*Supporting information*

# Cobalt-Catalyzed *Ortho*-C($sp^2$)-H Amidation of Benzaldehydes with Dioxazolones Using Transient Directing Groups

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## 1. General information

**Solvents:** Toluene was distilled and other solvents used in this manuscript were purchased in anhydrous form.

**Reagents:** All commercial materials, purchased from Aldrich, Adamas, Alfa Aesar, Energy, TCI and Acros, were used as received unless otherwise noted. The starting material of benzaldehyde [$D_5$]-**42**[1] was prepared according to reported methods.

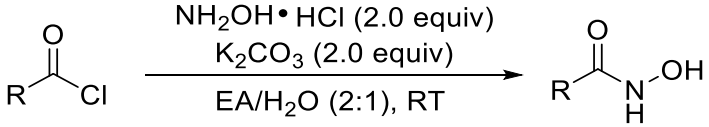
**Reactions:** All reactions were performed in oven-dried glassware under an atmosphere of argon unless otherwise noted.

**Chromatography:** Thin layer chromatography (TLC) was carried out on silica gel 60 F254 pre-coated glass plates. Visualization was detected by irradiation with UV light (254 nm), or by treatment with a solution of phosphomolybdic acid in ethanol followed by heating. Flash chromatography was carried out on 200-300 mesh silica gel, eluting with a mixture of petroleum ether (b.p. 60 -90 ℃) and ethyl acetate.

**NMR Spectroscope:** **$^1$H** NMR and **$^{13}$C** NMR spectra were recorded on a Bruker AVANCE III HD 500 spectrometer, operating at 400 MHz and 100 MHz respectively. Chemical shifts (δ) were given in parts permillion (ppm), and referenced relative to residual solvent $CHCl_3$ (7.26 ppm) in $CDCl_3$, or tetramethylsilane (0.00 ppm) as an internal standard for **$^1$H** NMR spectra and deuterated solvent $CDCl_3$ (77.16 ppm) for **$^{13}$C** NMR spectra. Coupling constants (J) were reported in hertz (Hz). The following abbreviations are used to indicate the multiplicity of the signals: s = singlet, d = doublet, t = triplet, m = multiplet, and associated combinations, e.g. dd = doublet of doublets.

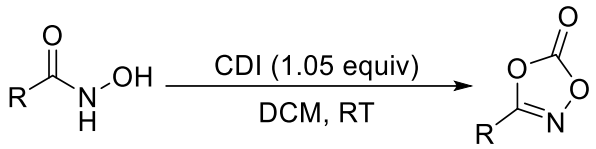
**Mass Spectrometry:** High resolution mass spectra (HRMS) were obtained on a Bruker Daltonics SolariX 7.0 Tesla Fourier Transform Ion Cyclotron Resonance (FT-ICR) Mass Spectrometer using the electrospray ionization (ESI) technique.

## 2. General procedure for the preparation of dioxazolones




Following a modified procedure[2], hydroxylamine hydrochloride (20.0 mmol, 2.0 equiv) ethyl cetate (60 mL), $H_2O$ (40 mL) and $K_2CO_3$ (20.0 mmol, 2.0 equiv) were added to a 250 mL flask at 0 $^o$C. Then acyl chloride (10.0 mmol, 1.0 equiv) dissolved in 20 mL ethyl acetate was added to the resulting mixture dropwise. The solution was warmed up to room temperature and stirred overnight. After that, the reaction mixture was extracted with ethyl acetate, washed with water and brine and dried over anhydrous $Na_2SO_4$. The solvent was evaporated under the reduced pressure to afford the desired

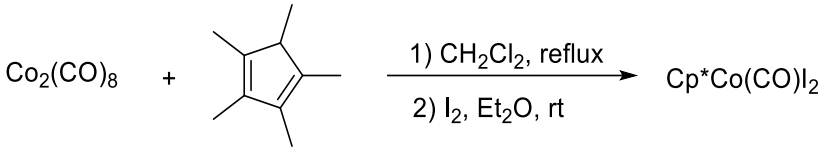
product(s) for the next step without further purification.




Following a modified procedure[3], to a stirred solution of hydoxamic acid (8 mmol, 1.0 equiv) in freshly distilled dichloromethane (60 mL) in a 250 mL flask was added 1,1'-carbonyldiimidazole (8.4 mmol, 1.05 equiv) in one portion at room temperature. After stirring for 20-30 min, the reaction mixture was quenched with 1 N aqueous solution of HCl (50 mL) and extracted with dichloromethane. The combined organic layers was washed with water and brine, dried over anhydrous $Na_2SO_4$, and then concentrated in vacuo. The resulting residue was further purified by recrystallization with ethyl acetate and hexane to give the desired 3-substituted-1,4,2-dioxazol-5-ones.

## 3. General procedure for the preparation of catalyst

### 3.1 Preparation of [Cp*Co(CO)$I_2$] catalyst[4]

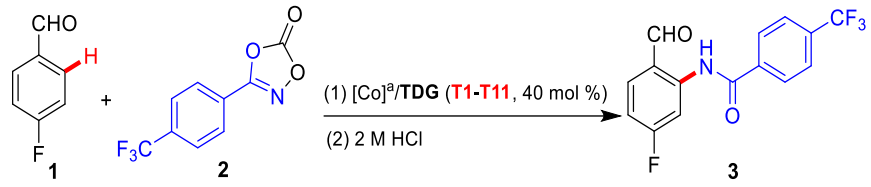


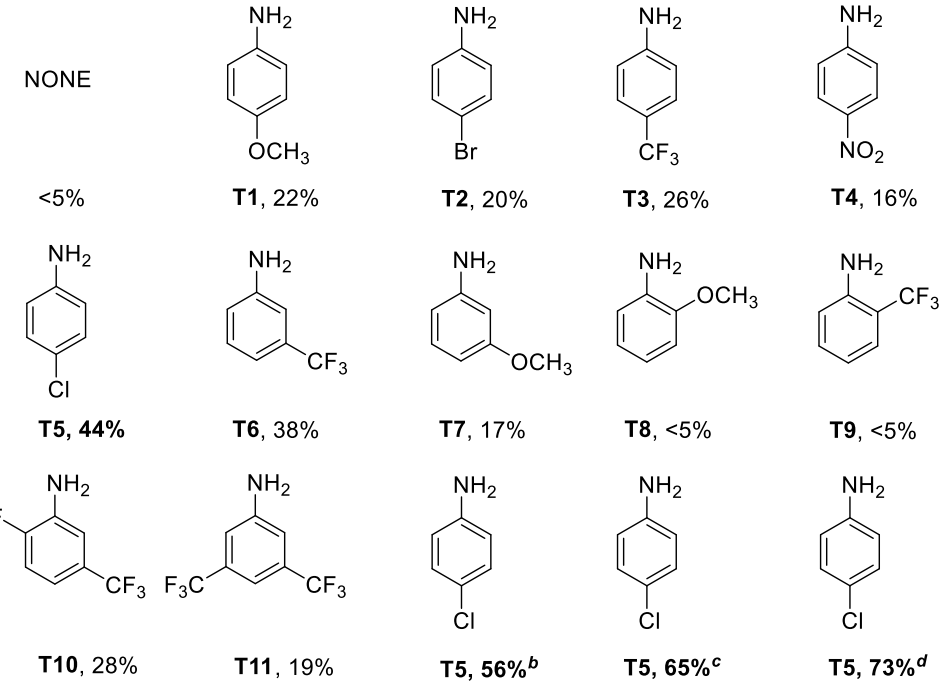

To a well-dried 2-necked 500-mL flask were successively added $Co_2(CO)_8$ (5.0 g, 14.6 mmol), degassed $CH_2Cl_2$ (100 mL) and pentamethylcyclopentadiene (5.55 mL, 35.4 mmol). The mixture was refluxed under argon stream for 6 h and then cooled to room temperature. The solvent was removed in vacuo. The residue was dissolved in degassed $Et_2O$ (50 mL) and then iodine (9.0 g, 35.5 mmol) in degassed $Et_2O$ (50 mL) was added dropwisely at room temperature with stirring. [Caution: During the addition, the mixture was refluxed due to the exothermic reaction and CO gas evolution was observed.] After the mixture was stirred at room temperature for 1 h, the solvent was evaporated. Resulting residue was purified by silica gel column chromatography (hexane then $CH_2Cl_2$/hexane=4/1) to afford deep purple crystalline solid.

### 3.2 Preparation of [Cp*Co($CH_3CN$)$_3$][$SbF_6$]$_2$ catalyst[5]

To a suspension of [Cp*Co(CO)$I_2$] (220 mg, 0.46 mmol) in dried $CH_3CN$ (3.6 mL), a solution of $AgSbF_6$ (600 mg, 1.75 mmol) in dried $CH_3CN$ (4.6 mL) was added within 2 min. Then a solid precipitated immediately. The reaction was stirred at rt for another 3 h. Then the solid was filtered through celite and washed with $CH_3CN$ (20 mL x 3). The filtrate was evaporated in vacuo to 15 mL, $Et_2O$ (50 mL) was added dropwise and a purple solid precipitated. The purple solid was collected by filtration, washed with $Et_2O$ (50 mL), dried in vacuo to afford [Cp*Co($CH_3CN$)$_3$][$SbF_6$]$_2$ (***Cat.*A**).

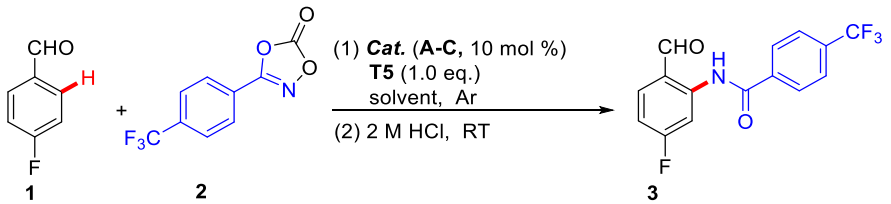
## 4. Evaluation of Aniline Promoters for *ortho*-C-H Amidation[a]




[a]Reaction conditions: **1** (0.2 mmol), **2** (0.4 mmol), ***Cat.*A** $[Cp^*Co(CH_3CN)_3][SbF_6]_2$ (10 mol%), TDG (0.4 equiv.) in DCE (1 mL) at 120 ℃ under Ar for 12 h. Isolated yield. [b]0.6 eq. *p*-chloroaniline. [c]0.8 eq. *p*-chloroaniline. [d]1.0 eq. *p*-chloroaniline.

## 5.Optimization of the Co-catalyzed *ortho*-amidation of benzaldehyde[a]




| entry | *cat.* | solvent | T (°C) | t (h) | yield (%)[b] |
|---|---|---|---|---|---|
| 1 | $CoCl_2$(***Cat.*B**) | DCE | 120 | 12 | ND |
| 2 | $Co(acac)_2$(***Cat.*C**) | DCE | 120 | 12 | ND |
| 3 | ***Cat.*A** | DCE | 120 | 12 | 73 |
| 4 | ***Cat.*A** | MeCN | 120 | 12 | <5 |
| 5 | ***Cat.*A** | dioxane | 120 | 12 | <5 |
| 6 | ***Cat.*A** | MTBE | 120 | 12 | <5 |

| | | | | | |
|---|---|---|---|---|---|
| 7 | ***Cat.*A** | toluene | 120 | 12 | <5 |
| 8 | ***Cat.*A** | THF | 120 | 12 | <5 |
| 9 | ***Cat.*A** | PhCl | 120 | 12 | <5 |
| 10 | ***Cat.*A** | DCE | 120 | 6 | **84** |
| 11 | ***Cat.*A** | DCE | 110 | 6 | 56 |

[a]Reaction conditions: All the reactions were run on a 0.2 mmol scale at 0.2 M concentration. [b]Isolated yield.

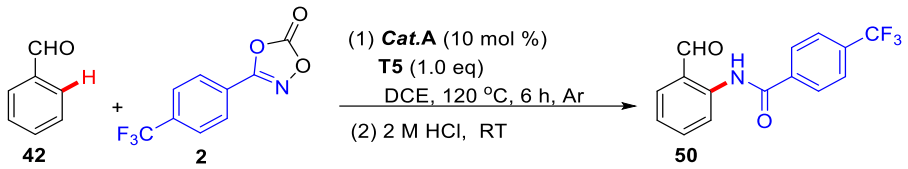
## 6. General procedure for the Co-catalyzed *ortho*-amidation reactions

A mixture of benzaldehyde substrate (0.2 mmol, 1.0 equiv), dioxazolones (0.4 mmol, 2.0 equiv), Cp*Co($CH_3CN$)$_3$[$SbF_6$]$_2$ (0.02 mmol, 10 mol %) and arylamine (0.2 mmol, 1.0 equiv) in 1 mL DCE in a 10 mL glass vial was purged with Ar and sealed with PTFE cap. After heated at 120 °C for 6 h and cooled to room temperature, the solution was removed to a 50 mL flask with 5 mL of THF, 5 mL of hydrochloric acid (2 M) was added, the mixture was stirred at rt for 3 h, extracted with DCM (3 x 15 mL). The combined organic phase was dried over anhydrous $Na_2SO_4$, concentrated, and crude product was further purified by flash chromatography (petroleum ether/ethyl acetate = 50/1~30/1) on silica gel to give the product.

## 7. Preliminary mechanistic experiments

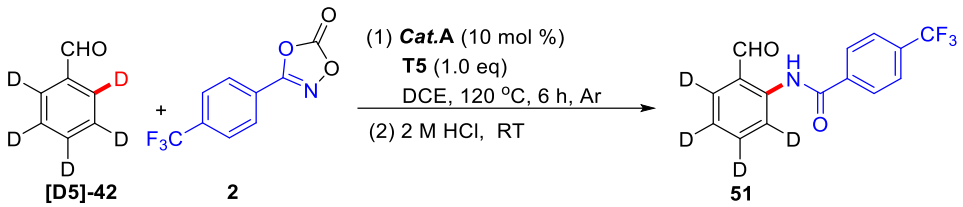
### 7.1 Parellel kinetic isotope effect

One mixture of benzaldehyde **42** (22 μL, 0.2 mmol, 1.0 equiv), dioxazolones **2** (92.5 mg, 0.4 mmol, 2.0 equiv), Cp*Co($CH_3CN$)$_3$[$SbF_6$]$_2$ (16 mg, 0.02 mmol, 10 mol %) and *p*-Chloroaniline (25.6 mg, 0.2 mmol, 1.0 equiv) in 1 mL DCE in a 10 mL glass vial was purged with Ar and sealed with PTFE cap.



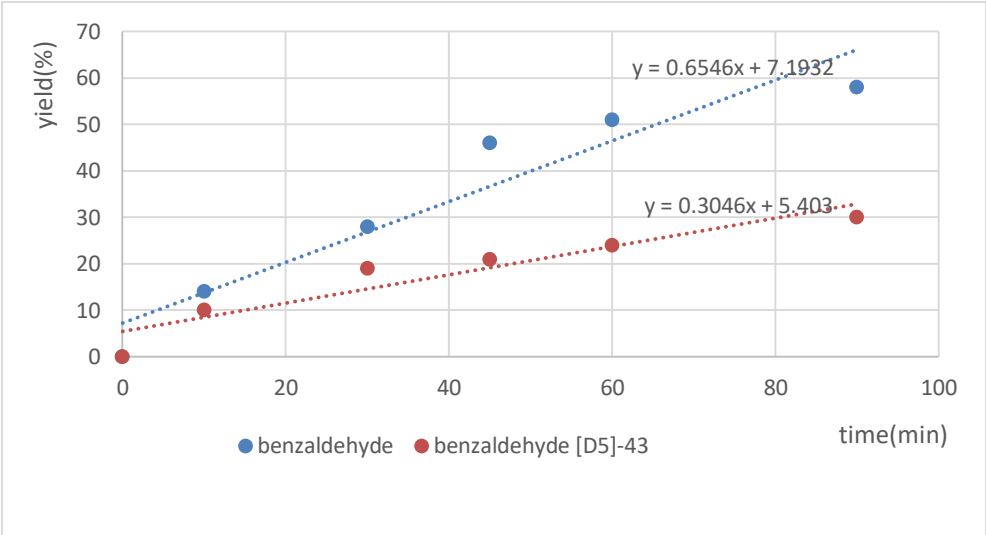

| Entry | t (min) | Yield (%) |
|---|---|---|
| 1 | 10 | 14 |
| 2 | 30 | 28 |
| 3 | 45 | 46 |
| 4 | 60 | 51 |
| 5 | 90 | 58 |

The other mixture of benzaldehyde [$D_5$]-**42** (22 μL, 0.2 mmol, 1.0 equiv), dioxazolones **2** (92.5 mg, 0.4 mmol, 2.0 equiv), Cp*Co($CH_3CN$)$_3$[$SbF_6$]$_2$ (16 mg, 0.02 mmol, 10 mol %) and *p*-Chloroaniline (25.6 mg, 0.2 mmol, 1.0 equiv) in 1 mL DCE in a 10 mL glass vial was purged with Ar and sealed with PTFE cap.



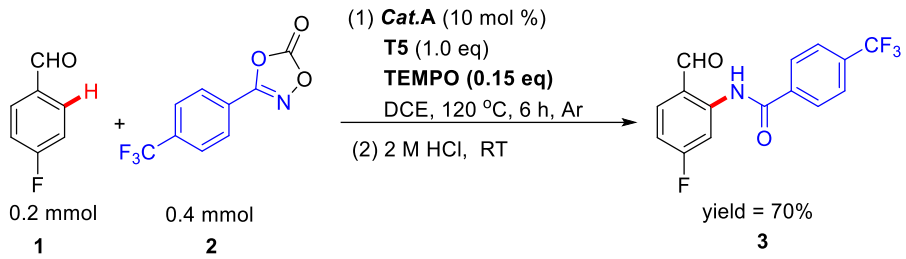

| Entry | t (min) | Yield (%) |
|---|---|---|
| 1 | 10 | 10 |
| 2 | 30 | 19 |
| 3 | 45 | 21 |
| 4 | 60 | 24 |
| 5 | 90 | 30 |

After heated at 120 °C and cooled to room temperature, the solution was removed to a 50 mL flask with 5 mL of THF, 5 mL of hydrochloric acid (2 M) was added, the mixture was stirred at rt for 3 h, extracted with DCM (3 x 15 mL). The combined organic phase was dried over anhydrous $Na_2SO_4$, concentrated, and crude product was further purified by flash chromatography (petroleum ether/ethyl acetate = 50/1) on silica gel to give the amidated product **50** and the amidated product **51**, respectively.




KIE = $k_H/k_D$ ≈2.15

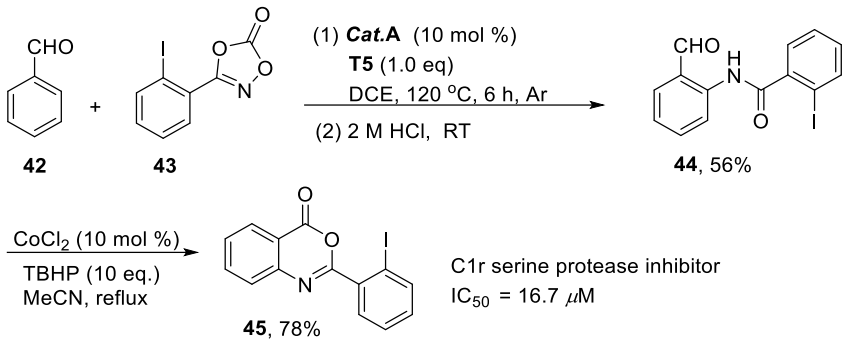
### 7.2 Radical capture experiment




A mixture of 4-fluorobenzaldehyde **1** (21.5 μL, 0.2 mmol, 1.0 equiv), dioxazolone **2** (92.5 mg, 0.4 mmol, 2.0 equiv), $Cp^*Co(CH_3CN)_3[SbF_6]_2$ (16 mg, 0.02 mmol, 10 mol %), *p*-chloroaniline (25.6 mg, 0.2 mmol, 1.0 equiv) and TEMPO (4.7 mg, 0.03 mmol, 0.15 equiv) in 1 mL DCE in a 10 mL glass vial was purged with Ar and sealed with PTFE cap. After heated at 120 °C for 6 h and cooled to room temperature, the solution was removed to a 50 mL flask with 5 mL of THF, 5 mL of hydrochloric acid (2 M) was added, the mixture was stirred at rt for 3 h, extracted with DCM (3 x 15 mL). The combined organic phase was dried over anhydrous $Na_2SO_4$, concentrated, and crude product was further purified by flash chromatography (petroleum ether/ethyl acetate = 50/1) on silica gel to give the product **3** (43.5 mg) in 70 % yield.

## 8. Synthetic utilities of the C−H amidation method

### 8.1 Preparation of compound C1r serine protease inhibitor

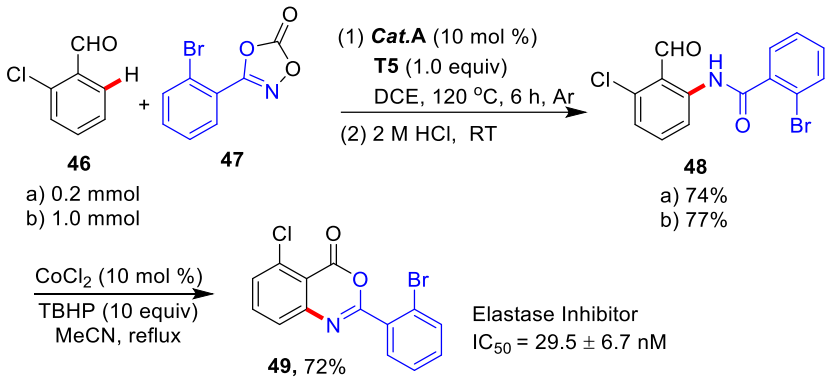



Compound **44:** A mixture of benzaldehyde **42** (22 μL, 0.2 mmol, 1.0 equiv), dioxazolones **43** (115.7 mg, 0.4 mmol, 2.0 equiv), $Cp^*Co(CH_3CN)_3[SbF_6]_2$ (16 mg, 0.02 mmol, 10 mol %) and *p*-chloroaniline (25.6 mg, 0.2 mmol, 1.0 equiv) in 1 mL DCE in a 10 mL glass vial was purged with Ar and sealed with PTFE cap. After heated at 120 °C for 6 h and cooled to room temperature, the solution was removed to a 50 mL flask with 5 mL of THF, 5 mL of hydrochloric acid (2 M) was added, the mixture was stirred at rt for 3 h, extracted with DCM (3 x 15 mL). The combined organic phase was dried over anhydrous $Na_2SO_4$, concentrated, and crude product was further purified by flash chromatography (petroleum ether/ethyl acetate = 50/1) on silica gel to give the product **44** (39.3 mg) in 56 % yield.

Compound **45:** To a suspension of amide **44** (70.2 mg, 0.2 mmol, 1.0 equiv) and $CoCl_2$ (2.6 mg, 0.02 mmol, 10 mol %) in MeCN (1 mL) was added TBHP (180.2 mg, 2.0 mmol, 10.0 equiv) dropwise at room temperature over a period of 3 min. The reaction mixture was then heated at reflux for 8 h and monitored by TLC analysis. After completion of the reaction, the solvent was evaporated under reduced pressure, and the

reaction mixture was purified by flash column chromatography (petroleum ether/ethyl acetate = 20~10/1) to give the desired amide product **45** (54.4 mg) in 78 % yield[6].

### 8.2 Preparation of compound Elastase Inhibitor

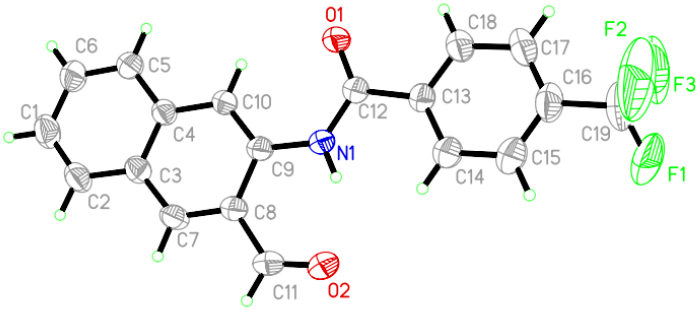



Compound **48:** A mixture of 2-chlorobenzaldehyde **46** (22.6 μL, 0.2 mmol, 1.0 equiv), dioxazolones **47** (96.8 mg, 0.4 mmol, 2.0 equiv), $Cp^*Co(CH_3CN)_3[SbF_6]_2$ (16 mg, 0.02 mmol, 10 mol %) and *p*-chloroaniline (25.6 mg, 0.2 mmol, 1.0 equiv) in 1 mL DCE in a 10 mL glass vial was purged with Ar and sealed with PTFE cap. After heated at 120 °C for 6 h and cooled to room temperature, the solution was removed to a 50 mL flask with 5 mL of THF, 5 mL of hydrochloric acid (2 M) was added, the mixture was stirred at rt for 3 h, extracted with DCM (3 x 15 mL). The combined organic phase was dried over anhydrous $Na_2SO_4$, concentrated, and crude product was further purified by flash chromatography (petroleum ether/ethyl acetate = 30/1) on silica gel to give the product **48** (50.1 mg) in 74 % yield.

***1 mmol scale experiment:*** A mixture of 2-chlorobenzaldehyde **46** (113 μL, 1.0 mmol, 1.0 equiv), dioxazolones **47** (484.0 mg, 2.0 mmol, 2.0 equiv), $Cp^*Co(CH_3CN)_3[SbF_6]_2$ (80.0 mg, 0.1 mmol, 10 mol %) and *p*-chloroaniline (128.0 mg, 1.0 mmol, 1.0 equiv) in 5 mL DCE in a 35 mL tube sealing was purged with Ar and sealed with PTFE cap. After heated at 120 °C for 6 h and cooled to room temperature, the solution was removed to a 100 mL flask with 10 mL of THF, 20 mL of hydrochloric acid (2 M) was added, the mixture was stirred at rt for 3 h, extracted with DCM (3 x 20 mL). The combined organic phase was dried over anhydrous $Na_2SO_4$, concentrated, and crude product was further purified by flash chromatography (petroleum ether/ethyl acetate = 30/1) on silica gel to give the product **48** (260.7 mg) in 77 % yield.

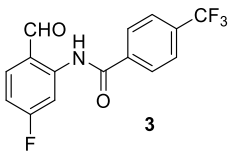
Compound **49:** To a suspension of amide **48** (67.8 mg, 0.2 mmol, 1.0 equiv) and $CoCl_2$ (2.6 mg, 0.02 mmol, 10 mol %) in MeCN (1 mL) was added TBHP (180.2 mg, 2.0 mmol, 10.0 equiv) dropwise at room temperature over a period of 3 min. The reaction mixture was then heated at reflux for 8 h and monitored by TLC analysis. After completion of the reaction, the solvent was evaporated under reduced pressure, and the reaction mixture was purified by flash column chromatography (petroleum ether/ethyl acetate = 20~10/1) to give the desired amide product **49** (48.5 mg) in 72 % yield[6].

## 9. X-ray single crystal structures of product 35




*X-Ray* of **35**
***CCDC 1940485***

## 10. Characterization data for the products

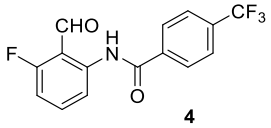



**3**

Compound **3** (52.3 mg) was isolated in 84 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^{1}$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.32 (s, 1H), 9.90 (s, 1H), 8.65 (dd, *J* = 12.0, 2.5 Hz, 1H), 8.12 (d, *J* = 8.0 Hz, 2H), 7.77 (d, *J* = 8.0 Hz, 2H), 7.72 (dd, *J* = 9.0, 6.5 Hz, 1H), 6.98-6.89 (m, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.59, 167.49 (d, *J* = 255.9 Hz), 164.79, 143.26 (d, *J* = 13.7 Hz), 138.76 (d, *J* = 11.7 Hz), 137.09, 134.10 (q, *J* = 32.5 Hz), 128.06, 126.06 (q, *J* = 3.7 Hz), 123.68 (q, *J* = 271.0 Hz), 119.05 (d, *J* = 2.3 Hz), 111.05 (d, *J* = 23.0 Hz), 107.69 (d, *J* = 28.7 Hz).

**HRMS**: calculated for $C_{15}H_{10}F_4NO_2$ [M+H$^+$]: 312.0642; **found**: 312.0638.

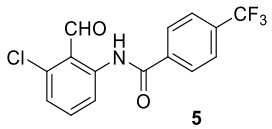



**4**

Compound **4** (44.8 mg) was isolated in 72 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^{1}$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.34 (s, 1H), 10.41 (s, 1H), 8.68 (d, *J* = 8.6 Hz, 1H), 8.13 (d, *J* = 8.1 Hz, 2H), 7.77 (d, *J* = 8.2 Hz, 2H), 7.71-7.52 (m, 1H), 6.97-6.75 (m, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 191.37 (d, *J* = 12.9 Hz), 166.18 (d, *J* = 257.2 Hz), 164.79, 142.12 (d, *J* = 2.5 Hz), 138.56 (d, *J* = 11.2 Hz), 137.31, 134.04 (q, *J* = 32.6 Hz), 128.08, 126.06 (q, *J* = 3.6 Hz), 123.71 (q, *J* = 271.1 Hz), 115.91 (d, *J* = 3.9 Hz), 111.09 (d, *J* = 8.4 Hz), 110.20 (d, *J* = 20.4 Hz).

**HRMS**: calculated for $C_{15}H_{10}F_4NO_2$ [M+H$^+$]: 312.0642; **found**: 312.0638



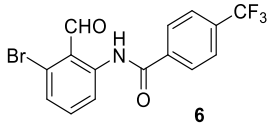

**5**

Compound **5** (52.4 mg) was isolated in 80 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.59 (s, 1H), 10.66 (s, 1H), 8.89 (d, *J* = 8.5 Hz, 1H), 8.17 (d, *J* = 8.0 Hz, 2H), 7.81 (d, *J* = 8.5 Hz, 2H), 7.59 (t, *J* = 8.0 Hz, 1H), 7.23 (dd, *J* = 8.0, 1.0 Hz, 1H).

**$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 195.06, 164.97, 143.16, 140.56, 137.56, 137.24, 134.13 (q, *J* = 32.7 Hz), 128.17, 126.15 (q, *J* = 3.7 Hz), 125.37, 122.66(q, *J* = 271.0 Hz), 119.29, 118.08.

**HRMS**: calculated for $C_{15}H_{10}ClF_3NO_2$ [M+H$^+$]: 328.0347; **found**: 328.0346.



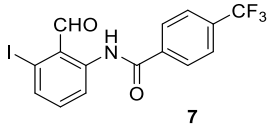

**6**

Compound **6** (58.1 mg) was isolated in 78 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.58 (s, 1H), 10.53 (s, 1H), 8.91 (d, *J* = 8.5 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.47 (t, *J* = 8.0 Hz, 1H), 7.42 (dd, *J* = 8.0, 1.0 Hz, 1H).

**$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 197.54, 164.78, 143.18, 137.50, 137.22, 134.08 (q, *J* = 32.6 Hz), 130.21, 128.87, 128.14, 126.11 (q, *J* = 3.6 Hz), 123.72 (q, *J* = 270.7 Hz), 120.01, 118.72.

**HRMS**: calculated for $C_{15}H_{10}BrF_3NO_2$ [M+H$^+$]: 371.9842; **found**: 371.9838.



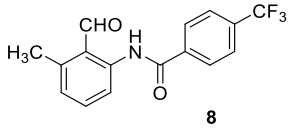

**7**

Compound **7** (63.7 mg) was isolated in 76 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.55 (s, 1H), 10.21 (s, 1H), 8.92 (d, *J* = 8.5 Hz, 1H), 8.13 (d, *J* = 8.0 Hz, 2H), 7.77 (d, *J* = 8.0 Hz, 2H), 7.72 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.22 (t, *J* = 8.0 Hz, 1H).

**$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 202.22, 164.45, 142.52, 137.45, 137.15, 136.10, 133.99 (q, *J* = 32.5 Hz), 128.10, 126.05 (q, *J* = 3.7 Hz), 123.68 (q, *J* = 271.0 Hz), 121.00, 119.55, 105.06.

**HRMS**: calculated for $C_{15}H_{10}F_3INO_2$ [M+H$^+$]: 419.9703; **found**: 419.9702.



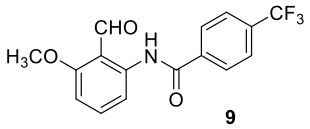

**8**

Compound **8** (49.8 mg) was isolated in 81 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.65 (s, 1H), 10.52 (d, *J* = 2.5 Hz, 1H), 8.79 (d, *J* = 8.5 Hz, 1H), 8.18 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.54 (t, *J* = 8.0 Hz, 1H), 7.00 (d, *J* = 7.5 Hz,

1H), 2.71 (s, 3H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 195.06, 164.93, 143.68, 141.81, 138.03, 136.86, 133.77 (q, *J* = 32.5 Hz), 128.12, 126.56, 126.02 (q, *J* = 3.7 Hz), 123.81 (q, *J* = 271.0 Hz), 119.79, 118.70, 19.36.

**HRMS**: calculated for $C_{16}H_{13}F_3NO_2$ [M+H$^+$]: 308.0893; **found**: 308.0889.

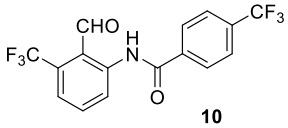



**9**

Compound **9** (50.4 mg) was isolated in 78 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 30/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.73 (s, 1H), 10.55 (s, 1H), 8.47 (d, *J* = 8.5 Hz, 1H), 8.17 (d, *J* = 8.0 Hz, 2H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.58 (t, *J* = 8.5 Hz, 1H), 6.70 (d, *J* = 8.5 Hz, 1H), 3.93 (s, 3H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.03, 164.96, 163.51, 142.39, 138.37, 137.87, 133.75 (q, *J* = 32.4 Hz), 128.13, 125.97 (q, *J* = 3.6 Hz), 123.80 (q, *J* = 270.97 Hz), 112.27, 111.34, 105.88, 56.10.

**HRMS**: calculated for $C_{16}H_{13}F_3NO_3$ [M+H$^+$]: 324.0842; **found**: 324.0835.



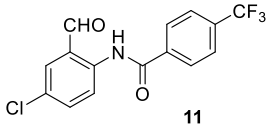

**10**

Compound **10** (5.8 mg) was isolated in 9 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 30/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.69 (s, 1H), 10.45 (s, 1H), 9.22 (d, *J* = 9.0 Hz, 1H), 8.17 (d, *J* = 8.0 Hz, 2H), 7.82 (d, *J* = 8.5 Hz, 2H), 7.77 (t, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 7.5 Hz, 1H).

**$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 193.89 (q, *J* = 3.7 Hz), 165.15, 142.97, 137.38, 135.76, 134.24 (q, *J* = 32.6 Hz), 133.32 (q, *J* = 31.5 Hz), 128.18, 126.19 (q, *J* = 3.6 Hz), 124.67, 123.71 (q, *J* = 271.0 Hz), 123.66 (q, *J* = 273.5 Hz), 121.20 (q, *J* = 6.1 Hz), 118.13.

