Supporting information

Experimental and Computational Studies on H_2O-Promoted, Rh-Catalyzed Transient-Ligand-Free *Ortho*-C(sp^2)−H Amidation of Benzaldehydes with Dioxazolones

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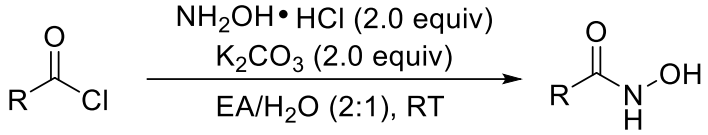
1 General considerations

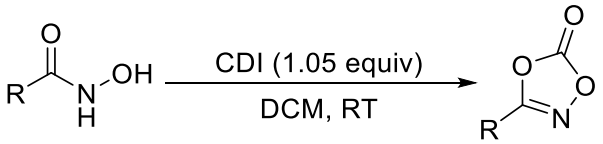
All ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker AVANCE III HD 400 and 500 instruments and calibrated using residual solvent peaks as internal reference. Multiplicities are recorded as: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, m = multiplet, br = broad. High resolution ESI mass experiments were operated on a SolariX-70FT-MS.

All chemicals and materials in the experiments were purchased from commercial suppliers and used as received unless otherwise noted. Flash Column chromatography was performed using 200-300 mesh silica gel, SiO_2. The starting material of product **12**[1], the starting material (**60**) of product **61**[2] and benzaldehyde [D_5]-**1**[3] were prepared according to reported methods.

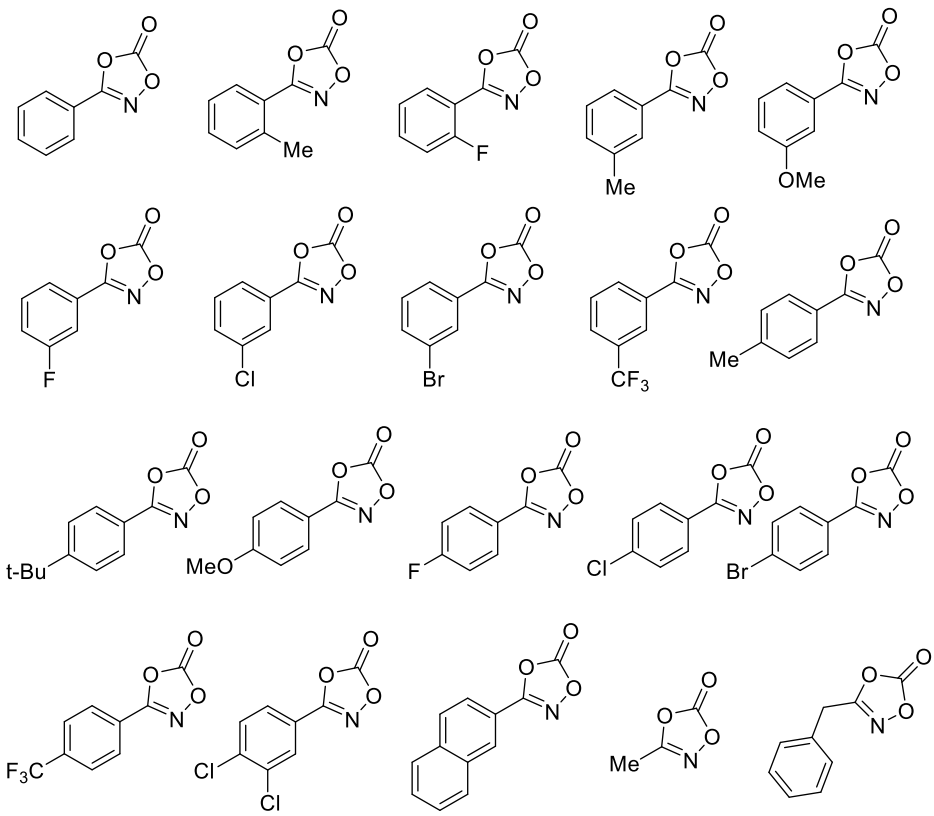
2 General procedure for the preparation of dioxazolones



Following a modified procedure[4], hydroxylamine hydrochloride (20.0 mmol), ethyl acetate (60 mL), H_2O (40 mL) and K_2CO_3 (20.0 mmol) were added to a 250 mL flask at 0 ^{o}C. Then acyl chloride (10.0 mmol) 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.

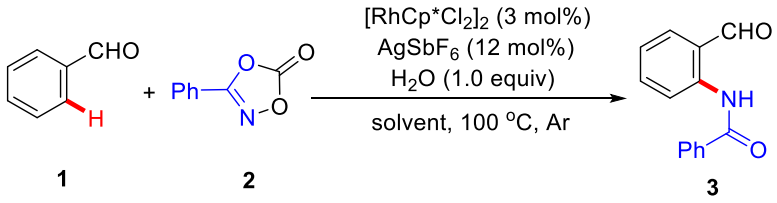


Following a modified procedure[5], to a stirred solution of hydoxamic acid (8 mmol) in freshly distilled dichloromethane (60 mL) in a 250 mL flask was added 1,1'-carbonyldiimidazole (8.4 mmol) in one portion at room temperature. After stirring for 20-30 min, the reaction mixture was quenched with 1 N 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.



List of prepared dioxazolones

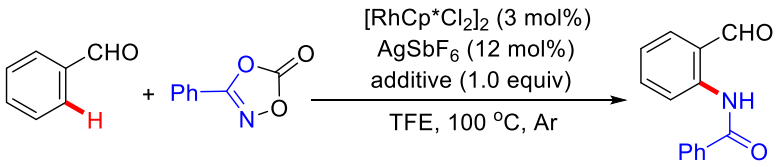
3 Optimization of the Rh-catalyzed *ortho*-amidation of benzaldehydes



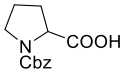
1 **2** **3**

entry	solvent	Yield (%)
1	TFE	81
2	HFIP	65
3	DCE	68
4	DCM	14
5	THF	51
6	1,4-dioxane	trace
7	MeCN	trace
8	MeOH	NR
9	Toluene	NR

Reaction conditions: benzaldehyde **1** (0.2 mmol), dioxazolone **2** (0.4 mmol), $[RhCp^*Cl_2]_2$ (3 mol%), $AgSbF_6$ (12 mol%), and H_2O (1.0 equiv) in solvent (1 mL) at 100 °C under Ar for 12 h. Isolated yields are given.



1 2 3

entry	additive	Yield (%)
1	AcOH	trace
2	PivOH	trace
3	MesCOOH	18
4	1-AdCOOH	58
5	PhCOOH	73
6	$(BnO)_2POOH$	NR
7		48
8	H_2O	81

Reaction conditions: benzaldehyde **1** (0.2 mmol), dioxazolone **2** (0.4 mmol), $[RhCp^*Cl_2]_2$ (3 mol%), $AgSbF_6$ (12 mol%), and additive (1.0 equiv) in TFE (1 mL) at 100 °C under Ar for 12 h. Isolated yields are given.

4 General procedure for the Rh-catalyzed *ortho*-amidation reactions

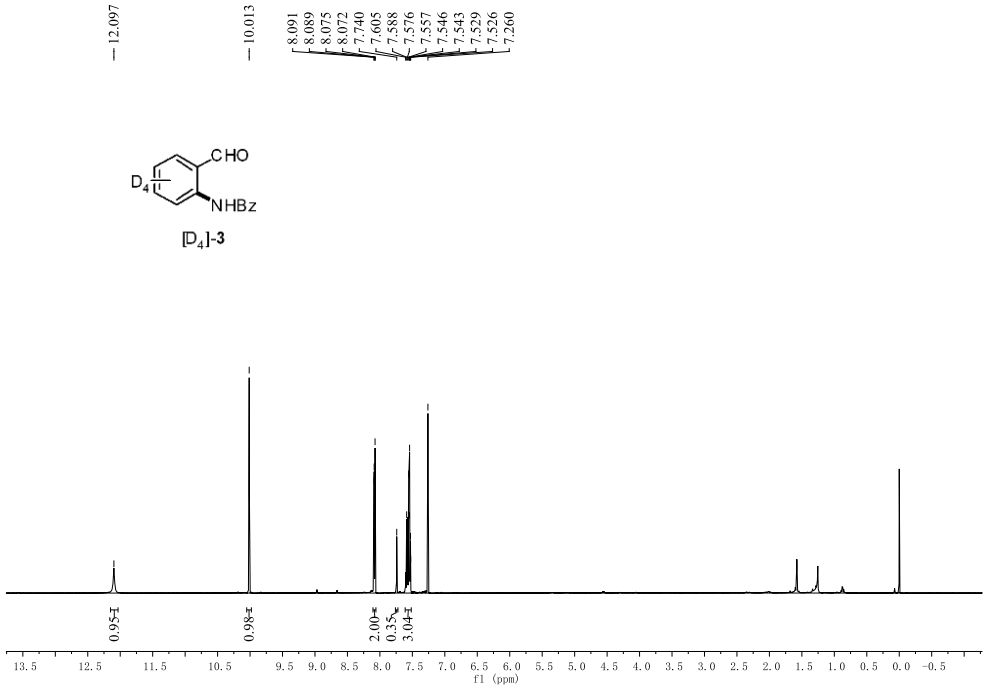
A mixture of benzaldehyde substrate (0.2 mmol, 1.0 equiv), dioxazolones (0.4 mmol, 2.0 equiv), $[RhCp^*Cl_2]_2$ (0.006 mmol, 3 mol%), $AgSbF_6$ (0.024 mmol, 12 mol%) and H_2O (0.4 mmol, 2.0 equiv) in 1 mL TFE in a 10 mL glass vial was purged with Ar and sealed with PTFE cap. After heated at 100 °C for 12 h and cooled to room temperature, the reaction mixture was diluted with EA, filtered through a pad of Celite and concentrated *in vacuo*. The resulting residue was purified by flash column chromatography to give the desired amidated product.

5 Preliminary mechanistic experiments

a) Parellel kinetic isotope effect

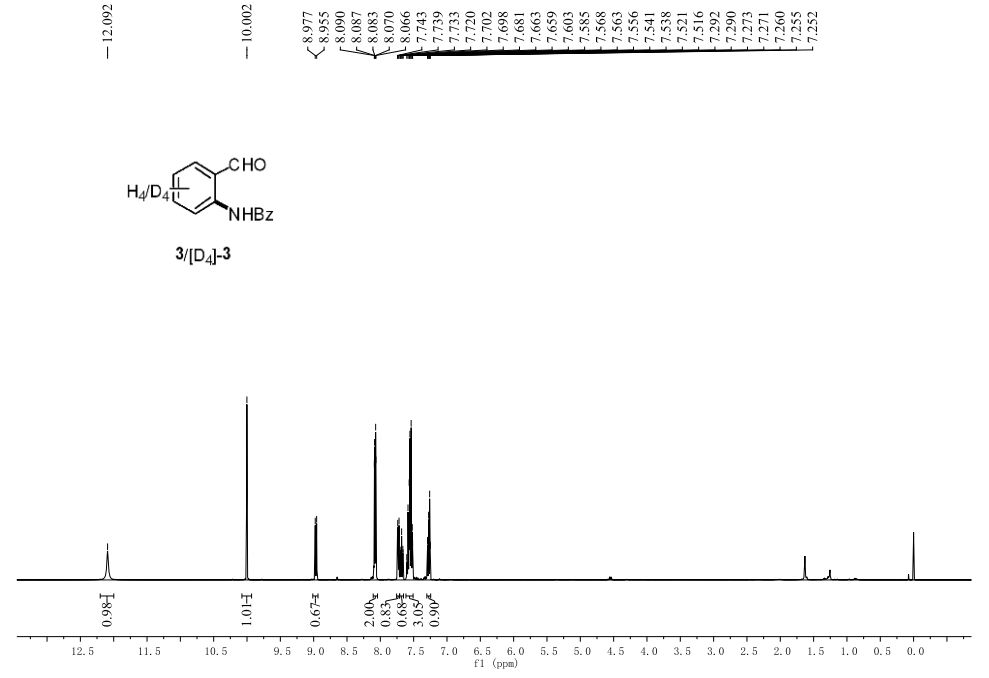
One mixture of benzaldehyde **1** (0.2 mmol, 1.0 equiv), dioxazolones **2** (0.4 mmol, 2.0 equiv), $[RhCp^*Cl_2]_2$ (0.006 mmol, 3 mol%), $AgSbF_6$ (0.024 mmol, 12 mol%) and H_2O (0.4 mmol, 2.0 equiv) in 1 mL TFE in a 10 mL glass vial was purged with Ar and sealed with PTFE cap. The other mixture of benzaldehyde $[D_5]$-**1** (0.2 mmol, 1.0 equiv), dioxazolones **2** (0.4 mmol, 2.0 equiv), $[RhCp^*Cl_2]_2$ (0.006 mmol, 3 mol%), $AgSbF_6$ (0.024 mmol, 12 mol%) and H_2O (0.4 mmol, 2.0 equiv) in 1 mL TFE in a 10 mL glass vial was also purged with Ar and sealed with PTFE cap. After heated at 100 °C for 6 h and cooled to room temperature, the reaction mixtures were diluted with EA, filtered through a pad of Celite and concentrated *in vacuo*. The resulting residues were purified by flash column chromatography to give the amidated product **3** as a white solid (18 mg, 40% yield) and the amidated product $[D_4]$-**3** as a white solid (7.0 mg, 16% yield) respectively. By the yield of the product, KIE=40%/16%=2.5, and the

35% D/H exchange in the product [D_4]-**3** can be observed in the ^{1}H NMR of [D_4]-**3**.

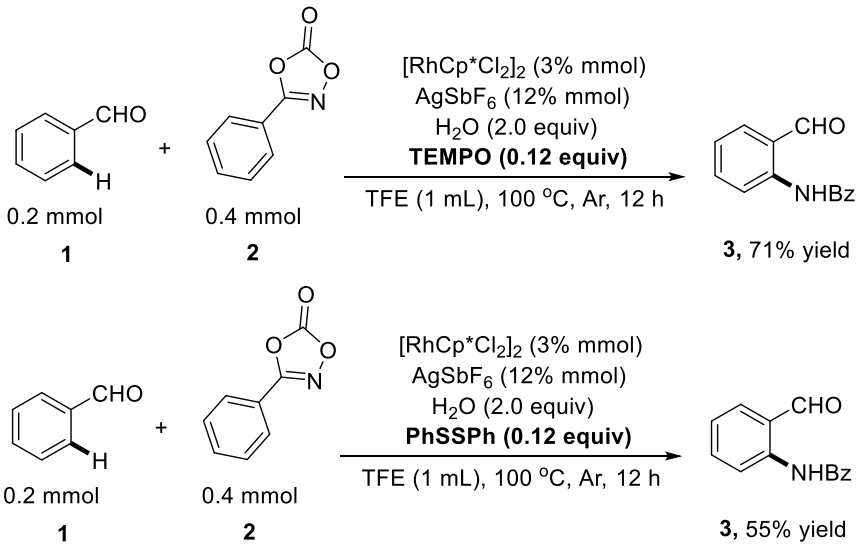


b) Intermoleculr kinetic isotope effect

A mixture of benzaldehyde **1** (0.2 mmol, 1.0 equiv), benzaldehyde [D_5]-**1** (0.2 mmol, 1.0 equiv), dioxazolones **2** (0.8 mmol, 2.0 equiv), [$RhCp^*Cl_2$]$_2$ (0.012 mmol, 3 mol%), $AgSbF_6$ (0.048 mmol, 12 mol%) and H_2O (0.8 mmol, 2.0 equiv) in 2 mL TFE in a 10 mL glass vial was purged with Ar and sealed with PTFE cap. After heated at 100 ^{o}C for 6 h and cooled to room temperature, the reaction mixture was diluted with EA, filtered through a pad of Celite and concentrated *in vacuo*. The resulting residue was purified by flash column chromatography to give the amidated product **3**/[D_4]-**3** as a white solid (23 mg). By the analysis of the ^{1}H NMR of **3**/ [D_4]-**3**, KIE=0.68/0.32=2.2.



c) **Radical capture experiment**



6 Synthetic utilities of the C−H amidation method

a) Gram-scale reaction

A mixture of benzaldehyde **1** (1.06 g, 10 mmol, 1.0 equiv), dioxazolones **2** (15 mmol, 1.5 equiv), $[RhCp^*Cl_2]_2$ (0.2 mmol, 2 mol%), $AgSbF_6$ (0.8 mmol, 8 mol%) and H_2O (20 mmol, 2.0 equiv) in 35 mL TFE in a 75 mL sealed tube was purged with Ar and sealed with PTFE cap. After heated at 100 °C for 16 h and cooled to room temperature, the reaction mixture was diluted with EA, filtered through a pad of Celite and concentrated *in vacuo*. The resulting residue was purified by flash column chromatography to give the amidated product **3** as a white solid (1.46 g, 66% yield).

b) Late-stage C(sp^2)−H amidation of complex molecule

A mixture of **60** (57 mg, 0.2 mmol, 1.0 equiv), dioxazolones **2** (0.4 mmol, 2.0 equiv), $[RhCp^*Cl_2]_2$ (0.008 mmol, 4 mol%), $AgSbF_6$ (0.032 mmol, 16 mol%) and H_2O (0.4 mmol, 2.0 equiv) in 1 mL TFE in a 10 mL glass vial was purged with Ar and sealed with PTFE cap. After heated at 100 °C for 12 h and cooled to room temperature, the reaction mixture was diluted with EA, filtered through a pad of Celite and concentrated *in vacuo*. The resulting residue was purified by flash column chromatography to give the amidated product **61** as a white solid (41 mg, 51% yield).

c) Direct synthesis of substituted quinoline[6]

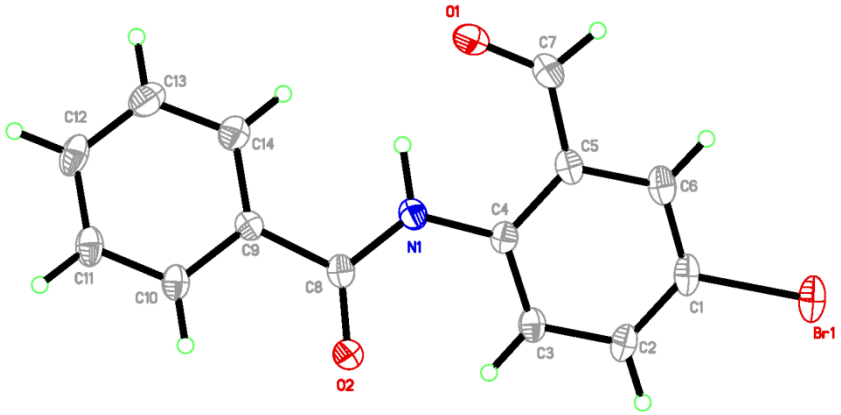
A mixture of the amidated product **3** (113 mg, 0.5 mmol, 1.0 equiv), α-Me-γ-Me-allenoate (87.6 mg, 0.625 mmol, 1.25 equiv) and K_2CO_3 (69.1 mg , 0.5 mmol, 1.0 equiv) in 2.5 mL DMSO in a 10 mL glass vial reacted in a preheated oil bath at 100 °C for 15 min. After cooled to room temperature, the reaction was quenched by 25 mL sat. aq. NH_4Cl, and the aqueous phase was extracted with Et_2O three times. The combined organic layers were washed with water and brine, dried over anhydrous Na_2SO_4 and evaporated under the reduced pressure. The resulting residue was purified by flash column chromatography to give **62** as a colorless oil (169 mg, 97% yield).

d) Diversification of aldehyde group[7]

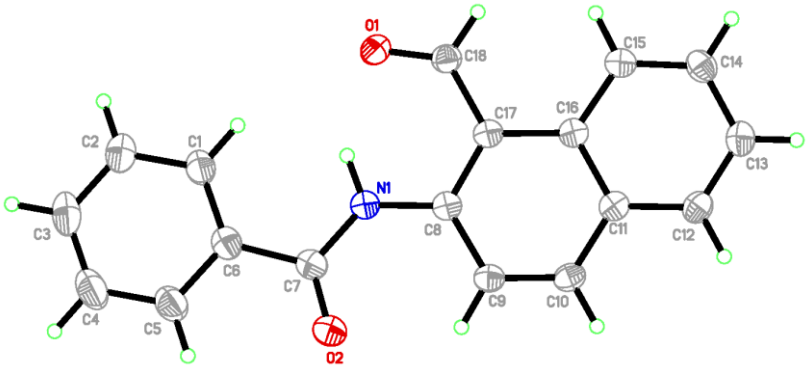
A mixture of the amidated product **3** (45 mg, 0.2 mmol, 1.0 equiv), morpholine (35 uL, 0.4 mmol, 2.0 equiv), $NaBH(OAc)_3$ (170 mg, 0.8 mmol, 4.0 equiv) and AcOH (1 drop) in 2.0 mL DCE in a 10 mL glass vial was stirred at room temperature for 6 h. Then the reaction mixture was diluted with 15 mL DCM, washed with 15 mL sat. aq. $NaHCO_3$ and dried over anhydrous Na_2SO_4. The solvent was evaporated under the reduced pressure and the resulting residue was purified by flash column chromatography to give **63** as a white solid (46 mg, 78% yield).

A mixture of the amidated product **3** (45 mg, 0.2 mmol, 1.0 equiv), Ylide (100 mg, 0.3 mmol, 1.5 equiv), 4Å molecular sieve (40 mg) in 1.0 mL DCE in a 10 mL glass vial was purged with Ar and sealed with PTFE cap. After stirred at room temperature for 4 h, the reaction mixture was diluted with DCM, filtered through a pad of Celite and concentrated *in vacuo*. The resulting residue was purified by flash column chromatography to give **64** as a white solid (53 mg, 94% yield).

7 X-ray single crystal structures of product 16 and 40

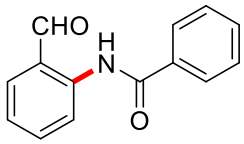


X-Ray of **16** (CCDC 1819612)



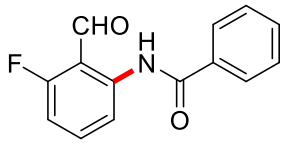
X-Ray of **40** (CCDC 1819622)

8 Characterization data for the products



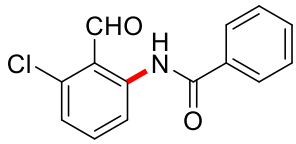
3

***N*-(2-Formylphenyl)benzamide:** white solid; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 12.09 (s, 1H), 10.00 (s, 1H), 8.96 (d, J = 8.5 Hz, 1H), 8.09 – 8.07 (m, 2H), 7.73 (d, J = 8.0 Hz, 1H), 7.68 (t, J = 7.8 Hz, 1H), 7.60 – 7.52 (m, 3H), 7.29 – 7.25 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 196.0, 166.3, 141.4, 136.5, 136.3, 134.5, 132.3, 129.0 (2C), 127.6 (2C), 123.2, 122.1, 120.1. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{12}NO_2$ [M+H] 226.0868, found 226.0870.



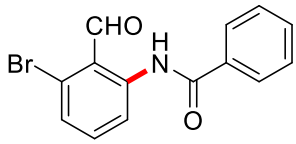
4

***N*-(3-Fluoro-2-formylphenyl)benzamide**: white solid, 39 mg, 79% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 12.27 (s, 1H), 10.44 (s, 1H), 8.74 (d, J = 8.5 Hz, 1H), 8.06 – 8.04 (m, 2H), 7.65 – 7.51 (m, 4H), 6.88 – 6.84 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 191.2 (d, J = 13.0 Hz), 166.3, 166.2 (d, J = 256.8 Hz), 142.6 (d, J = 2.4 Hz), 138.4 (d, J = 11.3 Hz), 134.1, 132.5, 129.0 (2C), 127.7 (2C), 115.9 (d, J = 3.8 Hz), 111.1 (d, J = 8.3 Hz), 109.7 (d, J = 20.6 Hz). **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}FNO_2$ [M+H] 244.0774, found 244.0775.



5

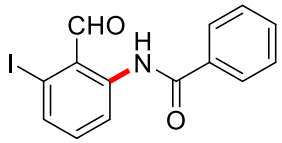
***N*-(3-Chloro-2-formylphenyl)benzamide**: white solid, 46 mg, 88% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 12.47 (s, 1H), 10.63 (s, 1H), 8.90 (d, J = 8.5 Hz, 1H), 8.06 – 8.04 (m, 2H), 7.60 – 7.51 (m, 4H), 7.17 (d, J = 8.5 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 194.8, 166.3, 143.5, 140.3, 137.0, 134.2, 132.5, 129.0 (2C), 127.7 (2C), 124.8, 119.2, 117.9. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}ClNO_2$ [M+H] 260.0478, found 260.0486.



6

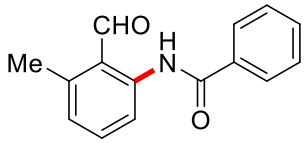
***N*-(3-Bromo-2-formylphenyl)benzamide**: white solid, 54 mg, 89% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 12.47 (s, 1H), 10.52 (s, 1H), 8.95 (d, J = 8.5 Hz, 1H), 8.06 – 8.03 (m, 2H), 7.60 – 7.50 (m, 3H), 7.44 (t, J = 8.5 Hz, 1H) , 7.39 – 7.36 (m, 1H). **^{13}C**

NMR (125 MHz, $CDCl_3$) δ: 197.3, 166.2, 143.6, 137.1, 134.3, 132.5, 130.0, 129.0 (2C), 128.3, 127.7 (2C), 120.0, 118.6. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}BrNO_2$ [M+H] 303.9973, found 303.9981.



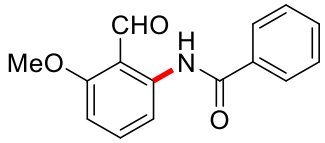
7

***N*-(2-Formyl-3-iodophenyl)benzamide**: white solid, 57 mg, 81% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 12.51 (s, 1H), 10.27 (s, 1H), 9.01 (d, J = 8.5 Hz, 1H), 8.08 – 8.05 (m, 2H), 7.76 – 7.74 (m, 1H), 7.61 – 7.53 (m, 3H), 7.26 (t, J = 8.5 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 202.2, 166.1, 143.1, 137.2, 135.7, 134.4, 132.5, 129.1 (2C), 127.7 (2C), 121.1, 119.5, 105.0. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}INO_2$ [M+H] 351.9835, found 351.9835.



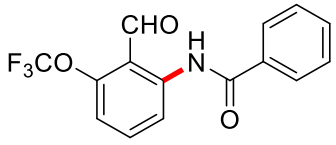
8

***N*-(2-Formyl-3-methylphenyl)benzamide**: white solid, 35 mg, 72% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.57 (s, 1H), 10.53 (s, 1H), 8.83 (d, J = 8.4 Hz, 1H), 8.10 – 8.07 (m, 2H), 7.60 – 7.51 (m, 4H), 6.97 (d, J = 7.6 Hz, 1H), 2.71(s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 194.9, 166.4, 143.5, 142.2, 136.8, 134.8, 132.2, 129.0 (2C), 127.7 (2C), 126.1, 120.0, 118.7, 19.4. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{14}NO_2$ [M+H] 240.1024, found 240.1023.



9

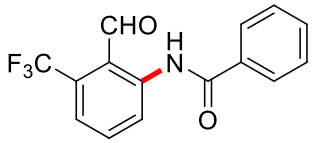
***N*-(2-Formyl-3-methoxyphenyl)benzamide:** white solid, 35 mg, 68% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.64 (s, 1H), 10.58 (s, 1H), 8.52 (d, J = 8.8 Hz, 1H), 8.10 – 8.07 (m, 2H), 7.60 – 7.50 (m, 4H), 6.68 (d, J = 7.6 Hz, 1H), 3.93 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 193.9, 166.5, 163.5, 142.8, 138.3, 134.7, 132.2, 129.0 (2C), 127.7 (2C), 112.3, 111.3, 105.4, 56.1. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{14}NO_3$ [M+H] 256.0973, found 256.0977.



10

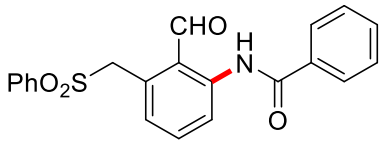
***N*-(2-Formyl-3-(trifluoromethoxy)phenyl)benzamide**: white solid, 36 mg, 58% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 12.42 (s, 1H), 10.48 (s, 1H), 8.94 (d, J = 9.0 Hz, 1H), 8.08 – 8.05 (m, 2H), 7.69 (t, J = 8.5 Hz, 1H), 7.62 – 7.52 (m, 3H) , 7.08 – 7.05

(m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 192.3, 166.5, 152.5, 143.2, 137.6, 134.2, 132.6, 129.1 (2C), 127.7 (2C), 120.5 (q, J = 258.4 Hz), 118.8, 114.5, 114.2. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{11}F_3NO_3$ [M+H] 310.0691, found 310.0692.



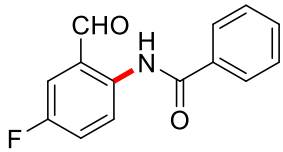
11

***N*-(2-Formyl-3-(trifluoromethyl)phenyl)benzamide:** white solid, 36 mg, 61% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 12.59 (s, 1H), 10.45 (s, 1H), 9.25 (d, J = 8.5 Hz, 1H), 8.08 – 8.06 (m, 2H), 7.74 (t, J = 8.0 Hz, 1H), 7.61 – 7.53 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 193.7 (q, J = 3.8 Hz), 166.5, 143.4, 135.5, 134.1, 133.1 (q, J = 31.3 Hz), 132.7, 129.1 (2C), 127.7 (2C), 124.7, 123.7 (q, J = 273.3 Hz), 120.7 (q, J = 6.3 Hz), 118.0. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{11}F_3NO_2$ [M+H] 294.0742, found 294.0740.



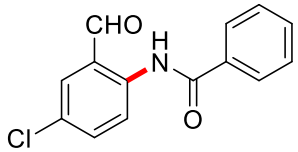
12

***N*-(2-Formyl-3-((phenylsulfonyl)methyl)phenyl)benzamide**: pale yellow solid, 42 mg, 55% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.57 (s, 1H), 10.38 (s, 1H), 9.02 (d, J = 8.4 Hz, 1H), 8.09 – 8.06 (m, 2H), 7.70 – 7.65 (m, 3H), 7.60 – 7.45 (m, 6H), 6.65 (d, J = 7.6 Hz, 1H), 4.73 (s, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 193.2, 166.5, 143.0, 137.5, 135.9, 134.6, 134.5, 132.8, 132.5, 129.5 (2C), 129.1 (2C), 128.8 (2C), 128.0, 127.7 (2C), 121.8, 120.2, 59.0. **HRMS**(ESI) *m/z* calculated for $C_{21}H_{18}NO_4S$ [M+H] 380.0957, found 380.0954.



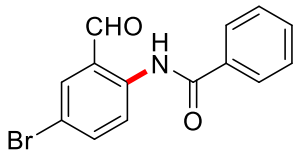
14

***N*-(4-Fluoro-2-formylphenyl)benzamide**: white solid, 33 mg, 68% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 11.92 (s, 1H), 9.94 (s, 1H), 8.99 (dd, J_1= 9.2 Hz, J_2 = 4.8 Hz, 1H), 8.06 – 8.03 (m, 2H), 7.61 – 7.51 (m, 3H), 7.43 – 7.37 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 194.7 (d, J = 1.9 Hz), 166.1, 157.9 (d, J = 243.8 Hz), 137.8 (d, J = 2.5 Hz), 134.2, 132.4, 129.0 (2C), 127.6 (2C), 123.6 (d, J = 21.7 Hz), 122.9 (d, J = 5.3 Hz), 122.2 (d, J = 6.7 Hz), 121.3 (d, J = 22.3 Hz). **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}FNO_2$ [M+H] 244.0774, found 244.0775.



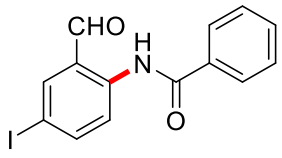
15

***N*-(4-Chloro-2-formylphenyl)benzamide**: white solid, 32 mg, 61% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 11.99 (s, 1H), 9.95 (s, 1H), 8.96 (d, J = 8.8 Hz, 1H), 8.07 – 8.04 (m, 2H), 7.70 (d, J = 2.4 Hz, 1H), 7.62 (dd, J_1= 8.8 Hz, J_2 = 2.4 Hz, 1H), 7.61 – 7.52 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 194.8, 166.2, 139.9, 136.3, 135.3, 134.1, 132.6, 129.1 (2C), 128.2, 127.6 (2C), 123.1, 121.8. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}ClNO_2$ [M+H] 260.0478, found 260.0481.



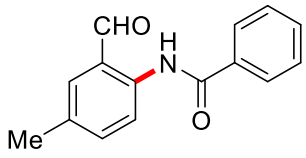
16

***N*-(4-Bromo-2-formylphenyl)benzamide**: white solid, 38 mg, 62% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 11.98 (s, 1H), 9.93 (s, 1H), 8.90 (d, J = 9.2 Hz, 1H), 8.06 – 8.03 (m, 2H), 7.83 (d, J = 2.4 Hz, 1H), 7.76 (dd, J_1= 9.2 Hz, J_2 = 2.4 Hz, 1H), 7.62 – 7.52 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 194.8, 166.2, 140.3, 139.2, 138.3, 134.1, 132.6, 129.1 (2C), 127.6 (2C), 123.4, 122.0, 115.3. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}BrNO_2$ [M+H] 303.9973, found 303.9969.



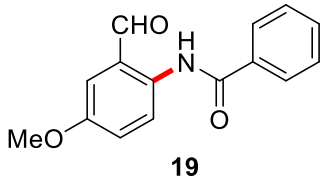
17

***N*-(2-Formyl-4-iodophenyl)benzamide**: white solid, 49 mg, 70% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 11.98 (s, 1H), 9.91 (s, 1H), 8.76 (d, J = 8.8 Hz, 1H), 8.06 – 8.03 (m, 2H), 8.00 (d, J = 2.0 Hz, 1H), 7.93 (dd, J_1= 8.8 Hz, J_2 = 2.0 Hz, 1H), 7.61 – 7.52 (m, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 194.7, 166.2, 144.9, 144.4, 140.9, 134.1, 132.6, 129.1 (2C), 127.6 (2C), 123.8, 122.2, 85.0. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}INO_2$ [M+H] 351.9835, found 351.9834.



18

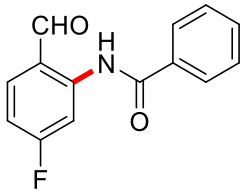
***N*-(2-Formyl-4-methylphenyl)benzamide**: white solid, 34 mg, 71% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 11.99 (s, 1H), 9.95 (s, 1H), 8.85 (d, J = 8.4 Hz, 1H), 8.08 – 8.05 (m, 2H), 7.57 – 7.47 (m, 5H) , 2.41 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 196.1, 166.1, 139.0, 137.3, 136.5, 134.6, 132.9, 132.2, 129.0 (2C), 127.6 (2C), 122.1, 120.1, 20.7. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{14}NO_2$ [M+H] 240.1024, found 240.1024.



19

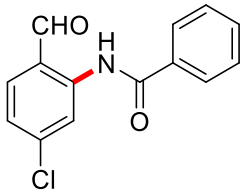
***N*-(2-Formyl-4-methoxyphenyl)benzamide**: white solid, 28 mg, 55% yield; **^{1}H**

NMR (400 MHz, $CDCl_3$) δ: 11.84 (s, 1H), 9.96 (s, 1H), 8.91 (d, J = 8.8 Hz, 1H), 8.07 – 8.04 (m, 2H), 7.57 – 7.50 (m, 3H), 7.26 – 7.21 (m, 2H), 3.88 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 195.7, 166.0, 155.3, 135.1, 134.6, 132.2, 129.0 (2C), 127.5 (2C), 122.9, 122.5, 121.9, 120.0, 55.9. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{14}NO_3$ [M+H] 256.0973, found 256.0977.



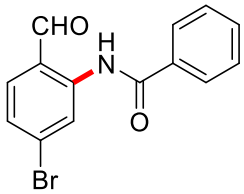
20

***N*-(5-Fluoro-2-formylphenyl)benzamide**: white solid, 40 mg, 81% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 12.27 (s, 1H), 9.92 (s, 1H), 8.74 (dd, J_1= 12.0 Hz, J_2 = 2.5 Hz, 1H), 8.06 – 8.04 (m, 2H), 7.71 (dd, J_1= 8.5 Hz, J_2 = 6.0 Hz, 1H), 7.60 – 7.52 (m, 3H), 6.95 – 6.91 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 194.5, 167.5 (d, J = 255.5 Hz), 166.3, 143.7 (d, J = 13.9 Hz), 138.8 (d, J = 12.0 Hz), 133.9, 132.6, 129.1 (2C), 127.6 (2C), 119.0 (d, J = 6.0 Hz), 110.6 (d, J = 23.0 Hz), 107.6 (d, J = 28.9 Hz). **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}FNO_2$ [M+H] 244.0774, found 244.0771.



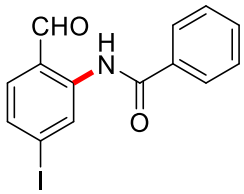
21

***N*-(5-Chloro-2-formylphenyl)benzamide**: white solid, 45 mg, 87% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.14 (s, 1H), 9.95 (s, 1H), 9.05 (d, J= 2.0 Hz, 1H), 8.07 – 8.04 (m, 2H), 7.65 (d, J= 8.4 Hz, 1H), 7.62 – 7.52 (m, 3H), 7.23 (dd, J_1= 8.0 Hz, J_2 = 2.0 Hz, 1H),. **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 194.9, 166.3, 143.3, 142.1, 137.2, 133.9, 132.6, 129.1 (2C), 127.7 (2C), 123.5, 120.4, 120.2. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}ClNO_2$ [M+H] 260.0478, found 260.0479.



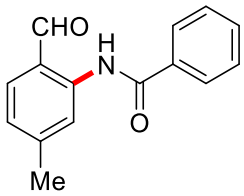
22

***N*-(5-Bromo-2-formylphenyl)benzamide**: white solid, 52 mg, 86% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 12.10 (s, 1H), 9.94 (s, 1H), 9.22 (d, J= 2.0 Hz, 1H), 8.07 – 8.04 (m, 2H), 7.62 – 7.52 (m, 4H), 7.40 (dd, J_1= 8.0 Hz, J_2 = 2.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 195.1, 166.2, 142.0, 137.1, 134.0, 132.6, 132.3, 129.1 (2C), 127.7 (2C), 126.5, 123.2, 120.8. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}BrNO_2$ [M+H] 303.9973, found 303.9976.



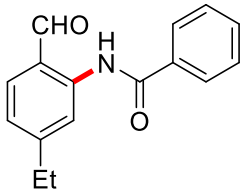
23

***N*-(2-Formyl-5-iodophenyl)benzamide**: white solid, 60 mg, 85% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.05 (s, 1H), 9.92 (s, 1H), 9.43 (s, 1H), 8.06 – 8.04 (m, 2H), 7.64 (dd, J_1= 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.61 – 7.52 (m, 3H), 7.38 (d, J= 8.0 Hz, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 195.4, 166.2, 141.4, 136.8, 134.0, 132.7, 132.6, 129.2, 129.1 (2C), 127.6 (2C), 121.2, 105.6. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}INO_2$ [M+H] 351.9835, found 351.9841.



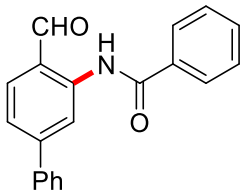
24

***N*-(2-Formyl-5-methylphenyl)benzamide**: white solid, 39 mg, 81% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.12 (s, 1H), 9.92 (s, 1H), 8.80 (s, 1H), 8.09 – 8.06 (m, 2H), 7.61 – 7.51 (m, 4H), 7.08 – 7.06 (m, 1H) , 2.48 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 195.4, 166.3, 148.4, 141.4, 136.4, 134.5, 132.3, 129.0 (2C), 127.6 (2C), 124.2, 120.5, 120.2, 22.7. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{14}NO_2$ [M+H] 240.1024, found 240.1027.



25

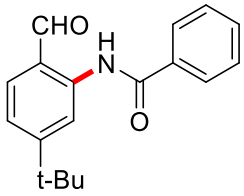
***N*-(5-Ethyl-2-formylphenyl)benzamide**: white solid, 40 mg, 78% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 12.14 (s, 1H), 9.93 (s, 1H), 8.84 (s, 1H), 8.09 – 8.07 (m, 2H), 7.62 (d, J = 8.0 Hz, 1H), 7.60 – 7.52 (m, 3H), 7.11 – 7.09 (m, 1H), 2.76 (q, J = 7.5 Hz, 2H), 1.31 (d, J = 7.5 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 195.4, 166.3, 154.4, 141.5, 136.5, 134.5, 132.3, 129.0 (2C), 127.6 (2C), 123.0, 120.3, 119.4, 29.9, 15.2. **HRMS**(ESI) *m/z* calculated for $C_{16}H_{16}NO_2$ [M+H] 254.1181, found 254.1181.



26

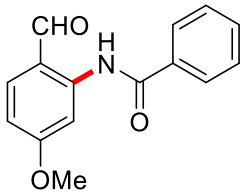
***N*-(4-Formyl-[1,1'-biphenyl]-3-yl)benzamide**: white solid, 41 mg, 68% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 12.17 (s, 1H), 9.99 (s, 1H), 9.29 (d, J = 1.5 Hz, 1H), 8.12

– 8.09 (m, 2H), 7.77 – 7.72 (m, 3H), 7.61 – 7.52 (m, 3H) , 7.50 – 7.46 (m, 3H) , 7.45 – 7.41 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 195.4, 166.3, 149.1, 141.8, 139.5, 136.7, 134.4, 132.4, 129.1 (2C), 129.0 (2C), 129.0, 127.7 (2C), 127.6 (2C), 121.7, 120.9, 118.6. **HRMS**(ESI) *m/z* calculated for $C_{20}H_{16}NO_2$ [M+H] 302.1181, found 302.1183.



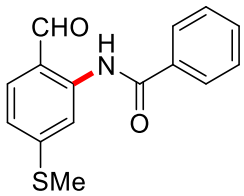
27

***N*-(5-(*Tert*-butyl)-2-formylphenyl)benzamide**：white solid, 36 mg, 63% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.12 (s, 1H), 9.95 (s, 1H), 9.09 (d, J = 1.6 Hz, 1H), 8.10 – 8.07 (m, 2H), 7.65 (d, J = 8.4 Hz, 1H), 7.58 – 7.51 (m, 3H), 7.30 (dd, J_1= 8.4 Hz, J_2 = 1.6 Hz, 1H), 1.40 (s, 9H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 195.4, 166.4, 161.2, 141.4, 136.2, 134.6, 132.3, 129.0 (2C), 127.6 (2C), 120.6, 120.1, 117.3, 36.0, 31.1 (3C). **HRMS**(ESI) *m/z* calculated for $C_{18}H_{20}NO_2$ [M+H] 282.1494, found 282.1493.



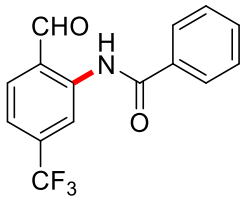
28

***N*-(2-Formyl-5-methoxyphenyl)benzamide**：white solid, 37 mg, 72% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.39 (s, 1H), 9.82 (s, 1H), 8.60 (d, J = 2.4 Hz, 1H), 8.09 – 8.06 (m, 2H), 7.61 – 7.51 (m, 4H), 6.75 (dd, J_1= 8.8 Hz, J_2 = 2.4 Hz, 1H), 3.95 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 194.0, 166.5, 166.2, 143.9, 138.1, 134.3, 132.4, 129.0 (2C), 127.6 (2C), 116.2, 110.7, 103.8, 56.0. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{14}NO_3$ [M+H] 256.0973, found 256.0975.



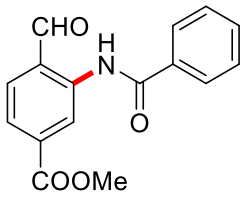
29

***N*-(2-Formyl-5-(methylthio)phenyl)benzamide**: white solid, 17 mg, 31% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.25 (s, 1H), 9.86 (s, 1H), 8.88 (d, J = 1.6 Hz, 1H), 8.08 – 8.06 (m, 2H), 7.61 – 7.52 (m, 4H), 7.06 (dd, J_1= 8.4 Hz, J_2 = 1.6 Hz, 1H), 2.60 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 194.5, 166.5, 151.4, 141.6, 136.0, 134.3, 132.4, 129.1 (2C), 127.6 (2C), 119.7, 118.7, 114.8, 14.7. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{14}NO_2S$ [M+H] 272.0745, found 272.0747.



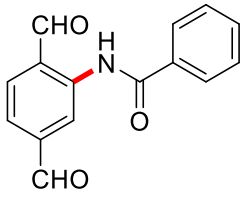
30

***N*-(2-Formyl-5-(trifluoromethyl)phenyl)benzamide**: white solid, 42 mg, 71% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.12 (s, 1H), 10.09 (s, 1H), 9.34 (s, 1H), 8.08 – 8.06 (m, 2H), 7.88 (d, J= 8.0 Hz, 1H), 7.64 – 7.50 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 195.5, 166.4, 141.7, 137.4 (q, J = 32.6 Hz), 136.5, 133.8, 132.8, 129.2 (2C), 127.7 (2C), 123.6, 123.3 (q, J = 271.9 Hz), 119.6 (q, J = 3.7 Hz), 117.4 (q, J =4.0 Hz). **HRMS**(ESI) *m/z* calculated for $C_{15}H_{11}F_3NO_2$ [M+H] 294.0742, found 294.0739.



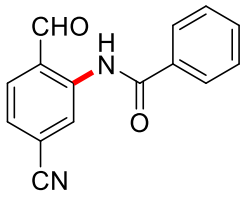
31

Methyl 3-benzamido-4-formylbenzoate: white solid, 40 mg, 71% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 12.01 (s, 1H), 10.06 (s, 1H), 9.55 (s, 1H), 8.07 – 8.05 (m, 2H), 7.90 (dd, J_1= 7.5 Hz, J_2 = 1.5 Hz, 1H), 7.80 (d, J= 8.0 Hz, 1H), 7.60 – 7.51 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 195.7, 166.2, 166.0, 141.3, 136.8, 136.0, 134.1, 132.5, 129.1 (2C), 127.6 (2C), 124.3, 123.9, 121.2, 52.8. **HRMS**(ESI) *m/z* calculated for $C_{16}H_{14}NO_4$ [M+H] 284.0923, found 284.0921.



32

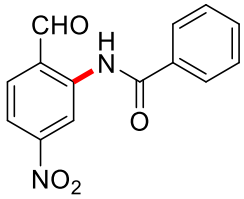
***N*-(2,5-Diformylphenyl)benzamide**: yellow solid, 31 mg, 61% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.12 (s, 1H), 10.14 (s, 1H), 10.12 (s, 1H), 9.49 (s, 1H), 8.10 – 8.07 (m, 2H), 7.91 (d, J= 8.0 Hz, 1H), 7.79 (dd, J_1= 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.64 – 7.54 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 195.9, 191.8, 166.5, 142.1, 141.3, 136.6, 133.9, 132.8, 129.2 (2C), 127.7 (2C), 124.8, 123.4, 121.6. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{12}NO_3$ [M+H] 254.0817, found 254.0820.



33

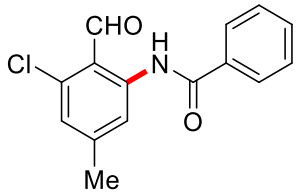
***N*-(5-Cyano-2-formylphenyl)benzamide**: white solid, 21 mg, 42% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.07 (s, 1H), 10.08 (s, 1H), 9.36 (s, 1H), 8.07 – 8.04 (m, 2H),

7.86 (d, *J*= 8.0 Hz, 1H), 7.64 – 7.52 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) *δ*: 195.2, 166.4, 141.6, 136.3, 133.6, 132.9, 129.2 (2C), 127.7 (2C), 126.0, 123.8, 123.7, 119.4, 117.7. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{11}N_2O_2$ [M+H] 251.0821, found 251.0822.



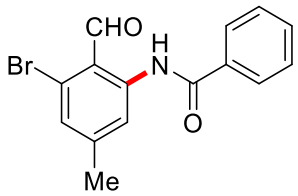
34

***N*-(2-Formyl-5-nitrophenyl)benzamide**: yellow solid, 21 mg, 38% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) *δ*: 12.12 (s, 1H), 10.15 (s, 1H), 9.84 (d, *J*= 2.4 Hz, 1H), 8.09 – 8.04 (m, 3H), 7.94 (d, *J*= 8.4 Hz, 1H), 7.65 – 7.60 (m, 1H) , 7.59 – 7.54 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) *δ*: 195.0, 166.3, 152.2, 142.3, 136.9, 133.6, 133.0, 129.2 (2C), 127.7 (2C), 124.9, 117.3, 115.5. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}N_2O_4$ [M+H] 271.0719, found 271.0719.



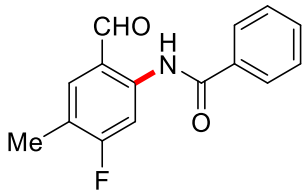
35

***N*-(3-Chloro-2-formyl-5-methylphenyl)benzamide**: white solid, 47 mg, 85% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) *δ*: 12.52 (s, 1H), 10.55 (s, 1H), 8.75 (s, 1H), 8.07 – 8.05 (m, 2H), 7.61 – 7.51 (m, 3H) , 7.00 (s, 1H), 2.42 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) *δ*: 194.3, 166.3, 149.3, 143.4, 140.2, 134.3, 132.5, 129.0 (2C), 127.7 (2C), 125.7, 119.5, 115.8, 22.5. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{13}ClNO_2$ [M+H] 274.0635, found 274.0636.



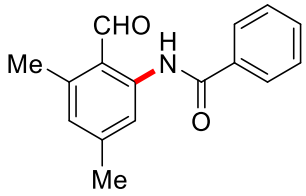
36

***N*-(3-Bromo-2-formyl-5-methylphenyl)benzamide**: white solid, 55 mg, 86% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) *δ*: 12.54 (s, 1H), 10.47 (s, 1H), 8.80 (s, 1H), 8.08 – 8.05 (m, 2H), 7.61 – 7.51 (m, 3H) , 7.23 (s, 1H) , 2.42 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) *δ*: 196.8, 166.3, 149.3, 143.4, 134.3, 132.5, 130.1, 129.3, 129.1 (2C), 127.7 (2C), 120.3, 116.5, 22.3. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{13}BrNO_2$ [M+H] 318.0130, found 318.0132.



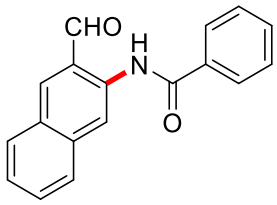
37

***N*-(5-Fluoro-2-formyl-4-methylphenyl)benzamide**: white solid, 43 mg, 84% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.17 (s, 1H), 9.90 (s, 1H), 8.69 (d, *J*= 12.4 Hz, 1H), 8.07 – 8.04 (m, 2H), 7.61 – 7.51 (m, 4H), 2.32 (d, *J*= 1.6 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 194.6, 166.2, 166.0 (d, *J*= 254.7 Hz), 141.5 (d, *J*= 13.7 Hz), 139.5 (d, *J*= 9.0 Hz), 134.1, 132.5, 129.1 (2C), 127.6 (2C), 120.3 (d, *J*= 19.1 Hz), 118.9 (d, *J*= 2.5 Hz), 107.5 (d, *J*= 29.8 Hz), 14.1 (d, *J*= 2.9 Hz). **HRMS**(ESI) *m/z* calculated for $C_{15}H_{13}FNO_2$ [M+H] 258.0930, found 258.0936.



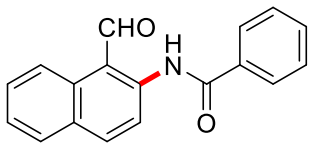
38

***N*-(2-Formyl-3,5-dimethylphenyl)benzamide**：white solid, 44 mg, 87% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.61 (s, 1H), 10.43 (s, 1H), 8.68 (s, 1H), 8.09 – 8.06 (m, 2H), 7.59 – 7.50 (m, 3H), 6.78 (s, 1H), 2.64 (s, 3H), 2.40 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 194.1, 166.3, 148.3, 143.3, 142.2, 134.7, 132.1, 128.8 (2C), 127.6 (2C), 127.0, 118.8, 117.6, 22.5, 19.2. **HRMS**(ESI) *m/z* calculated for $C_{16}H_{16}NO_2$ [M+H] 254.1181, found 254.1180.



