Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Rh(III)-catalyzed C–C coupling of unactivated C(sp^3)–H bonds with iodonium ylides for access to all-carbon quaternary carbon centers

Pengfei Xie, Huixing Gao, Xingwei Li, Yuqin Jiang,* and Bingxian Liu*

NMPA Key Laboratory for Research and Evaluation of Innovative Drug, Collaborative Innovation Center of Henan Province for Green Manufacturing of Fine Chemicals, School of Chemistry and Chemical Engineering, Henan Normal University, Xinxiang, Henan453007, China.

E-mail: liubx1120@163.com

Table of Contents

1. General Information

All chemicals were obtained from commercial sources and were used as received unless otherwise noted. All the reactions were carried out under Ar atmosphere. The ^{1}H NMR spectra were recorded on a 400 MHz or 600 MHz NMR spectrometer. The ^{13}C NMR spectra were recorded at 100 MHz or 150 MHz. The ^{19}F NMR spectra were recorded at 376 MHz. Chemical shifts were expressed in parts per million (δ) downfield from the internal standard tetramethylsilane (TMS), and were reported as s (singlet), d (doublet), t (triplet), dd (doublets of doublet), dt (doublets of triplet), and m (multiplet). The residual solvent signals were used as references and the chemical shifts were converted to the TMS scale ($CDCl_3$: δ H = 7.26 ppm, δ C = 77.16 ppm, DMSO-d_6: δ H = 2.50 ppm, δ C = 39.52 ppm). The coupling constants *J* were given in Hz. High resolution mass spectra (HRMS) were obtained via ESI mode by using a MicroTOF mass spectrometer. The conversion of starting materials was monitored by thin layer chromatography (TLC) using silica gel plates (silica gel 60 F254 0.25 mm), and components were visualized by observation under UV light (254 and 365 nm). Column chromatography was performed on silica gel 200-300 mesh.

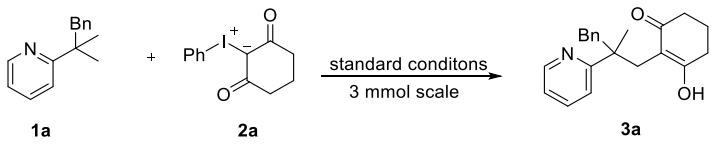
Pyridine derivatives[1] and iodonium ylides[2] were prepared according to the published procedures.

2. Experimental Section

(1) General procedures for pyridine-assisted fuctionalization of unactivated C(sp^3)−H bonds

A Schlenk tube with a magnetic stir bar was charged with pyridine derivatives (0.10 mmol), iodonium ylides (0.15 mmol), $[Cp^*RhCl_2]_2$ (0.004 mmol, 4.0 mol %), $AgSbF_6$ (16 mol %), 2,2-Dimethylbutyric acid (0.10 mmol), K_2CO_3 (0.10 mmol), NaOAc (0.10 mmol) and HFIP (0.5 mL) under an N_2 atmosphere. The resulting mixture was stirred at 100 ºC for 12 h. After the solvent was removed under reduced pressure, the residue was purified by column chromatography on silica gel to provide the desired product.

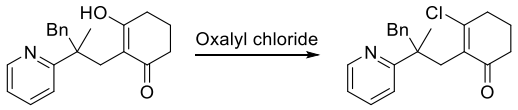
(2) Scale-up Synthesis of 3



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

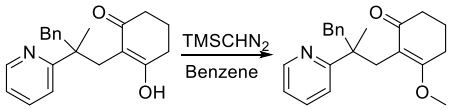
A Schlenk tube with a magnetic stir bar was charged with pyridine derivatives (3.00 mmol), iodonium ylides (4.50 mmol), $[Cp^*RhCl_2]_2$ (0.120 mmol, 4.0 mol %), $AgSbF_6$ (16 mol %), 2,2-Dimethylbutyric acid (3.0 mmol), K_2CO_3 (3.0 mmol), NaOAc (3.0 mmol) and HFIP (15 mL) under an N_2 atmosphere. The resulting mixture was stirred at 100 ºC for 12 h. Afterwards, it was evaporated under reduced pressure, and the residue was purified by silica gel chromatography (petroleum ether:Acetone = 5:1) to afford **3a** (724.6 mg, 75%).

(3) Diversification of the Products



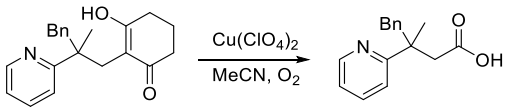
3a **4**, 99%

Compound **3** (0.1 mmol) was dissolved in oxalyl chloride (0.1 mL) and the reaction mixture was stirred at room temperature for 3 h. Then the reaction mixture was diluted with diethyl ether (3.0 mL) and washed with water (3.0 mL) and brine (3.0 mL). The filtrate was concentrated in vacuo, and the crude product was purified by silica gel chromatography (petroleum ether:ethyl acetate = 10:1).



3a **5**, 82%

To a solution of the **3** (0.1 mmol) in benzene (2 mL) was dropwise added trimethylsilyldiazomethane ($TMSCHN_2$, 0.15 mL, 0.3 mmol, 2.0 M solution in hexane) at r.t..The resulting mixture was stirred at room temperature for 12 h. The reaction was quenched by the addition of AcOH (10 μL), and the solvent was removed by vaporation, and the crude product was purified by silica gel chromatography (petroleum ether:ethyl acetate = 1:1) to afford **5** (27.4 mg, 82%).



3a **6**, 90%

A Schlenk tube with a magnetic stir bar was charged with **3** (0.1 mmol), $Cu(ClO_4)_2$ (0.15 mmol) and MeCN (0.5 mL) under an O_2 atmosphere. The resulting mixture was stirred at room temperature for 12 h. Afterwards, it was evaporated under reduced pressure, and the residue was purified by silica gel chromatography (MeOH:DCM = 1:20) to afford **6** (22.9 mg, 90%).

(4) Mechanistic Studies

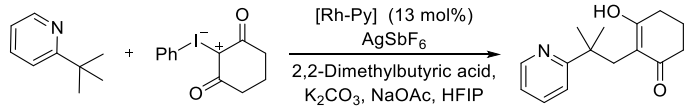
Synthesis of rhodacycle [Rh-Py] complex

1p [Rh-Py], 25%

A Schlenk tube with a magnetic stir bar was charged with $[RhCp^*Cl_2]_2$ (31.3 mg, 0.05 mmol), $AgSbF_6$ (70.4 mg, 0.20 mmol, 4 equiv), 2-(tert-butyl)pyridine (67.6 μL, 0.50 mmol, 10 equiv), and CH_2Cl_2 (0.75 mL) under an N_2 atmosphere. The resulting mixture was stirred at room temperature for 24 h and then diluted with 3 mL of dichloromethane. The solution was filtered through a celite pad and washed with

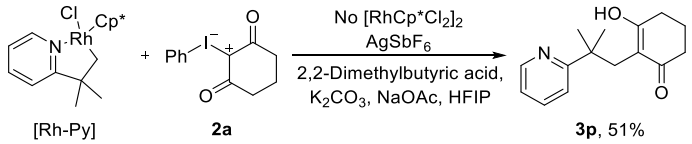
10-20 mL of dichloromethane. The filtrate was concentrated and the residue was purified by column chromatography on alumina to provide the complex as a orange solid.

[Rh-Py] complex catalyzed alkylation of 2-(tert-butyl)pyridine



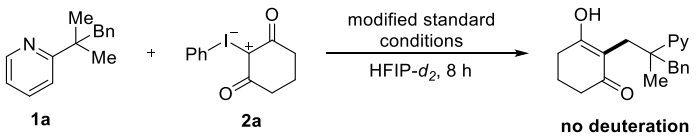
A Schlenk tube with a magnetic stir bar was charged with 2-(tert-butyl)pyridine (0.10 mmol), iodonium ylides (0.15 mmol), [Rh-Py] complex (0.013 mmol, 13.0 mol %), $AgSbF_6$ (13 mol %), 2,2-Dimethylbutyric acid (0.10 mmol), K_2CO_3 (0.10 mmol), NaOAc (0.10 mmol) and HFIP (0.5 mL) under an N_2 atmosphere. The resulting mixture was stirred at 100 ºC for 12 h. After the solvent was removed under reduced pressure, the residue was purified by column chromatography on silica gel to provide the desired product.

The reaction of stoichiometric amounts of [Rh-Py] complex with iodonium ylides

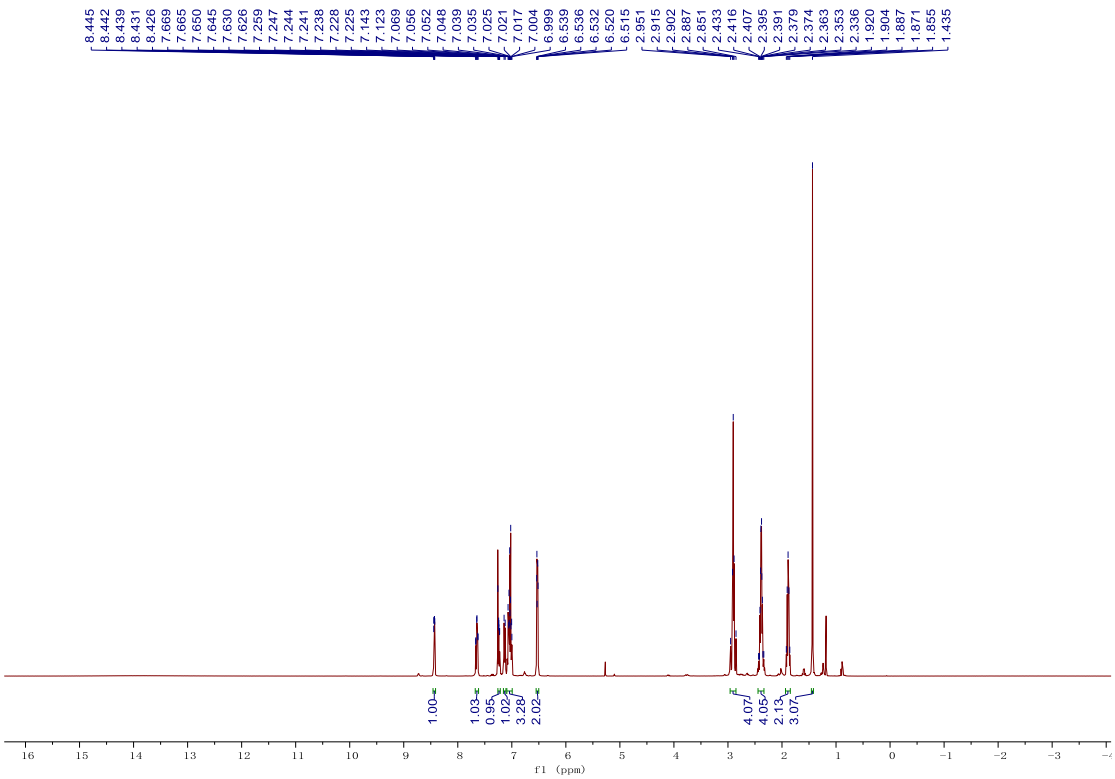


A Schlenk tube with a magnetic stir bar was charged with [Rh-Py] complex (0.05 mmol), iodonium ylides (0.075 mmol), $AgSbF_6$ (16 mol %), 2,2-Dimethylbutyric acid (0.05 mmol), K_2CO_3 (0.05 mmol), NaOAc (0.05 mmol) and HFIP (0.25 mL) under an N_2 atmosphere. The resulting mixture was stirred at 100 ºC for 12 h. After the solvent was removed under reduced pressure, the residue was purified by column chromatography on silica gel to provide the desired product.

H/D Exchange experiment



A Schlenk tube with a magnetic stir bar was charged with **1a** (0.10 mmol), **2a** (0.15 mmol), $[Cp^*RhCl_2]_2$ (0.004 mmol, 4.0 mol %), $AgSbF_6$ (16 mol %), AdCOOD (0.10 mmol), K_2CO_3 (0.10 mmol), NaOAc (0.10 mmol) and HFIP-d_2 (0.5 mL) under an N_2 atmosphere. The resulting mixture was stirred at 100 ºC for 8 h. After the solvent was removed under reduced pressure, the residue was purified by column chromatography on silica gel to provide the desired product, giving the product in 80% yield.



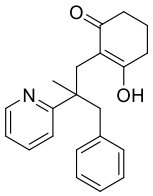
^{1}H NMR of product **3a-*d*$_n$** in the H/D Exchange experiment

3. References

[1] a) X. Huang, Y. Wang, J. Lan and J. You, *Angew. Chem., Int. Ed*., 2015, **54**, 9404–9408; b) J. Dong, Z. Wang, X. Wang, H. Song, Y. Liu and Q. Wang, *J. Org. Chem.* 2019, **84**. 7532–7540.

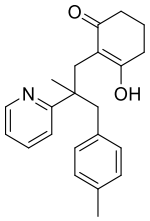
[2] R. M. Moriarty, S. Tyagi, D. Inanov and M. Constantinescu, *J. Am. Chem. Soc.*, 2008, **130**. 7564–7565.

4. Characterization Data



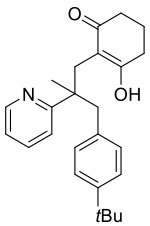
3-hydroxy-2-(2-methyl-3-phenyl-2-(pyridin-2-yl)propyl)cyclohex-2-en-1-one (**3a**).

Yellow solid (28.2 mg, 88%, m.p. 78 - 79 °C), eluent: PE/Acetone = 5:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 14.26 (s, 1H), 8.76 – 8.00 (m, 1H), 7.64 (td, *J* = 7.8, 1.9 Hz, 1H), 7.23 (ddd, *J* = 7.4, 5.1, 1.1 Hz, 1H), 7.13 (d, *J* = 8.2 Hz, 1H), 7.10 – 7.06 (m, 1H), 7.03 (dd, *J* = 8.2, 6.6 Hz, 2H), 2.99 – 2.77 (m, 4H), 2.55 – 2.29 (m, 4H), 1.92 – 1.89 (m, 2H), 1.45 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 199.5, 176.0, 166.7, 145.9, 137.9, 137.6, 130.3, 127.6, 126.2, 123.4, 121.9, 112.8, 50.4, 46.7, 37.2, 32.0, 30.4, 26.4, 21.1. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{24}NO_2^+$ 322.1802, Found: 322.1804.



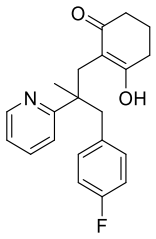
3-hydroxy-2-(2-methyl-2-(pyridin-2-yl)-3-(p-tolyl)propyl)cyclohex-2-en-1-one (**3b**).

Red oil (24.1 mg, 72%), eluent: PE/Acetone = 5:1. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.43 (dd, *J* = 5.1, 1.7 Hz, 1H), 7.64 (td, *J* = 7.8, 1.9 Hz, 1H), 7.23 (ddd, *J* = 7.5, 5.0, 1.0 Hz, 1H), 7.15 (d, *J* = 8.1 Hz, 1H), 6.85 (d, *J* = 7.7 Hz, 2H), 6.42 (d, *J* = 7.9 Hz, 2H), 2.97 – 2.78 (m, 4H), 2.39 (m, 4H), 2.23 (s, 3H), 1.95 – 1.85 (m, 2H), 1.43 (s, 3H).^{13}C NMR (100 MHz, Chloroform-*d*) δ 199.5, 176.0, 166.9, 145.9, 137.5, 135.6, 134.7, 130.2, 128.3, 123.5, 121.9, 112.9, 50.1, 46.7, 37.2, 31.8, 30.4, 26.4 , 21.1. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{26}NO_2^+$ 336.1958, Found: 336.1961.



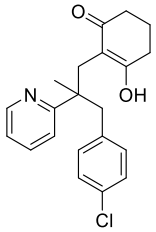
2-(3-(4-(tert-butyl)phenyl)-2-methyl-2-(pyridin-2-yl)propyl)-3-hydroxycyclohex-2-en-1-one (**3c**).

Colorless oil (26.4 mg, 70%), eluent: PE/Acetone = 5:1. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 14.27 (s, 1H), 8.43 (ddd, *J* = 5.1, 1.9, 0.9 Hz, 1H), 7.68 – 7.62 (m, 1H), 7.26 – 7.22 (m, 1H), 7.19 (d, *J* = 8.2 Hz, 1H), 7.07 – 7.03 (m, 2H), 6.50 – 6.42 (m, 2H), 2.93 – 2.81 (m, 4H), 2.46 – 2.33 (m, 4H), 1.93 – 1.87 (m, 2H), 1.44 (s, 3H), 1.23 (s, 9H).^{13}C NMR (150 MHz, Chloroform-*d*) δ 199.5, 175.9, 166.9, 149.0, 145.8, 137.6, 134.7, 129.9, 124.5, 123.5, 121.9, 112.9, 50.1, 46.8, 37.2, 34.4, 31.7, 31.4, 30.4, 26.6, 21.1. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{25}H_{32}NO_2^+$ 378.2428, Found: 378.2425.



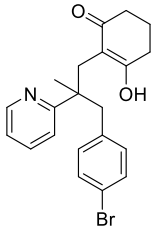
2-(3-(4-fluorophenyl)-2-methyl-2-(pyridin-2-yl)propyl)-3-hydroxycyclohex-2-en-1-one (**3d**).

Yellow oil (27.1 mg, 80%), eluent: PE/Acetone = 5:1. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.44 (d, *J* = 3.6 Hz, 1H), 7.65 (td, *J* = 7.8, 1.9 Hz, 1H), 7.24 (ddd, *J* = 7.5, 5.1, 1.1 Hz, 1H), 7.12 (d, *J* = 8.1 Hz, 1H), 6.72 (t, *J* = 8.7 Hz, 2H), 6.47 (dd, *J* = 8.5, 5.6 Hz, 2H), 2.95 – 2.80 (m, 4H), 2.43 –2.36 (m, 4H), 1.95 – 1.86 (m, 2H), 1.43 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 199.4, 176.0, 166.5, 161.5 (d, *J* = 244.3 Hz), 146.0, 137.6, 133.5 (d, *J* = 3.5 Hz), 131.5 (d, *J* = 7.9 Hz), 123.3, 122.0, 114.4 (d, *J* = 20.9 Hz), 112.6, 49.4, 46.6, 37.2, 31.9, 30.3, 26.2, 21.0. ^{19}F NMR (377 MHz, Chloroform-*d*) δ -117.09. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{23}FNO_2^+$ 340.1707, Found: 340.1702.



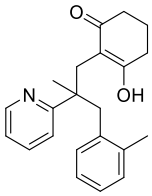
2-(3-(4-chlorophenyl)-2-methyl-2-(pyridin-2-yl)propyl)-3-hydroxycyclohex-2-en-1-one (**3e**).

Red oil (23.8 mg, 71%), eluent: PE/Acetone = 5:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 14.02 (s, 1H), 8.45 (dd, *J* = 5.2, 1.7 Hz, 1H), 7.66 (td, *J* = 7.8, 1.8 Hz, 1H), 7.26 – 7.23 (m, 1H), 7.13 (d, *J* = 8.2 Hz, 1H), 7.01 (d, *J* = 8.4 Hz, 2H), 6.44 (d, *J* = 8.4 Hz, 2H), 2.93 – 2.82 (m, 4H), 2.47 – 2.34 (m, 4H), 1.94 – 1.88 (m, 2H), 1.44 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 199.3, 175.9, 166.3, 146.0, 137.5, 136.2, 132.0, 131.4, 127.6, 123.1, 121.9, 112.5, 49.5, 46.4, 37.1, 31.9, 30.2, 26.1, 20.9. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{23}ClNO_2^+$ 356.1412, Found: 356.1400.



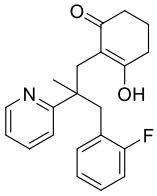
2-(3-(4-bromophenyl)-2-methyl-2-(pyridin-2-yl)propyl)-3-hydroxycyclohex-2-en-1-one (**3f**).

Colorless oil (30.7 mg, 77%), eluent: PE/Acetone = 5:1. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 14.07 (s, 1H), 8.45 (d, *J* = 3.4 Hz, 1H), 7.67 (td, *J* = 7.8, 1.9 Hz, 1H), 7.27 – 7.23 (m, 1H), 7.17 (s, 1H), 7.16 – 7.13 (m, 2H) 6.39 (d, *J* = 8.3 Hz, 2H), 2.94 – 2.82 (m, 4H), 2.47 – 2.34 (m, 4H), 1.95 – 1.88 (m, 2H), 1.44 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 199.4, 176.0, 166.3, 146.1, 137.7, 136.8, 131.9, 130.7, 123.2, 122.0, 120.2, 112.5, 49.6, 46.4, 37.1, 31.9, 30.3, 26.2, 21.0. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{24}BrNO_2^+$ 400.0907, Found: 400.0895.



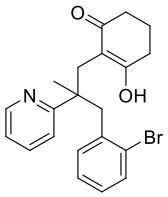
3-hydroxy-2-(2-methyl-2-(pyridin-2-yl)-3-(o-tolyl)propyl)cyclohex-2-en-1-one (**3g**).

Brown oil (29.2 mg, 87%), eluent: PE/Acetone = 5:1. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.48 (d, *J* = 3.9 Hz, 1H), 7.53 (td, *J* = 7.9, 1.9 Hz, 1H), 7.24 (ddd, *J* = 7.4, 5.1, 1.1 Hz, 1H), 7.05 – 7.00 (m, 1H), 6.96 (dd, *J* = 7.7, 1.6 Hz, 1H), 6.91 (td, *J* = 7.4, 1.6 Hz, 1H), 6.82 (d, *J* = 8.2 Hz, 1H), 6.49 (dd, *J* = 7.7, 1.3 Hz, 1H), 3.12 – 3.08 (m, 1H), 2.94 – 2.84 (m, 3H), 2.49 – 2.33 (m, 4H), 1.96 – 1.88 (m, 2H), 1.74 (s, 3H), 1.46 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 199.3, 175.9, 166.4, 145.9, 137.6, 137.3, 136.1, 131.0, 130.0, 126.2, 124.9, 123.5, 121.9, 112.8, 47.0, 45.1, 37.1, 32.7, 30.2, 26.4, 20.9, 19.4. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{26}NO_2^+$ 336.1958, Found: 336.1961.



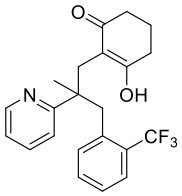
2-(3-(2-fluorophenyl)-2-methyl-2-(pyridin-2-yl)propyl)-3-hydroxycyclohex-2-en-1-one (**3h**).

Dark red oil (24.8 mg, 73%), eluent: PE/Acetone = 5:1. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 14.24 (s, 1H), 8.45 (d, *J* = 3.5 Hz, 1H), 7.63 (td, *J* = 7.8, 1.8 Hz, 1H), 7.28 – 7.24 (m, 1H), 7.12 – 7.05 (m, 2H), 6.86 (td, *J* = 7.5, 1.2 Hz, 1H), 6.79 (dd, *J* = 9.6, 8.1, 1H), 6.62 (td, *J* = 7.6, 1.8 Hz, 1H), 3.05 – 2.86 (m, 4H), 2.46 – 2.33(m, 4H), 1.93 – 1.87 (m, 2H), 1.45 (s, 3H). NMR (150 MHz, Chloroform-d) δ 199.2, 175.9, 166.2, 162.5 (d, *J* = 242.4 Hz), 145.9, 140.2 (d, *J* = 6.9 Hz), 137.4, 128.8 (d, *J* = 8.7 Hz), 125.8 , 123.0, 121.9, 116.7 (d, *J* = 20.8 Hz), 112.9 (d, *J* = 20.8 Hz), 112.4, 49.9, 46.4, 37.0, 31.7, 30.1, 26.2, 20.8. ^{19}F NMR (565 MHz, Chloroform-*d*) δ -115.88. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{23}FNO_2^+$ 340.1707, Found: 340.1703.

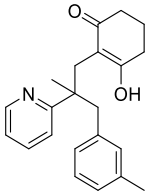


2-(3-(2-bromophenyl)-2-methyl-2-(pyridin-2-yl)propyl)-3-hydroxycyclohex-2-en-1-one (**3i**).

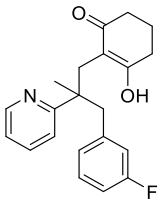
Yellow solid (23.5 mg, 59%, m.p. 75 - 76 °C), eluent: PE/Acetone = 5:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 14.45 (s, 1H), 8.47 (d, *J* = 3.4 Hz, 1H), 7.55 (td, *J* = 7.8, 1.8 Hz, 1H), 7.37 (d, *J* = 6.6 Hz, 1H), 7.26 – 7.23 (m, 1H), 7.06 (td, *J* = 7.5, 1.3 Hz, 1H), 6.98 (td, *J* = 7.7, 1.7 Hz, 1H), 6.85 (d, *J* = 8.1 Hz, 1H), 6.69 (dd, *J* = 7.6, 1.7 Hz, 1H), 3.11 – 2.95 (m, 4H), 2.50 – 2.41 (m, 2H), 2.39 – 2.34 (m, 2H), 1.94 – 1.89 (m, 2H), 1.49 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 199.4, 176.3, 165.8, 146.0, 137.7, 137.6, 132.8, 132.3, 127.9, 126.9, 126.6, 123.5, 122.2, 112.6, 47.6, 47.1, 37.2, 32.5, 30.4, 26.5, 21.0. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{23}BrNO_2^+$ 400.0907, Found: 400.0897.



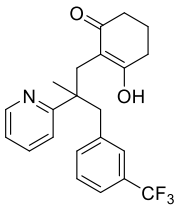
3-hydroxy-2-(2-methyl-2-(pyridin-2-yl)-3-(2-(trifluoromethyl)phenyl)propyl)cyclohex-2-en-1-one (**3j**). Yellow solid (21.8 mg, 56%, m.p. 109 - 110 °C), eluent: PE/Acetone = 5:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 14.38 (s, 1H), 8.54 – 8.43 (m, 1H), 7.56 – 7.50 (m, 2H), 7.30 – 7.19 (m, 3H), 6.86 (d, *J* = 8.1 Hz, 1H), 6.76 (d, *J* = 7.5 Hz, 1H), 3.21 (m, 2H), 3.02 – 2.93 (m, 2H), 2.41 (m, 4H), 1.94 – 1.90 (m, 2H), 1.45 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 199.3, 176.1, 166.4, 146.0, 137.7, 137.1, 132.0, 130.8, 129.8 (q, *J* = 28.9 Hz), 126.4, 126.3 (q, *J* = 5.9 Hz), 124.3 (q, *J* = 274.2 Hz), 123.1, 121.5, 112.7, 46.8, 44.2, 37.2, 32.5, 30.4, 27.8, 21.0. ^{19}F NMR (565 MHz, Chloroform-*d*) δ -58.44. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{23}F_3NO_2^+$ 390.1675, Found: 390.1674.



3-hydroxy-2-(2-methyl-2-(pyridin-2-yl)-3-(m-tolyl)propyl)cyclohex-2-en-1-one (**3k**).
Colorless oil (29.2 mg, 87%), eluent: PE/Acetone = 5:1. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 14.19 (s, 1H), 8.44 (d, *J* = 4.2 Hz, 1H), 7.65 (td, *J* = 7.8, 1.9 Hz, 1H), 7.24 (ddd, *J* = 7.4, 5.3, 1.3 Hz, 1H), 7.15 (d, *J* = 8.1 Hz, 1H), 6.93 – 6.87 (m, 2H), 6.33 (s, 1H), 6.29 (dt, *J* = 6.9, 2.0 Hz, 1H), 2.92 – 2.81 (m, 4H), 2.43 – 2.35 (m, 4H), 2.14 (s, 3H), 1.94 – 1.87 (m, 2H), 1.44 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 199.5, 176.0, 166.9, 145.8, 137.7, 137.4, 137.0, 131.2, 127.4, 127.2, 126.9, 123.5, 121.8, 112.8, 50.4, 46.7, 37.2, 31.9, 30.4, 26.4, 21.3, 21.1. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{26}NO_2^+$ 336.1958, Found: 336.1955.

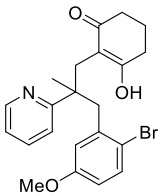


2-(3-(3-fluorophenyl)-2-methyl-2-(pyridin-2-yl)propyl)-3-hydroxycyclohex-2-en-1-one (**3l**).
Brown solid (28.2 mg, 83%, m.p. 111 - 112 °C), eluent: PE/Acetone = 5:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 14.11 (s, 1H), 8.46 (dd, *J* = 5.2, 1.7 Hz, 1H), 7.68 (td, *J* = 7.8, 1.8 Hz, 1H), 7.28 – 7.25 (m, 1H), 7.17 (d, *J* = 8.1 Hz, 1H), 7.01 (td, *J* = 8.0, 6.2 Hz, 1H), 6.79 (td, *J* = 8.5, 2.5 Hz, 1H), 6.37 (d, *J* = 7.6 Hz, 1H), 6.16 (dt, *J* = 10.3, 2.0 Hz, 1H), 2.96 – 2.83 (m, 4H), 2.49 – 2.33 (m, 4H), 1.94 – 1.89 (m, 2H), 1.46 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 199.4, 176.0, 166.3, 162.2 (d, *J* = 245.3 Hz), 146.1, 140.4 (d, *J* = 6.8 Hz), 137.7, 128.9 (d, *J* = 8.7 Hz), 126.0 (d, *J* = 2.3 Hz), 123.2, 122.1, 116.8 (d, *J* = 20.9 Hz), 113.1 (d, *J* = 20.9 Hz), 112.6, 50.0, 46.6, 37.1, 31.9, 30.3, 26.3, 21.0. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -114.36. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{23}FNO_2^+$ 340.1707, Found: 340.1707.



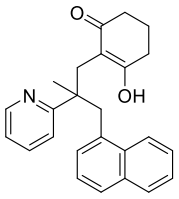
3-hydroxy-2-(2-methyl-2-(pyridin-2-yl)-3-(3-(trifluoromethyl)phenyl)propyl)cyclohex-2-en-1-one (**3m**).

Dark red oil (26.5 mg, 68%), eluent: PE/Acetone = 5:1. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 (dd, *J* = 5.6, 1.6 Hz, 1H), 7.65 (td, *J* = 7.8, 1.8 Hz, 1H), 7.37 – 7.32 (m, 1H), 7.28 – 7.24 (m, 1H), 7.20 (t, *J* = 7.7 Hz, 1H), 7.09 (d, *J* = 8.2 Hz, 1H), 6.87 (d, *J* = 7.7 Hz, 1H), 6.49 (s, 1H), 2.96 – 2.84 (m, 4H), 2.44 – 2.34 (m, 4H), 1.94 – 1.88 (m, 2H), 1.46 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 199.5, 176.1, 166.1, 146.2, 138.8, 137.7, 133.7, 129.8 (q, *J* = 31.8 Hz), 128.0, 126.6 (q, *J* = 3.4 Hz), 124.1 (d, *J* = 271.7 Hz), 123.0 (q, *J* = 3.8 Hz), 122.2, 112.5, 106.1, 50.0, 46.5, 37.1, 32.0, 30.3, 26.1, 21.0. ^{19}F NMR (377 MHz, Chloroform-*d*) δ -62.80. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{23}F_3NO_2^+$ 390.1675, Found: 390.1678.



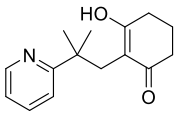
2-(3-(2-bromo-5-methoxyphenyl)-2-methyl-2-(pyridin-2-yl)propyl)-3-hydroxycyclohex-2-en-1-one (**3n**).

Yellow oil (29.1 mg, 68%), eluent: PE/Acetone = 5:1. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 14.31 (s, 1H), 8.49 (ddd, *J* = 5.1, 1.9, 0.9 Hz, 1H), 7.65 – 7.46 (m, 1H), 7.32 – 7.17 (m, 2H), 6.93 (d, *J* = 8.1 Hz, 1H), 6.57 (dd, *J* = 8.8, 3.0 Hz, 1H), 6.17 (d, *J* = 3.0 Hz, 1H), 3.60 (s, 3H), 3.14 – 2.89 (m, 4H), 2.42 (m, 4H), 1.94 – 1.91 (m, 2H), 1.51 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 199.4, 176.3, 166.0, 158.1, 146.1, 138.6, 137.8, 133.2, 123.6, 122.2, 117.4, 117.2, 114.4, 112.7, 55.3, 47.9, 47.2, 37.2, 32.6, 30.5, 26.6, 21.1. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{25}BrNO_3^+$ 430.1012, Found: 430.1007.



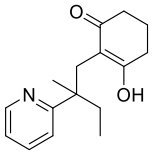
3-hydroxy-2-(2-methyl-3-(naphthalen-1-yl)-2-(pyridin-2-yl)propyl)cyclohex-2-en-1-one (**3o**).

White solid (25.2 mg, 68%, m.p. 49 - 50 °C), eluent: PE/Acetone = 5:1. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 14.51 (s, 1H), 8.48 (dd, *J* = 5.1, 1.8 Hz, 1H), 7.71 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.63 (d, *J* = 8.2 Hz, 1H), 7.43 (d, *J* = 8.6 Hz, 1H), 7.30 (ddd, *J* = 8.1, 6.6, 1.1 Hz, 1H), 7.26 – 7.15 (m, 3H), 7.12 (ddd, *J* = 7.5, 5.1, 1.1 Hz, 1H), 6.73 – 6.64 (m, 1H), 6.59 (d, *J* = 8.1 Hz, 1H), 3.31 – 3.30 (m, 2H), 3.22 – 3.18 (m, 1H), 3.00 – 2.96 (m, 1H), 2.55 – 2.34 (m, 4H), 1.97 – 1.90 (m, 2H), 1.49 (s, 3H).^{13}C NMR (150 MHz, Chloroform-*d*) δ 199.4, 176.1, 166.3, 145.9, 137.1, 134.2,133.4, 133.2, 128.6, 128.3, 126.9, 125.3, 124.9, 124.6, 124.0, 123.5, 121.8, 112.8, 46.9, 44.1, 37.1, 33.4, 30.3, 26.7, 21.0. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{25}H_{26}NO_2^+$ 372.1958, Found: 372.1958.



