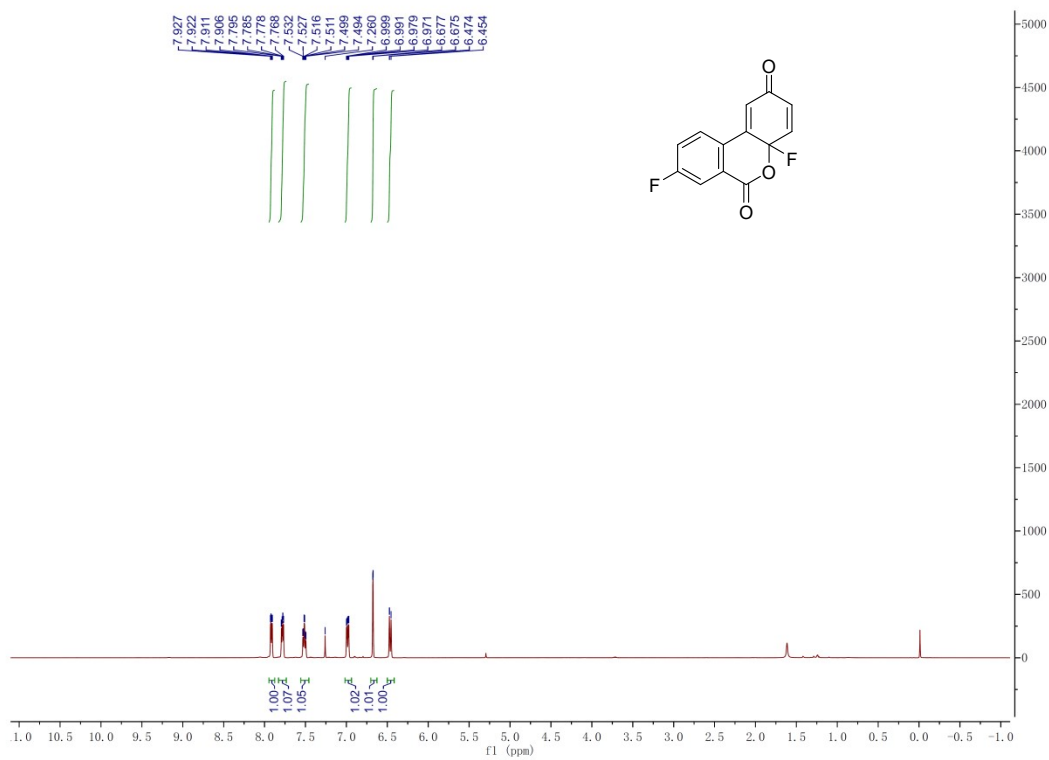
Polarity	Negative	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	200.7 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Wed Jun 17 02:41:42
Pulse Program	basic	n/a	n/a	Data Acquisition Size	2028576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.200 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec	n/a	n/a		



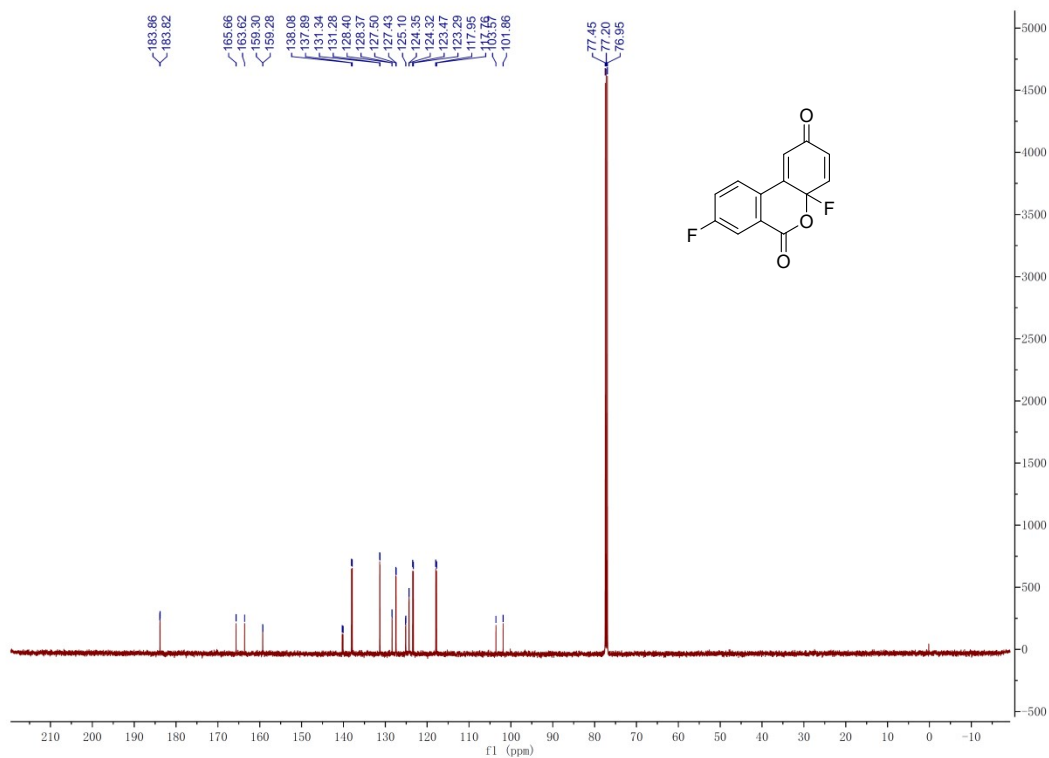
Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
274.01520	1	C ₁₃ H ₅ FNO ₅	100.00	274.01572	1.92	1.82	26.9	11.5	even	ok

4a,8-difluoro-6H-benzo[c]chromene-2,6(4aH)-dione (**2f**)

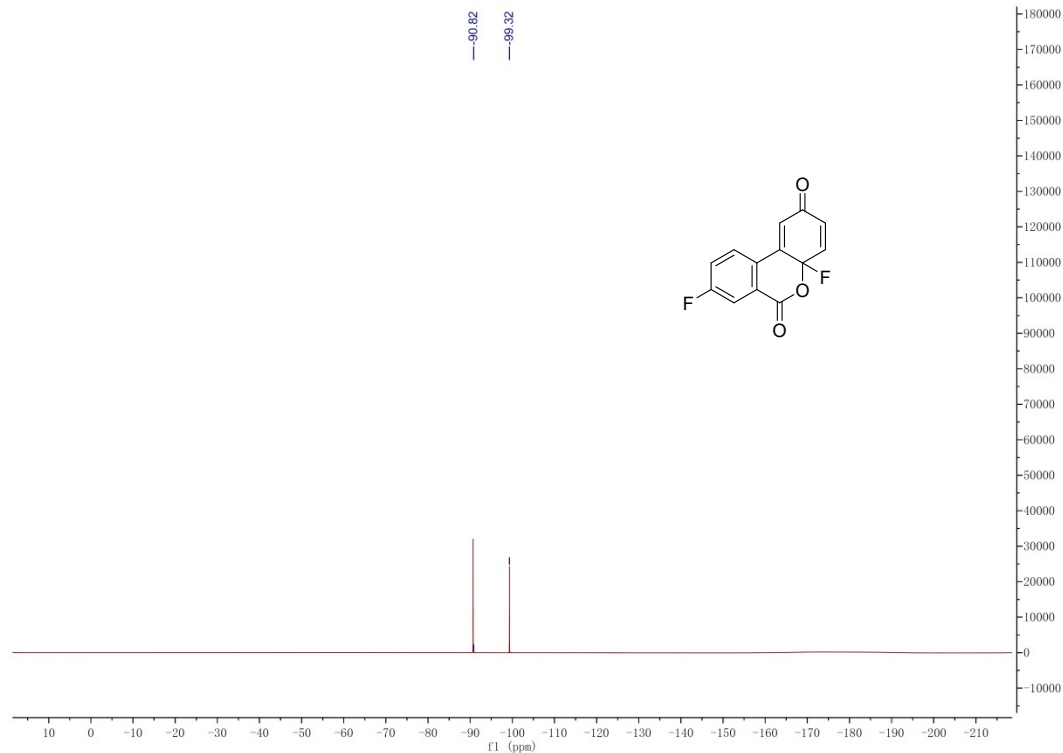
¹H NMR (500 MHz, CDCl₃)



¹³C {¹H} NMR (126 MHz, CDCl₃)



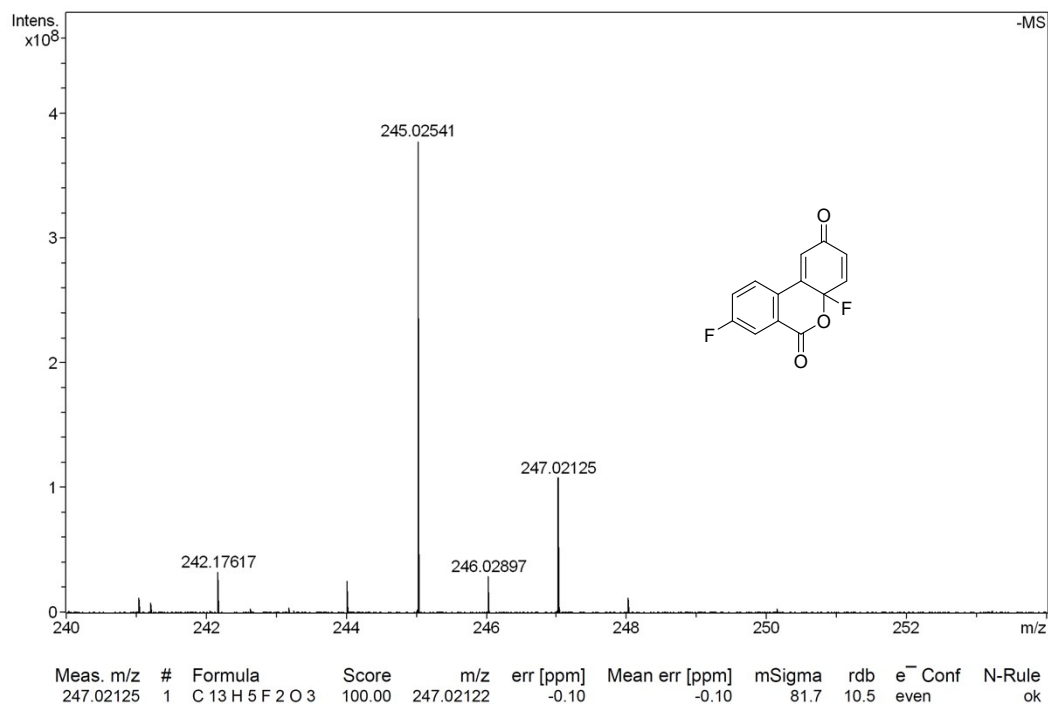
¹⁹F NMR (376 MHz, CDCl₃)



HRMS (ESI-TOF) m/z calcd for $C_{13}H_6F_2O_3$ (M-H)⁻ 247.0212, found 247.0213.

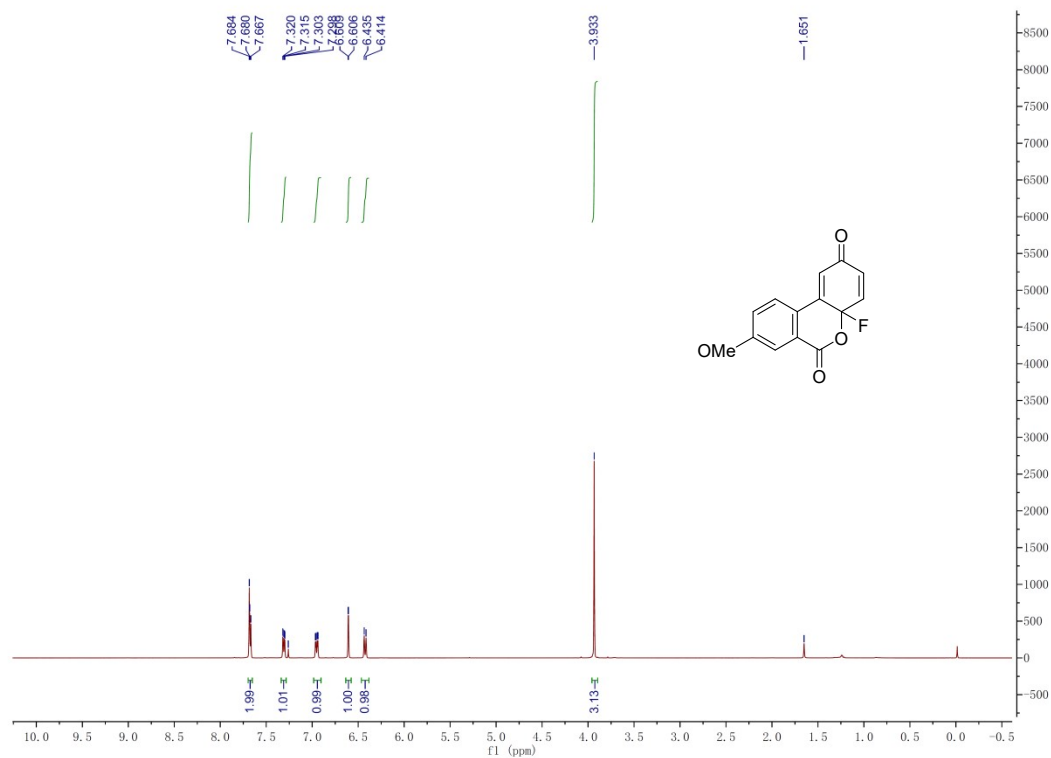
Acquisition Parameter

Polarity	Negative	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	200.7 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Wed Jun 17 02:41:42
Pulse Program	basic	n/a	n/a	Data Acquisition Size	2020576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.100 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec				

