

Supporting Information

For

Metal-Free Iodination of Arylaldehydes for Total Synthesis of Aristogins A–F and Hernandial

Fufang Wu,^{1*} Chunmei Tang,¹ Xuejian Li,¹ Nan Li,¹ Miao Liu,¹ Danqin Li,¹ Rongrong Dai,¹ Xiaobao Shen,^{1*} and Hongbin Zhai^{2*}

* Corresponding author.

E-mail address: fufang_wu@foxmail.com (F. Wu)

* Corresponding author.

E-mail address: zhaihb@pku.edu.cn (H. Zhai)

* Corresponding author.

E-mail address: shnxiaobao@foxmail.com (X. Shen)

Table of contents

1. General Information.....	S1
2. General procedure of reactions.....	S1-S3
3. Characterization Data.....	S3-S17
4. ¹H NMR and ¹³C NMR spectra.....	S17-S75

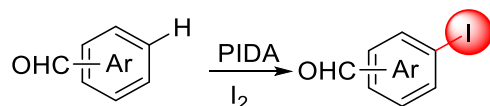
1. General Information

All chemical reagents were purchased from commercial suppliers and can be used without further purification. Unless otherwise specified, all reactions were run under nitrogen atmosphere. ^1H NMR and ^{13}C NMR spectra were recorded on a Bruker spectrometer (at 400 and 101 MHz, respectively). TMS was used as reference for chemical shifts. The high-resolution mass spectra (HRMS) were recorded on a Waters UPLC G2-XS Qt of instrument.

Note: The reactions and subsequent workup were conducted behind a blast shield with the sash positioned as low as possible. Although no issues were encountered during the synthesis, appropriate precautions were taken.

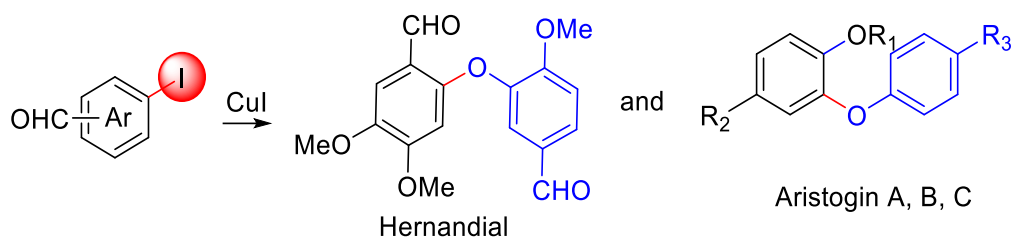
2. General procedure of reactions

I. General experimental procedure for the Iodination of Arylaldehydes



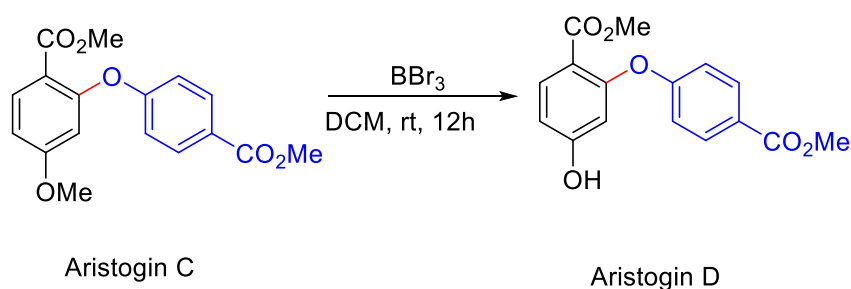
Arylaldehyde (1 mmol), PIDA (1.5 mmol), I₂ (1 mmol), and DCM (2 mL) were combined in a Schlenk tube. The mixture was stirred for 3 hours at 60 °C using a heating mantle under N₂. Subsequently, the reaction mixture was quenched by adding Na₂SO₃(aq) (15 mL), and then extracted with DCM three times. The resulting solution was dried with anhydrous Na₂SO₄ and concentrated. The crude residue obtained was purified by column chromatography on silica gel using petroleum ether : ethyl acetate = 30 : 1–15 : 1 as eluent to yield the desired products.

II. General experimental procedure for Hernandial and Aristogin A, B, C



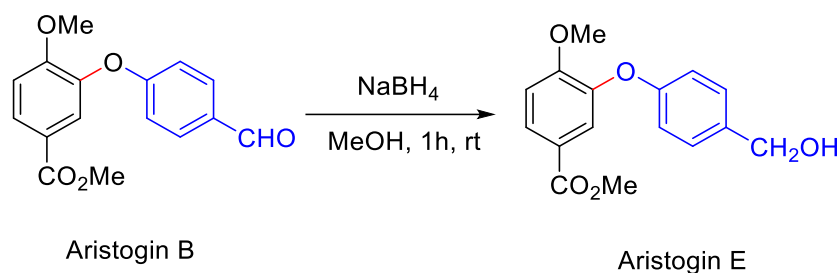
Iodo arylaldehyde (1 mmol) and substituted phenol compounds (1 mmol), CuI (0.1 mmol), DMG [N,N-Dimethylglycine] (0.1 mmol), K_3PO_4 (2 mmol), and DMSO (2 mL) were added to a Schlenk tube, and the mixture was stirred for 24 hours at 120 °C using a heating mantle under N_2 . After reaction, the mixture was quenched by water, and extracted with EtOAc for 3 times, dried with anhydrous Na_2SO_4 , and concentrated. The crude residue was purified by column chromatography on silica gel using petroleum ether/EtOAc (10:1) as eluent to afford the desired product Hernandial and Aristogin A, B, C.

III. Synthesis of Aristogin D

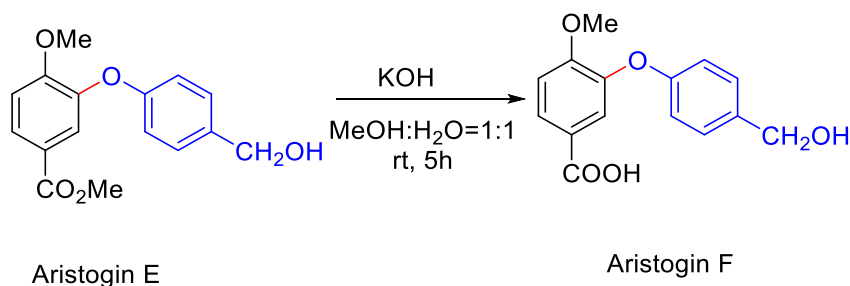


BBr_3 (1 M in DCM, 2 mL) was added to the solution of Aristogin C (12.0 mg 37.9 μmol) in DCM, and the mixture was stirred at room temperature for 12h. Then the solvent was removed under reduced pressure. the crude residue was purified by thinlayer chromatography to obtain the desired Aristogin D using petroleum ether/EtOAc (3:1) as the developing agent.

IV. Synthesis of Aristogin E and F

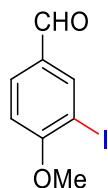


NaBH₄ (6.6 mg, 0.17 mmol, 1 equiv) was added to a solution of Aristogin B (50.0 mg, 0.17 mmol) in MeOH (2.5 mL), and the mixture was stirred for 1 h at room temperature. Then, the reaction was quenched with water, and extracted with EtOAc for 3 times, dried with anhydrous Na₂SO₄, and concentrated in vacuo to give the crude product Aristogin E which can be changed to Aristogin F directly. The crude product could also be purified by column chromatography on silica gel using petroleum ether/EtOAc (10:1) as eluent to afford the desired product Aristogin E.

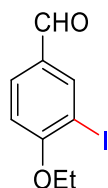


KOH (80 mg, 1.43 mmol, 14.3 equiv) was added to the solution of Aristogin E (crude) in MeOH (5 mL), and the mixture was stirred for 5 h at room temperature. Then, the reaction was extracted with EtOAc for 3 times, dried with anhydrous Na₂SO₄, and concentrated in vacuo to give the crude product. The crude product could also be purified by column chromatography on silica gel using petroleum ether/EtOAc (1:1) as eluent to afford the desired product Aristogin F.

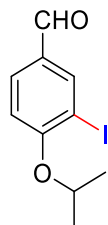
3. Characterization Data



3-iodo-4-methoxybenzaldehyde (2)¹. Product **2** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 15 : 1). white solid (236 mg, 0.9 mmol, 90% yield); mp 115–116 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.82 (s, 1H), 8.31 (d, *J* = 1.9 Hz, 1H), 7.86 (dd, *J* = 8.5, 2.0 Hz, 1H), 6.93 (d, *J* = 8.5 Hz, 1H), 3.98 (s, 3H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 189.4, 162.8, 141.1, 132.1, 131.4, 110.5, 86.5, 56.8; HRMS (ESI) *m/z* [M+H]⁺ calcd for C₈H₈O₂I: 262.9464; found: 262.9576.



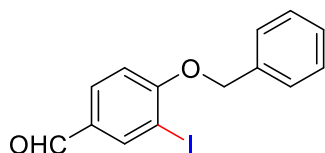
4-ethoxy-3-iodobenzaldehyde (3)². Product **3** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 15 : 1). white solid (262 mg, 0.95 mmol, 95% yield); mp 78–81 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.81 (s, 1H), 8.30 (d, *J* = 2.0 Hz, 1H), 7.83 (dd, *J* = 8.5, 2.1 Hz, 1H), 6.88 (d, *J* = 8.5 Hz, 1H), 4.20 (q, *J* = 7.0 Hz, 2H), 1.54 (t, *J* = 7.0 Hz, 3H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 189.5, 162.3, 141.2, 132.0, 131.2, 111.3, 87.0, 65.4, 14.5; HRMS (ESI) *m/z* [M+H]⁺ calcd for C₉H₁₀O₂I: 276.9720; found: 276.9722.



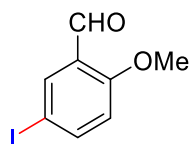
3-iodo-isopropoxybenzaldehyde (4). Product **4** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 10 : 1). white oil (203 mg, 0.7 mmol, 70% yield); ¹H NMR (400 MHz, CDCl₃) δ 9.79 (s, 1H), 8.29 (d, *J* = 2.0 Hz, 1H), 7.80 (dd, *J* = 8.5, 1.9 Hz, 1H), 6.87 (d, *J* = 8.5 Hz, 1H), 4.70 (m, *J* = 6.1 Hz, 1H), 1.43 (s, 3H), 1.42 (s, 3H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 189.4, 161.6, 141.5, 131.7, 131.0, 115.6, 112.4, 88.2, 72.4, 21.9; HRMS (ESI) *m/z* [M+H]⁺ calcd for C₁₀H₁₂O₂I: 290.9877; found: 290.9890.

¹ Kinsinger T, Kazmaier U. *Org. Lett.* **2018**, 20(23): 7726-7730.

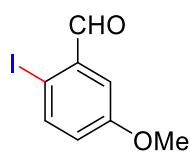
² Racys D T, Warrilow C E, Pimlott S L, Sutherland A. *Org. Lett.* **2015**, 17 (19), 4782-4785.



4-(benzyloxy)-3-iodobenzaldehyde (5). Product **5** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 15 : 1). white solid (321 mg, 0.93 mmol, 93% yield); mp 164–165 °C. ^1H NMR (400 MHz, CDCl_3) δ 9.81 (s, 1H), 8.33 (d, J = 2.0 Hz, 1H), 7.81 (dd, J = 8.5, 2.0 Hz, 1H), 7.5–7.47 (m, 2H), 7.44–7.39 (m, 2H), 7.36 (d, J = 7.3 Hz, 1H), 6.95 (d, J = 8.5 Hz, 1H), 5.25 (s, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 189.4, 161.8, 141.2, 135.5, 131.9, 131.6, 128.8, 128.3, 127.0, 112.0, 87.1, 71.2; HRMS (ESI) m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{14}\text{H}_{12}\text{O}_2\text{I}$: 338.9877; found: 338.9886.

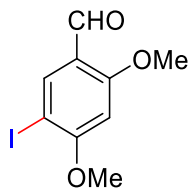


5-iodo-2-methoxybenzaldehyde (6)². Product **6** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 15 : 1). white solid (249 mg, 0.95 mmol, 95% yield); mp 142–143 °C. ^1H NMR (400 MHz, CDCl_3) δ 10.32 (s, 1H), 8.06 (d, J = 2.4 Hz, 1H), 7.78 (dd, J = 8.8, 2.4 Hz, 1H), 6.77 (d, J = 8.8 Hz, 1H), 3.90 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 188.3, 161.4, 144.2, 137.0, 126.5, 114.2, 83.0, 55.9. HRMS (ESI) m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_8\text{H}_8\text{O}_2\text{I}$: 262.9564; found: 262.9576; HRMS (ESI) m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_8\text{H}_8\text{O}_2\text{I}$: 262.9564; found: 262.9576.

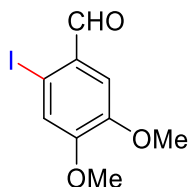


2-iodo-5-methoxybenzaldehyde (7)³. Product **7** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 15 : 1). white solid (244 mg, 0.93 mmol, 93% yield); mp 112–113 °C. ^1H NMR (400 MHz, CDCl_3) δ 10.00 (s, 1H), 7.78 (d, J = 8.7 Hz, 1H), 7.40 (d, J = 3.2 Hz, 1H), 6.90 (dd, J = 8.7, 3.2 Hz, 1H), 3.83 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 195.7, 160.2, 141.0, 135.6, 123.5, 113.5, 89.9, 55.7; HRMS (ESI) m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_8\text{H}_8\text{O}_2\text{I}$: 262.9564; found: 262.9573.

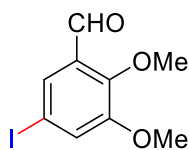
³ Whyte A, Olson M E, Lautens M. *Org. Lett.* **2017**, *20* (2), 345-348.



5-iodo-3,4-dimethoxybenzaldehyde (8)². Product **8** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 15 : 1). white solid (248 mg, 0.85 mmol, 85% yield); mp 171–172 °C. ¹H NMR (400 MHz, CDCl₃) δ 10.18 (s, 1H), 8.20 (s, 1H), 6.38 (s, 1H), 3.96 (s, 3H), 3.94 (s, 3H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 187.1, 164.1, 163.8, 139.3, 120.3, 94.8, 75.6, 56.7, 55.9; HRMS (ESI) m/z [M+Na]⁺ calcd for C₉H₉O₃NaI: 314.9489; found: 314.9487.

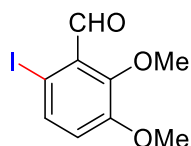


2-iodo-4,5-dimethoxybenzaldehyde (9)⁴. Product **9** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 15 : 1). yellow solid (254 mg, 0.87 mmol, 87% yield); mp 137–139 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.86 (s, 1H), 7.41 (s, 1H), 7.30 (s, 1H), 3.95 (s, 3H), 3.91 (s, 3H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 194.9, 154.5, 149.8, 128.4, 121.8, 111.1, 92.8, 56.5, 56.1; HRMS (ESI) m/z [M+H]⁺ calcd for C₉H₁₀O₃I: 292.9670; found: 292.9667.

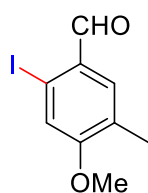


5-iodo-2,3-dimethoxybenzaldehyde (10a)². Product **10a** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 15 : 1). white solid (254 mg, 0.87 mmol, 87% yield); mp 97–98 °C. ¹H NMR (400 MHz, CDCl₃) δ 10.28 (s, 1H), 7.70 (d, *J* = 2.3 Hz, 1H), 7.36 (d, *J* = 2.1 Hz, 1H), 3.96 (s, 3H), 3.88 (s, 3H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 188.6, 153.8, 152.6, 130.9, 128.1, 126.6, 87.1, 62.4, 56.3; HRMS (ESI) m/z [M+Na]⁺ calcd for C₉H₉O₃NaI: 314.9489; found: 314.9499.

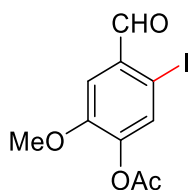
⁴ La M, Liu D, Chen X, Zhang F L, Zhou Y. *Org. Lett.* **2021**, *23* (23), 9184-9188.



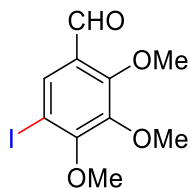
6-iodo-2,3-dimethoxybenzaldehyde (10b)⁴. Product **10b** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 20 : 1). white solid (35 mg, 0.12 mmol, 12% yield); mp 97–99 °C. ¹H NMR (400 MHz, CDCl₃) δ 10.16 (s, 1H), 7.65 (d, *J* = 8.6 Hz, 1H), 6.81 (d, *J* = 8.6 Hz, 1H), 3.92 (s, 3H), 3.88 (s, 3H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 191.8, 153.8, 152.58, 136.5, 130.1, 118.2, 82.3, 62.5, 56.2; HRMS (ESI) *m/z* [M+Na]⁺ calcd for C₉H₉O₃NaI: 314.9489; found: 314.9501.



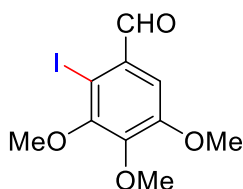
2-iodo-4-methoxy-5-methylbenzaldehyde (11)⁴. Product **11** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 15 : 1). yellow solid (232 mg, 0.84 mmol, 84% yield); mp 90–91 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.84 (s, 1H), 8.13 (d, *J* = 2.0 Hz, 1H), 7.68 (dd, *J* = 2.0, 0.9 Hz, 1H), 3.84 (s, 3H), 2.41 (s, 3H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 190.0, 163.1, 139.1, 134.0, 133.2, 132.8, 92.6, 60.3, 17.1; HRMS (ESI) *m/z* [M+H]⁺ calcd for C₉H₁₀O₂I: 276.9720; found: 276.9729.



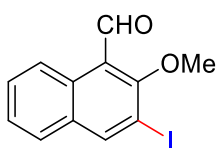
4-formyl-5-iodo-2-methoxyphenyl acetate (12). Product **12** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 15 : 1). white solid (259 mg, 0.81 mmol, 81% yield); mp 95–96 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.95 (s, 1H), 7.61 (s, 1H), 7.51 (s, 1H), 3.88 (s, 3H), 2.33 (s, 3H). 3.88 (s, 3H), 2.33 (s, 3H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 194.9, 168.0, 152.1, 145.0, 134.2, 133.3, 112.7, 89.6, 56.2, 20.6; HRMS (ESI) *m/z* [M+Na]⁺ calcd for C₁₀H₉O₄INa: 342.9439; found: 342.9441.



5-iodo-2,3,4-trimethoxybenzaldehyde (13). Product **13** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 15 : 1). yellow solid (251 mg, 0.78 mmol, 78% yield); mp 36–37 °C. ^1H NMR (400 MHz, CDCl_3) δ 10.17 (s, 1H), 7.98 (s, 1H), 4.02 (s, 3H), 3.97 (s, 3H), 3.89 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 187.7, 158.9, 157.9, 146.0, 132.6, 126.9, 85.9, 62.4, 61.2, 61.1; HRMS (ESI) m/z $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{10}\text{H}_{11}\text{O}_4\text{NaI}$: 344.9595; found: 344.9606.



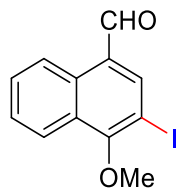
2-iodo-3,4,5-trimethoxybenzaldehyde (14)⁵. Product **14** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 15 : 1). yellow solid (306 mg, 0.95 mmol, 95% yield); mp 66–67 °C. ^1H NMR (400 MHz, CDCl_3) δ 10.03 (s, 1H), 7.34 (s, 1H), 3.97 (s, 3H), 3.92 (s, 3H), 3.90 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 195.3, 154.0, 153.0, 147.8, 130.5, 108.6, 91.6, 61.2, 61.0, 56.3; HRMS (ESI) m/z $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{10}\text{H}_{11}\text{O}_4\text{NaI}$: 344.9595; found: 344.9605.



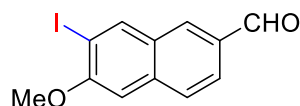
3-iodo-2-methoxy-1-naphthaldehyde (15). Product **15** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 40 : 1). white solid (243 mg, 0.78 mmol, 78% yield); mp 125–126 °C. ^1H NMR (400 MHz, CDCl_3) δ 10.86 (s, 1H), 9.03 (d, $J = 9.1$ Hz, 1H), 8.16 (d, $J = 1.9$ Hz, 1H), 7.94 (d, $J = 9.2$ Hz, 1H), 7.84 – 7.81 (m, 1H), 7.32 (d, $J = 9.2$ Hz, 1H), 4.06 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 191.7, 164.0, 138.2, 136.7, 136.4, 130.4,

⁵ Nicolaus N, Strauss S, Neudörfel J M, Prokop A, Schmalz H G. *Org. Lett.* **2009**, *11* (2), 341-344.

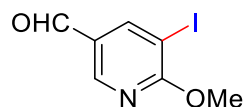
130.2, 126.8, 116.6, 113.4, 89.9, 56.6; HRMS (ESI) m/z $[M+H]^+$ calcd for $C_{12}H_{10}O_2I$: 312.9720; found: 312.9733.



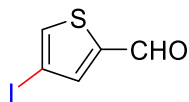
3-iodo-4-methoxy-1-naphthaldehyde (16). Product **16** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 40 : 1). yellow solid (175 mg, 0.56 mmol, 56% yield); mp 177–178 °C. 1H NMR (400 MHz, $CDCl_3$) δ 10.22 (s, 1H), 9.21 (dt, J = 8.6, 1.0 Hz, 1H), 8.25 (s, 1H), 8.17 (ddd, J = 8.3, 1.4, 0.7 Hz, 1H), 7.71 (ddd, J = 8.5, 6.9, 1.4 Hz, 1H), 7.62 (ddd, J = 8.3, 6.9, 1.3 Hz, 1H), 4.03 (s, 3H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 191.3, 162.2, 146.5, 132.0, 129.7, 129.5, 128.7, 127.8, 125.4, 122.8, 85.3, 62.1; HRMS (ESI) m/z $[M+H]^+$ calcd for $C_{12}H_{10}O_2I$: 312.9720; found: 312.9733.



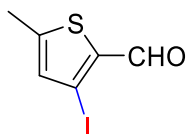
7-iodo-6-methoxy-2-naphthaldehyde (17). Product **17** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 30 : 1). yellow solid (193 mg, 0.62 mmol, 62% yield); mp 244–245 °C. 1H NMR (400 MHz, $CDCl_3$) δ 10.16 (s, 1H), 8.26 (d, J = 6.9 Hz, 2H), 8.00 (dd, J = 8.8, 4.8 Hz, 2H), 7.31 (d, J = 9.1 Hz, 1H), 4.09 (s, 3H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 191.6, 159.1, 139.0, 134.4, 132.6, 132.4, 132.2, 128.8, 125.1, 113.4, 87.6, 57.2; HRMS (ESI) m/z $[M+H]^+$ calcd for $C_{12}H_{10}O_2I$: 312.9720; found: 312.9733.



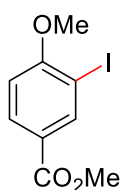
5-iodo-6-methoxynicotinaldehyde (18). Product **18** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 5 : 1). yellow solid (139 mg, 0.53 mmol, 53% yield); mp 142–143 °C. 1H NMR (400 MHz, $CDCl_3$) δ 9.54 (s, 1H), 8.45 (d, J = 2.3 Hz, 1H), 7.95 (d, J = 2.3 Hz, 1H), 3.70 (s, 3H); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 184.6, 160.2, 146.8, 145.2, 119.2, 92.9, 40.0; HRMS (ESI) m/z $[M+Na]^+$ calcd for $C_7H_6NO_2NaI$: 285.9336; found: 285.9349.



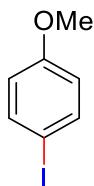
4-iodothiophene-2-carbaldehyde (19). Product **19** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 20 : 1). Yellow oil (174 mg, 0.73 mmol, 73% yield); ^1H NMR (400 MHz, CDCl_3) δ 9.89 (d, J = 1.3 Hz, 1H), 7.80 (t, J = 1.3 Hz, 1H), 7.75 (d, J = 1.3 Hz, 1H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 181.6, 145.0, 143.0, 137.8; HRMS (ESI) m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_5\text{H}_4\text{OSI}$: 238.9023; found: 238.9028.



3-iodo-5-methylthiophene-2-carbaldehyde (20). Product **20** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 20: 1). yellow solid (202 mg, 0.80 mmol, 80% yield); mp 77–78 °C. ^1H NMR (400 MHz, CDCl_3) δ 9.78 (s, 1H), 7.65 (s, 1H), 2.50 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 181.5, 149.9, 144.0, 142.2, 82.0, 19.1; HRMS (ESI) m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_5\text{H}_6\text{OSI}$: 252.9179; found: 252.9184.

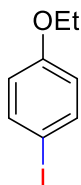


Methyl 3-iodo-4-methoxybenzoate (21)⁶. Product **21** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 5 : 1). white solid (274 mg, 0.94 mmol, 94% yield); mp 93-95 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.45 (d, J = 2.1 Hz, 1H), 8.02 (dd, J = 8.6, 2.1 Hz, 1H), 6.83 (d, J = 8.7 Hz, 1H), 3.94 (s, 3H), 3.89 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 165.6, 161.6, 141.0, 131.7, 124.3, 110.0, 56.6, 52.2; HRMS (ESI) m/z $[\text{M}+\text{H}]^+$ calcd for $\text{C}_9\text{H}_{10}\text{O}_3\text{I}$: 292.9670; found: 292.9680.

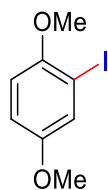


⁶ Tu G, Ju G, Ji S J, Zhao Y. *Org. Lett.* **2022**, *24* (11), 2155-2159

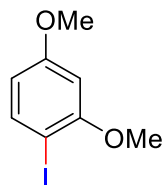
1-iodo-4-methoxybenzene (22)⁷. Product **22** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 150 : 1). white oil (211 mg, 0.91 mmol, 91% yield); ¹H NMR (400 MHz, CDCl₃) δ 7.61 – 7.50 (m, 2H), 6.71 – 6.64 (m, 2H), 3.78 (s, 3H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 159.4, 138.2, 116.8, 82.7, 55.3; HRMS (ESI) m/z [M+Na]⁺ calcd for C₇H₇ONaI: 256.9434; found: 256.9444.



1-ethoxy-4-iodobenzene (23)⁸. Product **23** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 150: 1). white oil (206 mg, 0.83 mmol, 83% yield); ¹H NMR (400 MHz, CDCl₃) δ 7.54 (d, *J* = 8.9 Hz, 2H), 6.67 (d, *J* = 8.9 Hz, 2H), 3.99 (q, *J* = 7.0 Hz, 2H), 1.40 (t, *J* = 7.0 Hz, 3H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 158.8, 138.2, 116.9, 82.5, 63.6, 14.8; HRMS (ESI) m/z [M+Na]⁺ calcd for C₈H₉ONaI: 270.9591; found: 270.9598.



2-iodo-1,4-dimethoxybenzene (24)⁹. Product **24** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 150 : 1). yellow oli (219 mg, 0.83 mmol, 83% yield).¹H NMR (400 MHz, CDCl₃) δ 7.34 (d, *J* = 3.0 Hz, 1H), 6.87 (dd, *J* = 8.9, 3.0 Hz, 1H), 6.76 (d, *J* = 9.0 Hz, 1H), 3.83 (s, 3H), 3.76 (s, 3H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 154.2, 152.7, 124.8, 114.8, 111.6, 86.0, 57.0, 56.0. HRMS (ESI) m/z [M+H]⁺ calcd for C₈H₁₀O₂I: 264.9720; found: 264.9722.

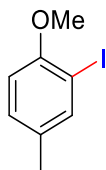


⁷ Bergström M, Suresh G, Naidu V R, Unelius C R. *Eur. J. Org. Chem.* **2017**, 2017 (22), 3234-3239.

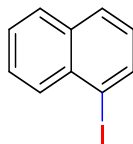
⁸ Tale R H, Toradmal G K, Gopula V B, Rodge A H, Pawar R P, Patil K M. *Tetrahedron Lett.* **2015**, 56 (21), 2699-2703.

⁹ Wu Z, Wei F, Wan B, Zhang Y. *J. Am. Chem. Soc.* **2021**, 143 (12), 4524-4530.

1-iodo-2,4-dimethoxybenzene (25)¹⁰. Product **25** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 100 : 1). yellow oil (230mg, 0.87 mmol, 87 % yield). ¹H NMR (400 MHz, CDCl₃) δ 7.61 (d, *J* = 8.6 Hz, 1H), 6.42 (d, *J* = 2.6 Hz, 1H), 6.31 (dd, *J* = 8.6, 2.7 Hz, 1H), 3.84 (s, 3H), 3.79 (s, 3H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 161.4, 158.8, 139.2, 107.0, 99.2, 74.8, 56.3, 55.6. HRMS (ESI) *m/z* [M+H]⁺ calcd for C₈H₁₀O₂I: 264.9720; found: 264.9716.



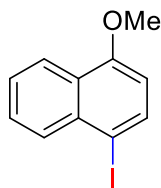
2-iodo-1-methoxy-4-methylbenzene (26)⁷. Product **26** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 100 : 1). yellow oil (211 mg, 0.85 mmol, 85% yield); ¹H NMR (400 MHz, CDCl₃) δ 7.60 (d, *J* = 1.4 Hz, 1H), 7.10 (ddd, *J* = 8.3, 2.1, 0.8 Hz, 1H), 6.72 (d, *J* = 8.3 Hz, 1H), 3.85 (s, 3H), 2.26 (s, 3H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 156.0, 139.8, 132.0, 130.0, 110.8, 85.8, 56.4, 20.0; HRMS (ESI) *m/z* [M+Na]⁺ calcd for C₈H₉ONaI: 270.9591; found: 270.9600.



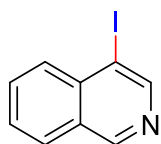
1-iodonaphthalene (27)¹¹. Product **27** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 200: 1). white oil (191 mg, 0.75 mmol, 75% yield); ¹H NMR (400 MHz, CDCl₃) δ 8.13 – 8.07 (m, 2H), 7.85 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.78 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.59 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.52 (ddd, *J* = 8.0, 6.8, 1.4 Hz, 1H), 7.19 (dd, *J* = 8.2, 7.3 Hz, 1H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 137.5, 134.4, 134.2, 132.2, 129.0, 128.6, 127.7, 126.9, 126.8, 99.6; HRMS (ESI) *m/z* [M+Na]⁺ calcd for C₁₀H₇NaI: 276.9485; found: 276.9488.

¹⁰ Bedrač L, Iskra J. *Tetrahedron Lett.* **2012**, 53 (41), 5555-5558.

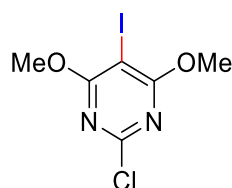
¹¹ Iwai K, Nishiguchi N, Nishiwaki N. *J. Org. Chem.* **2023**, 88 (13), 9409-9412.



1-iodo-4-methoxynaphthalene (28)¹². Product **28** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 100: 1). yellow oli (224mg, 0.79 mmol, 79 % yield). ¹H NMR (400 MHz, CDCl₃) δ 8.27 – 8.22 (m, 1H), 8.05 – 8.02 (m, 1H), 7.95 (d, *J* = 8.2 Hz, 1H), 7.60 (ddd, *J* = 8.4, 6.9, 1.4 Hz, 1H), 7.52 (ddd, *J* = 8.2, 6.9, 1.3 Hz, 1H), 6.58 (d, *J* = 8.2 Hz, 1H), 3.98 (s, 3H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 156.3, 136.9, 134.7, 131.8, 128.2, 126.6, 126.0, 122.5, 105.6, 88.2, 55.7; HRMS (ESI) *m/z* [M+H]⁺ calcd for C₁₁H₁₀OI: 284.9771; found: 284.9778.



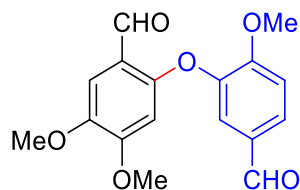
4-iodoisoquinoline (29)¹³. Product **29** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 15 : 1). white solid (206mg, 0.81 mmol, 81% yield); mp 94–95 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.14 (s, 1H), 8.94 (s, 1H), 8.00 (dd, *J* = 8.5, 1.1 Hz, 1H), 7.90 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.80 (ddd, *J* = 8.4, 6.9, 1.3 Hz, 1H), 7.67 (ddd, *J* = 8.1, 6.9, 1.1 Hz, 1H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 152.6, 151.0, 137.2, 132.0, 130.8, 129.8, 128.4, 128.2, 96.8; HRMS (ESI) *m/z* [M+H]⁺ calcd for C₉H₇NI: 255.9618; found: 255.9628.



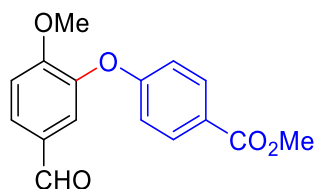
2-chloro-5-iodo-4,6-dimethoxypyrimidine (30). Product **30** was synthesized according to experimental procedure I and purified by column chromatography (petroleum ether : ethyl acetate= 20: 1). white solid (237 mg, 0.79 mmol, 79% yield); mp 183–185 °C. ¹H NMR (400 MHz, CDCl₃) δ 4.03 (s, 6H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 170.1, 159.1, 59.6, 56.1; HRMS (ESI) *m/z* [M+H]⁺ calcd for C₆H₇Cl₂N₂O₂: 300.9235; found: 300.9230.

¹² Racys D T, Sharif S A I, Pimlott S L, Sutherland A. *J. Org. Chem.* **2016**, 81 (3), 772-780.

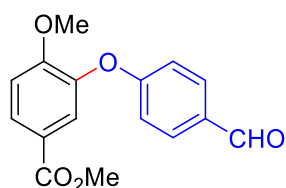
¹³ Sun K, Lv Y, Wang J, Sun J, Liu L, Jia M, Liu X, Li Z, Wang X. *Org. Lett.* **2015**, 17 (18), 4408-4411.



2-(2-formyl-6-methoxyphenoxy)-4,5-dimethoxybenzaldehyde (Hernandial)⁴. Product **Hernandial** was synthesized according to experimental procedure II and purified by column chromatography (petroleum ether : ethyl acetate= 15 : 1). White solid (155 mg, 0.49 mmol, 49% yield); mp 138-140 °C ¹H NMR (400 MHz, CDCl₃) δ 10.28 (s, 1H), 9.83 (s, 1H), 7.69-7.66 (m, 1H), 7.40 (s, 1H), 7.39 (d, *J* = 2.0 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 1H), 6.39 (s, 1H), 3.98 (s, 3H), 3.94 (s, 3H), 3.81 (s, 3H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 190.1, 187.6, 155.6, 155.6, 154.7, 147.2, 146.3, 130.2, 128.6, 120.0, 118.0, 112.1, 108.5, 102.3, 56.4, 56.3; HRMS (ESI) *m/z* [M+Na]⁺ calcd for C₁₇H₁₆O₆Na: 339.0840; found: 339.0846.



