Electronic supplementary information

A Ru(II)-Catalyzed C–H Activation and Annulation Cascade for the Construction of Highly Coumarin-fused Benzo[*a*]quinolizin-4-ones and Pyridin-2-ones

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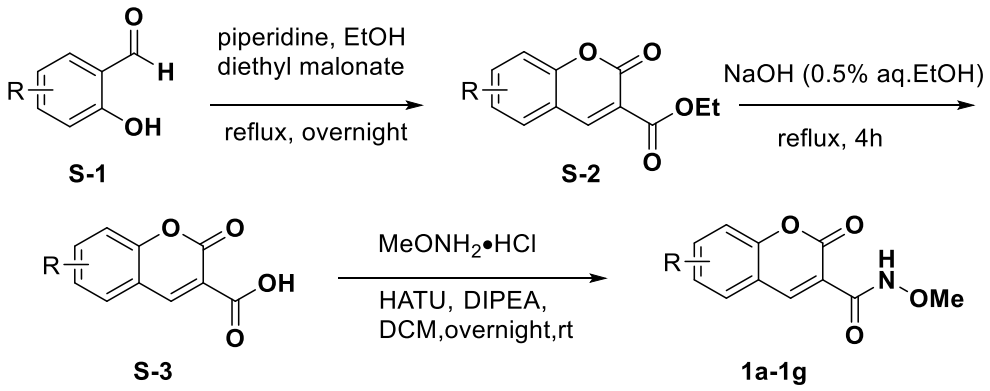
Contents

I.Genral Information

Unless otherwise specified, the reagents were purchased from commercial sources, and used without further purification. Analytical thin-layer chromatography (TLC) was performed on HSGF 254 (0.2-0.3 mm thickness). All products were characterized by their NMR and HRMS spectra. ^{1}H and ^{13}C NMR spectra were recorded on a 400 or 500 MHz instrument. The chemical shifts were reported in parts per million (ppm, δ) downfield from tetramethylsilane (TMS). Proton coupling patterns were described as singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), doublet of doublets (dd), and broad (br). High-resolution mass spectra (HRMS) were measured on a Micromass Ultra Q-TOF spectrometer. Column chromatography was performed on silica gel (300-400 mesh) using dichloromethane (DCM)/methanol (MeOH).

II.Synthesis of Substrates

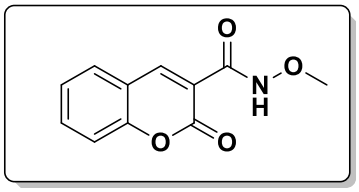
(1) General procedure for the synthesis of substrate **1a**-**1g**[1]



Firstly, salicylaldehyde compounds (S-**1**) (1 equiv), diethyl malonate (1 equiv) and catalytic amounts of piperidine were refluxed in ethanol overnight. After cooling to room temperature, the suspension was filtered off and S-2 was attained. Afterwards, compound S-**2** was hydrolyzed in ethanolic solution with 0.5% NaOH (aq.) at reflux for 1h. After reaction 10% HCl (aq.) was added and the desired S-**3** was then filtered off and washed with water to yield 89%. Next, solution of S-**3** (1 equiv), $MeONH_2$ • HCl (1.3 equiv), HATU (1.5 equiv) and DIPEA (2 equiv) in DCM, the mixture was stirred at r.t. overnight. After that, the solution was directly concentrated

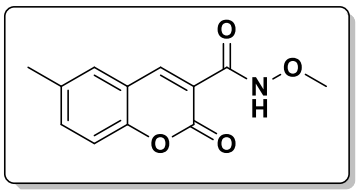
in vacuo then the crude product was purified by flash column chromatography on silica gel (PE/EA) to afford the pure product **1a-1g**.

N-methoxy-2-oxo-2H-chromene-3-carboxamide (**1a**)



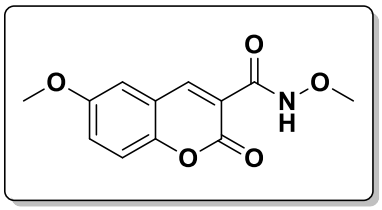
^{1}H NMR (500 MHz, $CDCl_3$) δ 11.05 (s, 1H), 8.93 (s, 1H), 7.76 – 7.60 (m, 2H), 7.44 – 7.36 (m, 2H), 3.90 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.87, 159.60, 154.50, 149.13, 134.63, 129.99, 125.62, 118.48, 117.78, 116.87, 64.75. HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{11}H_{10}NO_4^+$:220.0604, found: 220.0603.

N-methoxy-6-methyl-2-oxo-2H-chromene-3-carboxamide (**1b**)



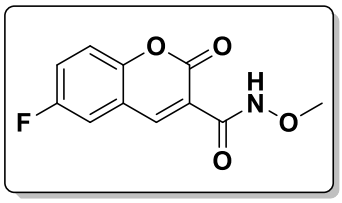
^{1}H NMR (500 MHz, $CDCl_3$) δ 11.07 (s, 1H), 8.86 (s, 1H), 7.51 – 7.45 (m, 2H), 7.29 (d, *J* = 8.4 Hz, 1H), 3.89 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.05, 159.74, 152.69, 149.08, 135.81, 135.54, 129.52, 118.24, 117.55, 116.55, 64.70, 20.87. HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{12}H_{12}NO_4^+$: 234.0761, found: 234.0766.

N,6-dimethoxy-2-oxo-2H-chromene-3-carboxamide (**1c**)



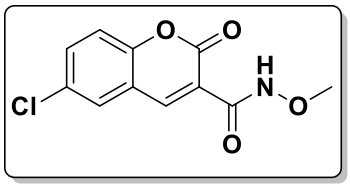
^{1}H NMR (500 MHz, DMSO-d_6) δ 11.38 (s, 1H), 8.72 (s, 1H), 7.51 (d, *J* = 2.0 Hz, 1H), 7.43 (d, *J* = 9.1 Hz, 1H), 7.36 – 7.30 (m, 1H), 3.81 (s, 3H), 3.72 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 159.13, 159.03, 155.93, 148.31, 147.08, 121.91, 119.14, 118.67, 117.32, 111.77, 63.44, 55.83. HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{12}H_{12}NO_5^+$: 250.071, found: 250.0712.

6-Fluoro-N-methoxy-2-oxo-2H-chromene-3-carboxamide (**1d**)



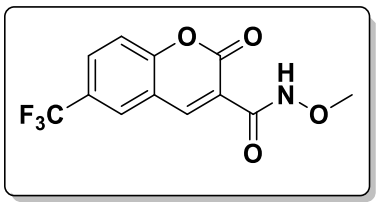
^{1}H NMR (500 MHz, DMSO-d_6) δ 11.39 (s, 1H), 8.72 (s, 1H), 8.00 – 7.70 (m, 1H), 7.70 – 7.40 (m, 2H), 3.70 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 159.03 (s), 158.64 (d, *J* = 241.7 Hz), 157.68 (s), 150.73 (s), 146.66 (s), 121.83 (d, *J* = 24.9 Hz), 120.64 (s), 119.60 (d, *J* = 9.9 Hz), 118.75 (d, *J* = 8.7 Hz), 115.45 (d, *J* = 24.4 Hz), 63.89 (s). HRMS (ESI) m/z [M + H]$^{+}$ calculated for $C_{11}H_9FNO_4^{+}$:238.051, found: 238.0512.

6-Chloro-N-methoxy-2-oxo-2H-chromene-3-carboxamide (**1e**)



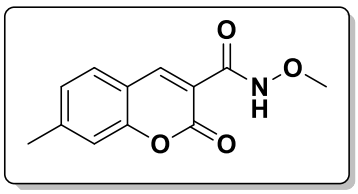
^{1}H NMR (500 MHz, DMSO-d_6) δ 11.40 (s, 1H), 8.71 (s, 1H), 8.06 (d, *J* = 2.4 Hz, 1H), 7.84 – 7.70 (m, 1H), 7.51 (d, *J* = 8.9 Hz, 1H), 3.70 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 158.79, 158.39, 152.47, 145.93, 133.51, 128.94, 128.79, 120.28, 119.61, 118.26, 63.43. HRMS (ESI) m/z [M + H]$^{+}$ calculated for $C_{11}H_9ClO_4^{+}$:254.0215, found:254.0215.

N-methoxy-2-oxo-6-(trifluoromethyl)-2H-chromene-3-carboxamide (**1f**)



^{1}H NMR (500 MHz, $CDCl_3$) δ 10.96 (s, 1H), 9.01 (s, 1H), 8.03 (s, 1H), 7.95 (d, *J* = 8.7 Hz, 1H), 7.57 (d, *J* = 8.7 Hz, 1H), 3.94 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.89 (s), 158.70 (s), 155.92 (s), 148.02 (s), 130.84 (d, *J* = 3.2 Hz), 128.19 (q, *J* = 33.9 Hz), 127.25 (d, *J* = 3.9 Hz), 123.10 (q, *J* = 272.4 Hz), 119.28 (s), 118.27 (s), 117.64 (s), 64.71 (s). HRMS (ESI) m/z [M + H]$^{+}$ calculated for $C_{12}H_9F_3NO_4^{+}$:288.0478, found: 288.0473.

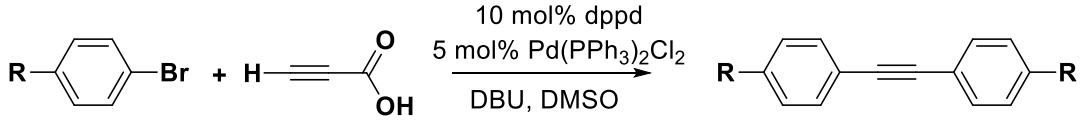
N-methoxy-7-methyl-2-oxo-2H-chromene-3-carboxamide (**1g**)



^{1}H NMR (500 MHz, $CDCl_3$) δ 11.03 (s, 1H), 8.87 (s, 1H), 7.56 (d, *J* = 8.3 Hz, 1H), 7.22 – 7.16 (m, 2H), 3.88 (s, 3H), 2.49 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ

161.08, 159.87, 154.67, 149.02, 146.68, 129.62, 126.93, 116.92, 116.44, 116.17, 64.69, 22.27. HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{12}H_{12}NO_4^+$: 234.0761, found: 234.0757.

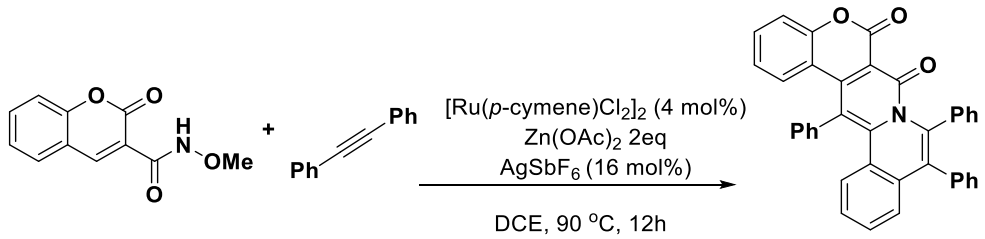
(2) General procedure for the synthesis of substrate **2a**-**2g**[2]



S-4 **S-5** **2a-2g**

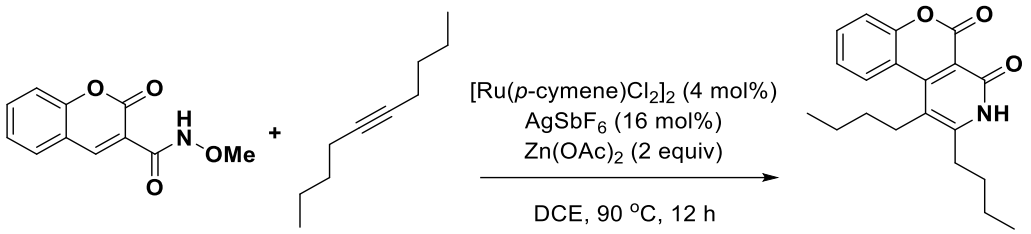
2.0 equiv of aryl halide (S-**4**), 1.0 equiv of propiolic acid (S-**5**), 5.0 mol % $Pd(PPh_3)_2Cl_2$, 10.0 mol % 1,4-bis(diphenylphosphino)butane (dppb), 2.0 equiv of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU), and dimethyl sulfoxide (DMSO) as the solvent, the mixture was stirred at 80 ^{0}C for 3 h. After that, the solution was directly concentrated in vacuo then the crude product was purified by flash column chromatography on silica gel (PE) to afford the pure product **2a-2g**.

III. Genral procedure for the Reaction



1a **2a** **3aa**

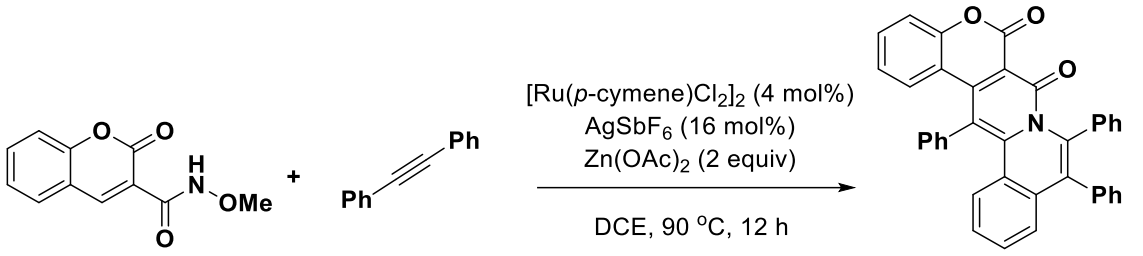
A mixture of **1a** (0.40 mmol, 1.0equiv.), **2a** (1.2 mmol, 3.0 equiv.), $AgSbF_6$ (0.16 mmol,0.4 equiv.), $Zn(OAc)_2$ (0.8 mmol, 2 equiv.) and $[Ru(p\text{-cymene})Cl_2]_2$ (0.04 mmol, 0.1 equiv.) was combined in DCE (1.0 mL) in a dried tube. The mixture was stirred at 90 ℃ and monitored by TLC. After the reaction was finished, the volatiles were removed under reduced pressure and the residue was purified by flash chromatography on silica gel to afford the desired products.



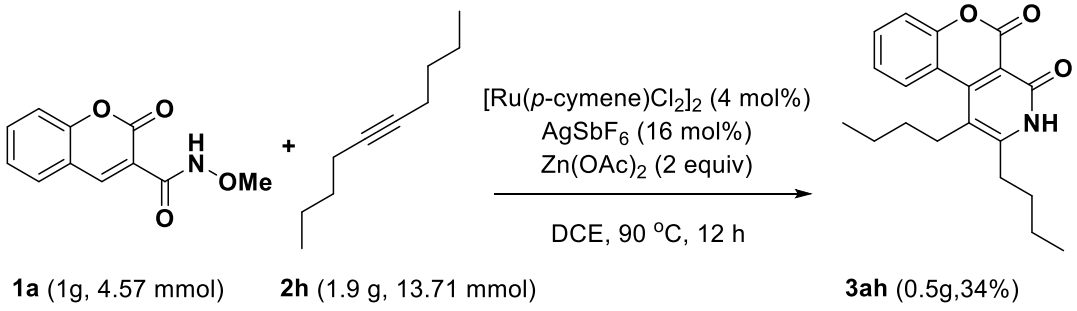
A mixture of **1a** (0.40 mmol, 1.0 equiv.), **2h** (1.2 mmol, 3.0 equiv.), $AgSbF_6$ (0.16 mmol, 0.4 equiv.), Zn(OAc)2 (0.8 mmol, 2 equiv.) and [Ru(*p*-cymene)Cl_2]$_2$ (0.04 mmol, 0.1 equiv.) was combined in DCE (1.0 mL) in a dried tube. The mixture was stirred at 90 ℃ and monitored by TLC. After the reaction was finished, the volatiles were removed under reduced pressure and the residue was purified by flash chromatography on silica gel to afford the desired products **3ah**.

IV. Synthesis application

(a) Gram-scale Preparation

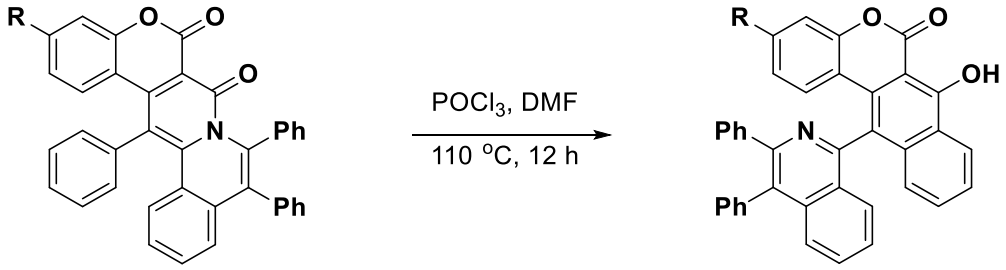


In a 100 mL reaction tube, the mixture of **1a** (1g, 4.57 mmol, 1.0 equiv.), **2a** (2.44g, 13.71 mmol, 3 equiv.), [Ru(*p*-cymene)Cl_2]$_2$ (111.8 mg, 4 mol %), $AgSbF_6$ (250 mg, 16 mol %), $Zn(OAc)_2$ (1.68 g, 9.14 mmol) and DCE (50 mL). Then the resulting mixture was stirred at 90 °C for 12 h. After that, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using DCM/MeOH to afford the product **3aa** (1.59g, yield: 65%).



In a 100 mL reaction tube, the mixture of **1a** (1g, 4.57 mmol, 1.0 equiv.), **2h** (1.9 g, 13.71 mmol, 3 equiv.), [Ru(*p*-cymene)Cl_2]$_2$ (111.8 mg, 4 mol %), $AgSbF_6$ (250 mg, 16 mol %), $Zn(OAc)_2$ (1.68 g, 9.14 mmol) and DCE (50 mL). Then the resulting mixture was stirred at 90 ^oC for 12 h. After that, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using DCM/MeOH to afford the product **3ah** (0.5 g, yield: 34%).

(b) Transformation of **3aa** and **3ga**

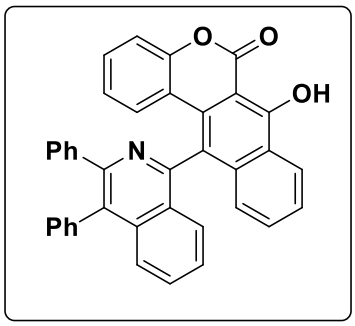


R = H, 3aa
R = CH_3, 3ga

R = H, 4a
R = CH_3, 4b

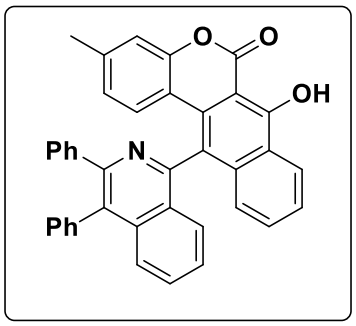
To a 25 mL round-bottom flask was added 1.5 mL *N*, *N*-dimethyllformamide (DMF)，and then was added 0.5 mL phosporus oxychoride ($POCl_3$) drop by drop under 0 °C ice bath. After stirring for 15 min, the mixed solvent was added a solution of **3aa** (108 mg, 0.2 mmoL in 1 mL DMF). Then the reaction was heated to 110 °C and stirred for 12 h. The reaction was removed to 0 ℃ ice bath and was added saturated Na_2CO_3 solution dropwise until the pH to 7~9. Then the reaction mixture was extracted with EtOAc (5 mL×3），the organic phase was collected and washed with brine, dried over anhydrous Na_2SO_4 , filtered, and concentrated under vacuum. The resulting residue was purified by column chromatography (PE/EA = 5/1, v/v) to afford **4a** as white solid (71.3 mg, 66% yield). Following thel procedure for synthesis of **4b**, afford **4b** as white solid (57% yield).

12-(3,4-Diphenylisoquinolin-1-yl)-7-hydroxy-6H-naphtho[2,3-c]chromen-6-one (**4a**)



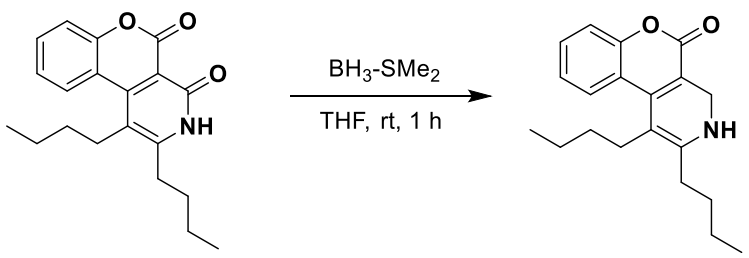
^{1}H NMR (600 MHz, DMSO-d_6) δ(600 MHz, DMSO) δ 13.45 (s, 1H), 8.58 (d, J = 8.1 Hz, 1H), 7.77 – 7.66 (m, 4H), 7.62 – 7.46 (m, 5H), 7.47 – 7.31 (m, 6H), 7.17 (d, J = 7.7 Hz, 4H), 6.87 (t, J = 7.5 Hz, 1H), 6.33 (d, J = 8.3 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 168.42, 164.00, 160.18, 152.08, 151.97, 142.06, 139.05, 138.58, 138.23, 133.48, 133.36, 133.17, 133.02, 132.87, 132.22, 132.02, 130.52, 130.38, 129.88, 129.67, 129.39, 129.17, 128.78, 128.75, 128.72, 128.44, 128.10, 127.92, 127.65, 126.54, 125.55, 125.15, 124.86, 120.26, 119.84, 102.63. HRMS (ESI) m/z [M + H]$^+$ calculated for $C_{38}H_{24}NO_3^+$: 542.1751, found:542.1752.

12-(3,4-diphenylisoquinolin-1-yl)-7-hydroxy-3-methyl-6H-naphtho[2,3-c]chromen-6-one (**4b**)



^{1}H NMR (600 MHz, DMSO-d_6) δ 13.47 (s, 1H), 8.58 (d, J = 7.6 Hz, 1H), 7.78 – 7.67 (m, 4H), 7.63 – 7.51 (m, 3H), 7.51 – 7.41 (m, 3H), 7.37 – 7.29 (m, 5H), 7.25 – 7.17 (m, 5H), 1.83 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 174.51, 166.83, 162.34, 158.74, 150.55, 148.35, 140.43, 137.23, 136.85, 136.54, 133.21, 131.80, 131.46, 131.16, 131.04, 131.00, 130.22, 129.86, 129.00, 128.87, 128.27, 128.04, 127.83, 127.52, 127.40, 127.19, 127.03, 126.47, 126.19, 125.76, 123.89, 123.36, 123.11, 118.08, 117.73, 100.96, 55.12. HRMS (ESI) m/z [M + H]$^+$ calculated for $C_{39}H_{26}NO_3^+$: 556.1907, found:556.191.

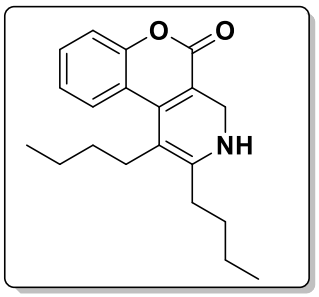
(c) Transformation of **3ah**



3ah **5**

To a 25 mL round-bottom flask was added 65 mg **3ah**（0.2 mmol）and dissolved in 1 mL dry tetrahydrofuran, after addition of 0.8 mL borane-methyl sulfide complex (2M solution in THF, 1.6 mmol) drop by drop under cooling in an ice bath, then ice-bath was removed, warmed to r.t. and stirred for 1 h. After TLC indicating full consumption of the starting material and the reaction mixture was added 4 mL water. Then the reaction mixture was extracted with 4 mL EtOAc, and the organic phase was collected and washed with brine, dried over anhydrous Na_2SO_4 , filtered, and concentrated under vacuum. The resulting residue was purified by column chromatography (DCM/MeOH = 10:1, v/v) to afford **5** as pale yellow solid (51 mg, 82% yield).

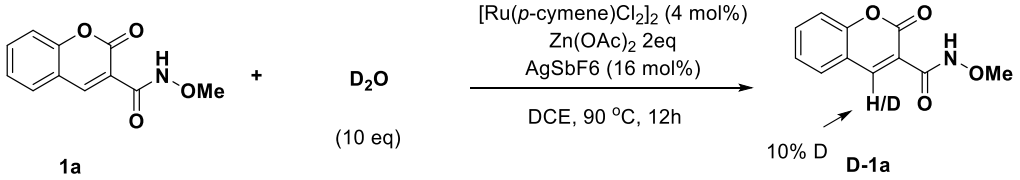
1,2-Dibutyl-3,4-dihydro-5H-chromeno[3,4-c]pyridin-5-one (**5**)



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.22 (m, 1H), 6.97 (d, *J* = 8.2 Hz, 1H), 6.89 (t, *J* = 7.3 Hz, 1H), 6.80 (d, *J* = 6.4 Hz, 1H), 4.45 (d, *J* = 13.1 Hz, 1H), 4.12 – 3.64 (m, 1H), 2.69 – 2.52 (m, 2H), 2.32 – 1.99 (m, 2H), 1.68 (d, *J* = 5.4 Hz, 2H), 1.47 – 0.76 (m, 10H), 0.63 (t, *J* = 7.2 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.86, 153.06, 150.31, 145.79, 130.02, 129.29, 126.21, 119.67, 119.38, 117.37, 60.68, 32.75, 32.16, 30.95, 27.45, 23.09, 22.68, 13.59, 13.46. HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{20}H_{26}NO_2^+$: 312.1958, found:312.1958.

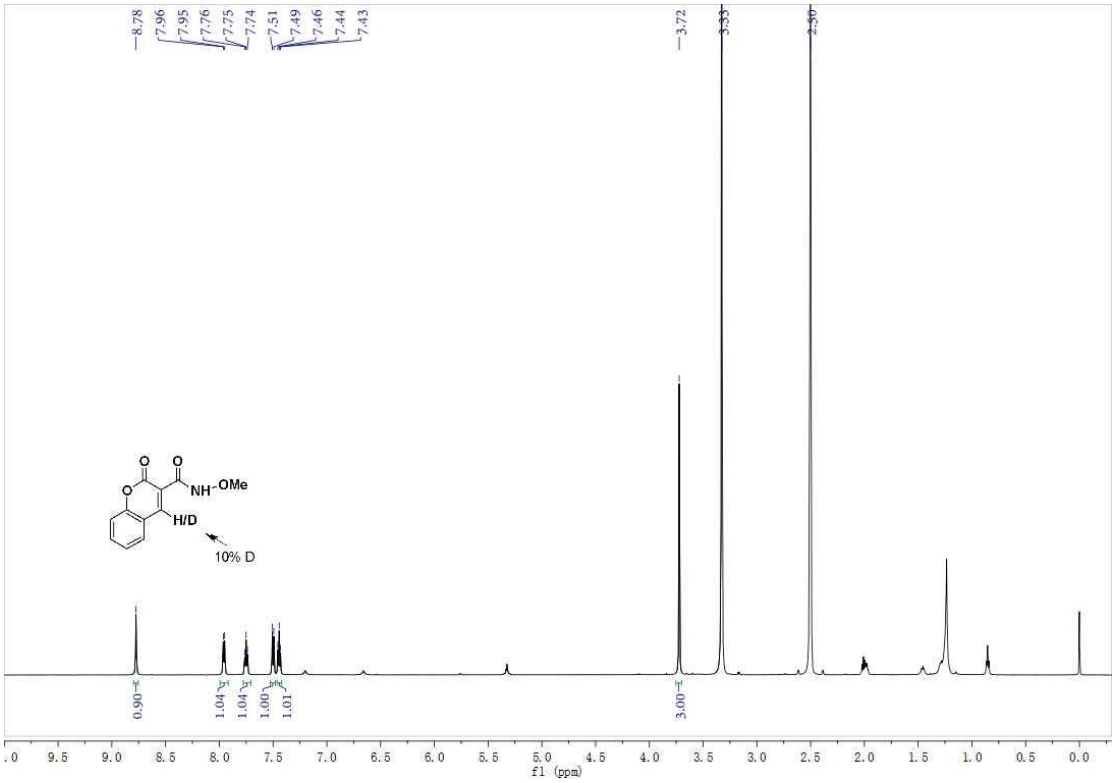
V. Mechanistic Studies

(a) H/D exchange experiment



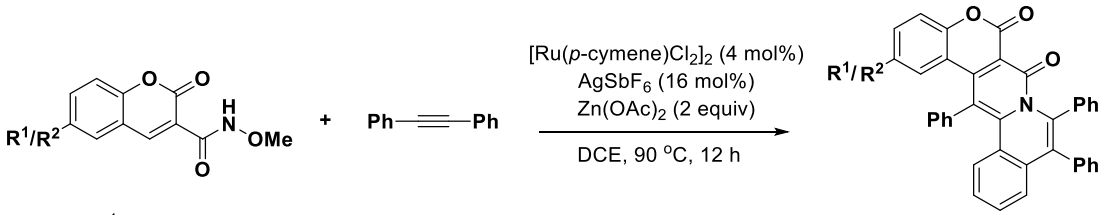
A pressure tube was charged with N-Methoxy-coumarin-3-carboxamide (**1a**, 21.9 mg, 0.1 mmol) and D_2O (20 mg, 1 mmol), $[Ru(p\text{-cymene})Cl_2]_2$ (2.4 mg, 4 mol %),

$AgSbF_6$ (5.5 mg, 16 mol %), $Zn(OAc)_2$ (36.7 mg, 0.2 mmol) and DCE (2 mL). The reaction mixture was stirred at 90 ºC in oil bath for 12 h. After that, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using DCM/MeOH to afford the product **D-1a.**



^{1}H NMR Spectrum of **D-1a** (DMSO-d_6, 500 MHz)

(b) Competition experiment



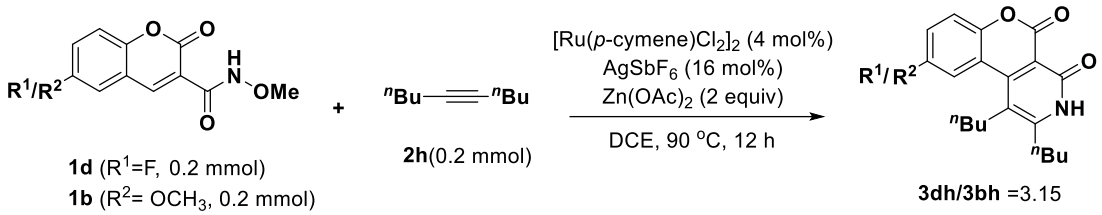
1d (R^1=F, 0.2 mmol)
1c (R^2= CH_3, 0.2 mmol)

2a (0.2 mmol)

3da/3ca =1.35

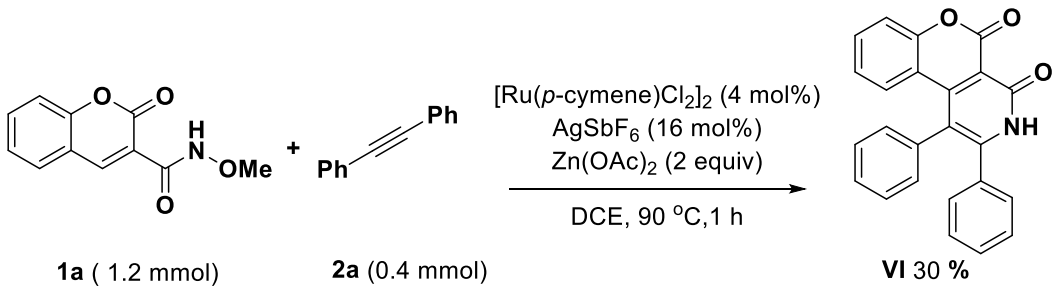
A pressure tube was charged with N,6-Dimethoxy-2-oxo-2H-chromene-3-carboxamide (**1d,** 47.4 mg, 0.2 mmol), N,6-dimethoxy-2-oxo-2H-chromene-3-carboxamide (**1c,** 49.8 mg, 0.2 mmol), 1,2-diphenylethyne (**2a,** 35.6 mg, 0.2 mmol), $[Ru(p\text{-cymene})Cl_2]_2$ (4.9 mg, 4 mol %), $AgSbF_6$ (11.0 mg, 16 mol %), $Zn(OAc)_2$ (73.4 mg, 0.4 mmol) and DCE (2 mL). The reaction mixture was stirred at 90 ºC in oil bath for 12 h. After that, the solvent was removed under reduced pressure and the residue was purified by silica gel

chromatography using DCM/MeOH to afford the product **3da** and **3ca.** The ratio of **3da**/**3ca** = 1.35.



A pressure tube was charged with N,6-Dimethoxy-2-oxo-2H-chromene-3-carboxa mide (**1d,** 47.4 mg, 0.2 mmol), N-methoxy-6-methyl-2-oxo-2H-chromene-3-carbo xamide (**1b,** 46.6 mg, 0.2 mmol), dec-5-yne (**2h,** 27.7 mg, 0.2 mmol), [Ru(*p*-c ymene)Cl_2]$_2$ (4.9 mg, 4 mol %), $AgSbF_6$ (11.0 mg, 16 mol %), $Zn(OAc)_2$ (73. 4 mg, 0.4 mmol) and DCE (2 mL). The reaction mixture was stirred at 90 °C in oil bath for 12 h. After that, the solvent was removed under reduced press ure and the residue was purified by silica gel chromatography using DCM/Me OH to afford the product **3dh** and **3bh.** The ratio of **3dh**/**3bh** = 3.15.

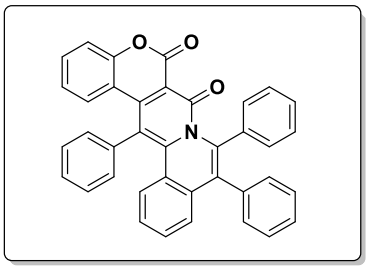
(c) Intermediate trapping experimen



A mixture of **1a** (1.2 mmol, 3.0 equiv.), **2a** (0.4 mmol, 1.0 equiv.), $AgSbF_6$ (0.48 mmol, 0.4 equiv.), $Zn(OAc)_2$ (2.4 mmol, 2 equiv.) and [Ru(*p*-cymene)Cl_2]$_2$ (0.12 mmol, 0.1 equiv.) was combined in DCE (4.0 mL) in a dried tube. The mixture was stirred at 90 ℃ for 1 h. After the reaction was finished, the volatiles were removed under reduced pressure and the residue was purified by flash chromatography on silica gel to afford the desired products **VI**.

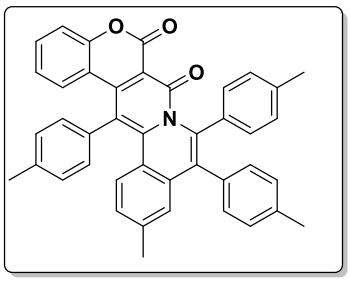
VI. Charaterization Date of Products

9,10,15-Triphenyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3aa**)



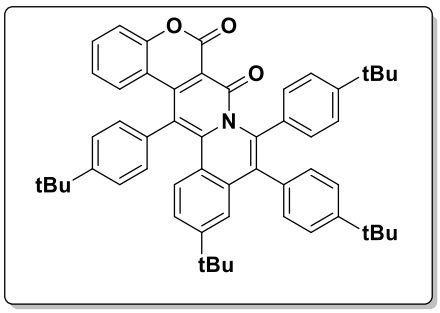
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.62 – 7.55 (m, 1H), 7.56 – 7.49 (m, 4H), 7.49 – 7.42 (m, 2H), 7.36 – 7.13 (m, 9H), 7.10 – 6.96 (m, 5H), 6.84 – 6.75 (m, 1H), 6.75 – 6.67 (m, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.70, 155.61, 153.58, 147.60, 144.78, 139.30, 136.40, 135.82, 134.92, 134.15, 132.56, 132.41, 131.15, 131.10, 130.35, 129.20, 129.11, 128.95, 128.68, 128.34, 128.05, 127.48, 127.32, 127.17, 126.30, 125.43, 125.06, 122.64, 117.19, 116.99, 115.39, 105.85. HRMS (ESI) m/z [M + H]$^+$ calculated for $C_{38}H_{24}NO_3^+$:542.1751, found: 542.1752.

12-Methyl-9,10,15-tri-p-tolyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ab**)



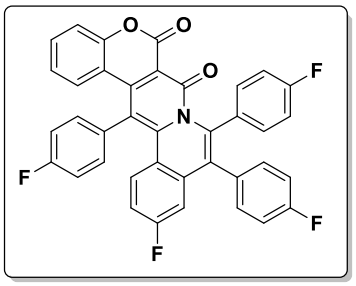
^{1}H NMR (600 MHz, DMSO-d_6) δ 7.50 – 7.42 (m, 1H), 7.40 – 7.29 (m, 5H), 7.18 – 7.03 (m, 6H), 6.99 – 6.80 (m, 6H), 6.79 – 6.72 (m, 1H), 2.45 (s, 3H), 2.29 (s, 3H), 2.21 (s, 3H), 2.18 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 158.33, 156.17, 153.97, 147.88, 145.74, 141.83, 138.96, 137.06, 136.94, 136.84, 135.06, 133.60, 132.87, 132.65, 132.51, 131.41, 129.46, 129.20, 129.15, 128.60, 128.32, 128.04, 125.65, 123.40, 123.10, 117.58, 115.14, 105.41, 21.60, 21.55, 21.31, 21.25. HRMS (ESI) m/z [M + Na]$^+$ calculated for $C_{42}H_{31}NNaO_3^+$: 620.2196, found: 620.2194.

12-(tert-Butyl)-9,10,15-tris(4-(tert-butyl)phenyl)-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ac**)



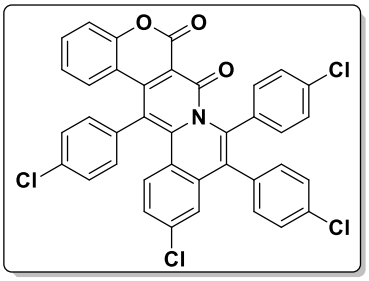
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.55 (d, J = 8.3 Hz,2H), 7.47 – 7.37 (m, 3H), 7.33 – 7.23 (m, 4H), 7.11 – 6.91 (m, 8H), 6.75 (t, J = 7.7 Hz, 1H), 6.69 (d, J = 7.4 Hz, 1H), 1.38 (s, 9H), 1.22 (s,9H), 1.14 (s, 9H), 1.09 (s, 9H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.73, 155.75, 153.80, 153.46, 152.11, 149.56, 149.02, 147.26, 144.87, 136.65, 136.44, 134.11, 133.26, 132.37, 131.99, 131.91, 130.78, 129.59, 128.88, 128.67, 128.62, 127.04, 124.31, 124.01, 123.54, 122.96, 122.45, 121.29, 117.07, 114.59, 104.71, 34.61, 34.60, 34.18, 34.06, 31.15, 30.96, 30.87, 30.32. HRMS (ESI) m/z [M + H]$^{+}$ calculated for $C_{54}H_{56}NO_3^{+}$: 766.4255, found: 766.4257.

12-Fluoro-9,10,15-tris(4-fluorophenyl)-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ad**)



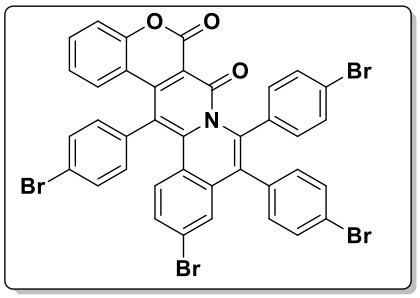
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.63 – 7.55 (m, 2H), 7.54 – 7.46 (m, 1H), 7.46 – 7.39 (m, 2H), 7.36 – 7.24 (m, 5H), 7.21 – 7.02 (m, 4H), 7.00 – 6.87 (m, 3H), 6.86 – 6.81 (m, 1H), 6.70 (d, J = 7.8 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 163.18 (d, J = 252.0 Hz), 163.09 (d, J = 247.5 Hz), 161.92 (d, J = 244.9 Hz), 161.61 (d, J = 245.0 Hz), 157.92 (s), 155.97 (s), 154.08 (s), 148.46 (s), 144.82 (s), 137.37 (s), 137.30 (s), 135.80 (d, J = 3.2 Hz), 134.94 (d, J = 8.0 Hz), 133.63 (d, J = 8.2 Hz), 133.18 (s), 132.51 (d, J = 9.8 Hz), 132.37 (d, J = 3.0 Hz), 131.72 (d, J = 8.3 Hz), 131.09 (d, J = 3.0 Hz), 128.90 (s), 127.24 (s), 123.26 (s), 122.26 (d, J = 1.4 Hz), 118.05 (d, J = 21.5 Hz), 117.73 (s), 117.25 (s), 115.76 (d, J = 21.6 Hz), 115.26 (d, J = 23.0 Hz), 114.76 (d, J = 17.1 Hz), 114.65 (s), 110.99 (d, J = 22.8 Hz), 106.43 (s). HRMS (ESI) m/z [M + H]$^{+}$ calculated for $C_{38}H_{20}F_4NO_3^{+}$: 614.1374, found: 614.1371.

12-Chloro-9,10,15-tris(4-chlorophenyl)-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ae**)



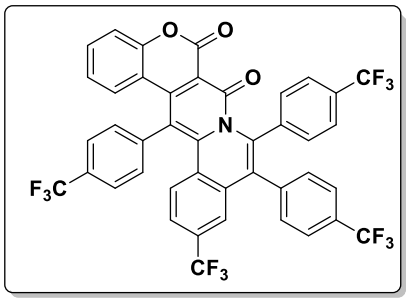
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.11 – 7.85 (m, 2H), 7.80 – 7.71 (m, 1H), 7.68 – 7.38 (m, 7H), 7.38 – 7.16 (m, 6H), 7.08 – 6.84 (m, 2H), 6.74 – 6.64 (m, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.64, 160.45, 157.43, 155.57, 154.16, 153.76, 148.17, 148.13, 147.94, 144.13, 137.80, 136.76, 136.21, 135.65, 134.28, 134.22, 133.11, 133.01, 132.36, 131.07, 130.69, 130.38, 128.60, 128.52, 127.58, 127.52, 126.31, 125.21, 124.31, 123.91, 123.02, 119.41, 118.57, 117.45, 116.76, 116.24, 114.77, 106.74. HRMS (ESI) m/z [M +Na]$^+$ calculated for $C_{38}H_{19}Cl_4NNaO_3^+$: 700.0011, found: 700.0023

12-Bromo-9,10,15-tris(4-bromophenyl)-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3af**)



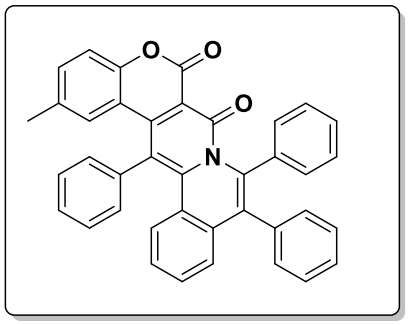
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.76 (d, J = 8.4 Hz, 2H), 7.59 – 7.46 (m, 5H), 7.41 – 7.29 (m, 4H), 7.28 – 7.14 (m, 5H), 6.95 – 6.87 (m, 2H), 6.72 – 6.65 (m, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.29, 155.44, 153.64, 148.02, 144.03, 138.03, 136.58, 135.57, 134.65, 134.41, 133.49, 133.42, 133.29, 132.91, 131.40, 131.22, 130.88, 130.37, 129.52, 128.45, 127.25, 126.05, 125.14, 124.10, 122.91, 122.81, 121.49, 121.03, 117.34, 116.63, 114.74, 106.66. HRMS (ESI) m/z [M + H]$^+$ calculated for $C_{38}H_{20}Br_4NO_3^+$: 853.8171, found: 853.8169

12-(Trifluoromethyl)-9,10,15-tris(4-(trifluoromethyl)phenyl)-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ag**)



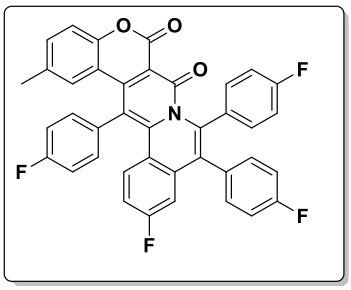
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.95 (d, J = 8.2 Hz, 2H), 7.85 (d, J = 8.1 Hz, 2H), 7.74 (d, J = 8.2 Hz, 2H), 7.60 (d, J = 8.0 Hz, 2H), 7.55 – 7.46 (m, 6H), 7.43 – 7.31 (m, 2H), 7.14 (d, J = 8.7 Hz, 1H), 6.96 – 6.83 (m, 1H), 6.64 – 6.52 (m, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.05, 155.30, 153.69, 148.43, 143.13, 142.91, 139.27, 138.25, 136.45, 133.84, 133.26, 133.16, 132.17, 130.68, 130.52, 130.42, 129.98, 129.62, 128.69, 128.38, 128.06, 127.77, 127.24, 126.55, 125.21, 125.04, 124.20, 123.04, 122.91, 122.10, 121.35, 117.40, 116.38, 115.74, 108.07. HRMS (ESI) m/z [M +Na]$^+$ calculated for $C_{42}H_{19}F_{12}NNaO_3^+$: 836.1066, found: 836.1065

2-Methyl-9,10,15-triphenyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ba**)



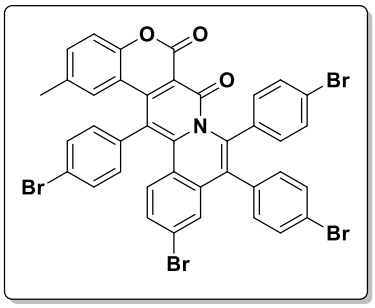
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.63 – 7.57 (m, 1H), 7.58 – 7.49 (m, 4H), 7.49 – 7.42 (m, 1H), 7.37 – 7.29 (m, 2H), 7.29 – 7.25 (m, 1H), 7.25 – 7.21 (m, 2H), 7.22 – 7.17 (m, 3H), 7.16 (s, 1H), 7.10 – 7.06 (m, 3H), 7.06 – 6.99 (m, 2H), 6.66 (d, J = 8.6 Hz, 1H), 6.57 (d, J = 8.5 Hz, 1H), 2.30 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.67, 155.66, 153.61, 147.74, 144.53, 143.56, 139.32, 136.34, 135.81, 134.91, 134.10, 132.33, 131.05, 131.02 , 130.28, 129.08, 129.05, 128.87, 128.35, 128.12, 127.98, 127.39, 127.22 , 127.10, 126.21, 125.34, 125.00, 123.76, 117.03, 115.17, 114.30, 105.37, 20.69. HRMS (ESI) m/z [M + H]$^+$ calculated for $C_{39}H_{26}Br_4NO_3^+$: 556.1907, found: 556.1902

12-Fluoro-9,10,15-tris(4-fluorophenyl)-2-methyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3bd**)



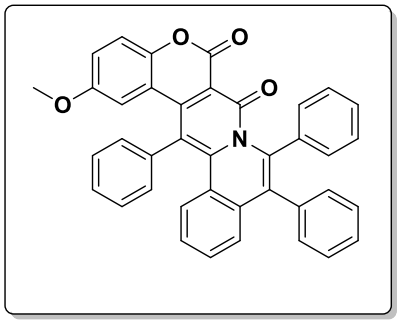
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.60 – 7.54 (m, 2H), 7.47 – 7.37 (m,2H), 7.34 – 7.28 (m, 2H), 7.28 – 7.22 (m, 2H), 7.21 – 7.15 (m, 3H), 7.14 – 7.07 (m, 1H), 7.07 – 7.01 (m, 1H), 7.00 – 6.92 (m, 2H), 6.82 (dd, *J* = 9.9, 2.7 Hz, 1H), 6.77 – 6.72 (m, 1H), 6.54 (d, *J* = 8.5 Hz, 1H), 2.31 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.93 (d, *J* = 251.9 Hz), 162.84 (d, *J* = 247.4 Hz), 161.69 (d, *J* = 245.1 Hz), 161.38 (d, *J* = 245.0 Hz), 157.74 (s), 155.88 (s), 153.95 (s), 148.43 (s), 144.41 (s), 144.07 (s), 137.15 (s), 137.08 (s), 135.65 (d, *J* = 3.3 Hz), 134.69 (d, *J* = 8.0 Hz), 133.42 (d, *J* = 8.1 Hz), 132.27 (d, *J* = 9.8 Hz), 132.20 (d, *J* = 3.0 Hz), 131.49 (d, *J* = 8.4 Hz), 130.91 (d, *J* = 2.9 Hz), 128.39 (s), 126.87 (d, *J* = 2.1 Hz), 124.23 (s), 122.02 (s), 117.82 (d, *J* = 21.5 Hz), 117.41 (s), 115.53 (d, *J* = 21.3 Hz), 115.00 (d, *J* = 23.1 Hz), 114.51 (d, *J* = 22.3 Hz), 114.40 (s), 114.32 (s), 110.74 (d, *J* = 23.2 Hz), 105.77 (s), 21.00 (s). HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{39}H_{22}F_4NO_3^+$: 628.153, found: 628.1527

12-Bromo-9,10,15-tris(4-bromophenyl)-2-methyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3bf**)



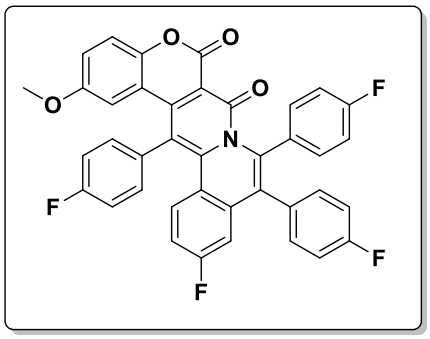
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.76 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.42 – 7.37 (m, 1H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.21 – 7.13 (m, 4H), 6.90 (d, *J* = 9.0 Hz, 1H), 6.80 – 6.71 (m, 1H), 6.53 (d, *J* = 8.5 Hz, 1H), 2.31 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ157.34, 155.58, 153.73, 148.20, 144.09, 143.86, 138.12, 136.58, 135.59, 134.70, 134.40, 133.48, 133.30, 131.39, 131.21, 130.88, 130.36, 129.50, 128.16, 127.22, 125.89, 125.06, 124.10, 122.75, 121.46, 120.98, 117.24, 114.60, 114.01, 106.17, 20.80. HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{39}H_{22}Br_4NO_3^+$: 867.8323, found: 867.8329