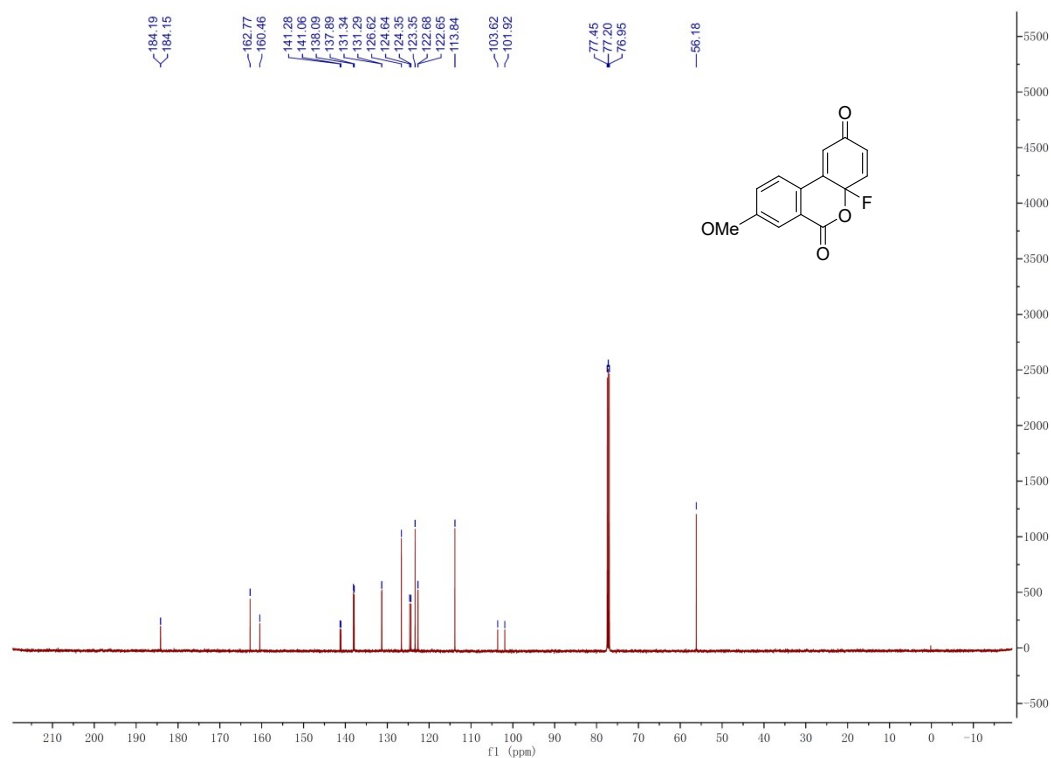


4a-fluoro-8-methoxy-6H-benzo[c]chromene-2,6(4aH)-dione (**2g**)

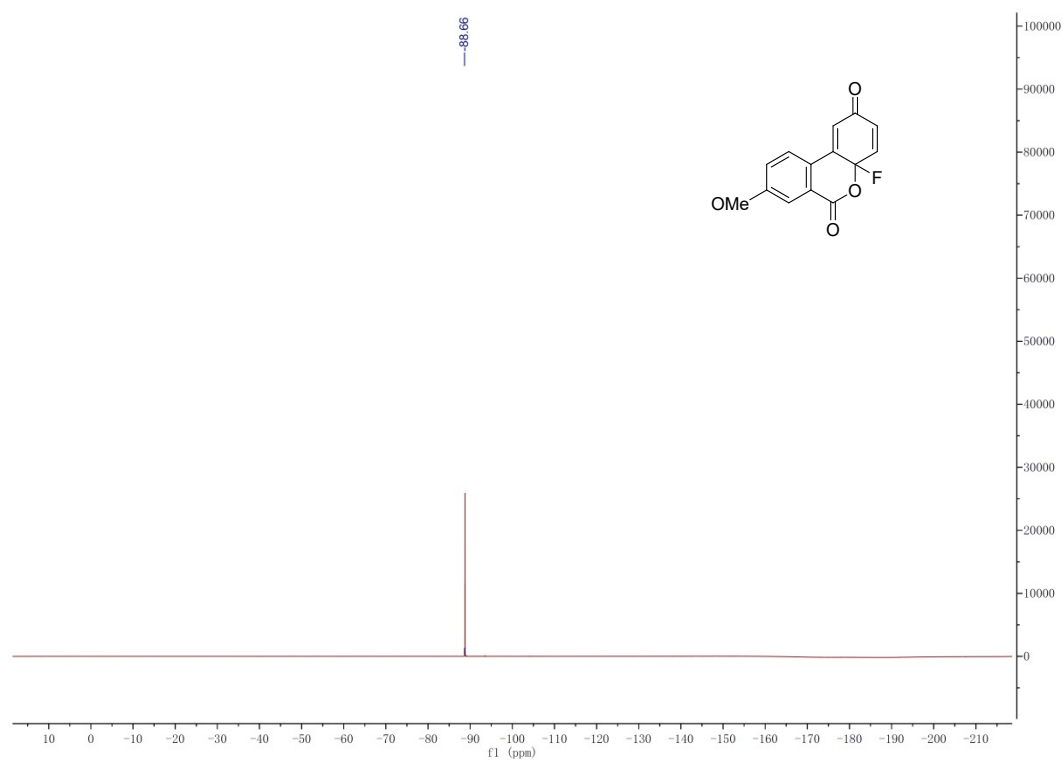
¹H NMR (500 MHz, CDCl₃)



¹³C {¹H} NMR (126 MHz, CDCl₃)



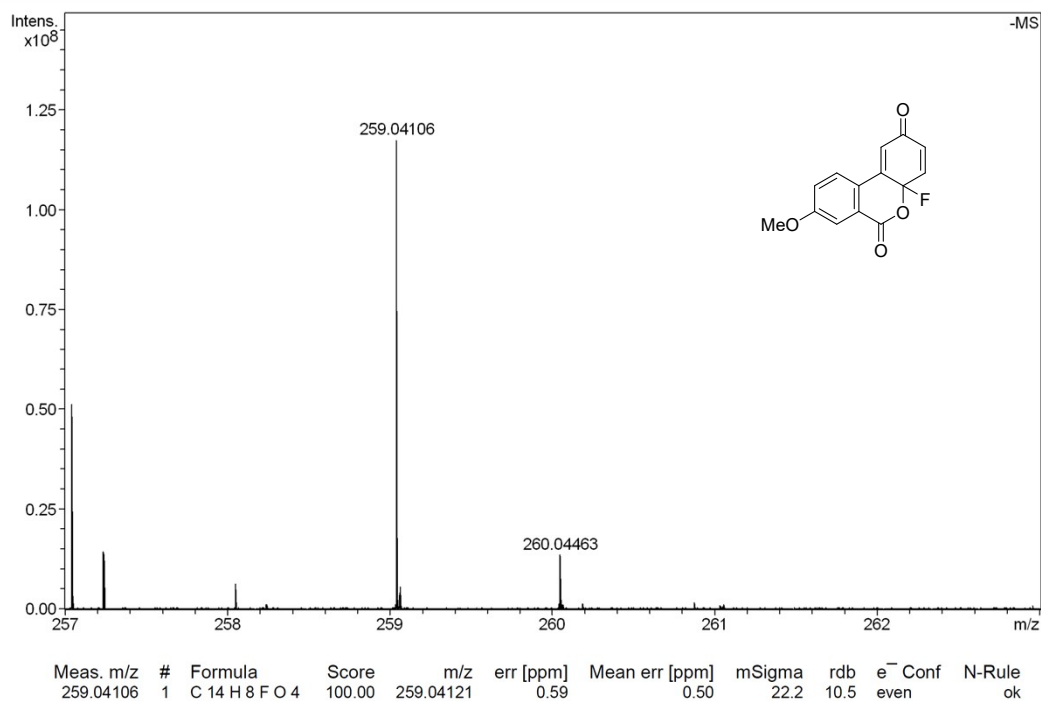
¹⁹F NMR (376 MHz, CDCl₃)



HRMS (ESI-TOF) m/z calcd for $C_{14}H_9FO_4$ (M-H)⁻ 259.0412, found 259.0411.

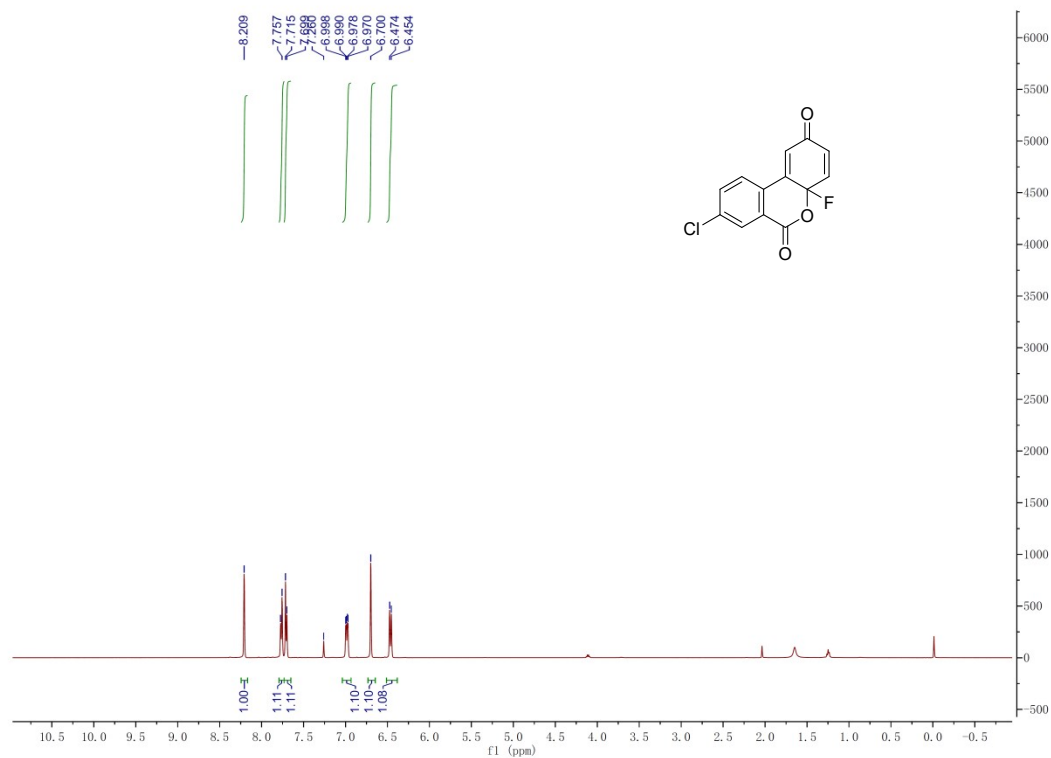
Acquisition Parameter

Polarity	Negative	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	200.7 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Wed Jun 17 02:41:42
Pulse Program	basic	n/a	n/a	Data Acquisition Size	2029576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.200 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec				

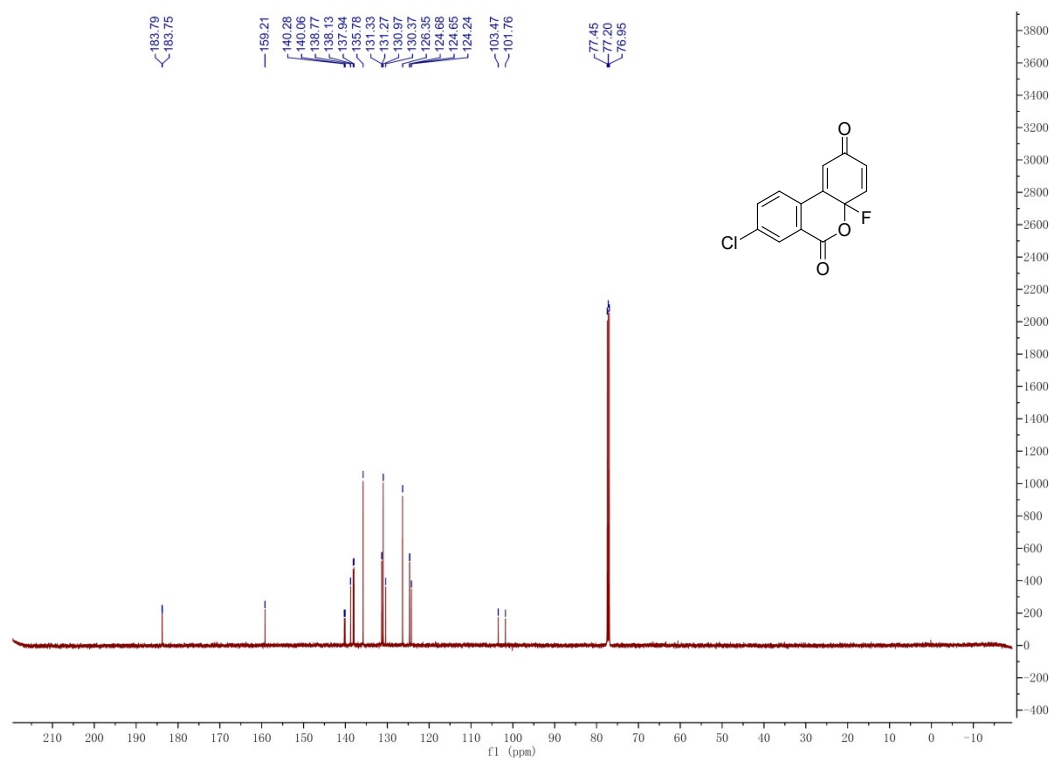


7-chloro-4a-fluoro-6H-benzo[c]chromene-2,6(4aH)-dione (**2h**)

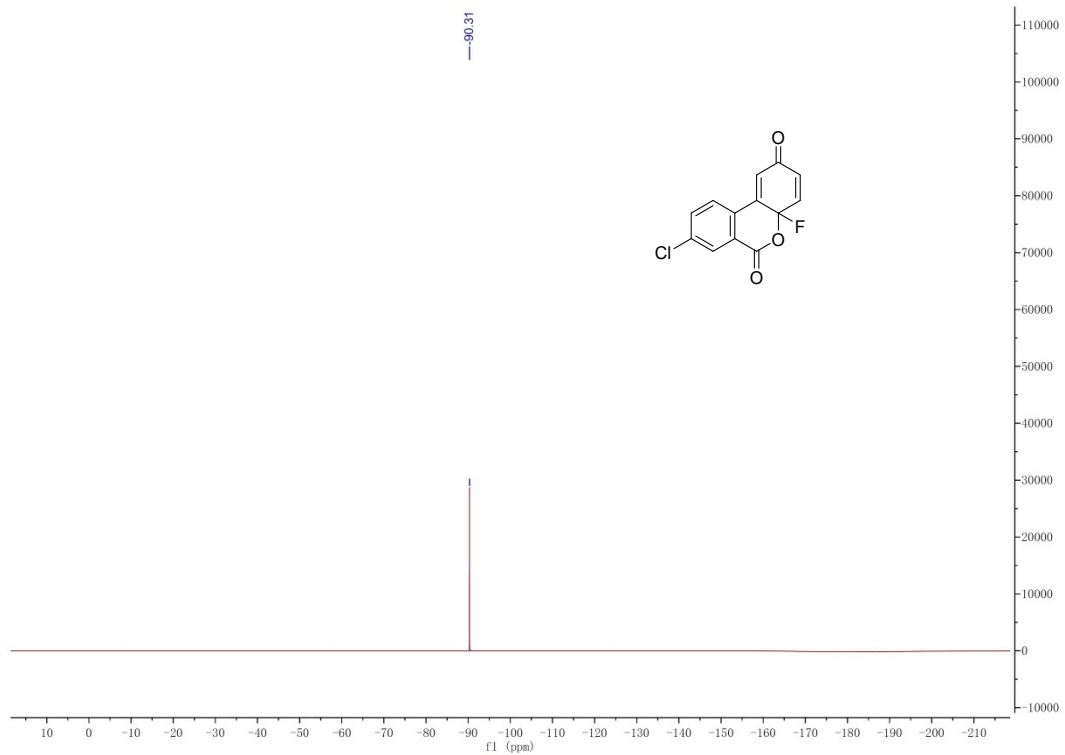
^1H NMR (500 MHz, CDCl_3)