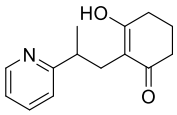
3-hydroxy-2-(2-methyl-2-(pyridin-2-yl)propyl)cyclohex-2-en-1-one (**3p**).

Yellow oil (17.7 mg, 72%), eluent: PE/Acetone = 4:1. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 14.19 (s, 1H), 8.40 (dd, *J* = 5.1, 1.9, 1H), 7.74 (ddd, *J* = 8.1, 7.4, 1.9 Hz, 1H), 7.48 (dt, *J* = 8.2, 1.1 Hz, 1H), 7.21 (dd, *J* = 7.5, 5.1 Hz, 1H), 2.82 (m, 2H), 2.39 (m, 4H), 1.93 – 1.87 (m, 2H), 1.31 (s, 6H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 199.5 , 175.9 , 169.4 , 145.6 , 138.4 , 122.0 , 121.7 , 113.4 , 42.8 , 37.2 , 32.3 , 30.4 , 21.1 .HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{15}H_{20}NO_2^+$ 246.1489, Found: 246.1491.



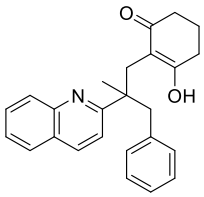
3-hydroxy-2-(2-methyl-2-(pyridin-2-yl)butyl)cyclohex-2-en-1-one (**3q**).

Yellow solid (21.5 mg, 83%, m.p. 57 - 58 °C), eluent: PE/Acetone = 5:1. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.43 (dd, *J* = 5.2, 1.9 Hz, 1H), 7.75 (ddd, *J* = 8.2, 7.4, 1.9 Hz, 1H), 7.43 (dt, *J* = 8.2, 1.0 Hz, 1H), 7.22 (dd, *J* = 7.4, 5.2 Hz, 1H), 2.89 – 2.79 (m, 2H), 2.43 – 2.34 (m, 4H), 1.94 – 1.87 (m, 2H), 1.84 – 1.87 (m, 2H), 1.25 (s, 3H), 0.64 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 199.4, 175.8, 167.9, 145.6, 138.1, 122.5, 121.6, 113.1, 46.0, 37.8, 37.2, 30.5, 29.9, 27.3, 21.1, 8.9. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{16}H_{22}NO_2^+$ 260.1645, Found: 260.1640.



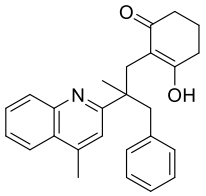
3-hydroxy-2-(2-(pyridin-2-yl)propyl)cyclohex-2-en-1-one (**3r**).

Yellow oil (6.9 mg, 30%), eluent: PE/Acetone = 3:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.42 (d, *J* = 4.4 Hz, 1H), 7.70 (td, *J* = 7.7, 1.8 Hz, 1H), 7.28 (d, *J* = 8.0 Hz, 1H), 7.22 – 7.19 (m, 1H), 3.32 – 3.26 (m, 1H), 2.84 – 2.80 (m, 1H), 2.65 – 2.62 (m, 1H), 2.35 (m, 4H), 1.91 – 1.87 (m, 2H), 1.28 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 207.1, 177.2, 165.6, 146.4, 138.1, 124.2, 121.8, 114.4, 40.4, 26.7, 23.3, 20.8. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{14}H_{18}NO_2^+$ 232.1332, Found: 232.1333.



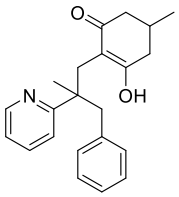
3-hydroxy-2-(2-methyl-3-phenyl-2-(quinolin-2-yl)propyl)cyclohex-2-en-1-one (**3s**).

Yellow solid (19.3 mg, 52%, m.p. 139 - 140 °C), eluent: PE/Acetone = 5:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 14.37 (s, 1H), 8.12 (d, *J* = 8.6 Hz, 2H), 7.84 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.76 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 7.59 (ddd, *J* = 8.0, 6.8, 1.0 Hz, 1H), 7.39 (d, *J* = 8.8 Hz, 1H), 7.09 – 7.04 (m, 1H), 6.99 (t, *J* = 7.5 Hz, 2H), 6.59 (dd, *J* = 7.8, 1.3 Hz, 2H), 3.15 – 3.04 (m, 2H), 3.03 – 2.97 (m, 2H), 2.39 – 2.38 (m, 4H), 1.91 – 1.89 (m, 2H), 1.54 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 199.3, 175.8, 167.6, 144.8, 137.6, 137.2, 130.4, 130.1, 127.6, 127.5, 126.8, 126.7, 126.7, 126.1, 120.9, 112.7, 50.9, 47.6, 37.1, 30.8, 30.2, 26.2, 21.0. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{25}H_{26}NO_2^+$ 372.1958, Found: 372.1961.



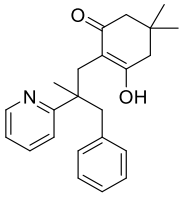
3-hydroxy-2-(2-methyl-2-(4-methylquinolin-2-yl)-3-phenylpropyl)cyclohex-2-en-1-one (**3t**).

White solid (20.0 mg, 57%, m.p. 159 - 160 ºC), eluent: PE/Acetone = 5:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 14.82 (s, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.99 (dd, *J* = 8.5, 1.3 Hz, 1H), 7.74 (ddd, *J* = 8.3, 6.8, 1.3 Hz, 1H), 7.60 (ddd, *J* = 8.2, 6.9, 1.2 Hz, 1H), 7.18 (s, 1H), 7.10 – 7.04 (m, 1H), 7.00 (t, *J* = 7.5 Hz, 2H), 6.64 – 6.55 (m, 2H), 3.16 – 3.02 (m, 1H), 3.00 – 2.95 (m, 2H), 2.66 (s, 3H), 2.47 – 2.35 (m, 4H), 1.91 – 1.86 (m, 2H), 1.52 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 199.4, 176.1, 167.0, 145.7, 144.6, 137.8, 130.2, 130.1, 127.6, 127.2, 127.8, 126.6, 126.2, 123.8, 121.6, 112.7, 50.9, 47.5, 37.2, 30.7, 30.4, 26.3, 21.1, 19.1. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{26}H_{28}NO_2^+$ 386.2115, Found: 386.2116.



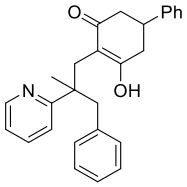
3-hydroxy-5-methyl-2-(2-methyl-3-phenyl-2-(pyridin-2-yl)propyl)cyclohex-2-en-1-one (**3u**).

Yellow oil (25.1 mg, 75%), eluent: PE/Acetone = 5:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 14.18 (s, 1H), 8.42 (dd, *J* = 36.2, 5.0 Hz, 1H), 7.63 (dt, *J* = 31.2, 7.8 Hz, 1H), 7.24 – 7.19 (m, 2H), 7.09 – 7.01(m, 3H), 6.52 (dd, *J* = 31.7, 7.4 Hz, 2H), 2.99 – 2.80 (m, 4H), 2.48 – 2.38 (m, 2H), 2.22 – 2.02 (m, 3H), 1.45 – 1.42 (m, 3H), 1.04 – 1.00 (m, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 199.4, 175.5, 166.8, 145.9, 137.8, 137.5, 130.2, 127.6, 126.2, 123.5, 121.9, 112.3, 51.2, 47.0, 45.2, 38.6, 31.3, 28.7, 26.4, 21.0. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{26}NO_2^+$ 336.1958, Found: 336.1959.



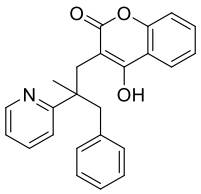
3-hydroxy-5,5-dimethyl-2-(2-methyl-3-phenyl-2-(pyridin-2-yl)propyl)cyclohex-2-en-1-one (**3v**).

Yellow oil (28.9 mg, 83%), eluent: PE/Acetone = 5:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 14.13 (s, 1H), 8.44 (d, *J* = 3.5 Hz, 1H), 7.64 (td, *J* = 7.8, 1.9 Hz, 1H), 7.24 (ddd, *J* = 7.5, 5.1, 1.1 Hz, 1H), 7.13 (d, *J* = 8.1 Hz, 1H), 7.10 – 7.07 (m, 1H), 7.04 (dd, *J* = 8.2, 6.5 Hz, 2H), 6.56 – 6.49 (m, 2H), 2.95 – 2.86 (m, 4H), 2.29 – 2.26 (m, 4H), 1.44 (s, 3H), 1.02 (s, 6H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 198.9, 174.0, 166.6, 145.8, 137.7, 137.4, 130.1, 127.5, 126.1, 123.3, 121.8, 111.4, 51.0, 50.4, 46.7, 44.0, 31.6, 28.8, 28.0, 26.4. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{23}H_{28}NO_2^+$ 350.2115, Found: 350.2116.



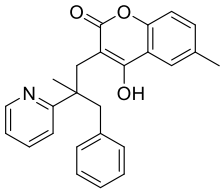
5-hydroxy-4-(2-methyl-3-phenyl-2-(pyridin-2-yl)propyl)-1 ,6-dihydro-[1,1'-biphenyl]-3(2*H*)-one (**3w**).

Yellow oil (21.4 mg, 54%), eluent: PE/Acetone = 5:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 14.32 (s, 1H), 8.43 (d, *J* = 28.5 Hz, 1H), 7.72 – 7.55 (m, 1H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.23 (dq, *J* = 14.4, 7.5, 6.7 Hz, 5H), 7.10 – 7.03 (m, 3H), 6.57 – 6.57(m, 2H), 3.30 (m, 1H), 2.96 – 2.89 (m, 4H), 2.69 – 2.64 (m, 4H), 1.50 – 1.47 (m, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 198.1, 175.0, 166.4, 145.8, 143.5, 137.7, 137.6, 130.2, 128.6, 127.5, 126.7, 126.7, 126.2, 123.4, 121.9, 112.4, 51.2, 47.1, 44.4, 39.2, 37.8, 31.3, 26.50. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{27}H_{28}NO_2^+$ 398.2115, Found: 398.2117.



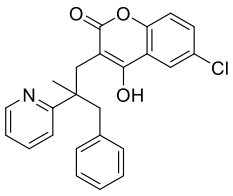
4-hydroxy-3-(2-methyl-3-phenyl-2-(pyridin-2-yl)propyl)-2*H*-chromen-2-one (**3x**).

Yellow solid (13.0 mg, 35%, m.p. 125 - 126 ºC), eluent: PE/Acetone = 5:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 15.50 (s, 1H), 8.51 (d, *J* = 3.5 Hz, 1H), 7.90 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.72 (td, *J* = 7.7, 1.8 Hz, 1H), 7.46 (ddd, *J* = 8.7, 7.2, 1.7 Hz, 1H), 7.33 – 7.29 (m, 1H), 7.28 – 7.25 (m, 2H), 7.24 – 7.21 (m, 1H), 7.13 – 7.10 (m, 1H), 7.07 (dd, *J* = 8.1, 6.5 Hz, 2H), 6.60 – 6.56 (m, 2H), 3.25 – 3.24 (m, 1H), 3.12 – 3.10 (m, 2H), 2.98 – 2.96 (m, 1H), 1.64 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 165.8, 165.6, 164.5, 153.0, 145.6, 138.1, 137.3, 131.3, 130.2, 127.8, 126.5, 123.8, 123.4, 122.3, 117.6, 116.2, 102.0, 50.9, 47.8, 34.1, 26.7. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{22}NO_3^+$ 372.1594, Found: 372.1593.



4-hydroxy-6-methyl-3-(2-methyl-3-phenyl-2-(pyridin-2-yl)propyl)-2*H*-chromen-2-one (**3y**).

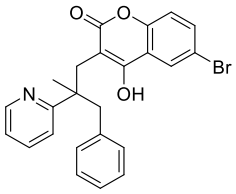
Yellow solid (25.8 mg, 67%, m.p. 105 - 106 ºC), eluent: PE/Acetone = 5:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 15.41 (s, 1H), 8.52 (d, *J* = 3.4 Hz, 1H), 7.72 (t, *J* = 6.9 Hz, 1H), 7.70 (d, *J* = 2.1 Hz, 1H), 7.31 (dd, *J* = 7.4, 5.3 Hz, 1H), 7.28 – 7.24 (m, 2H), 7.16 (d, *J* = 8.4 Hz, 1H), 7.13 – 7.09 (m, 1H), 7.07 (dd, *J* = 8.1, 6.5 Hz, 2H), 6.60 – 6.55 (m, 2H), 3.26 – 3.24 (m, 1H), 3.14 – 3.09 (m, 2H), 2.99 – 2.97 (m, 1H), 2.39 (s, 3H), 1.63 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 165.7, 165.7, 164.3, 151.0, 145.5, 138.0, 137.2, 132.9, 132.2, 130.1, 127.6, 126.3, 123.7, 123.4, 122.2, 117.1, 115.9, 101.8, 50.7, 47.6, 34.0, 26.5, 20.9. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{25}H_{24}NO_3^+$ 386.1751, Found: 386.1749.



6-chloro-4-hydroxy-3-(2-methyl-3-phenyl-2-(pyridin-2-yl)propyl)-2*H*-chromen-2-one (**3z**).

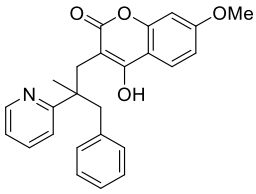
Yellow solid (16.6 mg, 41%, m.p. 94 - 95 ºC), eluent: PE/Acetone = 5:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 15.67 (s, 1H), 8.50 (d, *J* = 4.0 Hz, 1H), 7.88 (d, *J* = 2.6 Hz, 1H), 7.75 (td, *J* = 7.8, 1.8 Hz, 1H), 7.39 (dd, *J* = 8.7, 2.6 Hz, 1H), 7.34 (ddd, *J* = 7.5, 5.2, 1.1 Hz, 1H), 7.28 (d, *J* = 8.2 Hz, 1H), 7.20 (d, *J* = 8.7 Hz, 1H), 7.14 – 7.11 (m, 1H), 7.10 – 7.05 (m, 2H), 3.24 – 3.21 (m, 1H), 3.13 – 3.08 (m,

2H), 2.97 – 2.95 (m, 1H), 1.63 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 165.6, 165.2, 163.7, 151.4, 145.4, 138.4, 137.1, 131.3, 130.2, 128.9, 127.8, 126.6, 124.0, 123.5, 122.5, 119.0, 117.7, 102.6, 50.8, 47.9, 34.1, 26.8. HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $C_{24}H_{21}ClNO_3^+$ 406.1204, Found: 406.1204.



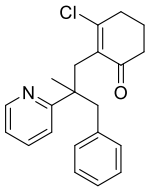
6-bromo-4-hydroxy-3-(2-methyl-3-phenyl-2-(pyridin-2-yl)propyl)-2*H*-chromen-2-one (**3aa**).

Yellow solid (17.5 mg, 39%, m.p. 131 - 132 ºC), eluent: PE/Acetone = 5:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 15.59 (s, 1H), 8.50 (d, *J* = 4.5 Hz, 1H), 8.07 – 8.01 (m, 1H), 7.75 (t, *J* = 7.3 Hz, 1H), 7.54 (d, *J* = 8.6 Hz, 1H), 7.37 – 7.31 (m, 1H), 7.28 (d, *J* = 8.1 Hz, 1H), 7.13 (dd, *J* = 15.2, 7.9 Hz, 2H), 7.08 (t, *J* = 7.3 Hz, 2H), 6.58 (d, *J* = 7.3 Hz, 2H), 3.24 – 3.21 (m, 1H), 3.13 – 3.08 (m, 2H), 2.97 – 2.95 (m, 1H), 1.63 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 165.4, 165.0, 163.5, 151.8, 145.3, 138.3, 137.0, 133.9, 130.1, 127.7, 126.4, 123.8, 122.4, 119.3, 117.9, 116.1, 102.5, 50.7, 47.7, 34.0, 26.7. HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $C_{24}H_{21}BrNO_3^+$ 450.0699, Found: 450.0700.



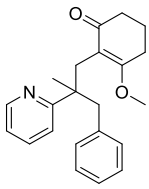
4-hydroxy-7-methoxy-3-(2-methyl-3-phenyl-2-(pyridin-2-yl)propyl)-2*H*-chromen-2-one (**3ab**).

Yellow solid (16.4 mg, 41%, m.p. 102 - 103 ºC), eluent: PE/Acetone = 5:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 15.28 (s, 1H), 8.50 (d, *J* = 3.5 Hz, 1H), 7.78 (d, *J* = 8.8 Hz, 1H), 7.71 (td, *J* = 7.8, 1.8 Hz, 1H), 7.30 (ddd, *J* = 7.4, 5.2, 1.0 Hz, 1H), 7.25 (d, *J* = 7.7 Hz, 1H), 7.13 – 7.09 (m, 1H), 7.06 (dd, *J* = 8.2, 6.5 Hz, 2H), 6.80 (dd, *J* = 8.7, 2.5 Hz, 1H), 6.76 (d, *J* = 2.4 Hz, 1H), 6.60 – 6.56 (m, 2H), 3.84 (s, 3H), 3.23 – 3.21 (m, 1H), 3.11 – 3.06 (m, 2H), 2.98 – 2.95 (m, 1H), 1.63 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 166.0, 165.9, 164.9, 162.5, 154.7, 145.6, 138.0, 137.4, 130.2, 127.7, 126.4, 124.9, 123.8, 122.3, 111.7, 111.0, 100.0, 99.4, 55.7, 50.9, 47.7, 34.0, 26.6. HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $C_{25}H_{24}NO_4^+$ 402.1700, Found: 402.1702.



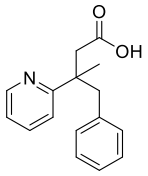
3-chloro-2-(2-methyl-3-phenyl-2-(pyridin-2-yl)propyl)cyclohex-2-en-1-one (**4**).

Dark red oil (34.0 mg, 99%), eluent: PE/EA = 10:1. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.65 (ddd, *J* = 4.8, 1.9, 0.9 Hz, 1H), 7.48 (td, *J* = 7.8, 1.9 Hz, 1H), 7.09 (ddd, *J* = 7.6, 4.8, 1.1 Hz, 1H), 7.06 – 7.00 (m, 4H), 6.78 – 6.74 (m, 2H), 3.76 – 3.73 (m, 1H), 3.11 – 3.00 (m, 2H), 2.80 – 2.77 (m, 1H), 2.72 – 2.69 (m, 2H), 2.43 – 2.30 (m, 2H), 2.04 – 1.96 (m, 2H), 1.22 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 196.2, 165.1, 154.8, 148.4, 139.1, 135.9, 135.7, 130.5, 127.5, 125.8, 121.4, 121.2, 47.5, 46.6, 39.1, 37.3, 35.7, 22.4, 21.9. HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $C_{21}H_{23}ClNO^+$ 340.1463, Found: 340.1460.



3-methoxy-2-(2-methyl-3-phenyl-2-(pyridin-2-yl)propyl)cyclohex-2-en-1-one (**5**).

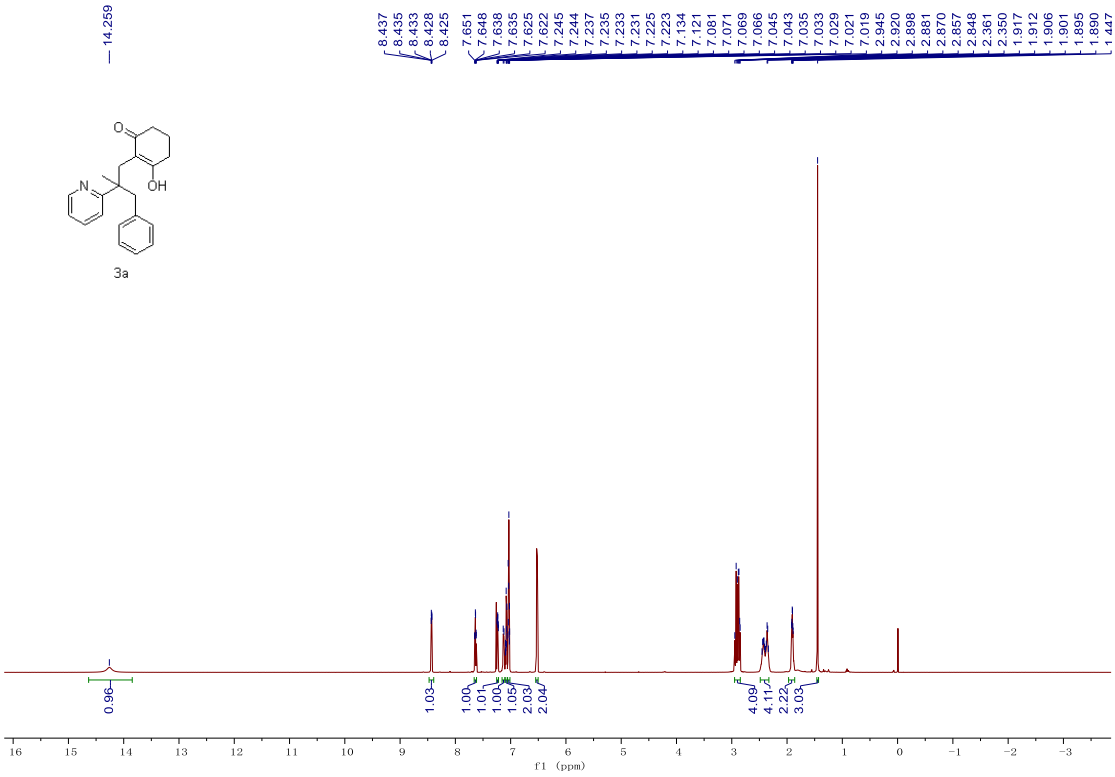
Yellow oil (27.4 mg, 82%), eluent: PE/EA = 1:1. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.67 (ddd, *J* = 4.8, 1.9, 0.9 Hz, 1H), 7.47 (td, *J* = 7.7, 1.9 Hz, 1H), 7.08 – 6.98 (m, 5H), 6.82 – 6.71 (m, 2H), 3.71 – 3.68 (m, 1H), 3.43 (s, 3H), 2.93 – 2.91 (m, 1H), 2.85 – 2.83 (m, 1H), 2.74 – 2.71 (m, 1H), 2.46 – 2.43 (m, 2H), 2.35 – 2.25 (m, 2H), 1.97 – 1.91 (m, 2H), 1.14 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 198.2, 173.1, 166.5, 148.0, 140.0, 135.3, 130.4, 127.4, 125.5, 121.6, 120.6, 116.5, 54.8, 47.5, 46.5, 36.5, 34.8, 25.0, 21.7, 20.7. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{26}NO_2^+$ 336.1958, Found: 336.1960.

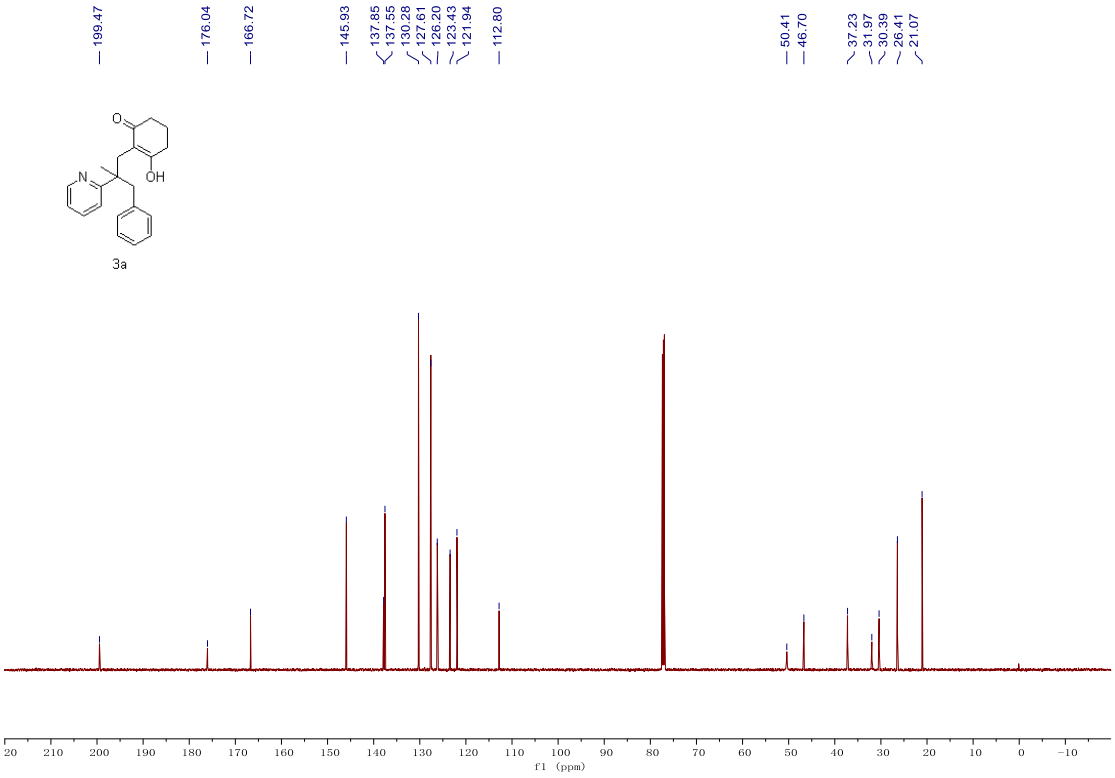


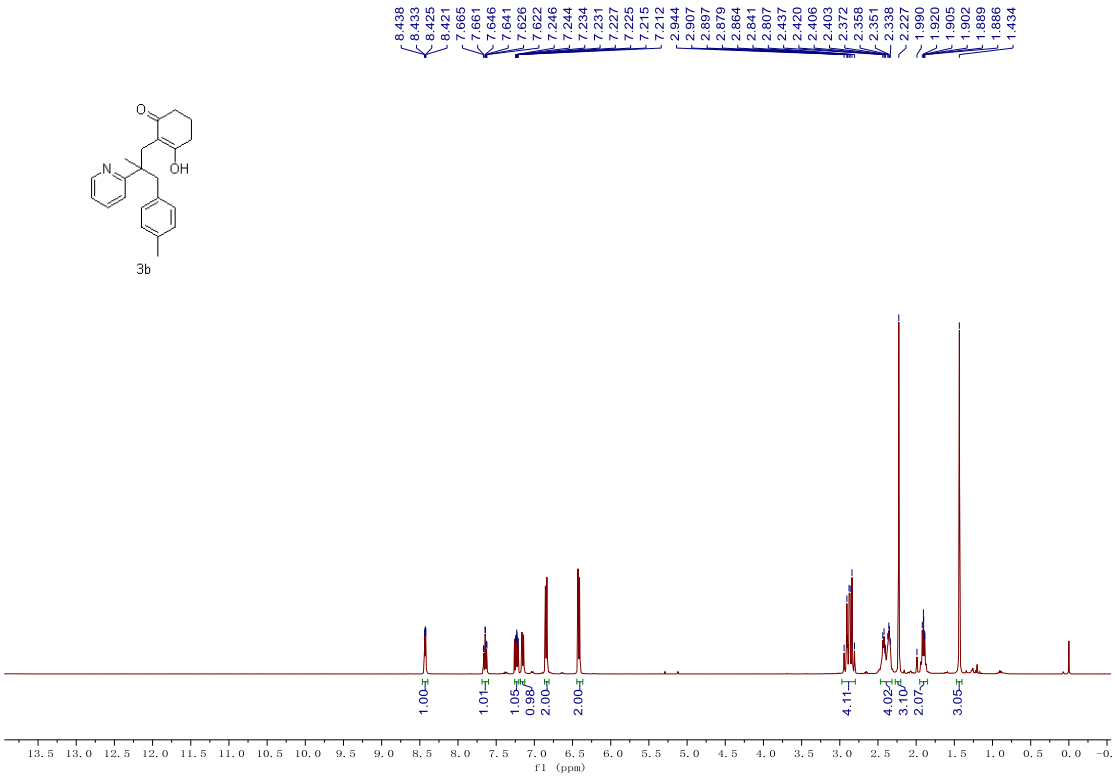
3-methyl-4-phenyl-3-(pyridin-2-yl)butanoic acid (**6**).

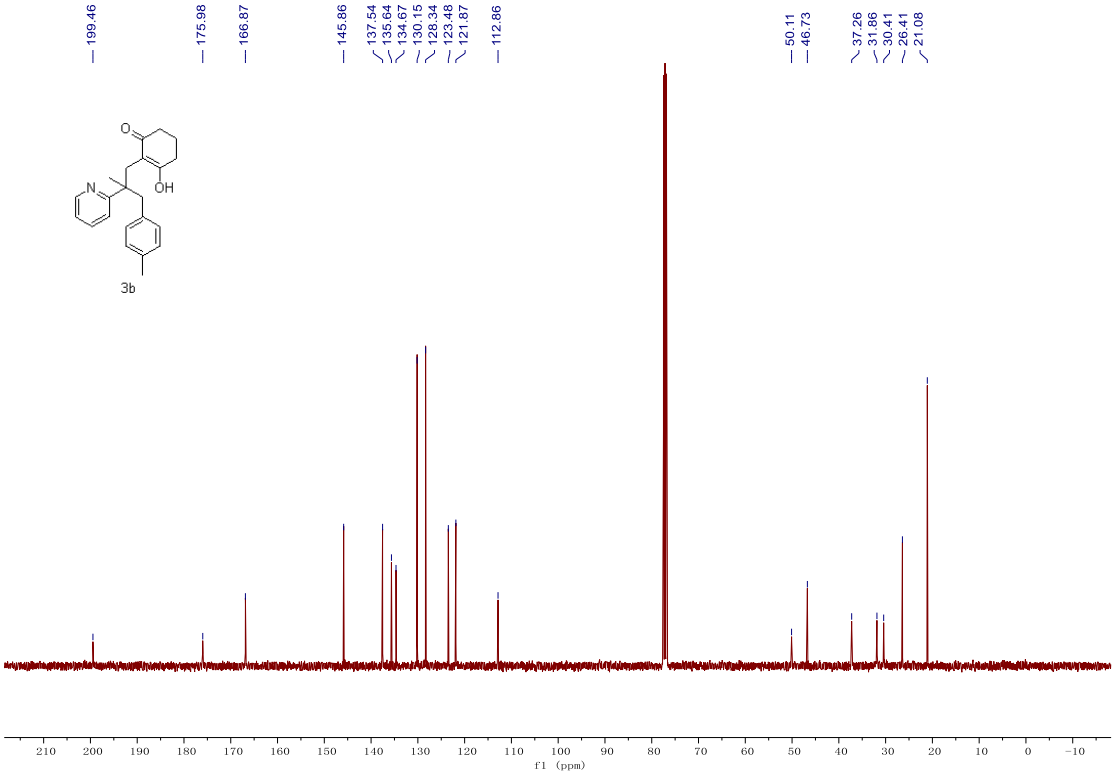
Yellow oil (22.9 mg, 90%), eluent: CH_2Cl_2/MeOH = 20:1. ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.88 (s, 1H), 8.60 – 8.31 (m, 1H), 7.59 (td, *J* = 7.7, 1.9 Hz, 1H), 7.17 – 7.10 (m, 2H), 7.08 – 7.01 (m, 3H), 6.69 – 6.60 (m, 2H), 3.03 – 3.00 (m, 1H), 2.93 – 2.85 (m, 2H), 2.50 – 2.46 (m, 1H), 1.33 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 173.3, 165.0, 146.3, 138.3, 136.4, 130.3, 127.9, 126.7, 122.7, 122.6, 53.4, 48.2, 47.2, 43.5, 26.2. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{16}H_{18}NO_2^+$ 256.1332, Found: 256.1328.