2-Methoxy-9,10,15-triphenyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ca**)



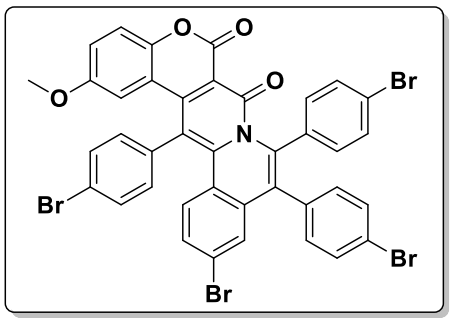
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.59 (s, 5H), 7.48 (t, J = 7.6 Hz, 1H), 7.36 – 7.16 (m, 9H), 7.15 – 6.95 (m, 6H), 6.38 (d, J = 2.8 Hz, 1H), 3.19 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ157.75, 155.80, 153.79, 147.94, 147.33, 144.66, 139.39, 136.40, 135.80, 134.93, 134.16, 132.53, 131.11, 130.50, 129.21, 129.10, 128.97, 128.31, 128.06, 127.48, 127.33, 127.20, 126.31, 125.43, 125.03, 120.95, 118.12, 117.11, 115.28, 114.42, 111.07, 106.04, 54.83. HRMS (ESI) m/z [M + H]$^{+}$ calculated for $C_{39}H_{26}NO_4^{+}$: 572.1856, found: 572.1854

12-Fluoro-9,10,15-tris(4-fluorophenyl)-2-methoxy-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3cd**)



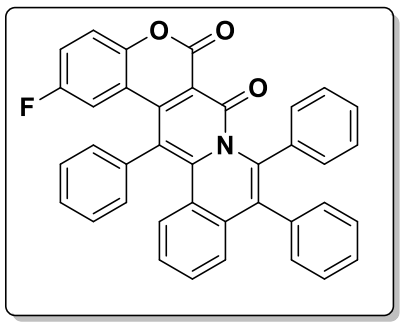
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.70 – 7.58 (m, 2H), 7.51 – 7.40 (m,2H), 7.36 – 7.24 (m, 5H), 7.22 – 7.09 (m, 4H), 7.08 – 7.01 (m, 1H), 7.01 – 6.94 (m,2H), 6.92 – 6.78 (m, 1H), 6.29 (d, J = 2.9 Hz,1H), 3.28 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) 162.45 (d, J = 252.1 Hz), 162.36 (d, J = 247.7 Hz), 161.20 (d, J = 245.2 Hz), 160.89 (d, J = 245.2 Hz), 157.99 (s), 156.16 (s), 154.28 (s), 148.47 (s), 148.16 (s), 144.70 (s), 137.37 (s), 137.31 (s), 135.86 (d, J = 3.3 Hz), 135.10 (d, J = 7.8 Hz), 133.65 (d, J = 8.2 Hz), 132.56 (d, J = 9.1 Hz), 132.35 (d, J = 3.0 Hz), 131.72 (d, J = 8.2 Hz), 131.10 (d, J = 2.8 Hz), 127.23 (d, J = 2.8 Hz), 122.24 (s), 121.40 (s), 118.71 (s), 118.15 (d, J = 21.4 Hz), 117.41 (s), 115.78 (d, J = 21.5 Hz), 115.29 (d, J = 22.7 Hz), 114.77 (d, J = 21.7 Hz), 114.56 (s), 111.44 (s), 111.00 (d, J = 23.0 Hz), 106.63 (s), 55.26 (s). HRMS (ESI) m/z [M + H]$^{+}$ calculated for $C_{39}H_{22}F_4NO_3^{+}$: 644.1479, found: 644.1481

12-Bromo-9,10,15-tris(4-bromophenyl)-2-methoxy-6H,7H-chromeno[4',3':4,5]pyrido [2,1-a]isoquinoline-6,7-dione (**3cf**)



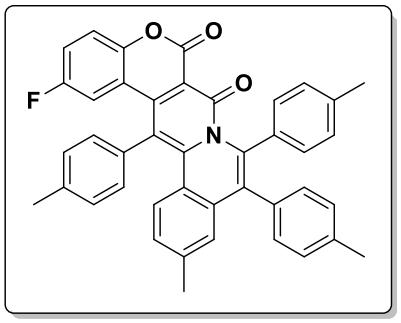
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.79 (d, J = 8.4 Hz, 2H), 7.59 – 7.51 (m,4H), 7.43 – 7.36 (m, 1H), 7.35 – 7.22 (m,5H), 7.22 – 7.09 (m,4H), 6.95 (d, J = 9.1 Hz, 1H), 6.19 (d, J =1 Hz, 1H), 3.24 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 174.31, 157.40, 155.65, 153.80, 148.06, 147.71, 143.86, 138.11, 136.58, 135.59, 134.65, 134.59, 133.61, 133.44, 133.30, 131.40, 131.21, 130.99, 130.38, 129.57, 127.25, 126.05, 125.14, 124.08, 122.92, 121.48, 121.01, 118.36, 116.74, 114.60, 110.60, 106.80, 54.61. HRMS (ESI) m/z [M + H]$^+$ calculated for $C_{39}H_{22}Br_4NO_4^+$: 883.8277, found: 883.8276

2-Fluoro-9,10,15-triphenyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3da**)



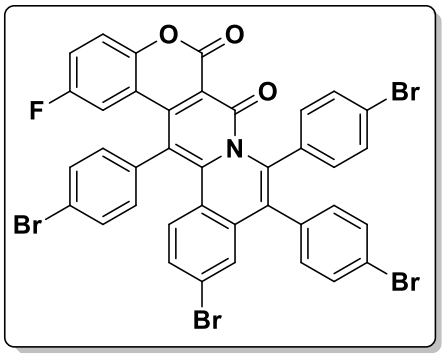
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.67 – 7.60 (m, 1H), 7.61 – 7.51 (m, 4H), 7.49 – 7.43 (m, 1H), 7.37 (M, 2H), 7.34 – 7.24 (m, 3H), 7.23 – 7.16 (m, 5H), 7.07 (m, 5H), 6.30 – 6.22 (m, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.78, 156.58 (d, J = 237.9 Hz), 155.66, 150.08, 146.48 (d, J = 1.9 Hz), 145.07, 138.94, 136.54, 135.86, 134.94, 134.28, 132.52, 131.44, 131.17, 130.66, 129.59, 129.22, 129.19, 128.80, 128.20, 127.66, 127.52, 127.32, 126.53, 125.60, 125.07, 119.98 (d, J = 24.4 Hz), 119.00 (d, J = 8.4 Hz), 118.08 (d, J = 9.1 Hz), 115.30, 114.40 (d, J = 28.2 Hz), 105.78. HRMS (ESI) m/z [M +Na]$^+$ calculated for $C_{38}H_{22}FNNaO_3^+$: 582.1476, found: 582.1477

2-Fluoro-12-methyl-9,10,15-tri-p-tolyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1a]isoquinoline-6,7-dione (**3db**)



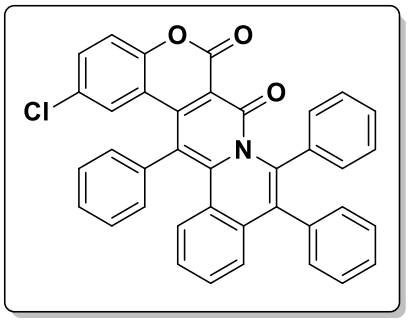
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.32 (m, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.22 (dd, *J* = 9.0, 5.1 Hz, 1H), 7.14 – 6.99 (m, 9H), 6.88 (d, *J* = 7.9 Hz, 2H), 6.84 – 6.78 (m, 1H), 6.43 – 6.35 (m, 1H), 2.52 (s, 3H), 2.35 (s, 3H), 2.27 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ159.14, 157.33 (d, *J* = 240.6 Hz), 156.92, 150.41, 146.36 (d, *J* = 2.4 Hz), 146.25, 141.84, 139.55, 137.61, 137.41, 137.14, 136.28, 135.32, 132.92, 132.35, 132.26, 131.49, 131.13, 129.41, 129.22, 128.94, 128.53, 127.85, 125.95, 123.14, 119.45 (d, *J* = 24.4 Hz), 118.78 (d, *J* = 8.4 Hz), 118.46 (d, *J* = 9.1 Hz), 115.26, 115.04, 114.64, 105.35, 21.80, 21.66, 21.46. HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{42}H_{31}FNO_3^+$: 616.2282, found: 616.2285

12-Bromo-9,10,15-tris(4-bromophenyl)-2-fluoro-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3df**)



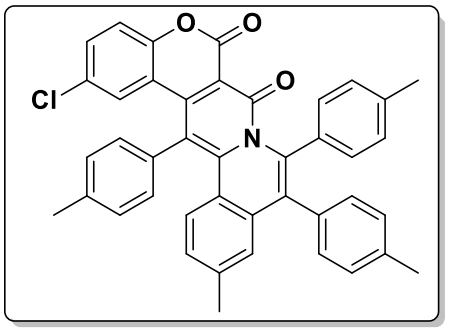
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.82 (d, *J* = 8.4 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.53 (d, *J* = 8.4 Hz, 2H), 7.48 – 7.41 (m,3H), 7.35 (d, *J* = 8.5 Hz, 2H), 7.29 – 7.16 (m, 5H), 7.00 (d, *J* = 9.0 Hz, 1H), 6.38 – 6.16 (m, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.90, 156.71 (d, *J* = 245.2 Hz), 156.00, 150.53, 147.24, 144.58, 138.03, 137.05, 136.02, 135.02, 134.90, 134.12, 133.81, 133.72, 131.87, 131.68, 131.45, 130.84, 130.13, 127.76, 126.79, 125.78, 124.44, 123.50, 121.98, 121.53, 120.68 (d, *J* = 22.5 Hz), 119.60 (d, *J* = 8.7 Hz), 118.05 (d, *J* = 9.1 Hz), 114.90, 114.42 (d, *J* = 27.8 Hz), 107.12. HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{38}H_{19}Br_4FNO_3^+$: 871.8077, found: 871.807

2-Chloro-9,10,15-triphenyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ea**)



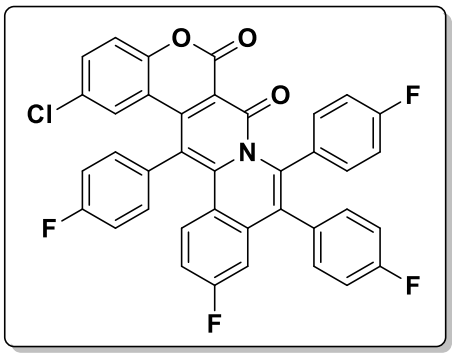
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.70 – 7.41 (m, 7H), 7.39 – 7.14 (m, 9H), 7.16 – 7.01 (m, 5H), 6.54 (d, J = 2.4 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.57, 155.27, 152.22, 146.16, 144.99, 138.93, 136.45, 135.75, 134.84, 134.17, 132.34, 132.00, 131.35, 131.07, 130.50, 129.65, 129.40, 129.11, 128.67, 128.25, 128.07, 127.52, 127.37, 127.18, 126.65, 126.42, 125.51, 124.95, 118.96, 118.37, 115.12, 105.71. HRMS (ESI) m/z [M + H]$^+$ calculated for $C_{38}H_{23}ClNO_3^+$: 576.1361, found: 576.1354

2-Chloro-12-methyl-9,10,15-tri-p-tolyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3eb**)



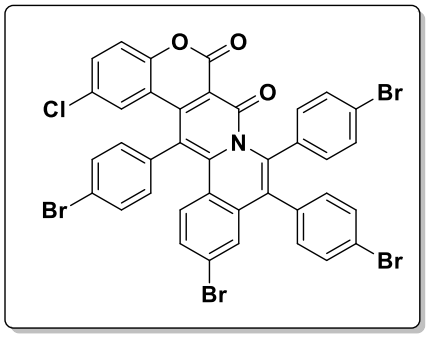
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.50 (dd, J = 8.8, 2.5 Hz, 1H), 7.38 (d, J = 2.8 Hz, 4H), 7.32 (d, J = 8.8 Hz, 1H), 7.15 – 7.01 (m, 7H), 6.99 – 6.91 (m, 2H), 6.88 (d, J = 8.0 Hz, 2H), 6.50 (d, J = 2.4 Hz, 1H), 2.45 (s, 3H), 2.28 (s, 3H), 2.20 (s, 3H), 2.17 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.71, 155.31, 152.09, 145.94, 145.35, 141.60, 138.87, 136.63, 136.48, 136.40, 136.01, 134.59, 133.03, 132.08, 131.93, 131.77, 130.99, 130.87, 128.95, 128.71, 128.43, 128.27, 127.82, 127.68, 126.60, 125.20, 122.78, 118.80, 118.43, 114.87, 114.35, 104.72, 21.12, 20.98, 20.80, 20.74. HRMS (ESI) m/z [M + H]$^+$ calculated for $C_{42}H_{31}ClNO_3^+$: 632.1987, found: 632.1989

2-Chloro-12-fluoro-9,10,15-tris(4-fluorophenyl)-6H,7H-chromeno[4',3':4,5]pyrido[2, 1-a]isoquinoline-6,7-dione (**3ed**)



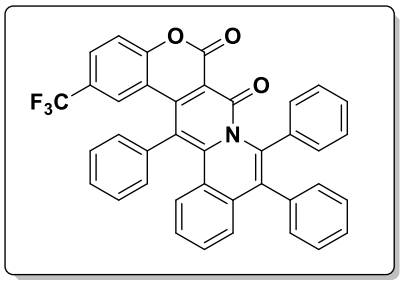
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.67 – 7.54 (m, 3H), 7.52 – 7.44 (m, 2H), 7.38 (d, J = 8.8 Hz, 1H), 7.33 – 7.23 (m, 4H), 7.21 – 7.14 (m, 4H), 7.07 – 6.93 (m, 2H), 6.89 – 6.78 (m, 1H), 6.51 (d, J = 2.4 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.87 (d, J = 247.7 Hz), 162.84 (d, J = 252.6 Hz), 161.50 (d, J = 244.9 Hz), 161.20 (d, J = 245.0 Hz), 157.35, 155.20, 152.27, 146.57, 144.59, 136.95, 136.89, 135.02 (d, J = 3.2 Hz), 134.51 (d, J = 7.9 Hz), 133.16 (d, J = 8.2 Hz), 132.22 (d, J = 9.5 Hz), 132.15, 131.85 (d, J = 2.9 Hz), 131.28 (d, J = 8.0 Hz), 130.56 (d, J = 2.6 Hz), 127.97, 127.16 (d, J = 1.9 Hz), 126.71, 121.73, 119.10, 118.18, 117.72 (d, J = 21.5 Hz), 115.35 (d, J = 21.5 Hz), 115.01 (d, J = 22.9 Hz), 114.32 (d, J = 21.6 Hz), 113.94, 110.62 (d, J = 23.0 Hz), 105.87. HRMS (ESI) m/z [M + H]$^+$ calculated for $C_{38}H_{19}F_4NO_3^+$: 648.0984, found: 648.0988

12-Bromo-9,10,15-tris(4-bromophenyl)-2-chloro-6H,7H-chromeno[4',3':4,5]pyrido[2, 1-a]isoquinoline-6,7-dione (**3ef**)



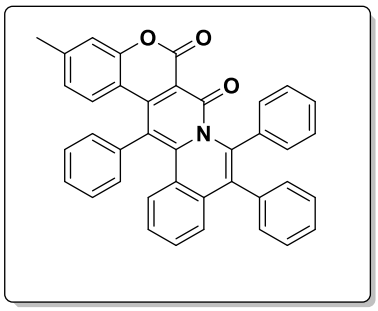
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.83 (d, J = 8.4 Hz, 2H), 7.61 – 7.56 (m, 3H), 7.52 (d, J = 8.4 Hz, 2H), 7.46 – 7.43 (m, 1H), 7.41 – 7.33 (m, 3H), 7.27 – 7.21 (m, 3H), 7.19 (d, J = 8.5 Hz, 2H), 7.06 (d, J = 9.0 Hz, 1H), 6.46 (d, J = 2.4 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.16, 155.11, 152.27, 146.58, 144.16, 137.69, 136.61, 135.54, 134.58, 134.36, 133.63, 133.33, 133.25, 132.29, 131.42, 131.21, 131.02, 130.38, 129.69, 127.96, 127.32, 126.78, 126.38, 125.38, 123.97, 123.09, 121.53, 121.08, 119.13, 117.98, 114.42, 106.59. HRMS (ESI) m/z [M + H]$^+$ calculated for $C_{38}H_{19}Br_4ClNO_3^+$: 887.7781, found: 887.7778

9,10,15-Triphenyl-2-(trifluoromethyl)-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3fa**)



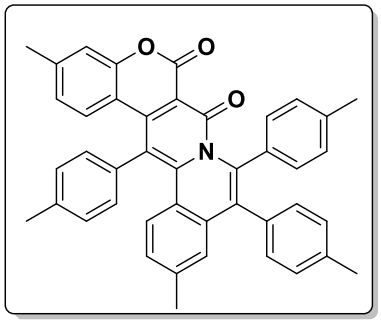
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.82 (dd, J = 8.7, 2.0 Hz, 1H), 7.65 – 7.55 (m, 5H), 7.55 – 7.47 (m, 2H), 7.37 – 7.20 (m, 8H), 7.17 – 7.07 (m, 5H), 7.01 (d, J = 1.0 Hz, 1H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.54, 155.80, 155.09, 146.23, 145.28, 138.90, 136.48, 135.73, 134.83, 134.20, 132.28, 132.22, 131.44, 131.06, 130.55, 129.66, 129.39, 129.13, 129.00, 128.78, 128.65, 128.08, 127.54, 127.39, 127.18, 126.44, 126.35, 125.54, 124.96, 118.44, 117.41, 115.19, 105.75. HRMS (ESI) m/z [M + H]$^+$ calculated for $C_{39}H_{23}F_3NO_3^+$: 610.1625, found: 610.1625

3-Methyl-9,10,15-triphenyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ga**)



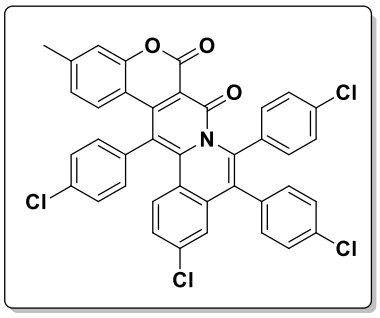
^{1}H NMR (600 MHz, DMSO-d_6) δ 7.62 (t, J = 7.2 Hz, 1H), 7.59 – 7.51 (m, 4H), 7.51 – 7.45 (m, 1H), 7.32 (t, J = 7.2 Hz, 3H), 7.30 – 7.25 (m, 1H), 7.25 – 7.17 (m, 6H), 7.16 – 7.13 (m, 1H), 7.11 – 7.05 (m, 4H), 6.39 (d, J = 1.0 Hz, 1H), 1.88 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d_6) δ 157.71, 155.72, 151.59, 147.55, 144.54, 139.46, 136.38, 135.83, 134.90, 134.11, 133.23, 132.43, 131.33, 131.12, 131.07, 130.20, 129.05, 128.97, 128.28, 128.02, 127.44, 127.27, 127.15, 126.28, 125.41, 125.02, 116.68, 116.47, 115.29, 105.83, 20.42. HRMS (ESI) m/z [M + H]$^+$ calculated for $C_{39}H_{26}NO_3^+$: 556.1907, found: 556.1908

3,12-Dimethyl-9,10,15-tri-p-tolyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoli ne-6,7-dione (**3gb**)



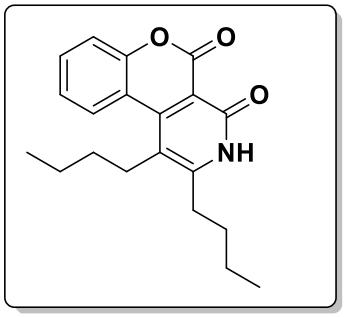
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.35 (s,4H), 7.23 – 7.01 (m, 7H), 7.00 – 6.80 (m, 5H), 6.75 – 6.53 (m, 2H), 2.45 (s, 3H), 2.29 (s, 3H), 2.28 (s,3H), 2.20 (s, 3H), 2.18 (s, 3H). ^{13}C NMR (126 MHz, DMSO) δ 157.90, 155.83, 153.59, 147.62, 145.09, 143.43, 141.28, 138.45, 136.59, 136.46, 136.34, 134.59, 133.19, 132.16, 132.09, 130.95, 128.99, 128.73, 128.42, 127.97, 127.85, 127.54, 125.17, 123.80, 122.93, 117.03, 116.88, 114.51, 114.48, 104.56, 21.13, 21.09, 20.85, 20.79, 20.73. HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{43}H_{34}NO_3^+$: 612.2553, found: 612.2534

12-Chloro-9,10,15-tris(4-chlorophenyl)-3-methyl-6H,7H-chromeno[4',3':4,5]pyrido[2 ,1-a]isoquinoline-6,7-dione (**3ge**)



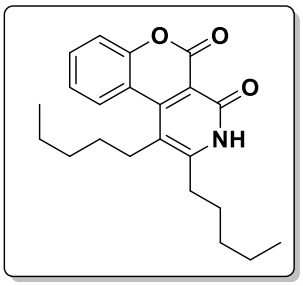
^{1}H NMR (500 MHz, DMSO-d_6) δ 7.65 – 7.61 (m, 2H), 7.58 – 7.51 (m,2H), 7.43 (d, J = 8.5 Hz,2H), 7.32 (d, J = 8.4 Hz,2H), 7.30 – 7.26 (m, 1H), 7.25 – 7.22 (m, 2H), 7.26 – 7.16 (m, 3H), 7.06 (d, J = 2.2 Hz, 1H), 6.99 (d, J = 9.0 Hz, 1H), 6.79 – 6.71 (m, 1H), 6.54 (d, J = 8.5 Hz, 1H), 2.31 (s,3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 157.35, 155.59, 153.73, 148.24, 144.07, 143.84, 137.77, 136.64, 136.01, 135.55, 134.35, 134.14, 134.11, 133.09, 133.01, 132.75, 132.21, 130.93, 130.57, 128.48, 128.16, 127.45, 126.72, 126.03, 124.16, 124.08, 123.79, 117.23, 114.52, 114.02, 106.14, 20.80. HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{39}H_{22}Cl_4NO_3^+$: 692.0348, found: 692.0348

1,2-Dibutyl-4H-chromeno[3,4-c]pyridine-4,5(3H)-dione (**3ah**)



^{1}H NMR (500 MHz, DMSO-d_6) δ 12.28 (s, 1H),8.00 (dd, J = 17.0, 4.3 Hz, 1H), 7.54 (d, J = 6.9 Hz, 1H), 7.27 (s, 2H), 2.69 (d, J = 62.2 Hz, 4H), 1.77 – 1.30 (m, 8H), 1.07 – 0.84 (m, 6H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 159.13, 156.74, 156.04, 152.61, 150.63, 132.03, 127.27, 123.12, 117.05, 111.60, 107.31, 31.90, 31.17, 30.60, 28.02, 22.04, 21.96, 13.32, 13.27. HRMS (ESI) m/z [M + H]$^+$ calculated for $C_{20}H_{24}NO_3^+$: 326.1751, found:326.1751

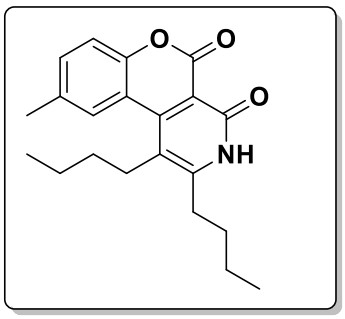
1,2-Dipentyl-4H-chromeno[3,4-c]pyridine-4,5(3H)-dione (**3ai**)



^{1}H NMR (500 MHz, DMSO-d_6) δ 12.22 (s, 1H), 8.03 (d, J = 7.9 Hz, 1H), 7.62 (t, J = 7.6 Hz, 1H), 7.33 (d, J = 7.7 Hz, 2H), 2.67 (d, J = 54.3 Hz, 4H), 1.58 (d, J = 5.6 Hz, 4H), 1.41 – 1.26 (m, 8H), 0.87 (t, J = 6.3 Hz, 6H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 158.64, 156.26, 153.08, 152.69, 150.58, 132.63, 127.59, 123.66, 117.35, 117.04, 111.50, 107.40, 31.10, 31.03, 29.41, 28.82, 28.27, 21.70, 21.59, 13.85, 13.77.

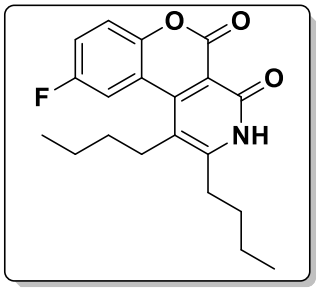
HRMS (ESI) m/z [M + H]$^+$ calculated for $C_{22}H_{28}NO_3^+$: 354.2064, found:354.2062

1,2-Dibutyl-9-methyl-4H-chromeno[3,4-c]pyridine-4,5(3H)-dione (**3bh**)



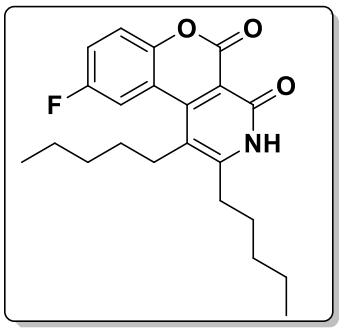
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, J = 8.4 Hz, 1H), 7.23 – 7.16 (m, 2H), 3.04 – 2.80 (m,4H), 2.47 (s, 3H), 1.83 – 1.65 (m, 4H), 1.63 – 1.44 (m, 4H), 1.10 – 0.95 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.54, 152.23, 143.33, 127.46, 125.88, 118.44, 115.28, 31.75, 31.68, 29.71, 29.30, 22.98, 22.84, 21.29, 13.92, 13.77. HRMS (ESI) m/z [M + H]$^+$ calculated for $C_{21}H_{26}NO_3^+$: 340.1907, found:340,1901

1,2-Dibutyl-9-fluoro-4H-chromeno[3,4-c]pyridine-4,5(3H)-dione (**3dh**)



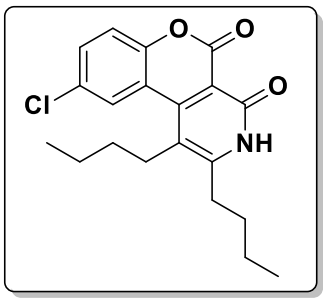
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 – 7.78 (m, 1H), 7.36 (ddd, *J* = 15.7, 11.2, 6.1 Hz, 2H), 3.07 – 2.80 (m, 4H), 1.86 – 1.69 (m, 4H), 1.66 – 1.47 (m, 4H), 1.14 – 0.94 (m, 6H). ^{13}C NMR (126 MHz, DMSO-d_6) 163.03, 158.32 (d, *J* = 242.9 Hz), 147.95, 119.20 (d, *J* = 8.6 Hz), 118.89 (d, *J* = 23.8 Hz), 113.59 (d, *J* = 27.1 Hz), 34.61, 31.27, 31.14, 28.54, 22.50, 22.23, 13.43, 13.21. HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{20}H_{23}FNO_3^+$: 344.1656, found:344.16551.

9-Fluoro-1,2-dipentyl-4H-chromeno[3,4-c]pyridine-4,5(3H)-dione (**3di**)



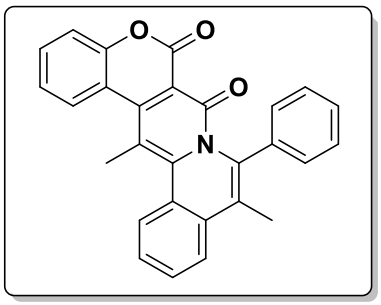
^{1}H NMR (500 MHz, DMSO-d_6) δ 12.32 (s, 1H), 7.73 (d, *J* = 11.0 Hz, 1H), 7.54 (t, *J* = 7.0 Hz, 1H), 7.41 (d, *J* = 4.7 Hz, 1H), 2.67 (d, *J* = 40.2 Hz, 4H), 1.58 (s,4H), 1.47 – 1.25 (m, 8H), 0.92 – 0.80 (m,6H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 175.35, 159.40, 158.57 (d, *J* = 268.5 Hz), 157.71, 157.14, 150.45 (d, *J* = 42.1 Hz), 120.97 (d, *J* = 23.6 Hz), 120.22 (d, *J* = 7.8 Hz), 118.87 (d, *J* = 8.0 Hz), 114.50 (d, *J* = 26.8 Hz), 112.53, 108.62, 32.17, 32.04, 30.23, 29.93, 29.80, 29.01, 22.79, 22.59, 14.90, 14.85. HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{22}H_{27}FNO_3^+$: 372.1969, found:372.1971.

1,2-Dibutyl-9-chloro-4H-chromeno[3,4-c]pyridine-4,5(3H)-dione (**3eh**)



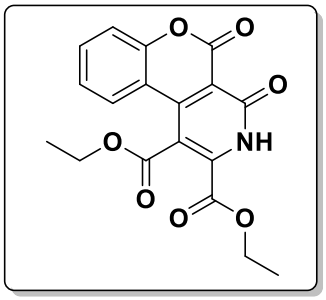
^{1}H NMR (500 MHz, DMSO-d_6) δ 12.31 (s, 1H), 7.95 (s, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 7.6 Hz, 1H), 2.65 (d, *J* = 26.6 Hz, 4H), 1.74 – 1.32 (m, 8H), 0.98 – 0.80 (m, 6H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 158.48, 156.87, 155.82, 151.54, 149.37, 132.21, 127.48, 127.02, 119.29, 118.36, 111.31, 107.52, 31.72, 31.31, 30.64, 27.87, 22.13, 21.95, 13.58, 13.49. HRMS (ESI) m/z $[M + H]^+$ calculated for $C_{20}H_{23}ClNO_3^+$: 360.1361, found:360.1364.

10,15-Dimethyl-9-phenyl-6*H*,7*H*-chromeno[4',3':4,5]pyrido[2,1-*a*]isoquinoline-6,7-di one (**3aj**)



^{1}H NMR (600 MHz, DMSO) δ 8.60 (d, *J* = 8.3 Hz, 1H), 8.44 (d, *J* = 8.2 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.87 (t, *J* = 7.5 Hz, 1H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.70 – 7.63 (m, 1H), 7.49 – 7.19 (m, 7H), 3.00 (s, 3H), 2.20 (s, 3H). ^{13}C NMR (126 MHz, DMSO) δ 157.84, 156.07, 153.15, 148.45, 146.78, 136.72, 134.80, 134.22, 132.69, 132.05, 130.04, 129.51, 128.57, 127.74, 127.53, 127.37, 125.82, 124.28, 123.60, 121.85, 117.29, 117.16, 106.01, 104.44, 24.55, 15.03. HRMS (ESI) m/z [M + H]+ calculated for $C_{28}H_{20}NO_3$+: 418.1438,found:418.1442.

Diethyl 4,5-dioxo-3,5-dihydro-4*H*-chromeno[3,4-*c*]pyridine-1,2-dicarboxylate (**3ak**)

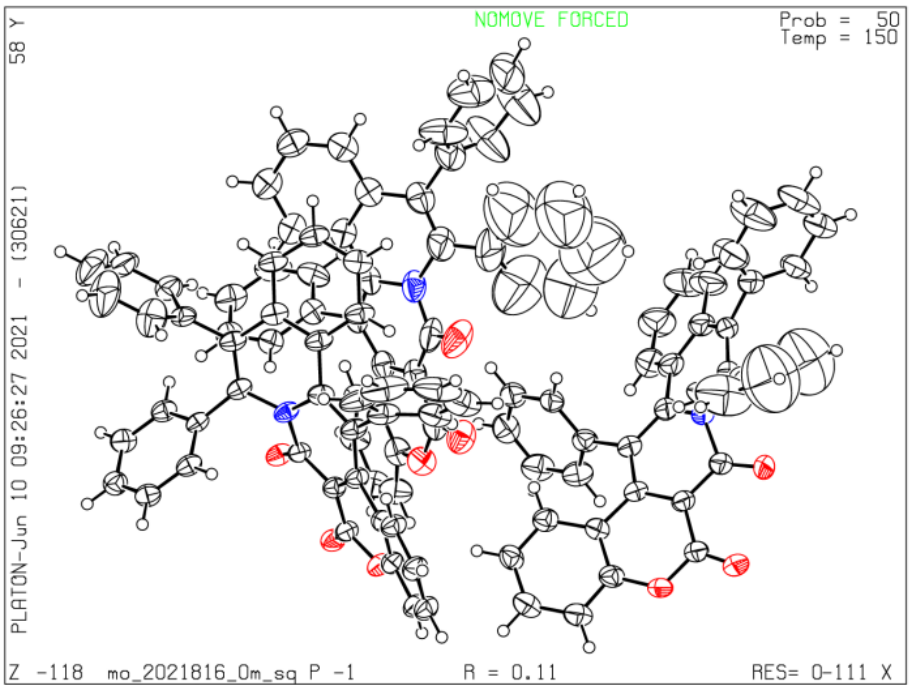


^{1}H NMR (500 MHz, DMSO-*d*6) δ 8.15 – 7.84 (m, 1H), 7.82 – 7.60 (m, 1H), 7.56 – 7.30 (m, 2H), 4.59 – 3.91 (m, 2H), 3.33 (s, 2H), 1.57 – 1.26 (m, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.84, 160.32, 133.57, 125.91, 125.16, 118.04, 114.90, 93.18, 90.50, 89.10, 63.68, 62.52, 21.59. HRMS (ESI) m/z [M + Na]+ calculated for $C_{18}H_{15}NNaO_7$+: 380.0741,found:380.0744.

VII. X-ray Crystallographic Data

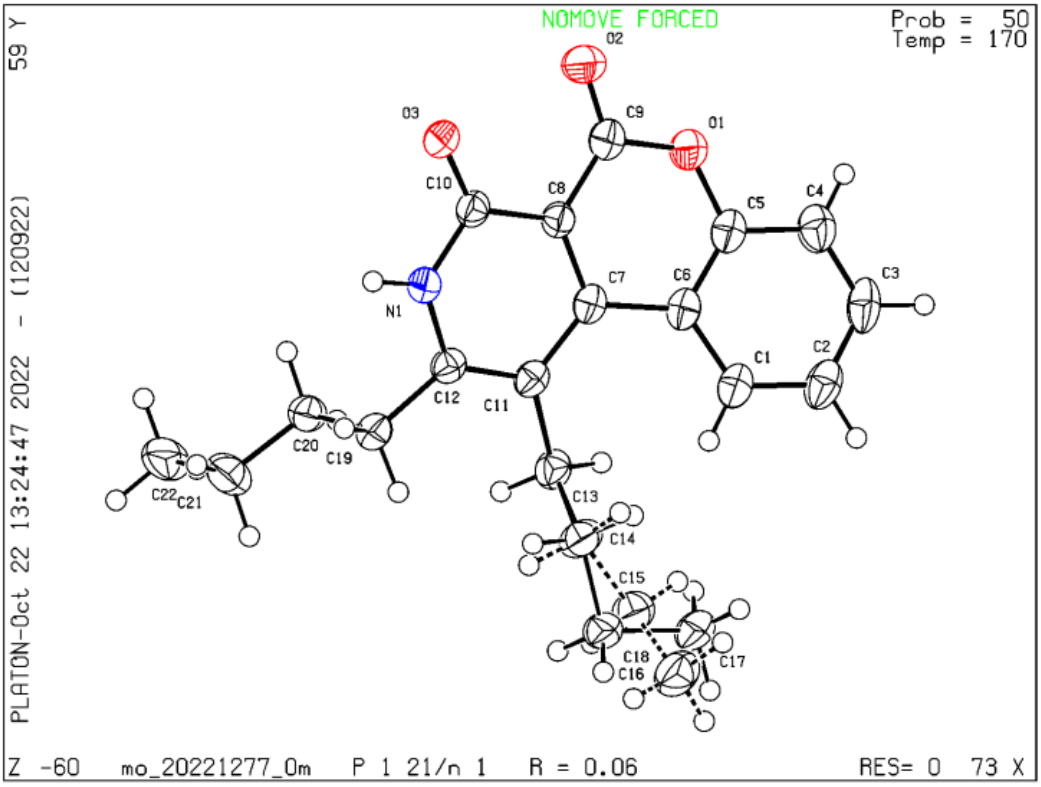
(1) The Single Crystal Structure of **3aa** (*Deposition No.* CCDC 2240822)

Crystal Data for $C_{38}H_{23}NO_3$ (M =541.57 g/mol): triclinic, space group P-1 (no. 2), a = 12.1985(15) Å, b =13.3130(18) Å, c =28.790(5) Å, α =78.149(7) °, β = 79.050 (5) °, γ = 84.650(7) °, V = 4485.3(12) Å^3, Z = 6, T = 150 K, μ(MoKα) = 0.076 m m^{-1}, *Dcalc* = 1.203 g/cm^3, 45382 reflections measured (3.938° ≤ 2Θ ≤ 50.212°), 15810 unique (R_{int} = 0.0801, R_{sigma} = 0.0967) which were used in all calculati ons. The final R_1 was 0.1104 (I > 2σ(I)) and wR_2 was 0.3675 (all data).



(2) The Single Crystal Structure of **3ah** (*Deposition No.* CCDC 2240823)

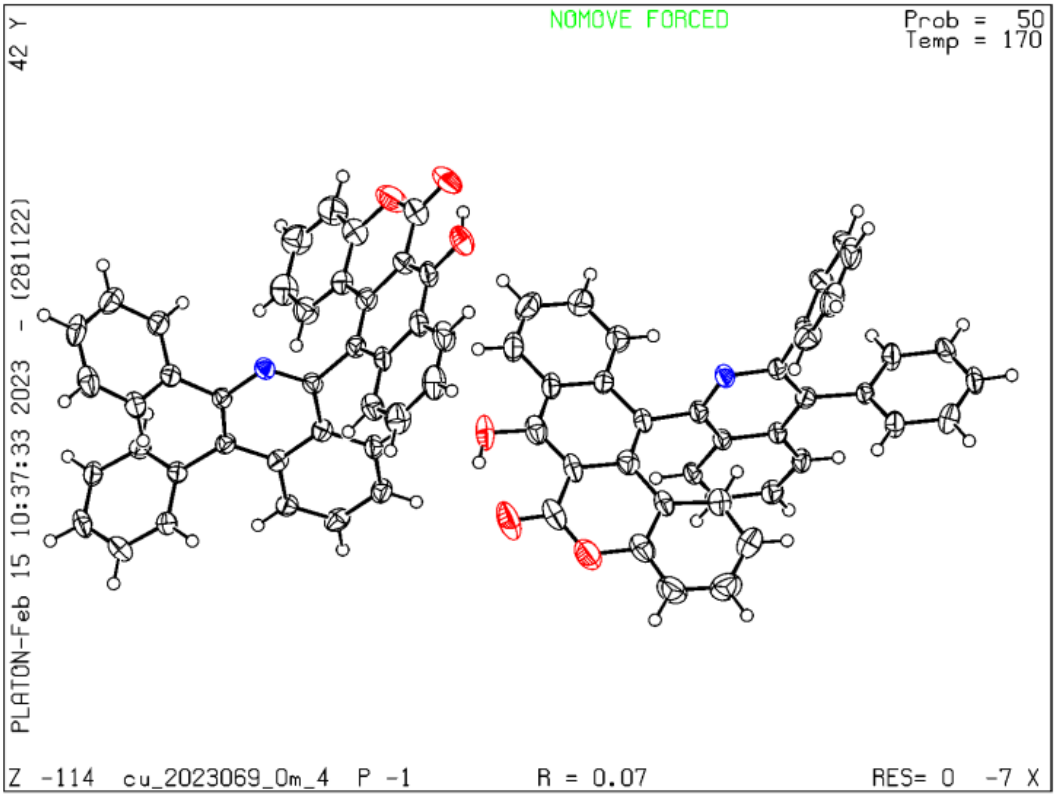
Crystal Data for $C_{20}H_{23}NO_3$ (M =325.39 g/mol): monoclinic, space group $P2_1/n$, a = 8.607(2) Å, b = 17.289(5) Å, c = 11.344(4) Å, α = 90 °, β = 95.054(10) °, γ = 90 °, V = 1681.6(9) Å^3, Z = 4, T = 170 K, μ(MoKα) = 0.086 mm^{-1}, *Dcalc* = 1.28 5 g/cm^3, 18747 reflections measured (4.306° ≤ 2Θ ≤ 52.716 °), 3436 unique (R_{in} $_t$ = 0.0944, R_{sigma} = 0.0788) which were used in all calculations. The final R_1 w as 0.0605 (I > 2σ(I)) and wR_2 was 0.1419 (all data).



(3) The Single Crystal Structure of **4a** (*Deposition No.* CCDC 2241973)

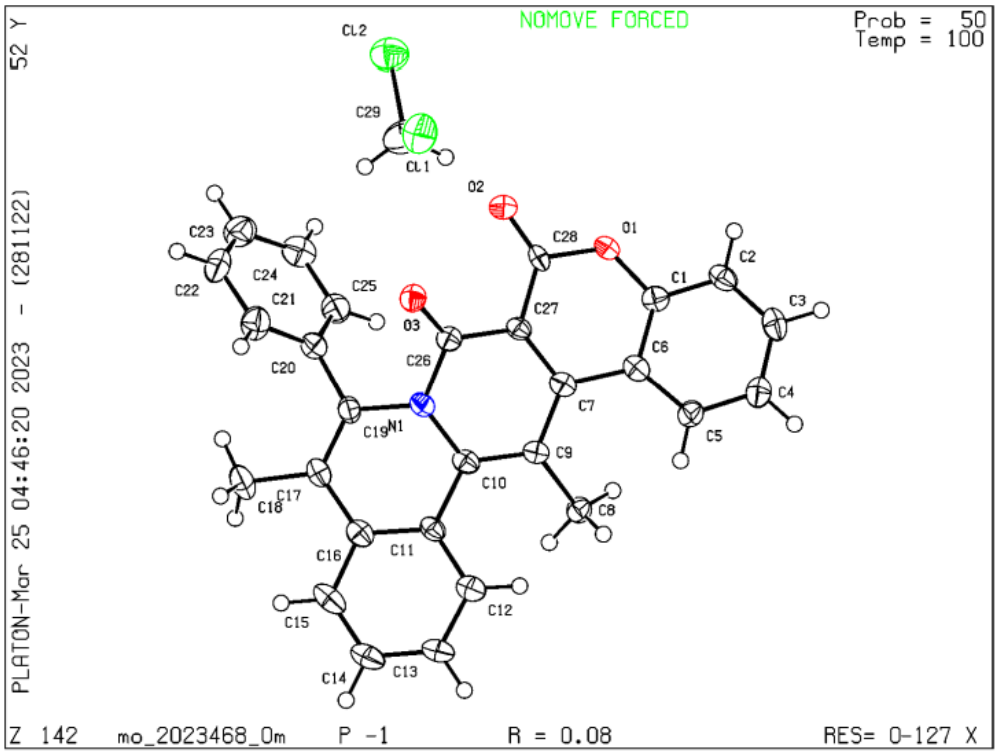
Crystal Data for C38H23NO3 (M =541.57 g/mol): triclinic, space group P-1 (no. 2), a = 8.4094(3) Å, b = 16.0205(6) Å, c = 22.2191(10) Å, α = 69.889(3)°, β = 85.532(2)°, γ = 77.428(2)°, V = 2743.5(2) Å3, Z = 4, T = 170.0 K, μ(CuKα) = 0.658 mm-1, Dcalc = 1.311 g/cm3, 8732 reflections measured (6° ≤ 2Θ ≤ 127.364°), 8732 unique (Rint = ?, Rsigma = 0.1358) which were used in all calculations.

The final R1 was 0.0719 (I > 2σ(I)) and wR2 was 0.1928 (all data).



(4) The Single Crystal Structure of **3aj** (*Deposition No.* CCDC 2254040)

Crystal Data for $C_{29}H_{21}Cl_2NO_3$ (M =502.37 g/mol): triclinic, space group P-1 (no. 2), a = 9.501(4) Å, b = 10.350(8) Å, c = 12.608(7) Å, α = 69.54(2)°, β = 78.40(2)°, γ = 76.82(2)°, V = 1120.9(12) Å3, Z = 2, T = 100 K, μ(MoKα) = 0.325 mm-1, Dcalc = 1.488 g/cm3, 12903 reflections measured (4.264° ≤ 2θ ≤ M =502.37 g/mol): triclinic, space group P-1 (no. 2), a = 9.501(4) Å, b = 10.350(8) Å, c = 12.608(7) Å, α = 69.54(2 (I > 2σ(I)) and wR2 was 0.1917 (all data).



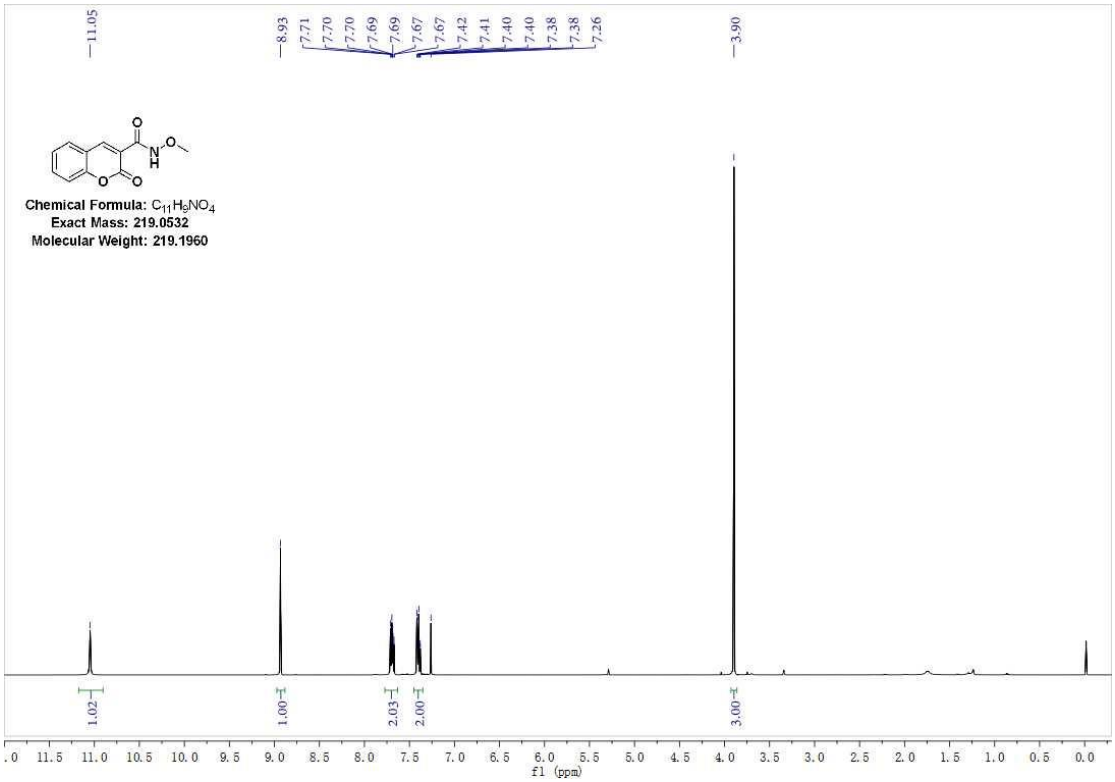
VIII. Reference

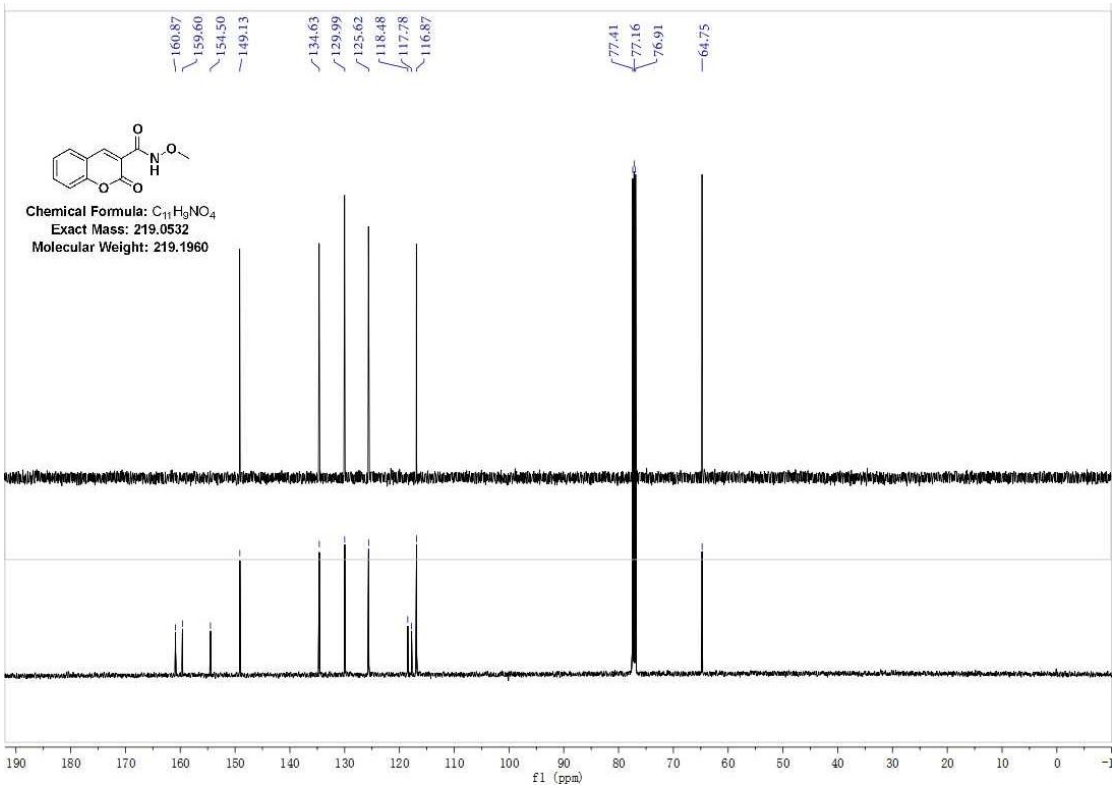
(1) Fonseca, A.; Matos, M. J.; Reis, J.; Duarte, Y.; Gutiérrez, M.; Santana, L.; Uriarte, E.; Borges, F. *RSC Advances* **2016**, *6*, 49764.