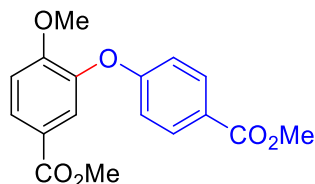
Methyl 4(5-formyl-2-methoxyphenoxy)benzoate (Aristogin A)¹⁴. Product **Aristogin A** was synthesized according to experimental procedure II and purified by column chromatography (petroleum ether : ethyl acetate= 8 : 1). white solid (232 mg, 0.81 mmol, 81% yield); mp 118-120 °C ¹H NMR (400 MHz, CDCl₃) δ 9.87 (s, 1H), 8.00 (d, *J* = 8.5 Hz, 2H), 7.75 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.59 (d, *J* = 2.0 Hz, 1H), 7.13 (s, 1H), 6.93 (d, *J* = 8.5 Hz, 2H), 3.90 (s, 6H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 190.1, 166.6, 161.3, 156.8, 144.4, 131.7, 130.4, 129.2, 124.7, 121.9, 116.3, 112.4, 56.3, 52.1; HRMS (ESI) *m/z* [M+Na]⁺ calcd for C₁₆H₁₄O₅Na: 309.0734; found: 309.0740.



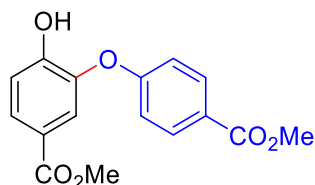
Methyl 3-(4-formylphenoxy)-4-methoxybenzoate (Aristogin B)¹⁴. Product **Aristogin B** was synthesized according to experimental procedure II and purified by column chromatography (petroleum ether : ethyl acetate= 8 : 1). white solid (166 mg, 0.58 mmol, 58% yield); mp 64-66 °C ¹H NMR (400 MHz, CDCl₃) δ 9.91 (s, 1H), 7.97 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 2H), 7.78 (d, *J* = 2.1 Hz,

¹⁴ Jung N, Bräse, S. *Eur. J. Org. Chem.* **2009**, 2009 (26), 4494-4502.

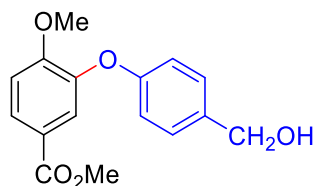
1H), 7.06 (d, $J = 8.6$ Hz, 1H), 6.99 (d, $J = 8.3$ Hz, 2H), 3.88 (s, 3H), 3.86 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 190.8, 166.2, 163.0, 155.6, 142.6, 132.0, 131.2, 128.5, 123.8, 123.4, 116.4, 112.2, 56.1, 52.2; HRMS (ESI) m/z $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{17}\text{H}_{16}\text{O}_6\text{Na}$: 309.0734; found: 309.0742.



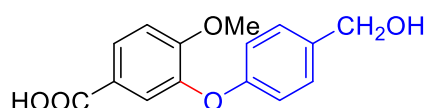
Methyl 4-methoxy-3-(4-(methoxycarbonyl)phenoxy)benzoate (Aristogin C)¹⁴. Product **Aristogin C** was synthesized according to experimental procedure II and purified by thin-layer chromatography (petroleum ether : ethyl acetate = 3 : 1). yellow solid (167 mg, 0.53 mmol, 53% yield); mp 93-94 °C ^1H NMR (400 MHz, CDCl_3) δ 7.98 (d, $J = 8.8$ Hz, 2H), 7.94 (dd, $J = 8.6, 2.1$ Hz, 1H), 7.74 (d, $J = 2.1$ Hz, 1H), 7.04 (d, $J = 8.6$ Hz, 1H), 6.91 (d, $J = 8.8$ Hz, 2H), 3.89 (s, 3H), 3.87 (s, 3H), 3.86 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 166.7, 166.2, 161.7, 155.6, 143.1, 131.6, 128.2, 124.4, 123.4, 123.3, 116.0, 112.1, 56.1, 52.1, 52.0; HRMS (ESI) m/z $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{17}\text{H}_{16}\text{O}_6\text{Na}$: 339.0840; found: 339.0852.



Methyl 4-hydroxy-3-(4-(methoxycarbonyl)phenoxy)benzoate (Aristogin D)¹⁴. Product **Aristogin D** was synthesized according to experimental procedure III and purified by thin-layer chromatography (petroleum ether : ethyl acetate = 5 : 1). white solid (9.1 mg, 0.03 mmol, 81% yield); mp 93-94 °C ^1H NMR (400 MHz, CDCl_3) δ 8.02 (d, $J = 8.4$ Hz, 2H), 7.83 (dd, $J = 8.6, 2.0$ Hz, 1H), 7.63 (s, 1H), 7.10 (d, $J = 8.5$ Hz, 1H), 7.03 (d, $J = 8.5$ Hz, 2H), 6.15 (s, 1H), 3.91 (s, 3H), 3.84 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 166.4, 166.1, 160.4, 151.9, 142.1, 132.0, 127.8, 125.7, 123.2, 121.2, 117.2, 116.5, 52.2, 52.1; HRMS (ESI) m/z $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{16}\text{H}_{14}\text{O}_6\text{Na}$: 325.0683; found: 325.0694.



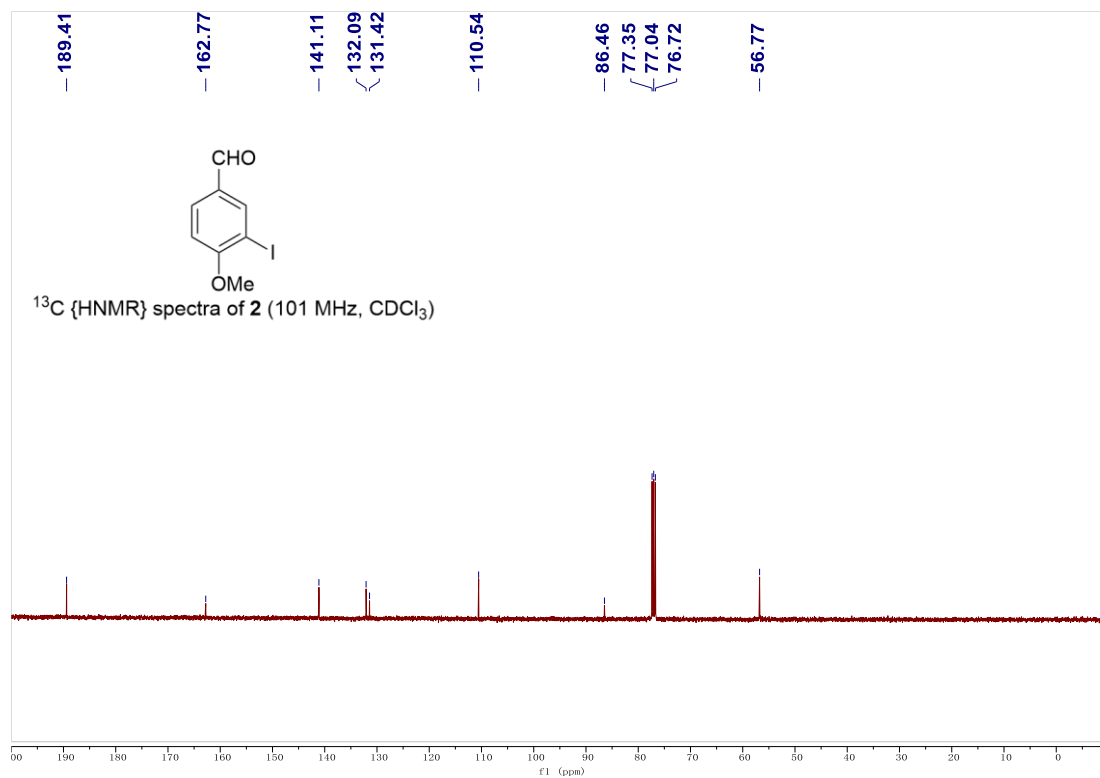
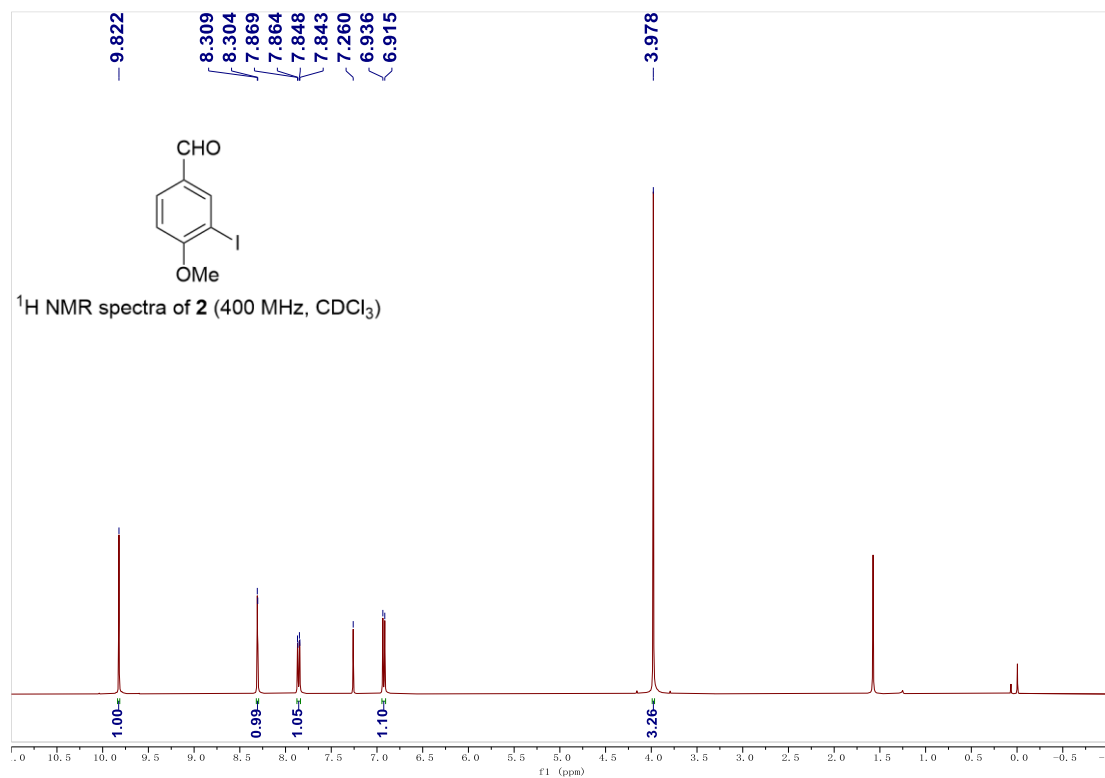
Methyl 3-(4-(hydroxymethyl)phenoxy)-4-methoxybenzoate (Aristogin E)¹⁵. Product **Aristogin E** was synthesized according to experimental procedure IV and purified by thin-layer chromatography (petroleum ether : ethyl acetate= 5 : 1). yellow oil (30 mg, 0.105 mmol, 62% yield); ¹H NMR (400 MHz, CDCl₃) δ 7.86 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.62 (d, *J* = 2.1 Hz, 1H), 7.31 (d, *J* = 8.6 Hz, 2H), 7.02 (d, *J* = 8.6 Hz, 1H), 6.94 (d, *J* = 8.6 Hz, 2H), 4.66 (s, 2H), 3.90 (s, 3H), 3.85 (s, 3H); ¹³C {¹H} NMR (101 MHz, CDCl₃) δ 166.4, 157.0, 155.2, 144.8, 135.5, 128.7, 127.0, 123.1, 121.8, 117.6, 111.8, 64.9, 56.1, 52.0; HRMS (ESI) *m/z* [M+Na]⁺ calcd for C₁₆H₁₆O₅Na: 297.0734; found: 311.0899.



3-(4-(hydroxymethyl)phenoxy)-4-methoxybenzoic acid (Aristogin F)¹⁴. Product **Aristogin F** was synthesized according to experimental procedure IV and purified by thin-layer chromatography (petroleum ether : ethyl acetate= 3 : 1). yellow oil (16 mg, 0.06 mmol, 58% yield); ¹H NMR (400 MHz, DMSO) δ 7.78 (dd, *J* = 8.5, 2.1 Hz, 1H), 7.40 (d, *J* = 2.1 Hz, 1H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.25 (d, *J* = 8.6 Hz, 1H), 6.89 (d, *J* = 8.6 Hz, 2H), 4.46 (s, 2H), 3.85 (s, 3H); ¹³C {¹H} NMR (101 MHz, DMSO) δ 167.1, 156.1, 155.0, 144.8, 137.8, 128.7, 127.1, 123.9, 121.0, 117.5, 113.2, 62.9, 56.4; HRMS (ESI) *m/z* [M+Na]⁺ calcd for C₁₆H₁₄O₅Na: 297.0734; found: 309.0742.

¹⁵ Morin É, Raymond M, Dubart A, Collins S K. *Org. Lett.* **2017**, 19 (11), 2889-2892.

4. ^1H NMR and ^{13}C NMR spectra



Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

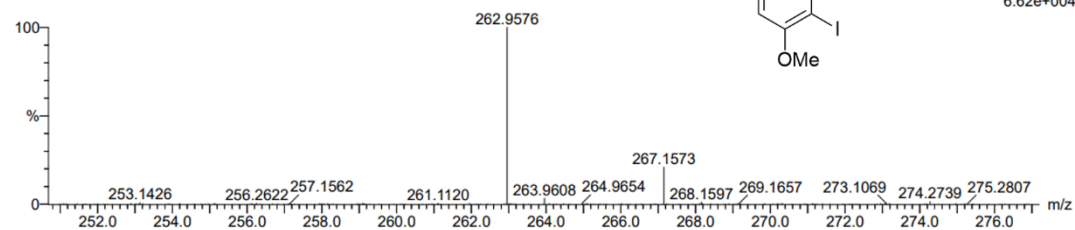
79 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 8-8 H: 8-8 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

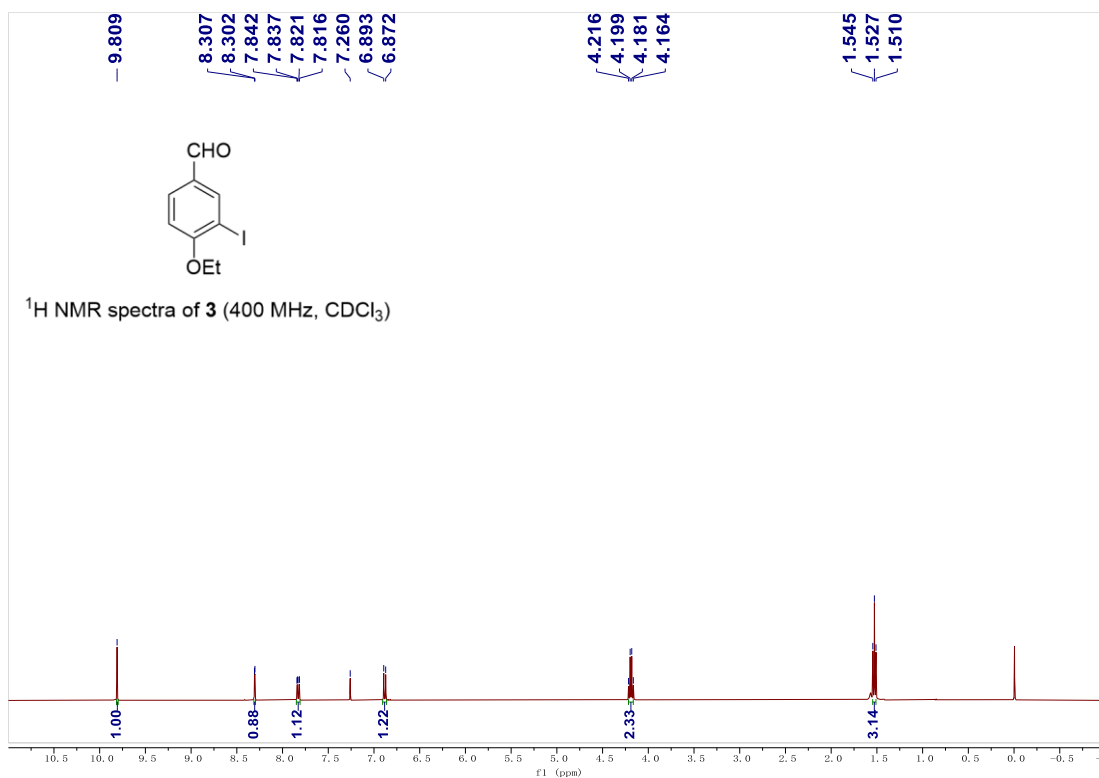
12

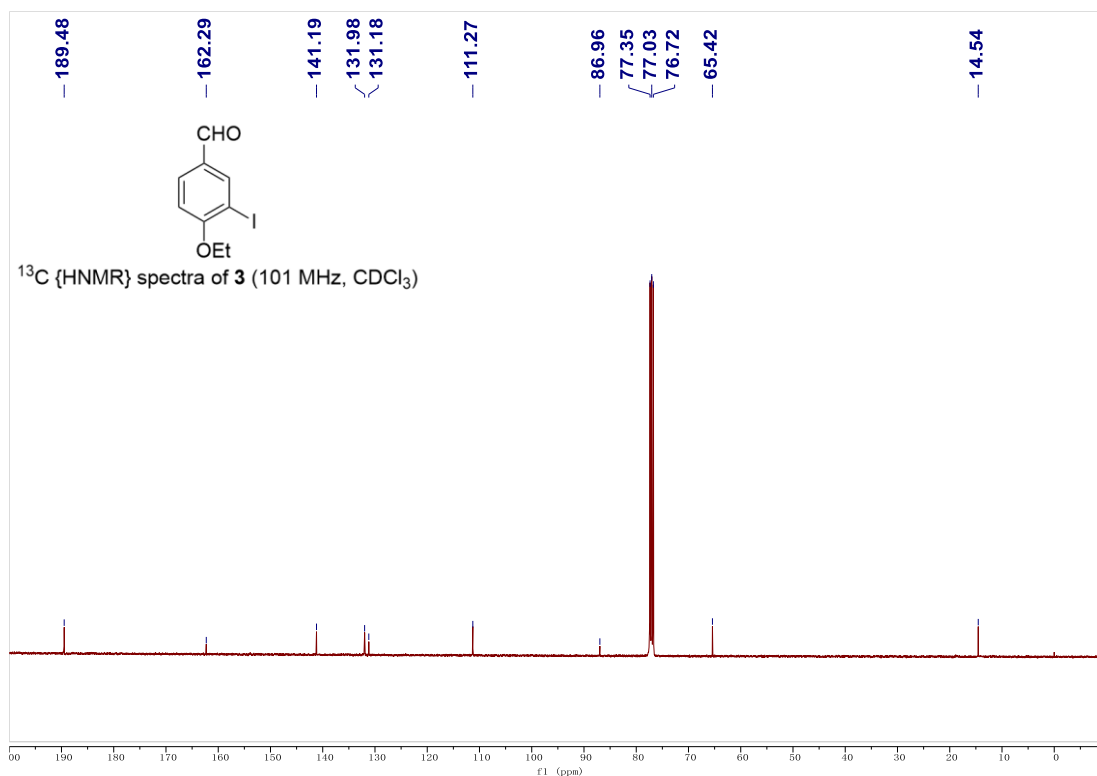
240405-1-2 11 (0.076)



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
262.9576	262.9569	0.7	2.7	4.5	206.7	n/a	n/a	C8 H8 O2 I





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

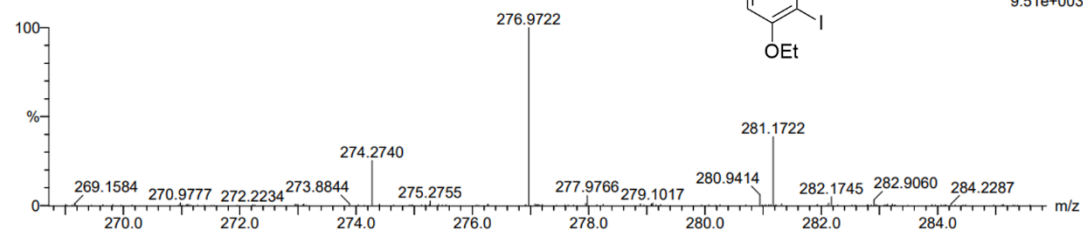
Monoisotopic Mass, Even Electron Ions

99 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 9-9 H: 10-10 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

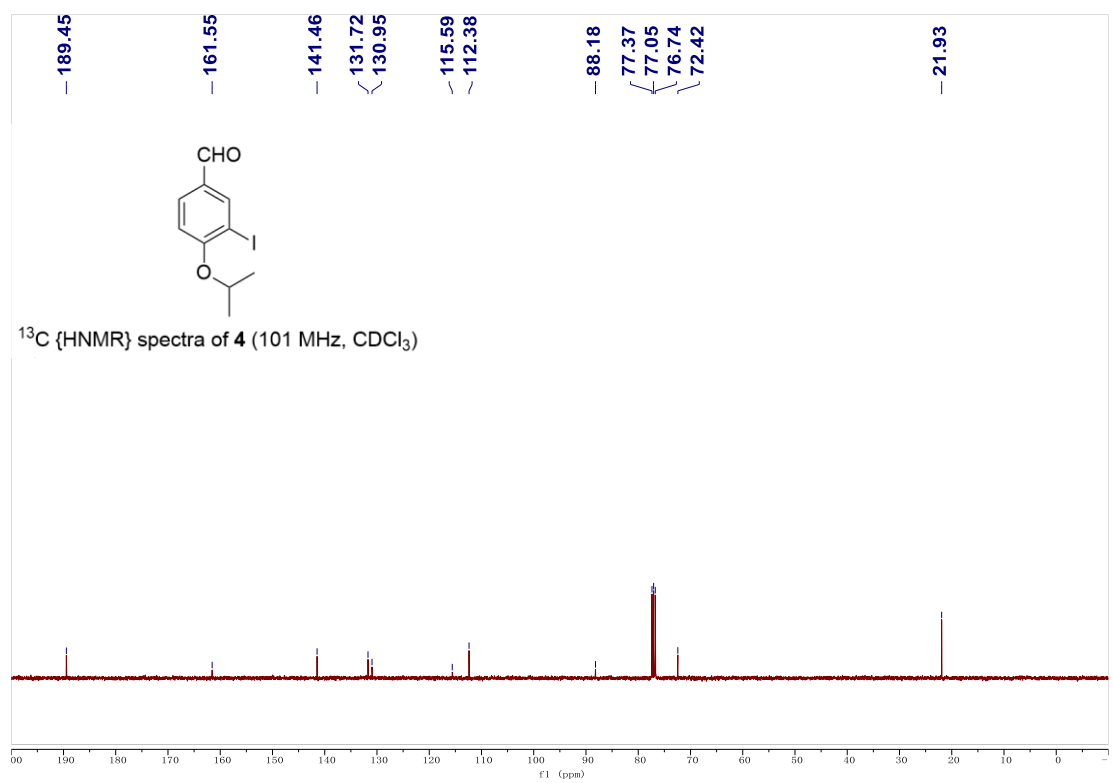
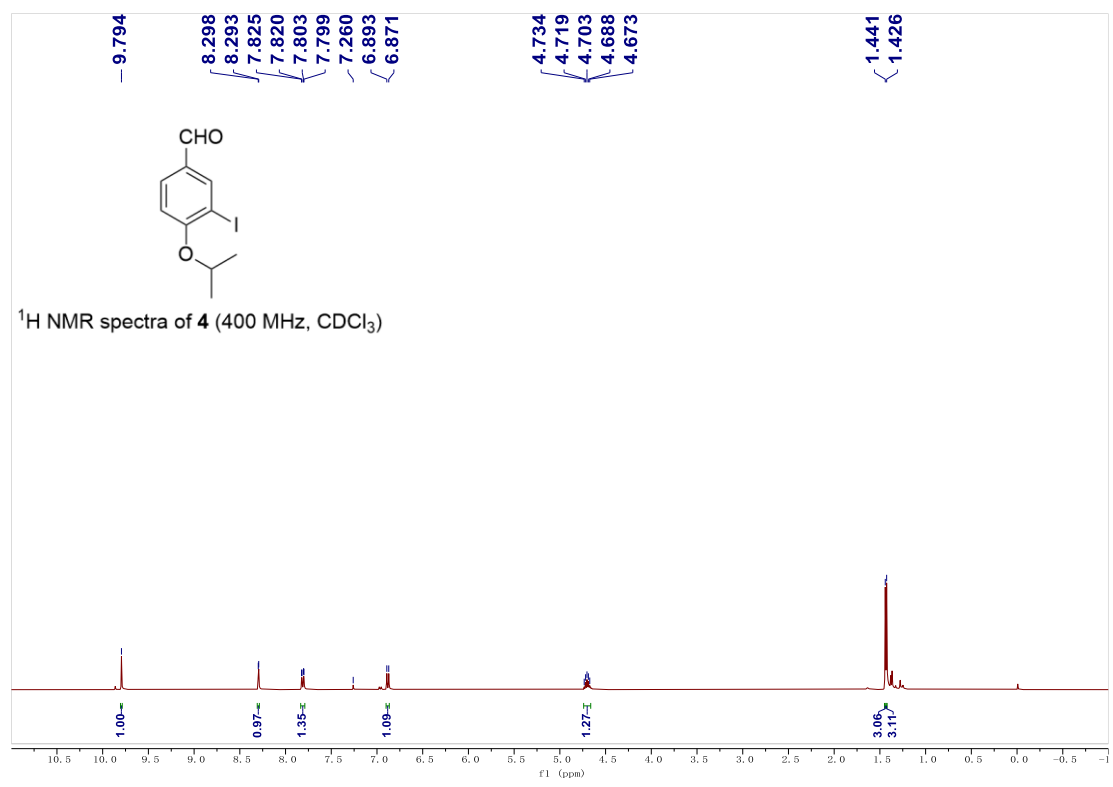
12
 240405-1-3 11 (0.076)



1: TOF MS ES+
 9.51e+003

Minimum: -1.5
 Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
276.9722	276.9725	-0.3	-1.1	4.5	167.9	n/a	n/a	C9 H10 O2 I



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

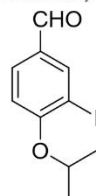
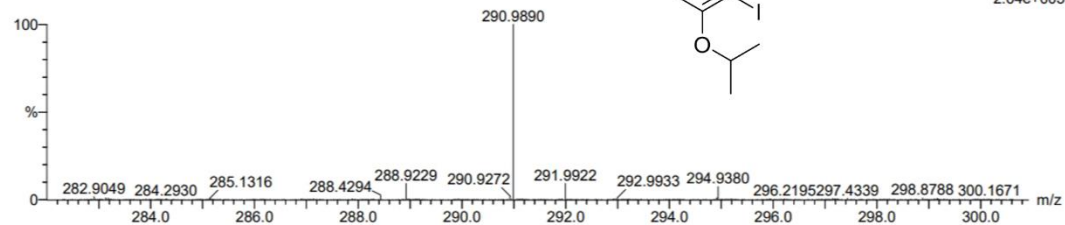
162 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 10-10 H: 12-12 N: 0-200 O: 0-100 Na: 0-2 I: 1-2

6

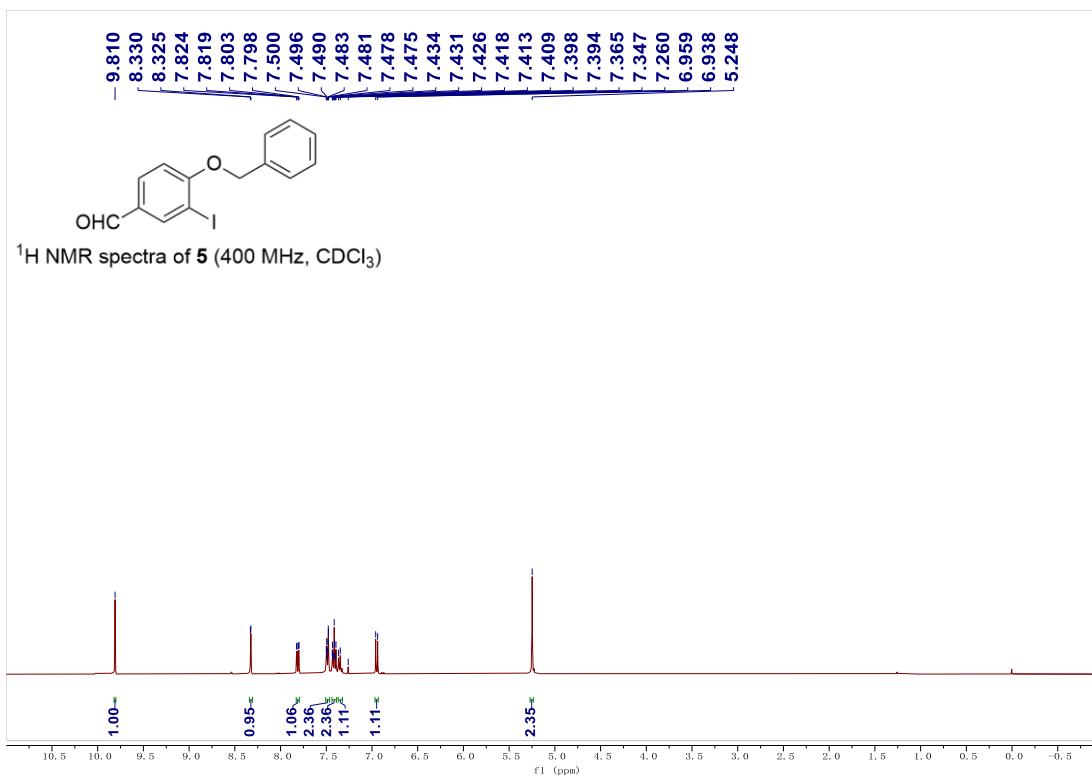
231208-3-9 25 (0.121)

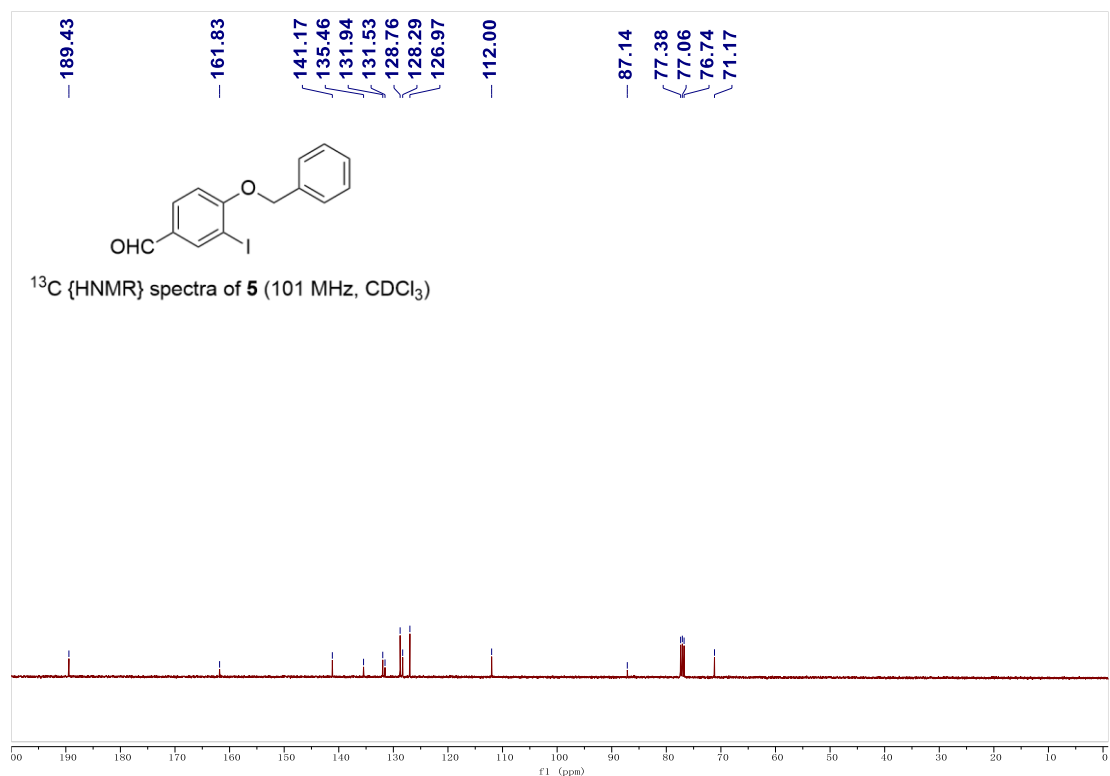


1: TOF MS ES+
2.64e+005

Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
290.9890	290.9882	0.8	2.7	4.5	947.1	n/a	n/a	C10 H12 O2 I





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

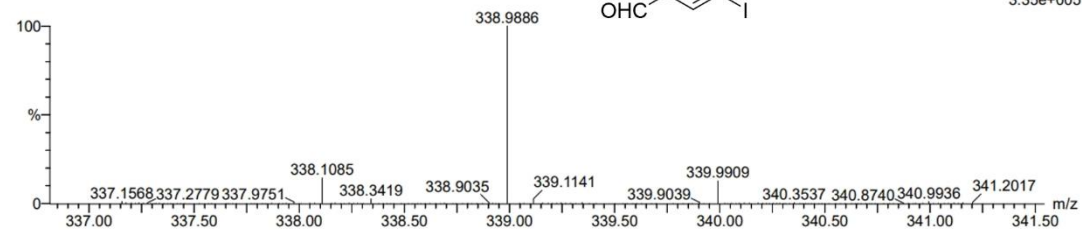
17 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 14-14 H: 12-12 O: 0-100 I: 1-2

6

231208-3-1 16 (0.083)