39

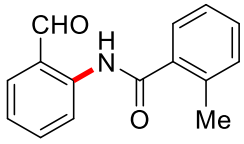
***N*-(3-Formylnaphthalen-2-yl)benzamide**: yellow solid, 40 mg, 73% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 11.92 (s, 1H), 10.14 (s, 1H), 9.35 (s, 1H), 8.25 (s, 1H), 8.12 – 8.10 (m, 2H), 7.91 (d, *J*= 9.2 Hz, 2H), 7.66 – 7.46 (m, 5H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 196.0, 166.2, 140.5, 137.4, 135.9, 134.6, 132.2, 130.6, 129.2, 129.0 (2C), 128.9, 128.3, 127.5 (2C), 126.1, 123.2, 117.5. **HRMS**(ESI) *m/z* calculated for $C_{18}H_{14}NO_2$ [M+H] 276.1025, found 276.1027.



40

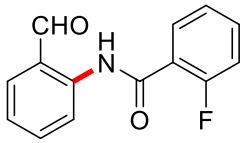
***N*-(1-Formylnaphthalen-2-yl)benzamide**: yellow solid, 42 mg, 76% yield;**^{1}H NMR**

(400 MHz, $CDCl_3$) δ: 13.14 (s, 1H), 11.09 (s, 1H), 9.16 (d, J= 9.2 Hz, 1H), 8.49 (d, J= 8.8 Hz, 1H), 8.16 – 8.11 (m, 3H), 7.88 (d, J= 8.0 Hz, 1H), 7.67 – 7.48 (m, 5H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 193.2, 166.8, 143.2, 138.0, 134.6, 133.8, 132.5, 129.8, 129.6, 129.2, 129.1 (2C), 127.9 (2C), 125.4, 119.9, 119.4, 113.0. **HRMS**(ESI) *m/z* calculated for $C_{18}H_{14}NO_2$ [M+H] 276.1025, found 276.1031.



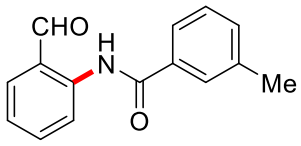
41

***N*-(2-Formylphenyl)-2-methylbenzamide:** white solid, 36 mg, 75% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 11.54 (s, 1H), 9.94 (s, 1H), 8.94 (d, J = 8.4 Hz, 1H), 7.72 – 7.62 (m, 3H), 7.41 – 7.37 (m, 1H), 7.33 – 7.25 (m, 3H), 2.57 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 195.6, 169.0, 141.1, 137.3, 136.4, 136.3, 135.9, 131.7, 130.8, 127.3, 126.2, 123.2, 122.0, 120.0, 20.4. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{14}NO_2$ [M+H] 240.1024, found 240.1028.



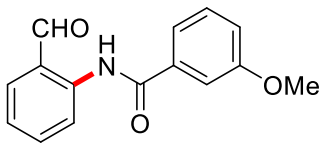
42

2-Fluoro-*N*-(2-formylphenyl)benzamide: white solid, 38 mg, 78% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 11.97 (d, J = 5.6 Hz, 1H), 9.97 (s, 1H), 8.96 (d, J = 8.4 Hz, 1H), 8.06 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.72 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.69 – 7.65 (m, 1H), 7.56 – 7.50 (m, 1H), 7.32 – 7.27 (m, 2H) , 7.25 – 7.20 (m, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 195.2, 163.1 (d, J = 2.6 Hz), 160.4 (d, J = 249.7 Hz), 140.5, 136.3, 136.2, 133.9 (d, J = 9.0 Hz), 131.8 (d, J = 2.0 Hz), 124.9 (d, J = 3.5 Hz), 123.6, 122.6, 122.5 (d, J = 12 Hz), 120.9, 116.7 (d, J = 23.4 Hz). **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}FNO_2$ [M+H] 244.0774, found 244.0772.



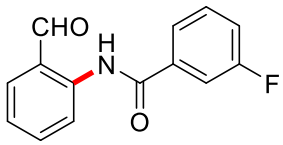
43

***N*-(2-Formylphenyl)-3-methylbenzamide:** white solid, 34 mg, 71% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.05 (s, 1H), 10.00 (s, 1H), 8.96 (d, J = 8.4 Hz, 1H), 7.88 – 7.85 (m, 2H), 7.74 – 7.72 (m, 1H), 7.70 – 7.66 (m, 1H), 7.44 – 7.38 (m, 2H), 7.27 (t, J = 7.6 Hz, 1H), 2.47 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 196.0, 166.6, 141.4, 138.9, 136.5, 136.3, 134.5, 133.1, 128.9, 128.5, 124.6, 123.1, 122.1, 120.1, 21.6. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{14}NO_2$ [M+H] 240.1024, found 240.1024.



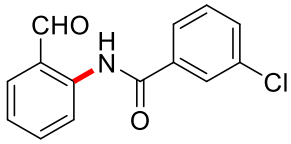
44

***N*-(2-Formylphenyl)-3-methoxybenzamide:** white solid, 26 mg, 52% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 12.06 (s, 1H), 9.97 (s, 1H), 8.93 (d, J = 8.0 Hz, 1H), 7.71 (dd, J_1 = 7.5 Hz, J_2 = 1.5 Hz, 1H), 7.68 – 7.59 (m, 3H), 7.43 (t, J = 8.0 Hz, 1H), 7.25 (td, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 7.12 – 7.09 (m, 1H), 3.89 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 195.9, 166.1, 160.1, 141.3, 136.5, 136.3, 135.9, 130.0, 123.2, 122.1, 120.0, 119.5, 118.9, 112.5, 55.5. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{14}NO_3$ [M+H] 256.0973, found 256.0974.



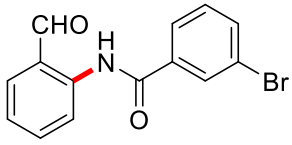
45

3-Fluoro-*N*-(2-formylphenyl)benzamide: white solid, 28 mg, 58% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.09 (s, 1H), 9.98 (s, 1H), 8.91 (d, J = 8.4 Hz, 1H), 7.84 – 7.82 (m, 1H), 7.78 – 7.72 (m, 2H), 7.69 – 7.65 (m, 1H), 7.53 – 7.48 (m, 1H) , 7.30 – 7.24 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 196.1, 164.9 (d, J = 2.5 Hz), 163.1 (d, J = 246.4 Hz), 141.0, 136.7 (d, J = 6.8 Hz), 136.6, 136.3, 130.7 (d, J = 7.9 Hz), 123.5, 122.9 (d, J = 3.0 Hz), 122.1, 120.1, 119.4 (d, J = 21.3 Hz), 115.1 (d, J = 23.0 Hz). **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}FNO_2$ [M+H] 244.0774, found 244.0773.



46

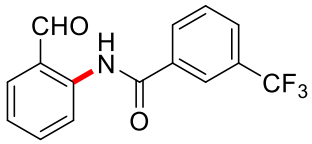
3-Chloro-*N*-(2-formylphenyl)benzamide: white solid, 40 mg, 65% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.08 (s, 1H), 9.99 (s, 1H), 8.91 (d, J = 8.4 Hz, 1H), 8.05 (t, J = 2.0 Hz, 1H), 7.93 – 7.91 (m, 1H), 7.73 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz,, 1H), 7.70 – 7.66 (m, 1H), 7.56 – 7.53 (m, 1H), 7.47 (t, J = 7.6 Hz, 1H), 7.28 (td, J_1 = 7.6 Hz, J_2 = 1.2 Hz,, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 196.1, 164.8, 141.0, 136.6, 136.3, 136.2, 135.3, 132.4, 130.3, 128.3, 125.3, 123.5, 122.1, 120.1. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}ClNO_2$ [M+H] 260.0478, found 260.0481.



47

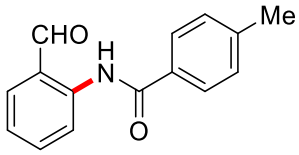
3-Bromo-*N*-(2-formylphenyl)benzamide: white solid, 46 mg, 75% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.08 (s, 1H), 9.99 (s, 1H), 8.90 (d, J = 8.8 Hz, 1H), 8.21 (t, J = 2.0 Hz, 1H), 7.98 – 7.95 (m, 1H), 7.73 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz,, 1H), 7.70 – 7.66

(m, 2H), 7.41 (t, J = 7.6 Hz, 1H), 7.28 (td, J_1 = 7.6 Hz, J_2 = 1.2 Hz,, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 196.1, 164.7, 141.0, 136.6, 136.4, 136.3, 135.3, 131.2, 130.5, 125.8, 123.5, 123.3, 122.1, 120.1. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}BrNO_2$ [M+H] 303.9973, found 303.9978.



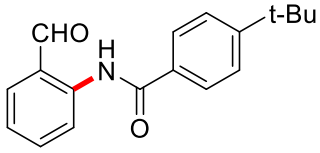
48

***N*-(2-Formylphenyl)-3-(trifluoromethyl)benzamide**: white solid, 30 mg, 51% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.08 (s, 1H), 10.00 (s, 1H), 8.92 (d, J = 8.4 Hz, 1H), 8.36 (s, 1H), 8.23 (d, J = 7.6 Hz, 1H), 7.84 (d, J = 7.6 Hz, 1H), 7.75 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz,, 1H), 7.72 – 7.66 (m, 2H), 7.30 (td, J_1 = 7.6 Hz, J_2 = 0.8 Hz,, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 196.2, 164.7, 141.0, 136.6, 136.4, 135.3, 131.7 (q, J = 32.8 Hz), 130.4, 129.6, 128.9 (q, J = 3.5 Hz), 123.8 (q, J = 270.9 Hz), 125.1 (q, J = 3.9 Hz), 123.7, 122.2, 120.1. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{11}F_3NO_2$ [M+H] 294.0742, found 294.0744.



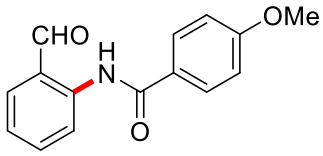
49

***N*-(2-Formylphenyl)-4-methylbenzamide**: white solid, 35 mg, 72% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.04 (s, 1H), 9.98 (s, 1H), 8.95 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 8.0 Hz, 2H), 7.71 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz,, 1H), 7.68 – 7.63 (m, 1H), 7.32 (d, J = 8.0 Hz, 2H), 7.26 – 7.22 (m, 1H), 2.43 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 196.0, 166.2, 142.9, 141.5, 136.5, 136.3, 131.6, 129.7 (2C), 127.6 (2C), 123.0, 122.0, 120.0, 21.6. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{14}NO_2$ [M+H] 240.1024, found 240.1021.



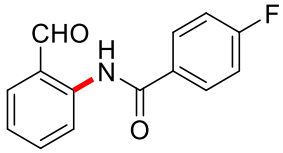
50

4-(*Tert*-butyl)-*N*-(2-formylphenyl)benzamide: colorless oil, 40 mg, 71% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 12.05 (s, 1H), 9.98 (s, 1H), 8.96 (d, J = 8.5 Hz, 1H), 8.03 – 7.99 (m, 2H), 7.70 (dd, J_1 = 7.5 Hz, J_2 = 1.5 Hz,, 1H), 7.68 – 7.63 (m, 1H), 7.57 – 7.53 (m, 2H), 7.26 – 7.22 (m, 1H), 1.37 (s, 9H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 195.9, 166.2, 155.9, 141.5, 136.4, 136.3, 131.6, 127.5 (2C), 125.9 (2C), 123.0, 122.1, 120.0, 35.1, 31.2. **HRMS**(ESI) *m/z* calculated for $C_{18}H_{20}NO_2$ [M+H] 282.1494, found 282.1493.



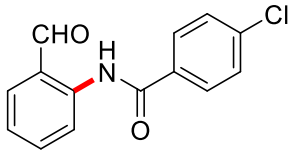
51

***N*-(2-Formylphenyl)-4-methoxybenzamide:** white solid, 21 mg, 41% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.02 (s, 1H), 9.99 (s, 1H), 8.94 (d, J = 8.4 Hz, 1H), 8.16 – 8.03 (m, 2H), 7.71 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz,, 1H), 7.68 – 7.64 (m, 1H), 7.26 – 7.22 (m, 1H), 7.04 – 7.00 (m, 2H), 3.88 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 196.0, 165.8, 162.9, 141.7, 136.5, 136.3, 129.6 (2C), 126.7, 122.9, 122.0, 120.0, 114.2 (2C), 55.6. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{14}NO_3$ [M+H] 256.0973, found 256.0972.



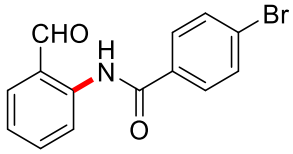
52

4-Fluoro-*N*-(2-formylphenyl)benzamide: white solid, 40 mg, 82% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.07 (s, 1H), 9.99 (s, 1H), 8.92 (d, J = 8.4 Hz, 1H), 8.11 – 8.06 (m, 2H), 7.73 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz,, 1H), 7.70 – 7.65 (m, 1H), 7.29 – 7.25 (m, 1H), 7.23 – 7.17 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 196.1, 165.3 (d, J = 251.6 Hz), 165.1, 141.3, 136.6, 136.3, 130.6 (d, J = 3.1 Hz), 130.1 (d, J = 9.1 Hz, 2C), 123.3, 122.1, 120.0, 116.1 (d, J = 21.9 Hz, 2C). **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}FNO_2$ [M+H] 244.0774, found 244.0774.



53

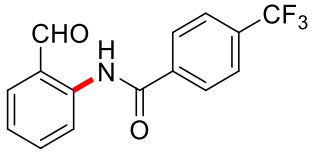
4-Chloro-*N*-(2-formylphenyl)benzamide: white solid, 44 mg, 84% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.08 (s, 1H), 9.99 (s, 1H), 8.92 (d, J = 8.4 Hz, 1H), 8.02 – 7.99 (m, 2H), 7.73 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz,, 1H), 7.70 – 7.66 (m, 1H), 7.52 – 7.48 (m, 2H), 7.30 – 7.26 (m, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 196.1, 165.2, 141.2, 138.7, 136.6, 136.4, 132.8, 129.3 (2C), 129.1 (2C), 123.4, 122.1, 120.1. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}ClNO_2$ [M+H] 260.0478, found 260.0474.



54

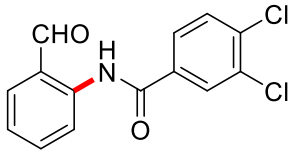
4-Bromo-*N*-(2-formylphenyl)benzamide: white solid, 52 mg, 86% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.09 (s, 1H), 10.00 (s, 1H), 8.92 (d, J = 8.8 Hz, 1H), 7.95 – 7.92 (m, 2H), 7.74 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz,, 1H), 7.71 – 7.66 (m, 3H), 7.31 – 7.27 (m, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 196.1, 165.3, 141.2, 136.6, 136.4,

133.3, 132.3 (2C), 129.2 (2C), 127.3, 123.4, 122.1, 120.1. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{11}BrNO_2$ [M+H] 303.9973, found 303.9978.



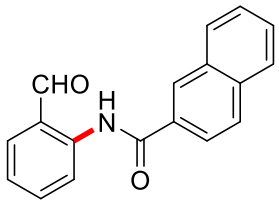
55

***N*-(2-Formylphenyl)-4-(trifluoromethyl)benzamide**: white solid, 35 mg, 59% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.18 (s, 1H), 10.00 (s, 1H), 8.93 (d, J = 8.8 Hz, 1H), 8.18 (d, J = 8.0 Hz, 2H), 7.80 (d, J = 8.4 Hz, 2H), 7.75 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz,, 1H), 7.72 – 7.68 (m, 1H), 7.33 – 7.29 (m, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 196.2, 164.9, 141.0, 137.7, 136.6, 136.4, 133.9 (q, J = 32.5 Hz), 128.1 (2C), 126.1 (q, J = 3.7 Hz, 2C), 123.8 (q, J = 271.0 Hz), 123.7, 122.2, 120.2. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{11}F_3NO_2$ [M+H] 294.0742, found 294.0745.



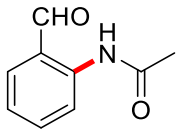
56

3,4-Dichloro-*N*-(2-formylphenyl)benzamide: white solid, 49 mg, 83% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 12.11 (s, 1H), 10.00 (s, 1H), 8.88 (d, J = 8.4 Hz, 1H), 8.16 (d, J = 2.0 Hz, 1H), 7.87 (dd, J_1 = 8.4 Hz, J_2 = 2.0 Hz,, 1H), 7.75 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz,, 1H), 7.71 – 7.67 (m, 1H), 7.61 (d, J = 8.4 Hz, 1H), 7.32 – 7.28 (m, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 196.2, 163.9, 140.9, 136.9, 136.7, 136.4, 134.3, 133.7, 131.0, 130.2, 126.3, 123.7, 122.1, 120.1. **HRMS**(ESI) *m/z* calculated for $C_{14}H_{10}Cl_2NO_2$ [M+H] 294.0088, found 294.0091.



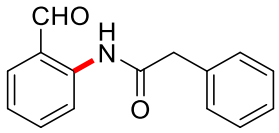
57

***N*-(2-Formylphenyl)-2-naphthamide:** white solid, 25 mg, 45% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 12.22 (s, 1H), 9.98 (s, 1H), 8.99 (d, J = 8.5 Hz, 1H), 8.58 (s, 1H), 8.11 (dd, J_1 = 8.5 Hz, J_2 = 2.0 Hz, 1H), 8.01 (d, J = 8.5 Hz, 1H), 7.96 (d, J = 9.0 Hz, 1H), 7.88 (d, J = 8.5 Hz, 1H), 7.70 – 7.64 (m, 2H), 7.60 – 7.53 (m, 2H), 7.26 – 7.22 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 195.9, 166.2, 141.4, 136.4, 136.2, 135.1, 132.8, 131.6, 129.5, 128.8, 128.6, 128.1, 127.8, 126.9, 123.7, 123.1, 122.1, 120.1. **HRMS**(ESI) *m/z* calculated for $C_{18}H_{14}NO_2$ [M+H] 276.1025, found 276.1028.



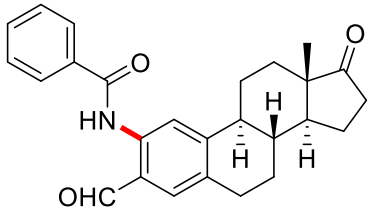
58

***N*-(2-Formylphenyl)acetamide**: white solid, <2% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 11.13 (s, 1H), 9.92 (s, 1H), 8.73 (d, J = 8.4 Hz, 1H), 7.67 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz,, 1H), 7.64 – 7.59 (m, 1H), 7.25 – 7.21 (m, 1H), 2.26 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 195.7, 169.8, 141.1, 136.4, 136.2, 123.0, 121.6, 120.0, 25.6. **HRMS**(ESI) *m/z* calculated for $C_9H_{10}NO_2$ [M+H] 164.0711, found 164.0713.



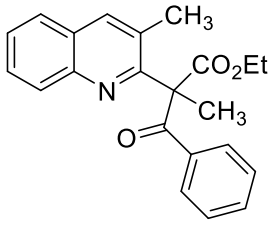
59

***N*-(2-Formylphenyl)-2-phenylacetamide**: colorless oil, <2% yield; **^{1}H NMR** (400 MHz, $CDCl_3$) δ: 11.10 (s, 1H), 9.82 (s, 1H), 8.75 (d, J = 8.8 Hz, 1H), 7.63 – 7.57 (m, 2H), 7.43 – 7.33 (m, 5H), 7.23 – 7.19 (m, 1H), 3.79 (s, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 195.4, 170.9, 140.9, 136.2, 136.1, 134.1, 129.8 (2C), 129.1 (2C), 127.6, 123.1, 121.9, 120.0, 45.9. **HRMS**(ESI) *m/z* calculated for $C_{15}H_{14}NO_2$ [M+H] 240.1024, found 240.1020.



61

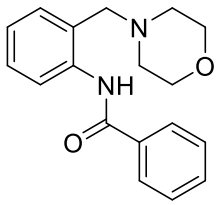
***N*-((8R,9S,13S,14S)-3-formyl-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-2-yl)benzamide**: white solid, 41 mg, 51% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 11.96 (s, 1H), 9.90 (s, 1H), 8.98 (s, 1H), 8.07 – 8.05 (m, 2H), 7.59 – 7.51 (m, 3H), 7.41 (s, 1H), 3.00 – 2.89 (m, 2H), 2.62 – 2.49 (m, 2H), 2.39 – 2.34 (m, 1H), 2.20 – 1.99 (m, 4H), 1.70 – 1.45 (m, 6H), 0.93 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 200.5, 195.5, 166.1, 149.6, 139.0, 136.5, 134.5, 132.2, 131.8, 129.0 (2C), 127.5 (2C), 120.5, 117.2, 50.7, 48.0, 45.4, 37.8, 35.9, 31.6, 28.6, 26.3, 25.8, 21.7, 13.9. **HRMS**(ESI) *m/z* calculated for $C_{26}H_{28}NO_3$ [M+H] 402.2069, found 402.2065.



62

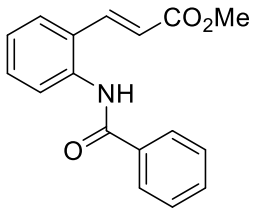
Ethyl 2-methyl-2-(3-methylquinolin-2-yl)-3-oxo-3-phenylpropanoate: colorless oil, 169 mg, 97% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 7.94 (d, J = 8.5 Hz, 1H), 7.86 (s, 1H), 7.72 – 7.69 (m, 3H), 7.63 – 7.59 (m, 1H), 7.51 – 7.48 (m, 1H), 7.41 – 7.37 (m, 1H), 7.24 – 7.21 (m, 2H), 4.33 – 4.20 (m, 2H), 2.33 (s, 3H), 2.10 (s, 3H), 1.20 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ: 197.9, 171.4, 159.9, 145.4, 138.3, 136.8,

132.2, 130.1, 129.7 (2C), 129.3, 128.7, 127.9 (2C), 127.5, 126.9, 126.5, 68.0, 61.8, 21.9, 20.3, 14.0. **HRMS**(ESI) *m/z* calculated for $C_{22}H_{22}NO_3$ [M+H] 348.1600, found 348.1601.



63

***N*-(2-(Morpholinomethyl)phenyl)benzamide**: white solid, 46 mg, 78% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 11.20 (s, 1H), 8.44 (d, J = 8.0 Hz, 1H), 7.99 – 7.97 (m, 2H), 7.57 – 7.54 (m, 1H), 7.51 – 7.48 (m, 2H), 7.38 – 7.35 (m, 1H), 7.16 – 7.14 (m, 1H), 7.06 – 7.03 (m, 1H), 3.76 – 3.75 (m, 4H), 3.65 (s, 2H), 2.53 (s, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 165.3, 138.8, 135.5, 131.8, 130.2, 128.9, 128.7 (2C), 127.2 (2C), 124.9, 123.6, 121.1, 66.9 (2C), 62.8, 53.2 (2C). **HRMS**(ESI) *m/z* calculated for $C_{18}H_{21}N_2O_2$ [M+H] 297.1603, found 297.1601.



64

Methyl (*E*)-3-(2-benzamidophenyl)acrylate: white solid, 53 mg, 94% yield; **^{1}H NMR** (500 MHz, $CDCl_3$) δ: 8.02 (s, 1H), 7.90 (d, J = 7.5 Hz, 2H), 7.85 (d, J = 16.0 Hz, 1H), 7.81 (d, J = 8.0 Hz, 1H), 7.58 – 7.54 (m, 2H), 7.48 (t, J = 7.5 Hz, 2H), 7.43 – 7.40 (m, 1H), 7.24 (t, J = 7.5 Hz, 1H), 6.41 (d, J = 16.0 Hz, 1H), 3.75 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ: 167.2, 166.3, 139.7, 136.1, 134.3, 132.2, 131.0, 129.0 (2C), 128.3, 127.4, 127.3 (2C), 126.2, 125.5, 120.5, 51.9. **HRMS**(ESI) *m/z* calculated for $C_{17}H_{16}NO_3$ [M+H] 282.1130, found 282.1130.

9 Computational Details

The M06 density functional method[8] was used to carry out all the calculations. The LANL2DZ basis set in conjunction with the LANL2DZ pseudo potential was employed for Rh and Sb atoms,[9] and the 6-31G(d) basis setwas used for other atoms in geometry optimizations.[10] For each optimized stationary point, vibrational frequency analyses at the same level of theory were performed on all optimized structures to characterize stationary points as local minima (no imaginary frequency) or transition states (one imaginary frequency). Intrinsic reaction coordinate calculations confirmed that the optimized transition states connect to their respective reactants and products. To consider solvation effects, single-point energy computations using the SMD model[11] with TFE as the solvent were performed based on the optimized gas-phase geometries of all species. The basis sets (SDD for Rh and Sb and 6-311++G(d,p) for other atoms) were employed for such single-point energy calculations. The solution-phase Gibbs free energy was determined by adding the solvation single-point energy and the gas-phase thermal correction to the Gibbs free energy obtained from the vibrational frequency analyses. All calculations were carried out with the Gaussian 09 suite of programs.[12]

The cationic $[CpRh(SbF_6)]^+$ catalyst model was employed in the computational study. The additive, water molecule, could coordinate with Rh center to form **INT1**. With the assistance of substrate **2**, behaving as a Lewis base, the coordinated water molecule could dissociate to form **INT3**. After a ligand exchange step with substrate **1**, a complex **INT5** might be formed via the coordination of O atom of **1** with Rh (**Figure S1**). Subsequently, the yielded hydroxide anion in **INT5** could lead to the concerted metalation-deprotonation (CMD) with the *ortho* C−H group of **1** to afford **INT6**. The optimized transition state (TS) of the formation of **INT6** is shown as **TS2**, in which the C…H bond distance is lengthened to 1.27 Å while the O…H bond distance is shortened to 1.41 Å. The predicted overall free energy barrier to form **INT6** is ca. 40 kcal/mol relative to **INT2**. Next, the aminating agent **2** could undergo a ligand exchange step with water to form **INT7**, from which the dissociation of CO_2

may occur to afford the intermediate **INT8**. The calculated $\Delta G^{\neq}$ of the dissociation of CO_2 is ca. 27 kcal/mol relative to **INT7**. The generated **INT8** is ready to undergo intramolecular migratory insertion *via* **TS4** to yield **INT9**. Finally, the formed **INT9** can be protonated with water to produce the desired product **3** and the proposed active catalyst model **INT5** is regenerated after a ligand exchange step. Computational results suggest that the CMD step is the rate-limiting step, which is consistent with the experimental KIE results.

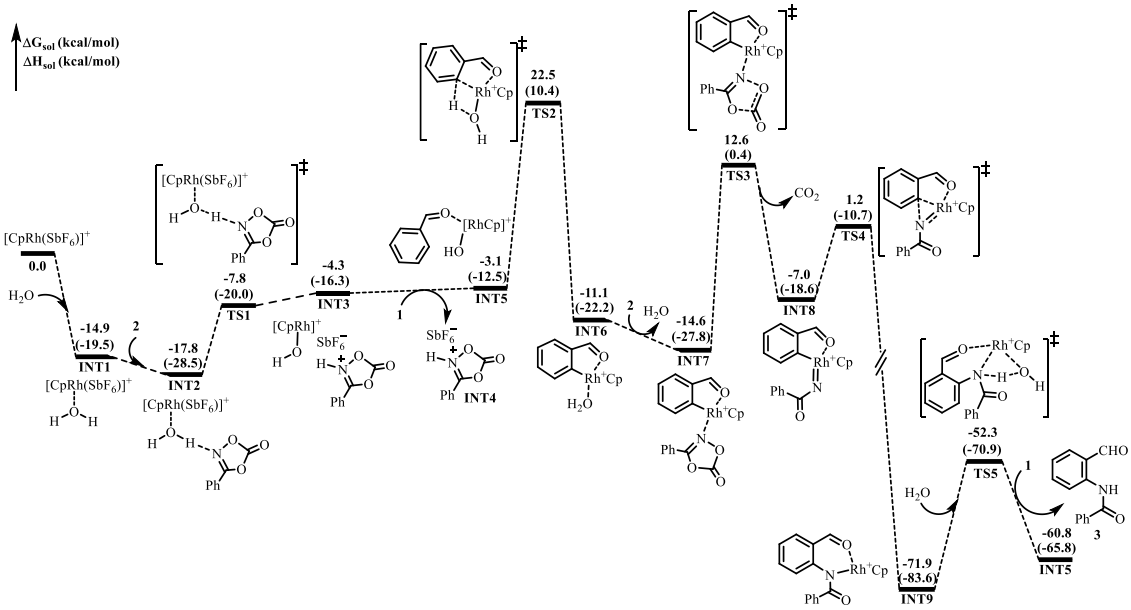


Figure S1. Energy profile for the H_2O-promoted, Rh-catalyzed *ortho*-C−H amidation of benzaldehydes with dioxazolones.

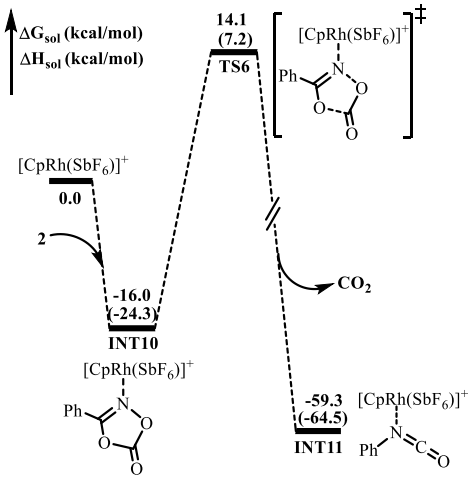


Figure S2. Energy profile for the Rh-mediated dissociation of **2** to form the corresponding isocyanate derivative and CO_2.

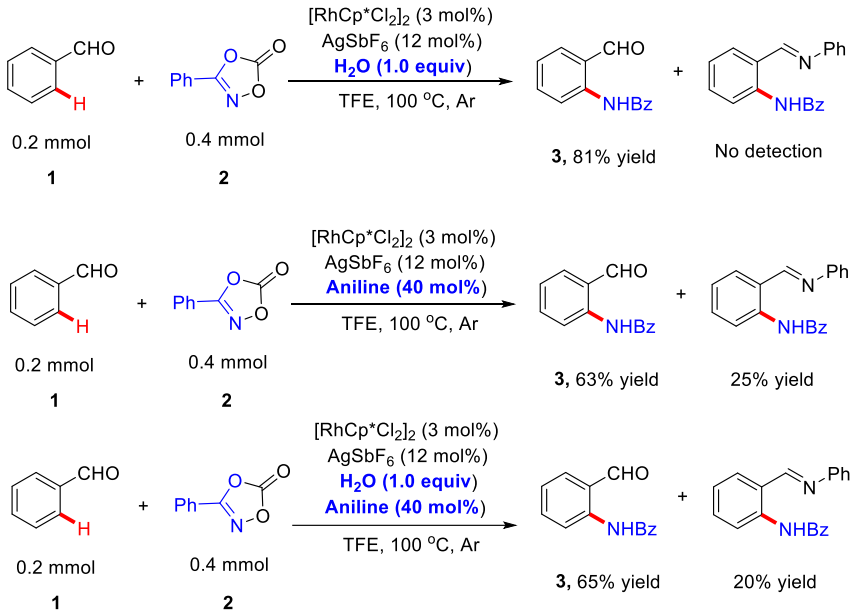


Figure S3. Control experiments.

10 References

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11 CartesianCoordinates and Energies

[CpRh(SbF$_6$)]$^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.313699	0.003902	-0.000351
2	6	0	3.068669	0.544705	1.089528
3	6	0	3.066039	-0.875111	0.854235
4	6	0	3.070813	-1.087979	-0.556937
5	6	0	3.087096	1.199150	-0.180933
6	6	0	3.064627	0.195035	-1.202906
7	51	0	-1.715047	-0.000553	0.000182
8	9	0	-2.575749	-1.535883	0.397739
9	9	0	-2.569050	0.422072	-1.532138
10	9	0	-0.345678	-0.987154	-0.998645
11	9	0	-0.352452	-0.374734	1.356531
12	9	0	-0.346166	1.360412	-0.354421
13	9	0	-2.569450	1.117627	1.129283
14	1	0	3.018555	2.271568	-0.343312
15	1	0	3.015275	0.372308	-2.273297
16	1	0	2.993012	-2.051131	-1.054418
17	1	0	2.993685	-1.647196	1.615230
18	1	0	3.013825	1.031207	2.059223

Zero-point correction= 0.100099 (Hartree/Particle)
Thermal correction to Energy= 0.114246
Thermal correction to Enthalpy= 0.115191
Thermal correction to Gibbs Free Energy= 0.057543
Sum of electronic and zero-point Energies= -906.886471
Sum of electronic and thermal Energies= -906.872323
Sum of electronic and thermal Enthalpies= -906.871379
Sum of electronic and thermal Free Energies= -906.929027
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-908.37601377

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.728689	1.057181	0.000002
2	6	0	0.358836	1.287892	0.000000
3	6	0	-0.530604	0.213524	-0.000002
4	6	0	-0.047297	-1.097518	-0.000003
5	6	0	1.319274	-1.327610	-0.000001
6	6	0	2.205781	-0.250260	0.000002
7	1	0	2.425059	1.893441	0.000004
8	1	0	-0.033601	2.305940	0.000001
9	1	0	-0.766167	-1.915043	-0.000005
10	1	0	1.702482	-2.346285	-0.000002
11	1	0	3.279116	-0.433242	0.000003
12	6	0	-1.981991	0.466273	-0.000005
13	1	0	-2.257688	1.549943	-0.000015
14	8	0	-2.833167	-0.393955	0.000007

Zero-point correction= 0.109844 (Hartree/Particle)
Thermal correction to Energy= 0.116135
Thermal correction to Enthalpy= 0.117079
Thermal correction to Gibbs Free Energy= 0.079380
Sum of electronic and zero-point Energies= -345.216511
Sum of electronic and thermal Energies= -345.210221
Sum of electronic and thermal Enthalpies= -345.209277
Sum of electronic and thermal Free Energies= -345.246975
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-345.42052444

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.639763	-0.275694	-0.000151
2	6	0	2.739019	0.310181	0.000097

3	8	0	1.453517	0.806140	-0.000002
4	8	0	2.625685	-1.036381	-0.000231
5	8	0	3.735253	0.953228	0.000343
6	6	0	-0.799969	-0.088553	0.000040
7	6	0	-1.641864	-1.205750	0.000250
8	6	0	-1.335853	1.200846	-0.000134
9	6	0	-3.015648	-1.025473	0.000210
10	1	0	-1.207376	-2.203524	0.000529
11	6	0	-2.713968	1.370323	-0.000134
12	1	0	-0.670577	2.061467	-0.000219
13	6	0	-3.552631	0.260703	-0.000007
14	1	0	-3.672954	-1.892379	0.000300
15	1	0	-3.134543	2.373574	-0.000262
16	1	0	-4.632507	0.396140	-0.000050
17	7	0	1.269887	-1.399810	-0.000316

Zero-point correction= 0.120171 (Hartree/Particle)
Thermal correction to Energy= 0.128926
Thermal correction to Enthalpy= 0.129870
Thermal correction to Gibbs Free Energy= 0.084912
Sum of electronic and zero-point Energies= -587.778440
Sum of electronic and thermal Energies= -587.769685
Sum of electronic and thermal Enthalpies= -587.768741
Sum of electronic and thermal Free Energies= -587.813699
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-588.04279255

H_2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.118603
2	1	0	0.000000	0.760019	-0.474413
3	1	0	0.000000	-0.760019	-0.474413

Zero-point correction= 0.021592 (Hartree/Particle)
Thermal correction to Energy= 0.024427
Thermal correction to Enthalpy= 0.025371
Thermal correction to Gibbs Free Energy= 0.003941
Sum of electronic and zero-point Energies= -76.354307
Sum of electronic and thermal Energies= -76.351472
Sum of electronic and thermal Enthalpies= -76.350528
Sum of electronic and thermal Free Energies= -76.371959
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-76.43003606

CO_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000068
2	8	0	0.000000	1.164100	-0.000026
3	8	0	0.000000	-1.164100	-0.000026

Zero-point correction= 0.010444 (Hartree/Particle)
Thermal correction to Energy= 0.013410
Thermal correction to Enthalpy= 0.014354
Thermal correction to Gibbs Free Energy= -0.004205
Sum of electronic and zero-point Energies= -188.491624
Sum of electronic and thermal Energies= -188.488659
Sum of electronic and thermal Enthalpies= -188.487715
Sum of electronic and thermal Free Energies= -188.506274
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-188.54989604

INT1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.067620	-0.466809	-1.198420
2	6	0	-2.388080	-1.588027	-0.596040
3	6	0	-2.486682	-1.453046	0.814781
4	6	0	-3.219130	-0.244839	1.101551
5	6	0	-3.601416	0.339718	-0.147991
6	45	0	-1.450224	0.236150	0.004490

7	1	0	0.107496	2.343295	-0.162782
8	8	0	-0.878721	2.326136	-0.082663
9	51	0	1.787879	-0.133327	0.000827
10	9	0	1.211306	-1.870462	0.017529
11	9	0	0.297852	0.145487	1.260824
12	9	0	2.939458	-0.266622	1.386574
13	9	0	1.781598	1.728440	-0.023613
14	9	0	2.939827	-0.303027	-1.380201
15	9	0	0.292685	0.130522	-1.252974
16	1	0	-1.995807	-2.089208	1.546588
17	1	0	-1.815477	-2.346980	-1.122554
18	1	0	-3.125788	-0.252584	-2.261458
19	1	0	-3.435718	0.149492	2.089462
20	1	0	-4.120049	1.285183	-0.278716
21	1	0	-1.093606	2.873614	0.690013

Zero-point correction= 0.126411 (Hartree/Particle)
Thermal correction to Energy= 0.142777
Thermal correction to Enthalpy= 0.143721
Thermal correction to Gibbs Free Energy= 0.082083
Sum of electronic and zero-point Energies= -983.287666
Sum of electronic and thermal Energies= -983.271300
Sum of electronic and thermal Enthalpies= -983.270356
Sum of electronic and thermal Free Energies= -983.331993
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-984.84033314

INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.838905	0.863260	-0.853436
2	6	0	-4.044998	0.141685	0.348795
3	6	0	-3.916242	1.063434	1.451613
4	6	0	-3.659795	2.361618	0.910955
5	6	0	-3.574585	2.239552	-0.510504
6	45	0	-2.075987	1.002385	0.371627
7	6	0	4.735535	2.216191	-2.245445
8	6	0	5.520948	1.485323	-1.358181
9	6	0	4.936855	0.864936	-0.262952
10	6	0	3.559055	0.989786	-0.058017
11	6	0	2.765226	1.713022	-0.956593
12	6	0	3.359641	2.326138	-2.047755
13	1	0	5.197112	2.695841	-3.106165
14	1	0	6.592064	1.395124	-1.522440
15	1	0	5.540008	0.288188	0.435160
16	1	0	1.685266	1.756506	-0.818096
17	1	0	2.749842	2.879949	-2.757967
18	6	0	2.689742	-1.125254	2.678026
19	6	0	2.943476	0.350626	1.082436
20	7	0	1.804963	0.645593	1.624630
21	8	0	3.545739	-0.680990	1.687261
22	8	0	1.609969	-0.301658	2.634418
23	8	0	2.872351	-2.031211	3.412058
24	1	0	0.448838	1.467480	1.282760
25	8	0	-0.399592	2.021823	1.139377
26	51	0	-0.461893	-1.548637	-0.848321
27	9	0	1.260838	-1.257888	-0.310383
28	9	0	-1.023751	-0.860004	0.897107
29	9	0	-0.611110	0.385385	-1.165057
30	9	0	-2.277815	-1.567725	-1.233990
31	9	0	-0.013609	-1.814524	-2.584433
32	9	0	-0.504174	-3.253132	-0.235567
33	1	0	-0.502793	2.574040	1.928813
34	1	0	-3.981116	0.808478	2.505044
35	1	0	-3.482450	3.268004	1.482321
36	1	0	-3.331873	3.035620	-1.207645
37	1	0	-3.769900	0.425529	-1.844553
38	1	0	-4.160606	-0.935403	0.423872

Zero-point correction= 0.247258 (Hartree/Particle)
Thermal correction to Energy= 0.273930
Thermal correction to Enthalpy= 0.274874
Thermal correction to Gibbs Free Energy= 0.188184
Sum of electronic and zero-point Energies= -1571.074292

Sum of electronic and thermal Energies= -1571.047620
Sum of electronic and thermal Enthalpies= -1571.046676
Sum of electronic and thermal Free Energies= -1571.133366
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-1572.89877546

TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.782490	0.839522	-0.823216
2	6	0	-3.968135	0.090678	0.357995
3	6	0	-3.842359	0.987266	1.482593
4	6	0	-3.614274	2.305135	0.975878
5	6	0	-3.534549	2.211226	-0.449515
6	45	0	-2.001926	1.009269	0.412402
7	6	0	4.440344	2.494923	-2.103372
8	6	0	5.251799	1.637048	-1.363853
9	6	0	4.716116	0.920924	-0.305330
10	6	0	3.360532	1.082800	0.011694
11	6	0	2.537716	1.938417	-0.736624
12	6	0	3.087607	2.642241	-1.794073
13	1	0	4.864465	3.049749	-2.937763
14	1	0	6.302803	1.523377	-1.617272
15	1	0	5.335718	0.242569	0.277236
16	1	0	1.474924	2.021279	-0.508820
17	1	0	2.461335	3.300329	-2.391489
18	6	0	2.596199	-1.283162	2.579211
19	6	0	2.801279	0.333356	1.098872
20	7	0	1.671933	0.534150	1.721264
21	8	0	3.428757	-0.714803	1.619447
22	8	0	1.488507	-0.489785	2.628892
23	8	0	2.819015	-2.242332	3.220436
24	1	0	0.734590	1.160622	1.503675
25	8	0	-0.367082	1.881294	1.184017
26	51	0	-0.388485	-1.536301	-0.907824
27	9	0	1.348299	-1.259925	-0.358145
28	9	0	-0.912901	-0.927655	0.858532
29	9	0	-0.519949	0.380348	-1.186798
30	9	0	-2.199690	-1.575190	-1.292630
31	9	0	0.086729	-1.775492	-2.642925
32	9	0	-0.387128	-3.263481	-0.350810
33	1	0	-0.514952	2.639928	1.766553
34	1	0	-3.896400	0.704648	2.529340
35	1	0	-3.469142	3.203544	1.567382
36	1	0	-3.314072	3.026021	-1.131977
37	1	0	-3.711271	0.427581	-1.824435
38	1	0	-4.062669	-0.989131	0.410790

Zero-point correction= 0.243626 (Hartree/Particle)
Thermal correction to Energy= 0.269651
Thermal correction to Enthalpy= 0.270595
Thermal correction to Gibbs Free Energy= 0.186174
Sum of electronic and zero-point Energies= -1571.072614
Sum of electronic and thermal Energies= -1571.046589
Sum of electronic and thermal Enthalpies= -1571.045645
Sum of electronic and thermal Free Energies= -1571.130065
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-1572.88084620

INT3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.717102	-0.887682	-0.855363
2	6	0	3.974731	-0.010501	0.217515
3	6	0	3.927864	-0.773057	1.441779
4	6	0	3.677632	-2.140785	1.105309
5	6	0	3.504264	-2.207979	-0.313741
6	45	0	2.017941	-0.926220	0.512710
7	6	0	-4.015386	-2.956742	-1.955024
8	6	0	-4.880910	-1.950817	-1.529463
9	6	0	-4.484626	-1.076983	-0.530839
10	6	0	-3.212441	-1.225354	0.042147
11	6	0	-2.334809	-2.233332	-0.389520

12	6	0	-2.746847	-3.096057	-1.389559
13	1	0	-4.330675	-3.639386	-2.741510
14	1	0	-5.864588	-1.847589	-1.980302
15	1	0	-5.146811	-0.283544	-0.191764
16	1	0	-1.337397	-2.320794	0.042730
17	1	0	-2.079020	-3.879533	-1.739163
18	6	0	-2.832883	1.486245	2.340412
19	6	0	-2.805280	-0.312445	1.065404
20	7	0	-1.733938	-0.351746	1.817154
21	8	0	-3.537815	0.739911	1.397105
22	8	0	-1.695721	0.778730	2.601818
23	8	0	-3.170124	2.502014	2.821997
24	1	0	-0.798901	-0.886398	1.725303
25	8	0	0.460814	-1.689774	1.476849
26	51	0	0.326895	1.499468	-0.963020
27	9	0	-1.392026	1.324860	-0.308349
28	9	0	0.937669	1.071329	0.822351
29	9	0	0.400984	-0.431899	-1.042902
30	9	0	2.109170	1.470829	-1.462510
31	9	0	-0.247311	1.571085	-2.684496
32	9	0	0.373433	3.275579	-0.591184
33	1	0	0.665651	-2.384184	2.119445
34	1	0	4.047279	-0.372709	2.443741
35	1	0	3.584170	-2.966793	1.803070
36	1	0	3.249445	-3.095470	-0.884242
37	1	0	3.578117	-0.592306	-1.889903
38	1	0	4.066348	1.067812	0.141920

Zero-point correction= 0.247438 (Hartree/Particle)
Thermal correction to Energy= 0.273694
Thermal correction to Enthalpy= 0.274638
Thermal correction to Gibbs Free Energy= 0.189803
Sum of electronic and zero-point Energies= -1571.069509
Sum of electronic and thermal Energies= -1571.043252
Sum of electronic and thermal Enthalpies= -1571.042308
Sum of electronic and thermal Free Energies= -1571.127144
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-1572.87897873

INT4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.557779	-3.630080	0.024945
2	6	0	3.657104	-2.857997	0.406528
3	6	0	3.588792	-1.478495	0.338272
4	6	0	2.408523	-0.875832	-0.131254
5	6	0	1.308314	-1.651652	-0.528240
6	6	0	1.388323	-3.029507	-0.436163
7	1	0	2.615929	-4.714710	0.093722
8	1	0	4.564637	-3.337363	0.765424
9	1	0	4.432287	-0.863943	0.644882
10	1	0	0.388866	-1.196036	-0.876405
11	1	0	0.521914	-3.623969	-0.715180
12	6	0	2.972961	2.651430	0.076753
13	6	0	2.331325	0.550126	-0.176816
14	7	0	1.365799	1.317530	-0.609991
15	8	0	3.342532	1.320196	0.230640
16	8	0	1.718305	2.636198	-0.449731
17	8	0	3.626607	3.592108	0.344652
18	1	0	0.351919	1.107007	-0.887666
19	9	0	-0.484290	0.049442	1.056015
20	51	0	-2.086223	0.037529	0.096113
21	9	0	-3.070973	-0.435278	1.557358
22	9	0	-0.909913	0.528620	-1.381656
23	9	0	-1.703178	-1.717518	-0.363224
24	9	0	-2.201934	1.844079	0.406658
25	9	0	-3.498273	0.068028	-1.064623

Zero-point correction= 0.148177 (Hartree/Particle)
Thermal correction to Energy= 0.166548
Thermal correction to Enthalpy= 0.167492
Thermal correction to Gibbs Free Energy= 0.099904
Sum of electronic and zero-point Energies= -1192.705997
Sum of electronic and thermal Energies= -1192.687626

Sum of electronic and thermal Enthalpies= -1192.686682
Sum of electronic and thermal Free Energies= -1192.754270
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-1193.21071413

INT5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.249093	0.138159	0.253702
2	6	0	-3.297718	-0.448203	0.571317
3	6	0	-2.571310	-1.550976	0.056748
4	6	0	-2.091582	-1.186441	-1.260384
5	6	0	-2.553926	0.117145	-1.562993
6	6	0	-3.251233	0.601613	-0.422467
7	6	0	3.113094	-1.695655	-0.144211
8	6	0	2.107606	-0.751339	-0.232606
9	6	0	4.445650	-1.285984	-0.037421
10	6	0	4.776932	0.066180	-0.028273
11	6	0	3.770918	1.014973	-0.126057
12	6	0	2.428711	0.615196	-0.218251
13	6	0	1.442827	1.664316	-0.332044
14	1	0	2.872327	-2.756177	-0.158964
15	1	0	5.232165	-2.034590	0.035452
16	1	0	5.816226	0.375332	0.049622
17	1	0	4.015125	2.077295	-0.126530
18	1	0	1.852229	2.688111	-0.419875
19	8	0	0.211492	1.568335	-0.376962
20	1	0	1.066178	-1.063207	-0.319436
21	8	0	-0.250249	0.207601	1.862764
22	1	0	-3.666445	1.597805	-0.306305
23	1	0	-2.309585	0.692439	-2.449023
24	1	0	-1.470281	-1.807168	-1.898074
25	1	0	-2.394535	-2.497569	0.556521
26	1	0	-3.780325	-0.384077	1.540654
27	1	0	-0.633650	-0.277796	2.612791

Zero-point correction= 0.210202 (Hartree/Particle)
Thermal correction to Energy= 0.224463
Thermal correction to Enthalpy= 0.225407
Thermal correction to Gibbs Free Energy= 0.166512
Sum of electronic and zero-point Energies= -723.544293
Sum of electronic and thermal Energies= -723.530032
Sum of electronic and thermal Enthalpies= -723.529088
Sum of electronic and thermal Free Energies= -723.587983
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-725.08400597

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.852175	0.147882	0.180744
2	6	0	-2.936491	-0.574567	0.309883
3	6	0	-2.017588	-1.654030	0.088222
4	6	0	-1.411327	-1.455391	-1.206772
5	6	0	-1.883620	-0.230682	-1.723993
6	6	0	-2.824067	0.324132	-0.775126
7	6	0	1.951783	-1.485163	0.618950
8	6	0	1.333218	-0.241070	0.493231
9	6	0	3.243686	-1.685111	0.123952
10	6	0	3.931577	-0.643769	-0.492159
11	6	0	3.334579	0.610748	-0.635331
12	6	0	2.039602	0.796454	-0.167610
13	6	0	1.312259	2.038508	-0.386287
14	1	0	1.444480	-2.296081	1.142087
15	1	0	3.722362	-2.656132	0.233425
16	1	0	4.941008	-0.806944	-0.863128
17	1	0	3.868879	1.424432	-1.125105
18	1	0	1.859569	2.952969	-0.672514
19	8	0	0.085346	2.091450	-0.283755
20	1	0	0.647267	0.156029	1.487531
21	8	0	-0.435464	0.799107	2.118068
22	1	0	-3.333716	1.276896	-0.870905
23	1	0	-1.579069	0.232029	-2.656507

24	1	0	-0.667843	-2.099559	-1.664416
25	1	0	-1.868441	-2.510426	0.737345
26	1	0	-3.532243	-0.418294	1.203033
27	1	0	-0.795096	0.165585	2.759418

Zero-point correction= 0.204721 (Hartree/Particle)
Thermal correction to Energy= 0.218159
Thermal correction to Enthalpy= 0.219103
Thermal correction to Gibbs Free Energy= 0.164316
Sum of electronic and zero-point Energies= -723.514103
Sum of electronic and thermal Energies= -723.500666
Sum of electronic and thermal Enthalpies= -723.499721
Sum of electronic and thermal Free Energies= -723.554508
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-725.04109840

INT6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.780820	0.166171	0.144076
2	6	0	-3.045407	-0.348453	0.382161
3	6	0	-2.155884	-1.501544	0.395479
4	6	0	-1.528808	-1.587864	-0.877425
5	6	0	-1.876930	-0.403396	-1.596912
6	6	0	-2.880749	0.315552	-0.825254
7	6	0	1.753679	-1.583426	0.253645
8	6	0	1.172951	-0.351737	-0.008768
9	6	0	3.143146	-1.727342	0.151742
10	6	0	3.963684	-0.656405	-0.202240
11	6	0	3.398922	0.585196	-0.451553
12	6	0	2.009424	0.735316	-0.354202
13	6	0	1.326440	1.979789	-0.558159
14	1	0	1.148399	-2.445340	0.535558
15	1	0	3.590911	-2.700589	0.347876
16	1	0	5.038982	-0.796392	-0.279001
17	1	0	4.021373	1.439516	-0.717816
18	1	0	1.879956	2.900971	-0.802554
19	8	0	0.089545	2.047171	-0.454359
20	1	0	0.336982	0.203048	2.680004
21	8	0	-0.122298	0.884461	2.165513
22	1	0	-3.343254	1.251838	-1.117229
23	1	0	-1.543890	-0.141989	-2.595950
24	1	0	-0.839227	-2.355741	-1.210575
25	1	0	-2.082238	-2.234473	1.192390
26	1	0	-3.675491	-0.033518	1.207257
27	1	0	-0.816372	1.247789	2.736319