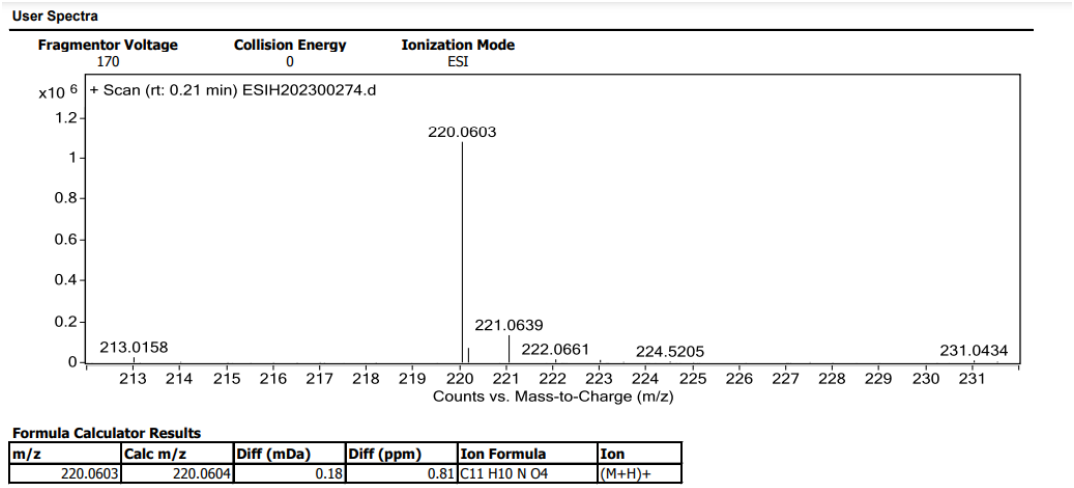
(2) Park, K.; Bae, G.; Moon, J.; Choe, J.; Song, K. H.; Lee, S. *The Journal of Organic Chemistry* **2010**, *75*, 6244.

IV. NMR Spectra and HR-MS Spectra of Substrates and Products

N-methoxy-2-oxo-2H-chromene-3-carboxamide (**1a**)



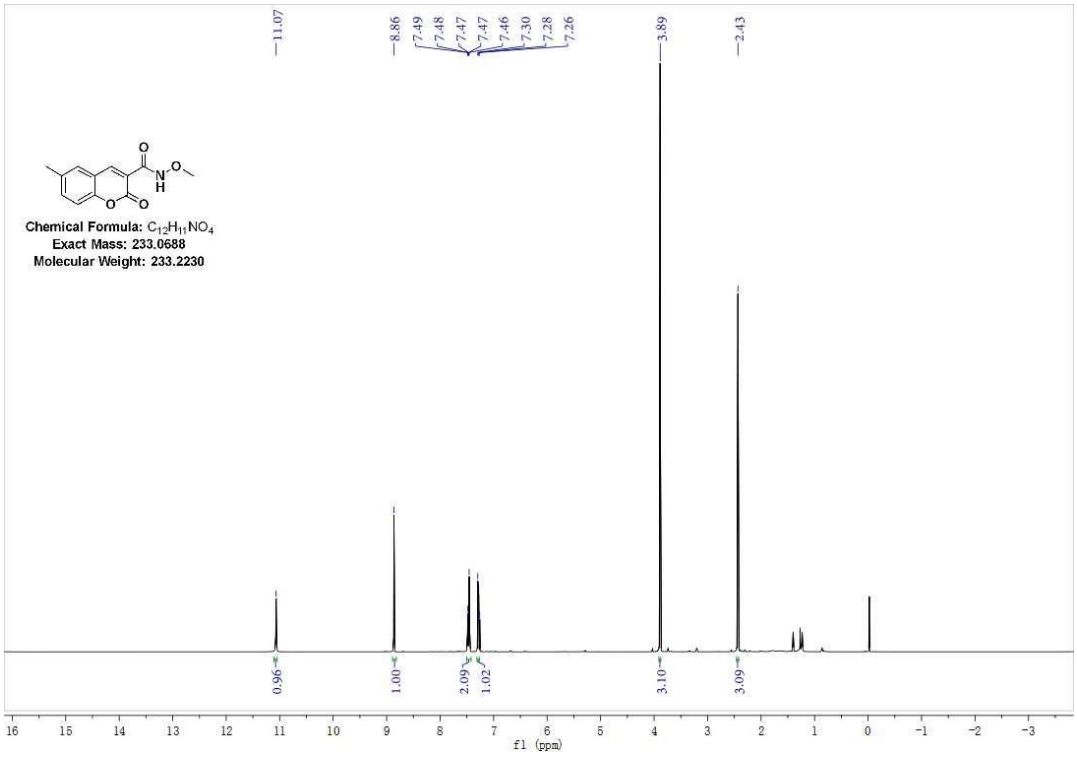


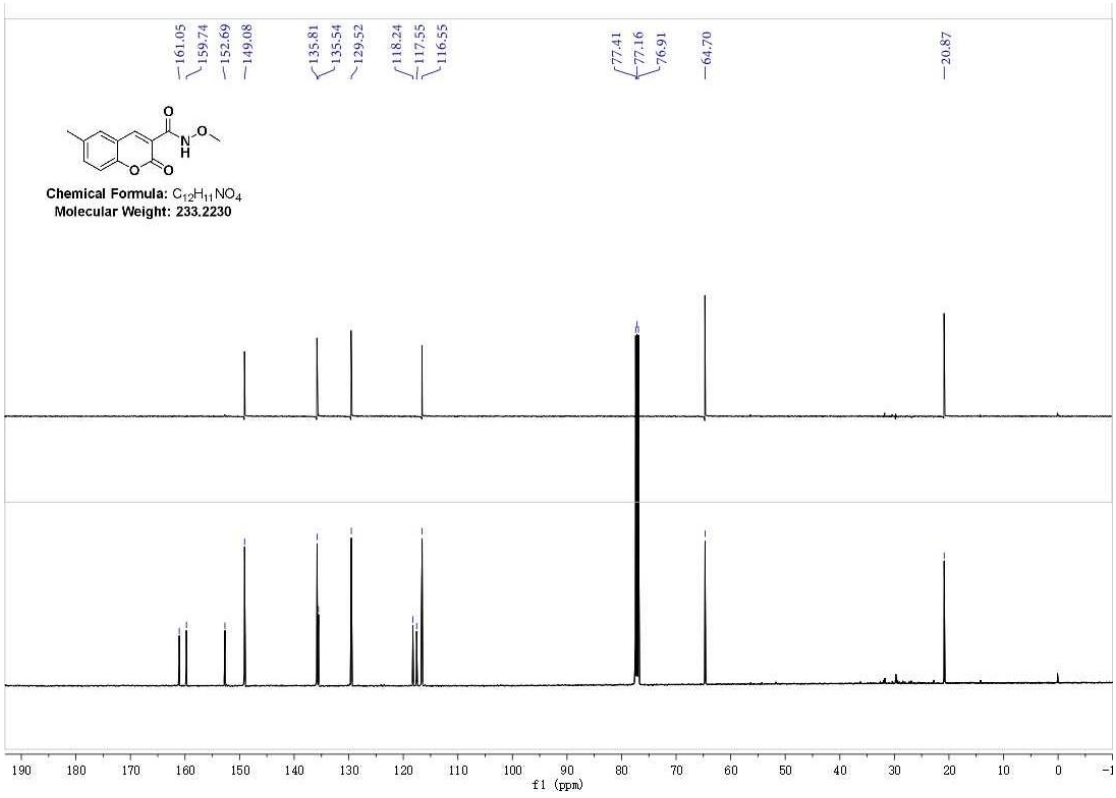


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
220.0603	220.0604	0.18	0.81	C11 H10 N O4	(M+H)+

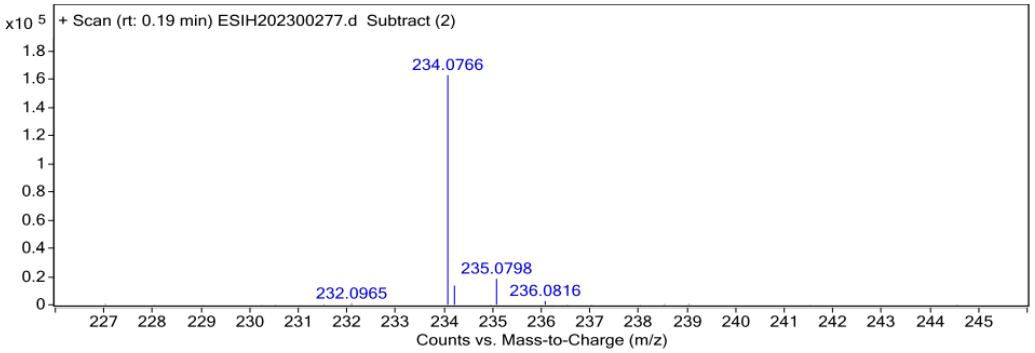
N-methoxy-6-methyl-2-oxo-2H-chromene-3-carboxamide (**1b**)





User Spectra

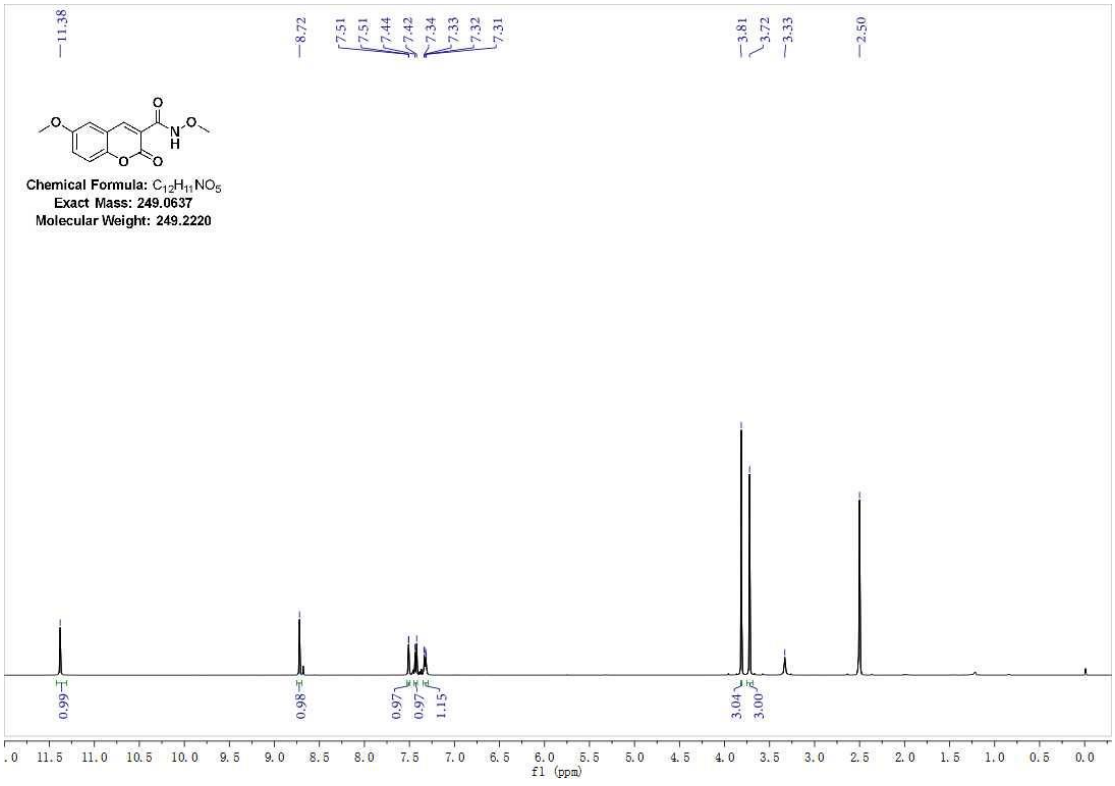
Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI

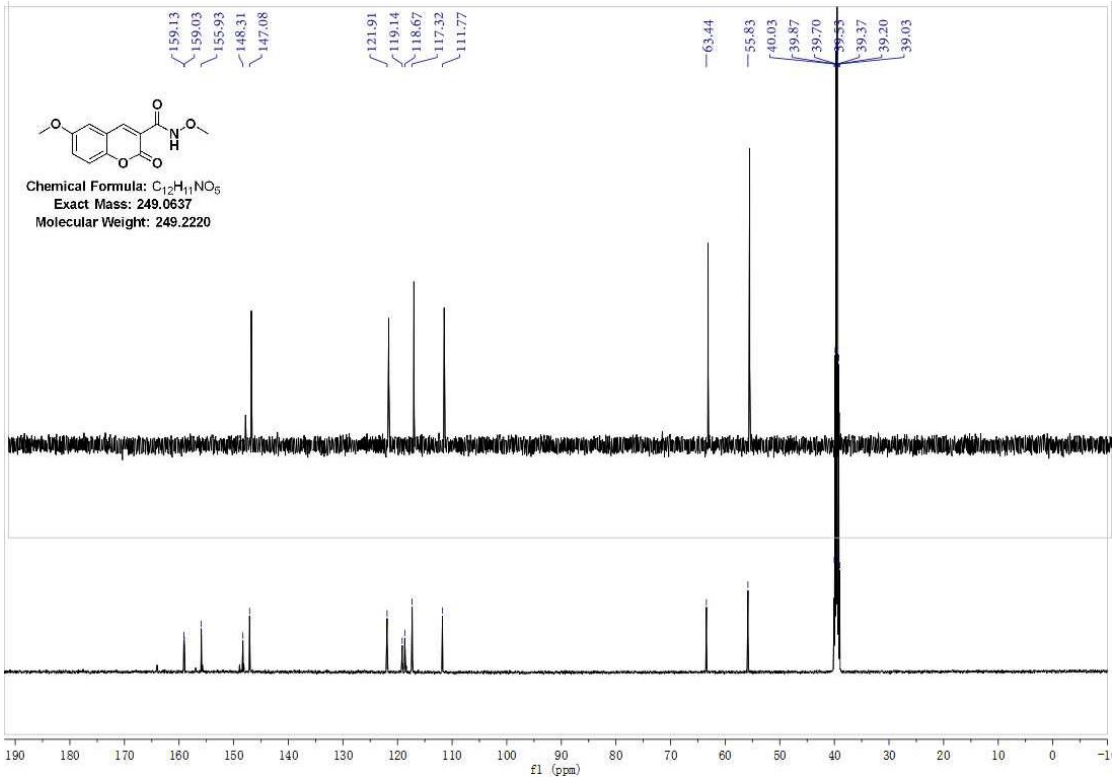


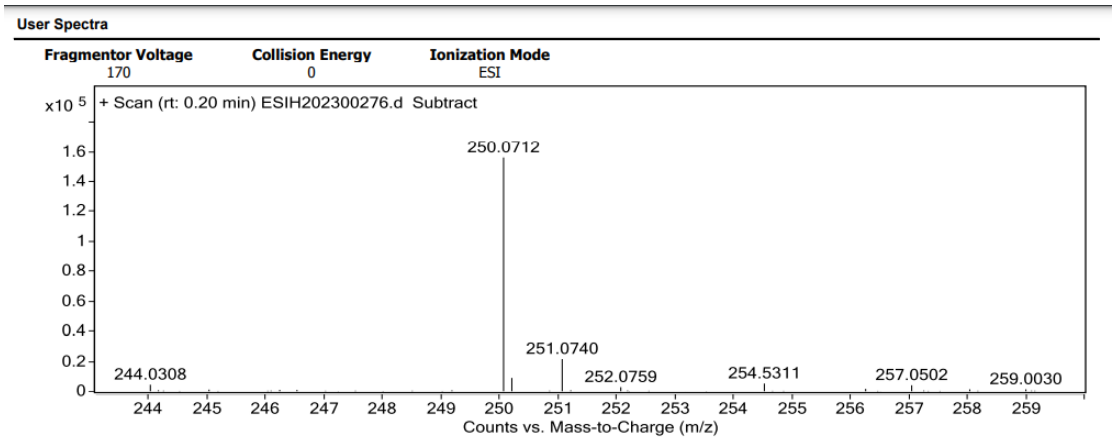
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
234.0766	234.0761	-0.54	-2.3	C12 H12 N O4	(M+H)+

N,6-dimethoxy-2-oxo-2H-chromene-3-carboxamide (**1c**)



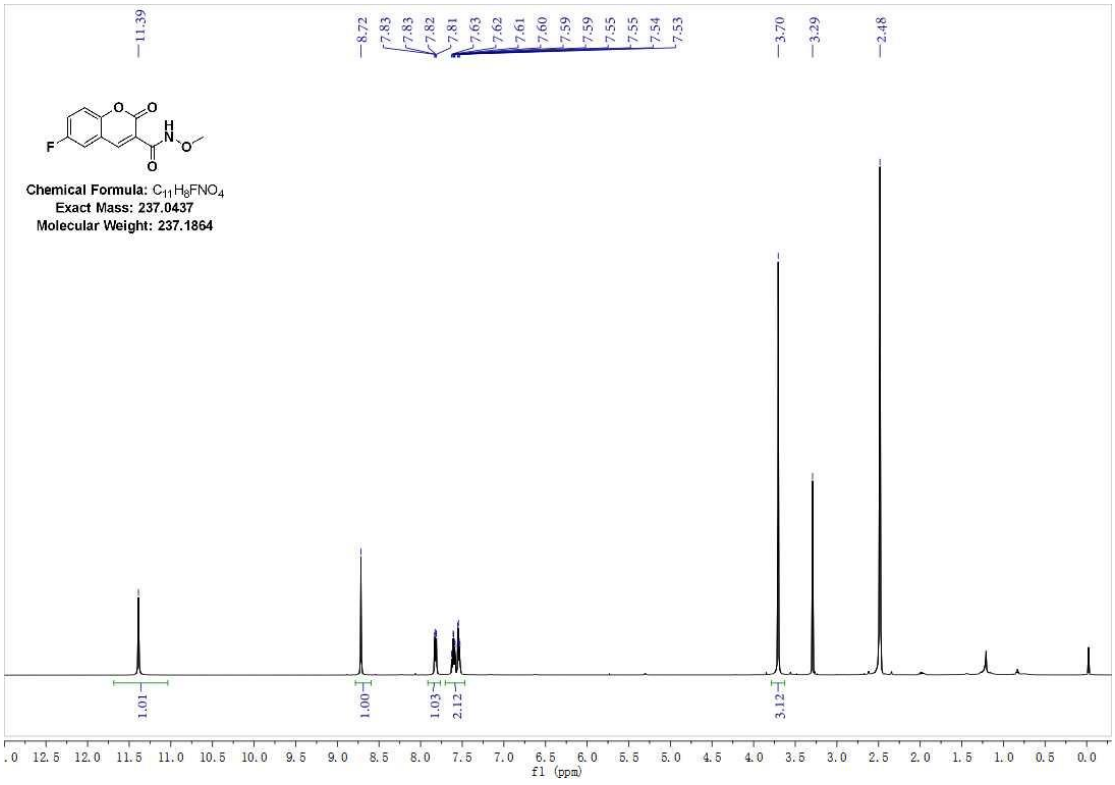


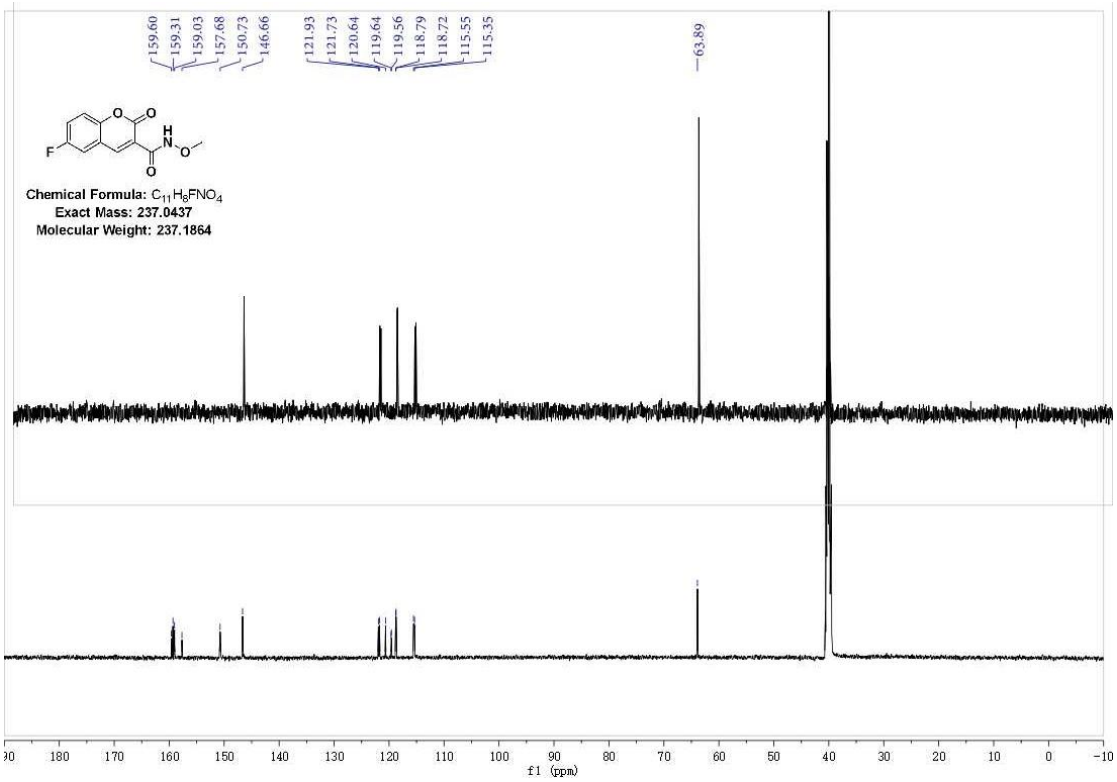


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
250.0712	250.071	-0.18	-0.73	C12 H12 N O5	(M+H)+

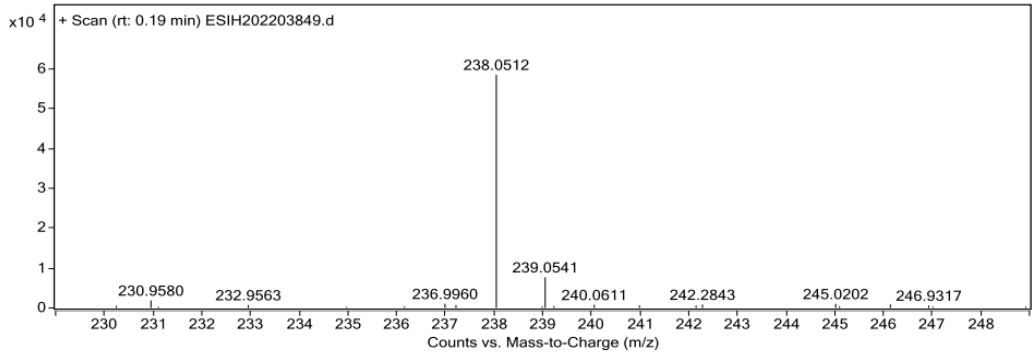
6-Fluoro-N-methoxy-2-oxo-2H-chromene-3-carboxamide (**1d**)





User Spectra

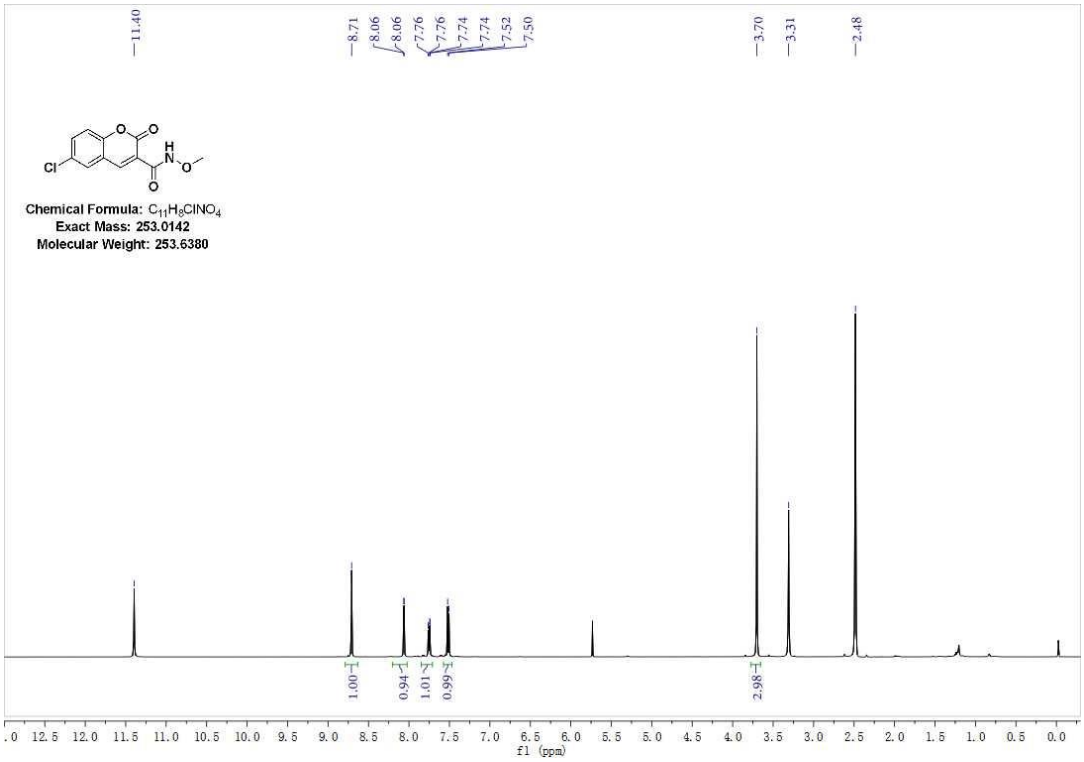
Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI

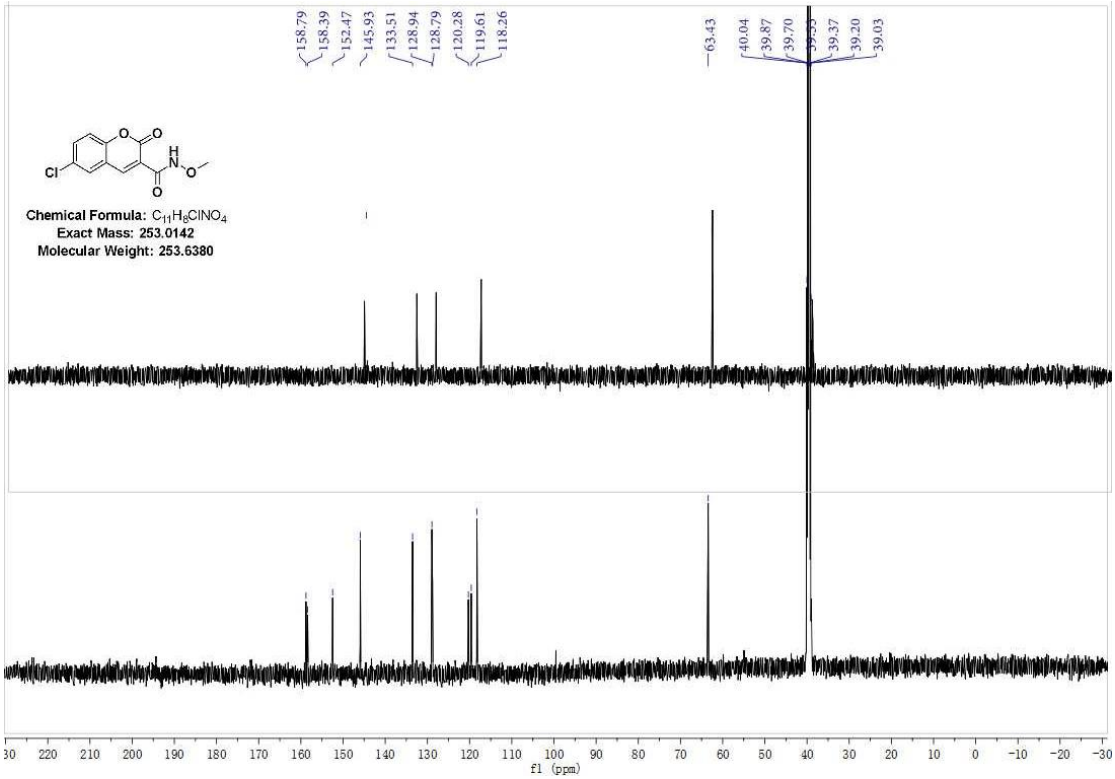


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
238.0512	238.051	-0.2	-0.83	C11 H9 F N O4	(M+H)+

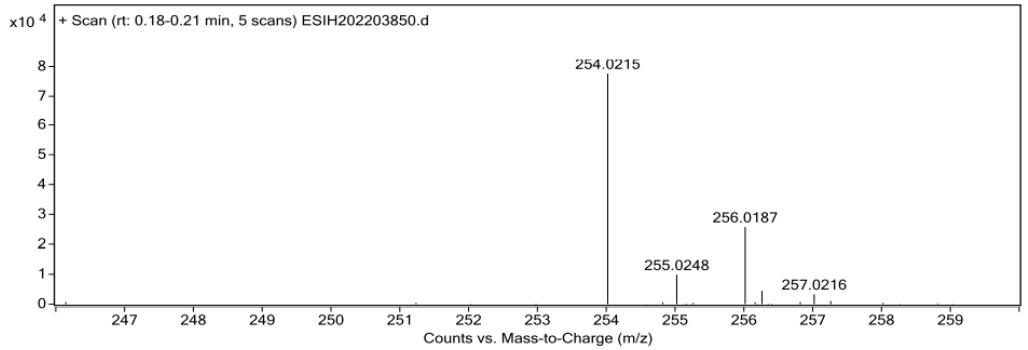
6-Chloro-N-methoxy-2-oxo-2H-chromene-3-carboxamide (**1e**)





User Spectra

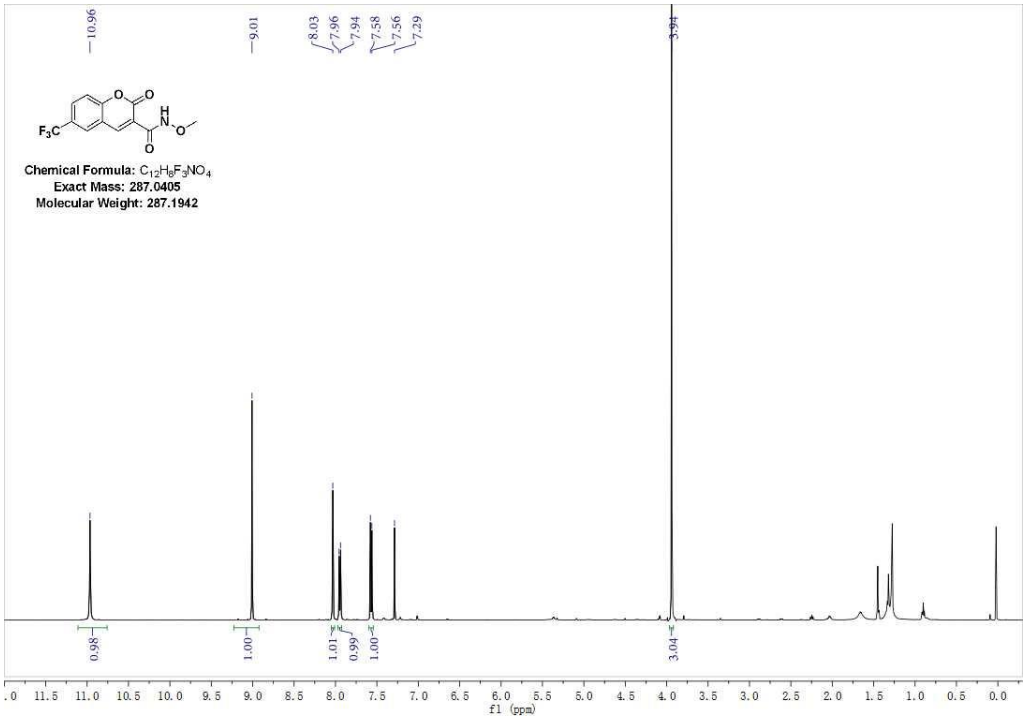
Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI

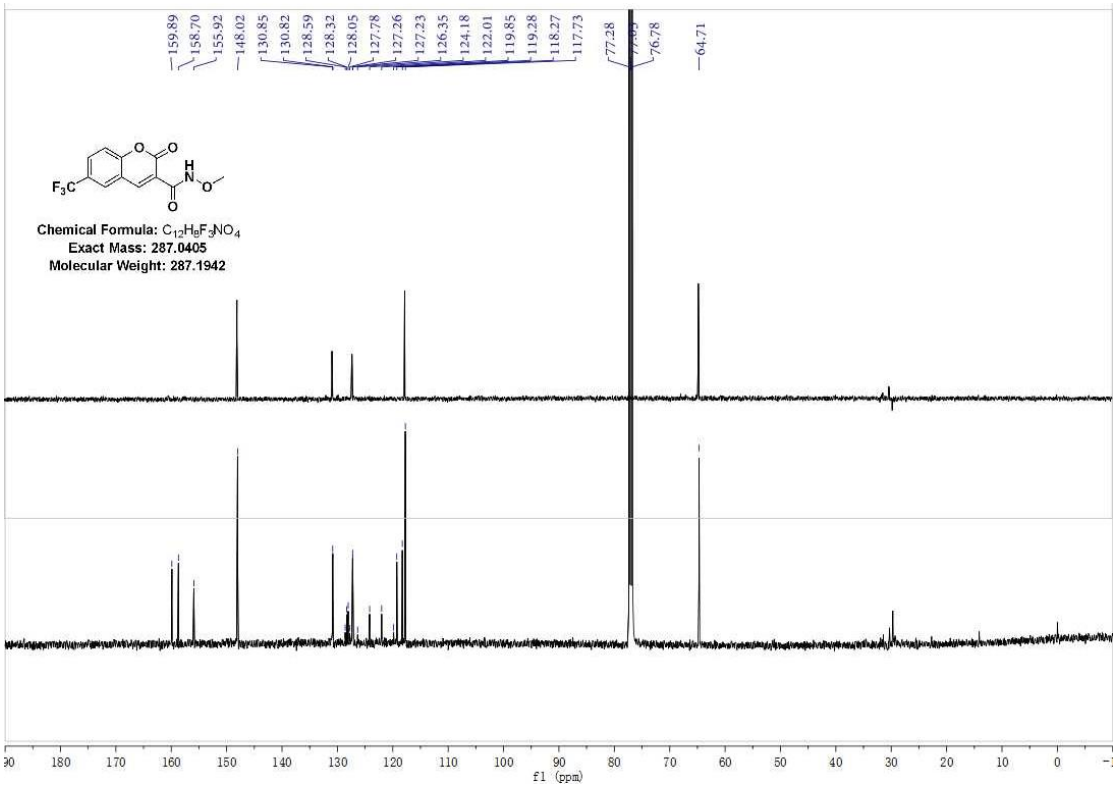


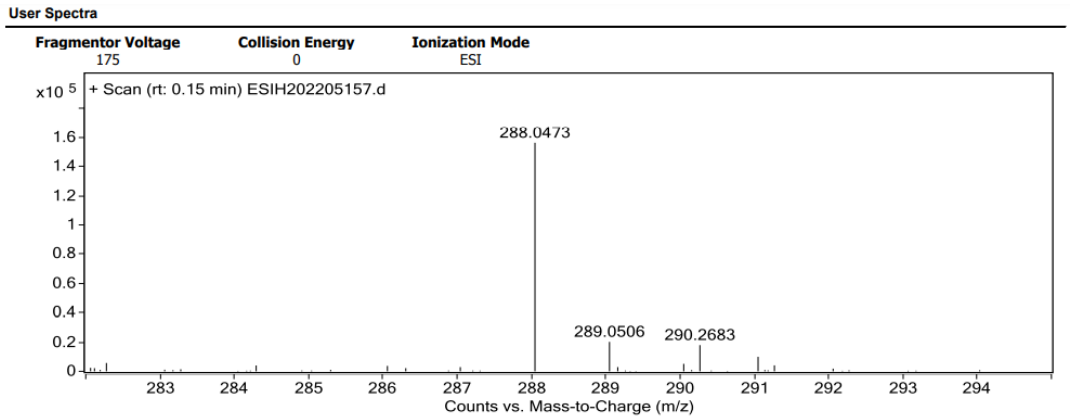
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
254.0215	254.0215	-0.08	-0.3	C11 H9 Cl N O4	(M+H)+

N-methoxy-2-oxo-6-(trifluoromethyl)-2H-chromene-3-carboxamide (**1f**)


10.96
9.01
8.03
7.96
7.94
7.58
7.56
7.29
3.94
Chemical Formula: C12H8F3NO4
Exact Mass: 287.0405
Molecular Weight: 287.1942
0.98
1.00
1.01
0.99
1.00
3.04
f1 (ppm)

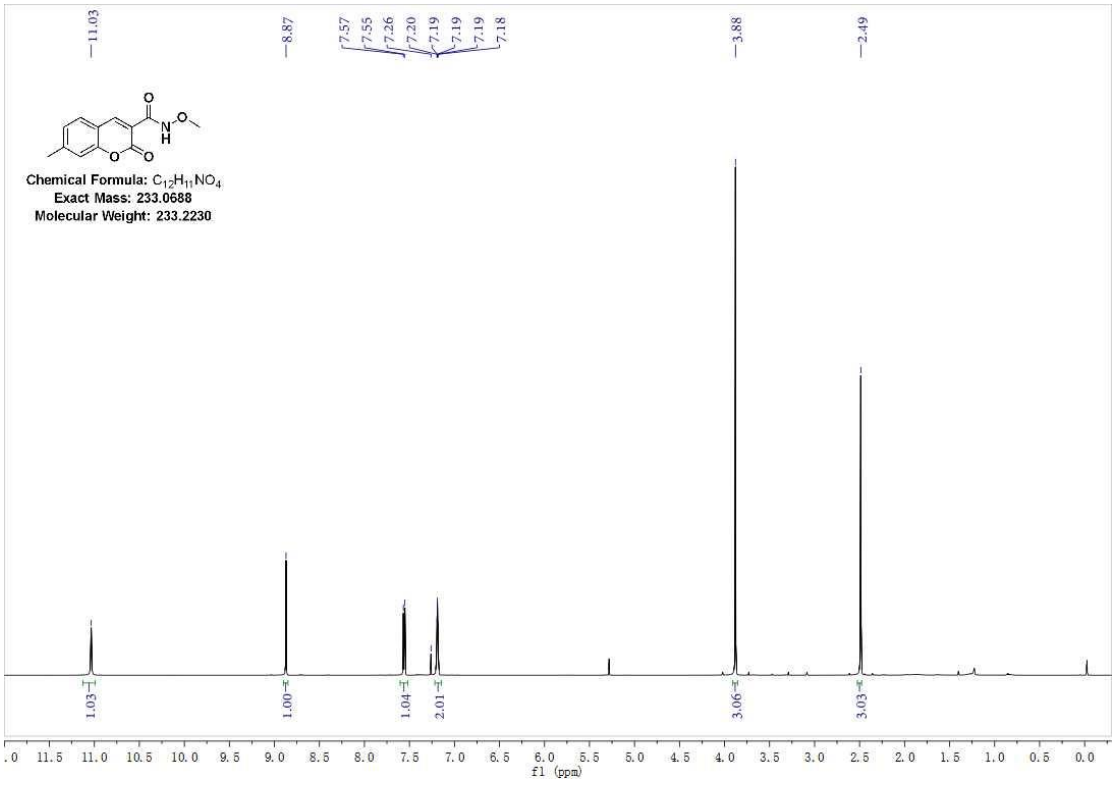

159.89
158.70
155.92
148.02
130.85
130.82
128.59
128.32
128.05
127.78
127.26
127.23
126.35
124.18
122.01
119.85
119.28
118.27
117.73
77.28
76.78
64.71
Chemical Formula: C12H8F3NO4
Exact Mass: 287.0405
Molecular Weight: 287.1942
f1 (ppm)

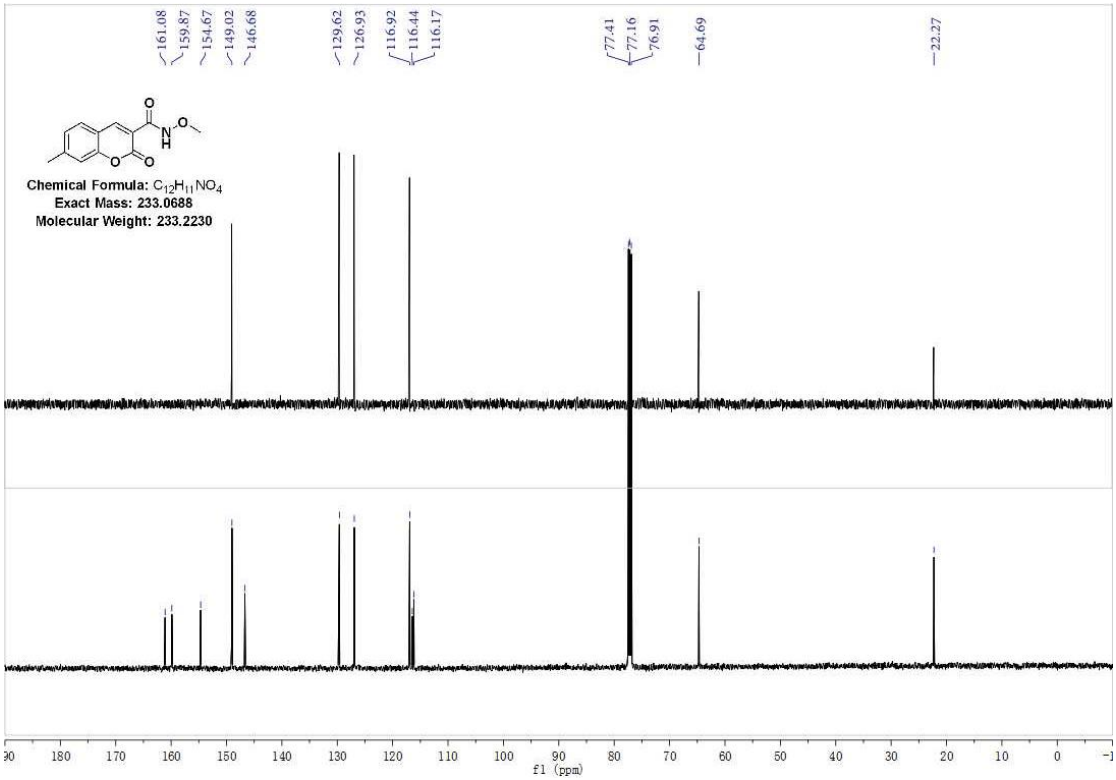


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
288.0473	288.0478	0.49	1.71	C12 H9 F3 N O4	(M+H)+

N-methoxy-7-methyl-2-oxo-2H-chromene-3-carboxamide (**1g**)

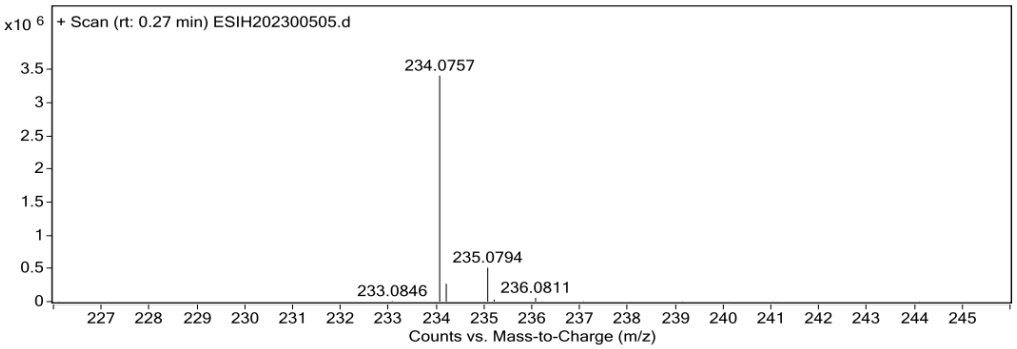




`

User Spectra

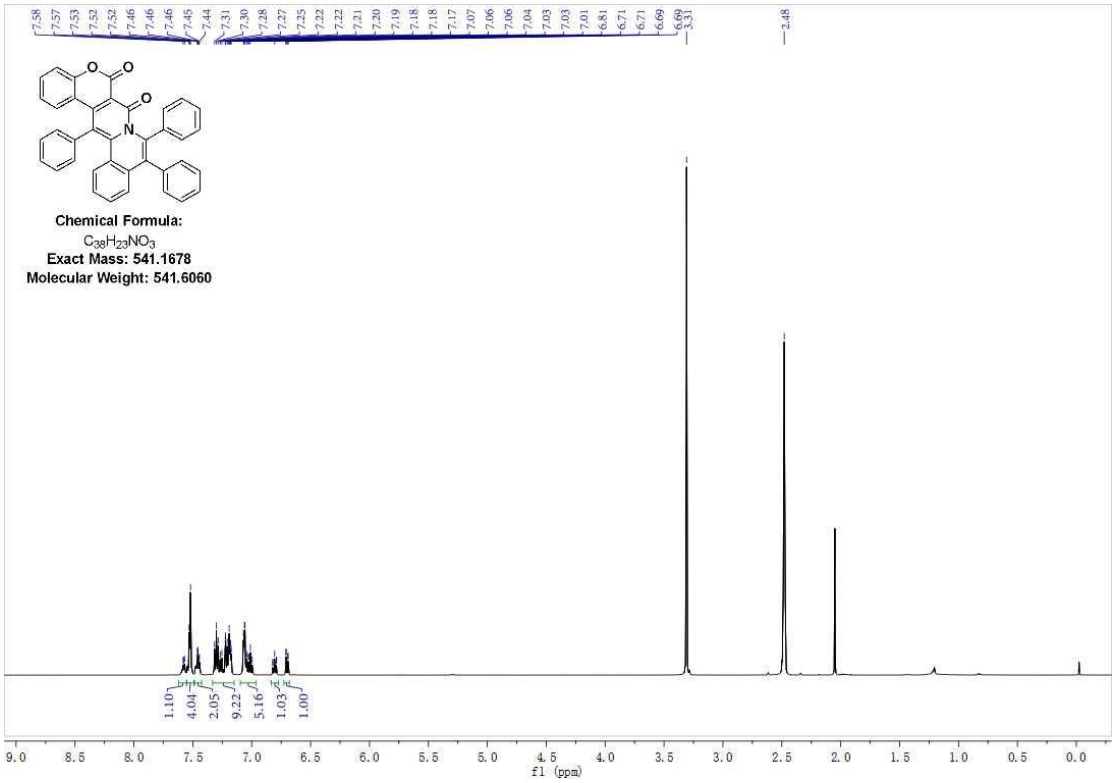
Fragmentor Voltage	Collision Energy	Ionization Mode
90	0	ESI

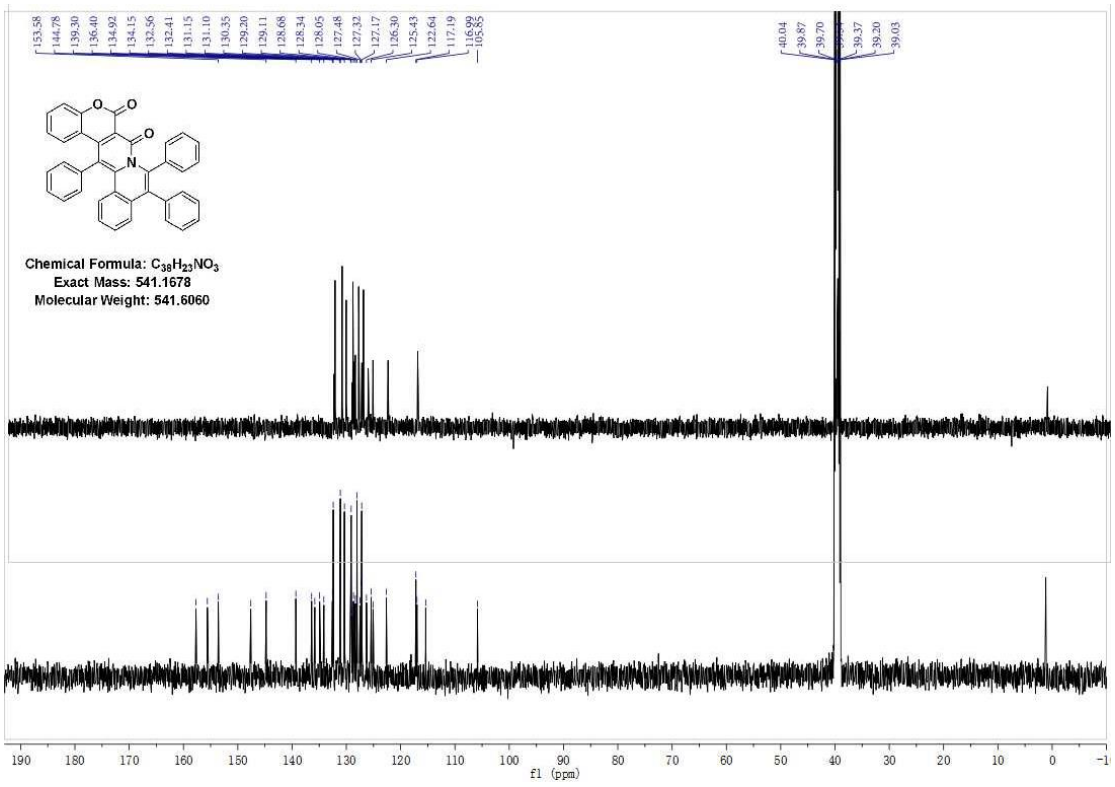


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
234.0757	234.0761	0.4	1.71	C12 H12 N O4	(M+H)+