^{13}C { ^1H } NMR (126 MHz, CDCl_3)



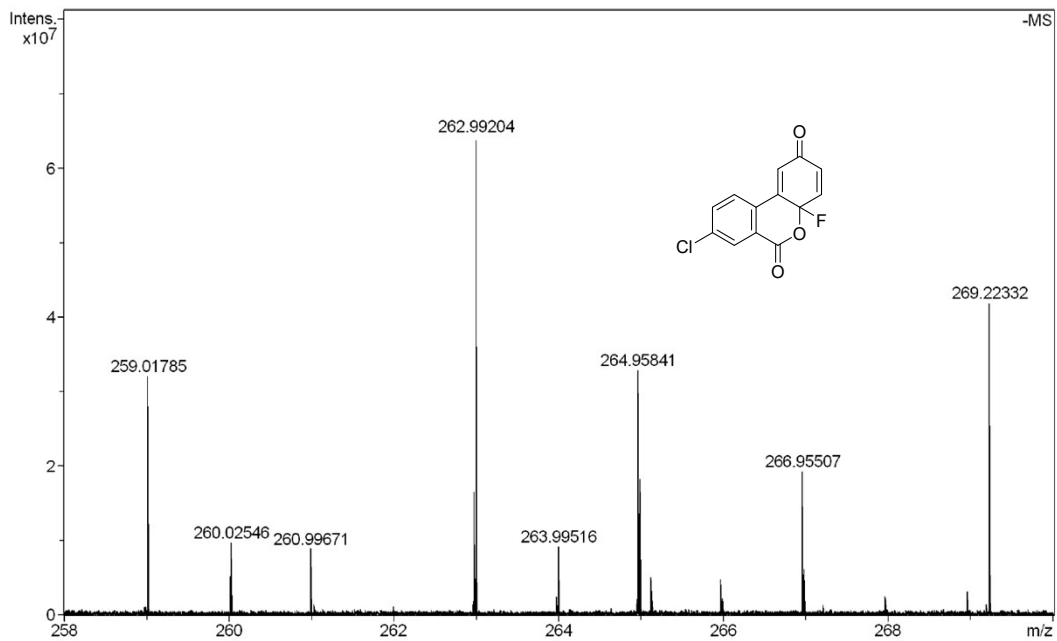
^{19}F NMR (376 MHz, CDCl_3)



HRMS (ESI-TOF) m/z calcd for $C_{13}H_6ClFO_3$ (M-H)⁻ 262.9917, found 262.9920.

Acquisition Parameter

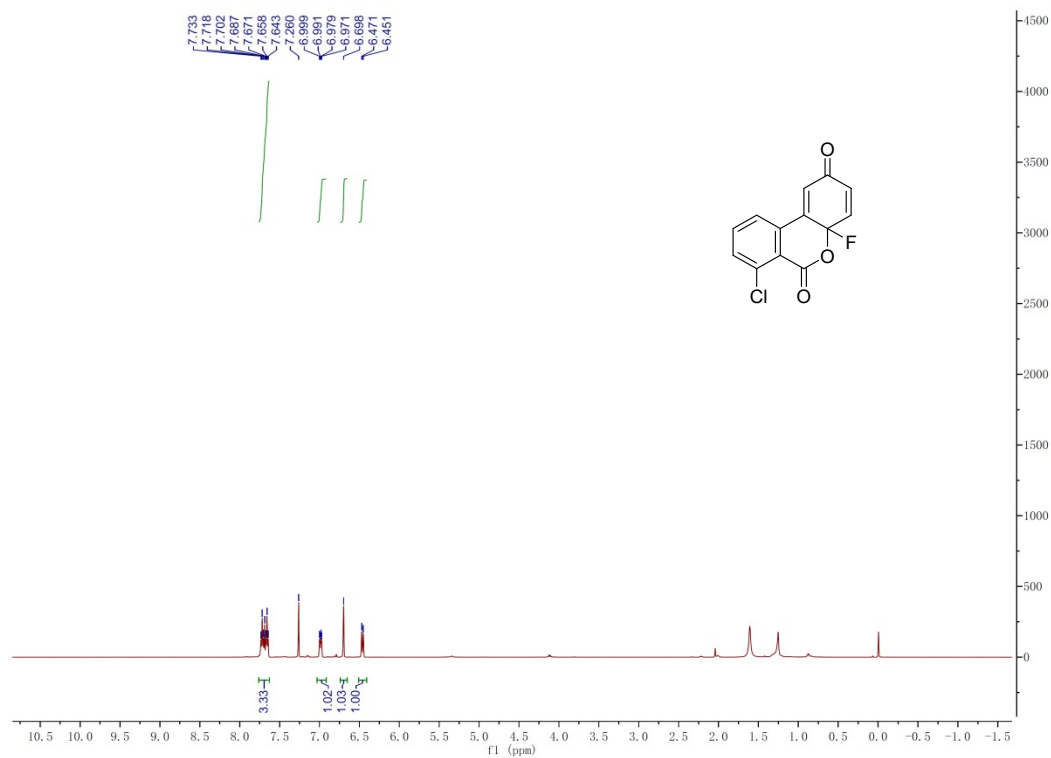
Polarity	Negative	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	100.4 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Wed Jun 17 02:41:42
Pulse Program	basic	n/a	n/a	Data Acquisition Size	2020576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.200 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec	n/a	n/a		



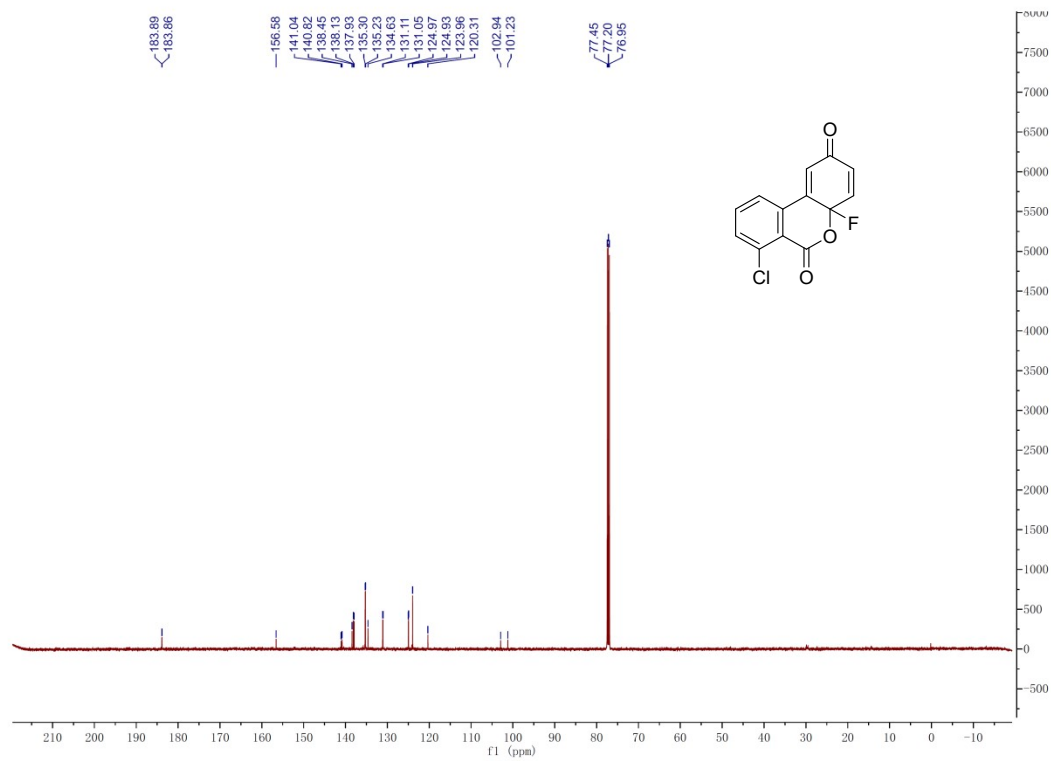
Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-R ulation
262.99204	1	C ₁₃ H ₅ ClFO ₃	100.00	262.99167	-1.39	-1.28	169.0	10.5	even	ok

7-chloro-4a-fluoro-6H-benzo[*c*]chromene-2,6(4a*H*)-dione (**2i**)

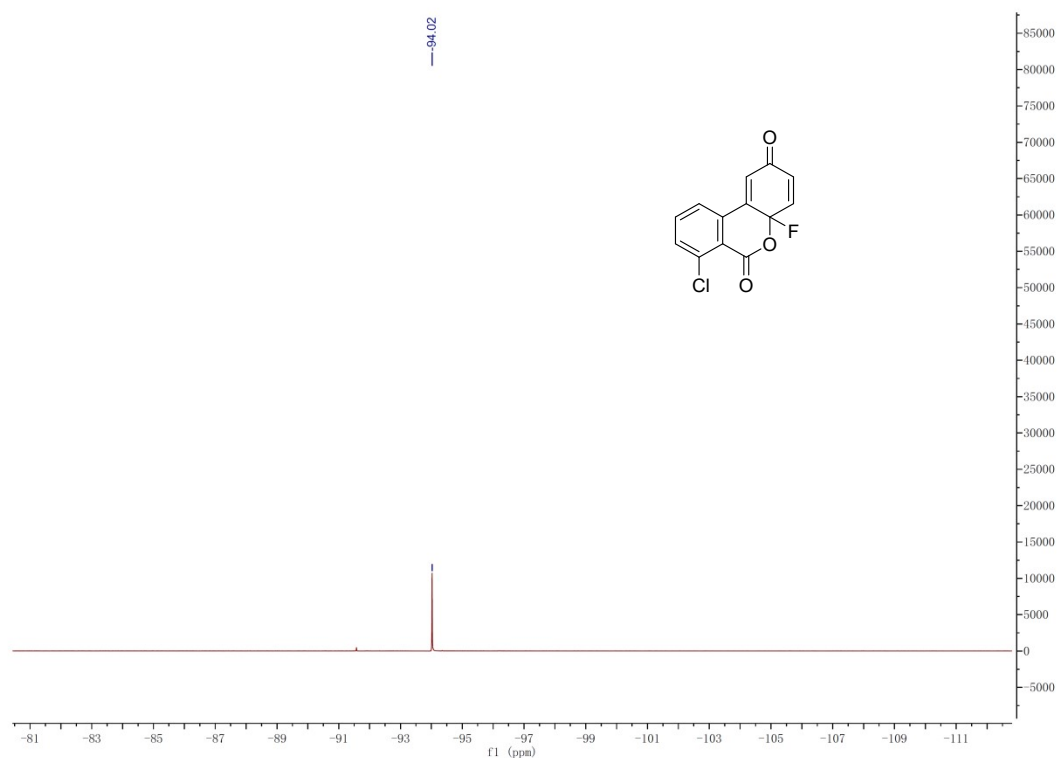
^1H NMR (500 MHz, CDCl_3)



^{13}C { ^1H } NMR (126 MHz, CDCl_3)



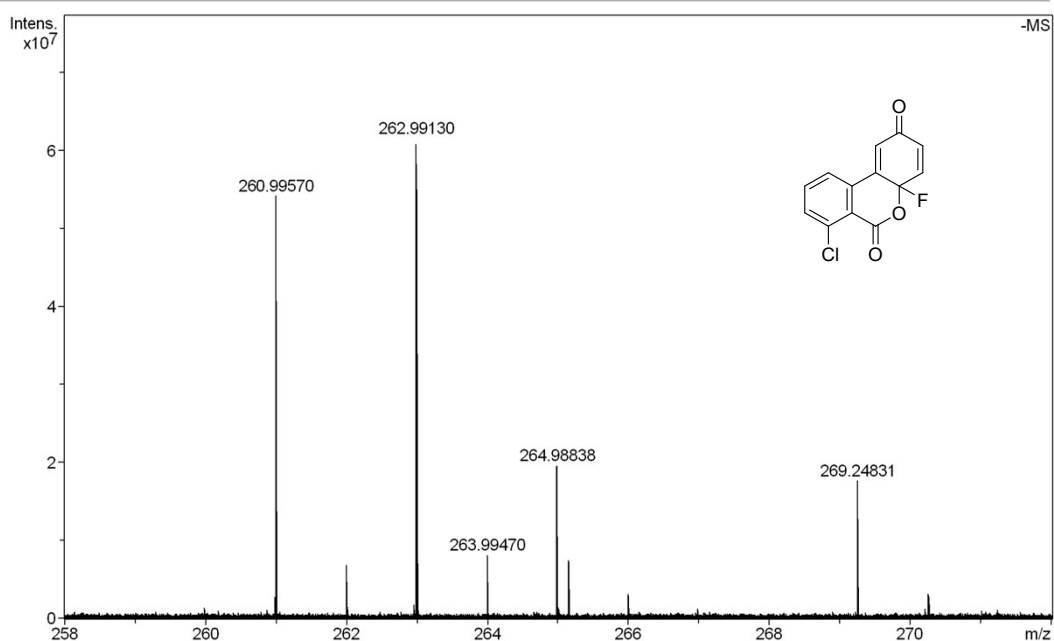
^{19}F NMR(376 MHz, CDCl_3)



HRMS (ESI-TOF) m/z calcd for $\text{C}_{13}\text{H}_6\text{ClFO}_3$ (M-H) $^-$ 262.9917, found 262.9913.