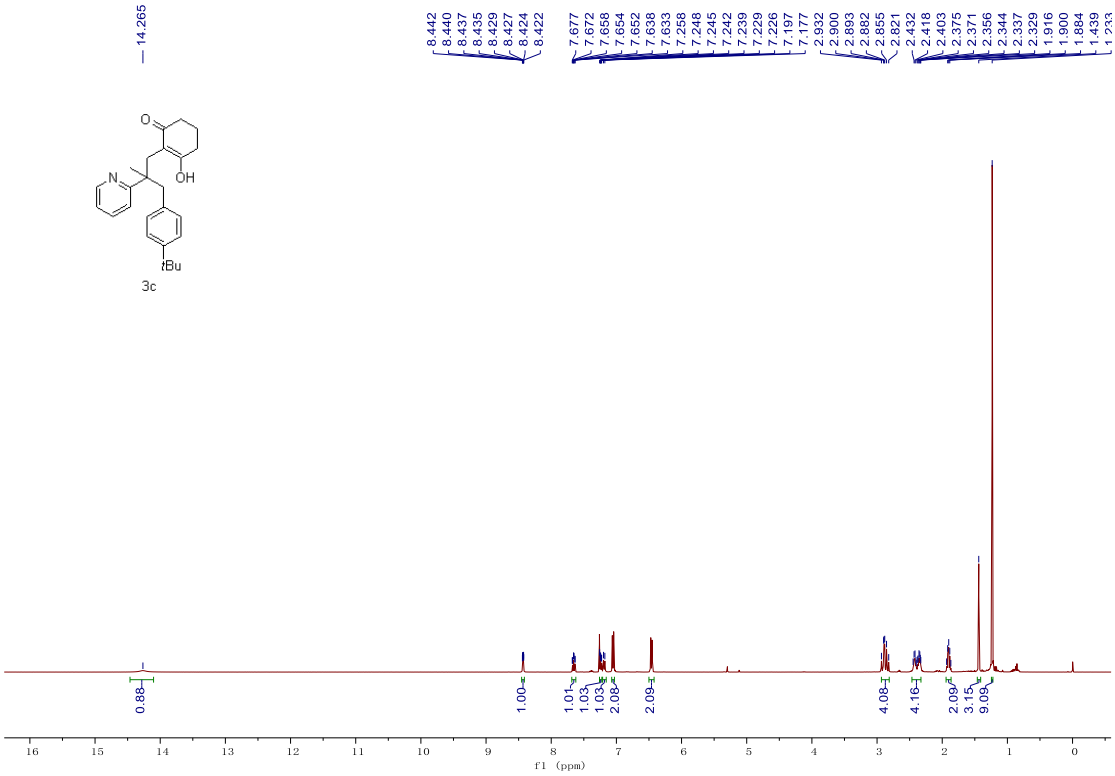
5. NMR Spectrum and NRMS Data

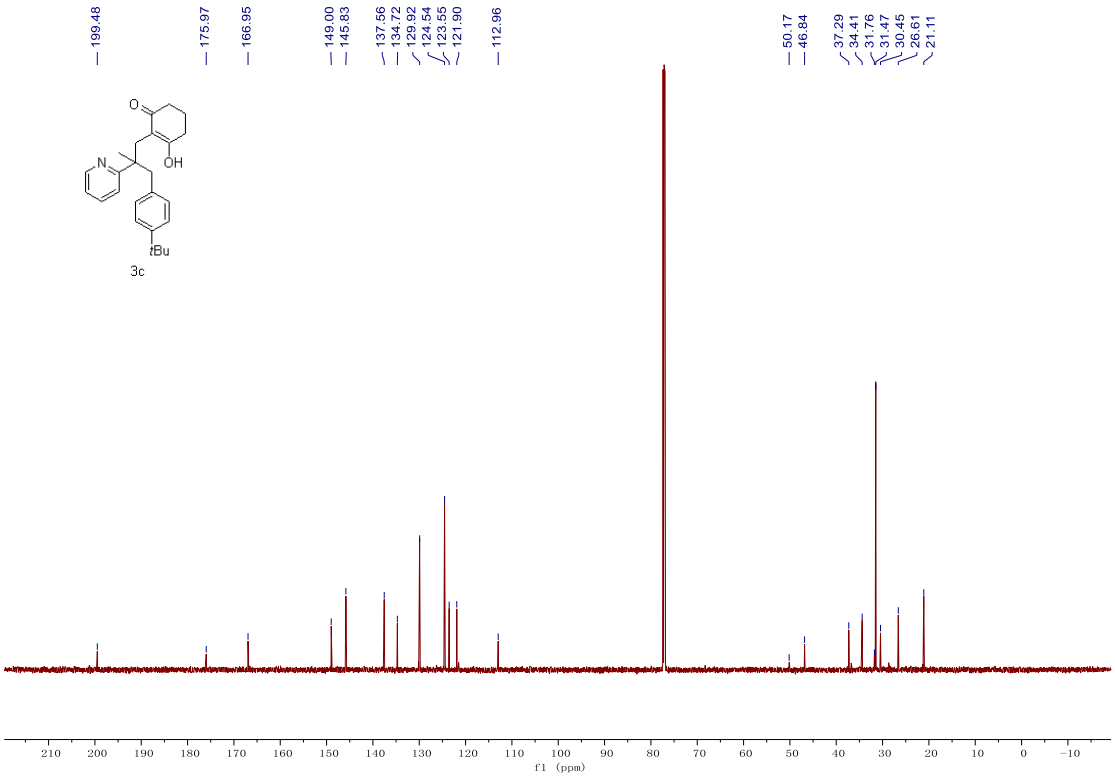


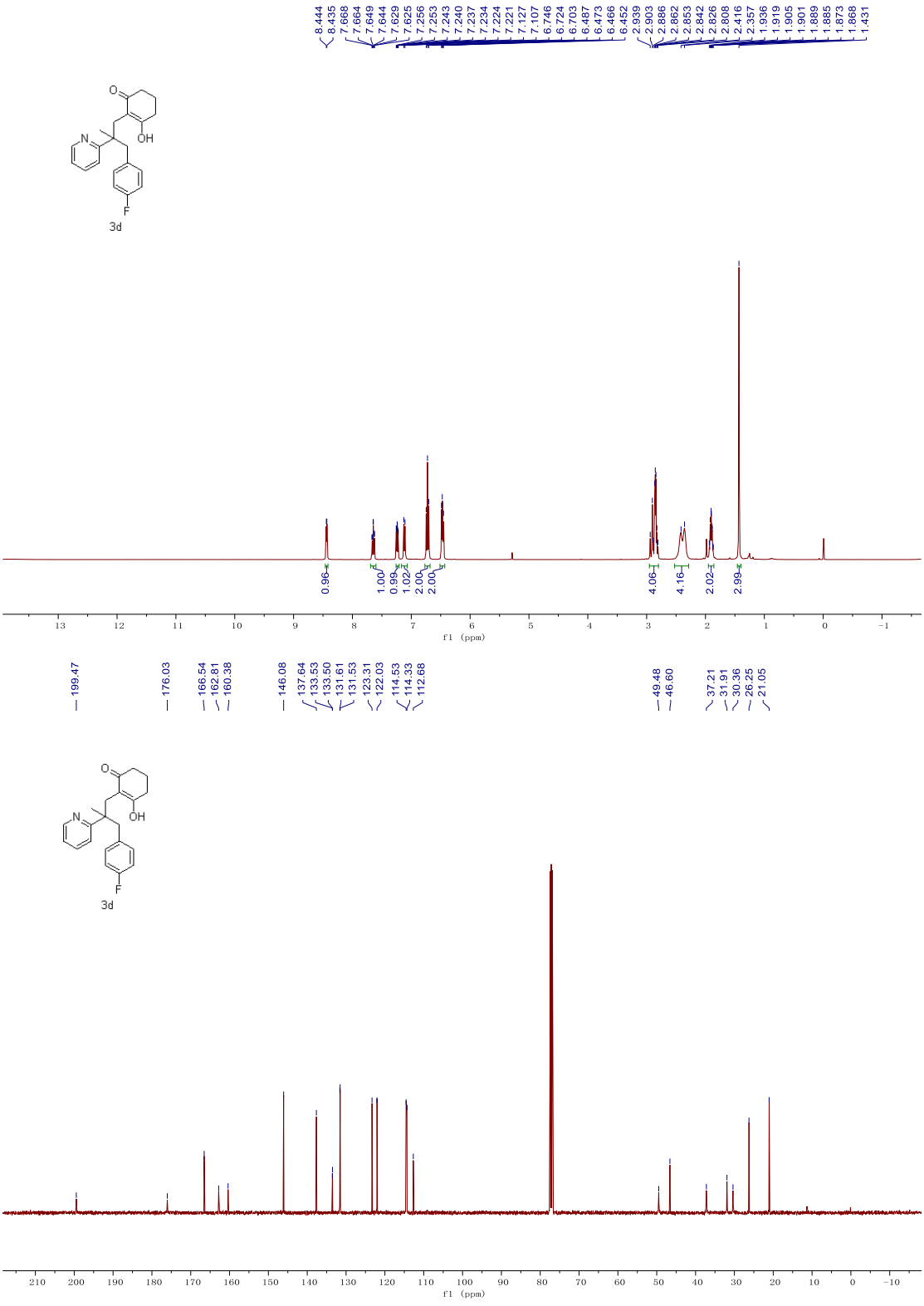


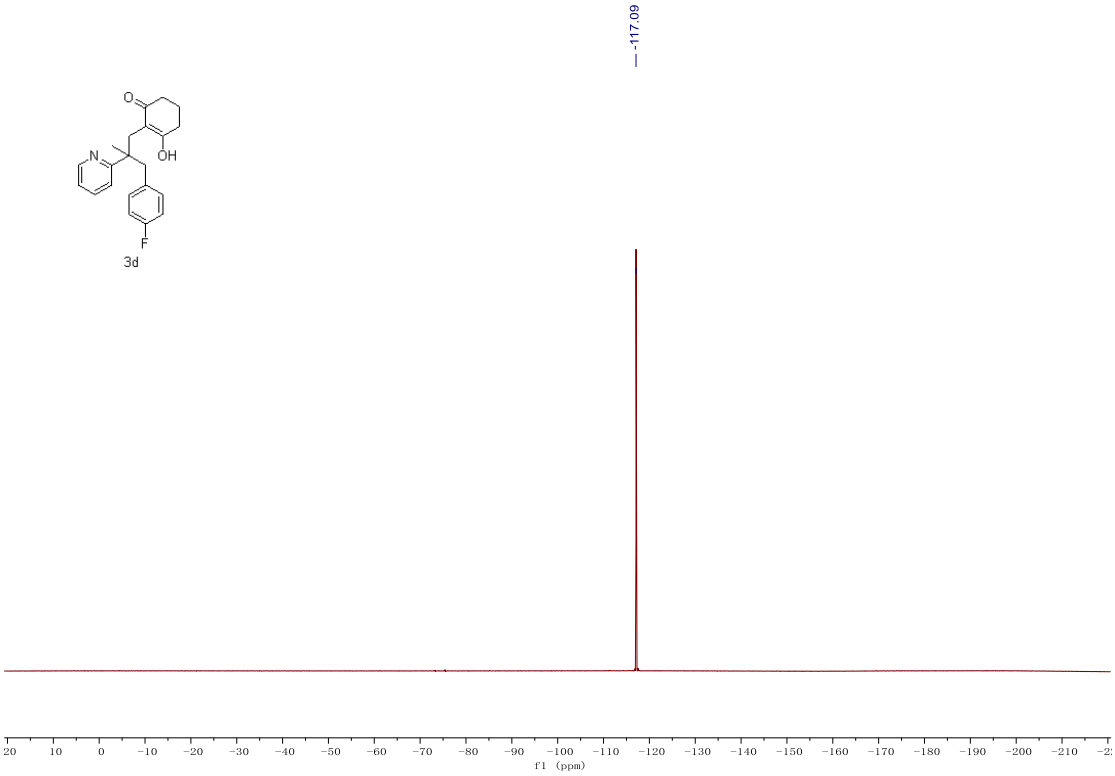

8.438
8.433
8.425
8.421
7.665
7.661
7.646
7.641
7.626
7.622
7.246
7.244
7.234
7.231
7.227
7.225
7.215
7.212
2.944
2.907
2.897
2.879
2.864
2.841
2.807
2.437
2.420
2.406
2.403
2.372
2.358
2.351
2.338
2.227
1.990
1.920
1.905
1.902
1.889
1.886
1.434
O
OH
N
3b
1.00
1.01
1.05
0.98
2.00
2.00
4.11
4.02
3.10
2.07
3.05
f1 (ppm)

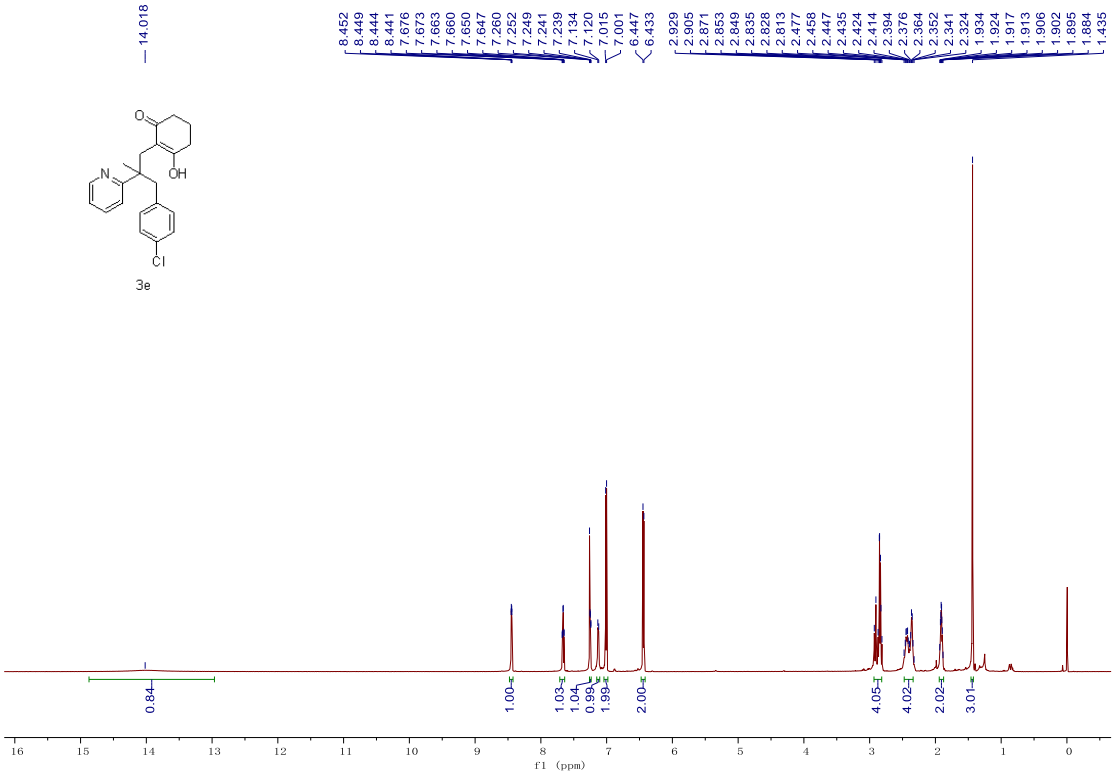

199.46
175.98
166.87
145.86
137.54
135.64
134.67
130.15
128.34
123.48
121.87
112.86
50.11
46.73
37.26
31.86
30.41
26.41
21.08
O
OH
N
3b
f1 (ppm)

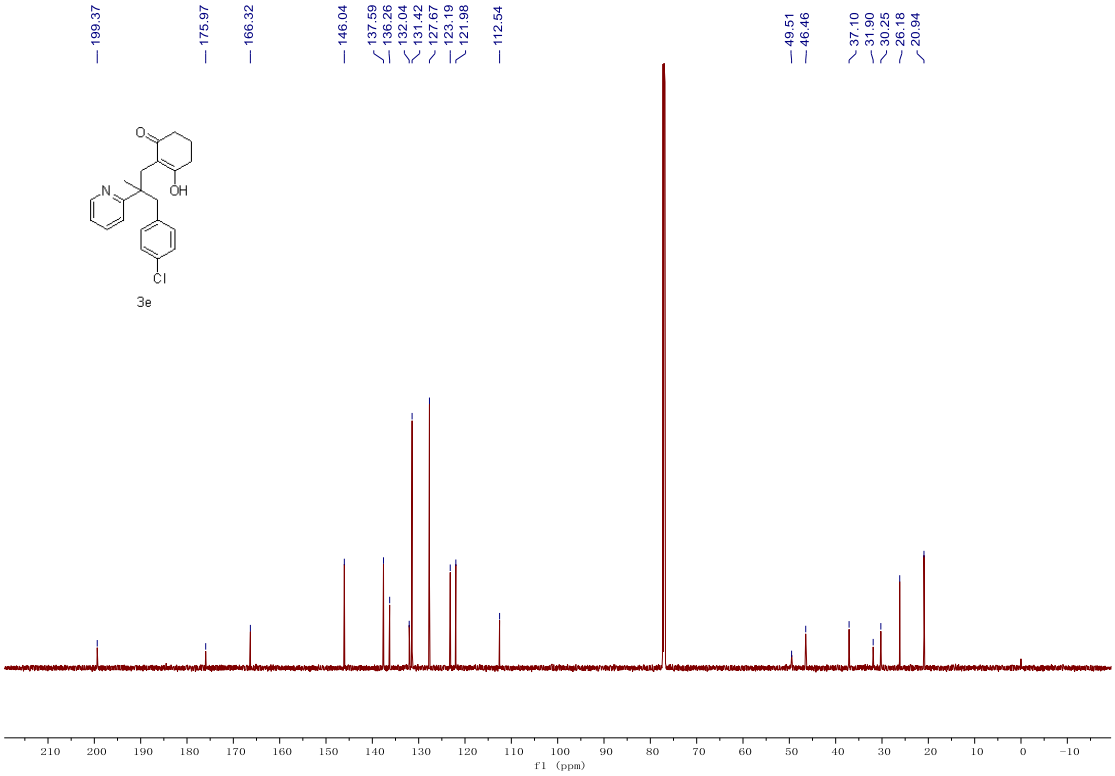

14.265
8.442
8.440
8.437
8.435
8.429
8.427
8.424
8.422
7.677
7.672
7.658
7.654
7.652
7.638
7.633
7.258
7.248
7.245
7.242
7.239
7.229
7.226
7.197
7.177
2.932
2.900
2.893
2.882
2.855
2.821
2.432
2.418
2.403
2.375
2.371
2.356
2.344
2.337
2.329
1.916
1.900
1.884
1.439
O
OH
N
tBu
3c
0.88
1.00
1.01
1.03
1.03
2.08
2.09
4.08
4.16
2.09
3.15
9.09
f1 (ppm)

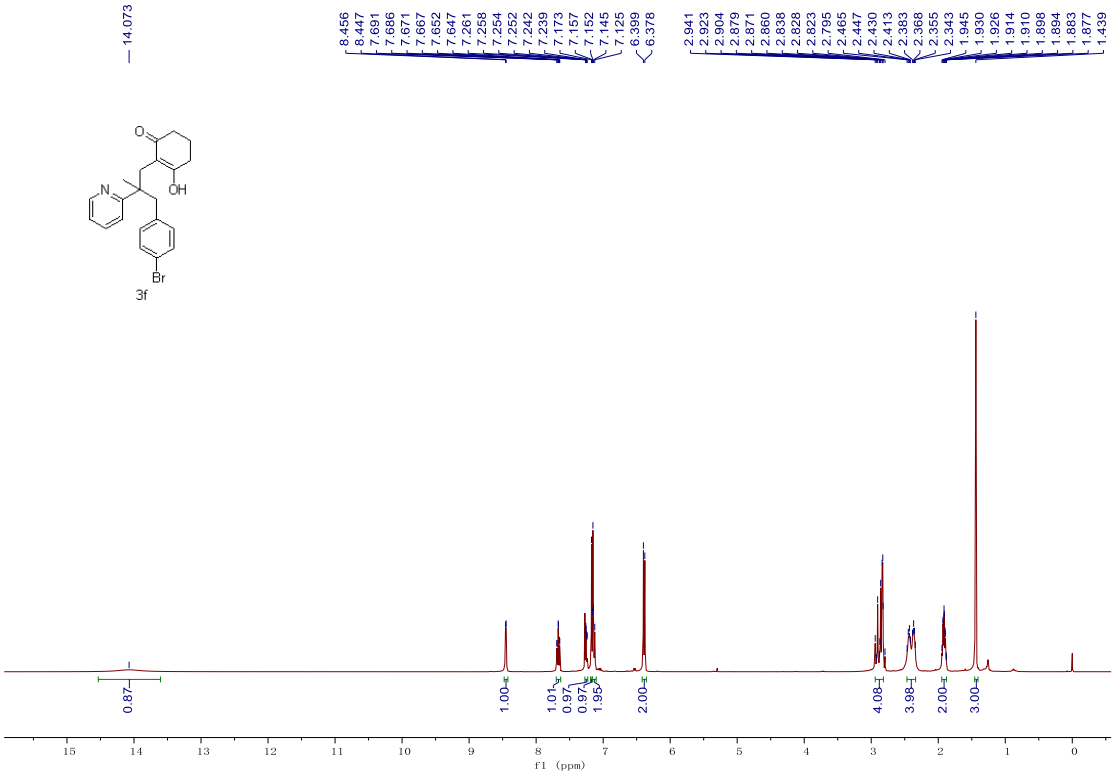

199.48
175.97
166.95
149.00
145.83
137.56
134.72
129.92
124.54
123.55
121.90
112.96
50.17
46.84
37.29
34.41
31.76
31.47
30.45
26.61
21.11
O
OH
N
tBu
3c
f1 (ppm)

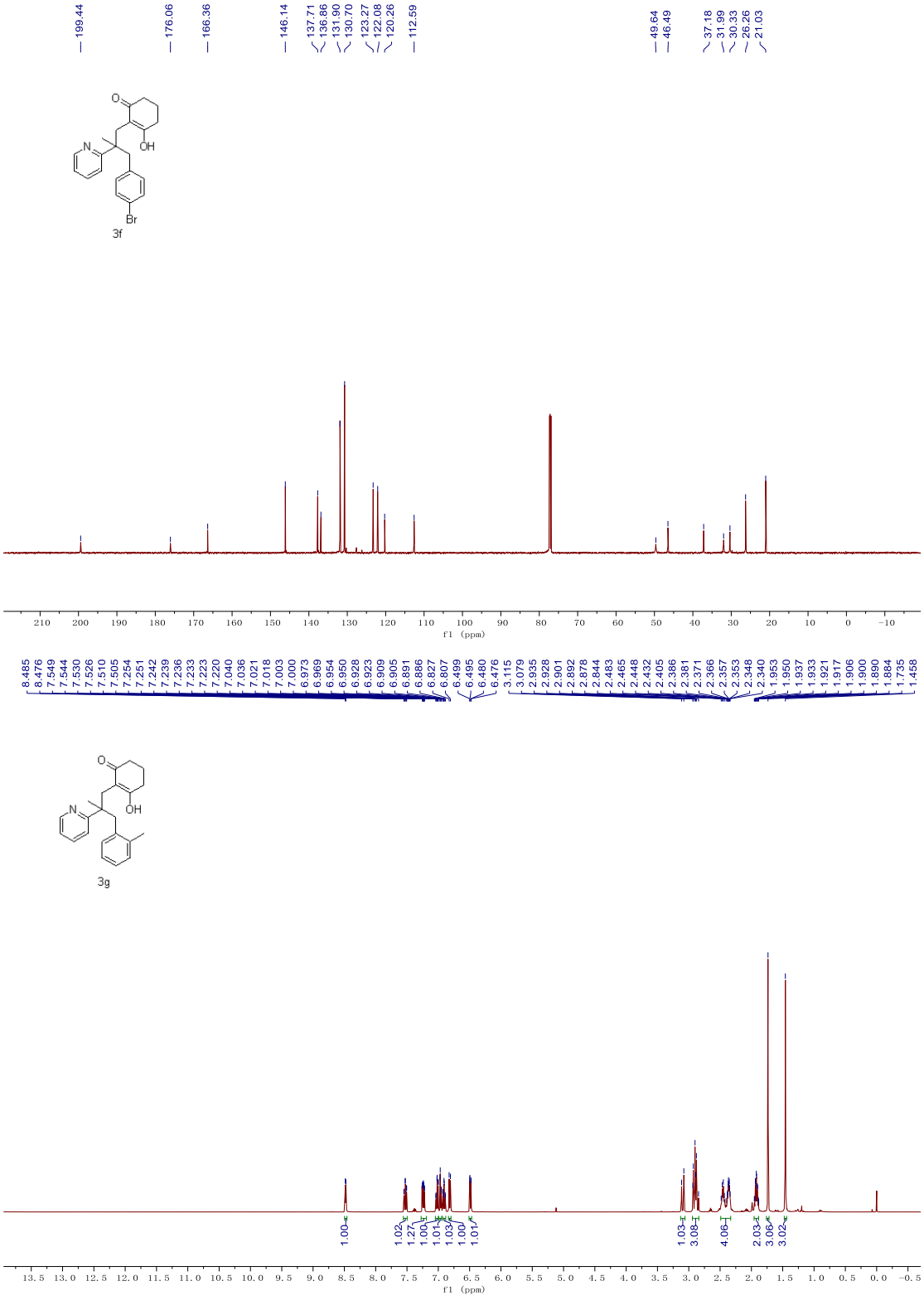

8.444
8.435
7.668
7.664
7.649
7.644
7.629
7.625
7.256
7.253
7.243
7.240
7.237
7.234
7.224
7.221
7.127
7.107
6.746
6.724
6.703
6.487
6.473
6.466
6.452
2.939
2.903
2.886
2.862
2.853
2.842
2.826
2.808
2.416
2.357
1.936
1.919
1.905
1.901
1.889
1.885
1.873
1.868
1.431
O
OH
N
F
3d
0.96
1.00
0.99
1.02
2.00
2.00
4.06
4.16
2.02
2.99
f1 (ppm)
199.47
176.03
166.54
162.81
160.38
146.08
137.64
133.53
133.50
131.61
131.53
123.31
122.03
114.53
114.33
112.68
49.48
46.60
37.21
31.91
30.36
26.25
21.05
f1 (ppm)

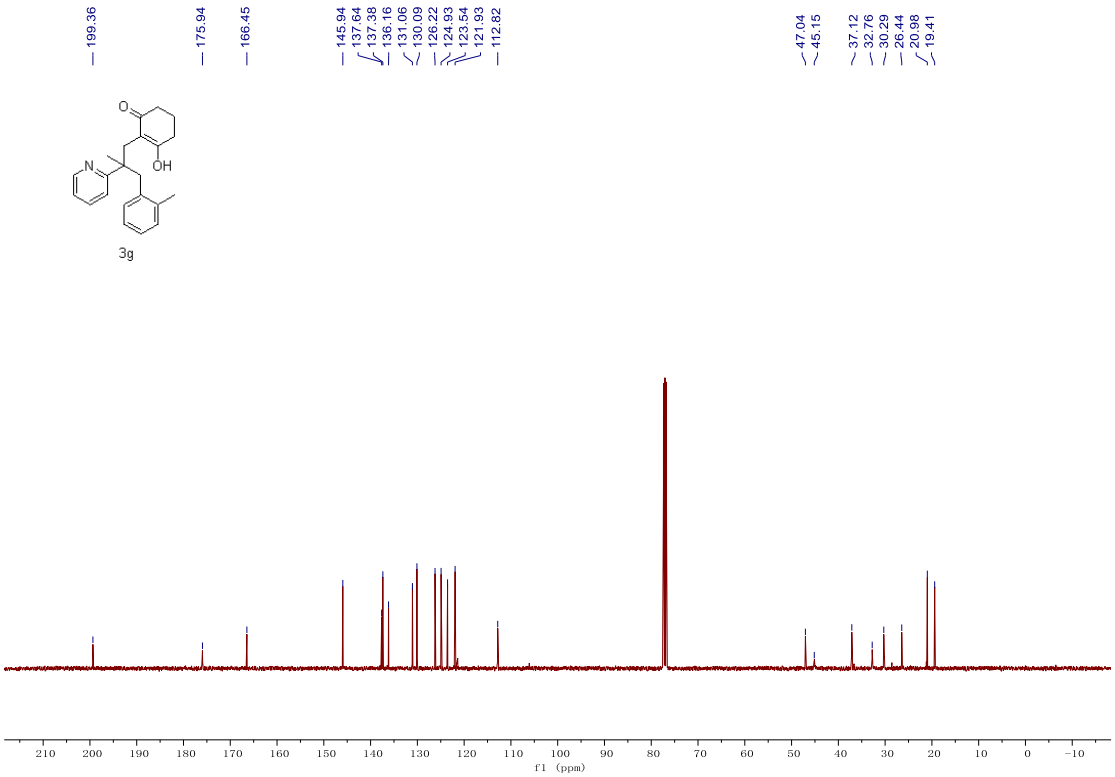

-117.09
O
OH
N
F
3d
f1 (ppm)

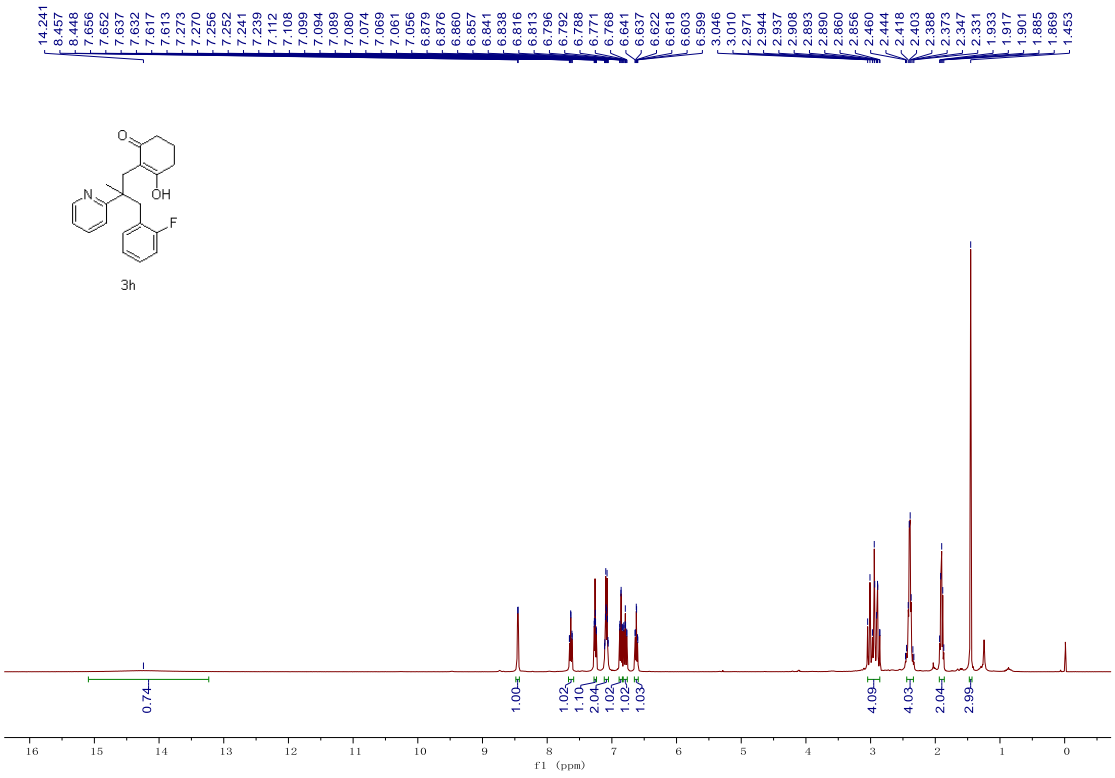

14.018
8.452
8.449
8.444
8.441
7.676
7.673
7.663
7.660
7.650
7.647
7.260
7.252
7.249
7.241
7.239
7.134
7.120
7.015
7.001
6.447
6.433
2.929
2.905
2.871
2.853
2.849
2.835
2.828
2.813
2.477
2.458
2.447
2.435
2.424
2.414
2.394
2.376
2.364
2.352
2.341
2.324
1.934
1.924
1.917
1.913
1.906
1.902
1.895
1.884
1.435
O
OH
N
Cl
3e
0.84
1.00
1.03
1.04
0.99
1.99
2.00
4.05
4.02
2.02
3.01
f1 (ppm)

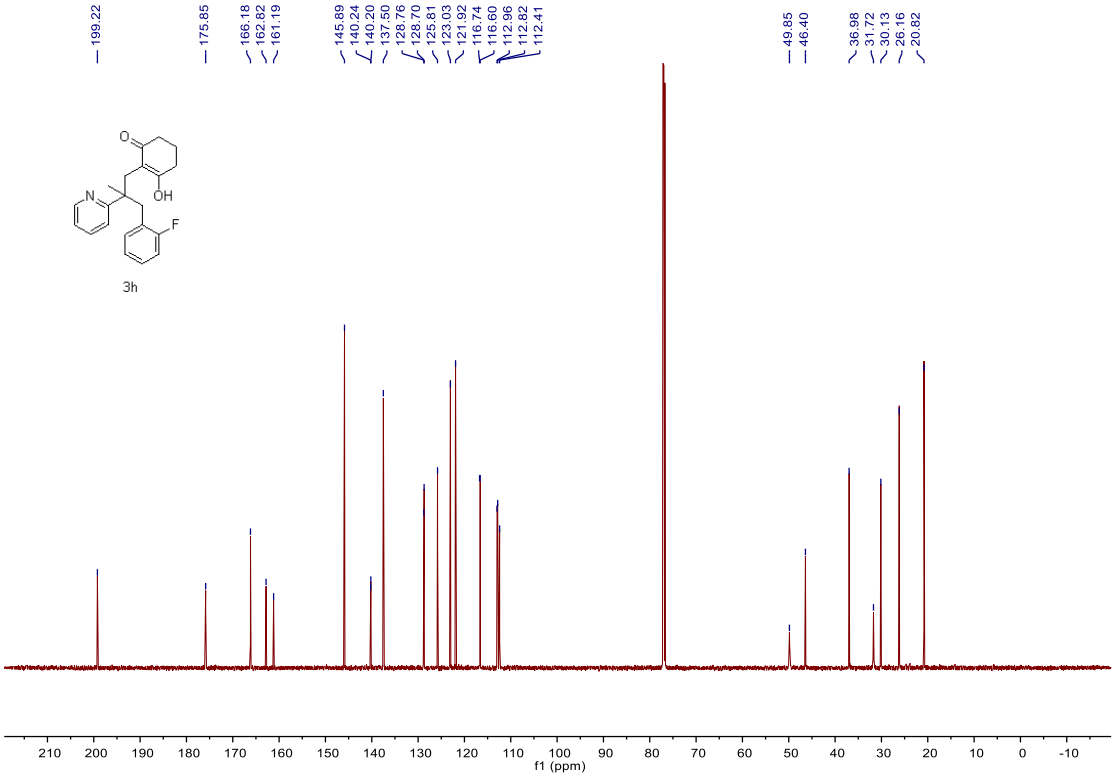

199.37
175.97
166.32
146.04
137.59
136.26
132.04
131.42
127.67
123.19
121.98
112.54
49.51
46.46
37.10
31.90
30.25
26.18
20.94
O
OH
N
Cl
3e
f1 (ppm)