**HRMS**: calculated for $C_{16}H_{10}F_6NO_2$ [M+H$^+$]: 362.0610; **found**: 362.0613.



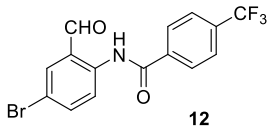

**11**

Compound **11** (28.2 mg) was isolated in 43 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.05 (s, 1H), 9.94 (s, 1H), 8.91 (d, *J* = 8.5 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 2H), 7.80 (d, *J* = 8.5 Hz, 2H), 7.71 (d, *J* = 2.5 Hz, 1H), 7.63 (dd, *J* = 9.0, 2.5 Hz, 1H).

**$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.98, 164.74, 139.43, 137.30, 136.39, 135.37, 134.10 (q, *J* = 32.5 Hz), 128.80, 128.07, 126.13 (q, *J* = 3.7 Hz), 123.71 (q, *J* = 271.1 Hz), 123.16, 121.80.

**HRMS**: calculated for $C_{15}H_{10}ClF_3NO_2$ [M+H$^+$]: 328.0347; **found**: 328.0349.

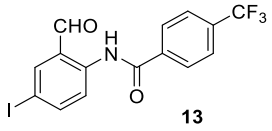



**12**

Compound **12** (30.5 mg) was isolated in 41 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.05 (s, 1H), 9.93 (s, 1H), 8.85 (d, *J* = 9.0 Hz, 1H), 8.14 (d, *J* = 8.0 Hz, 2H), 7.85 (d, *J* = 2.5 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 2H), 7.77 (dd, *J* = 9.0, 2.5 Hz, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.91, 164.76, 139.89, 139.27, 138.40, 137.31, 134.13 (q, *J* = 32.7 Hz), 128.08, 126.15 (q, *J* = 3.6 Hz), 123.72 (q, *J* = 270.7 Hz), 123.52, 122.04, 115.91.

**HRMS**: calculated for $C_{15}H_{10}BrF_3NO_2$ [M+H$^+$]: 371.9842; **found**: 371.9837.

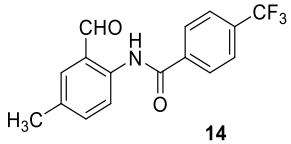



**13**

Compound **13** (40.2 mg) was isolated in 48 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.06 (s, 1H), 9.92 (s, 1H), 8.72 (dd, *J* = 8.5, 2.5 Hz, 1H), 8.14 (d, *J* = 7.5 Hz, 2H), 8.03 (d, *J* = 2.5 Hz, 1H), 7.95 (dd, *J* = 9.0, 2.5 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 2H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.89, 164.81, 145.03, 144.47, 140.49, 137.33, 134.13 (q, *J* = 32.6 Hz), 128.09, 126.15 (q, *J* = 3.7 Hz), 123.86, 123.71 (q, *J* = 271.0 Hz), 122.17, 85.67.

**HRMS**: calculated for $C_{15}H_{10}F_3INO_2$ [M+H$^+$]: 419.9703; **found**: 419.9703.

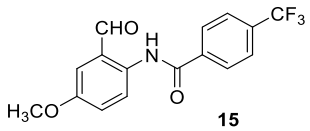



**14**

Compound **14** (38.7 mg) was isolated in 63 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.06 (s, 1H), 9.94 (s, 1H), 8.80 (d, *J* = 8.5 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 2H), 7.78 (d, *J* = 8.5 Hz, 2H), 7.57-7.36 (m, 2H), 2.42 (s, 3H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 196.23, 164.61, 138.57, 137.78, 137.32, 136.52, 133.76 (q, *J* = 32.6 Hz), 133.44, 128.02, 126.01 (q, *J* = 3.7 Hz), 123.79 (q, *J* = 271.1 Hz), 122.17, 120.14, 20.66.

**HRMS**: calculated for $C_{16}H_{13}F_3NO_2$ [M+H$^+$]: 308.0893; **found**: 308.0887.

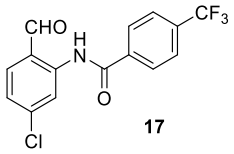



**15**

Compound **15** (18.1 mg) was isolated in 28 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 30/1).

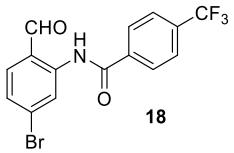
**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 11.88 (s, 1H), 9.92 (s, 1H), 8.84 (d, *J* = 8.5 Hz, 1H), 8.12 (d,

*J* = 8.0 Hz, 2H), 7.76 (d, *J* = 8.5 Hz, 2H), 7.23-7.15 (m, 2H), 3.85 (s, 3H).
**$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 195.76, 164.30, 155.59, 137.80, 134.47, 133.65 (q, *J* = 32.5 Hz), 127.92, 125.96 (q, *J* = 3.7 Hz), 123.78 (q, *J* = 270.9 Hz), 122.99, 122.31, 121.80, 120.00, 55.81.
**HRMS**: calculated for $C_{16}H_{13}F_3NO_3$ [M+H$^+$]: 324.0842; **found**: 324.0834.



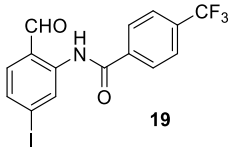
**17**

Compound **17** (52.4 mg) was isolated in 80 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).
**$^{1}$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.19 (s, 1H), 9.92 (s, 1H), 8.95 (t, *J* = 2.2 Hz, 1H), 8.12 (d, *J* = 8.0 Hz, 2H), 7.77 (d, *J* = 8.0 Hz, 2H), 7.64 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.25-7.21 (m, 1H).
**$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.95, 164.68, 143.31, 141.64, 137.13, 137.07, 134.09 (q, *J* = 32.6 Hz), 128.05, 126.08 (q, *J* = 3.6 Hz), 123.93, 123.67 (q, *J* = 271.0 Hz), 120.46, 120.21.
**HRMS**: calculated for $C_{15}H_{10}ClF_3NO_2$ [M+H$^+$]: 328.0347; **found**: 328.0341.



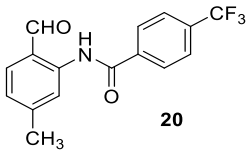
**18**

Compound **18** (60.3 mg) was isolated in 81 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).
**$^{1}$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.18 (s, 1H), 9.94 (s, 1H), 9.15 (s, 1H), 8.14 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.58 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.46-7.35 (m, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 195.23, 164.75, 141.52, 137.13, 134.14 (q, *J* = 32.6 Hz), 132.32, 128.09, 126.99, 126.13 (q, *J* = 3.6 Hz), 123.69 (q, *J* = 271.0 Hz), 123.24, 120.80
**HRMS**: calculated for $C_{15}H_{10}BrF_3NO_2$ [M+H$^+$]: 371.9842; **found**: 371.9839.



**19**

Compound **19** (62.9 mg) was isolated in 75 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).
**$^{1}$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.11 (s, 1H), 9.91 (s, 1H), 9.35 (d, *J* = 1.5 Hz, 1H), 8.13 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.66 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H).
**$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 195.53, 164.65, 140.94, 137.13, 136.83, 134.09 (q, *J* = 32.5 Hz), 133.06, 129.14, 128.07, 126.12 (q, *J* = 3.6 Hz), 123.68 (q, *J* = 270.9 Hz), 121.21, 105.66.
**HRMS**: calculated for $C_{15}H_{10}F_3INO_2$ [M+H$^+$]: 419.9703; **found**: 419.9705.

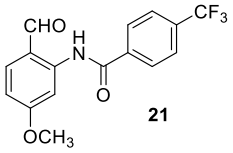



**20**

Compound **20** (45.5 mg) was isolated in 74 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.18 (s, 1H), 9.90 (s, 1H), 8.74 (s, 1H), 8.16 (d, *J* = 8.5 Hz, 2H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 7.5 Hz, 1H), 7.08 (d, *J* = 8.0 Hz, 1H), 2.47 (s, 3H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 195.46, 164.75, 148.48, 140.89, 137.69, 136.40, 133.81 (q, *J* = 32.6 Hz), 128.04, 126.01 (q, *J* = 3.6 Hz), 124.85(q, *J* = 270.9 Hz), 124.61, 120.49, 120.20, 22.64.

**HRMS**: calculated for $C_{16}H_{13}F_3NO_2$ [M+H$^+$]: 308.0893; **found**: 308.0890.

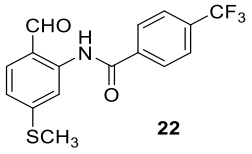



**21**

Compound **21** (38.8 mg) was isolated in 60 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 30/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.47 (s, 1H), 9.81 (s, 1H), 8.53 (d, *J* = 2.5 Hz, 1H), 8.17 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.60 (d, *J* = 8.5 Hz, 1H), 6.76 (dd, *J* = 8.5, 2.0 Hz, 1H), 3.94 (s, 3H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.10, 166.25, 165.02, 143.42, 138.20, 137.55, 133.91 (q, *J* = 32.6 Hz), 128.08, 126.06 (q, *J* = 3.6 Hz), 123.75 (q, *J* = 271.0 Hz), 116.27, 110.84, 104.13, 56.00.

**HRMS**: calculated for $C_{16}H_{13}F_3NO_3$ [M+H$^+$]: 324.0842; **found**: 324.0836.

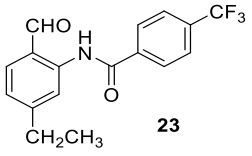



**22**

Compound **22** (55.0 mg) was isolated in 81 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.32 (s, 1H), 9.84 (s, 1H), 8.81 (d, *J* = 1.5 Hz, 1H), 8.16 (d, *J* = 8.5 Hz, 2H), 7.79 (d, *J* = 8.5 Hz, 2H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.07 (dd, *J* = 8.0, 2.0 Hz, 1H), 2.58 (s, 3H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.59, 164.94, 151.66, 141.18, 137.48, 135.99, 133.94 (q, *J* = 32.5 Hz), 128.06, 126.07 (q, *J* = 3.8 Hz), 123.74 (q, *J* = 271.3 Hz), 119.96, 118.74, 114.84, 14.70.

**HRMS**: calculated for $C_{16}H_{13}F_3NO_2S$ [M+H$^+$]: 340.0614; **found**: 340.0615.

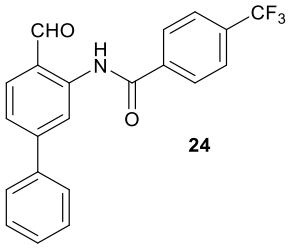



**23**

Compound **23** (49.5 mg) was isolated in 77 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.20 (s, 1H), 9.90 (s, 1H), 8.78 (s, 1H), 8.16 (d, *J* = 8.0 Hz, 2H), 7.78 (d, *J* = 8.5 Hz, 2H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.11 (d, *J* = 7.5 Hz, 1H), 2.75 (q, *J* = 7.5 Hz, 2H), 1.29 (t, *J* = 7.5 Hz, 3H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 195.48, 164.73, 154.54, 141.04, 137.70, 136.52, 133.77 (q, *J* = 32.5 Hz), 128.02, 126.00 (q, *J* = 3.8 Hz), 123.91 (q, *J* = 270.9 Hz), 123.39, 120.35, 119.46, 29.82, 15.07.

**HRMS**: calculated for $C_{17}H_{15}F_3NO_2$ [M+H$^+$]: 322.1049; **found**: 322.1043.



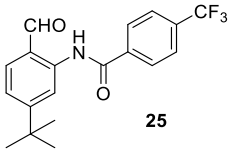

**24**

Compound **24** (39.2 mg) was isolated in 53 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.27 (s, 1H), 10.00 (s, 1H), 9.26 (s, 1H), 8.21 (d, *J* = 9.0 Hz, 2H), 7.82 (d, *J* = 7.5 Hz, 2H), 7.80-7.76 (m, 1H), 7.75 (d, *J* = 7.0 Hz, 2H), 7.57-7.43 (m, 4H).

**$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 195.55, 164.84, 149.21, 141.33, 139.28, 137.60, 136.75, 133.89 (q, *J* = 32.5 Hz), 129.14, 129.13, 128.06, 127.68, 126.07 (q, *J* = 3.6 Hz), 123.77 (q, *J* = 270.9 Hz), 122.14, 120.96, 118.57.

**HRMS**: calculated for $C_{21}H_{15}F_3NO_2$ [M+H$^+$]: 370.1049; **found**: 370.1046.

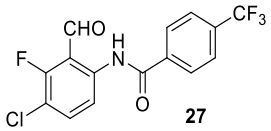



**25**

Compound **25** (32.1 mg) was isolated in 46 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.19 (s, 1H), 9.93 (s, 1H), 9.05 (d, *J* = 2.0 Hz, 1H), 8.18 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.32 (dd, *J* = 8.0, 1.5 Hz, 1H), 1.40 (s, 9H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 195.49, 164.88, 161.36, 140.96, 137.84, 136.19, 133.82 (q, *J* = 32.5 Hz), 128.04, 126.06 (q, *J* = 3.6 Hz), 123.79 (q, *J* = 270.9 Hz), 121.00, 120.14, 117.35, 36.03, 31.06.

**HRMS**: calculated for $C_{19}H_{19}F_3NO_2$ [M+H$^+$]: 350.1362; **found**: 350.1358.

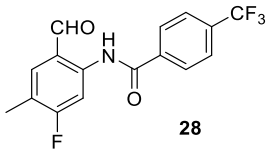



**27**

Compound **27** (52.5 mg) was isolated in 76 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

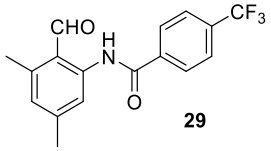
**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.26 (s, 1H), 10.43 (s, 1H), 8.70 (d, *J* = 9.5 Hz, 1H), 8.12 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 8.5 Hz, 2H), 7.66 (t, *J* = 8.5 Hz, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 190.84 (d, *J* = 12.5 Hz), 164.83, 161.32 (d, *J* = 258.5 Hz), 140.63 (d, *J* = 1.8 Hz), 138.45 (d,

*J* = 2.4 Hz), 137.01, 134.26 (q, *J* = 32.6 Hz), 128.08, 126.16 (q, *J* = 3.6 Hz), 123.66 (q, *J* = 270.9 Hz), 116.61 (d, *J* = 4.7 Hz), 115.21 (d, *J* = 17.1 Hz), 112.03 (d, *J* = 8.5 Hz).
**HRMS**: calculated for $C_{15}H_9ClF_4NO_2$ [M+H$^+$]: 346.0252; **found**: 346.0255.



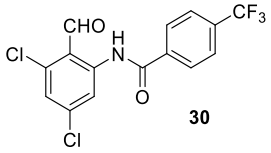
**28**

Compound **28** (43.6 mg) was isolated in 67 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).
**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.22 (s, 1H), 9.87 (s, 1H), 8.61 (dd, *J* = 12.5, 3.5 Hz, 1H), 8.13 (d, *J* = 8.5 Hz, 2H), 7.77 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 1H), 2.31 (s, 3H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.73, 165.95 (d, *J* = 255.0 Hz), 164.65, 141.00 (d, *J* = 12.2 Hz), 139.47 (d, *J* = 9.0 Hz), 137.27, 134.00 (q, *J* = 32.5 Hz), 128.04, 126.06 (q, *J* = 3.9 Hz), 123.72 (q, *J* = 271.1 Hz), 120.83 (d, *J* = 19.0 Hz), 118.94 (d, *J* = 2.6 Hz), 107.56 (d, *J* = 29.9 Hz), 14.05.
**HRMS**: calculated for $C_{16}H_{12}F_4NO_2$ [M+H$^+$]: 326.0799; **found**: 326.0800.



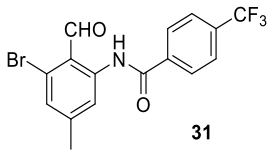
**29**

Compound **29** (56.5 mg) was isolated in 88 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).
**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.68 (s, 1H), 10.40 (s, 1H), 8.61 (s, 1H), 8.16 (d, *J* = 8.0 Hz, 2H), 7.77 (d, *J* = 8.0 Hz, 2H), 6.79 (s, 1H), 2.63 (s, 3H), 2.39 (s, 3H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.21, 164.71, 148.46, 143.45, 141.78, 137.91, 133.56 (q, *J* = 32.5 Hz), 127.96, 127.43, 125.84 (q, *J* = 4.0 Hz), 123.69 (q, *J* = 270.9 Hz), 118.83, 117.62, 22.42, 19.10.
**HRMS**: calculated for $C_{17}H_{15}F_3NO_2$ [M+H$^+$]: 322.1049; **found**: 322.1043.



**30**

Compound **30** (59.4 mg) was isolated in 82 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).
**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.66 (s, 1H), 10.57 (s, 1H), 9.36-8.83 (m, 2H), 8.16 (d, *J* = 8.0 Hz, 2H), 7.82 (d, *J* = 8.5 Hz, 2H), 7.24 (d, *J* = 2.0 Hz, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.05, 164.96, 143.60, 143.50, 141.20, 137.08, 134.37 (q, *J* = 32.6 Hz), 128.20, 126.23 (q, *J* = 3.6 Hz), 125.26, 123.68 (q, *J* = 270.5 Hz), 119.37, 116.39.
**HRMS**: calculated for $C_{15}H_9Cl_2F_3NO_2$ [M+H$^+$]: 361.9957; **found**: 361.9956.

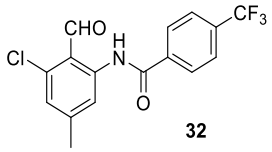



**31**

Compound **31** (61.8 mg) was isolated in 80 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.62 (s, 1H), 10.45 (s, 1H), 8.75 (s, 1H), 8.15 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.35-7.08 (m, 1H), 2.43 (s, 3H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 196.98, 164.80, 149.48, 142.99, 137.56, 134.02 (q, *J* = 32.6 Hz), 130.20, 129.71, 128.13, 126.09 (q, *J* = 3.7 Hz), 123.74 (q, *J* = 270.9 Hz), 120.30, 116.67, 22.31.

**HRMS**: calculated for $C_{16}H_{12}BrF_3NO_2$ [M+H$^+$]: 385.9998; **found**: 385.9993.

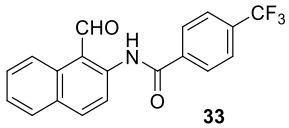



**32**

Compound **32** (54.7 mg) was isolated in 80 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.62 (s, 1H), 10.55 (s, 1H), 8.71 (s, 1H), 8.16 (d, *J* = 8.0 Hz, 2H), 7.80 (d, *J* = 8.0 Hz, 2H), 7.04 (d, *J* = 1.0 Hz, 1H), 2.44 (s, 3H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.47, 164.92, 149.50, 142.98, 140.41, 137.57, 134.03 (q, *J* = 32.5 Hz), 128.14, 126.10 (q, *J* = 3.6 Hz), 123.75 (q, *J* = 271.0 Hz), 119.57, 115.97, 22.53.

**HRMS**: calculated for $C_{16}H_{12}ClF_3NO_2$ [M+H$^+$]: 342.0503; **found**: 342.0505.

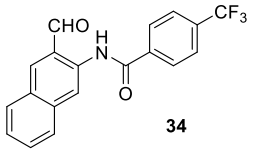



**33**

Compound **33** (29.5 mg) was isolated in 43 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 13.22 (s, 1H), 11.07 (s, 1H), 9.11 (d, *J* = 9.0 Hz, 1H), 8.48 (d, *J* = 8.5 Hz, 1H), 8.22 (d, *J* = 8.0 Hz, 2H), 8.12 (d, *J* = 9.0 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 2H), 7.70-7.61 (m, 1H), 7.55-7.47 (m, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 193.37, 165.34, 142.68, 138.18, 137.77, 134.01 (q, *J* = 32.6 Hz), 133.68, 129.94, 129.60, 129.33, 128.32, 126.08 (q, *J* = 3.7 Hz), 125.61, 123.77 (q, *J* = 271.0 Hz), 119.92, 119.14, 113.17.

**HRMS**: calculated for $C_{19}H_{13}F_3NO_2$ [M+H$^+$]: 344.0893; **found**: 346.0892.



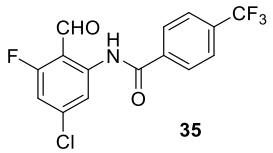

**34**

Compound **34** (60.4 mg) was isolated in 88 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 11.99 (s, 1H), 10.12 (s, 1H), 9.30 (s, 1H), 8.25 (s, 1H), 8.19

(d, *J* = 8.0 Hz, 2H), 7.91 (dd, *J* = 8.0, 4.0 Hz, 2H), 7.80 (d, *J* = 8.5 Hz, 2H), 7.69-7.62 (m, 1H), 7.54-7.46 (m, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 196.05, 164.64, 140.62, 137.86, 137.27, 135.51, 133.76 (q, *J* = 32.6 Hz), 130.81, 129.27, 129.07, 128.30, 127.94, 126.35, 126.06 (q, *J* = 3.6 Hz), 123.83 (q, *J* = 270.9 Hz), 123.09, 117.72.

**HRMS**: calculated for $C_{19}H_{13}F_3NO_2$ [M+H$^+$]: 344.0893; **found**: 344.0890.

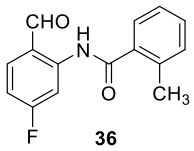



**35**

Compound **35** (56.7 mg) was isolated in 82 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.43 (s, 1H), 10.37 (s, 1H), 8.83 (s, 1H), 8.15 (d, *J* = 8.0 Hz, 2H), 7.81 (d, *J* = 8.0 Hz, 2H), 6.95 (dd, *J* = 10.5, 1.5 Hz, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 190.47 (d, *J* = 12.4 Hz), 166.98, 164.92 (d, *J* = 3.7 Hz), 144.64 (d, *J* = 14.0 Hz), 142.62 (d, *J* = 4.0 Hz), 136.92, 134.37 (q, *J* = 32.7 Hz), 128.16, 126.22 (q, *J* = 3.6 Hz), 123.67 (q, *J* = 271.1 Hz), 116.39 (d, *J* = 3.6 Hz), 111.25 (d, *J* = 24.2 Hz), 109.53 (d, *J* = 8.7 Hz).

**HRMS**: calculated for $C_{15}H_9ClF_4NO_2$ [M+H$^+$]: 346.0252; **found**: 346.0246.

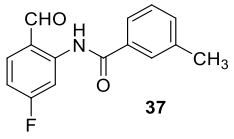



**36**

Compound **36** (40.1 mg) was isolated in 78 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 11.74 (s, 1H), 9.88 (s, 1H), 8.74 (dd, *J* = 12.0, 2.5 Hz, 1H), 7.70 (dd, *J* = 8.5, 6.0 Hz, 1H), 7.62 (d, *J* = 7.0 Hz, 1H), 7.43-7.36 (m, 1H), 7.35-7.27 (m, 2H), 6.98-6.90 (m, 1H), 2.56 (s, 3H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.14, 169.02, 167.49 (d, *J* = 255.4 Hz), 143.54 (d, *J* = 13.6 Hz), 138.71 (d, *J* = 12.0 Hz), 137.60, 135.36, 131.81, 131.08, 127.33, 126.32, 118.92 (d, *J* = 2.2 Hz), 110.66 (d, *J* = 23.0 Hz), 107.54 (d, *J* = 28.6 Hz), 20.45.

**HRMS**: calculated for $C_{15}H_{12}FNNaO_2$ [M+Na$^+$]: 280.0744; **found**: 280.0753.

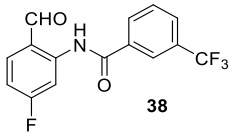



**37**

Compound **37** (38.6 mg) was isolated in 75 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.18 (s, 1H), 9.87 (s, 1H), 8.69 (dd, *J* = 12.0, 2.5 Hz, 1H), 7.87-7.77 (m, 2H), 7.67 (dd, *J* = 8.5, 6.0 Hz, 1H), 7.44-7.32 (m, 2H), 6.94-6.81 (m, 1H), 2.43 (s, 3H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.30, 168.42, 166.37, 143.63 (d, *J* = 13.7 Hz), 138.84, 138.64 (d, *J* = 12.0 Hz), 133.79, 133.30, 128.82, 128.34, 124.46, 118.89 (d, *J* = 2.2 Hz), 110.44 (d, *J* = 23.1 Hz), 107.42 (d, *J* = 28.6 Hz), 21.47.

**HRMS**: calculated for $C_{15}H_{12}FNNaO_2$ [M+Na$^+$]: 280.0744; **found**: 280.0753.

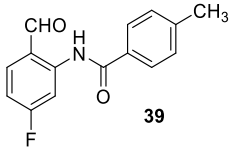



**38**

Compound **38** (41.7 mg) was isolated in 67 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.34 (s, 1H), 9.90 (s, 1H), 8.63 (dd, *J* = 12.0, 2.5 Hz, 1H), 8.29 (s, 1H), 8.17 (d, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 7.5 Hz, 1H), 7.71 (dd, *J* = 8.5, 6.0 Hz, 1H), 7.68-7.62 (m, 1H), 6.98-6.87 (m, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.59, 167.46 (d, *J* = 255.9 Hz), 164.61, 143.24 (d, *J* = 13.5 Hz), 138.74 (d, *J* = 11.9 Hz), 134.69, 131.65 (q, *J* = 32.6 Hz), 130.34, 129.68, 129.06 (q, *J* = 3.6 Hz), 125.01 (q, *J* = 3.7 Hz), 123.71 (q, *J* = 271.0 Hz), 119.01 (d, *J* = 2.4 Hz), 111.02 (d, *J* = 22.9 Hz), 107.63 (d, *J* = 28.6 Hz).

**HRMS**: calculated for $C_{15}H_9F_4NNaO_2$ [M+Na$^+$]: 334.0462; **found**: 334.0469.

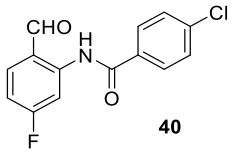



**39**

Compound **39** (36.5 mg) was isolated in 71 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.20 (s, 1H), 9.90 (s, 1H), 8.71 (dd, *J* = 12.0, 2.5 Hz, 1H), 8.07-7.86 (m, 2H), 7.68 (dd, *J* = 8.5, 6.5 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 2H), 6.94-6.86 (m, 1H), 2.42 (s, 3H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.39, 167.50 (d, *J* = 255.1 Hz), 166.26, 143.83 (d, *J* = 13.7 Hz), 143.26, 138.70 (d, *J* = 12.0 Hz), 131.10, 129.70, 127.64, 118.91 (d, *J* = 2.2 Hz), 110.44 (d, *J* = 23.0 Hz), 107.47 (d, *J* = 28.7 Hz), 21.64.

**HRMS**: calculated for $C_{15}H_{12}FNNaO_2$ [M+Na$^+$]: 280.0744; **found**: 280.0753.

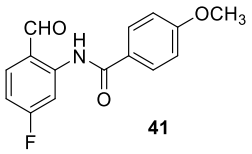



**40**

Compound **40** (37.8 mg) was isolated in 68 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.20 (s, 1H), 9.88 (s, 1H), 8.63 (dd, *J* = 12.0, 2.5 Hz, 1H), 7.99-7.86 (m, 2H), 7.68 (dd, *J* = 8.5, 6.5 Hz, 1H), 7.51-7.39 (m, 2H), 6.99-6.81 (m, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.48, 167.44 (d, *J* = 255.6 Hz), 165.01, 143.44 (d, *J* = 13.6 Hz), 138.95, 138.70 (d, *J* = 12.0 Hz), 132.18, 129.26, 128.98, 118.90 (d, *J* = 2.2 Hz), 110.75 (d, *J* = 23.0 Hz), 107.51 (d, *J* = 28.7 Hz).

**HRMS**: calculated for $C_{14}H_9ClFNNaO_2$ [M+Na$^+$]: 300.0198; **found**: 300.0207.

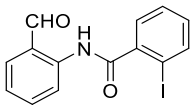



**41**

Compound **41** (42.6 mg) was isolated in 78 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.18 (s, 1H), 9.92 (s, 1H), 8.98-8.53 (m, 1H), 8.19-7.93 (m, 2H), 7.84-7.51 (m, 1H), 7.04-6.98 (m, 2H), 6.90 (t, *J* = 8.0 Hz, 1H), 3.88 (s, 3H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.49, 167.61 (d, *J* = 255.2 Hz), 165.92, 163.16, 144.07 (d, *J* = 14.0 Hz), 138.76 (d, *J* = 12.0 Hz), 129.67, 126.24, 118.91(d, *J* = 2.1 Hz), 114.30, 110.40 (d, *J* = 23.1 Hz), 107.48 (d, *J* = 28.6 Hz), 55.63.

**HRMS**: calculated for $C_{15}H_{12}FNNaO_3$ [M+$Na^+$]: 296.0693; **found**: 296.0698.

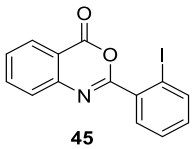



**44**

Compound **44** (39.3 mg) was isolated in 56 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 50/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 11.46 (s, 1H), 9.91 (s, 1H), 8.89 (d, *J* = 8.5 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.74-7.63 (m, 2H), 7.54 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.44 (t, *J* = 8.0 Hz, 1H), 7.32-7.24 (m, 1H), 7.19-7.11 (m, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 195.55, 168.11, 141.42, 140.59, 140.52, 136.32, 136.17, 131.78, 128.47, 128.23, 123.65, 122.05, 120.16, 92.78.

**HRMS**: calculated for $C_{14}H_{11}INO_2$ [M+$H^+$]: 351.9829; **found**: 351.9829.

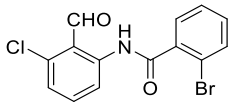



**45**

Compound **45** (54.4 mg) was isolated in 78 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 20~10/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 8.33-8.21 (m, 1H), 8.10-7.98 (m, 1H), 7.92-7.80 (m, 2H), 7.80-7.70 (m, 1H), 7.63-7.54 (m, 1H), 7.52-7.42 (m, 1H), 7.23-7.07 (m, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 159.33, 157.82, 146.28, 141.23, 136.80, 135.54, 132.41, 130.97, 129.09, 128.71, 128.30, 127.45, 117.05, 94.70.

**HRMS**: calculated for $C_{14}H_9INO_2$ [M+$H^+$]: 349.9672; **found**: 349.9669.



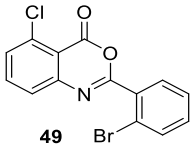

**48**

Compound **48** (50.1 mg) was isolated in 74 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 30/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 11.91 (s, 1H), 10.57 (s, 1H), 8.86 (d, *J* = 8.5 Hz, 1H), 7.67 (d,

*J* = 8.0 Hz, 1H), 7.61-7.53 (m, 2H), 7.47-7.39 (m, 1H), 7.38-7.31 (m, 1H), 7.25-7.18 (m, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 194.34, 166.93, 142.66, 140.31, 137.81, 136.96, 134.04, 131.95, 129.11, 127.85, 125.34, 119.86, 119.36, 117.98.

**HRMS**: calculated for $C_{14}H_{10}BrClNO_2$ [M+H$^+$]: 337.9578; **found**: 337.9577.

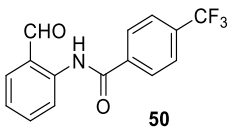



**49**

Compound **49** (48.5 mg) was isolated in 72 % yield. Flash silica gel chromatography (petroleum ether/ethyl acetate = 20~10/1).

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 7.86 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.76-7.69 (m, 2H), 7.63 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.59 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.49-7.43 (m, 1H), 7.41-7.35 (m, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 158.00, 155.95, 148.83, 136.26, 136.20, 134.57, 132.74, 131.90, 131.60, 131.55, 127.64, 126.59, 121.97, 114.92.

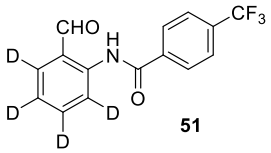
**HRMS**: calculated for $C_{14}H_8BrClNO_2$ [M+H$^+$]: 335.9421; **found**: 335.9418.




**50**

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.13 (s, 1H), 9.95 (s, 1H), 8.88 (d, *J* = 8.5 Hz, 1H), 8.13 (d, *J* = 8.5 Hz, 2H), 7.76 (d, *J* = 8.0 Hz, 2H), 7.70 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.67-7.62 (m, 1H), 7.30-7.22 (m, 1H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 196.08, 164.64, 140.86, 137.59, 136.50, 136.28, 133.78 (q, *J* = 32.5 Hz), 128.01, 125.97 (q, *J* = 3.7 Hz), 123.73 (q, *J* = 270.9 Hz), 123.57, 122.12, 120.04.

**HRMS**: calculated for $C_{15}H_{11}F_3NO_2$ [M+H$^+$]: 294.0736; **found**: 294.0745.




**51**

**$^1$H NMR** ($CDCl_3$, 500 MHz, ppm): δ 12.12 (s, 1H), 9.94 (s, 1H), 8.13 (d, *J* = 8.0 Hz, 2H), 7.75 (d, *J* = 8.5 Hz, 2H). **$^{13}$C NMR** ($CDCl_3$, 125 MHz, ppm) δ 196.07, 164.60, 140.77, 137.57, 136.16, 136.04, 133.76 (q, *J* = 32.6 Hz), 128.00, 125.95 (q, *J* = 3.7 Hz), 123.73 (q, *J* = 271.0 Hz), 122.10, 122.04, 119.91.