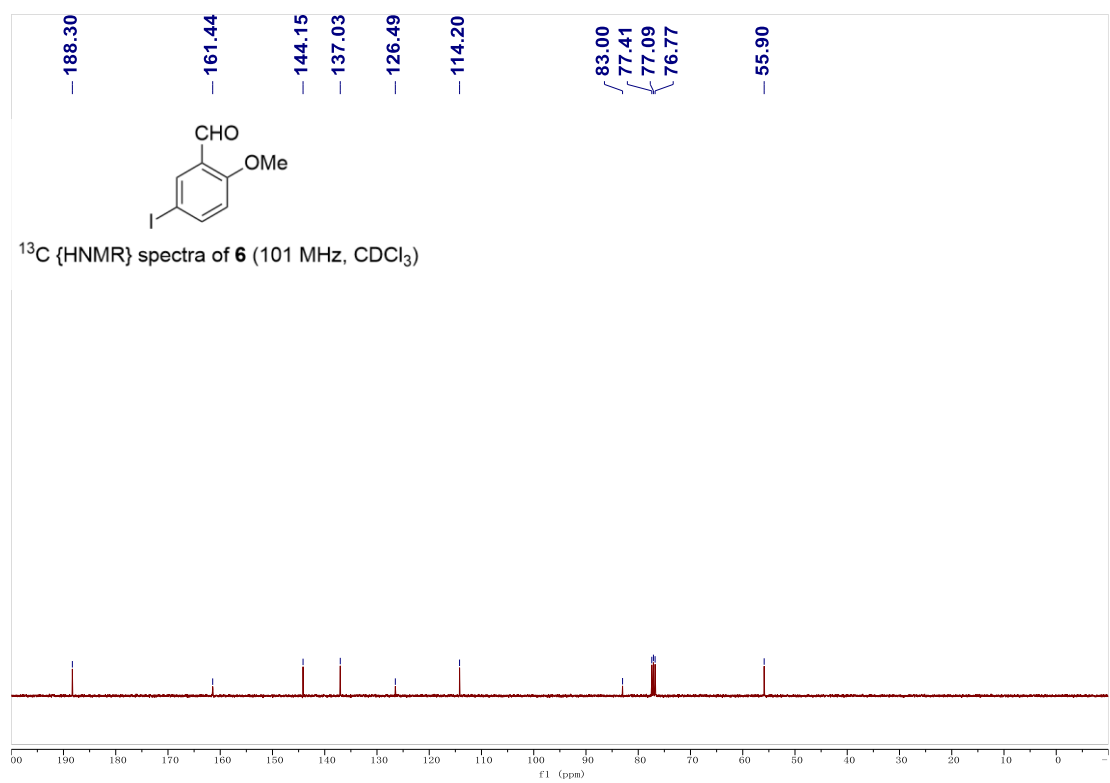
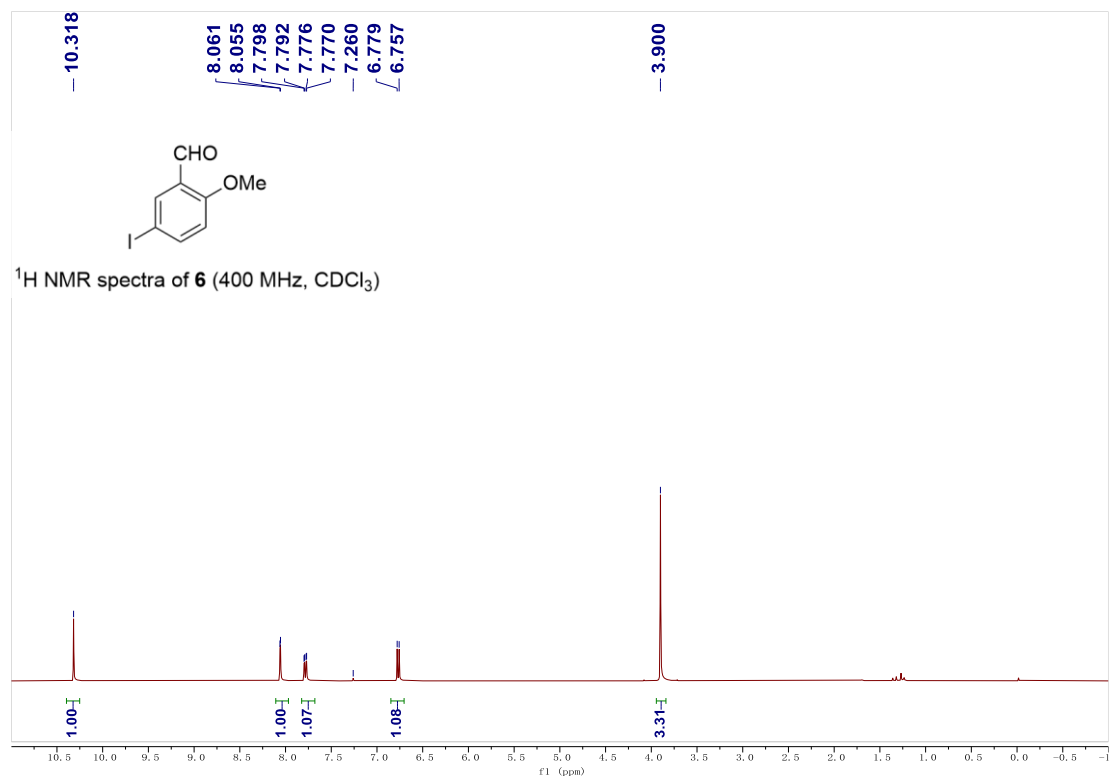


1: TOF MS ES+
3.35e+005

Minimum: -1.5

Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
338.9886	338.9882	0.4	1.2	8.5	894.9	n/a	n/a	C14 H12 O2 I



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

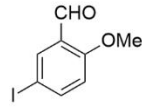
Monoisotopic Mass, Even Electron Ions

79 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

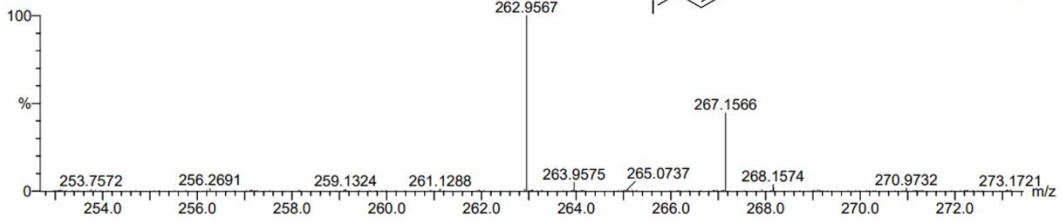
Elements Used:

C: 8-8 H: 8-8 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

12
240405-1-6 11 (0.076)

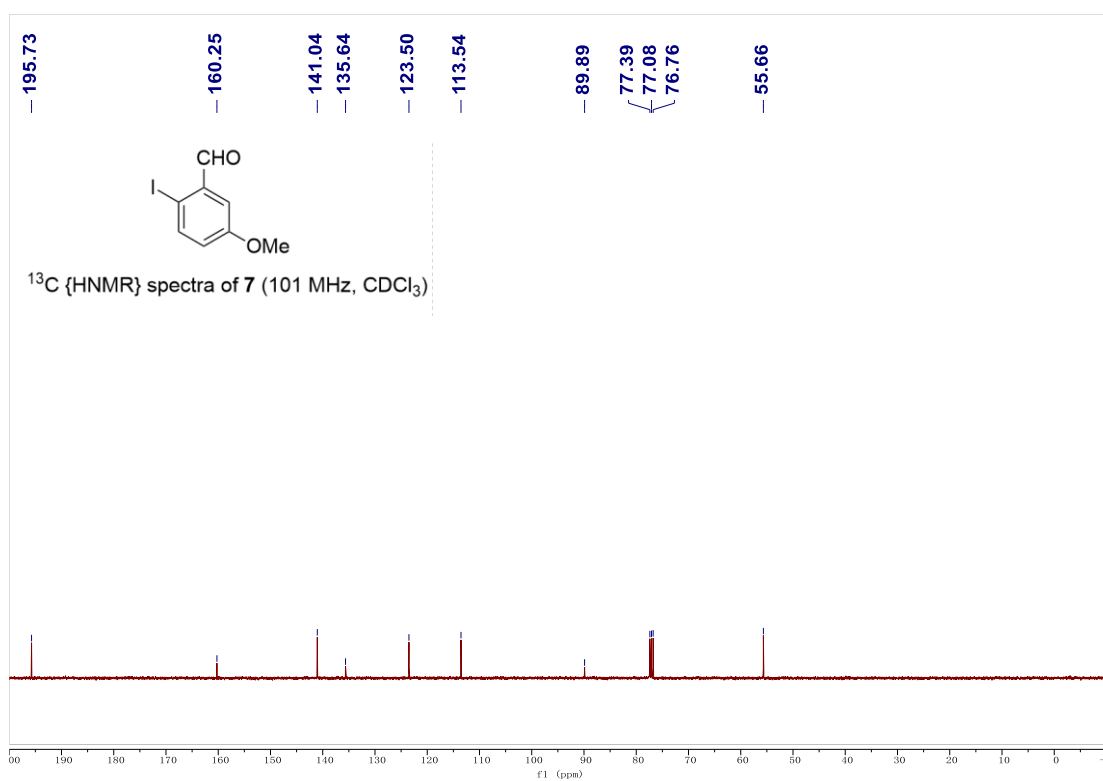
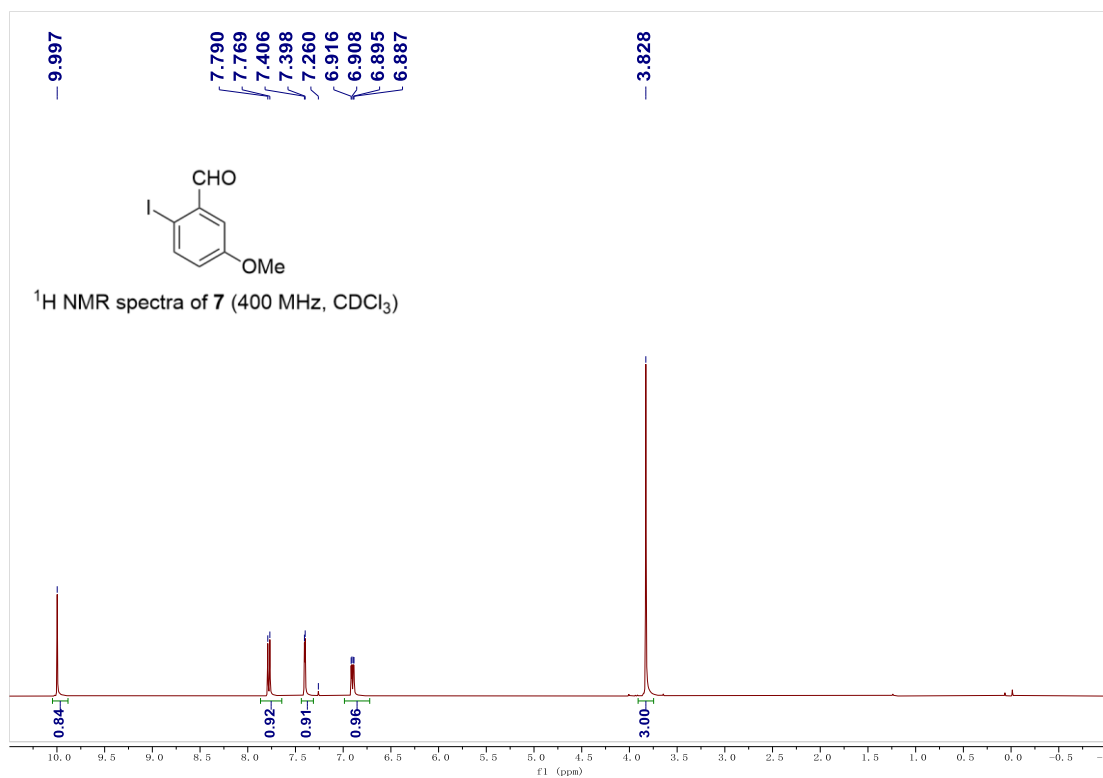


1: TOF MS ES+
1.20e+04



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
262.9567	262.9569	-0.2	-0.8	4.5	183.6	n/a	n/a	C8 H8 O2 I



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

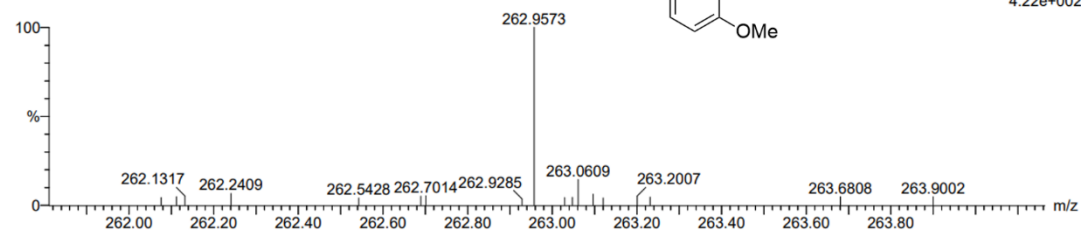
Monoisotopic Mass, Even Electron Ions

79 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

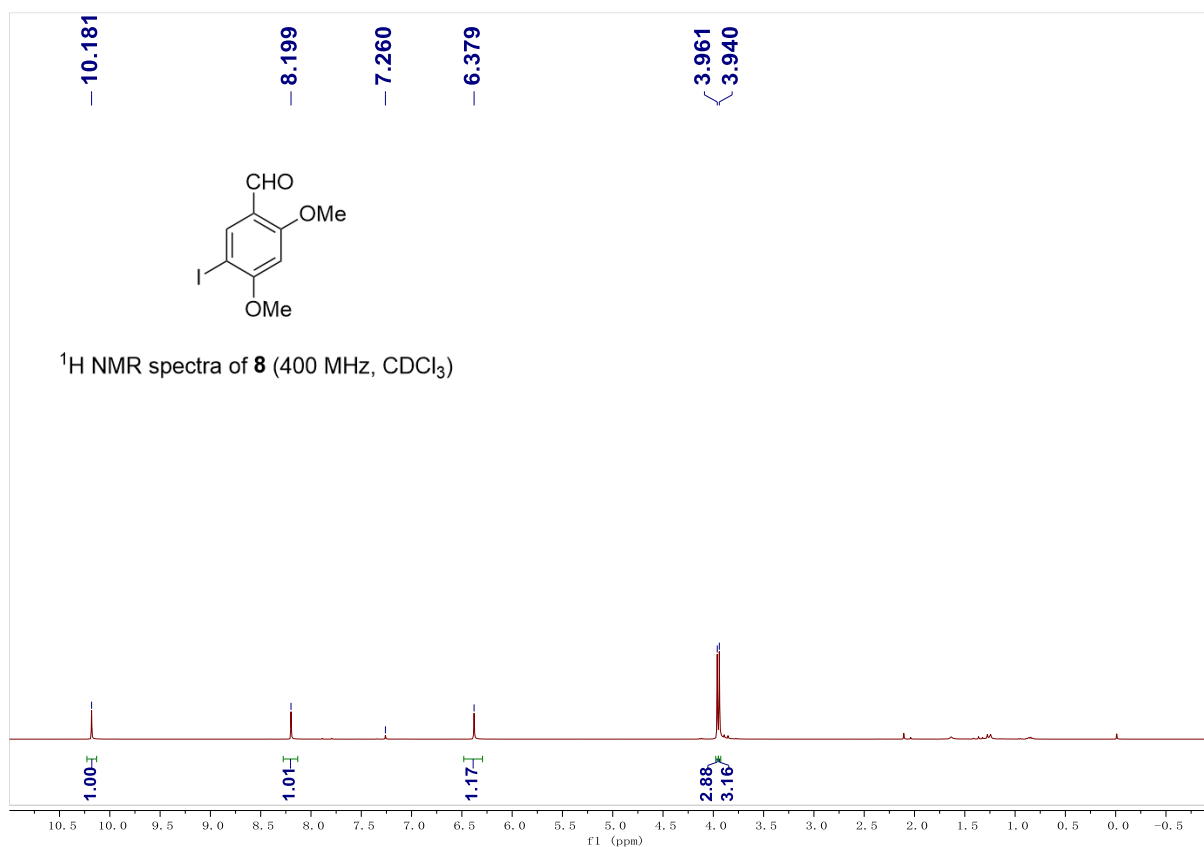
C: 8-8 H: 8-8 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

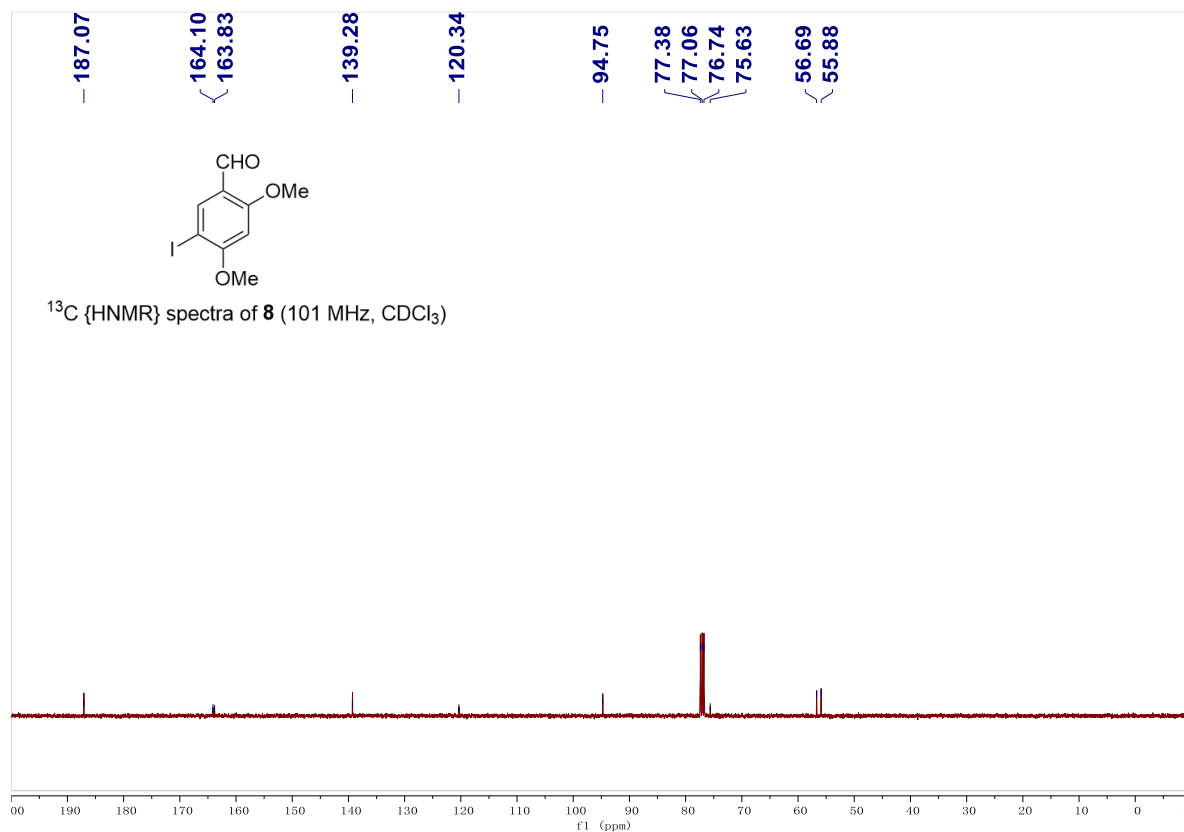
12
240405-1-7 10 (0.072)



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
262.9573	262.9569	0.4	1.5	4.5	71.3	n/a	n/a	C8 H8 O2 I





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

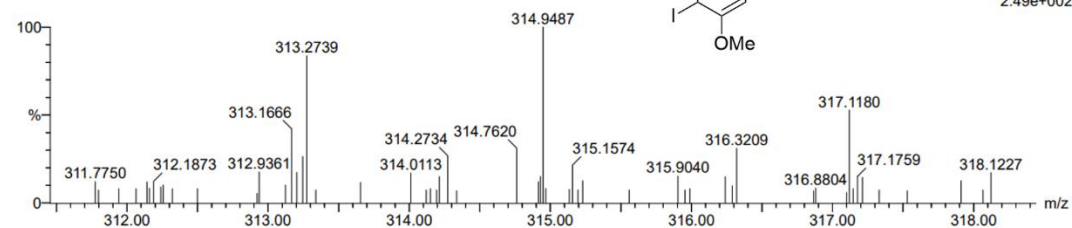
152 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 9-9 H: 9-9 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

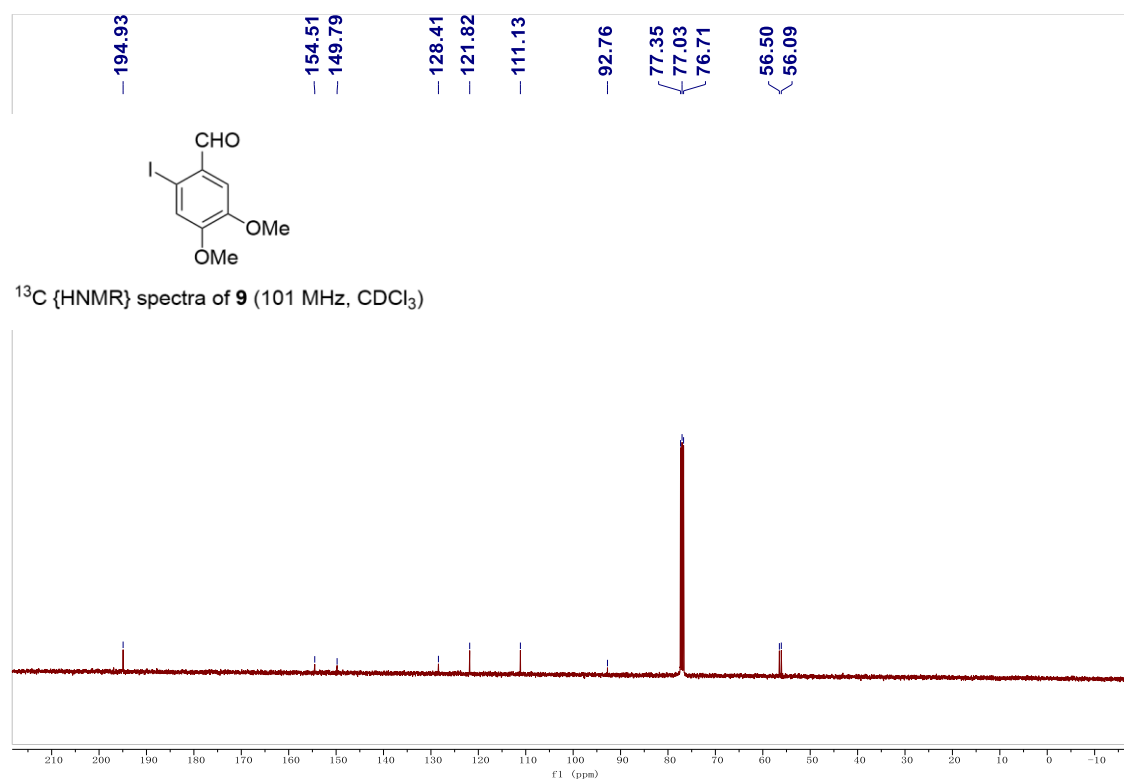
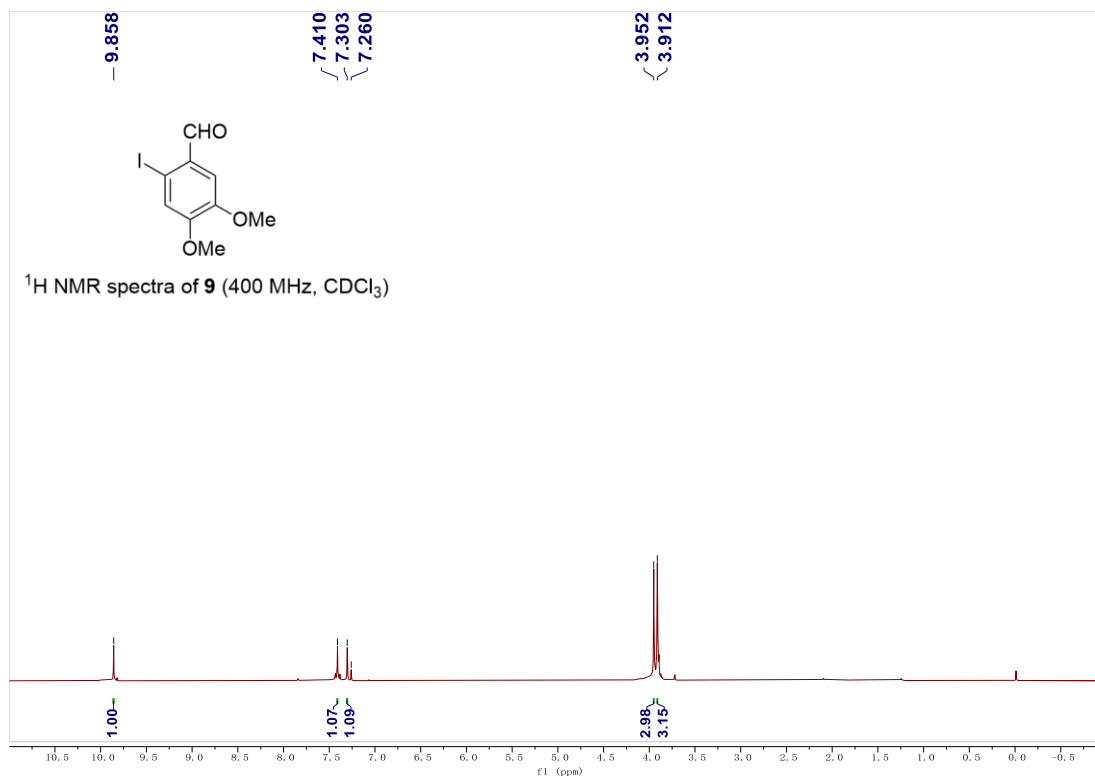
12

240405-1-8 13 (0.083)



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
314.9487	314.9494	-0.7	-2.2	4.5	136.2	n/a	n/a	C ₉ H ₉ O ₃ NaI



Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

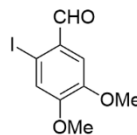
120 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

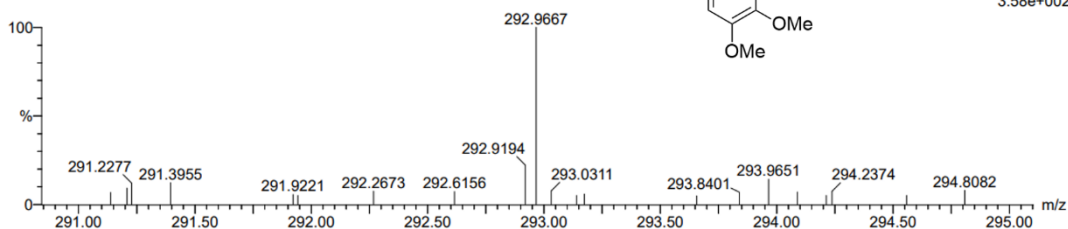
C: 9-9 H: 10-10 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

12

240405-1-9 12 (0.080)

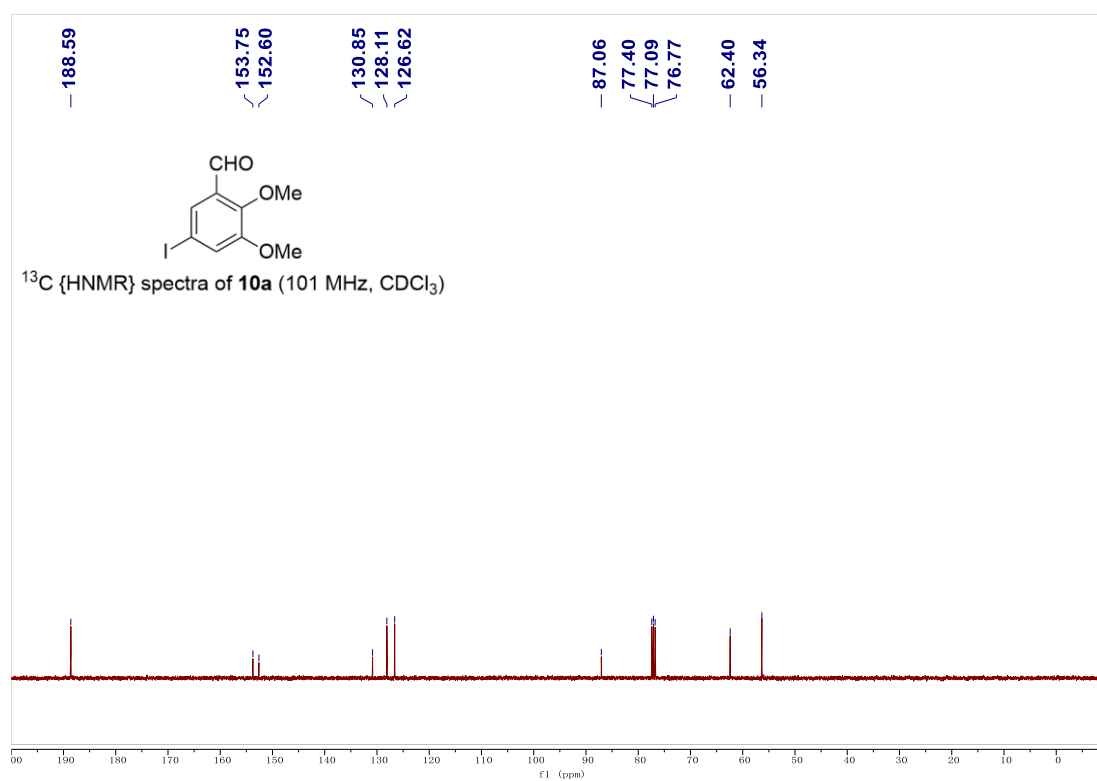
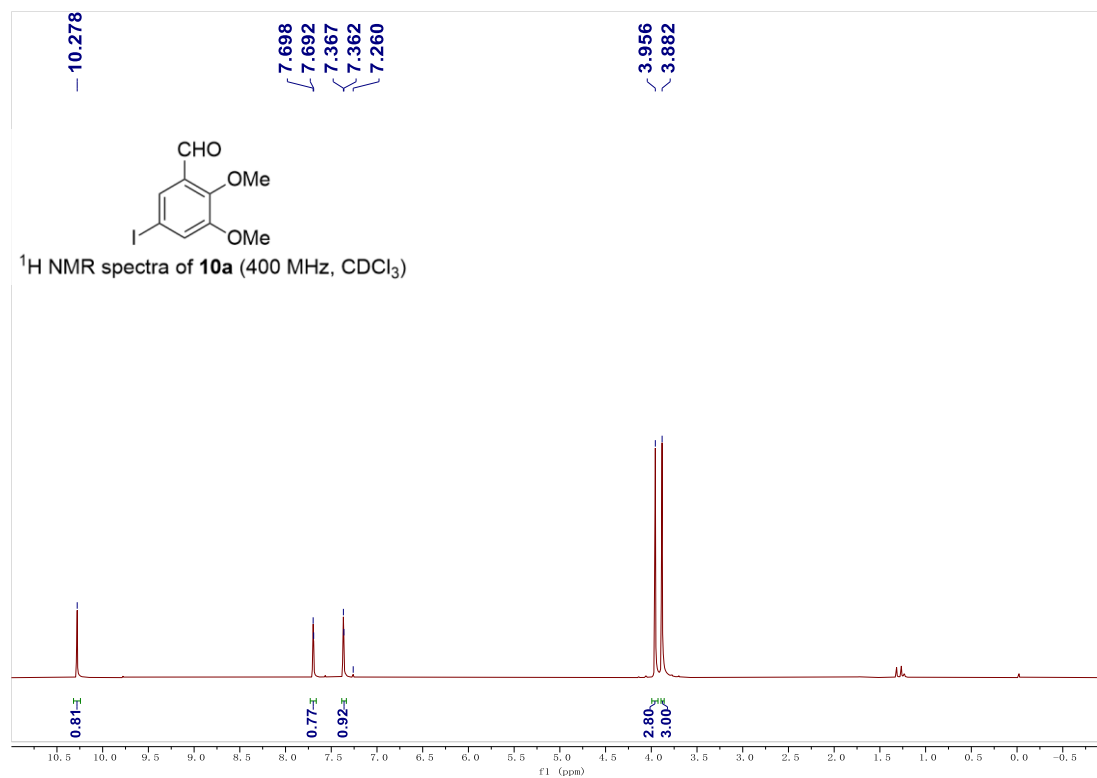


1: TOF MS ES+
3.58e+002



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
292.9667	292.9675	-0.8	-2.7	4.5	76.3	n/a	n/a	C9 H10 O3 I



Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

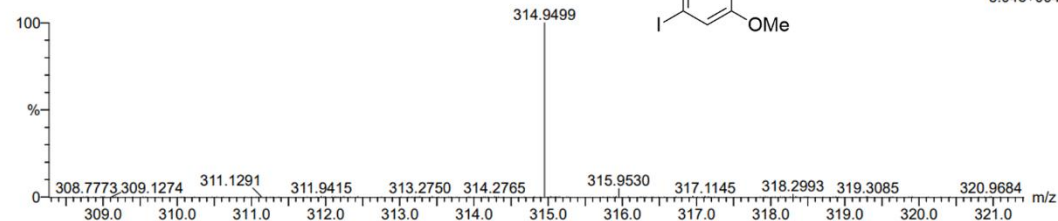
Monoisotopic Mass, Even Electron Ions

152 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

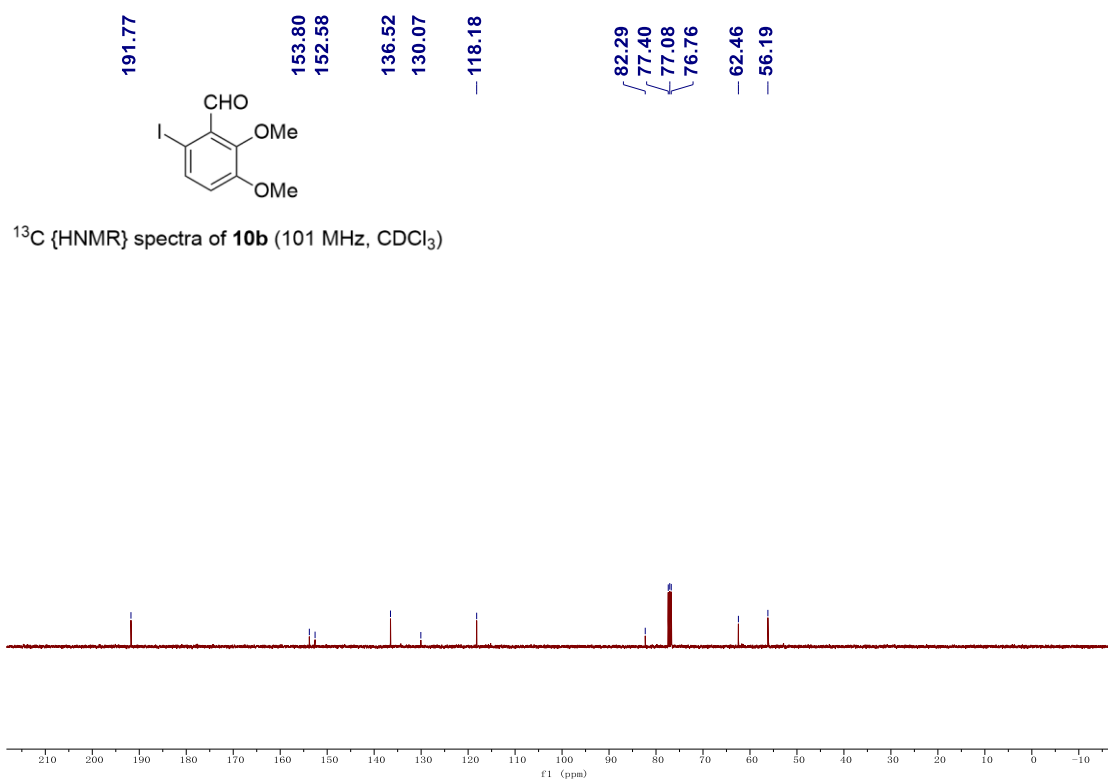
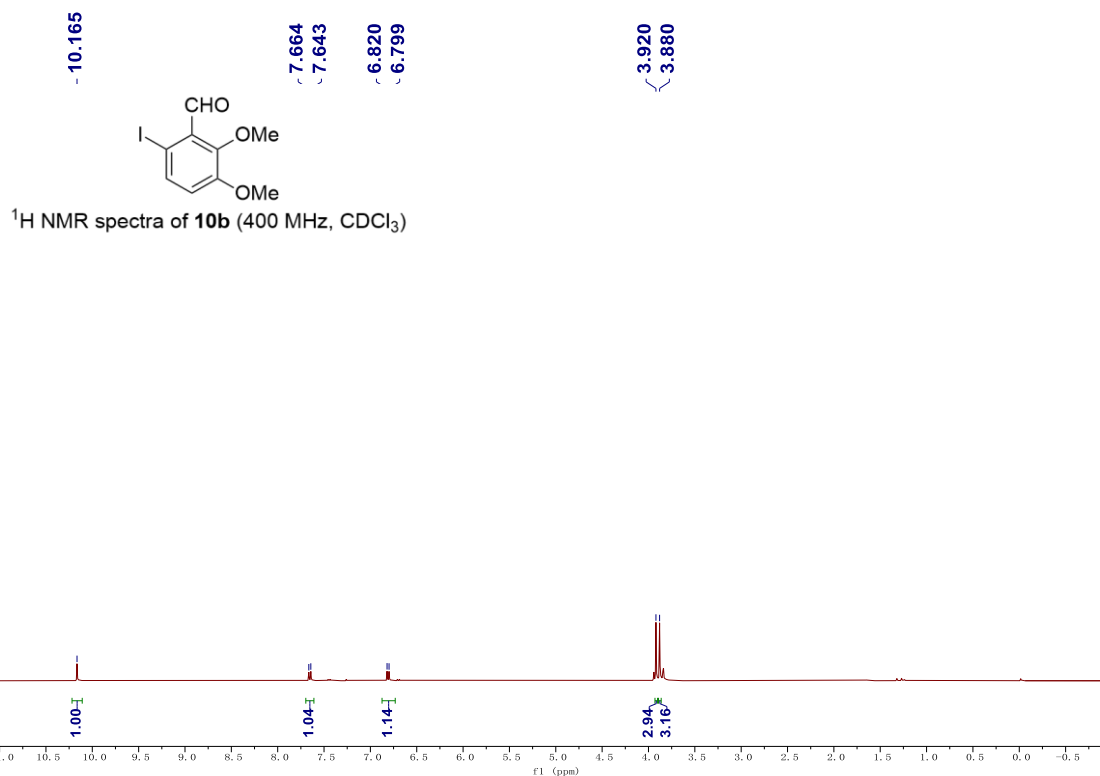
C: 9-9 H: 9-9 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