Zero-point correction= 0.210321 (Hartree/Particle)
Thermal correction to Energy= 0.224675
Thermal correction to Enthalpy= 0.225619
Thermal correction to Gibbs Free Energy= 0.169437
Sum of electronic and zero-point Energies= -723.567237
Sum of electronic and thermal Energies= -723.552883
Sum of electronic and thermal Enthalpies= -723.551939
Sum of electronic and thermal Free Energies= -723.608121
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-725.09970673

INT7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.864397	-0.987140	0.135590
2	6	0	0.577442	-2.669160	1.718241
3	6	0	1.720793	-1.799456	1.954416
4	6	0	2.649388	-1.998052	0.892155
5	6	0	2.009949	-2.819510	-0.077987
6	6	0	0.750810	-3.284022	0.484539
7	6	0	2.874830	1.343186	0.030424
8	6	0	1.902149	0.589582	-0.609801
9	6	0	3.475281	2.408432	-0.646528
10	6	0	3.113578	2.745364	-1.953665
11	6	0	2.128282	2.017605	-2.596927
12	6	0	1.523188	0.943382	-1.925071

13	6	0	0.471705	0.152948	-2.481251
14	1	0	3.167681	1.128836	1.058149
15	1	0	4.243120	2.990795	-0.139207
16	1	0	3.599473	3.578735	-2.454843
17	1	0	1.816426	2.269799	-3.610535
18	6	0	-1.717541	0.907691	0.774239
19	8	0	-1.935299	2.035475	1.471376
20	7	0	-0.491284	0.491519	0.909964
21	6	0	-0.762023	2.361637	2.120739
22	8	0	0.129032	1.390648	1.785660
23	8	0	-0.578785	3.290061	2.824421
24	1	0	0.077167	0.355803	-3.490317
25	8	0	-0.035563	-0.780300	-1.830051
26	6	0	-2.808575	0.326483	0.025684
27	6	0	-3.946625	1.108555	-0.218375
28	6	0	-2.749964	-0.999394	-0.424774
29	6	0	-5.008748	0.567543	-0.926501
30	1	0	-3.991478	2.132643	0.145345
31	6	0	-3.819863	-1.530019	-1.126328
32	1	0	-1.873084	-1.609468	-0.213256
33	6	0	-4.945386	-0.747569	-1.380620
34	1	0	-5.891186	1.172203	-1.121225
35	1	0	-3.782212	-2.559846	-1.473598
36	1	0	-5.782988	-1.169801	-1.931995
37	1	0	0.045458	-3.938358	-0.016426
38	1	0	2.434263	-3.139133	-1.023795
39	1	0	3.618435	-1.522449	0.787304
40	1	0	1.882668	-1.194490	2.841336
41	1	0	-0.289707	-2.753020	2.364854

Zero-point correction= 0.306269 (Hartree/Particle)
Thermal correction to Energy= 0.328317
Thermal correction to Enthalpy= 0.329261
Thermal correction to Gibbs Free Energy= 0.252826
Sum of electronic and zero-point Energies= -1234.988109
Sum of electronic and thermal Energies= -1234.966061
Sum of electronic and thermal Enthalpies= -1234.965117
Sum of electronic and thermal Free Energies= -1235.041551
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-1236.72043652

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.061608	-0.840722	0.134272
2	6	0	-2.341475	-2.387472	-1.057871
3	6	0	-2.991351	-1.104094	-0.872809
4	6	0	-3.259392	-0.938409	0.520535
5	6	0	-2.628763	-2.009796	1.196582
6	6	0	-2.104147	-2.931125	0.201708
7	6	0	-1.523758	2.158916	0.615837
8	6	0	-0.822901	1.006173	0.931388
9	6	0	-1.161609	3.366474	1.221669
10	6	0	-0.111786	3.439394	2.140629
11	6	0	0.592272	2.293513	2.467274
12	6	0	0.238615	1.076036	1.864068
13	6	0	0.904038	-0.164315	2.113239
14	1	0	-2.340862	2.143294	-0.105484
15	1	0	-1.711418	4.270806	0.965624
16	1	0	0.148464	4.392915	2.592996
17	1	0	1.415133	2.325857	3.181483
18	6	0	1.222299	0.459943	-1.378301
19	8	0	1.322084	1.642270	-1.755047
20	7	0	0.088158	-0.263032	-1.386777
21	6	0	-0.381407	2.140335	-2.404387
22	8	0	-0.945891	1.059400	-2.335489
23	8	0	-0.359721	3.279205	-2.651321
24	1	0	1.743973	-0.237178	2.822807
25	8	0	0.545759	-1.202482	1.523312
26	6	0	2.373470	-0.299250	-0.840646
27	6	0	3.330136	0.431488	-0.125793
28	6	0	2.482383	-1.687014	-0.976216
29	6	0	4.391515	-0.239072	0.465450
30	1	0	3.232593	1.513342	-0.053095

31	6	0	3.551659	-2.344704	-0.382958
32	1	0	1.746782	-2.238477	-1.558726
33	6	0	4.497306	-1.624707	0.342780
34	1	0	5.148755	0.320176	1.010898
35	1	0	3.653425	-3.421760	-0.493777
36	1	0	5.333924	-2.144830	0.804882
37	1	0	-1.571445	-3.850359	0.419281
38	1	0	-2.603586	-2.160721	2.270720
39	1	0	-3.760081	-0.093931	0.981652
40	1	0	-3.301922	-0.433660	-1.668110
41	1	0	-2.018967	-2.792783	-2.010648

Zero-point correction= 0.301470 (Hartree/Particle)
Thermal correction to Energy= 0.324239
Thermal correction to Enthalpy= 0.325184
Thermal correction to Gibbs Free Energy= 0.247247
Sum of electronic and zero-point Energies= -1234.937163
Sum of electronic and thermal Energies= -1234.914394
Sum of electronic and thermal Enthalpies= -1234.913450
Sum of electronic and thermal Free Energies= -1234.991387
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-1236.67150336

INT8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.444674	-0.325087	-0.003932
2	6	0	-3.221715	-1.351308	-1.008191
3	6	0	-3.003947	-0.038103	-1.539226
4	6	0	-3.298643	0.909971	-0.494004
5	6	0	-3.587731	0.187541	0.677445
6	6	0	-3.529038	-1.219695	0.364824
7	6	0	-0.208669	2.337815	-1.007240
8	6	0	-0.320614	1.392080	-0.003866
9	6	0	0.667584	3.414745	-0.830675
10	6	0	1.427144	3.557293	0.332475
11	6	0	1.319055	2.615124	1.342095
12	6	0	0.444986	1.531043	1.175486
13	6	0	0.283686	0.479371	2.130995
14	1	0	-0.772988	2.250388	-1.935080
15	1	0	0.758399	4.157615	-1.621705
16	1	0	2.100586	4.403565	0.441431
17	1	0	1.907022	2.701486	2.255537
18	6	0	0.961678	-1.907560	-0.194790
19	8	0	0.646259	-2.917480	0.433640
20	7	0	-0.148548	-1.400267	-0.832705
21	1	0	0.823505	0.481114	3.090416
22	8	0	-0.477321	-0.478388	1.894034
23	6	0	2.296558	-1.334641	-0.340545
24	6	0	3.355213	-1.952883	0.331819
25	6	0	2.516397	-0.196981	-1.124231
26	6	0	4.632931	-1.422545	0.227148
27	1	0	3.155199	-2.844280	0.924116
28	6	0	3.796481	0.327374	-1.225405
29	1	0	1.687226	0.267515	-1.659423
30	6	0	4.851112	-0.285272	-0.549392
31	1	0	5.463464	-1.898333	0.743809
32	1	0	3.977984	1.209419	-1.835919
33	1	0	5.855541	0.125295	-0.634043
34	1	0	-3.799179	0.609513	1.654010
35	1	0	-3.685422	-2.031046	1.067405
36	1	0	-3.062367	-2.282227	-1.541992
37	1	0	-2.761386	0.197954	-2.570050
38	1	0	-3.243724	1.989538	-0.582344

Zero-point correction= 0.288909 (Hartree/Particle)
Thermal correction to Energy= 0.308891
Thermal correction to Enthalpy= 0.309835
Thermal correction to Gibbs Free Energy= 0.239215
Sum of electronic and zero-point Energies= -1046.470909
Sum of electronic and thermal Energies= -1046.450927
Sum of electronic and thermal Enthalpies= -1046.449983
Sum of electronic and thermal Free Energies= -1046.520603
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-1048.15080472

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.603105	-0.289908	0.056423
2	6	0	-3.420918	-1.278888	-0.813556
3	6	0	-3.261692	0.064703	-1.294962
4	6	0	-3.445457	0.957350	-0.176922
5	6	0	-3.598876	0.173114	0.982430
6	6	0	-3.568406	-1.216975	0.589099
7	6	0	-0.074685	2.172991	-1.152769
8	6	0	-0.182073	1.248718	-0.126940
9	6	0	0.786931	3.264270	-0.989118
10	6	0	1.562408	3.404593	0.161903
11	6	0	1.490395	2.450859	1.172570
12	6	0	0.619578	1.368129	1.027473
13	6	0	0.481226	0.307226	1.995518
14	1	0	-0.643265	2.052464	-2.074048
15	1	0	0.859918	4.009071	-1.779736
16	1	0	2.230678	4.256237	0.263937
17	1	0	2.101509	2.542908	2.070313
18	6	0	0.954741	-1.575002	-0.685916
19	8	0	0.524307	-2.730438	-0.702435
20	7	0	-0.101866	-0.781114	-1.058746
21	1	0	1.131276	0.274684	2.885812
22	8	0	-0.350670	-0.597086	1.835640
23	6	0	2.339261	-1.172791	-0.456061
24	6	0	3.158608	-2.078316	0.228169
25	6	0	2.856782	0.038943	-0.924369
26	6	0	4.486226	-1.755232	0.468123
27	1	0	2.739147	-3.025637	0.562741
28	6	0	4.188657	0.349200	-0.691466
29	1	0	2.222159	0.719633	-1.490339
30	6	0	4.998996	-0.543146	0.009112
31	1	0	5.126526	-2.451210	1.005257
32	1	0	4.601506	1.283960	-1.065603
33	1	0	6.043180	-0.295701	0.190551
34	1	0	-3.706815	0.539614	1.997156
35	1	0	-3.639341	-2.065006	1.261540
36	1	0	-3.323990	-2.181176	-1.407762
37	1	0	-3.117249	0.355200	-2.330433
38	1	0	-3.391753	2.040304	-0.216735

Zero-point correction= 0.287778 (Hartree/Particle)
Thermal correction to Energy= 0.307365
Thermal correction to Enthalpy= 0.308309
Thermal correction to Gibbs Free Energy= 0.238243
Sum of electronic and zero-point Energies= -1046.462697
Sum of electronic and thermal Energies= -1046.443109
Sum of electronic and thermal Enthalpies= -1046.442165
Sum of electronic and thermal Free Energies= -1046.512231
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-1048.13672333

INT9

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.026762	-1.537334	0.043548
2	6	0	2.087087	-1.884824	0.489409
3	6	0	1.897022	-1.892042	-0.919650
4	6	0	1.012813	-2.978511	-1.231489
5	6	0	0.672454	-3.641789	-0.011190
6	6	0	1.324350	-2.969499	1.050873
7	6	0	-1.855272	2.308446	-0.693434
8	6	0	-1.715021	0.969945	-0.251670
9	6	0	-3.044828	2.985624	-0.538250
10	6	0	-4.162144	2.379458	0.061004
11	6	0	-4.058890	1.080001	0.495758
12	6	0	-2.856858	0.352715	0.353267
13	6	0	-2.856779	-0.984480	0.824038
14	1	0	-1.016203	2.806314	-1.174077
15	1	0	-3.115841	4.012174	-0.892240

16	1	0	-5.091921	2.930332	0.173616
17	1	0	-4.911277	0.584140	0.959253
18	6	0	0.550330	0.991566	-1.088455
19	8	0	0.622965	0.902000	-2.292139
20	7	0	-0.529408	0.314888	-0.392092
21	1	0	-3.794426	-1.350165	1.272824
22	8	0	-1.917256	-1.809116	0.790988
23	6	0	1.538497	1.687849	-0.242041
24	6	0	1.379503	1.841683	1.141495
25	6	0	2.667189	2.220577	-0.878243
26	6	0	2.344445	2.516396	1.877204
27	1	0	0.499164	1.437291	1.639344
28	6	0	3.630712	2.888807	-0.137594
29	1	0	2.764265	2.103242	-1.956050
30	6	0	3.469319	3.036106	1.239089
31	1	0	2.219405	2.642670	2.950497
32	1	0	4.507929	3.300741	-0.631580
33	1	0	4.223927	3.563744	1.819243
34	1	0	-0.023832	-4.467255	0.088330
35	1	0	1.232308	-3.200525	2.106392
36	1	0	2.670578	-1.160399	1.049285
37	1	0	2.320948	-1.192152	-1.632906
38	1	0	0.635860	-3.225540	-2.218456

Zero-point correction= 0.292173 (Hartree/Particle)
Thermal correction to Energy= 0.311473
Thermal correction to Enthalpy= 0.312417
Thermal correction to Gibbs Free Energy= 0.242106
Sum of electronic and zero-point Energies= -1046.576800
Sum of electronic and thermal Energies= -1046.557500
Sum of electronic and thermal Enthalpies= -1046.556556
Sum of electronic and thermal Free Energies= -1046.626867
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-1048.25705120

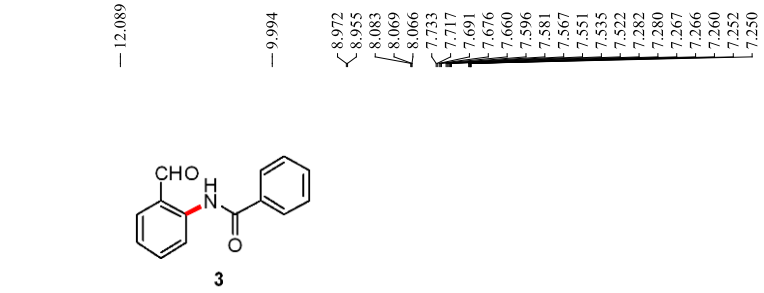
TS5

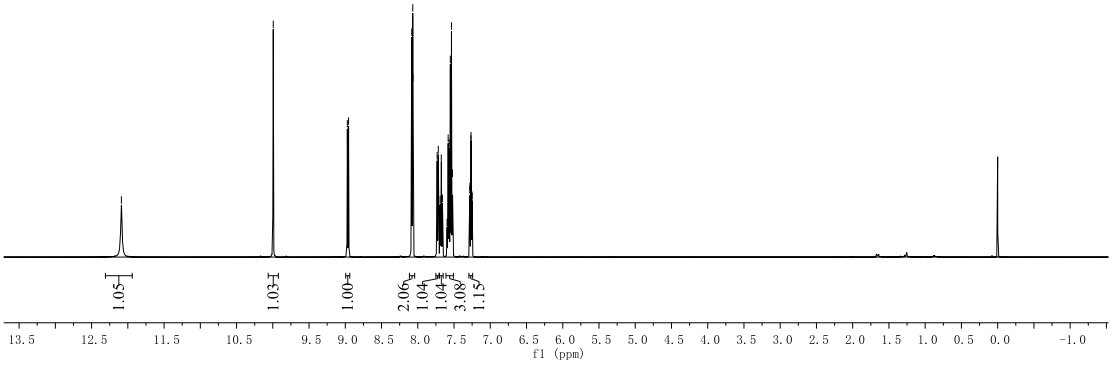
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.059873	-1.386307	-0.126633
2	6	0	-1.292407	-1.561935	1.683614
3	6	0	-2.114781	-1.593065	0.506307
4	6	0	-1.754889	-2.762709	-0.242229
5	6	0	-0.681263	-3.401491	0.429776
6	6	0	-0.392562	-2.655959	1.630123
7	6	0	2.915511	-1.114366	-0.677823
8	1	0	3.750778	3.879864	0.854003
9	6	0	3.557897	2.862817	0.518536
10	6	0	4.620232	2.045918	0.129007
11	1	0	5.643218	2.410516	0.161043
12	6	0	4.340706	0.766030	-0.295821
13	1	0	5.150172	0.101109	-0.595832
14	6	0	3.017392	0.273729	-0.334275
15	6	0	1.938955	1.120101	0.038104
16	7	0	0.588216	0.741045	-0.151672
17	6	0	2.246169	2.412289	0.473044
18	1	0	1.447320	3.085341	0.767934
19	1	0	3.864562	-1.590725	-0.981176
20	8	0	1.930380	-1.868863	-0.646773
21	6	0	-0.389192	1.372427	0.708565
22	8	0	-0.123157	1.566704	1.875971
23	6	0	-1.713265	1.685318	0.125407
24	6	0	-2.747433	1.939846	1.039387
25	6	0	-1.975670	1.753352	-1.247828
26	6	0	-4.029146	2.215429	0.588396
27	1	0	-2.521147	1.919101	2.104028
28	6	0	-3.260063	2.039402	-1.694315
29	1	0	-1.192710	1.578969	-1.980190
30	6	0	-4.287367	2.260231	-0.781308
31	1	0	-4.827707	2.403279	1.302898
32	1	0	-3.457943	2.094104	-2.762492
33	1	0	-5.291990	2.479659	-1.137577
34	1	0	0.384341	-2.880721	2.352060
35	1	0	-0.136636	-4.271483	0.077823
36	1	0	-2.161110	-3.046576	-1.207211

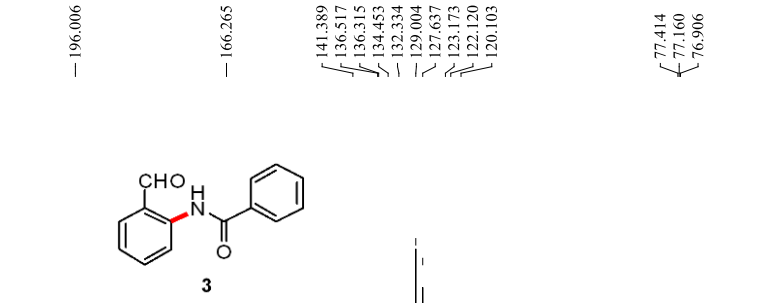
37	1	0	-2.882234	-0.871722	0.241290
38	1	0	-1.283548	-0.773756	2.431261
39	1	0	0.305905	0.427602	-1.282012
40	8	0	-0.150758	-0.540756	-2.050284
41	1	0	0.540835	-0.948933	-2.596955

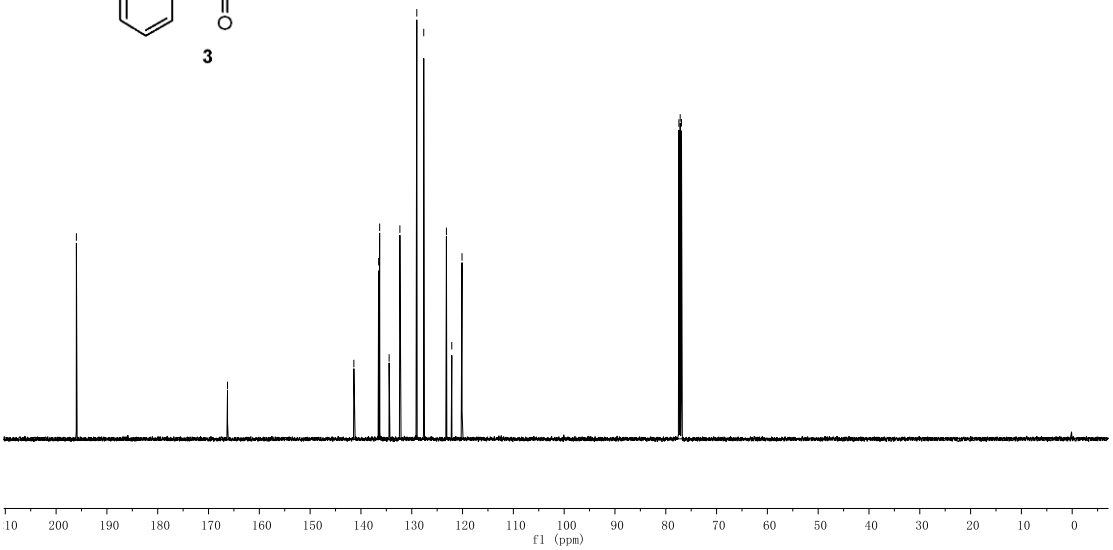
Zero-point correction= 0.314277 (Hartree/Particle)
Thermal correction to Energy= 0.334814
Thermal correction to Enthalpy= 0.335758
Thermal correction to Gibbs Free Energy= 0.265008
Sum of electronic and zero-point Energies= -1122.925381
Sum of electronic and thermal Energies= -1122.904844
Sum of electronic and thermal Enthalpies= -1122.903900
Sum of electronic and thermal Free Energies= -1122.974651
M06/6-311++G(d,p)-SDD/SMD//M06/6-31G(d)-LANL2DZ energy=-1124.66476460

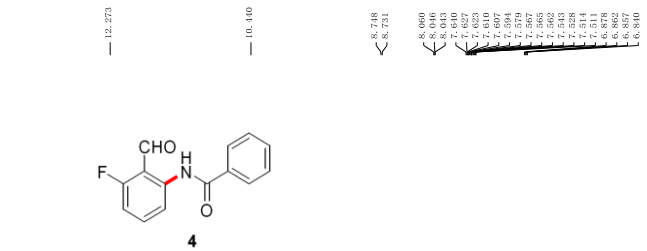
12 ^{1}H NMR and ^{13}C NMR Spectra of the products





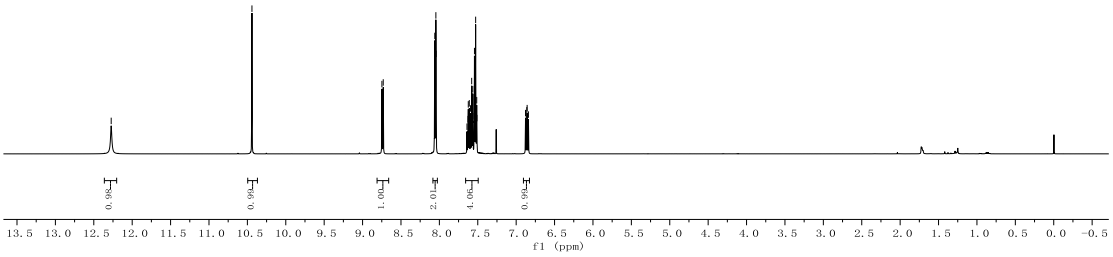


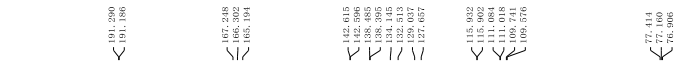


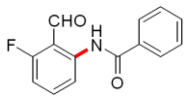

12.273
10.440
8.748
8.731
8.060
8.046
8.043
7.640
7.627
7.623
7.610
7.607
7.594
7.579
7.567
7.565
7.562
7.543
7.528
7.514
7.511
6.878
6.862
6.857
6.840

CHO
H
N
F
O

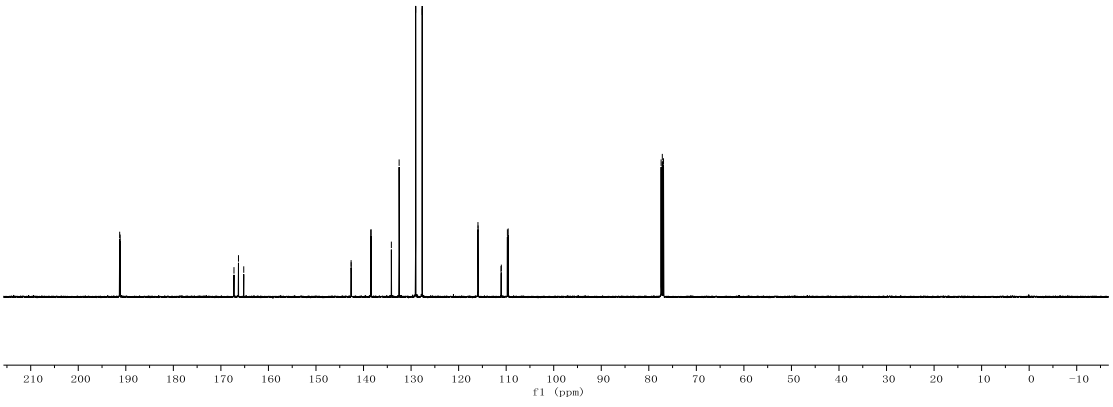
4

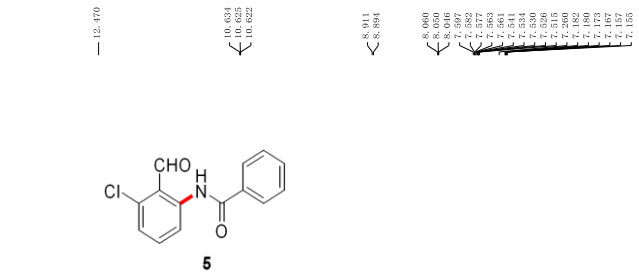

0.98
0.99
1.00
2.01
4.06
0.99
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)


191.290
191.186
167.248
166.302
165.194
142.615
142.596
138.485
138.395
134.145
132.513
129.037
127.657
115.932
115.902
111.084
111.018
109.741
109.576
77.414
77.160
76.906


CHO
H
N
F
O

4


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


12.470
10.634
10.625
10.622
8.911
8.894
8.060
8.056
8.046
7.597
7.582
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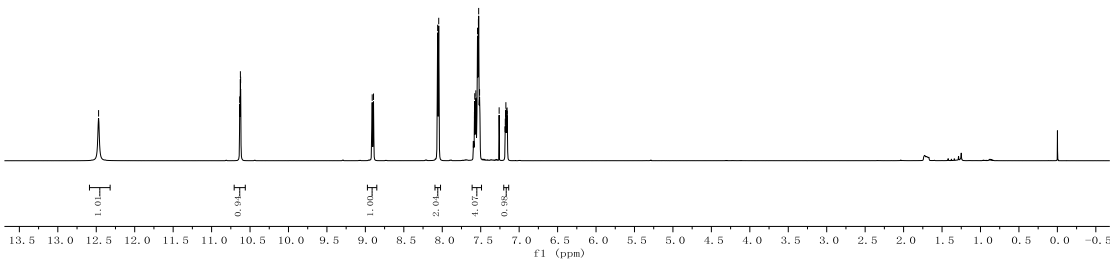
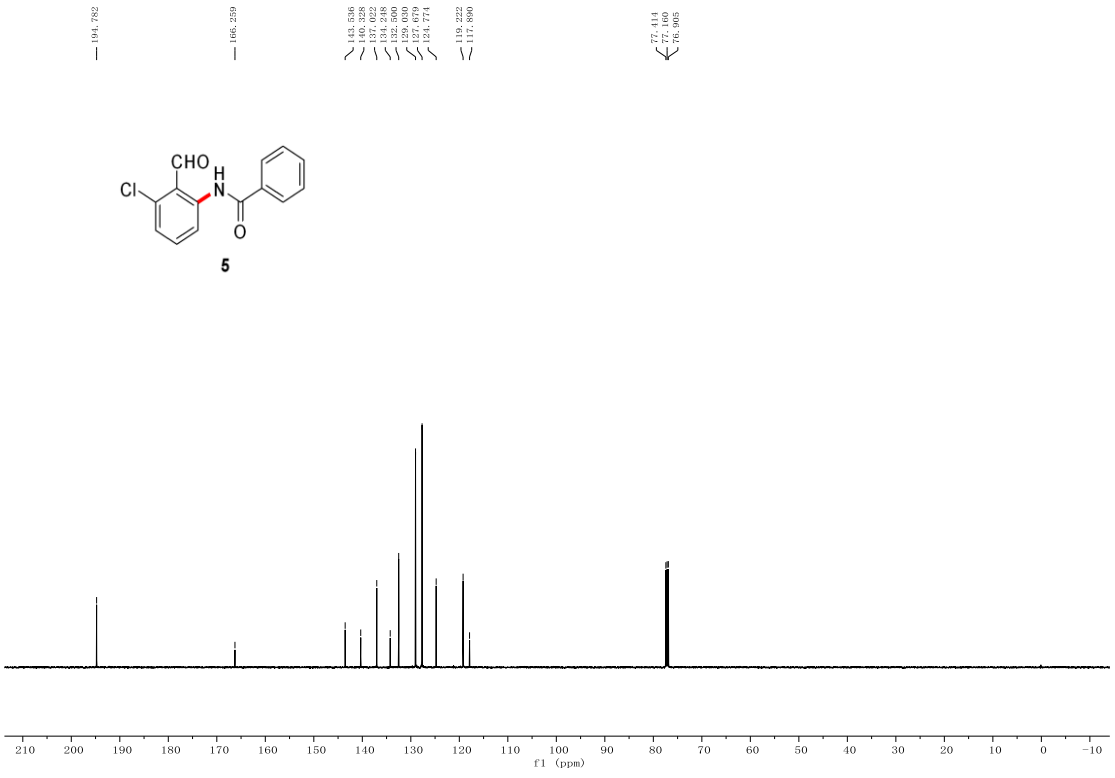
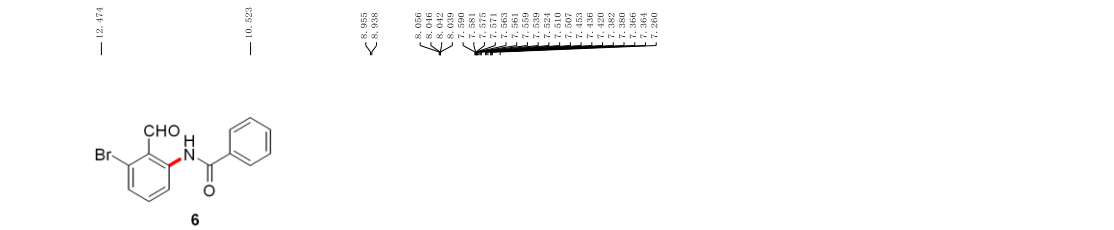
7.565
7.561
7.541
7.534
7.530
7.526
7.515
7.280
7.195
7.180
7.173
7.167
7.157
7.155
CHO
H
N
Cl
O

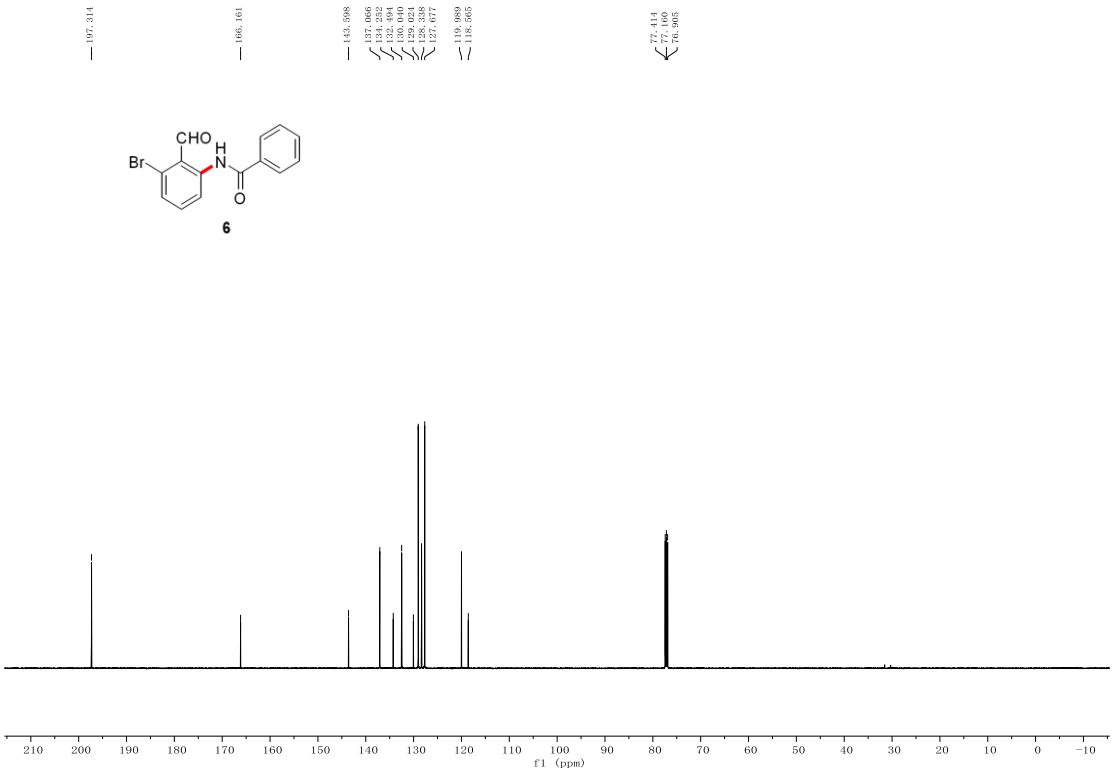
5

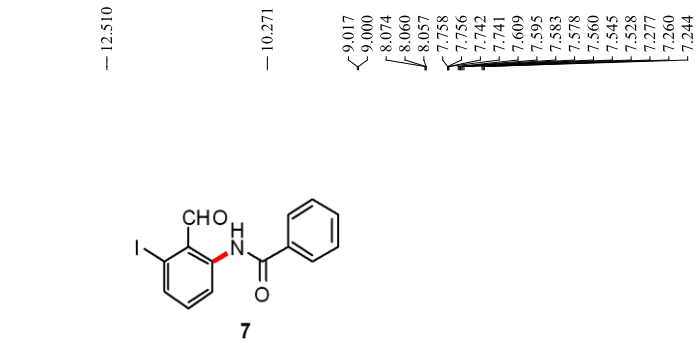

1.01
0.94
1.00
2.04
4.07
0.98
f1 (ppm)


194.782
166.259
143.536
140.328
137.022
134.248
132.580
129.030
127.679
124.774
119.222
117.890
77.414
77.160
76.905
CHO
H
N
Cl
O
f1 (ppm)

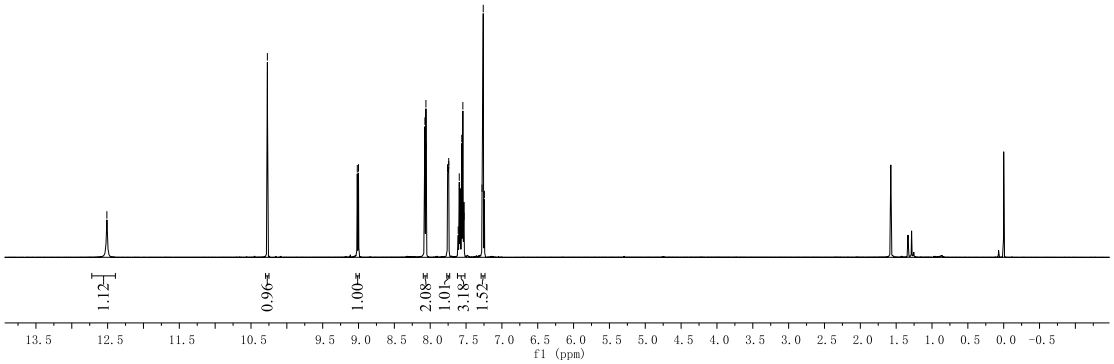
5

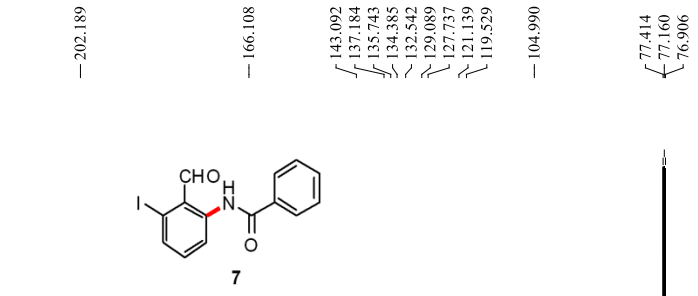

12.474
10.523
8.955
8.938
8.056
8.046
8.042
8.032
7.599
7.581
7.575
7.571
7.565
7.561
7.559
7.539
7.534
7.510
7.507
7.453
7.436
7.429
7.382
7.380
7.366
7.364
7.360
CHO
H
N
Br
O
6
1.04
0.93
1.00
2.06
3.10
1.03
1.01
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)


197.314
166.161
143.598
137.066
135.252
132.494
130.040
129.024
128.598
127.677
119.989
118.565
77.414
77.160
76.905
CHO
H
N
Br
O
6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


12.510
10.271
9.017
9.000
8.074
8.060
8.057
7.758
7.756
7.742
7.741
7.609
7.595
7.583
7.578
7.560
7.545
7.528
7.277
7.260
7.244
CHO
H
N
I
O

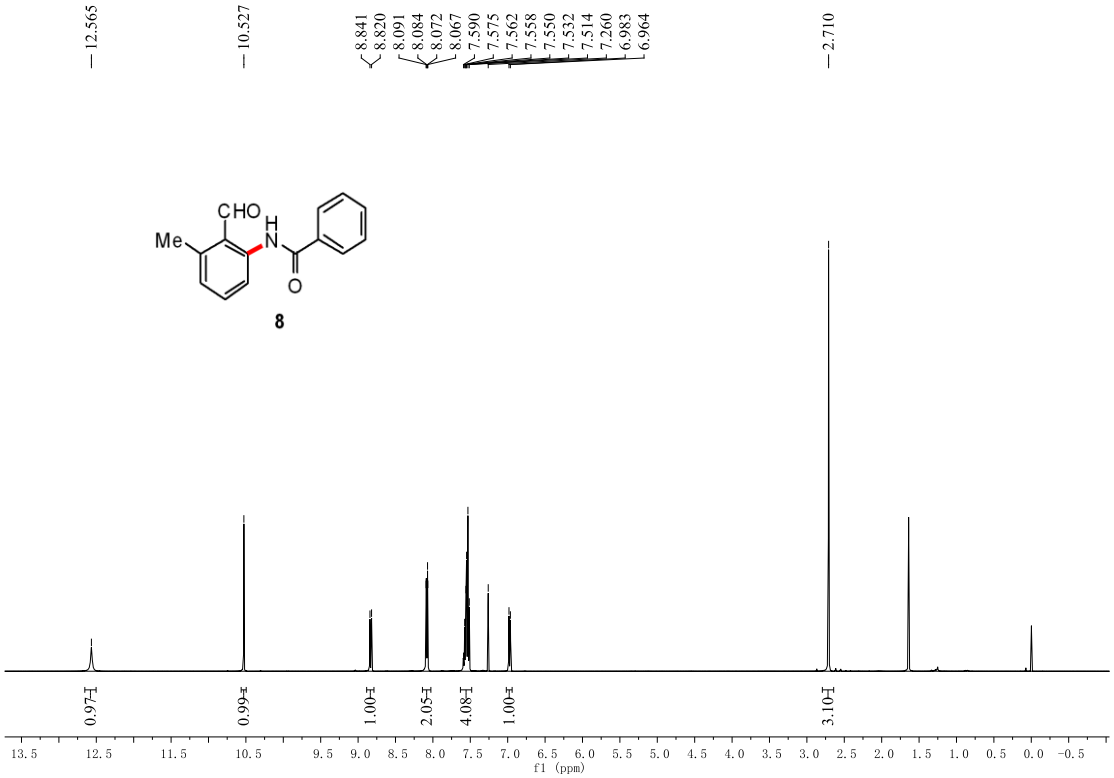
7

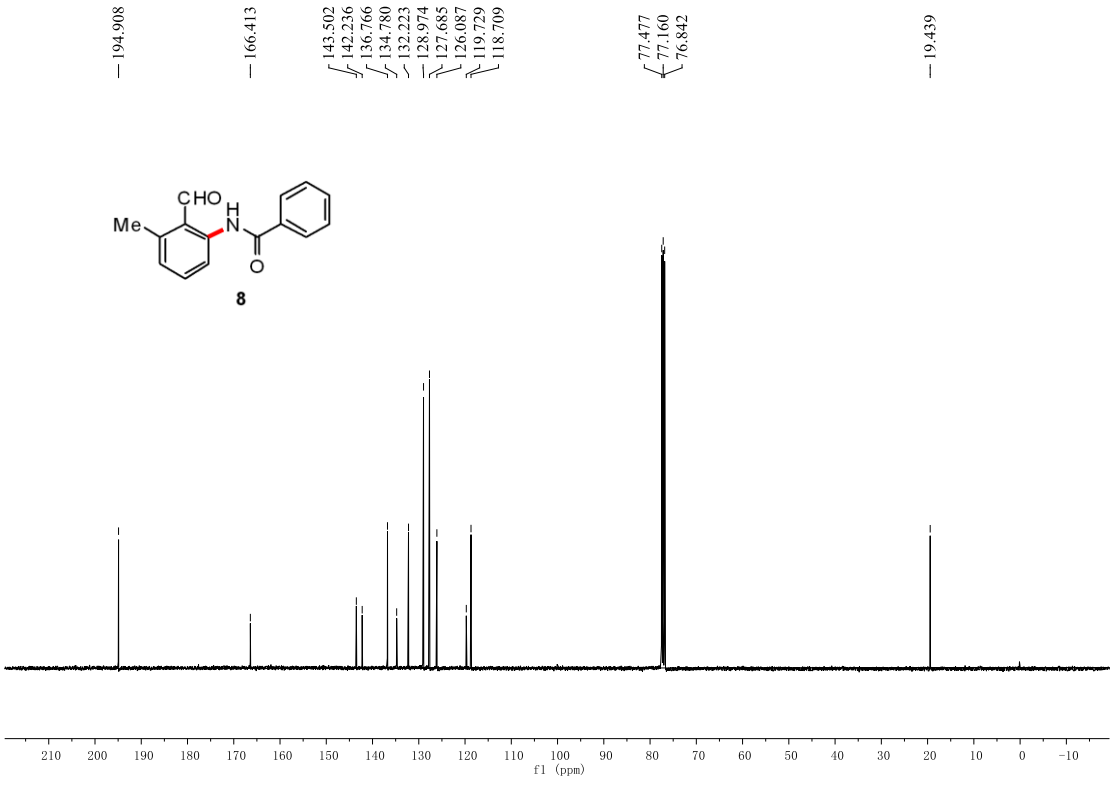

1.12
0.96
1.00
2.08
1.01
3.18
1.52
f1 (ppm)

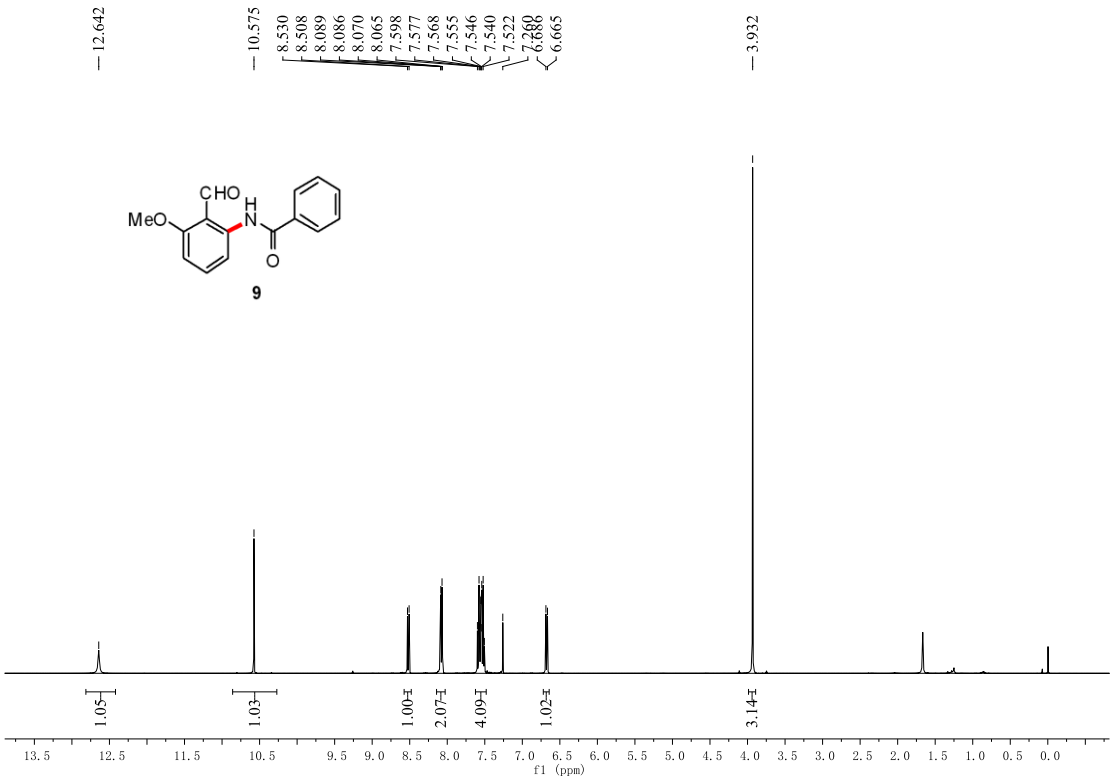

202.189
166.108
143.092
137.184
135.743
134.385
132.542
129.089
127.737
121.139
119.529
104.990
77.414
77.160
76.906
CHO
H
N
I
O

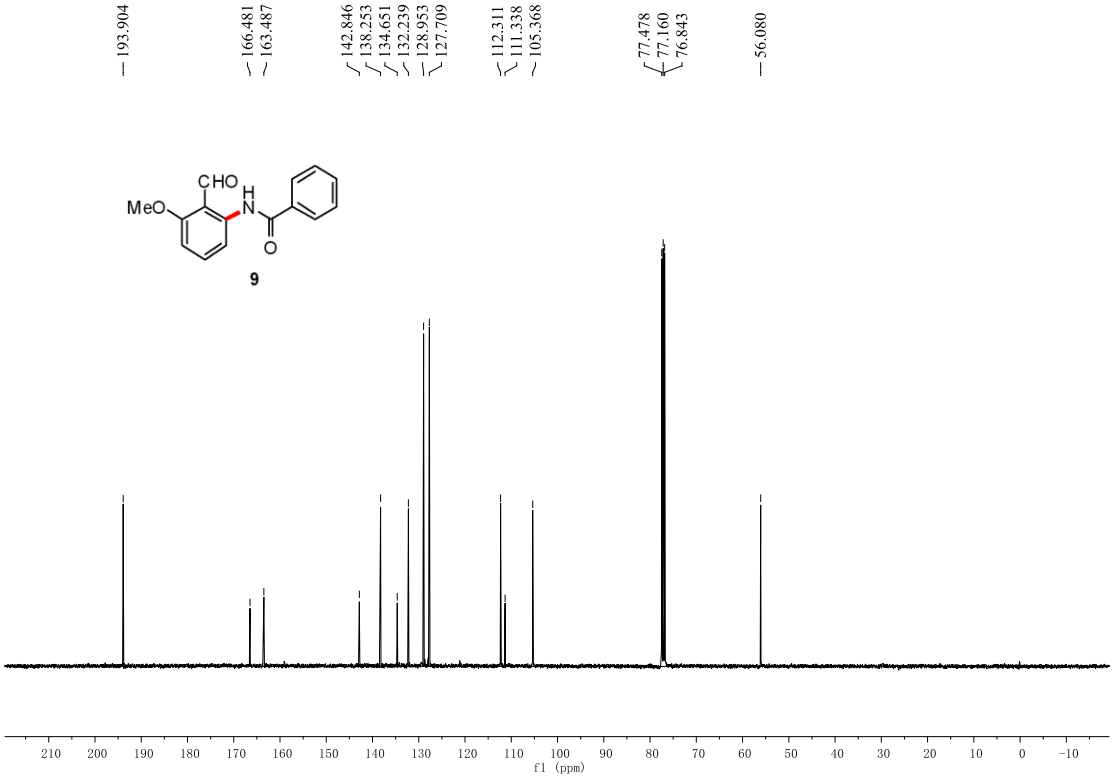
7

f1 (ppm)


12.565
10.527
8.841
8.820
8.091
8.084
8.072
8.067
7.590
7.575
7.562
7.558
7.550
7.532
7.514
7.260
6.983
6.964
2.710
CHO
Me
N
H
O
8
0.97
0.99
1.00
2.05
4.08
1.00
3.10
f1 (ppm)


194.908
166.413
143.502
142.236
136.766
134.780
132.223
128.974
127.685
126.087
119.729
118.709
77.477
77.160
76.842
19.439
CHO
Me
N
H
O
8
f1 (ppm)


12.642
10.575
8.530
8.508
8.089
8.086
8.070
8.065
7.598
7.577
7.568
7.555
7.546
7.540
7.522
7.260
6.686
6.665
3.932
CHO
MeO
H
N
O
9
1.05
1.03
1.00
2.07
4.09
1.02
3.14
f1 (ppm)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163.487
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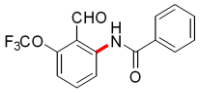
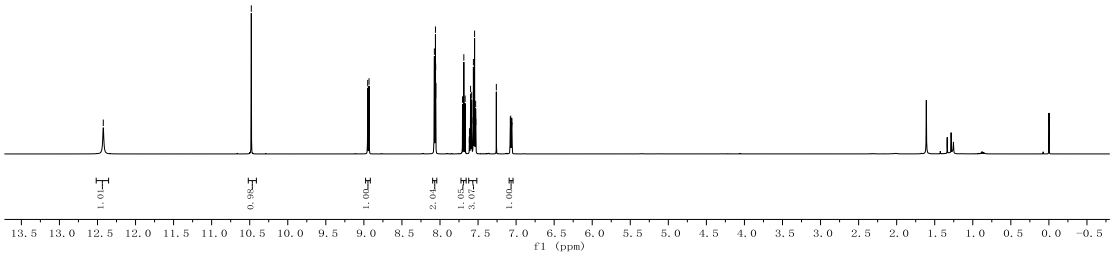
138.253
134.651
132.239
128.953
127.709
112.311
111.338
105.368
77.478
77.160
76.843
56.080
CHO
MeO
H
N
O
9
f1 (ppm)


12.424
10.479
8.950
8.932
8.074
8.060
8.057
7.704
7.695
7.670
7.615
7.613
7.610
7.603
7.598
7.593
7.586
7.584
7.581
7.561
7.538
7.540
7.545
7.535
7.532
7.509
7.260
7.076
7.071
7.066
7.055

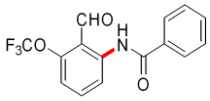

CHO
H
N
F3CO
O

10

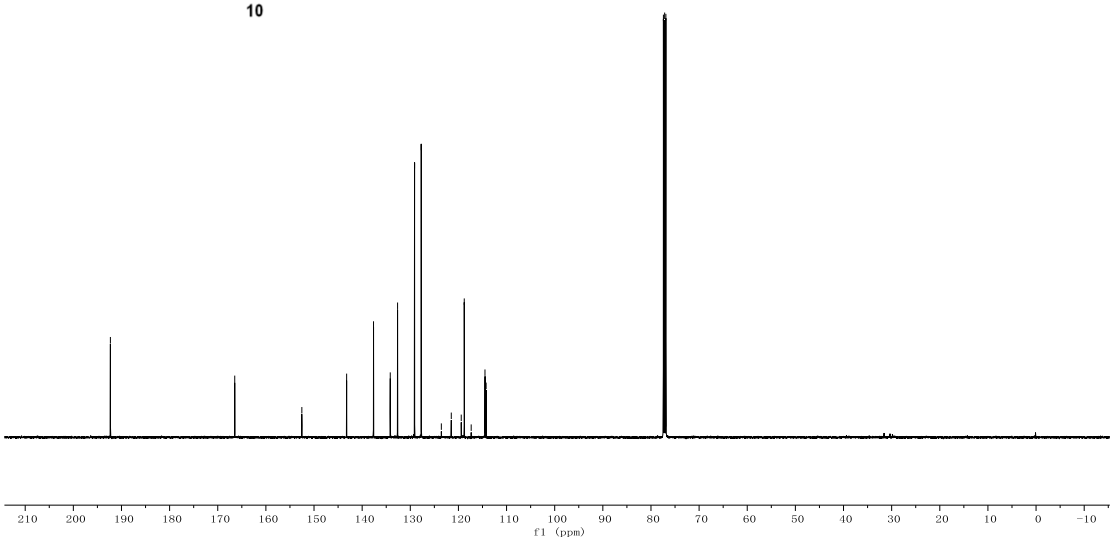

1.01
0.98
1.00
2.04
1.05
3.07
1.00
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