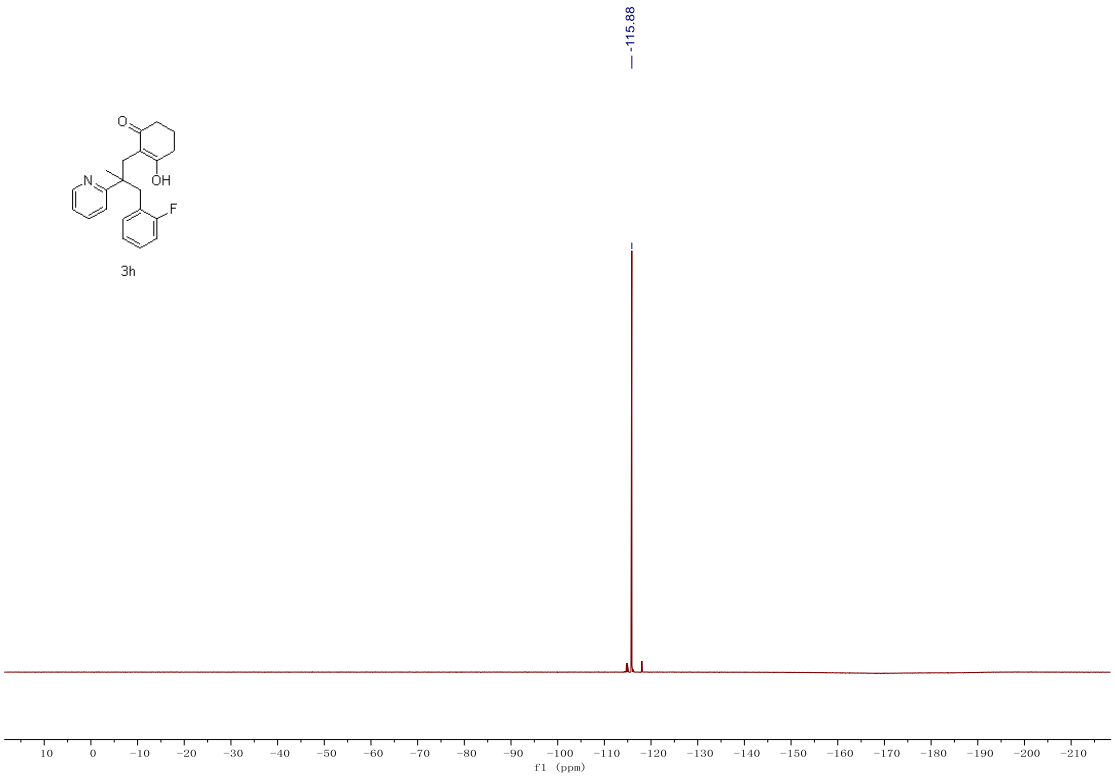

14.073
8.456
8.447
7.691
7.686
7.671
7.667
7.652
7.647
7.261
7.258
7.254
7.252
7.242
7.239
7.173
7.157
7.152
7.145
7.125
6.399
6.378
2.941
2.923
2.904
2.879
2.871
2.860
2.838
2.828
2.823
2.795
2.465
2.447
2.430
2.413
2.383
2.368
2.355
2.343
1.945
1.930
1.926
1.914
1.910
1.898
1.894
1.883
1.877
1.439
O
OH
N
Br
3f
0.87
1.00
1.01
0.97
0.97
1.95
2.00
4.08
3.98
2.00
3.00
f1 (ppm)

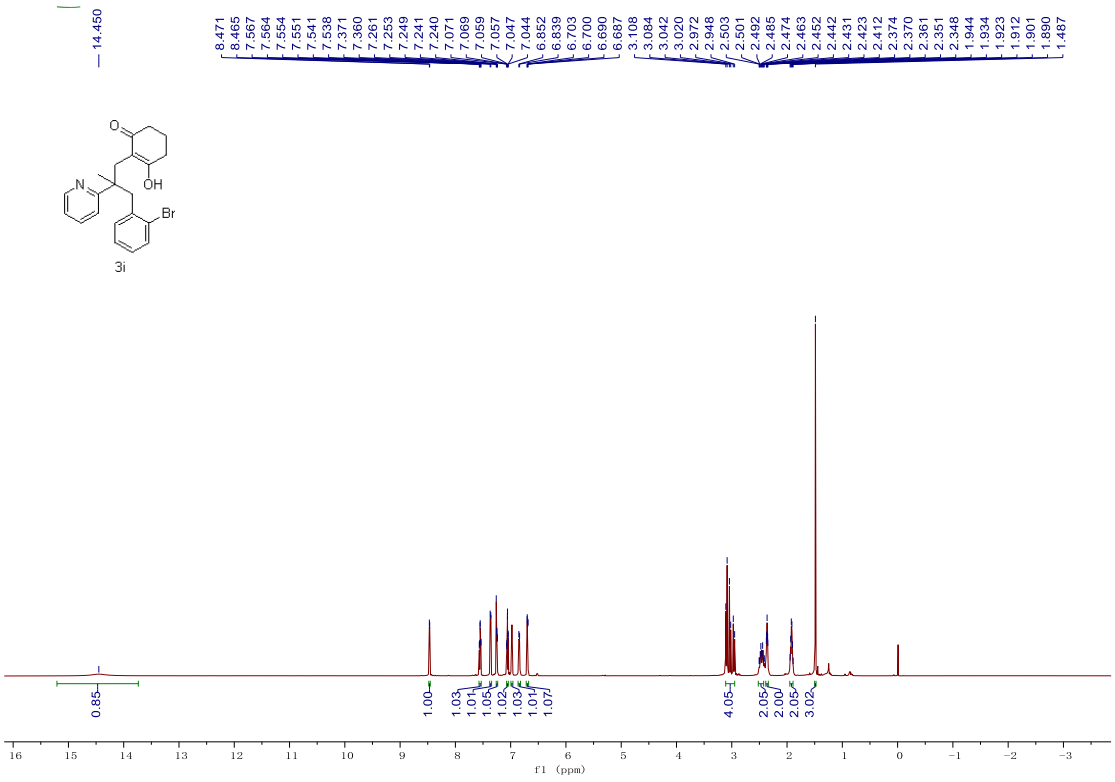

199.44
176.06
166.36
146.14
137.71
136.86
131.90
130.70
123.27
122.08
120.26
112.59
49.64
46.49
37.18
31.99
30.33
26.26
21.03
O
OH
N
Br
3f
f1 (ppm)
8.485
8.476
7.549
7.544
7.530
7.526
7.510
7.505
7.254
7.251
7.242
7.239
7.236
7.233
7.223
7.220
7.040
7.036
7.021
7.018
7.003
7.000
6.973
6.969
6.954
6.950
6.928
6.923
6.909
6.905
6.891
6.886
6.827
6.807
6.499
6.495
6.480
6.476
3.115
3.079
2.935
2.928
2.901
2.892
2.878
2.844
2.483
2.465
2.448
2.432
2.405
2.386
2.381
2.371
2.366
2.357
2.353
2.348
2.340
1.953
1.950
1.937
1.933
1.921
1.917
1.906
1.900
1.890
1.884
1.736
1.458
O
OH
N
3g
1.00
1.02
1.27
1.00
1.01
1.03
1.00
1.01
1.03
3.08
4.06
2.03
3.06
3.02
f1 (ppm)

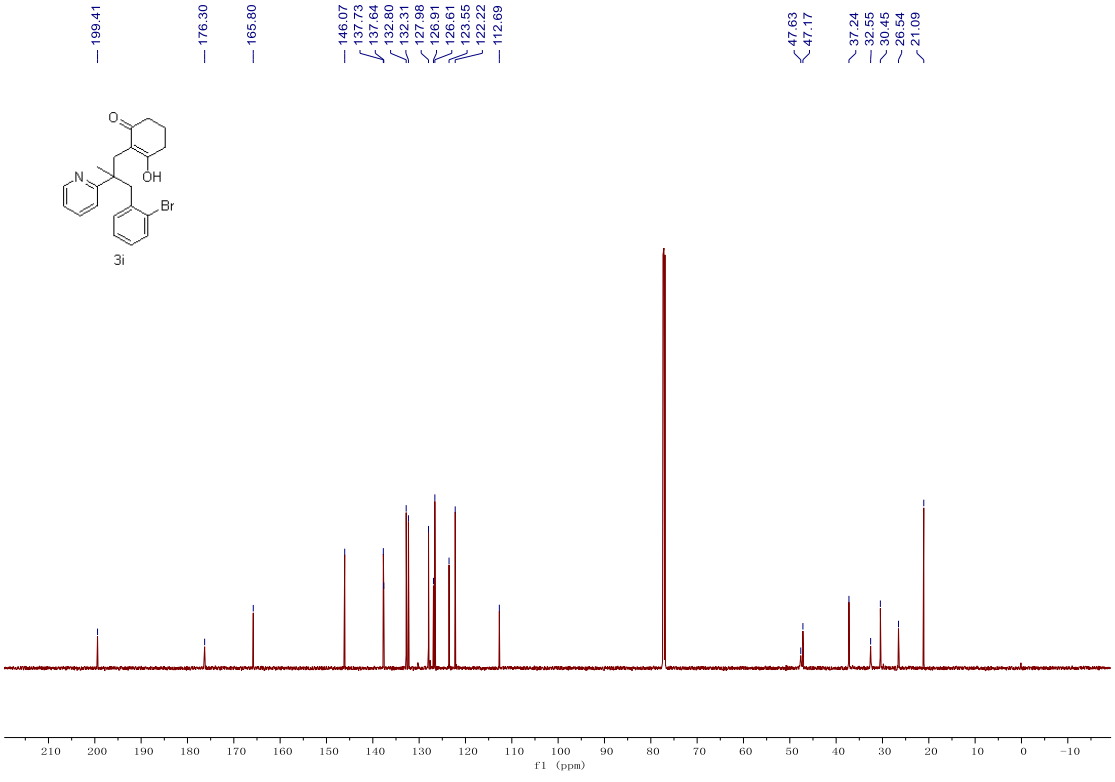

199.36
175.94
166.45
145.94
137.64
137.38
136.16
131.06
130.09
126.22
124.93
123.54
121.93
112.82
47.04
45.15
37.12
32.76
30.29
26.44
20.98
19.41
O
N
OH
3g
f1 (ppm)

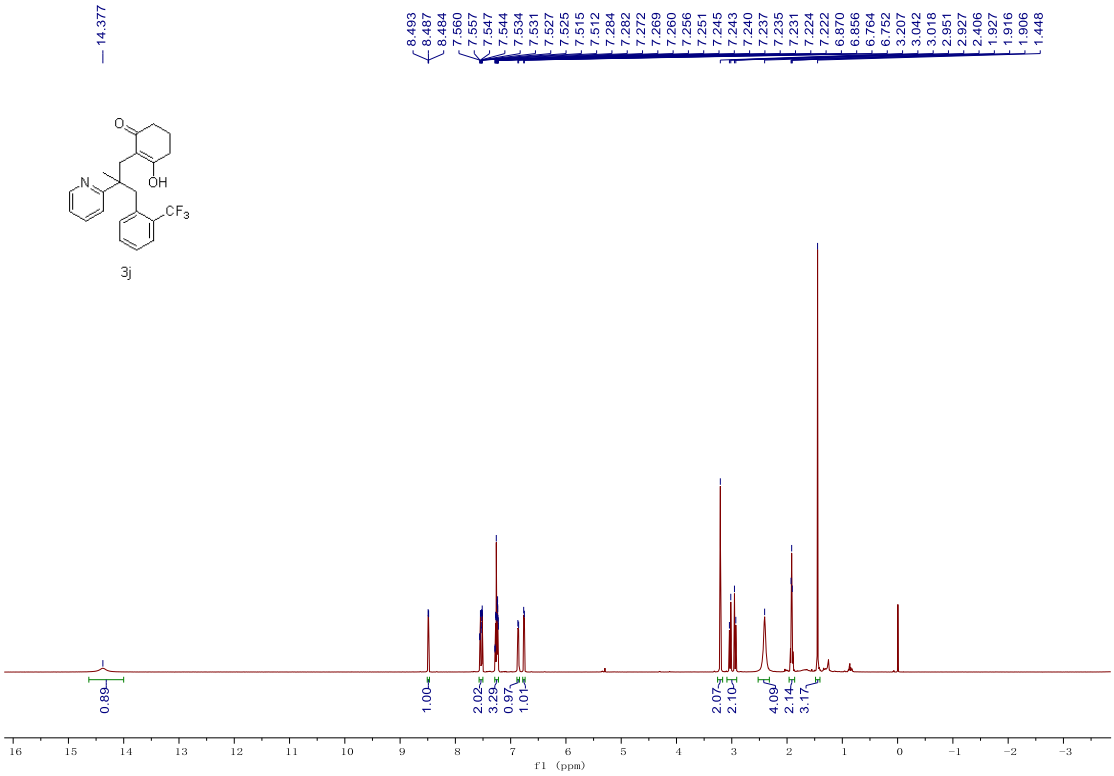

14.241
8.457
8.448
7.656
7.652
7.637
7.632
7.617
7.613
7.273
7.270
7.256
7.252
7.241
7.239
7.112
7.108
7.099
7.094
7.089
7.080
7.074
7.069
7.061
7.056
6.879
6.876
6.860
6.857
6.841
6.838
6.816
6.813
6.796
6.792
6.788
6.771
6.768
6.641
6.637
6.622
6.618
6.603
6.599
3.046
3.010
2.971
2.944
2.937
2.908
2.893
2.890
2.860
2.856
2.460
2.444
2.418
2.403
2.388
2.373
2.347
2.331
1.933
1.917
1.901
1.885
1.869
1.453
O
N
OH
F
3h
0.74
1.00
1.02
1.10
2.04
1.02
1.02
1.03
4.09
4.03
2.04
2.99
f1 (ppm)

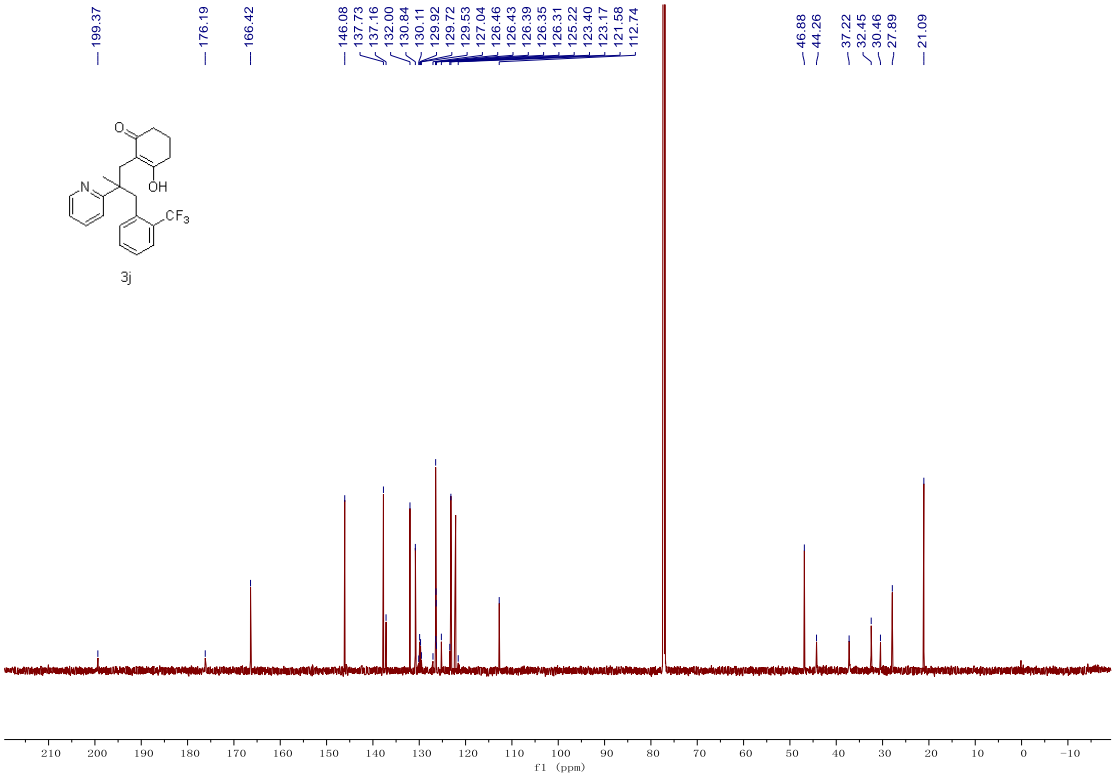

199.22
175.85
166.18
162.82
161.19
145.89
140.24
140.20
137.50
128.76
128.70
125.81
123.03
121.92
116.74
116.60
112.96
112.82
112.41
49.85
46.40
36.98
31.72
30.13
26.16
20.82
O
OH
N
F
3h
f1 (ppm)

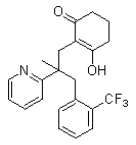

-115.88
O
OH
N
F
3h
f1 (ppm)


14.450
8.471
8.465
7.567
7.564
7.554
7.551
7.541
7.538
7.371
7.360
7.261
7.253
7.249
7.241
7.240
7.071
7.069
7.059
7.057
7.047
7.044
6.852
6.839
6.703
6.700
6.690
6.687
3.108
3.084
3.042
3.020
2.972
2.948
2.503
2.501
2.492
2.485
2.474
2.463
2.452
2.442
2.431
2.423
2.412
2.374
2.370
2.361
2.351
2.348
1.944
1.934
1.923
1.912
1.901
1.890
1.487
O
OH
N
Br
3i
0.85
1.00
1.03
1.01
1.05
1.02
1.03
1.01
1.07
4.05
2.05
2.00
2.05
3.02
f1 (ppm)


199.41
176.30
165.80
146.07
137.73
137.64
132.80
132.31
127.98
126.91
126.61
123.55
122.22
112.69
47.63
47.17
37.24
32.55
30.45
26.54
21.09
O
OH
N
Br
3i
f1 (ppm)


14.377
8.493
8.487
8.484
7.560
7.557
7.547
7.544
7.534
7.531
7.527
7.525
7.515
7.512
7.284
7.282
7.272
7.269
7.260
7.256
7.251
7.245
7.243
7.240
7.237
7.235
7.231
7.224
7.222
6.870
6.856
6.764
6.752
3.207
3.042
3.018
2.951
2.927
2.406
1.927
1.916
1.906
1.448
O
OH
N
CF3
3j
0.89
1.00
2.02
3.29
0.97
1.01
2.07
2.10
4.09
2.14
3.17
f1 (ppm)

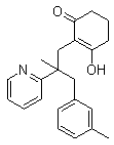

199.37
176.19
166.42
146.08
137.73
137.16
132.00
130.84
130.11
129.92
129.72
129.53
127.04
126.46
126.43
126.39
126.35
126.31
125.22
123.40
123.17
121.58
112.74
46.88
44.26
37.22
32.45
30.46
27.89
21.09
O
OH
N
CF3
3j
f1 (ppm)



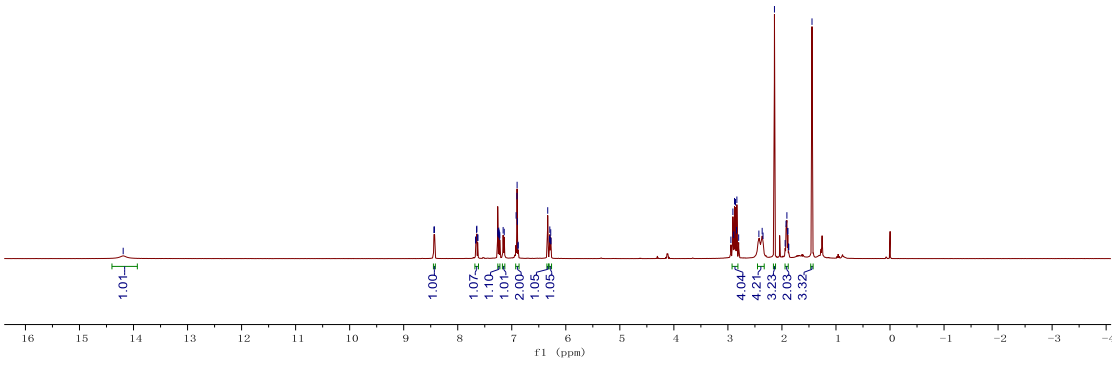
3j

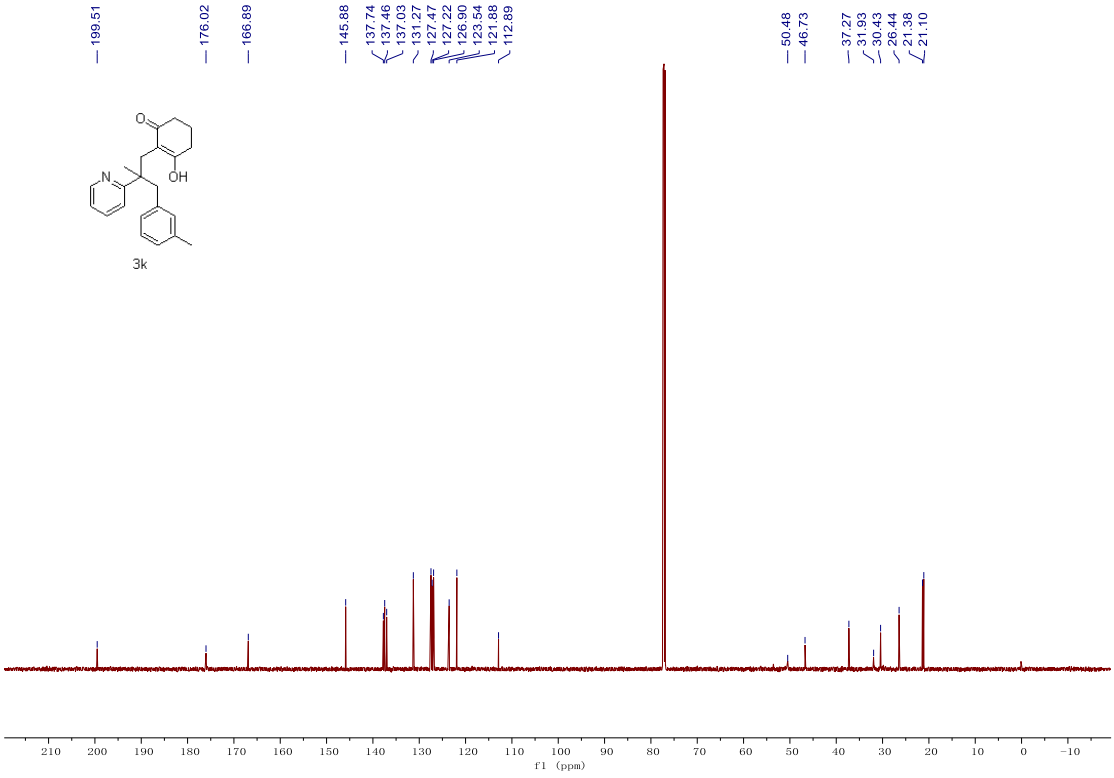
-58.44
f1 (ppm)


14.191
8.441
8.430
7.671
7.666
7.651
7.646
7.631
7.627
7.257
7.253
7.243
7.241
7.237
7.235
7.225
7.222
7.160
7.139
6.920
6.904
6.901
6.897
6.886
6.881
6.335
6.301
6.296
6.291
6.284
6.279
6.274
2.944
2.908
2.892
2.877
2.859
2.841
2.834
2.801
2.427
2.366
2.350
2.138
1.941
1.924
1.908
1.894
1.890
1.878
1.874
1.444

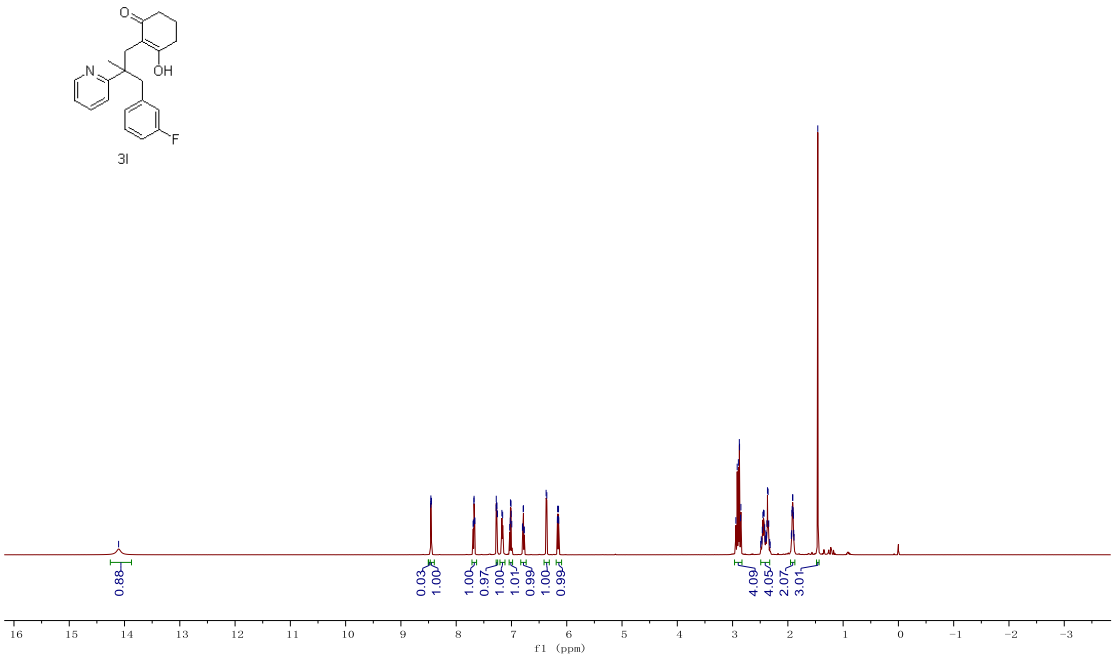


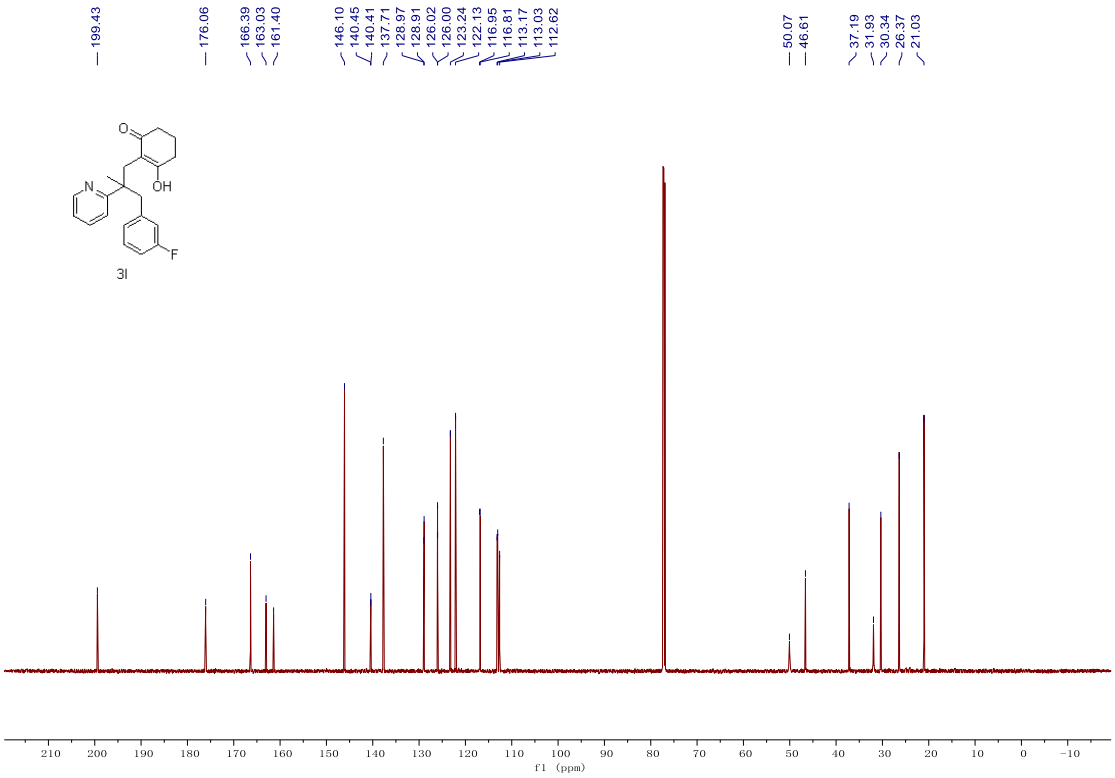
3k

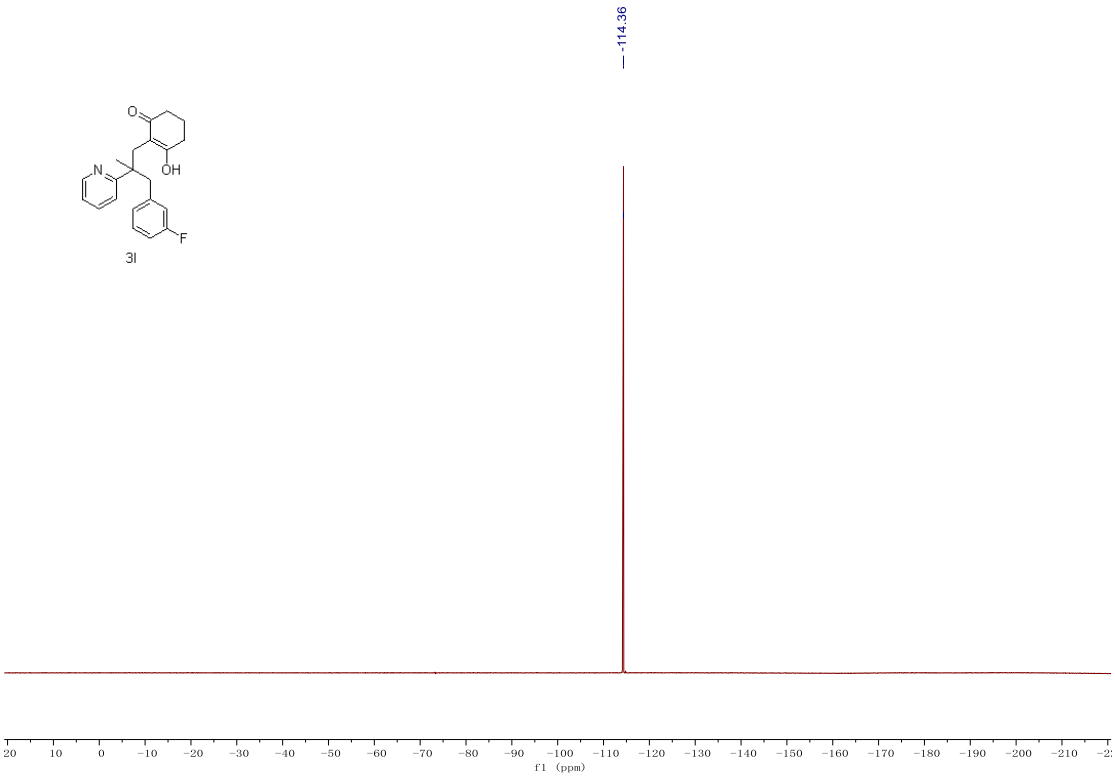

1.01
1.00
1.07
1.10
1.01
2.00
1.05
1.05
4.04
4.21
3.23
2.03
3.32
f1 (ppm)

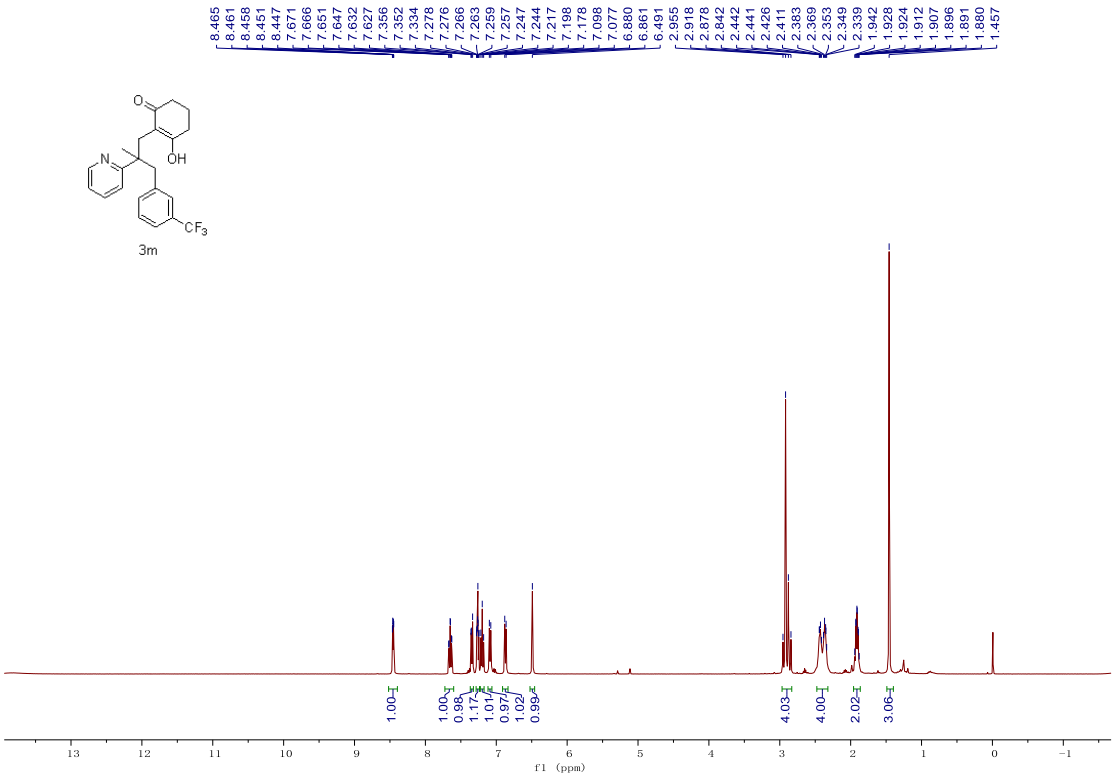

199.51
176.02
166.89
145.88
137.74
137.46
137.03
131.27
127.47
127.22
126.90
123.54
121.88
112.89
50.48
46.73
37.27
31.93
30.43
26.44
21.38
21.10
O
OH
N
3k
f1 (ppm)