Acquisition Parameter

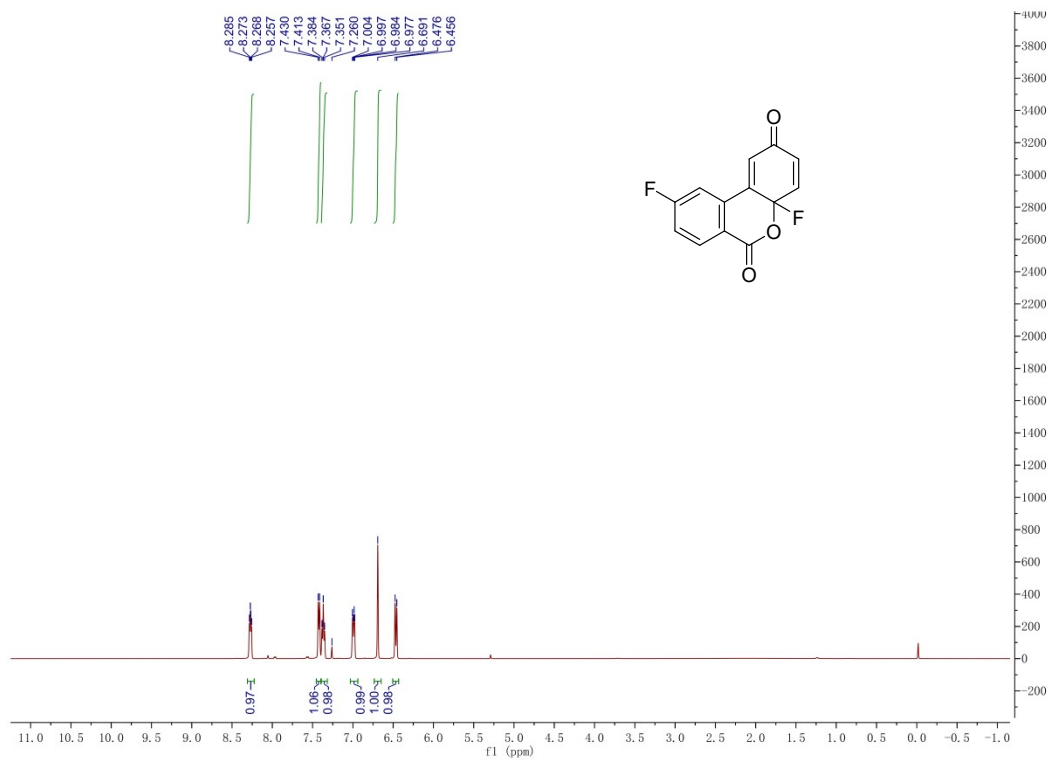
Polarity	Negative	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	200.7 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Wed Jun 17 02:41:42
Pulse Program	basic	n/a	n/a	Data Acquisition Size	2020576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.200 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec				



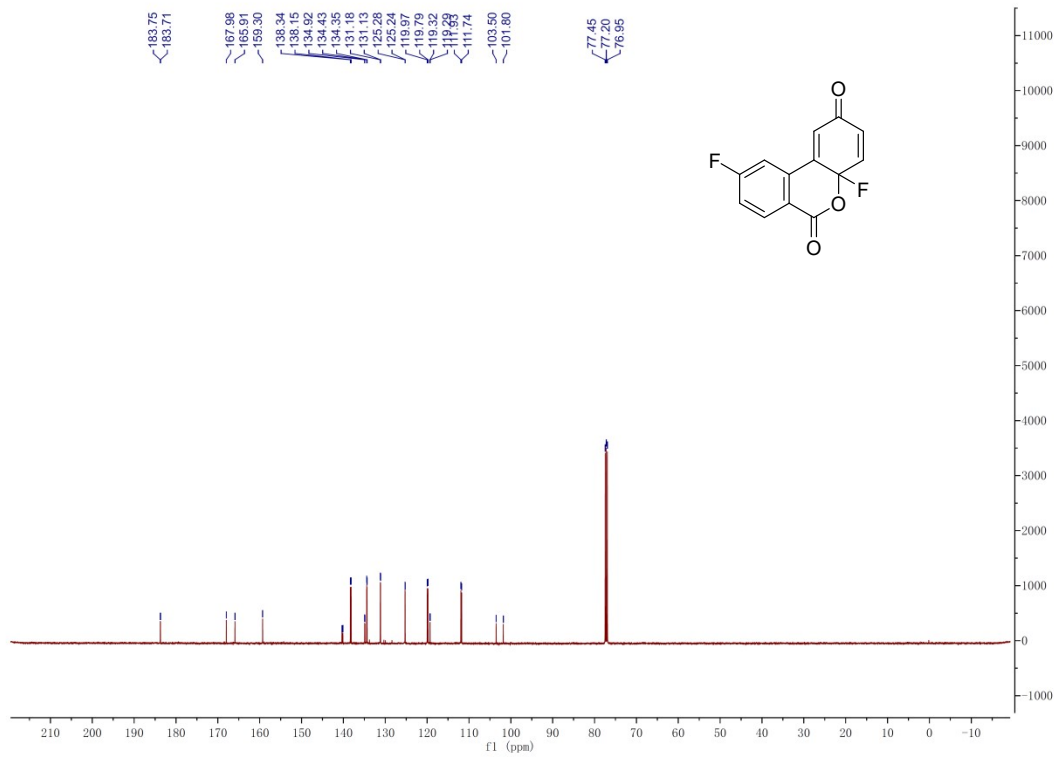
Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSig	rdb	e^- Conf	N-R rule
262.99130	1	$\text{C}_{13}\text{H}_5\text{ClFO}_3$	100.00	262.99167	1.42	1.45	24.2	10.5	even	ok

4a,9-difluoro-6H-benzo[c]chromene-2,6(4aH)-dione (**2j**)

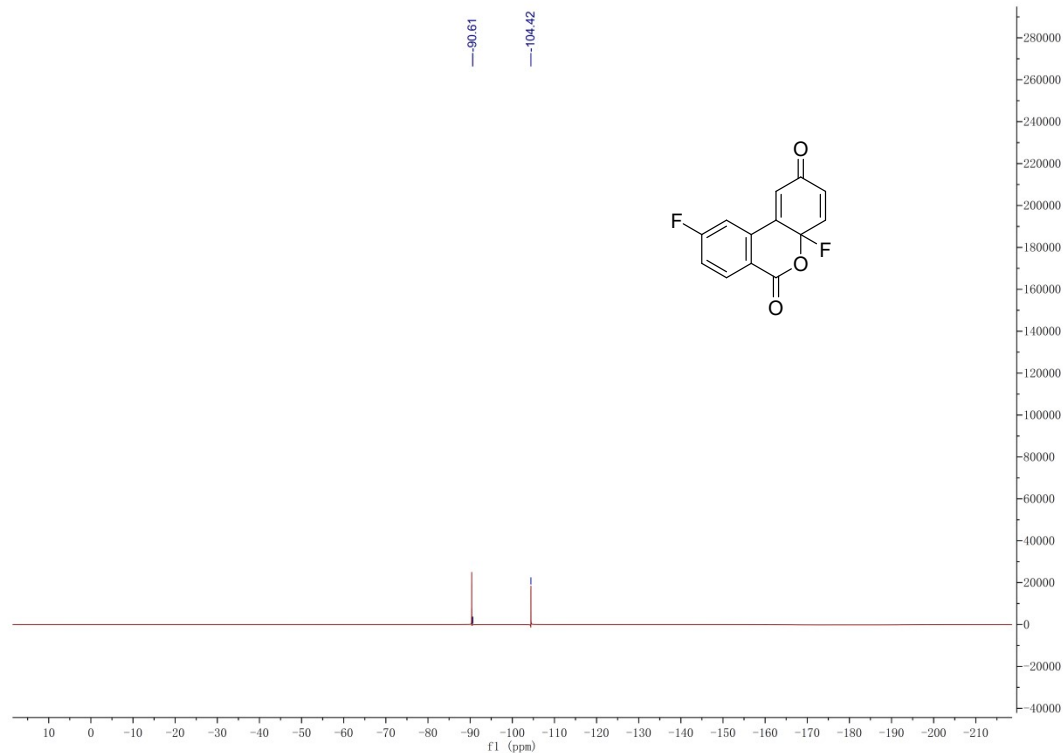
^1H NMR (500 MHz, CDCl_3)



^{13}C { ^1H } NMR (126 MHz, CDCl_3)



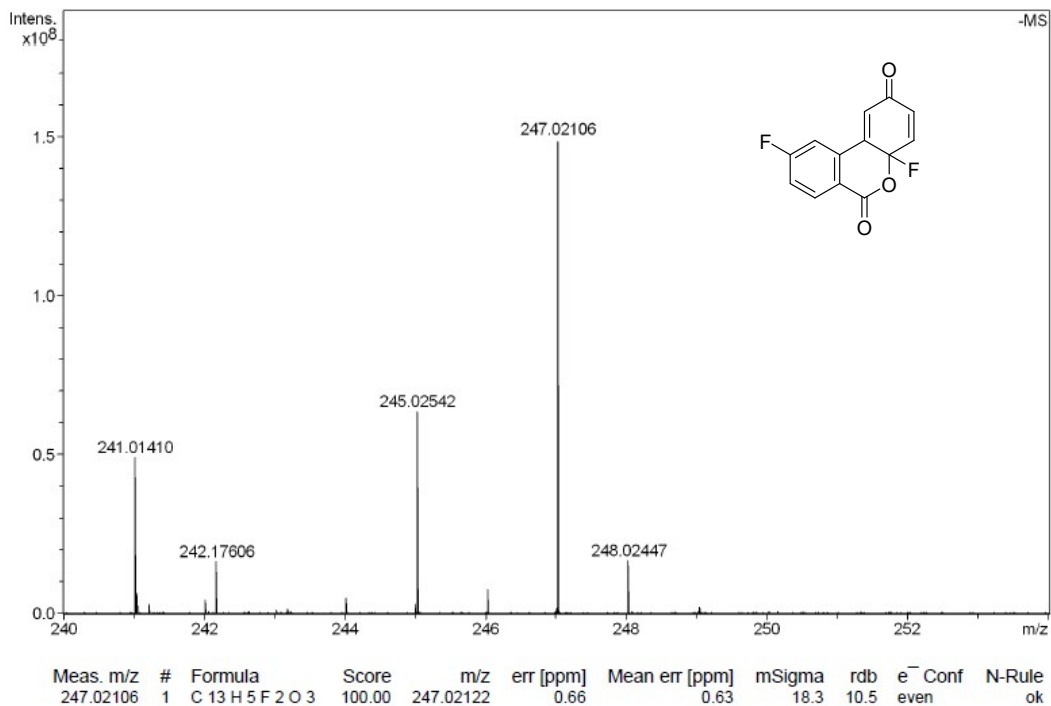
^{19}F NMR(376 MHz, CDCl_3)



HRMS (ESI-TOF) m/z calcd for $C_{13}H_6F_2O_3$ (M-H)⁻ 247.0212, found 247.0211.

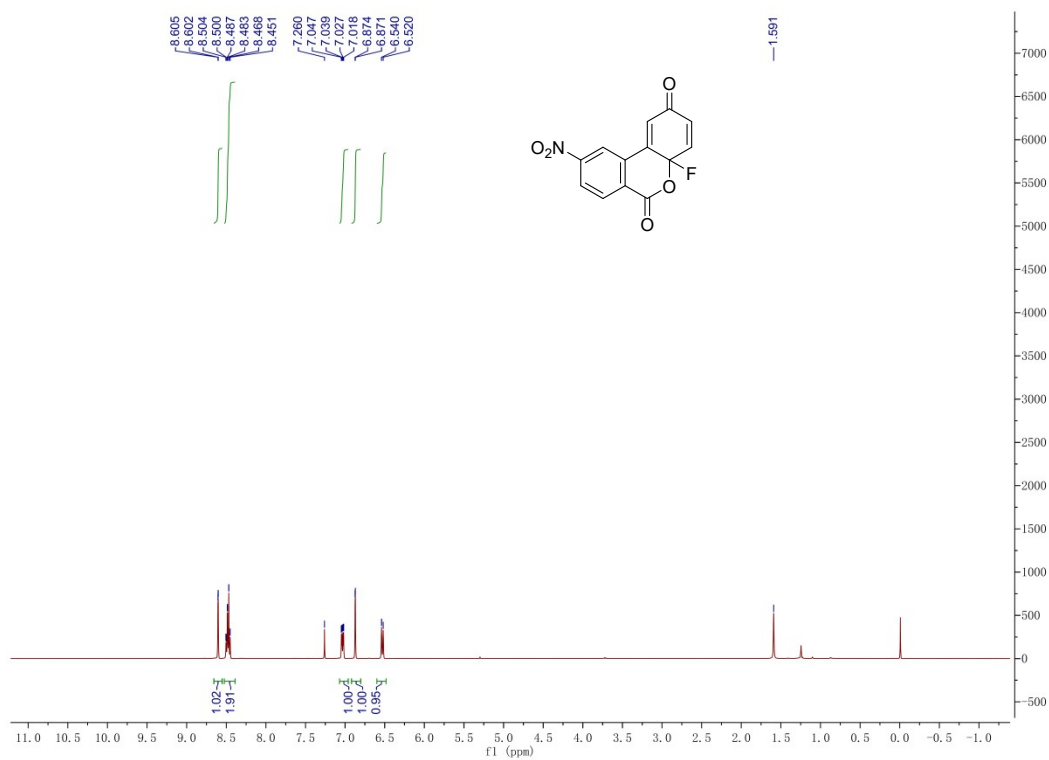
Acquisition Parameter

Polarity	Negative	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	200.7 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Wed Jun 17 02:41:42
Pulse Program	basic	n/a	n/a	Data Acquisition Size	2028576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.200 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec				

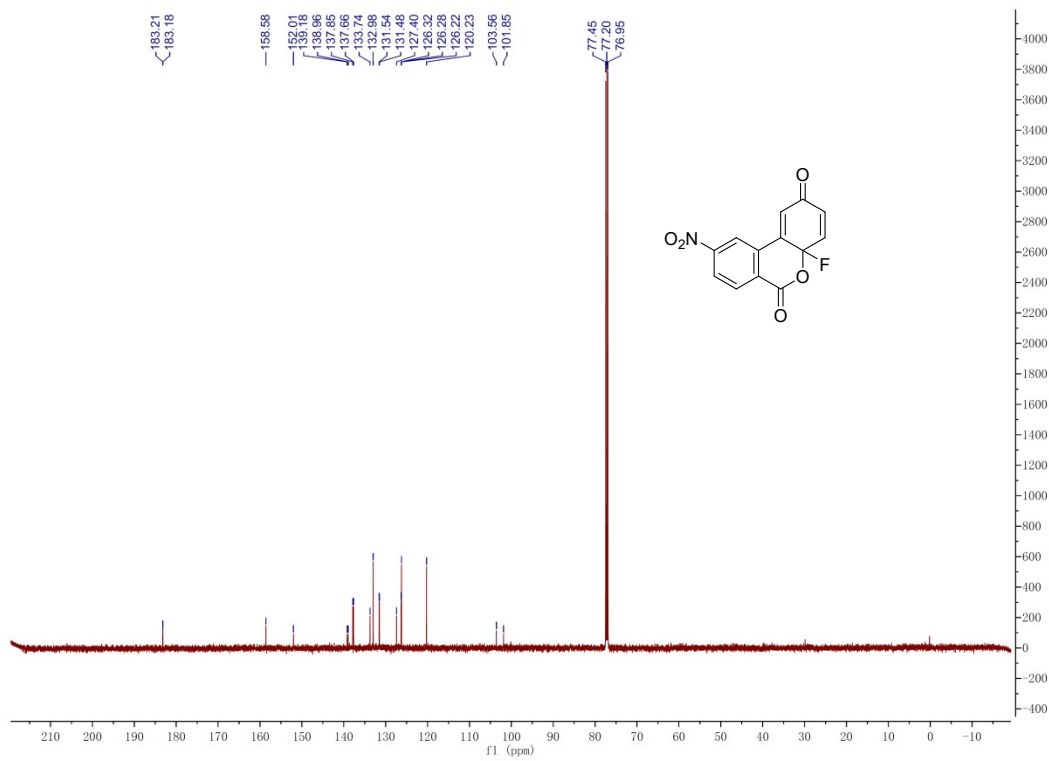


4a-fluoro-9-nitro-6H-benzo[c]chromene-2,6(4aH)-dione (**2k**)