**HRMS**: calculated for $C_{15}H_7D_4F_3NO_2$ [M+H$^+$]: 298.0987; **found**: 298.0984.

## 11. References

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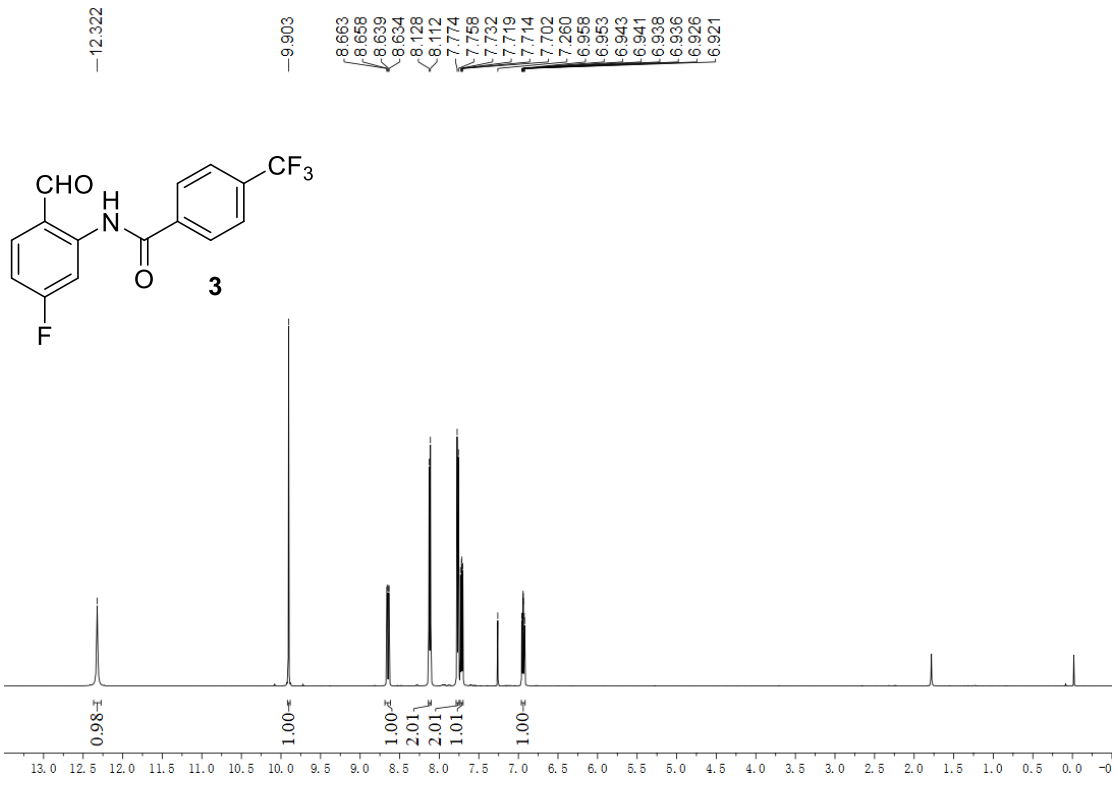
[6] (a) Yu, J.; Zhang-Negrerie, D.; Du, Y. *Eur. J. Org. Chem*. **2016**, 562. (b) Debbarma, S.; Maji, M. S. *Eur. J. Org. Chem.* **2017**, 3699–3706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6.941
6.938
6.936
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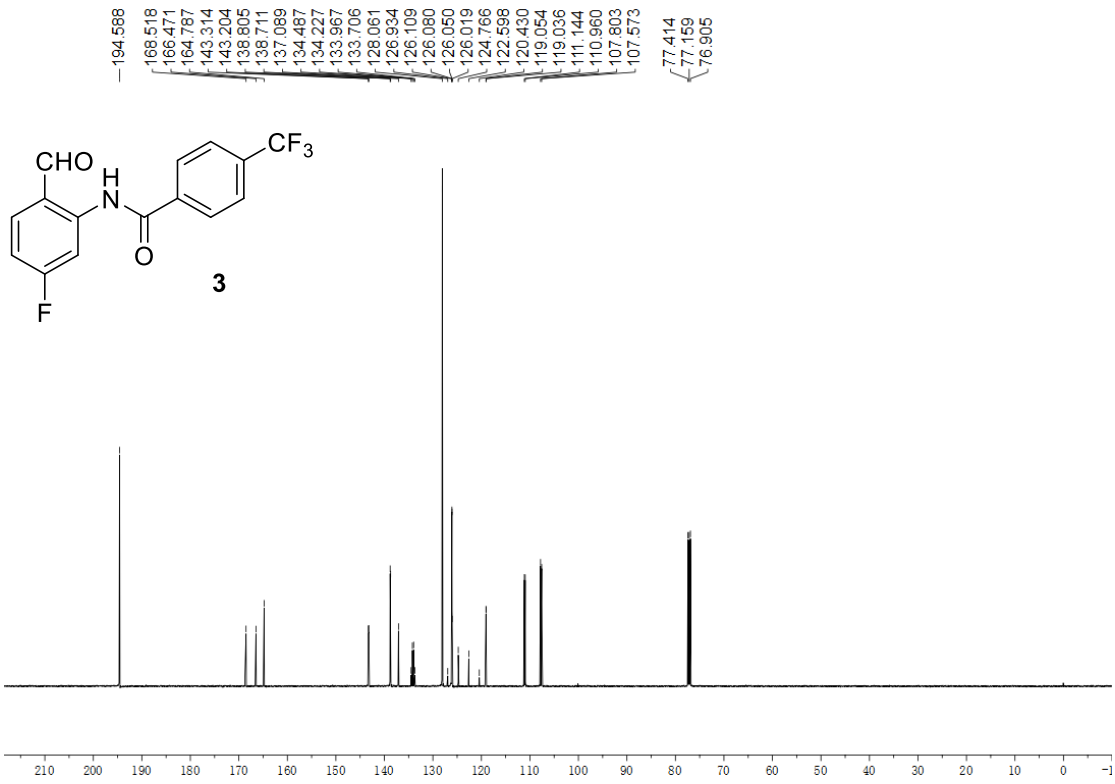
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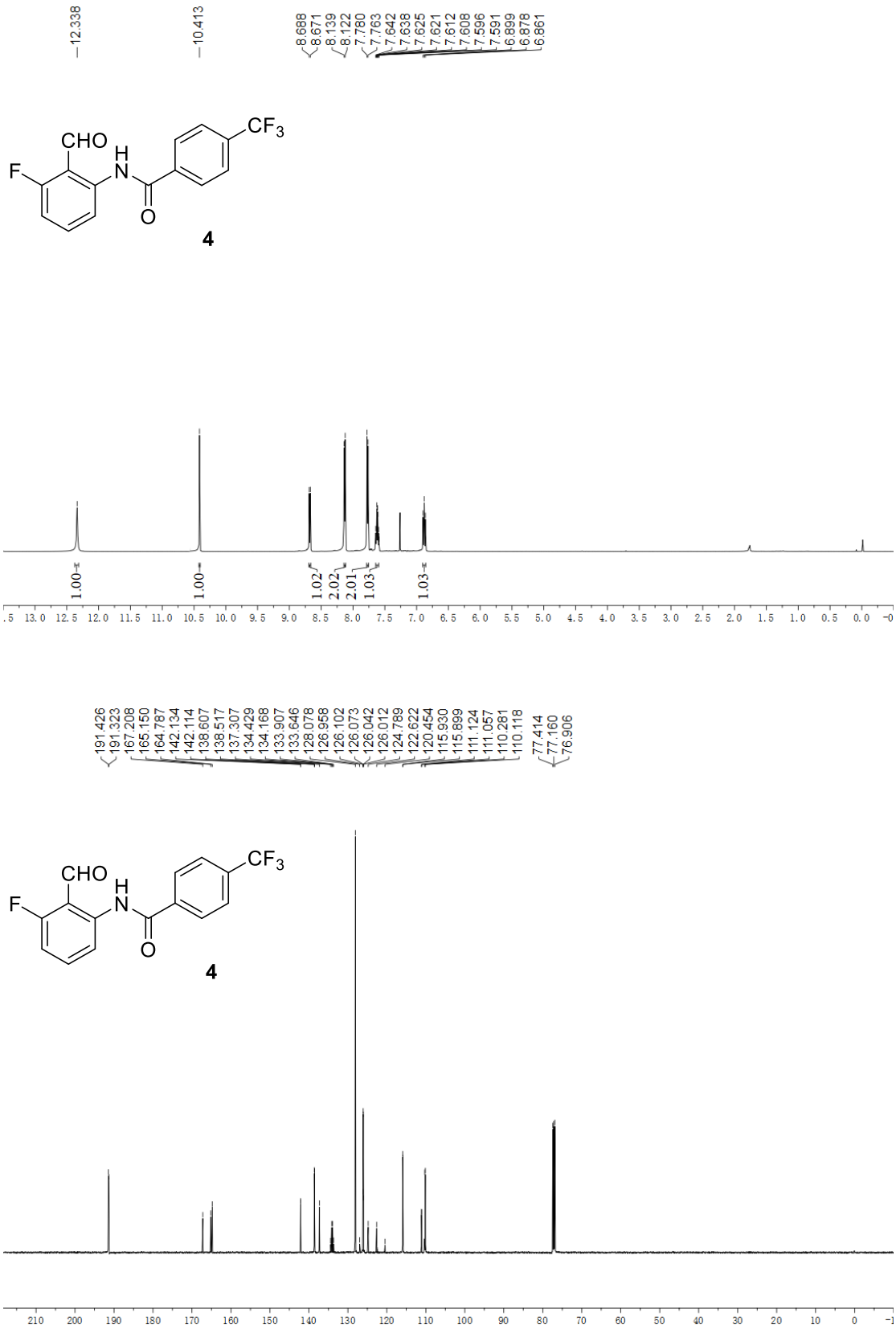
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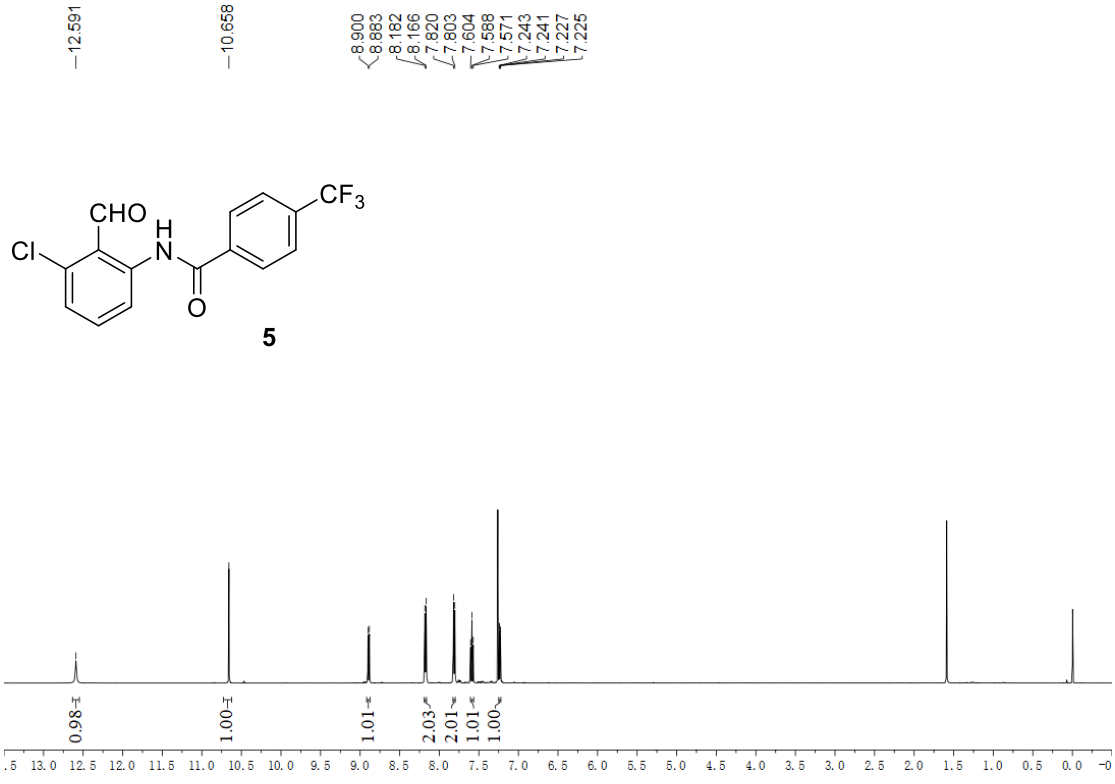
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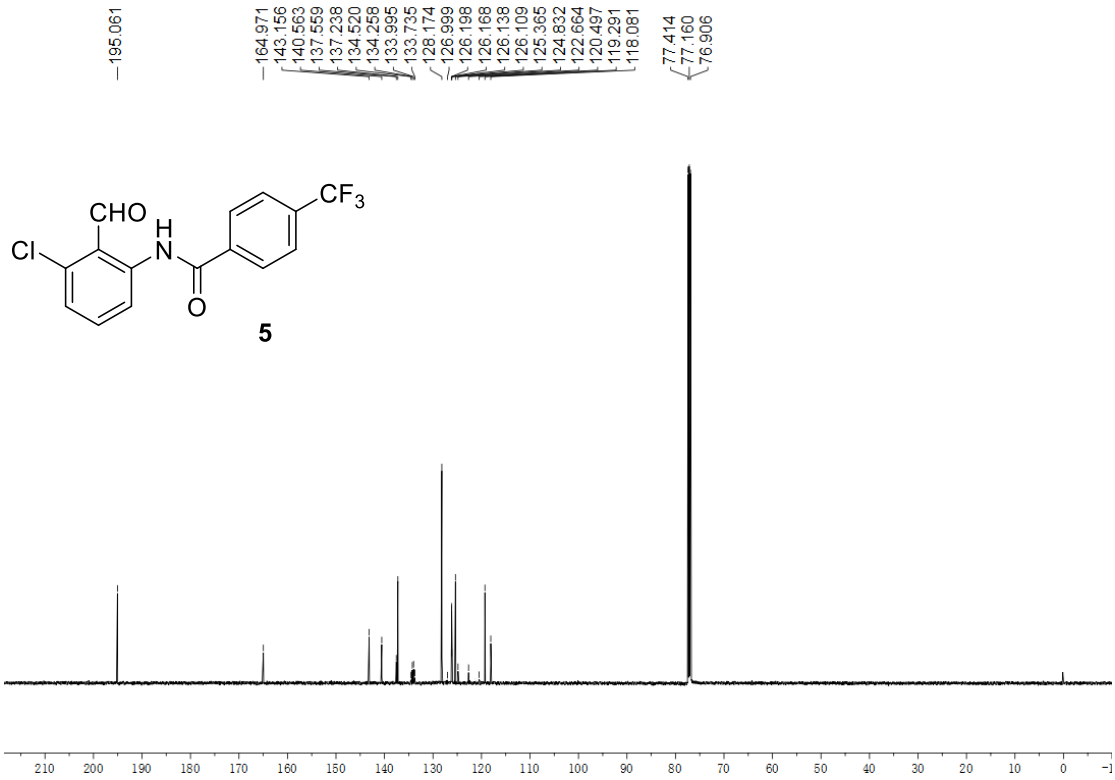
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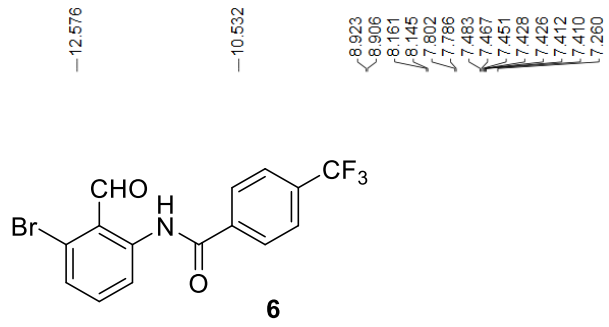
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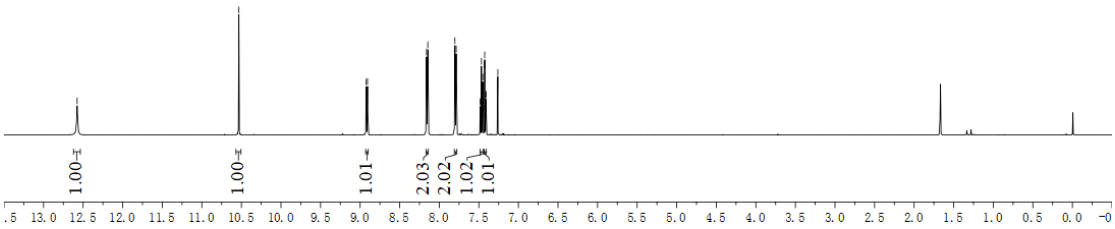
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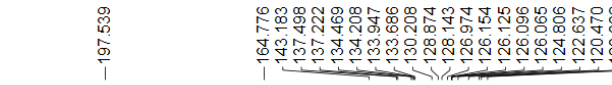
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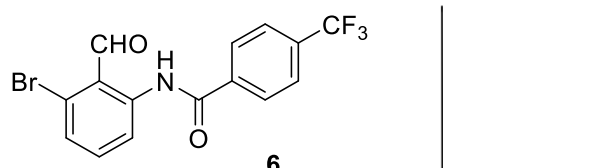
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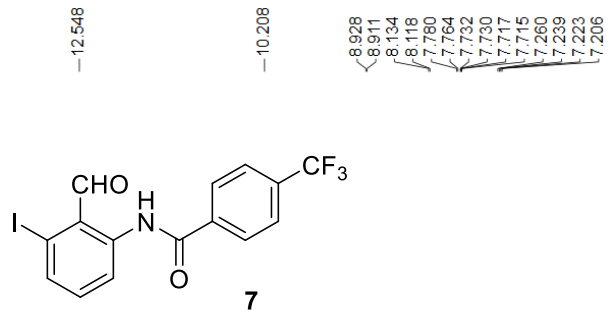
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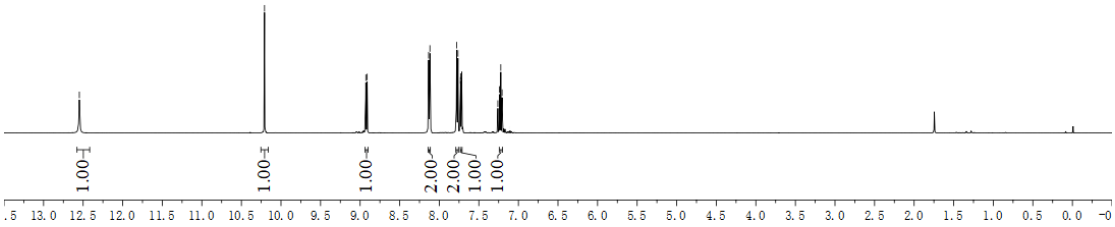
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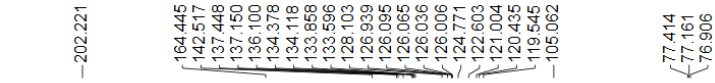
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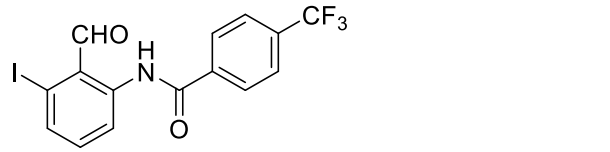
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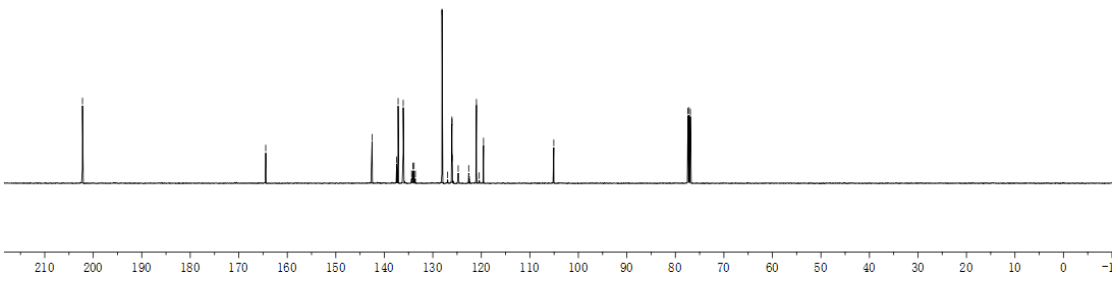

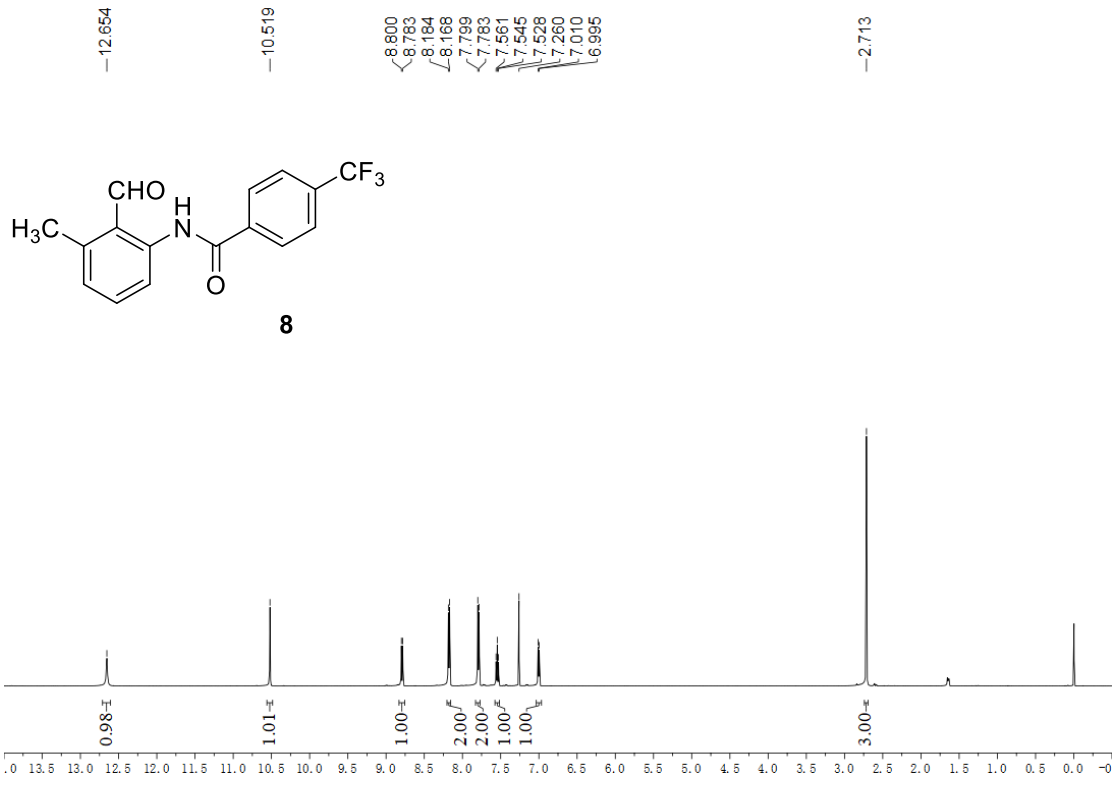
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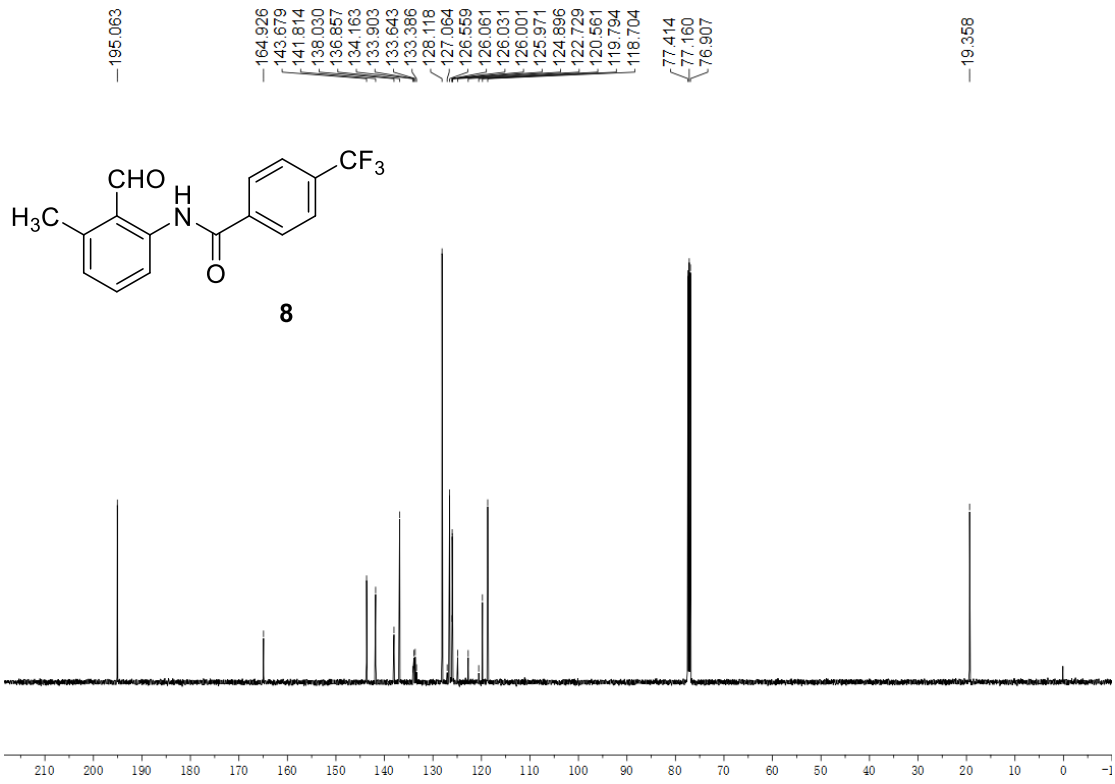
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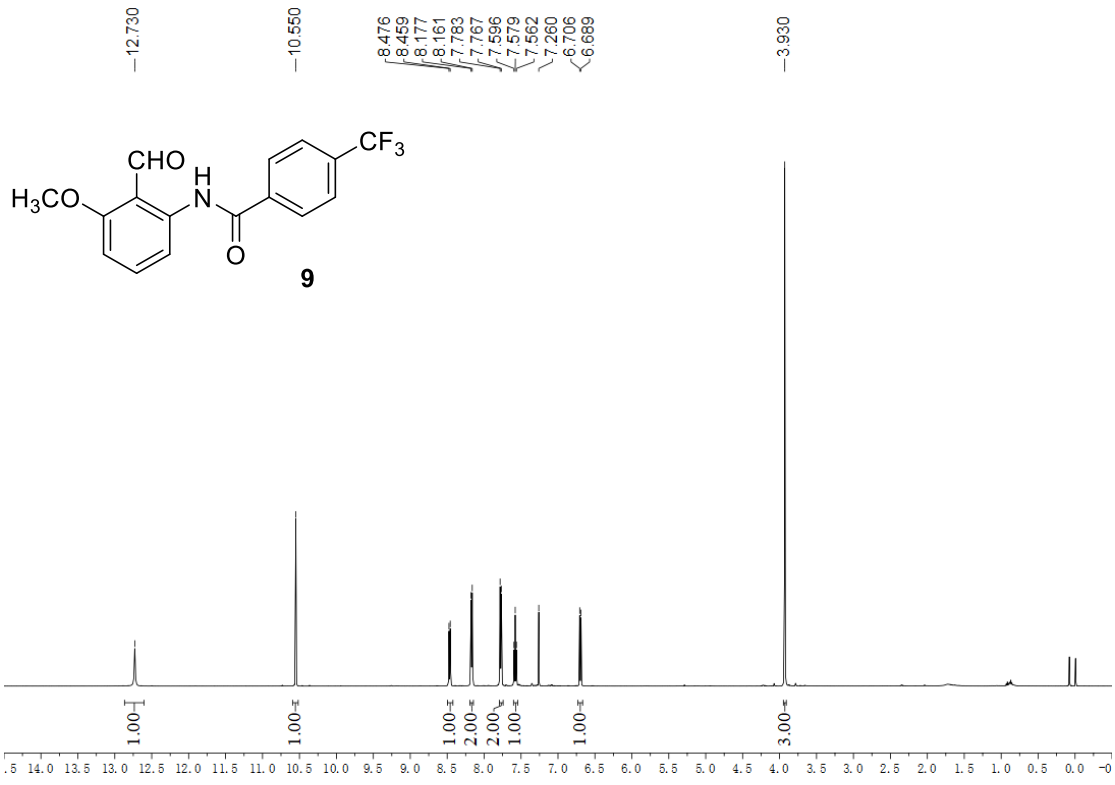
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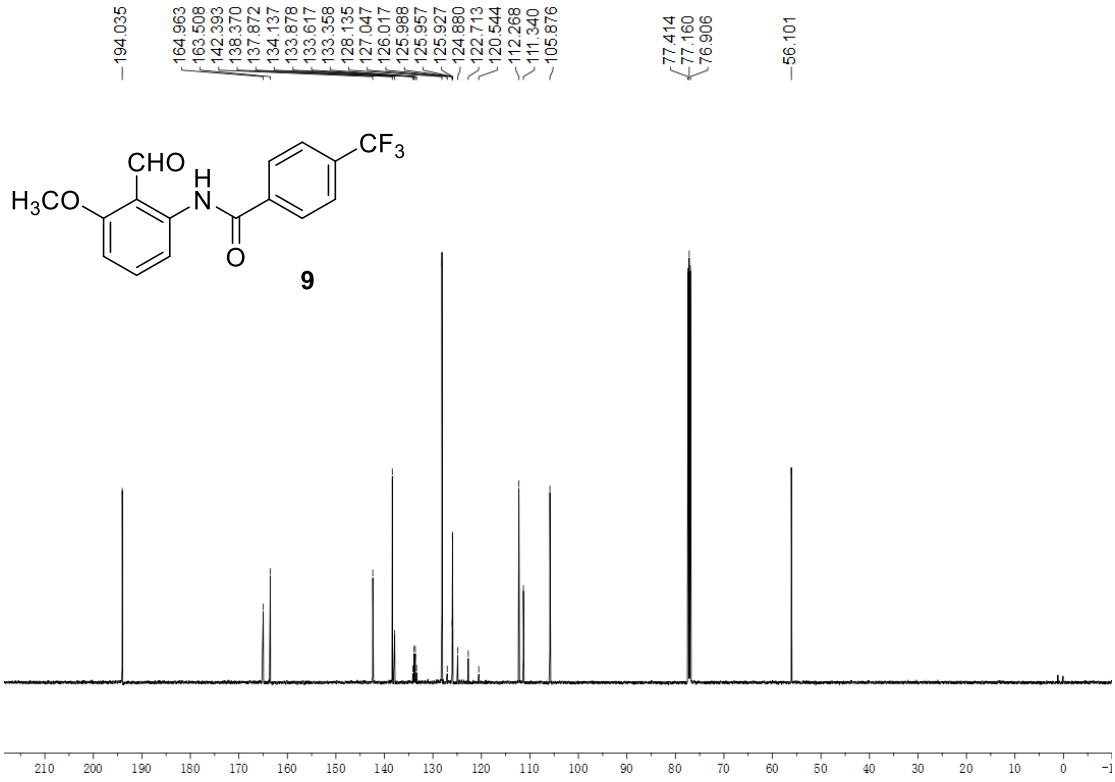
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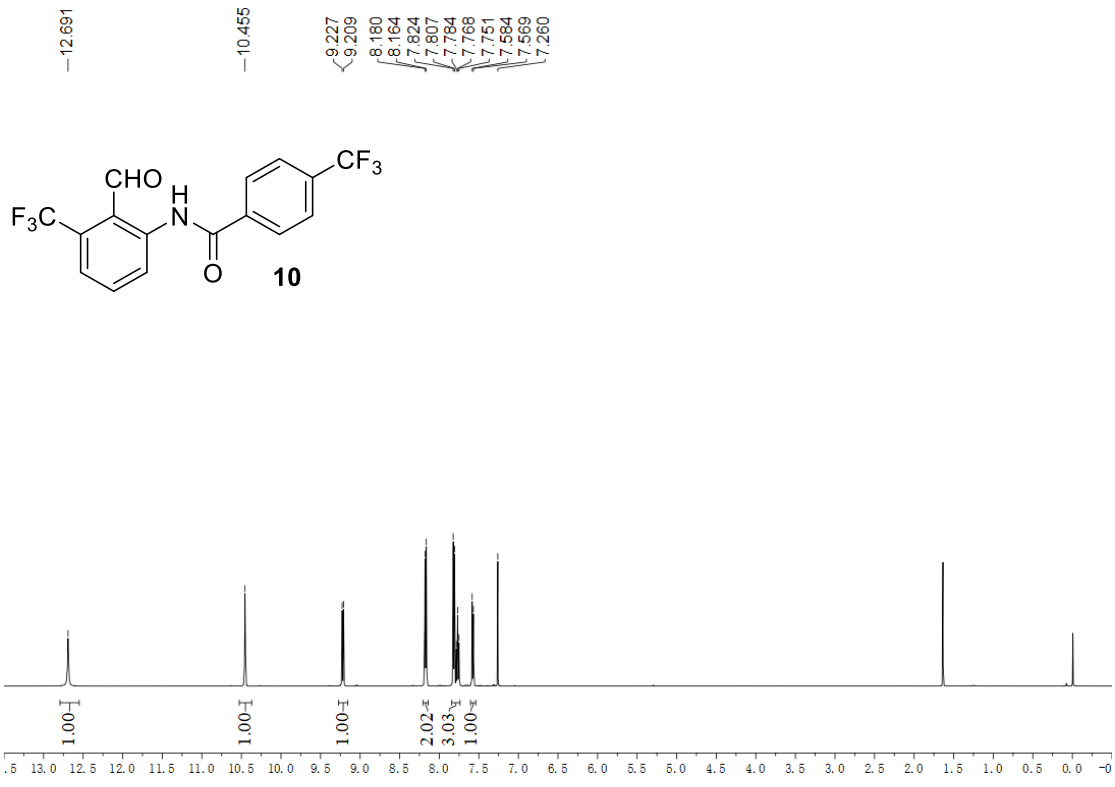
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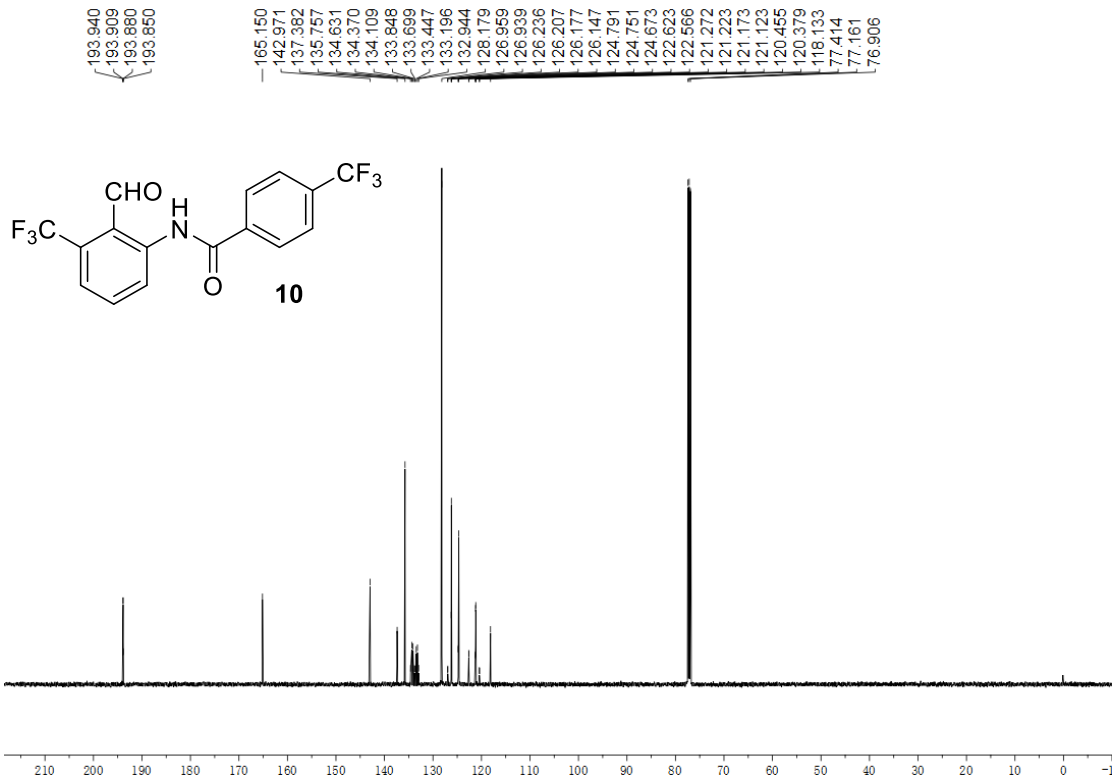
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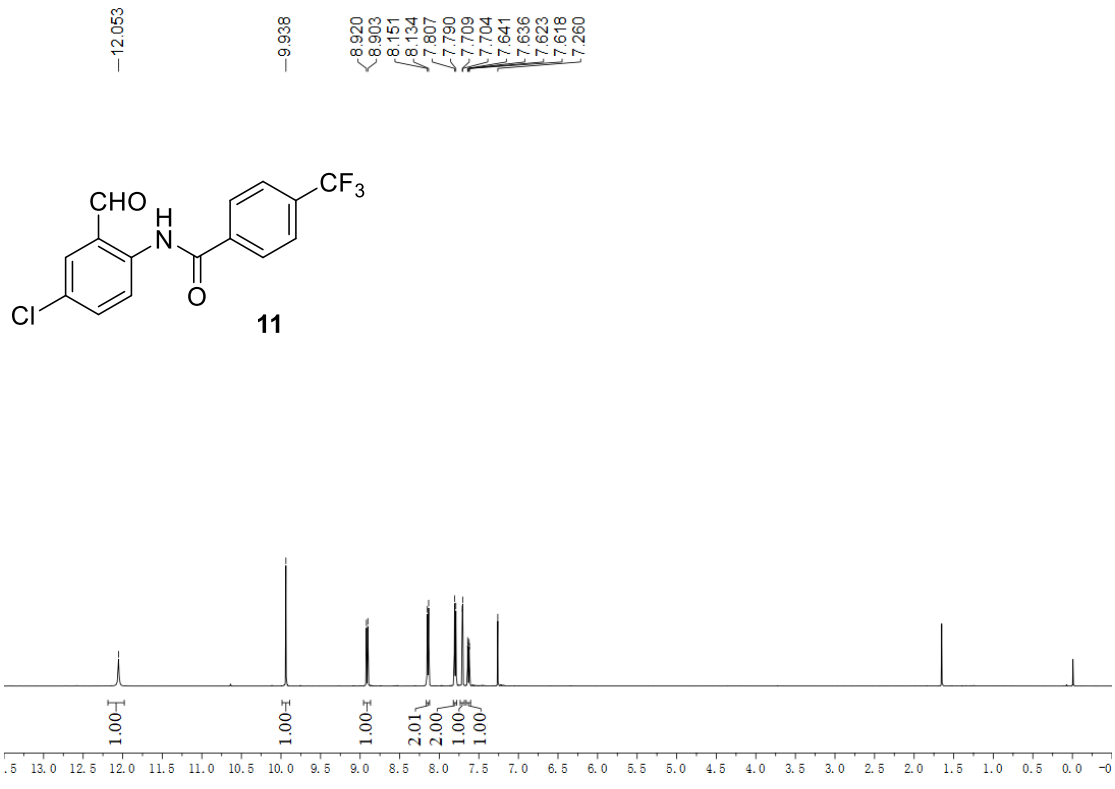
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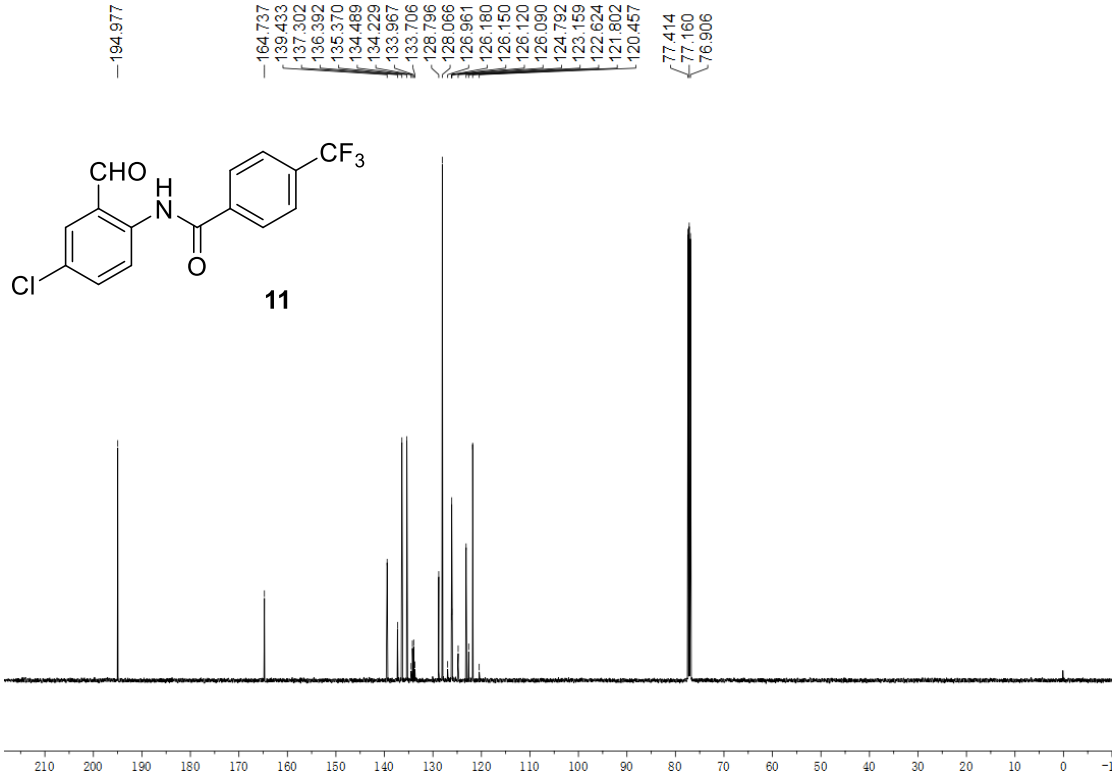
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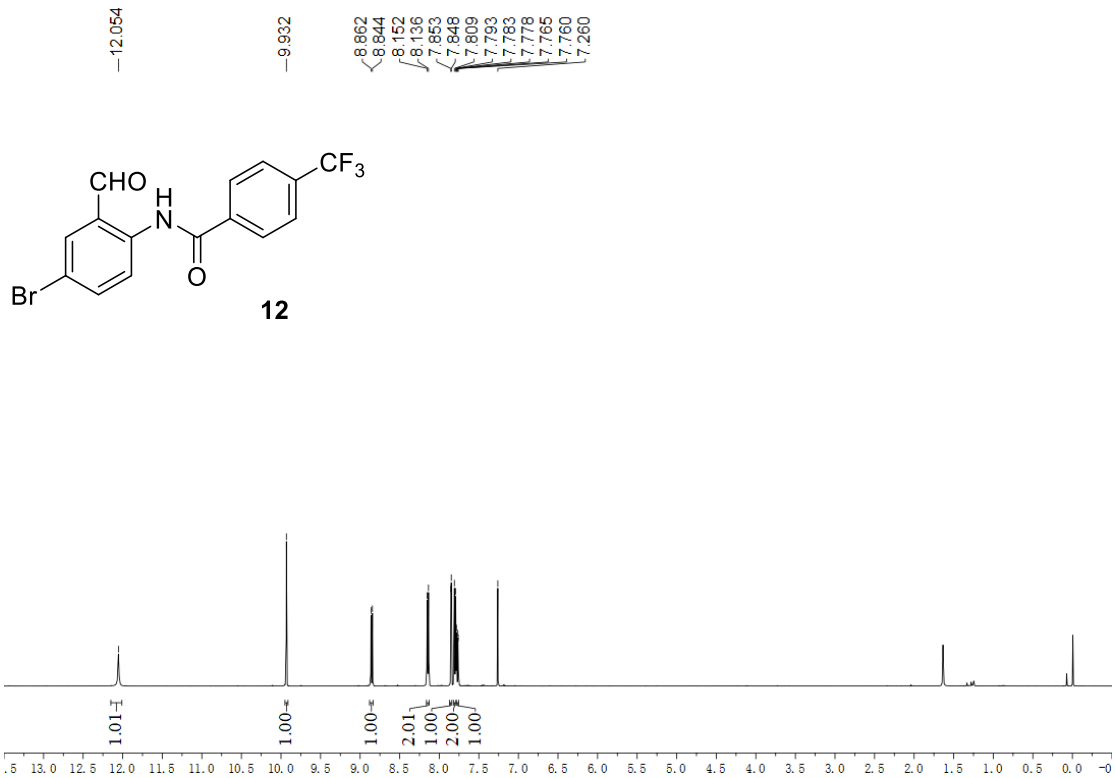
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7.793
7.783
7.778
7.765
7.760
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Br
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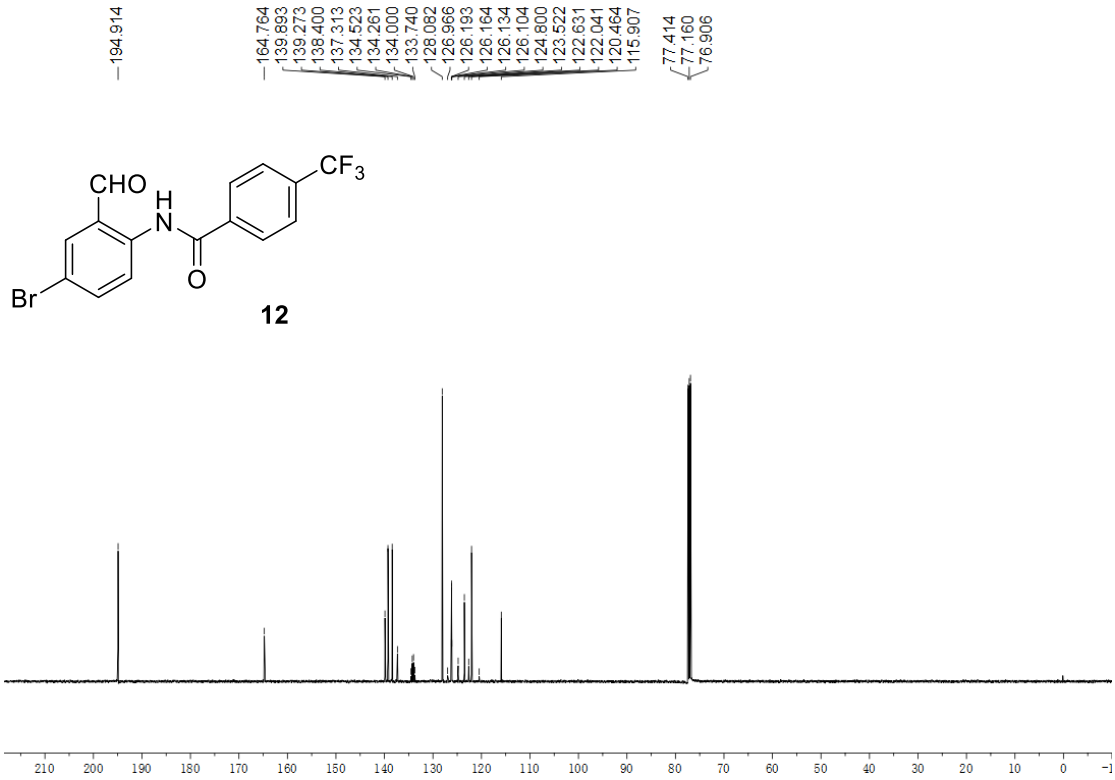
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126.164
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77.160
76.906
CHO
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O
Br
CF3
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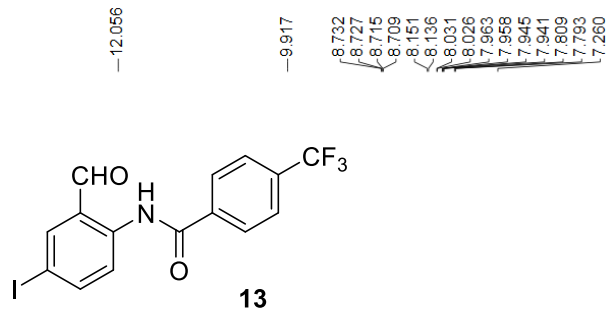
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7.793
7.260
CHO
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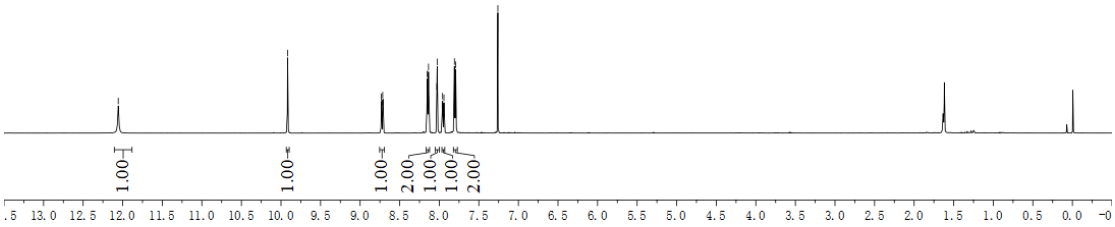
O
I
CF3