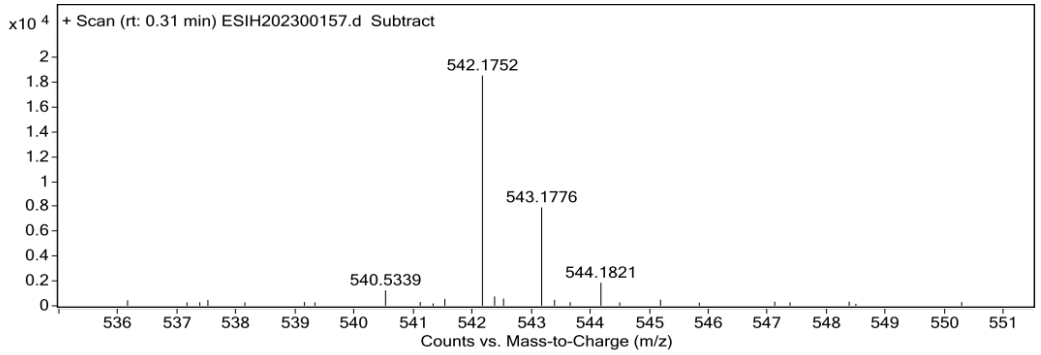
9,10,15-Triphenyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3aa**)


Chemical Formula:
$C_{38}H_{23}NO_3$
Exact Mass: 541.1678
Molecular Weight: 541.6060
f1 (ppm)


Chemical Formula: $C_{38}H_{23}NO_3$
Exact Mass: 541.1678
Molecular Weight: 541.6060
f1 (ppm)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
542.1752	542.1751	-0.15	-0.27	C38 H24 N O3	(M+H)+

--- End Of Report ---

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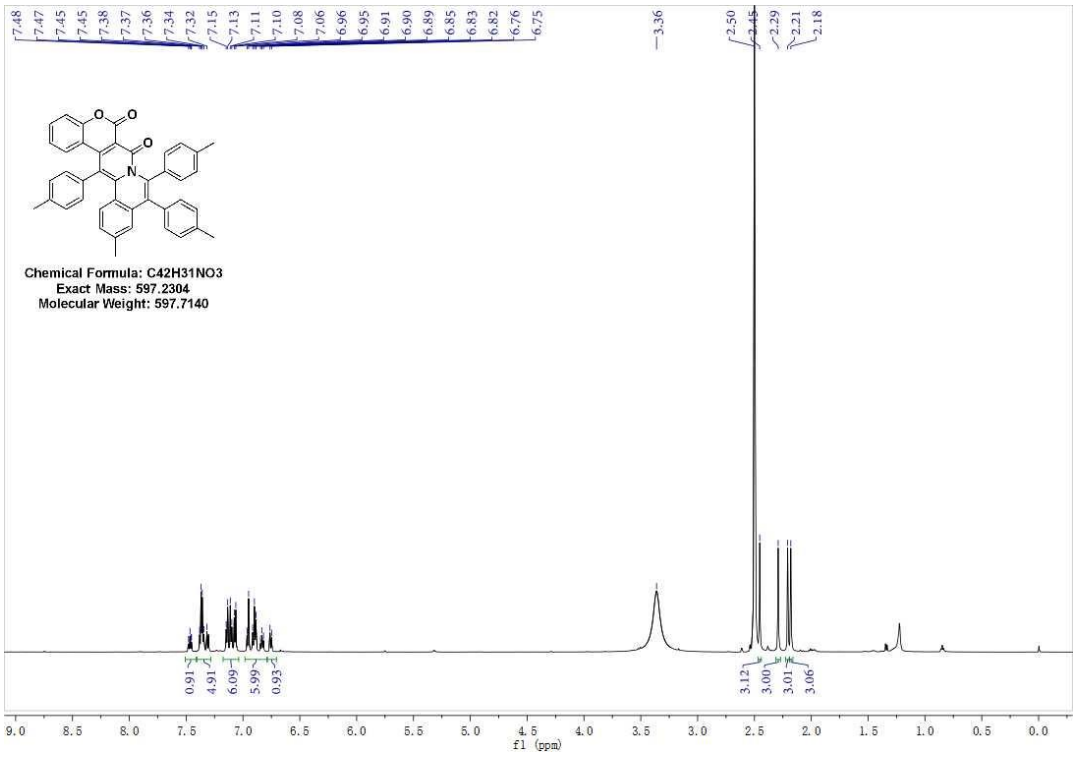
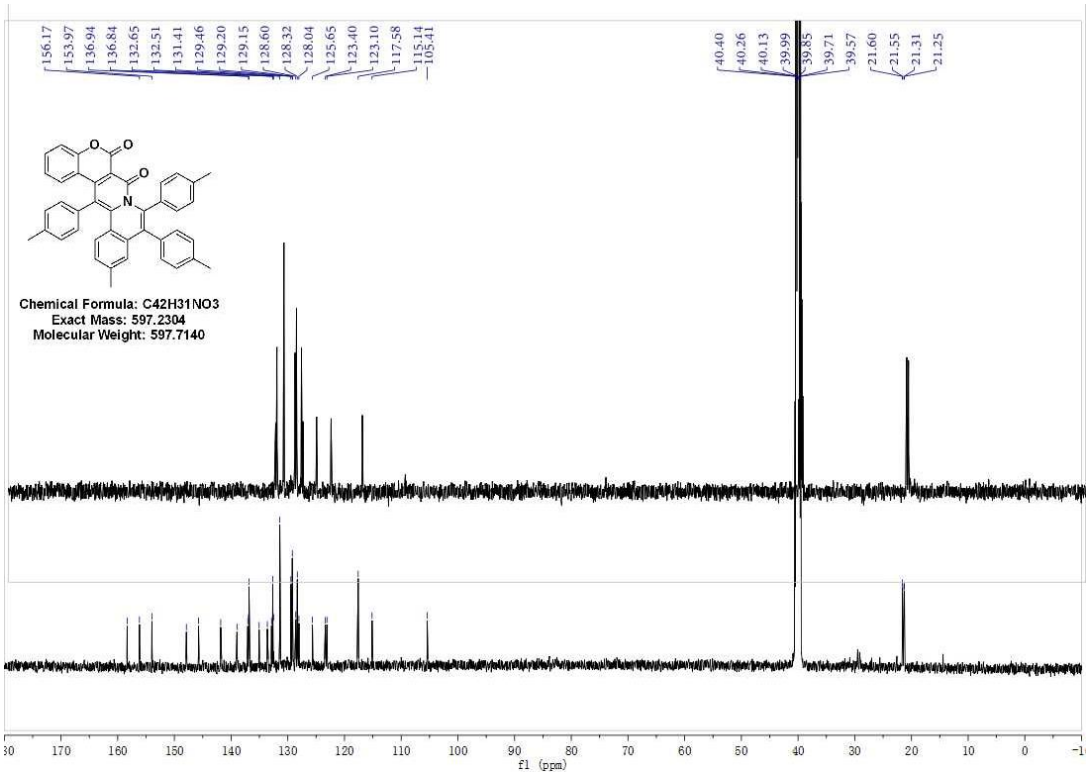
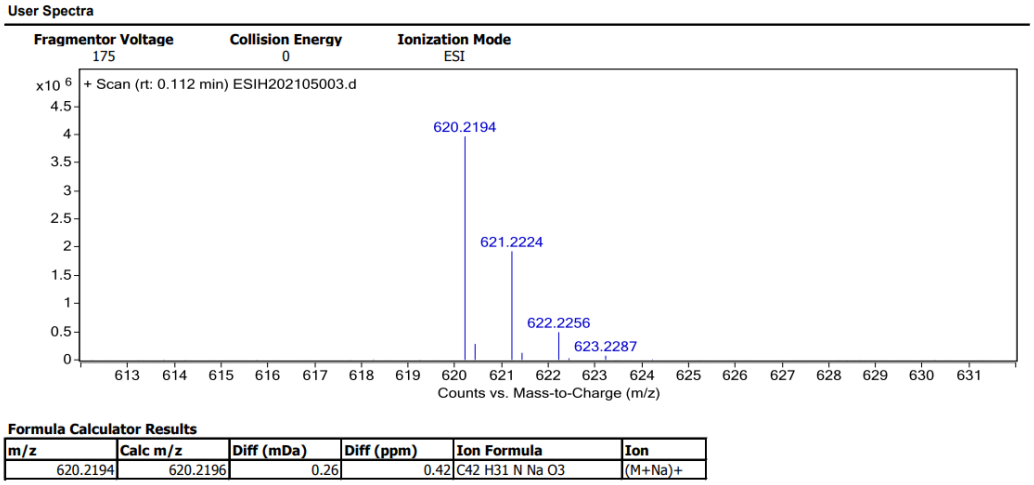
12-Methyl-9,10,15-tri-p-tolyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ab**)



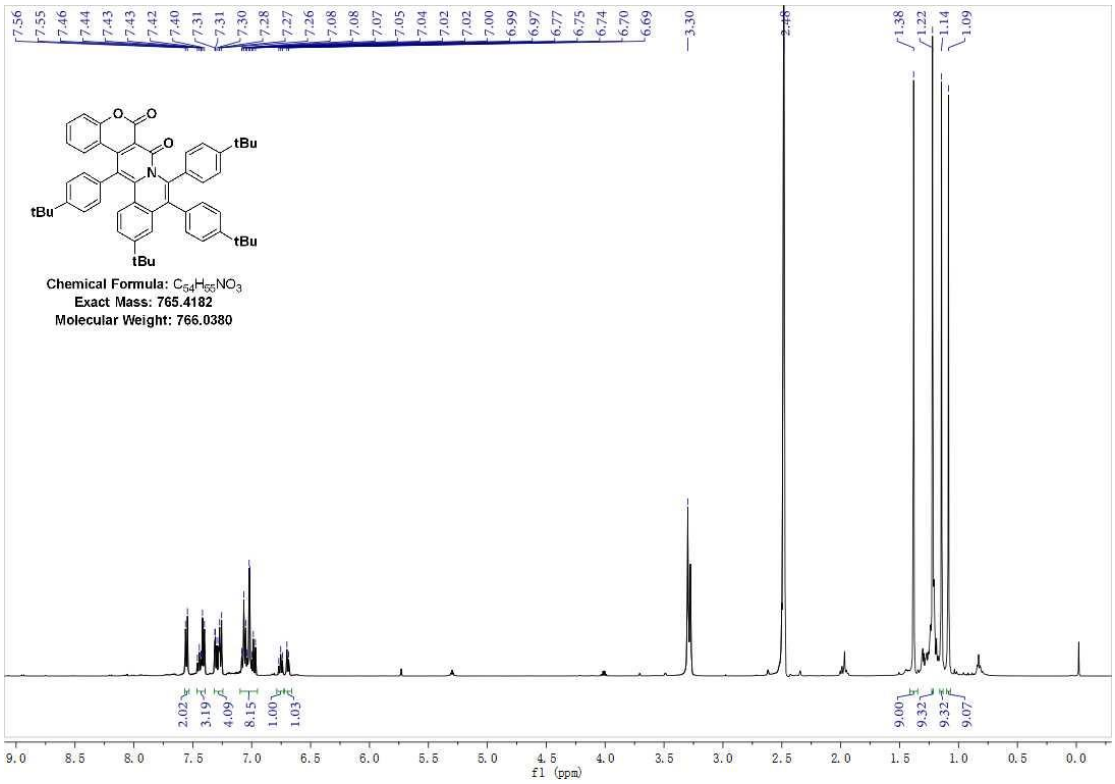


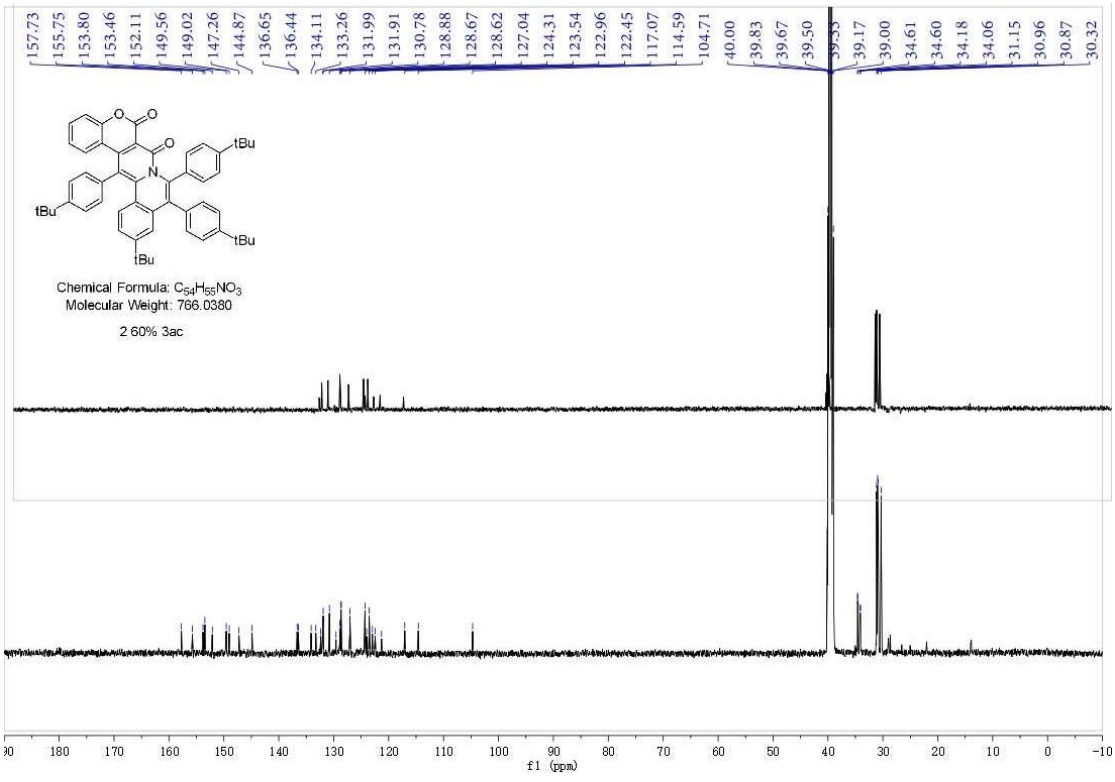


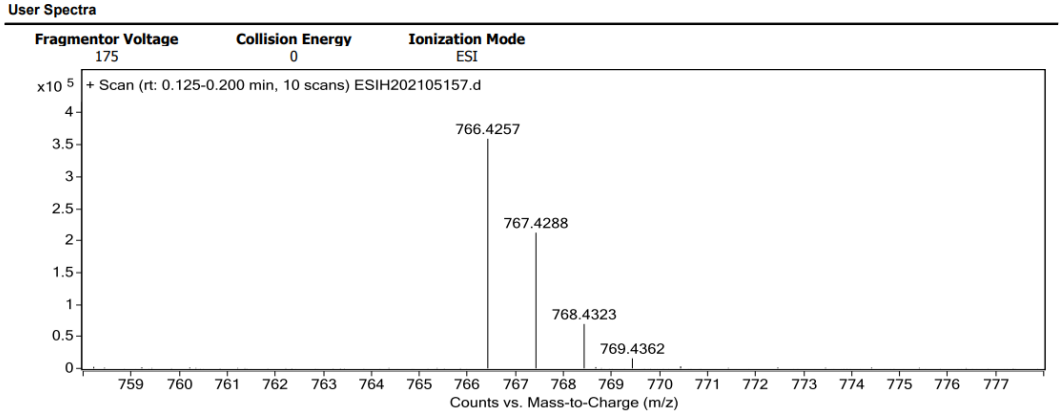
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
620.2194	620.2196	0.26	0.42	C42 H31 N Na O3	(M+Na)+

12-(tert-Butyl)-9,10,15-tris(4-(tert-butyl)phenyl)-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ac**)


Chemical Formula: C54H55NO3
Exact Mass: 765.4182
Molecular Weight: 766.0380
f1 (ppm)

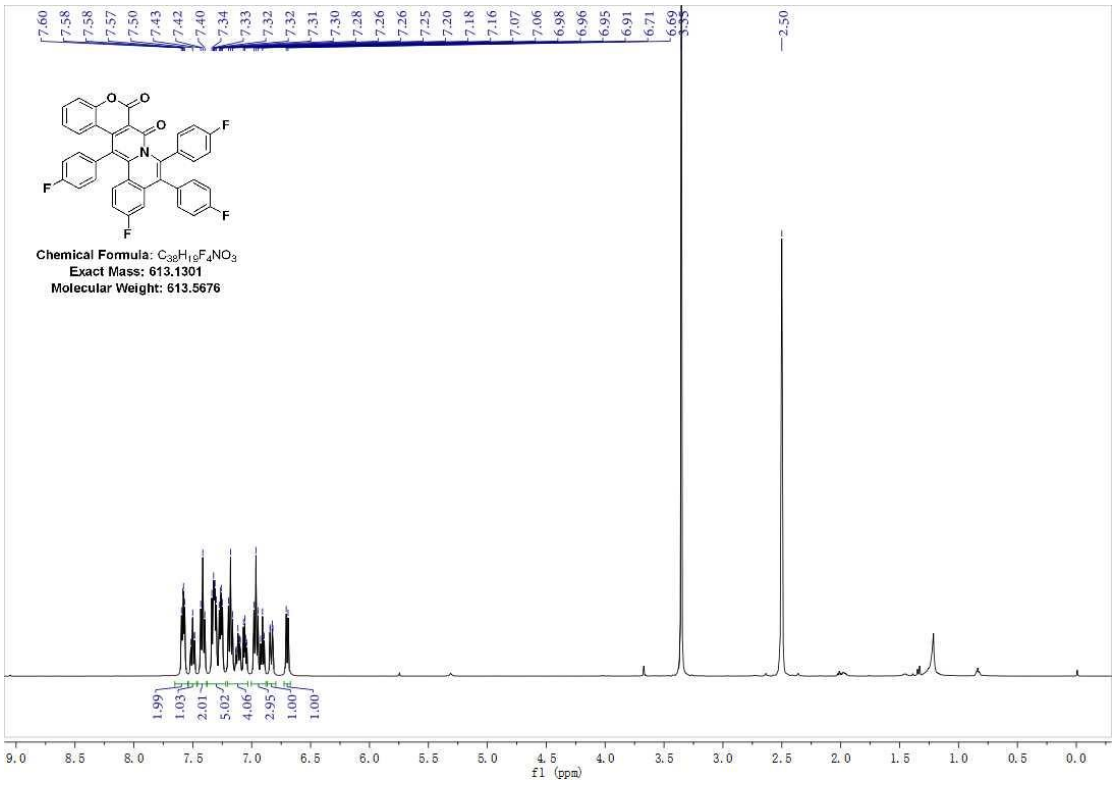

Chemical Formula: C54H55NO3
Molecular Weight: 766.0380
2.60% 3ac
f1 (ppm)

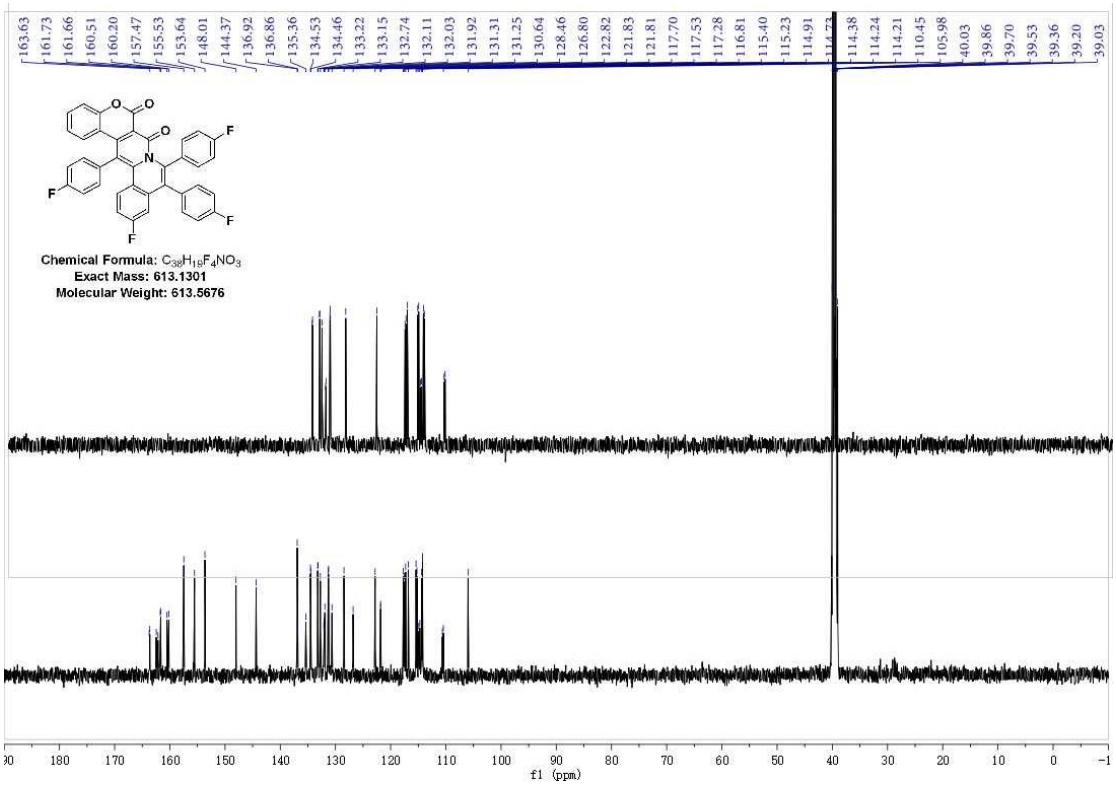


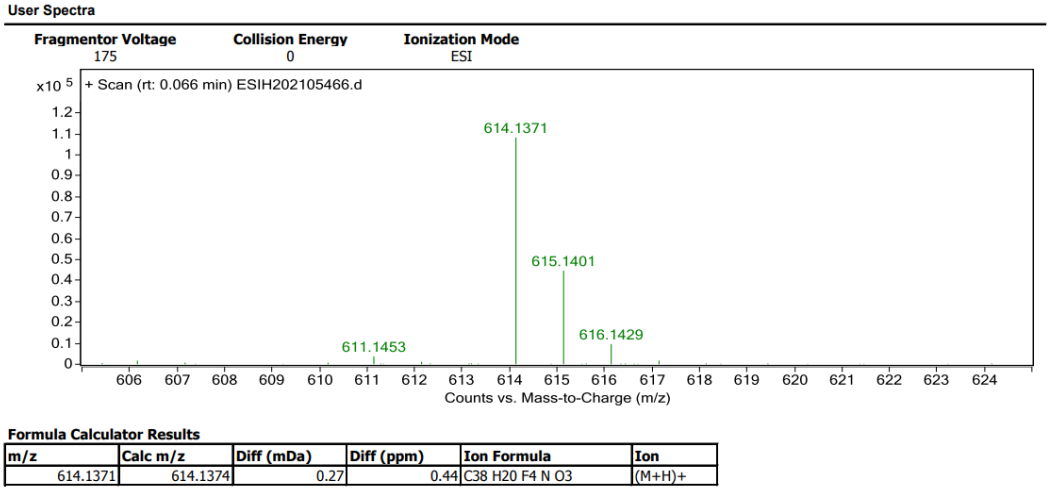
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
766.4257	766.4255	-0.18	-0.24	C54 H56 N O3	(M+H)+

12-Fluoro-9,10,15-tris(4-fluorophenyl)-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ad**)



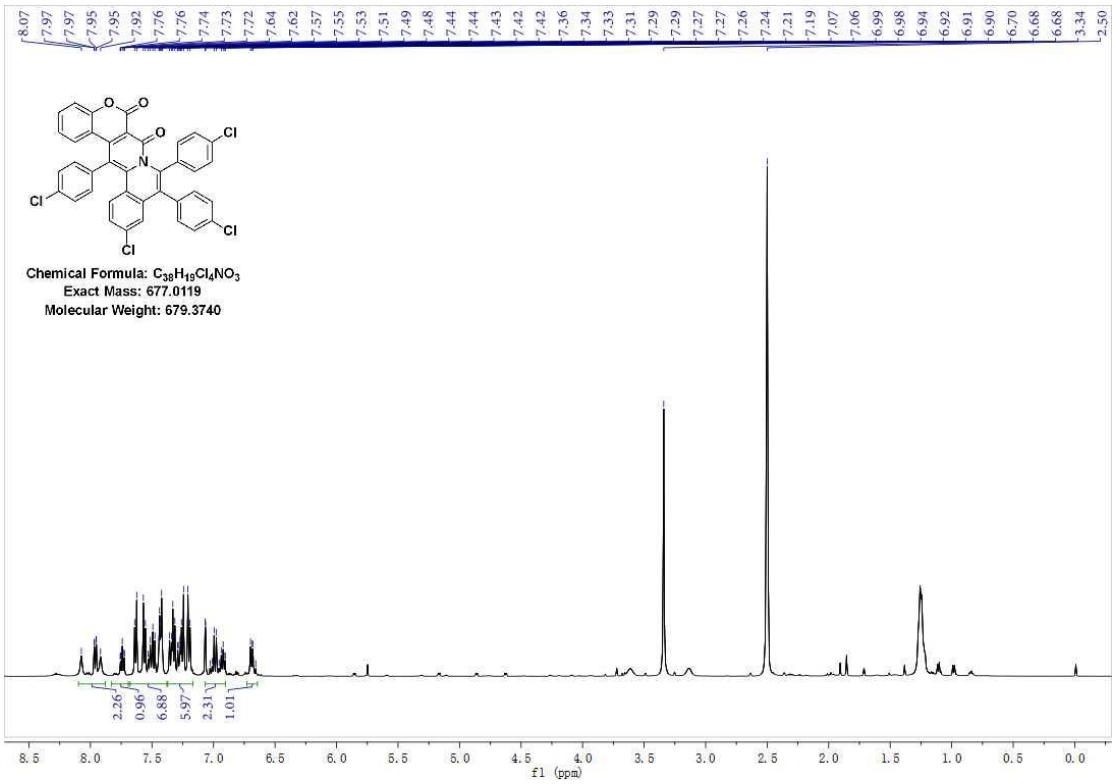


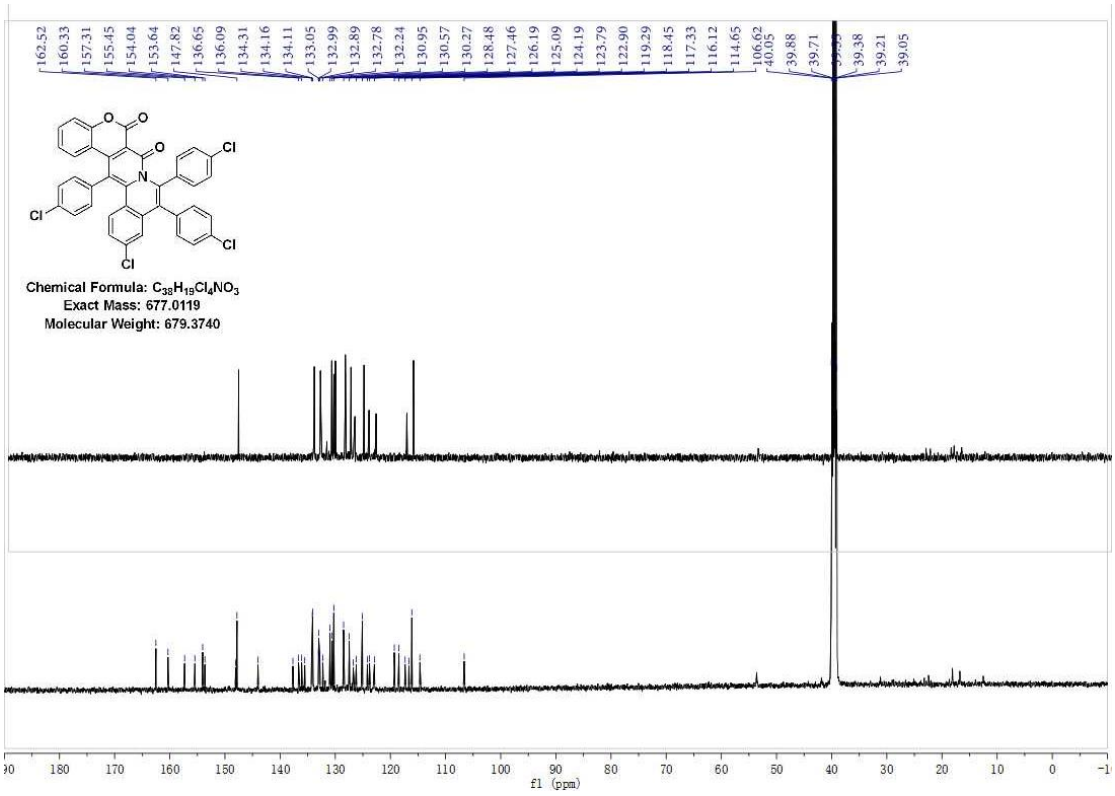


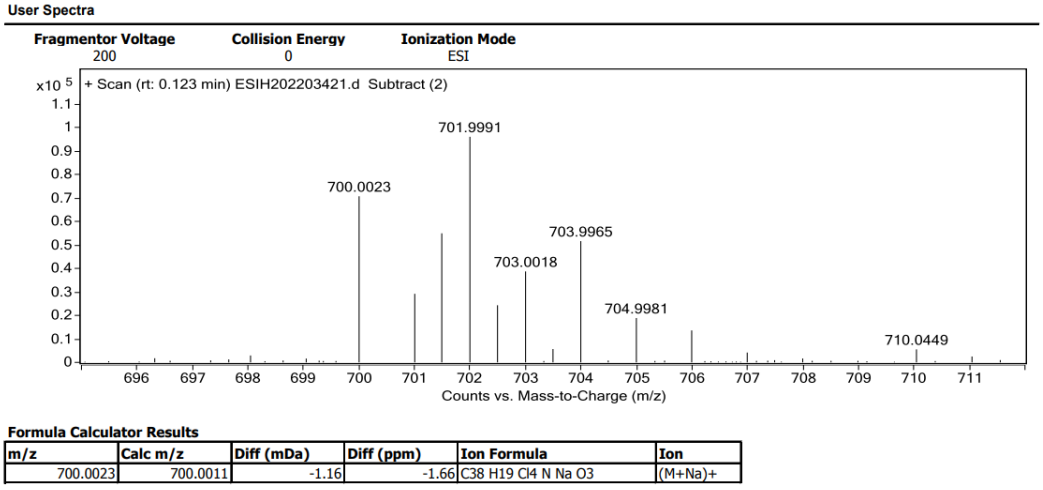
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
614.1371	614.1374	0.27	0.44	C38 H20 F4 N O3	(M+H)+

12-Chloro-9,10,15-tris(4-chlorophenyl)-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ae**)


Chemical Formula: $C_{38}H_{19}Cl_4NO_3$
Exact Mass: 677.0119
Molecular Weight: 679.3740
f1 (ppm)

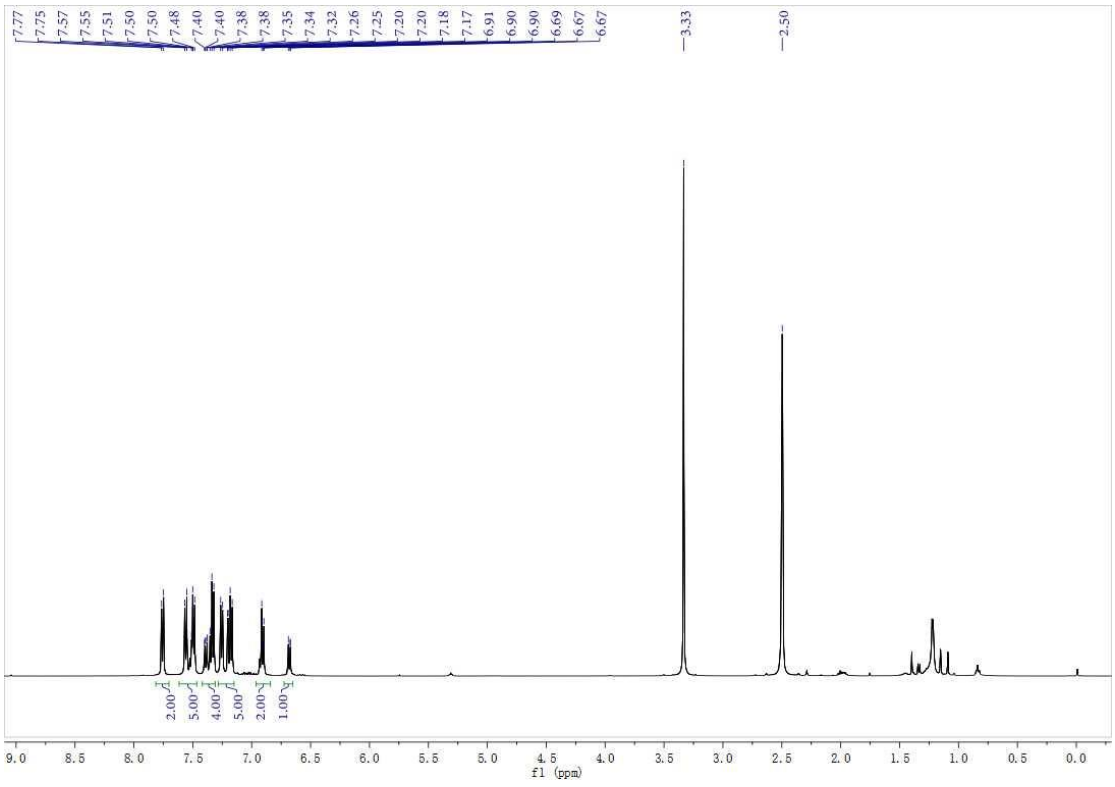

Chemical Formula: $C_{38}H_{19}Cl_4NO_3$
Exact Mass: 677.0119
Molecular Weight: 679.3740
f1 (ppm)

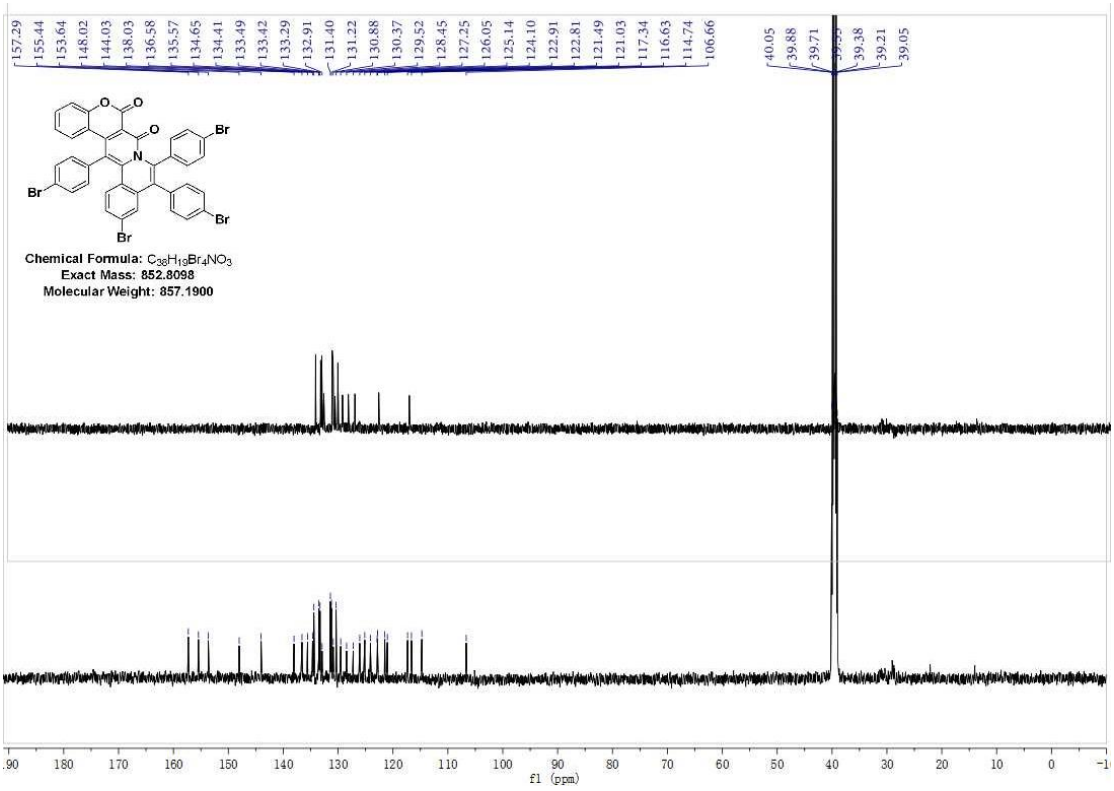


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
700.0023	700.0011	-1.16	-1.66	C38 H19 Cl4 N Na O3	(M+Na)+

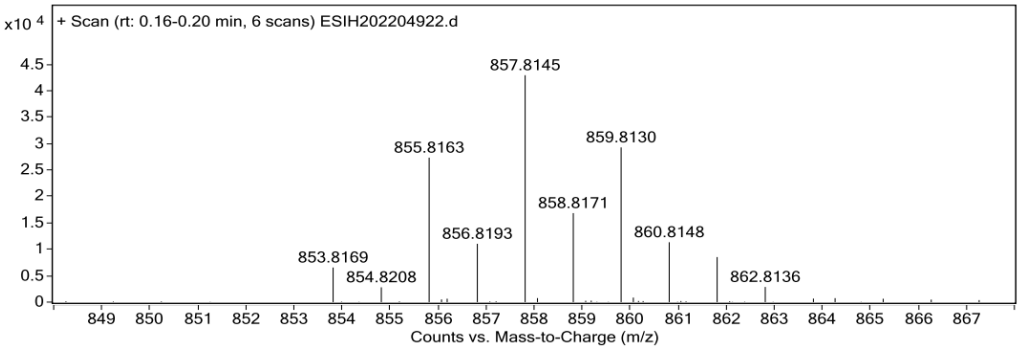
12-Bromo-9,10,15-tris(4-bromophenyl)-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3af**)





User Spectra

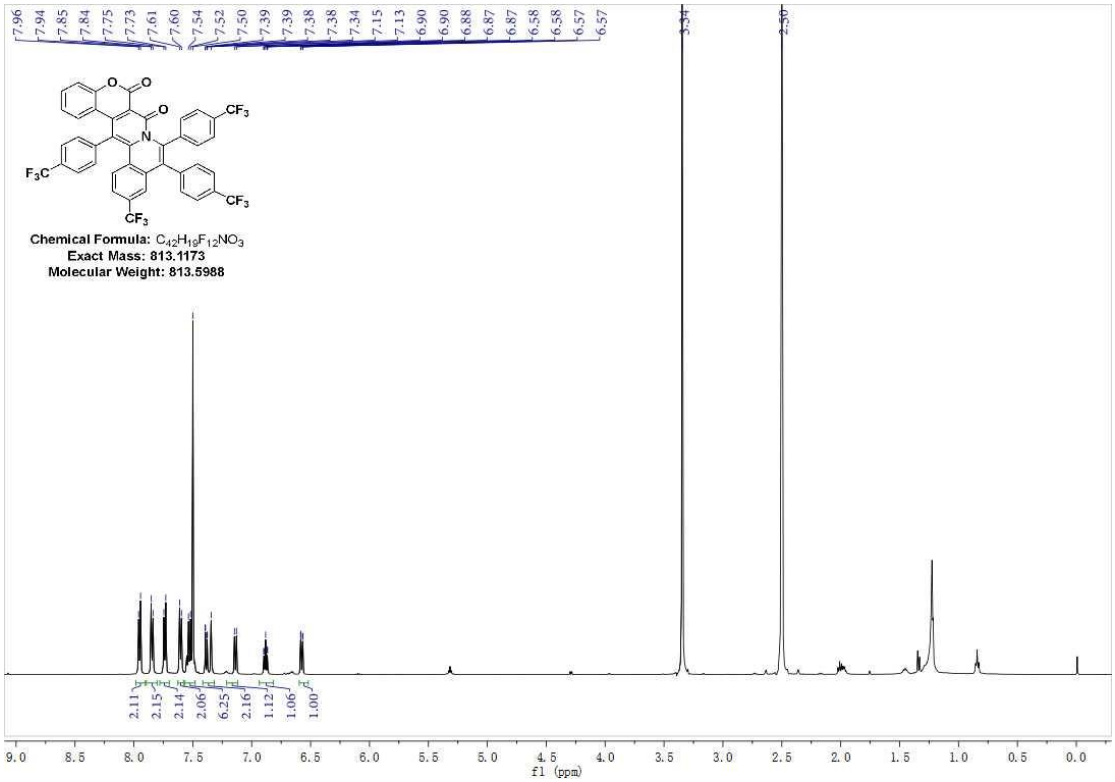
Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI

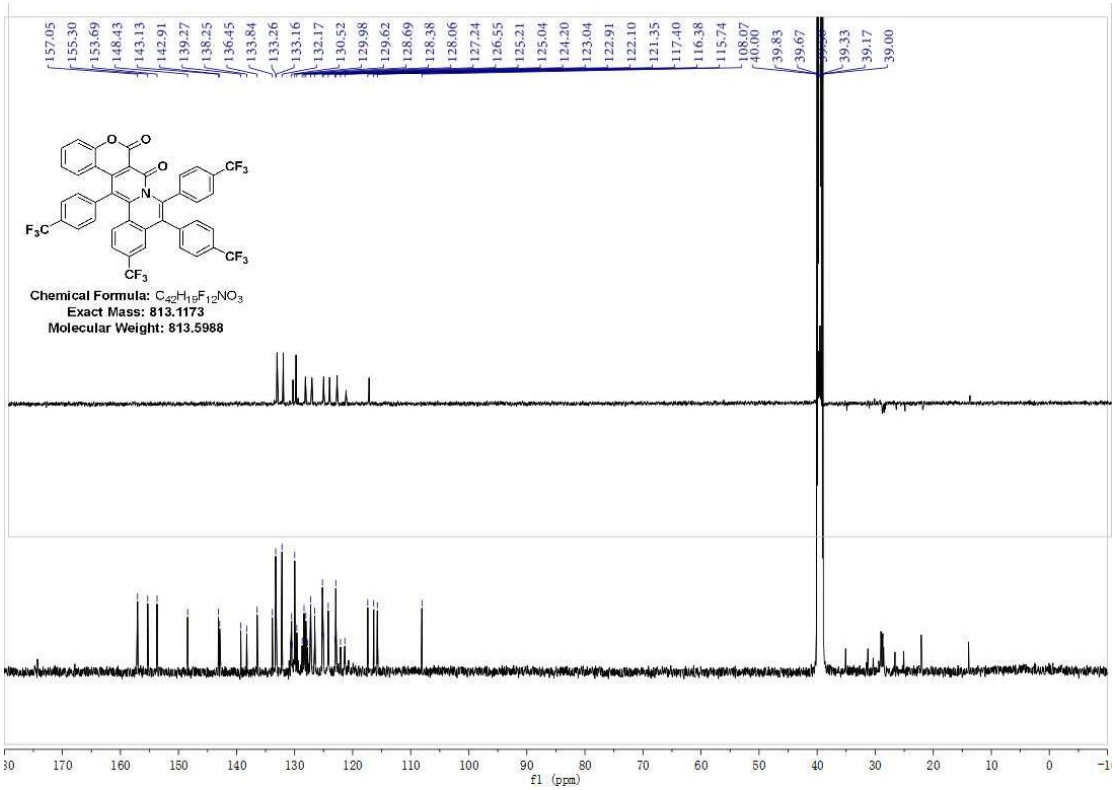


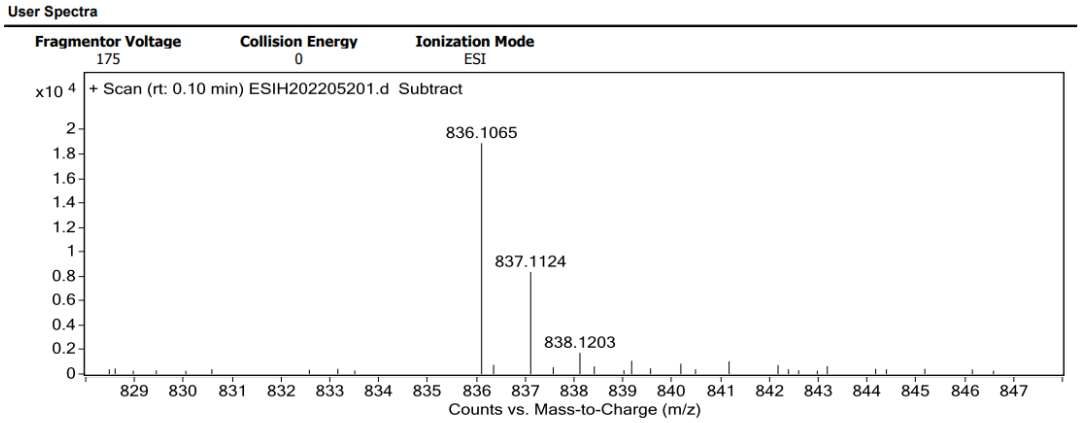
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
853.8169	853.8171	0.24	0.29	C38 H20 Br4 N O3	(M+H)+

12-(Trifluoromethyl)-9,10,15-tris(4-(trifluoromethyl)phenyl)-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ag**)



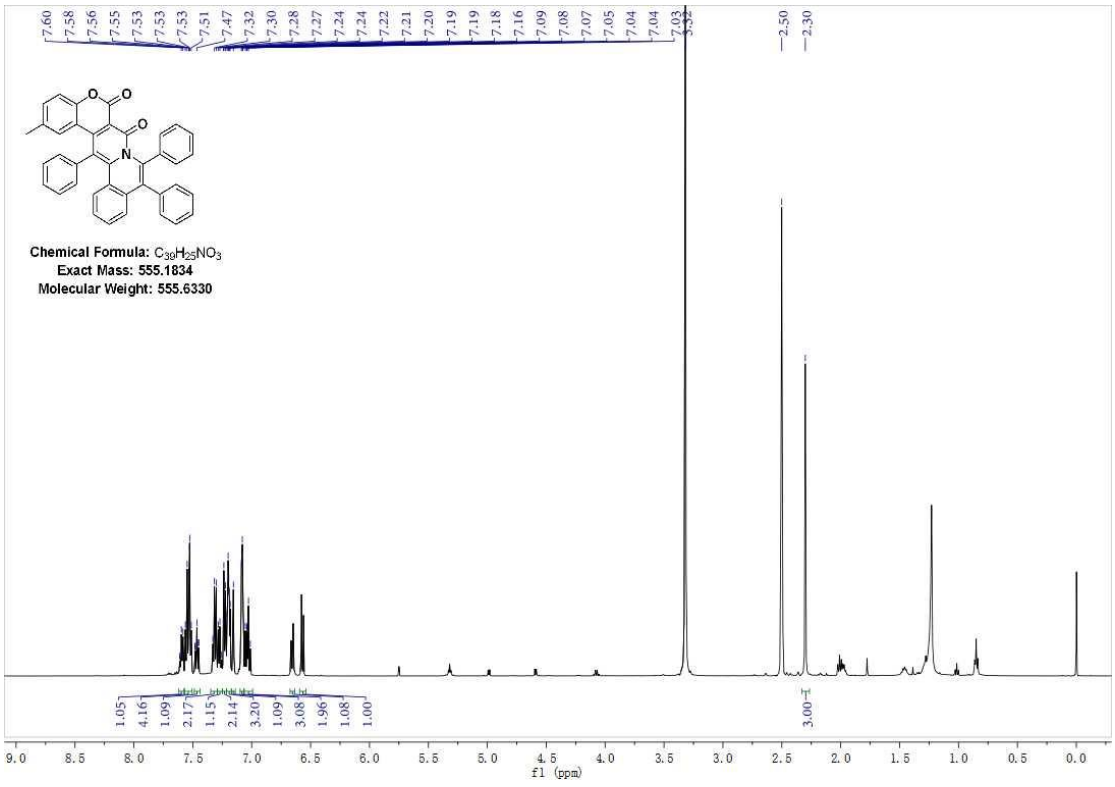


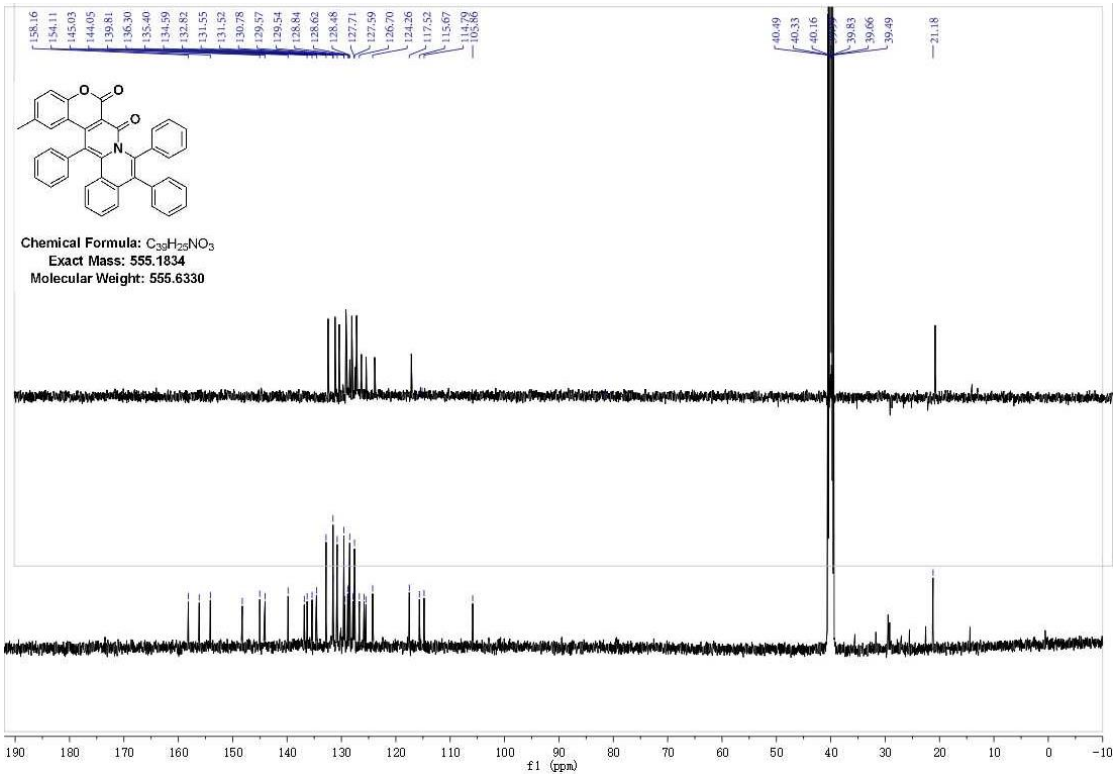


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
836.1065	836.1066	0.1	0.12	C42 H19 F12 N Na O3	(M+Na)+