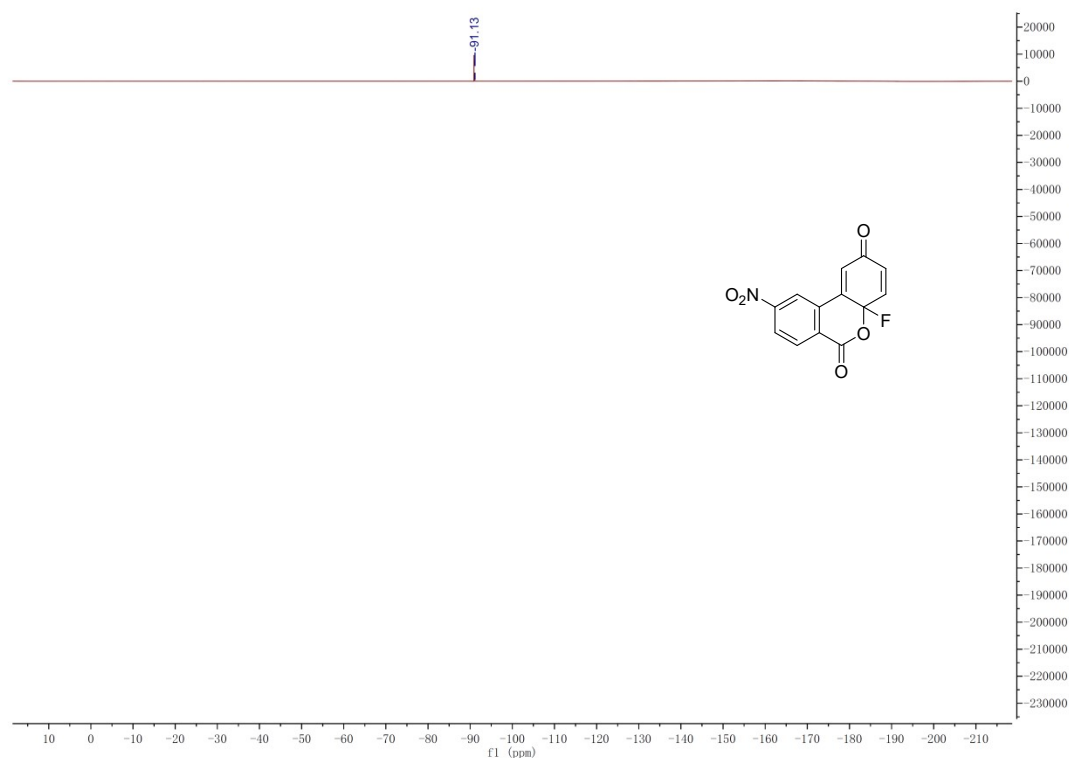
^1H NMR (500 MHz, CDCl_3)



^{13}C { ^1H } NMR (126 MHz, CDCl_3)



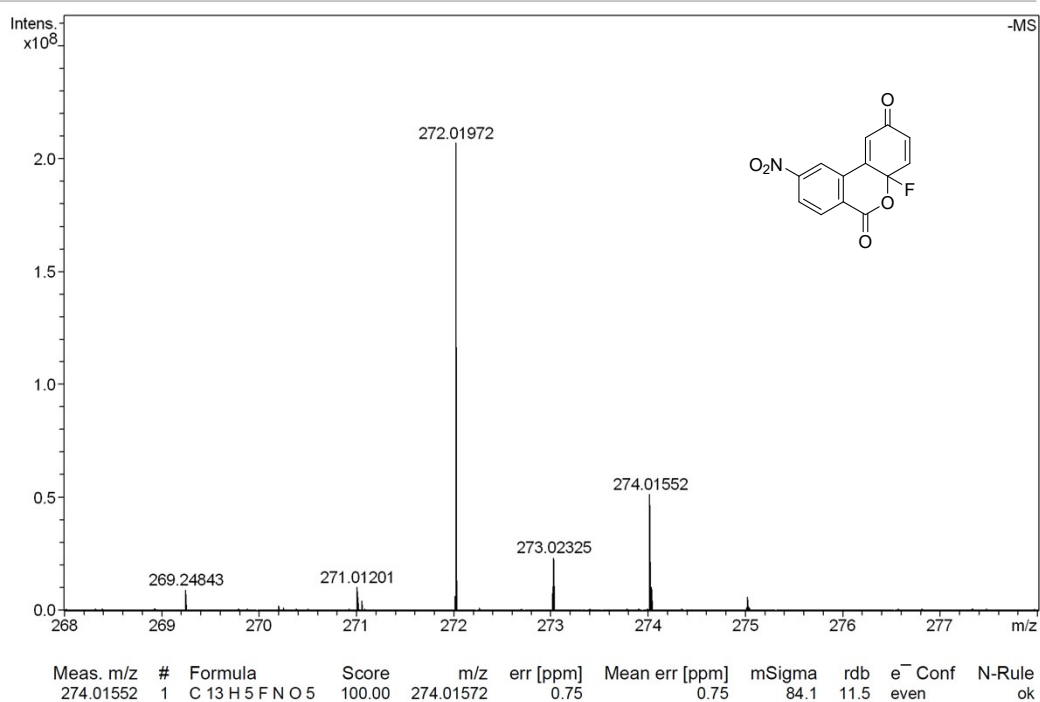
¹⁹F NMR(376 MHz, CDCl₃)



HRMS (ESI-TOF) m/z calcd for C₁₃H₆FNO₅ (M-H)⁻ 274.0157, found 274.0155.

Acquisition Parameter

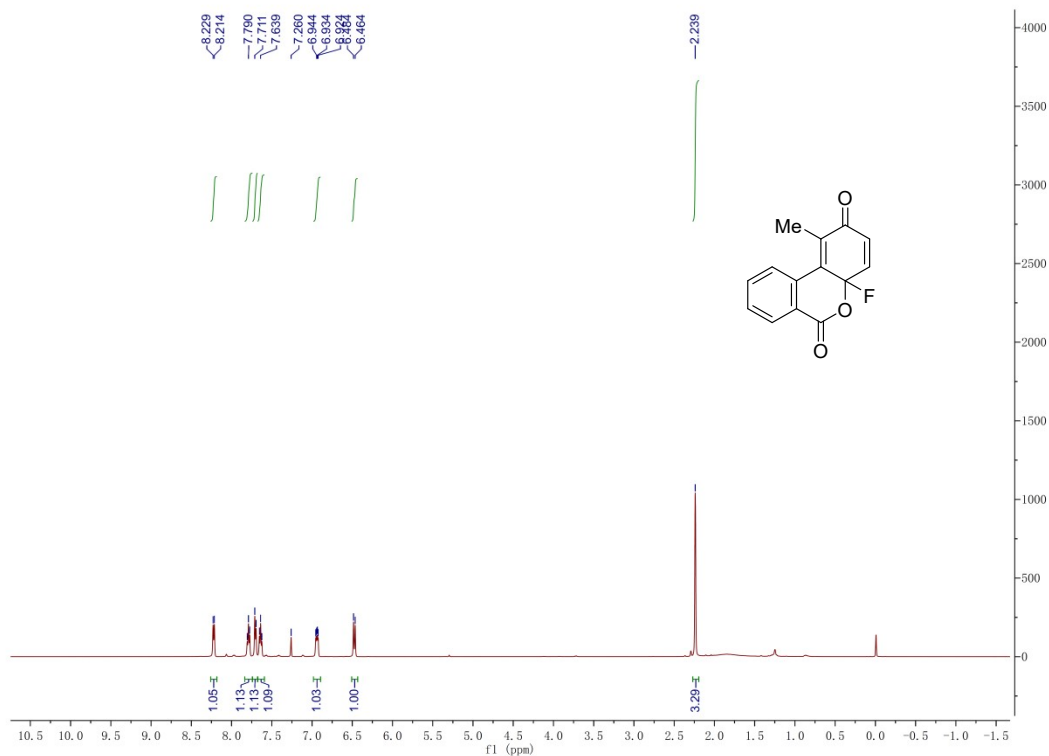
Polarity	Negative	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	200.7 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Wed Jun 17 02:41:42
Pulse Program	basic	n/a	n/a	Data Acquisition Size	2026576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.200 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec	n/a	n/a		



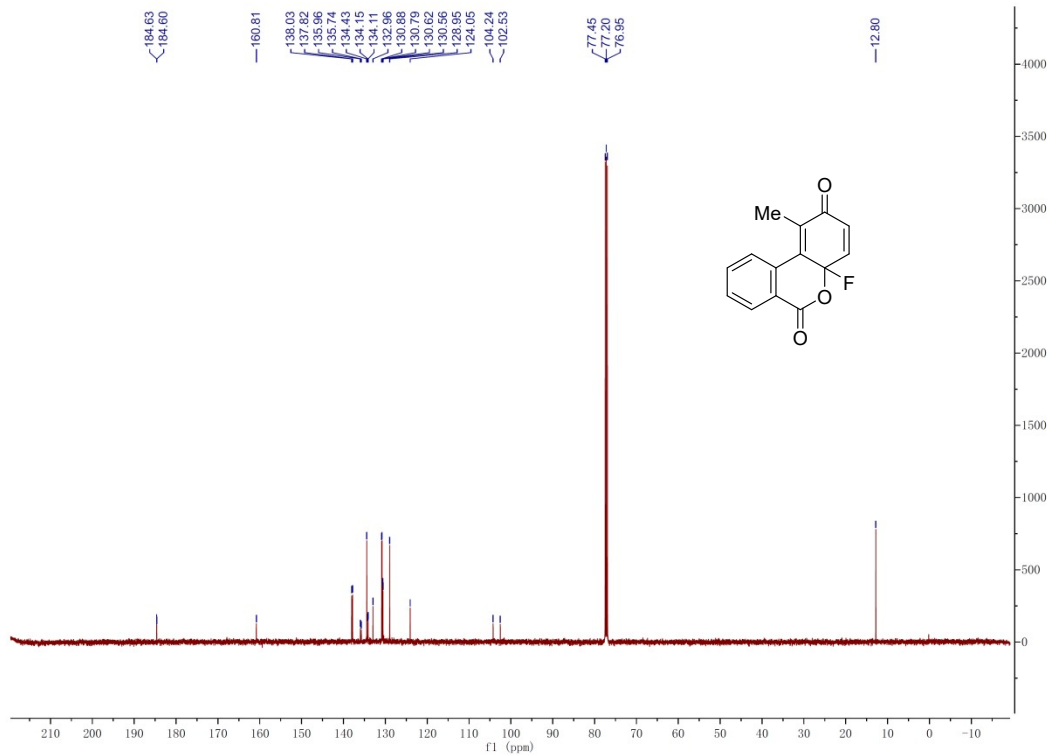
Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
274.01552	1	C ₁₃ H ₆ FNO ₅	100.00	274.01572	0.75	0.75	84.1	11.5	even	ok

4a-fluoro-1-methyl-6H-benzo[*c*]chromene-2,6(4aH)-dione (**21**)

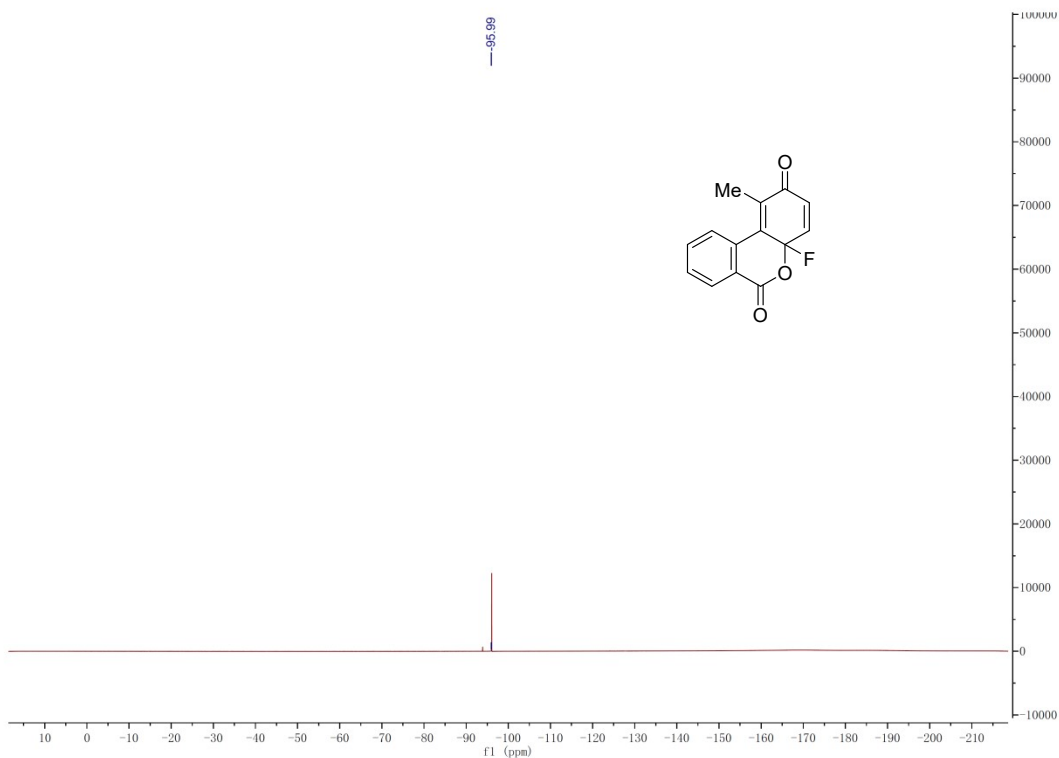
¹H NMR (500 MHz, CDCl₃)