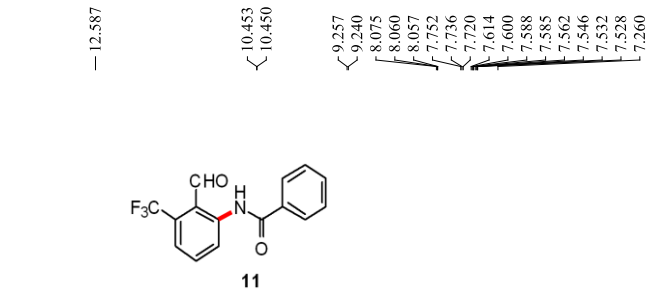

192.302
166.469
152.528
143.223
137.638
133.462
132.642
129.113
127.725
127.559
123.484
119.417
118.790
117.480
114.484
114.247


77.414
77.160
76.906


CHO
H
N
F3CO
O

10


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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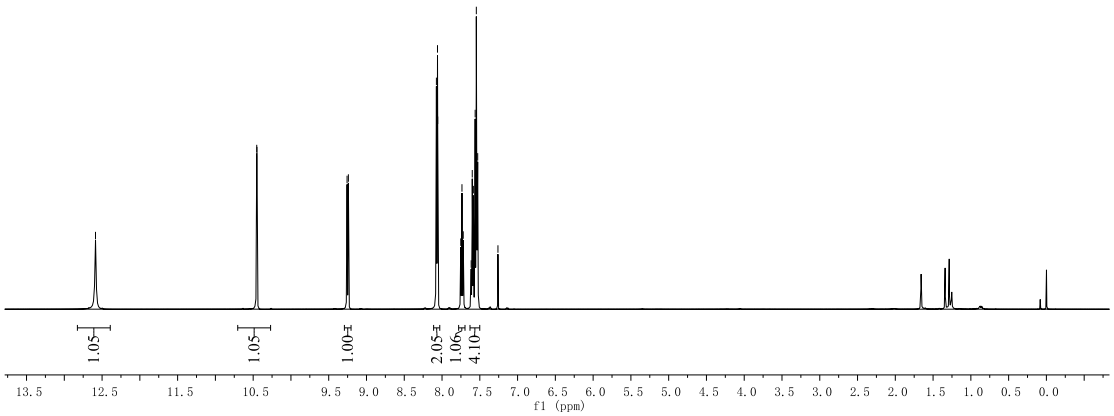
9.240
8.075
8.060
8.057
7.752
7.736
7.720
7.614
7.600
7.588
7.585
7.562
7.546
7.532
7.528
7.260
CHO
H
N
F3C
O

11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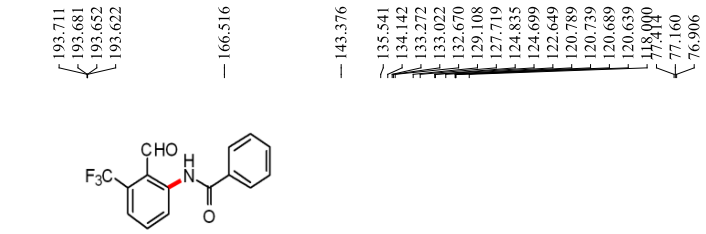
1.05
1.00
2.05
1.06
4.10
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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193.652
193.622
166.516
143.376
135.541
134.142
133.272
133.022
132.670
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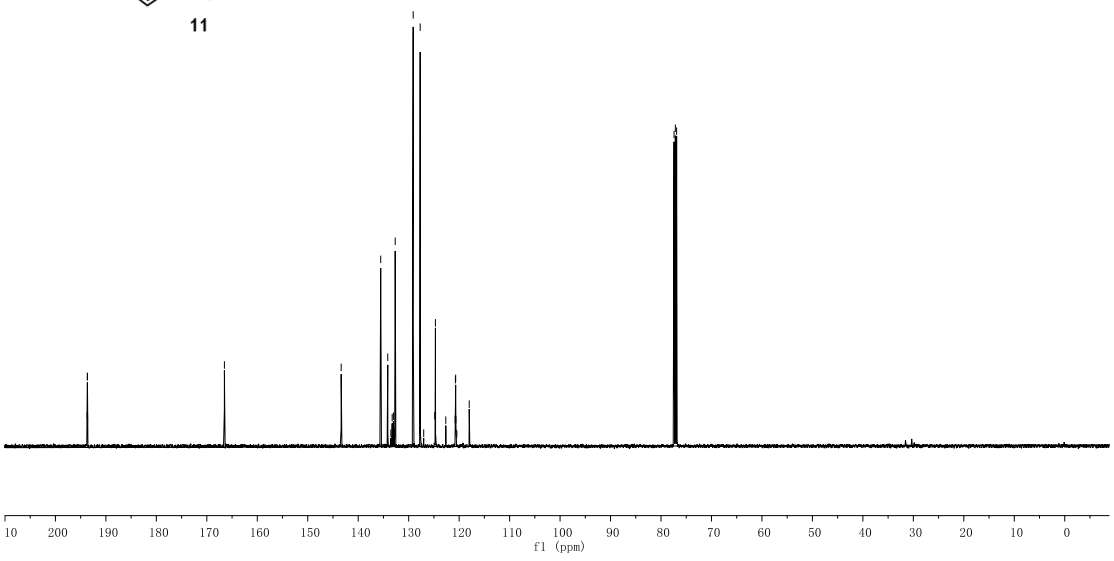
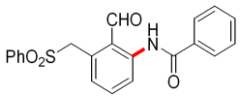
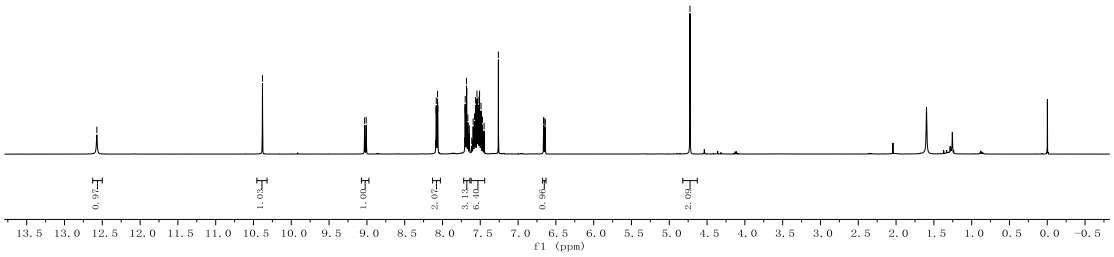
124.835
124.699
122.649
120.789
120.739
120.689
120.639
118.000
77.414
77.160
76.906
CHO
H
N
F3C
O

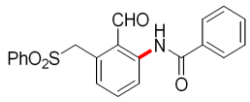
11


10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

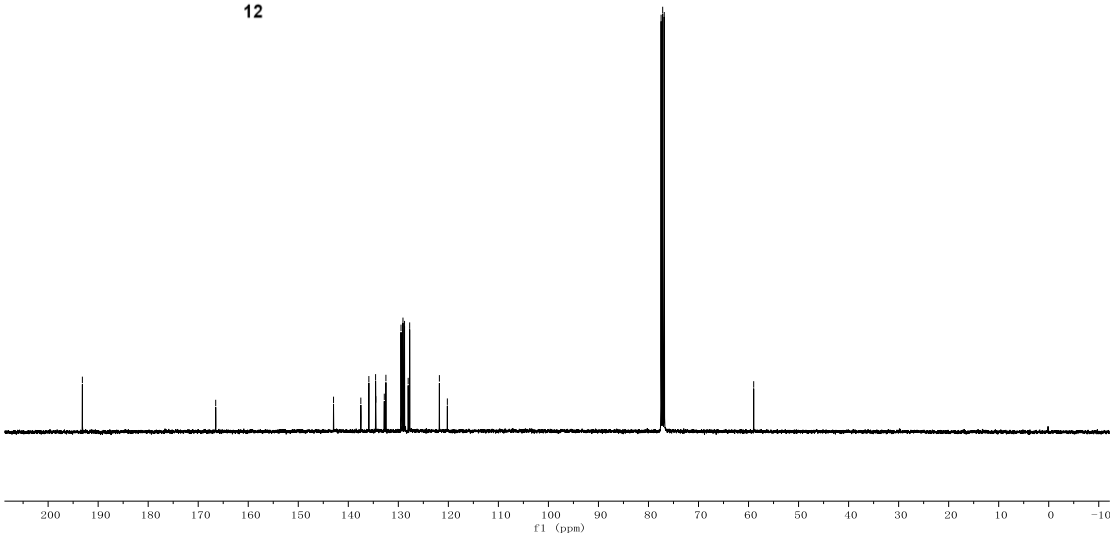


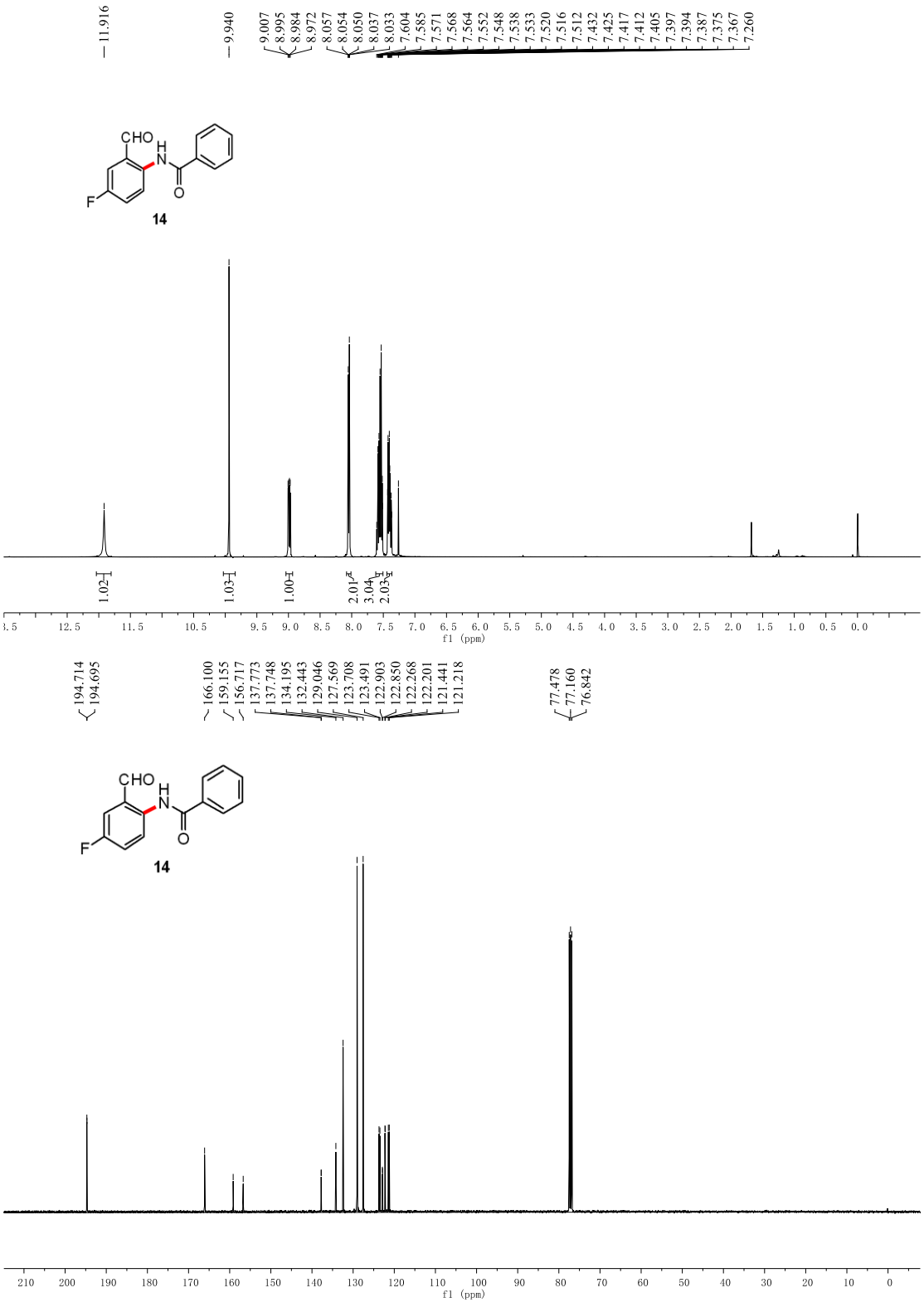
12

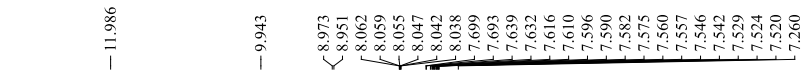




12




11.916
9.940
9.007
8.995
8.984
8.972
8.057
8.054
8.050
8.037
8.033
7.604
7.585
7.571
7.568
7.564
7.552
7.548
7.538
7.533
7.520
7.516
7.512
7.432
7.425
7.417
7.412
7.405
7.397
7.394
7.387
7.375
7.367
7.260
CHO
H
N
O
F
14
1.02
1.03
1.00
2.01
3.04
2.03
f1 (ppm)
194.714
194.695
166.100
159.155
156.717
137.773
137.748
134.195
132.443
129.046
127.569
123.708
123.491
122.903
122.850
122.268
122.201
121.441
121.218
77.478
77.160
76.842
CHO
H
N
O
F
14
f1 (ppm)


11.986
9.943
8.973
8.951
8.062
8.059
8.055
8.047
8.042
8.038
7.699
7.693
7.639
7.632
7.616
7.610
7.596
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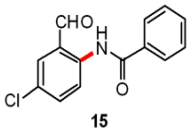
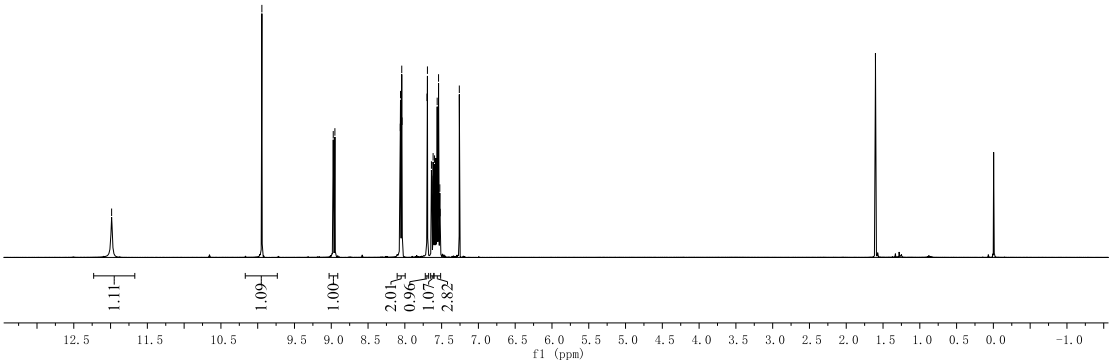
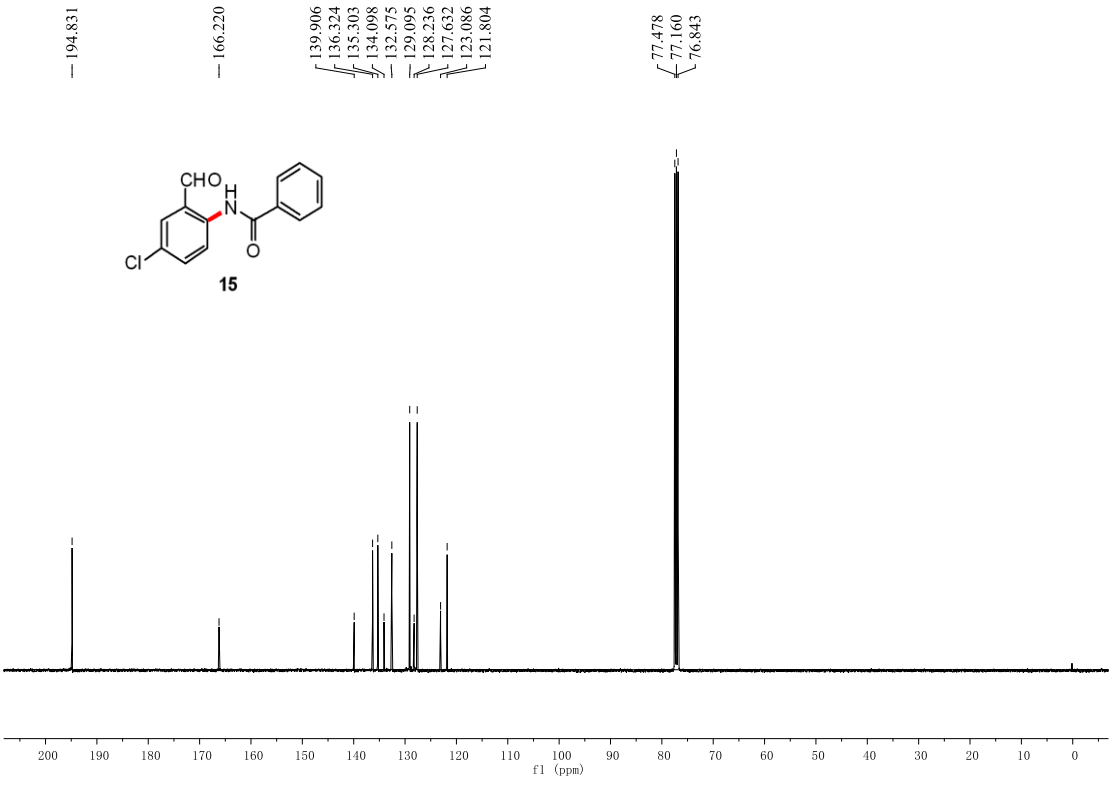
7.575
7.560
7.557
7.546
7.542
7.529
7.524
7.520
7.260


CHO
N
H
O
Cl

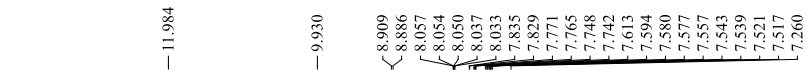
15

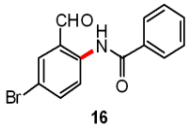

1.11
1.09
1.00
2.01
0.96
1.07
2.82
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-1.0
f1 (ppm)


194.831
166.220
139.906
136.324
135.303
134.098
132.575
129.095
128.236
127.632
123.086
121.804
77.478
77.160
76.843
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

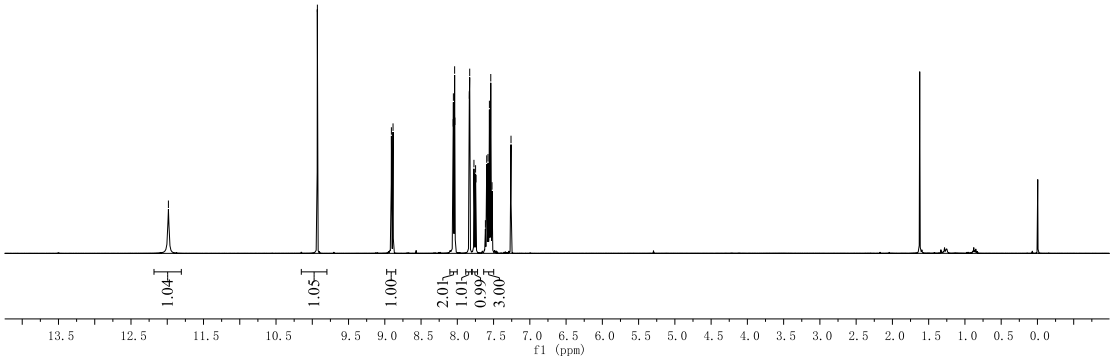
CHO
N
H
O
Cl

15

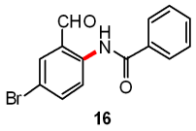

11.984
9.930
8.909
8.886
8.057
8.054
8.050
8.037
8.033
7.835
7.829
7.771
7.765
7.748
7.742
7.613
7.594
7.580
7.577
7.557
7.543
7.539
7.521
7.517
7.260


CHO
H
N
O
Br

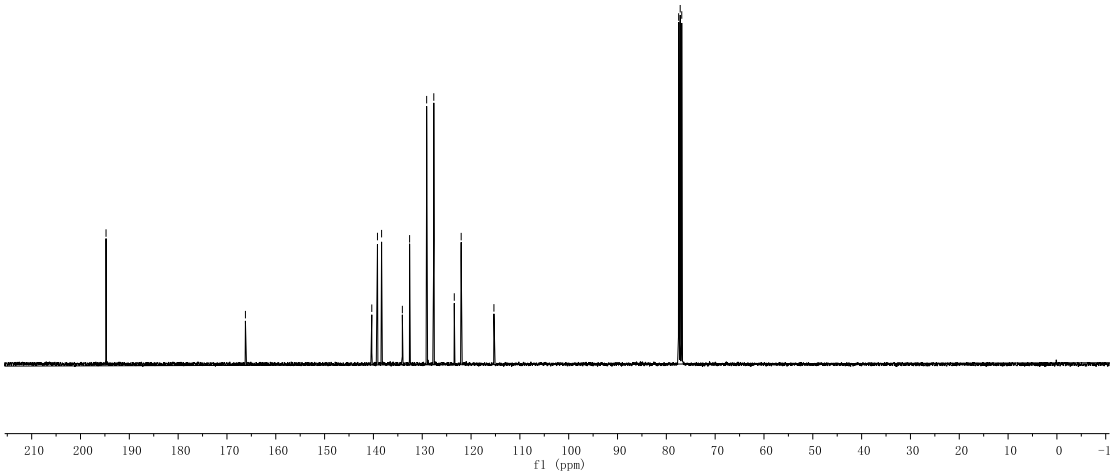
16


1.04
1.05
1.00
2.01
1.01
0.99
3.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

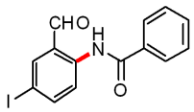

194.770
166.219
140.334
139.171
138.326
134.073
132.589
129.094
127.632
123.438
122.024
115.315
77.478
77.160
76.843


CHO
H
N
O
Br

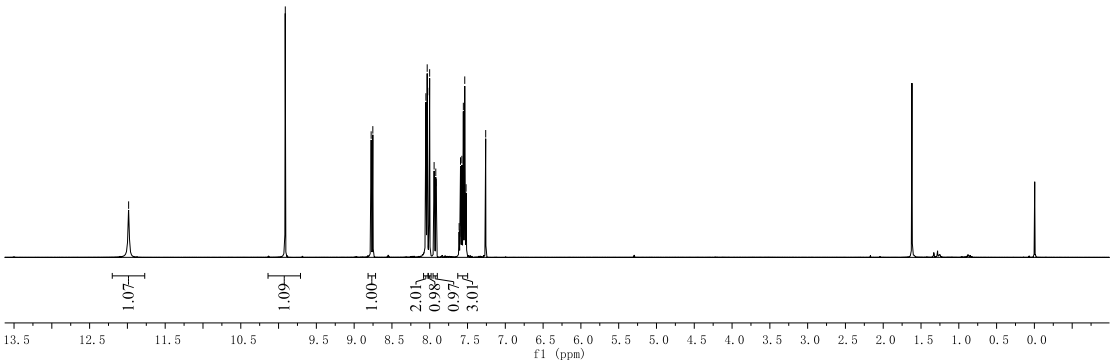
16

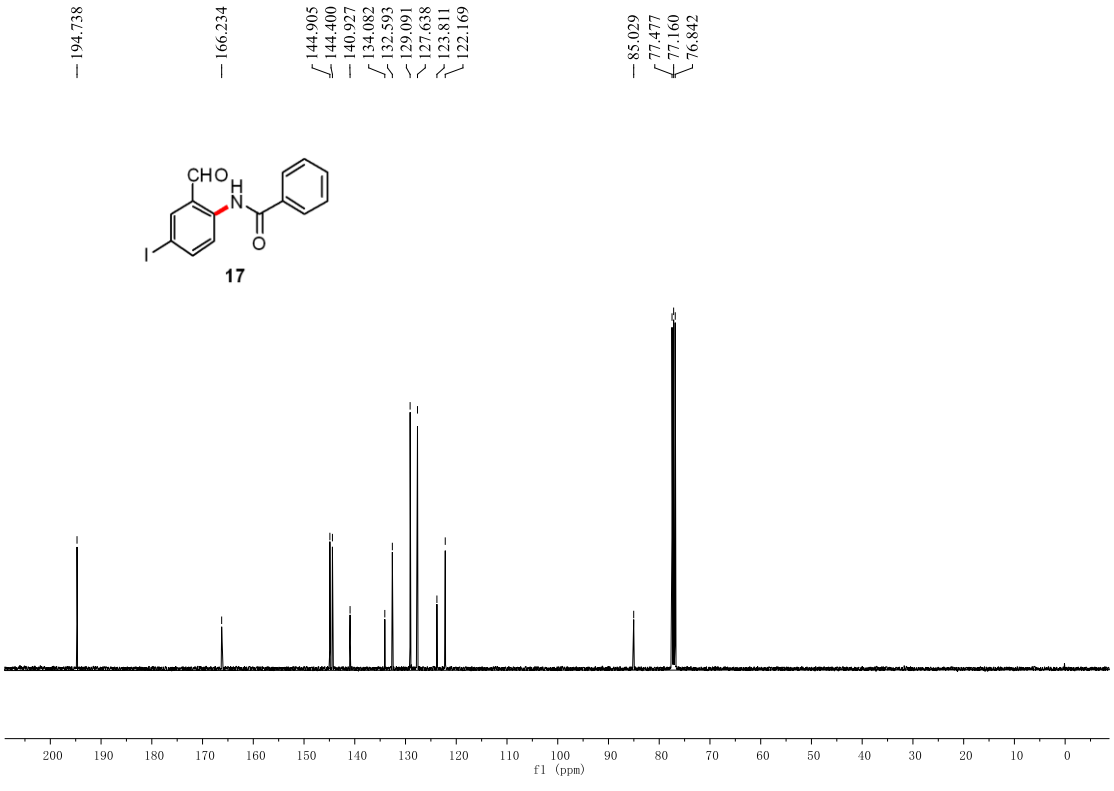

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


11.984
9.911
8.775
8.753
8.054
8.051
8.047
8.033
8.030
8.006
8.001
7.942
7.937
7.920
7.915
7.611
7.600
7.593
7.587
7.579
7.575
7.571
7.555
7.552
7.541
7.537
7.524
7.519
7.515
7.260


CHO
H
N
O
I

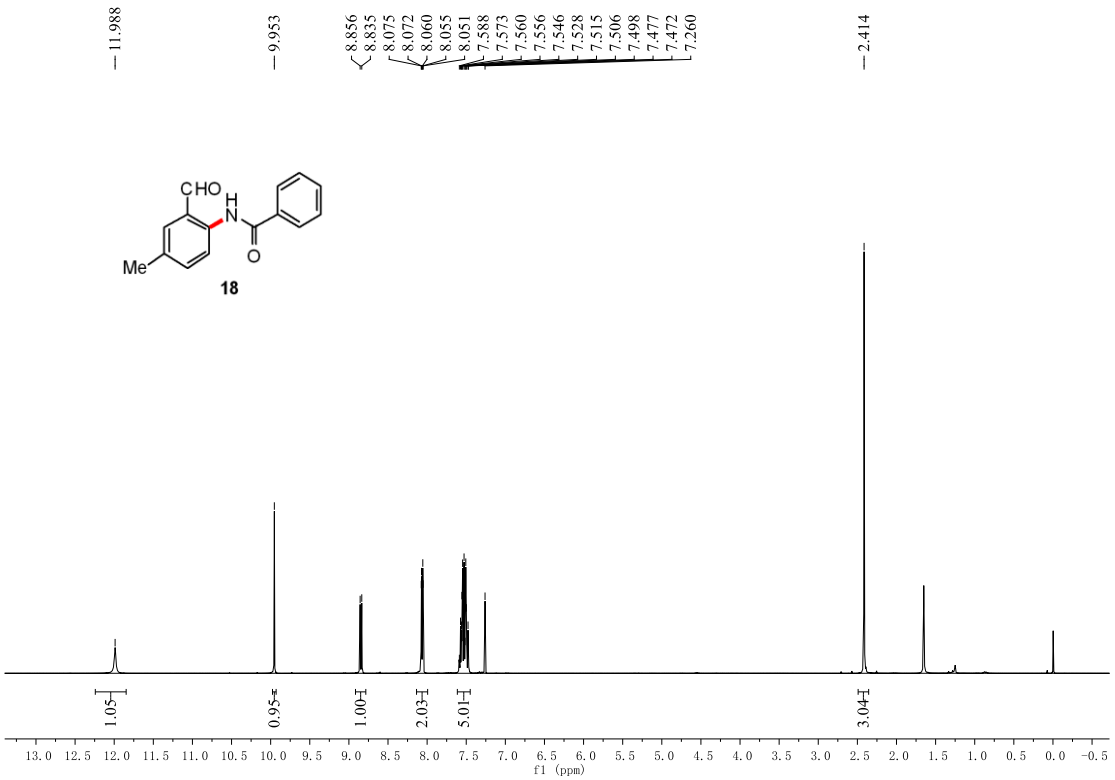
17

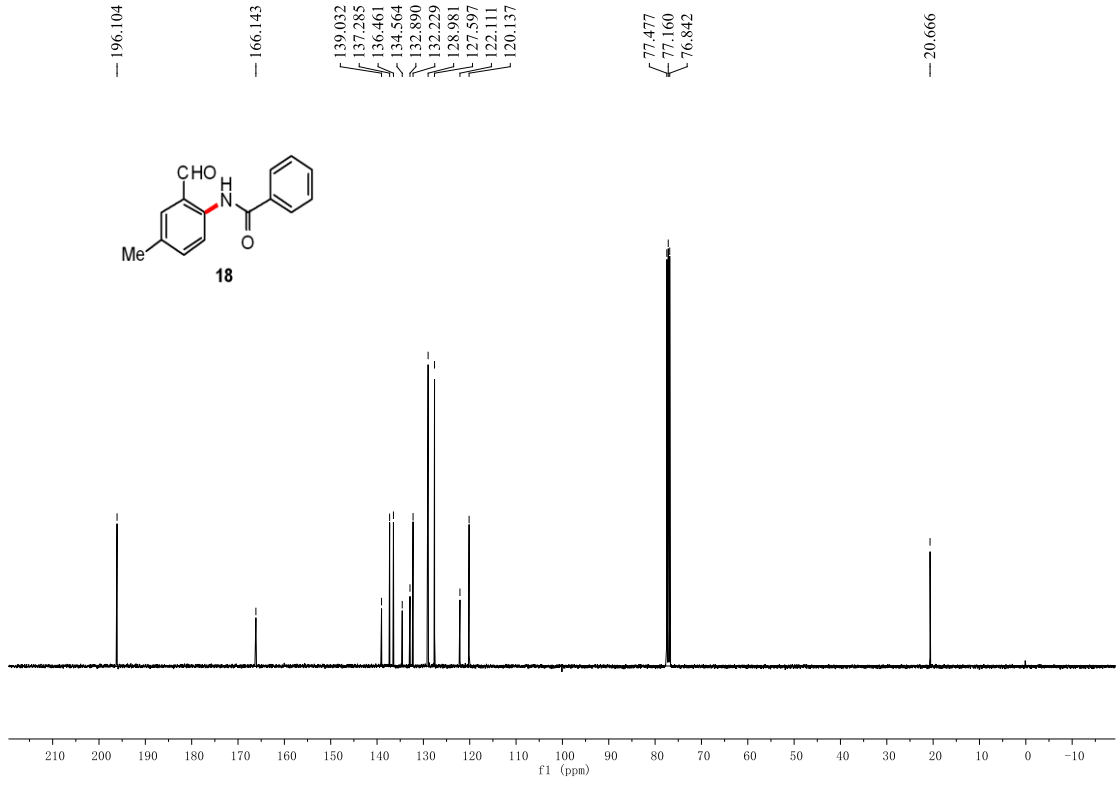

1.07
1.09
1.00
2.01
0.98
0.97
3.01
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

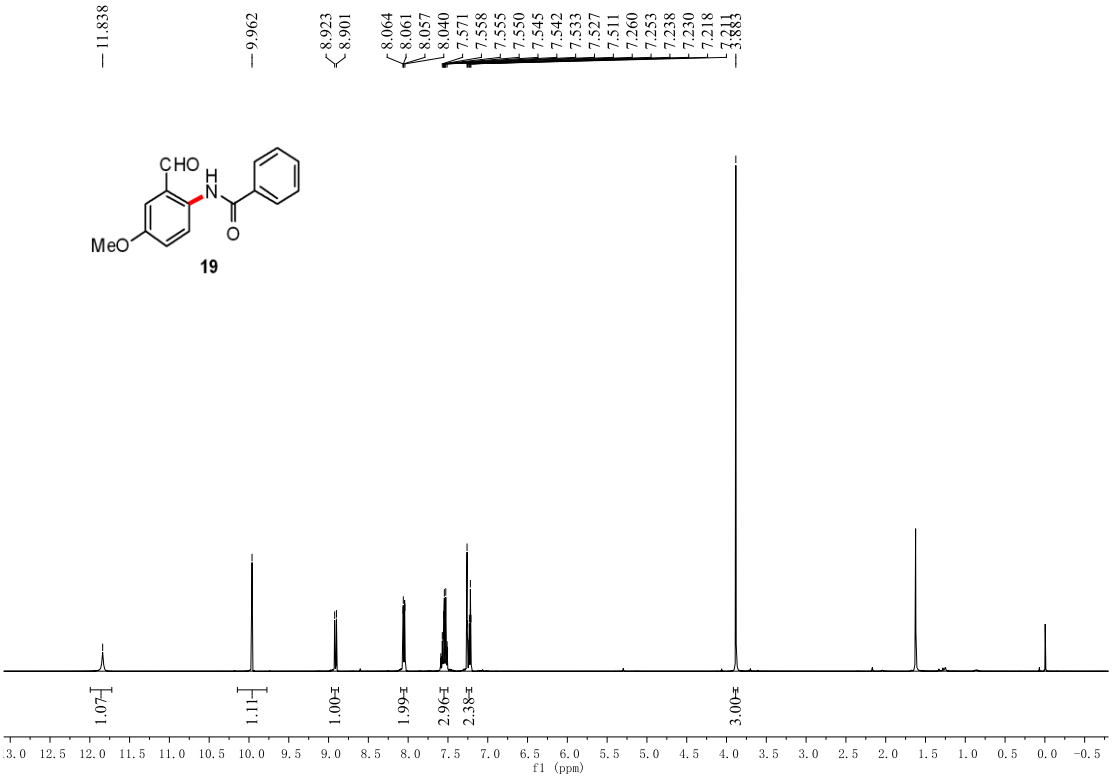

194.738
166.234
144.905
144.400
140.927
134.082
132.593
129.091
127.638
123.811
122.169
85.029
77.477
77.160
76.842
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

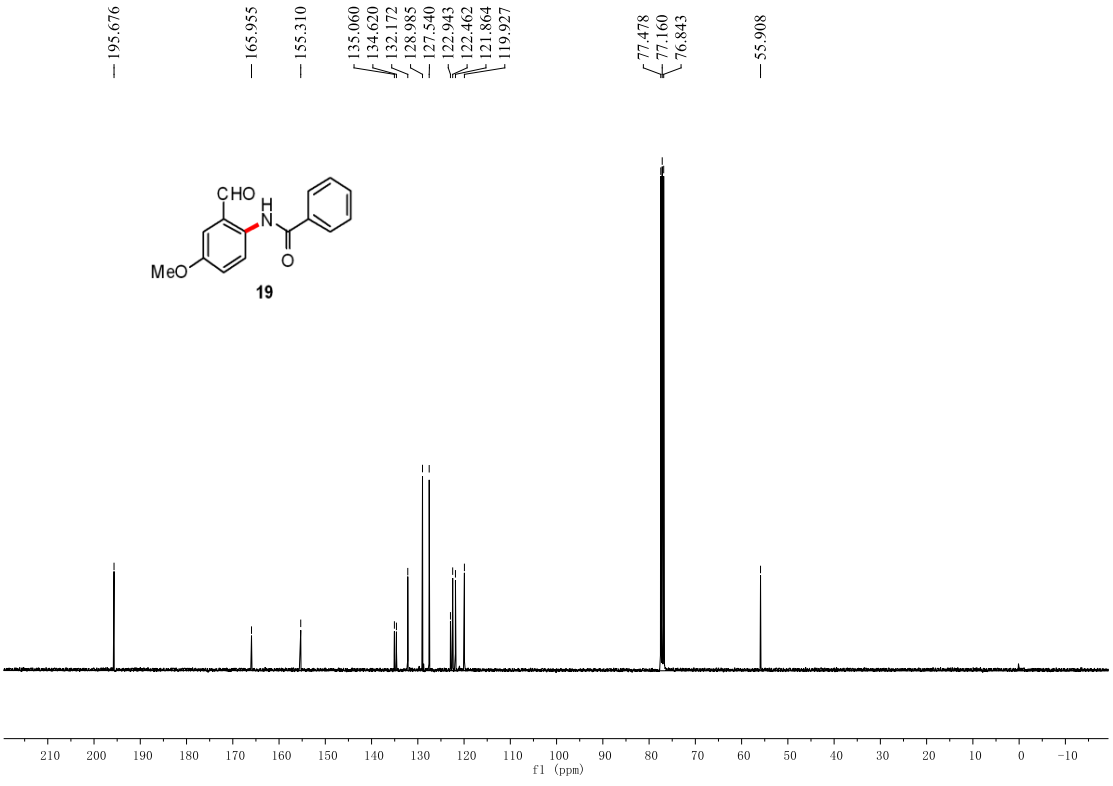
CHO
H
N
O
I

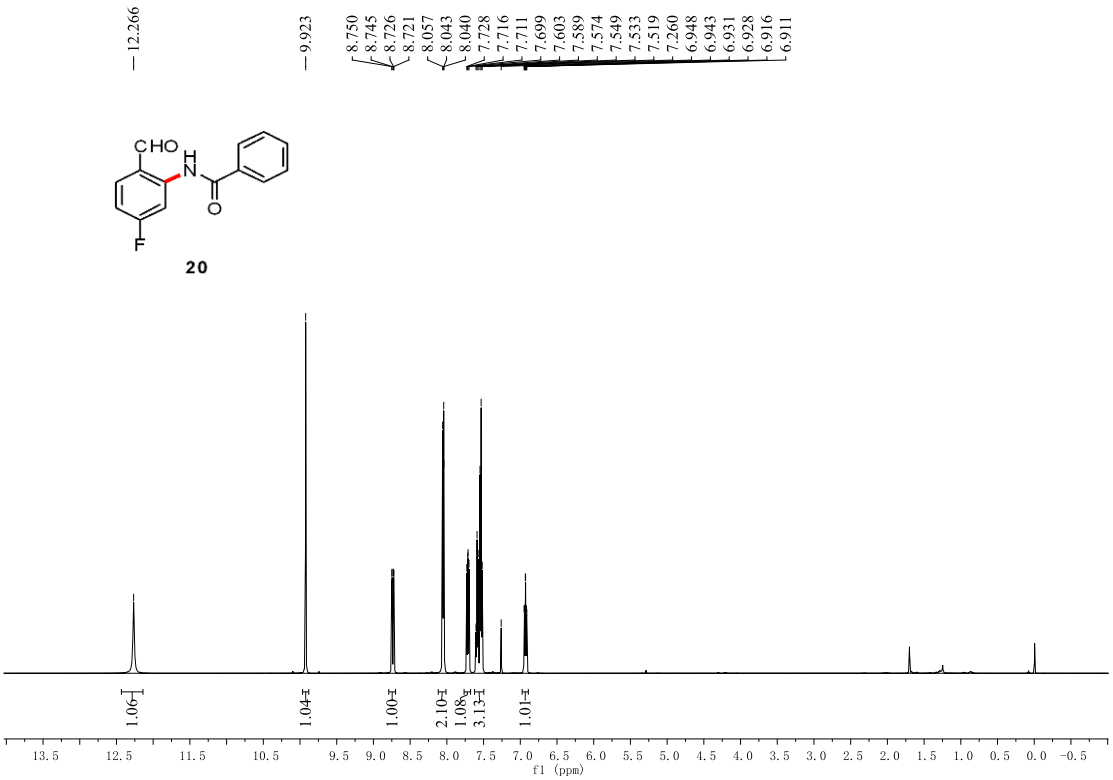
17

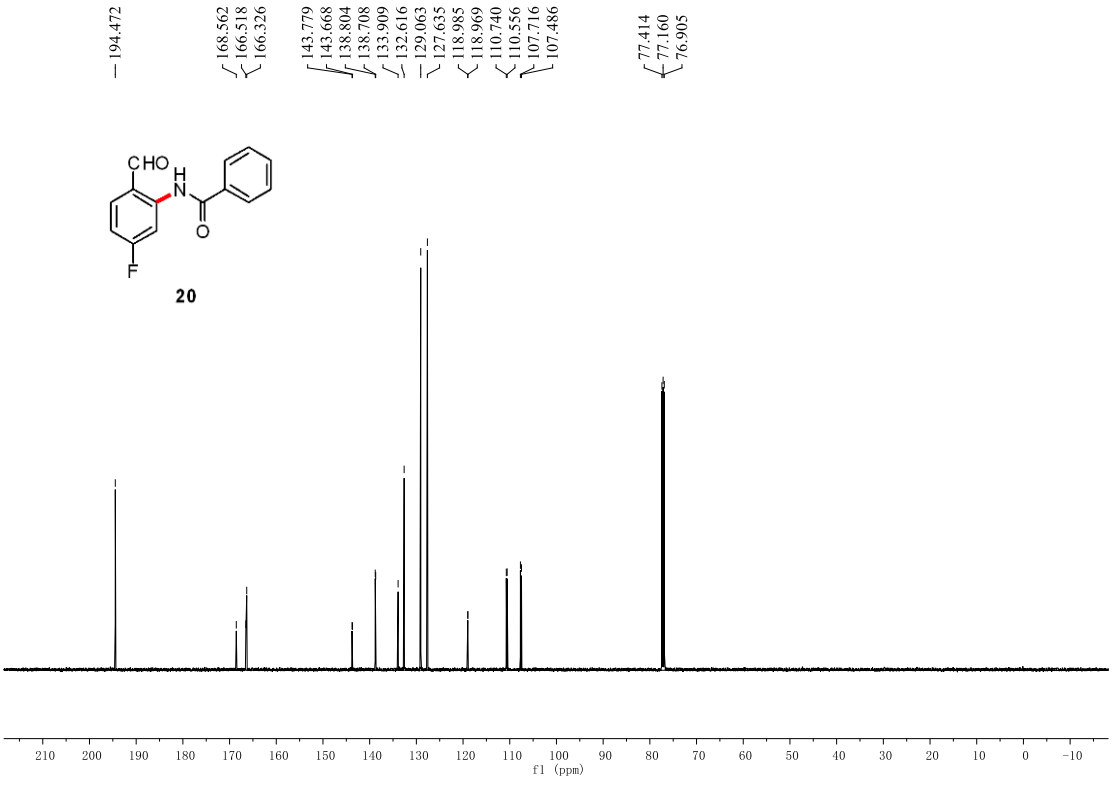

11.988
9.953
8.856
8.835
8.075
8.072
8.060
8.055
8.051
7.588
7.573
7.560
7.556
7.546
7.528
7.515
7.506
7.498
7.477
7.472
7.260
2.414
CHO
N
H
O
Me
18
1.05
0.95
1.00
2.03
5.01
3.04
f1 (ppm)

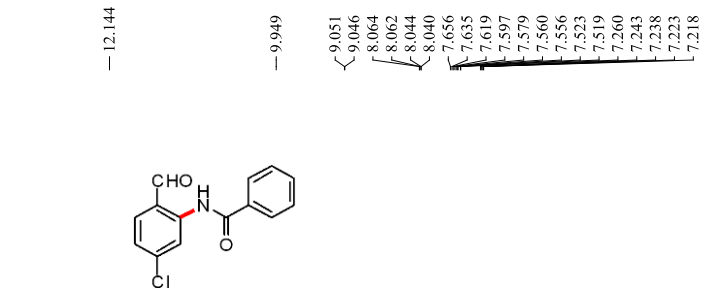

196.104
166.143
139.032
137.285
136.461
134.564
132.890
132.229
128.981
127.597
122.111
120.137
77.477
77.160
76.842
20.666
CHO
H
N
O
Me
18
f1 (ppm)


11.838
9.962
8.923
8.901
8.064
8.061
8.057
8.040
7.571
7.558
7.555
7.550
7.545
7.542
7.533
7.527
7.511
7.260
7.253
7.238
7.230
7.218
7.211
3.883
CHO
N
H
O
MeO
19
1.07
1.11
1.00
1.99
2.96
2.38
3.00
f1 (ppm)


195.676
165.955
155.310
135.060
134.620
132.172
128.985
127.540
122.943
122.462
121.864
119.927
77.478
77.160
76.843
55.908
CHO
N
H
O
MeO
19
f1 (ppm)

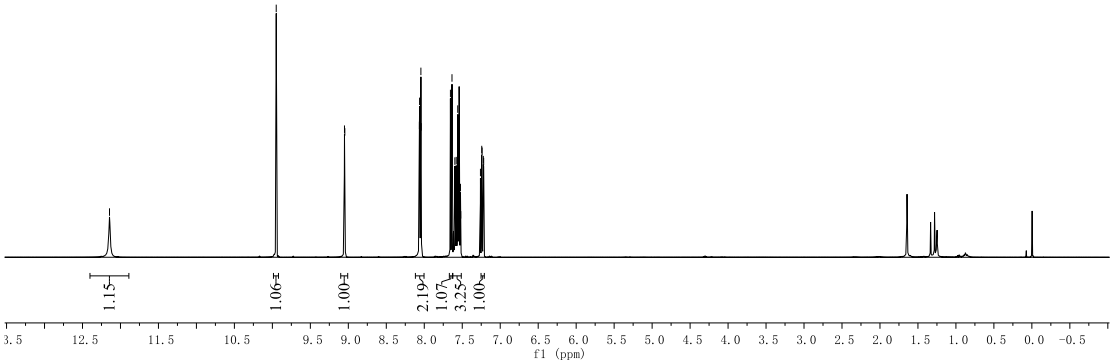

12.266
9.923
8.750
8.745
8.726
8.721
8.057
8.043
8.040
7.728
7.716
7.711
7.699
7.603
7.589
7.574
7.549
7.533
7.519
7.260
6.948
6.943
6.931
6.928
6.916
6.911
CHO
NH
O
F
20
1.06
1.04
1.00
2.10
1.08
3.13
1.01
f1 (ppm)


194.472
168.562
166.518
166.326
143.779
143.668
138.804
138.708
133.909
132.616
129.063
127.635
118.985
118.969
110.740
110.556
107.716
107.486
77.414
77.160
76.905
CHO
NH
O
F
20
f1 (ppm)

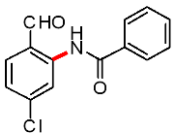

12.144
9.949
9.051
9.046
8.064
8.062
8.044
8.040
7.656
7.635
7.619
7.597
7.579
7.560
7.556
7.523
7.519
7.260
7.243
7.238
7.223
7.218

CHO
H
N
O
Cl

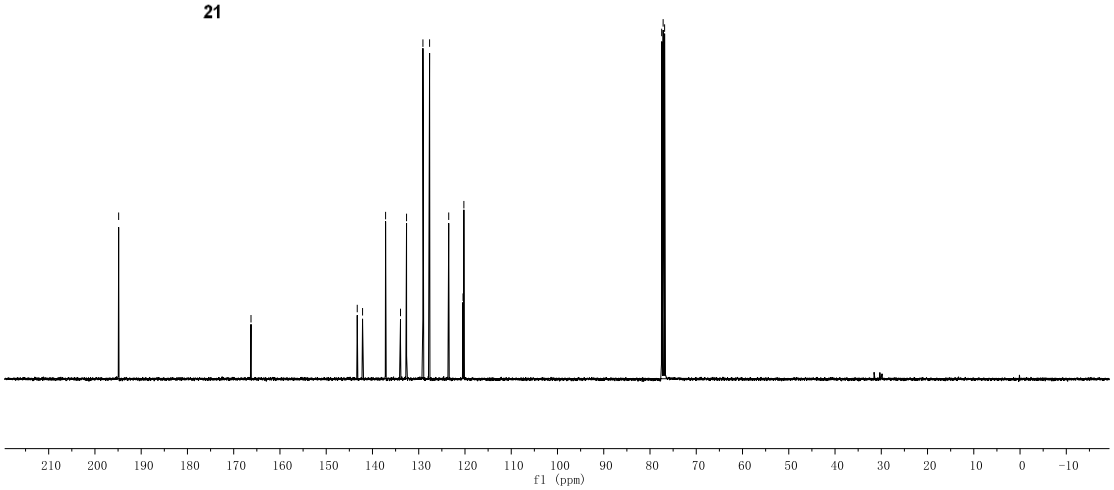
21

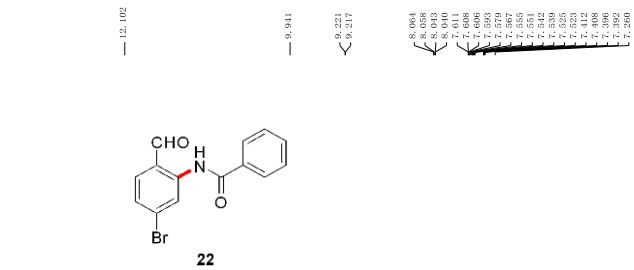

1.15
1.06
1.00
2.19
1.07
3.25
1.00
f1 (ppm)


194.874
166.260
143.293
142.142
137.163
133.939
132.634
129.093
127.651
123.517
120.425
120.239
77.478
77.160
76.843

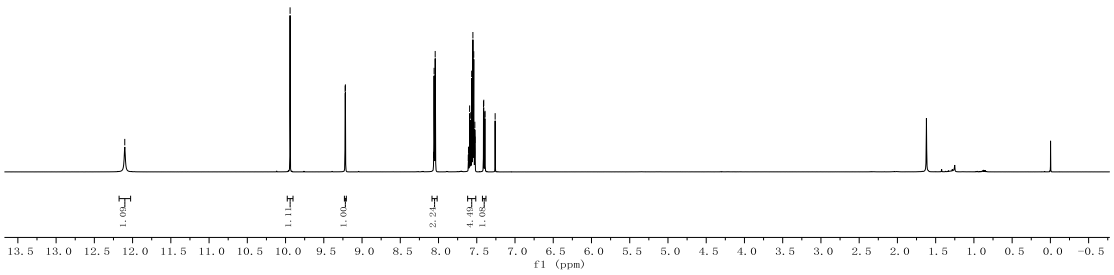

CHO
H
N
O
Cl

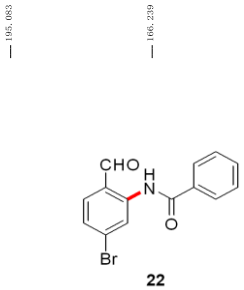
21


f1 (ppm)