**13**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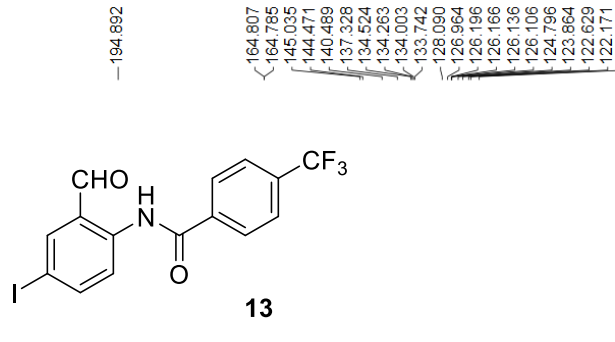
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126.136
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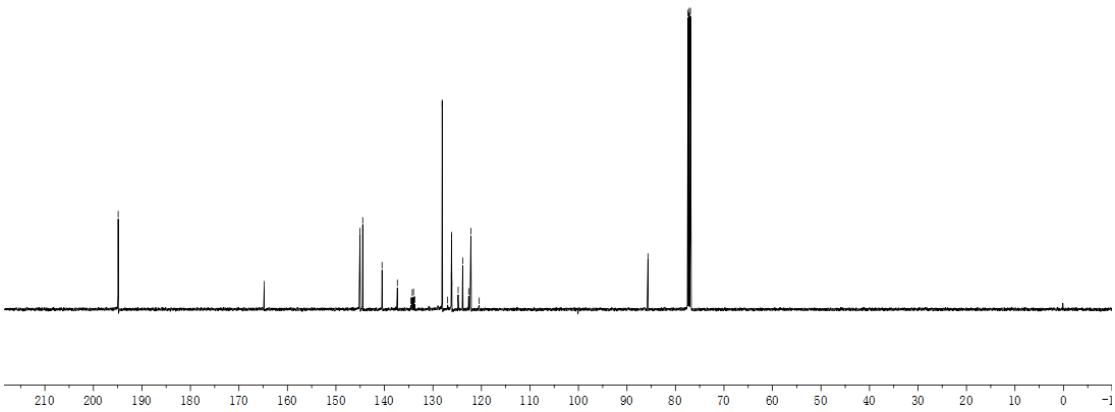
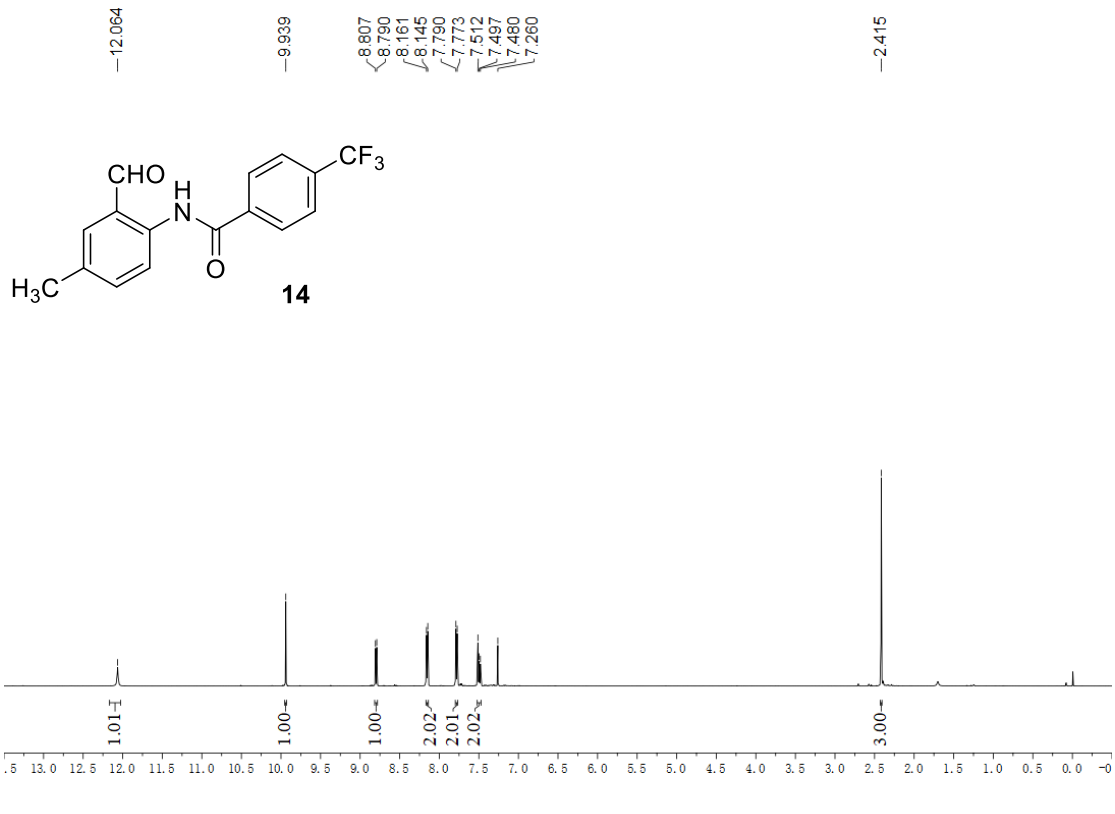
77.415
77.160
76.906
CHO
H
N
O
I
CF3

**13**

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7.260
2.415
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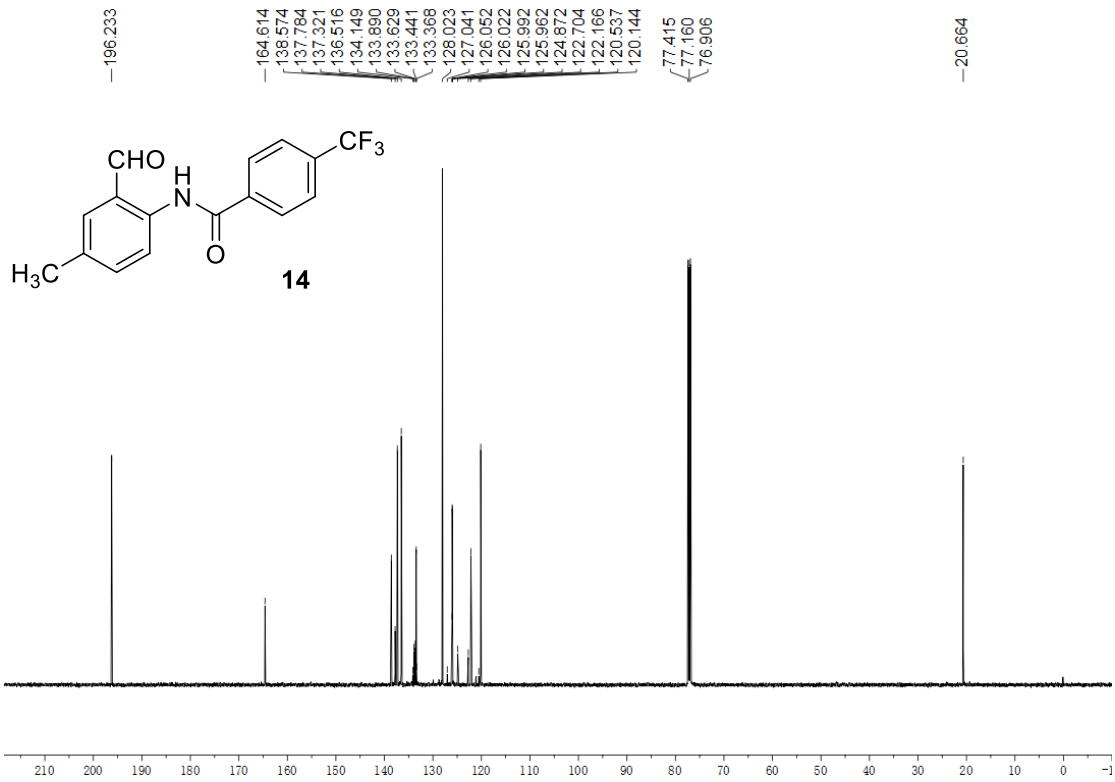
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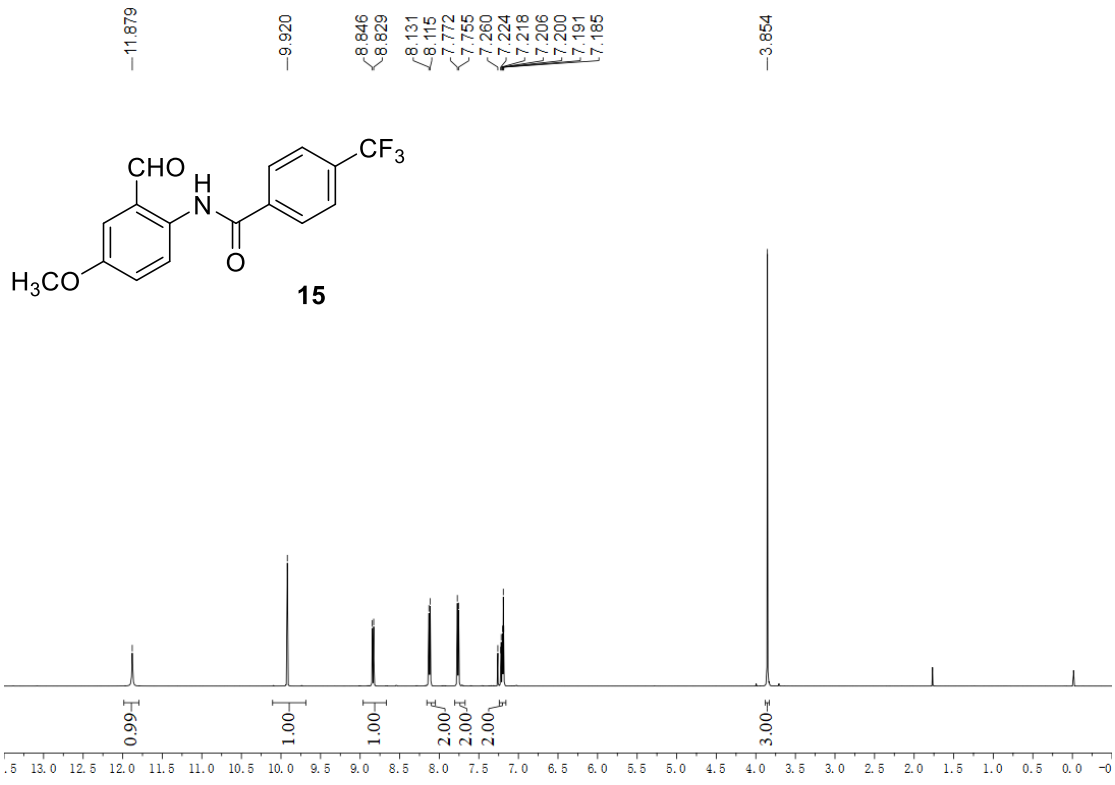
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7.200
7.191
7.185
3.854
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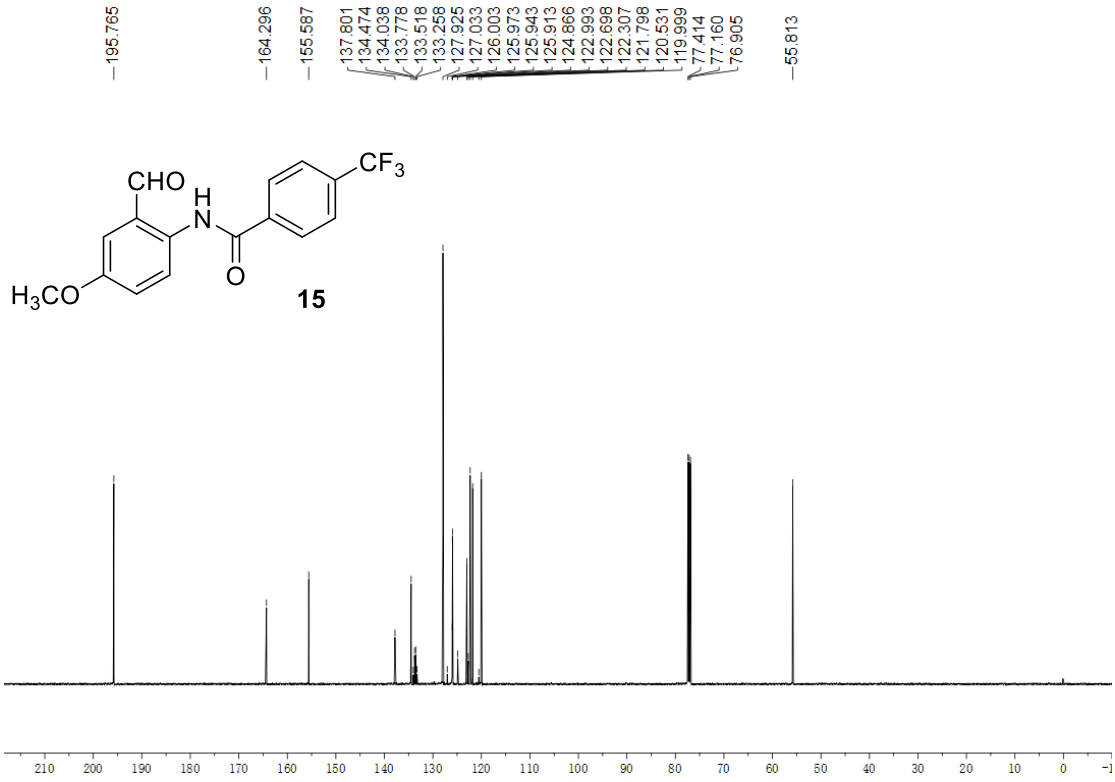
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CHO
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O
CF3
H3CO
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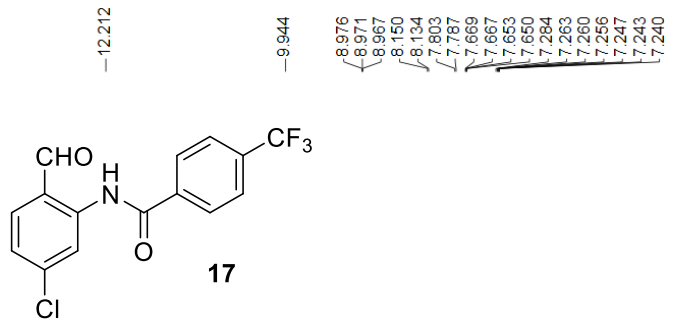
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Cl
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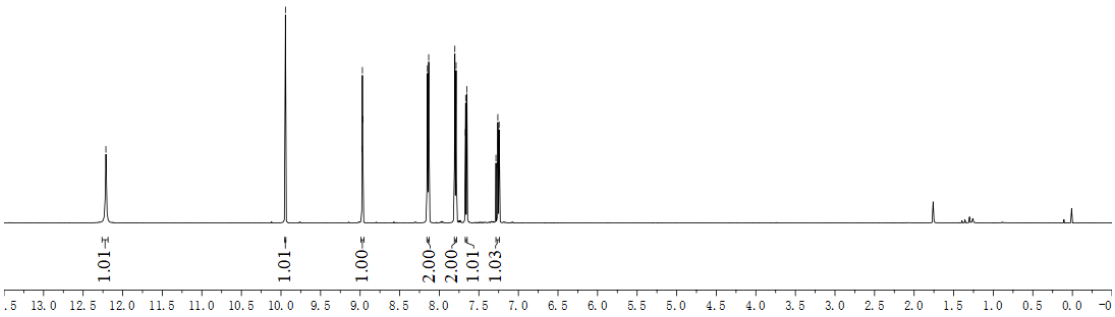
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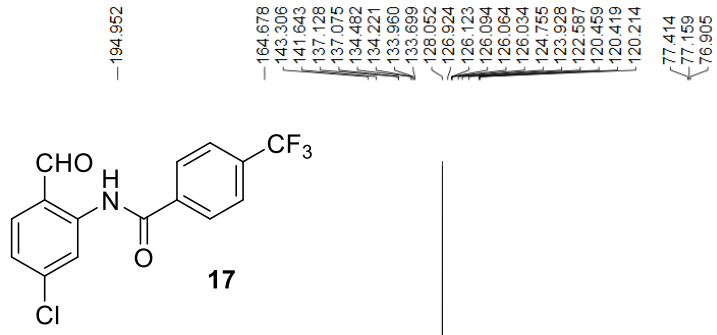
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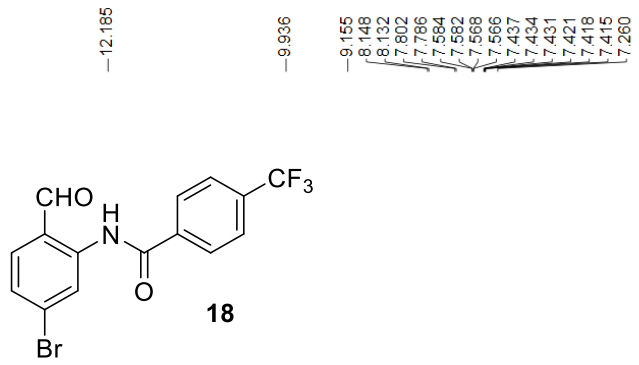
N
O
CF3
Cl
17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7.568
7.566
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7.431
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7.415
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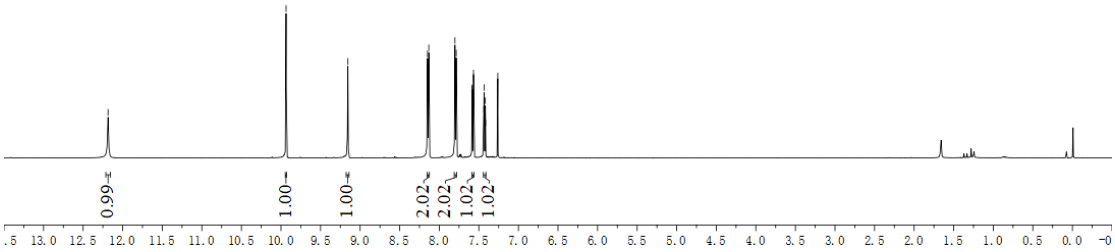
CHO
H
N
O
CF3
Br

**18**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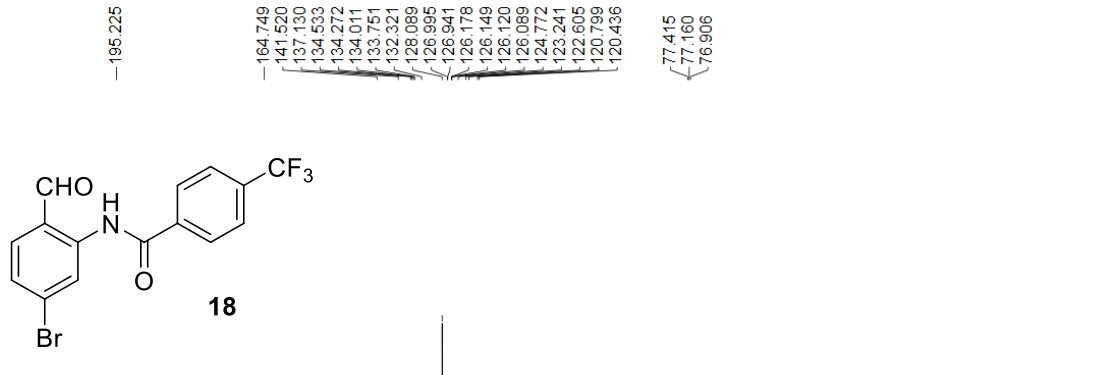
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126.089
124.772
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77.160
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CHO
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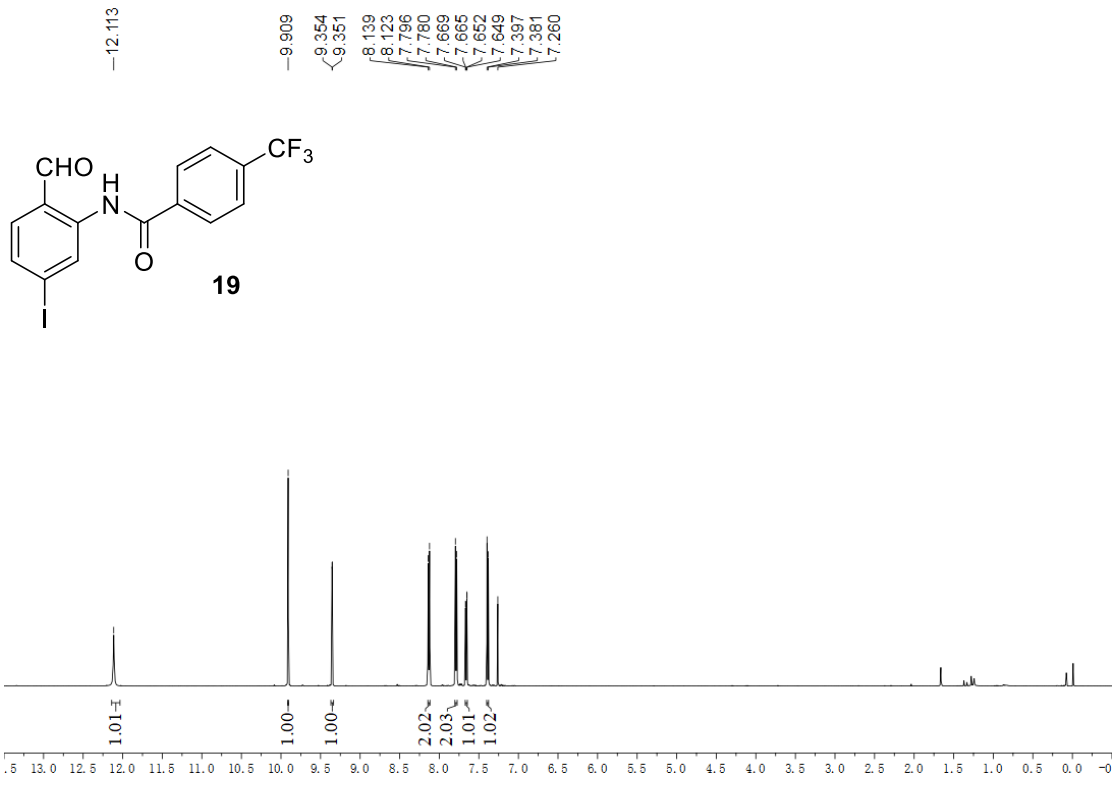
N
O
CF3
Br