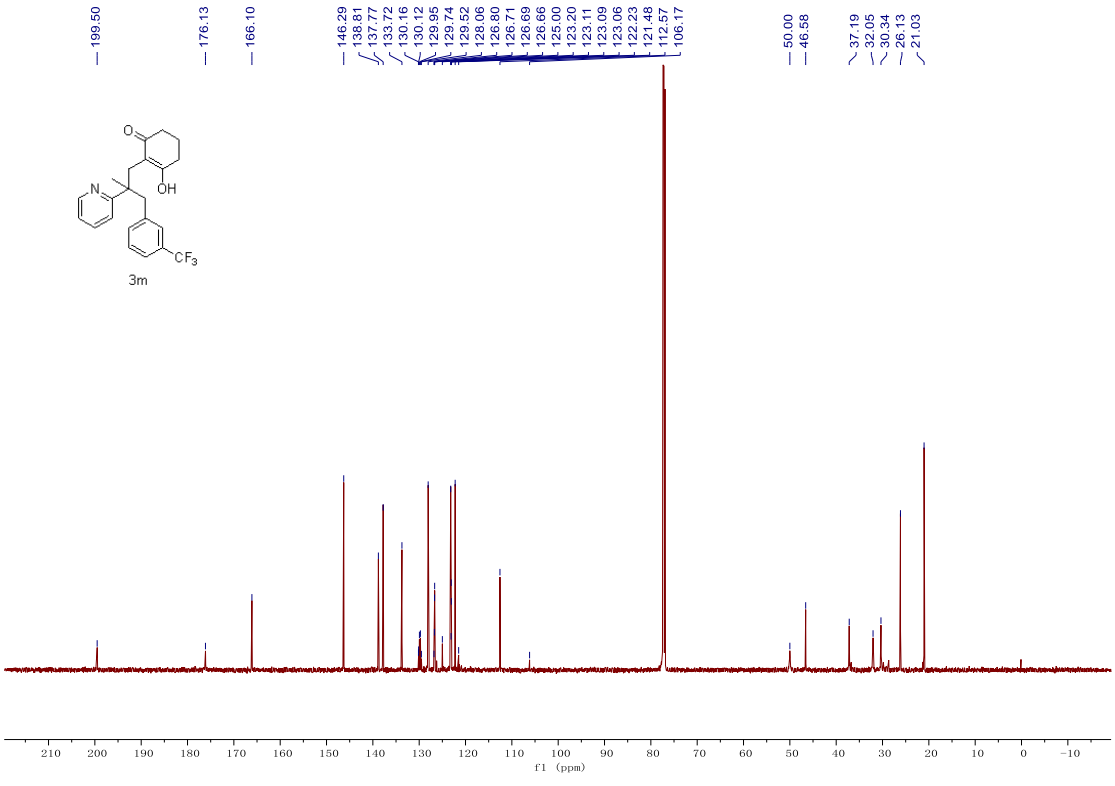

8.461
8.458
8.452
8.449
7.692
7.689
7.679
7.676
7.666
7.663
7.277
7.275
7.268
7.264
7.256
7.255
7.173
7.160
7.032
7.021
7.018
7.008
7.005
6.995
6.802
6.797
6.787
6.783
6.773
6.769
6.373
6.360
6.169
6.166
6.162
6.152
6.149
6.145
2.941
2.916
2.895
2.878
2.874
2.856
2.850
2.481
2.470
2.462
2.452
2.440
2.429
2.419
2.410
2.408
2.399
2.390
2.385
2.380
2.369
2.358
2.346
1.937
1.932
1.926
1.921
1.916
1.910
1.905
1.899
1.894
1.888
1.459

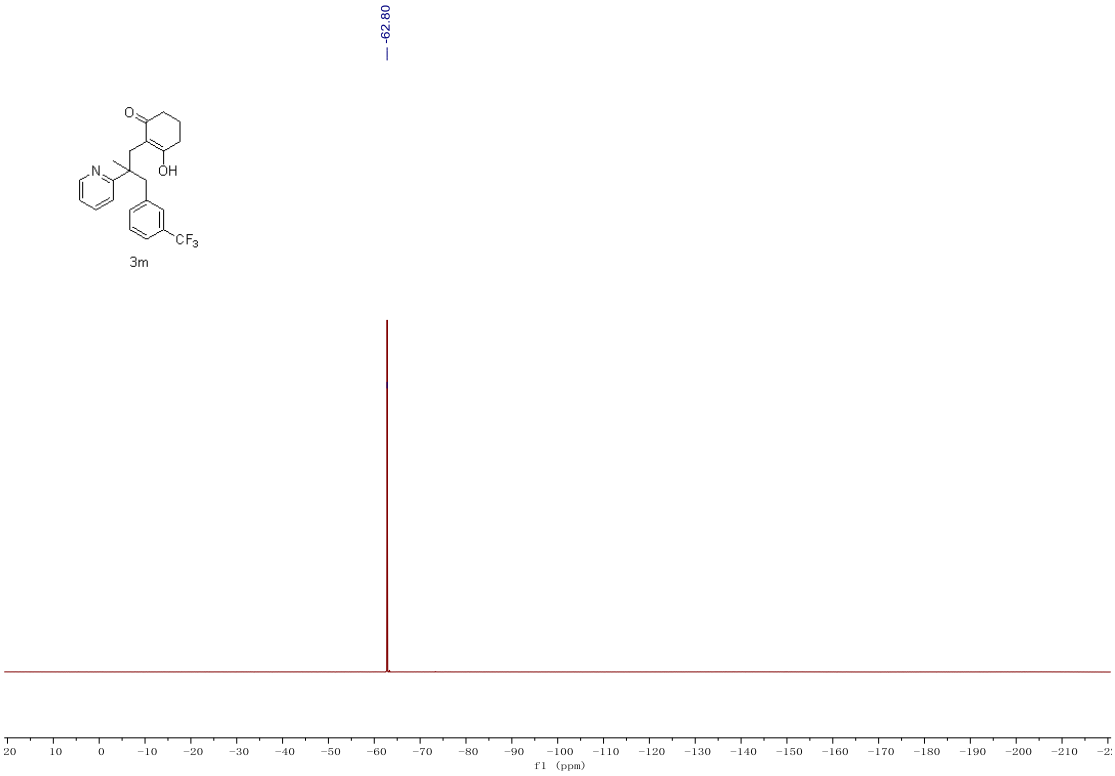

O
OH
N
F
3l
0.88
0.03
1.00
1.00
0.97
1.00
1.01
0.99
1.00
0.99
4.09
4.05
2.07
3.01
f1 (ppm)

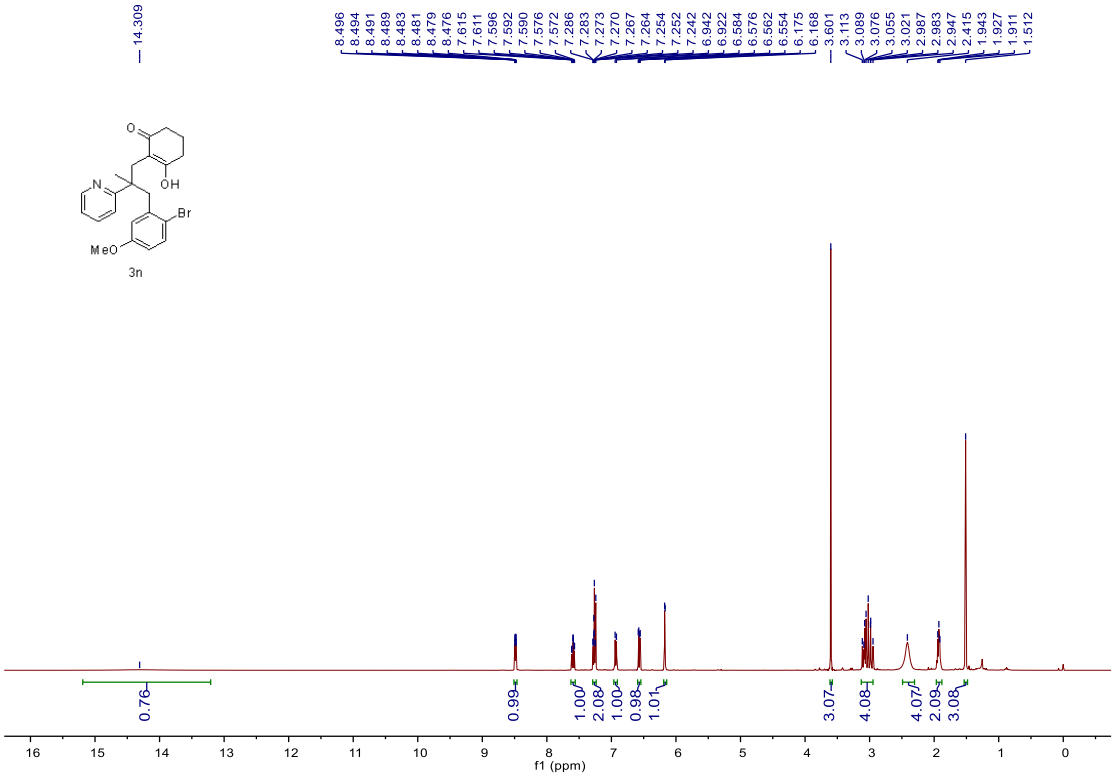

199.43
176.06
166.39
163.03
161.40
146.10
140.45
140.41
137.71
128.97
128.91
126.02
126.00
123.24
122.13
116.95
116.81
113.17
113.03
112.62
50.07
46.61
37.19
31.93
30.34
26.37
21.03
O
OH
N
F
3l
f1 (ppm)

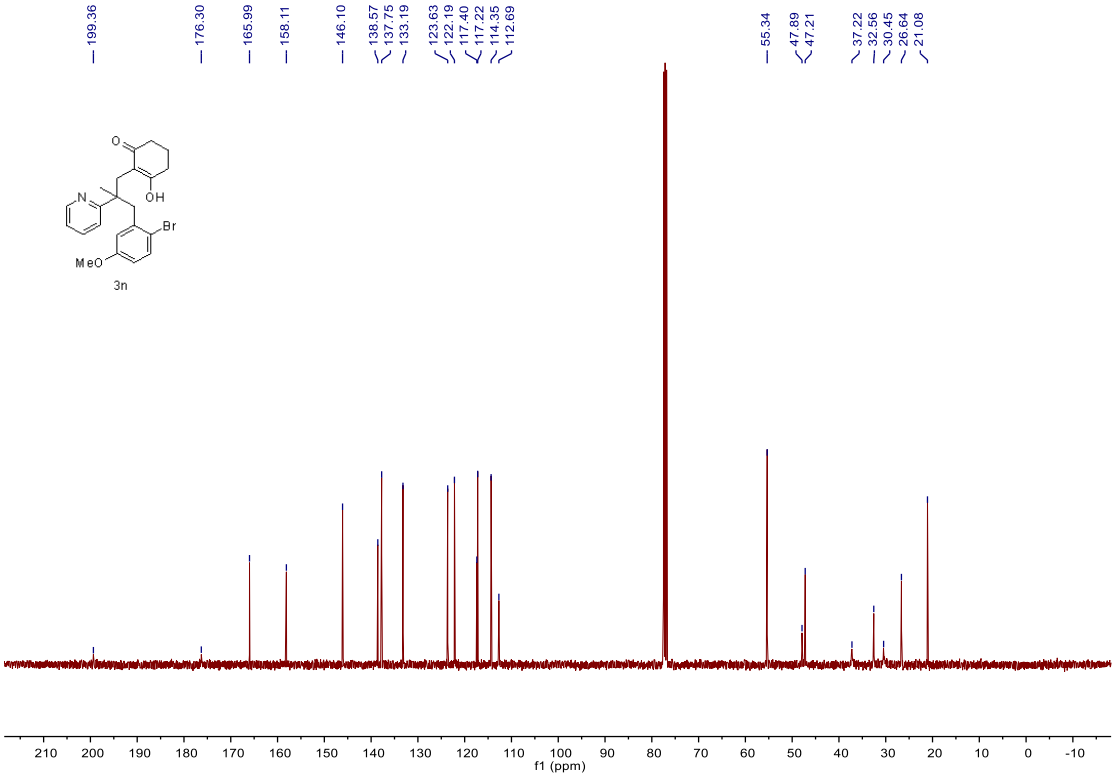

-114.36
O
OH
N
F
3l
f1 (ppm)

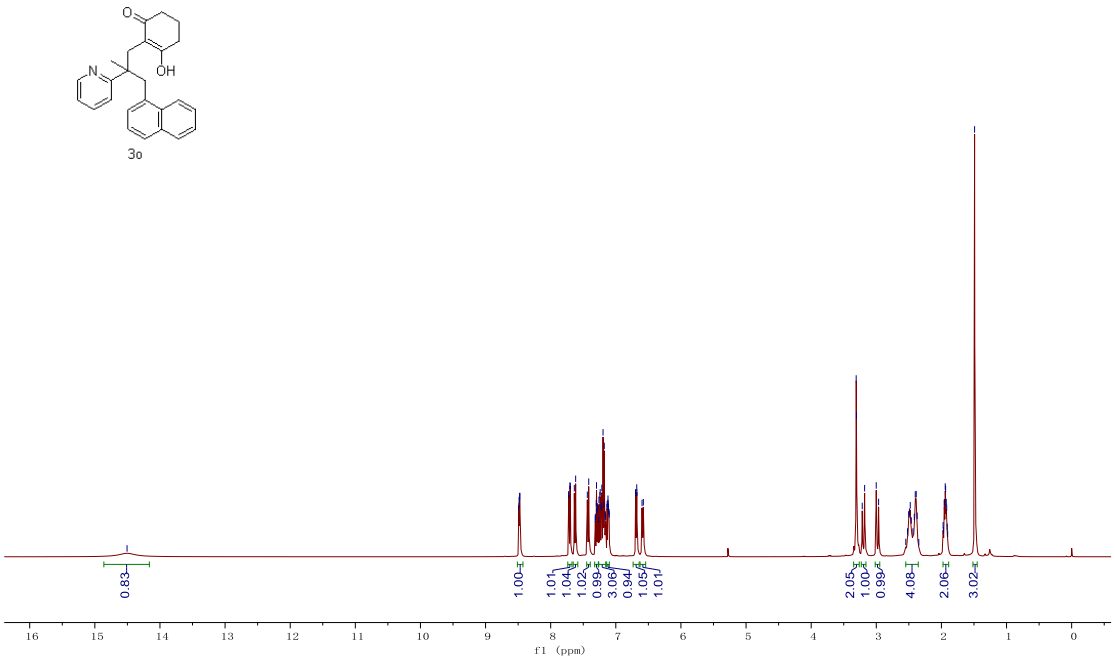

8.465
8.461
8.458
8.451
8.447
7.671
7.666
7.651
7.647
7.632
7.627
7.356
7.352
7.334
7.278
7.276
7.266
7.263
7.259
7.257
7.247
7.244
7.217
7.198
7.178
7.098
7.077
6.880
6.861
6.491
2.955
2.918
2.878
2.842
2.442
2.441
2.426
2.411
2.383
2.369
2.353
2.349
2.339
1.942
1.928
1.924
1.912
1.907
1.896
1.891
1.880
1.457
O
OH
N
CF3
3m
1.00
1.00
0.98
1.17
1.01
0.97
1.02
0.99
4.03
4.00
2.02
3.06
f1 (ppm)

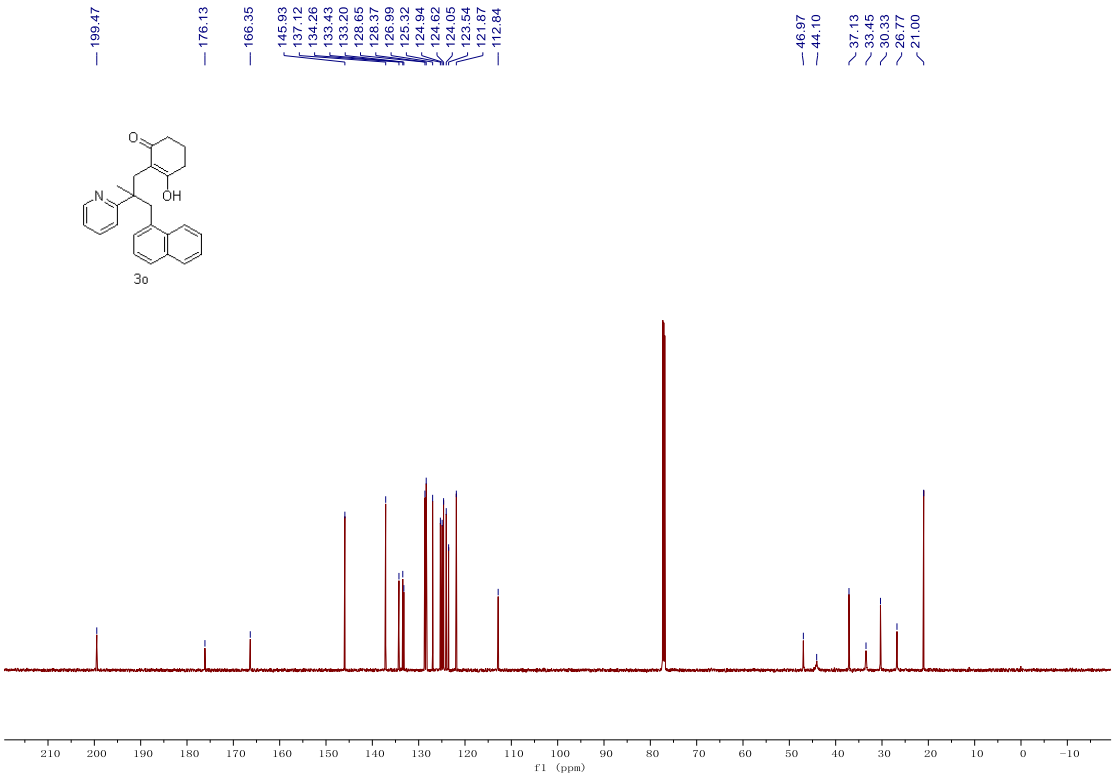

199.50
176.13
166.10
146.29
138.81
137.77
133.72
130.16
130.12
129.95
129.74
129.52
128.06
126.80
126.71
126.69
126.66
125.00
123.20
123.11
123.09
123.06
122.23
121.48
112.57
106.17
50.00
46.58
37.19
32.05
30.34
26.13
21.03
O
OH
N
CF3
3m
f1 (ppm)

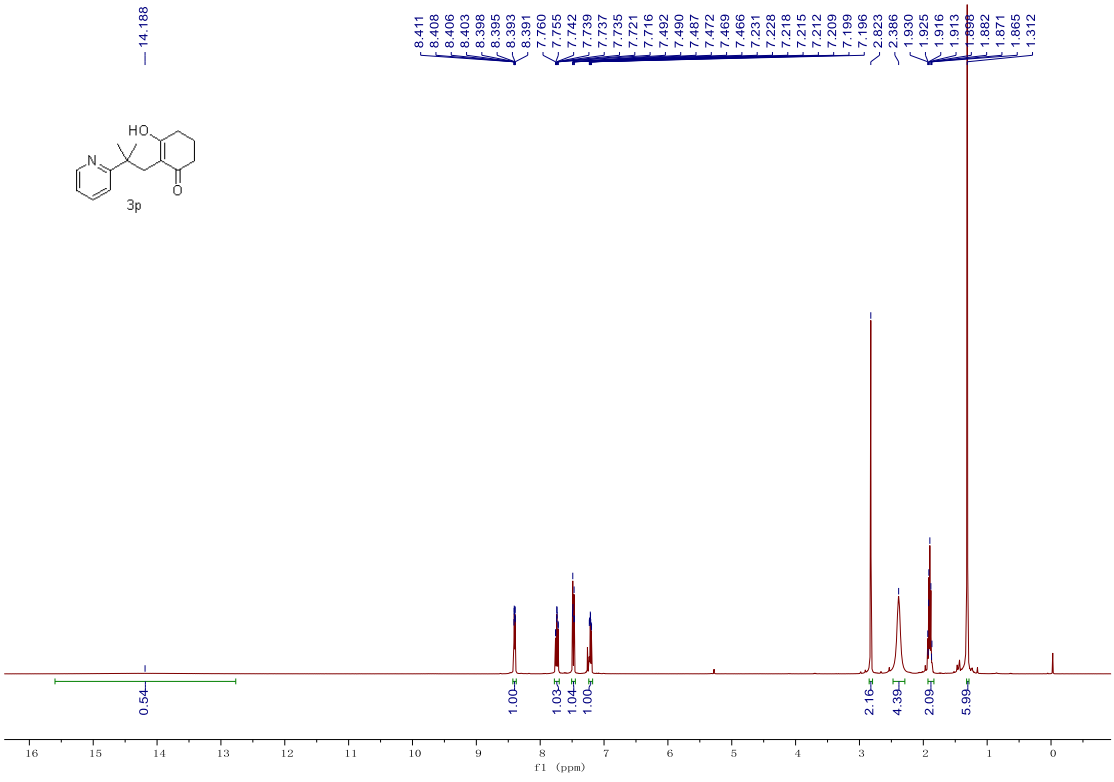

-62.80
O
OH
N
CF3
3m
f1 (ppm)

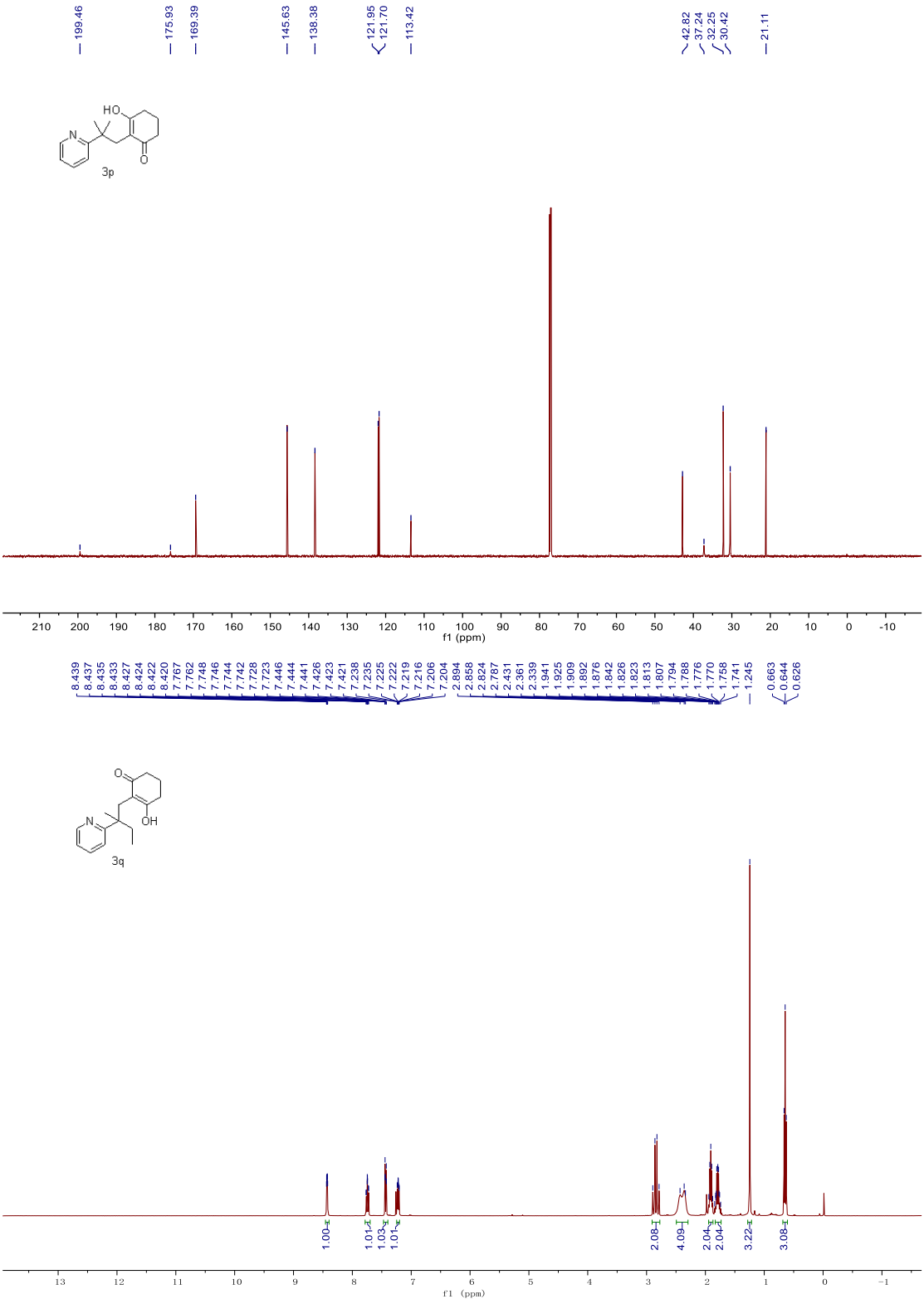

14.309
8.496
8.494
8.491
8.489
8.483
8.481
8.479
8.476
7.615
7.611
7.596
7.592
7.590
7.576
7.572
7.286
7.283
7.273
7.270
7.267
7.264
7.254
7.252
7.242
6.942
6.922
6.584
6.576
6.562
6.554
6.175
6.168
3.601
3.113
3.089
3.076
3.055
3.021
2.987
2.983
2.947
2.415
1.943
1.927
1.911
1.512
O
OH
N
Br
MeO
3n
0.76
0.99
1.00
2.08
1.00
0.98
1.01
3.07
4.08
4.07
2.09
3.08
f1 (ppm)

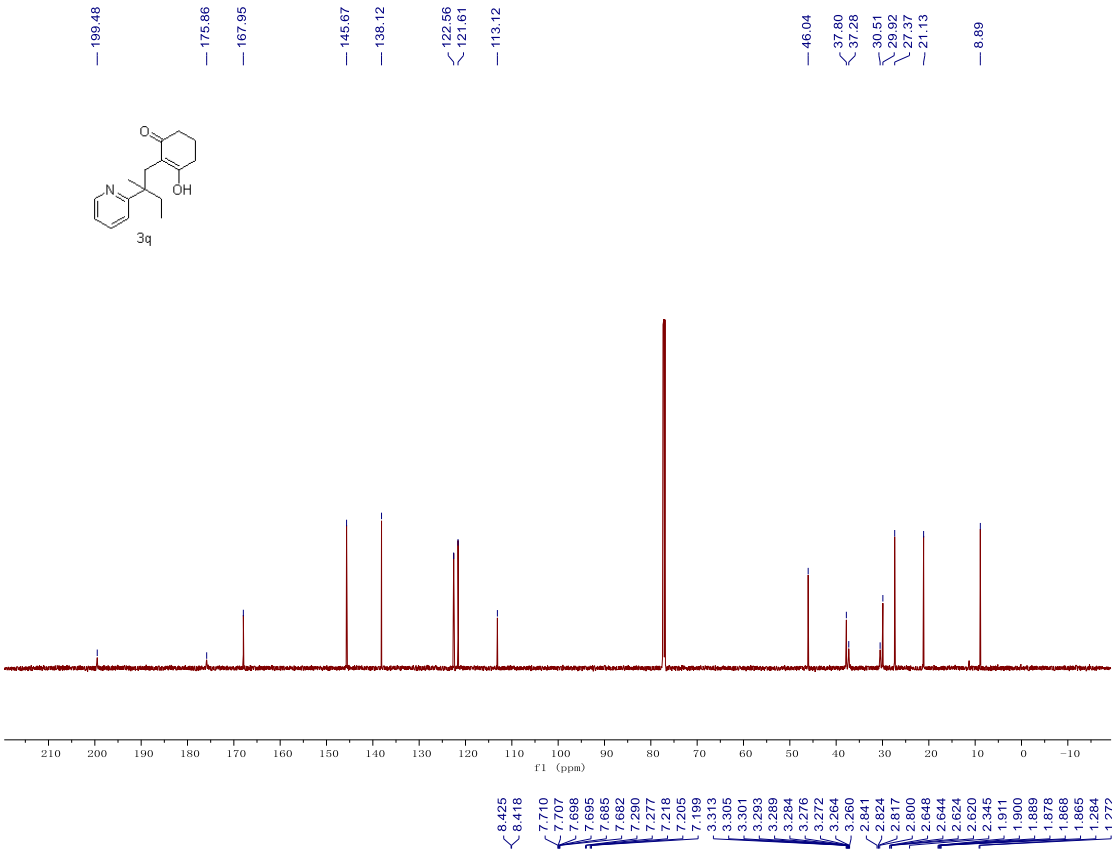

199.36
176.30
165.99
158.11
146.10
138.57
137.75
133.19
123.63
122.19
117.40
117.22
114.35
112.69
55.34
47.89
47.21
37.22
32.56
30.45
26.64
21.08
O
OH
N
Br
MeO
3n
f1 (ppm)

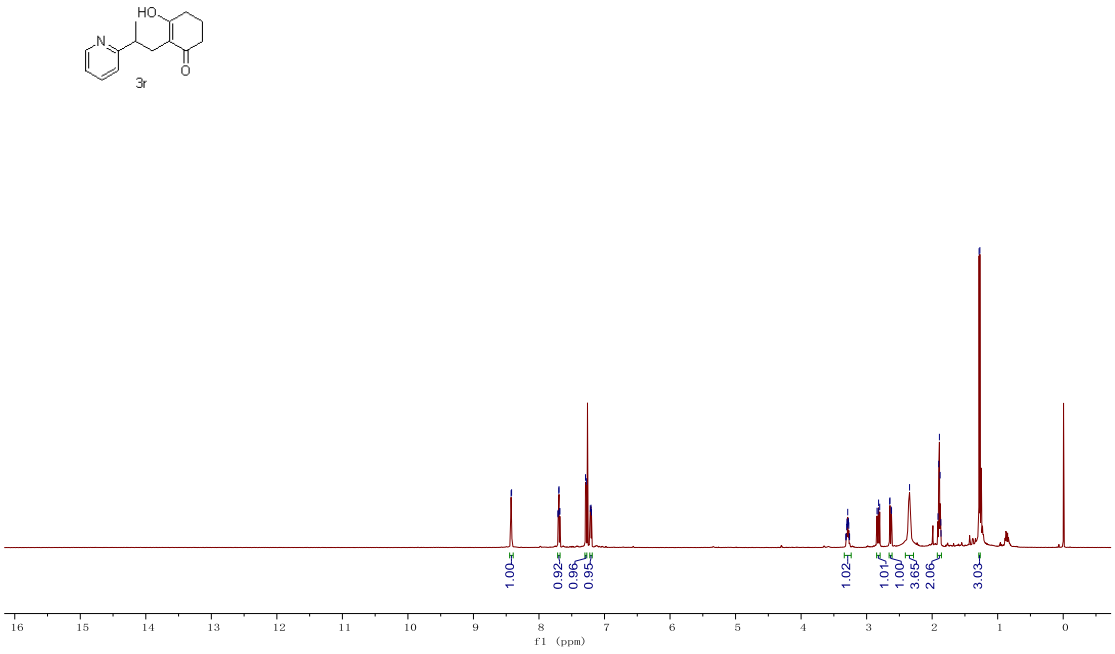

O
OH
N
3o
0.83
1.00
1.01
1.04
1.02
0.99
3.06
0.94
1.05
1.01
2.05
1.00
0.99
4.08
2.06
3.02
f1 (ppm)