¹³C {¹H} NMR (126 MHz, CDCl₃)



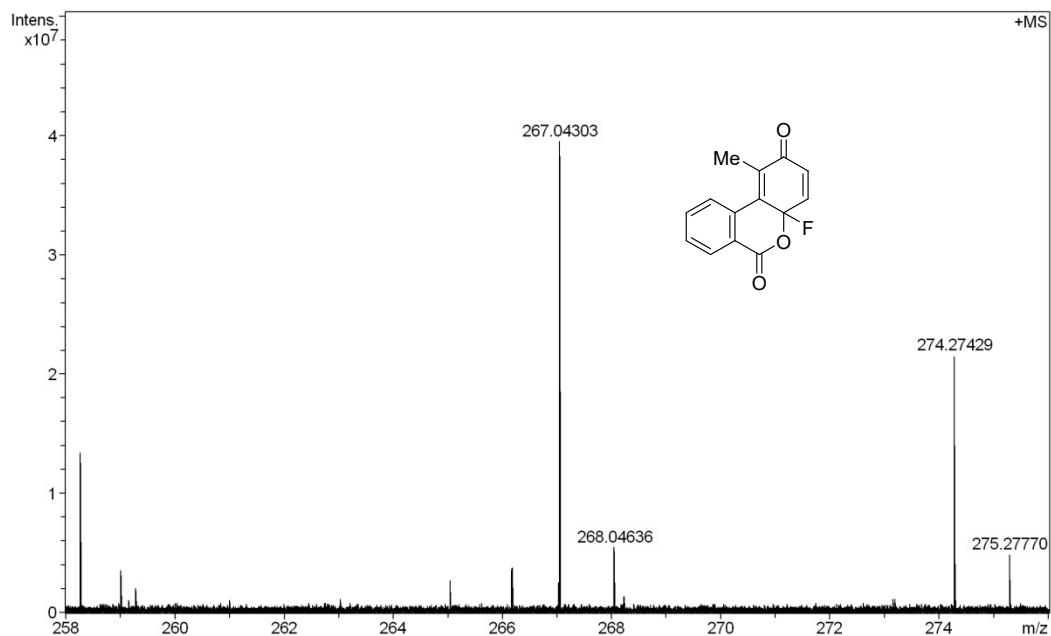
¹⁹F NMR(376 MHz, CDCl₃)



HRMS (ESI-TOF) m/z calcd for $C_{14}H_9FO_3$ (M+H)⁺ 267.0428, found 267.0430.

Acquisition Parameter

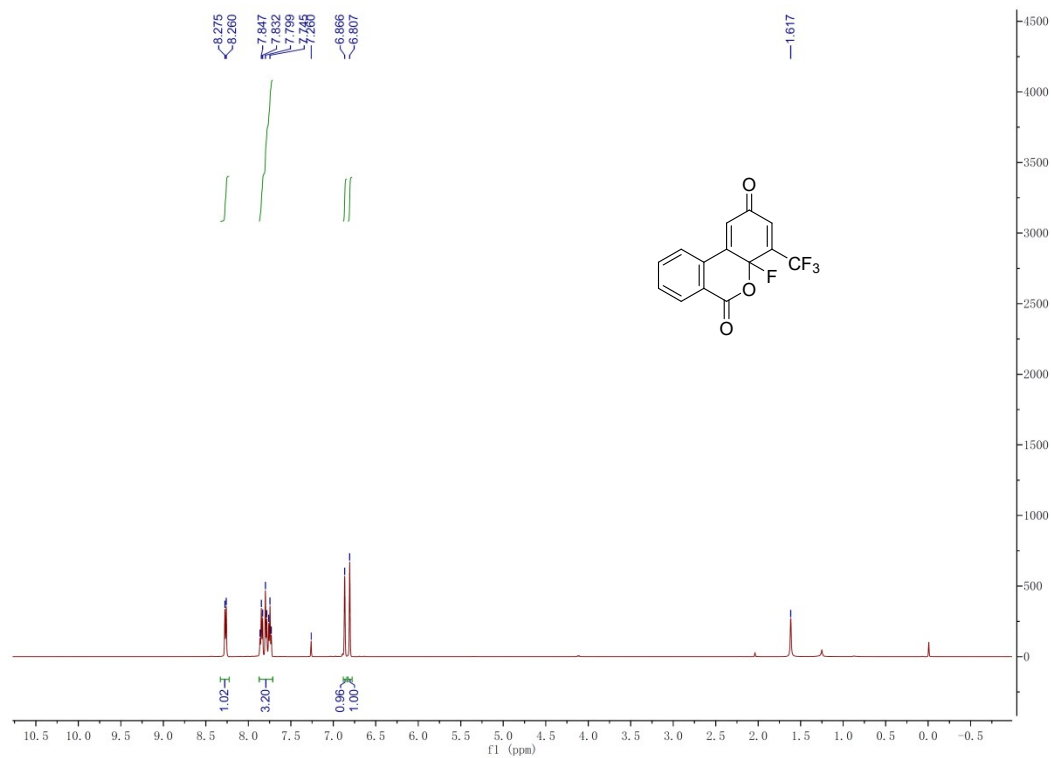
Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 Ip
Broadband Low Mass	100.4 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Wed Jun 17 02:41:42
Pulse Program	basic	n/a	n/a	Data Acquisition Size	2026576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.200 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec				



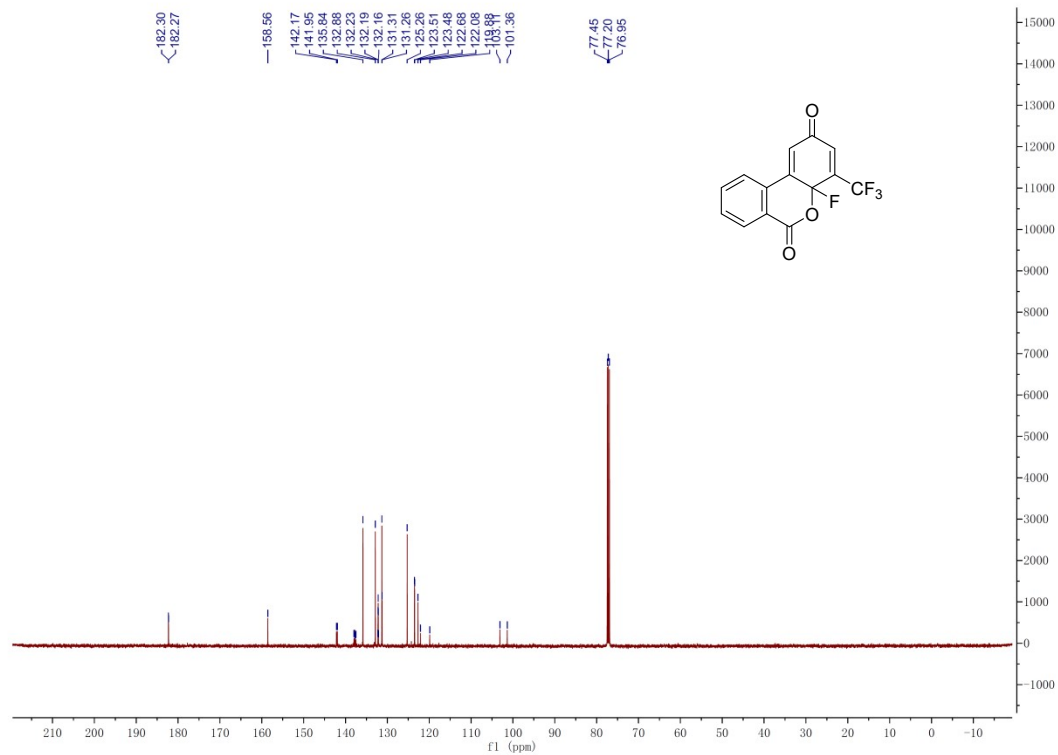
Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSig ma	rdb	e ⁻ Conf	N-R ulti
267.04303	1	C ₁₄ H ₉ FO ₃	100.00	267.04279	-0.89	-0.88	11.3	9.5	even	ok

4a-fluoro-4-(trifluoromethyl)-6H-benzo[c]chromene-2,6(4aH)-dione (**2m**)

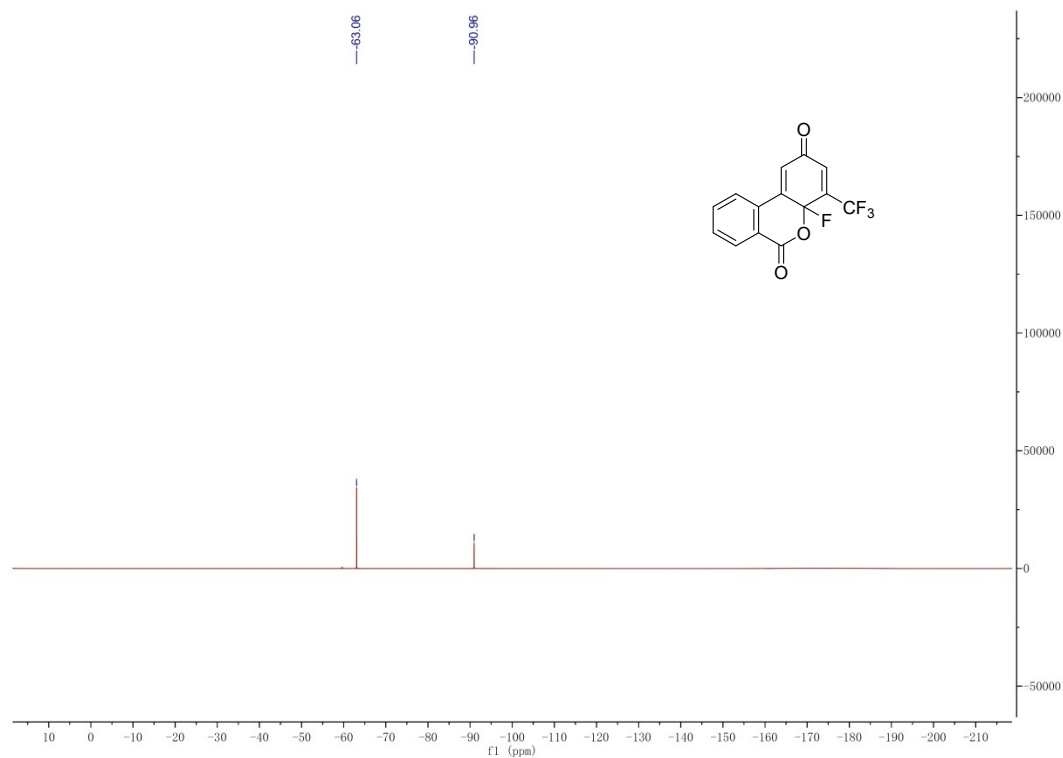
^1H NMR (500 MHz, CDCl_3)



^{13}C { ^1H } NMR (126 MHz, CDCl_3)



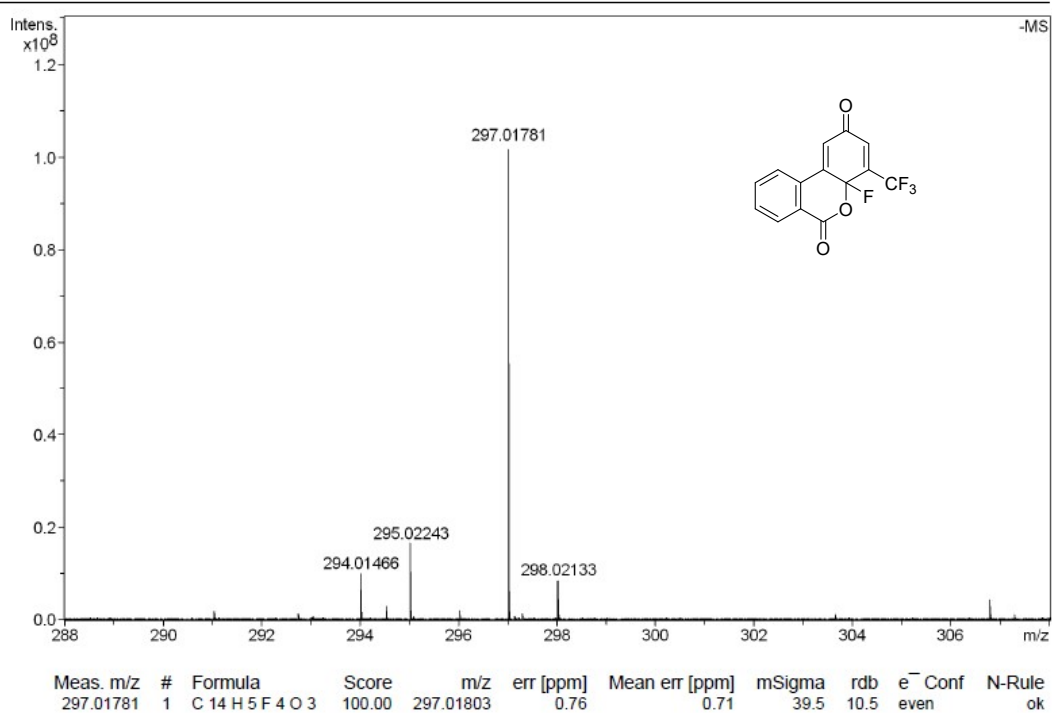
^{19}F NMR(376 MHz, CDCl_3)



HRMS (ESI-TOF) m/z calcd for $\text{C}_{14}\text{H}_6\text{F}_4\text{O}_3$ ($\text{M}-\text{H}$) $^-$ 297.0180, found 297.0178.