**18**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7.397
7.381
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CF3
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1.00
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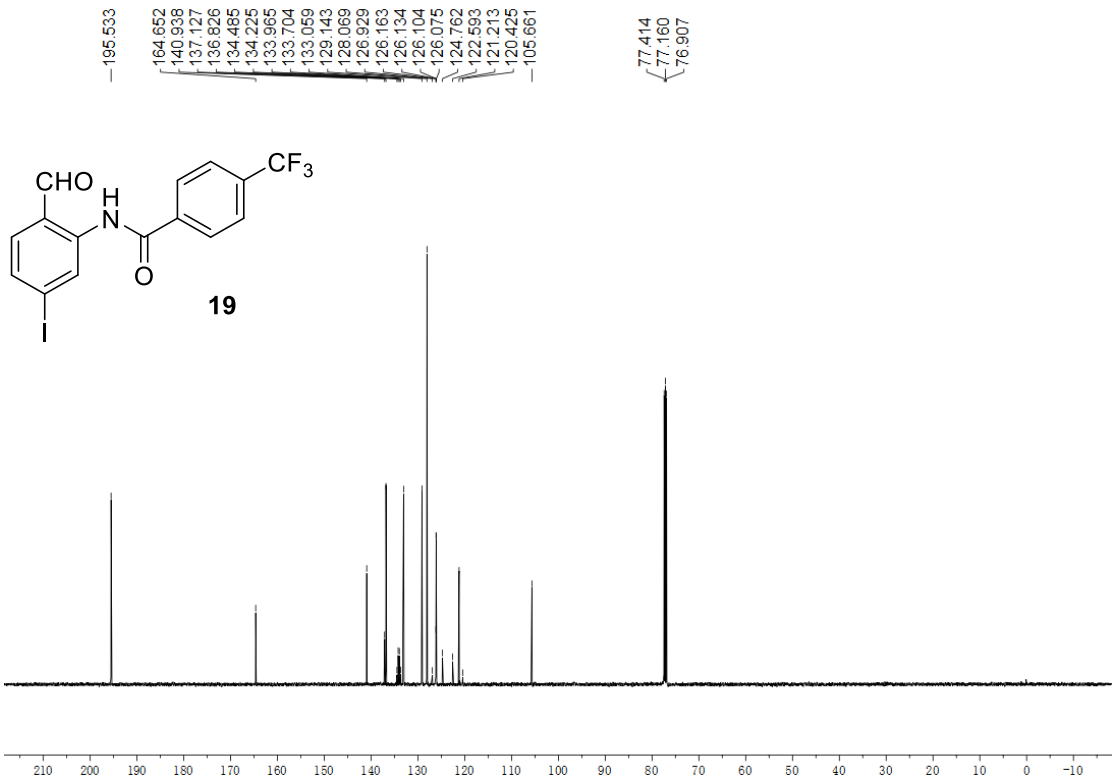
1.02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O
CF3
I
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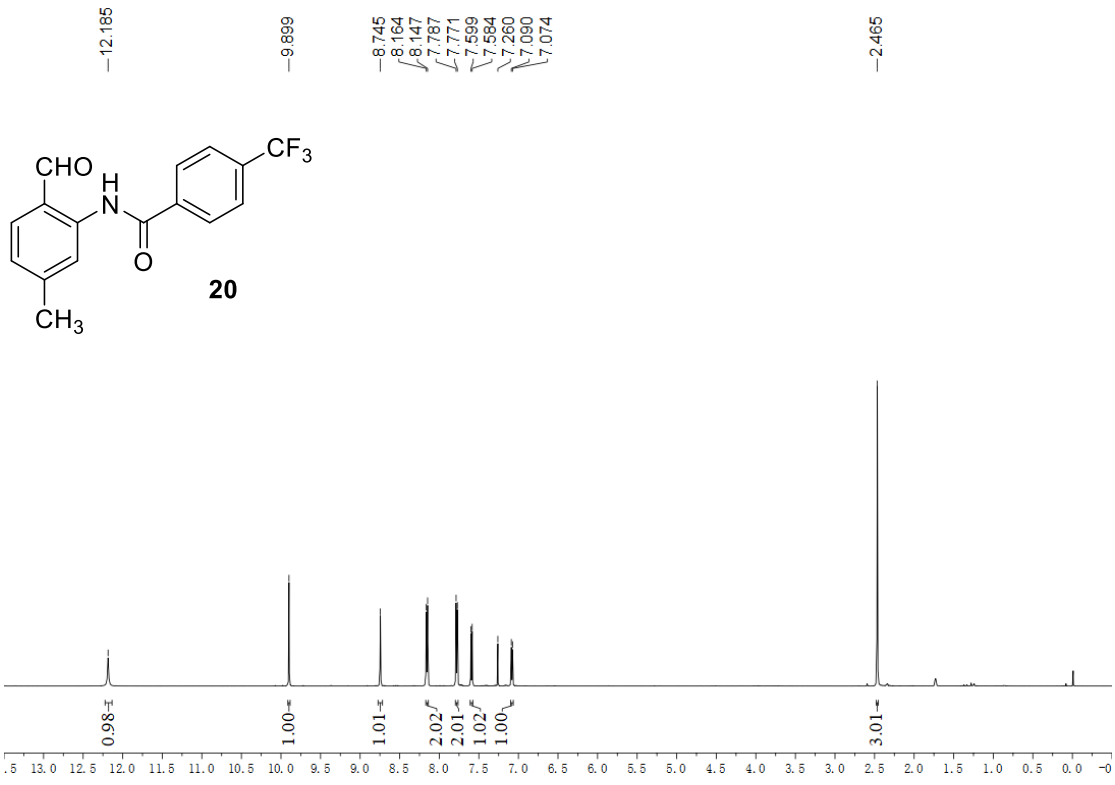
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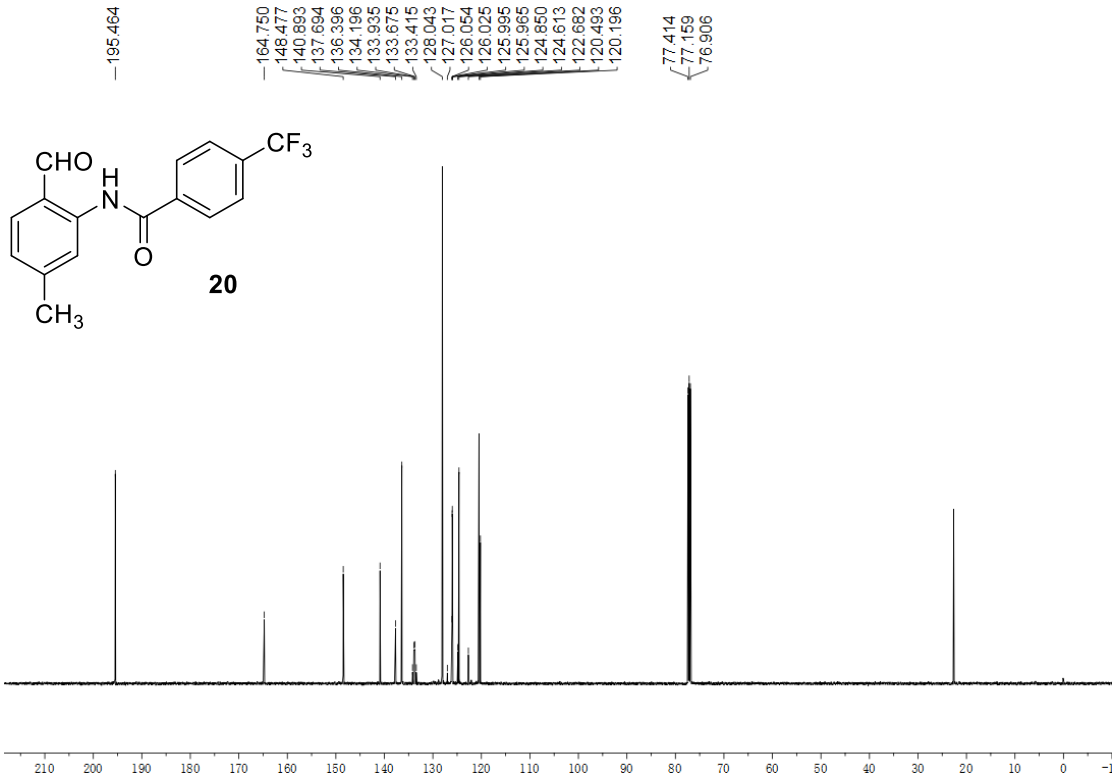
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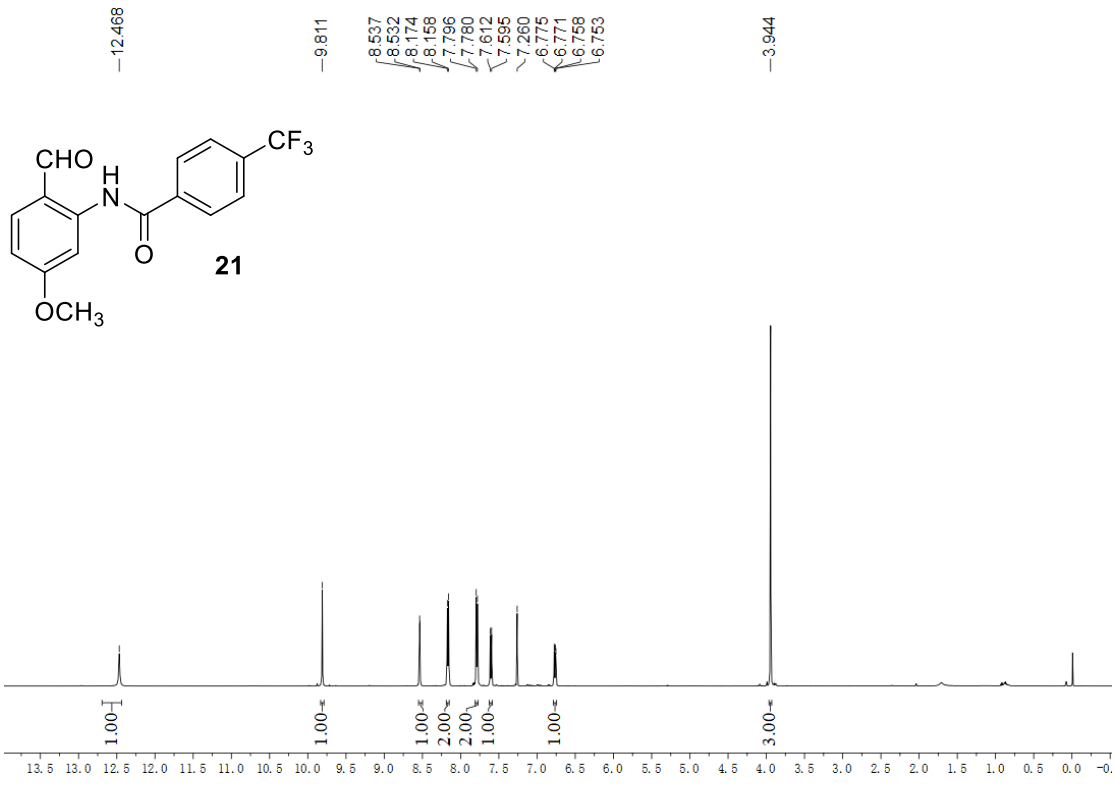
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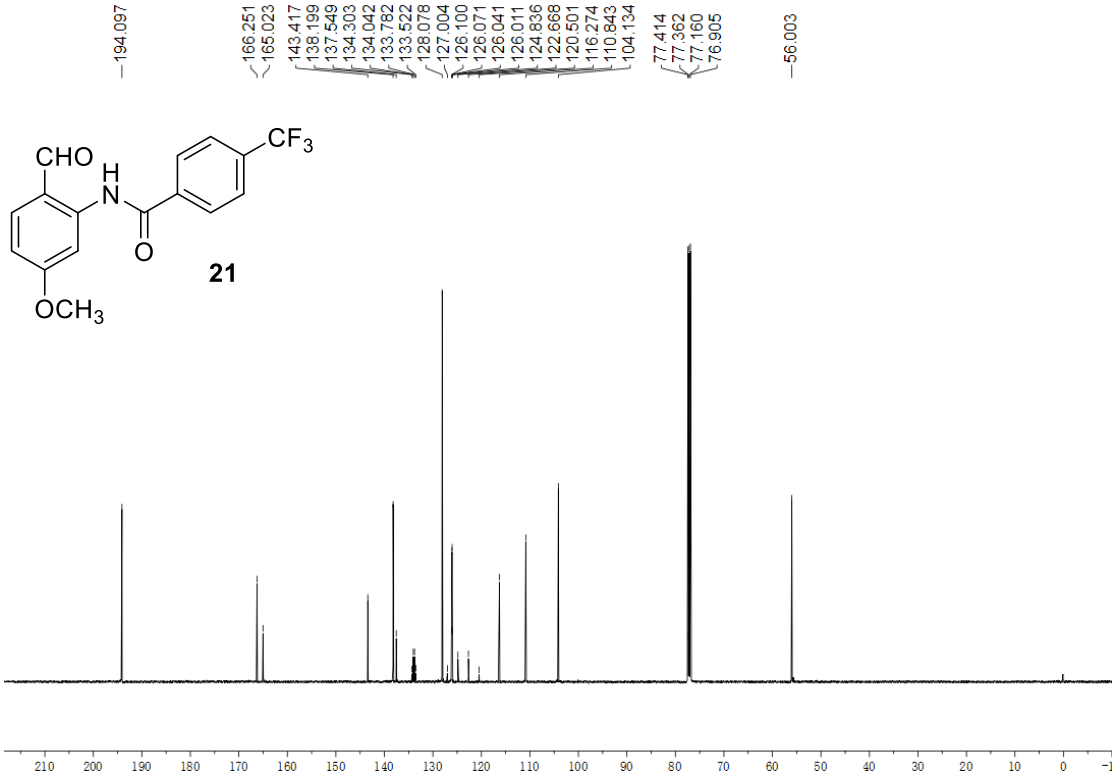
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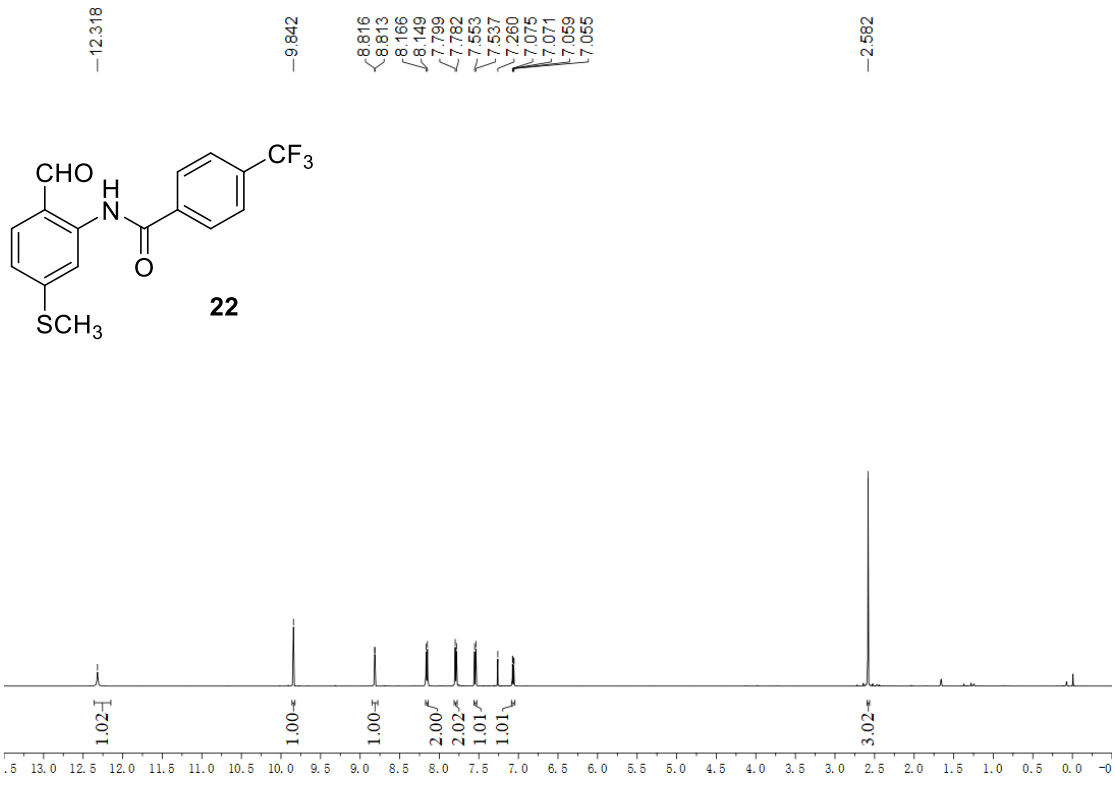
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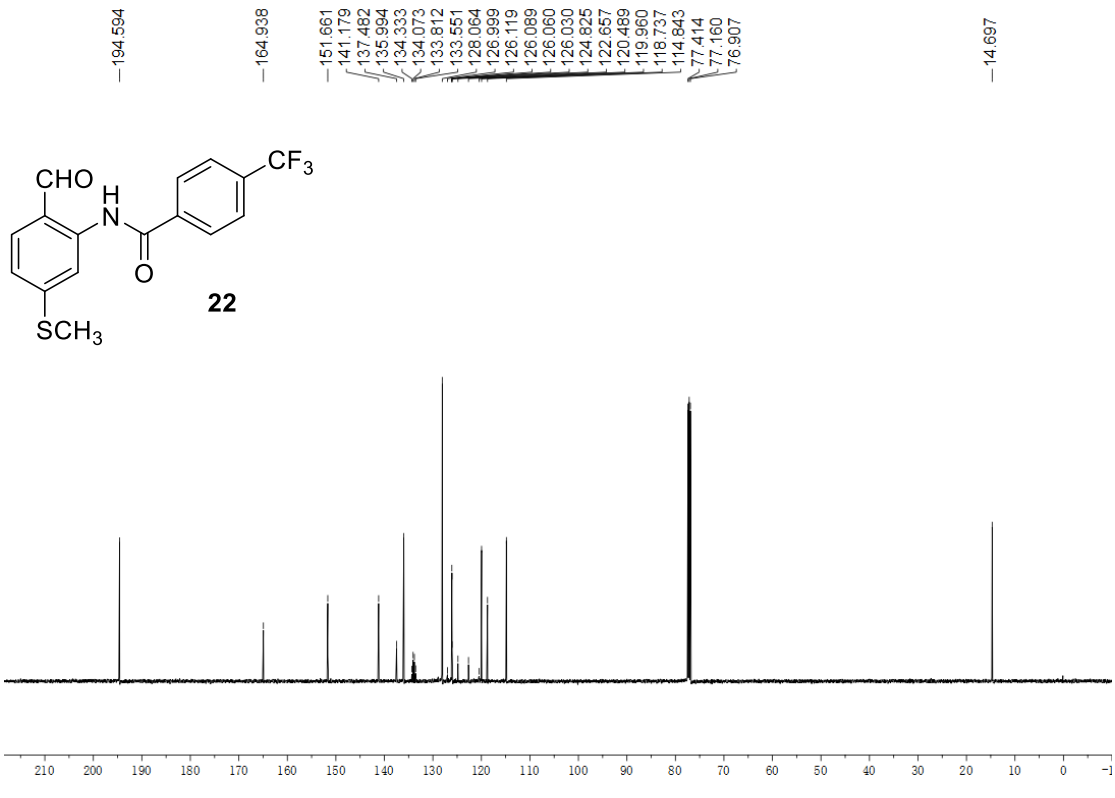
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SCH3
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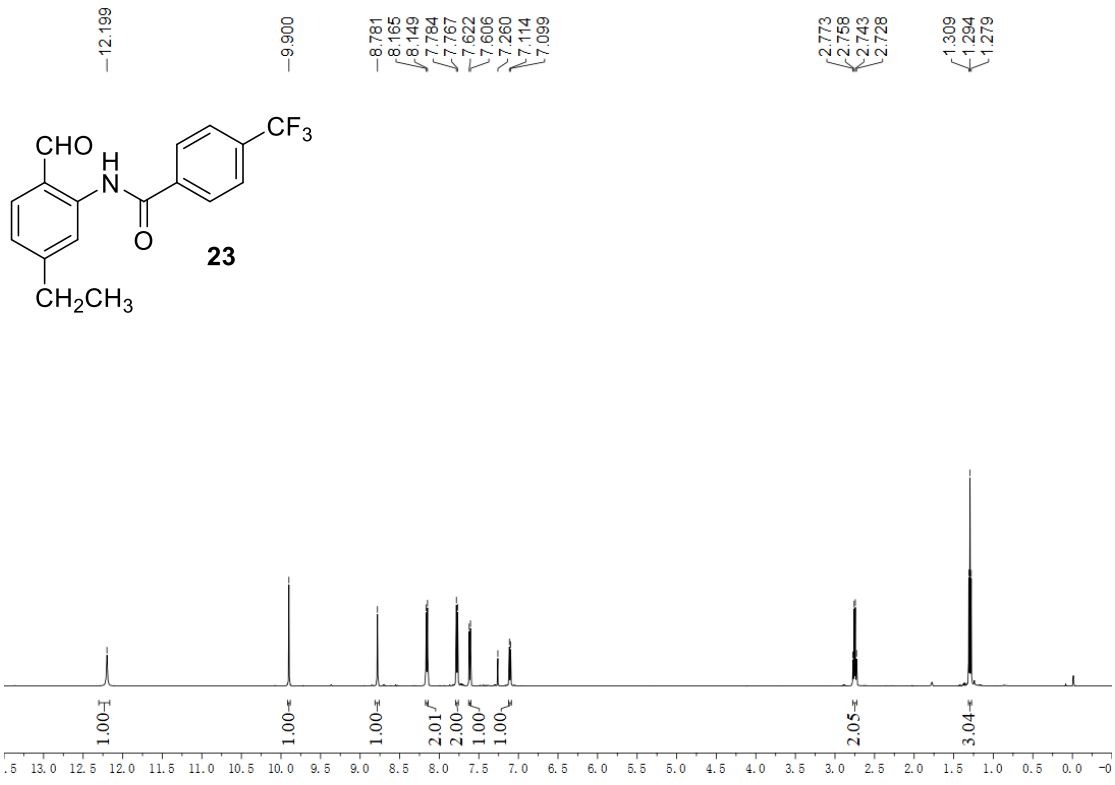
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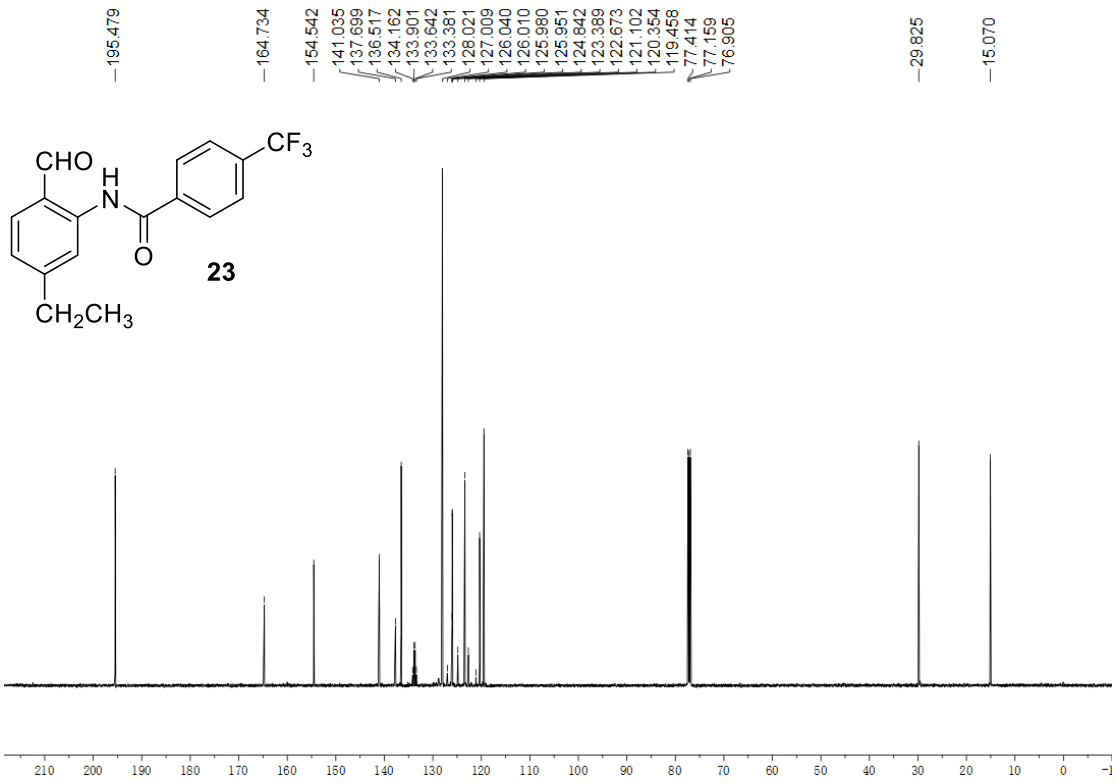
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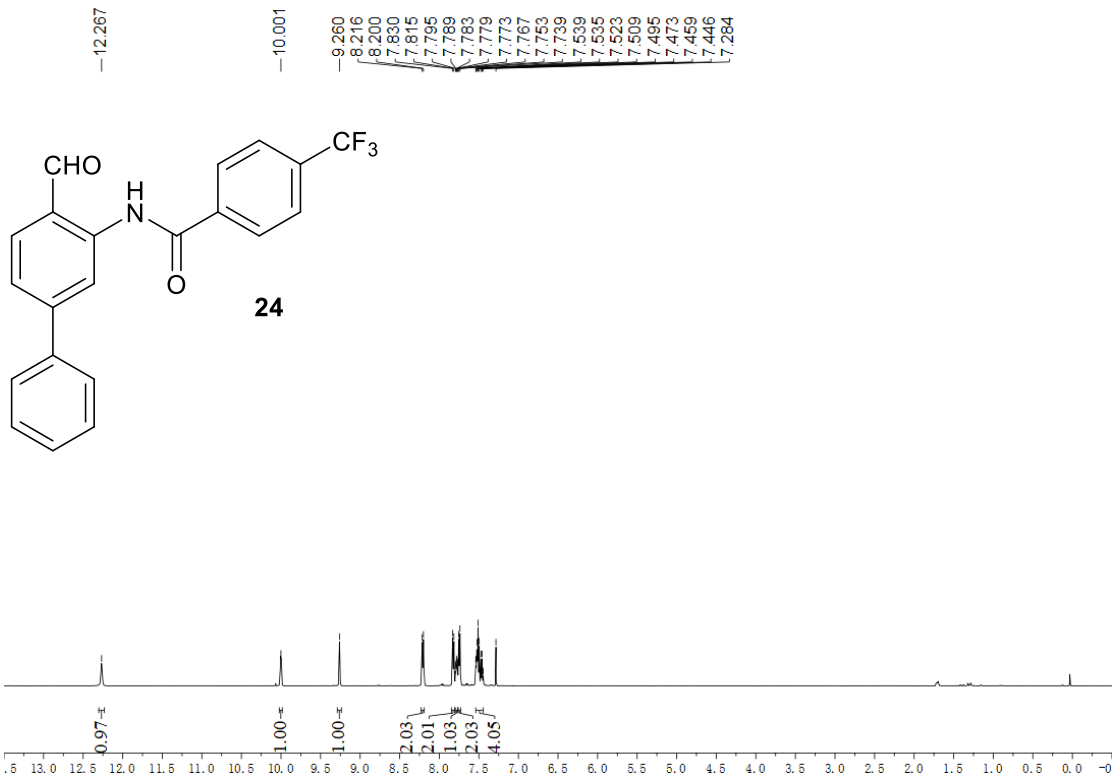
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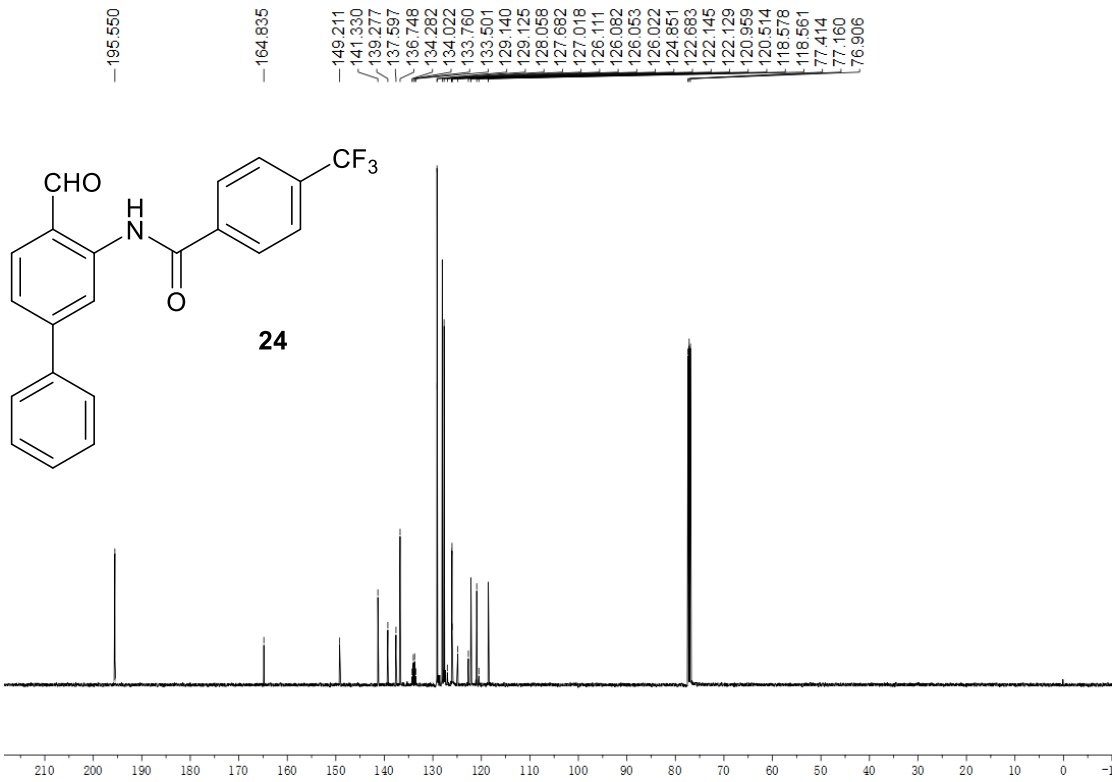
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CF3
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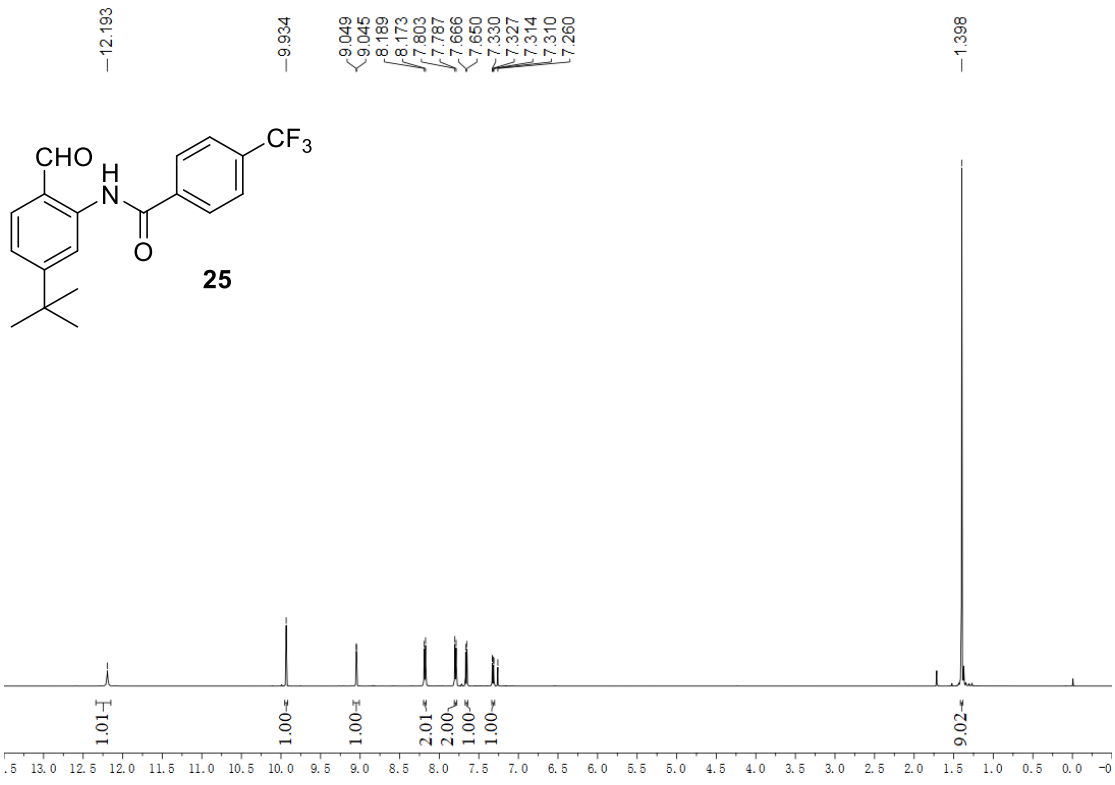
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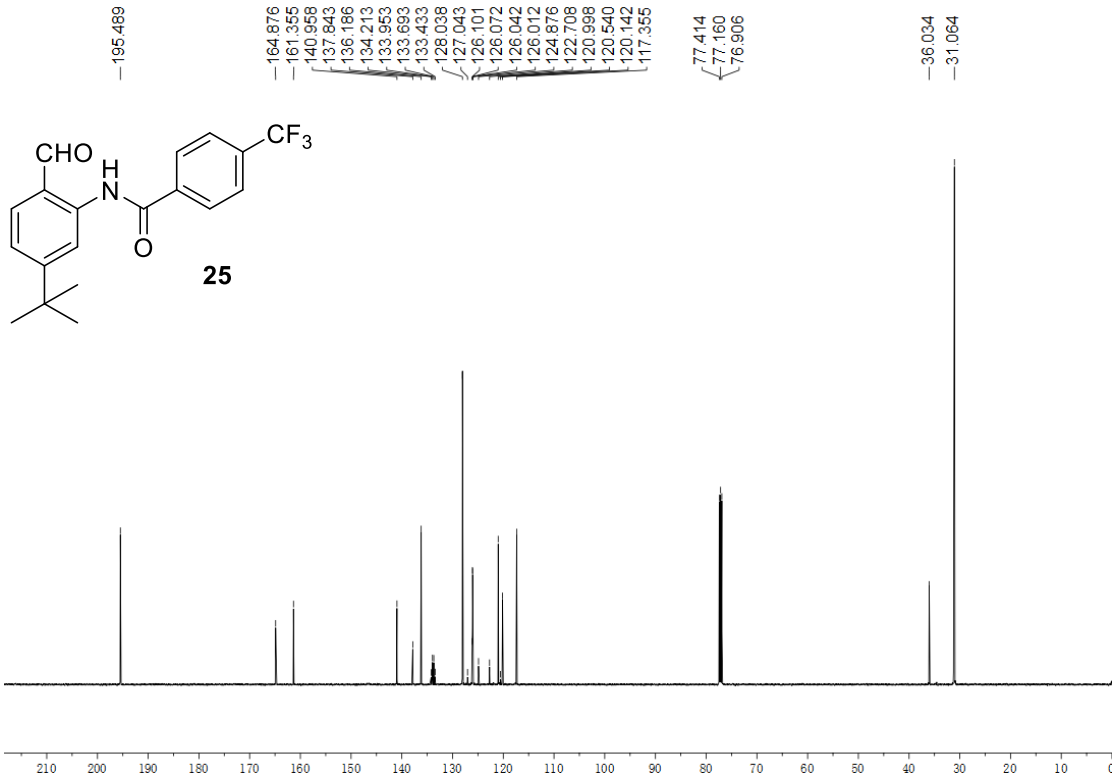