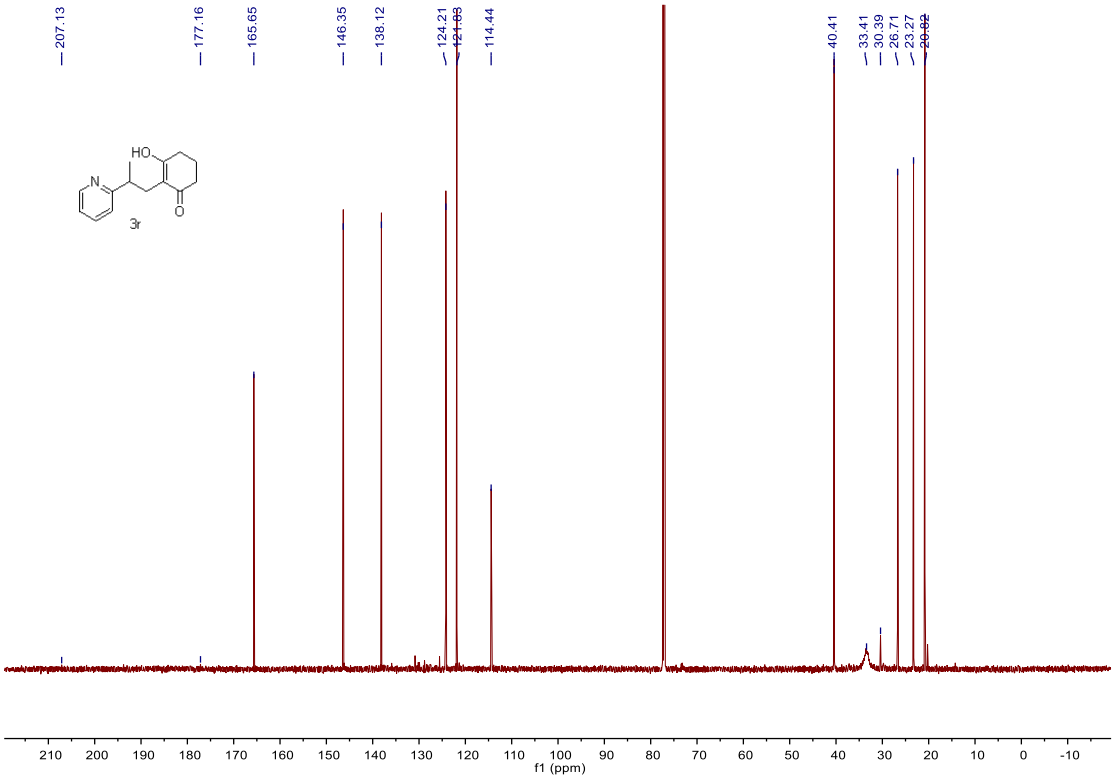

199.47
176.13
166.35
145.93
137.12
134.26
133.43
133.20
128.65
128.37
126.99
125.32
124.94
124.62
124.05
123.54
121.87
112.84
46.97
44.10
37.13
33.45
30.33
26.77
21.00
O
OH
N
3o
f1 (ppm)

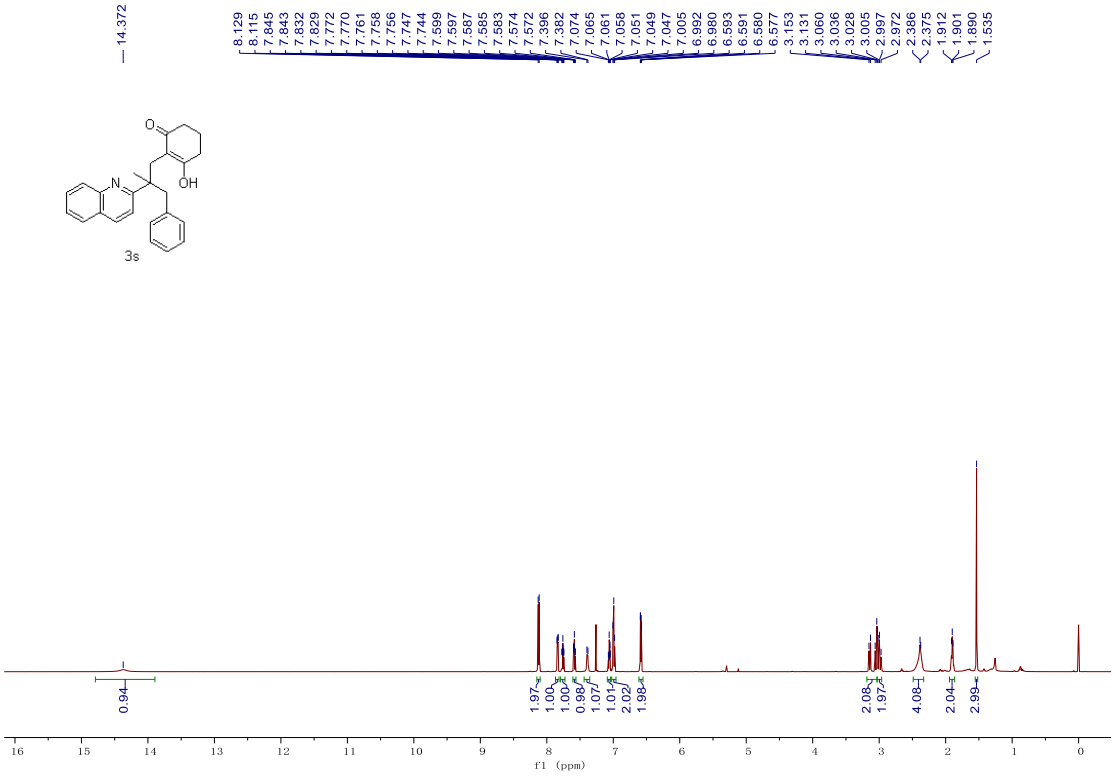

14.188
8.411
8.408
8.406
8.403
8.398
8.395
8.393
8.391
7.760
7.755
7.742
7.739
7.737
7.735
7.721
7.716
7.492
7.490
7.487
7.472
7.469
7.466
7.231
7.228
7.218
7.215
7.212
7.209
7.199
7.196
2.823
2.386
1.930
1.925
1.916
1.913
1.898
1.882
1.871
1.865
1.312
HO
N
O
3p
0.54
1.00
1.03
1.04
1.00
2.16
4.39
2.09
5.99
f1 (ppm)

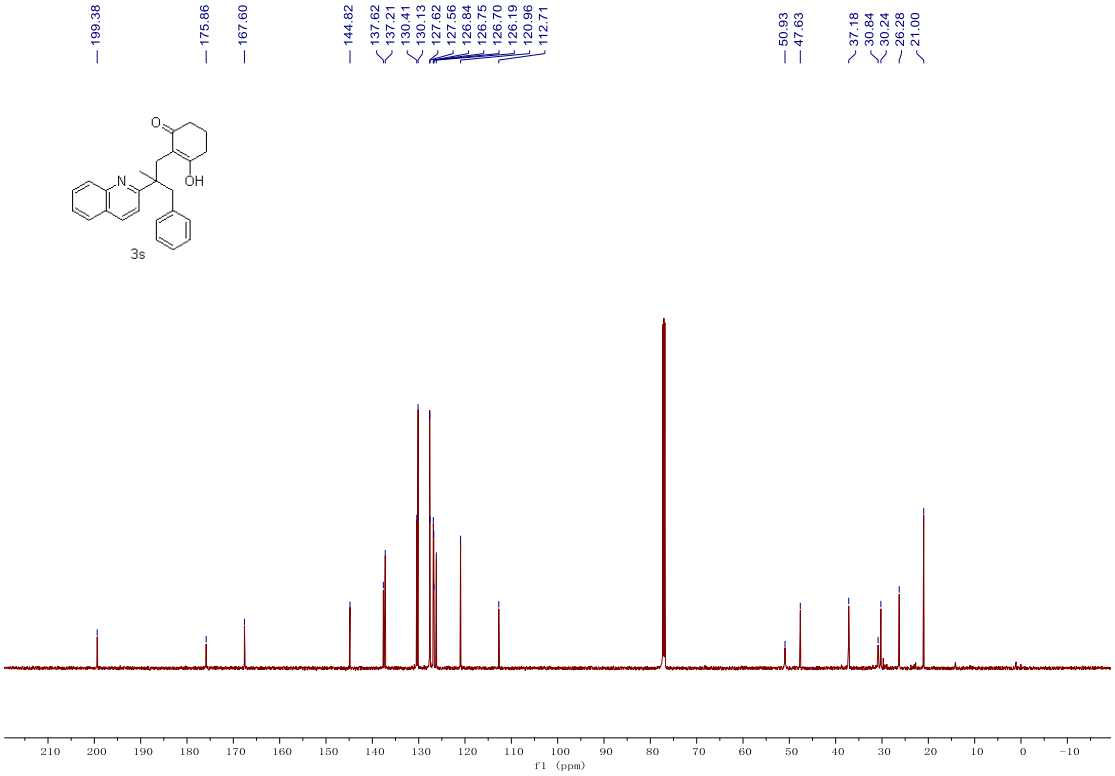

199.46
175.93
169.39
145.63
138.38
121.95
121.70
113.42
42.82
37.24
32.25
30.42
21.11
HO
N
O
3p
f1 (ppm)
8.439
8.437
8.435
8.433
8.427
8.424
8.422
8.420
7.767
7.762
7.748
7.746
7.744
7.742
7.728
7.723
7.446
7.444
7.441
7.426
7.423
7.421
7.238
7.235
7.225
7.222
7.219
7.216
7.206
7.204
2.894
2.858
2.824
2.787
2.431
2.361
2.339
1.941
1.925
1.909
1.892
1.876
1.842
1.826
1.823
1.813
1.807
1.794
1.788
1.776
1.770
1.758
1.741
1.245
0.663
0.644
0.626
O
N
OH
3q
1.00
1.01
1.03
1.01
2.08
4.09
2.04
2.04
3.22
3.08
f1 (ppm)

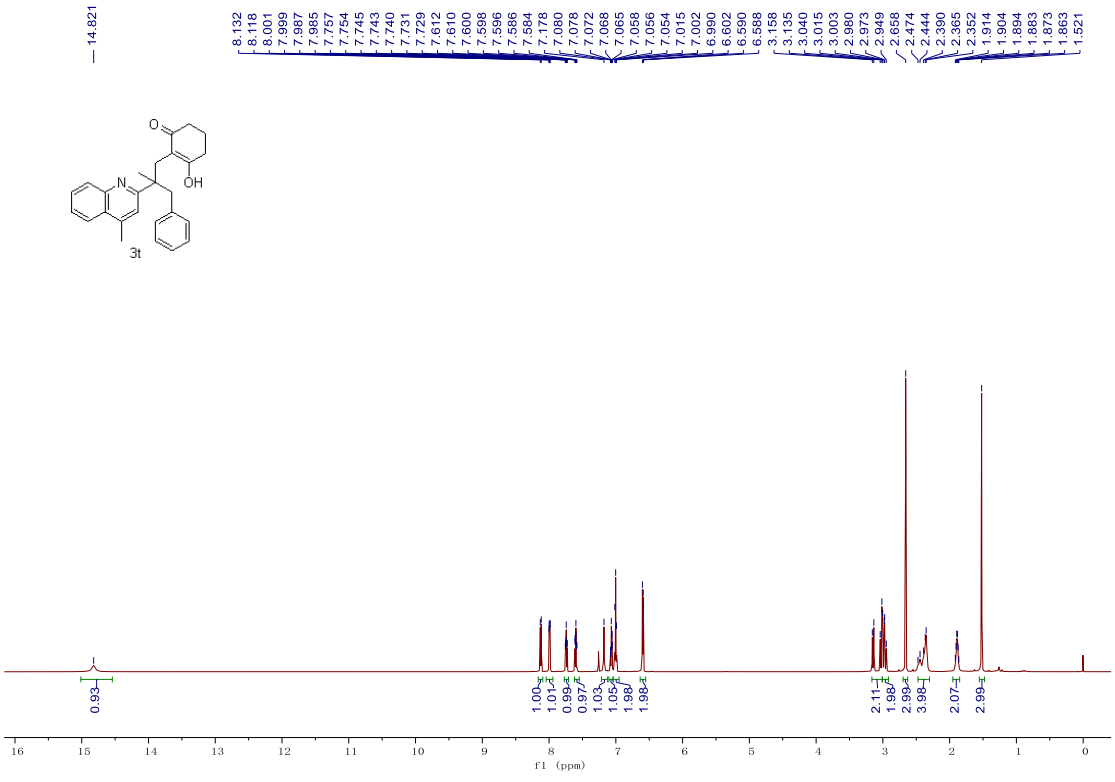

199.48
175.86
167.95
145.67
138.12
122.56
121.61
113.12
46.04
37.80
37.28
30.51
29.92
27.37
21.13
8.89
O
OH
N
3q
f1 (ppm)
8.425
8.418
7.710
7.707
7.698
7.695
7.685
7.682
7.290
7.277
7.218
7.205
7.199
3.313
3.305
3.301
3.293
3.289
3.284
3.276
3.272
3.264
3.260
2.841
2.824
2.817
2.800
2.648
2.644
2.624
2.620
2.345
1.911
1.900
1.889
1.878
1.868
1.865
1.284
1.277

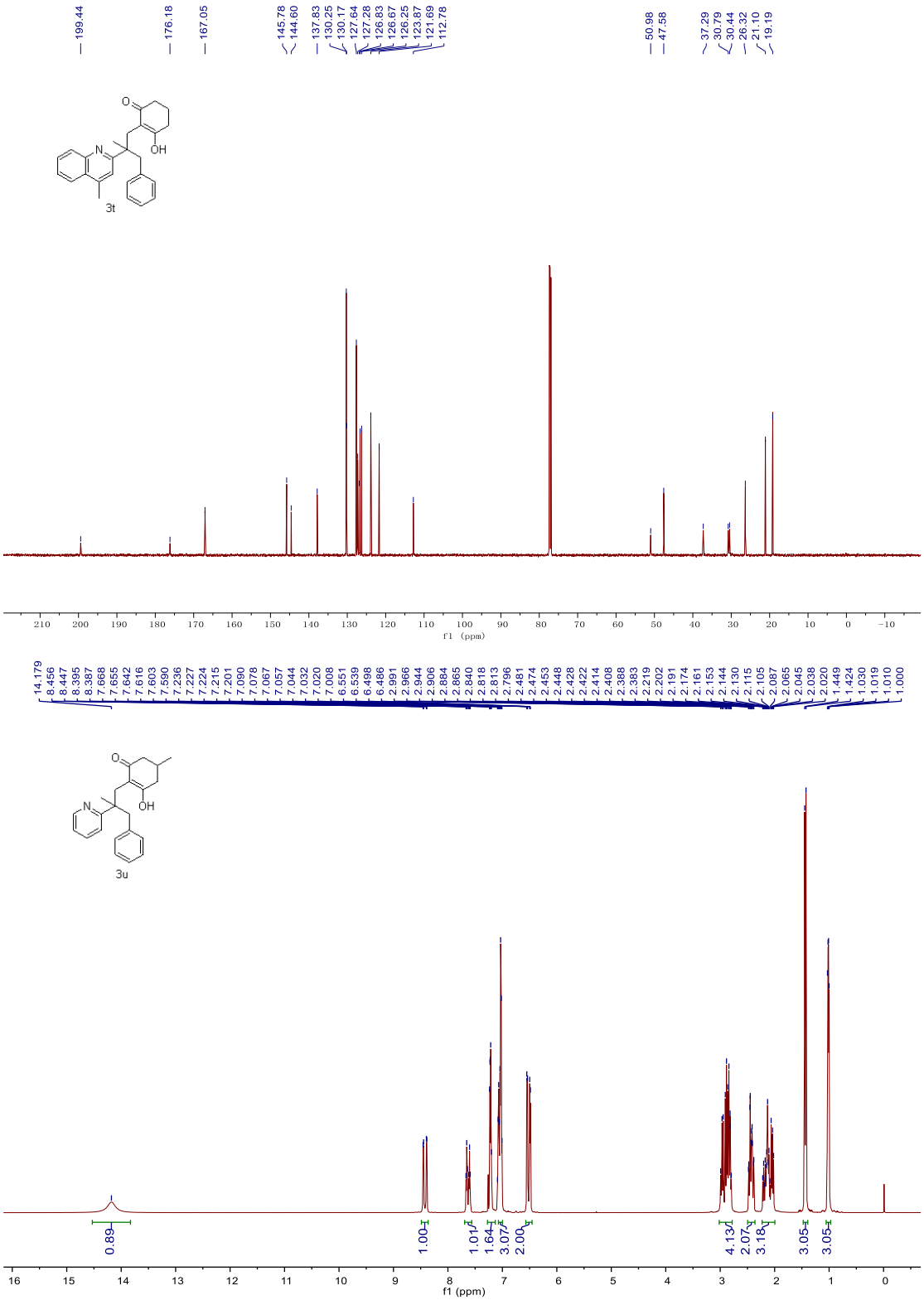

HO
N
O
3r
1.00
0.92
0.96
0.95
1.02
1.01
1.00
3.65
2.06
3.03
f1 (ppm)

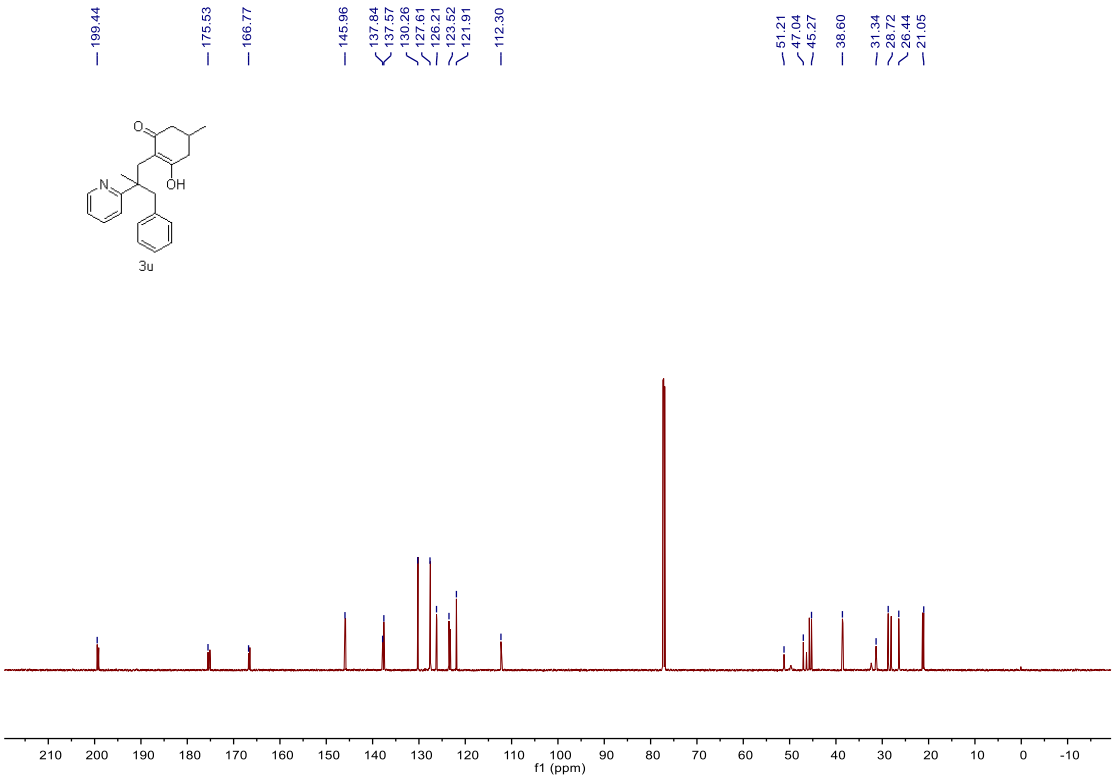

207.13
177.16
165.65
146.35
138.12
124.21
121.68
114.44
40.41
33.41
30.39
26.71
23.27
20.02
HO
N
O
3r
f1 (ppm)

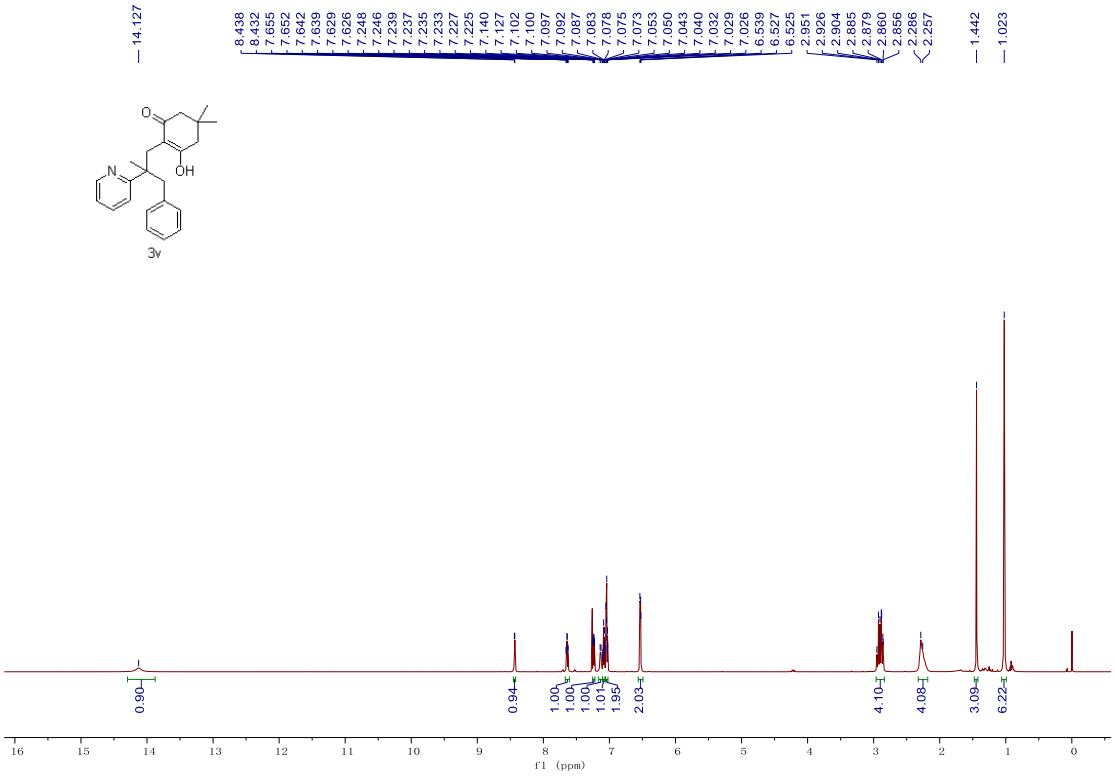

14.372
8.129
8.115
7.845
7.843
7.832
7.829
7.772
7.770
7.761
7.758
7.756
7.747
7.744
7.599
7.597
7.587
7.585
7.583
7.574
7.572
7.396
7.382
7.074
7.065
7.061
7.058
7.051
7.049
7.047
7.005
6.992
6.980
6.593
6.591
6.580
6.577
3.153
3.131
3.060
3.036
3.028
3.005
2.997
2.972
2.386
2.375
1.912
1.901
1.890
1.535
O
OH
N
3s
0.94
1.97
1.00
1.00
0.98
1.07
1.01
2.02
1.98
2.08
1.97
4.08
2.04
2.99
f1 (ppm)

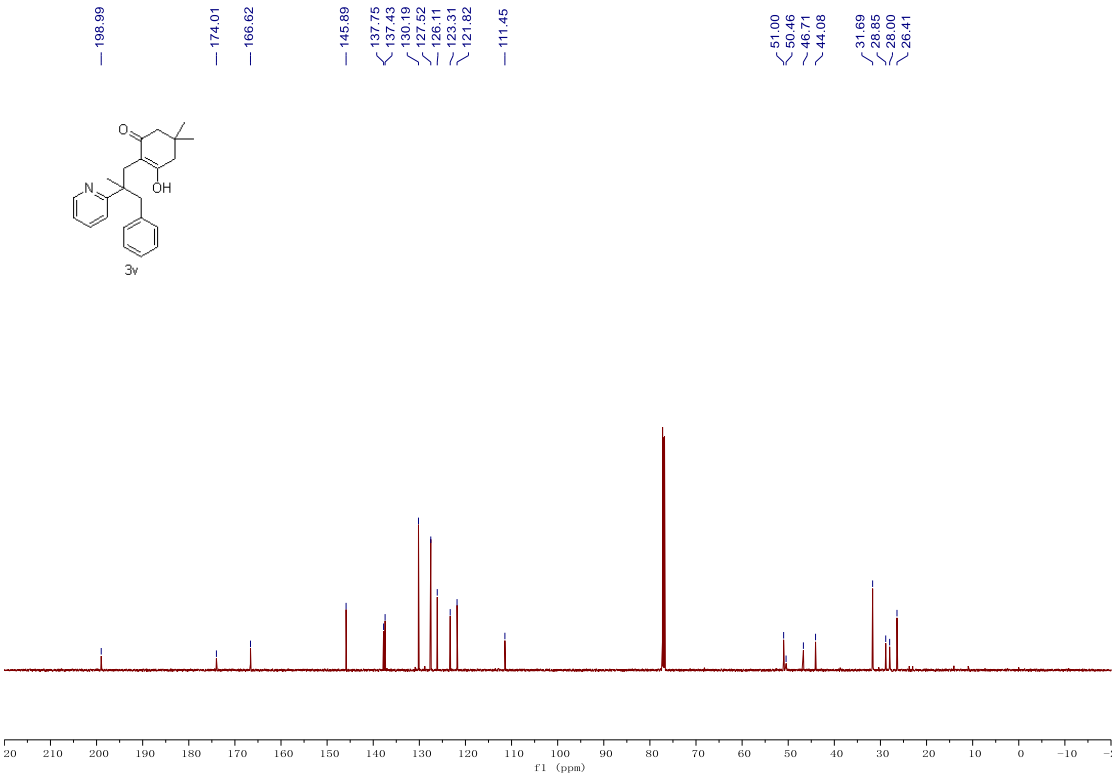

199.38
175.86
167.60
144.82
137.62
137.21
130.41
130.13
127.62
127.56
126.84
126.75
126.70
126.19
120.96
112.71
50.93
47.63
37.18
30.84
30.24
26.28
21.00
O
OH
N
3s
f1 (ppm)

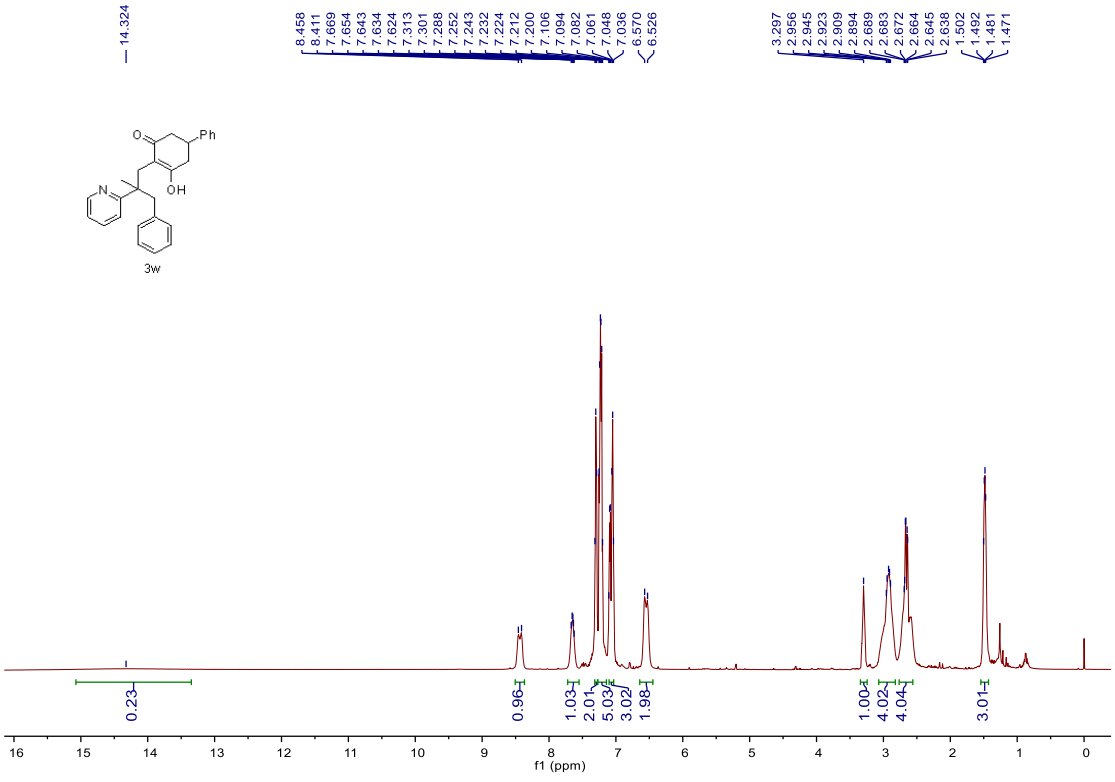

14.821
8.132
8.118
8.001
7.999
7.987
7.985
7.757
7.754
7.745
7.743
7.740
7.731
7.729
7.612
7.610
7.600
7.598
7.596
7.586
7.584
7.178
7.080
7.078
7.072
7.068
7.065
7.058
7.056
7.054
7.015
7.002
6.990
6.602
6.590
6.588
3.158
3.135
3.040
3.015
3.003
2.980
2.973
2.949
2.658
2.474
2.444
2.390
2.365
2.352
1.914
1.904
1.894
1.883
1.873
1.863
1.521
O
OH
N
3t
0.93
1.00
1.01
0.99
0.97
1.03
1.05
1.98
1.98
2.11
1.98
2.99
3.98
2.07
2.99
f1 (ppm)

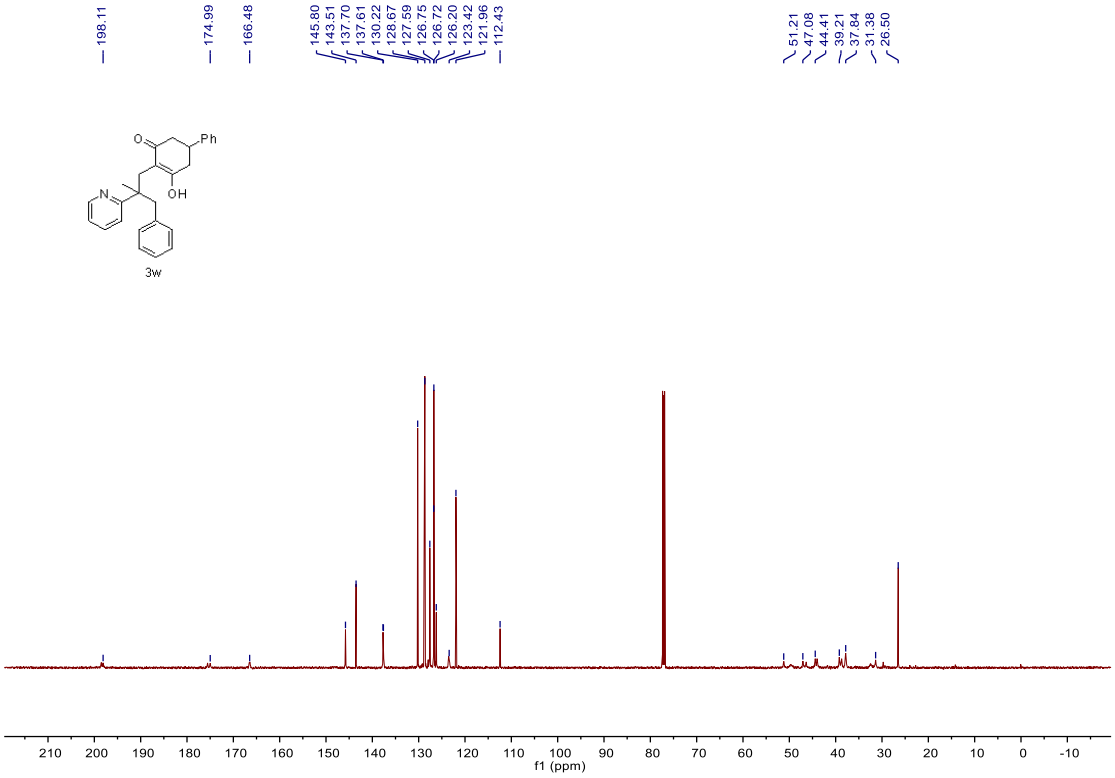

199.44
176.18
167.05
145.78
144.60
137.83
130.25
130.17
127.64
127.28
126.83
126.67
126.25
123.87
121.69
112.78
50.98
47.58
37.29
30.79
30.44
26.32
21.10
19.19
O
OH
N
3t
f1 (ppm)
14.179
8.456
8.447
8.395
8.387
7.668
7.655
7.642
7.616
7.603
7.590
7.236
7.227
7.224
7.215
7.201
7.090
7.078
7.067
7.057
7.044
7.032
7.020
7.008
6.551
6.539
6.498
6.486
2.991
2.966
2.944
2.906
2.884
2.865
2.840
2.818
2.813
2.796
2.481
2.474
2.453
2.448
2.428
2.422
2.414
2.408
2.388
2.383
2.219
2.202
2.191
2.174
2.161
2.153
2.144
2.130
2.115
2.105
2.087
2.065
2.045
2.038
2.020
1.449
1.424
1.030
1.019
1.010
1.000
O
OH
N
3u
0.89
1.00
1.01
1.64
3.07
2.00
4.13
2.07
3.18
3.05
3.05
f1 (ppm)