12
240405-1-10a 11 (0.076)



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
314.9499	314.9494	0.5	1.6	4.5	260.4	n/a	n/a	C9 H9 O3 Na I



Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

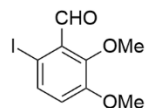
152 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

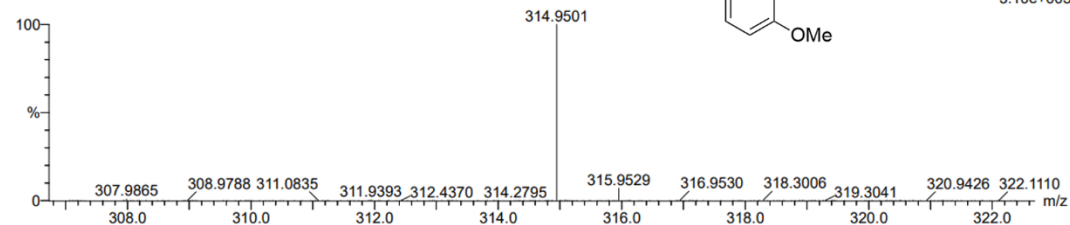
C: 9-9 H: 9-9 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

12

240405-1-11b 11 (0.076)

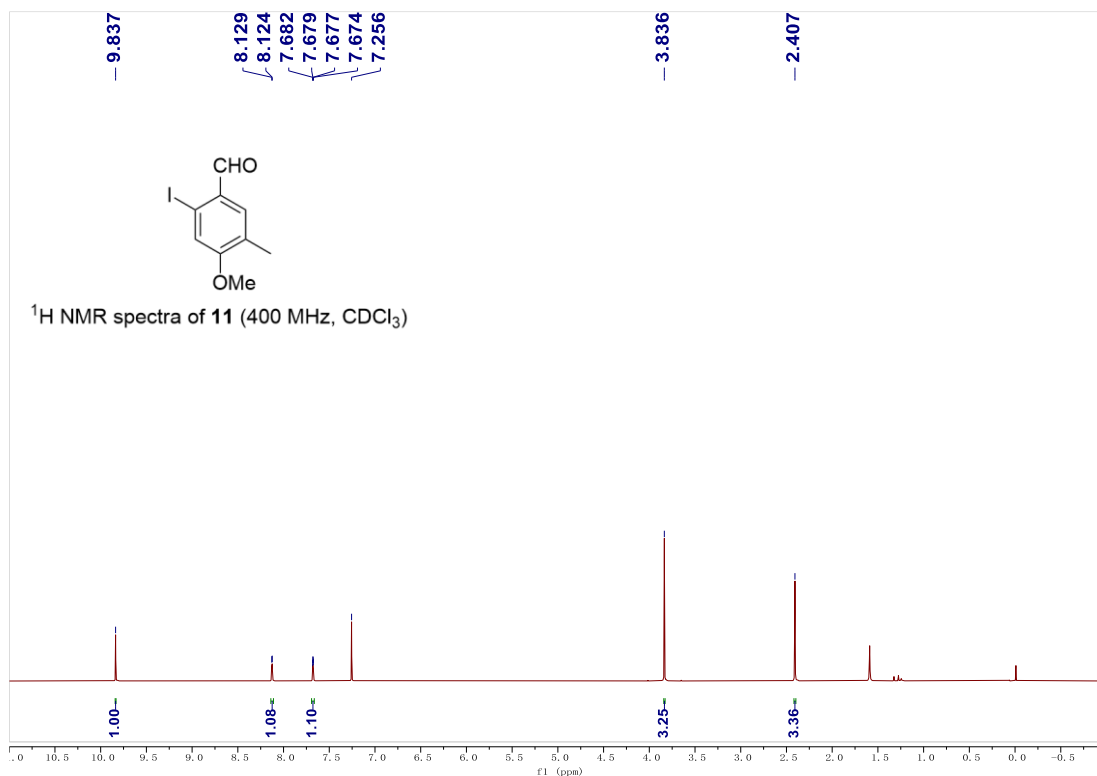


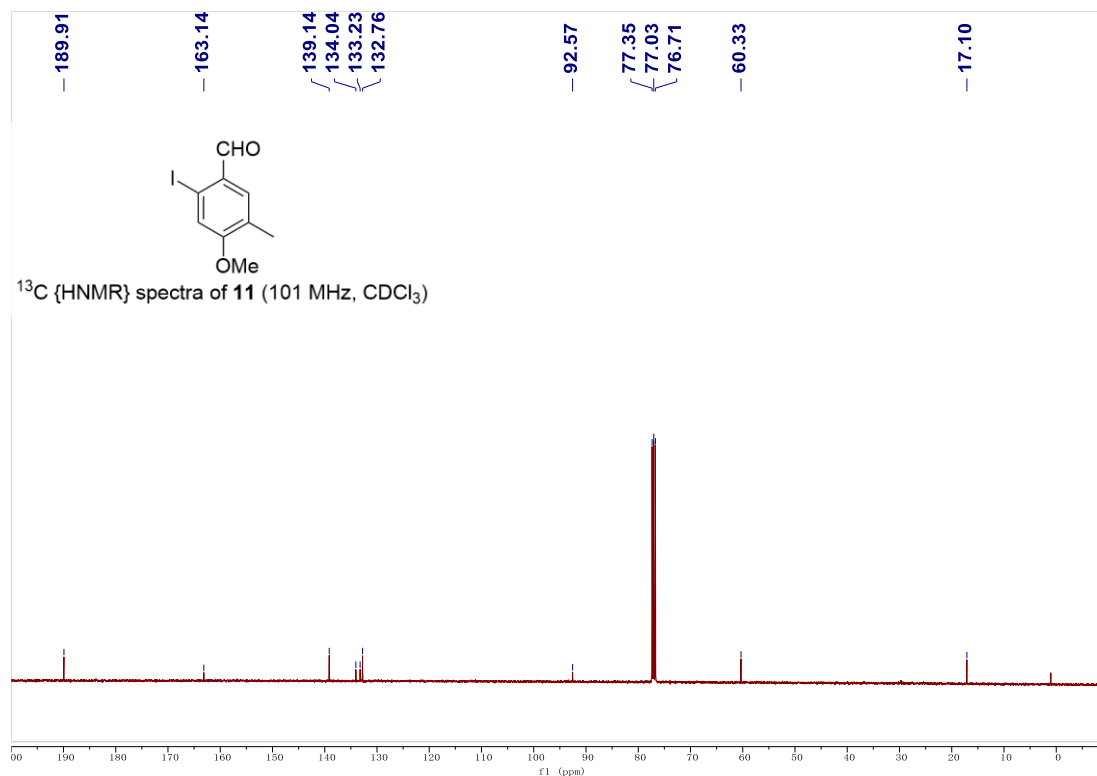
1: TOF MS ES+
3.10e+005



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
314.9501	314.9494	0.7	2.2	4.5	355.2	n/a	n/a	C9 H9 O3 Na I





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

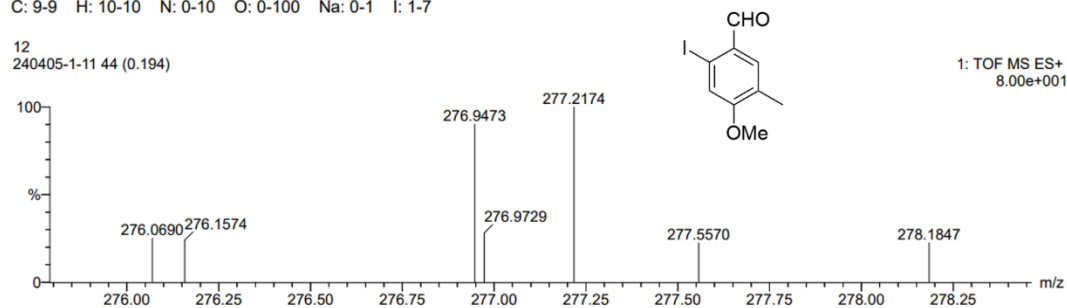
Monoisotopic Mass, Even Electron Ions

99 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

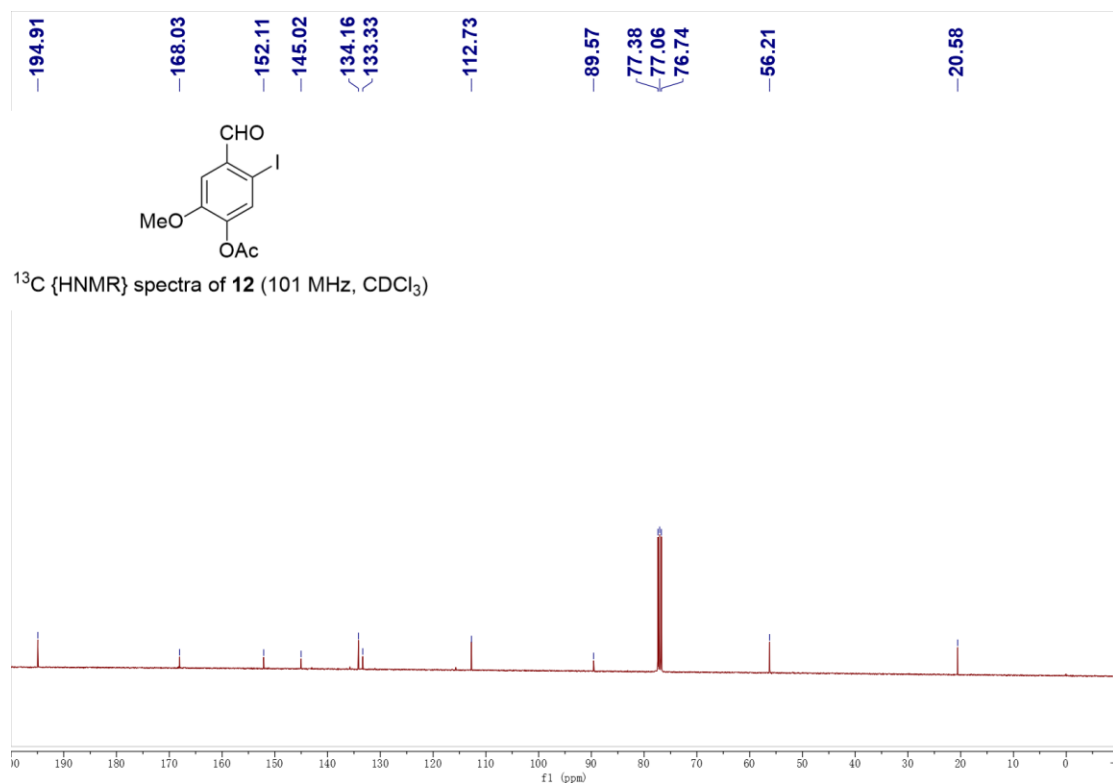
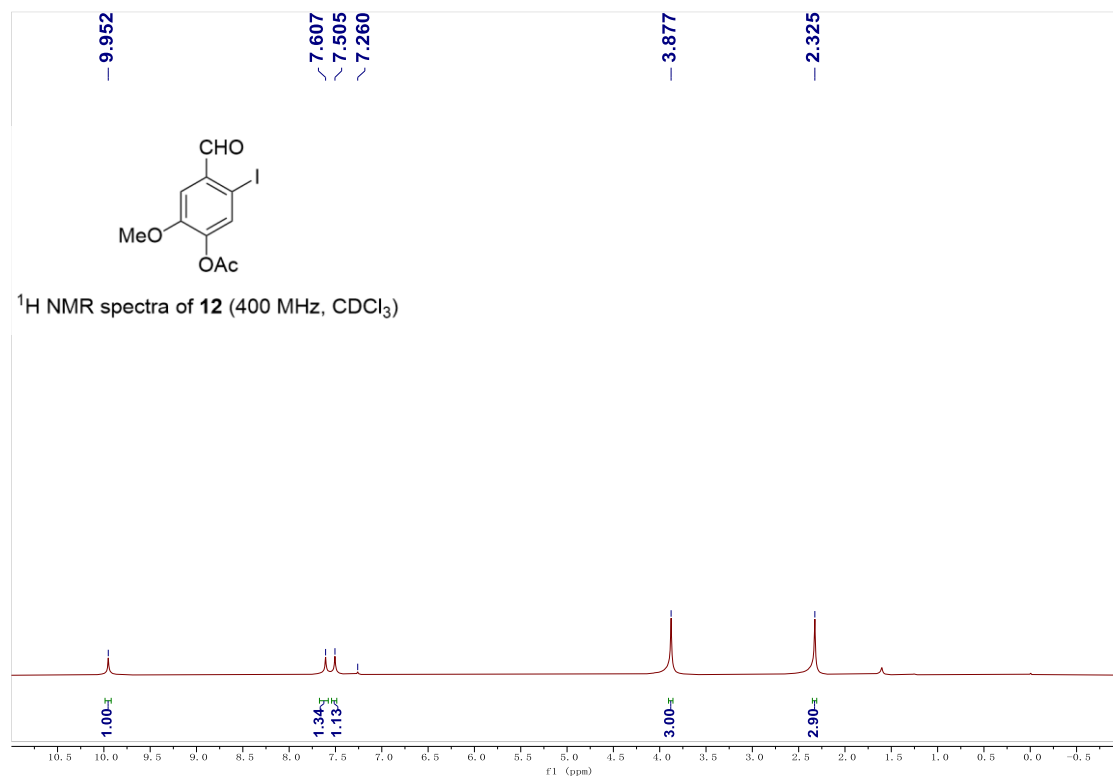
C: 9-9 H: 10-10 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

12
240405-1-11 44 (0.194)



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
276.9729	276.9725	0.4	1.4	4.5	31.4	n/a	n/a	C9 H10 O2 I



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

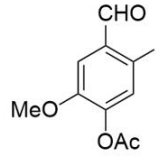
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

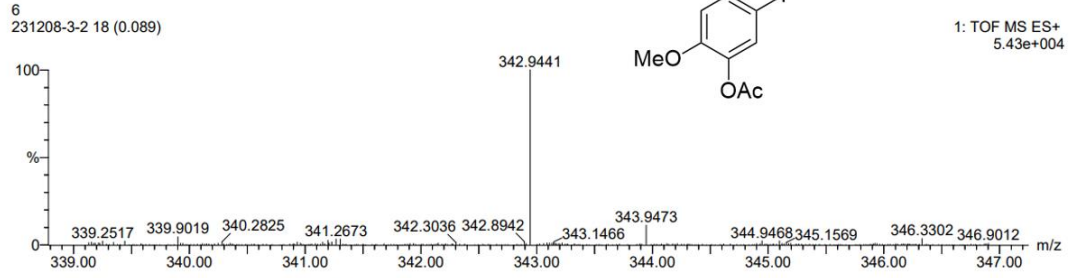
45 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 10-10 H: 9-9 O: 0-100 I: 1-2 Na: 0-2

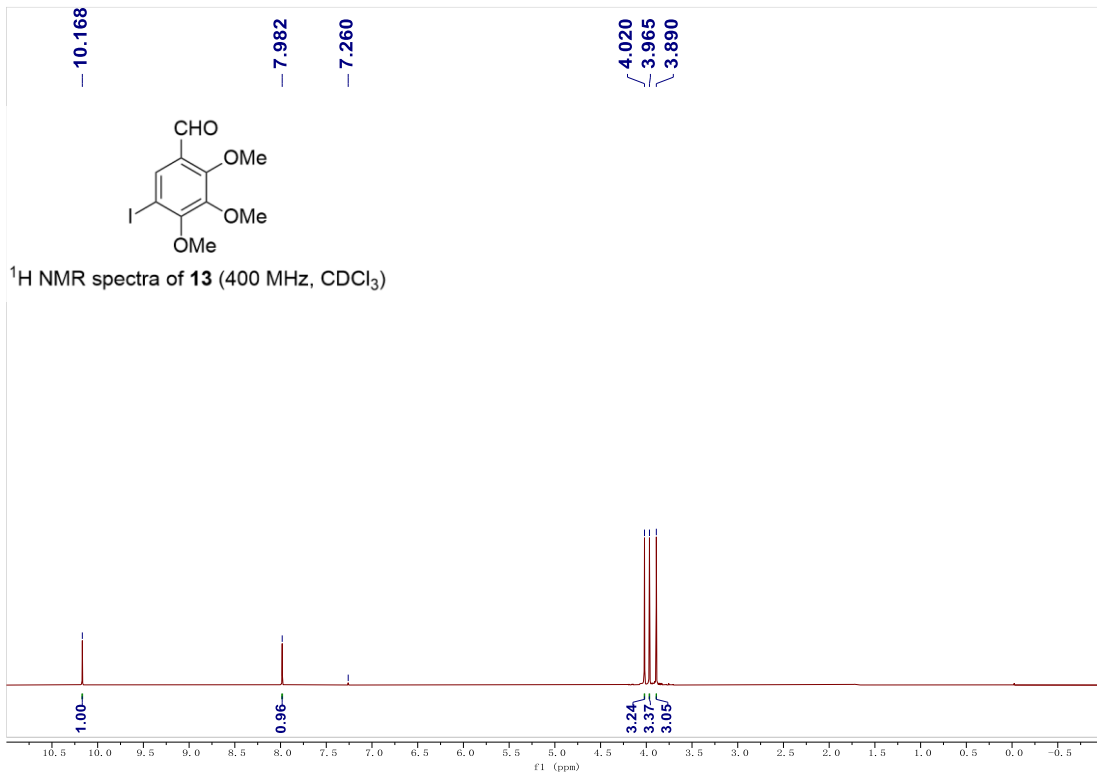


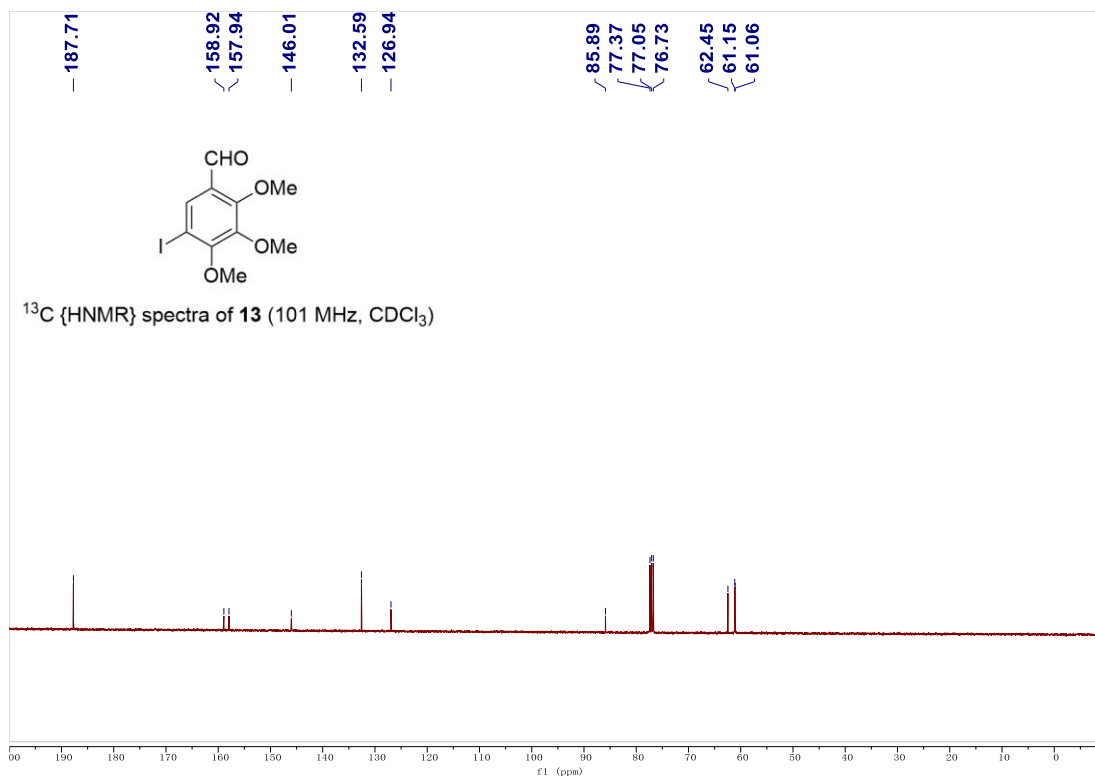
1: TOF MS ES+
5.43e+04



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
342.9441	342.9443	-0.2	-0.6	5.5	924.6	n/a	n/a	C10 H9 O4 I Na





Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

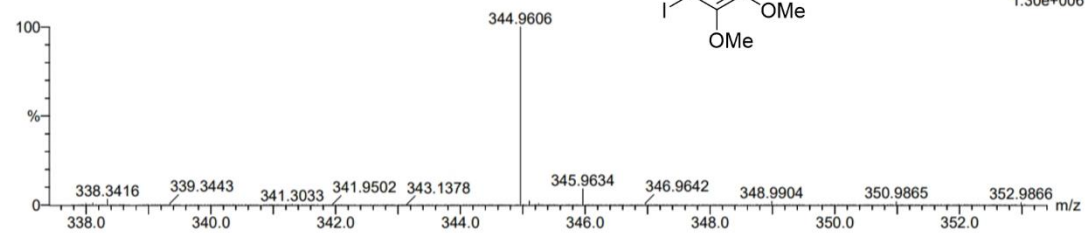
44 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 10-10 H: 11-11 O: 0-100 Na: 0-2 I: 1-2

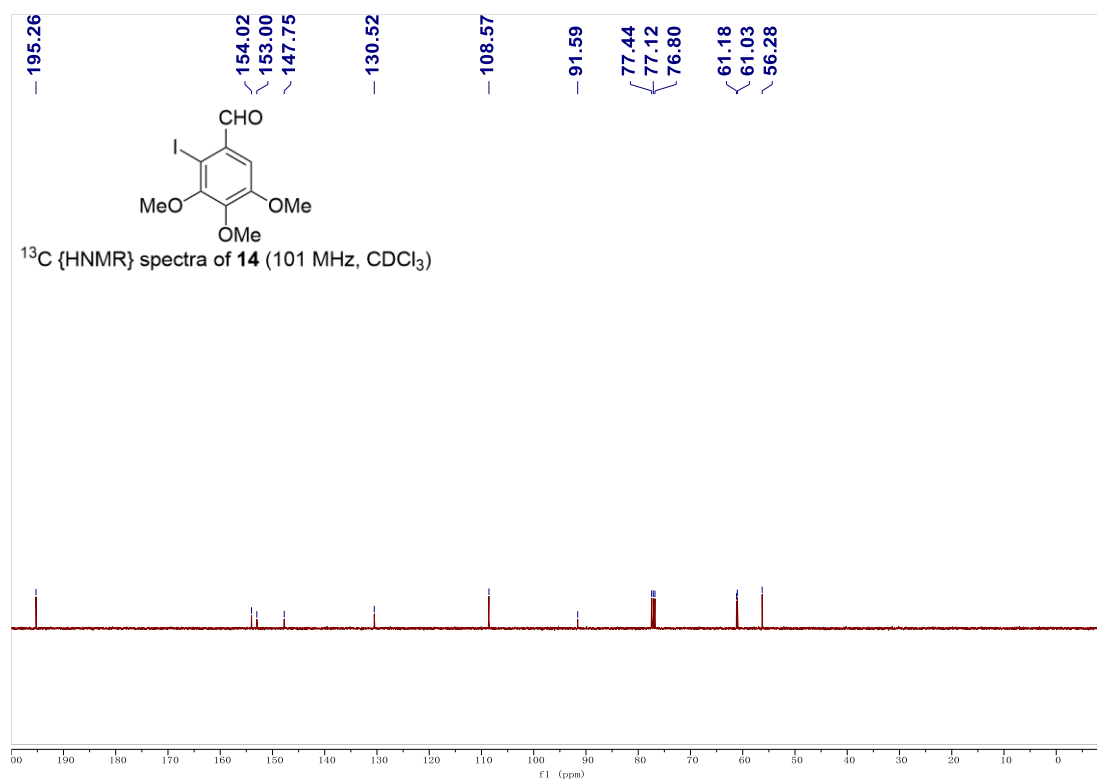
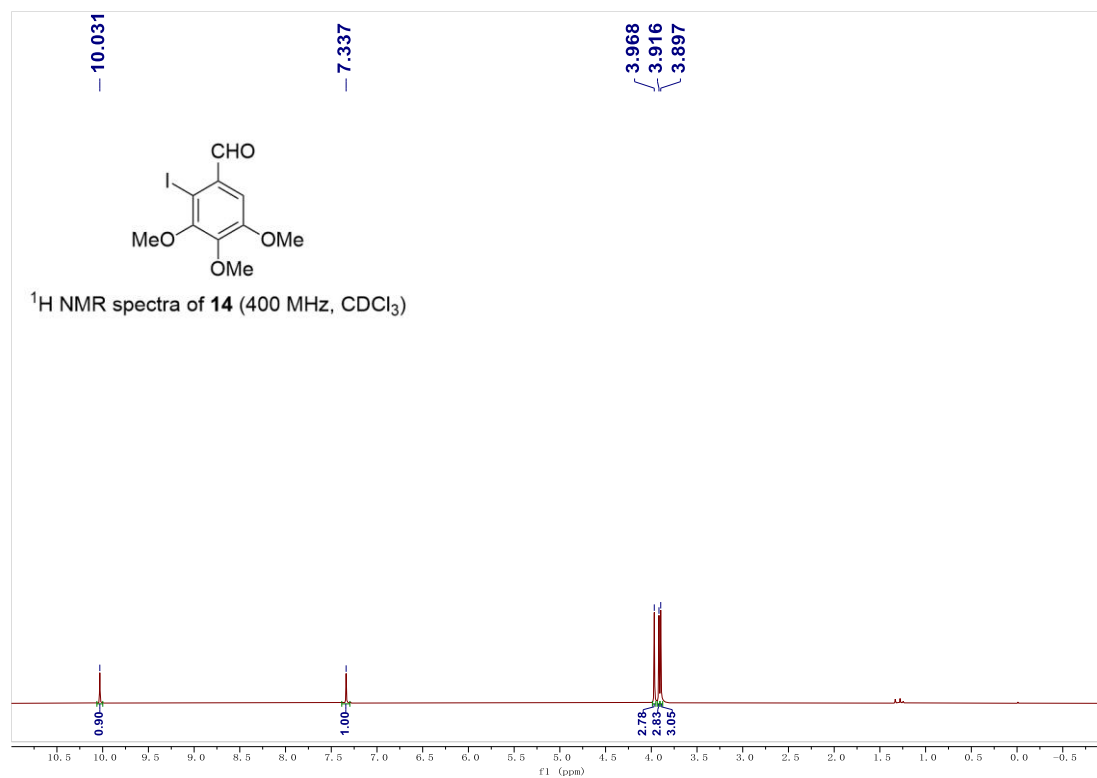
6

231208-3-3 21 (0.100)



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
344.9606	344.9600	0.6	1.7	4.5	1027.9	n/a	n/a	C10 H11 O4 Na I



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

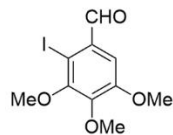
205 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

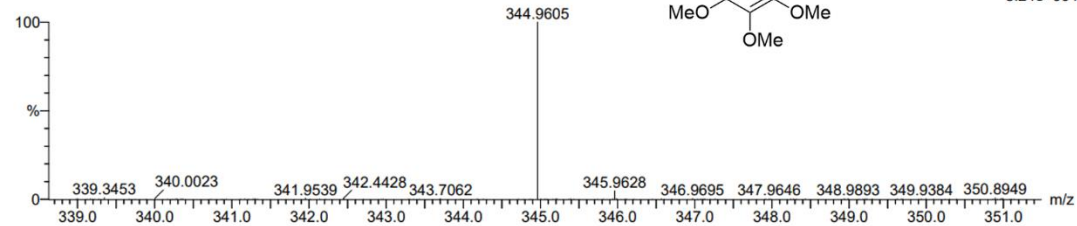
C: 10-10 H: 11-11 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

12

240405-1-14 15 (0.090)

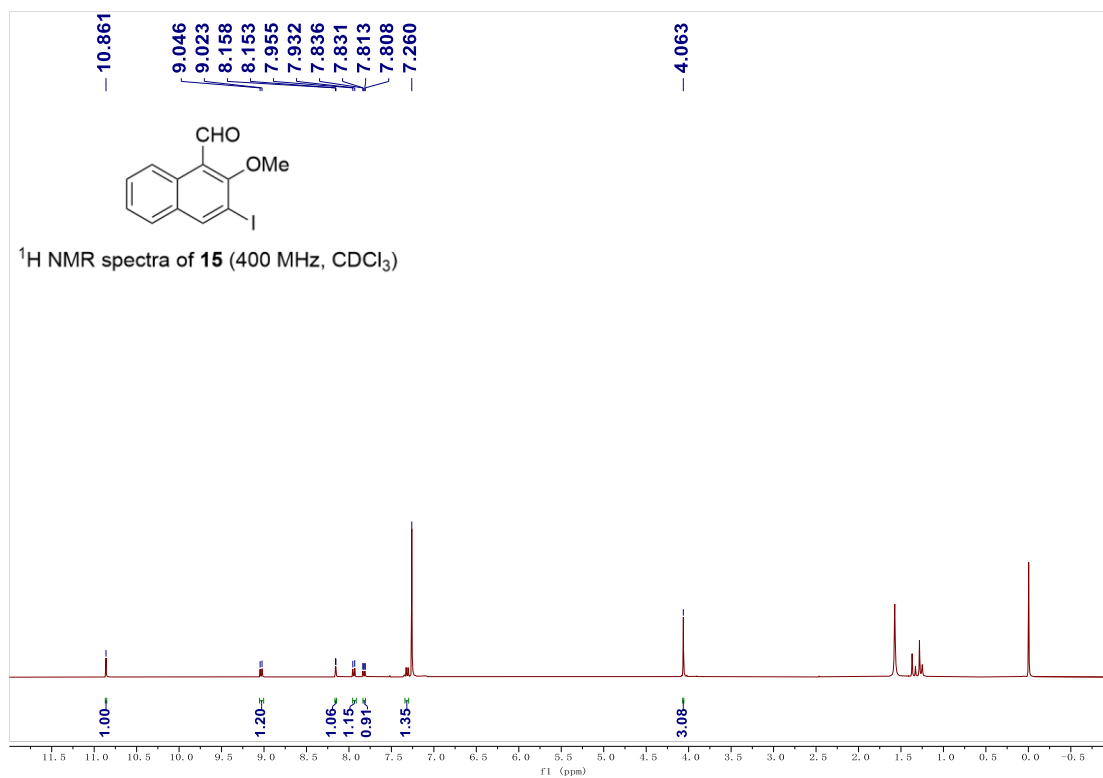


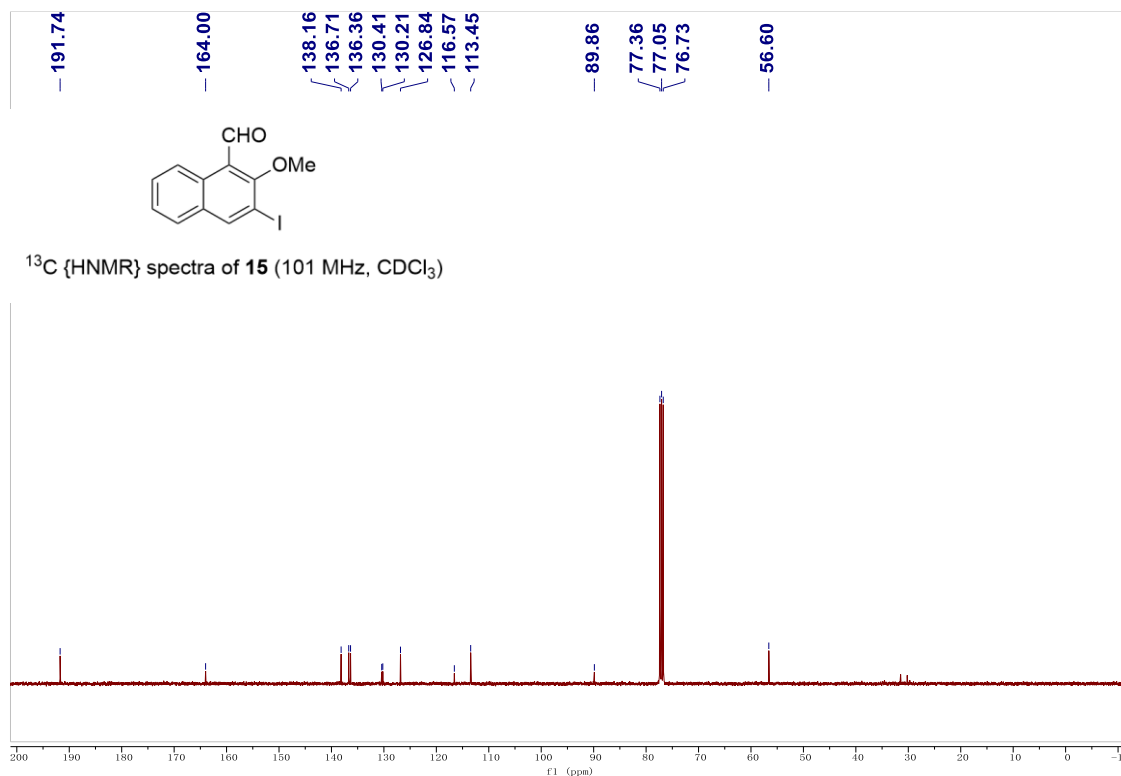
1: TOF MS ES+
5.24e+004



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
344.9605	344.9600	0.5	1.4	4.5	223.2	n/a	n/a	C10 H11 O4 Na I





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

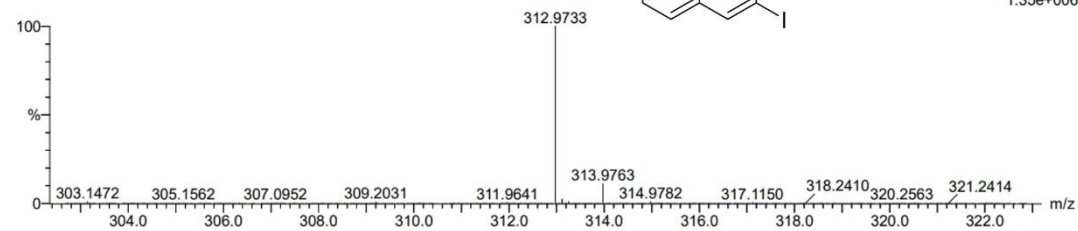
35 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 12-12 H: 10-10 O: 0-100 Na: 0-2 I: 1-2