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CF3
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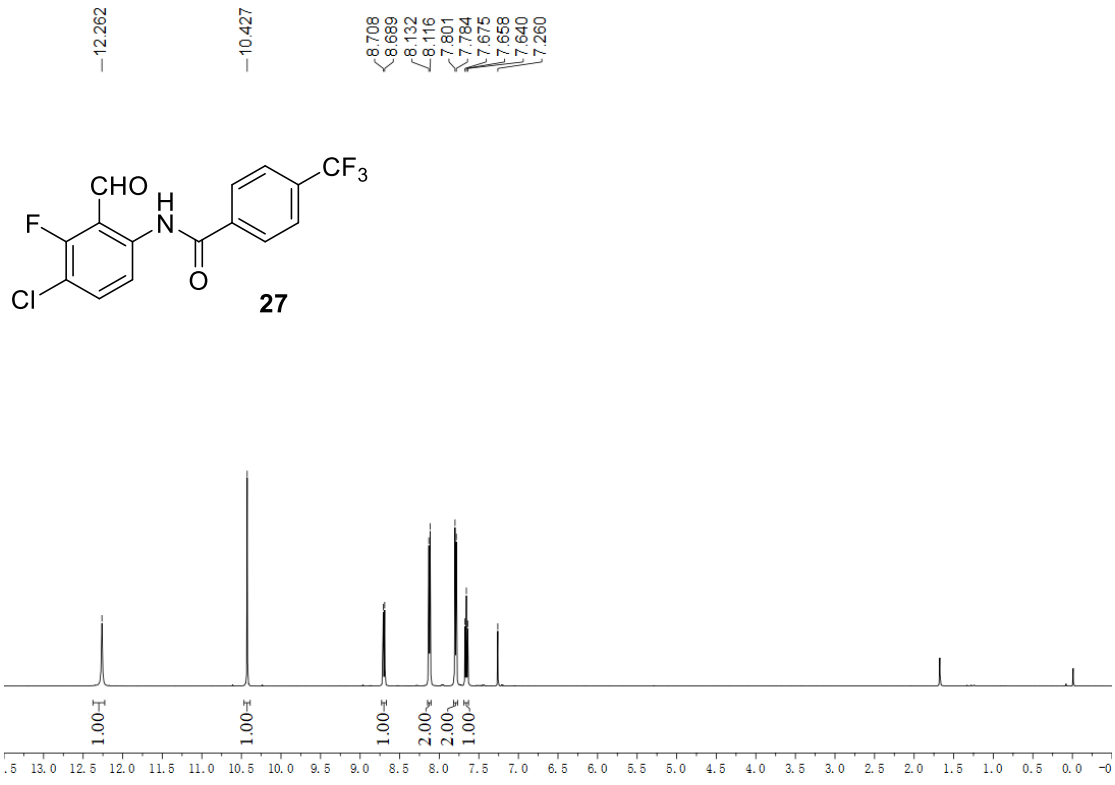
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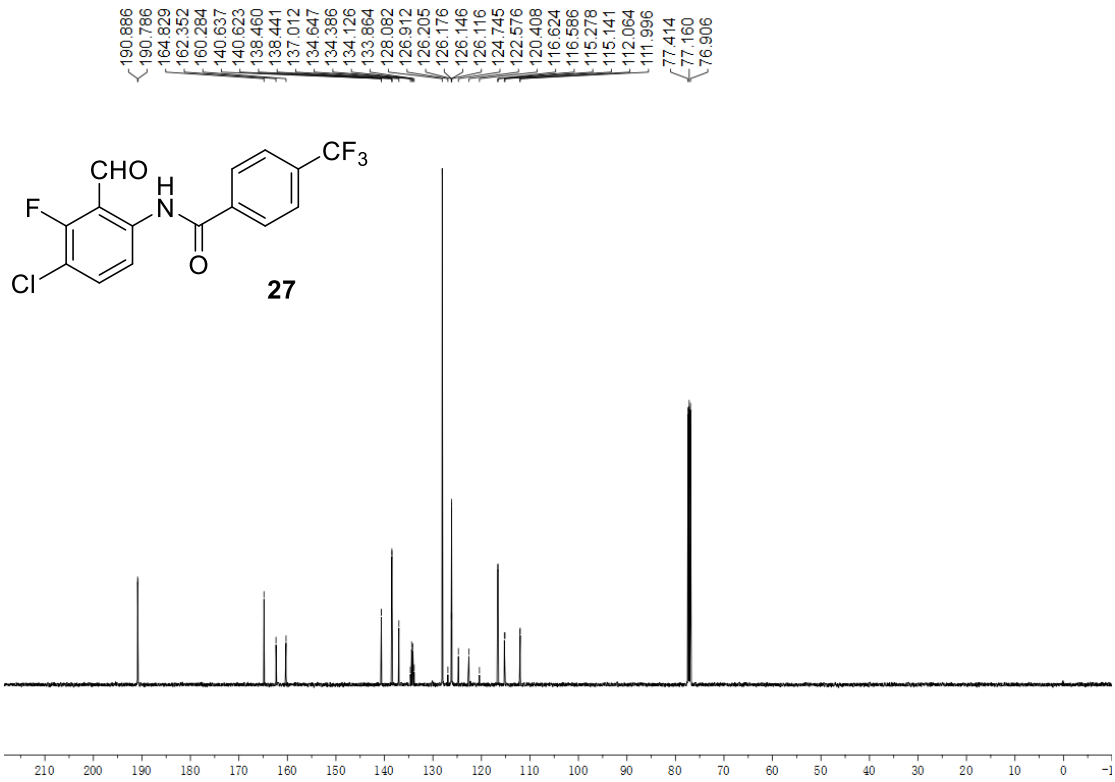
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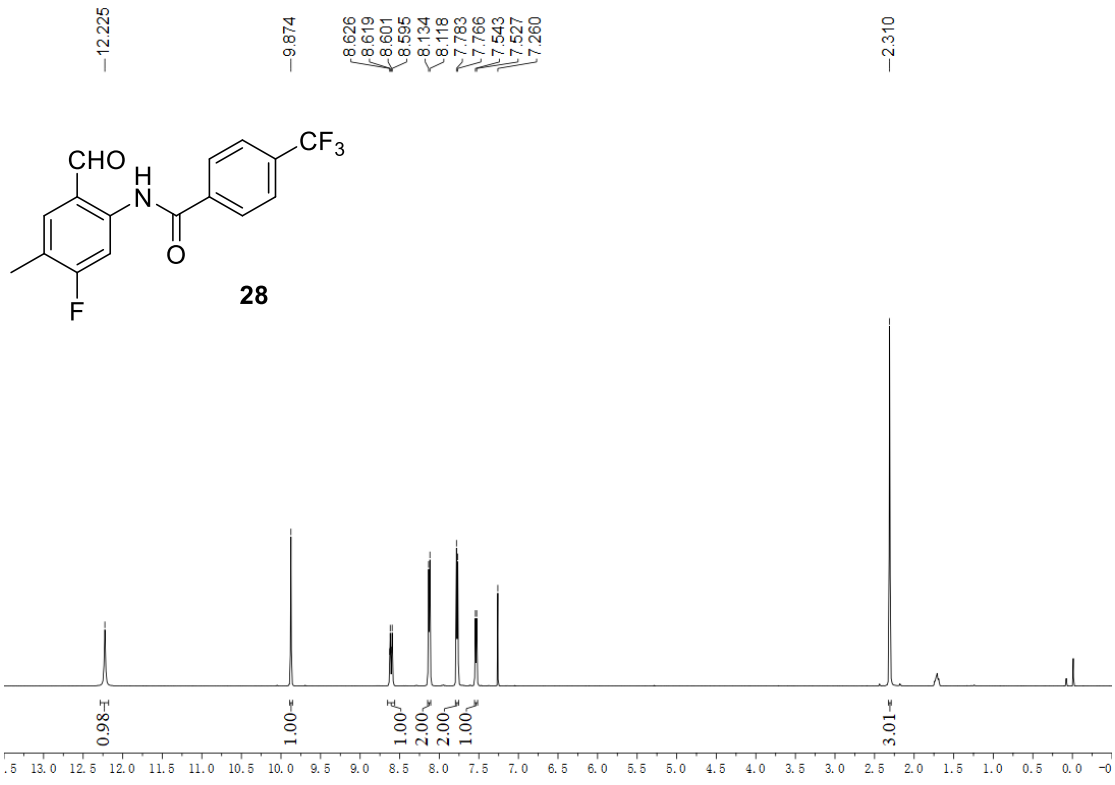
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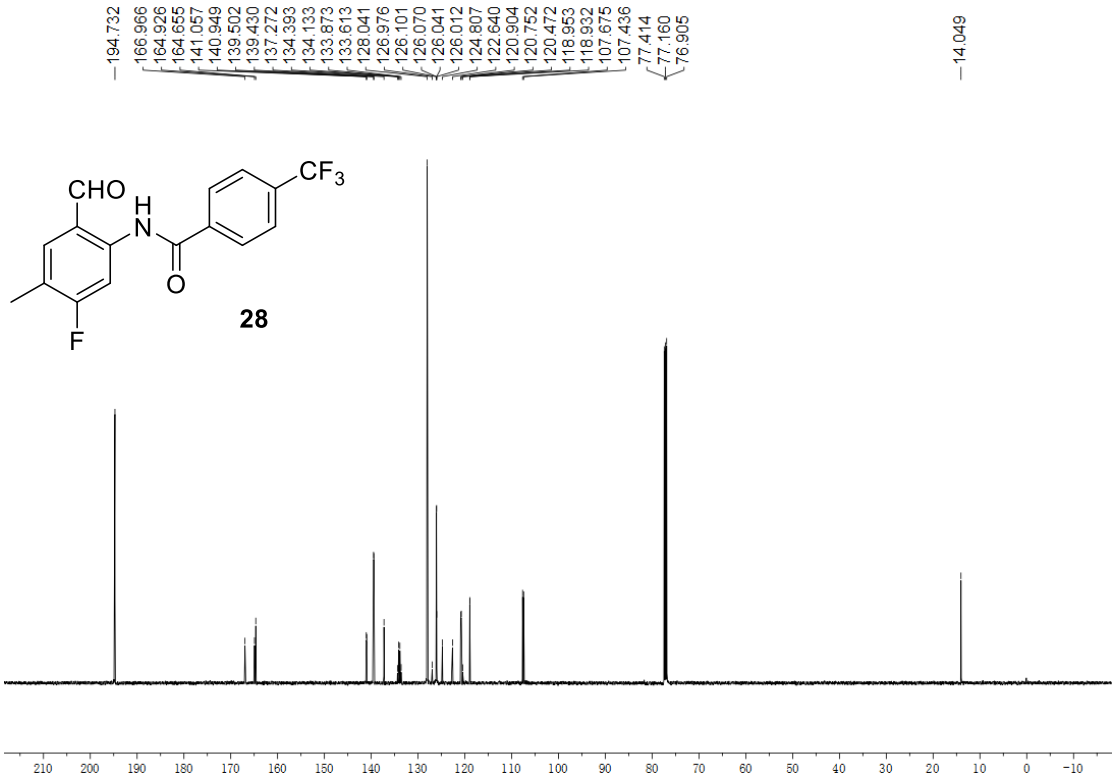
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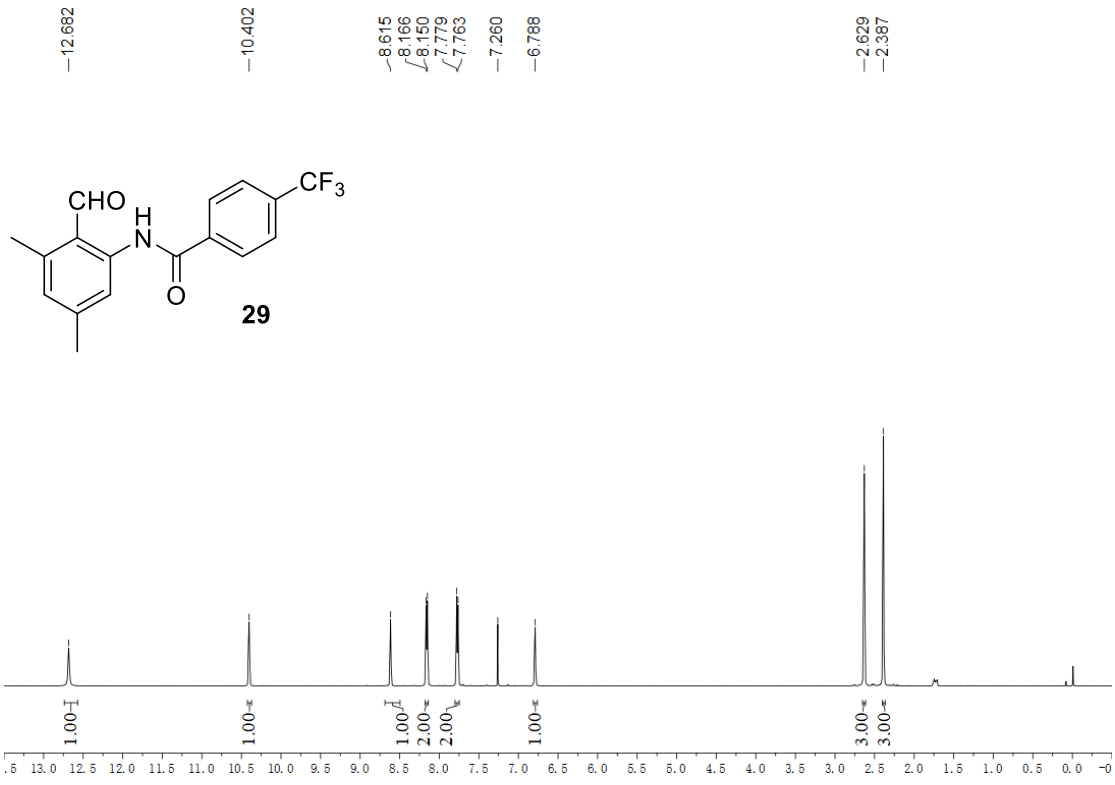
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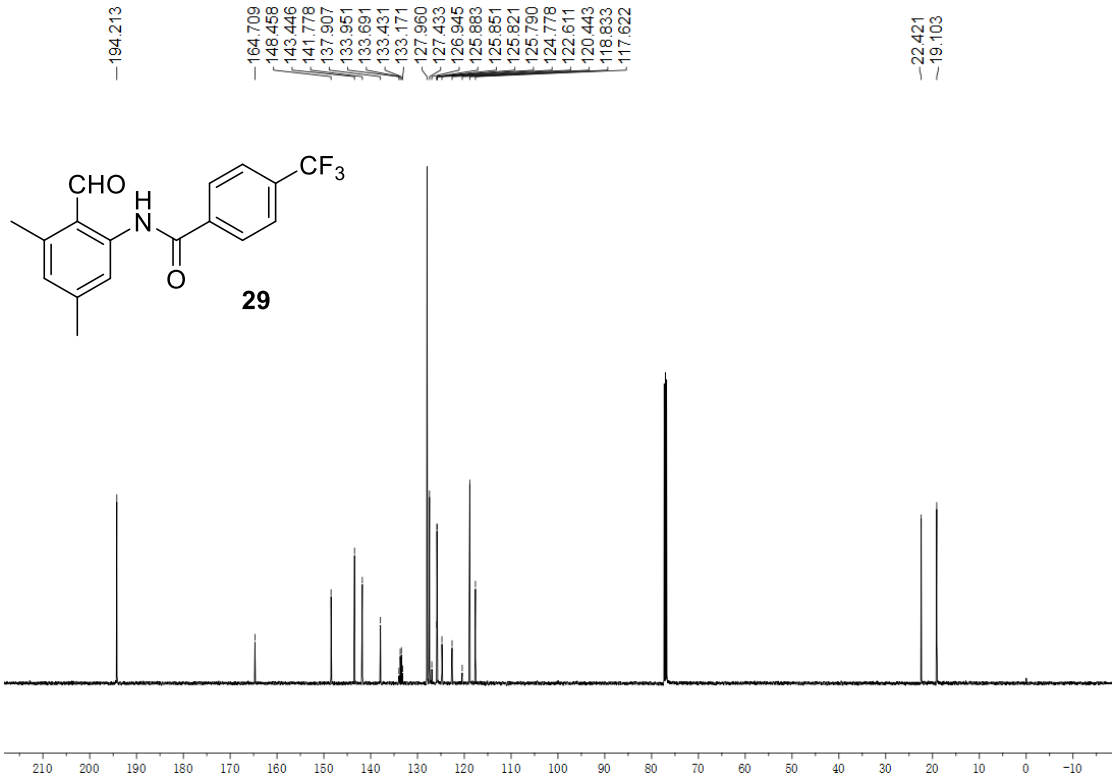
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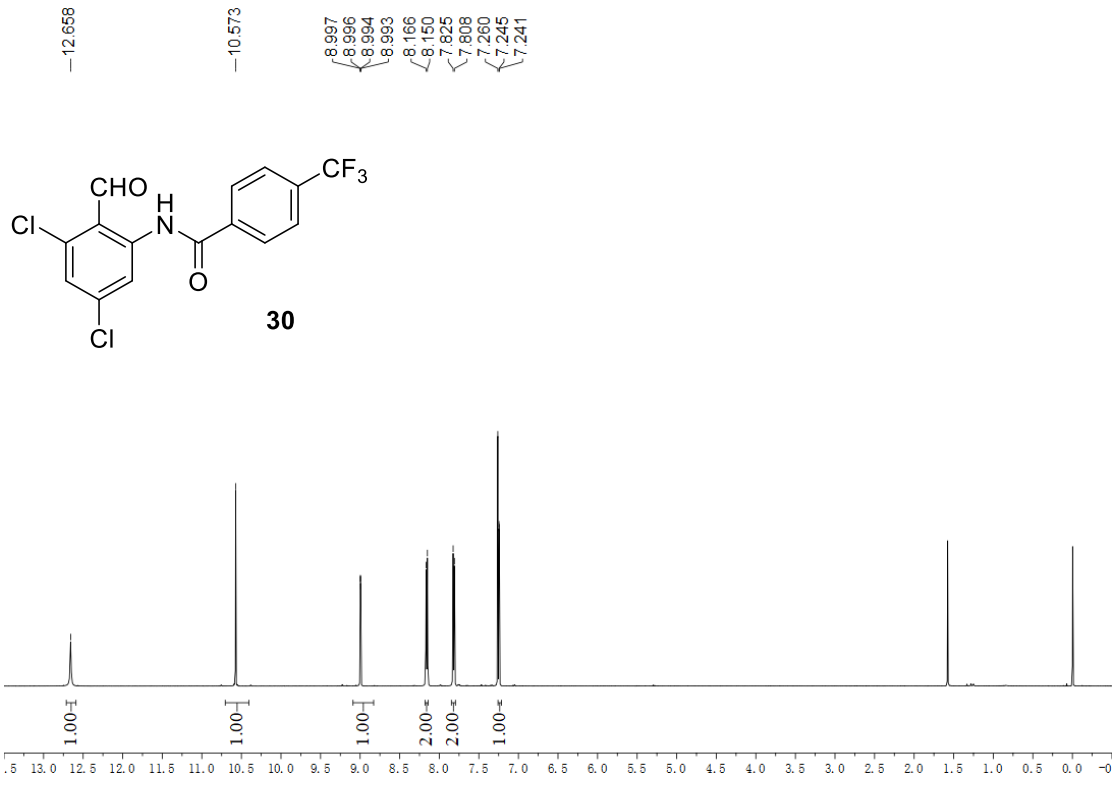
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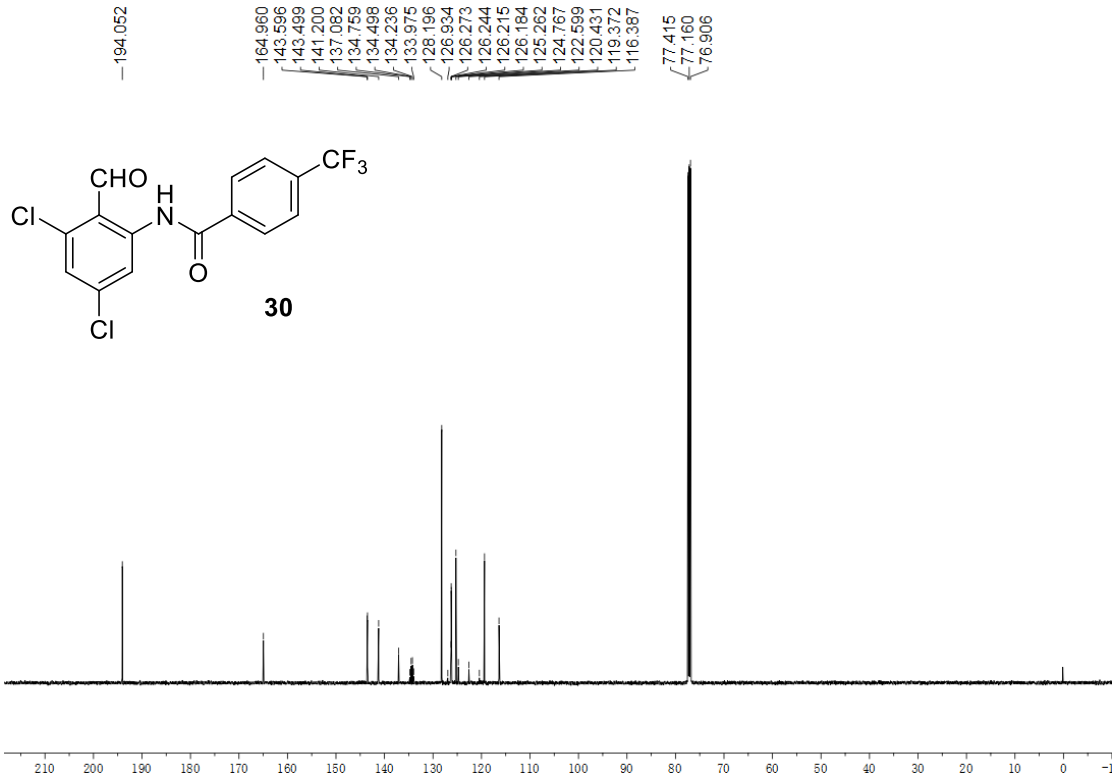
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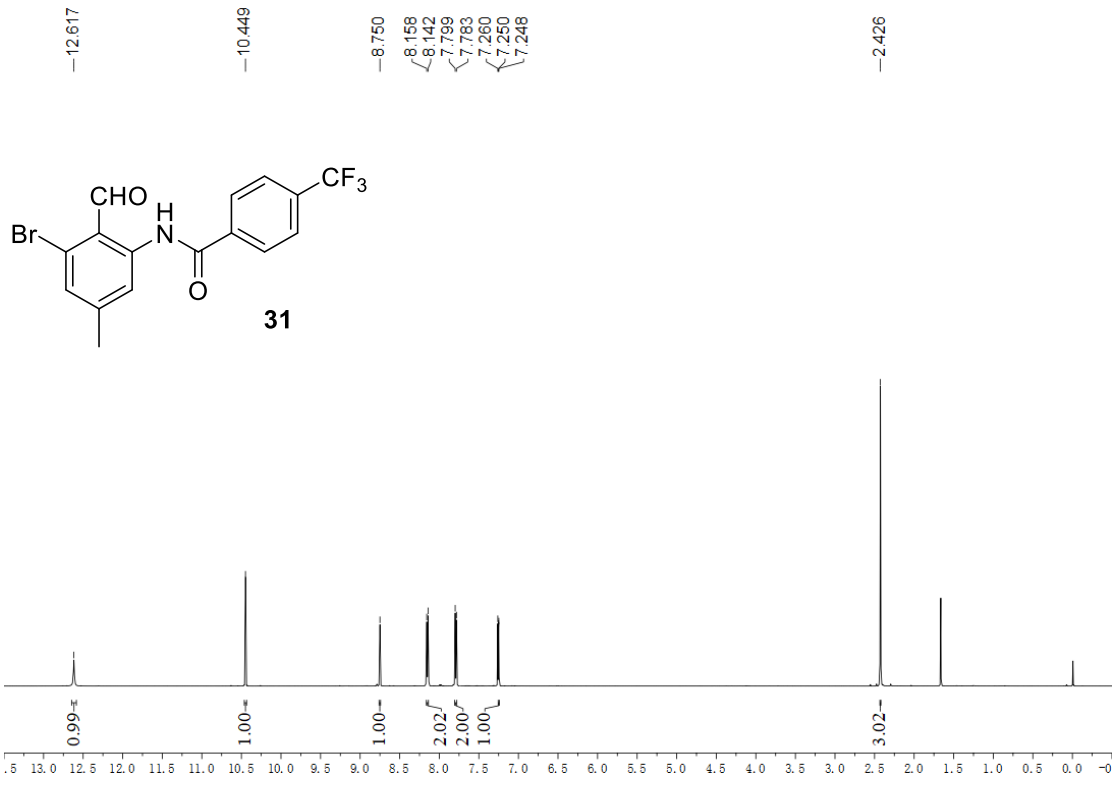
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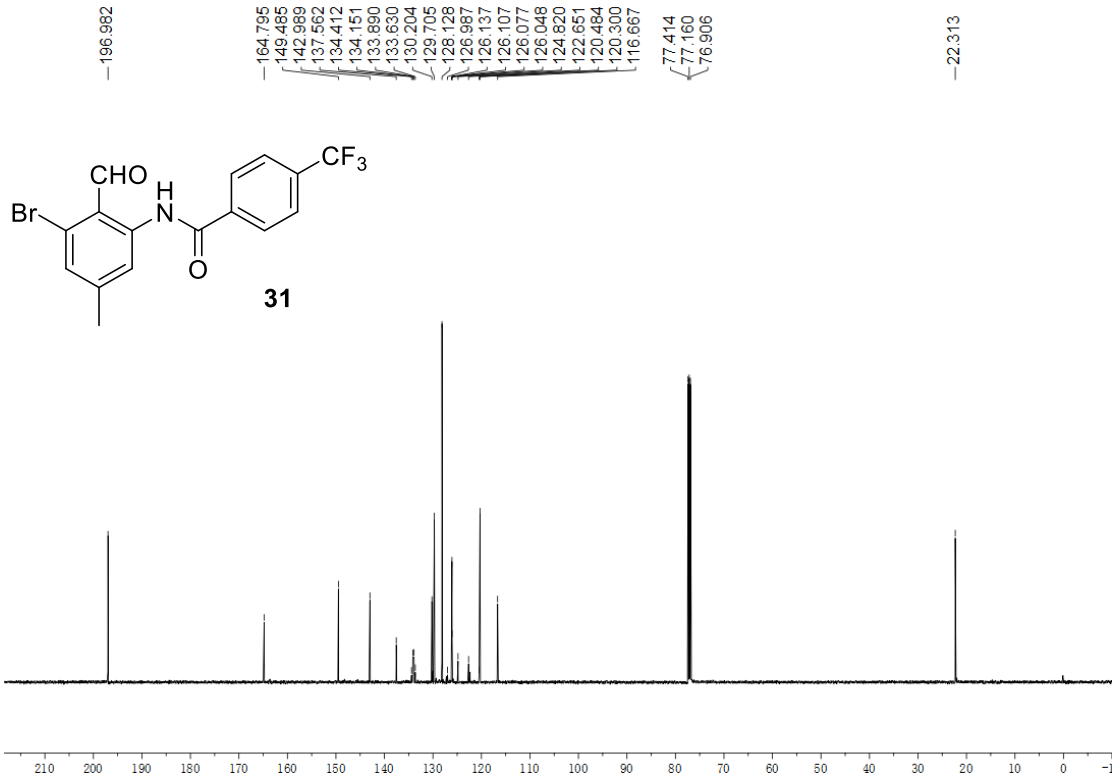
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77.160
76.906
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Br
O
CF3
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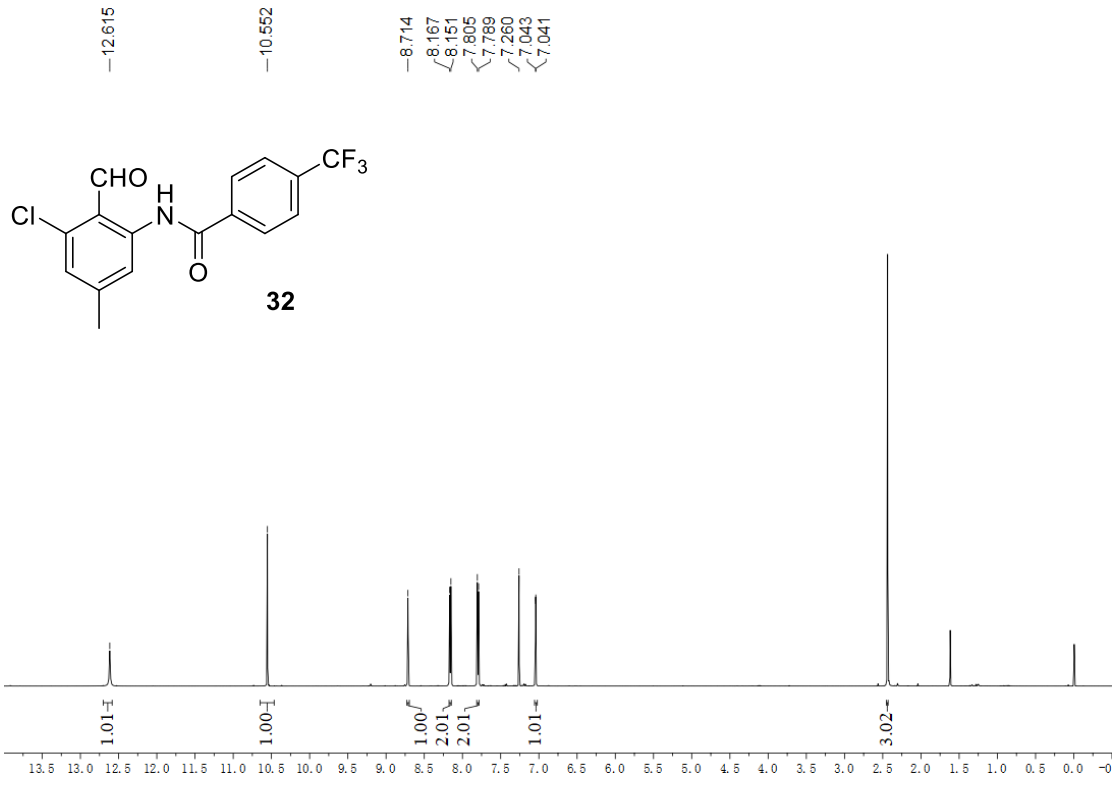
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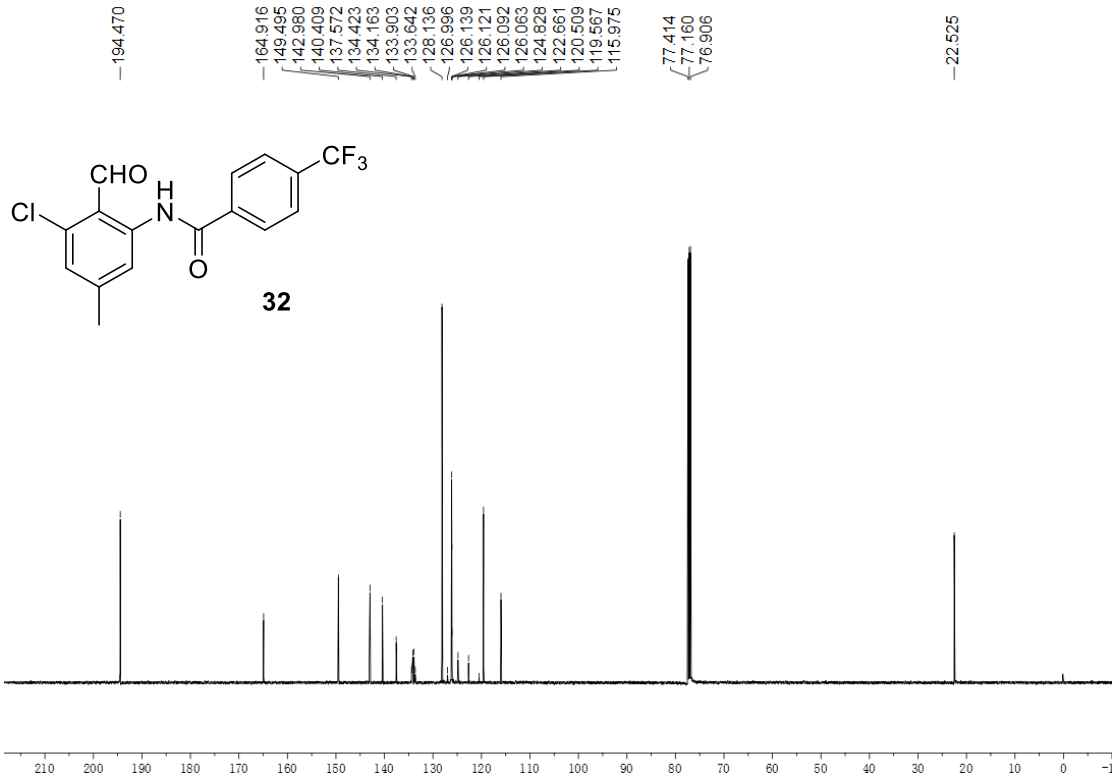
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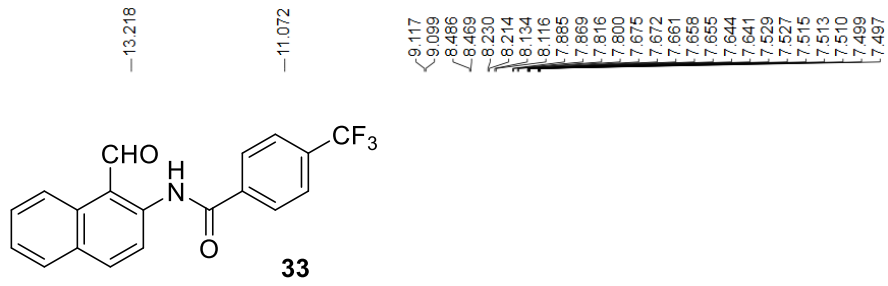
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7.510
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7.497