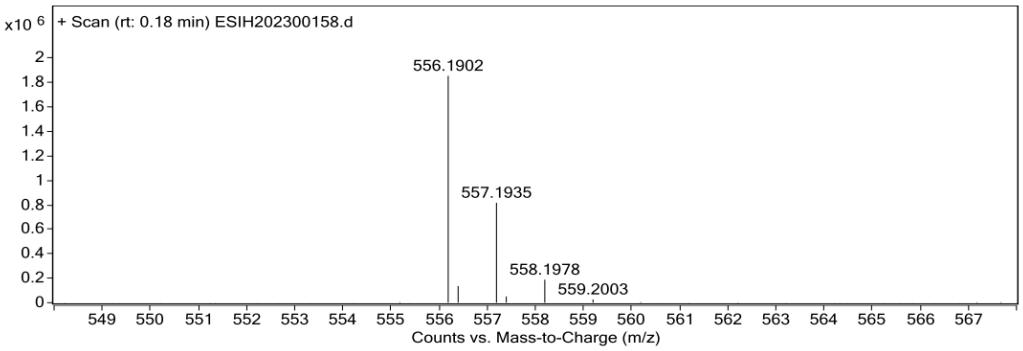
2-Methyl-9,10,15-triphenyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ba**)





User Spectra

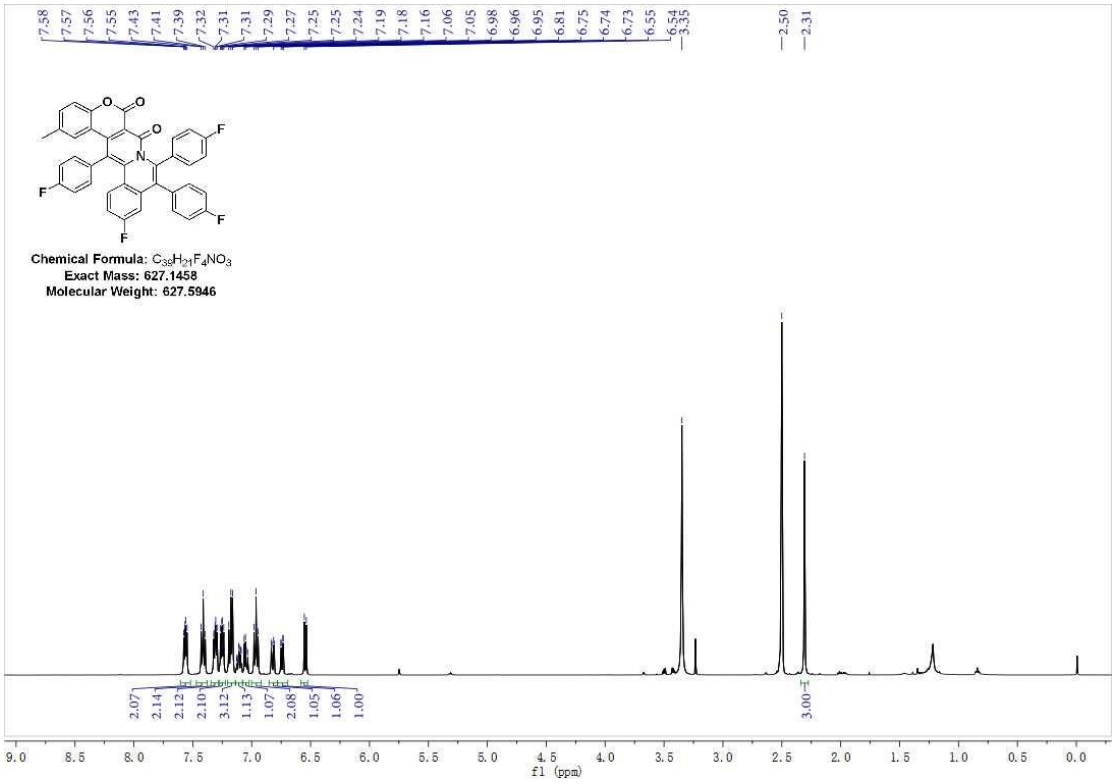
Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI

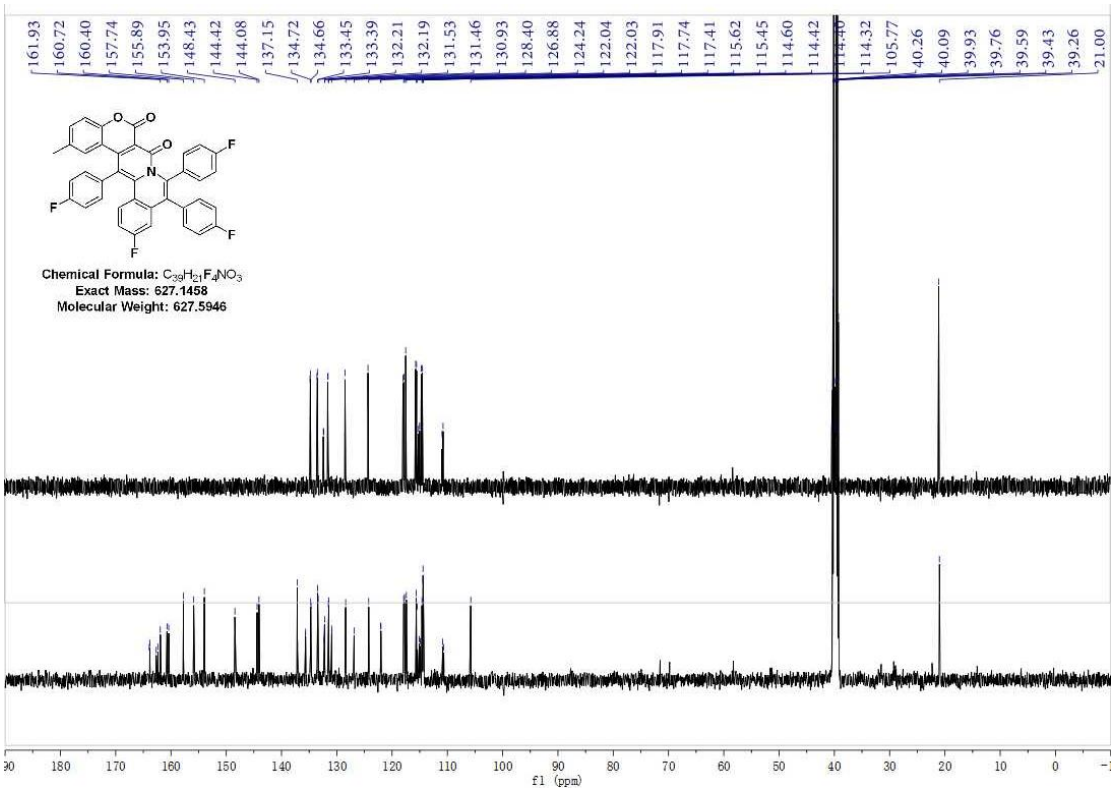


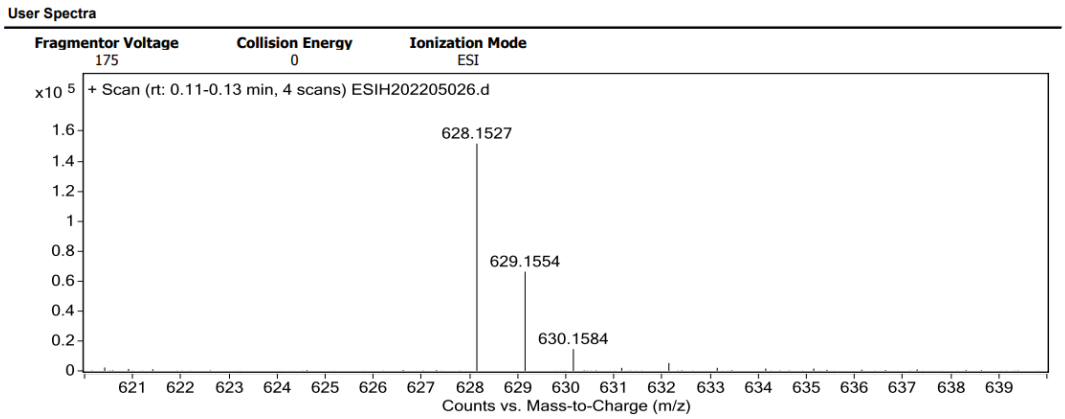
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
556.1902	556.1907	0.54	0.97	C39 H26 N O3	(M+H)+

12-Fluoro-9,10,15-tris(4-fluorophenyl)-2-methyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3bd**)



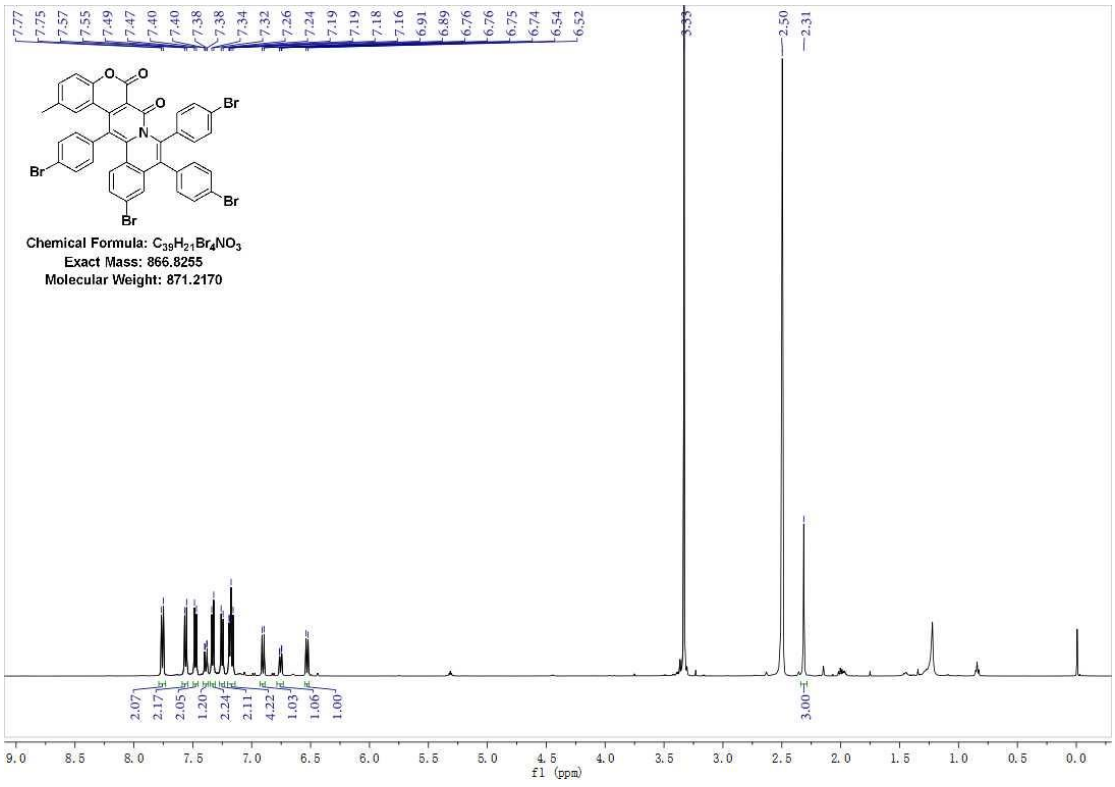


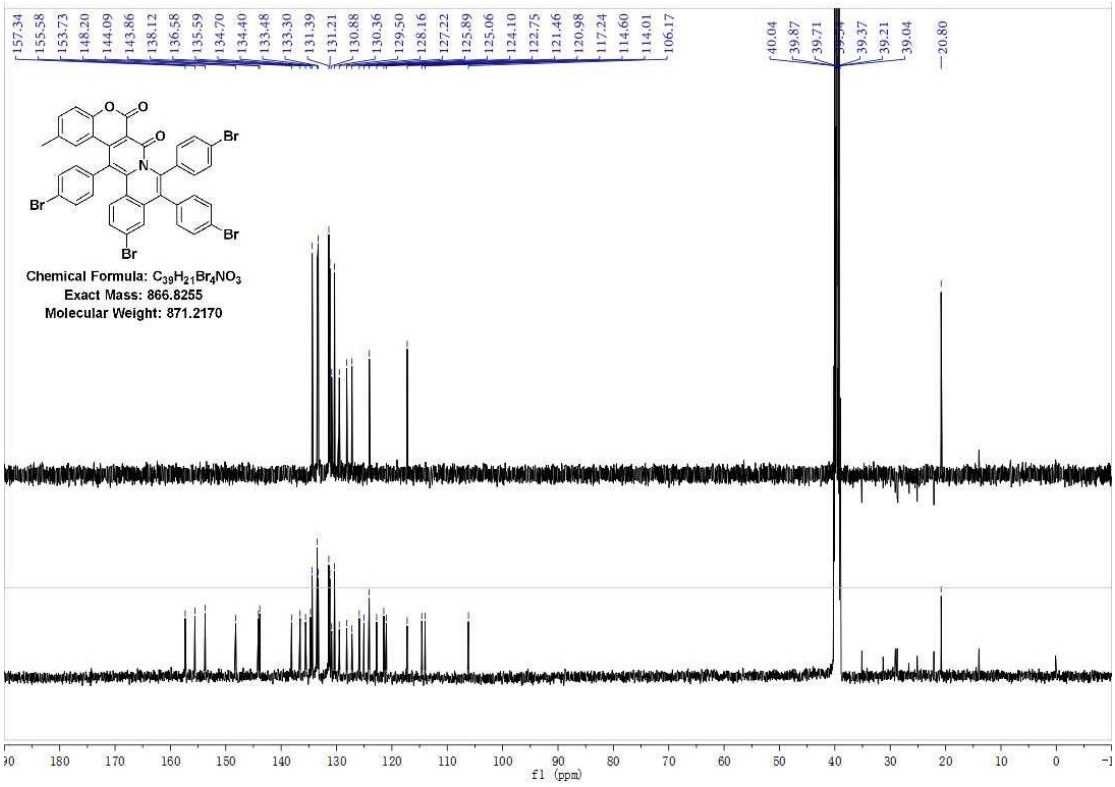


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
628.1527	628.153	0.34	0.54	C39 H22 F4 N O3	(M+H)+

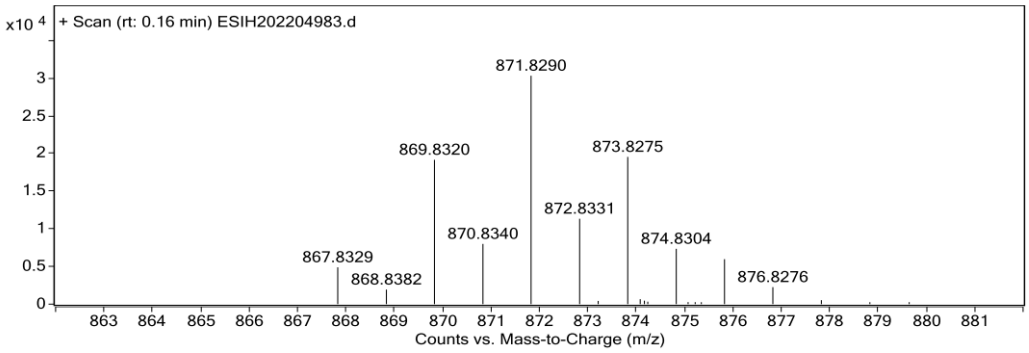
12-Bromo-9,10,15-tris(4-bromophenyl)-2-methyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3bf**)





User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI

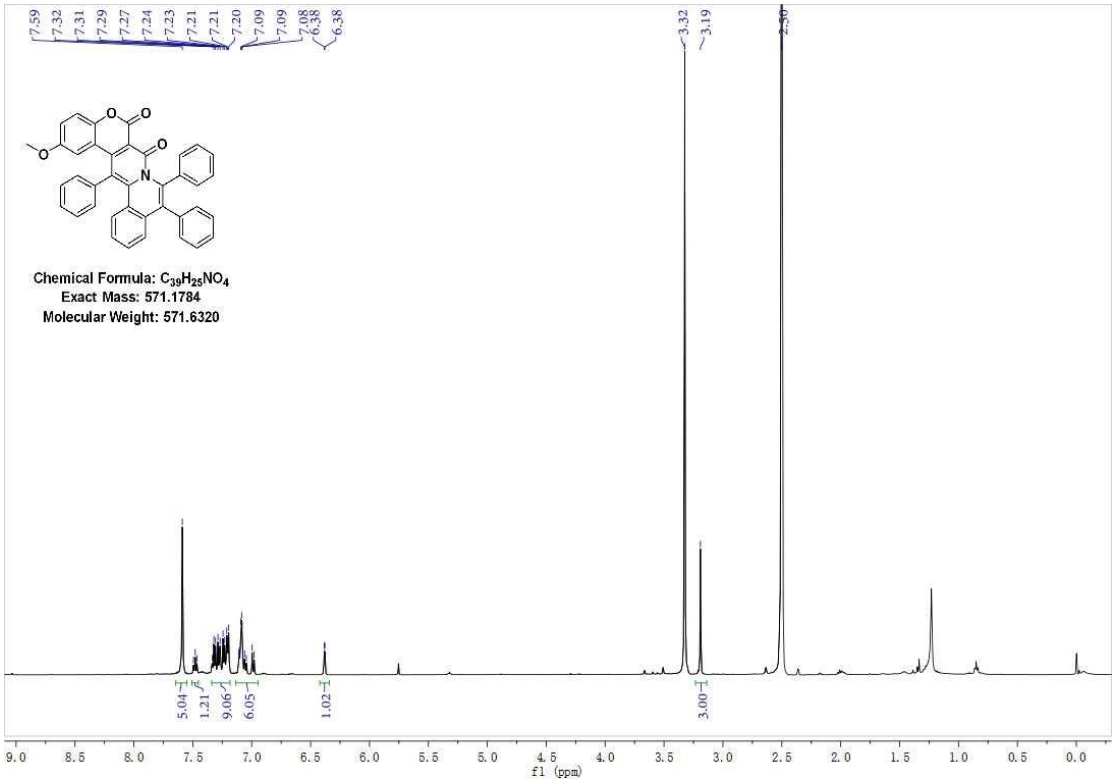


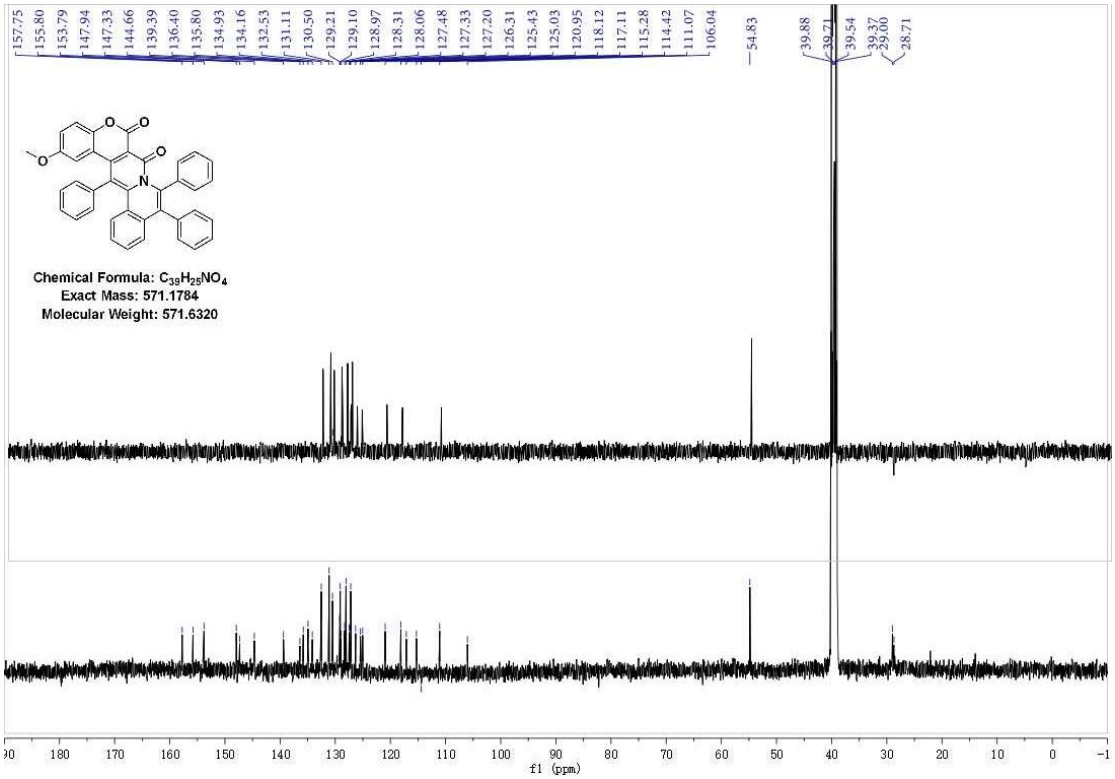
Formula Calculator Results

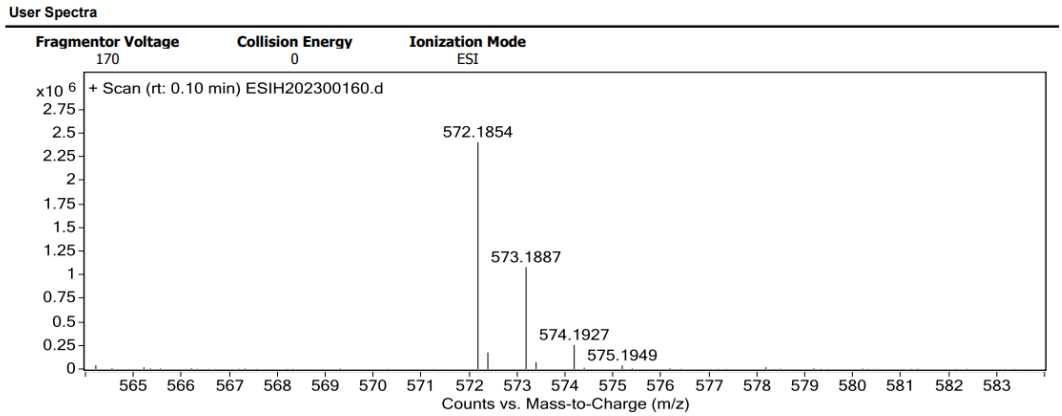
m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
867.8329	867.8328	-0.13	-0.15	C39 H22 Br4 N O3	(M+H)+

End Of Report

2-Methoxy-9,10,15-triphenyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ca**)



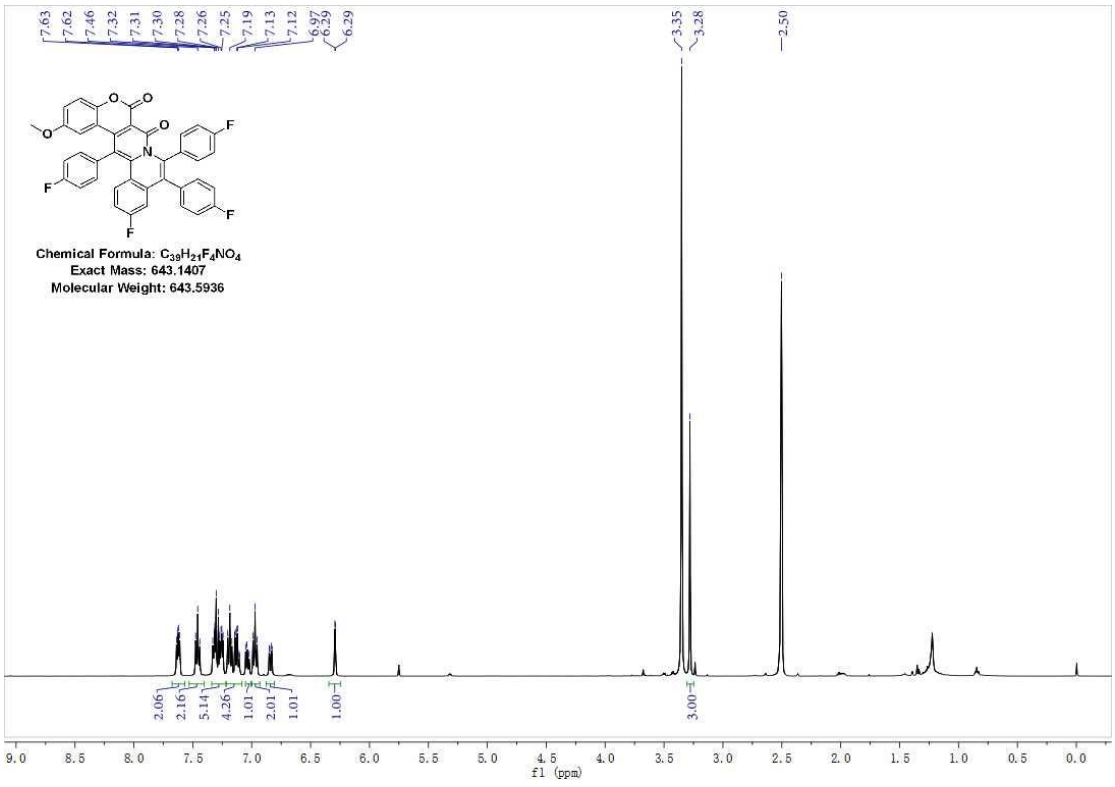


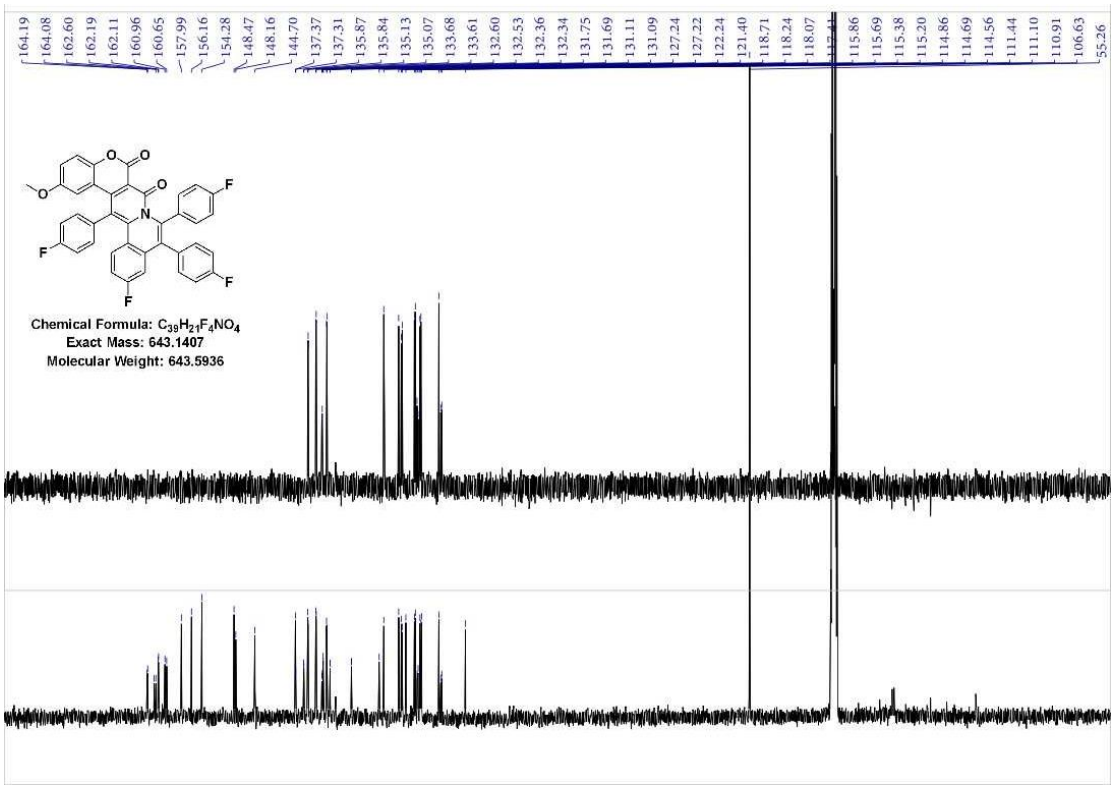


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
572.1854	572.1856	0.26	0.45	C39 H26 N O4	(M+H)+

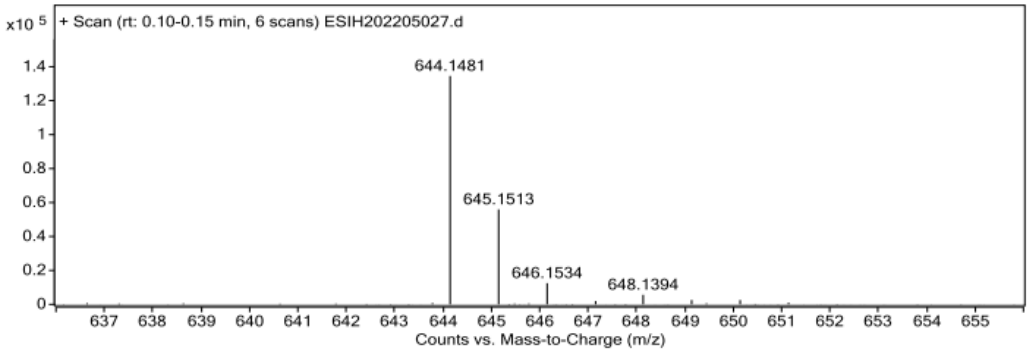
12-Fluoro-9,10,15-tris(4-fluorophenyl)-2-methoxy-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3cd**)





User Spectra

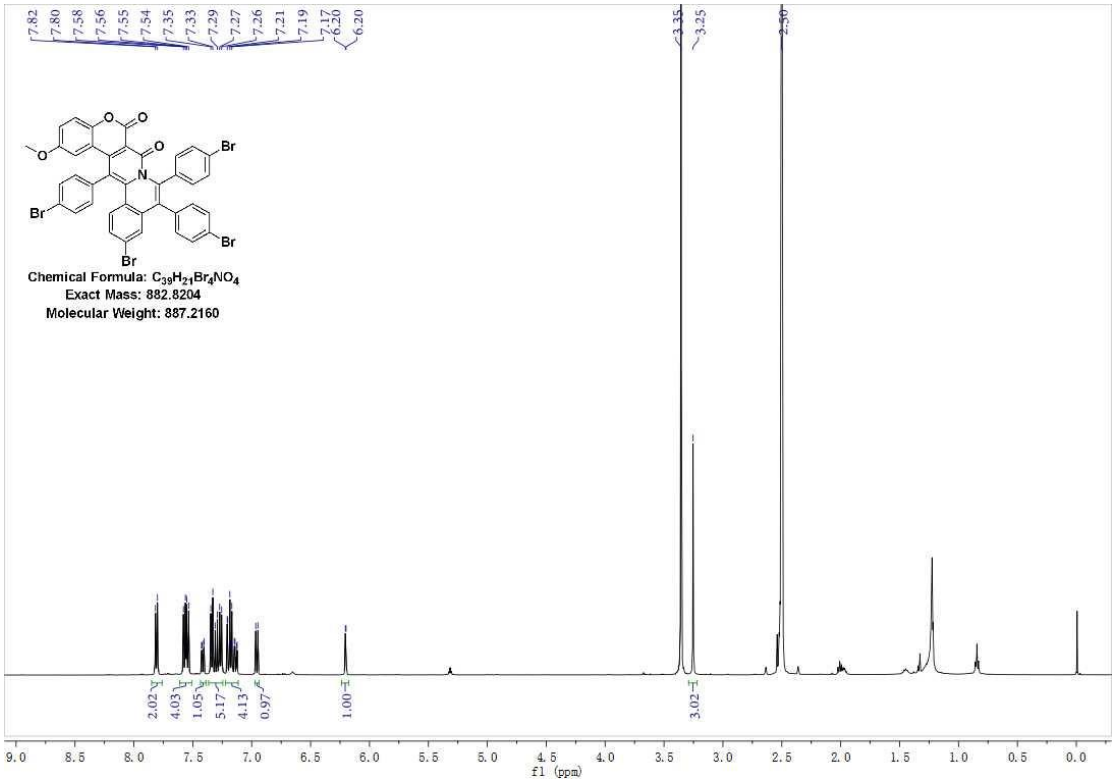
Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI

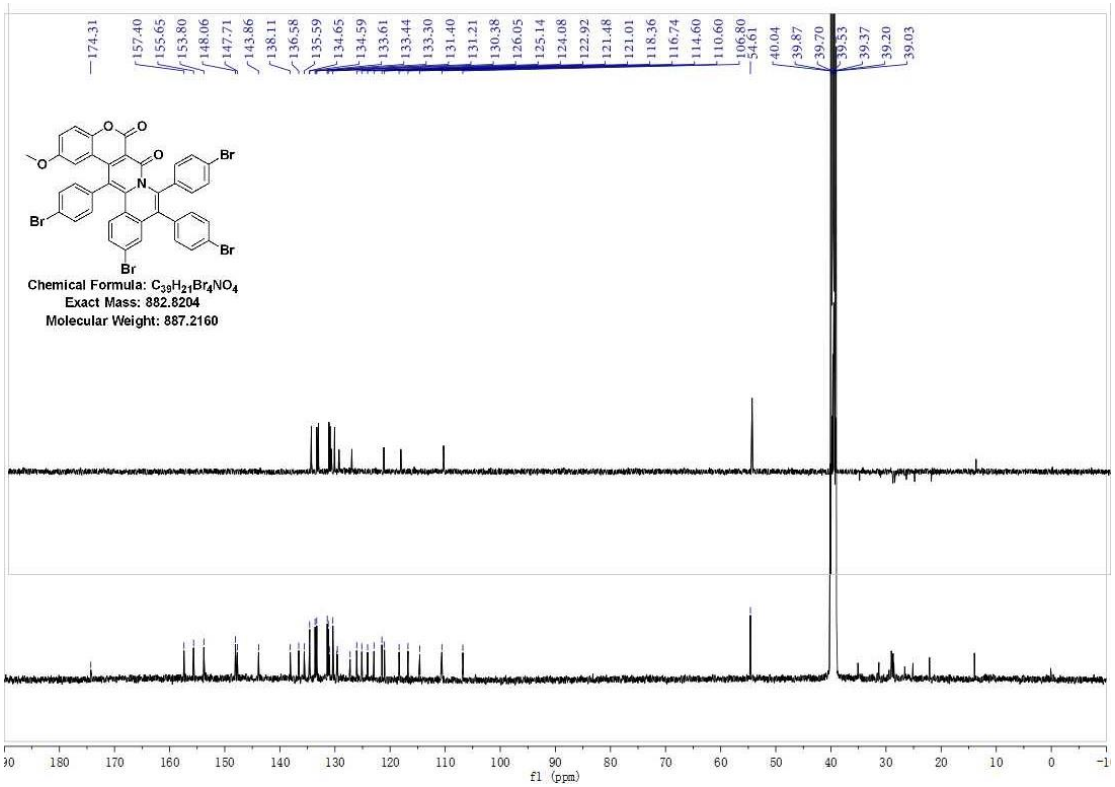


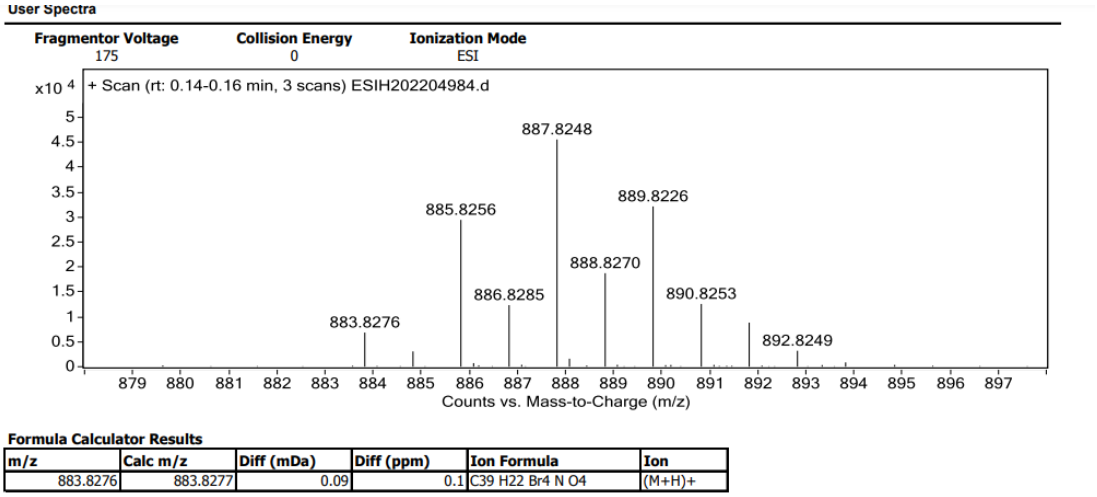
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
644.1481	644.1479	-0.13	-0.21	C39 H22 F4 N O4	(M+H)+

12-Bromo-9,10,15-tris(4-bromophenyl)-2-methoxy-6H,7H-chromeno[4',3':4,5]pyrido [2,1-a]isoquinoline-6,7-dione (**3cf**)



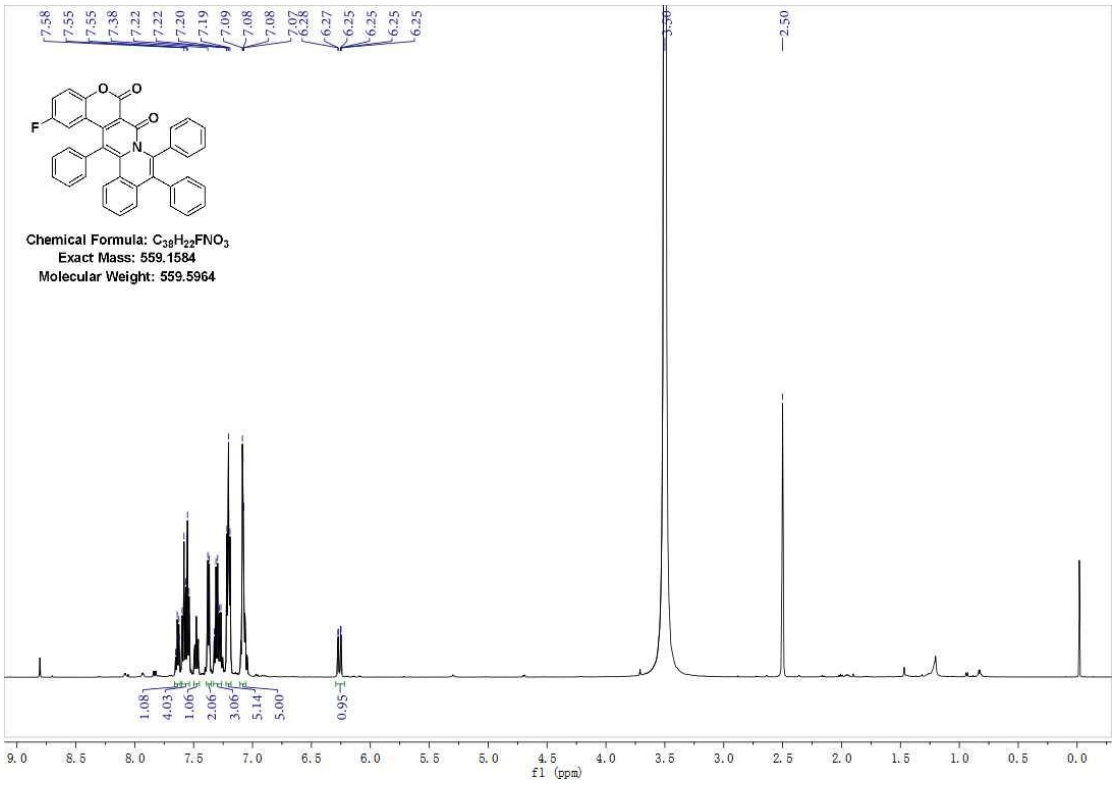


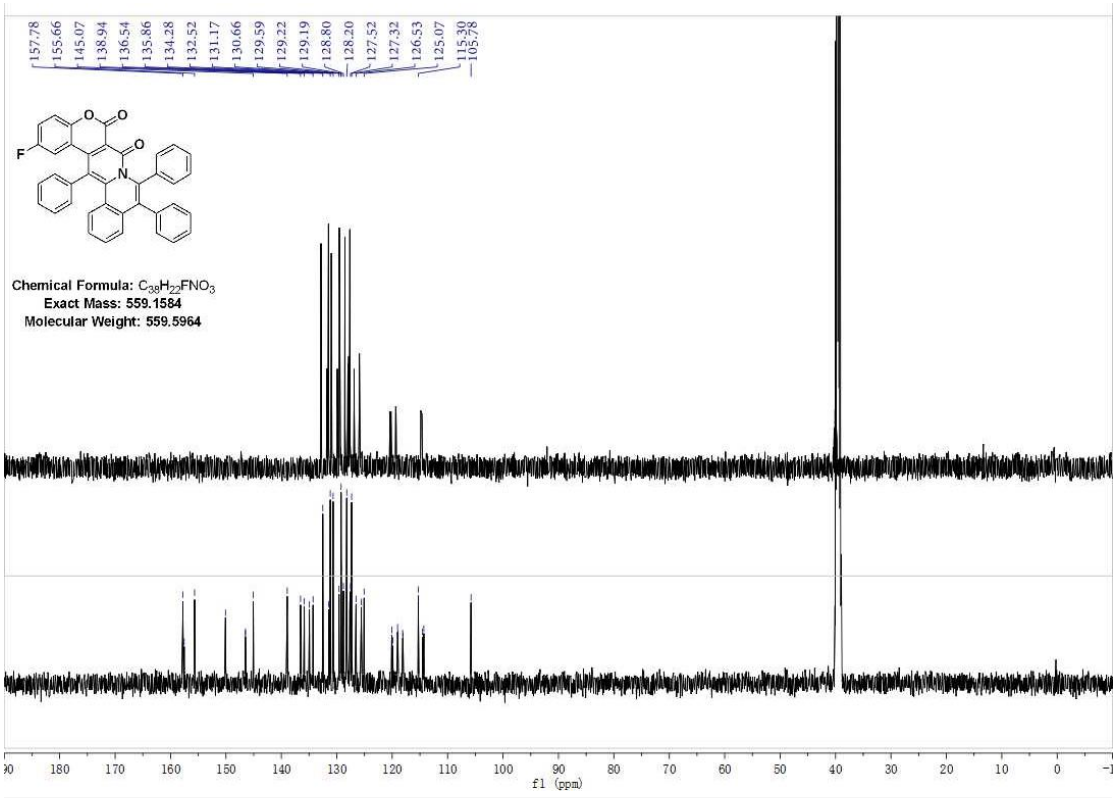


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
883.8276	883.8277	0.09	0.1	C39 H22 Br4 N O4	(M+H)+

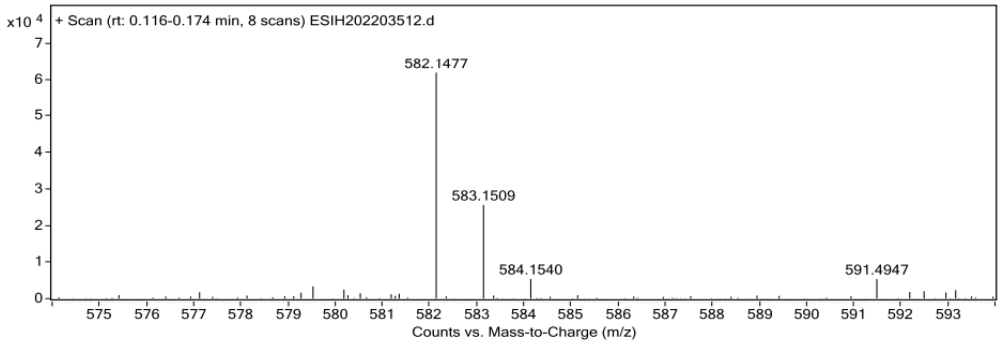
2-Fluoro-9,10,15-triphenyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3da**)





User Spectra

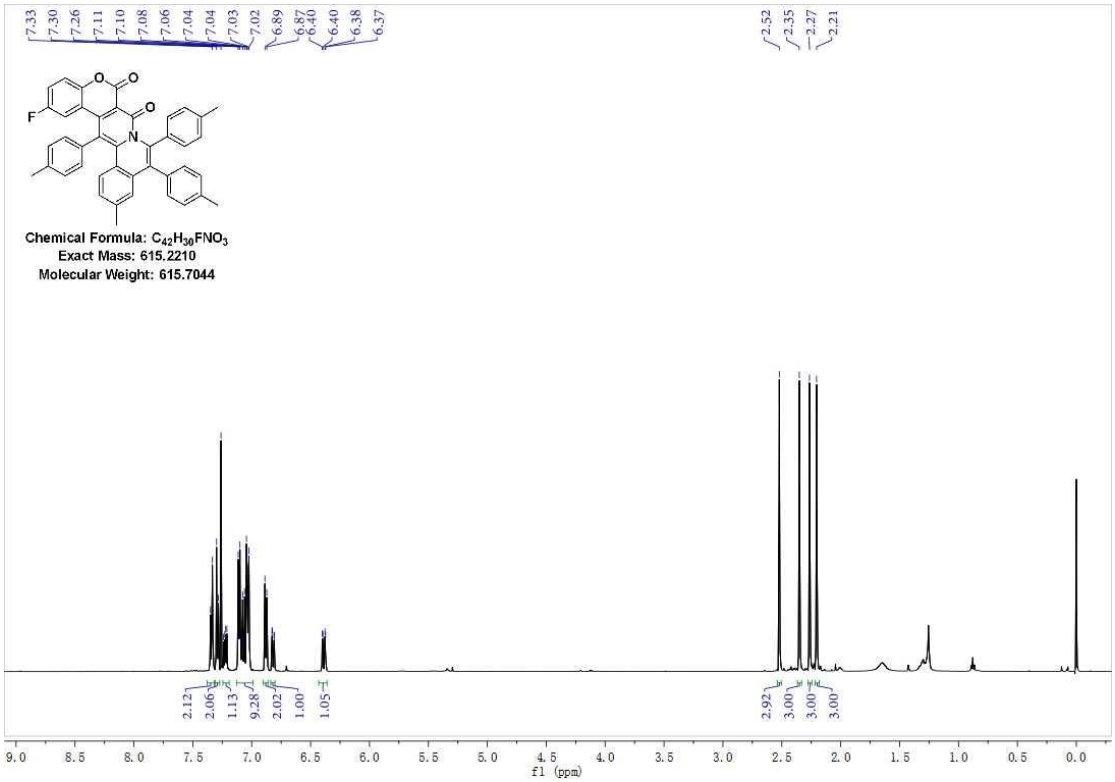
Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI

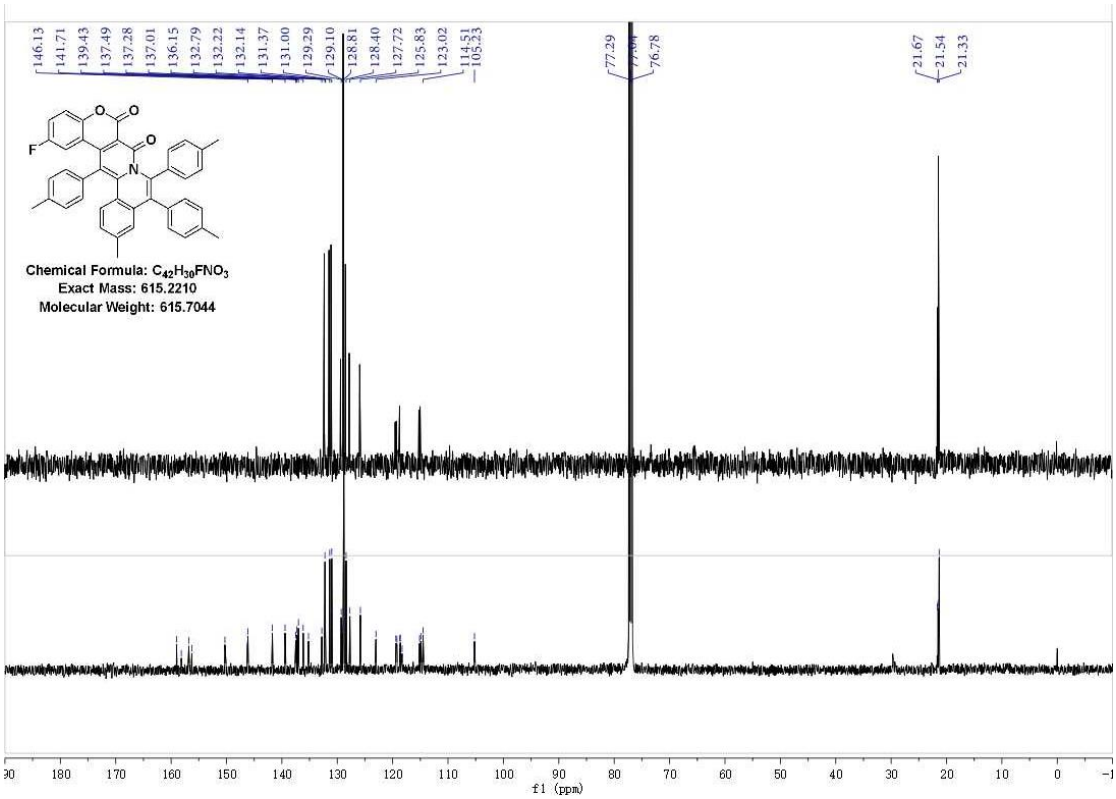


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
582.1477	582.1476	-0.12	-0.2	C38 H22 F N Na O3	(M+Na)+