6

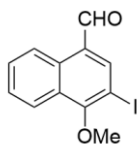
231208-3-4 16 (0.082)



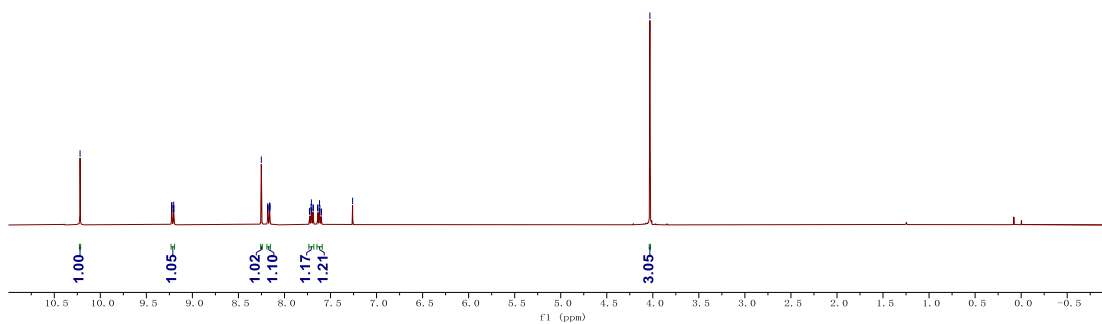
Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
312.9733	312.9725	0.8	2.6	7.5	1149.6	n/a	n/a	C12 H10 O2 I

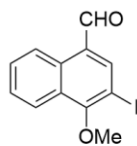
10.220
9.227
9.225
9.224
9.222
9.206
9.203
9.201
8.252
8.184
8.182
8.180
8.178
8.163
8.161
8.159
8.158
7.729
7.725
7.711
7.708
7.704
7.690
7.686
7.640
7.637
7.623
7.619
7.616
7.602
7.599
7.260
4.032



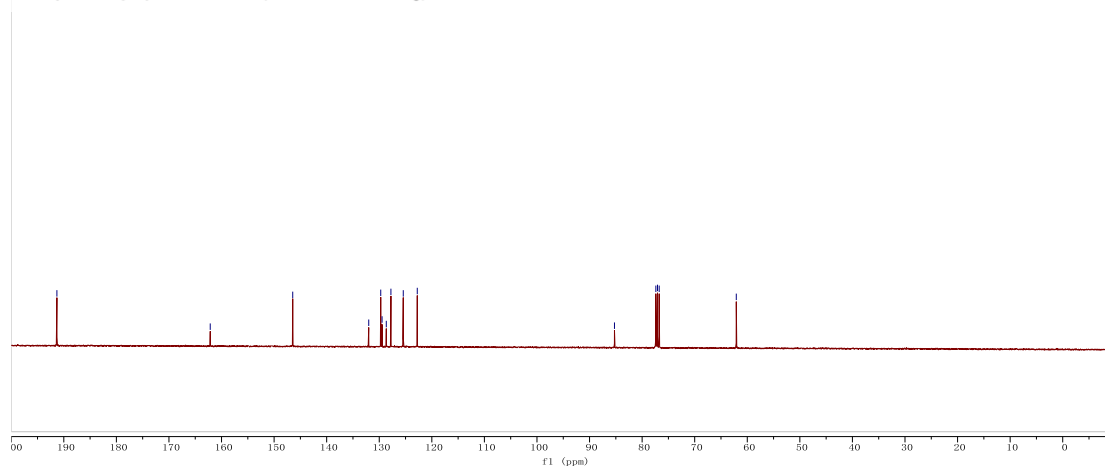
¹H NMR spectra of **16** (400 MHz, CDCl₃)



191.31
162.15
146.46
132.00
129.72
129.46
128.66
127.78
125.43
122.77
85.26
77.39
77.07
76.75
62.09



¹³C {HNMR} spectra of **16** (101 MHz, CDCl₃)



Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

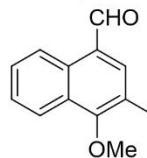
35 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

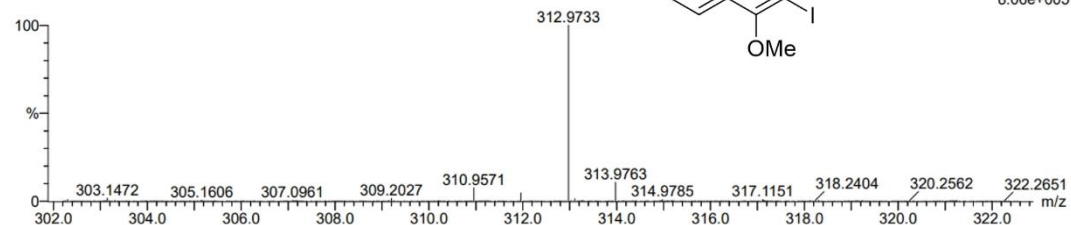
C: 12-12 H: 10-10 O: 0-100 Na: 0-2 I: 1-2

6

231208-3-5 16 (0.083)

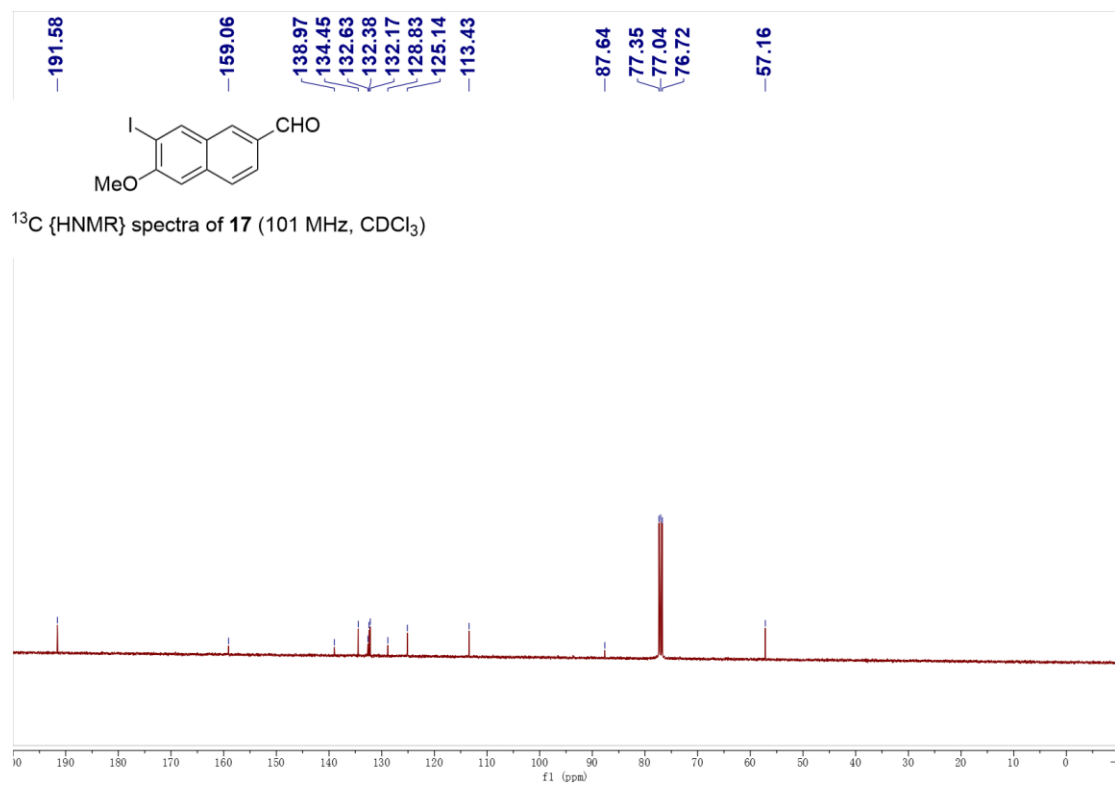
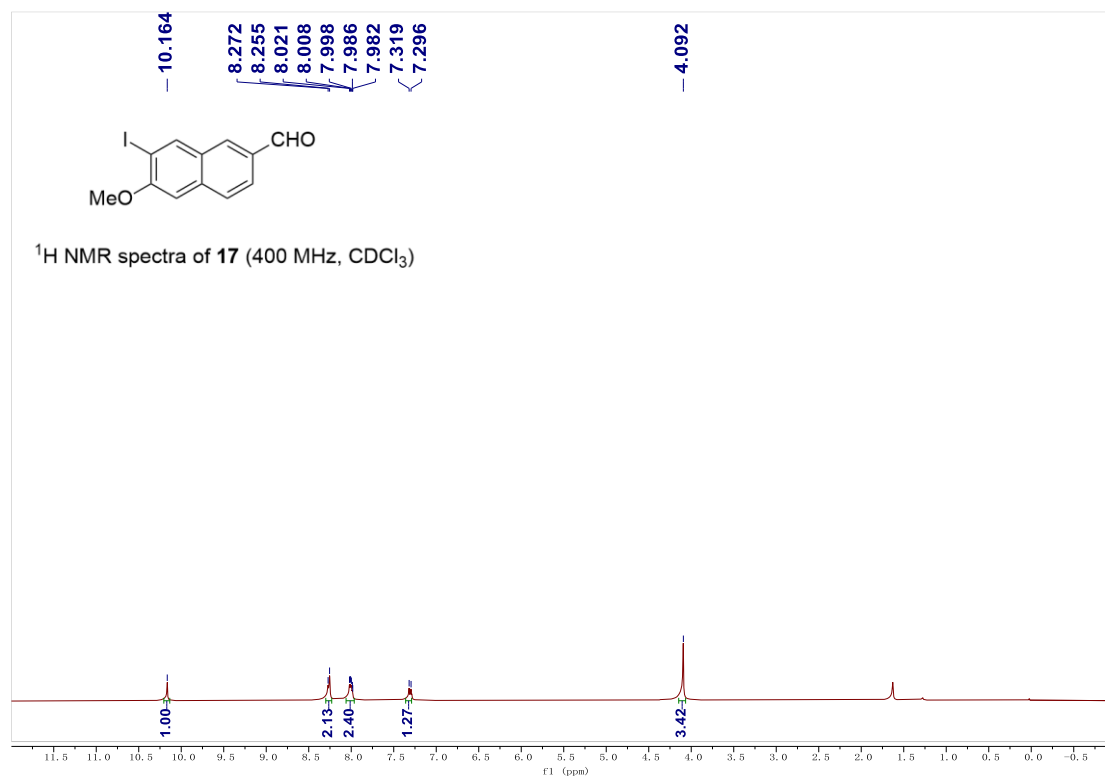


1: TOF MS ES+
8.06e+005



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
312.9733	312.9725	0.8	2.6	7.5	1081.4	n/a	n/a	C12 H10 O2 I



Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

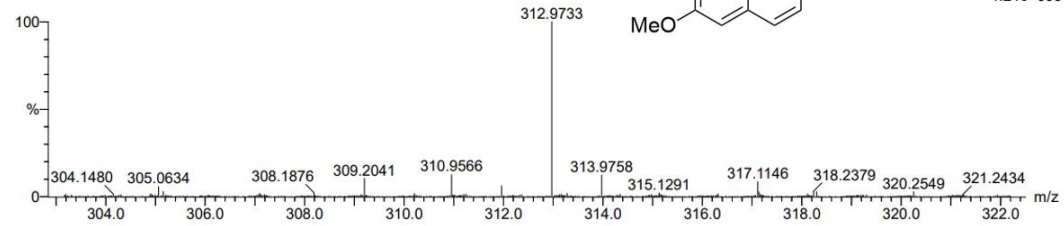
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

35 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

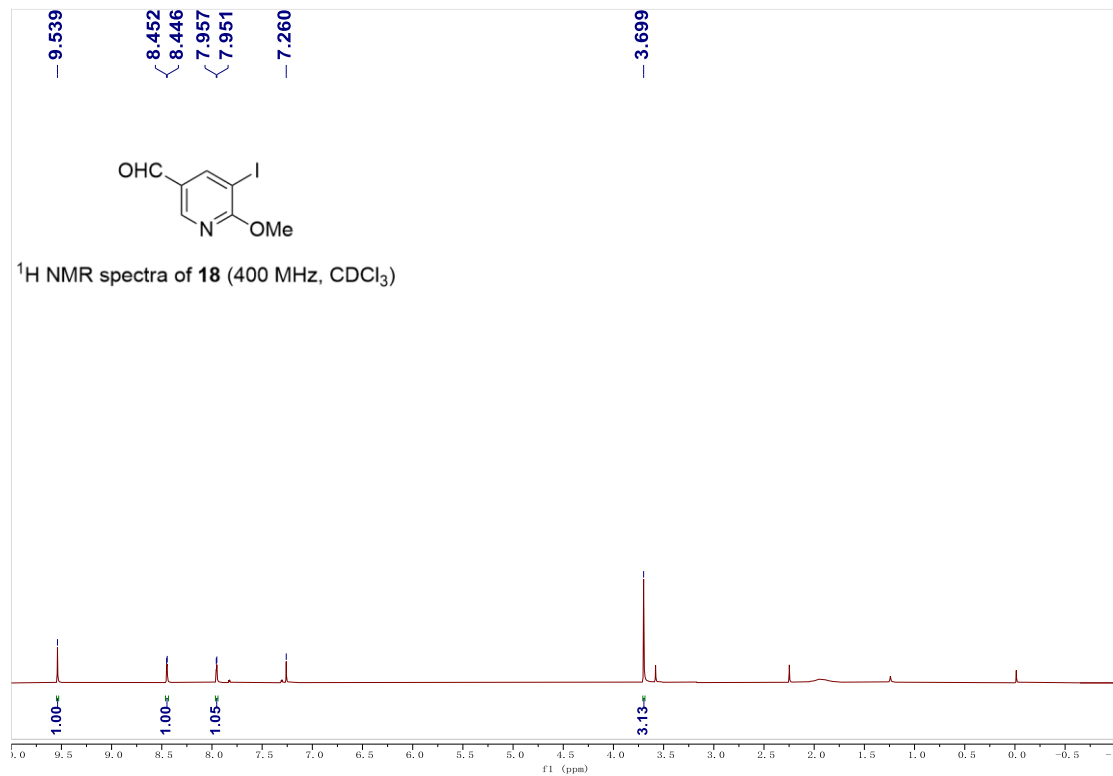
Elements Used:

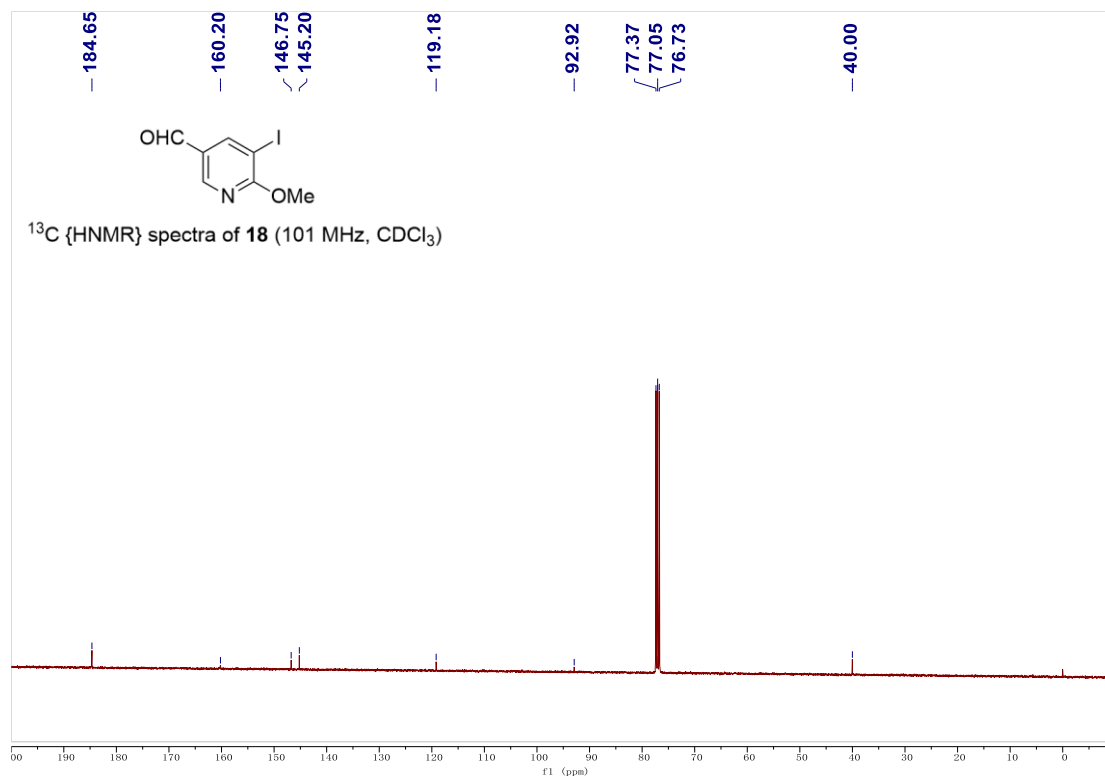
C: 12-12 H: 10-10 O: 0-100 Na: 0-2 I: 1-2

6
231208-3-6 16 (0.082)

Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
312.9733	312.9725	0.8	2.6	7.5	1010.7	n/a	n/a	C12 H10 O2 I





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

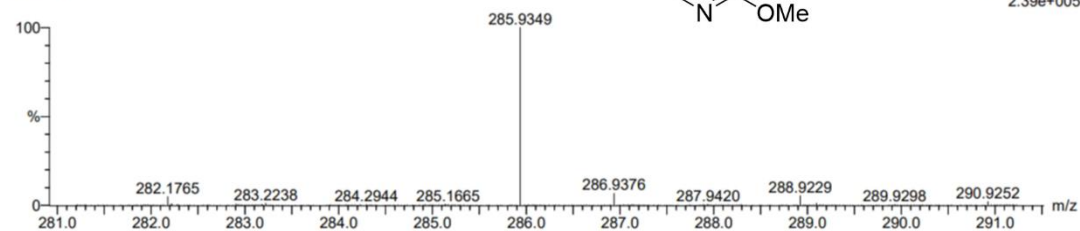
138 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 7-7 H: 6-6 N: 0-200 O: 0-100 Na: 0-2 I: 1-2

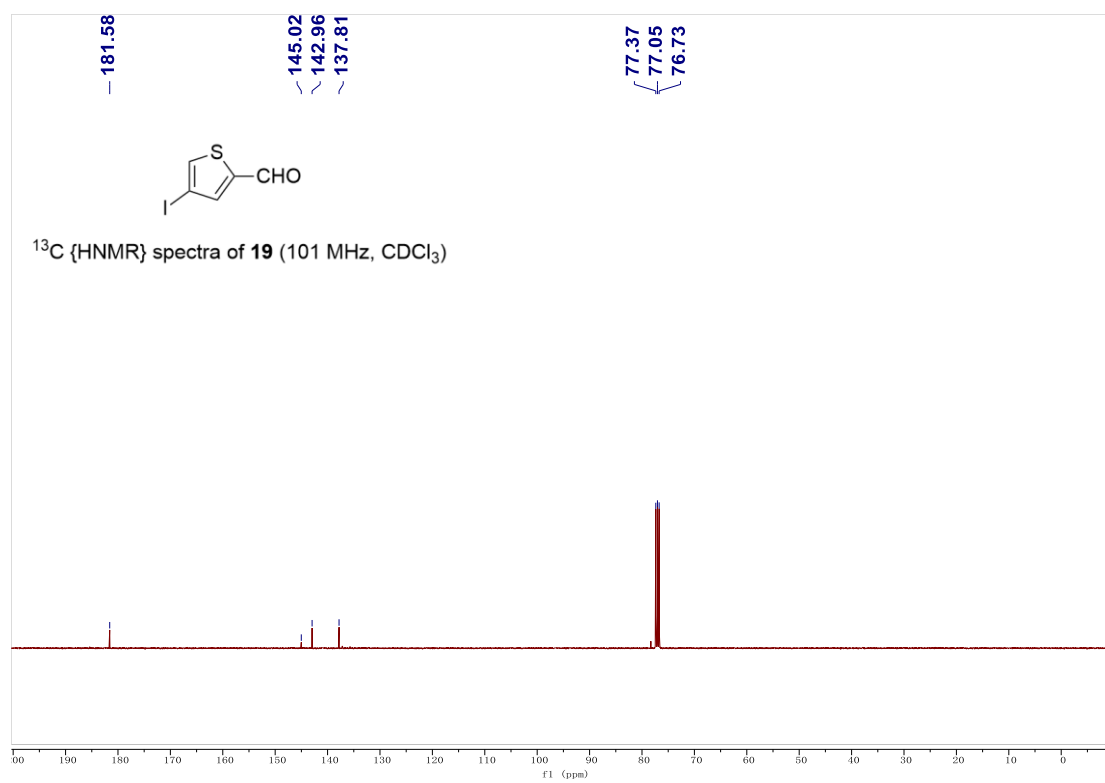
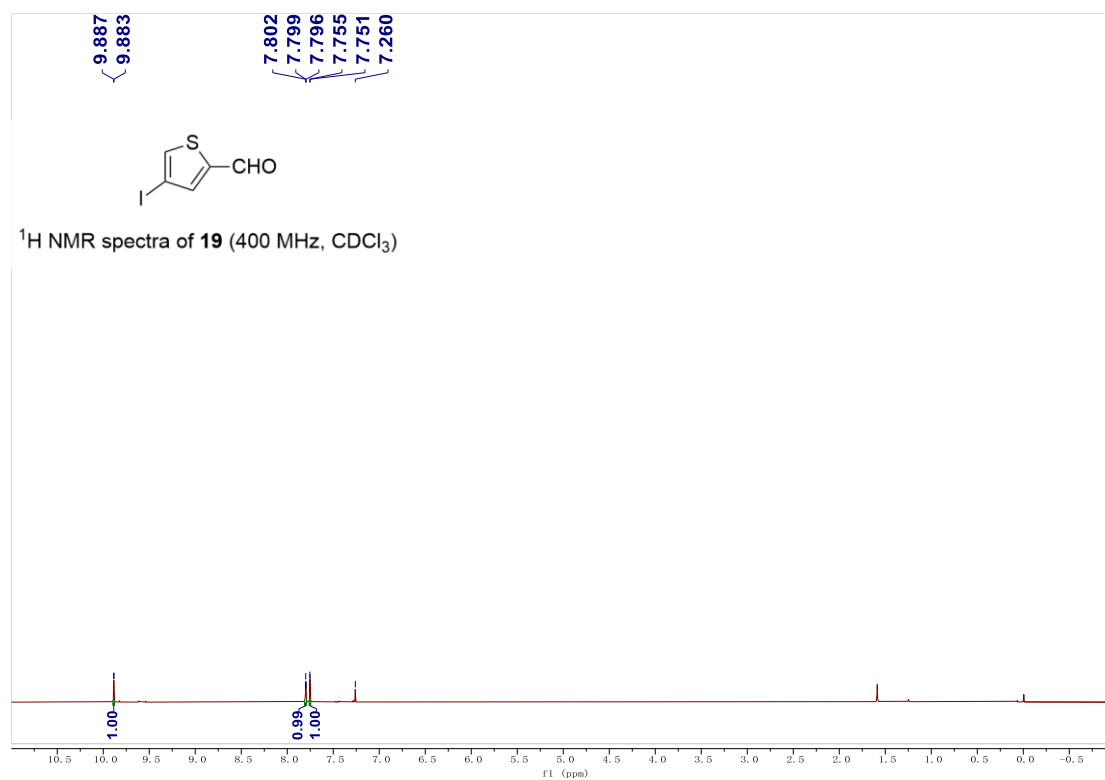
6

231208-3-7 21 (0.100)



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
285.9349	285.9341	0.8	2.8	4.5	954.3	n/a	n/a	C7 H6 N O2 Na I



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

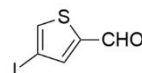
Monoisotopic Mass, Even Electron Ions

92 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

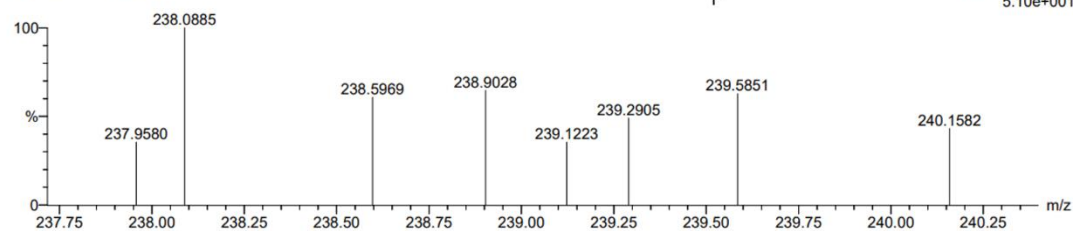
Elements Used:

C: 5-5 H: 4-4 N: 0-10 O: 0-100 Na: 0-1 S: 0-2 I: 1-7

12
240405-1-19 20 (0.108)

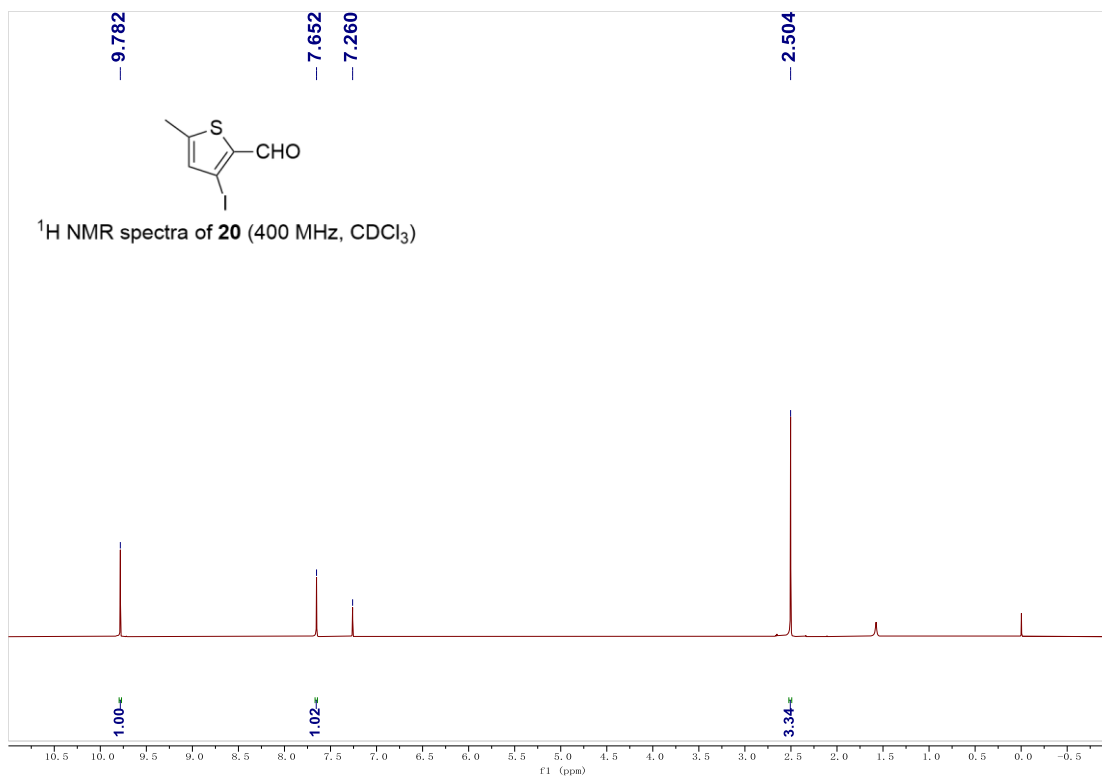


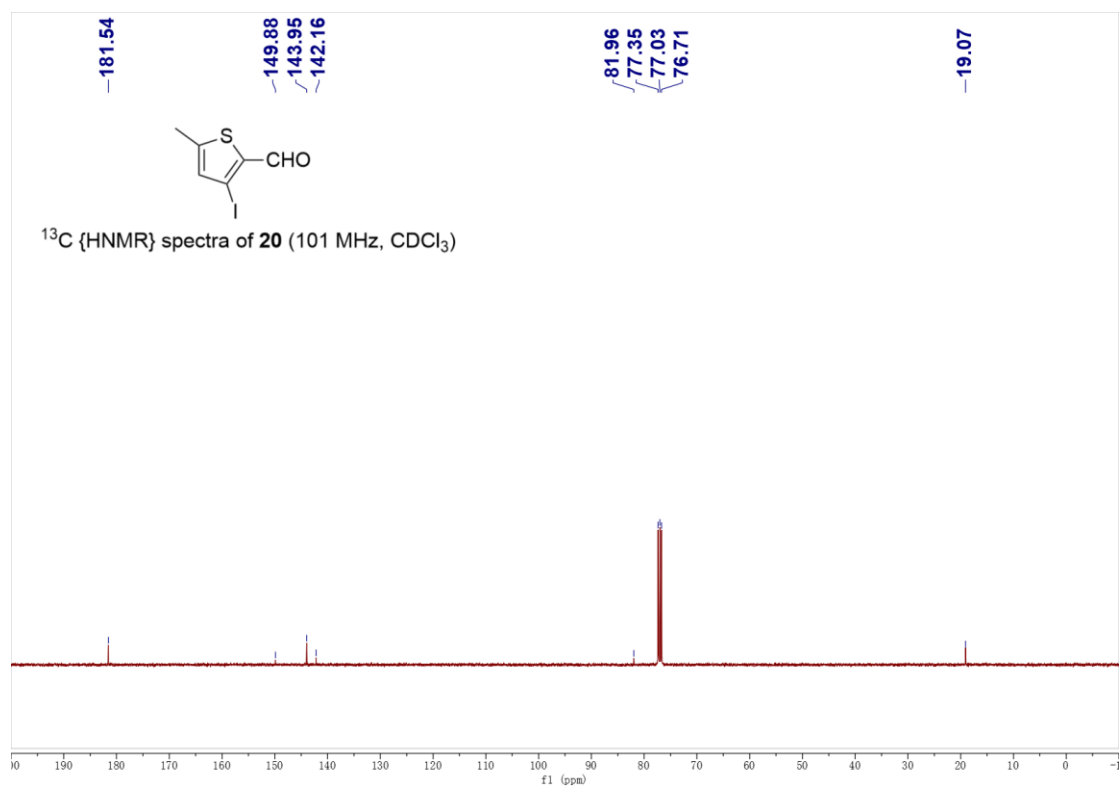
1: TOF MS ES+
5.10e+001



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
238.9028	238.9028	0.0	0.0	3.5	36.0	n/a	n/a	C5 H4 O S I





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

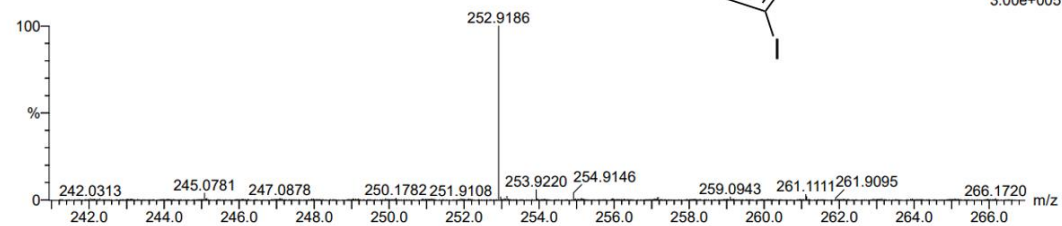
72 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 6-6 H: 6-6 N: 0-200 O: 0-100 Na: 0-2 S: 1-2 I: 1-2

6

231208-3-8 16 (0.082)

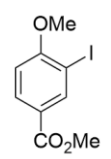


Minimum: -1.5
Maximum: 5.0 10.0 50.0

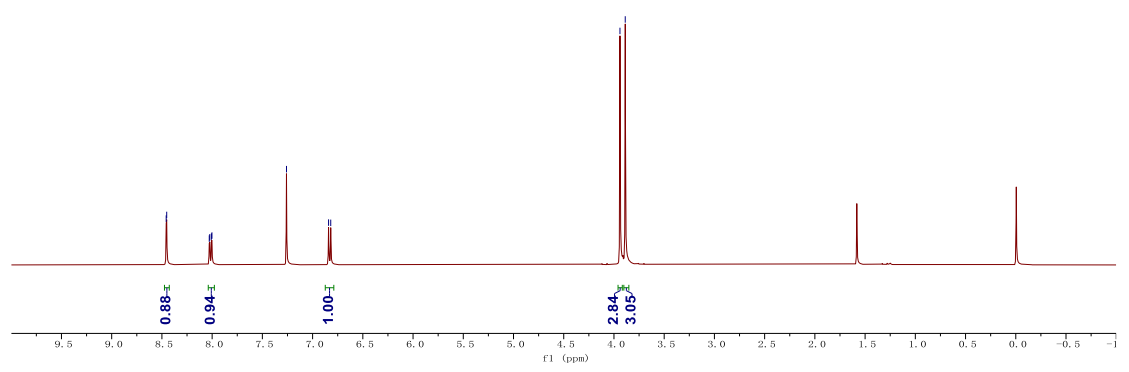
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
252.9186	252.9184	0.2	0.8	3.5	949.5	n/a	n/a	C6 H6 O S I

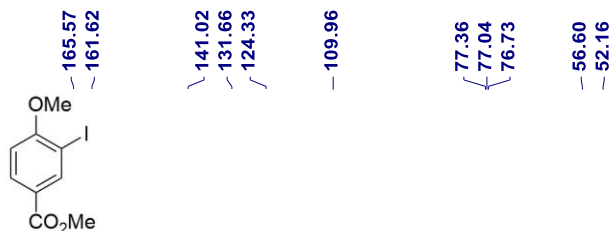
8.457
8.452
8.029
8.023
8.007
8.002
7.260
6.841
6.819

3.940
3.888

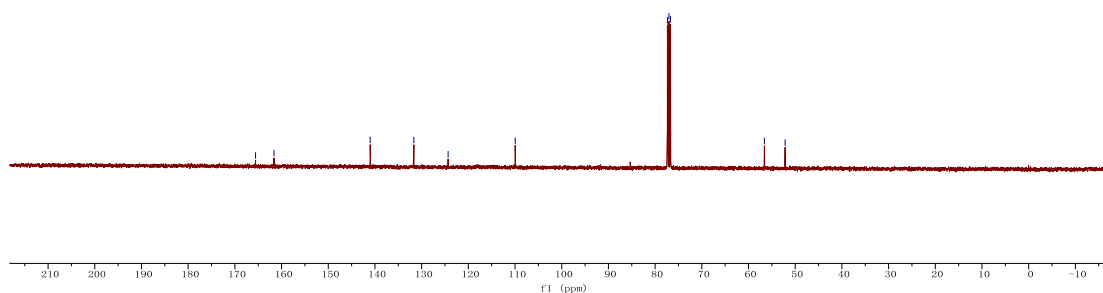


¹H NMR spectra of 21 (400 MHz, CDCl₃)





¹³C {HNMR} spectra of **21** (101 MHz, CDCl₃)



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

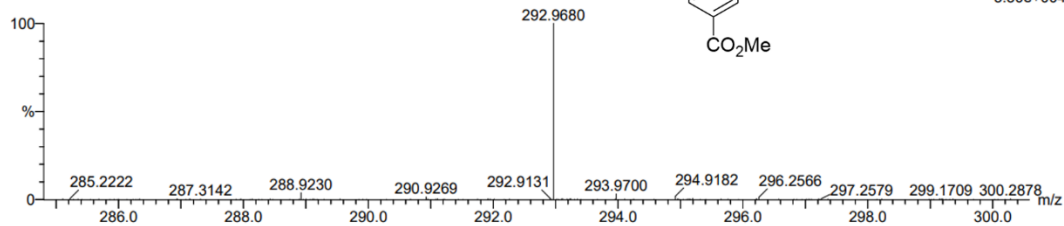
Monoisotopic Mass, Even Electron Ions

120 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 9-9 H: 10-10 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