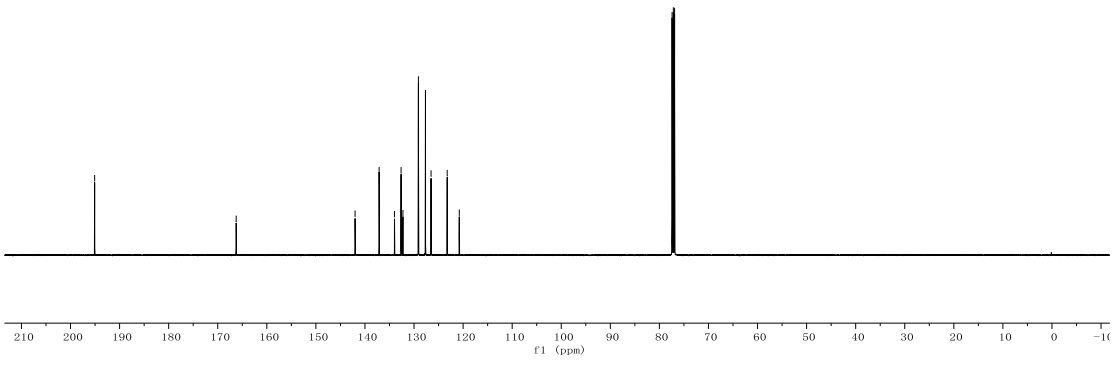

12.102
9.941
9.221
9.217
8.064
8.058
8.044
8.040
7.611
7.608
7.606
7.593
7.579
7.567
7.555
7.551
7.542
7.539
7.525
7.523
7.412
7.408
7.396
7.392
7.260
CHO
H
N
O
Br

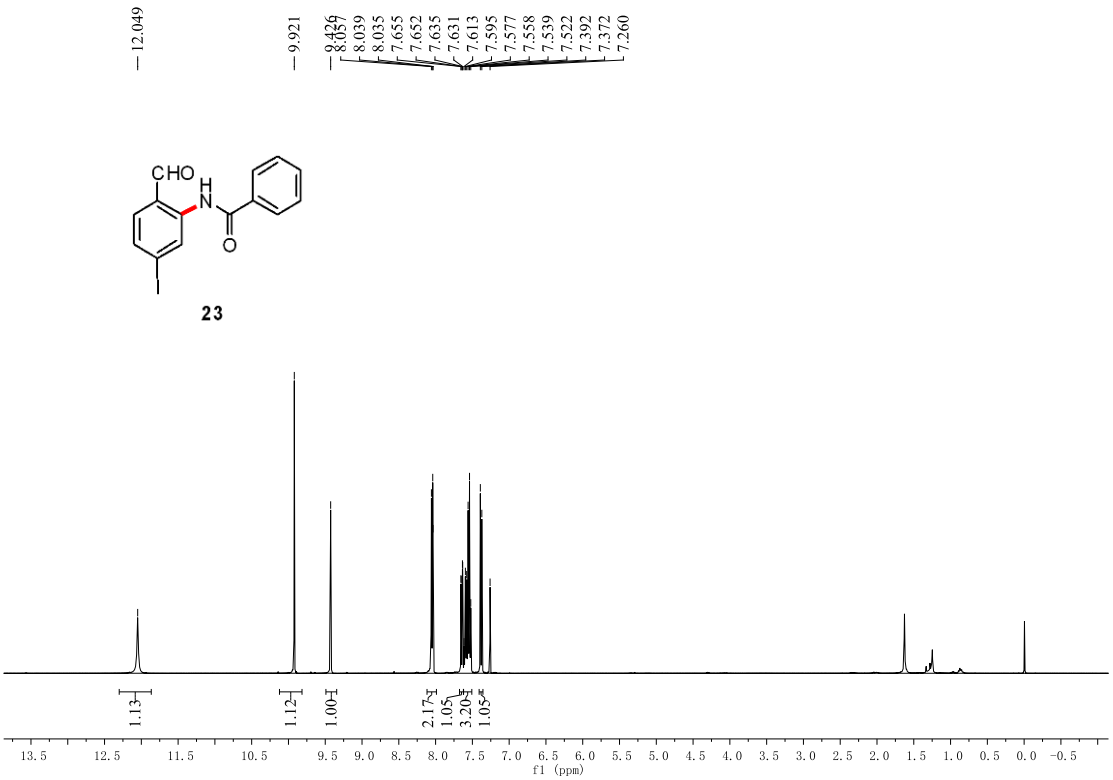
22

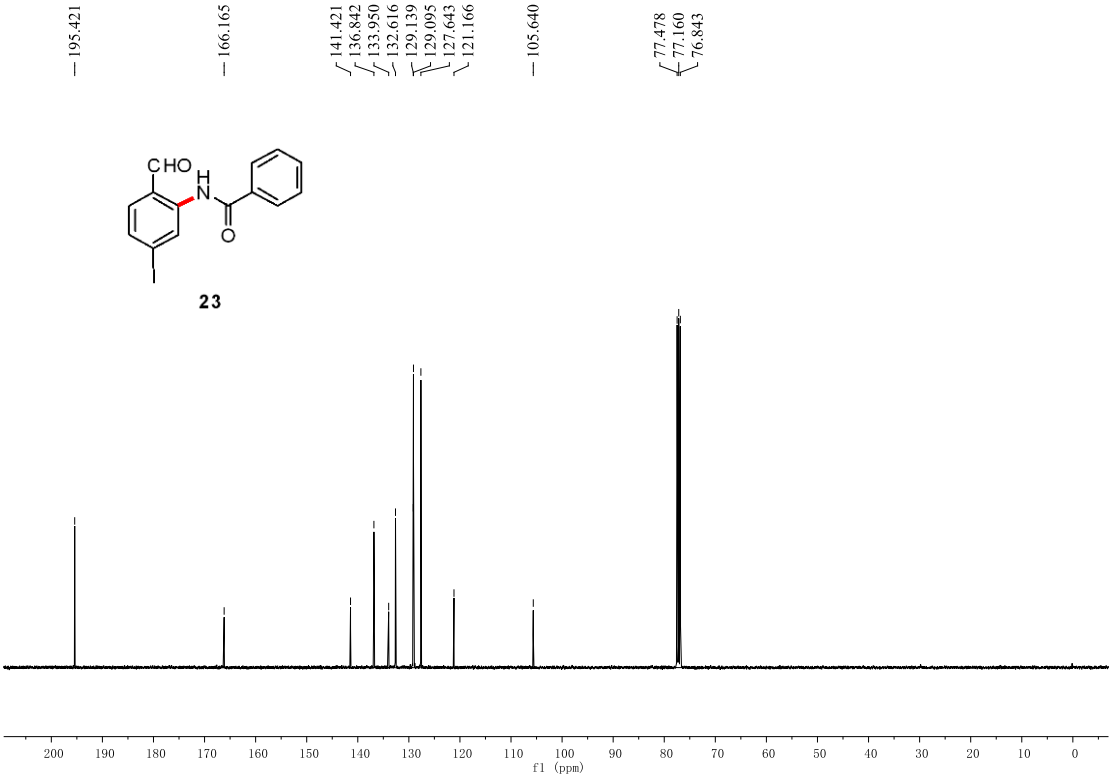

1.00
1.11
1.00
2.24
4.40
1.08
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

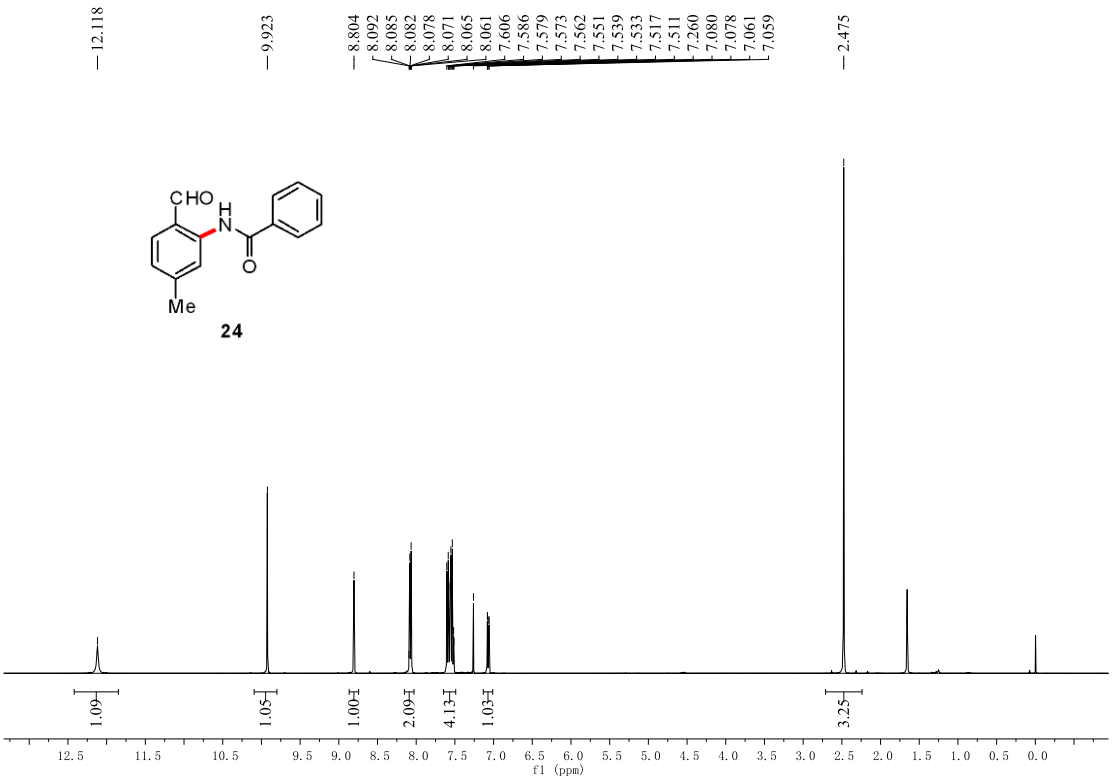

195.083
166.239
142.012
137.115
133.981
132.637
131.261
129.106
127.669
126.529
125.259
120.777
77.414
77.160
76.906
CHO
H
N
O
Br

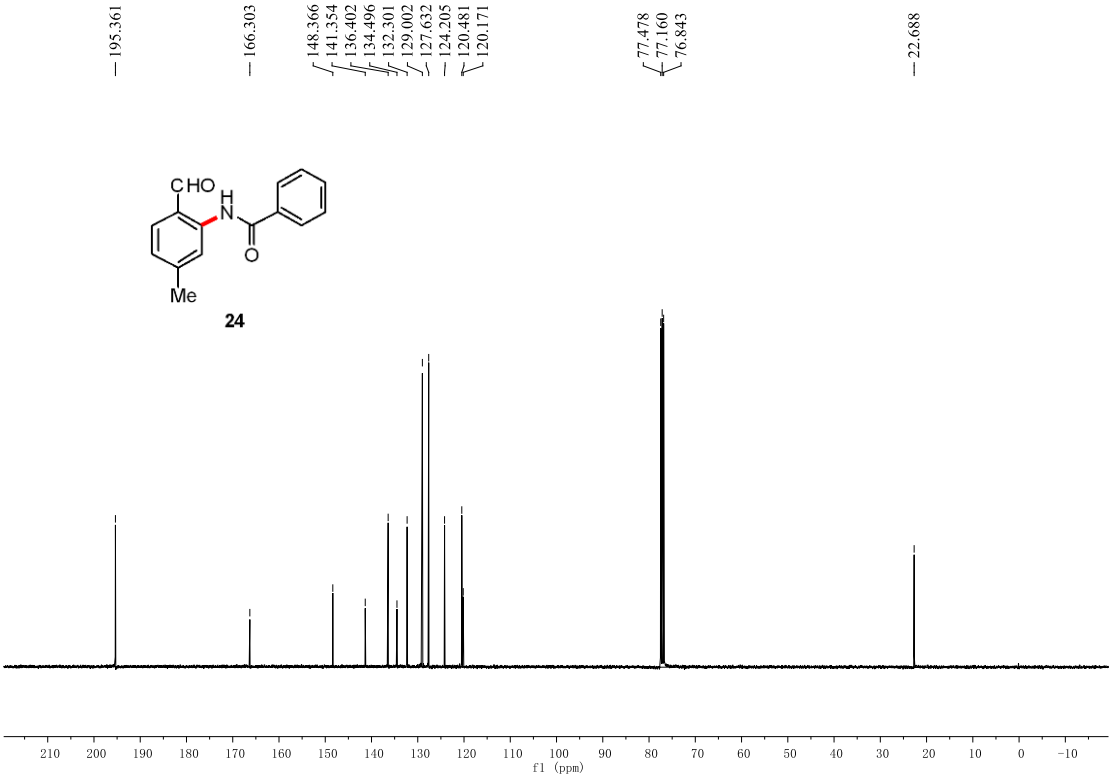
22

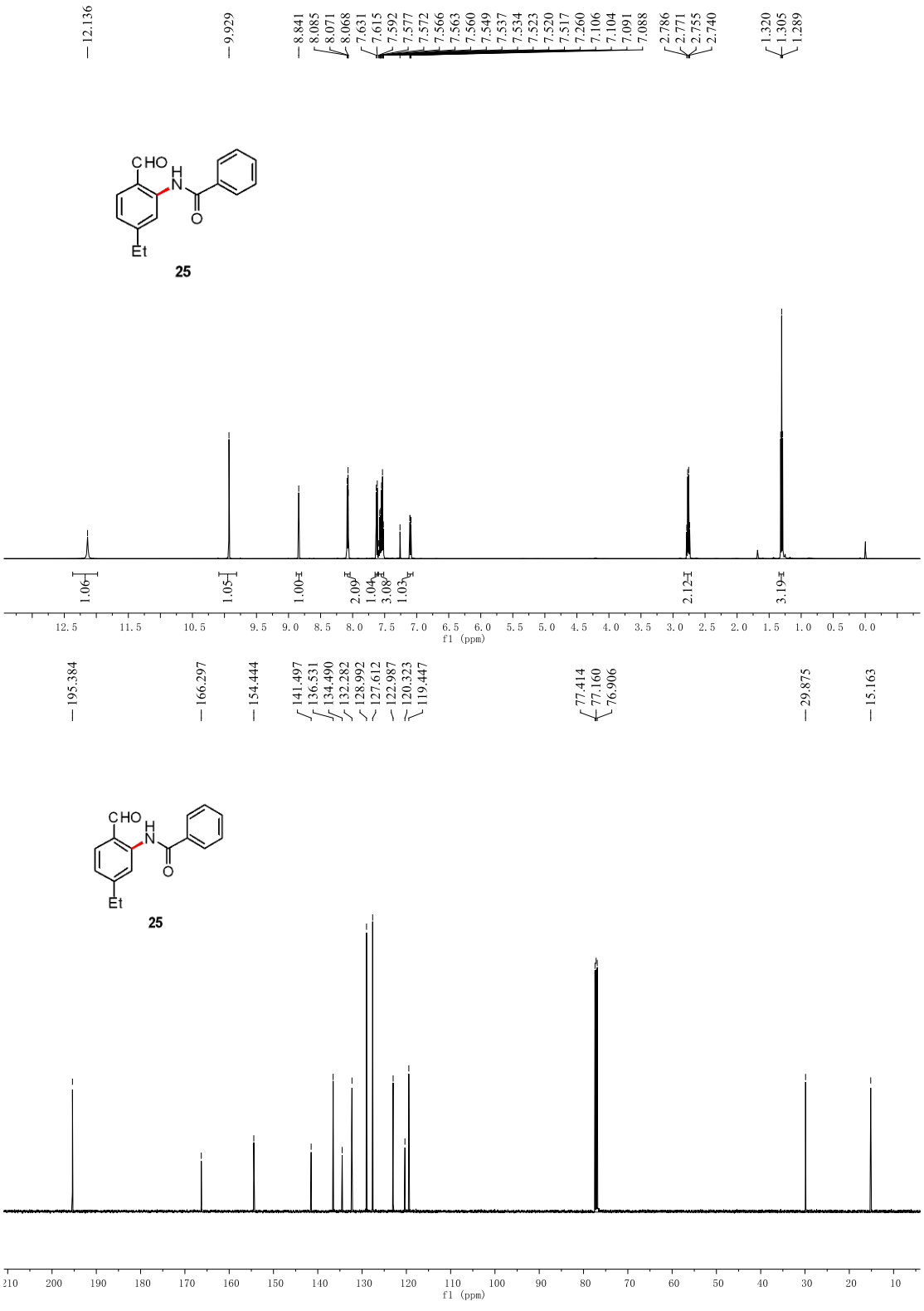

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


12.049
9.921
9.426
8.057
8.039
8.035
7.655
7.652
7.635
7.631
7.613
7.595
7.577
7.558
7.539
7.522
7.392
7.372
7.260
CHO
N
H
O
I
23
1.13
1.12
1.00
2.17
1.05
3.20
1.05
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


195.421
166.165
141.421
136.842
133.950
132.616
129.139
129.095
127.643
121.166
105.640
77.478
77.160
76.843
CHO
N
H
O
I
23
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


12.118
9.923
8.804
8.092
8.085
8.082
8.078
8.071
8.065
8.061
7.606
7.586
7.579
7.573
7.562
7.551
7.539
7.533
7.517
7.511
7.260
7.080
7.078
7.061
7.059
2.475
CHO
H
N
O
Me
24
1.09
1.05
1.00
2.09
4.13
1.03
3.25
f1 (ppm)


195.361
166.303
148.366
141.354
136.402
134.496
132.301
129.002
127.632
124.205
120.481
120.171
77.478
77.160
76.843
22.688
CHO
H
N
O
Me
24
f1 (ppm)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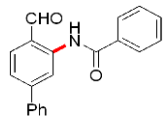
9.929
8.841
8.085
8.071
8.068
7.631
7.615
7.592
7.577
7.572
7.566
7.563
7.560
7.549
7.537
7.534
7.523
7.520
7.517
7.260
7.106
7.104
7.091
7.088
2.786
2.771
2.755
2.740
1.320
1.305
1.289
CHO
H
N
O
Et
25
1.06
1.05
1.00
2.09
1.04
3.08
1.03
2.12
3.19
f1 (ppm)
195.384
166.297
154.444
141.497
136.531
134.490
132.282
128.992
127.612
122.987
120.323
119.447
77.414
77.160
76.906
29.875
15.163
CHO
H
N
O
Et
25
f1 (ppm)



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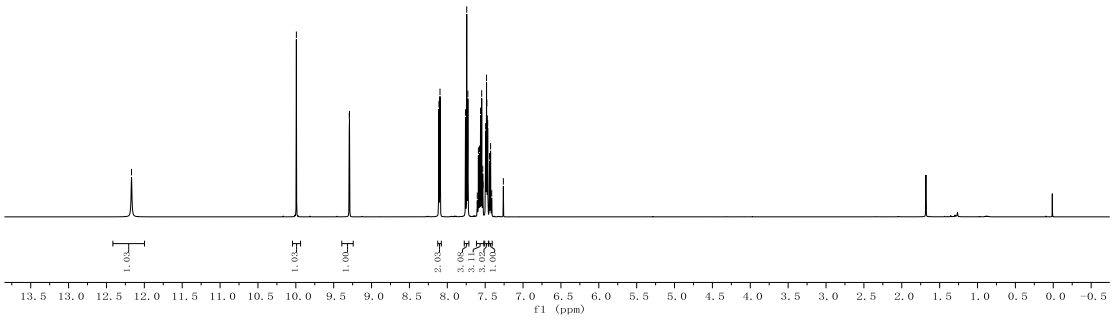

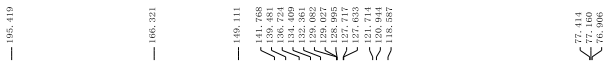

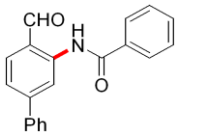

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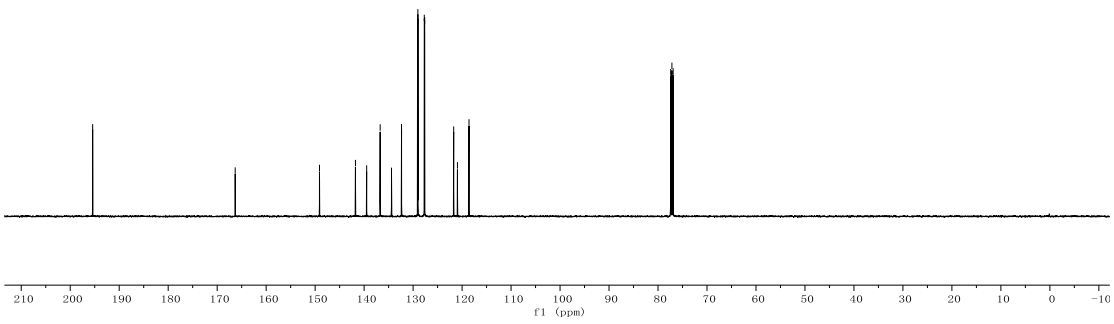

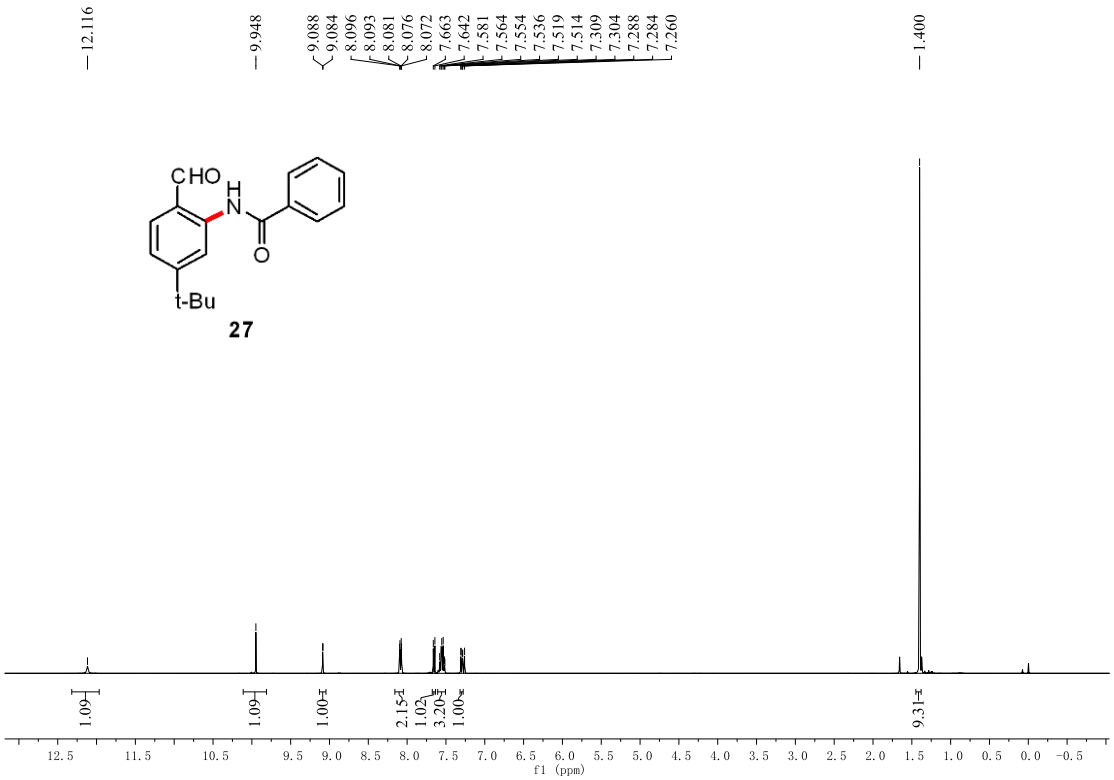
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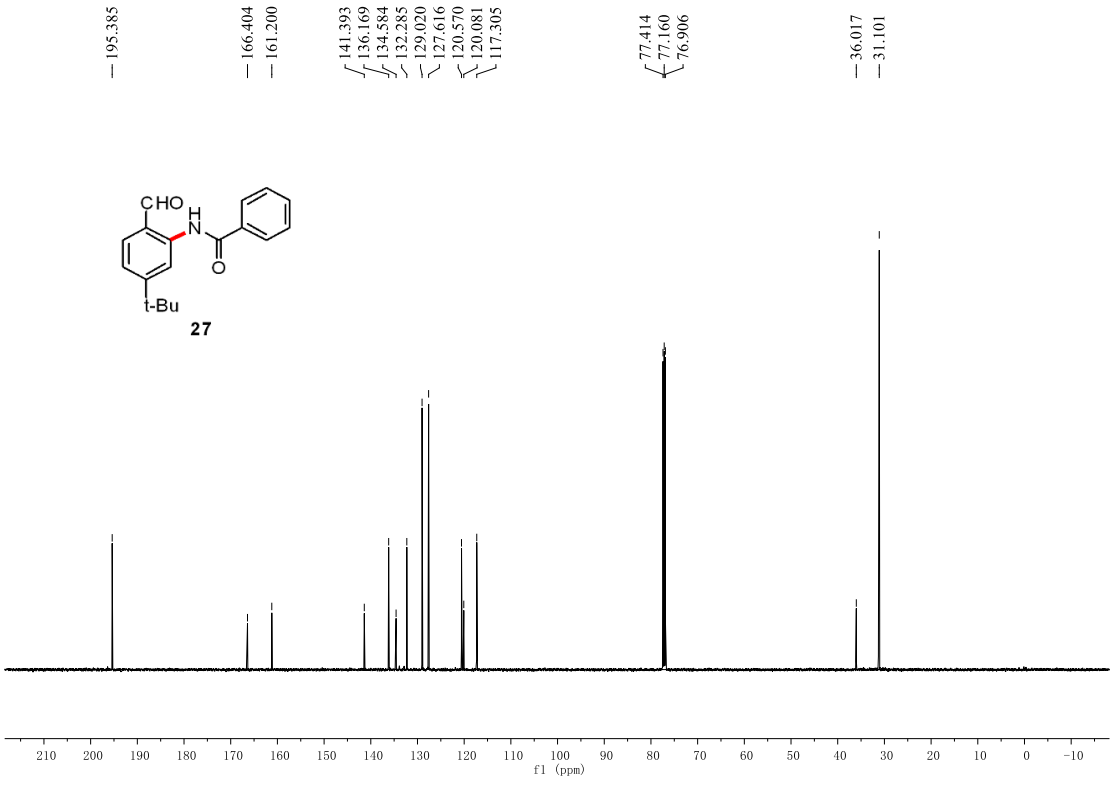
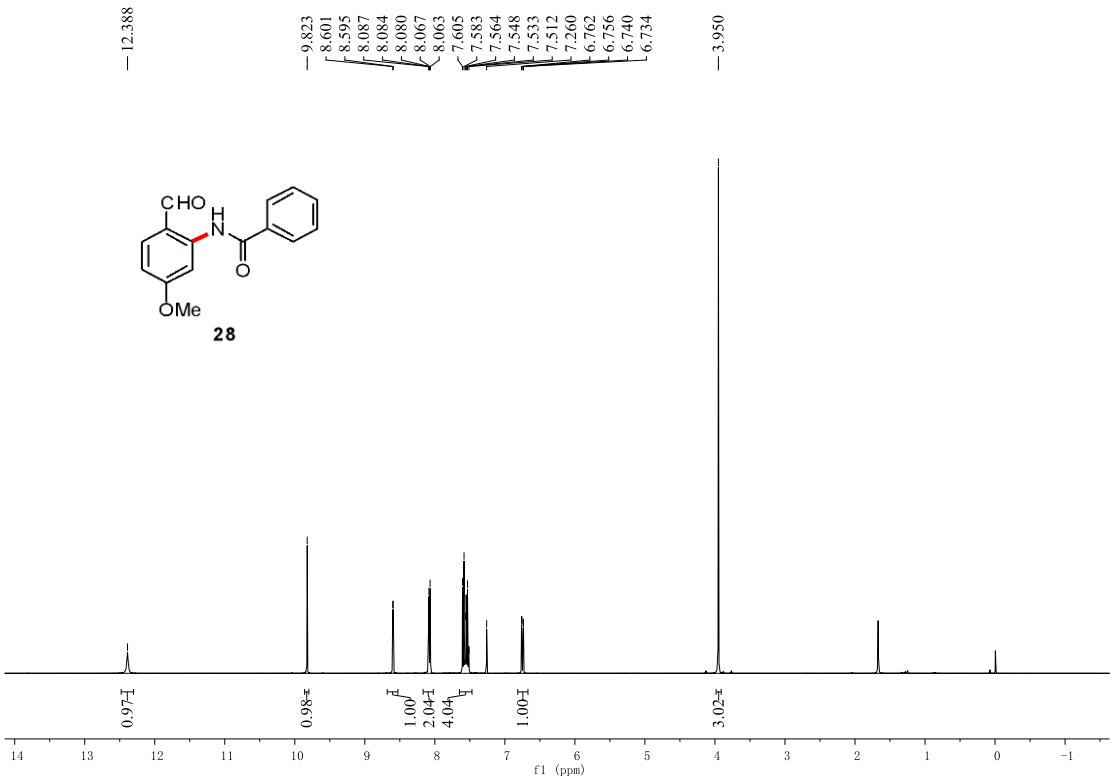
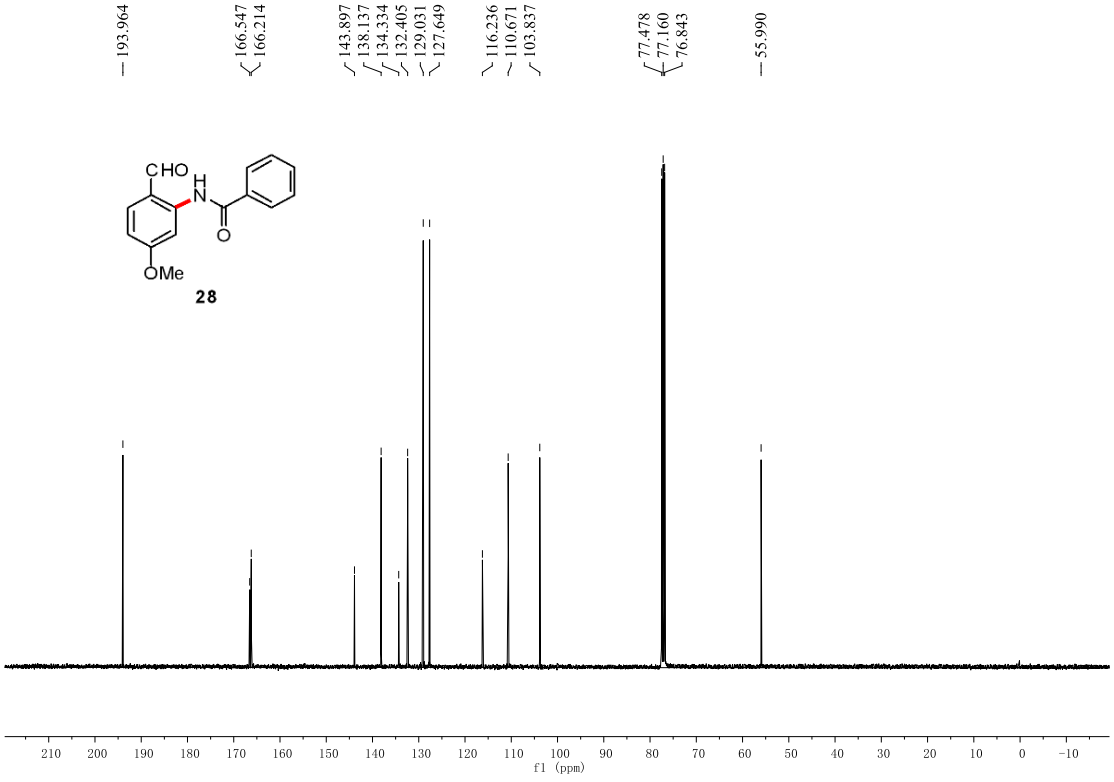
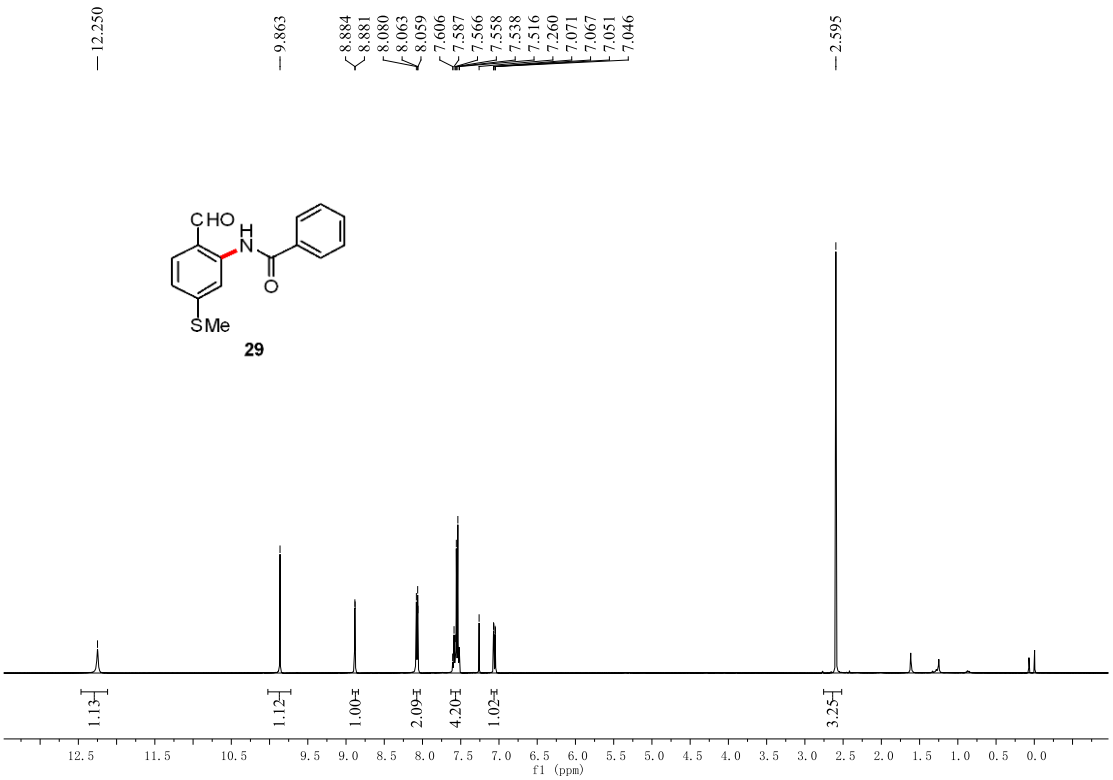
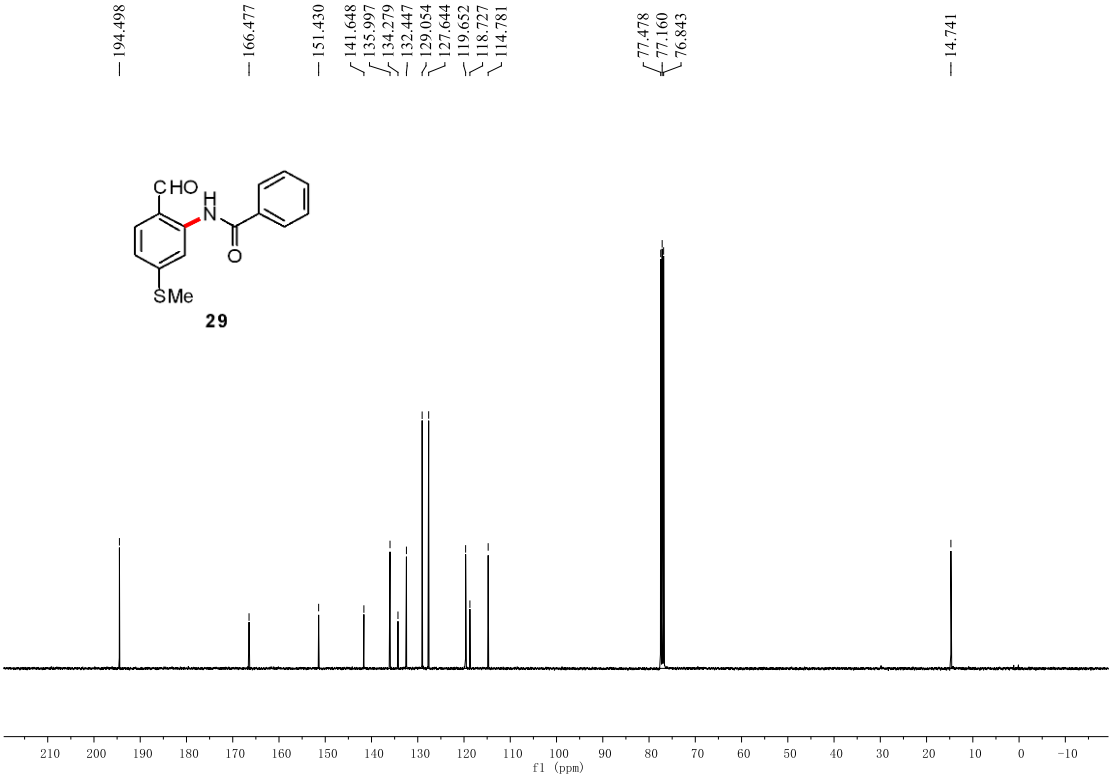
9.948
9.088
9.084
8.096
8.093
8.081
8.076
8.072
7.663
7.642
7.581
7.564
7.554
7.536
7.519
7.514
7.309
7.304
7.288
7.284
7.260
1.400
CHO
H
N
O
t-Bu
27
1.09
1.09
1.00
2.15
1.02
3.20
1.00
9.31
f1 (ppm)

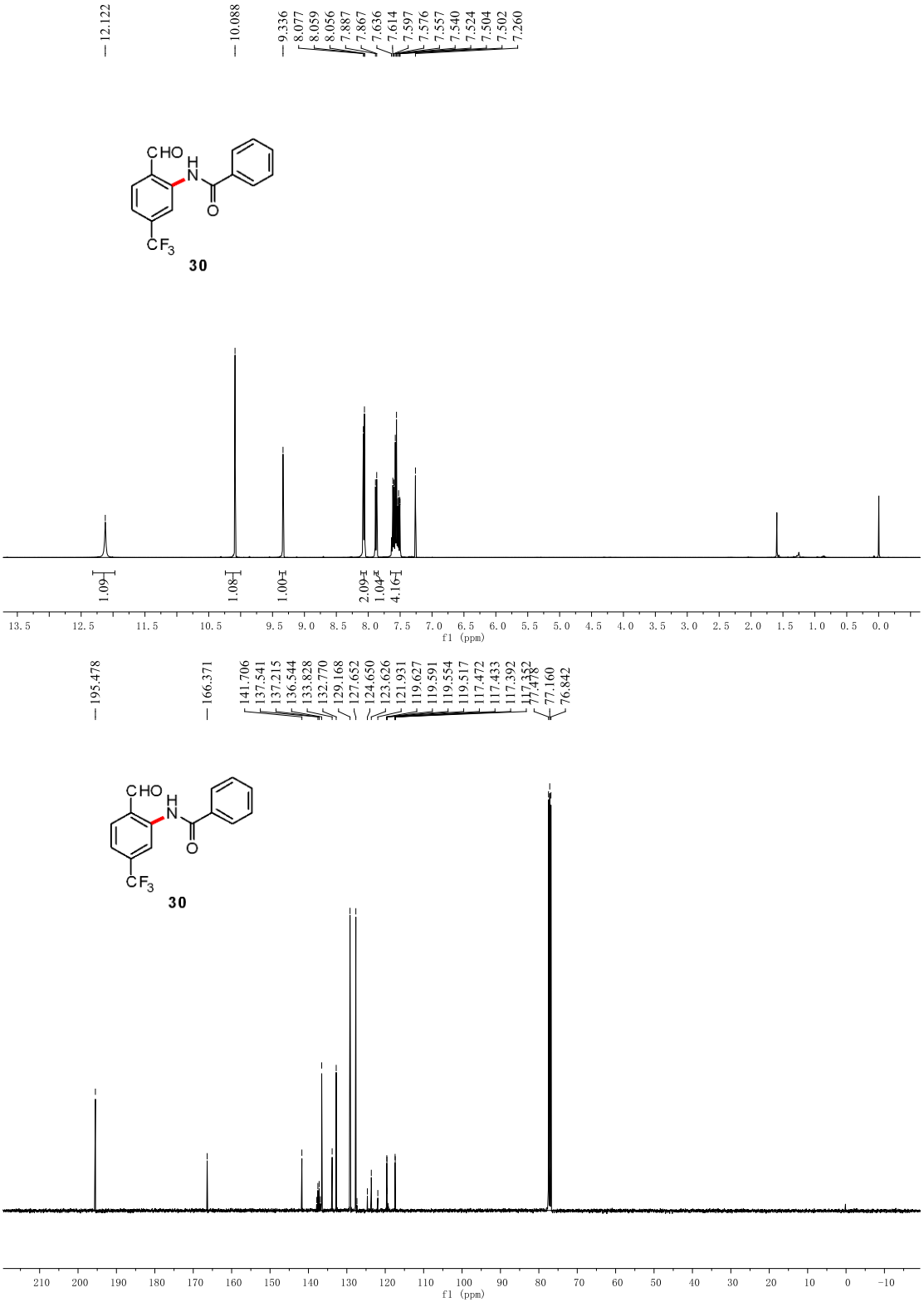

195.385
166.404
161.200
141.393
136.169
134.584
132.285
129.020
127.616
120.570
120.081
117.305
77.414
77.160
76.906
36.017
31.101
CHO
H
N
O
t-Bu
27
f1 (ppm)

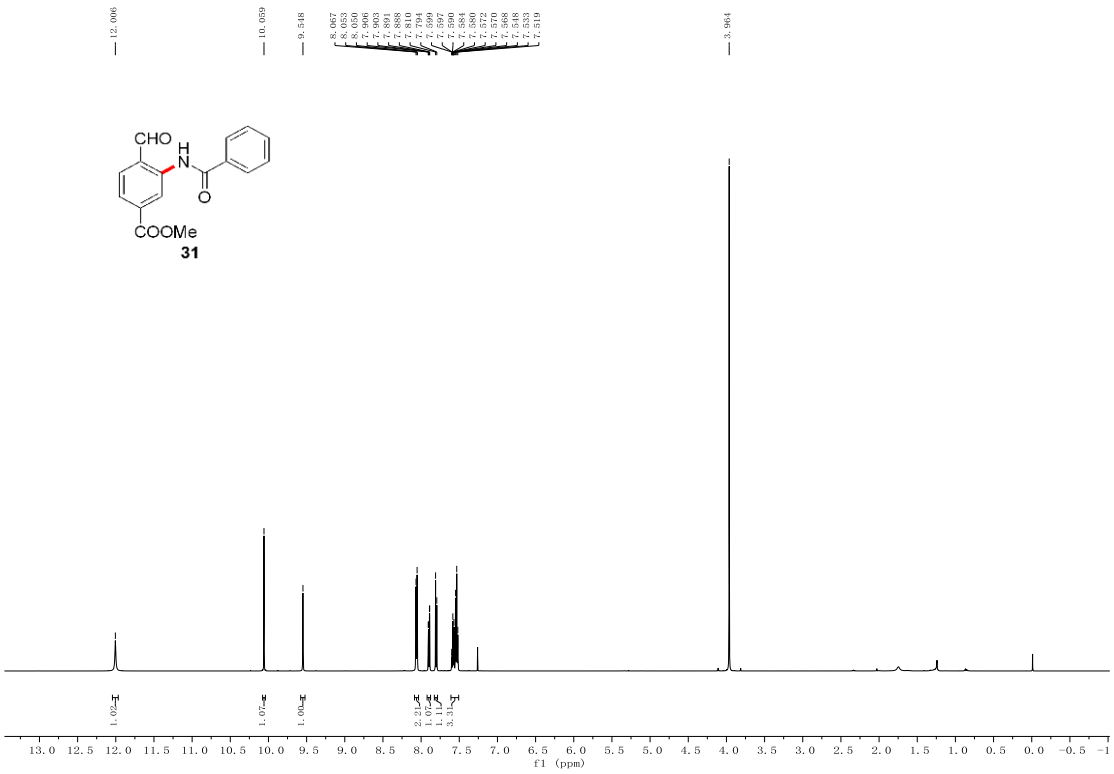

12.388
9.823
8.601
8.595
8.087
8.084
8.080
8.067
8.063
7.605
7.583
7.564
7.548
7.533
7.512
7.260
6.762
6.756
6.740
6.734
3.950
CHO
N
H
O
OMe
28
0.97
0.98
1.00
2.04
4.04
1.00
3.02
f1 (ppm)

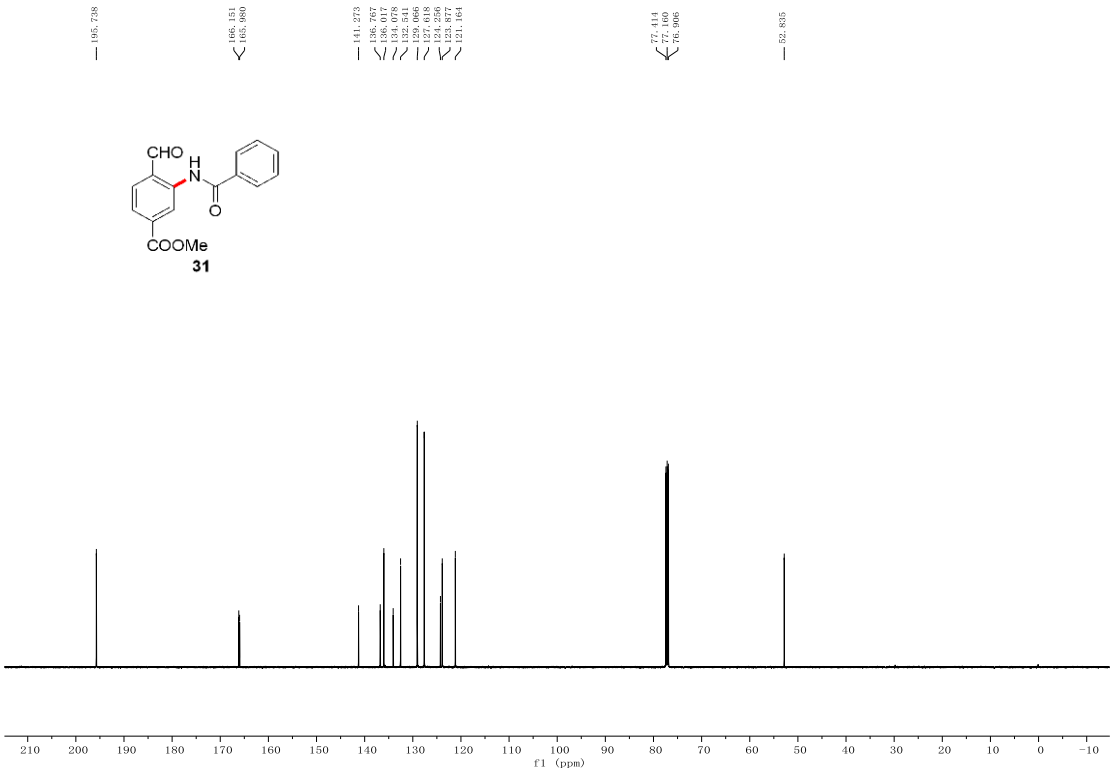

193.964
166.547
166.214
143.897
138.137
134.334
132.405
129.031
127.649
116.236
110.671
103.837
77.478
77.160
76.843
55.990
CHO
N
H
O
OMe
28
f1 (ppm)

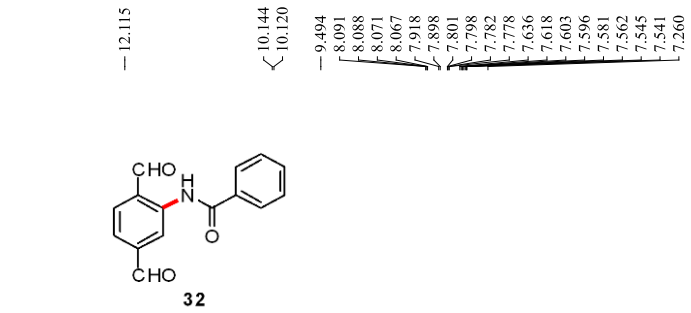

12.250
9.863
8.884
8.881
8.080
8.063
8.059
7.606
7.587
7.566
7.558
7.538
7.516
7.260
7.071
7.067
7.051
7.046
2.595
CHO
H
N
O
SMe
29
1.13
1.12
1.00
2.09
4.20
1.02
3.25
f1 (ppm)


194.498
166.477
151.430
141.648
135.997
134.279
132.447
129.054
127.644
119.652
118.727
114.781
77.478
77.160
76.843
14.741
CHO
H
N
O
SMe
29
f1 (ppm)

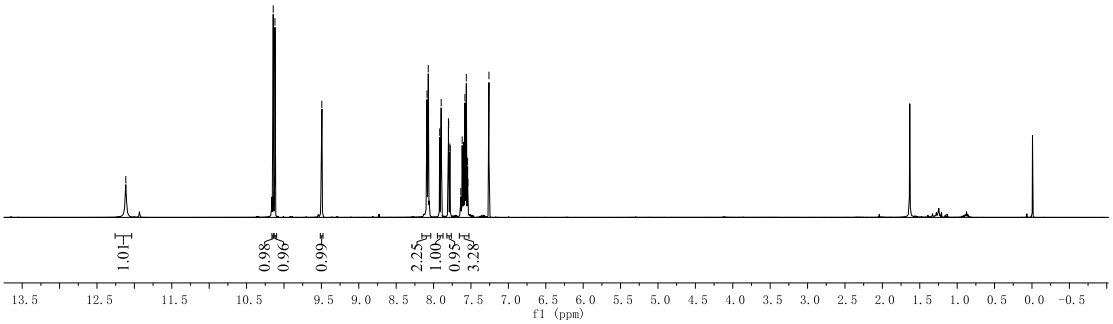

12.122
10.088
9.336
8.077
8.059
8.056
7.887
7.867
7.636
7.614
7.597
7.576
7.557
7.540
7.524
7.504
7.502
7.260
CHO
H
N
O
CF3
30
1.09
1.08
1.00
2.09
1.04
4.16
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
195.478
166.371
141.706
137.541
137.215
136.544
133.828
132.770
129.168
127.652
124.650
123.626
121.931
119.627
119.591
119.554
119.517
117.472
117.433
117.392
77.478
77.160
76.842
CHO
H
N
O
CF3
30
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

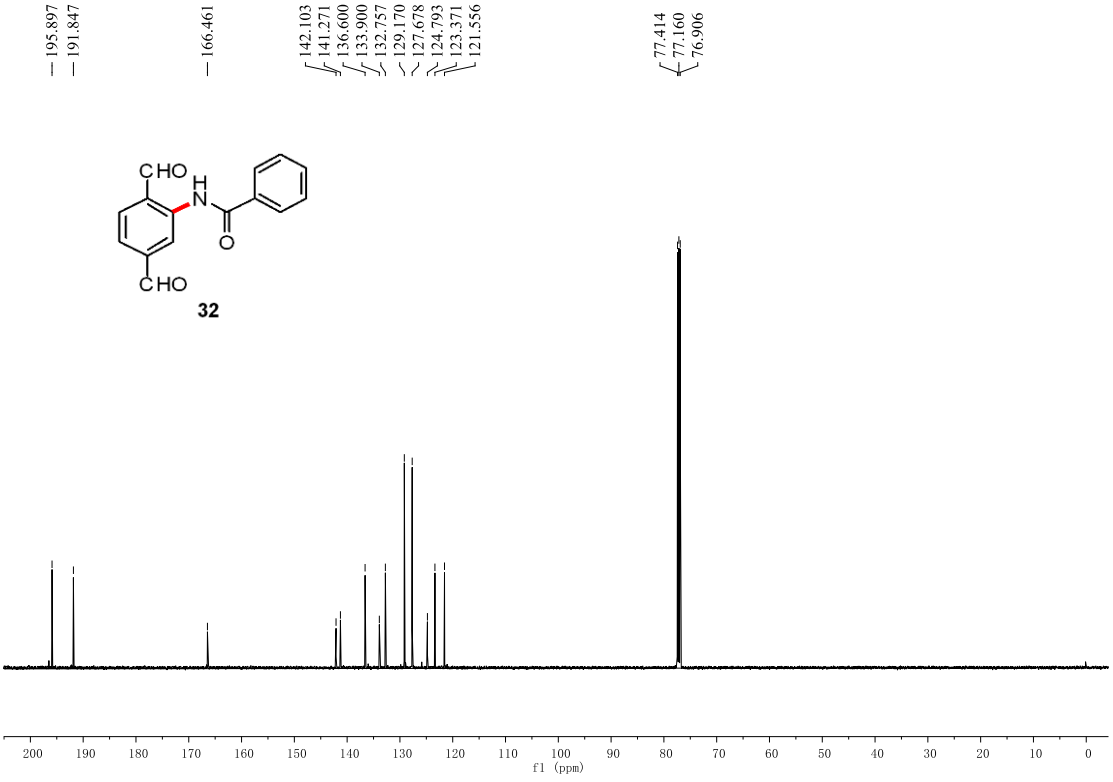

12.006
10.059
9.548
8.067
8.063
8.050
8.046
7.903
7.891
7.888
7.810
7.794
7.599
7.597
7.590
7.584
7.580
7.572
7.570
7.566
7.548
7.533
7.519
3.964
CHO
H
N
O
COOMe
31
1.00
1.07
1.00
2.21
1.07
1.11
5.31
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