CHO
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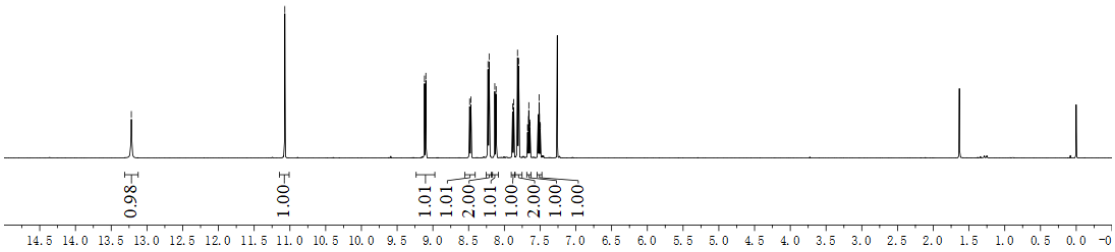
N
O
CF3

**33**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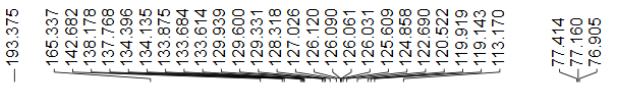
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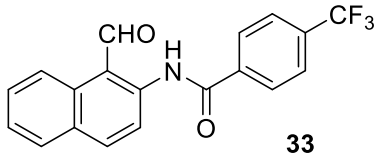
77.160
76.905


CHO
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**33**


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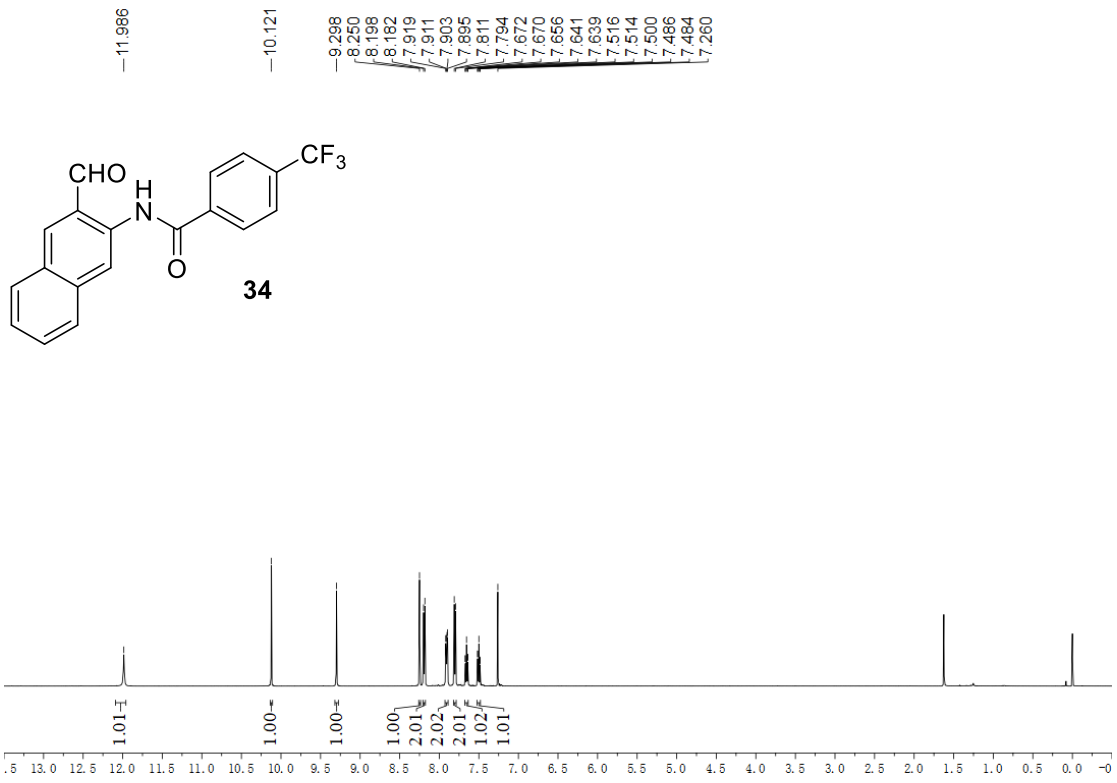
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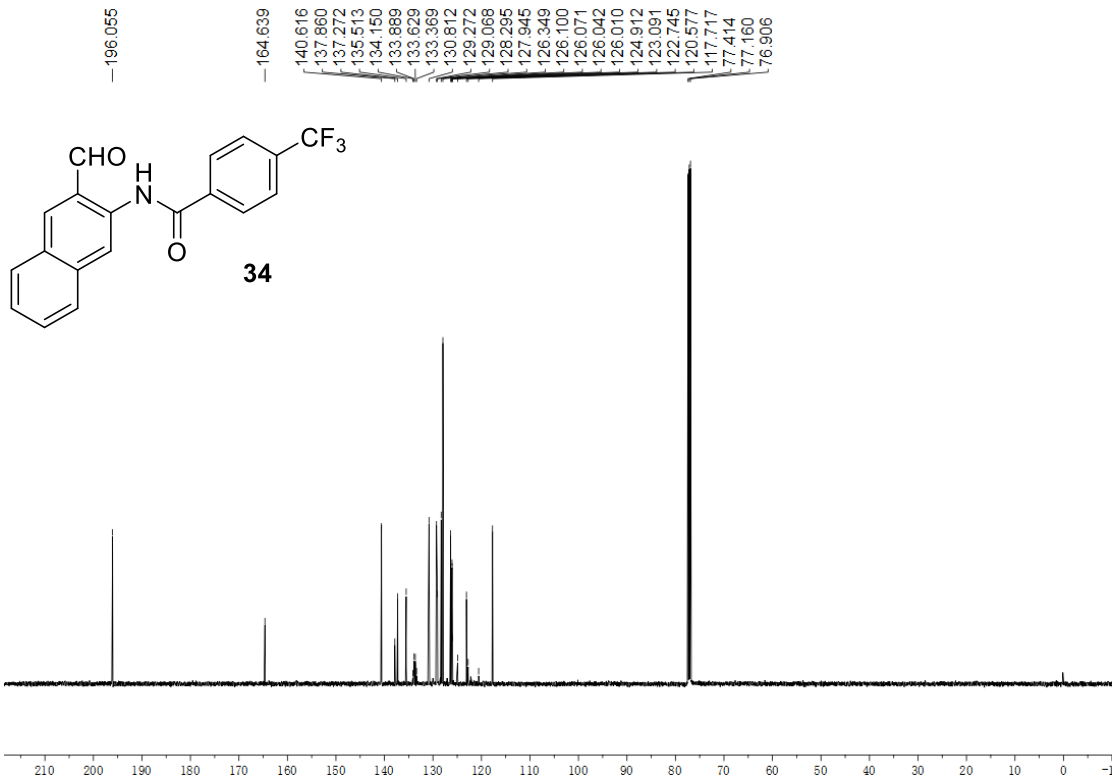
1.01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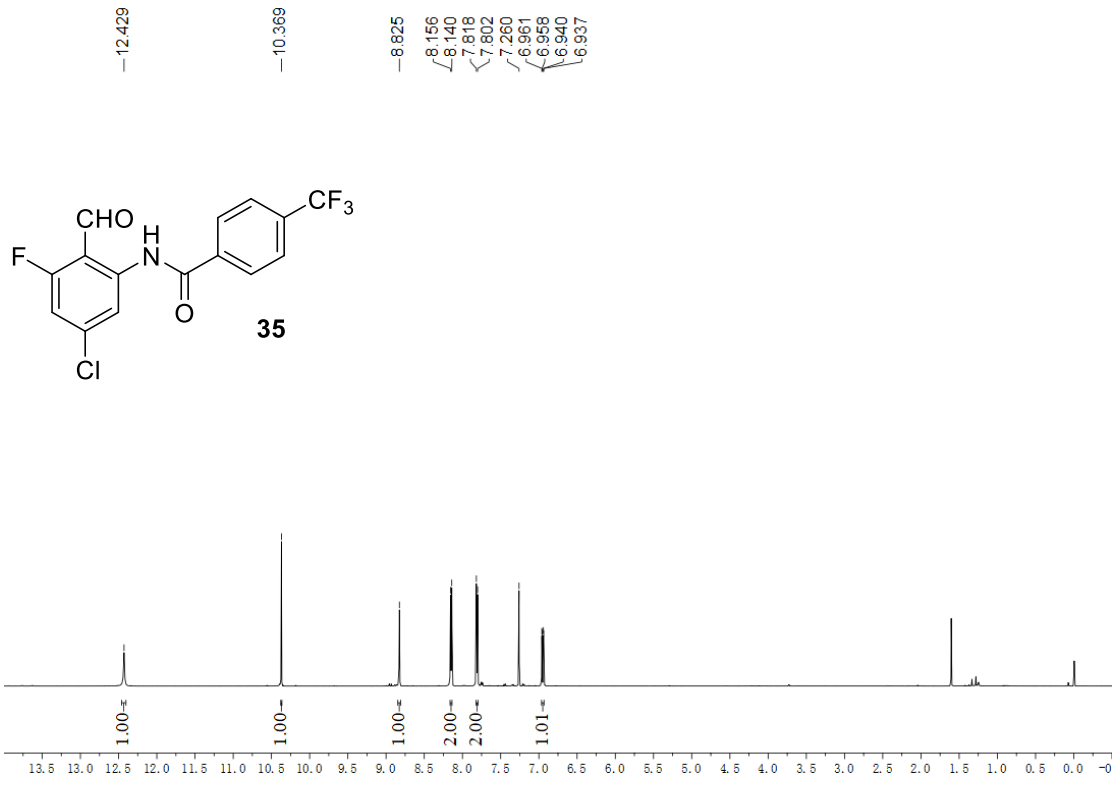
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1.00
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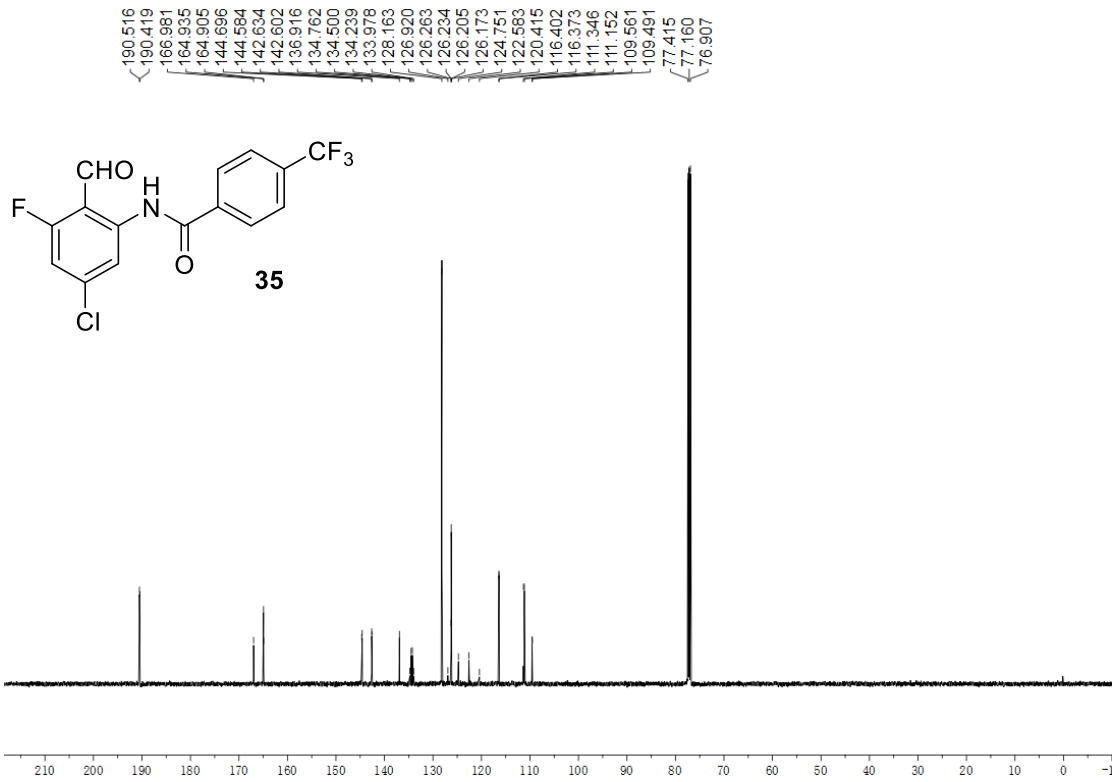
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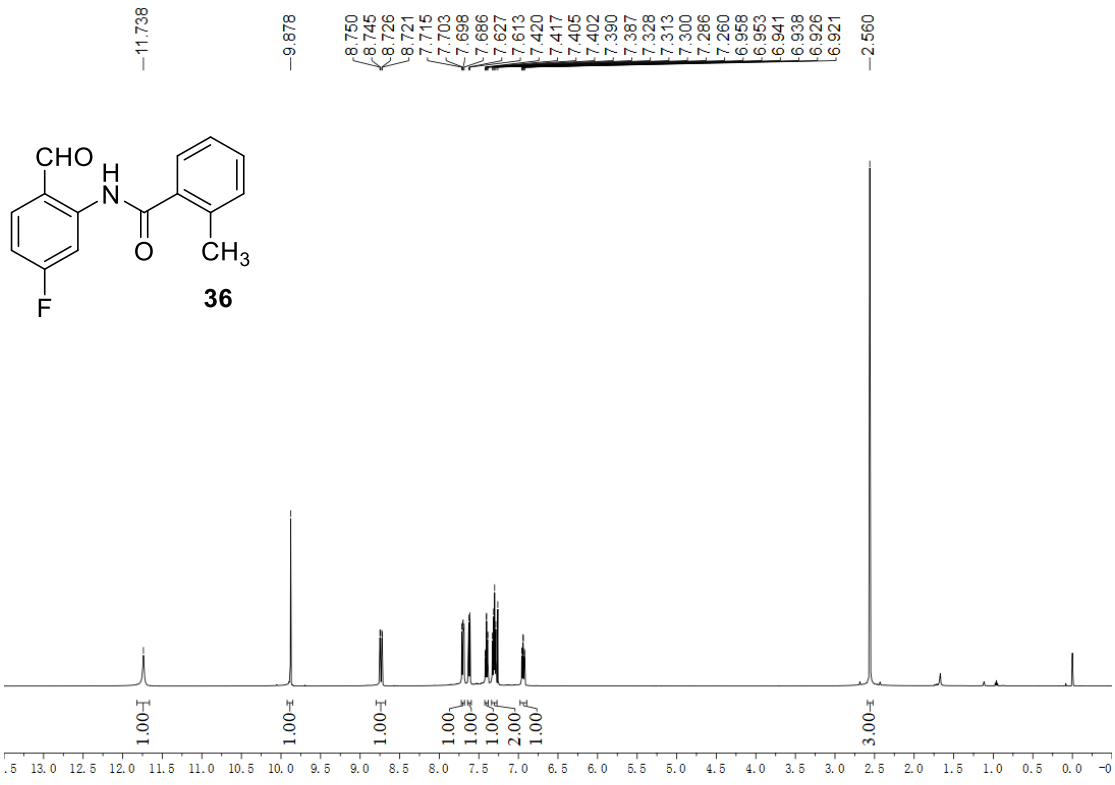
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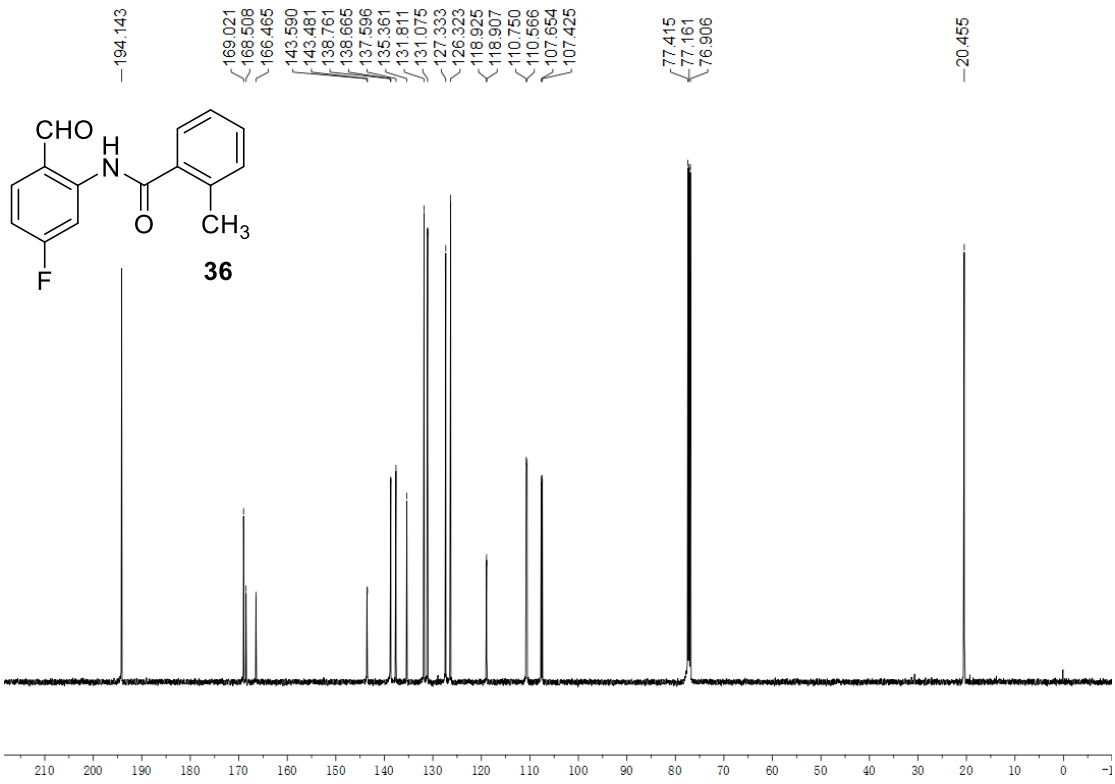
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CH3
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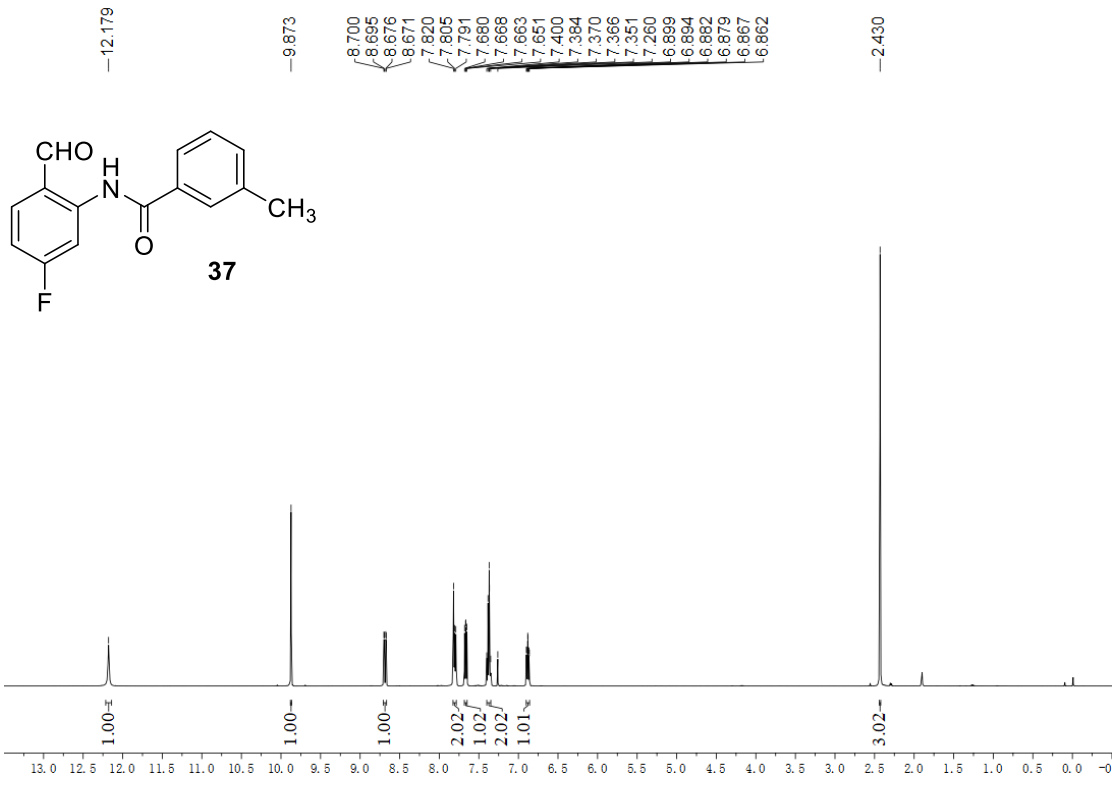
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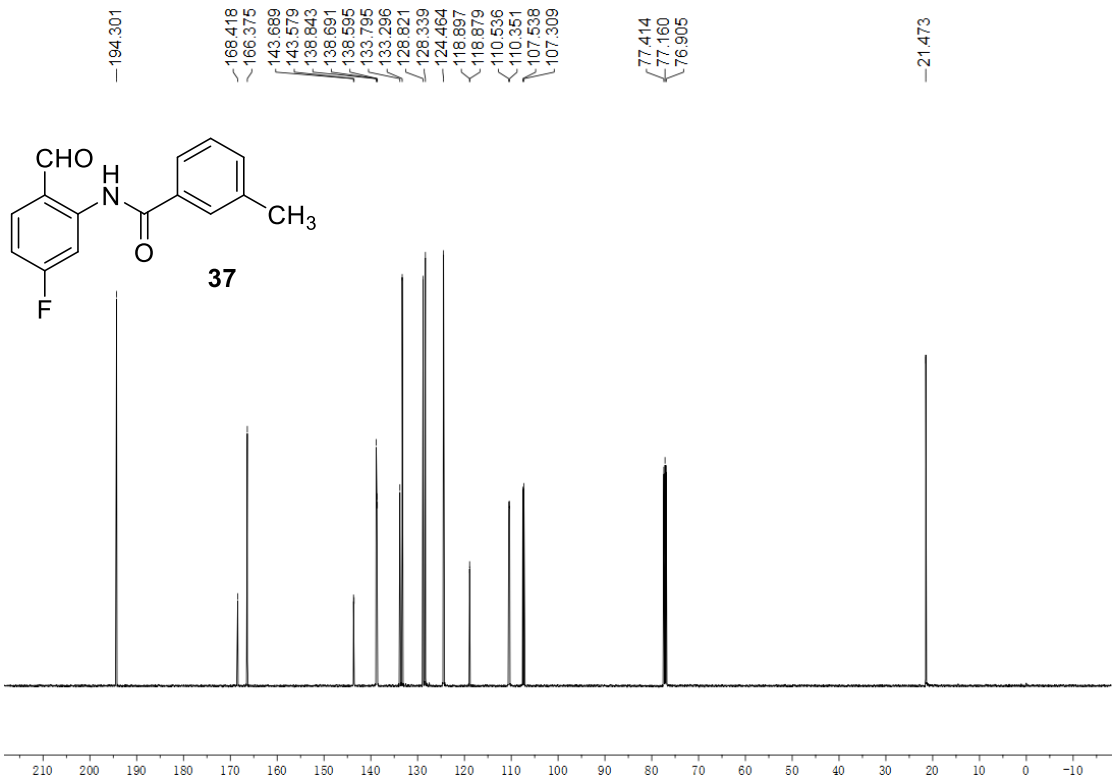
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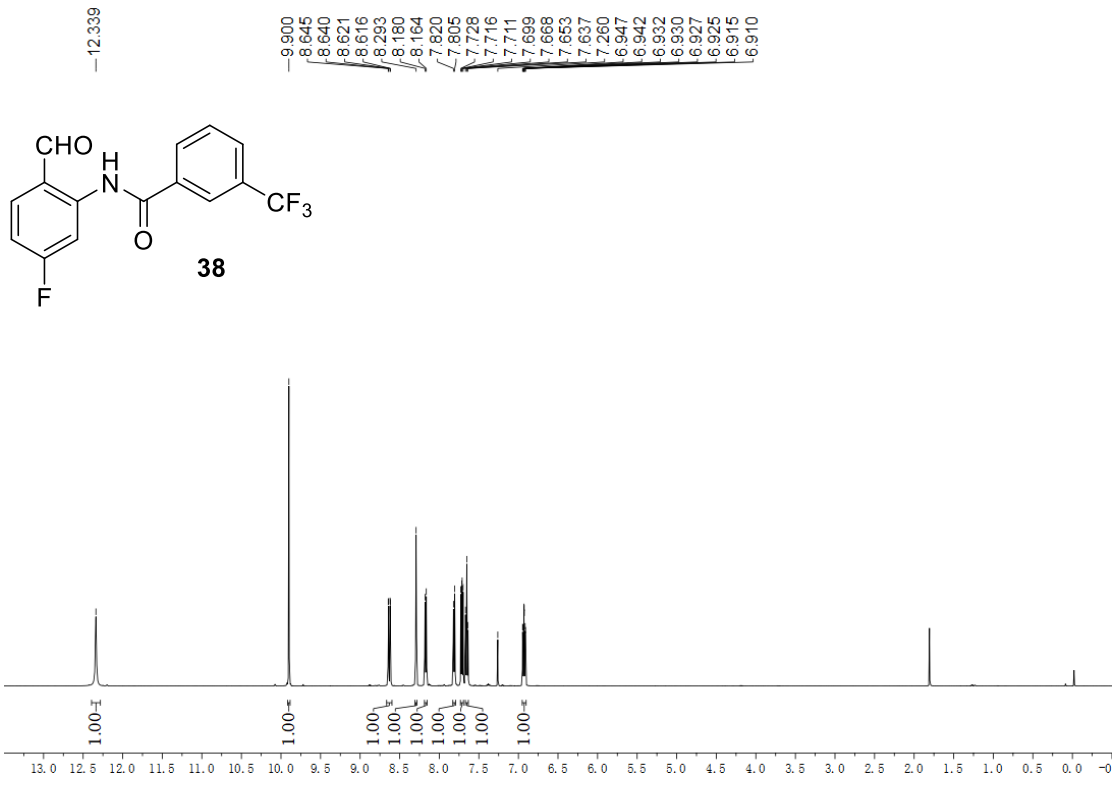
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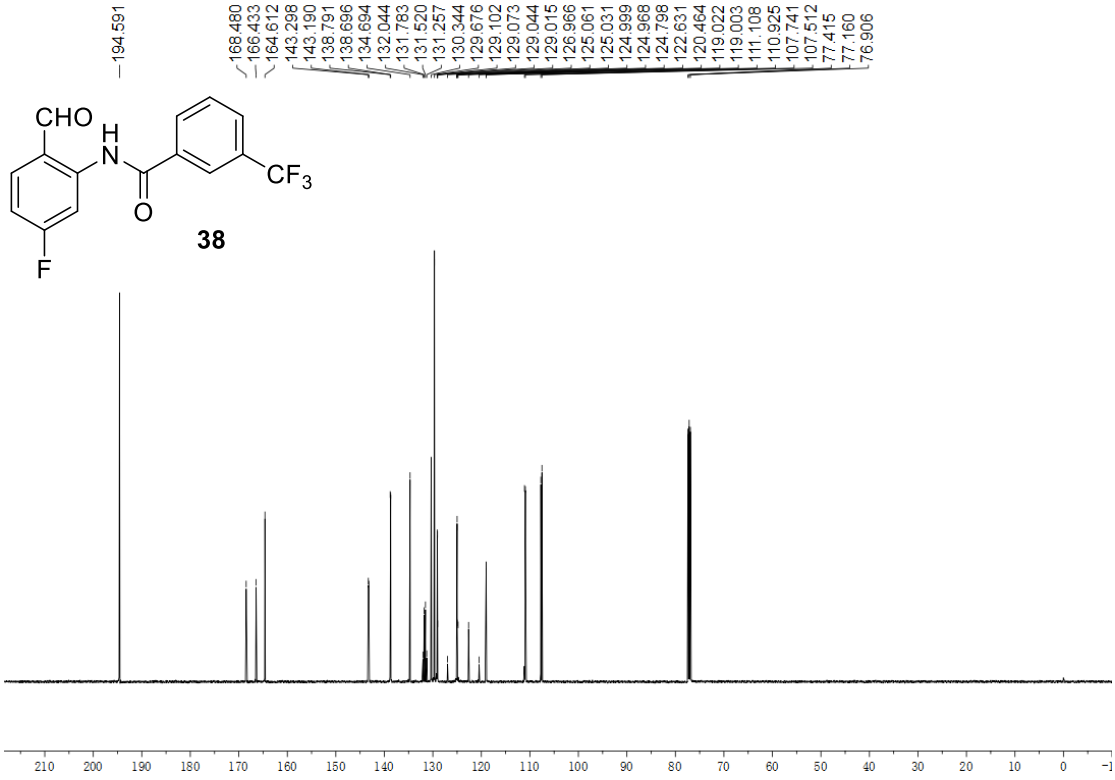
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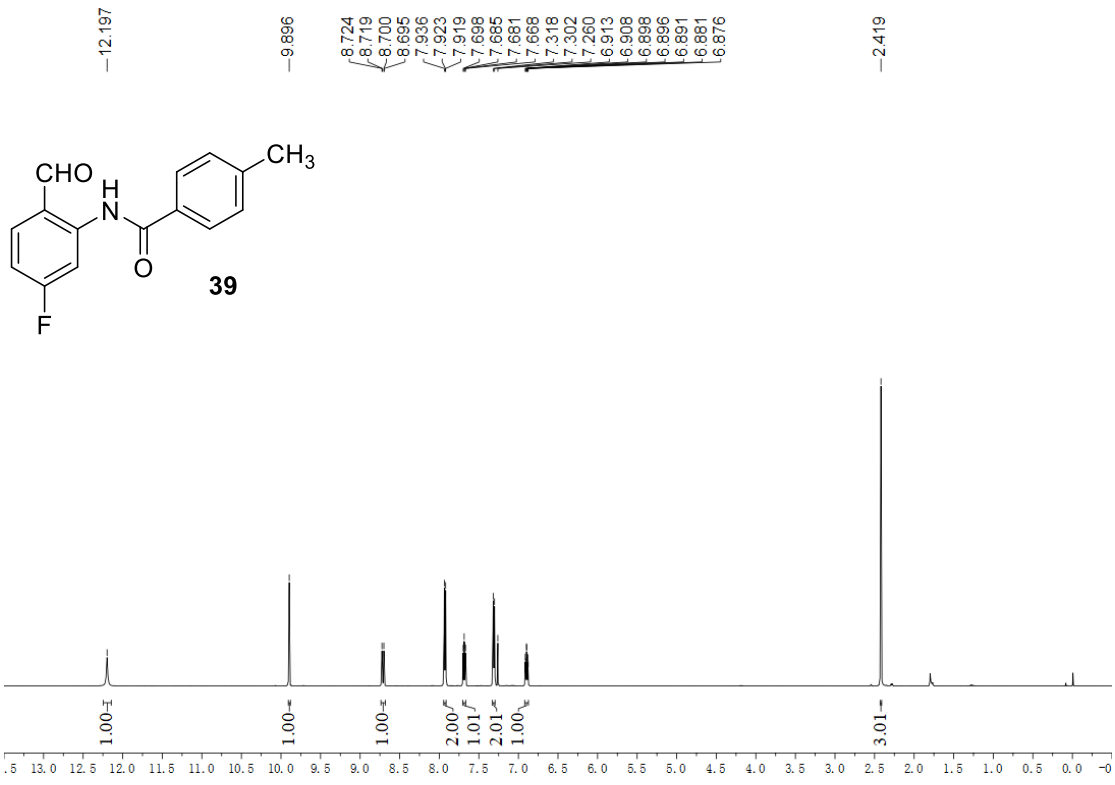
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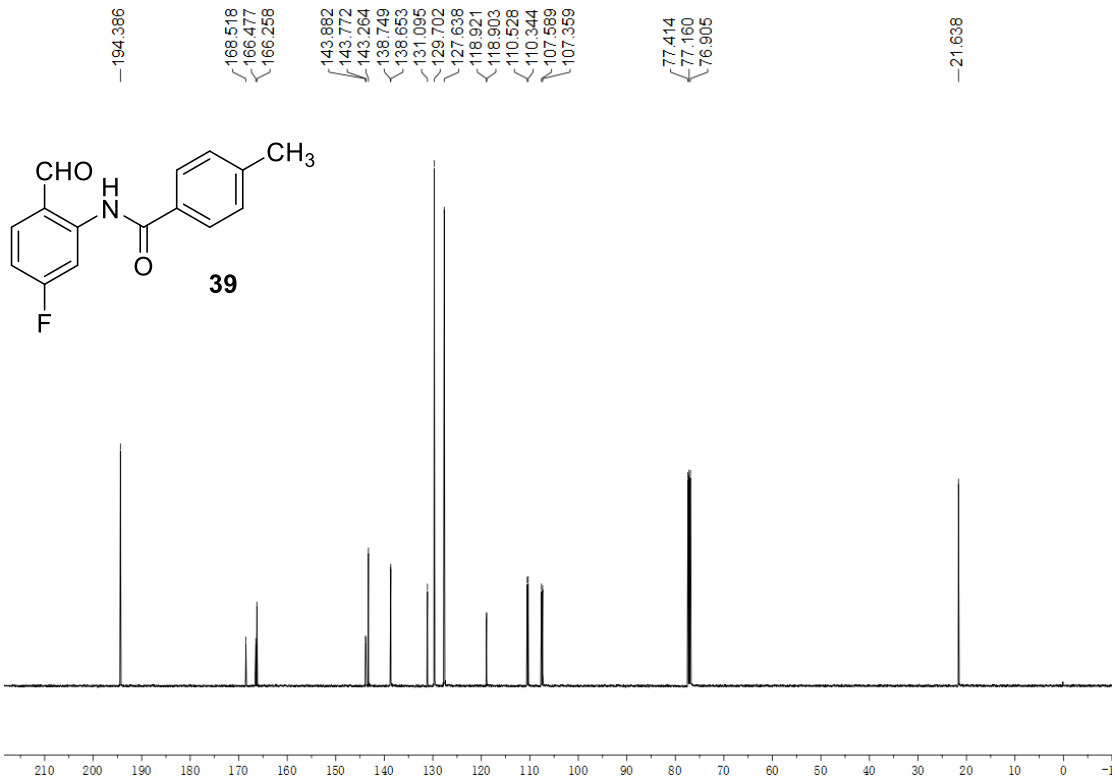
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CH3
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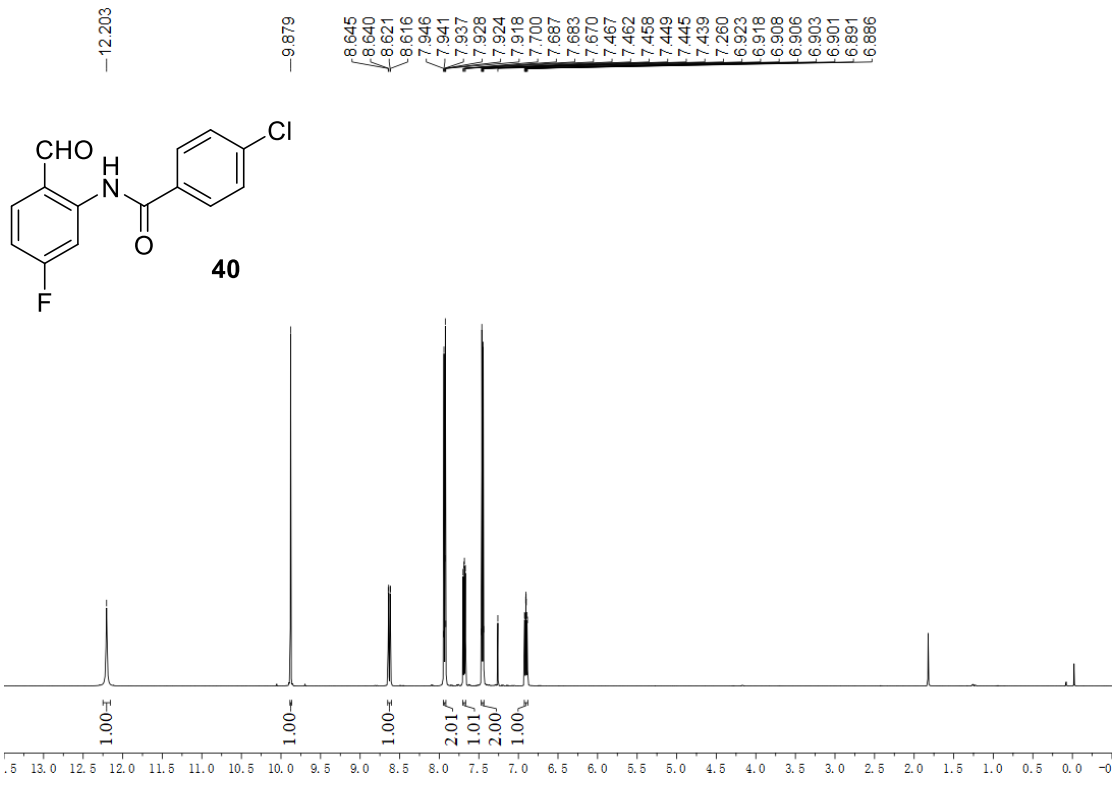
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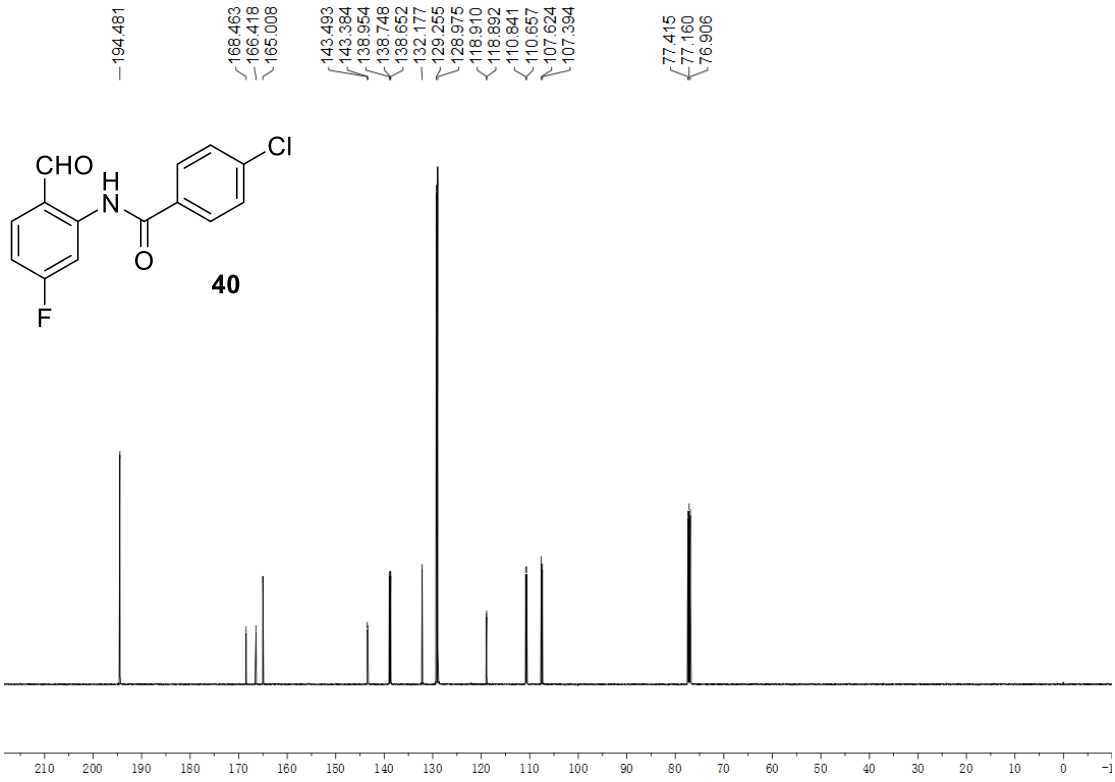
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107.624
107.394
77.415
77.160
76.906
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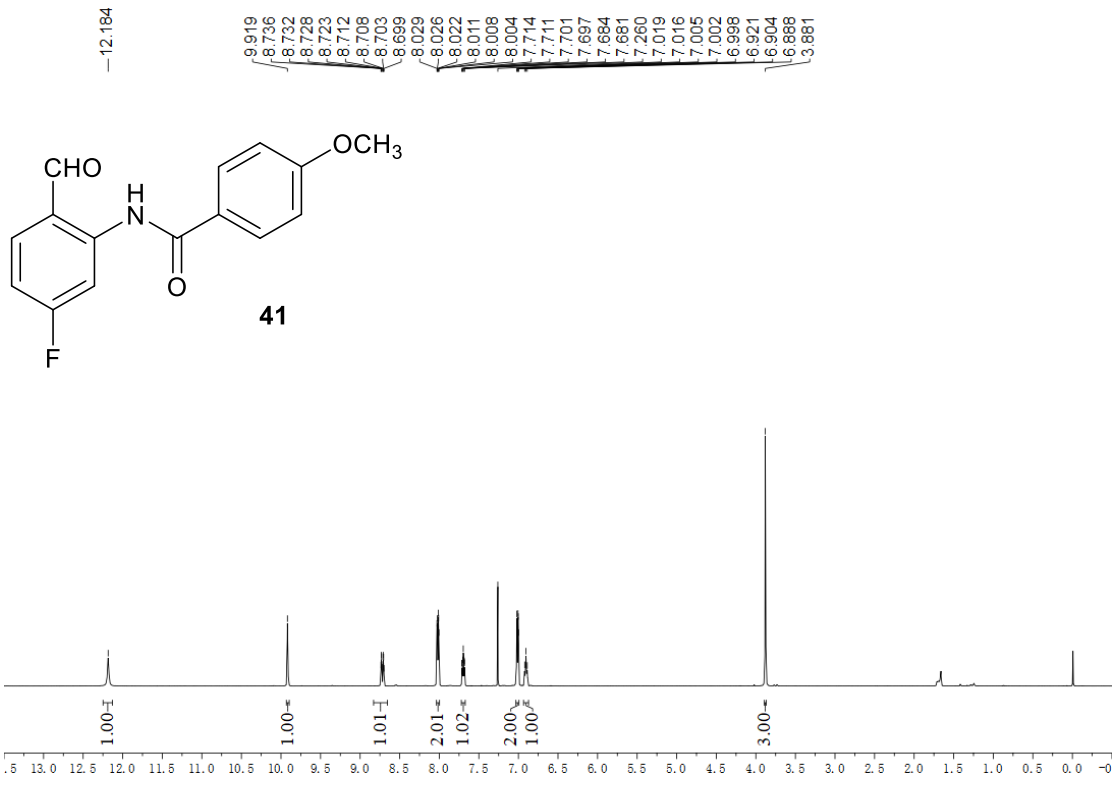
O
Cl
F
40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8.026
8.022
8.011
8.008
8.004
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7.711
7.701
7.697
7.684
7.681
7.260
7.019
7.016
7.005
7.002
6.998
6.921
6.904
6.888
3.881
CHO
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OCH3
F
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2.01
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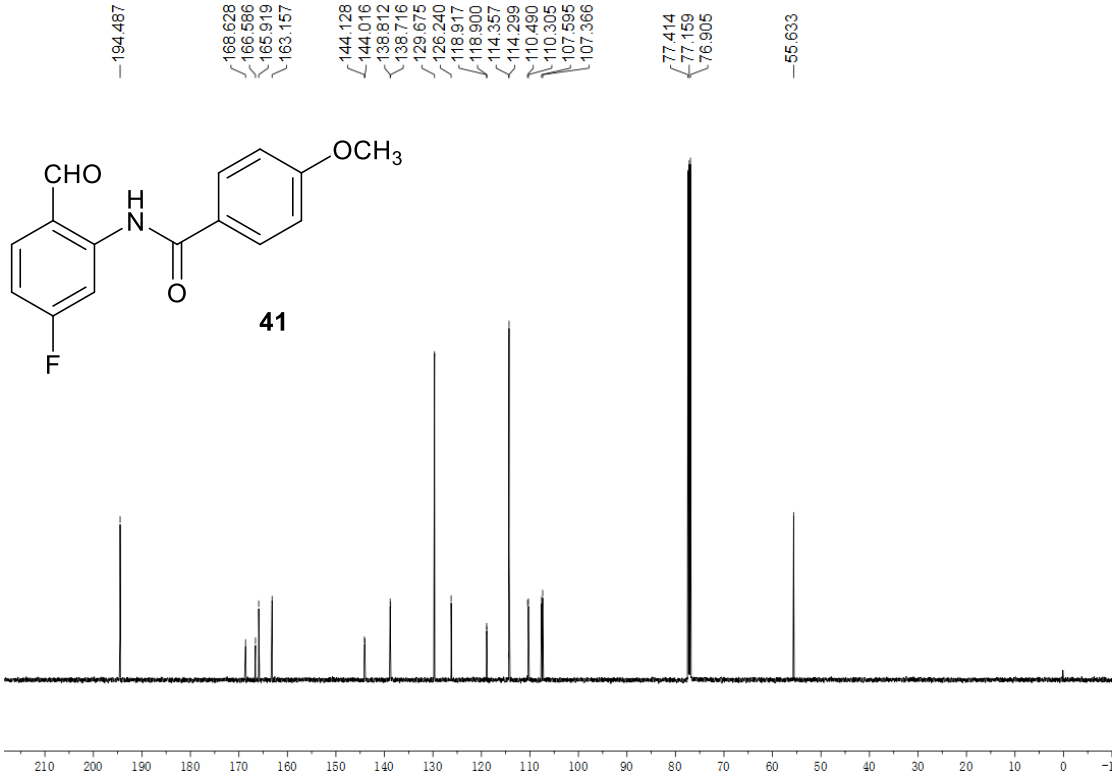
1.00
3.00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138.812
138.716
129.675
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118.900
114.357
114.299
110.490
110.305
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107.366
77.414
77.159
76.905
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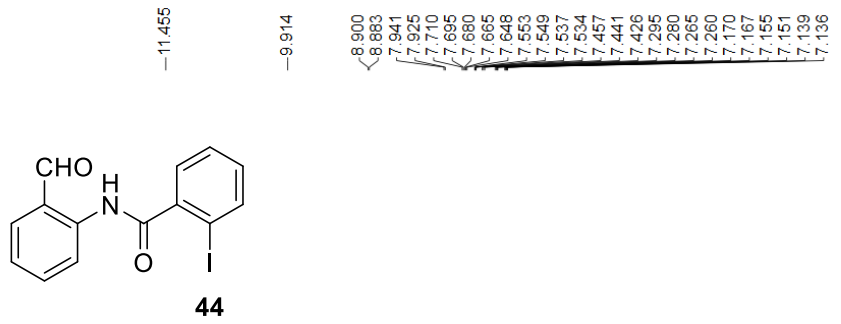
O
OCH3
F
41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8.900
8.883
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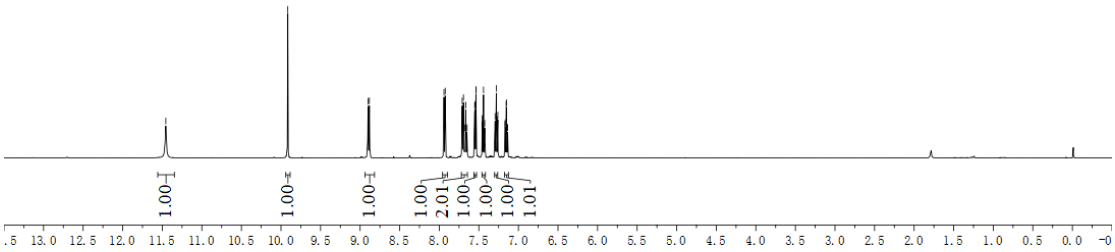
7.925
7.710
7.695
7.680
7.665
7.648
7.553
7.549
7.537
7.534
7.457
7.441
7.426
7.295
7.280
7.265
7.260
7.170
7.167
7.155
7.151
7.139
7.136