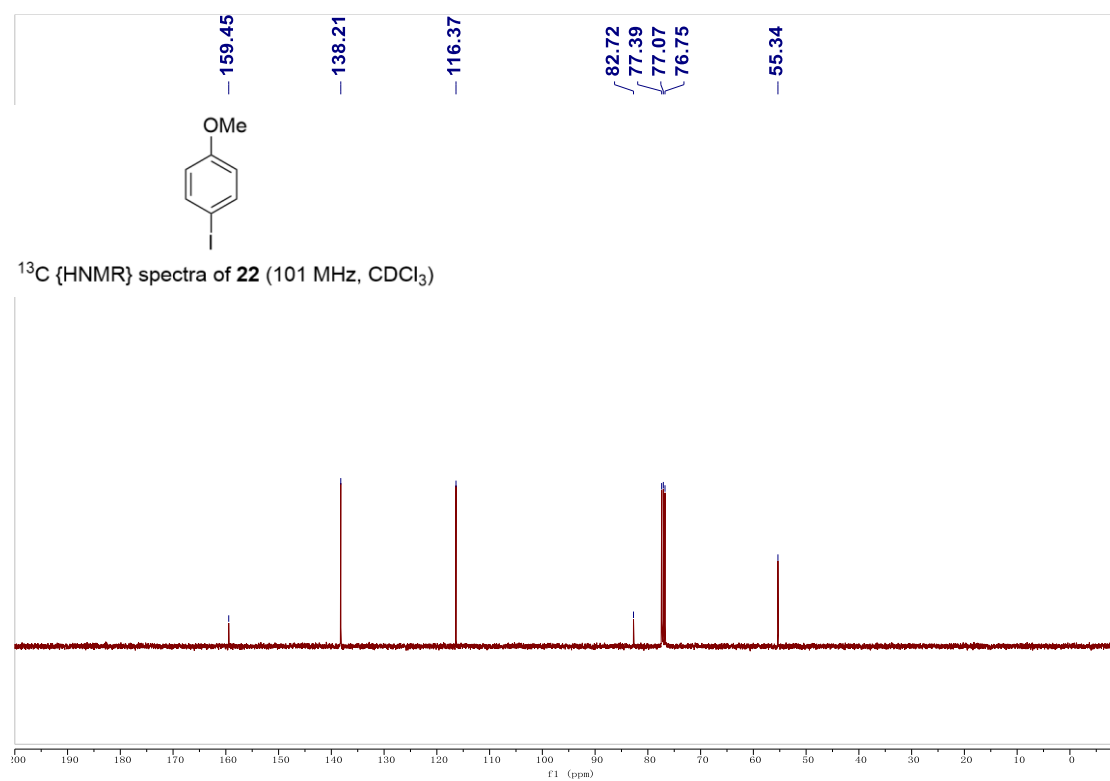
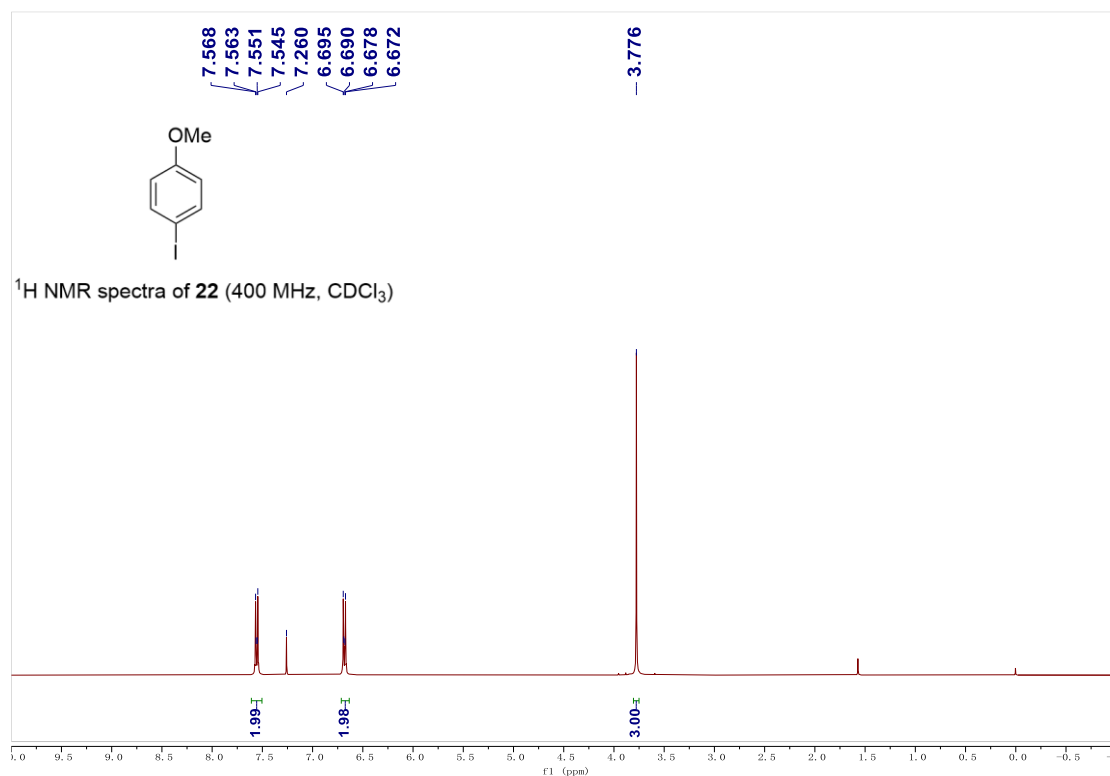
12
240405-1-21 11 (0.076)



1: TOF MS ES+
3.50e+004

Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
292.9680	292.9675	0.5	1.7	4.5	220.3	n/a	n/a	C9 H10 O3 I



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

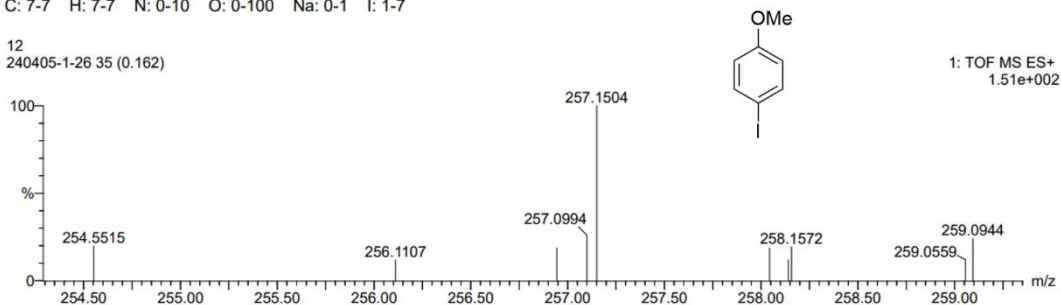
72 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 7-7 H: 7-7 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

12

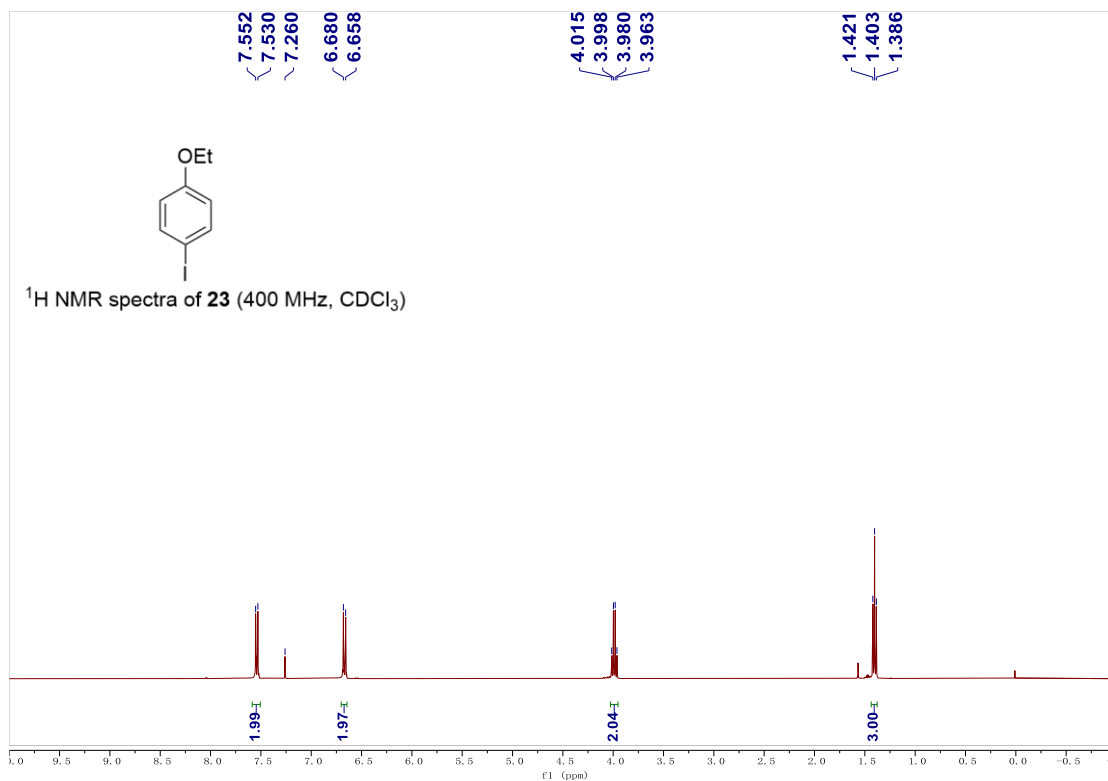
240405-1-26 35 (0.162)



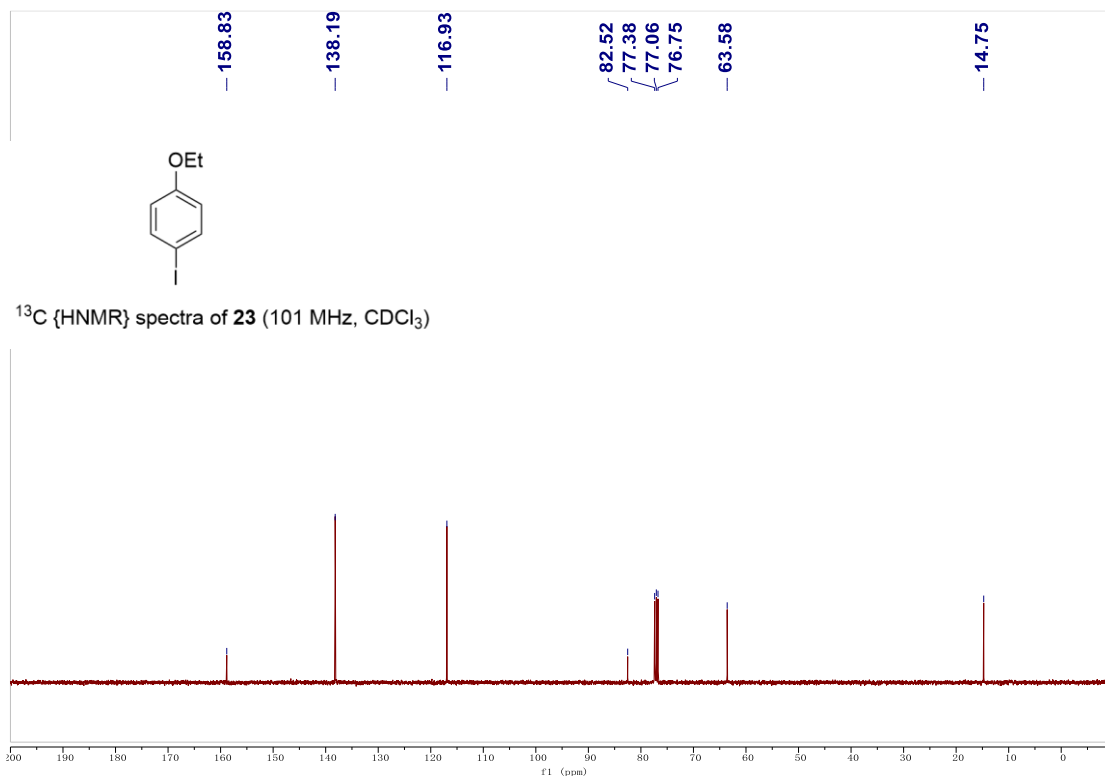
1: TOF MS ES+
1.51e+002

Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
256.9444	256.9439	0.5	1.9	3.5	60.7	n/a	n/a	C7 H7 O Na I



¹H NMR spectra of **23** (400 MHz, CDCl₃)



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

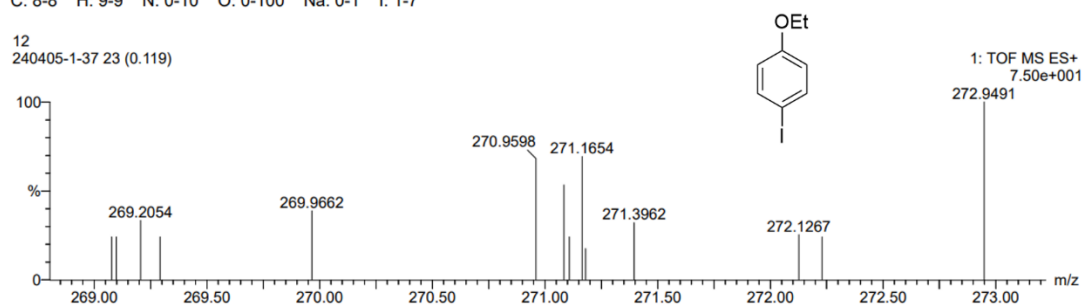
Monoisotopic Mass, Even Electron Ions

90 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

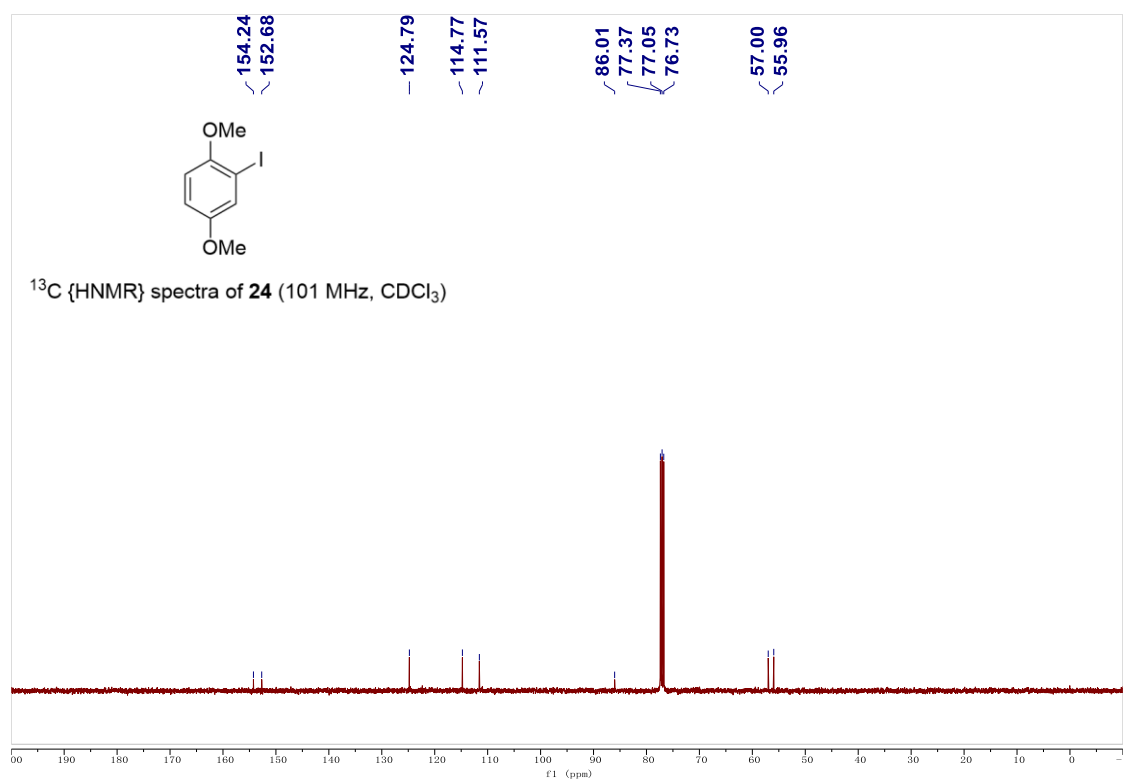
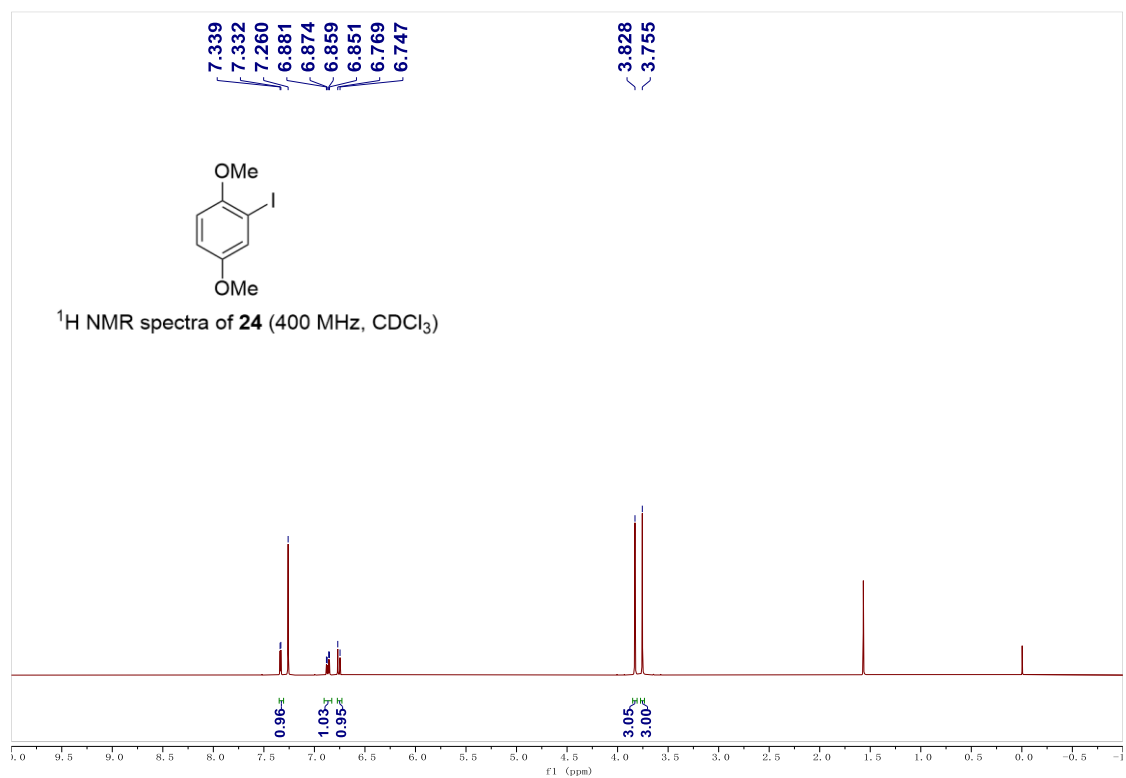
C: 8-8 H: 9-9 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

12
240405-1-37 23 (0.119)



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
270.9598	270.9596	0.2	0.7	3.5	66.1	n/a	n/a	C8 H9 O Na I



Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

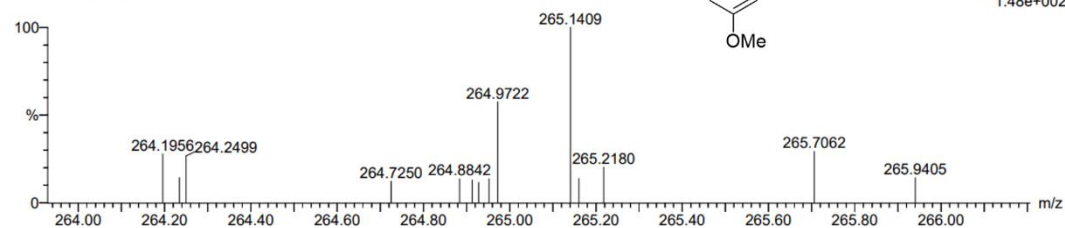
80 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 8-8 H: 10-10 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

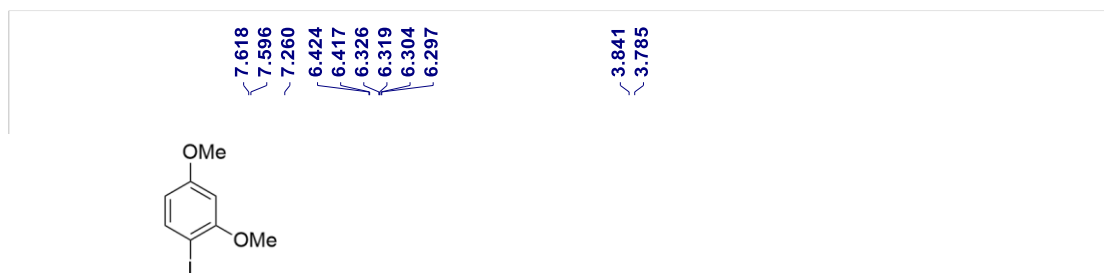
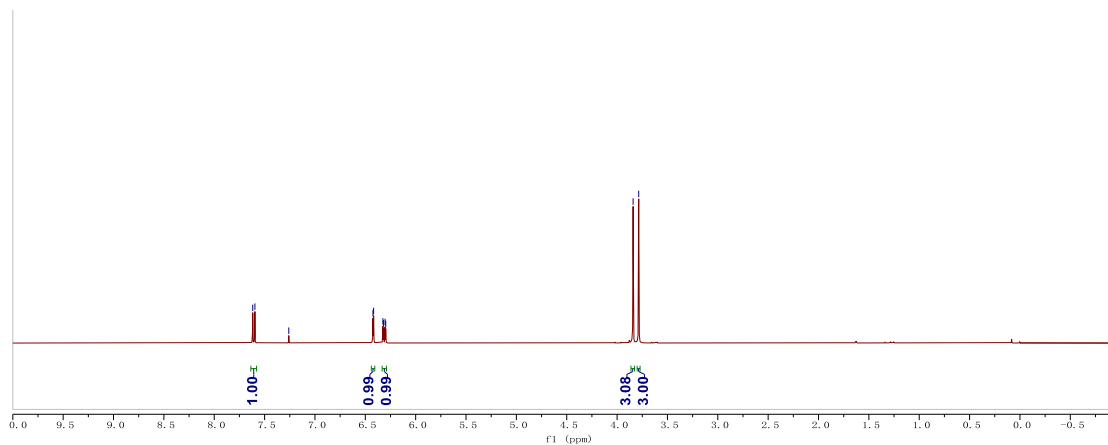
12

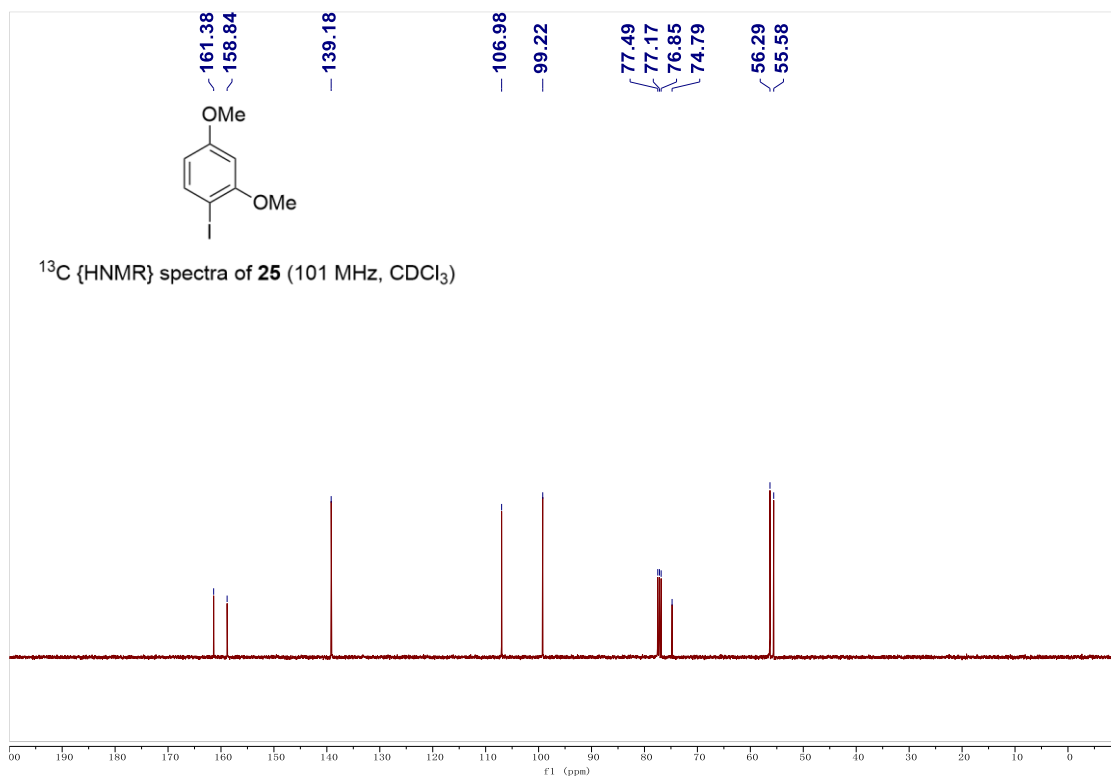
240405-1-22 15 (0.090)



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
264.9722	264.9725	-0.3	-1.1	3.5	48.2	n/a	n/a	C8 H10 O2 I

¹H NMR spectra of 25 (400 MHz, CDCl₃)



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

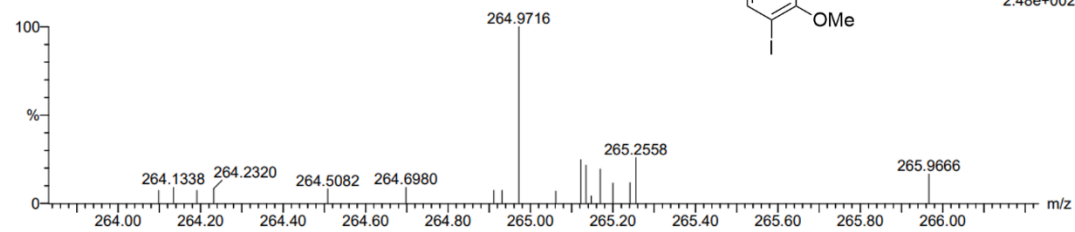
80 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 8-8 H: 10-10 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

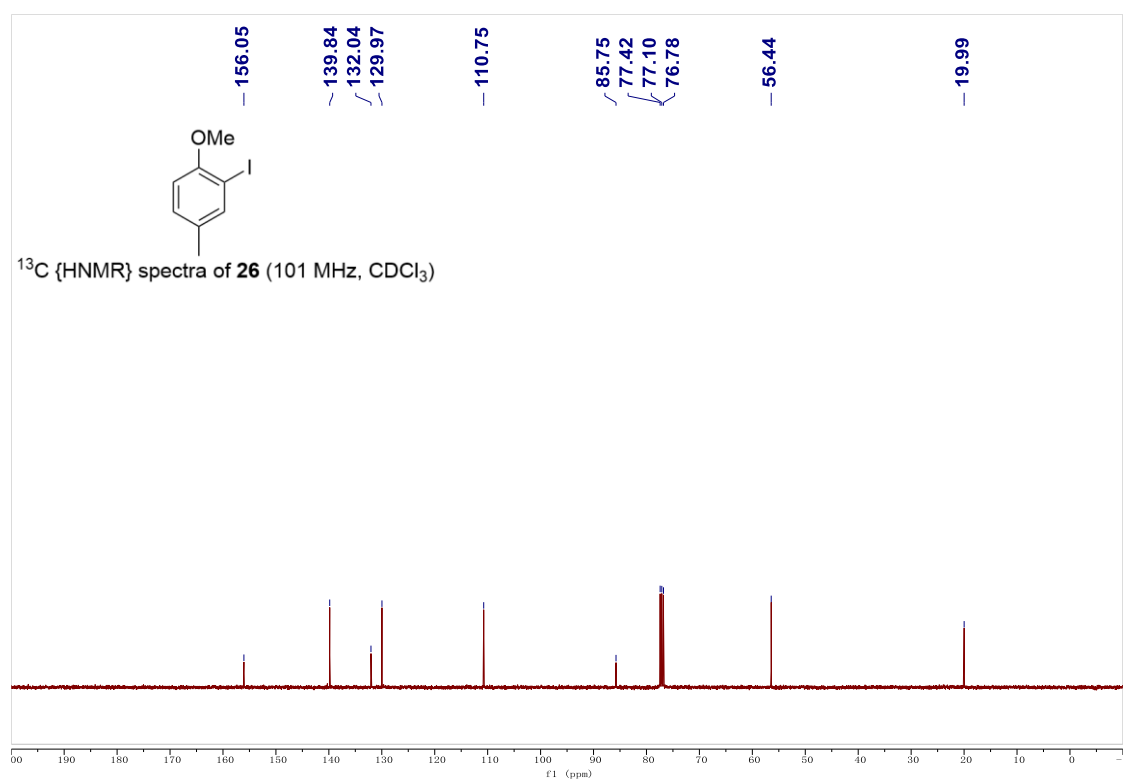
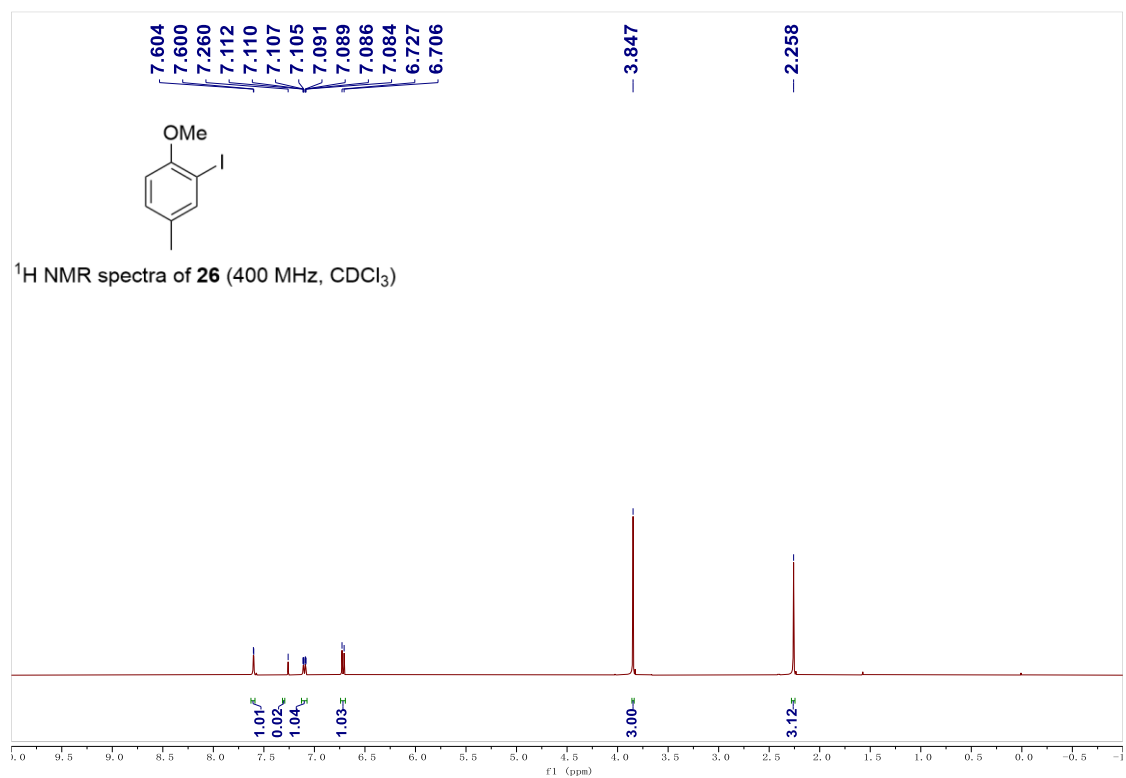
12

240405-1-23 14 (0.087)



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
264.9716	264.9725	-0.9	-3.4	3.5	71.0	n/a	n/a	C8 H10 O2 I



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

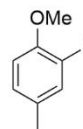
90 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

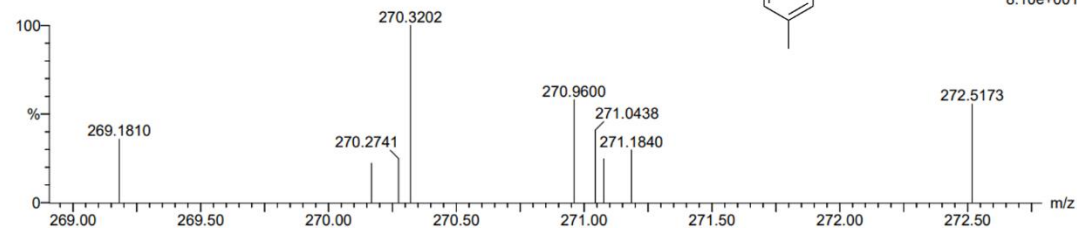
C: 8-8 H: 9-9 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

12

240405-1-24 52 (0.242)