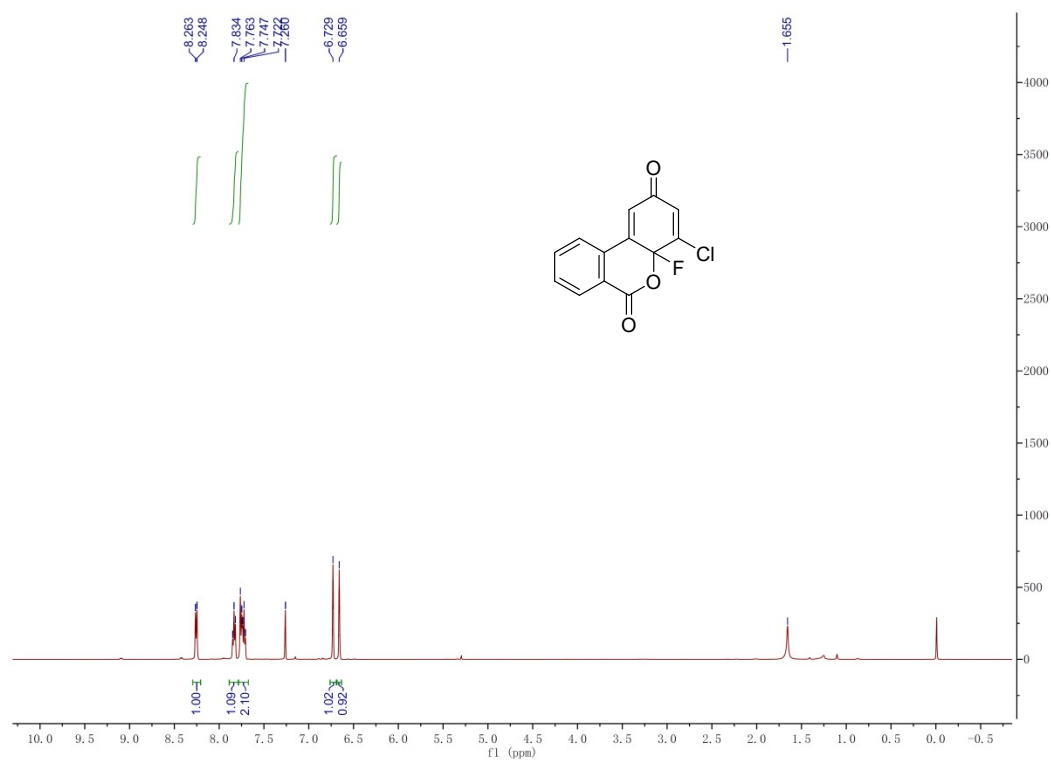
Acquisition Parameter

Polarity	Negative	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	200.7 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Wed Jun 17 02:41:42
Pulse Program	basic	n/a	n/a	Data Acquisition Size	2028576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.200 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec				

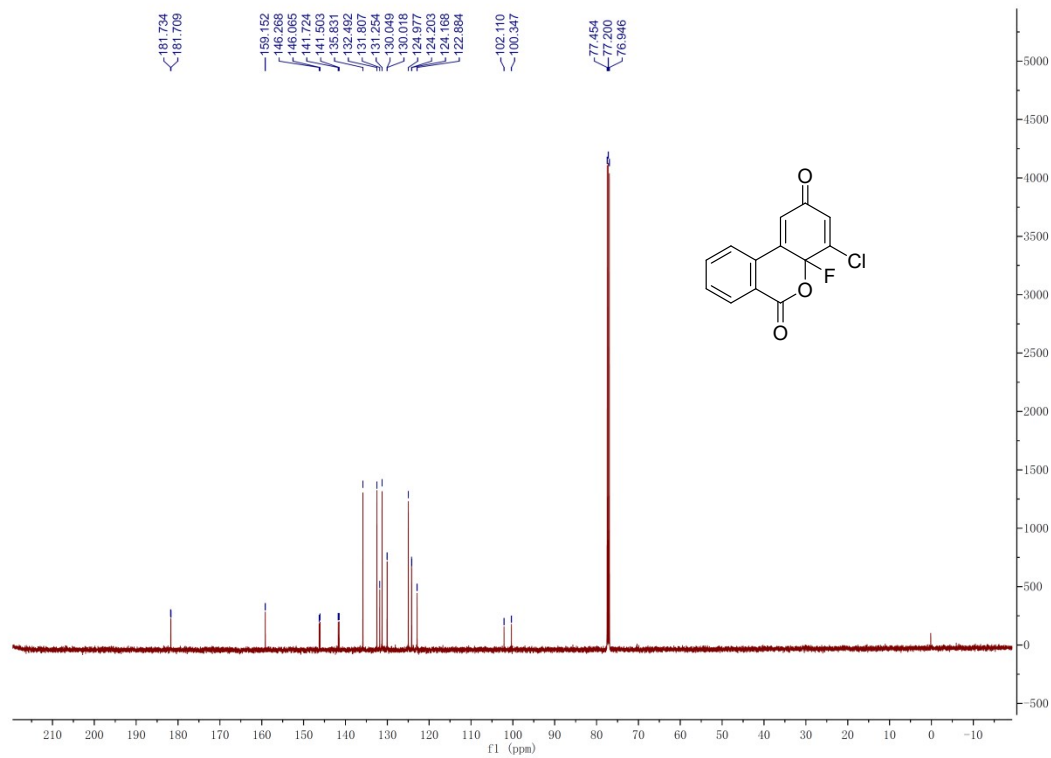


4-chloro-4a-fluoro-6H-benzo[*c*]chromene-2,6(4a*H*)-dione (**2n**)

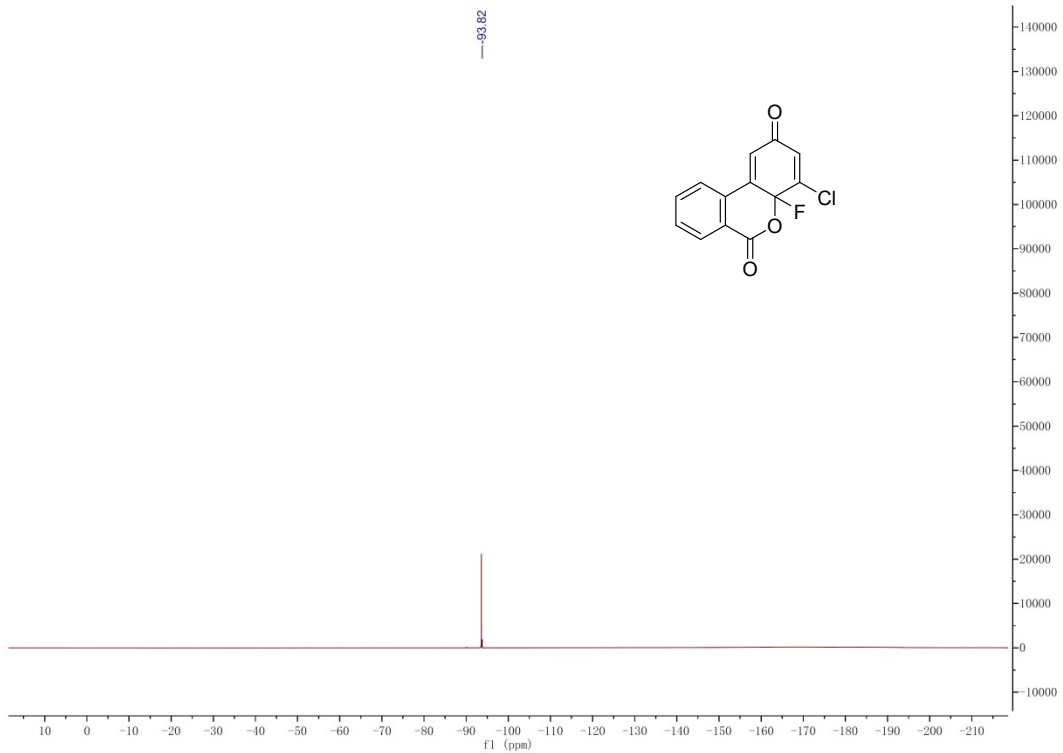
^1H NMR (500 MHz, CDCl_3)



^{13}C { ^1H } NMR (126 MHz, CDCl_3)



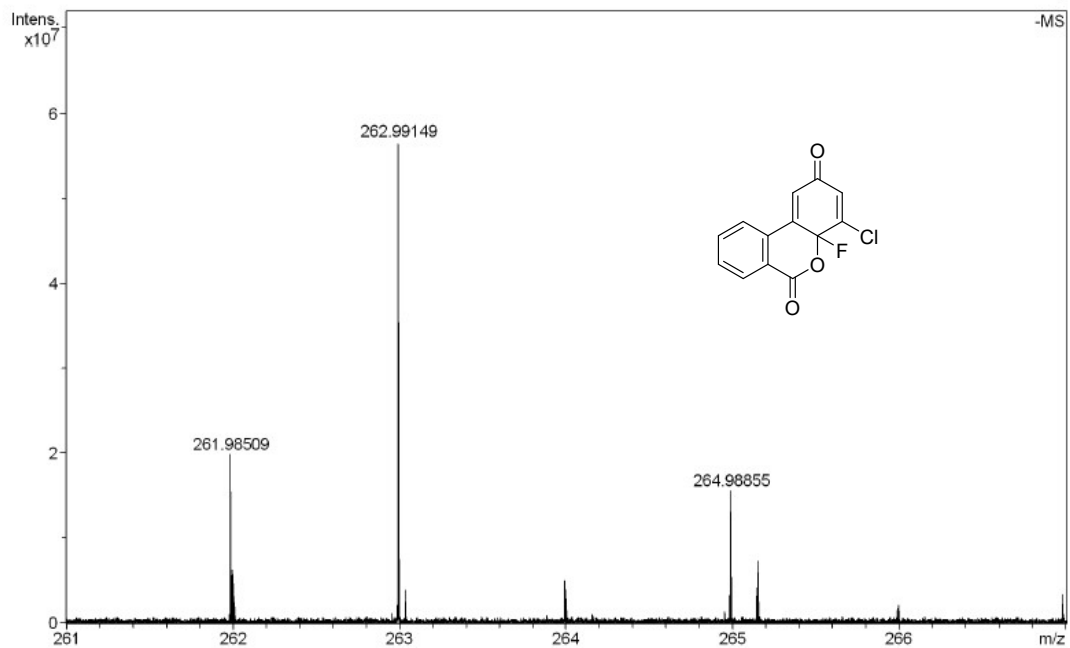
^{19}F NMR(376 MHz, CDCl_3)



HRMS (ESI-TOF) m/z calcd for $C_{13}H_6ClFO_3$ (M-H)⁻ 262.9917, found 262.9915.

Acquisition Parameter

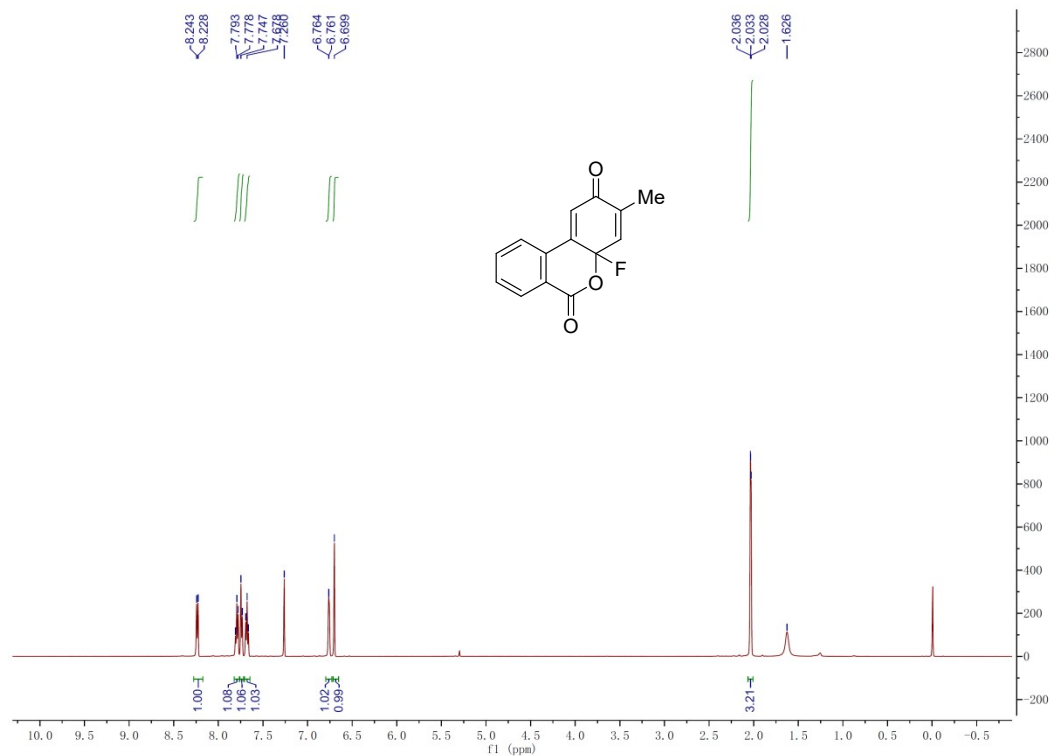
Polarity	Negative	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	200.7 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Wed Jun 17 02:41:42
Pulse Program	basic	n/a	n/a	Data Acquisition Size	2029576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.100 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec				



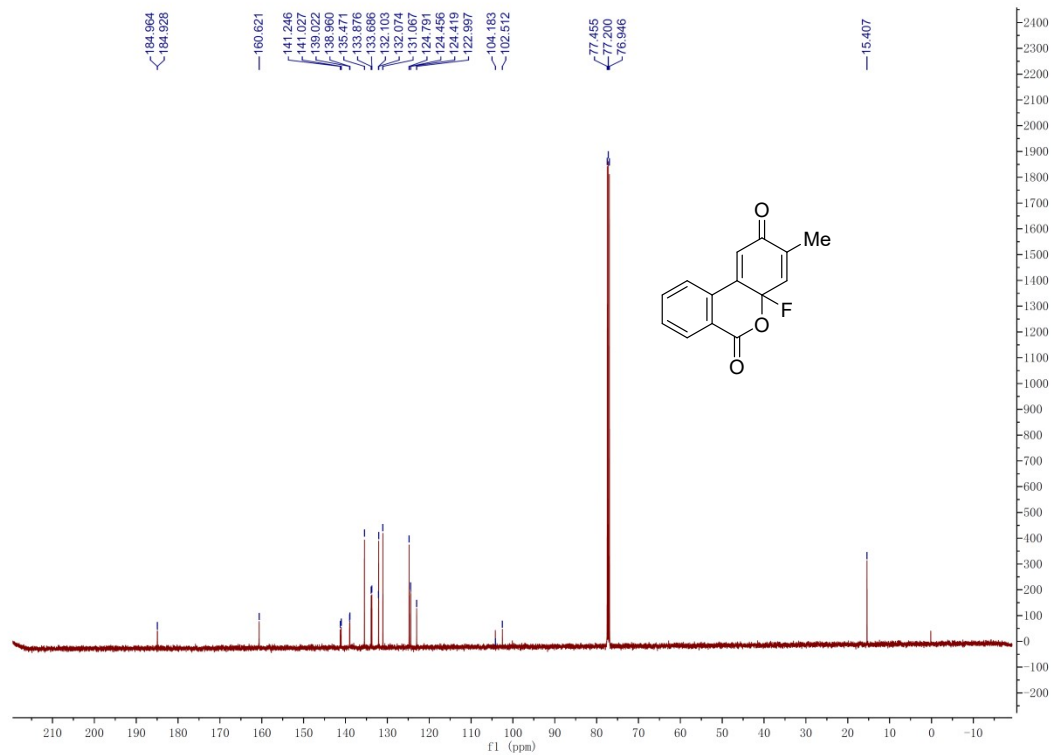
Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSig ma	rdb	e ⁻ Conf	N-R ule
262.99149	1	C ₁₃ H ₅ ClFO ₃	100.00	262.99167	0.69	0.75	79.6	10.5	even	ok