CHO
H
N
O
I

**44**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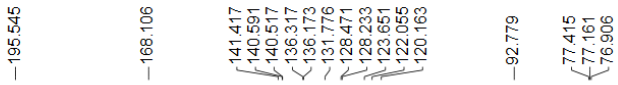
1.00
1.00
1.00
1.01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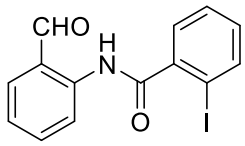
168.106
141.417
140.591
140.517
136.317
136.173
131.776
128.471
128.233
123.651
122.055
120.163
92.779
77.415
77.161
76.906


CHO
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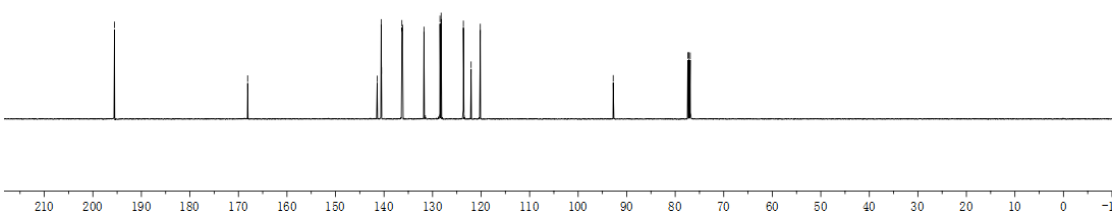
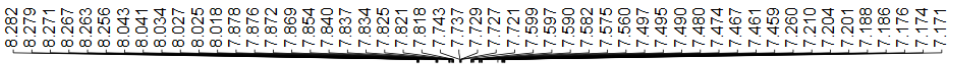
N
O
I

**44**

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8.041
8.034
8.027
8.025
8.018
7.878
7.876
7.872
7.869
7.854
7.840
7.837
7.834
7.825
7.821
7.818
7.743
7.737
7.729
7.727
7.721
7.599
7.597
7.590
7.582
7.575
7.560
7.497
7.495
7.490
7.480
7.474
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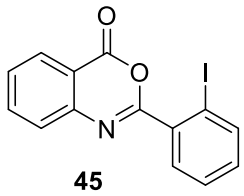
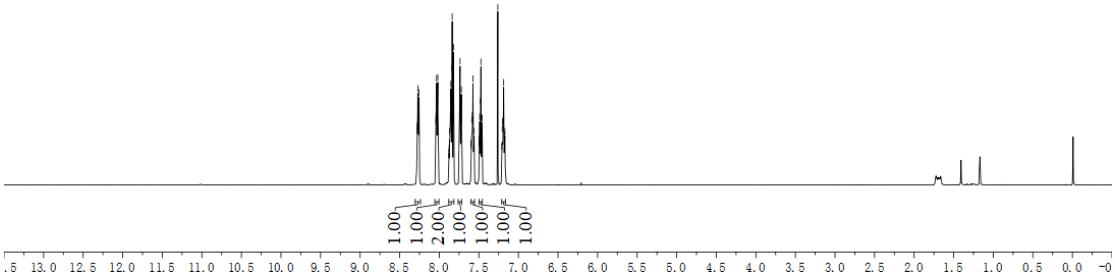
7.186
7.176
7.174
7.171


O
O
I
N

**45**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13.0
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12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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5.0
4.5
4.0
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3.0
2.5
2.0
1.5
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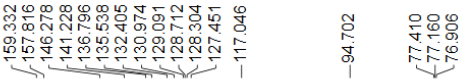
0.0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141.228
136.796
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130.974
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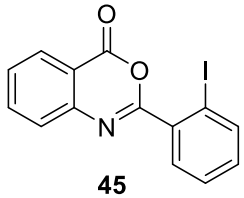
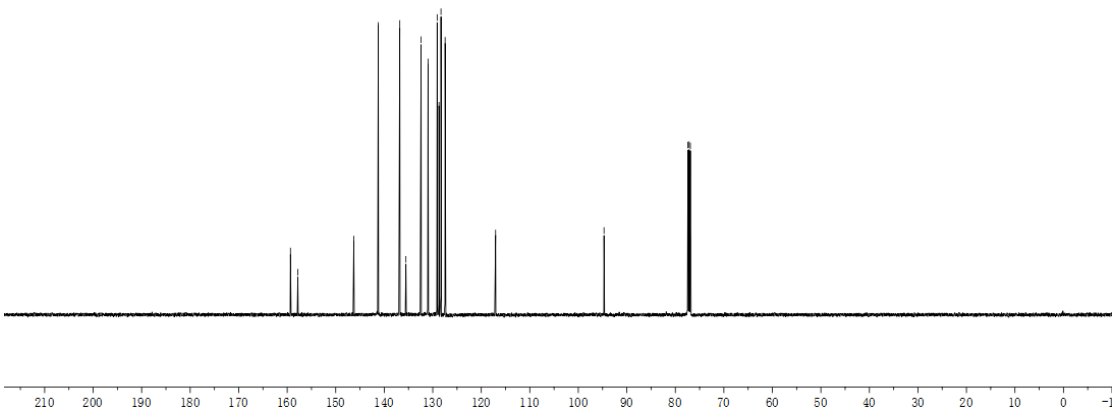
128.712
128.304
127.451
117.046
94.702
77.410
77.160
76.906


O
O
I
N

**45**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80
70
60
50
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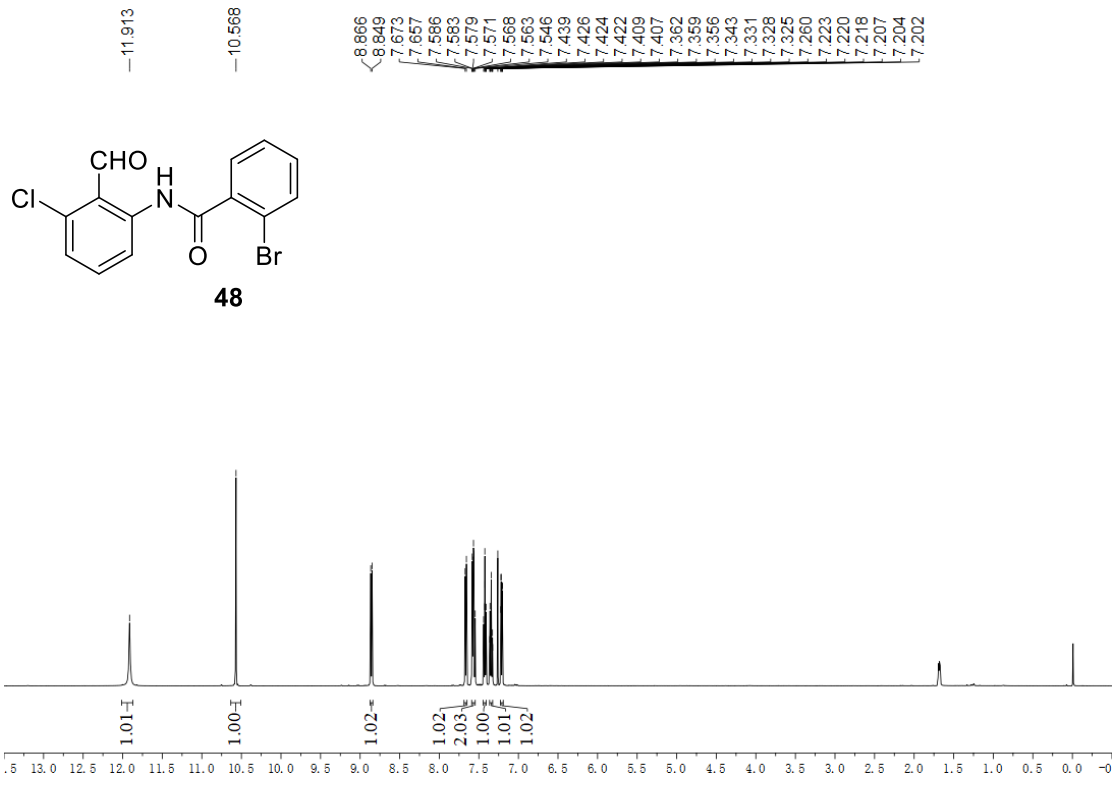
30
20
10
0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7.583
7.579
7.571
7.568
7.563
7.546
7.439
7.426
7.424
7.422
7.409
7.407
7.362
7.359
7.356
7.343
7.331
7.328
7.325
7.260
7.223
7.220
7.218
7.207
7.204
7.202
CHO
H
N
Cl
O
Br
48
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1.00
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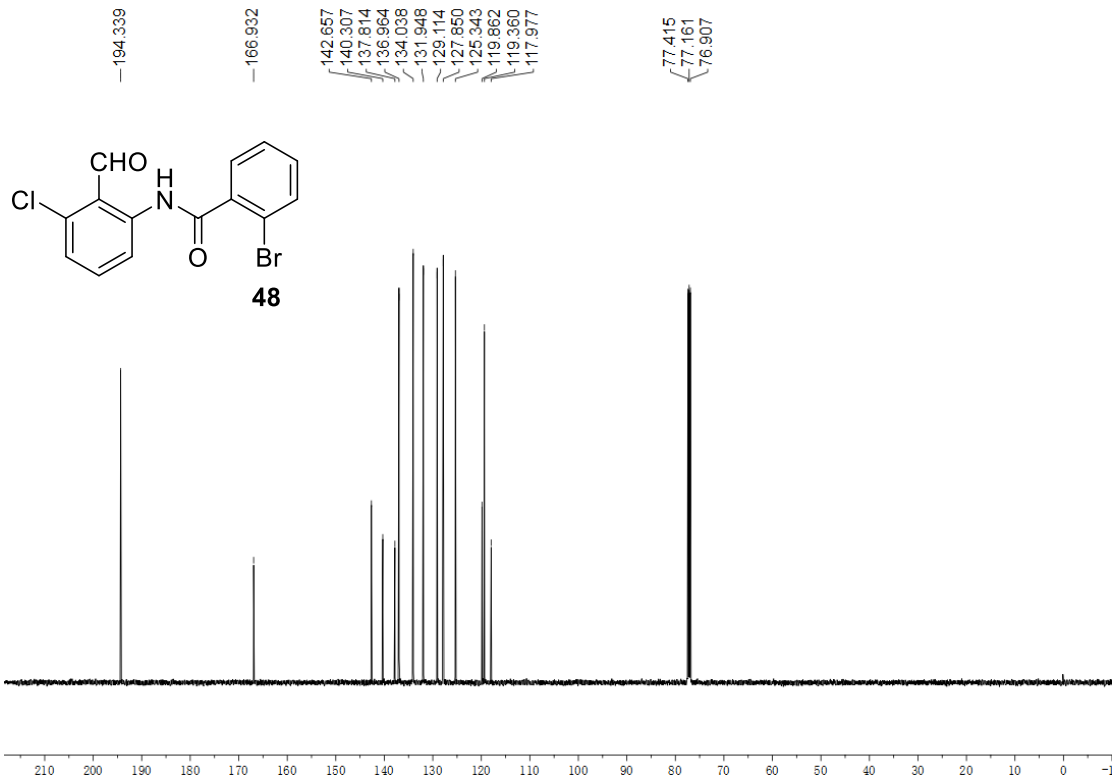
1.02
2.03
1.00
1.01
1.02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131.948
129.114
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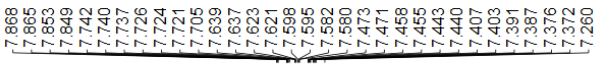
119.360
117.977
77.415
77.161
76.907
CHO
H
N
Cl
O
Br
48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7.639
7.637
7.623
7.621
7.598
7.595
7.582
7.580
7.473
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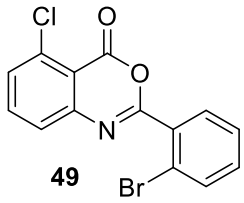
7.372
7.260


Cl
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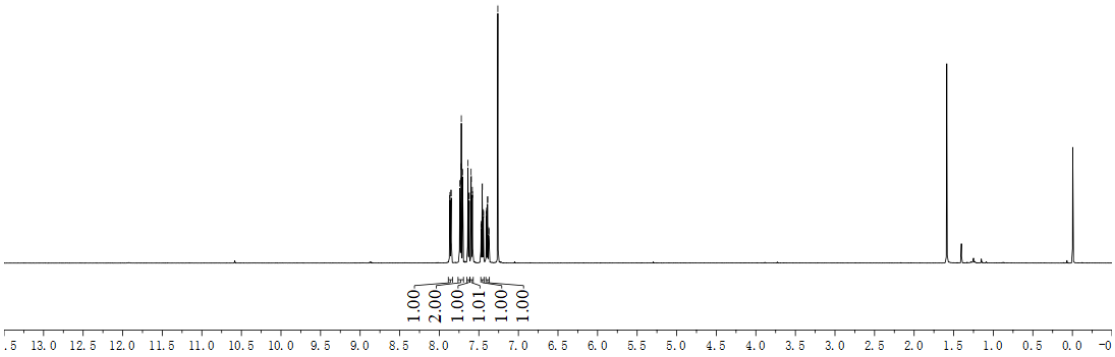
O
N
Br

**49**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12.5
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11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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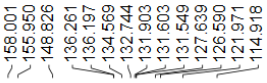
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131.603
131.549
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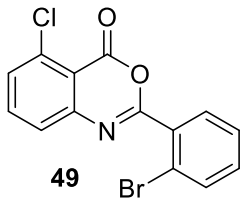
126.590
121.971
114.918


77.415
77.160
76.907


Cl
O
O
N
Br

**49**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200
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110
100
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70
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30
20
10
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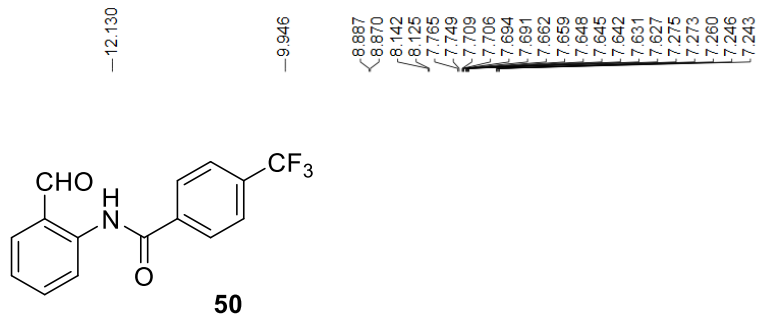
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7.706
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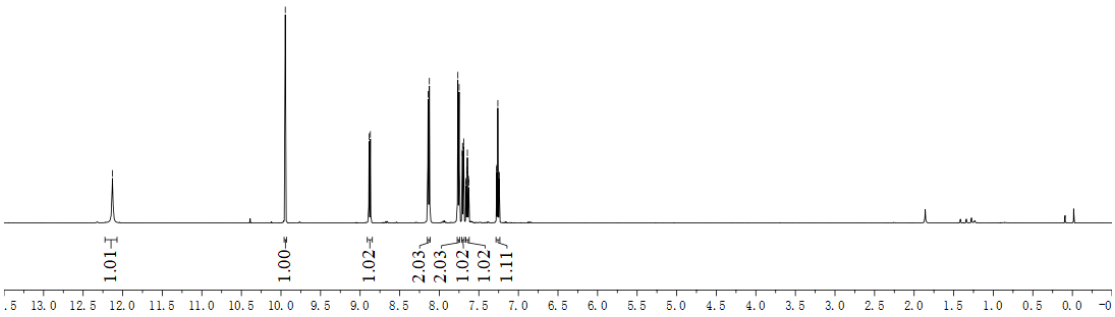
7.659
7.648
7.645
7.642
7.631
7.627
7.275
7.273
7.260
7.246
7.243
CHO
H
N
O
CF3

**50**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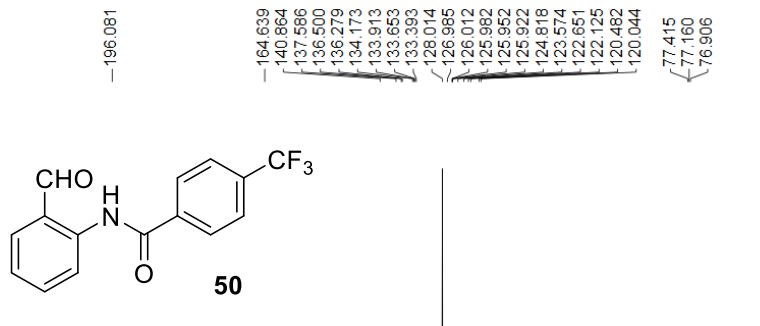
1.02
1.02
1.11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137.586
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134.173
133.913
133.653
133.393
128.014
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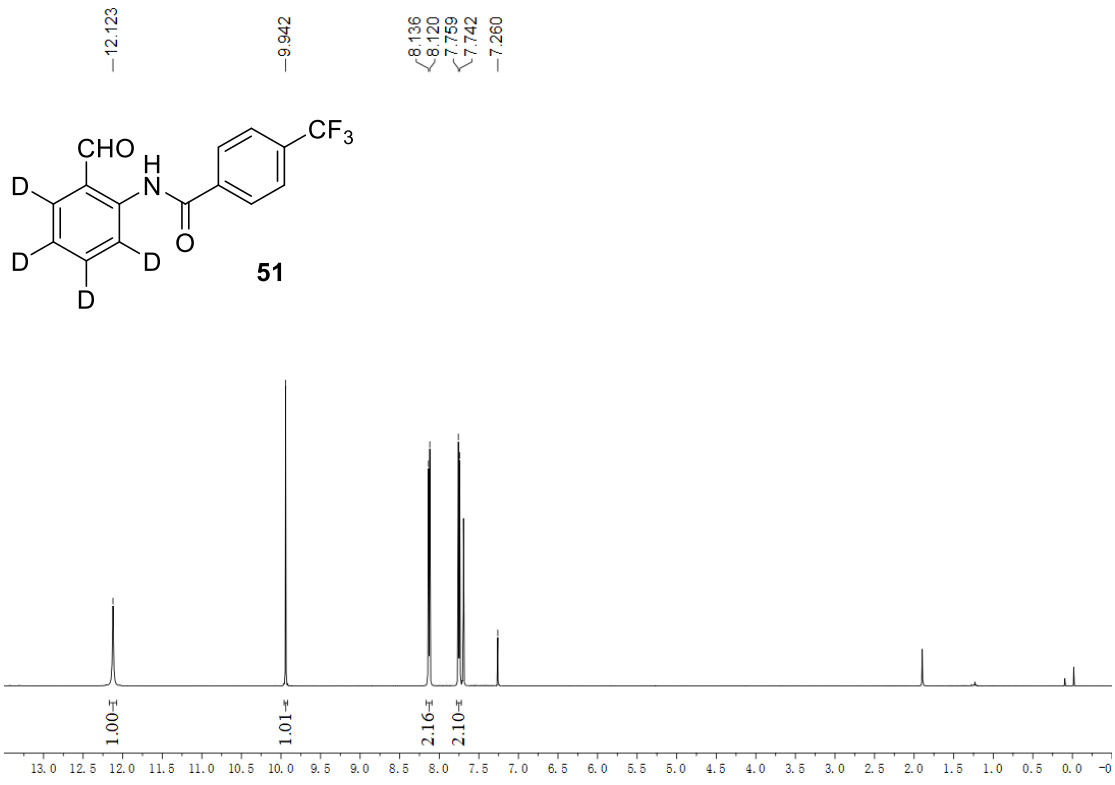
125.982
125.952
125.922
124.818
123.574
122.651
122.125
120.482
120.044
77.415
77.160
76.906
CHO
H
N
O
CF3

**50**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8.120
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D
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D
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D
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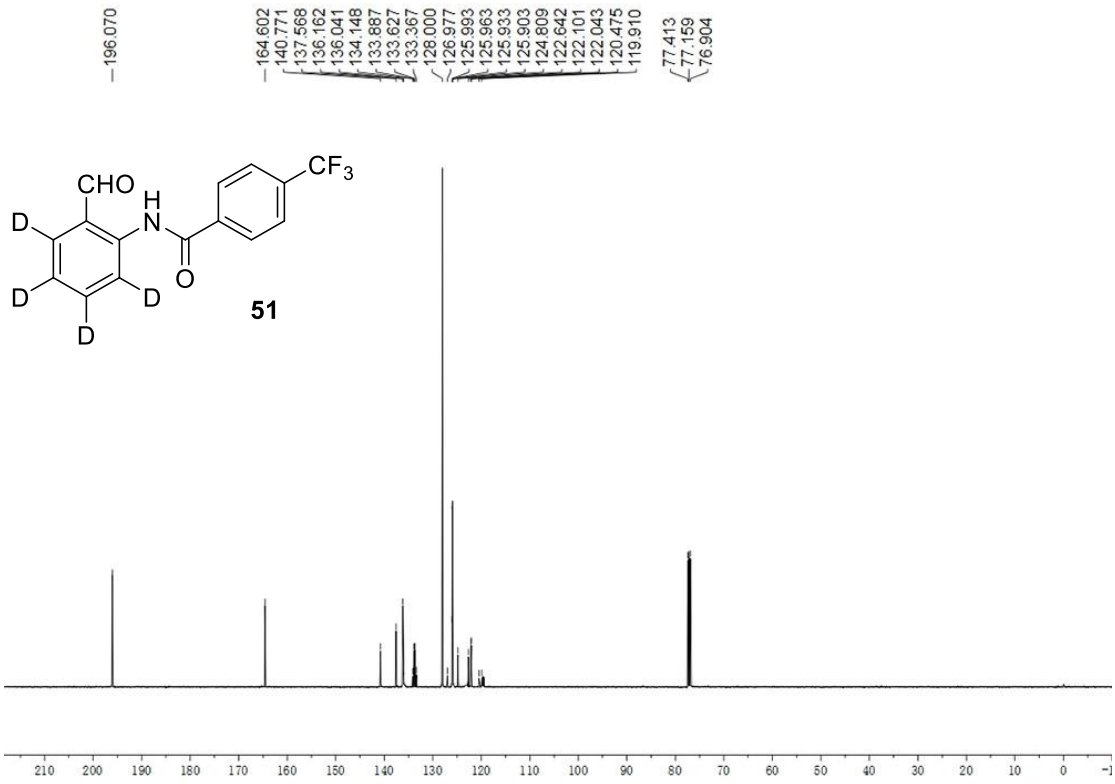
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133.367
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125.993
125.963
125.933
125.903
124.809
122.642
122.101
122.043
120.475
119.910
77.413
77.159
76.904
CHO
H
N
O
D
D
D
D
D
CF3
51