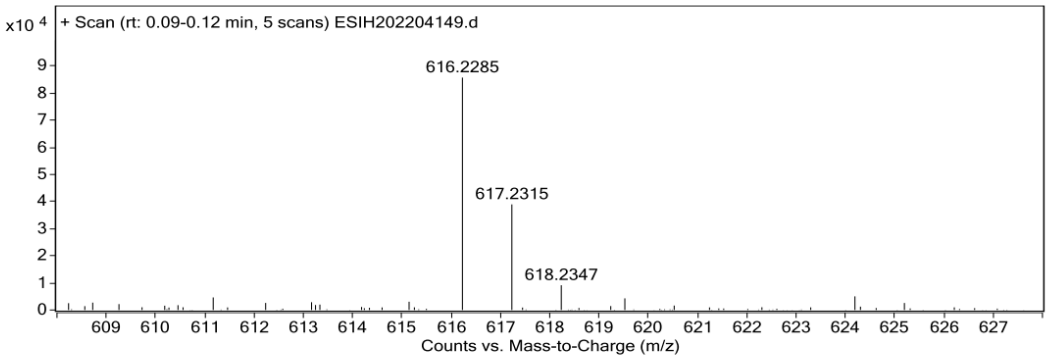
2-Fluoro-12-methyl-9,10,15-tri-p-tolyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1a]isoquinoline-6,7-dione (**3db**)





User Spectra

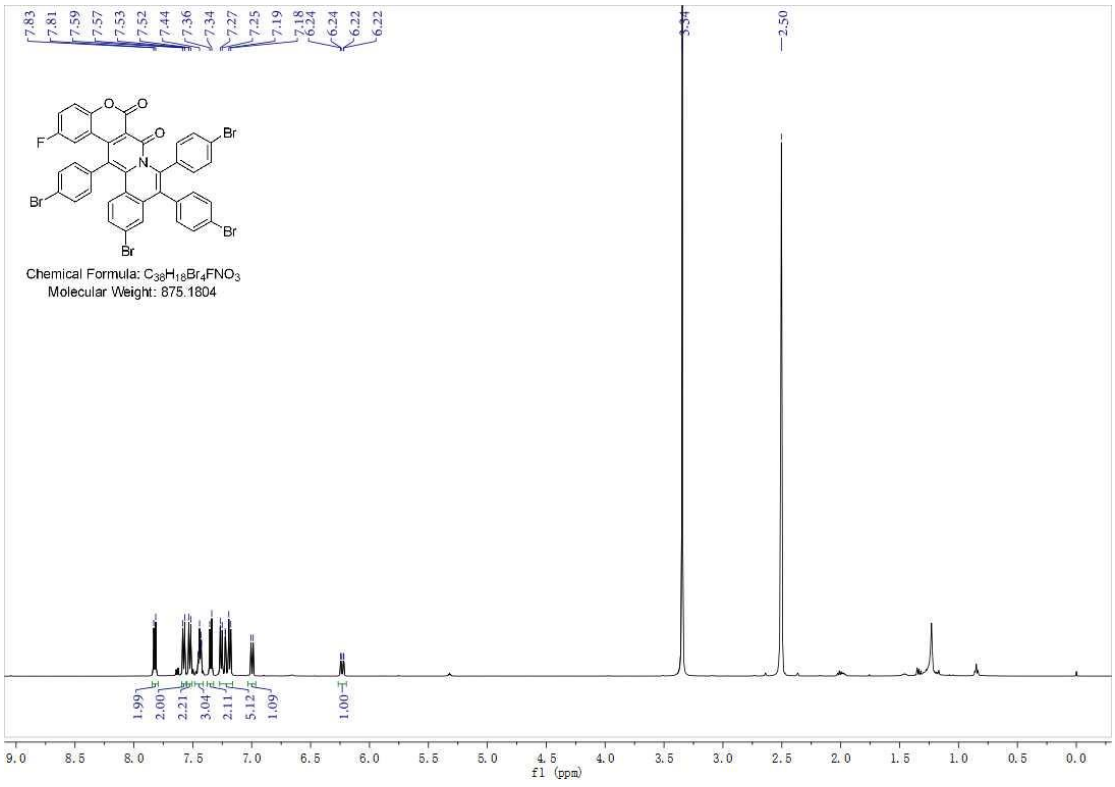
Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI

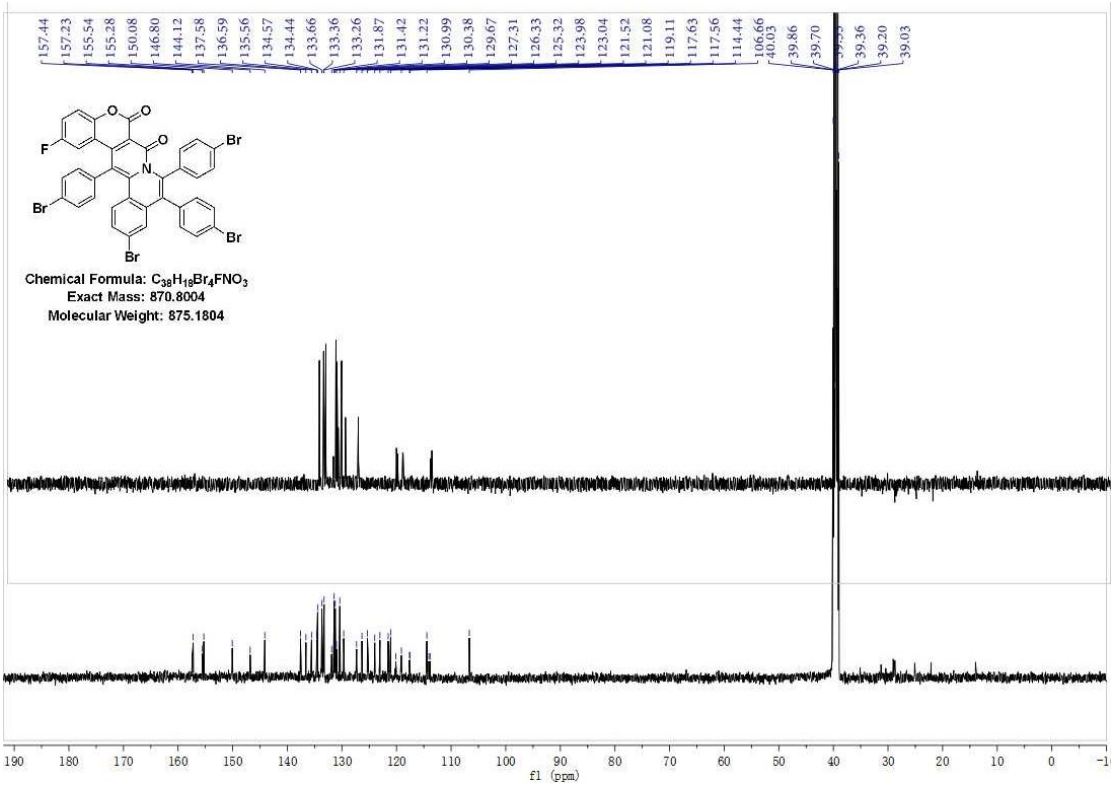


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
616.2285	616.2282	-0.3	-0.48	C42 H31 F N O3	(M+H)+

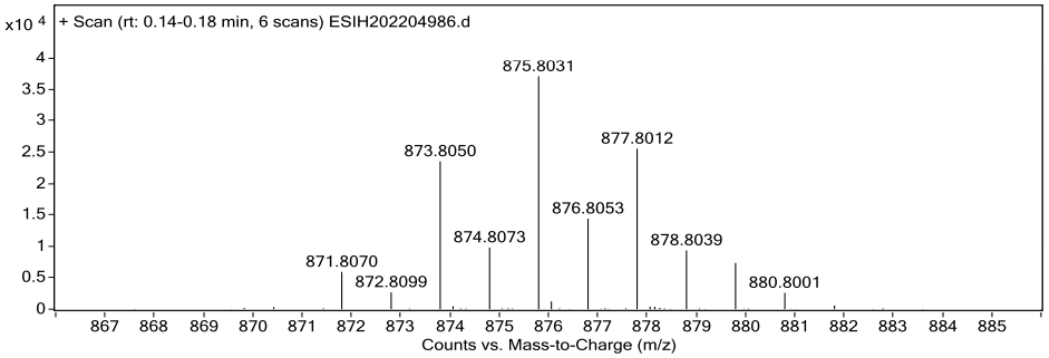
12-Bromo-9,10,15-tris(4-bromophenyl)-2-fluoro-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3df**)





User Spectra

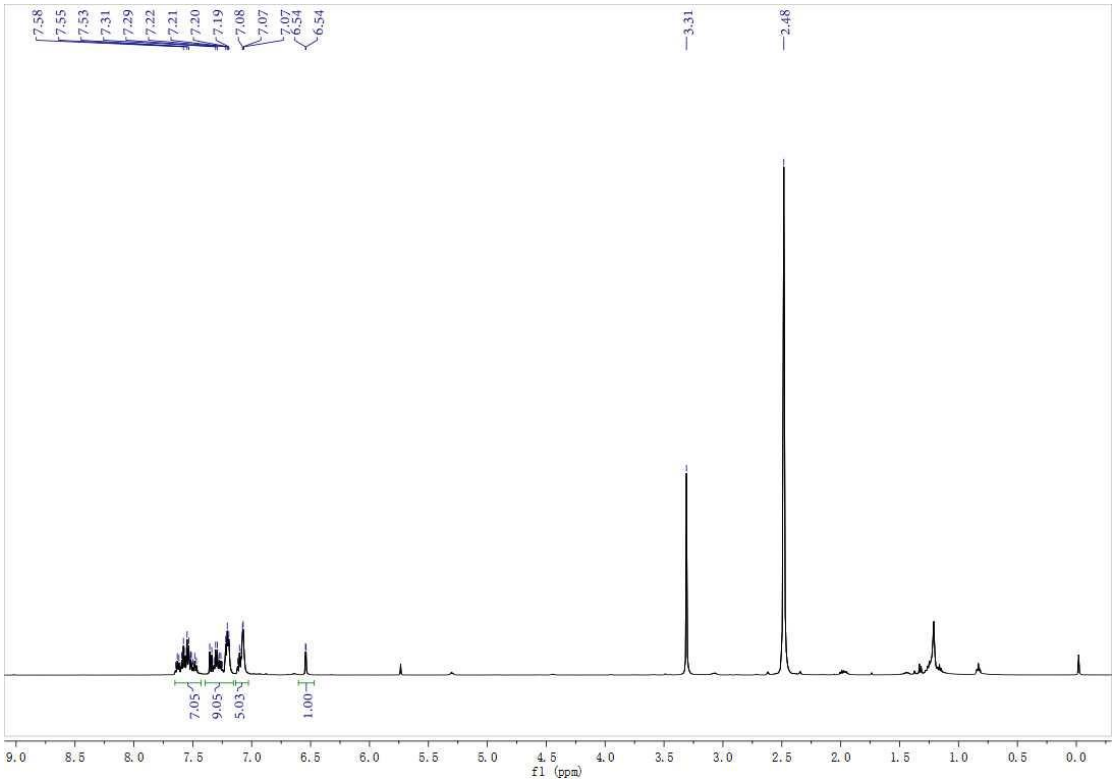
Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI

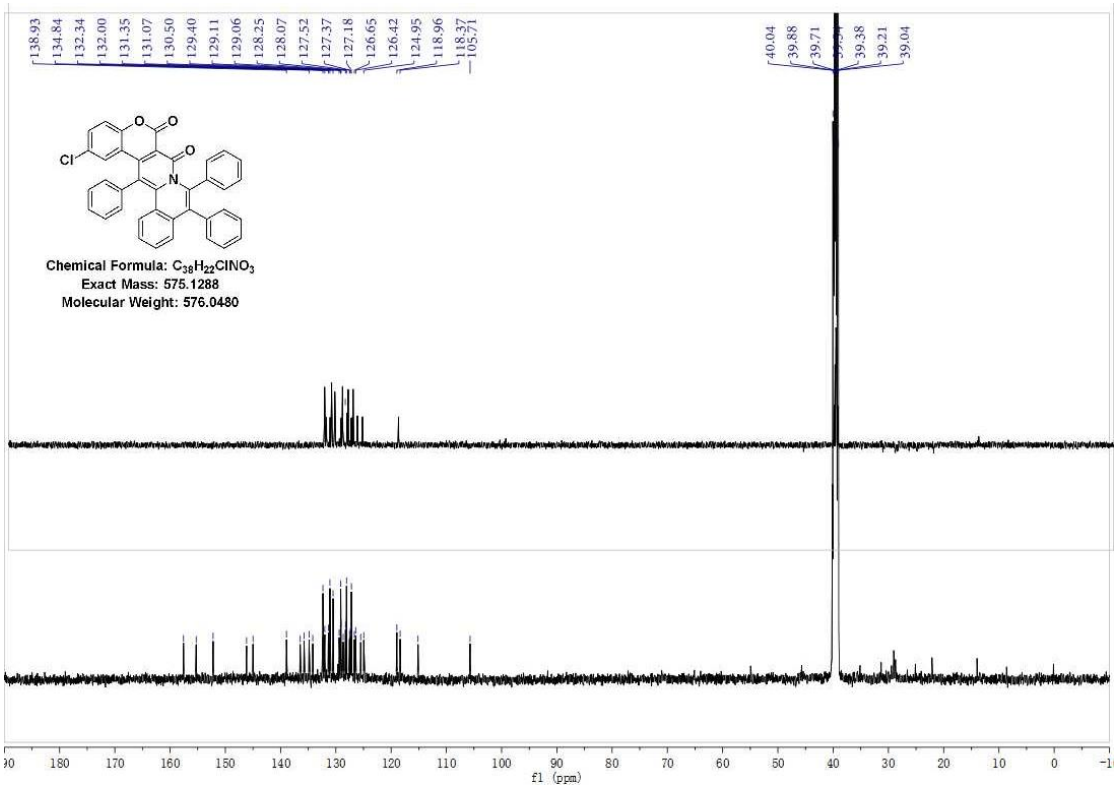


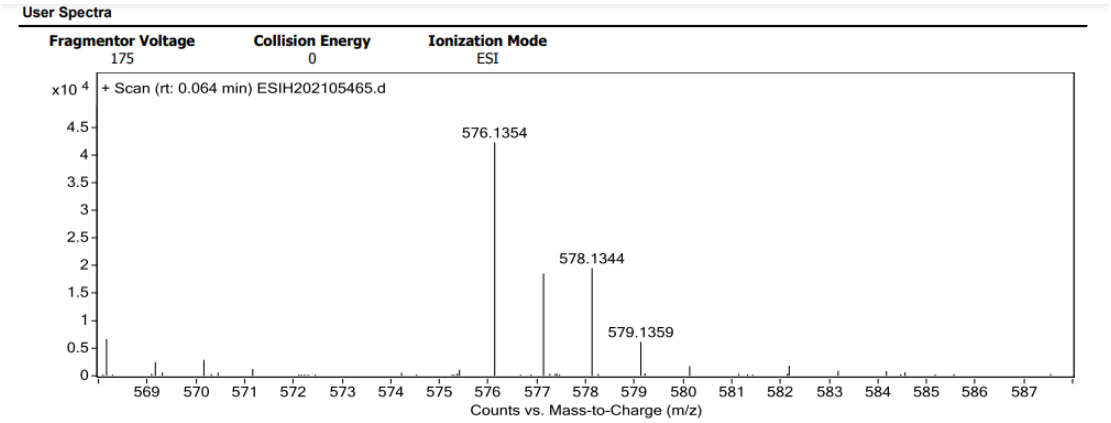
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
871.807	871.8077	0.74	0.85	C38 H19 Br4 F N O3	(M+H)+

2-Chloro-9,10,15-triphenyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ea**)



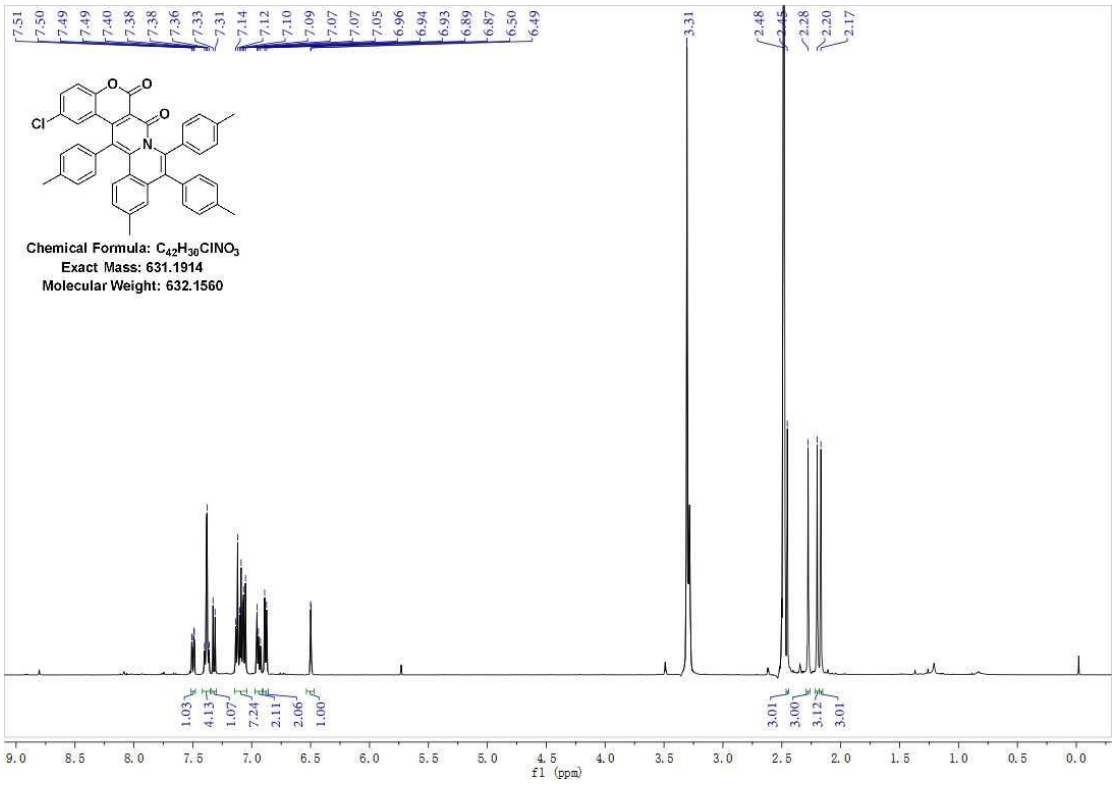


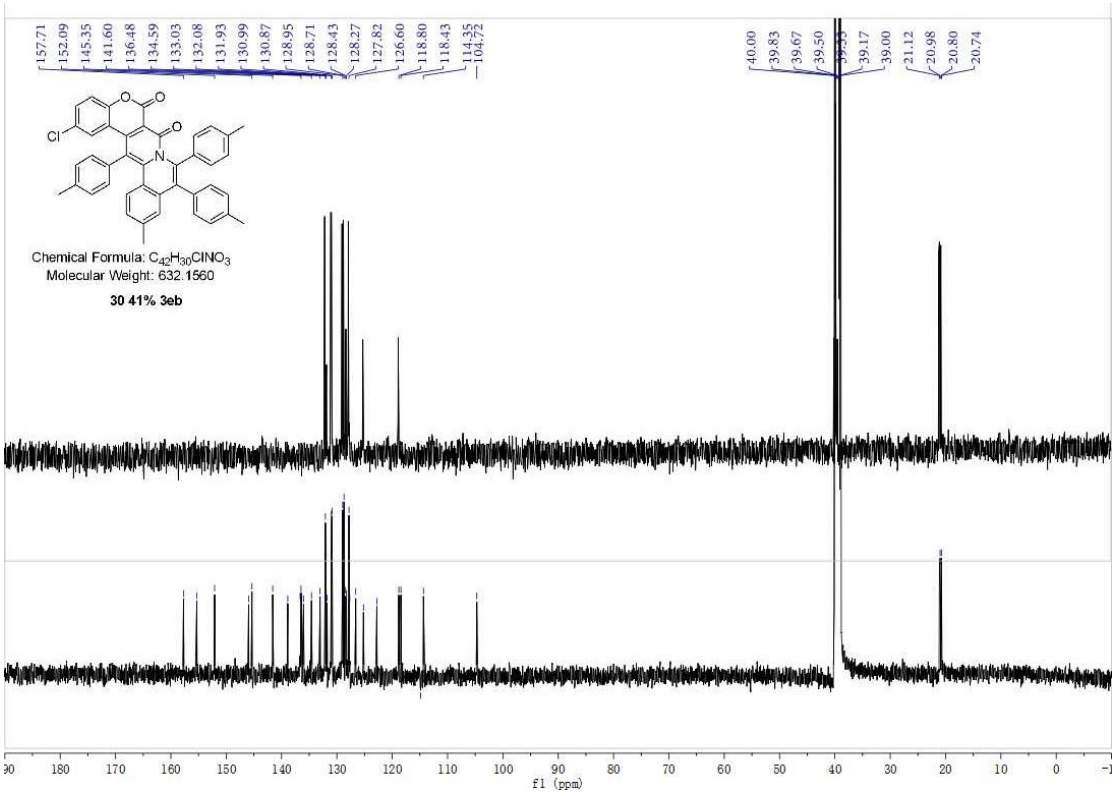


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
576.1354	576.1361	0.66	1.14	C38 H23 Cl N O3	(M+H)+

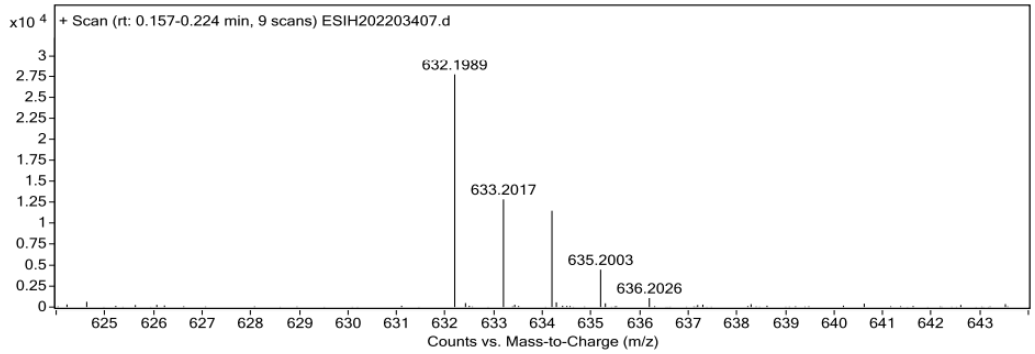
2-Chloro-12-methyl-9,10,15-tri-p-tolyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3eb**)





User Spectra

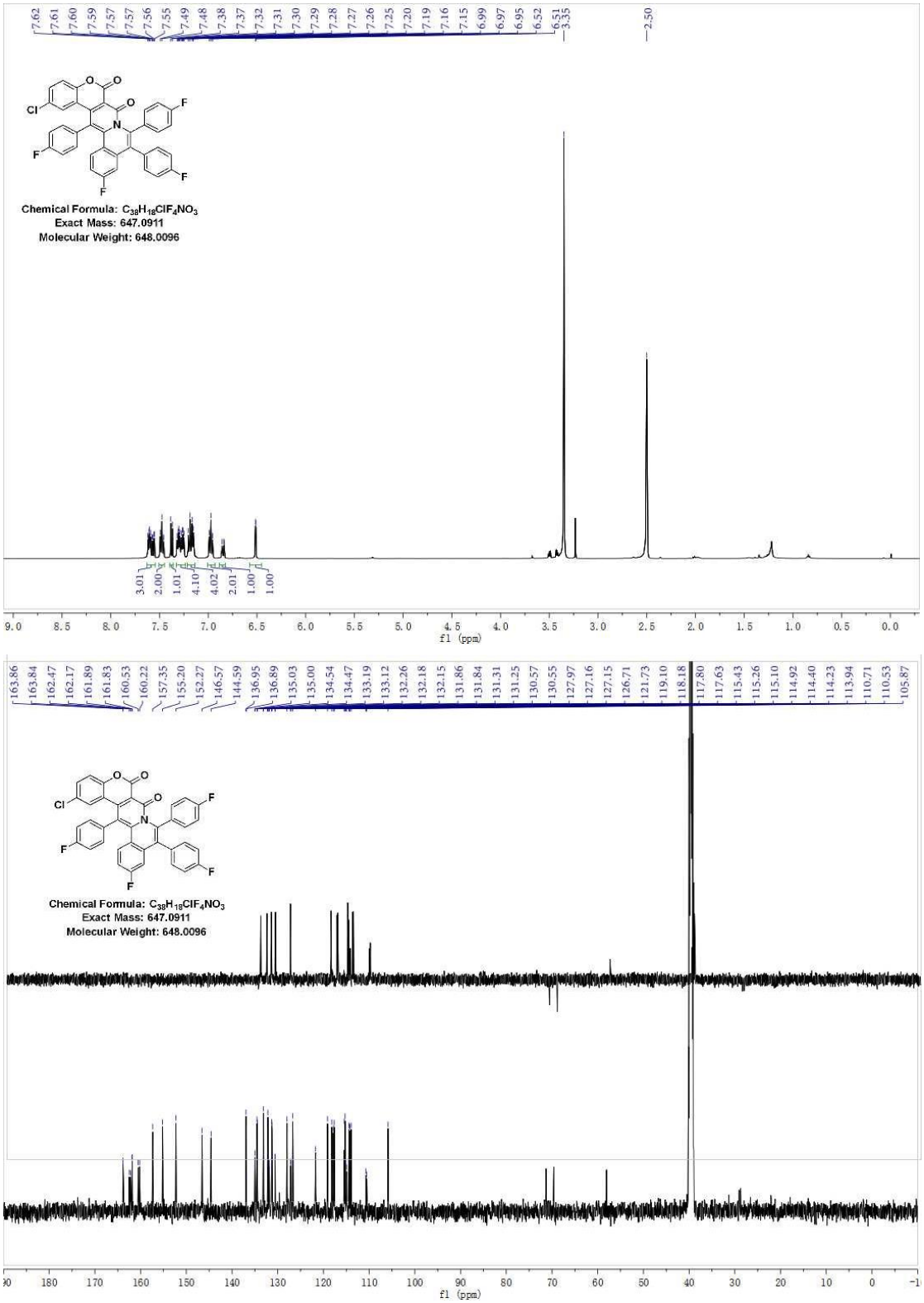
Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI

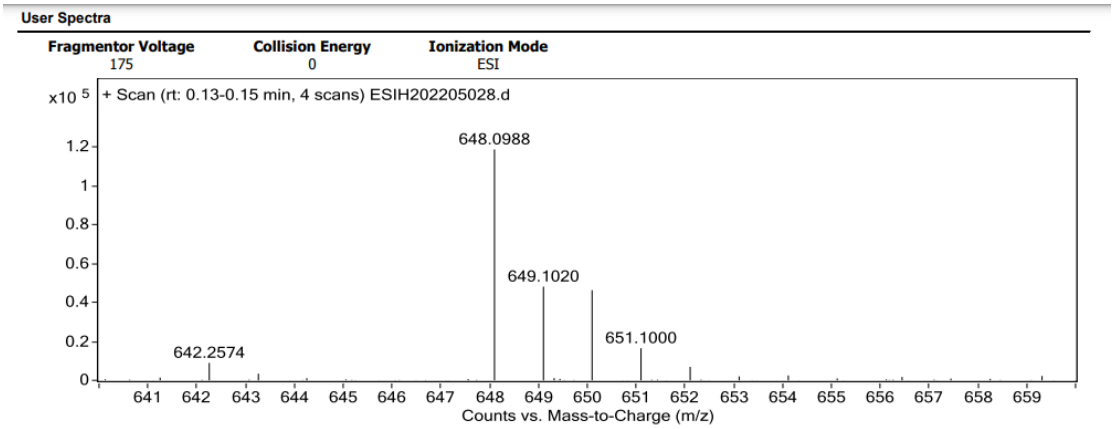


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
632.1989	632.1987	-0.16	-0.25	C42 H31 Cl N O3	(M+H)+

2-Chloro-12-fluoro-9,10,15-tris(4-fluorophenyl)-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ed**)

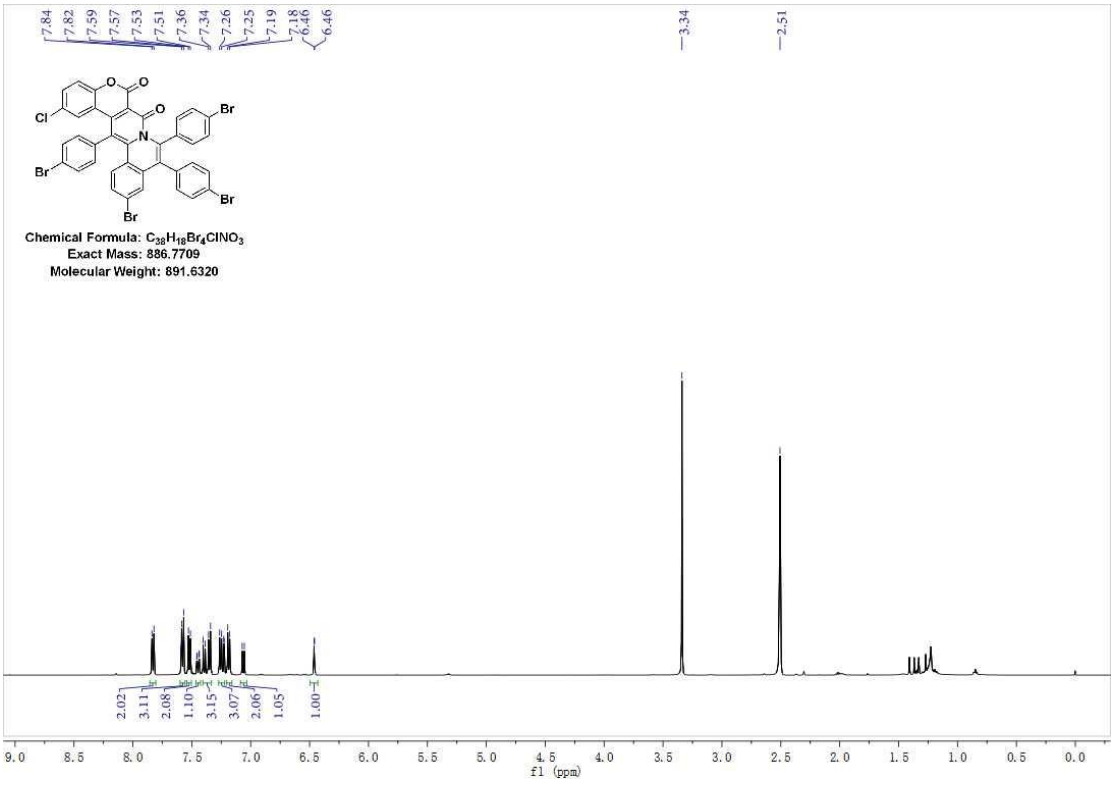


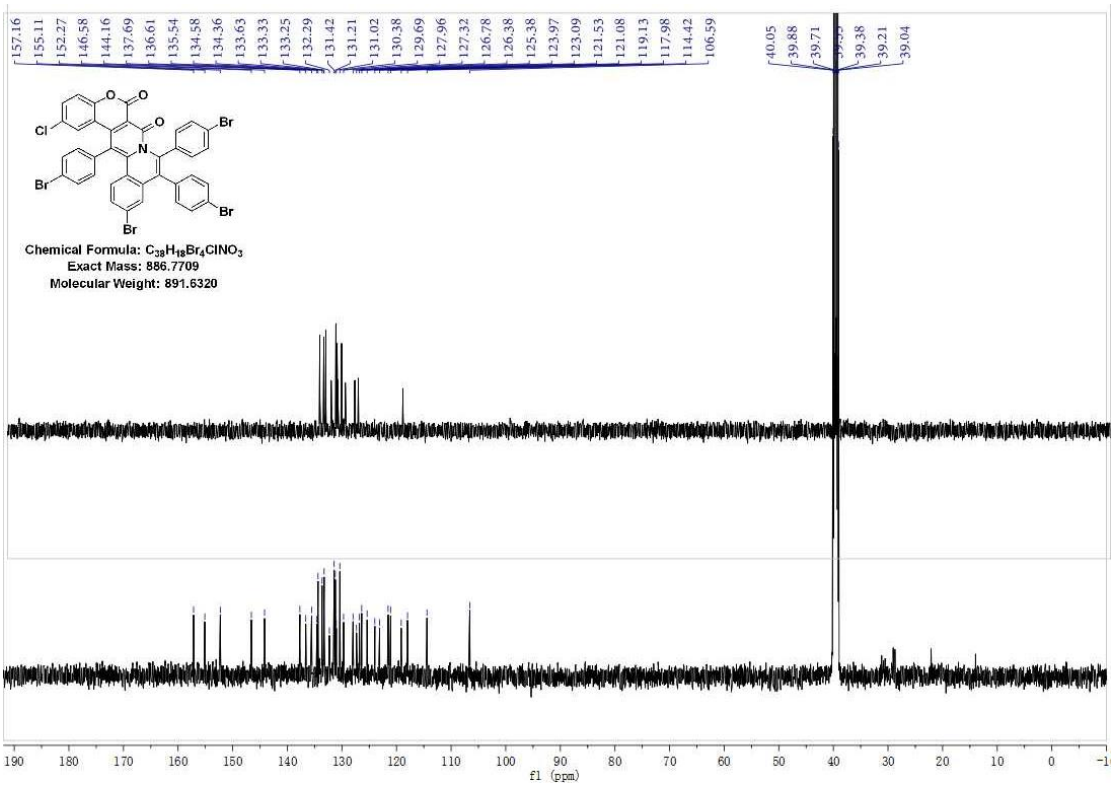


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
648.0988	648.0984	-0.43	-0.66	C38 H19 Cl F4 N O3	(M+H)+

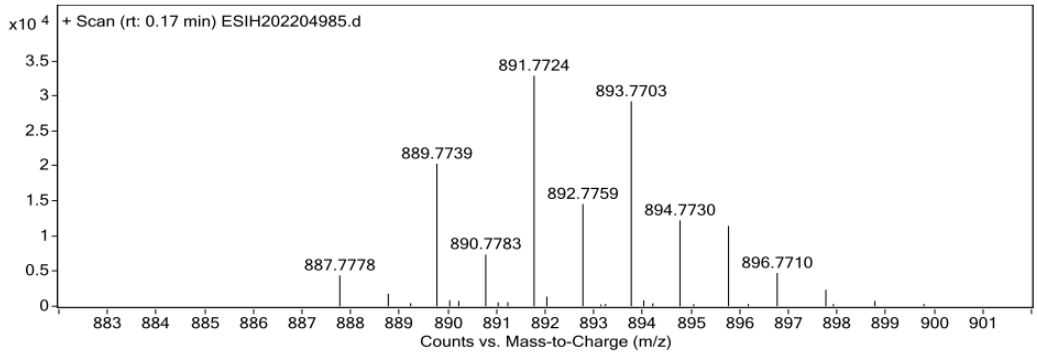
12-Bromo-9,10,15-tris(4-bromophenyl)-2-chloro-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (3ef)





User Spectra

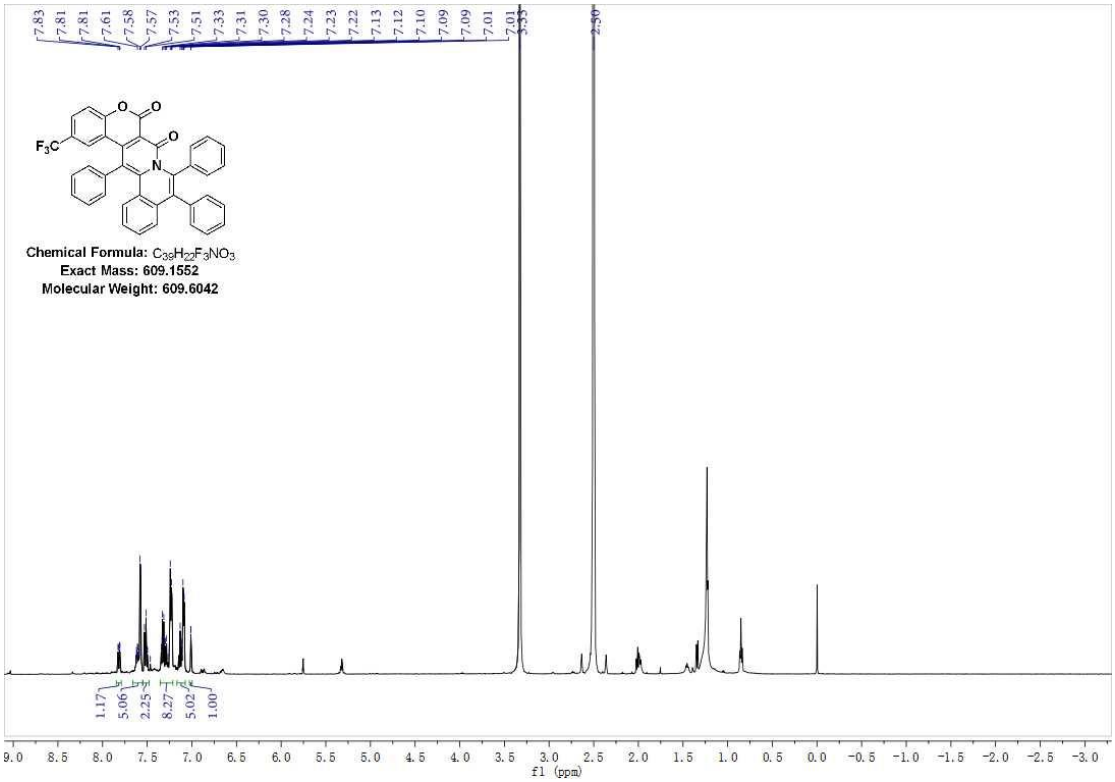
Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI

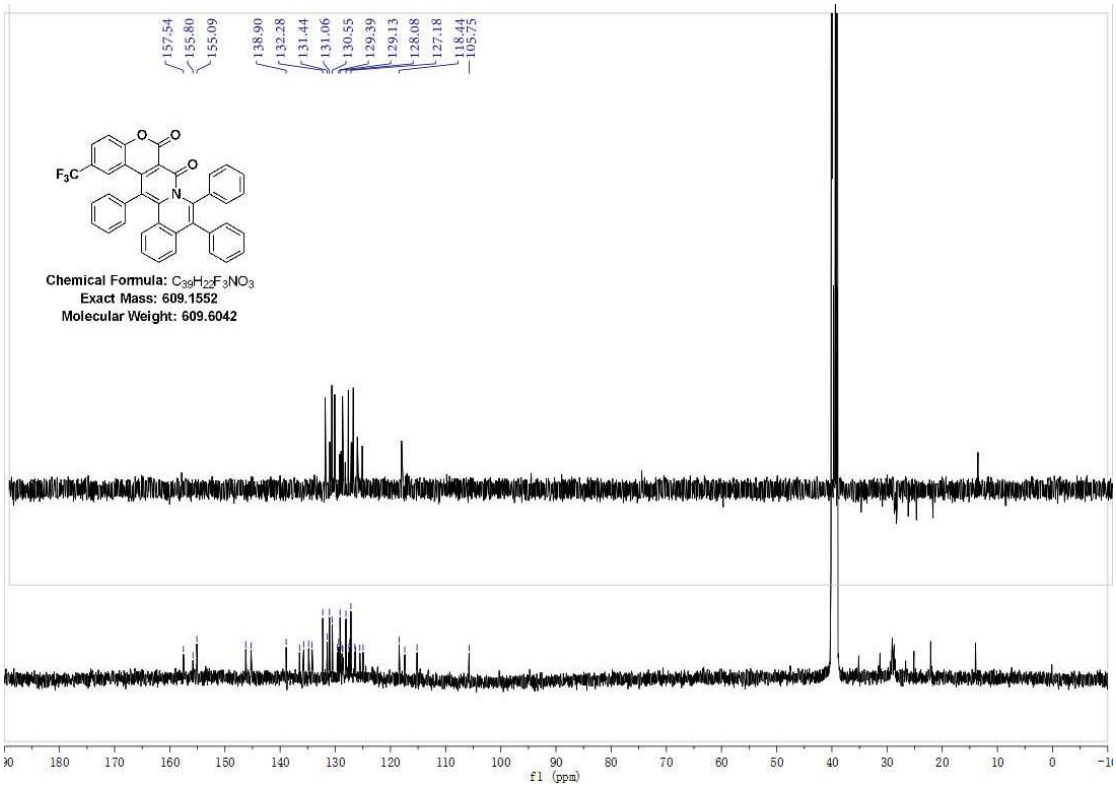


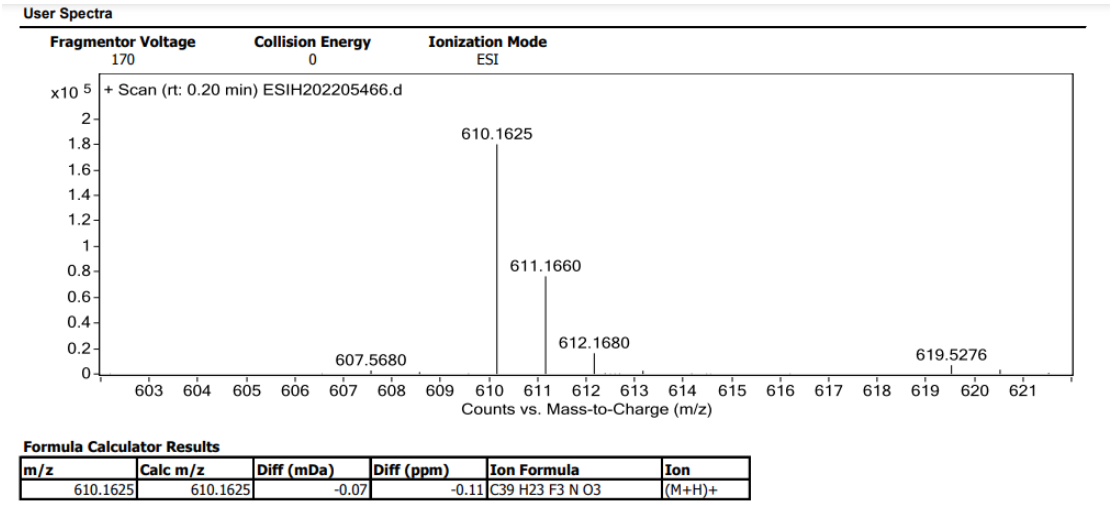
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
887.7778	887.7781	0.4	0.45	C38 H19 Br4 Cl N O3	(M+H)+

9,10,15-Triphenyl-2-(trifluoromethyl)-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3fa**)



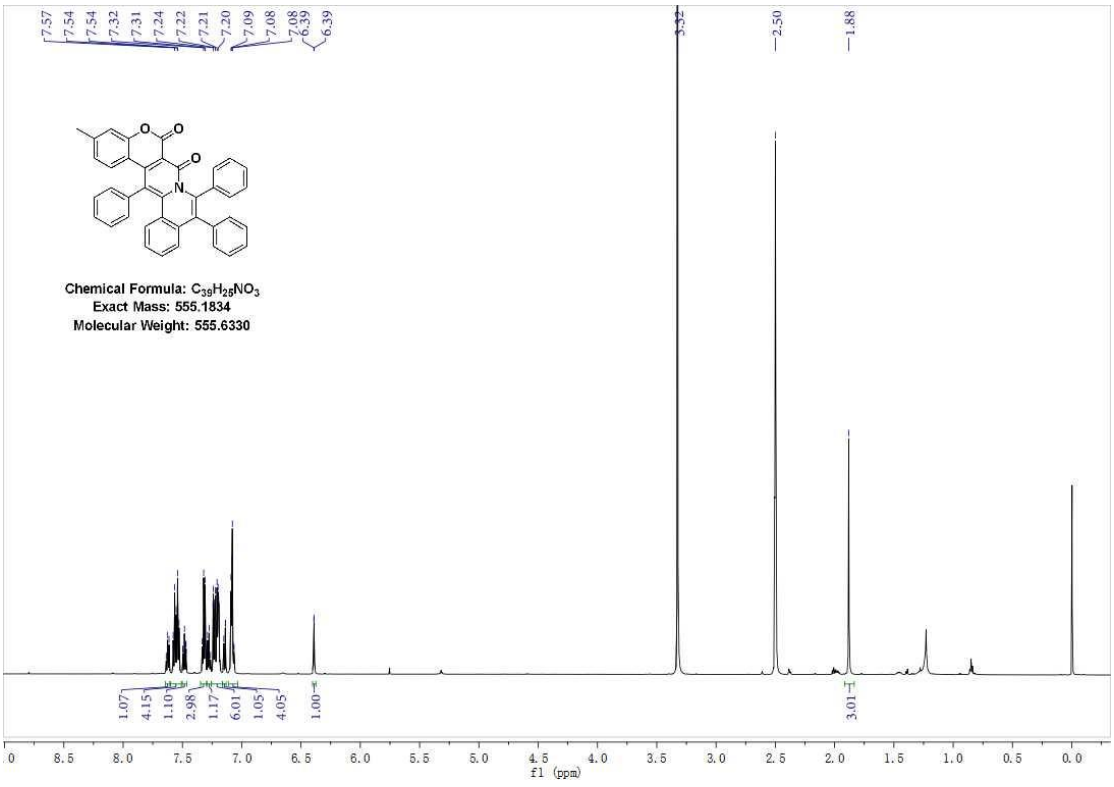


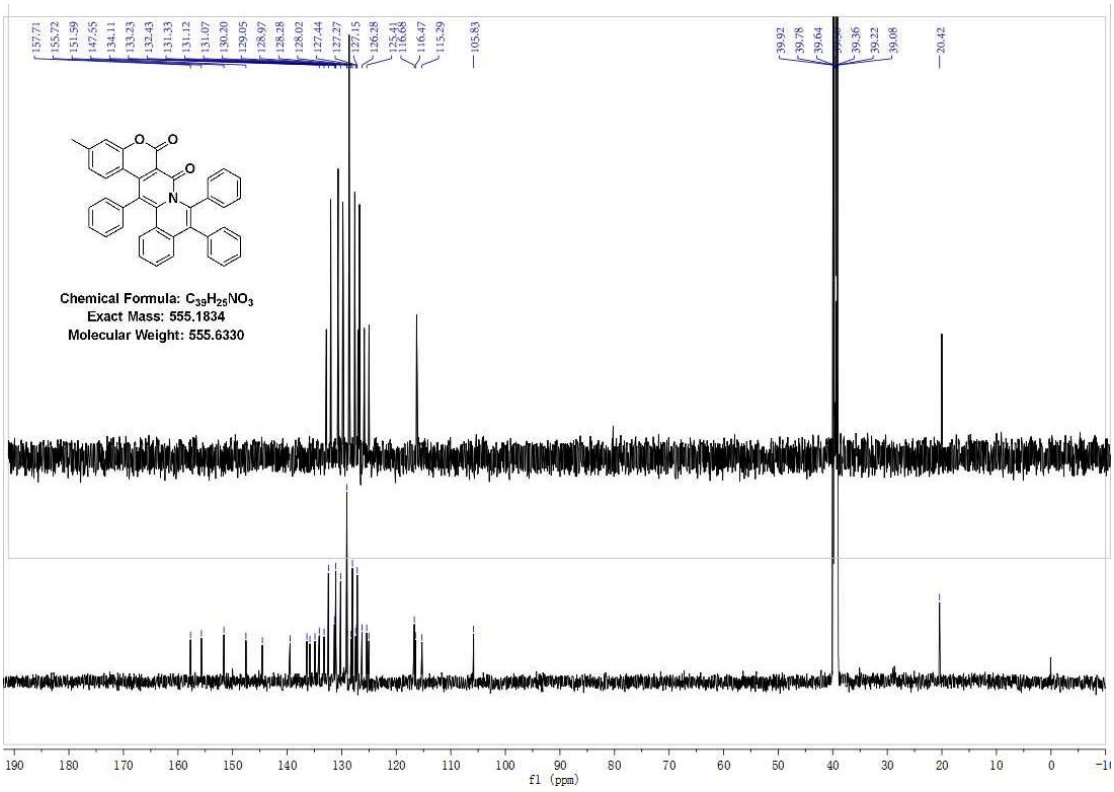


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
610.1625	610.1625	-0.07	-0.11	C39 H23 F3 N O3	(M+H)+