4a-fluoro-3-methyl-6H-benzo[*c*]chromene-2,6(4aH)-dione (**2o**)

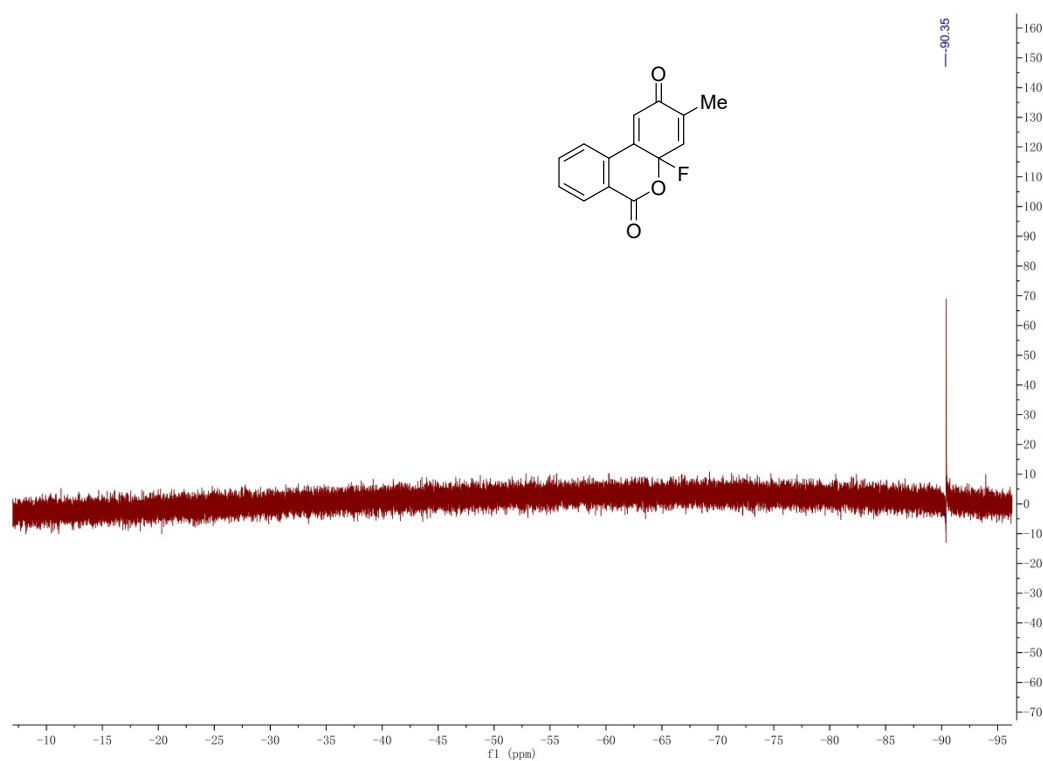
^1H NMR (500 MHz, CDCl_3)



^{13}C { ^1H } NMR (126 MHz, CDCl_3)



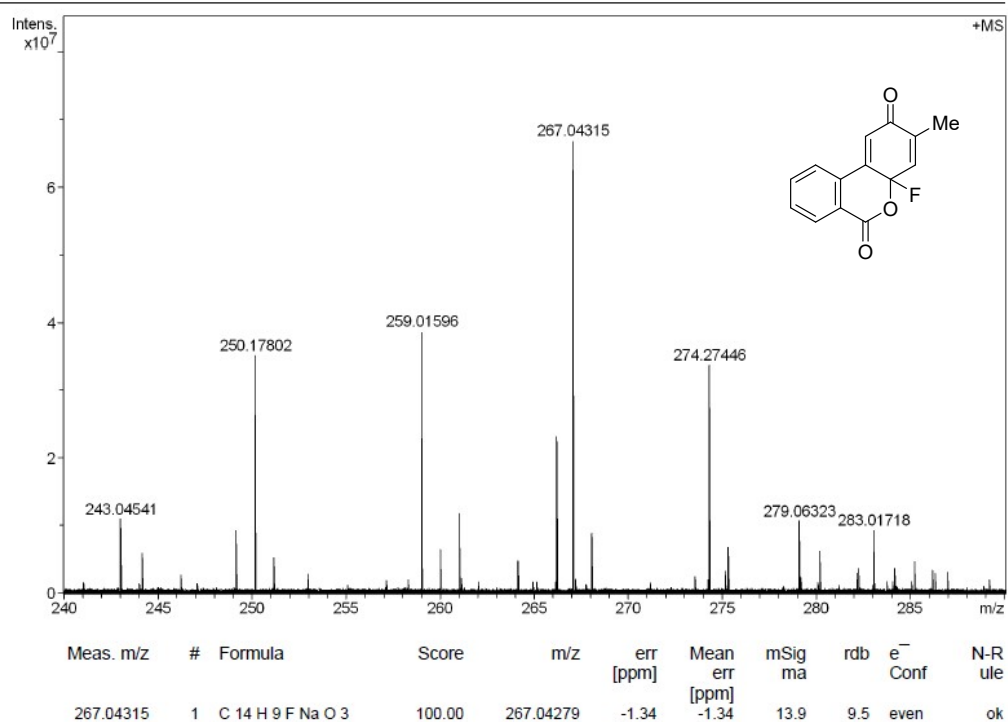
^{19}F NMR(376 MHz, CDCl_3)



HRMS (ESI-TOF) m/z calcd for $\text{C}_{14}\text{H}_9\text{FO}_3$ ($\text{M}+\text{Na}$) $^+$ 267.0428, found 267.0432.

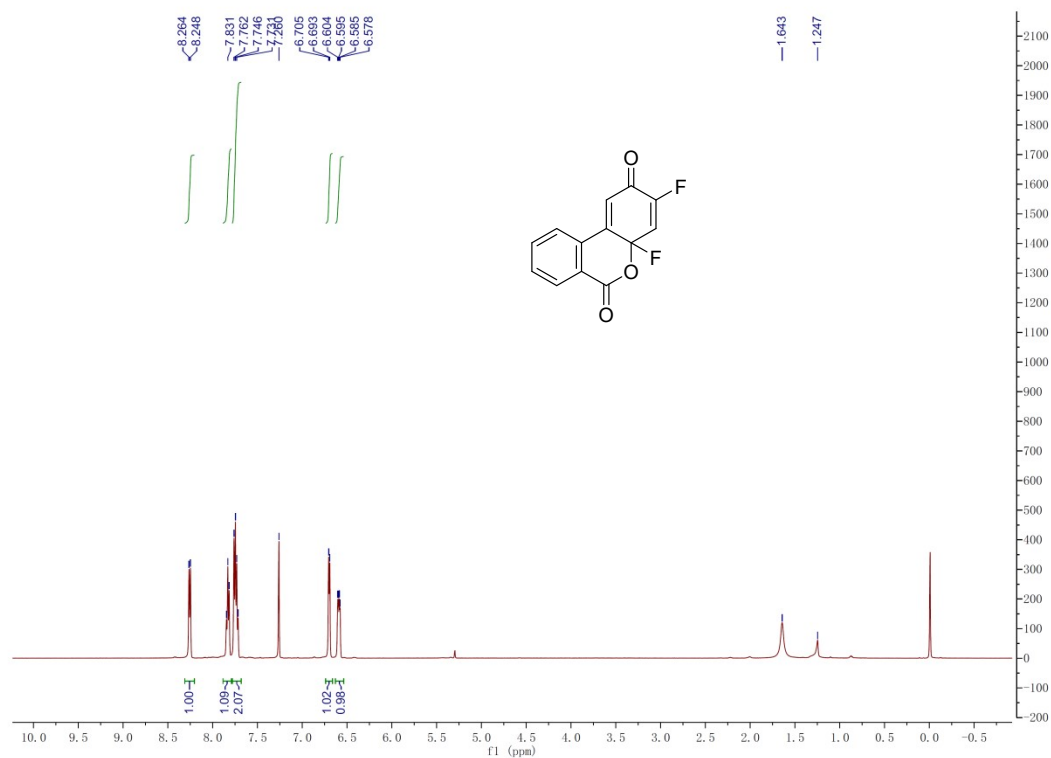
Acquisition Parameter

Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	200.7 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Tue Sep 29 10:34:51 2020
Pulse Program	basic	n/a	n/a	Data Acquisition Size	1048576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.100 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec				

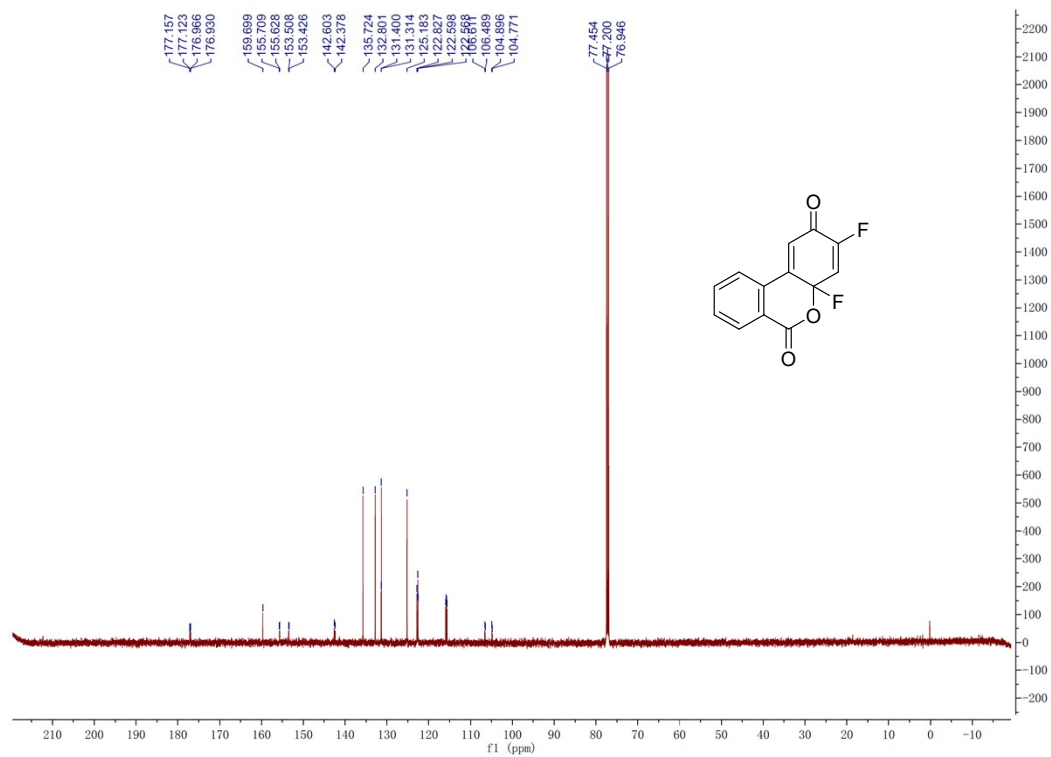


3,4a-difluoro-6H-benzo[c]chromene-2,6(4aH)-dione (**2p**)

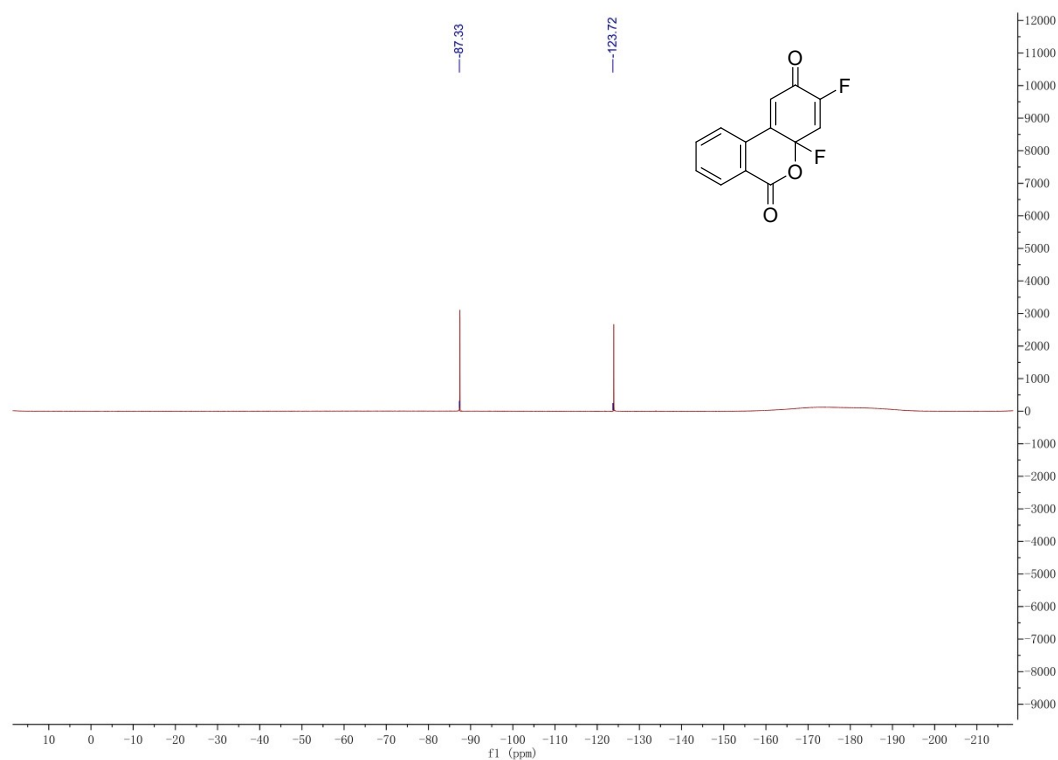
¹H NMR (500 MHz, CDCl₃)



¹³C {¹H} NMR (126 MHz, CDCl₃)



¹⁹F NMR(376 MHz, CDCl₃)



HRMS (ESI-TOF) m/z calcd for $C_{13}H_6F_2O_3$ (M-H)⁻ 247.0212, found 247.0211.

Acquisition Parameter

Polarity	Negative	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	200.7 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1000.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Wed Jun 17 02:41:42
Pulse Program	basic	n/a	n/a	Data Acquisition Size	2028576
Source Accumulation	0.500 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.200 sec	n/a	n/a		
Flight Time to Acq. Cell	0.001 sec				