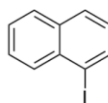
1: TOF MS ES+
8.10e+001



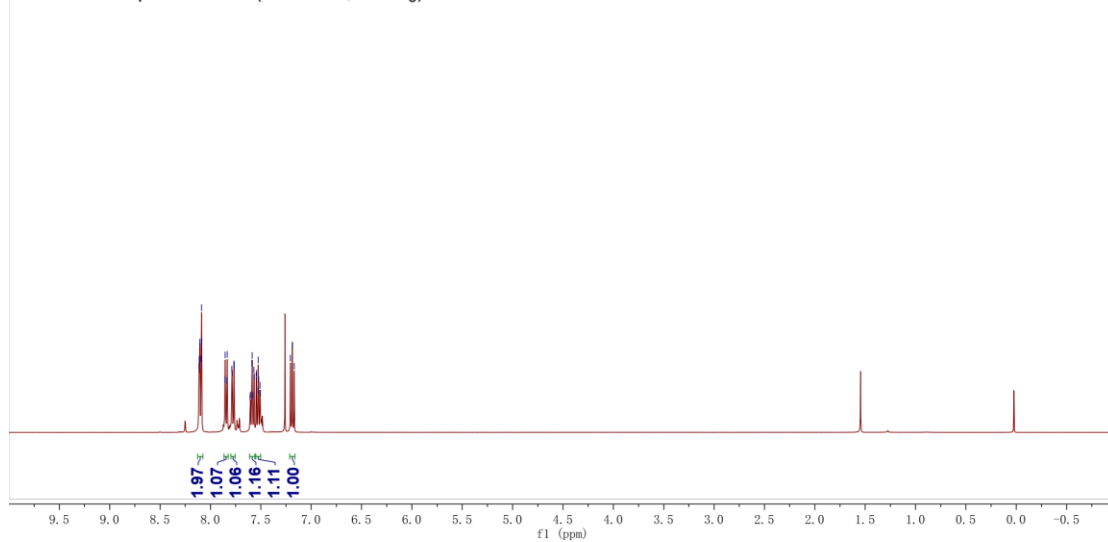
Minimum: -1.5
Maximum: 5.0 10.0 50.0

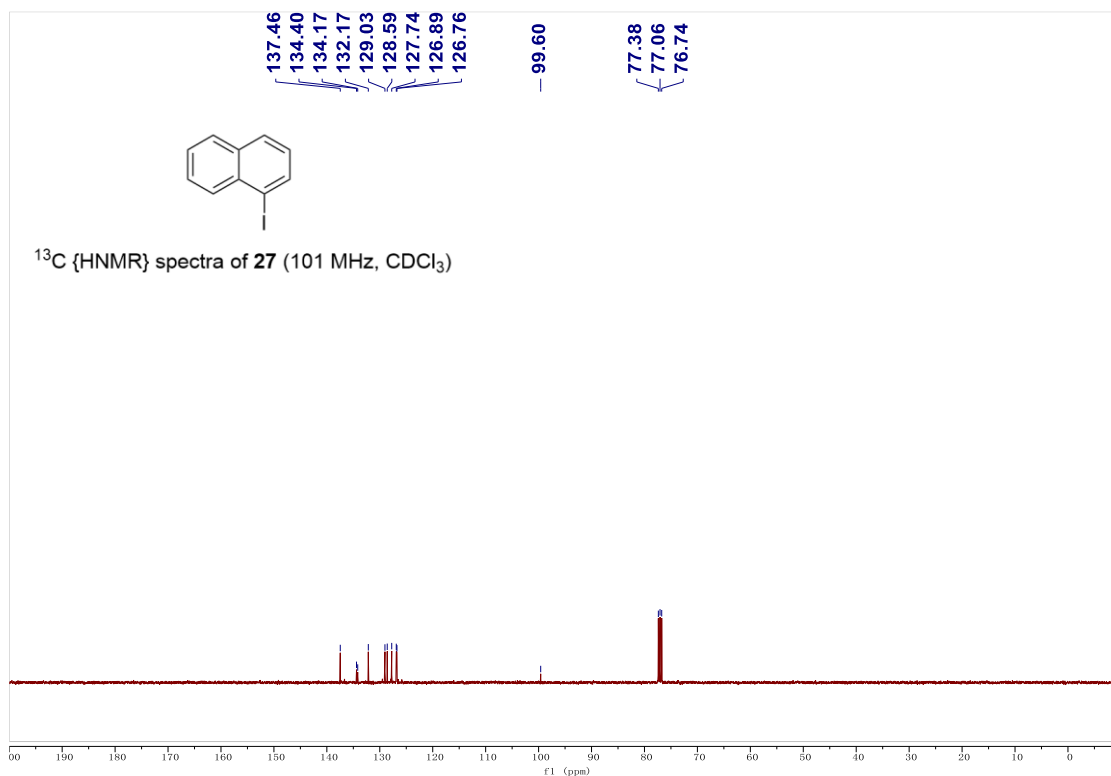
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
270.9600	270.9596	0.4	1.5	3.5	39.5	n/a	n/a	C8 H9 O Na I

8.114
8.111
8.107
8.104
8.093
8.089
8.086
7.857
7.854
7.836
7.833
7.787
7.784
7.767
7.764
7.606
7.603
7.589
7.586
7.582
7.568
7.565
7.545
7.542
7.528
7.525
7.522
7.508
7.505
7.206
7.188
7.186
7.167



¹H NMR spectra of 27 (400 MHz, CDCl₃)





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

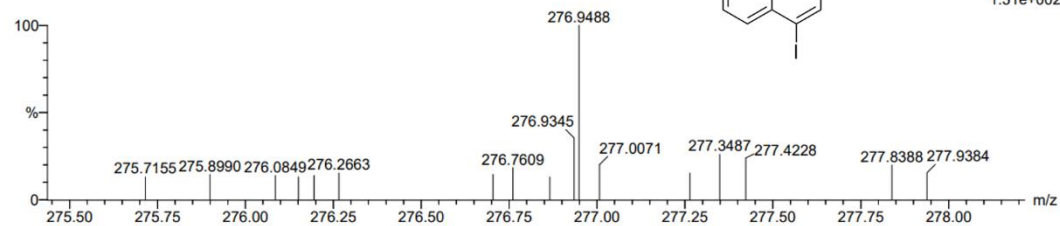
104 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 10-10 H: 7-7 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

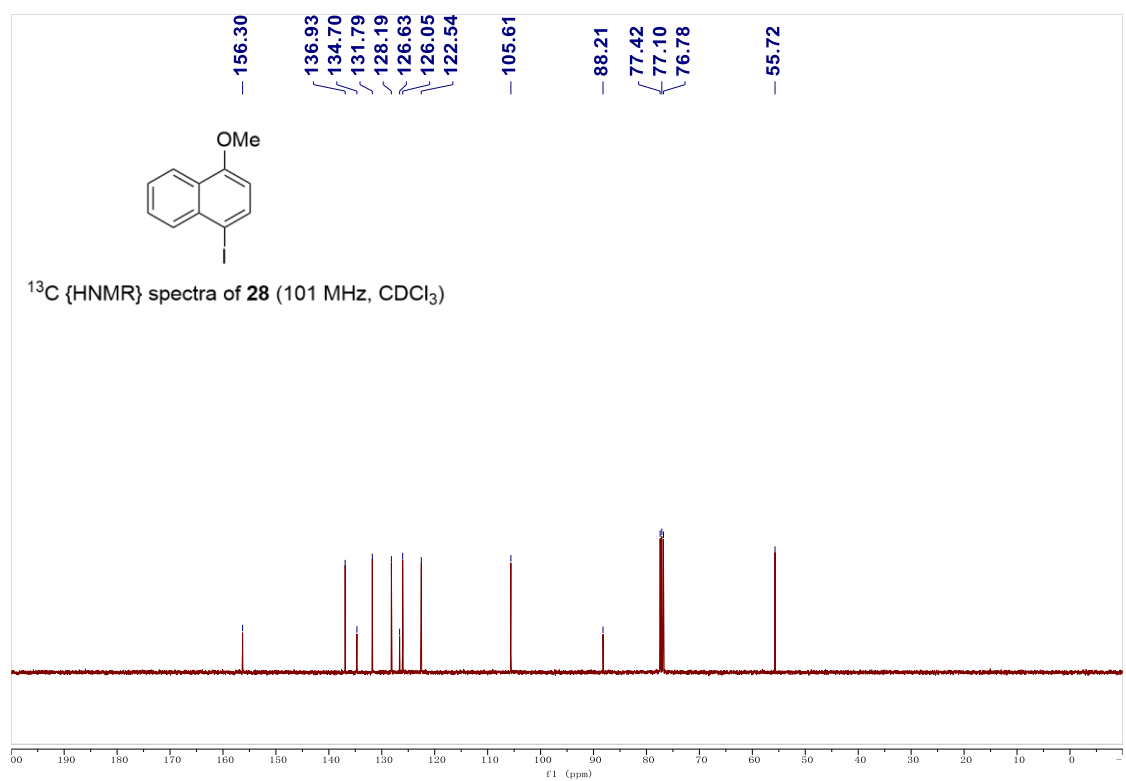
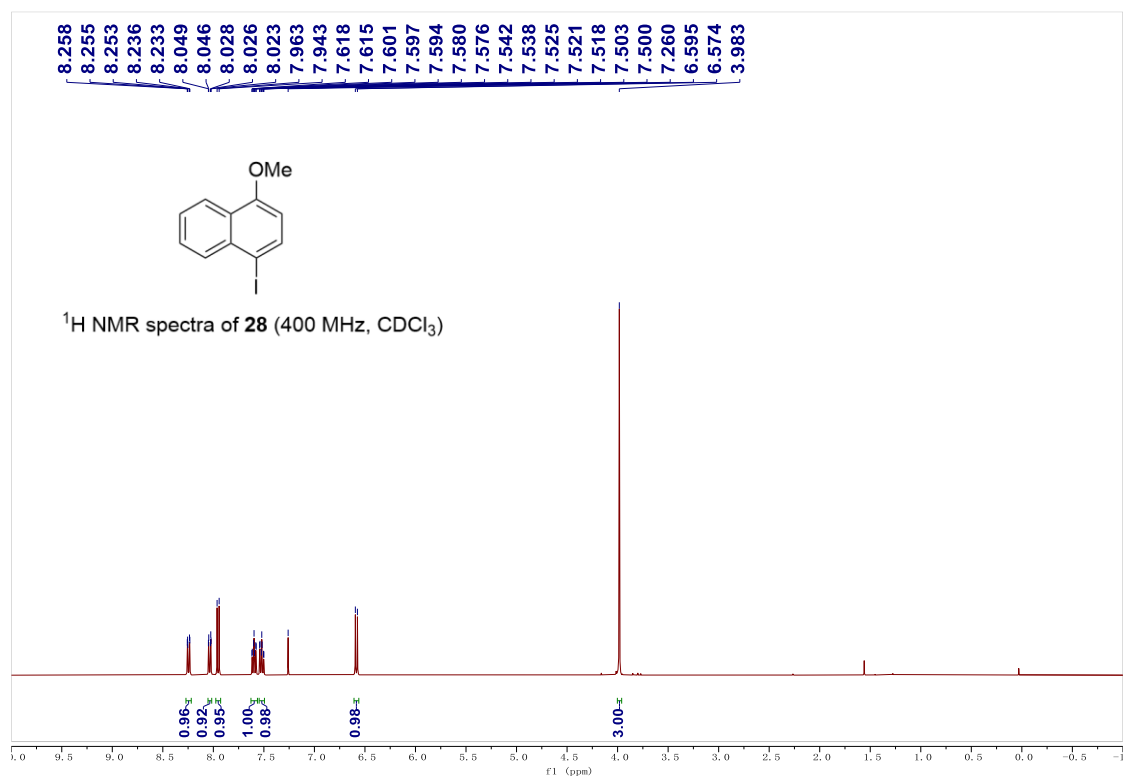
12

240405-1-35 9 (0.069)



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
276.9488	276.9490	-0.2	-0.7	6.5	46.3	n/a	n/a	C10 H7 Na I



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

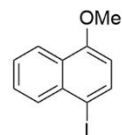
117 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

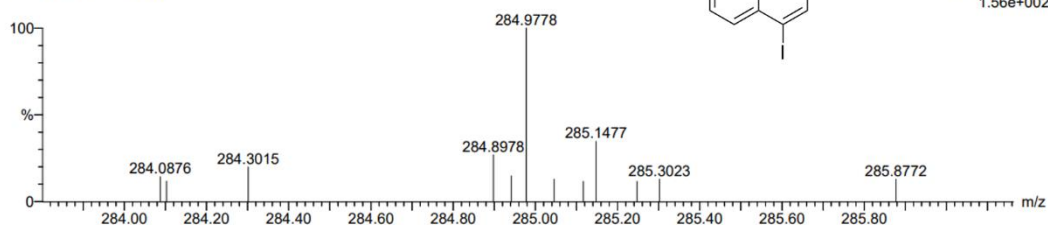
C: 11-11 H: 10-10 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

12

240405-1-25 18 (0.101)



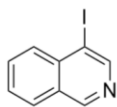
1: TOF MS ES+
1.56e+002



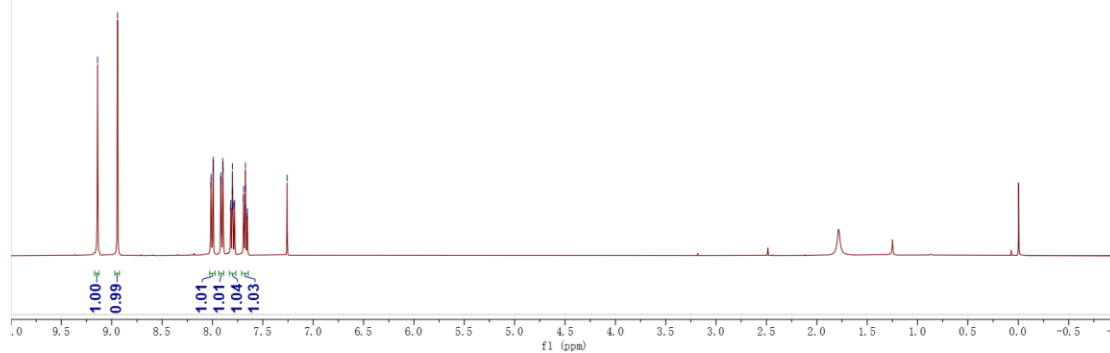
Minimum: -1.5
Maximum: 5.0 10.0 50.0

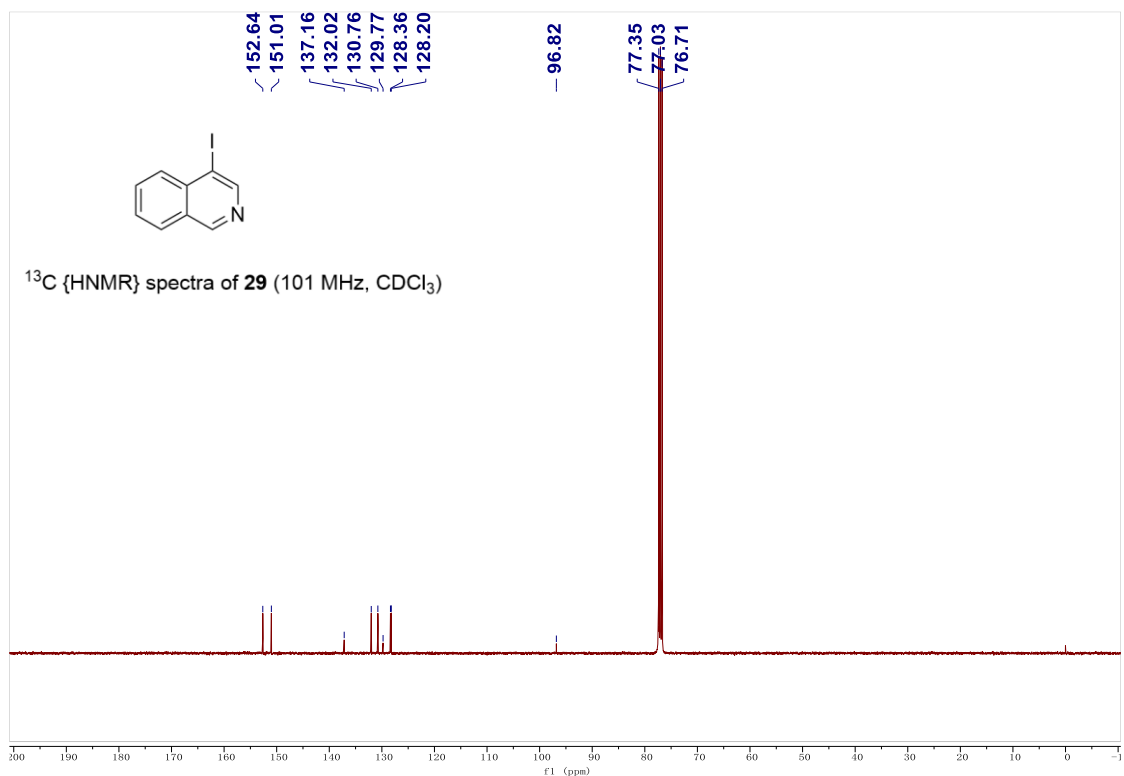
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
284.9778	284.9776	0.2	0.7	6.5	55.7	n/a	n/a	C11 H10 O I

9.141
8.943
8.016
8.013
7.995
7.992
7.917
7.914
7.896
7.893
7.821
7.818
7.804
7.800
7.796
7.782
7.779
7.779
7.693
7.690
7.676
7.673
7.670
7.656
7.653
7.260



¹H NMR spectra of **29** (400 MHz, CDCl₃)





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

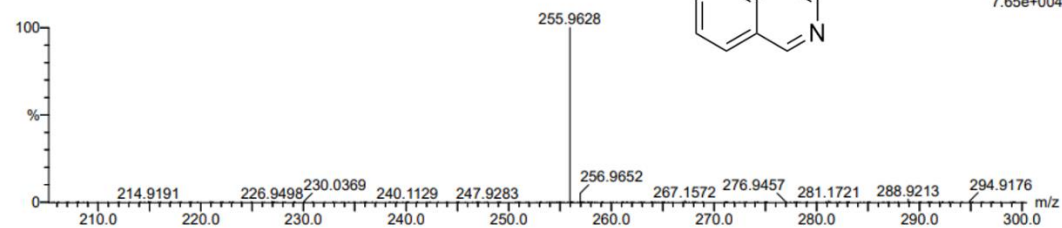
78 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 9-9 H: 7-7 N: 0-10 O: 0-100 Na: 0-1 I: 1-7

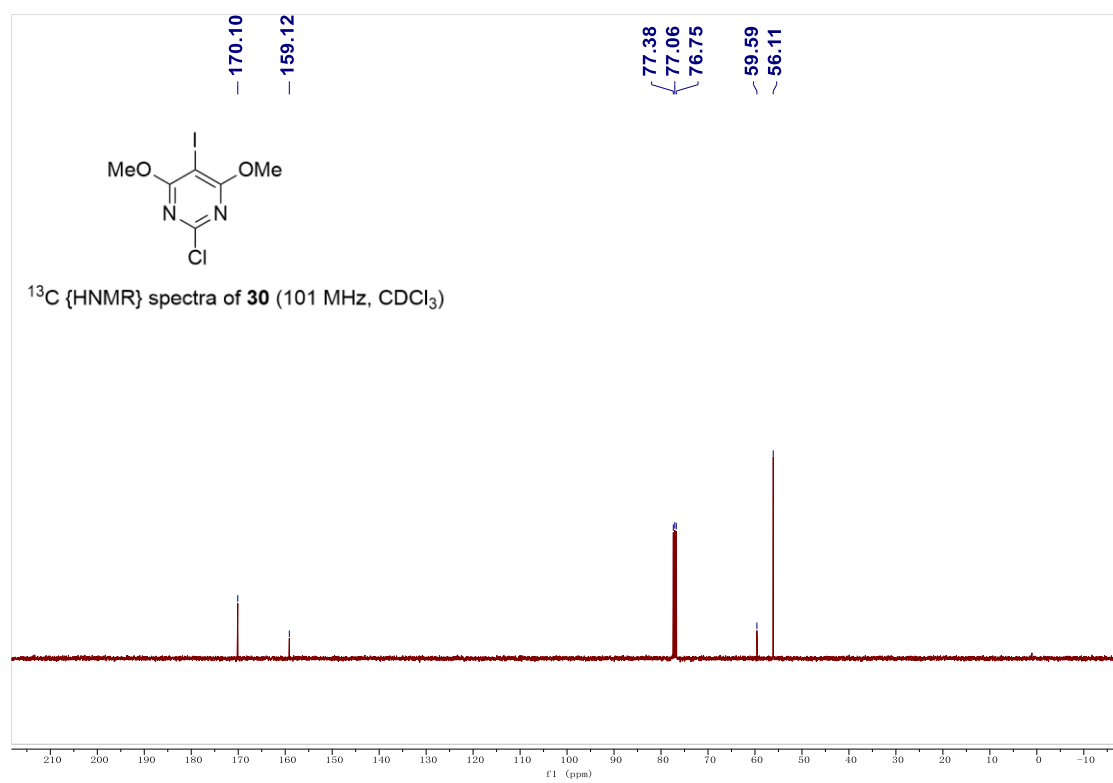
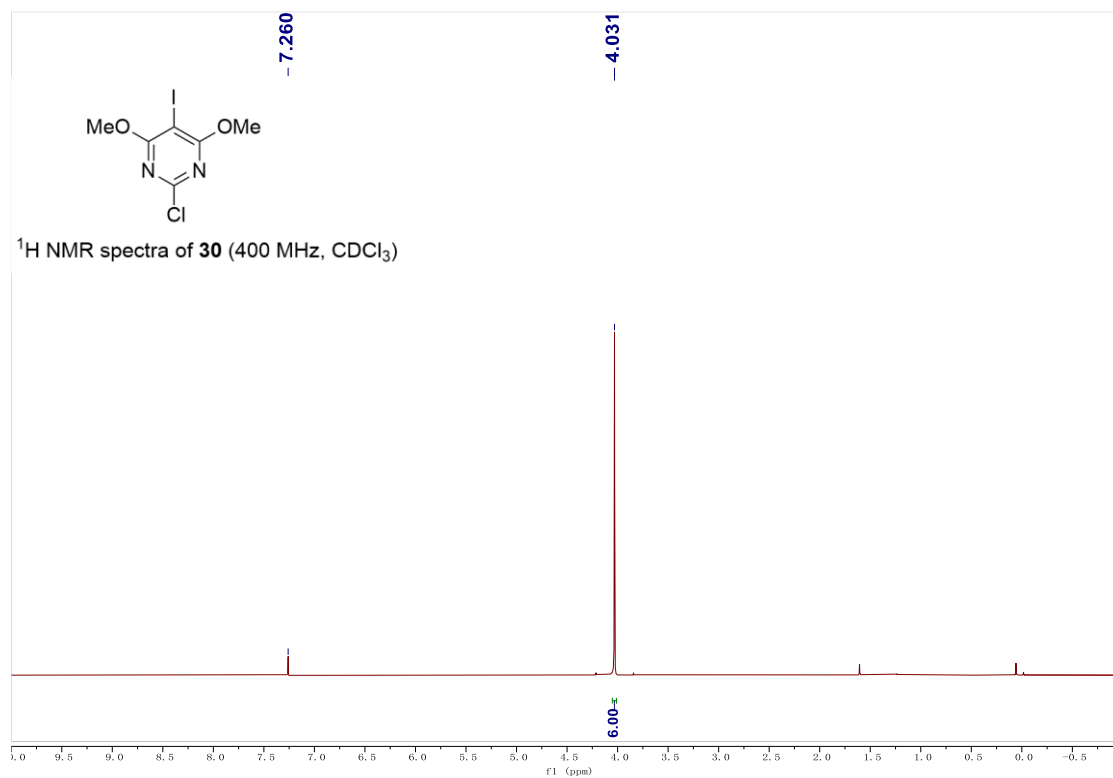
12

240405-1-38 29 (0.140)

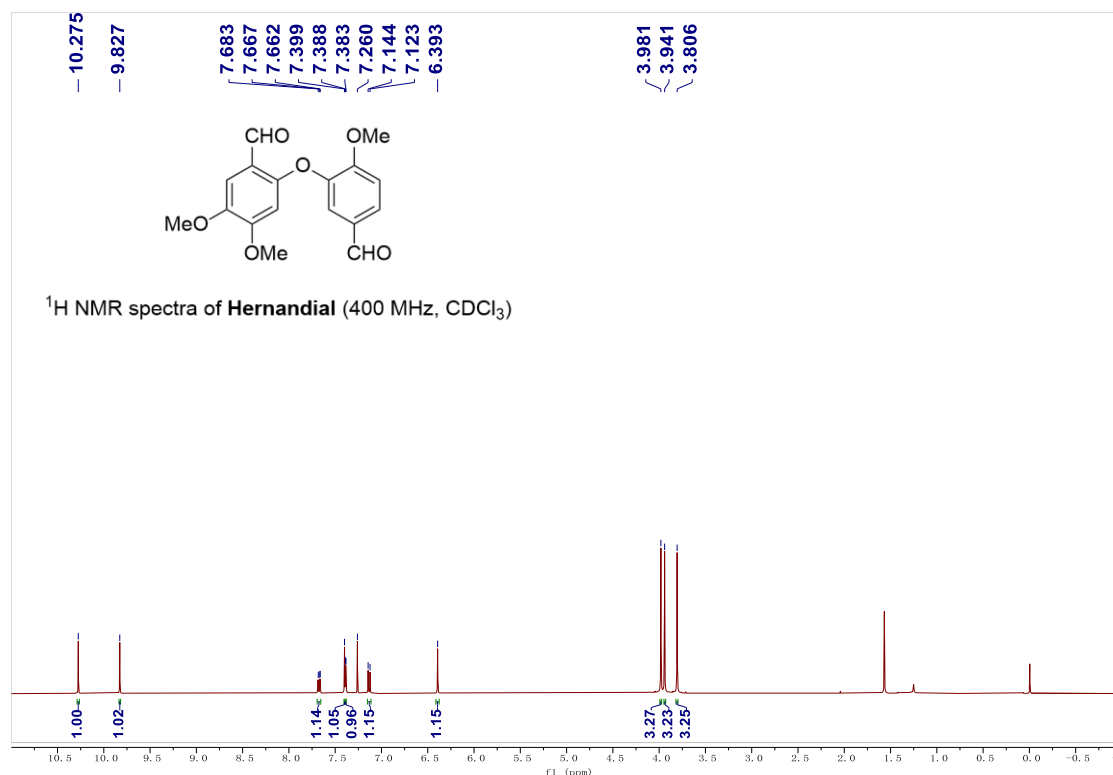
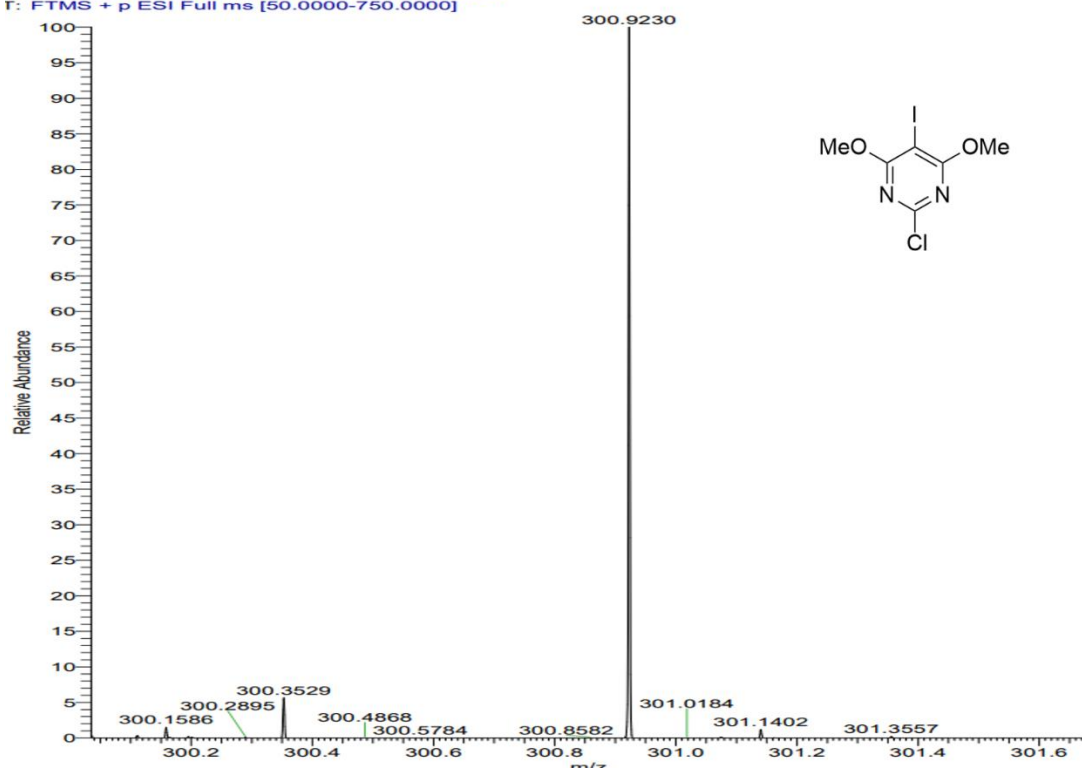


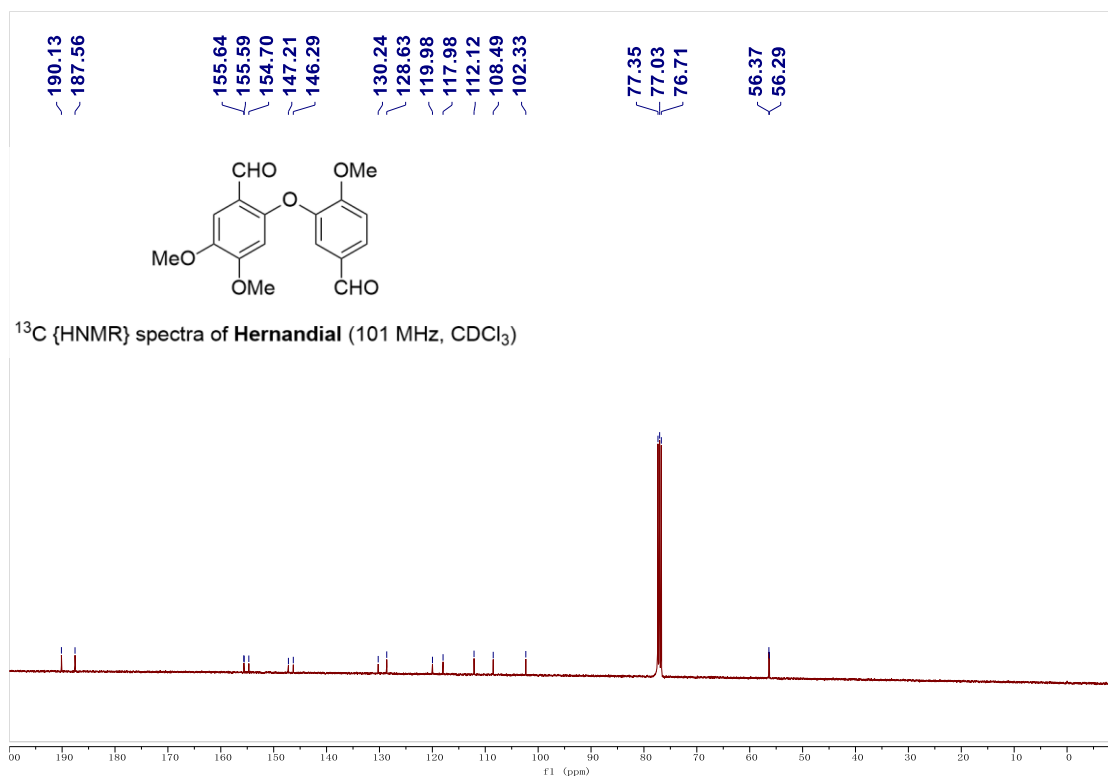
Minimum: -1.5
 Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	IPM	DBE	i-FIT	Norm	Conf (%)	Formula
255.9628	255.9623	0.5	2.0	6.5	160.7	n/a	n/a	C9 H7 N I



T-1 #1-202 RT: 0.00-1.96 AV: 202 NL: 2.28E6
 T: FTMS + p ESI Full ms [50.0000-750.0000]





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

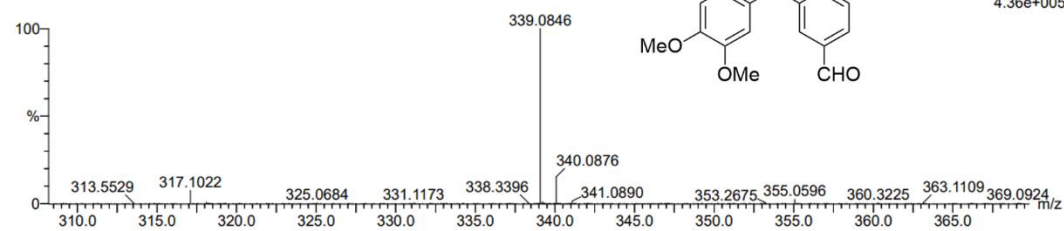
302 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 17-17 H: 16-16 N: 0-10 O: 0-100 Na: 0-1

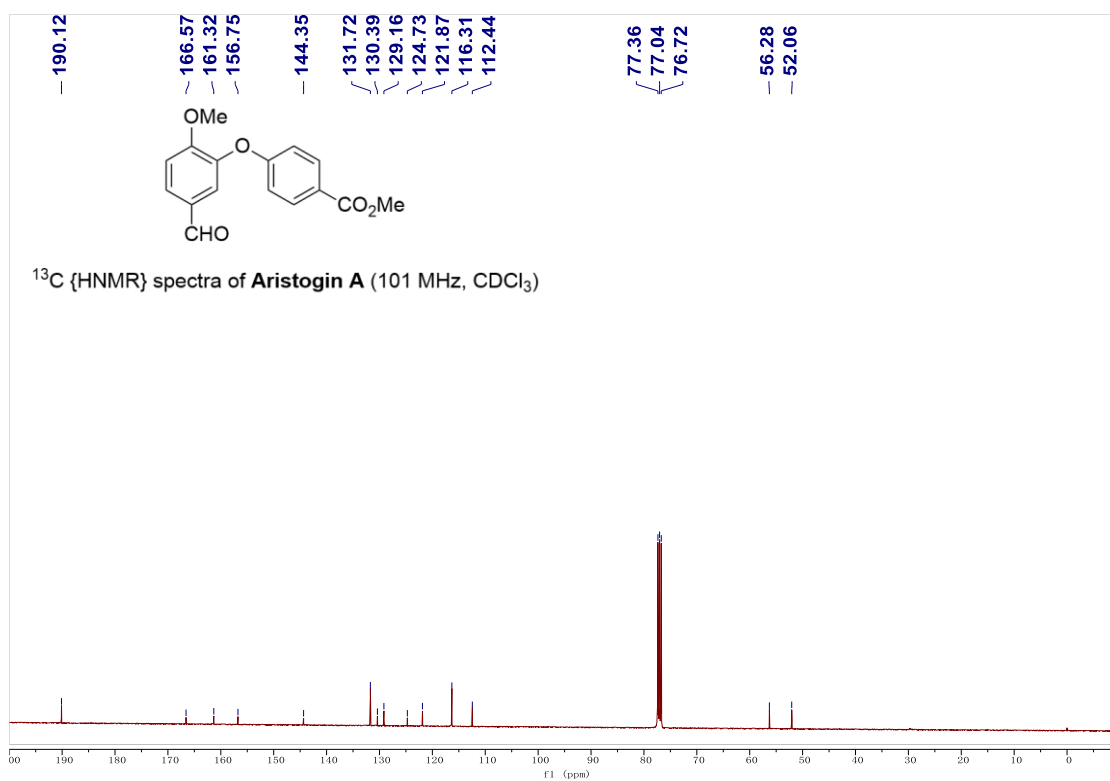
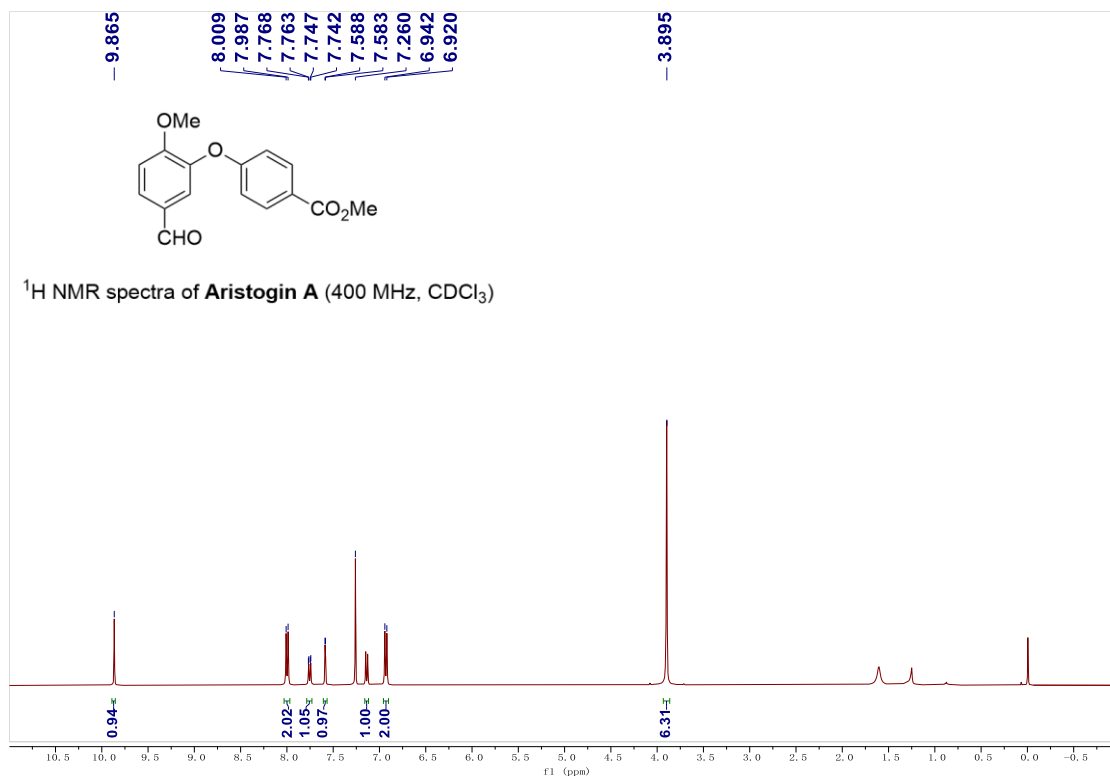
12