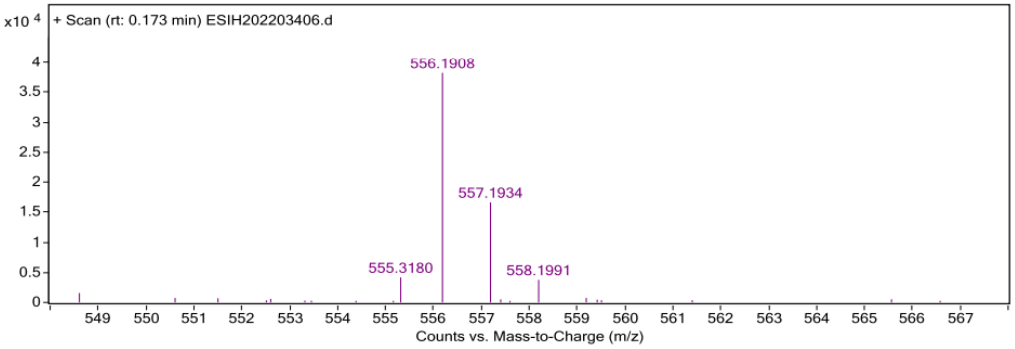
3-Methyl-9,10,15-triphenyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ga**)





User Spectra

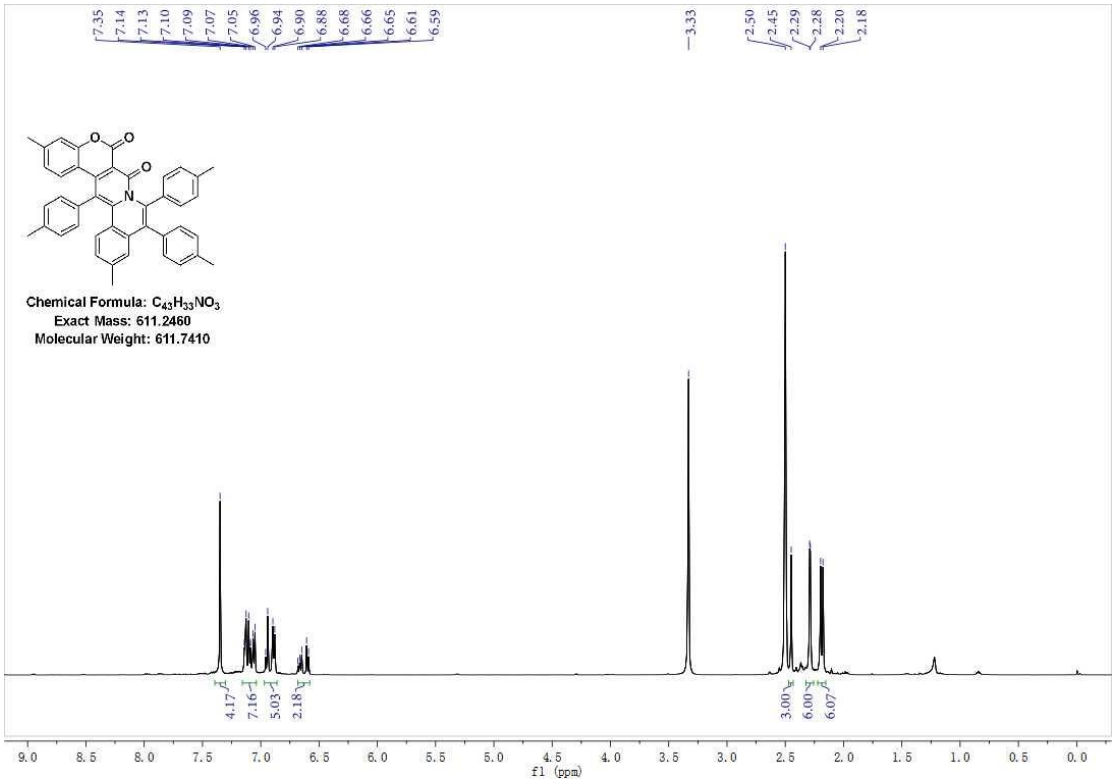
Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI

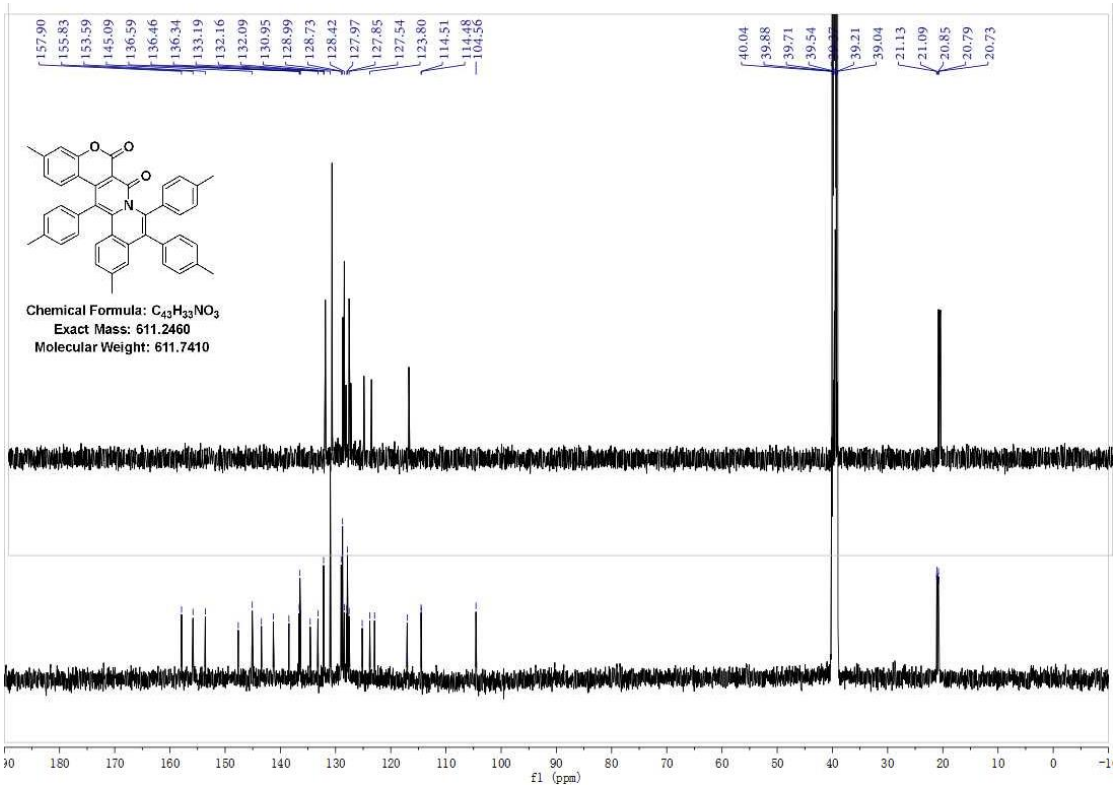


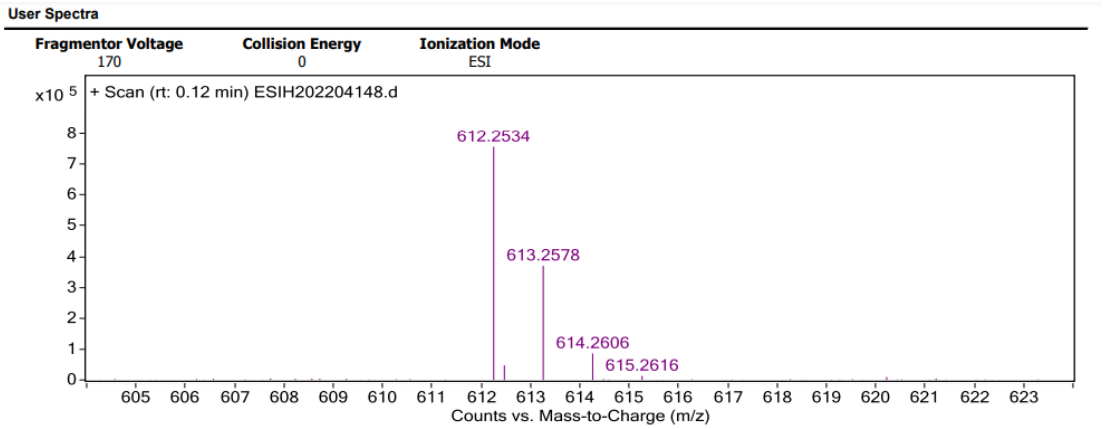
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
556.1908	556.1907	-0.09	-0.15	C39 H26 N O3	(M+H)+

3,12-Dimethyl-9,10,15-tri-p-tolyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoli ne-6,7-dione (**3gb**)



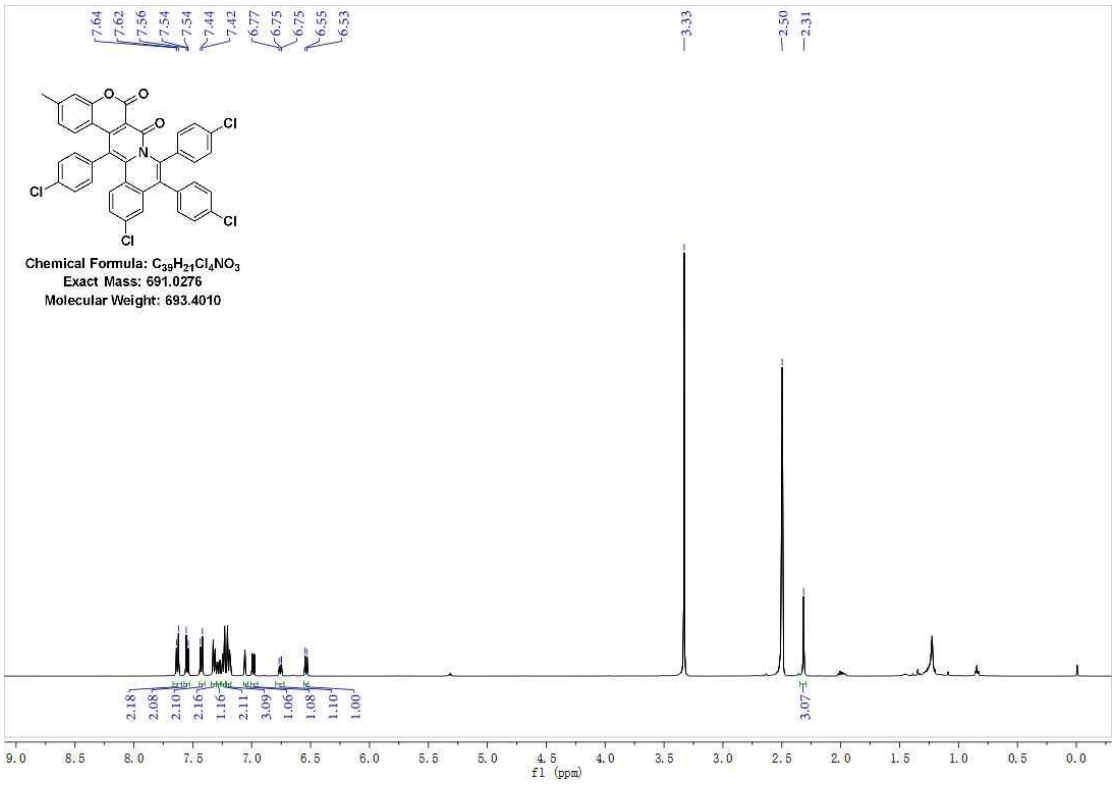


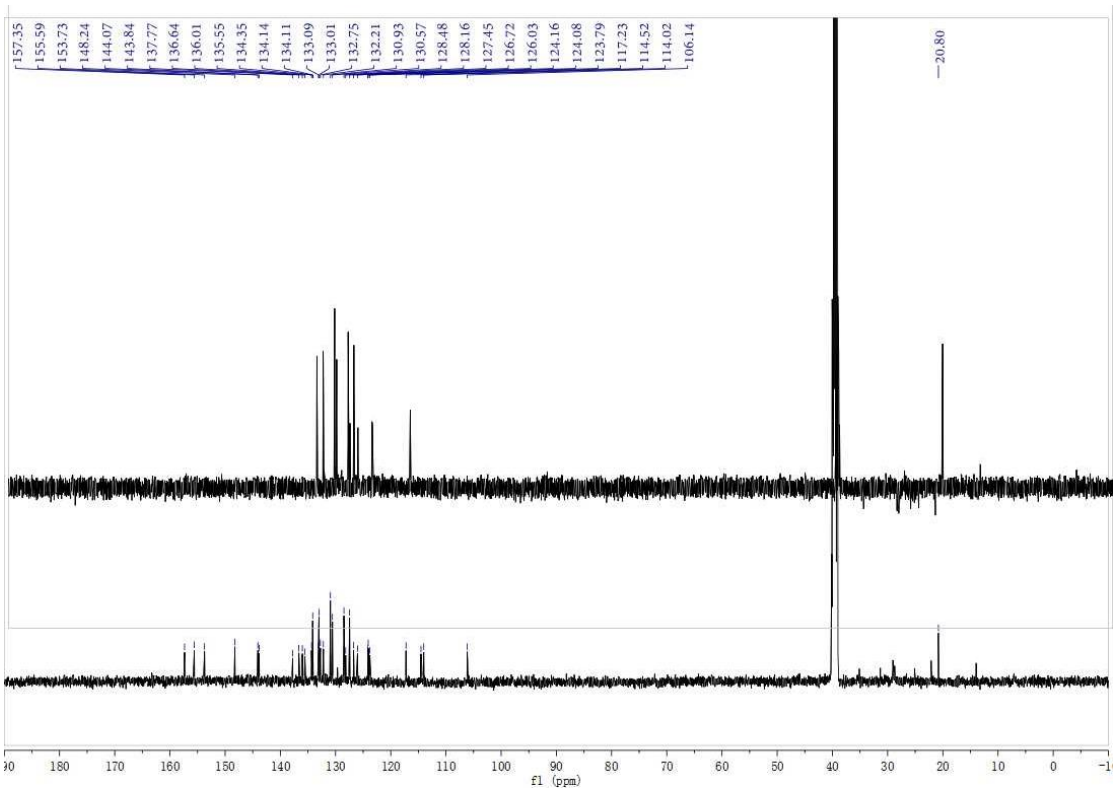


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
612.2534	612.2533	-0.1	-0.17	C43 H34 N O3	(M+H)+

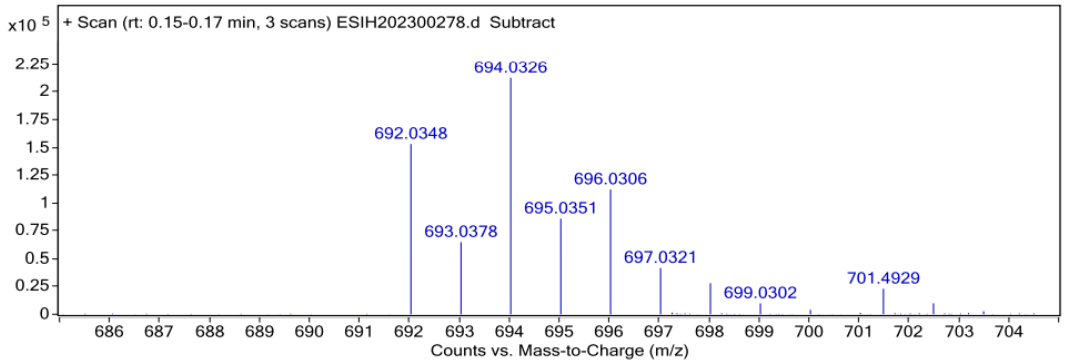
12-Chloro-9,10,15-tris(4-chlorophenyl)-3-methyl-6H,7H-chromeno[4',3':4,5]pyrido[2,1-a]isoquinoline-6,7-dione (**3ge**)





User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI

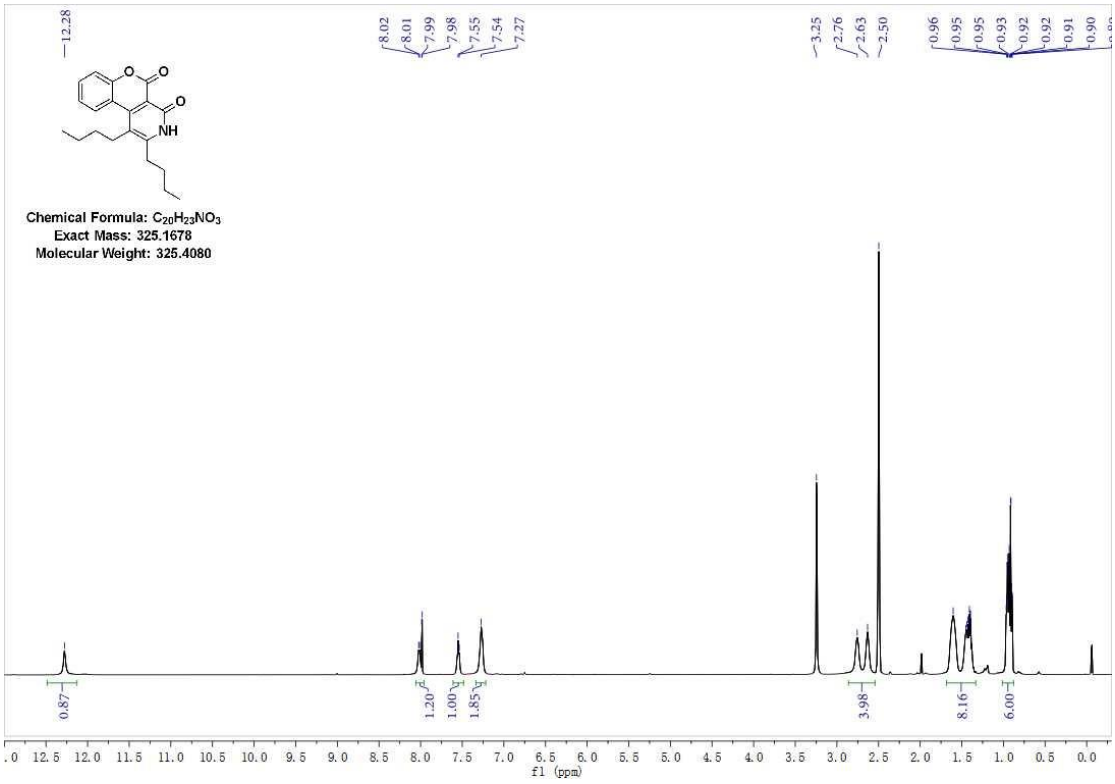


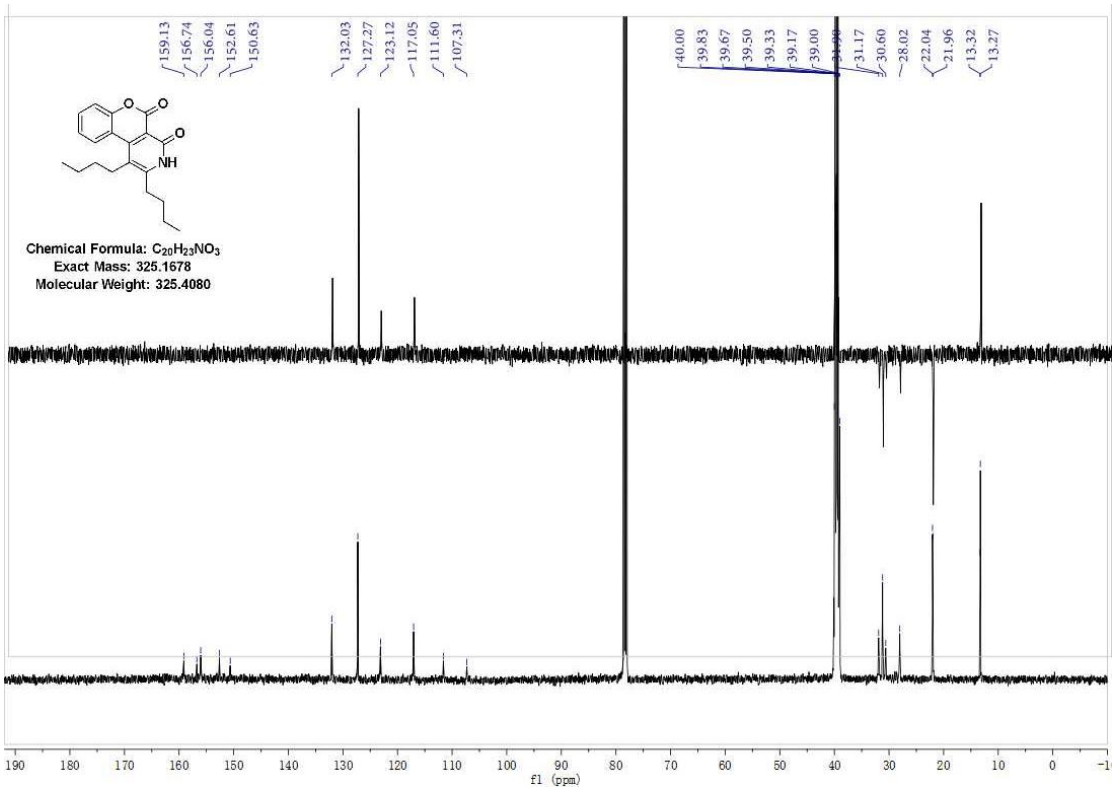
Formula Calculator Results

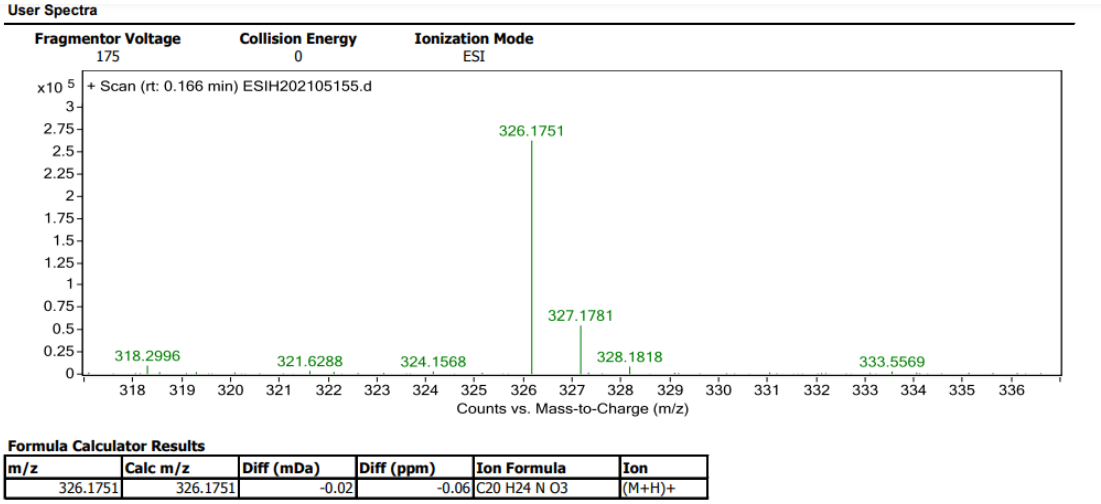
m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
692.0348	692.0348	0.06	0.08	C39 H22 Cl4 N O3	(M+H)+

End Of Report

1,2-Dibutyl-4H-chromeno[3,4-c]pyridine-4,5(3H)-dione (**3ah**)



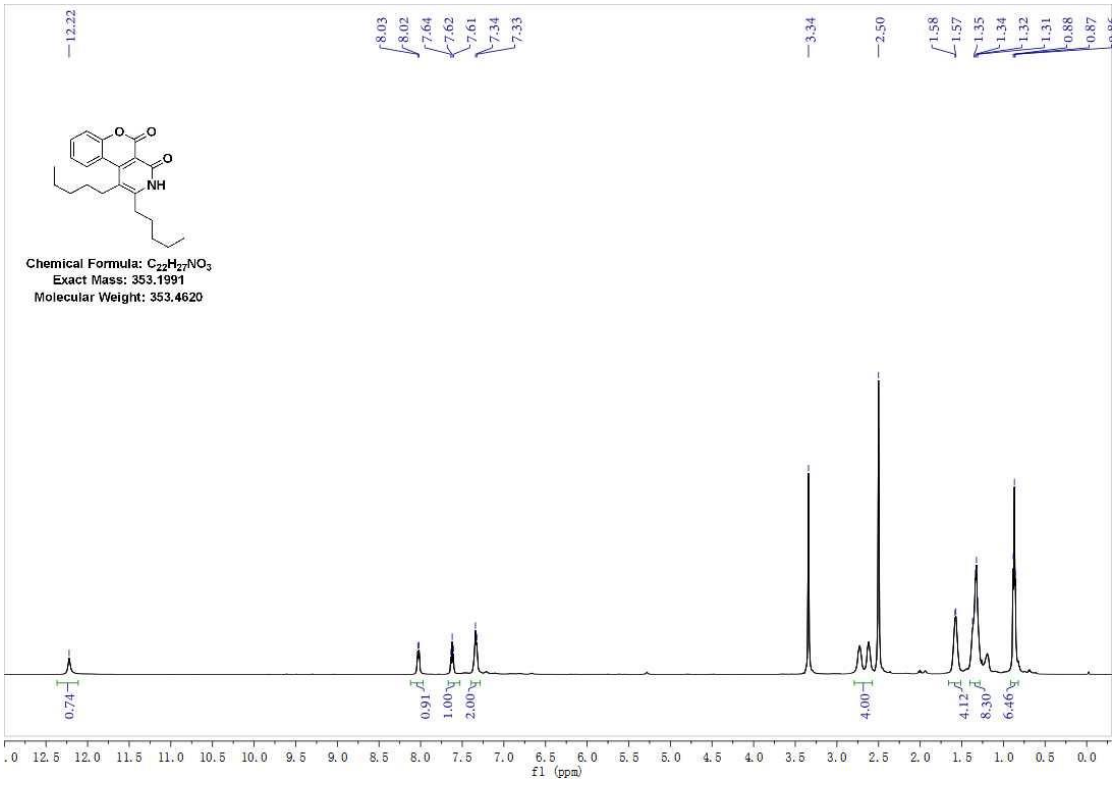


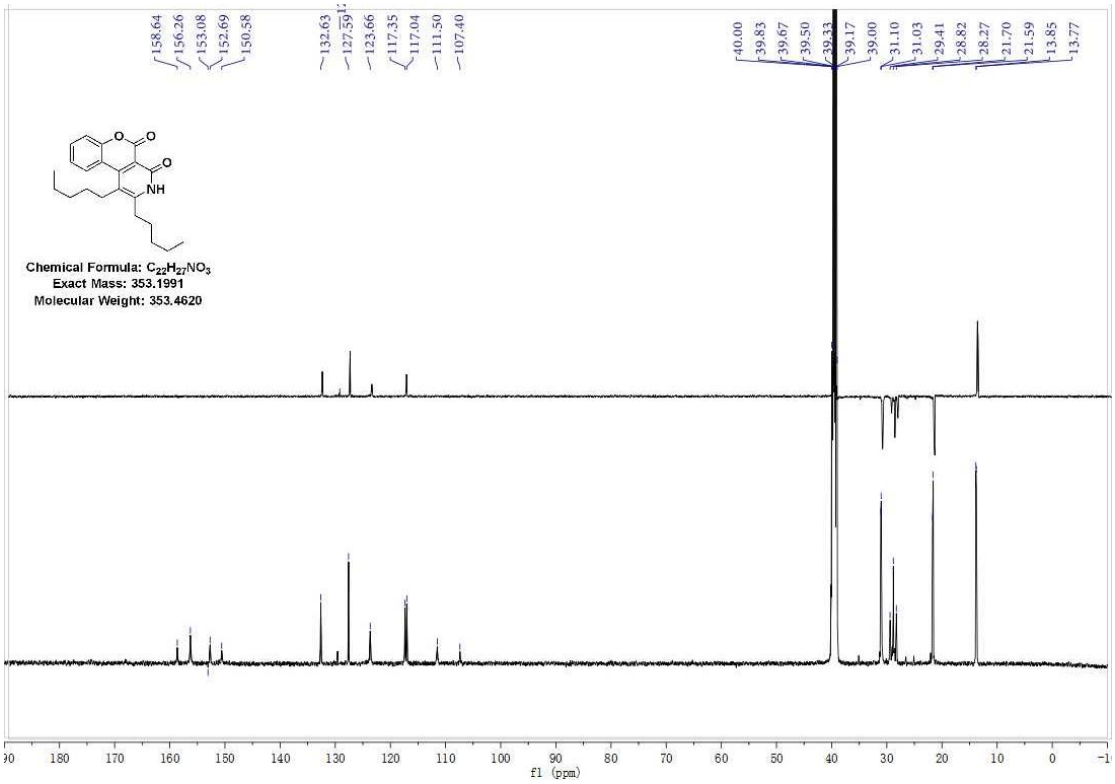


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
326.1751	326.1751	-0.02	-0.06	C20 H24 N O3	(M+H)+

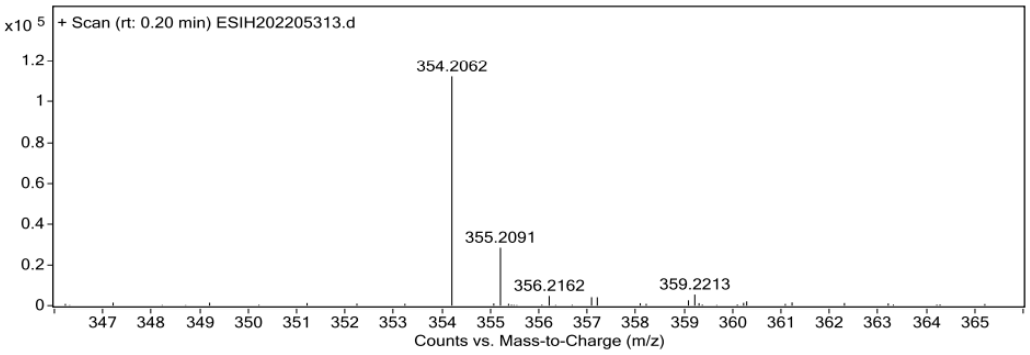
1,2-Dipentyl-4H-chromeno[3,4-c]pyridine-4,5(3H)-dione (**3ai**)





User Spectra

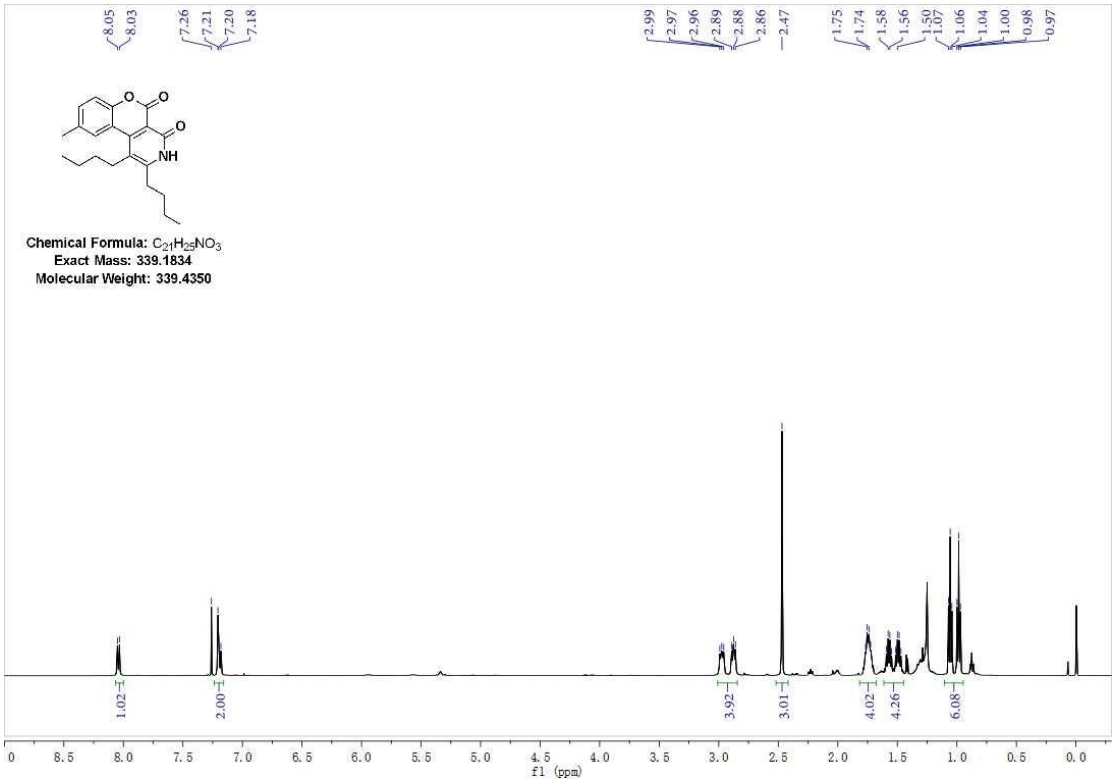
Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI

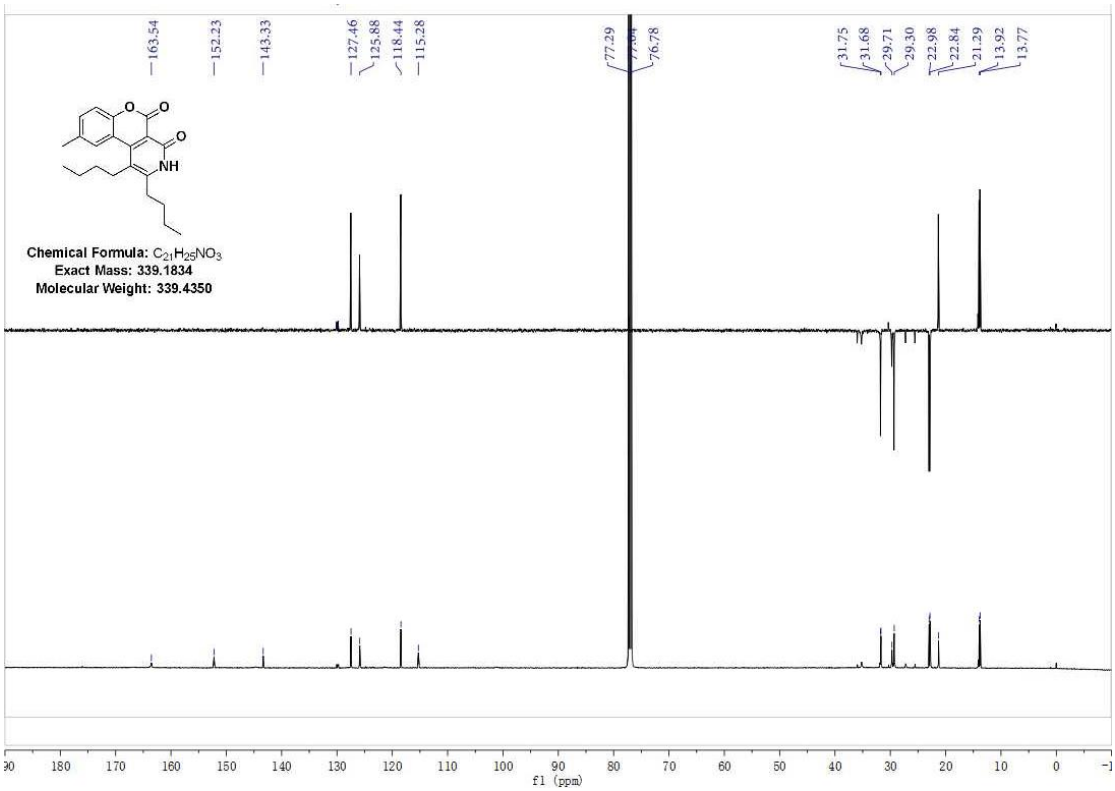


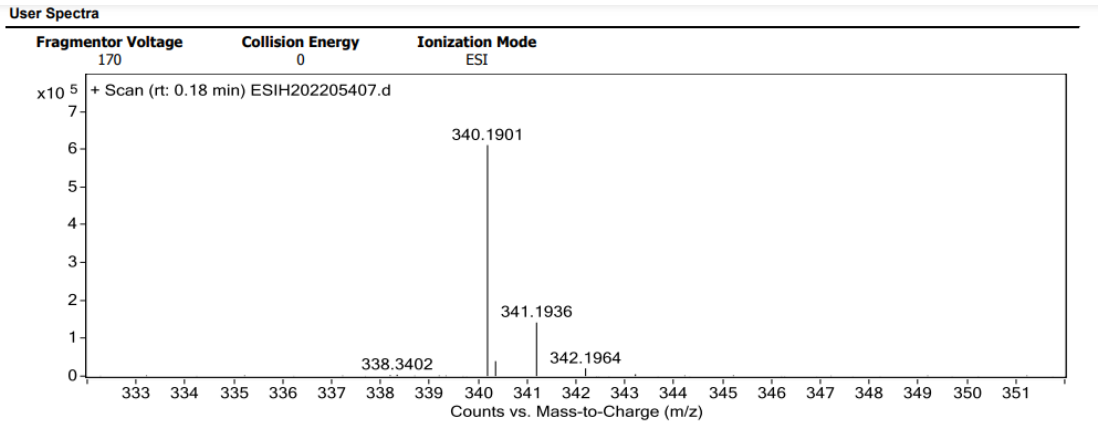
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
354.2062	354.2064	0.12	0.35	C22 H28 N O3	(M+H)+

1,2-Dibutyl-9-methyl-4H-chromeno[3,4-c]pyridine-4,5(3H)-dione (**3bh**)



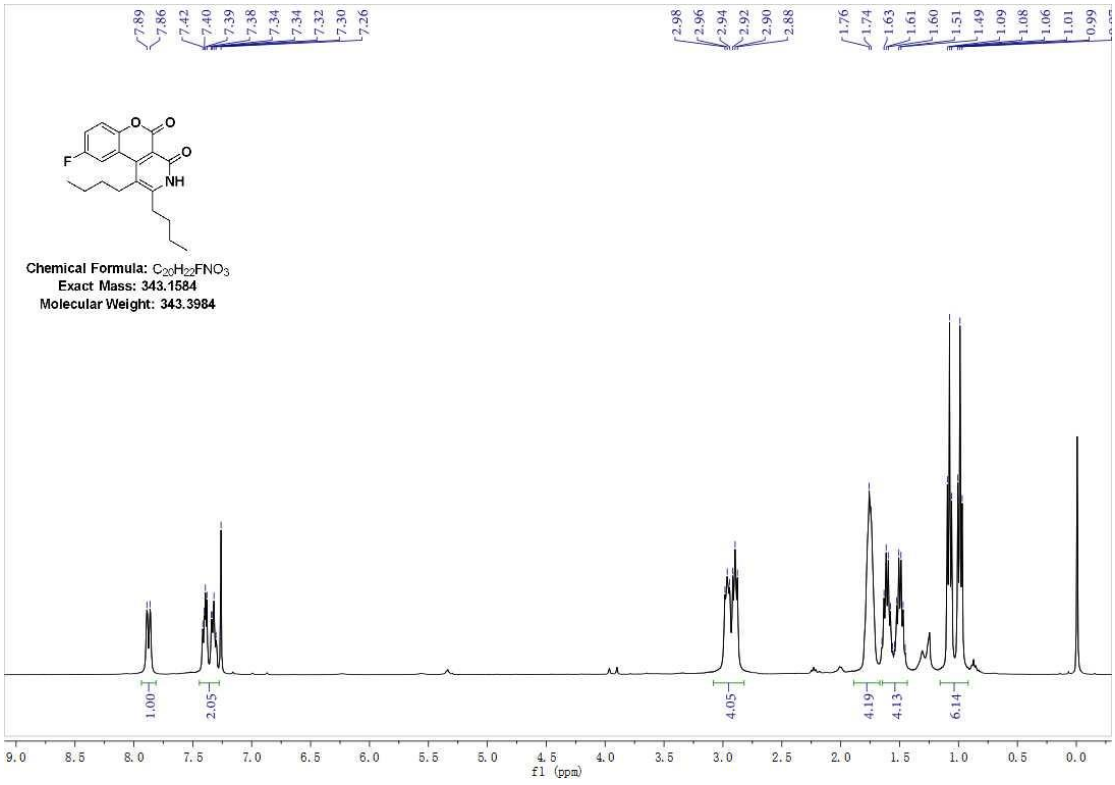


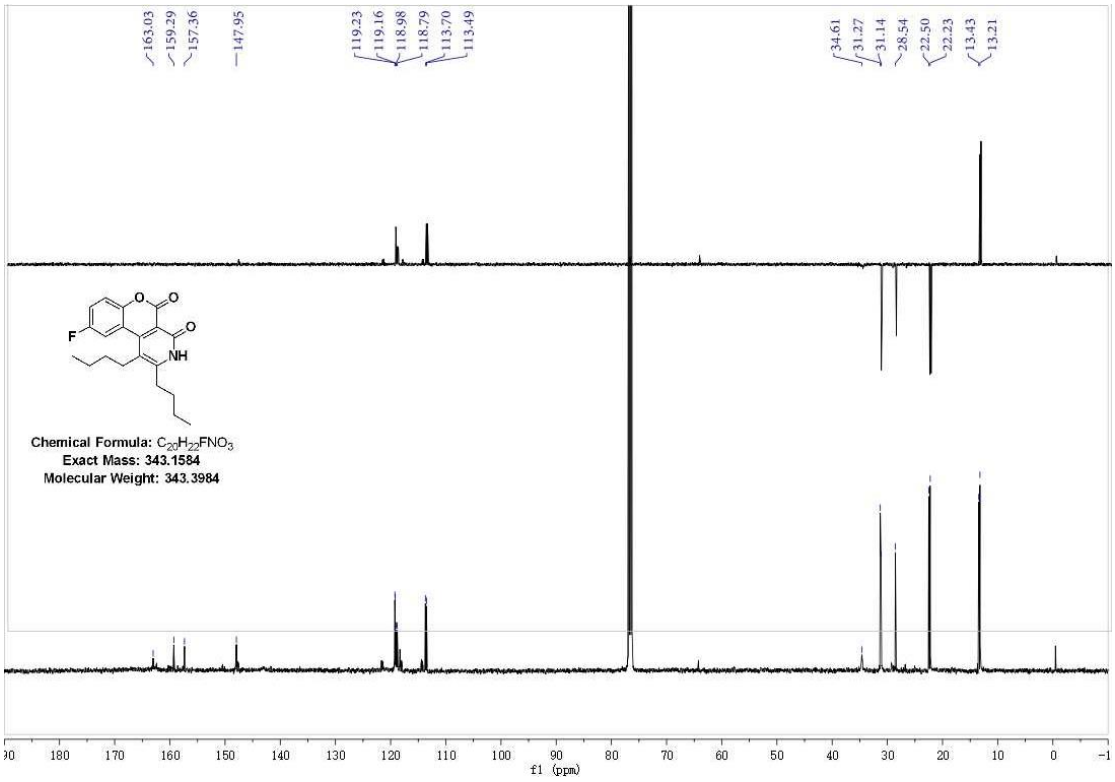


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
340.1901	340.1907	0.65	1.9	C21 H26 N O3	(M+H)+

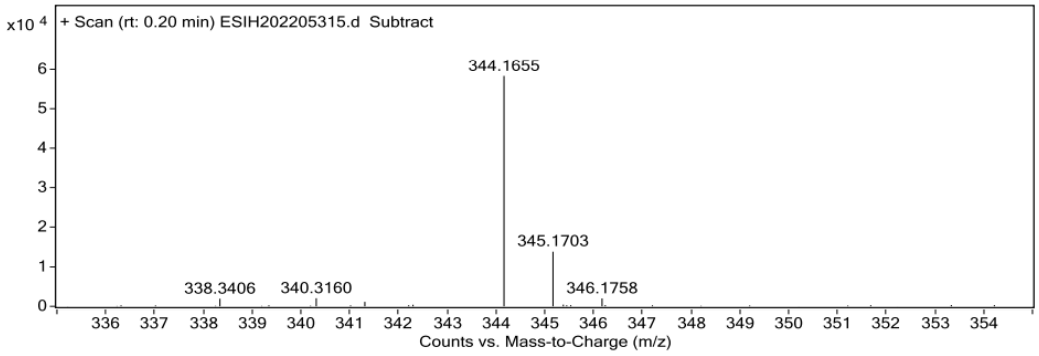
1,2-Dibutyl-9-fluoro-4H-chromeno[3,4-c]pyridine-4,5(3H)-dione (**3dh**)





User Spectra

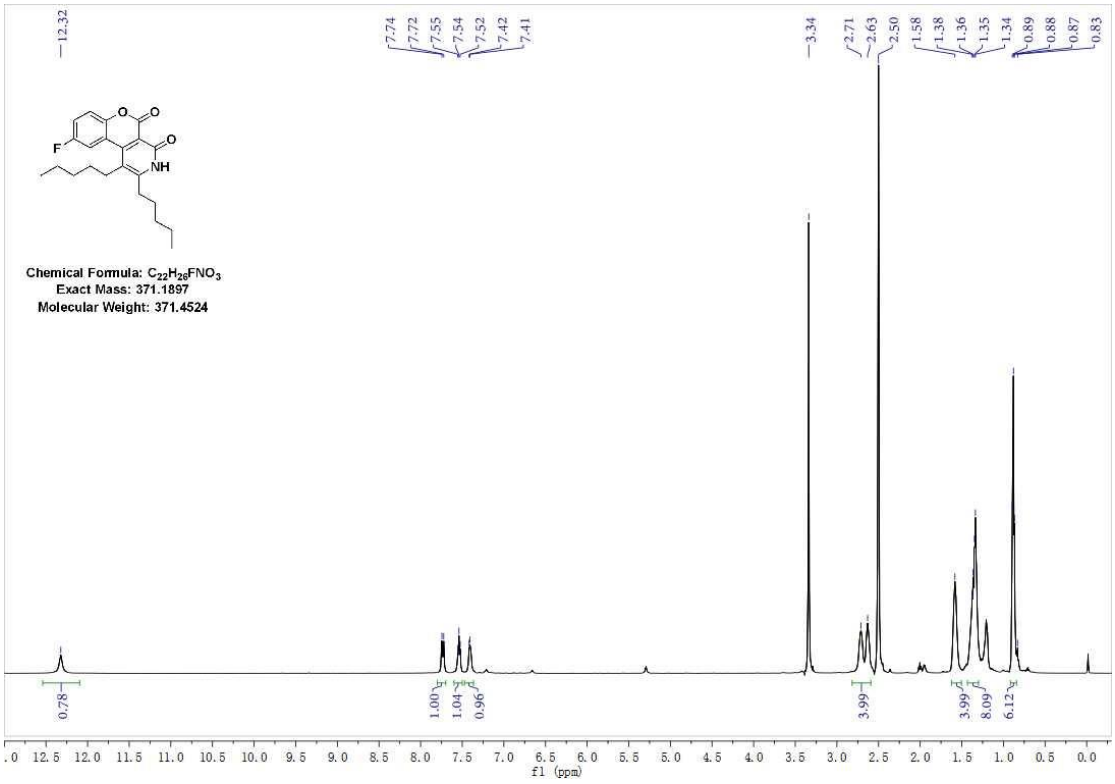
Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI

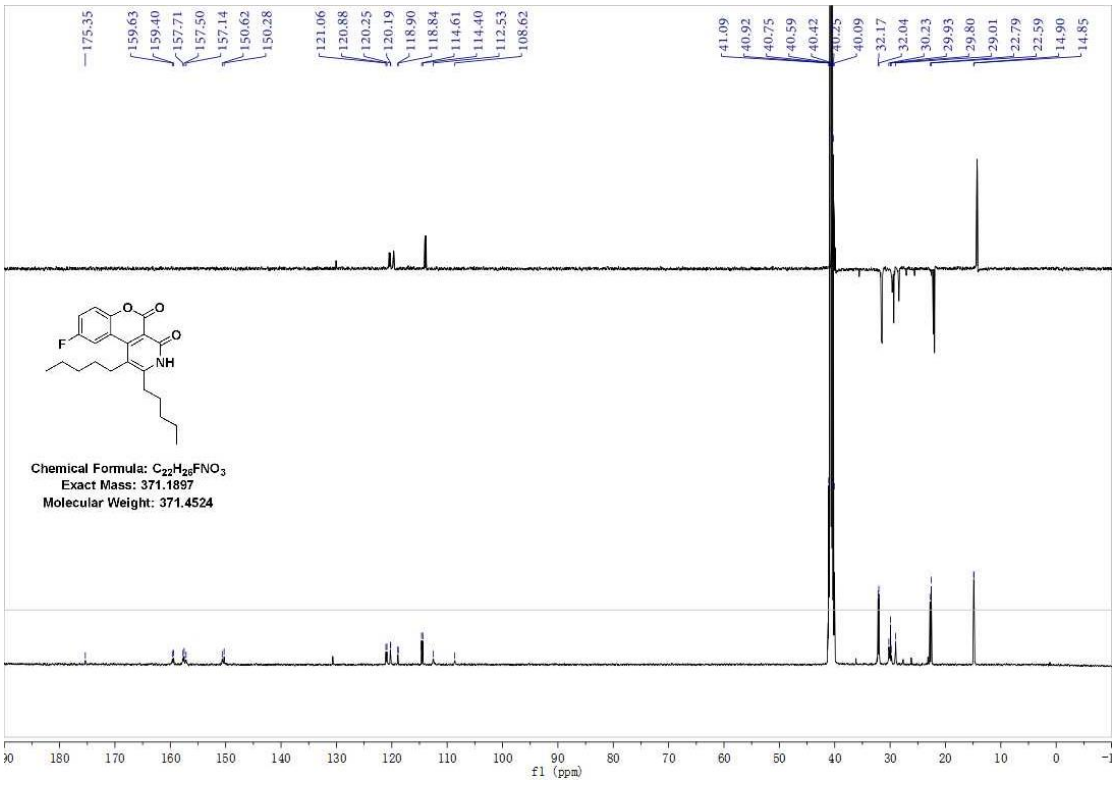


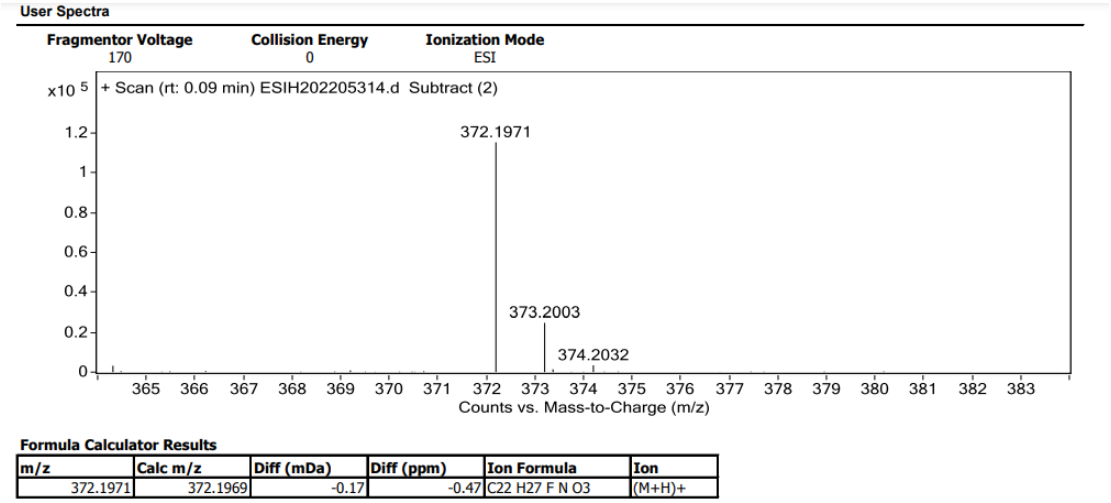
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
344.1655	344.1656	0.16	0.47	C20 H23 F N O3	(M+H)+