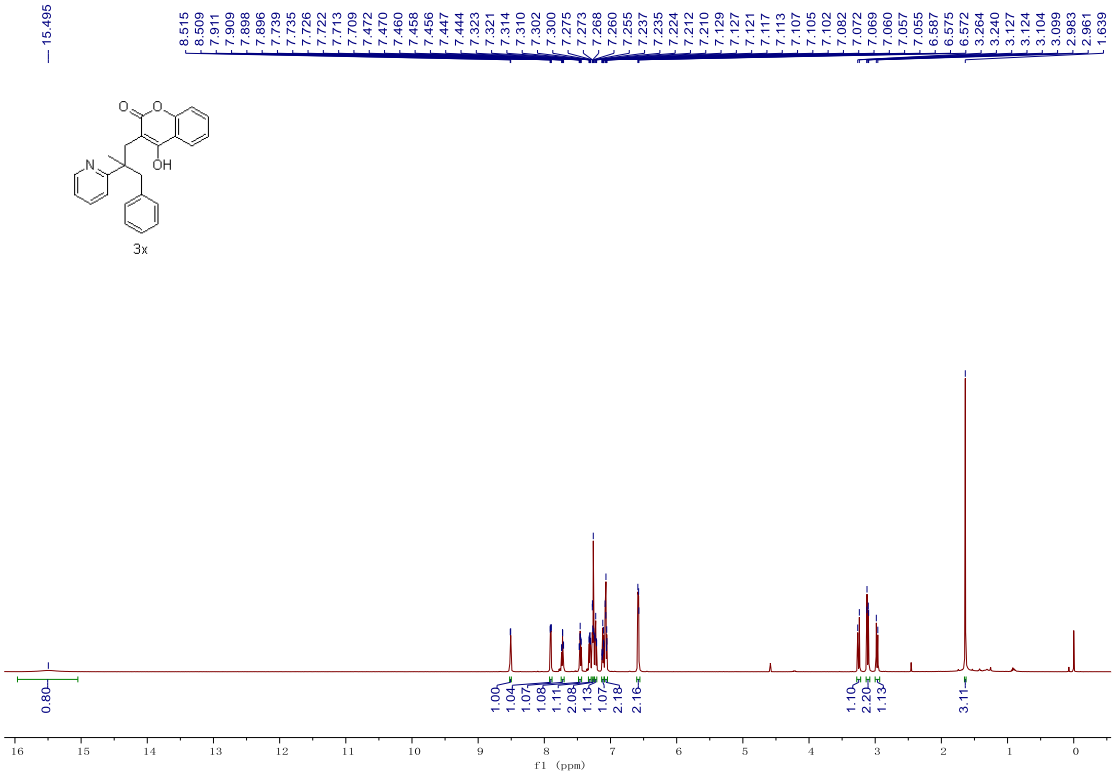

199.44
175.53
166.77
145.96
137.84
137.57
130.26
127.61
126.21
123.52
121.91
112.30
51.21
47.04
45.27
38.60
31.34
28.72
26.44
21.05
O
OH
N
3u
f1 (ppm)

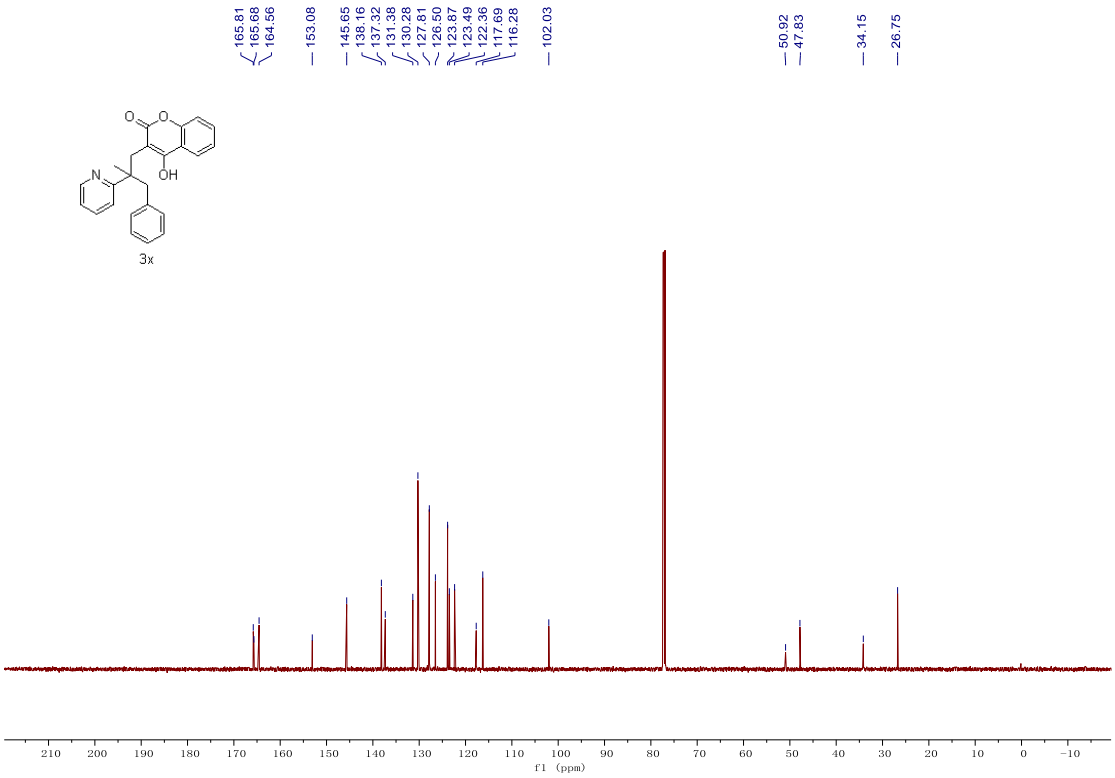

14.127
8.438
8.432
7.655
7.652
7.642
7.639
7.629
7.626
7.248
7.246
7.239
7.237
7.235
7.233
7.227
7.225
7.140
7.127
7.102
7.100
7.097
7.092
7.087
7.083
7.078
7.075
7.073
7.053
7.050
7.043
7.040
7.032
7.029
7.026
6.539
6.527
6.525
2.951
2.926
2.904
2.885
2.879
2.860
2.856
2.286
2.257
1.442
1.023
O
OH
N
3v
0.90
0.94
1.00
1.00
1.00
1.01
1.95
2.03
4.10
4.08
3.09
6.22
f1 (ppm)

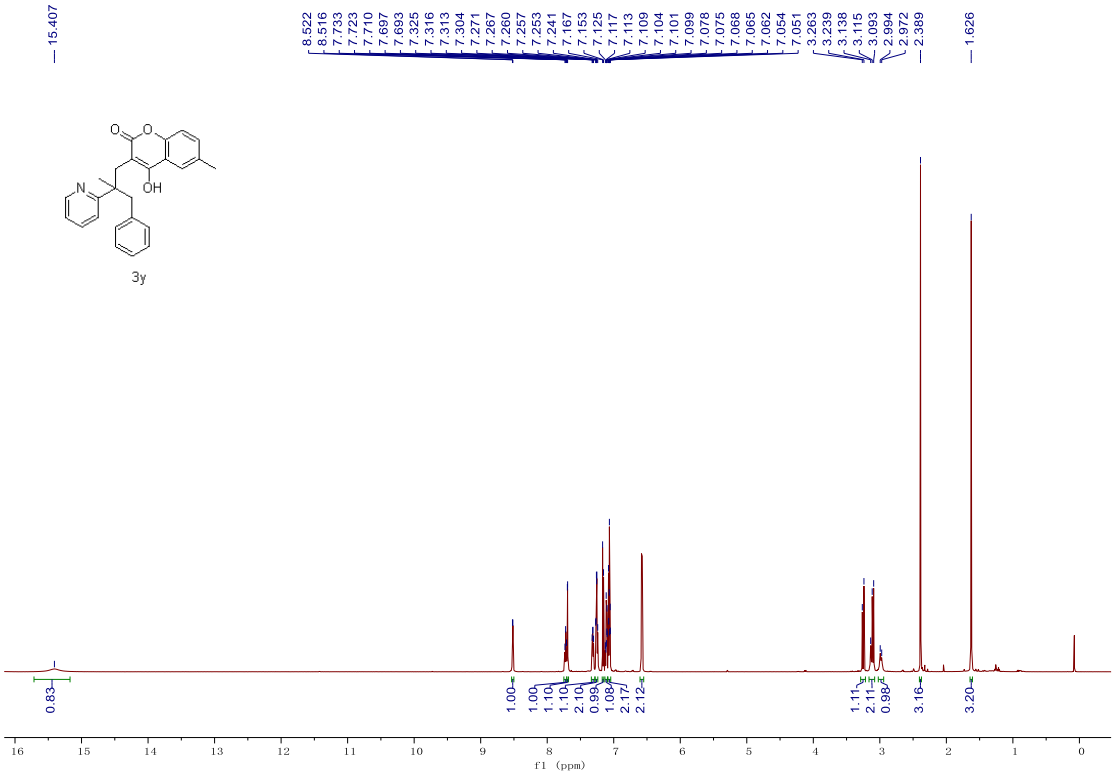

198.99
174.01
166.62
145.89
137.75
137.43
130.19
127.52
126.11
123.31
121.82
111.45
51.00
50.46
46.71
44.08
31.69
28.85
28.00
26.41
O
OH
N
3v
f1 (ppm)

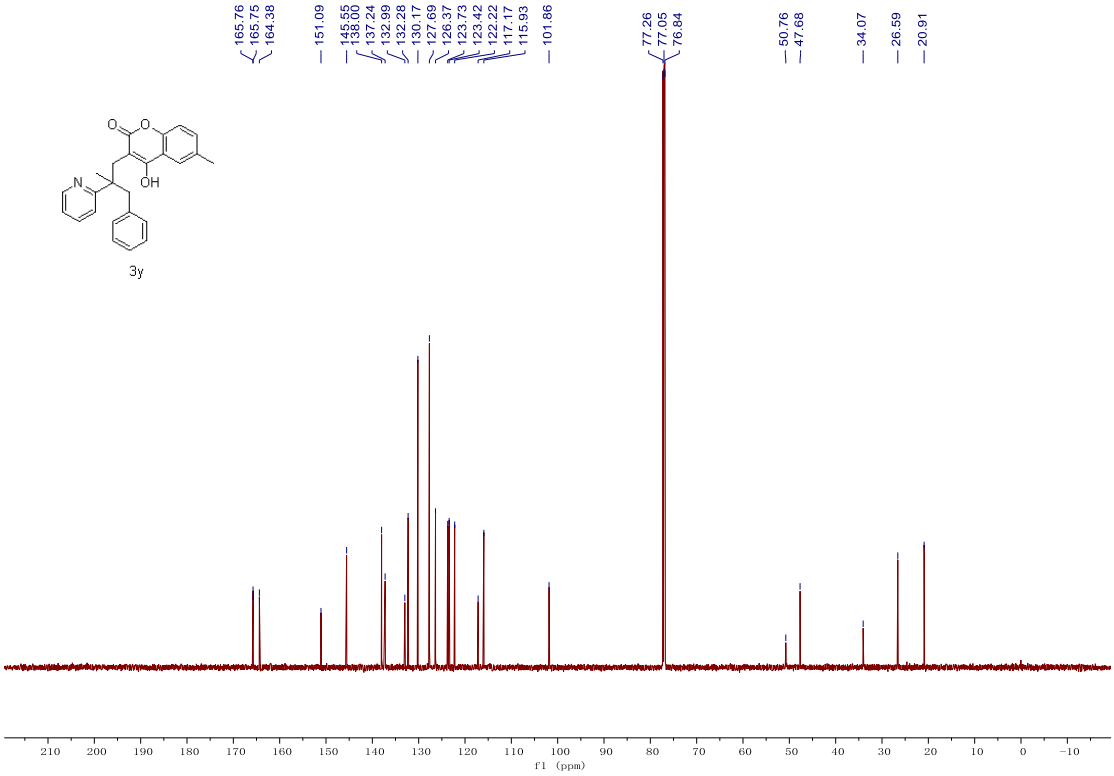

14.324
8.458
8.411
7.669
7.654
7.643
7.634
7.624
7.313
7.301
7.288
7.252
7.243
7.232
7.224
7.212
7.200
7.106
7.094
7.082
7.061
7.048
7.036
6.570
6.526
3.297
2.956
2.945
2.923
2.909
2.894
2.689
2.683
2.672
2.664
2.645
2.638
1.502
1.492
1.481
1.471
O
Ph
OH
N
3w
0.23
0.96
1.03
2.01
5.03
3.02
1.98
1.00
4.02
4.04
3.01
f1 (ppm)

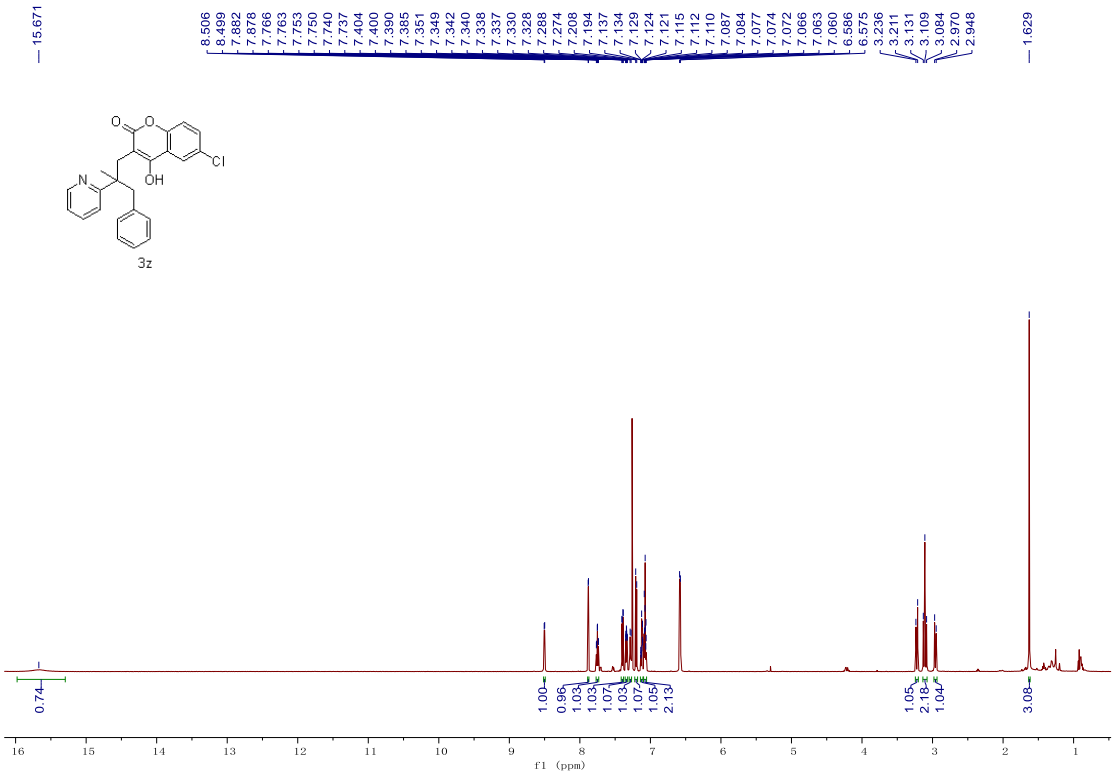

198.11
174.99
166.48
145.80
143.51
137.70
137.61
130.22
128.67
127.59
126.75
126.72
126.20
123.42
121.96
112.43
51.21
47.08
44.41
39.21
37.84
31.38
26.50
Ph
O
N
OH
3w
f1 (ppm)

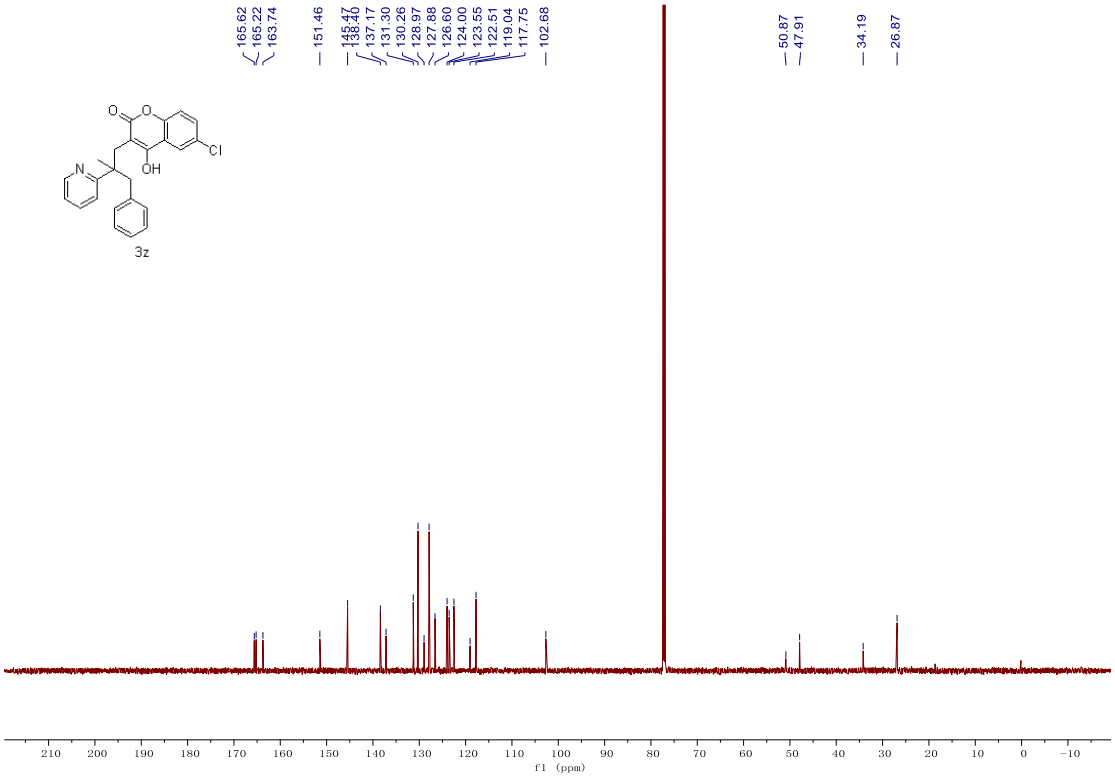

15.495
8.515
8.509
7.911
7.909
7.898
7.896
7.739
7.735
7.726
7.722
7.713
7.709
7.472
7.470
7.460
7.458
7.456
7.447
7.444
7.323
7.321
7.314
7.310
7.302
7.300
7.275
7.273
7.268
7.260
7.255
7.237
7.235
7.224
7.212
7.210
7.129
7.127
7.121
7.117
7.113
7.107
7.105
7.102
7.082
7.072
7.069
7.060
7.057
7.055
6.587
6.575
6.572
3.264
3.240
3.127
3.124
3.104
3.099
2.983
2.961
1.639
O
O
N
OH
3x
0.80
1.00
1.04
1.07
1.08
1.11
2.08
1.13
1.07
2.18
2.16
1.10
2.20
1.13
3.11
f1 (ppm)

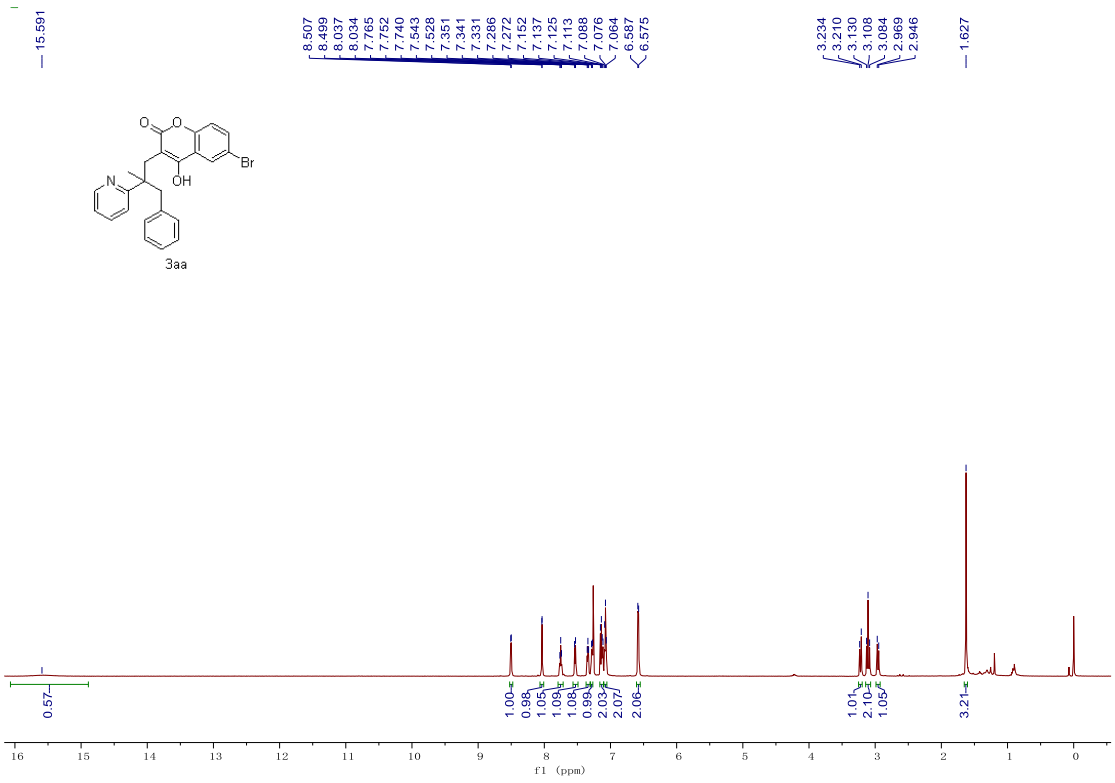

165.81
165.68
164.56
153.08
145.65
138.16
137.32
131.38
130.28
127.81
126.50
123.87
123.49
122.36
117.69
116.28
102.03
50.92
47.83
34.15
26.75
O
O
OH
N
3x
f1 (ppm)

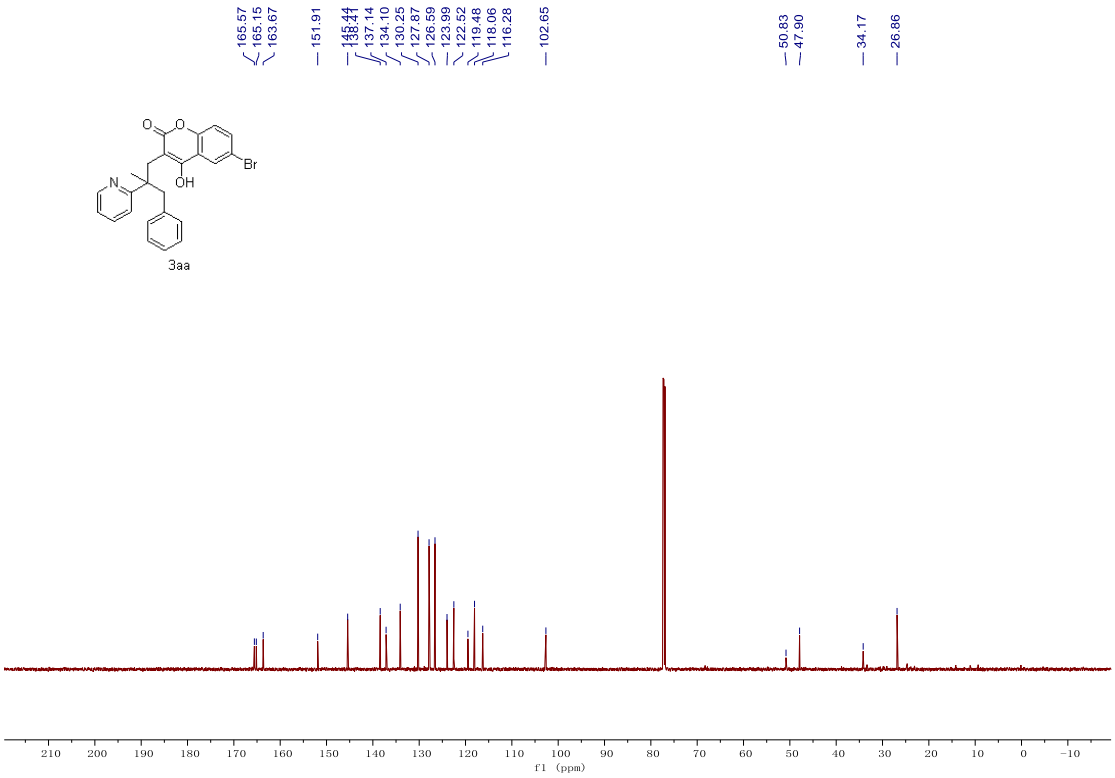

15.407
8.522
8.516
7.733
7.723
7.710
7.697
7.693
7.325
7.316
7.313
7.304
7.271
7.267
7.260
7.257
7.253
7.241
7.167
7.153
7.125
7.117
7.113
7.109
7.104
7.101
7.099
7.078
7.075
7.068
7.065
7.062
7.054
7.051
3.263
3.239
3.138
3.115
3.093
2.994
2.972
2.389
1.626
O
O
OH
N
3y
0.83
1.00
1.00
1.10
1.10
2.10
0.99
1.08
2.17
2.12
1.11
2.11
0.98
3.16
3.20
f1 (ppm)

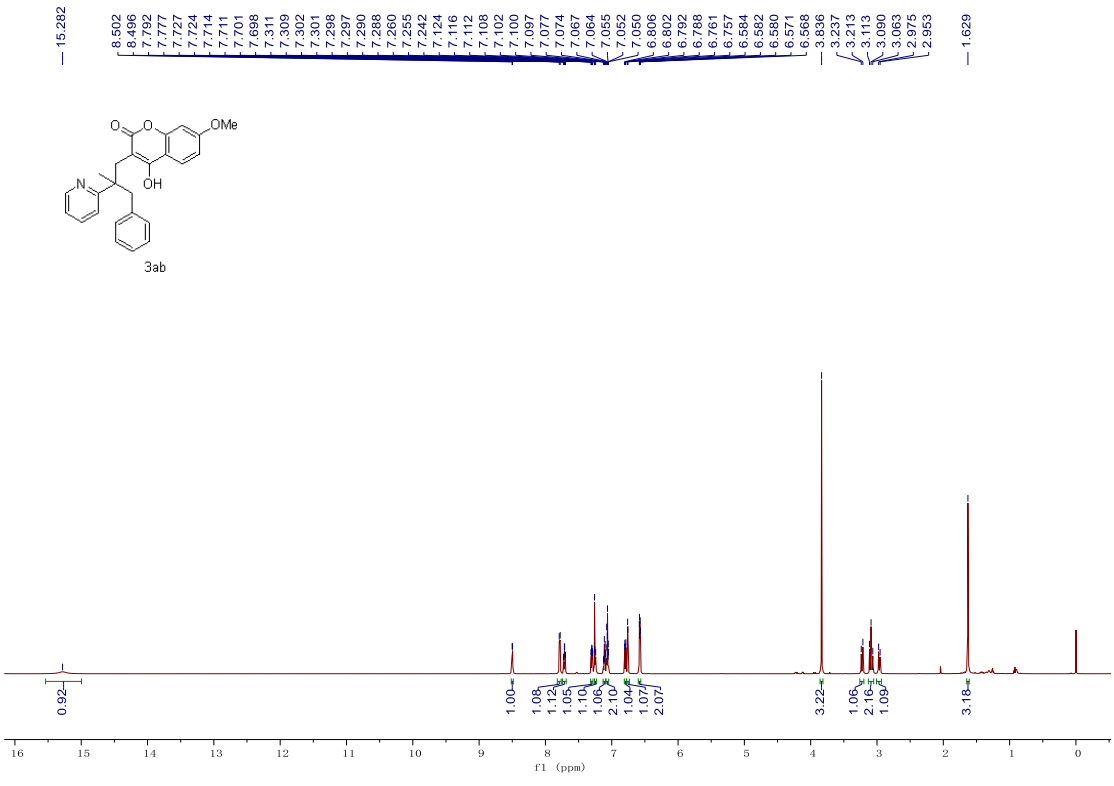

165.76
165.75
164.38
151.09
145.55
138.00
137.24
132.99
132.28
130.17
127.69
126.37
123.73
123.42
122.22
117.17
115.93
101.86
77.26
77.05
76.84
50.76
47.68
34.07
26.59
20.91
O
O
OH
N
3y
f1 (ppm)

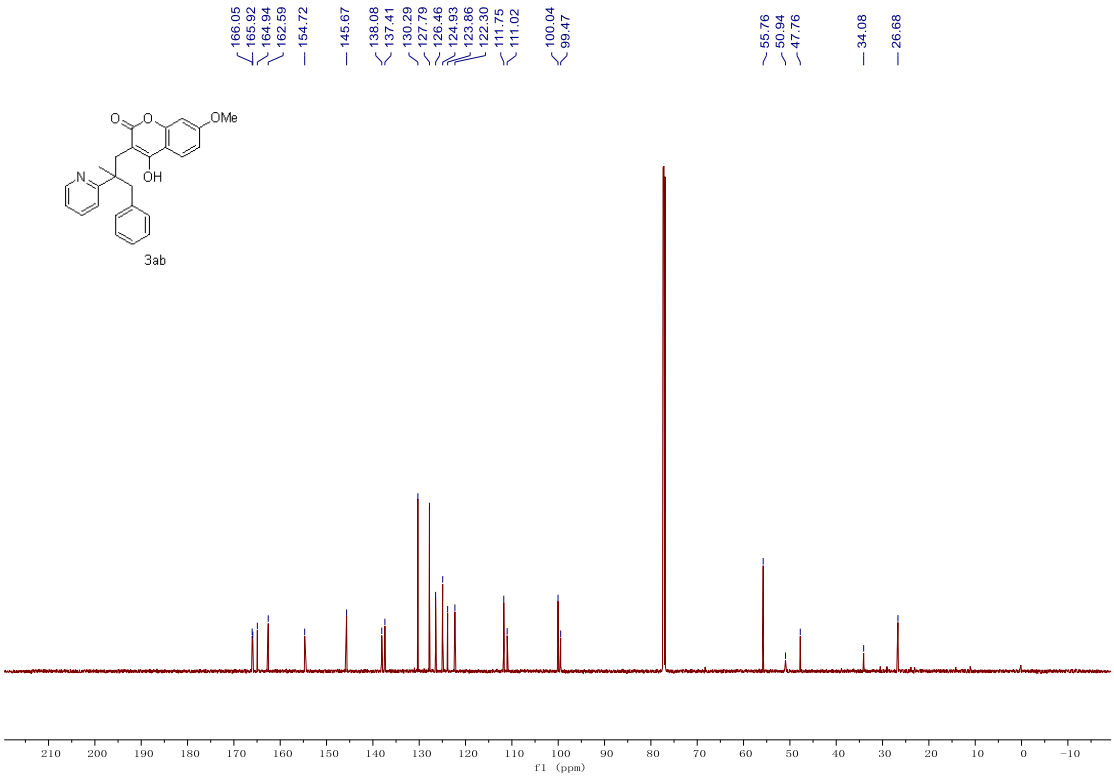

15.671
8.506
8.499
7.882
7.878
7.766
7.763
7.753
7.750
7.740
7.737
7.404
7.400
7.390
7.385
7.351
7.349
7.342
7.340
7.338
7.337
7.330
7.328
7.288
7.274
7.208
7.194
7.137
7.134
7.129
7.124
7.121
7.115
7.112
7.110
7.087
7.084
7.077
7.074
7.072
7.066
7.063
7.060
6.586
6.575
3.236
3.211
3.131
3.109
3.084
2.970
2.948
1.629
O
O
OH
Cl
N
3z
0.74
1.00
0.96
1.03
1.03
1.07
1.03
1.07
1.05
2.13
1.05
2.18
1.04
3.08
f1 (ppm)

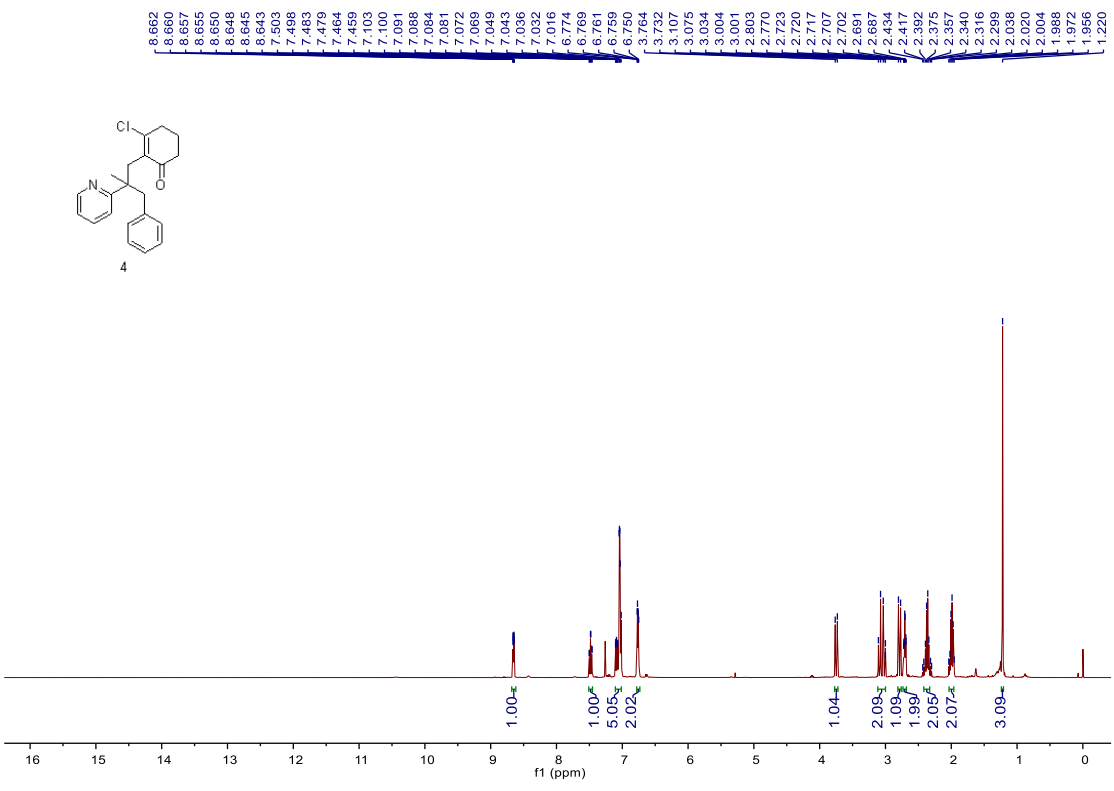

165.62
165.22
163.74
151.46
145.47
138.40
137.17
131.30
130.26
128.97
127.88
126.60
124.00
123.55
122.51
119.04
117.75
102.68
50.87
47.91
34.19
26.87
O
O
Cl
OH
N
3z
f1 (ppm)