240405-1-27 19 (0.105)



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
339.0846	339.0845	0.1	0.3	9.5	453.2	n/a	n/a	C17 H16 O6 Na



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

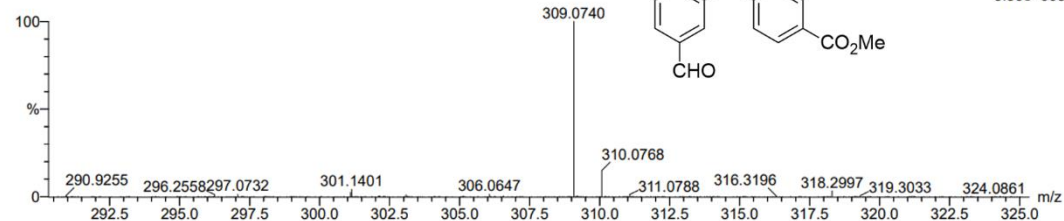
387 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 16-16 H: 14-14 N: 0-100 O: 0-100 Na: 0-1

30

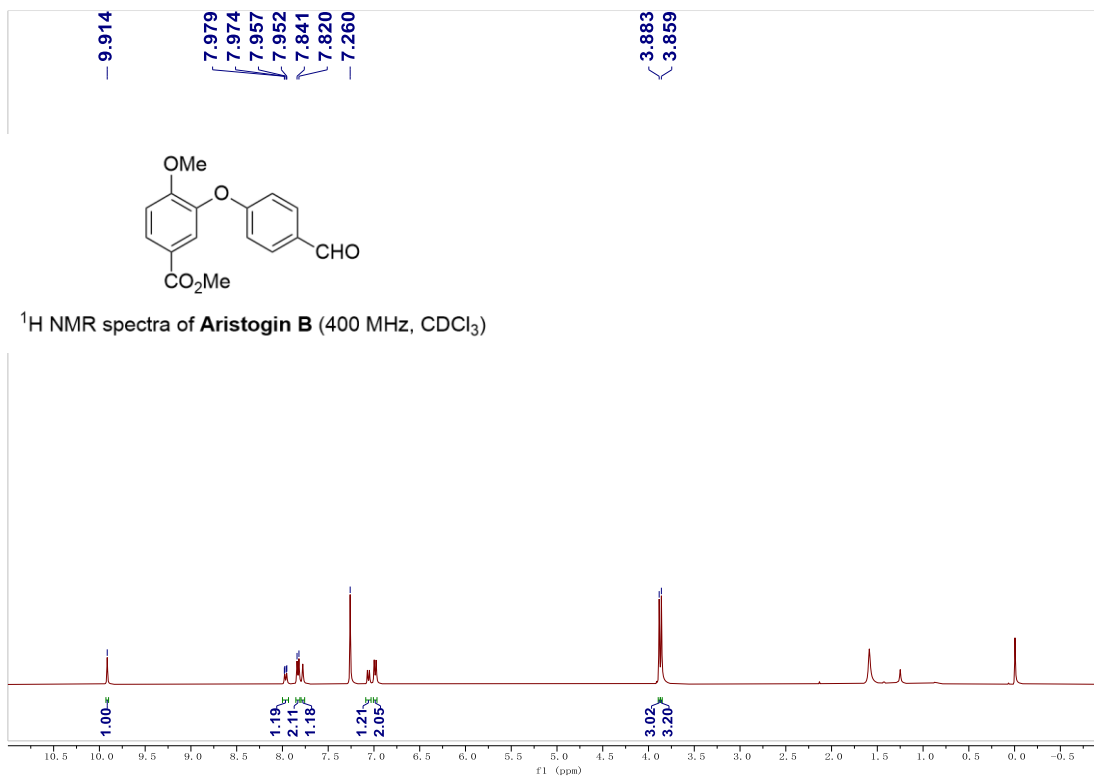
240411-3-28a 10 (0.072)

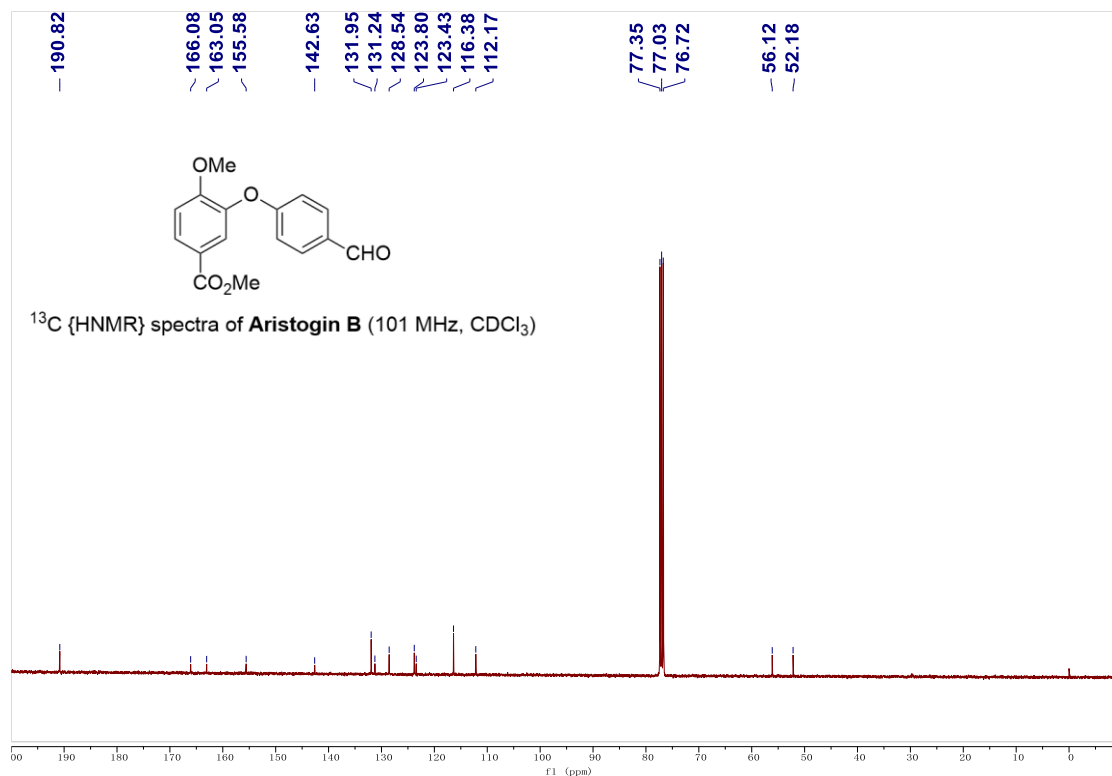


1: TOF MS ES+
3.56e+005

Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
309.0740	309.0739	0.1	0.3	9.5	365.0	n/a	n/a	C16 H14 O5 Na





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

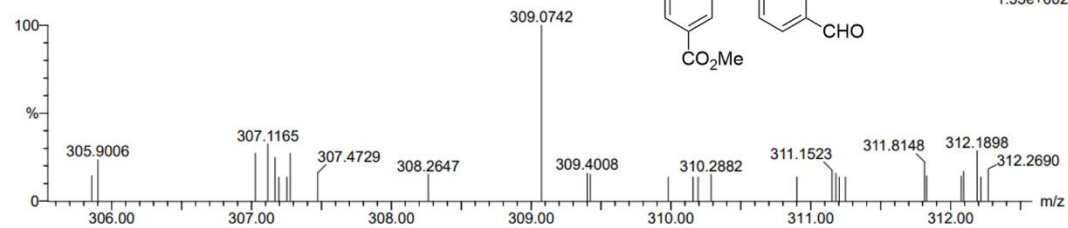
274 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 16-16 H: 14-14 N: 0-10 O: 0-100 Na: 0-1

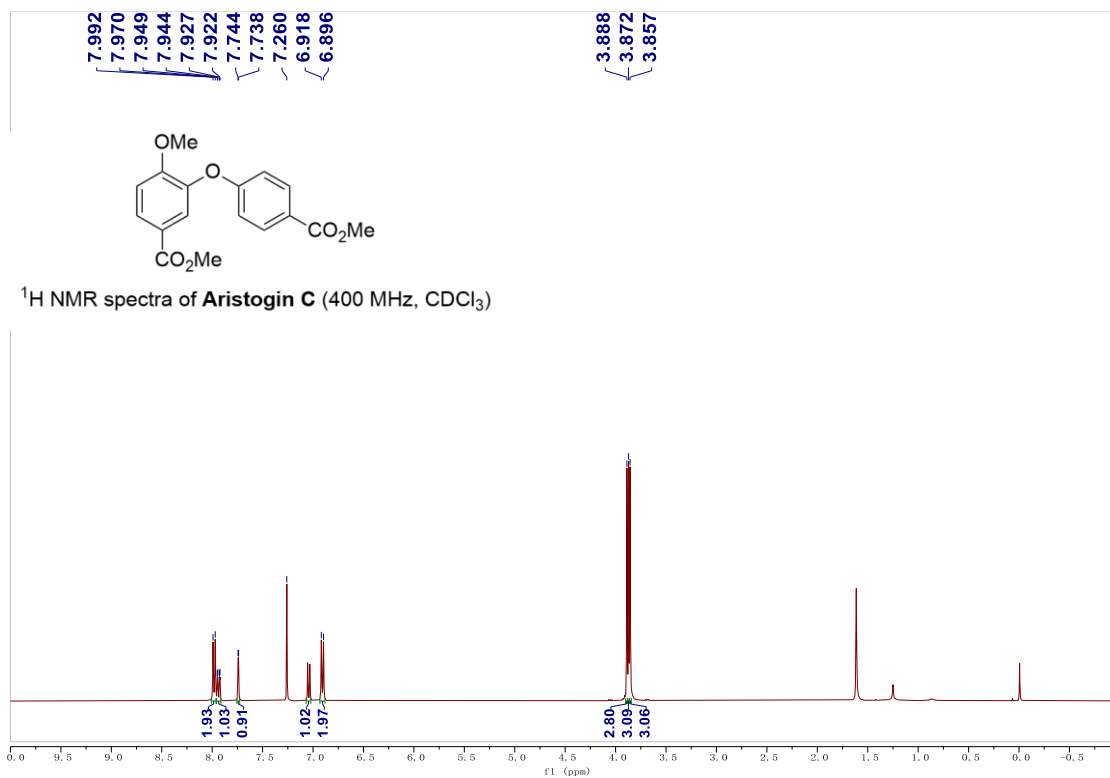
12

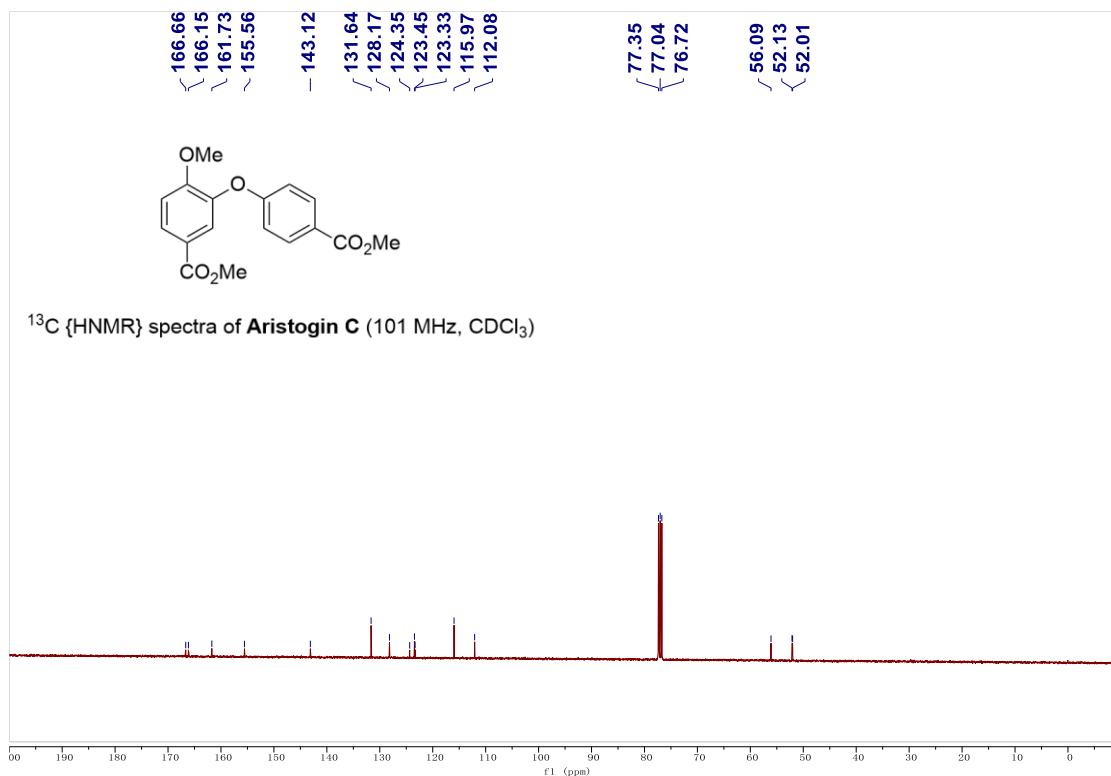
240405-1-29 85 (0.360)



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
309.0742	309.0739	0.3	1.0	9.5	75.8	n/a	n/a	C16 H14 O5 Na





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

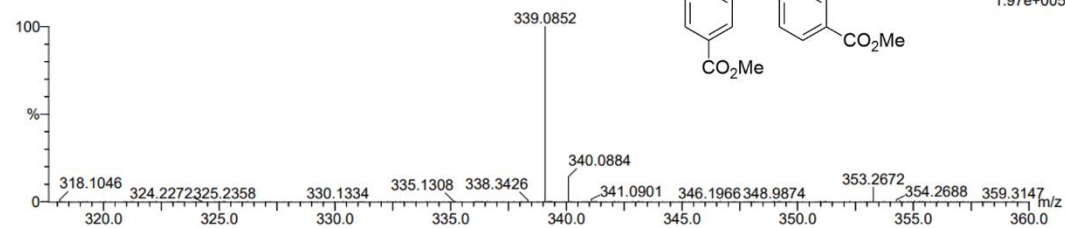
302 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 17-17 H: 16-16 N: 0-10 O: 0-100 Na: 0-1

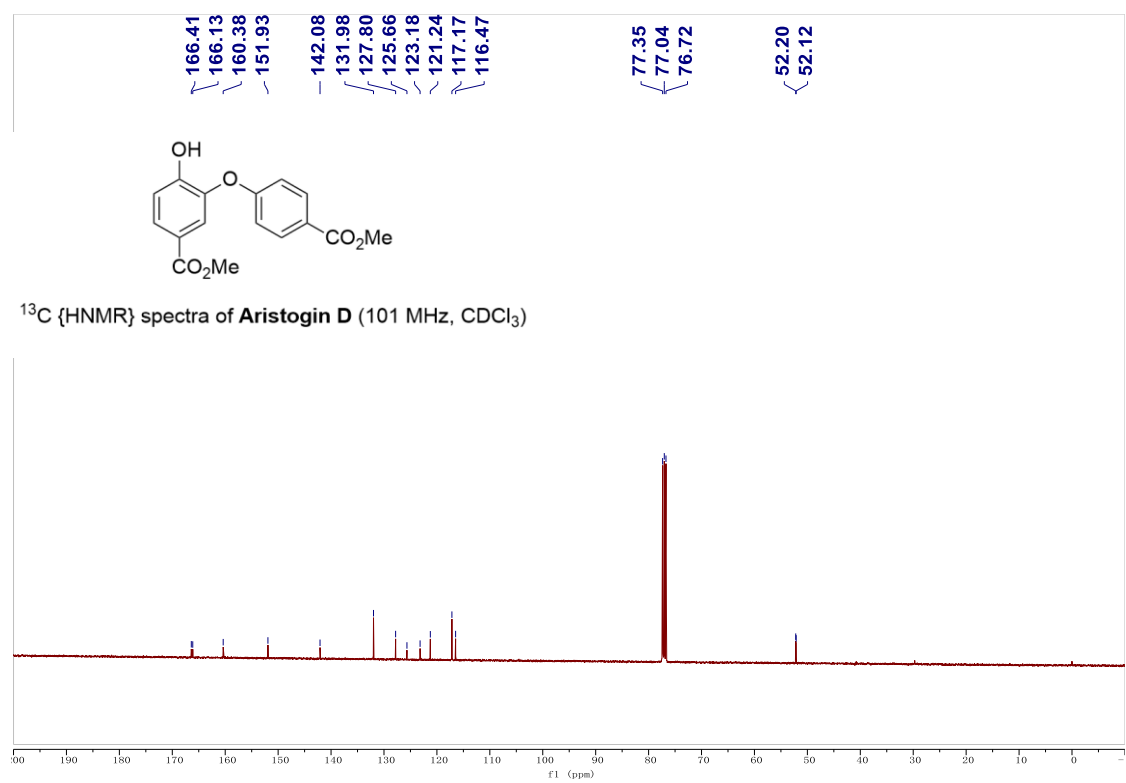
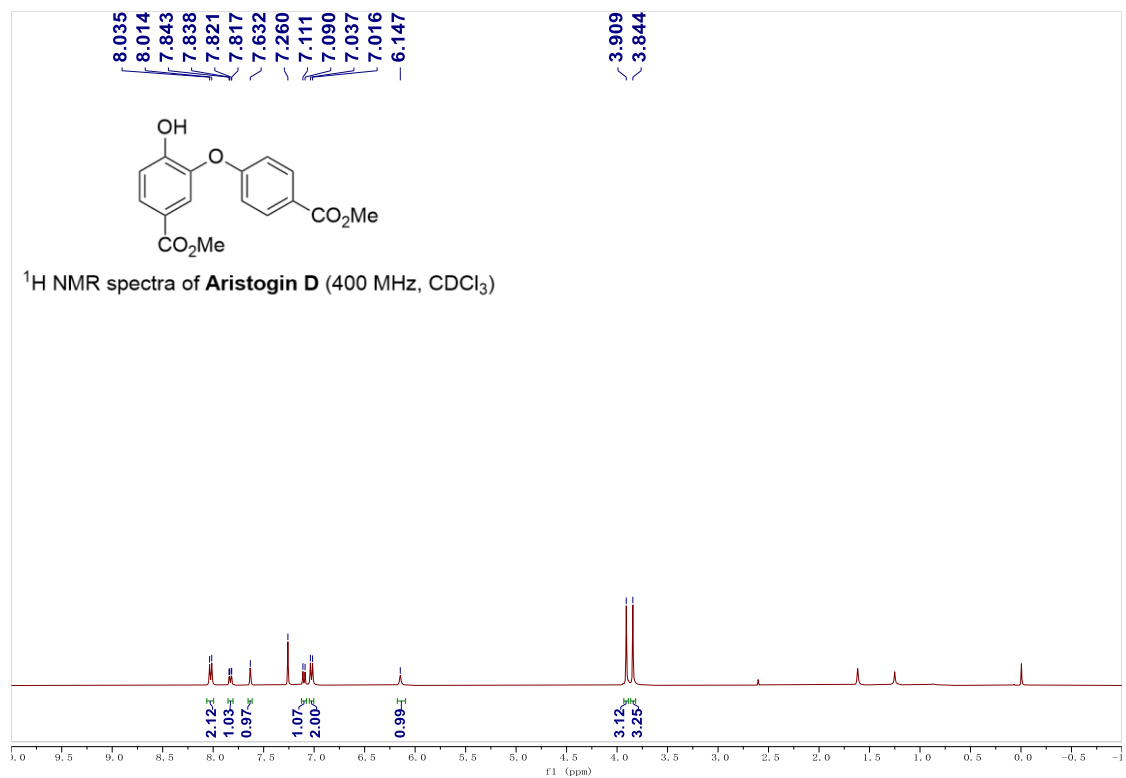
12

240405-1-28 16 (0.094)



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
339.0852	339.0845	0.7	2.1	9.5	316.9	n/a	n/a	C17 H16 O6 Na



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

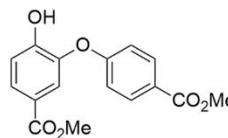
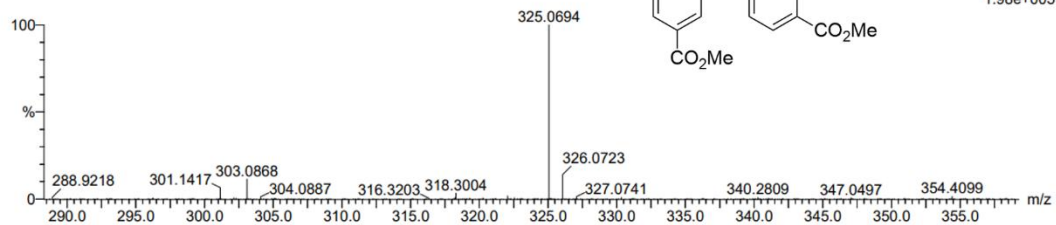
288 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 16-16 H: 14-14 N: 0-10 O: 0-100 Na: 0-1

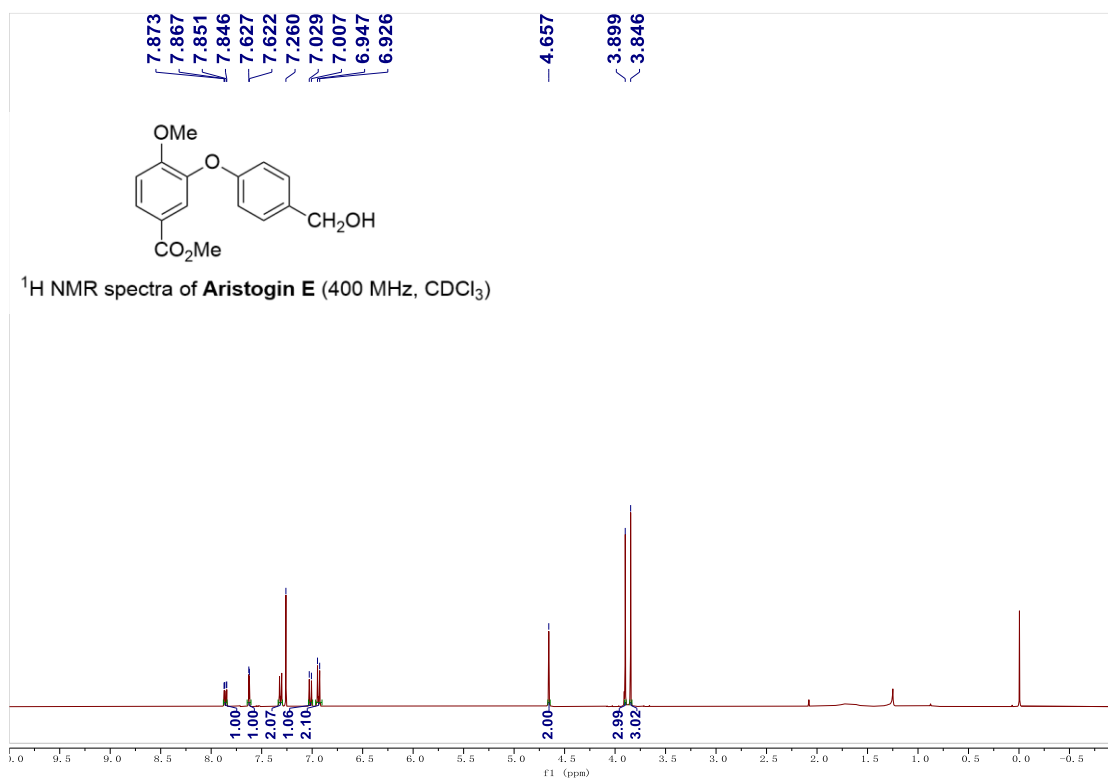
12

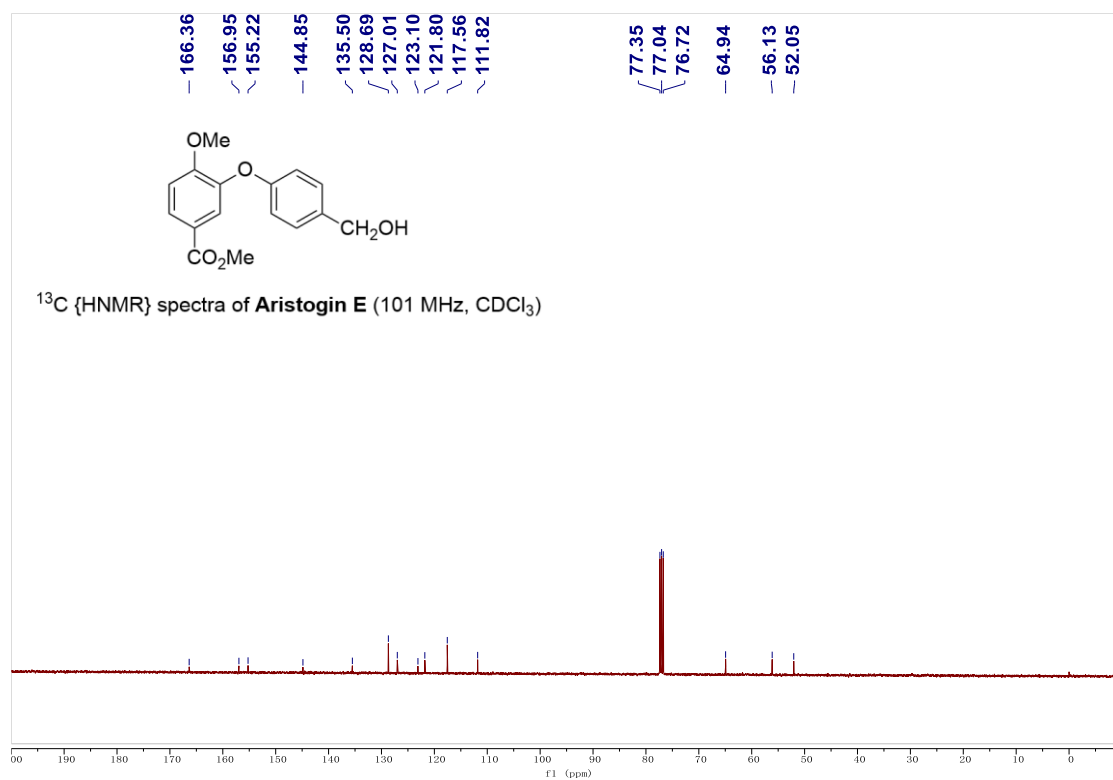
240405-1-31 8 (0.065)



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
325.0694	325.0688	0.6	1.8	9.5	282.5	n/a	n/a	C16 H14 O6 Na





Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

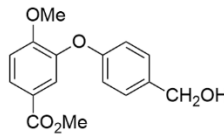
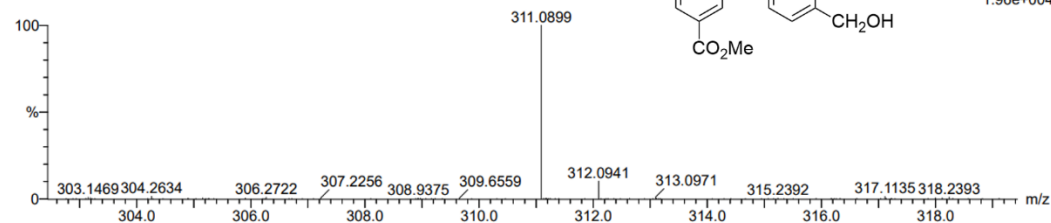
275 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 16-16 H: 16-16 N: 0-10 O: 0-100 Na: 0-1

12

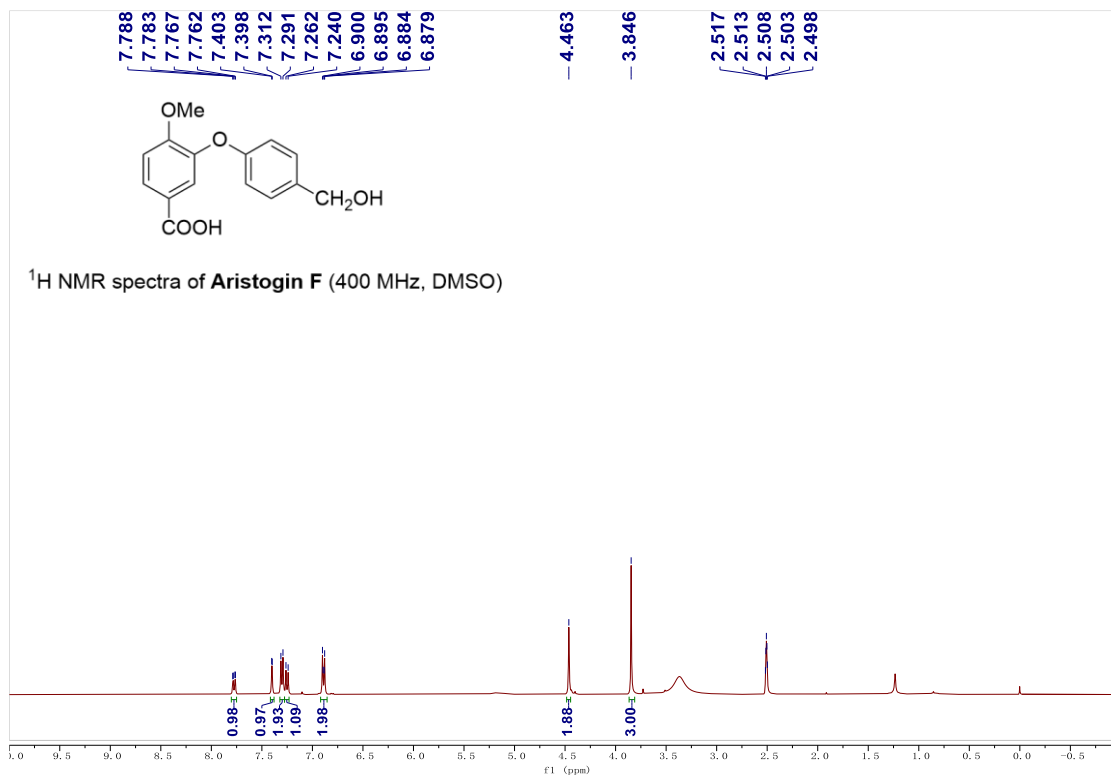
240405-1-32 45 (0.197)



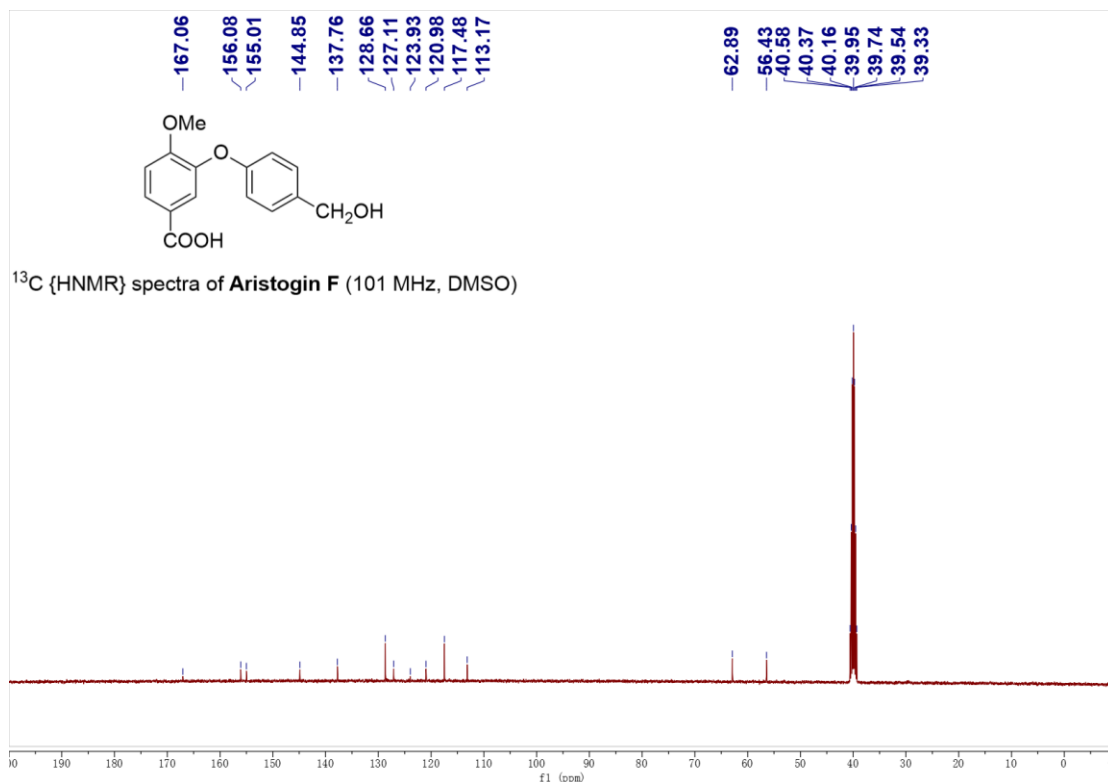
1: TOF MS ES+
1.96e+004

Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
311.0899	311.0895	0.4	1.3	8.5	151.9	n/a	n/a	C16 H16 O5 Na



¹H NMR spectra of Aristogin F (400 MHz, DMSO)



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

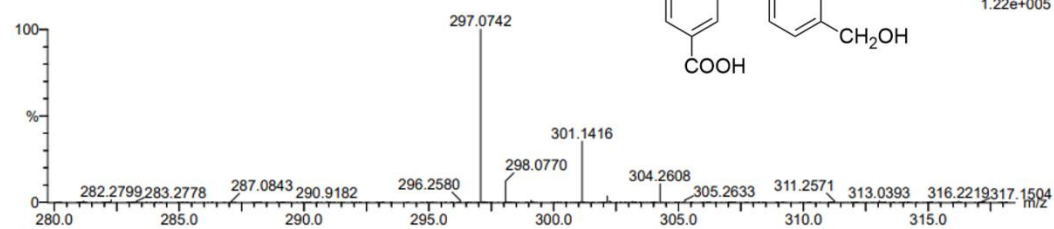
259 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 15-15 H: 14-14 N: 0-10 O: 0-100 Na: 0-1

12

240405-1-33 10 (0.072)



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
297.0742	297.0739	0.3	1.0	8.5	276.3	n/a	n/a	C ₁₅ H ₁₄ O ₅ Na