9-Fluoro-1,2-dipentyl-4H-chromeno[3,4-c]pyridine-4,5(3H)-dione (**3di**)



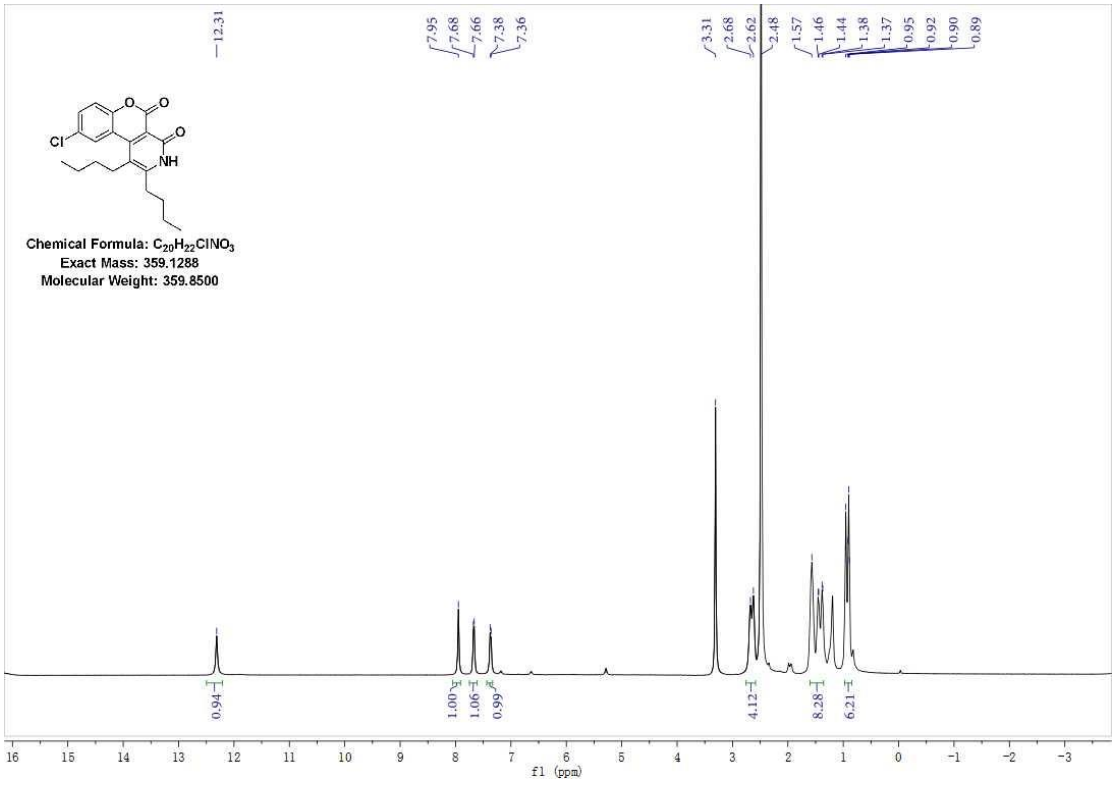


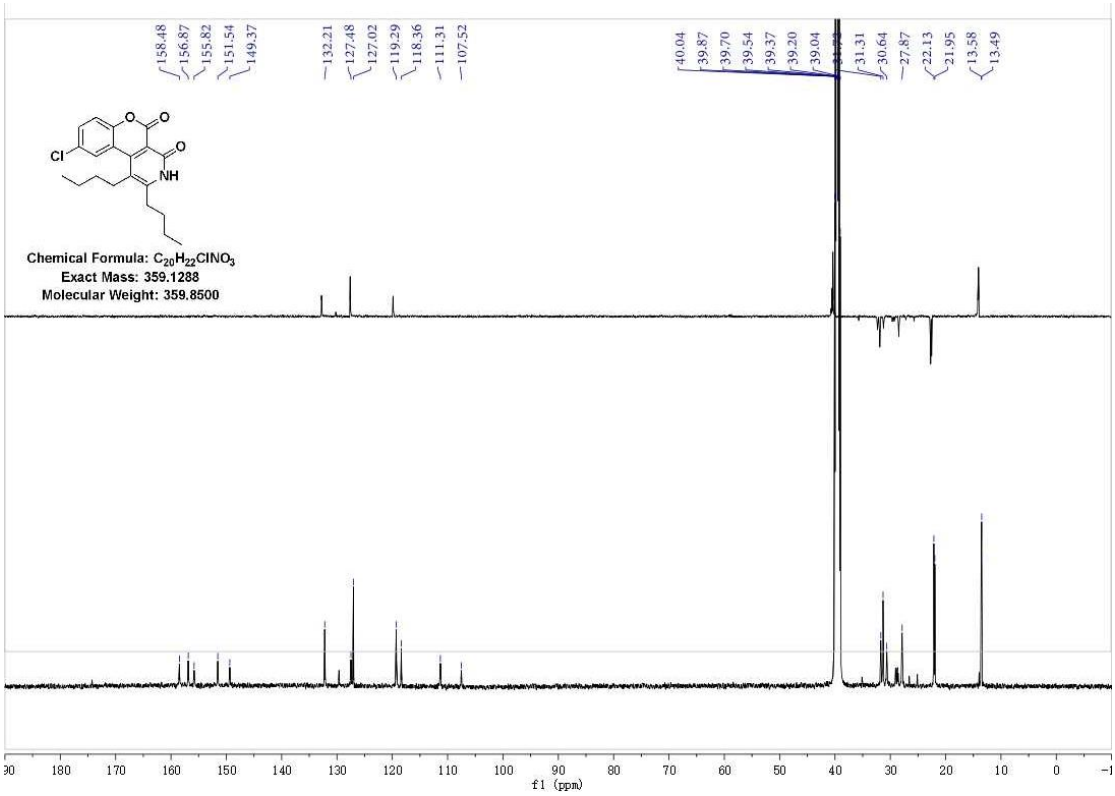


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
372.1971	372.1969	-0.17	-0.47	C22 H27 F N O3	(M+H)+

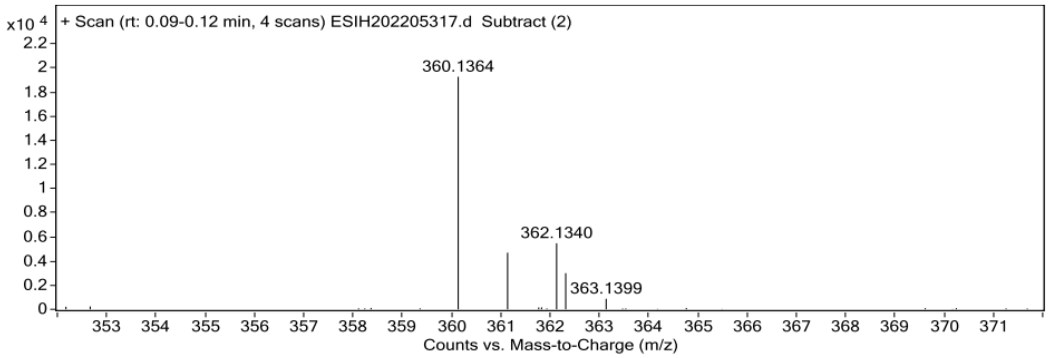
1,2-Dibutyl-9-chloro-4H-chromeno[3,4-c]pyridine-4,5(3H)-dione (**3eh**)





User Spectra

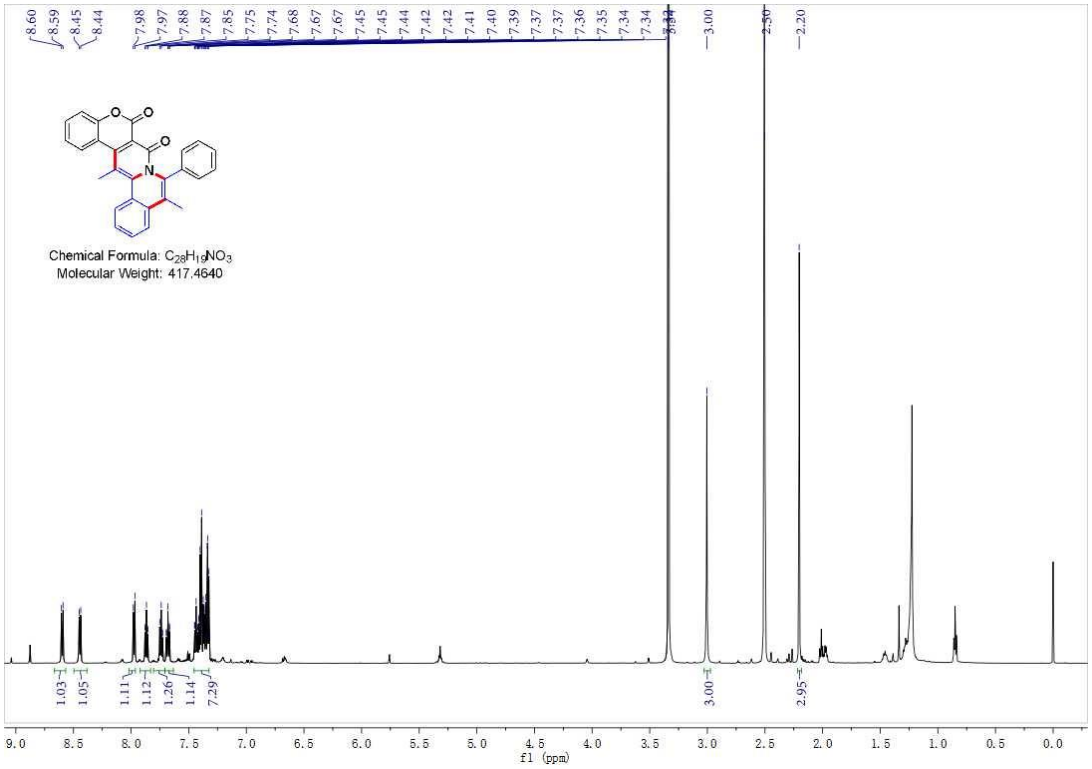
Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI

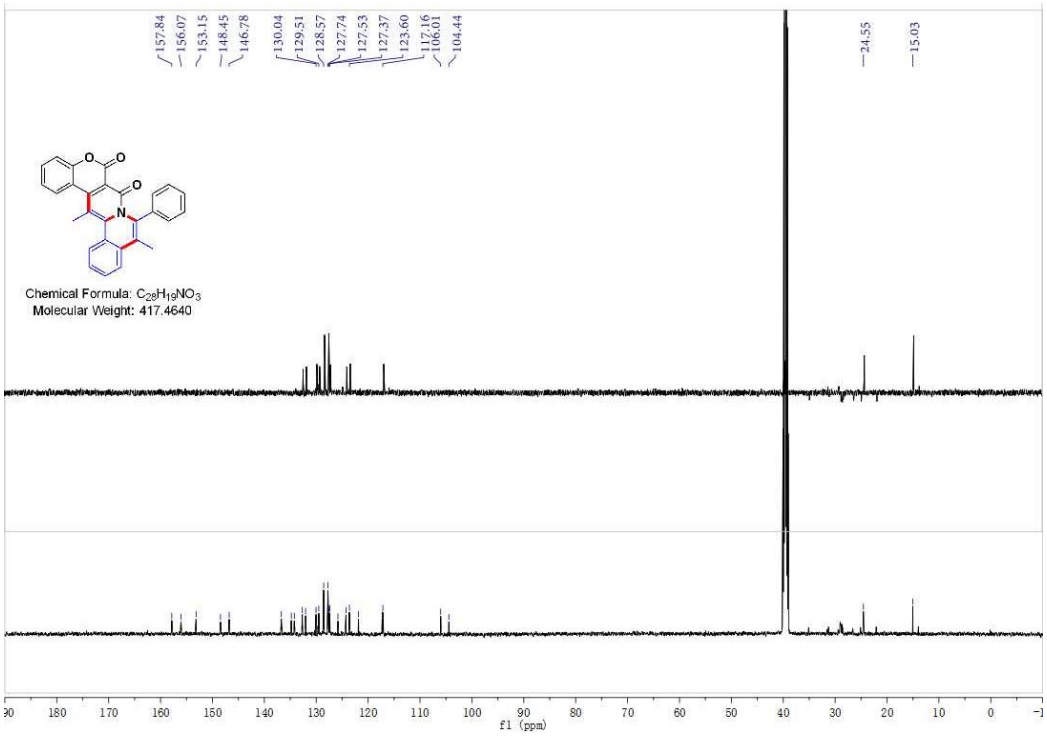


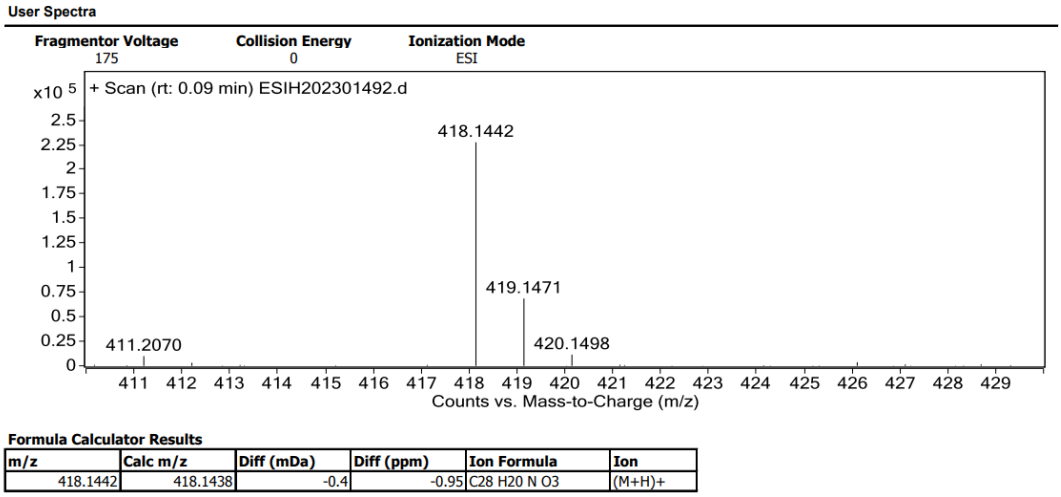
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
360.1364	360.1361	-0.25	-0.71	C20 H23 Cl N O3	(M+H)+

10,15-Dimethyl-9-phenyl-6*H*,7*H*-chromeno[4',3':4,5]pyrido[2,1-*a*]isoquinoline-6,7-dione (**3aj**)



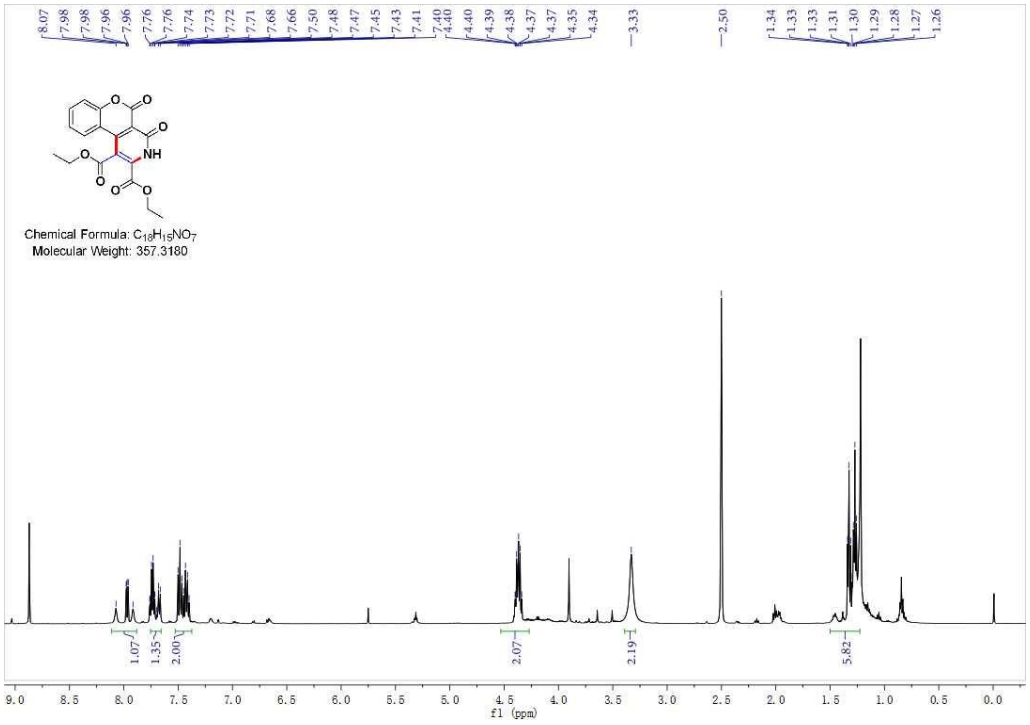


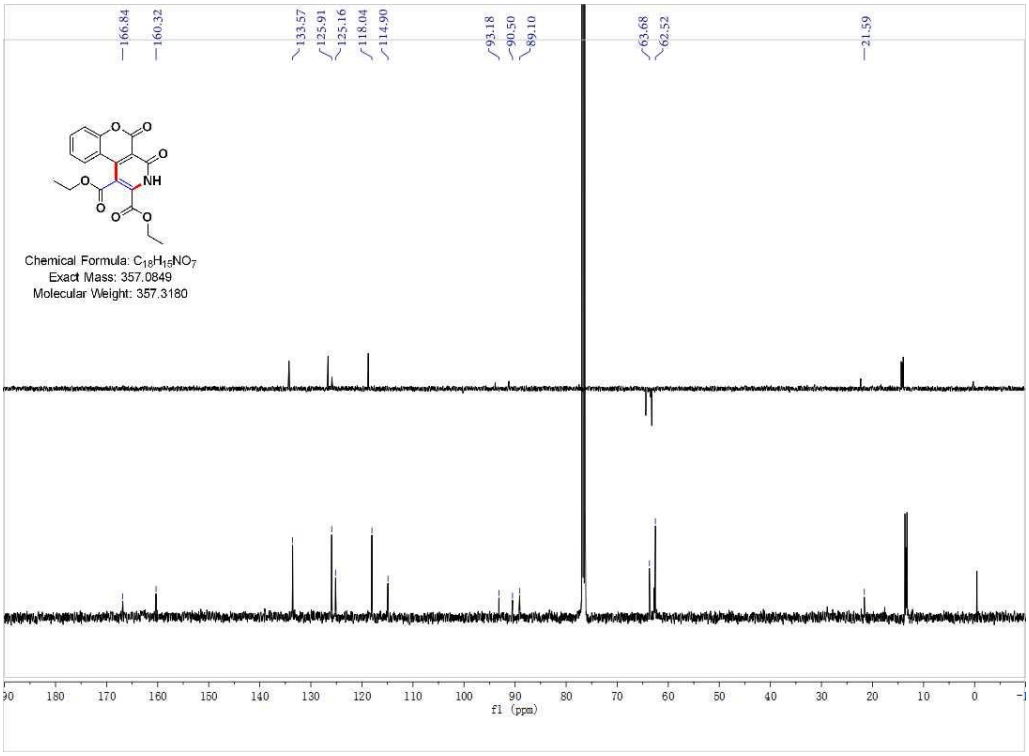


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
418.1442	418.1438	-0.4	-0.95	C28 H20 N O3	(M+H)+

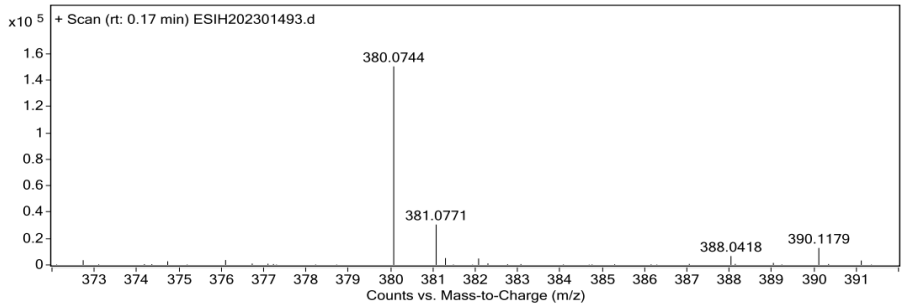
Diethyl 4,5-dioxo-3,5-dihydro-4*H*-chromeno[3,4-*c*]pyridine-1,2-dicarboxylate (**3ak**)





User Spectra

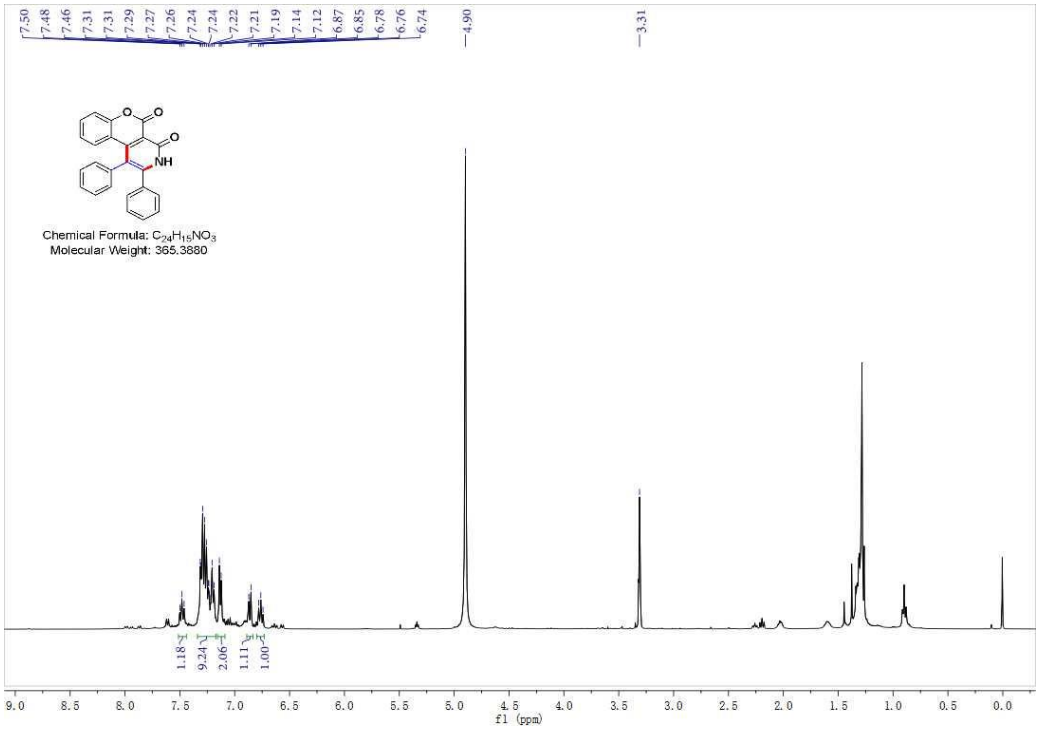
Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI

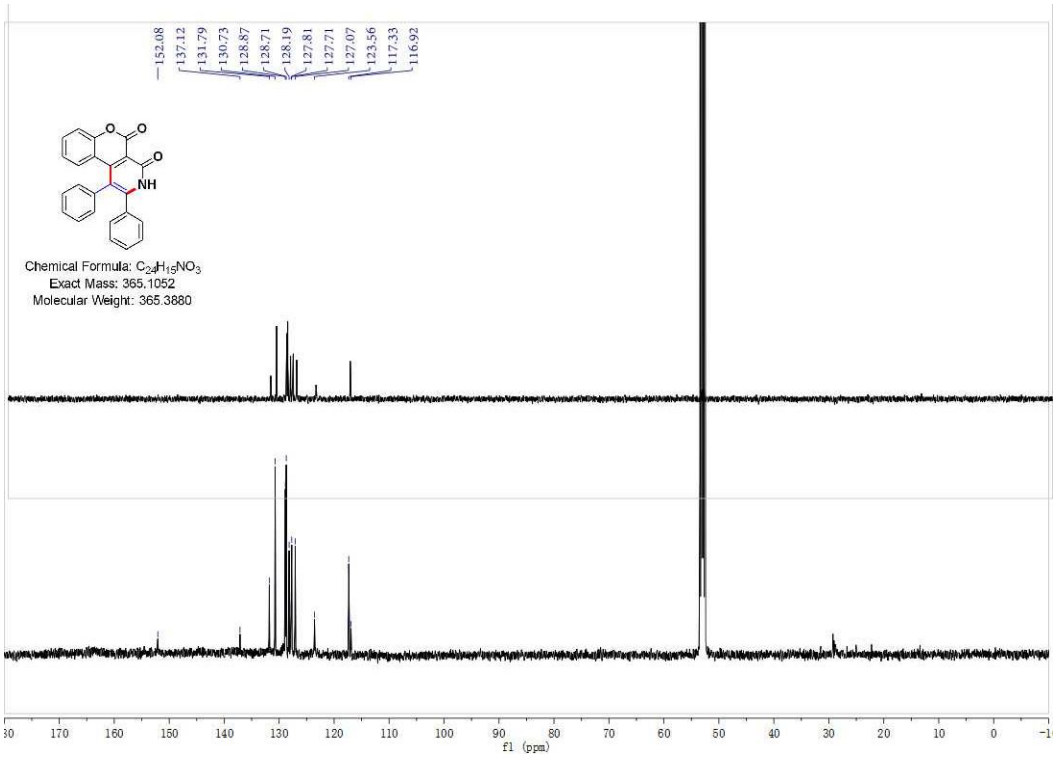


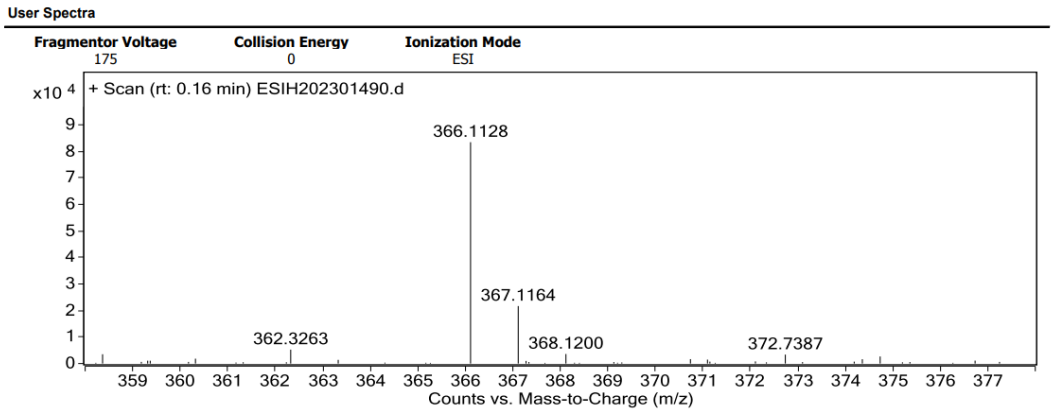
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
380.0744	380.0741	-0.3	-0.78	C18 H15 N Na O7	(M+Na)+

1,2-Diphenyl-4*H*-chromeno[3,4-*c*]pyridine-4,5(3H)-dione (**VI**)



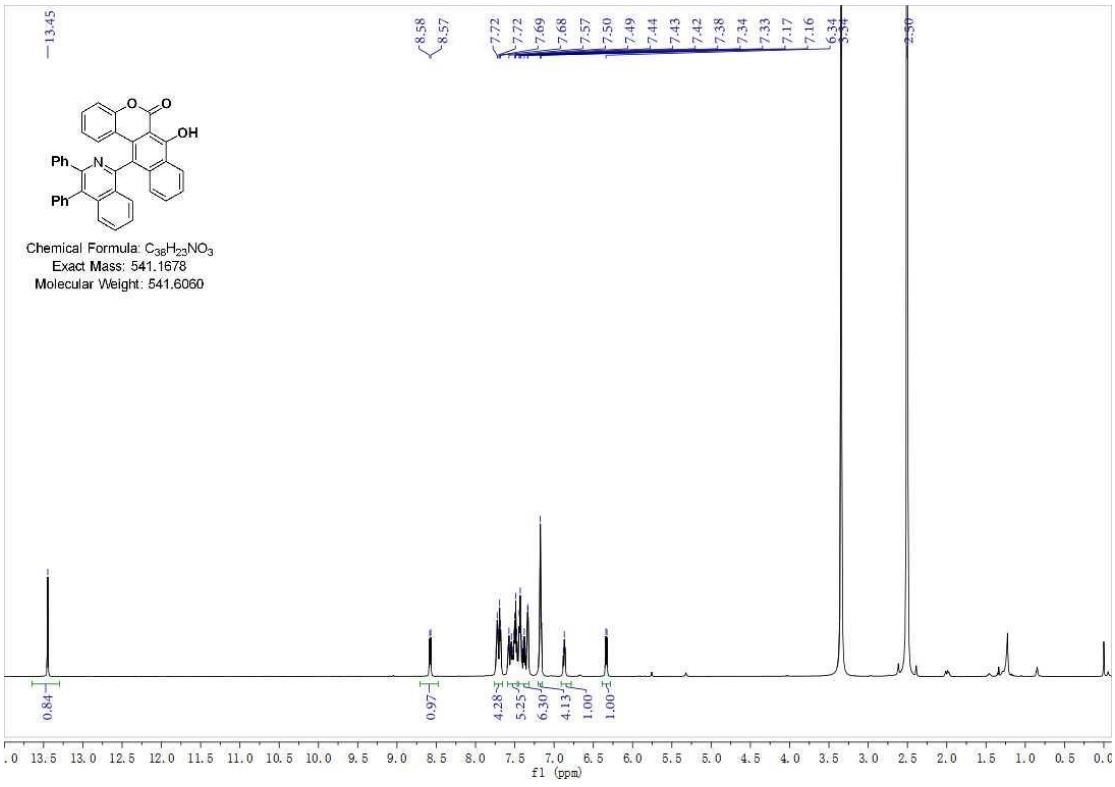


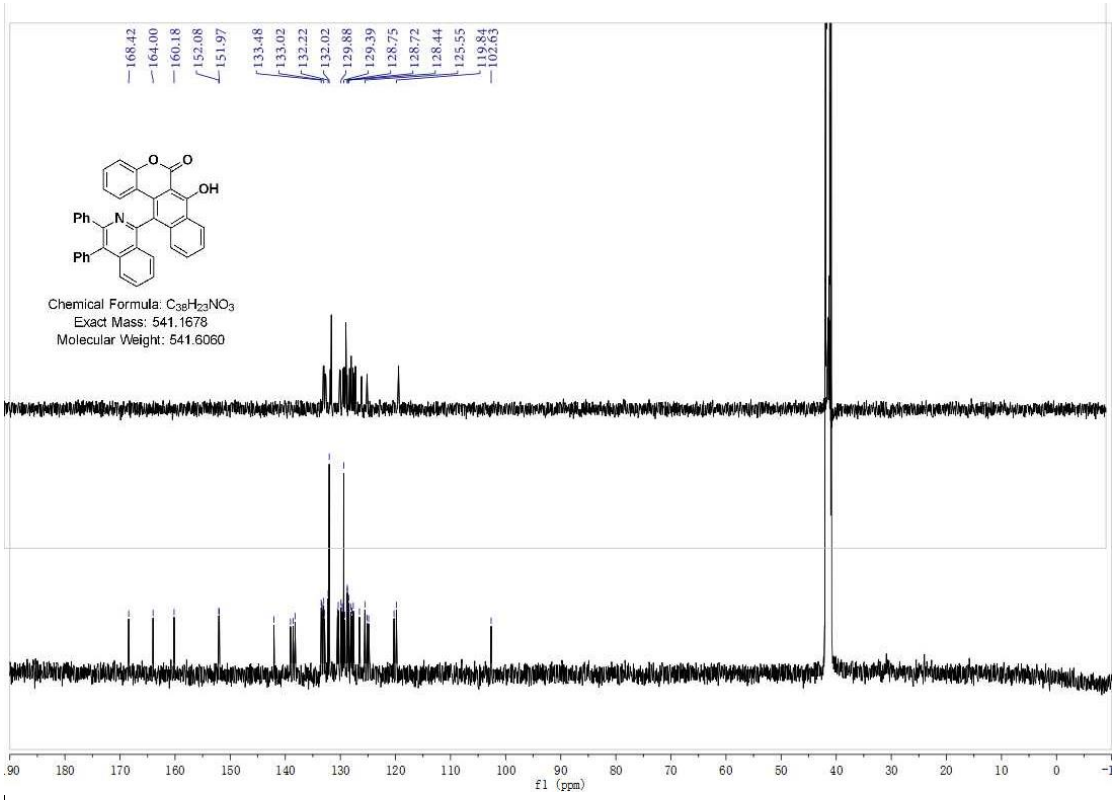


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
366.1128	366.1125	-0.3	-0.81	C24 H16 N O3	(M+H)+

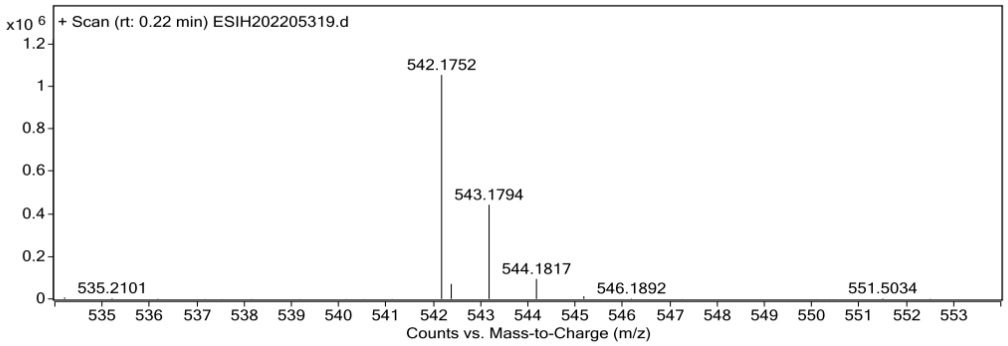
12-(3,4-Diphenylisoquinolin-1-yl)-7-hydroxy-6H-naphtho[2,3-c]chromen-6-one (**4a**)





User Spectra

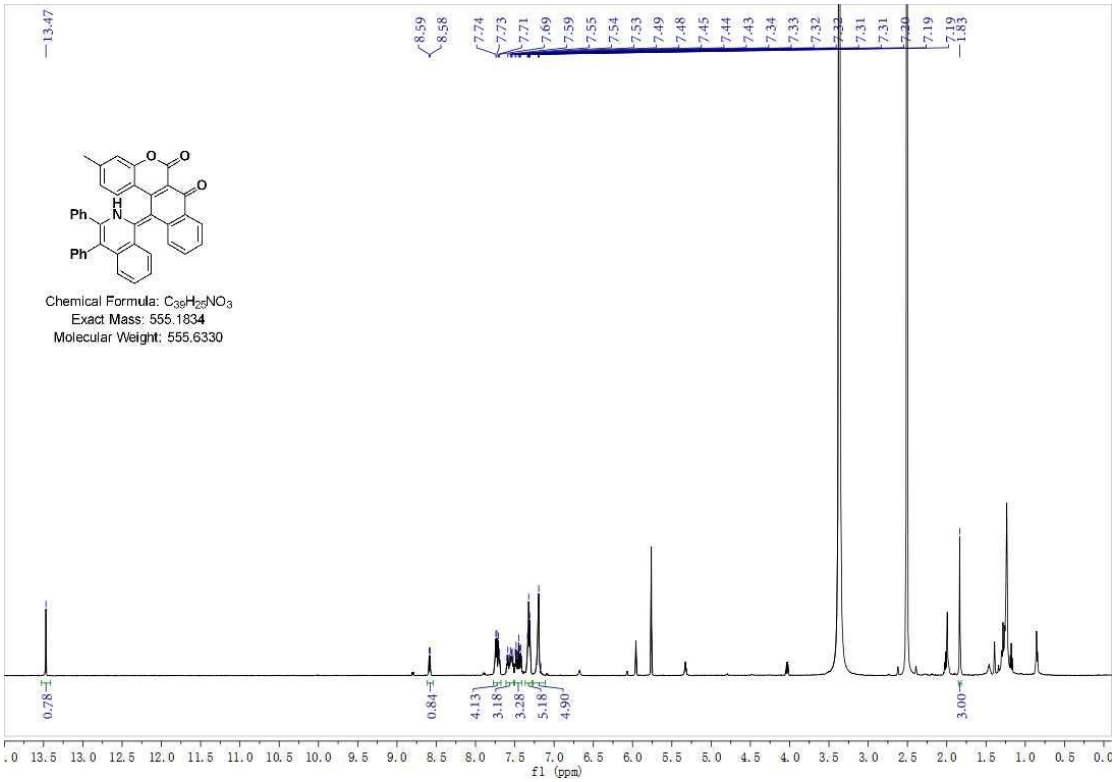
Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI

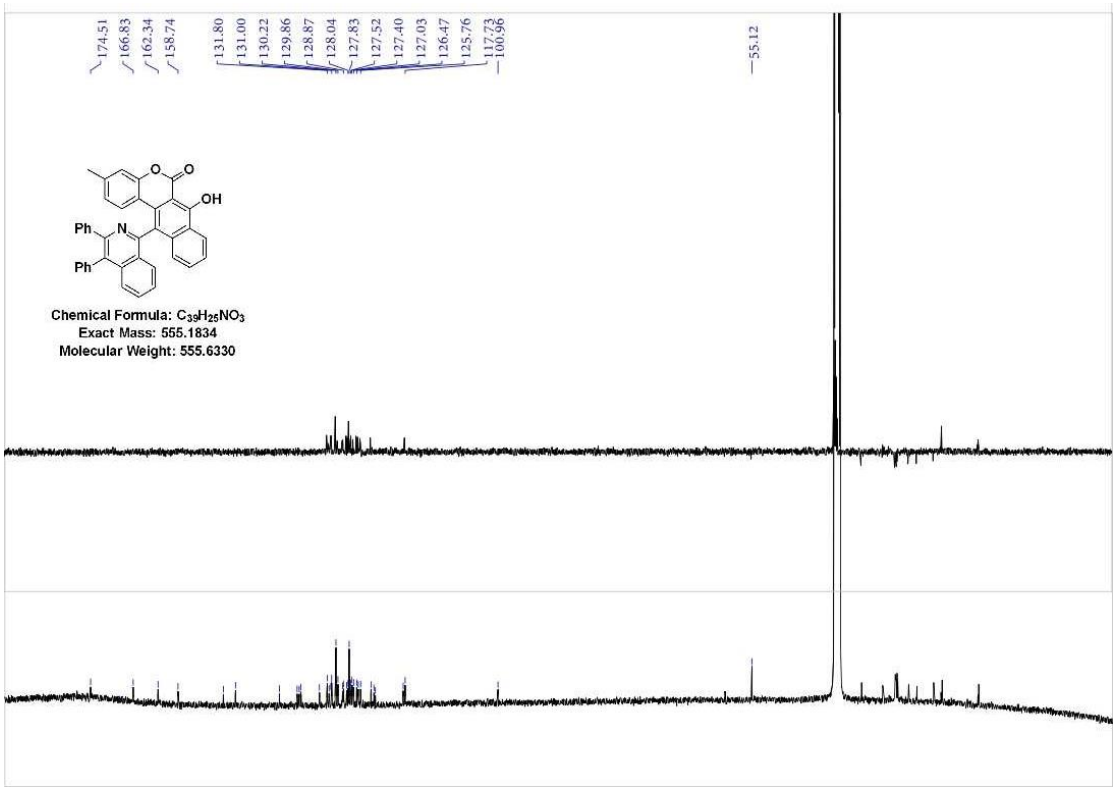


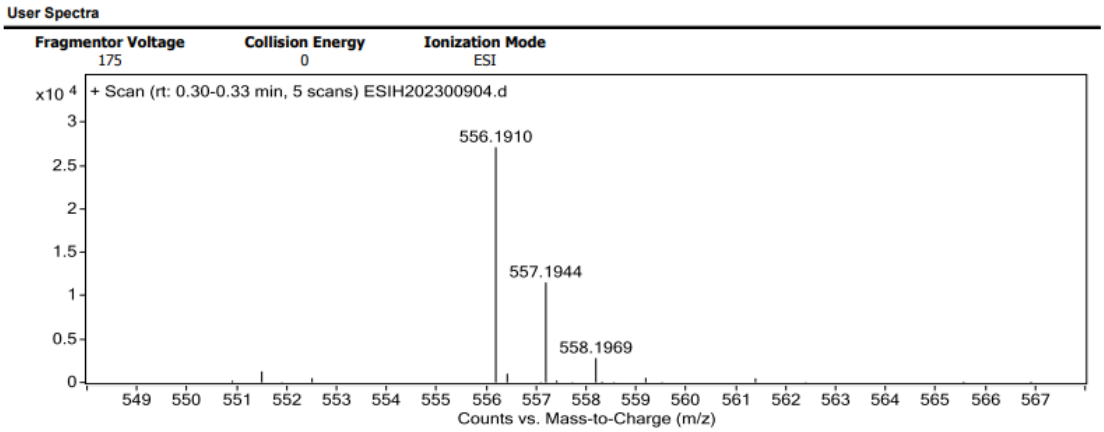
Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
542.1752	542.1751	-0.12	-0.22	C38 H24 N O3	(M+H)+

12-(3,4-diphenylisoquinolin-1-yl)-7-hydroxy-3-methyl-6H-naphtho[2,3-c]chromen-6-one (**4b**)



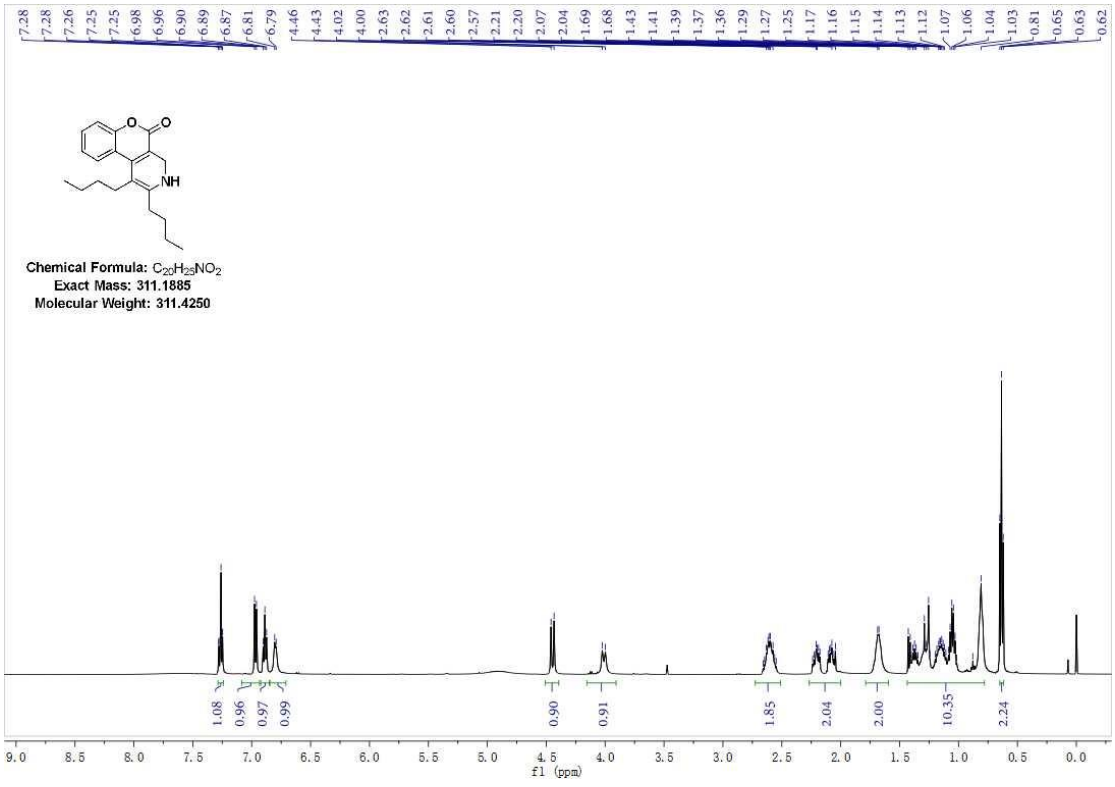


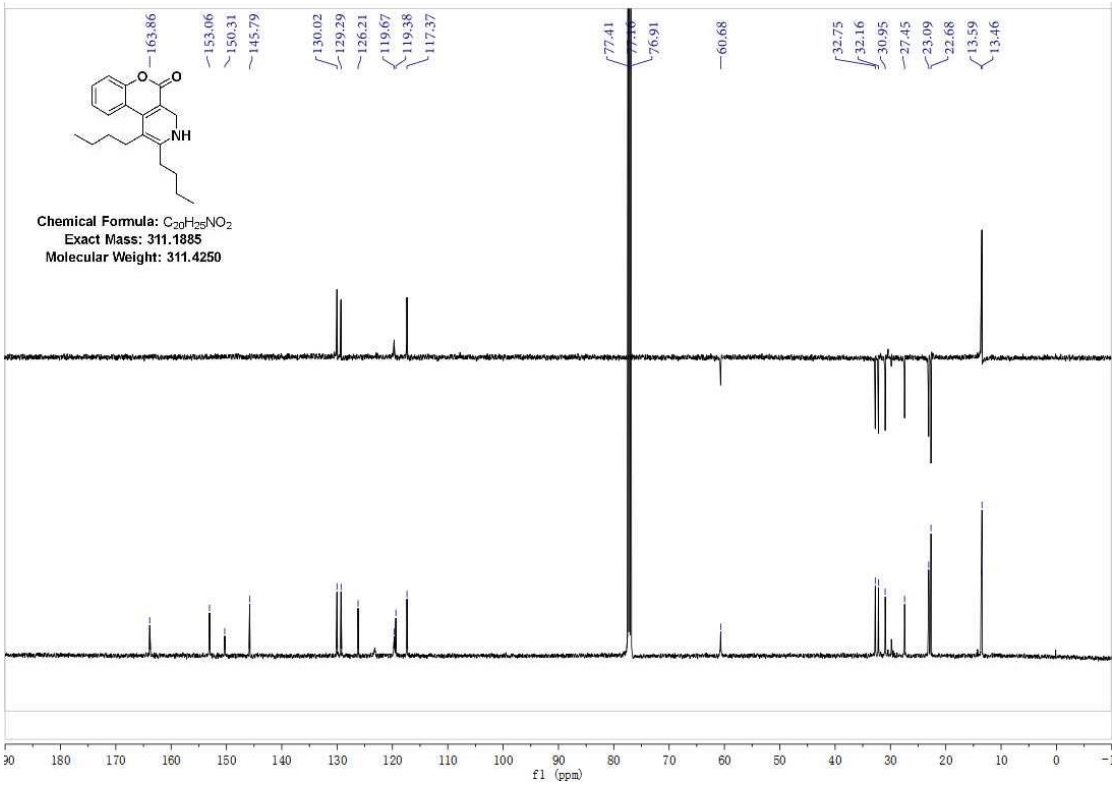


Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
556.191	556.1907	-0.27	-0.48	C39 H26 N O3	(M+H)+

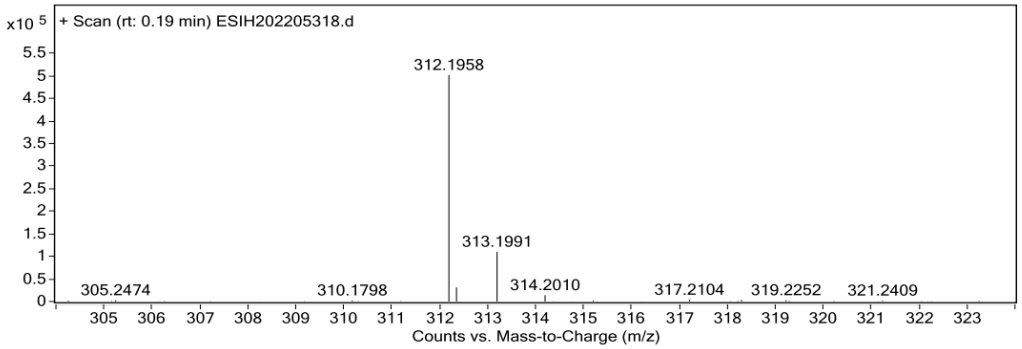
1,2-Dibutyl-3,4-dihydro-5H-chromeno[3,4-c]pyridin-5-one (**5**)





User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
312.1958	312.1958	0.02	0.05	C20 H26 N O2	(M+H)+