195.738
166.151
165.980
141.273
136.767
136.017
131.078
132.541
129.066
127.618
124.256
121.877
121.164
77.414
77.160
76.906
52.835
CHO
H
N
O
COOMe
31
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

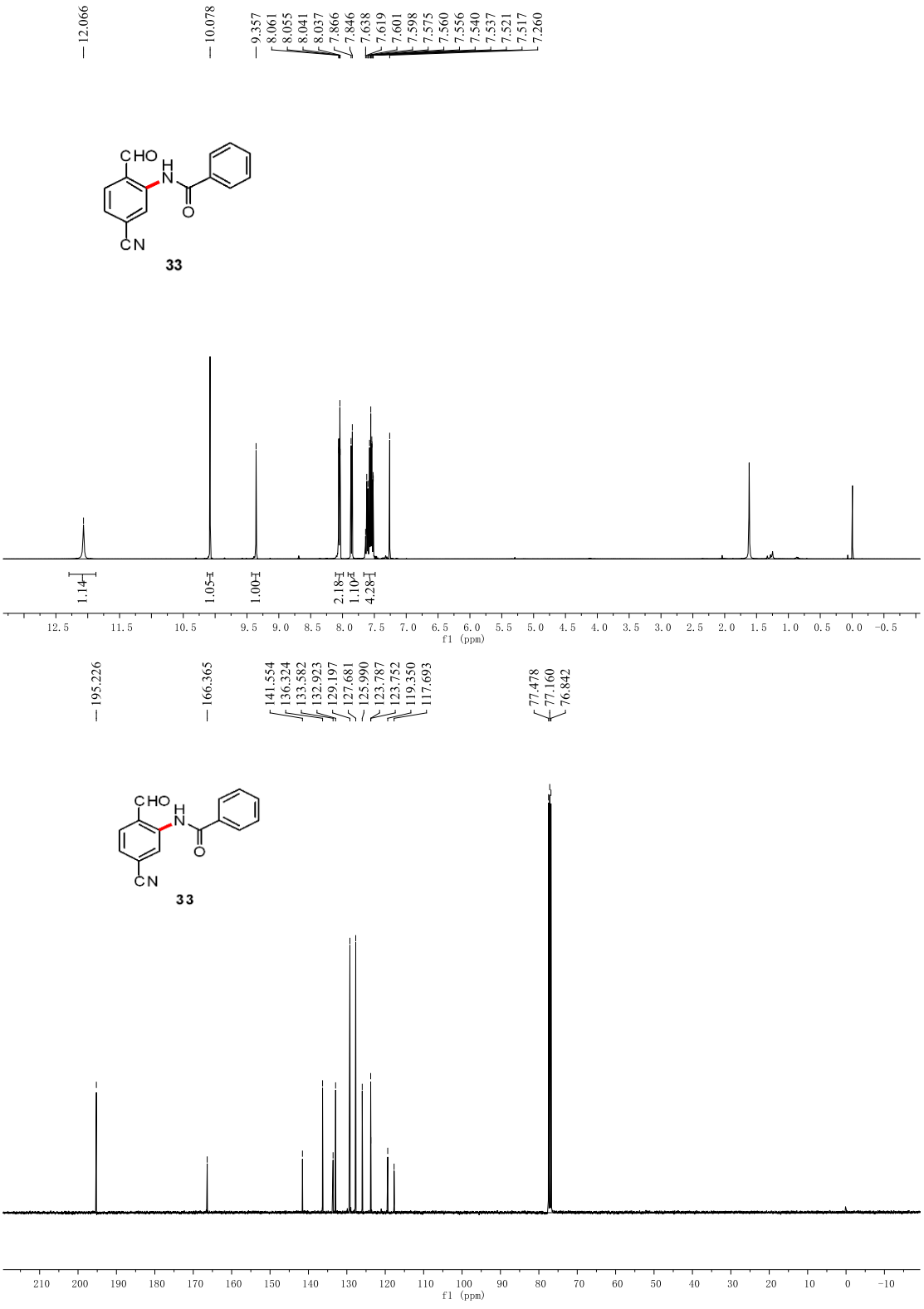

12.115
10.144
10.120
9.494
8.091
8.088
8.071
8.067
7.918
7.898
7.801
7.798
7.782
7.778
7.636
7.618
7.603
7.596
7.581
7.562
7.545
7.541
7.260
CHO
H
N
O
CHO

32


1.01
0.98
0.96
0.99
2.25
1.00
0.95
3.28
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


195.897
191.847
166.461
142.103
141.271
136.600
133.900
132.757
129.170
127.678
124.793
123.371
121.556
77.414
77.160
76.906
CHO
H
N
O
CHO
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

32


12.066
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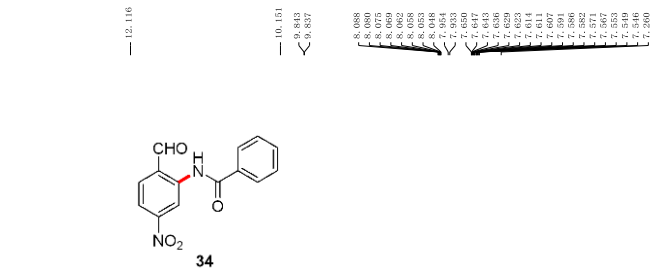
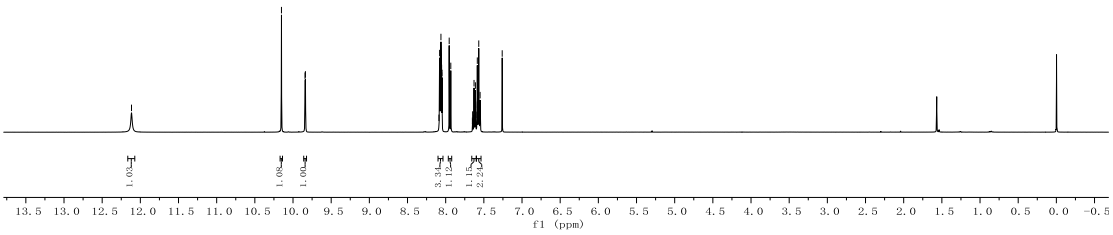
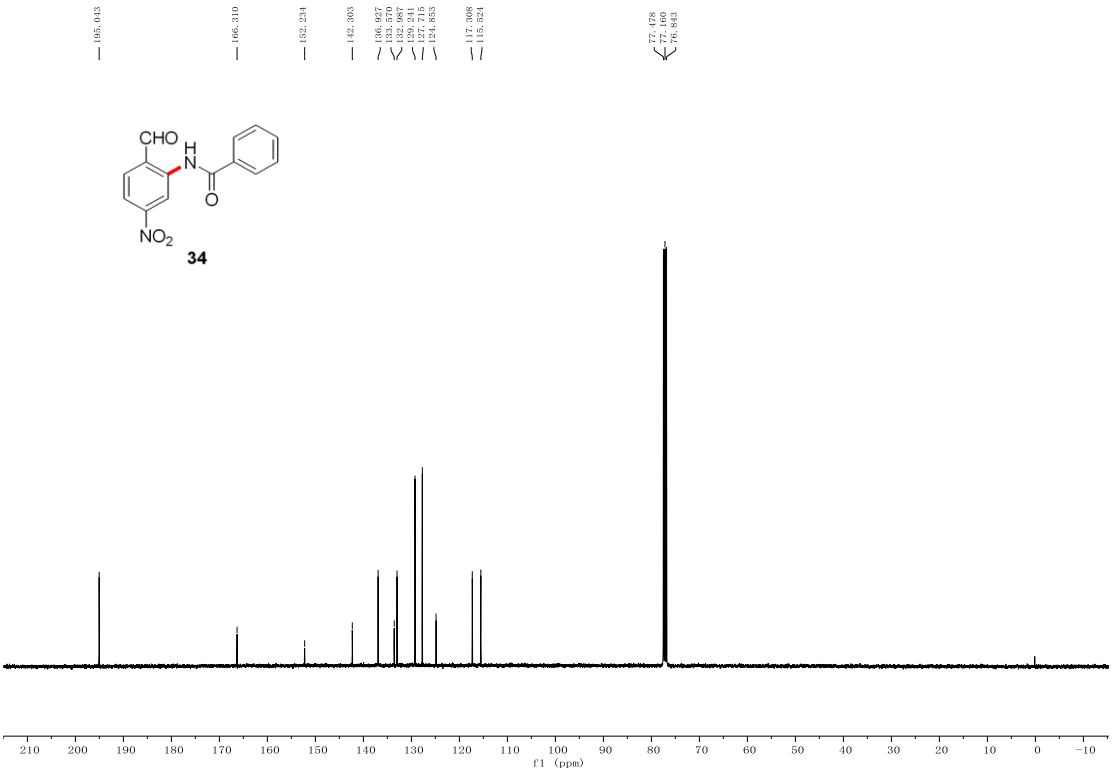
8.061
8.055
8.041
8.037
7.866
7.846
7.638
7.619
7.601
7.598
7.575
7.560
7.556
7.540
7.537
7.521
7.517
7.260
CHO
NH
O
CN
33
1.14
1.05
1.00
2.18
1.10
4.28
f1 (ppm)
195.226
166.365
141.554
136.324
133.582
132.923
129.197
127.681
125.990
123.787
123.752
119.350
117.693
77.478
77.160
76.842
CHO
NH
O
CN
33
f1 (ppm)

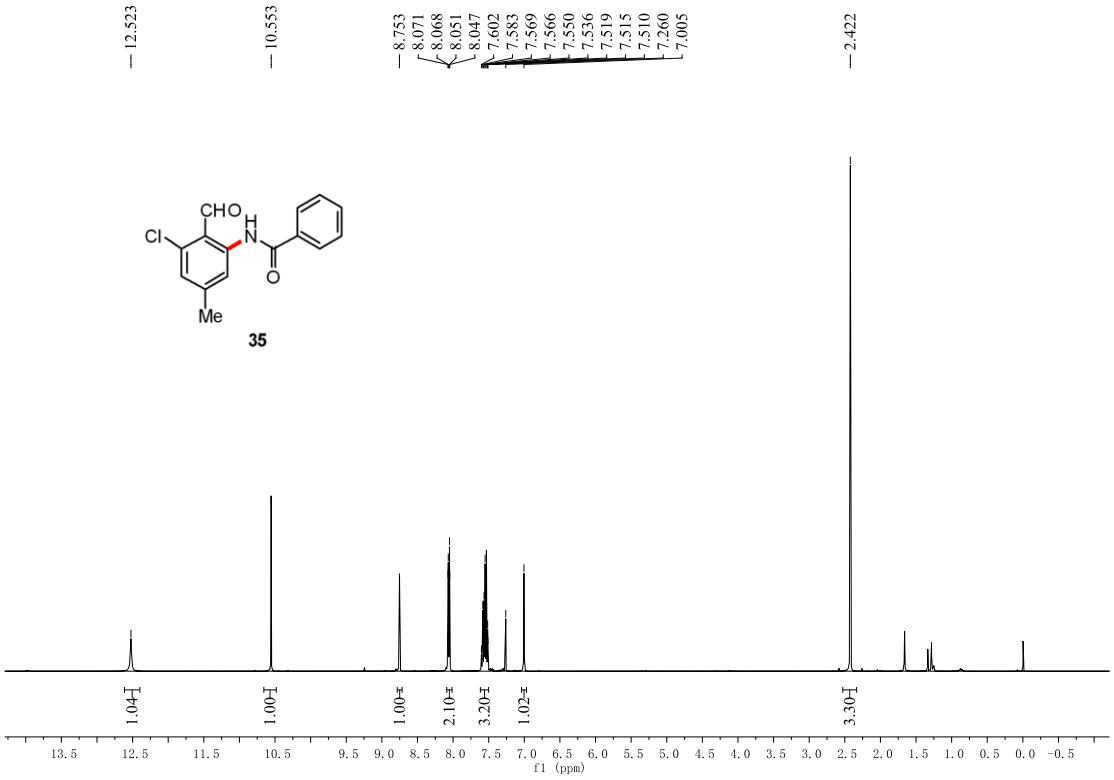


34





34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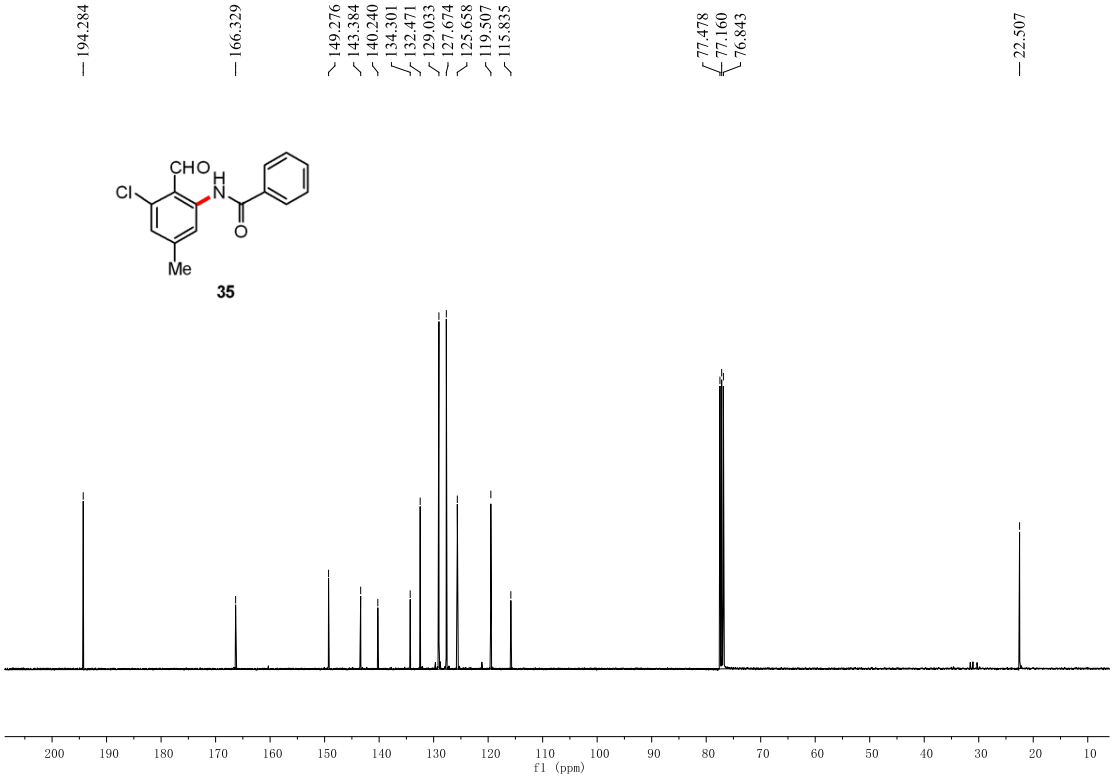
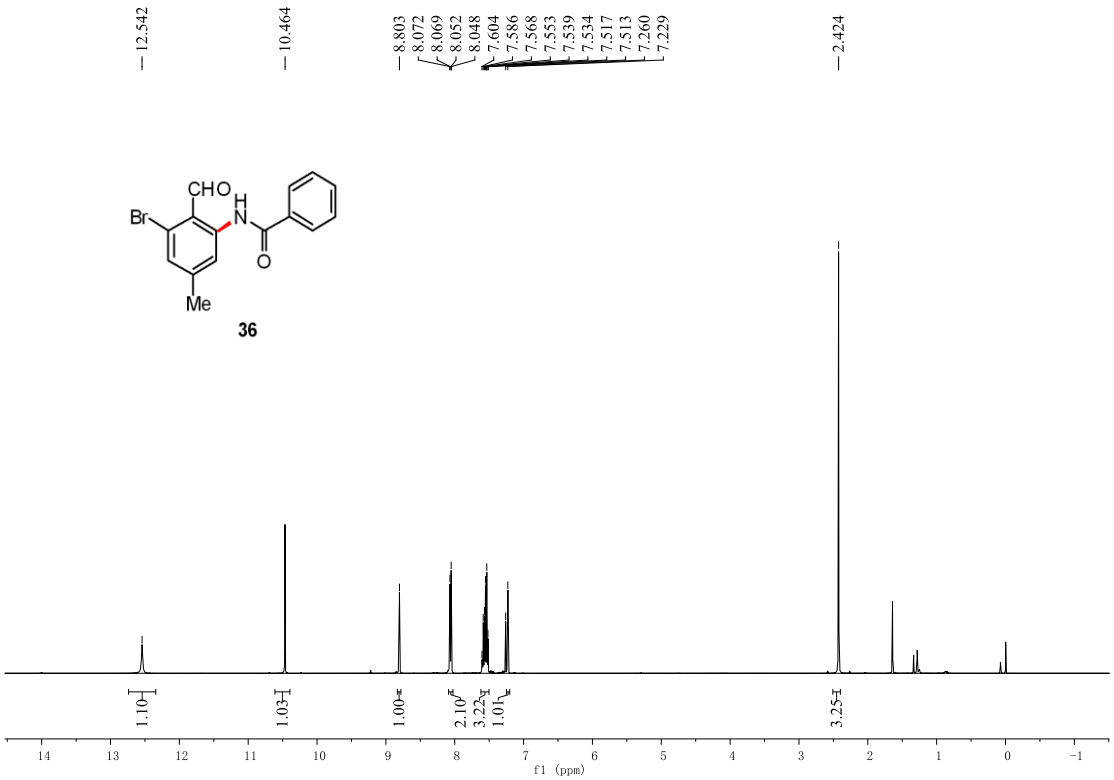
8.753
8.071
8.068
8.051
8.047
7.602
7.583
7.569
7.566
7.550
7.536
7.519
7.515
7.510
7.260
7.005
2.422
CHO
H
N
Cl
O
Me
35
1.04
1.00
1.00
2.10
3.20
1.02
3.30
f1 (ppm)


194.284
166.329
149.276
143.384
140.240
134.301
132.471
129.033
127.674
125.658
119.507
115.835
77.478
77.160
76.843
22.507
CHO
H
N
Cl
O
Me
35
f1 (ppm)


12.542
10.464
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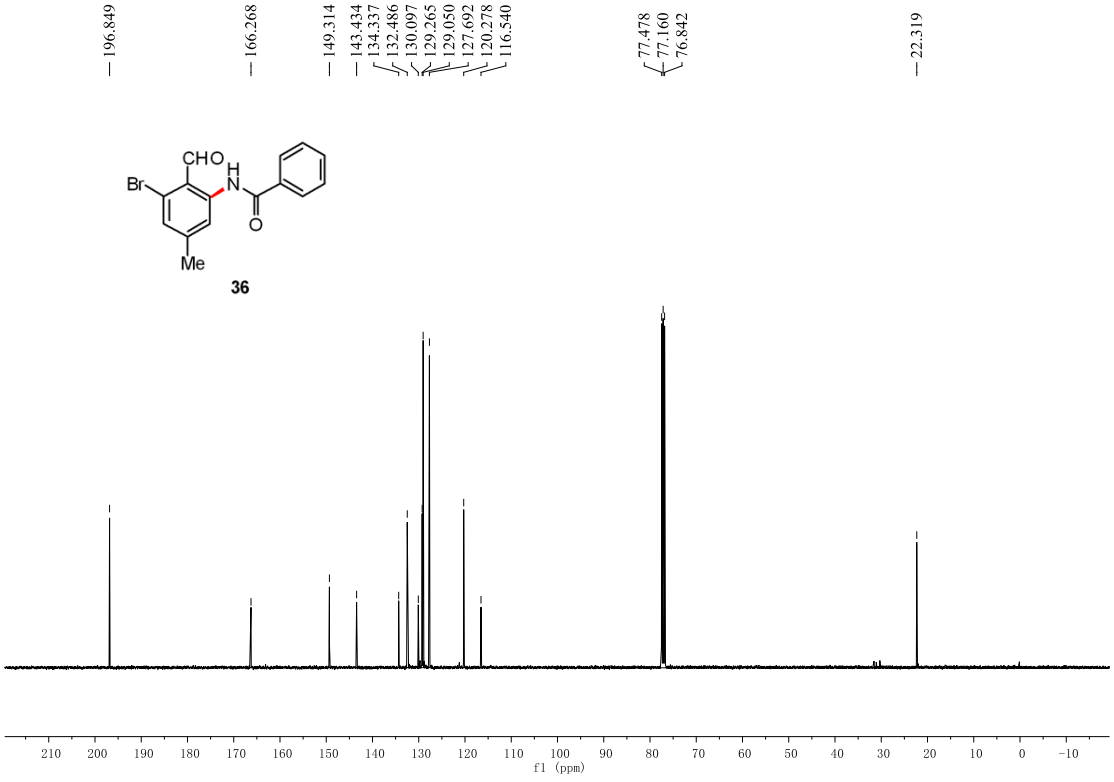
8.072
8.069
8.052
8.048
7.604
7.586
7.568
7.553
7.539
7.534
7.517
7.513
7.260
7.229
2.424
CHO
H
N
Br
O
Me
36
1.10
1.03
1.00
2.10
3.22
1.01
3.25
f1 (ppm)


196.849
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149.314
143.434
134.337
132.486
130.097
129.265
129.050
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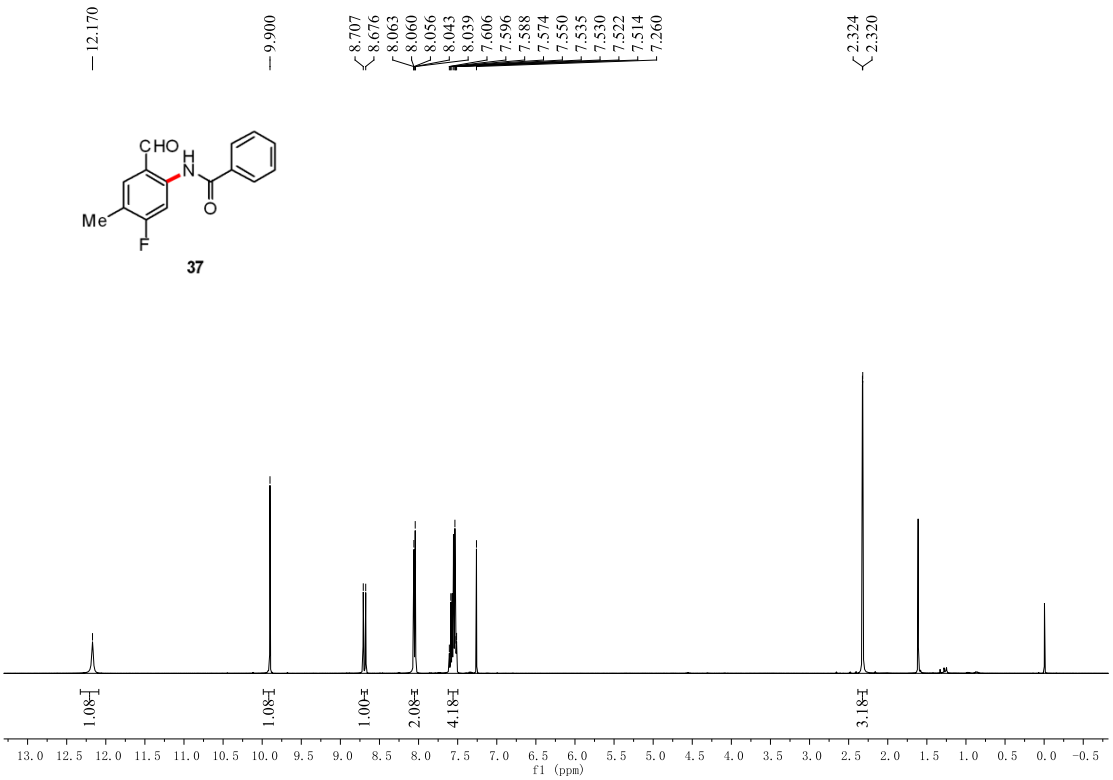
77.478
77.160
76.842
22.319
CHO
H
N
Br
O
Me
36
f1 (ppm)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8.676
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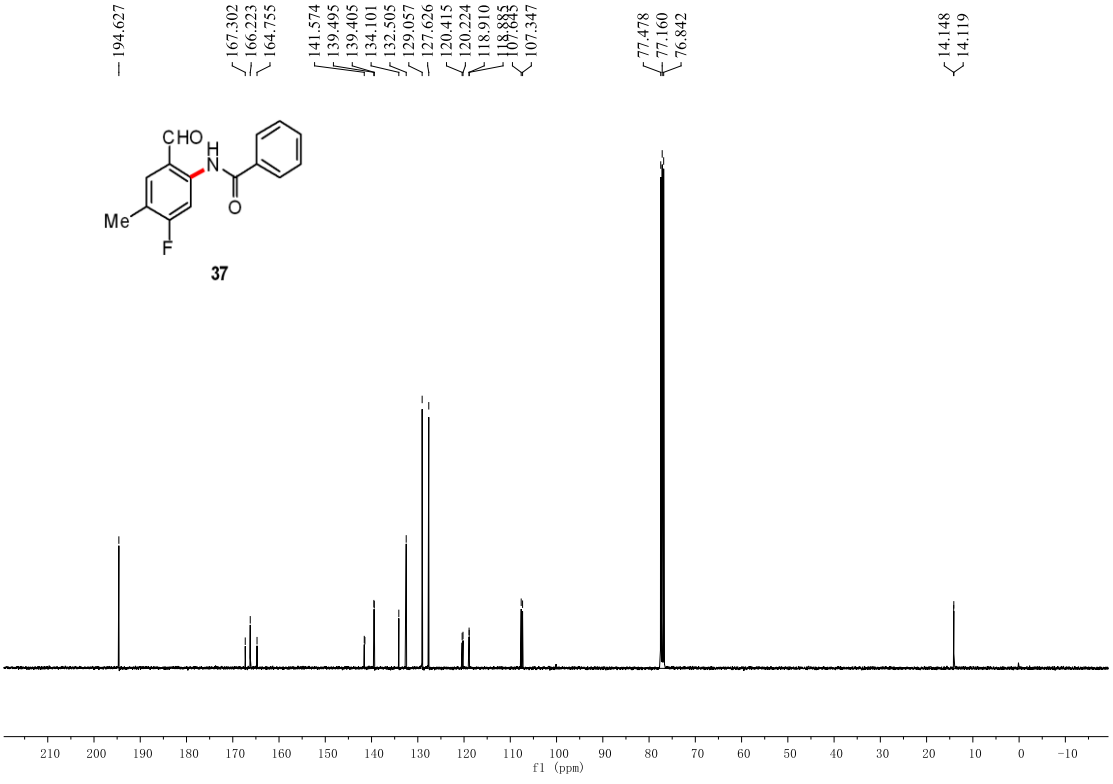
8.060
8.056
8.043
8.039
7.606
7.596
7.588
7.574
7.550
7.535
7.530
7.522
7.514
7.260
2.324
2.320
CHO
N
H
O
Me
F
37
1.08
1.08
1.00
2.08
4.18
3.18
f1 (ppm)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167.302
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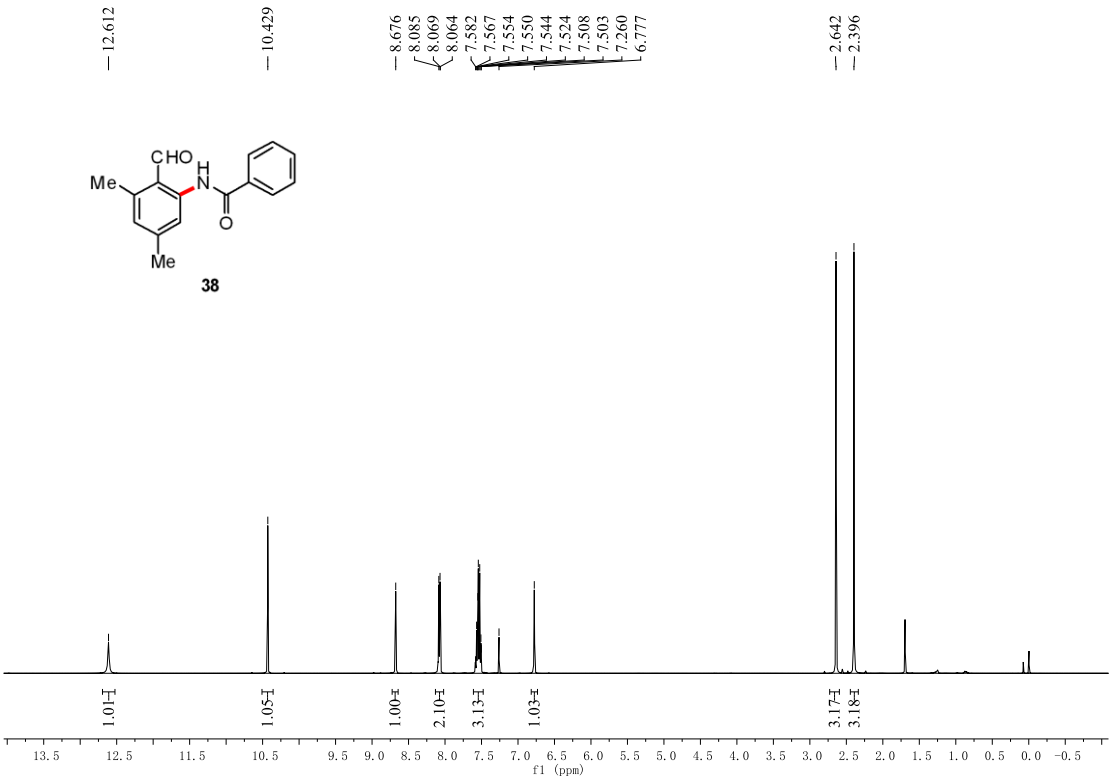
164.755
141.574
139.495
139.405
134.101
132.505
129.057
127.626
120.415
120.224
118.910
118.885
118.845
107.347
77.478
77.160
76.842
14.148
14.119
CHO
N
H
O
Me
F
37
f1 (ppm)


12.612
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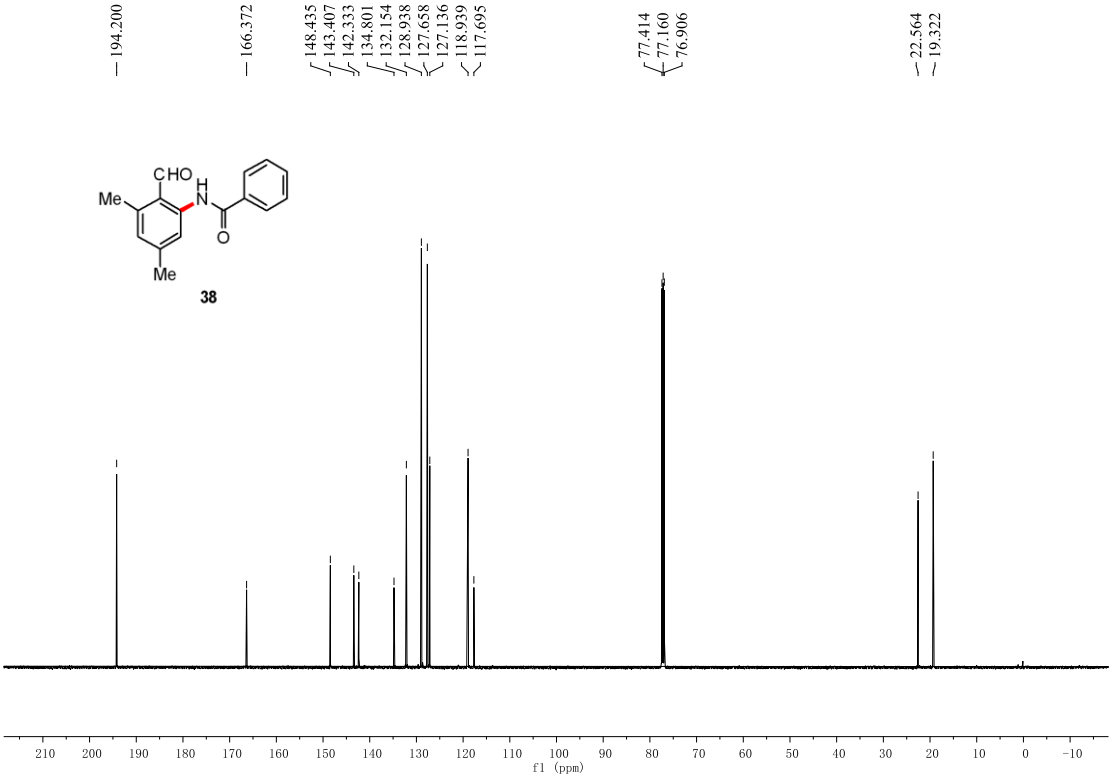
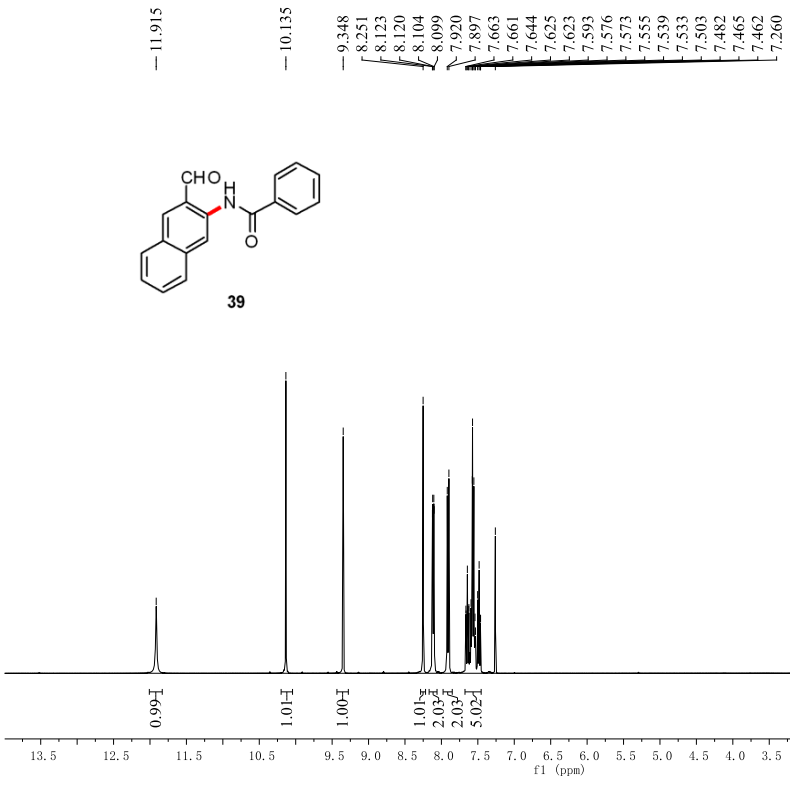
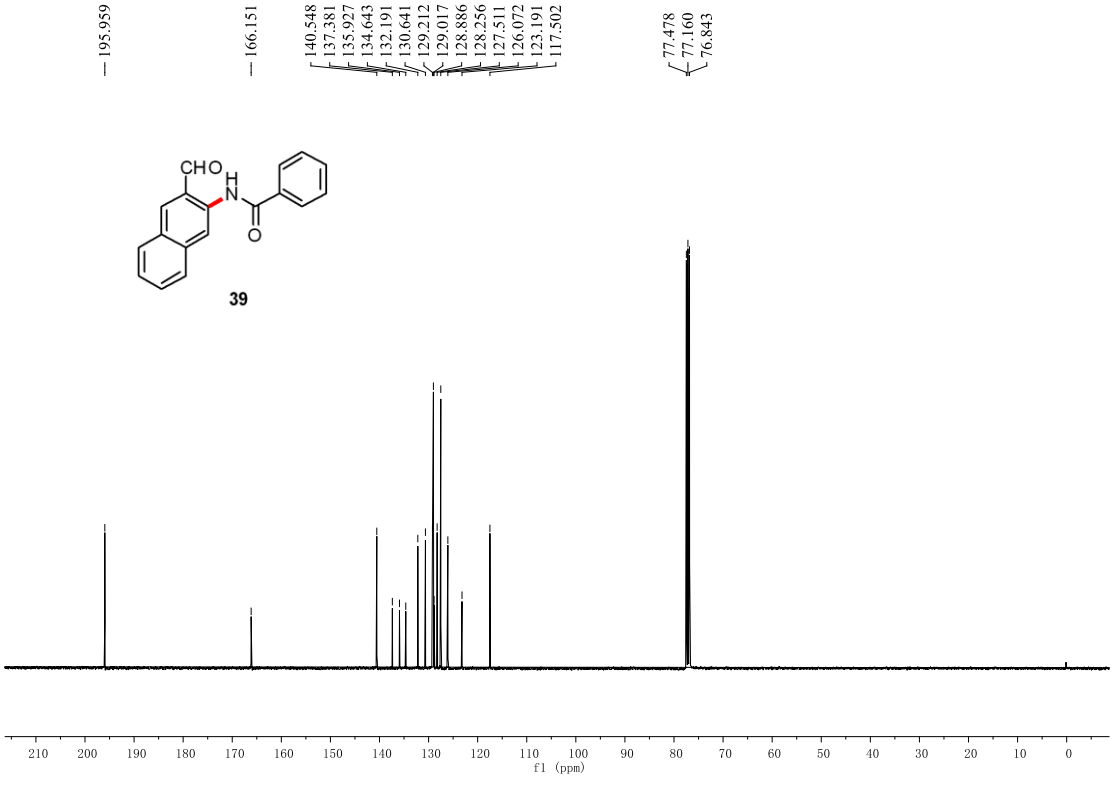
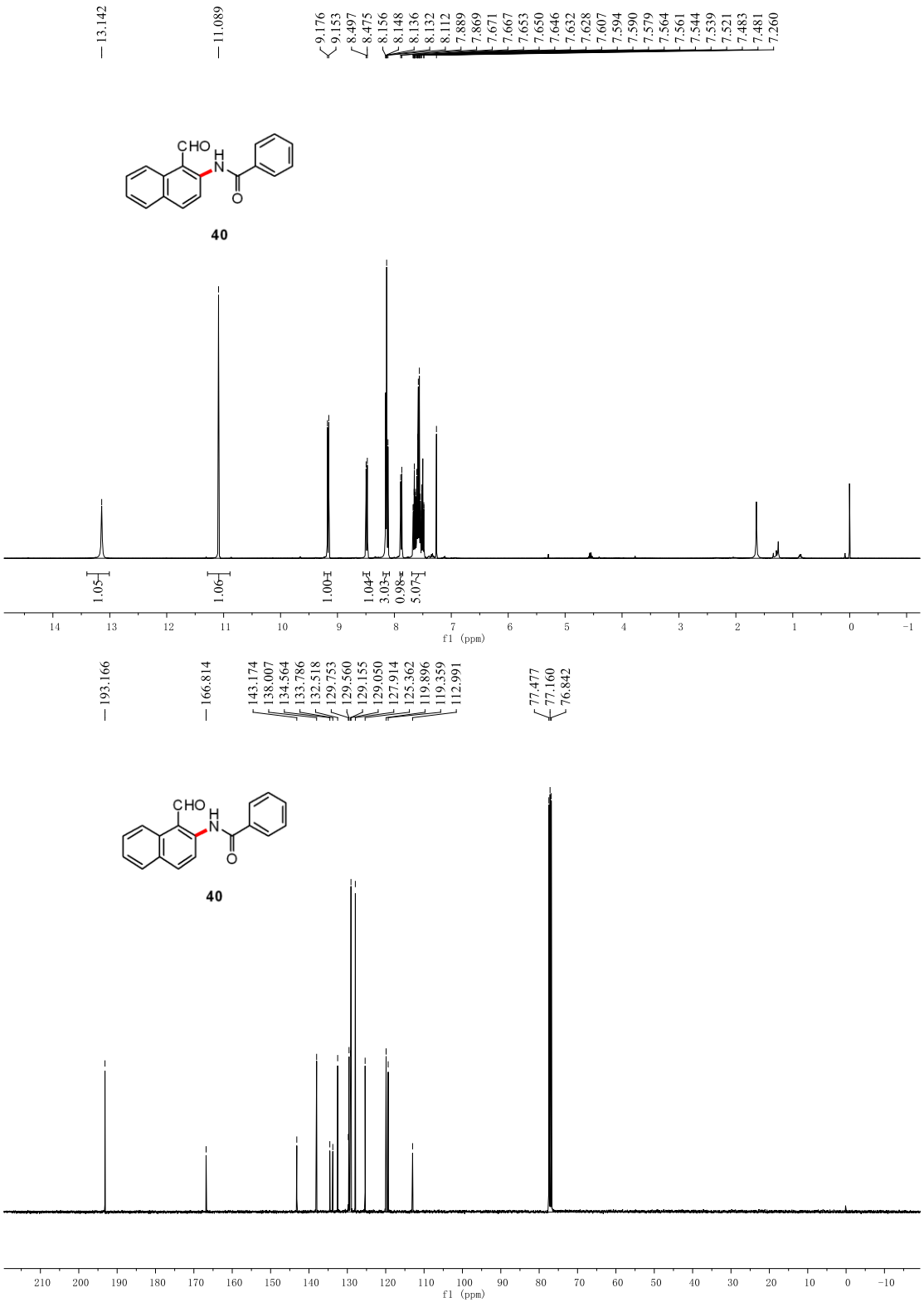
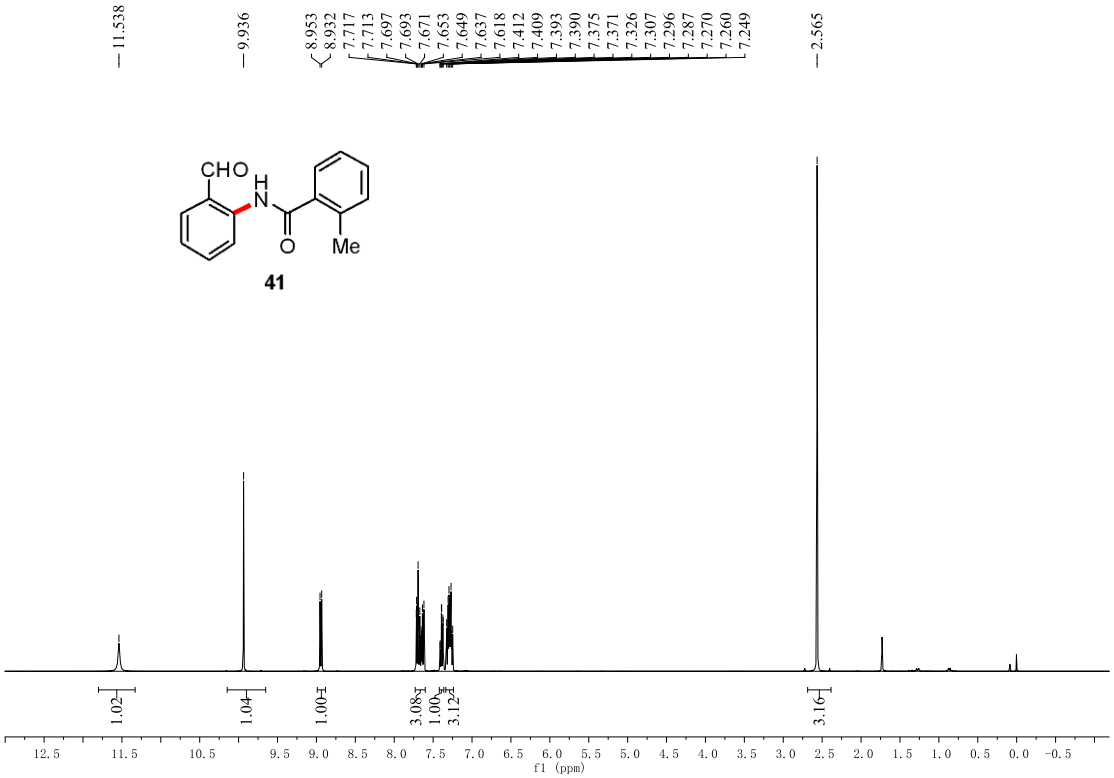
8.676
8.085
8.069
8.064
7.582
7.567
7.554
7.550
7.544
7.524
7.508
7.503
7.260
6.777
2.642
2.396
CHO
H
N
O
Me
Me
38
1.01
1.05
1.00
2.10
3.13
1.03
3.17
3.18
f1 (ppm)

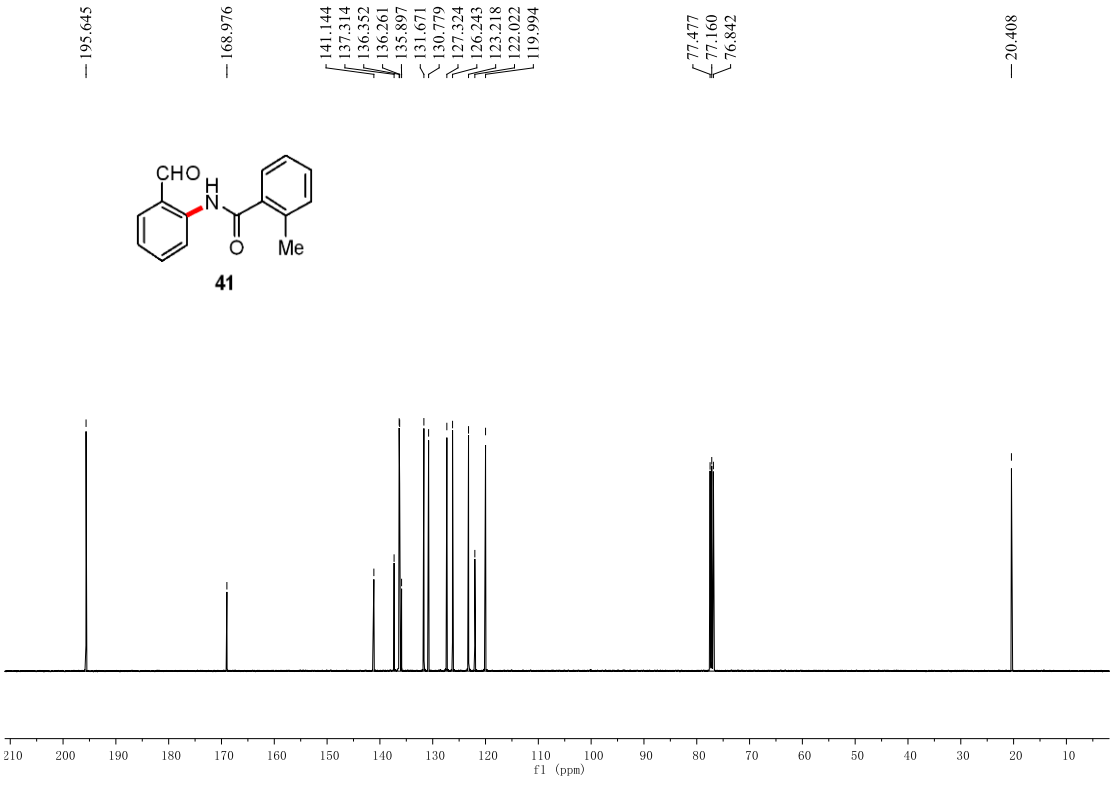

194.200
166.372
148.435
143.407
142.333
134.801
132.154
128.938
127.658
127.136
118.939
117.695
77.414
77.160
76.906
22.564
19.322
CHO
H
N
O
Me
Me
38
f1 (ppm)

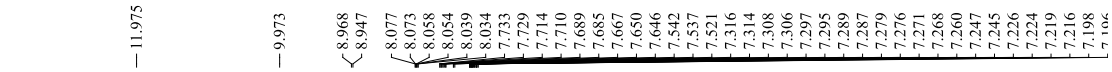

11.915
10.135
9.348
8.251
8.123
8.120
8.104
8.099
7.920
7.897
7.663
7.661
7.644
7.625
7.623
7.593
7.576
7.573
7.555
7.539
7.533
7.503
7.482
7.465
7.462
7.260
CHO
N
H
O
39
0.99
1.01
1.00
1.01
2.03
2.03
5.02
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

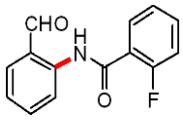

195.959
166.151
140.548
137.381
135.927
134.643
132.191
130.641
129.212
129.017
128.886
128.256
127.511
126.072
123.191
117.502
77.478
77.160
76.843
CHO
N
H
O
39
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


13.142
11.089
9.176
9.153
8.497
8.475
8.156
8.148
8.136
8.132
8.112
7.889
7.869
7.671
7.667
7.653
7.650
7.646
7.632
7.628
7.607
7.594
7.590
7.579
7.564
7.561
7.544
7.539
7.521
7.483
7.481
7.260
CHO
H
N
O
40
1.05
1.06
1.00
1.04
3.03
0.98
5.07
f1 (ppm)
193.166
166.814
143.174
138.007
134.564
133.786
132.518
129.753
129.560
129.155
129.050
127.914
125.362
119.896
119.359
112.991
77.477
77.160
76.842
CHO
H
N
O
40
f1 (ppm)

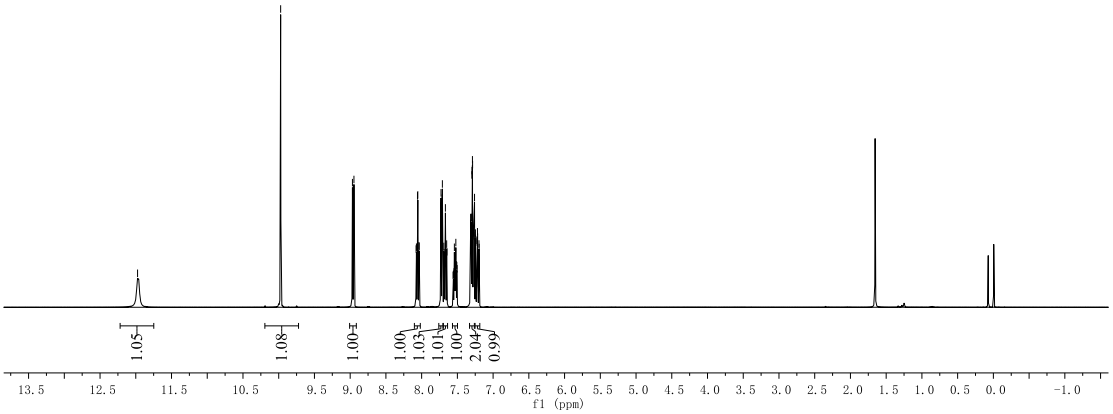

11.538
9.936
8.953
8.932
7.717
7.713
7.697
7.693
7.671
7.653
7.649
7.637
7.618
7.412
7.409
7.393
7.390
7.375
7.371
7.326
7.307
7.296
7.287
7.270
7.260
7.249
2.565
CHO
H
N
O
Me
41
1.02
1.04
1.00
3.08
1.00
3.12
3.16
f1 (ppm)


195.645
168.976
141.144
137.314
136.352
136.261
135.897
131.671
130.779
127.324
126.243
123.218
122.022
119.994
77.477
77.160
76.842
20.408
CHO
H
N
O
Me
41
f1 (ppm)

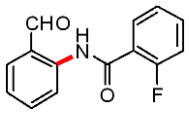

11.975
9.973
8.968
8.947
8.077
8.073
8.058
8.054
8.039
8.034
7.733
7.729
7.714
7.710
7.689
7.685
7.667
7.650
7.646
7.542
7.537
7.521
7.316
7.314
7.308
7.306
7.297
7.295
7.289
7.287
7.279
7.276
7.271
7.268
7.260
7.247
7.245
7.226
7.224
7.219
7.216
7.198


CHO
H
N
O
F

42

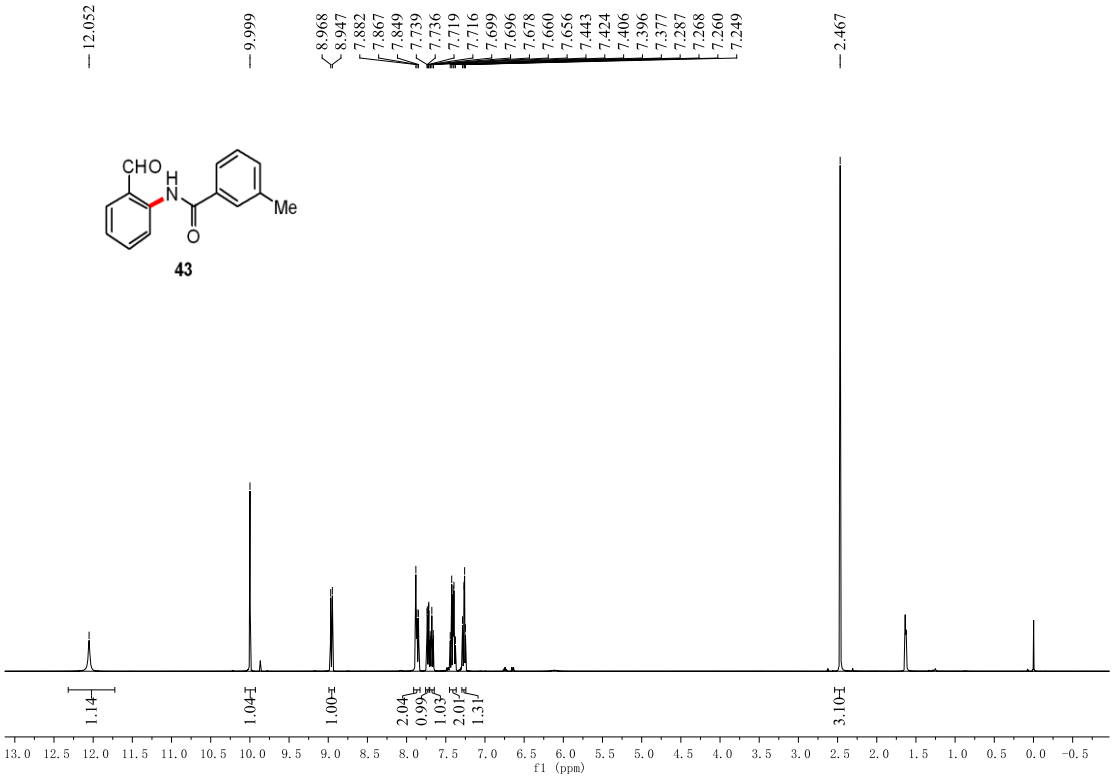

1.05
1.08
1.00
1.00
1.03
1.01
1.00
2.04
0.99
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−1.0
f1 (ppm)

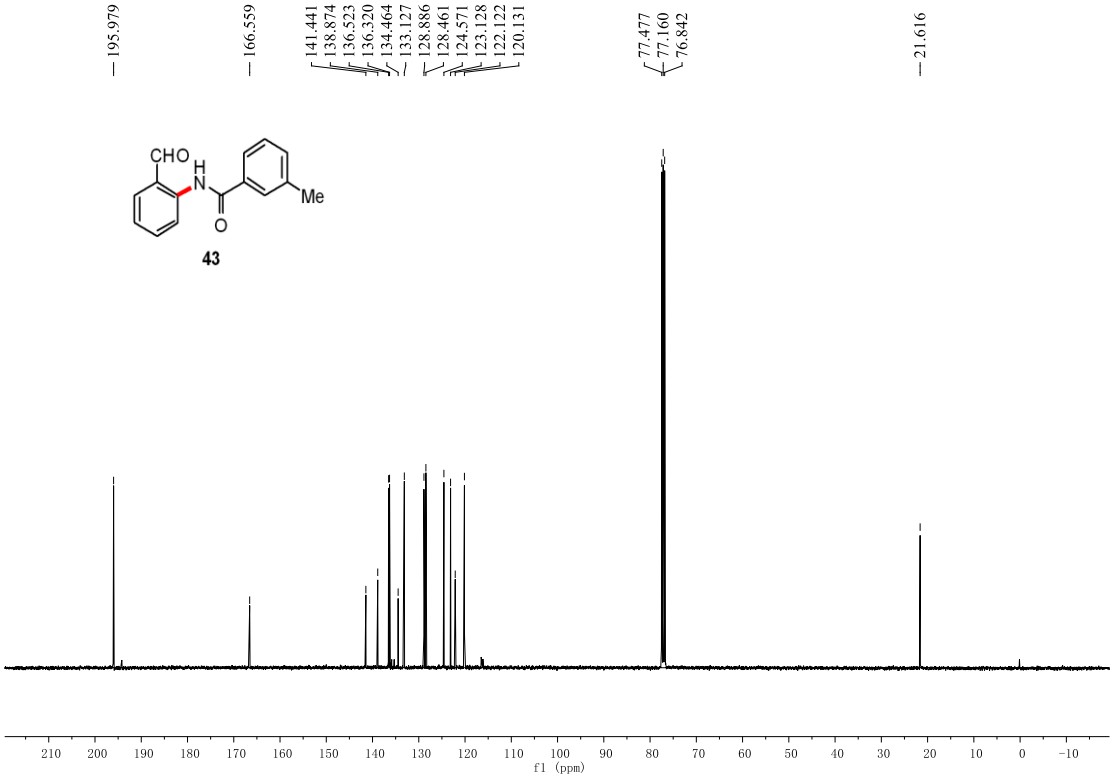

195.221
163.099
163.073
161.628
159.131
140.546
136.279
136.210
133.982
133.892
131.817
131.797
124.890
124.855
123.588
122.588
122.516
122.396
120.866
116.808
116.574
77.478
77.160
76.843

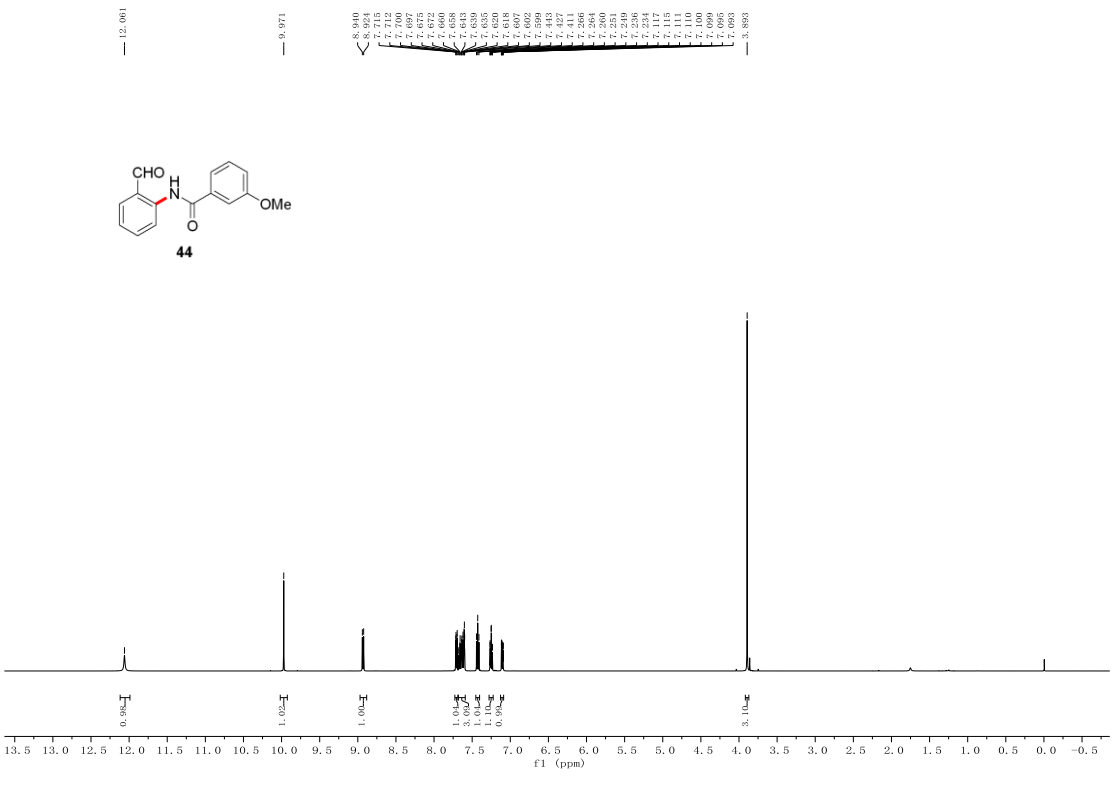

CHO
H
N
O
F

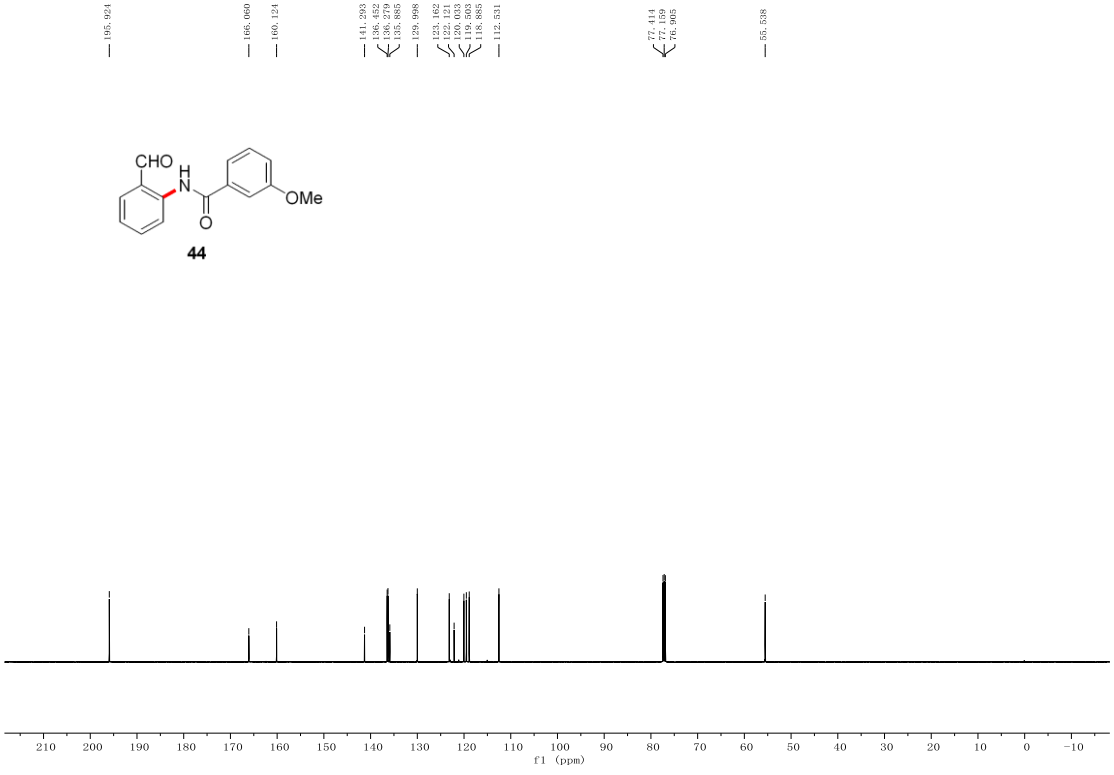
42

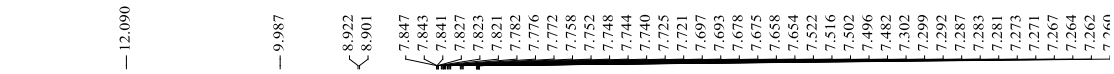
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

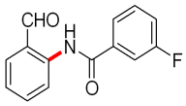

12.052
9.999
8.968
8.947
7.882
7.867
7.849
7.739
7.736
7.719
7.716
7.699
7.696
7.678
7.660
7.656
7.443
7.424
7.406
7.396
7.377
7.287
7.268
7.260
7.249
2.467
CHO
H
N
O
Me
43
1.14
1.04
1.00
2.04
0.99
1.03
2.01
1.31
3.10
f1 (ppm)


195.979
166.559
141.441
138.874
136.523
136.320
134.464
133.127
128.886
128.461
124.571
123.128
122.122
120.131
77.477
77.160
76.842
21.616
CHO
H
N
O
Me
43
f1 (ppm)

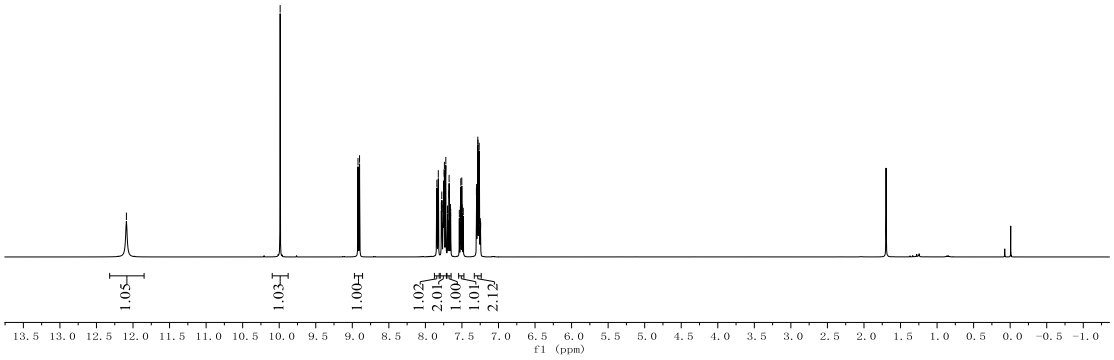

12.061
9.971
8.940
8.934
8.715
7.712
7.700
7.697
7.675
7.672
7.660
7.658
7.645
7.639
7.635
7.620
7.618
7.607
7.602
7.599
7.443
7.437
7.411
7.266
7.264
7.260
7.251
7.249
7.236
7.234
7.117
7.115
7.111
7.110
7.100
7.099
7.095
7.093
3.893
CHO
N
H
O
OMe
44
0.98
1.02
1.00
1.04
3.02
1.04
1.10
0.99
3.10
13.5 13.0 12.5 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 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)

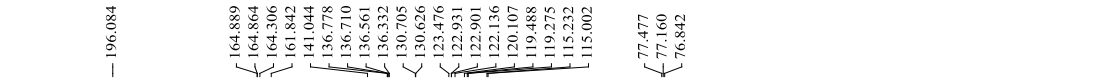

195.924
166.060
160.124
141.293
136.452
136.279
135.885
129.998
123.162
122.121
120.033
119.503
118.885
112.531
77.414
77.159
76.905
55.538
CHO
N
H
O
OMe
44
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

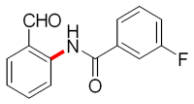

12.090
9.987
8.922
8.901
7.847
7.843
7.841
7.827
7.823
7.821
7.782
7.776
7.772
7.758
7.752
7.748
7.744
7.740
7.725
7.721
7.697
7.693
7.678
7.675
7.658
7.654
7.522
7.516
7.502
7.496
7.482
7.302
7.299
7.292
7.287
7.283
7.281
7.273
7.271
7.267
7.264
7.262


CHO
H
N
O
F

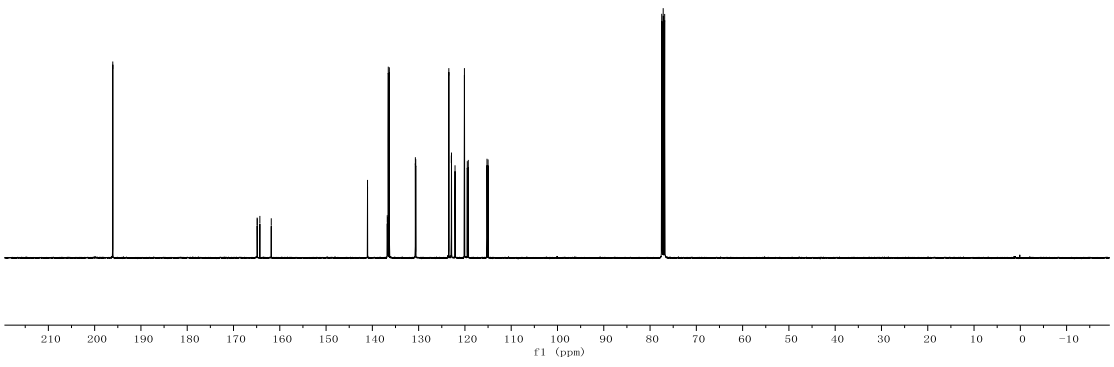
45


1.05
1.03
1.00
1.02
2.01
1.00
1.01
2.12
13.5 13.0 12.5 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 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


196.084
164.889
164.864
164.306
161.842
141.044
136.778
136.710
136.561
136.332
130.705
130.626
123.476
122.931
122.901
122.136
120.107
119.488
119.275
115.232
115.002
77.477
77.160
76.842


CHO
H
N
O
F

45


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


12.083
9.990
8.916
8.895
8.055
8.050
8.045
7.934
7.931
7.927
7.915
7.912
7.908
7.746
7.742
7.727
7.723
7.700
7.697
7.681
7.661
7.657
7.557
7.554
7.552
7.537
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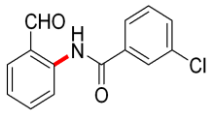
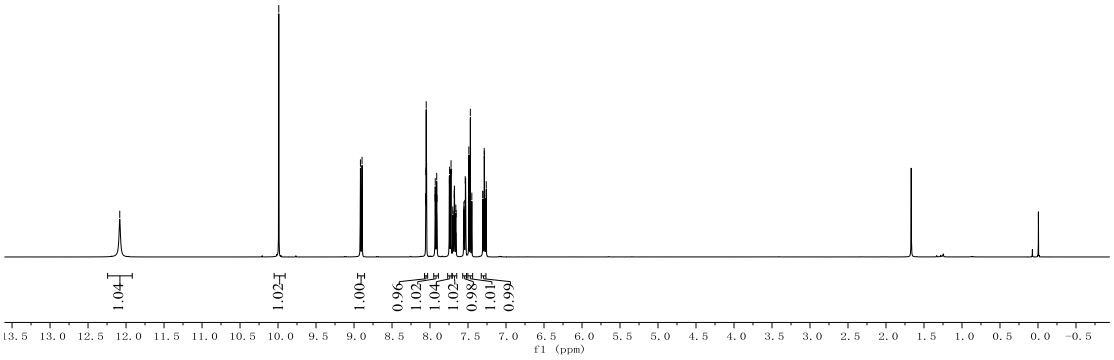
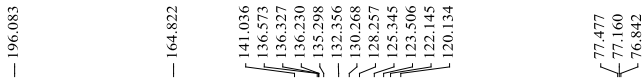
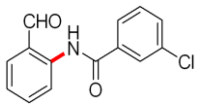
7.469
7.450
7.306
7.303
7.287
7.284
7.268
7.266
7.260


CHO
H
N
O
Cl

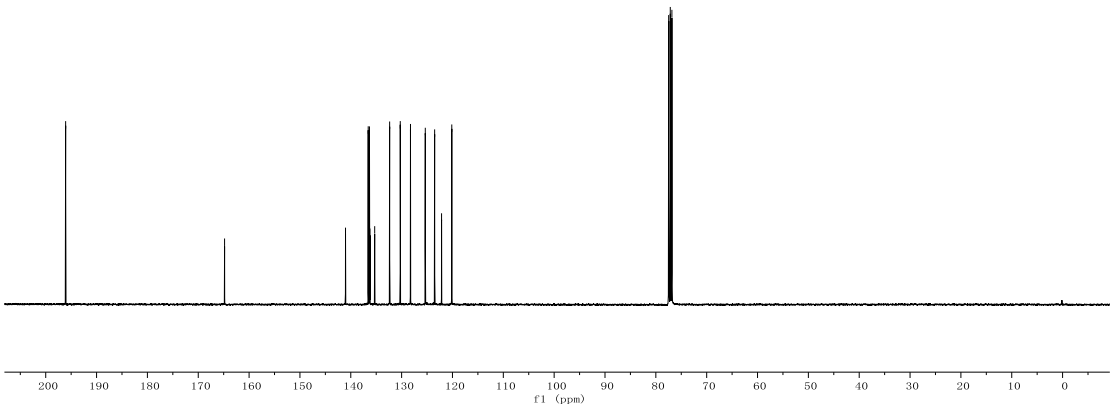
46

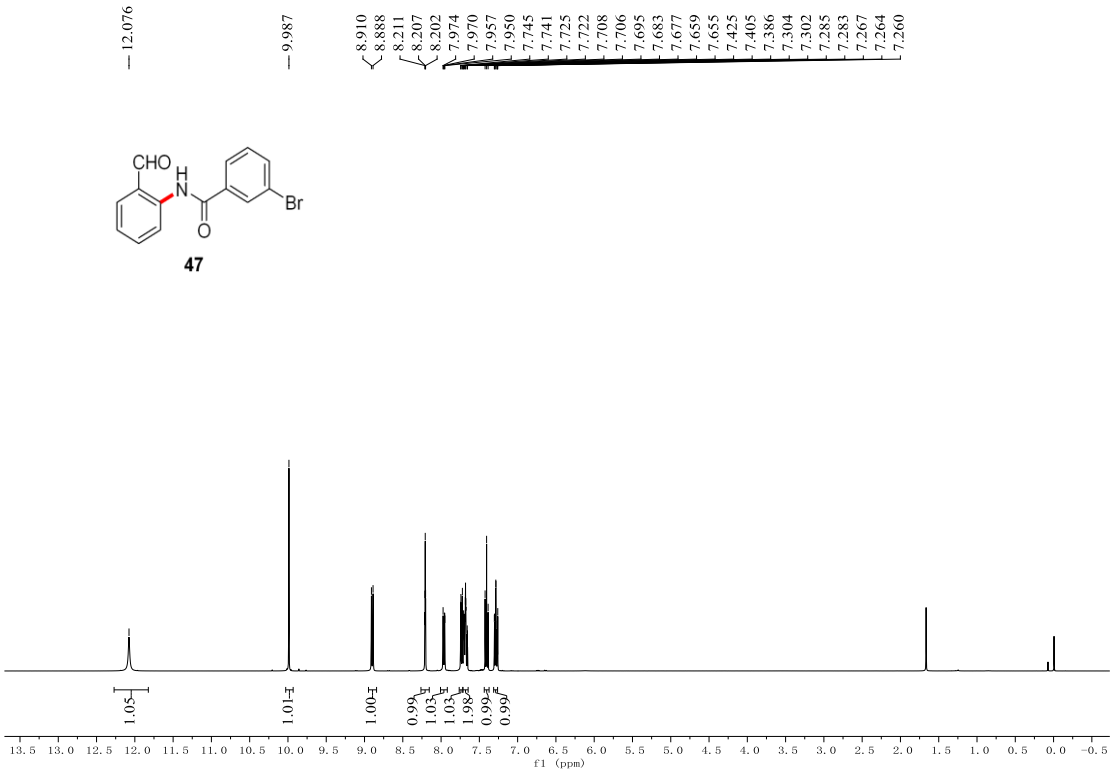

1.04
1.02
1.00
0.96
1.02
1.04
1.02
0.98
1.01
0.99
f1 (ppm)

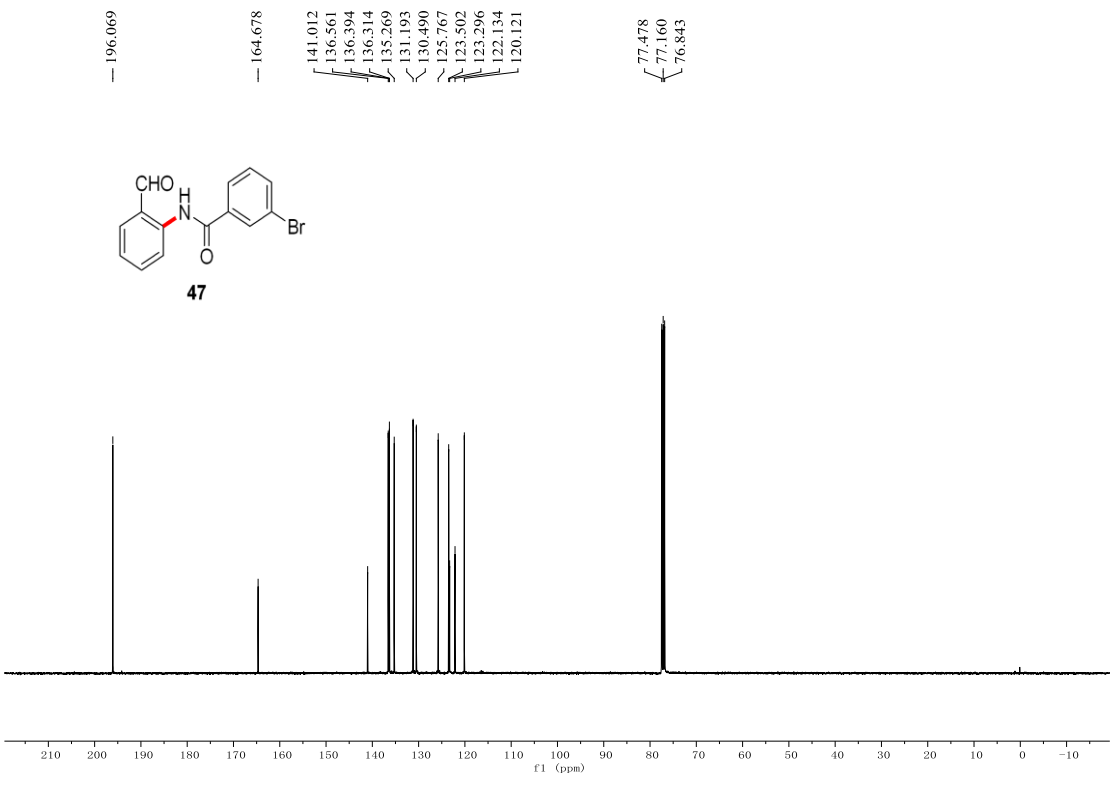

196.083
164.822
141.036
136.573
136.327
136.230
135.298
132.356
130.268
128.257
125.345
123.506
122.145
120.134
77.477
77.160
76.842

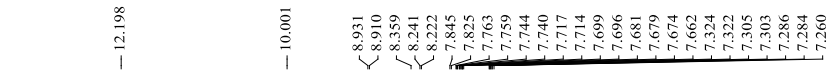

CHO
H
N
O
Cl

46


f1 (ppm)


12.076
9.987
8.910
8.888
8.211
8.207
8.202
7.974
7.970
7.957
7.950
7.745
7.741
7.725
7.722
7.708
7.706
7.695
7.683
7.677
7.659
7.655
7.425
7.405
7.386
7.304
7.302
7.285
7.283
7.267
7.264
7.260
CHO
H
N
O
Br
47
1.05
1.01
1.00
0.99
1.03
1.03
1.98
0.99
0.99
f1 (ppm)


196.069
164.678
141.012
136.561
136.394
136.314
135.269
131.193
130.490
125.767
123.502
123.296
122.134
120.121
77.478
77.160
76.843
CHO
H
N
O
Br
47
f1 (ppm)


12.198
10.001
8.931
8.910
8.359
8.241
8.222
7.845
7.825
7.763
7.759
7.744
7.740
7.717
7.714
7.699
7.696
7.681
7.679
7.674
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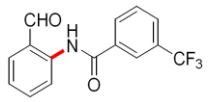
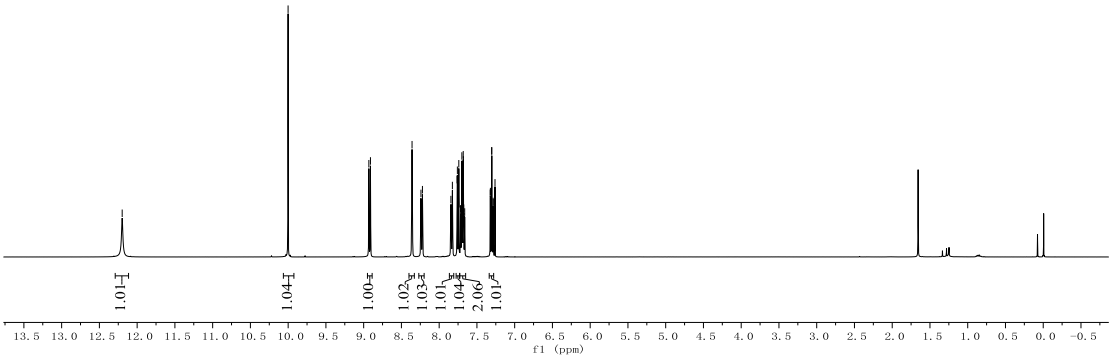
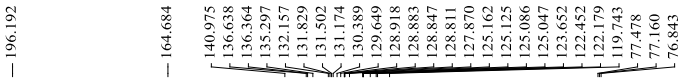
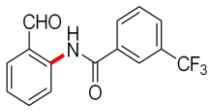
7.324
7.322
7.305
7.303
7.286
7.284
7.260


CHO
H
N
O
CF3

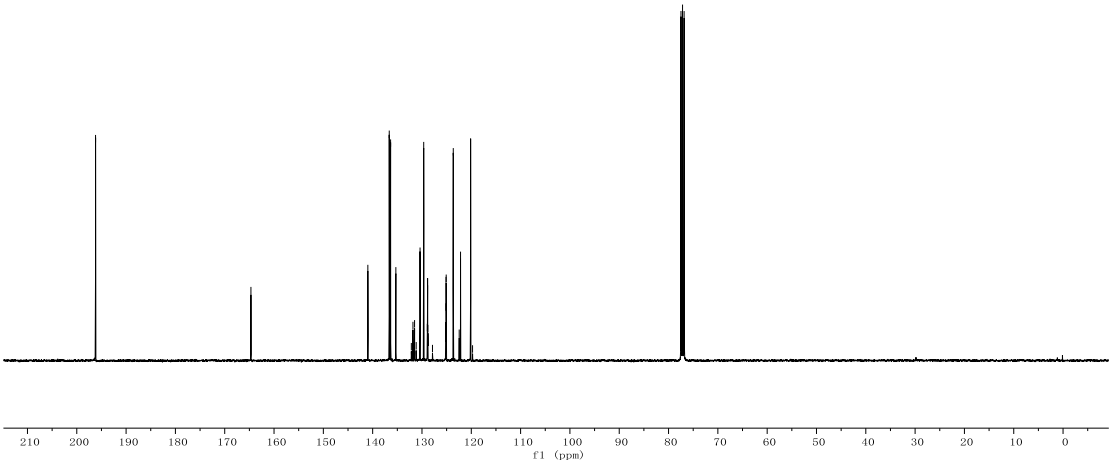
48

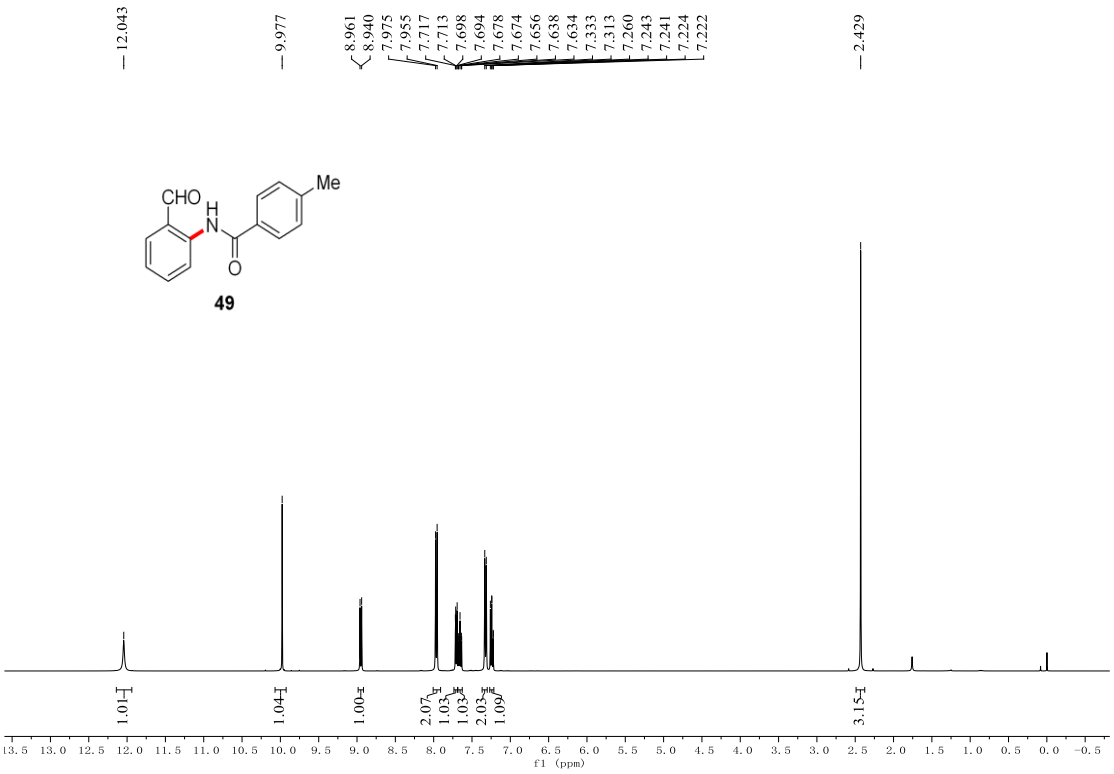

1.01
1.04
1.00
1.02
1.03
1.01
1.04
2.06
1.01
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

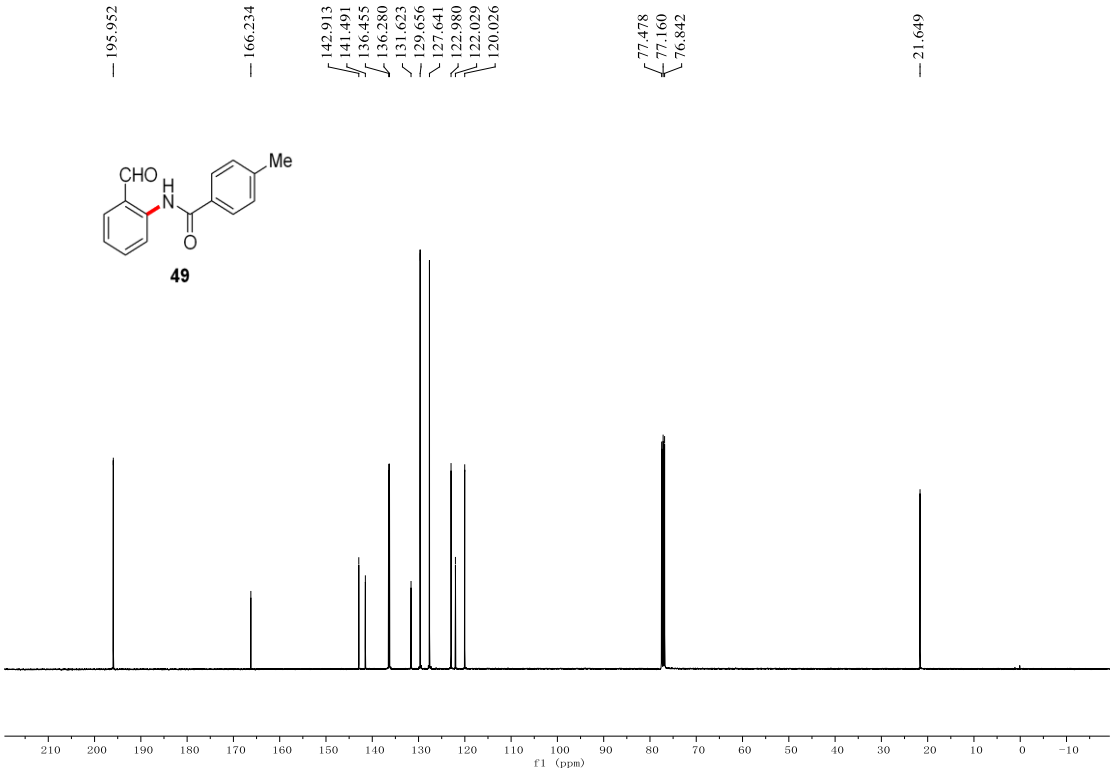

196.192
164.684
140.975
136.638
136.364
135.297
132.157
131.829
131.502
131.174
130.389
129.649
128.918
128.883
128.847
128.811
127.870
125.162
125.125
125.086
125.047
123.652
122.452
122.179
119.743
77.478
77.160
76.843

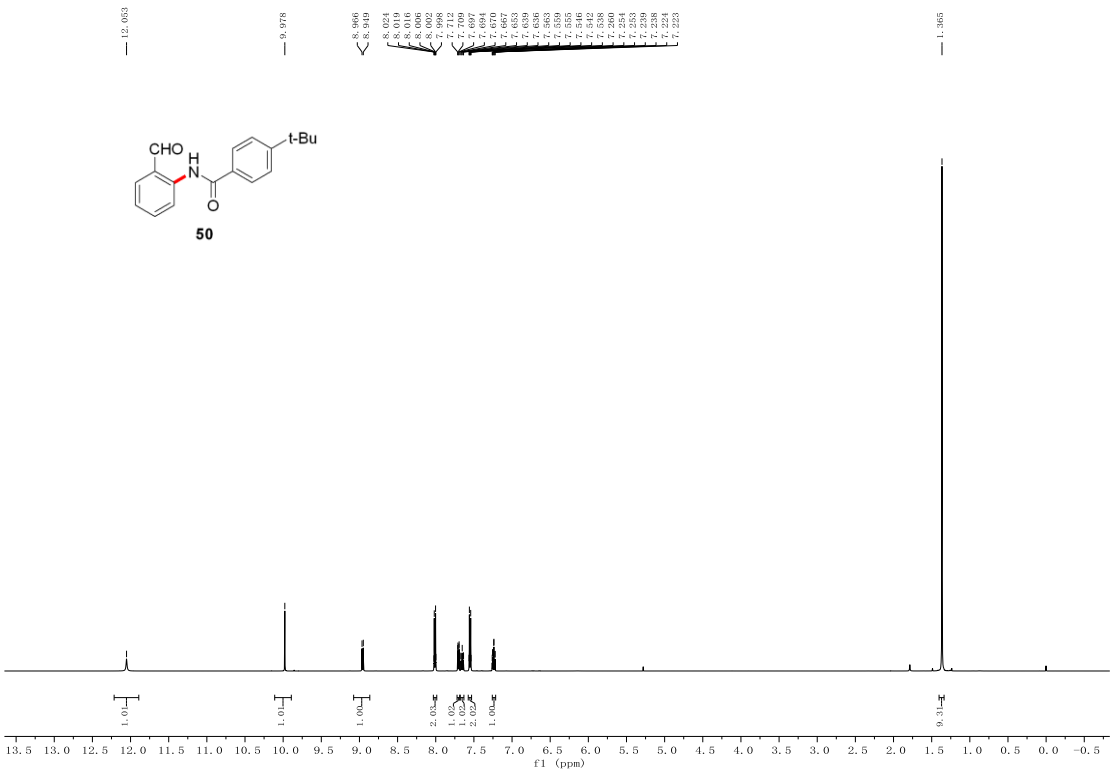

CHO
H
N
O
CF3

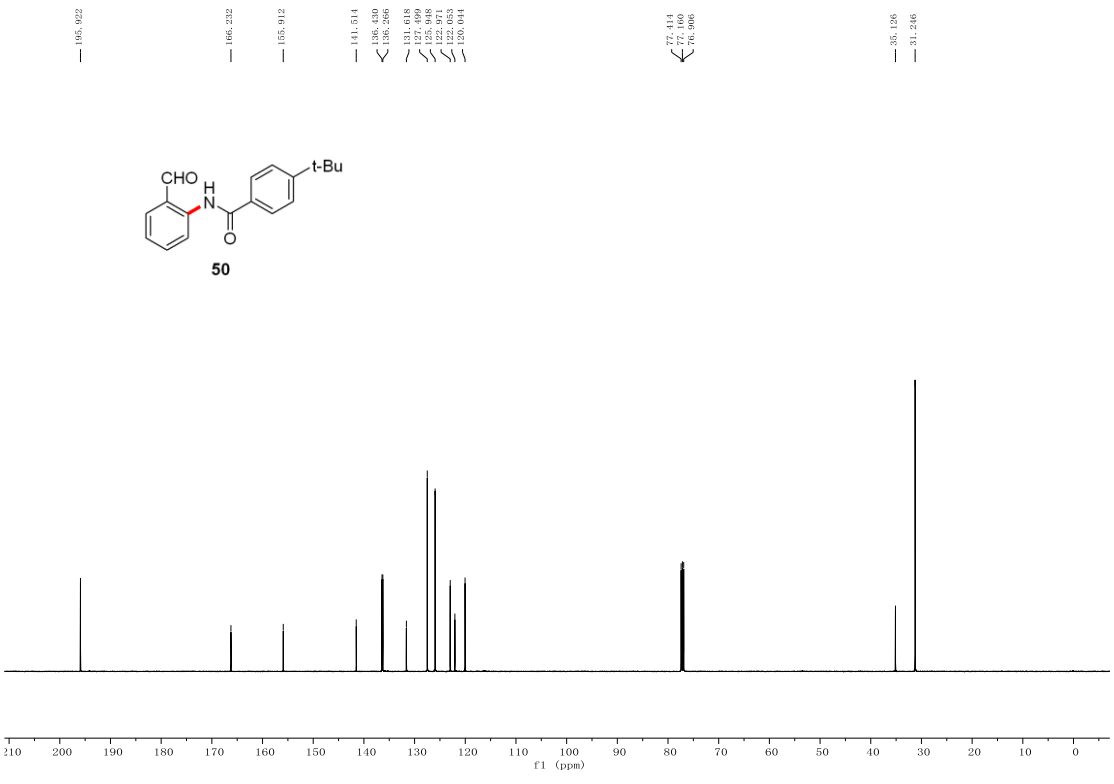
48

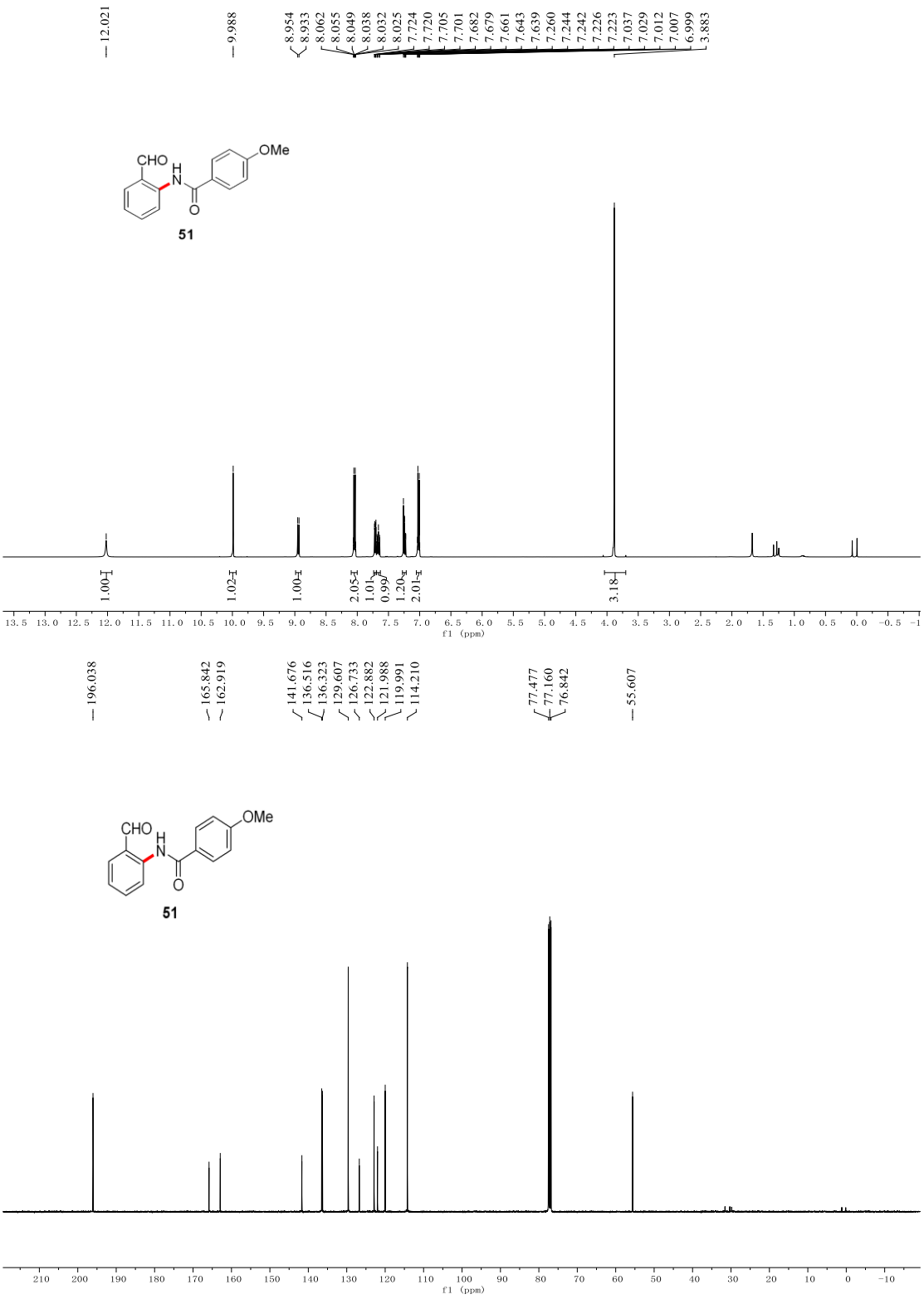

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

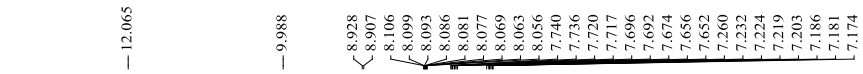

12.043
9.977
8.961
8.940
7.975
7.955
7.717
7.713
7.698
7.694
7.678
7.674
7.656
7.638
7.634
7.333
7.313
7.260
7.243
7.241
7.224
7.222
2.429
CHO
H
N
O
Me
49
1.01
1.04
1.00
2.07
1.03
1.03
2.03
1.09
3.15
f1 (ppm)

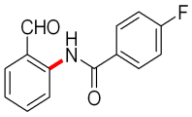

195.952
166.234
142.913
141.491
136.455
136.280
131.623
129.656
127.641
122.980
122.029
120.026
77.478
77.160
76.842
21.649
CHO
H
N
O
Me
49
f1 (ppm)


12.053
9.978
8.966
8.949
8.024
8.019
8.016
8.006
8.002
7.998
7.712
7.709
7.697
7.694
7.670
7.667
7.653
7.639
7.636
7.566
7.559
7.555
7.546
7.542
7.538
7.260
7.254
7.253
7.239
7.238
7.224
7.223
1.365
CHO
H
N
O
t-Bu
50
1.01
1.01
1.00
2.03
1.03
2.02
1.00
9.31
f1 (ppm)

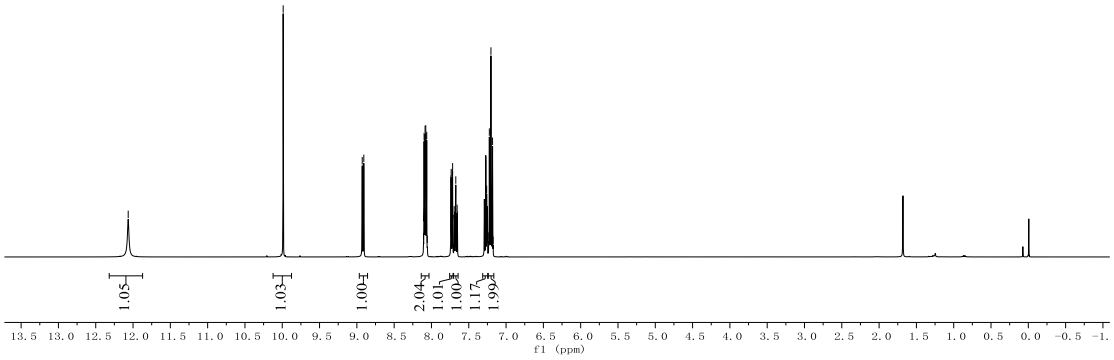

195.922
168.232
155.912
141.514
136.430
136.266
131.618
127.499
125.948
122.971
120.053
120.044
77.414
77.160
76.906
35.126
31.246
CHO
H
N
O
t-Bu
50
f1 (ppm)


12.021
9.988
8.954
8.933
8.062
8.055
8.049
8.038
8.032
8.025
7.724
7.720
7.705
7.701
7.682
7.679
7.661
7.643
7.639
7.260
7.244
7.242
7.226
7.223
7.037
7.029
7.012
7.007
6.999
3.883
CHO
H
N
O
OMe
51
1.00
1.02
1.00
2.05
1.01
0.99
1.20
2.01
3.18
f1 (ppm)
196.038
165.842
162.919
141.676
136.516
136.323
129.607
126.733
122.882
121.988
119.991
114.210
77.477
77.160
76.842
55.607
CHO
H
N
O
OMe
51
f1 (ppm)

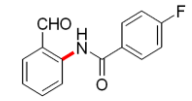

12.065
9.988
8.928
8.907
8.106
8.099
8.093
8.086
8.081
8.077
8.069
8.063
8.056
7.740
7.736
7.720
7.717
7.696
7.692
7.674
7.656
7.652
7.260
7.232
7.224
7.219
7.203
7.186
7.181
7.174


CHO
H
N
O
F

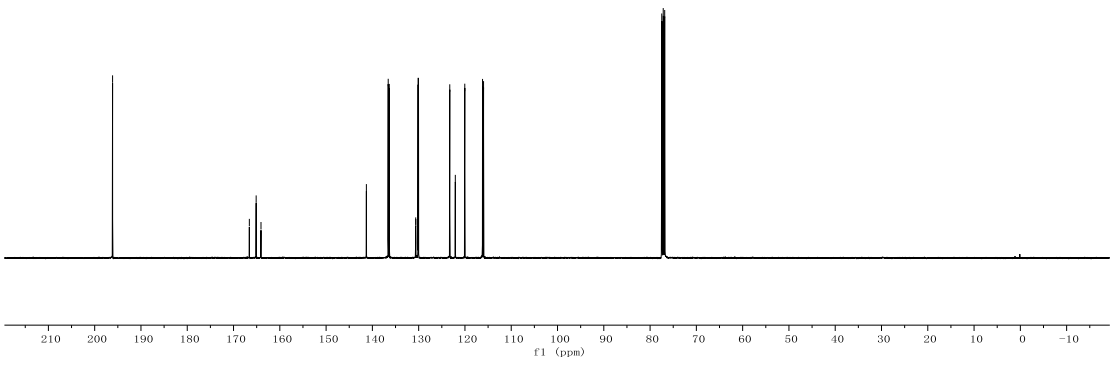
52

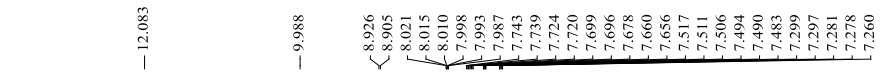

1.05
1.03
1.00
2.04
1.01
1.00
1.17
1.99
f1 (ppm)

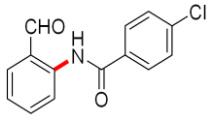

196.133
166.584
165.111
164.068
141.298
136.580
136.346
130.642
130.611
130.128
130.037
123.282
122.081
120.037
116.200
115.981
77.478
77.160
76.842


CHO
H
N
O
F

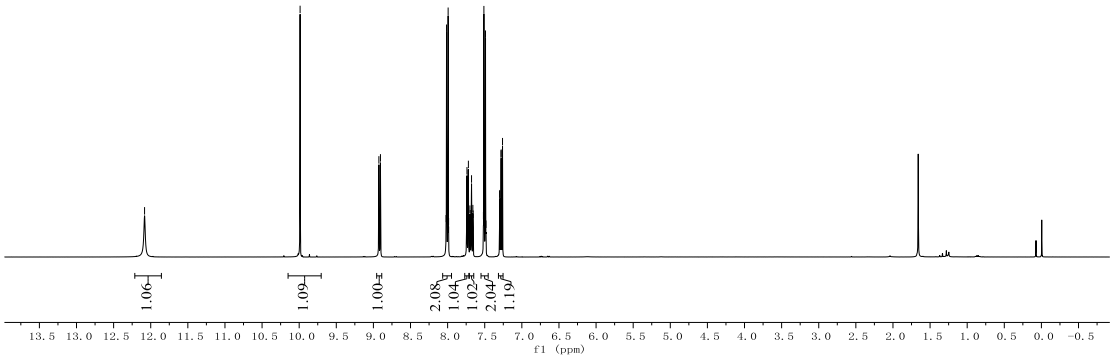
52


f1 (ppm)

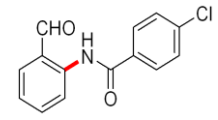

12.083
9.988
8.926
8.905
8.021
8.015
8.010
7.998
7.993
7.987
7.743
7.739
7.724
7.720
7.699
7.696
7.678
7.660
7.656
7.517
7.511
7.506
7.494
7.490
7.483
7.299
7.297
7.281
7.278
7.260


CHO
H
N
O
Cl

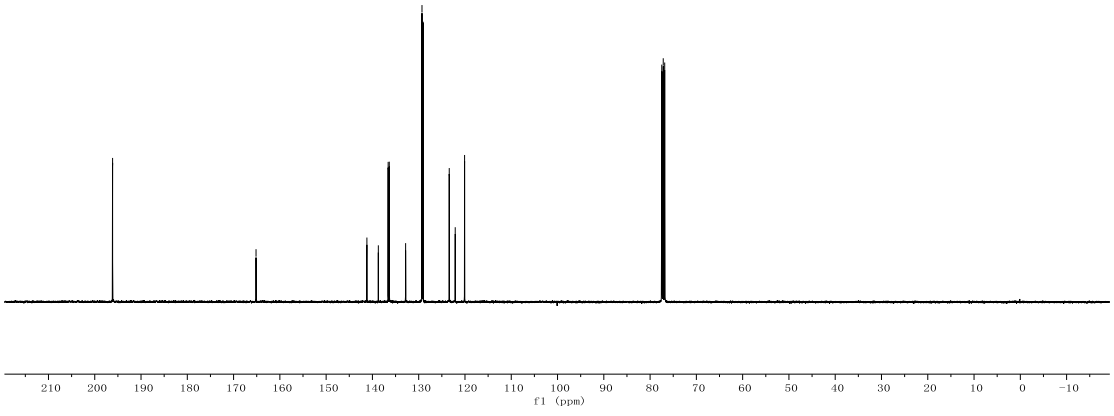
53

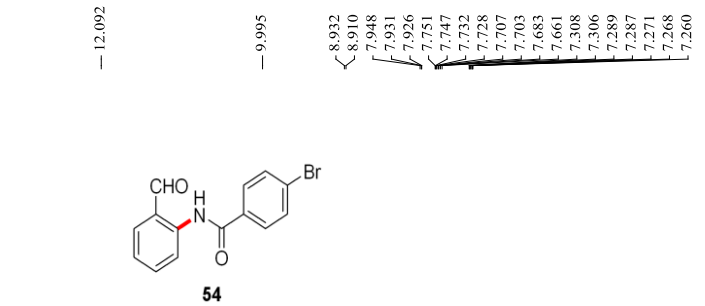

1.06
1.09
1.00
2.08
1.04
1.02
2.04
1.19
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


196.146
165.150
141.193
138.723
136.601
136.359
132.824
129.289
129.066
123.400
122.107
120.084
77.478
77.160
76.843

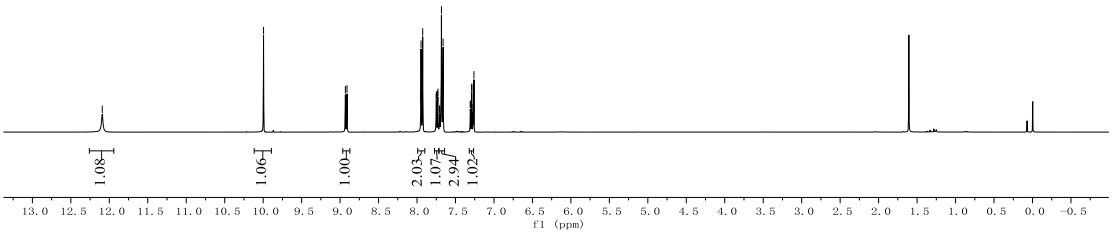

CHO
H
N
O
Cl

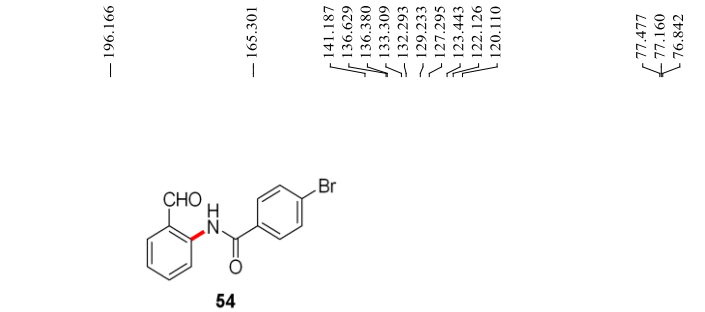
53


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

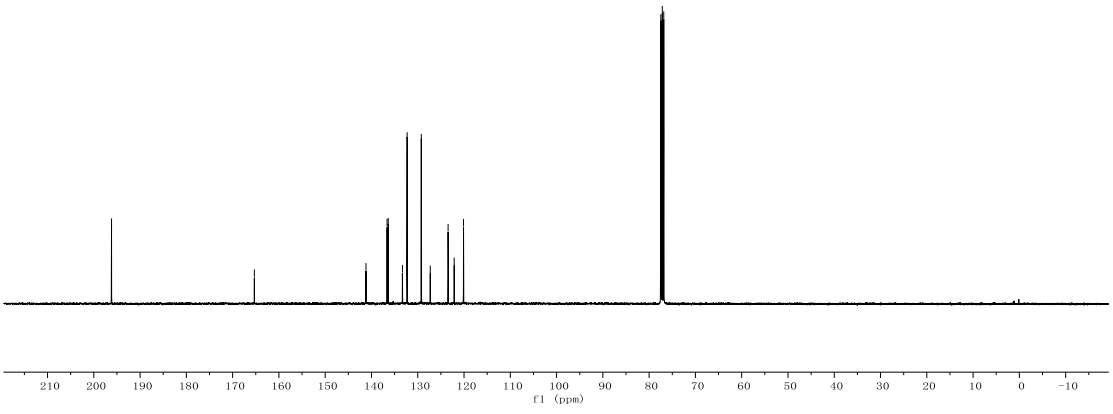

12.092
9.995
8.932
8.910
7.948
7.931
7.926
7.751
7.747
7.732
7.728
7.707
7.703
7.683
7.661
7.308
7.306
7.289
7.287
7.271
7.268
7.260
CHO
H
N
O
Br

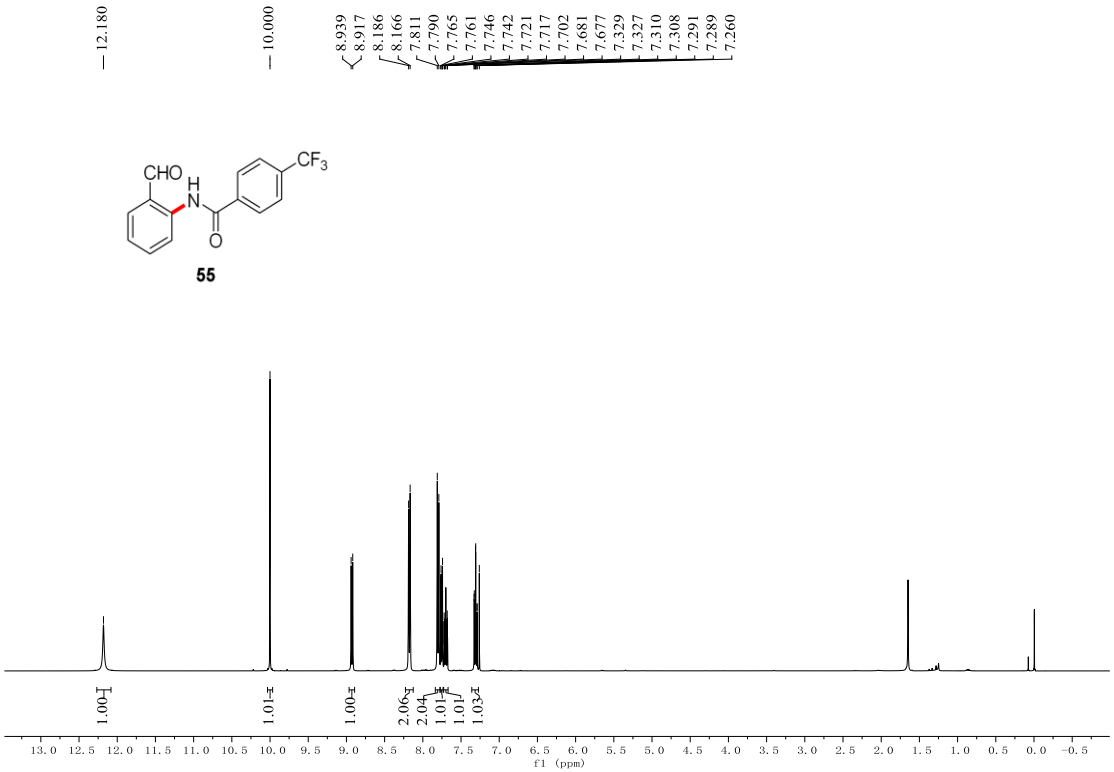
54

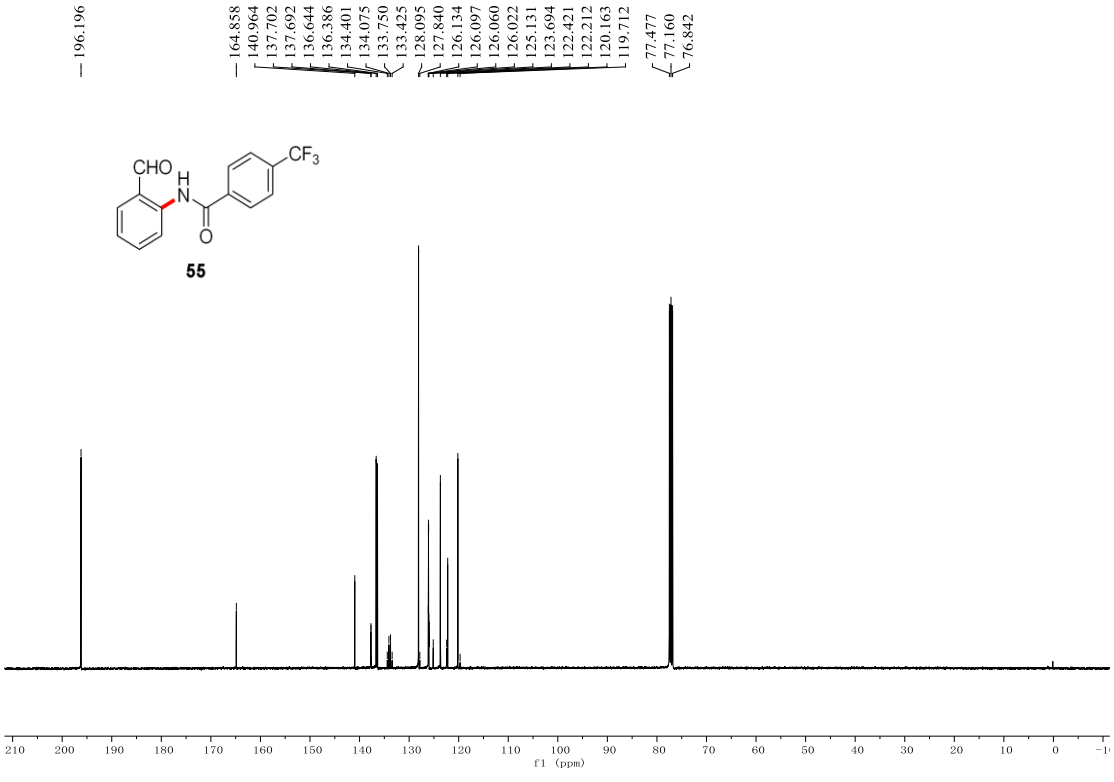

1.08
1.06
1.00
2.03
1.07
2.94
1.02
f1 (ppm)

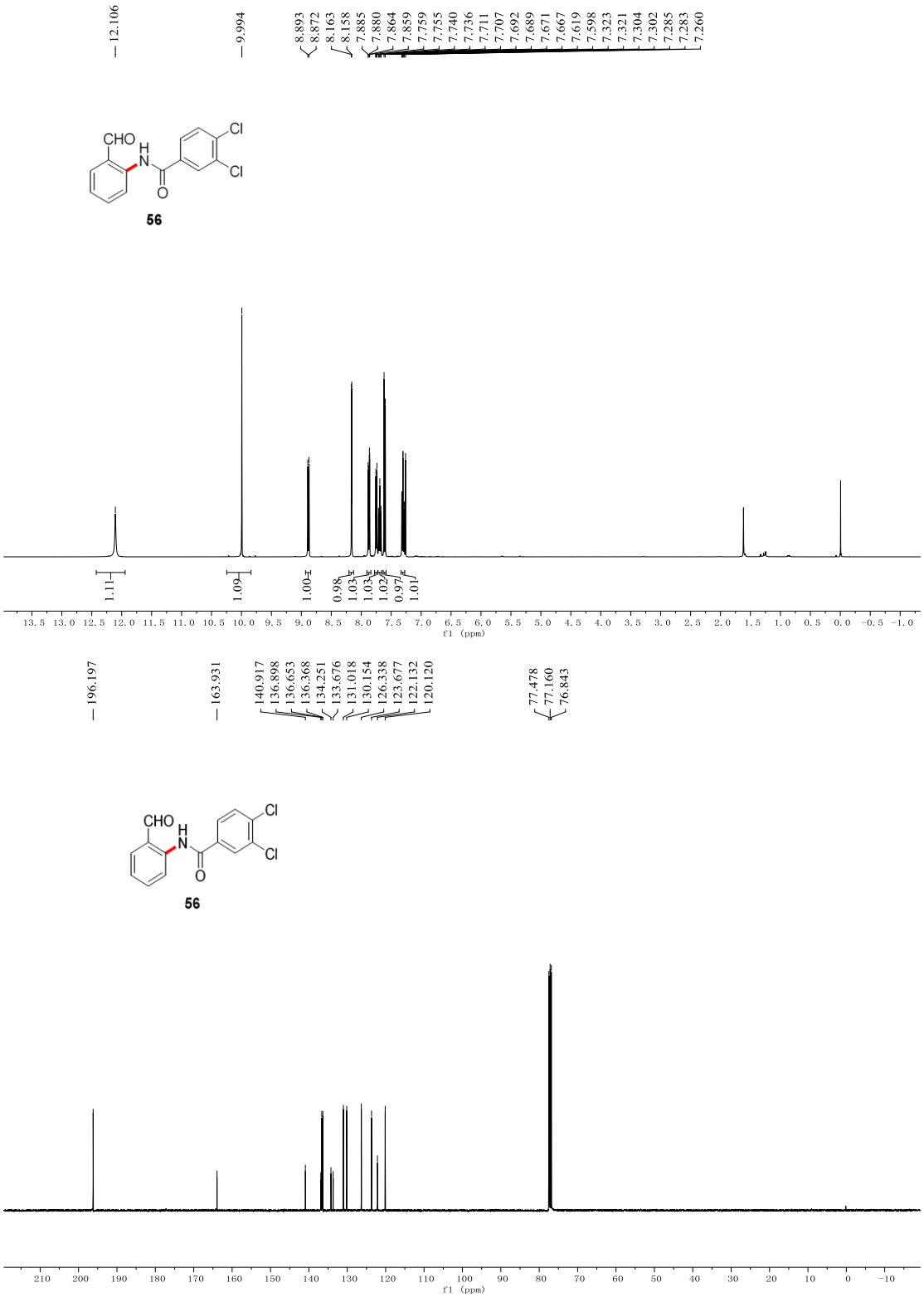

196.166
165.301
141.187
136.629
136.380
133.309
132.293
129.233
127.295
123.443
122.126
120.110
77.477
77.160
76.842
CHO
H
N
O
Br

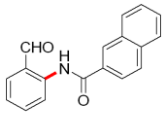
54


f1 (ppm)

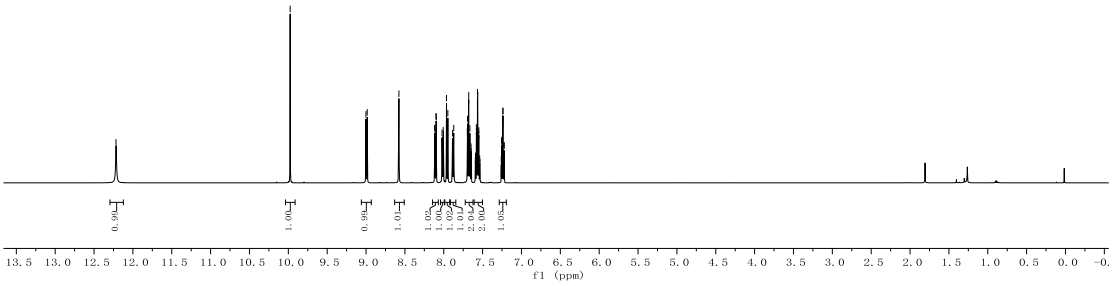

12.180
10.000
8.939
8.917
8.186
8.166
7.811
7.790
7.765
7.761
7.746
7.742
7.721
7.717
7.702
7.681
7.677
7.329
7.327
7.310
7.308
7.291
7.289
7.260
CHO
H
N
O
CF3
55
1.00
1.01
1.00
2.06
2.04
1.01
1.01
1.03
f1 (ppm)

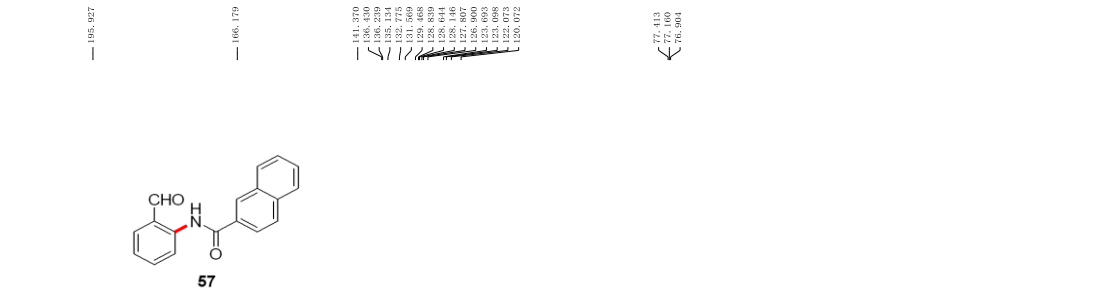

196.196
164.858
140.964
137.702
137.692
136.644
136.386
134.401
134.075
133.750
133.425
128.095
127.840
126.134
126.097
126.060
126.022
125.131
123.694
122.421
122.212
120.163
119.712
77.477
77.160
76.842
CHO
H
N
O
CF3
55
f1 (ppm)


12.106
9.994
8.893
8.872
8.163
8.158
7.885
7.880
7.864
7.859
7.759
7.755
7.740
7.736
7.711
7.707
7.692
7.689
7.671
7.667
7.619
7.598
7.323
7.321
7.304
7.302
7.285
7.283
7.260
CHO
H
N
O
Cl
Cl
56
1.11
1.09
1.00
0.98
1.03
1.03
1.02
0.97
1.01
f1 (ppm)
196.197
163.931
140.917
136.898
136.653
136.368
134.251
133.676
131.018
130.154
126.338
123.677
122.132
120.120
77.478
77.160
76.843
CHO
H
N
O
Cl
Cl
56
f1 (ppm)


CHO
H
N
O

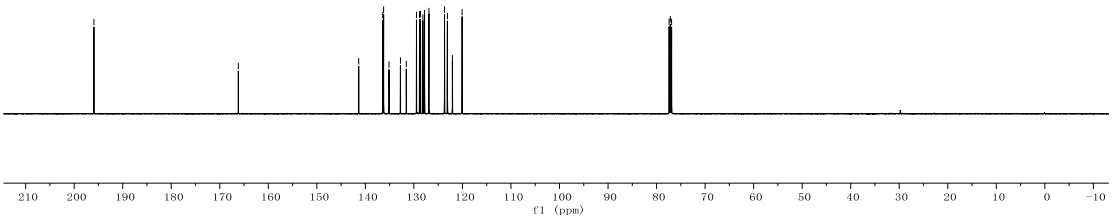
57

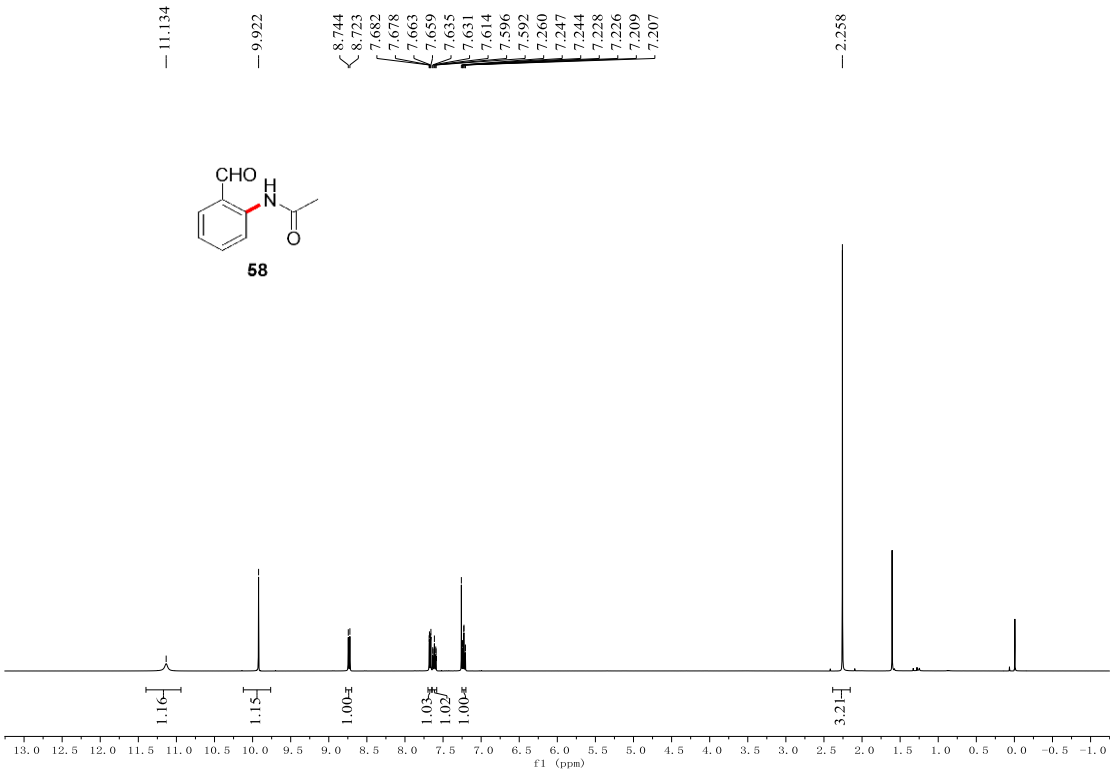

0.90
1.00
0.99
1.01
1.02
1.00
1.01
2.04
2.00
1.05
f1 (ppm)

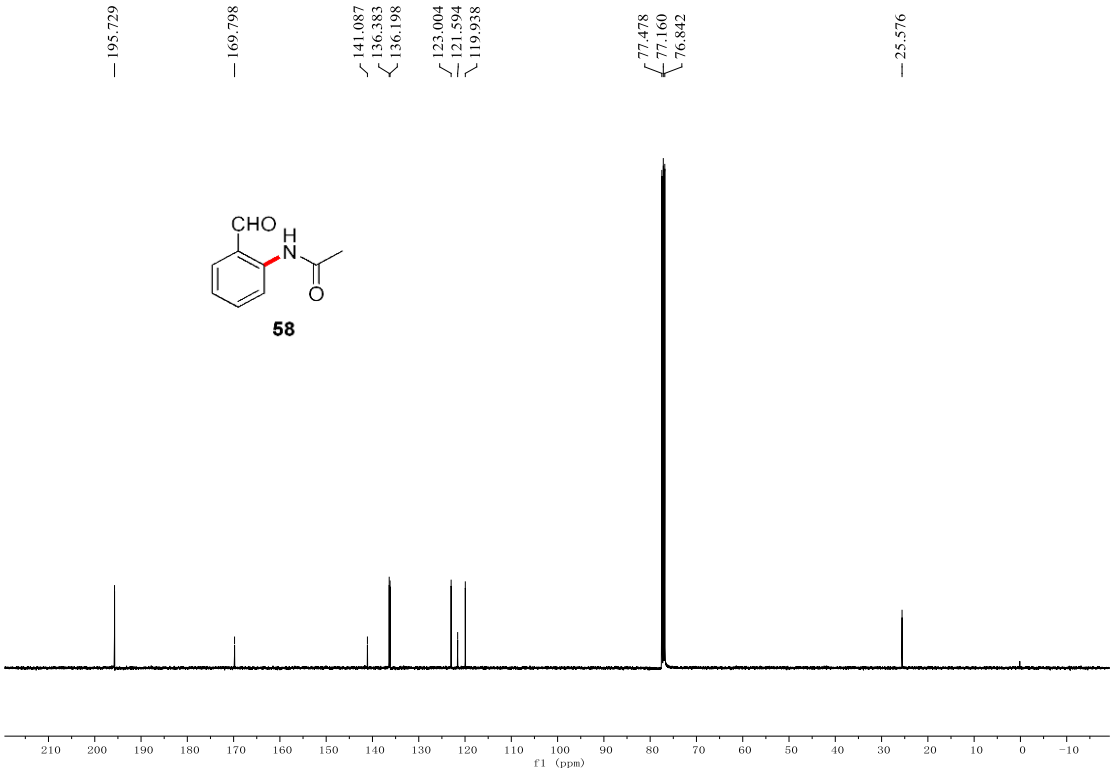

195.927
166.179
141.370
136.430
135.239
133.134
132.775
131.569
129.466
128.839
128.644
128.146
127.897
126.800
123.693
123.098
122.073
120.072
77.413
77.160
76.904

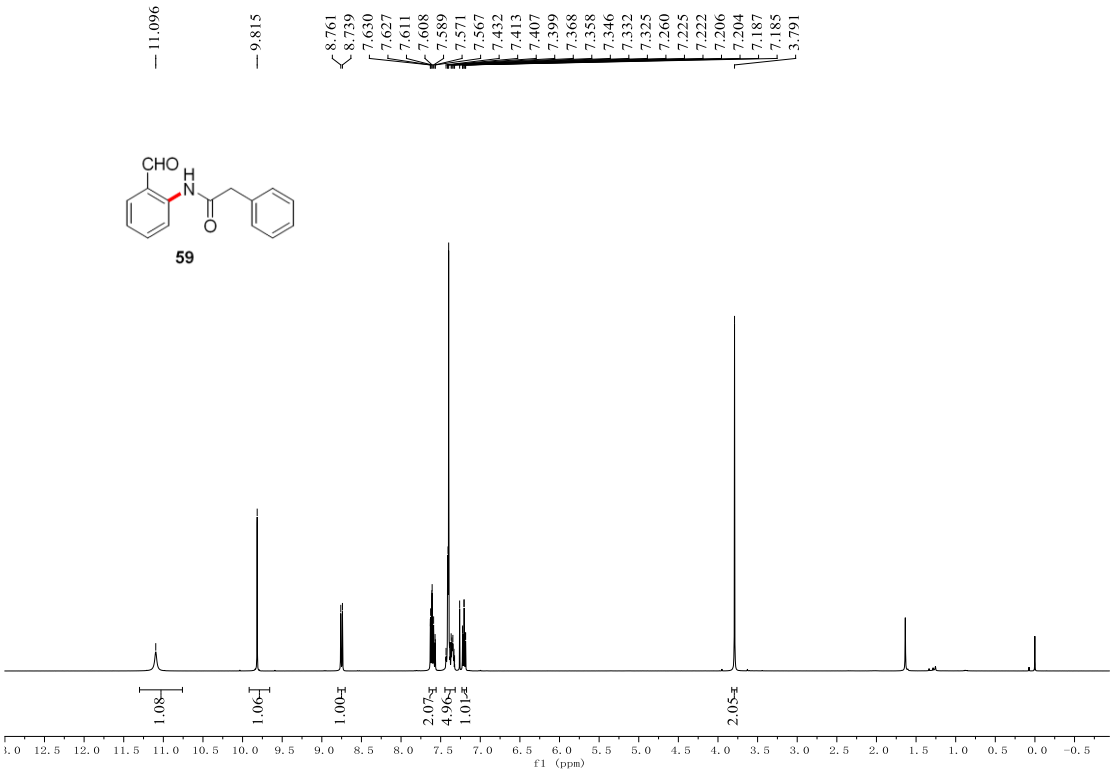
CHO
H
N
O

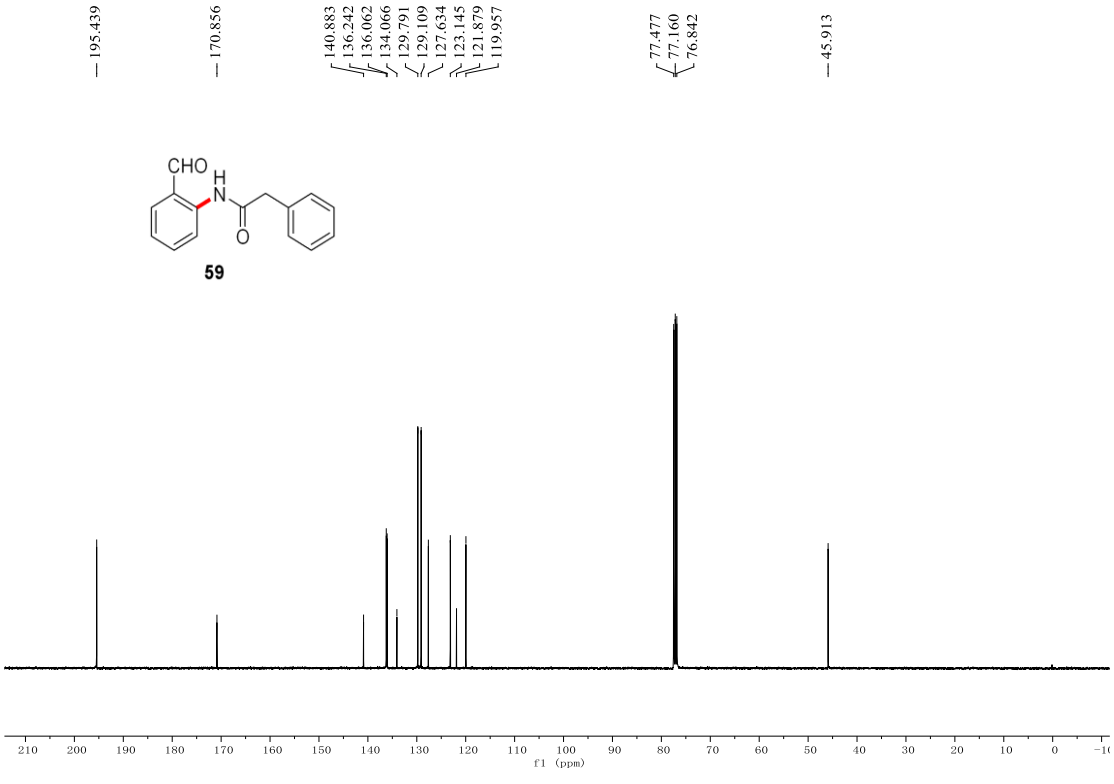
57

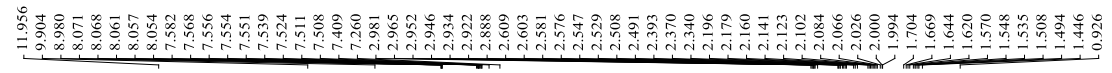

f1 (ppm)

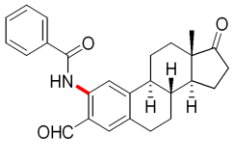

11.134
9.922
8.744
8.723
7.682
7.678
7.663
7.659
7.635
7.631
7.614
7.596
7.592
7.260
7.247
7.244
7.228
7.226
7.209
7.207
2.258
CHO
H
N
O
58
1.16
1.15
1.00
1.03
1.02
1.00
3.21
f1 (ppm)


195.729
169.798
141.087
136.383
136.198
123.004
121.594
119.938
77.478
77.160
76.842
25.576
CHO
H
N
O
58
f1 (ppm)


11.096
9.815
8.761
8.739
7.630
7.627
7.611
7.608
7.589
7.571
7.567
7.432
7.413
7.407
7.399
7.368
7.358
7.346
7.332
7.325
7.260
7.225
7.222
7.206
7.204
7.187
7.185
3.791
CHO
H
N
O
59
1.08
1.06
1.00
2.07
4.96
1.01
2.05
f1 (ppm)

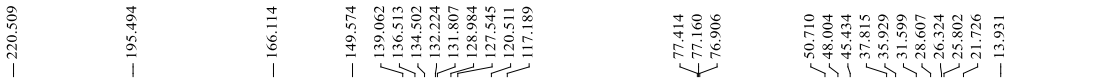

195.439
170.856
140.883
136.242
136.062
134.066
129.791
129.109
127.634
123.145
121.879
119.957
77.477
77.160
76.842
45.913
CHO
H
N
O
59
f1 (ppm)

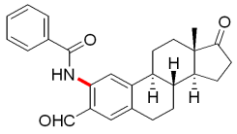

11.956
9.904
8.980
8.071
8.068
8.061
8.057
8.054
7.582
7.568
7.556
7.554
7.551
7.539
7.524
7.511
7.508
7.409
7.260
2.981
2.965
2.952
2.946
2.934
2.922
2.888
2.609
2.603
2.581
2.576
2.547
2.529
2.508
2.491
2.393
2.370
2.340
2.196
2.179
2.160
2.141
2.123
2.102
2.084
2.066
2.026
2.000
1.994
1.704
1.669
1.644
1.620
1.570
1.548
1.535
1.508
1.494
1.446
0.926


O
HN
OHC
H
H
H
O

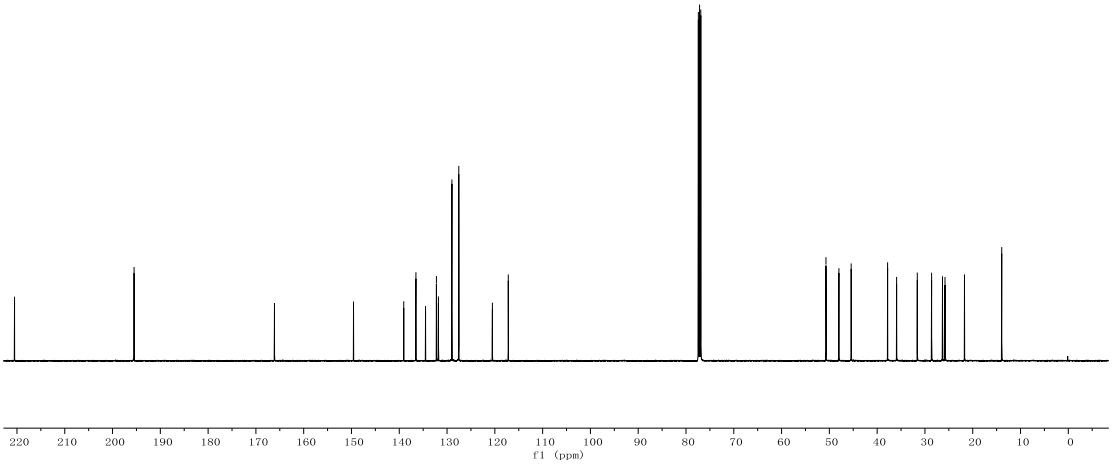
61

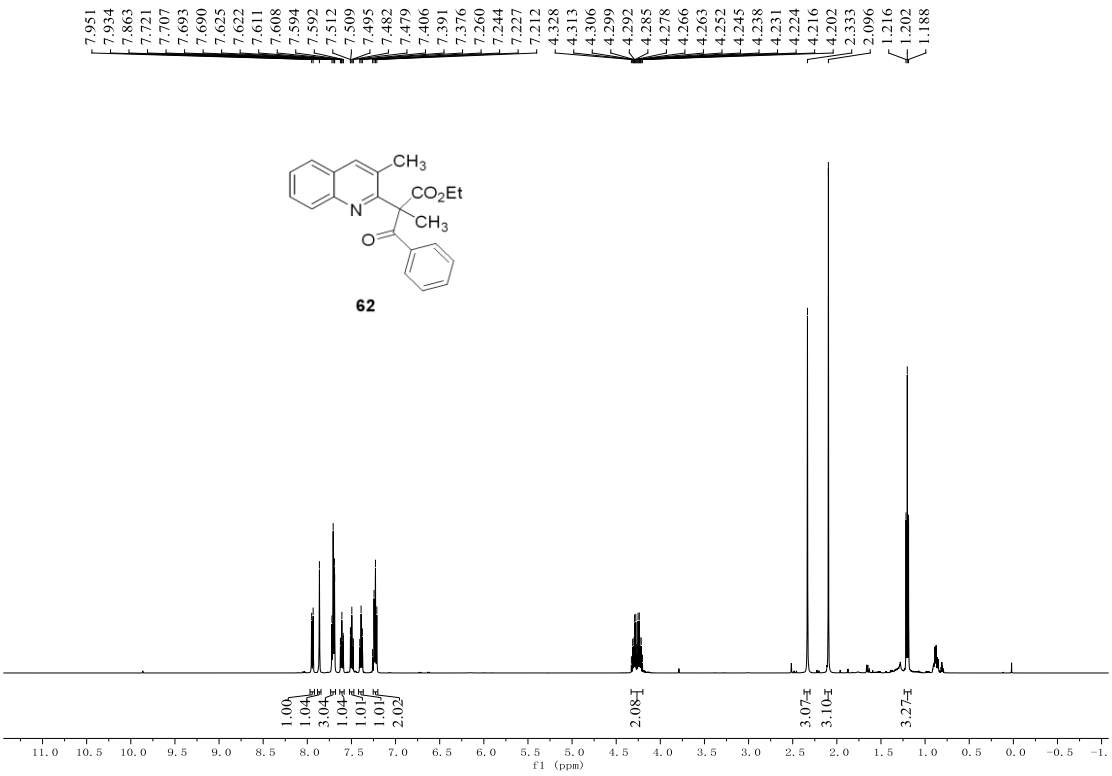
1.02
1.00
1.00
2.00
3.04
1.01
2.03
2.02
1.03
4.15
6.52
3.05
f1 (ppm)

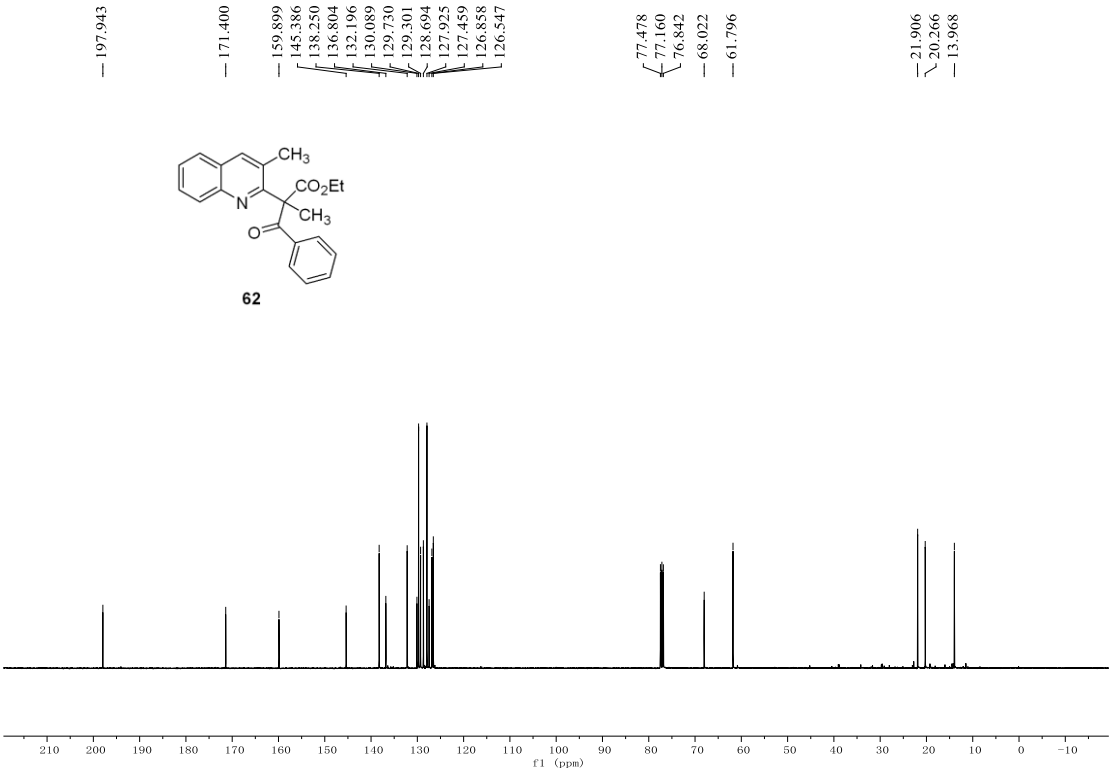

220.509
195.494
166.114
149.574
139.062
136.513
134.502
132.224
131.807
128.984
127.545
120.511
117.189
77.414
77.160
76.906
50.710
48.004
45.434
37.815
35.929
31.599
28.607
26.324
25.802
21.726
13.931

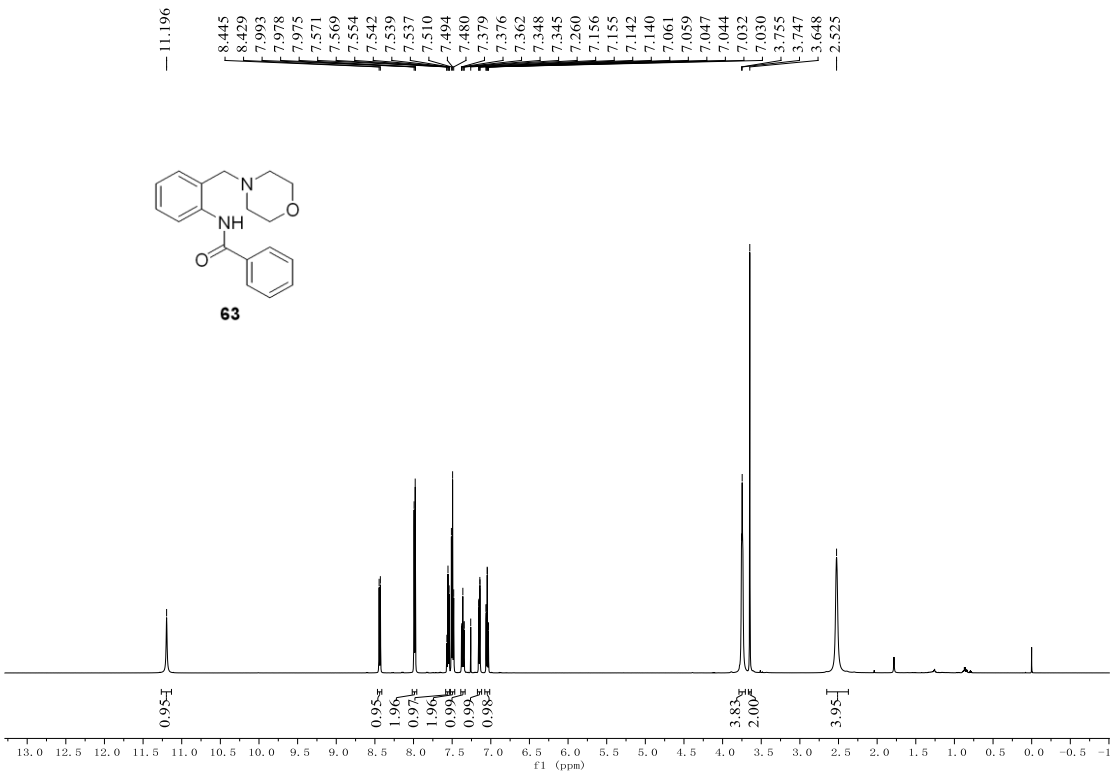

O
HN
OHC
H
H
H
O

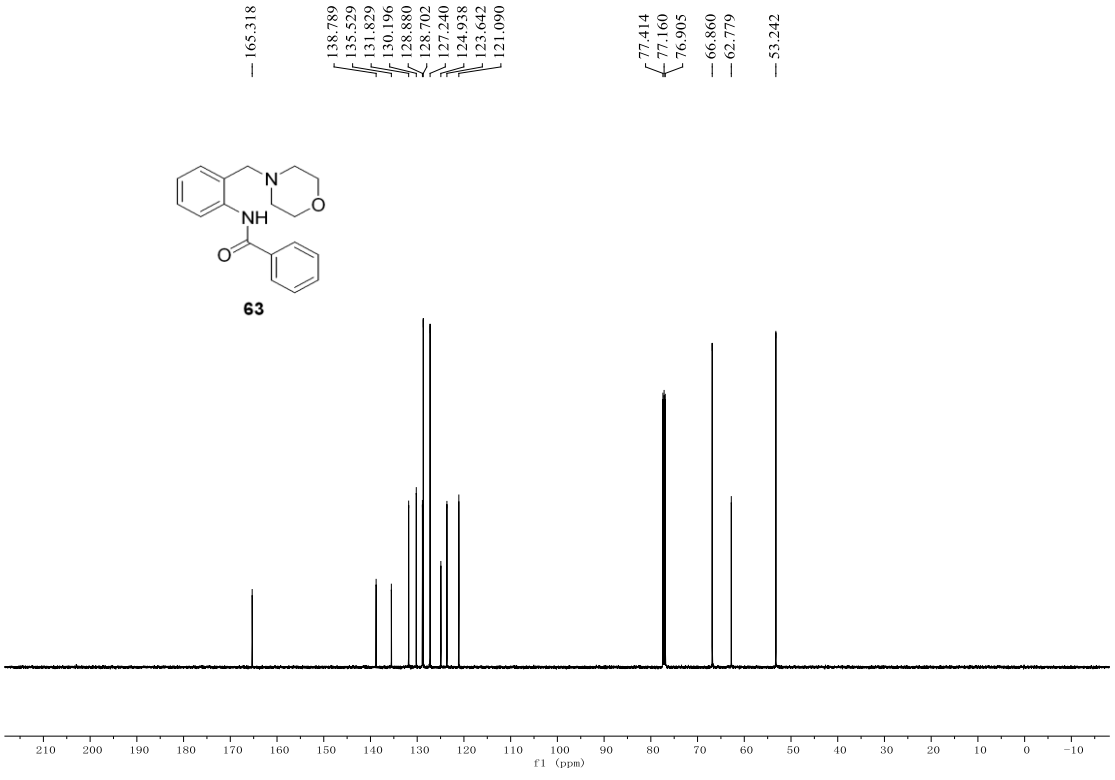
61

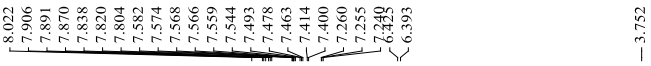

f1 (ppm)

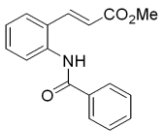

7.951
7.934
7.863
7.721
7.707
7.693
7.690
7.625
7.622
7.611
7.608
7.594
7.592
7.512
7.509
7.495
7.482
7.479
7.406
7.391
7.376
7.260
7.244
7.227
7.212
4.328
4.313
4.306
4.299
4.292
4.285
4.278
4.266
4.263
4.252
4.245
4.238
4.231
4.224
4.216
4.202
2.333
2.096
1.216
1.202
1.188
CH3
CO2Et
CH3
O
N
62
1.00
1.04
3.04
1.04
1.01
1.01
2.02
2.08
3.07
3.10
3.27
f1 (ppm)


197.943
171.400
159.899
145.386
138.250
136.804
132.196
130.089
129.730
129.301
128.694
127.925
127.459
126.858
126.547
77.478
77.160
76.842
68.022
61.796
21.906
20.266
13.968
CH3
CO2Et
CH3
O
N
62
f1 (ppm)

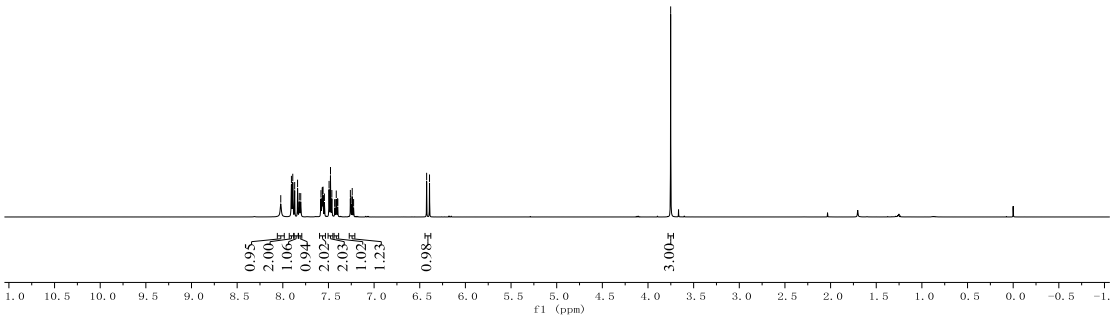

11.196
8.445
8.429
7.993
7.978
7.975
7.571
7.569
7.554
7.542
7.539
7.537
7.510
7.494
7.480
7.379
7.376
7.362
7.348
7.345
7.260
7.156
7.155
7.142
7.140
7.061
7.059
7.047
7.044
7.032
7.030
3.755
3.747
3.648
2.525
N
O
NH
O
63
0.95
1.96
0.97
1.96
0.99
0.99
0.98
3.83
2.00
3.95
f1 (ppm)


165.318
138.789
135.529
131.829
130.196
128.880
128.702
127.240
124.938
123.642
121.090
77.414
77.160
76.905
66.860
62.779
53.242
N
O
NH
O
63
f1 (ppm)

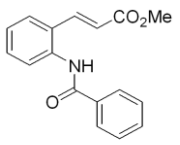

8.022
7.906
7.891
7.870
7.838
7.820
7.804
7.582
7.574
7.568
7.566
7.559
7.544
7.493
7.478
7.463
7.414
7.400
7.260
7.255
7.240
6.422
6.393
3.752


CO2Me
NH
O

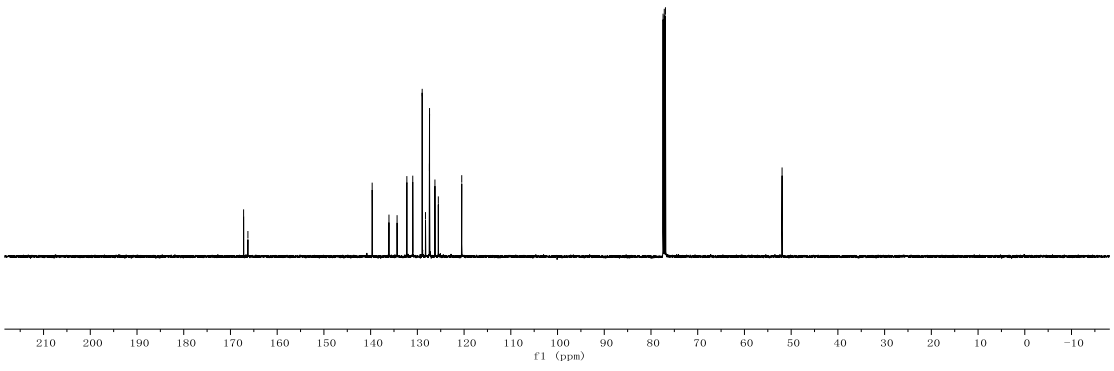
64


0.95
2.00
1.06
0.94
2.02
2.03
1.02
1.23
0.98
3.00
f1 (ppm)


167.187
166.264
139.671
136.078
134.338
132.248
130.986
128.966
128.260
127.417
127.394
126.239
125.513
120.503
77.414
77.160
76.906
51.945


CO2Me
NH
O

64


f1 (ppm)