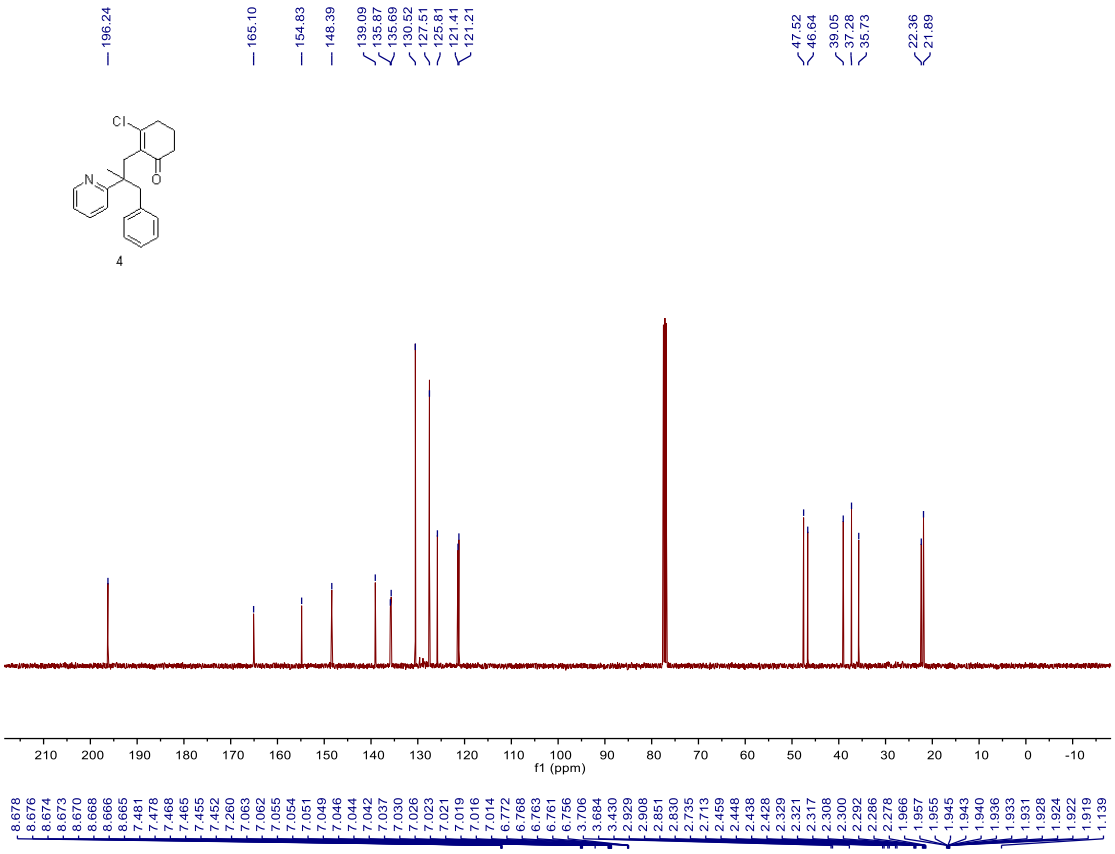

15.591
8.507
8.499
8.037
8.034
7.765
7.752
7.740
7.543
7.528
7.351
7.341
7.331
7.286
7.272
7.152
7.137
7.125
7.113
7.088
7.076
7.064
6.587
6.575
3.234
3.210
3.130
3.108
3.084
2.969
2.946
1.627
O
O
Br
OH
N
3aa
0.57
1.00
0.98
1.05
1.09
1.08
0.99
2.03
2.07
2.06
1.01
2.10
1.05
3.21
f1 (ppm)

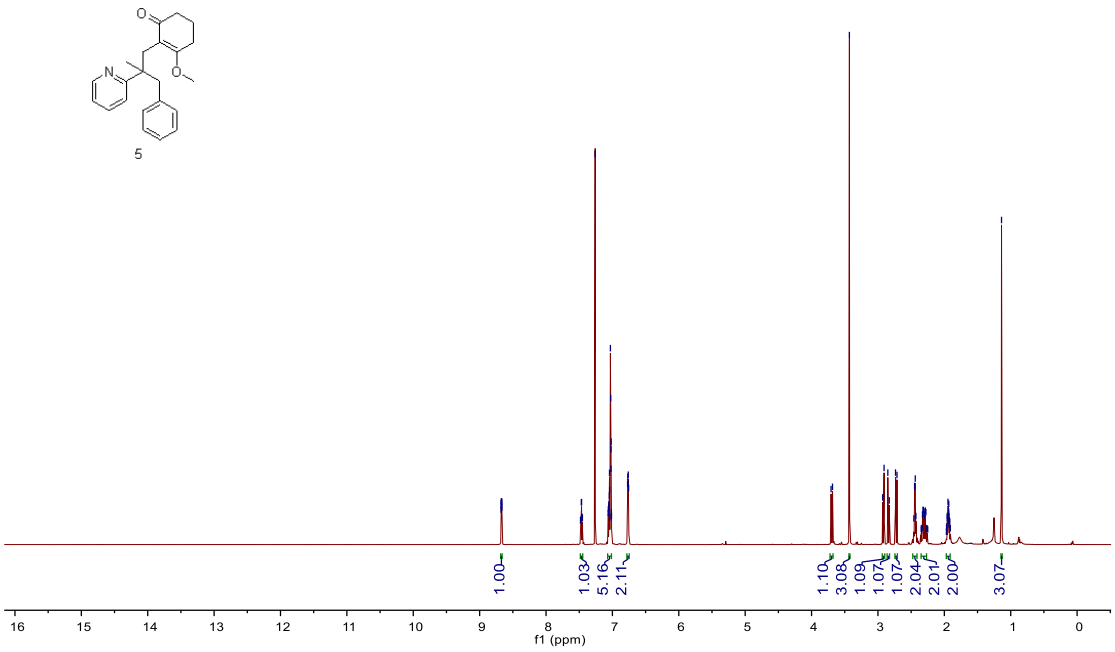

165.57
165.15
163.67
151.91
145.44
138.41
137.14
134.10
130.25
127.87
126.59
123.99
122.52
119.48
118.06
116.28
102.65
50.83
47.90
34.17
26.86
O
O
Br
OH
N
3aa
f1 (ppm)

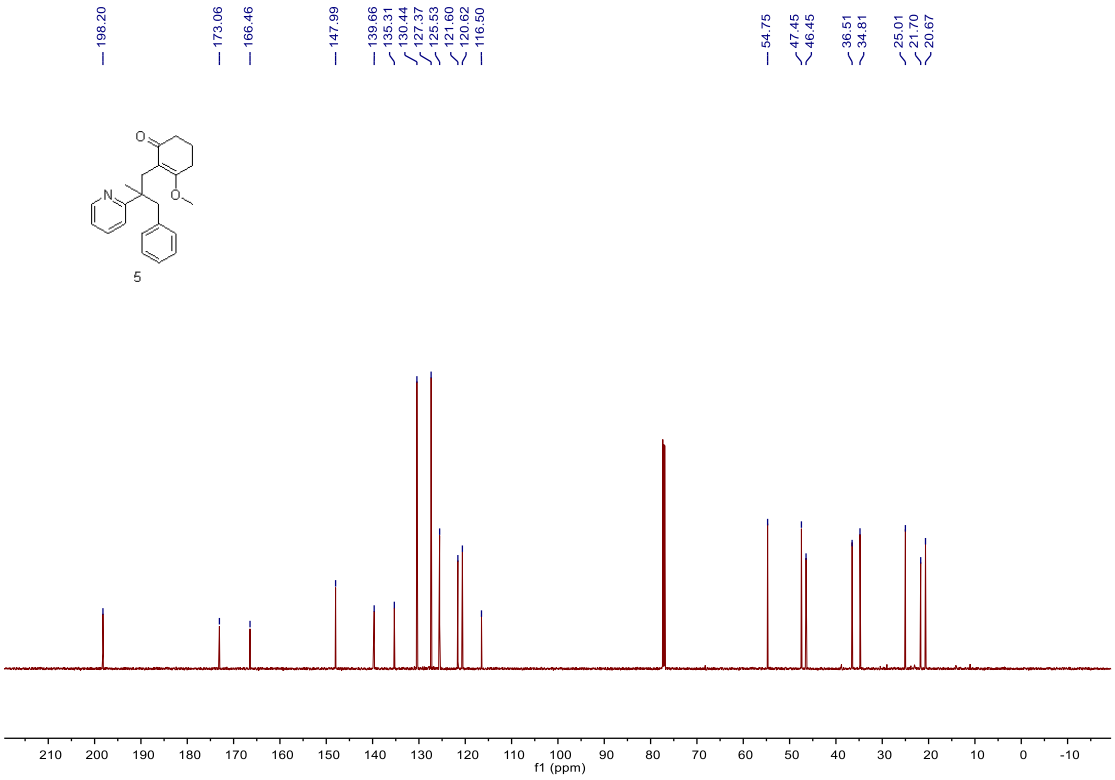

15.282
8.502
8.496
7.792
7.777
7.727
7.724
7.714
7.711
7.701
7.698
7.311
7.309
7.302
7.301
7.298
7.297
7.290
7.288
7.260
7.255
7.242
7.124
7.116
7.112
7.108
7.102
7.100
7.097
7.077
7.074
7.067
7.064
7.055
7.052
7.050
6.806
6.802
6.792
6.788
6.761
6.757
6.584
6.582
6.580
6.571
6.568
3.836
3.237
3.213
3.113
3.090
3.063
2.975
2.953
1.629
O
O
OMe
OH
N
3ab
0.92
1.00
1.08
1.12
1.05
1.10
1.06
2.10
1.04
1.07
2.07
3.22
1.06
2.16
1.09
3.18
f1 (ppm)

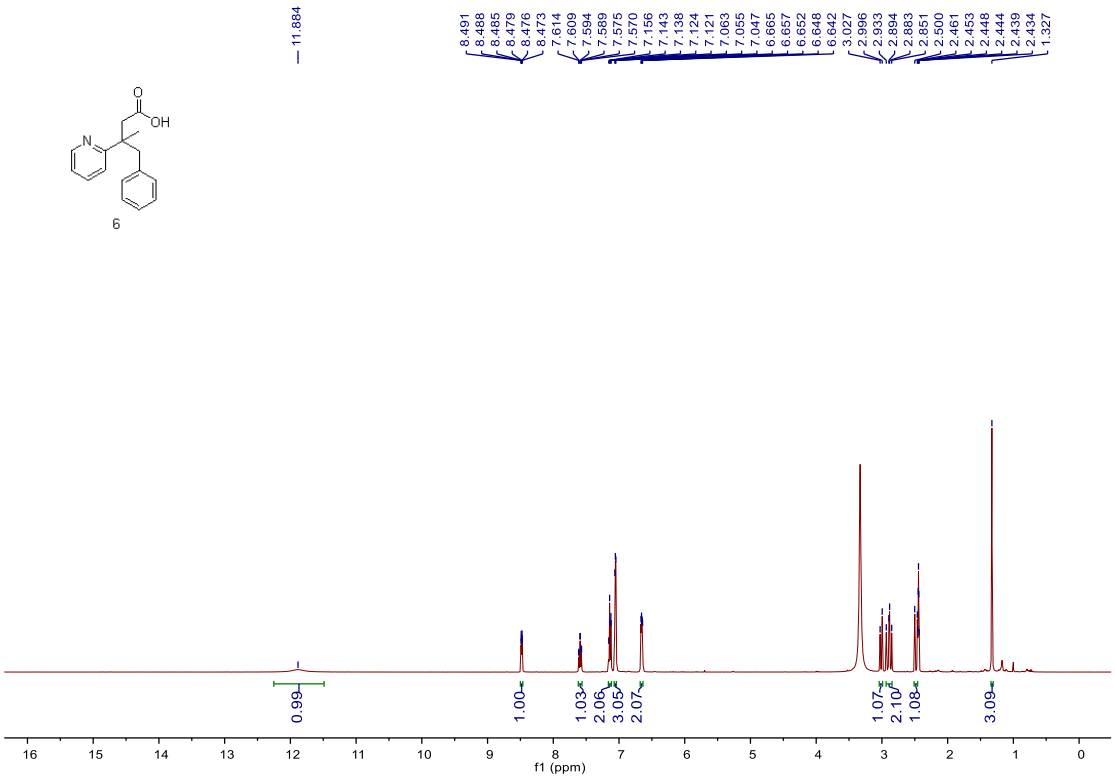

166.05
165.92
164.94
162.59
154.72
145.67
138.08
137.41
130.29
127.79
126.46
124.93
123.86
122.30
111.75
111.02
100.04
99.47
55.76
50.94
47.76
34.08
26.68
OMe
OH
N
O
3ab
f1 (ppm)

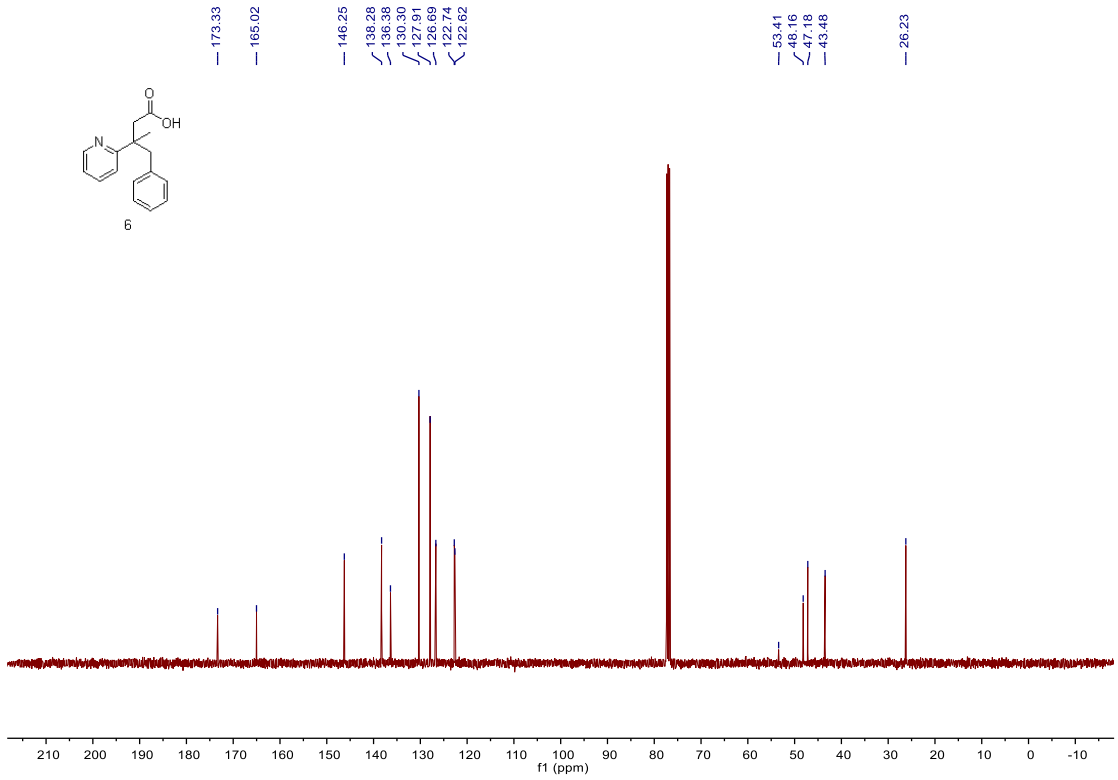

8.662
8.660
8.657
8.655
8.650
8.648
8.645
8.643
7.503
7.498
7.483
7.479
7.464
7.459
7.103
7.100
7.091
7.088
7.084
7.081
7.072
7.069
7.049
7.043
7.036
7.032
7.016
6.774
6.769
6.761
6.759
6.750
3.764
3.732
3.107
3.075
3.034
3.004
3.001
2.803
2.770
2.723
2.720
2.717
2.707
2.702
2.691
2.687
2.434
2.417
2.392
2.375
2.357
2.340
2.316
2.299
2.038
2.020
2.004
1.988
1.972
1.956
1.220
Cl
N
O
4
1.00
1.00
5.05
2.02
1.04
2.09
1.09
1.99
2.05
2.07
3.09
f1 (ppm)


196.24
165.10
154.83
148.39
139.09
135.87
135.69
130.52
127.51
125.81
121.41
121.21
47.52
46.64
39.05
37.28
35.73
22.36
21.89
Cl
N
O
4
f1 (ppm)


O
N
O
5
1.00
1.03
5.16
2.11
1.10
3.08
1.09
1.07
1.07
2.04
2.01
2.00
3.07
f1 (ppm)


198.20
173.06
166.46
147.99
139.66
135.31
130.44
127.37
125.53
121.60
120.62
116.50
54.75
47.45
46.45
36.51
34.81
25.01
21.70
20.67
O
N
O
5
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


11.884
8.491
8.488
8.485
8.479
8.476
8.473
7.614
7.609
7.594
7.589
7.575
7.570
7.156
7.143
7.138
7.124
7.121
7.063
7.055
7.047
6.665
6.657
6.652
6.648
6.642
3.027
2.996
2.933
2.894
2.883
2.851
2.500
2.461
2.453
2.448
2.444
2.439
2.434
1.327
O
OH
N
6
0.99
1.00
1.03
2.06
3.05
2.07
1.07
2.10
1.08
3.09
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


173.33
165.02
146.25
138.28
136.38
130.30
127.91
126.69
122.74
122.62
53.41
48.16
47.18
43.48
26.23
O
OH
N
6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2022-04-01 10:11:35

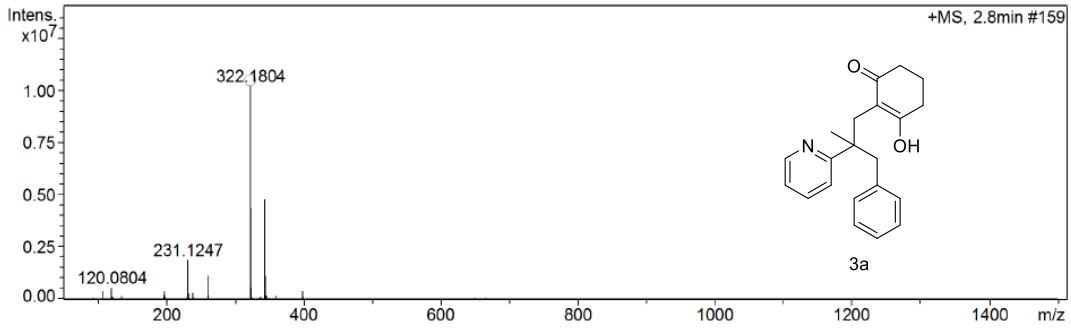
Analysis Name F:\gaofenbian(xiepengfei)\0331_RE5_01_12399.d

Method	LC_NO UV_P50-1500_6MIN.m	Operator	Demo User
Sample Name	0331	Instrumen compact	8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
322.1804	1	C21H24NO2	322.1802	-0.9	111.6	1	100.00	11.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2022-01-17 23:50:54

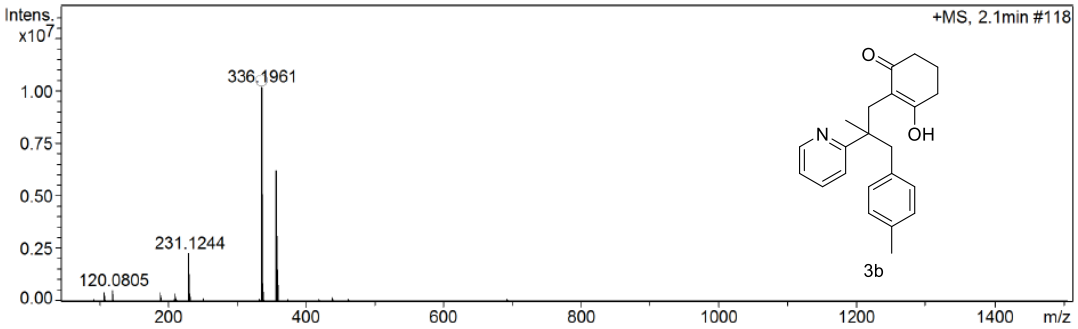
Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BD5_01_11138.d

Method	LC_NO UV_P50-1500_6MIN.m	Operator	Demo User
Sample Name	0114	Instrumen compact	8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
336.1961	1	C22H26NO2	336.1958	-0.8	229.4	1	100.00	11.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2022-01-18 0:20:34

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BE1_01_11142.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

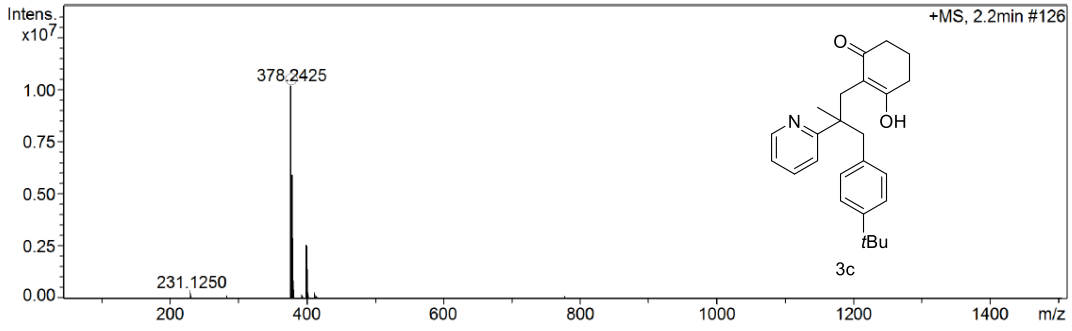
Sample Name 0114

Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
378.2425	1	C25H32NO2	378.2428	0.8	177.9	1	100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2022-01-17 23:43:33

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BD4_01_11137.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

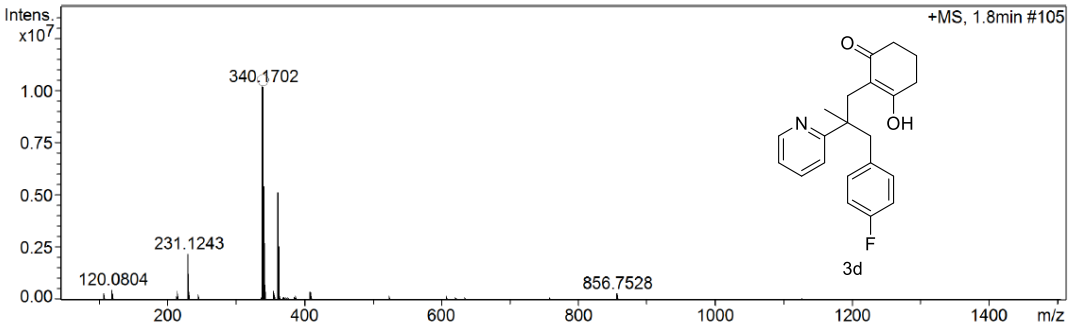
Sample Name 0114

Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
340.1702	1	C21H23FNO2	340.1707	1.5	174.9	1	100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-01-17 22:42:55

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BC4_01_11129.d

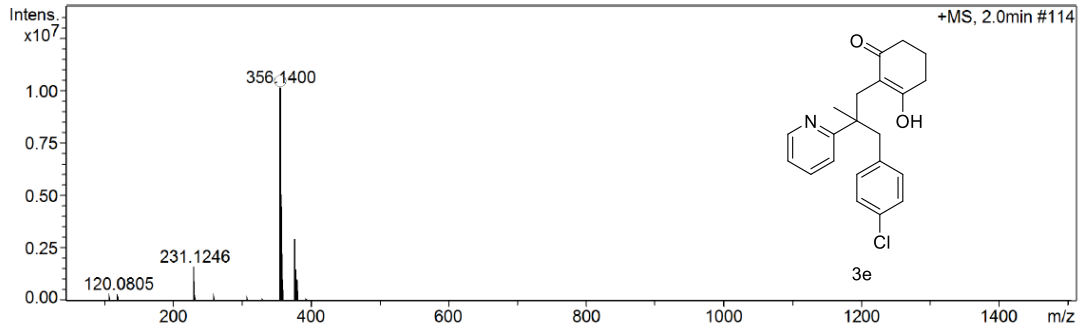
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0114 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
356.1400	1	C21H23ClNO2	356.1412	3.2	51.5	1		100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-01-17 22:51:02

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BC5_01_11130.d

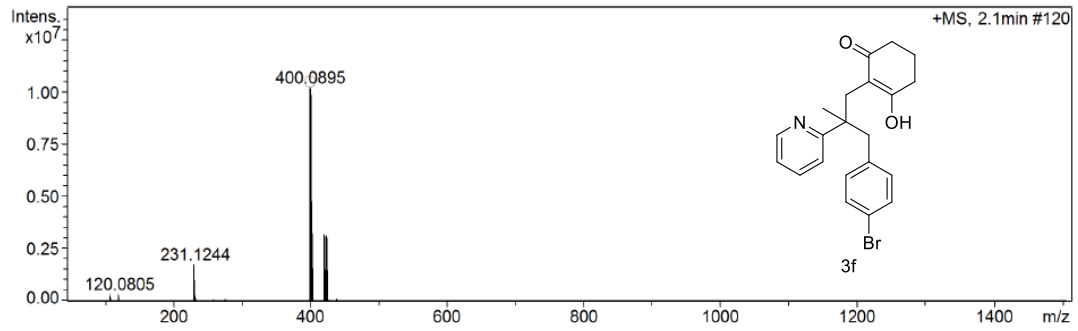
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0114 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
400.0895	1	C21H23BrNO2	400.0907	3.0	61.7	1		100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-01-17 23:06:32

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BC7_01_11132.d

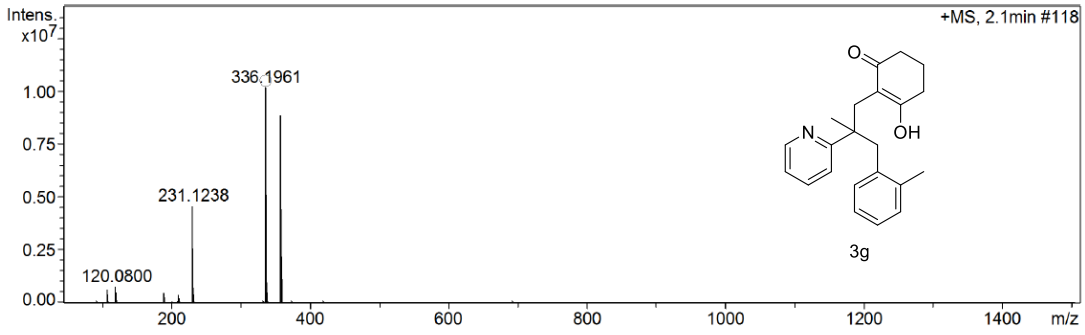
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0114 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
336.1961	1	C22H26NO2	336.1958	-0.9	286.0		1	100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-01-17 22:20:52

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BC1_01_11126.d

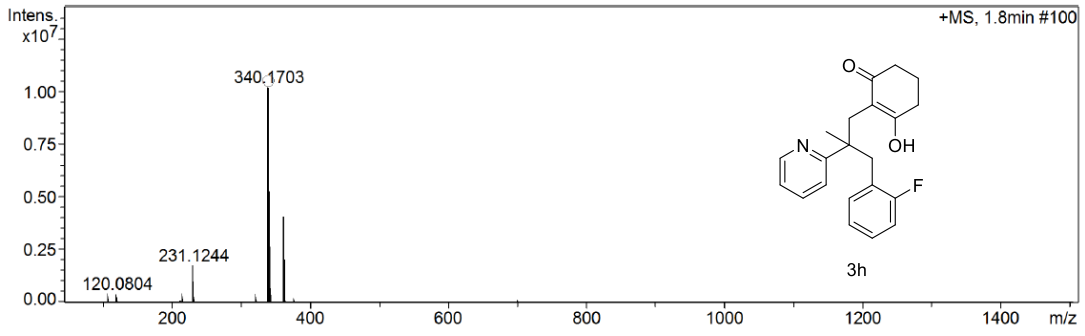
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0114 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
340.1703	1	C21H23FNO2	340.1707	1.3	163.9		1	100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-01-17 23:14:08

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BC8_01_11133.d

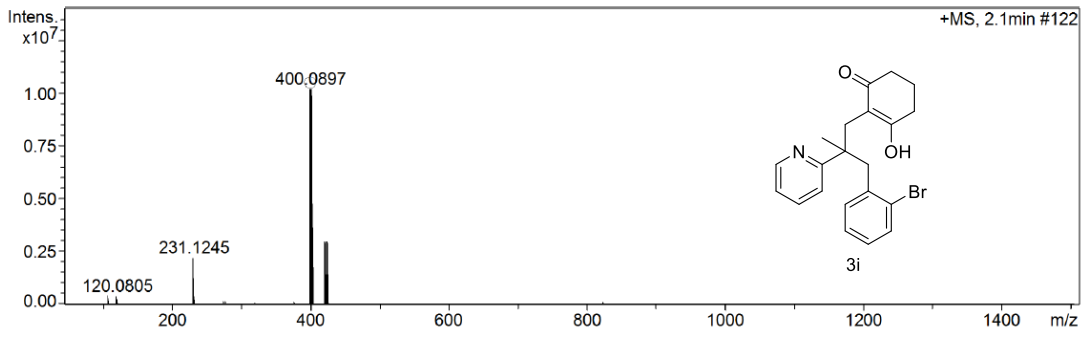
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0114 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
400.0897	1	C21H23BrNO2	400.0907	2.4	87.5	1		100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-01-17 23:58:16

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BD6_01_11139.d

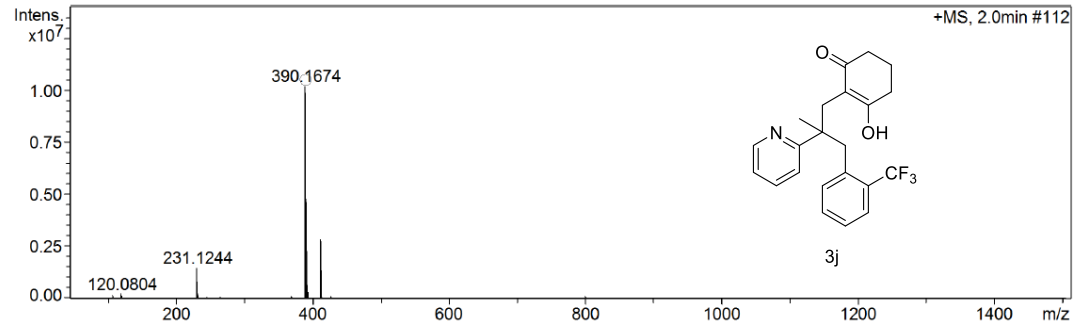
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0114 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
390.1674	1	C22H23F3NO2	390.1675	0.4	129.5	1		100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-01-18 0:13:14

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BD8_01_11141.d

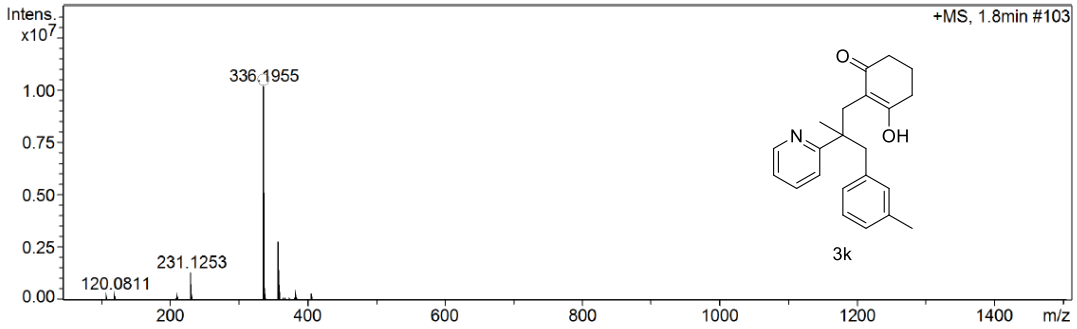
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0114 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
336.1955	1	C22H26NO2	336.1958	1.0	109.5	1	100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-01-17 22:13:30

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BB8_01_11125.d

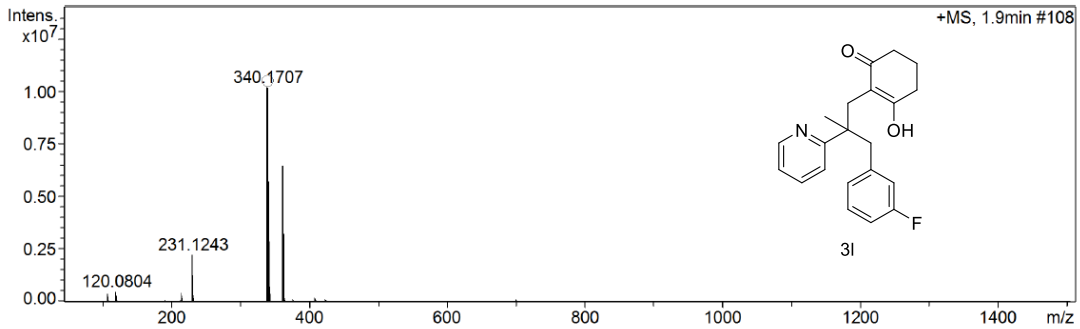
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0114 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
340.1707	1	C21H23FNO2	340.1707	0.1	190.9	1	100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-01-17 22:35:32

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BC3_01_11128.d

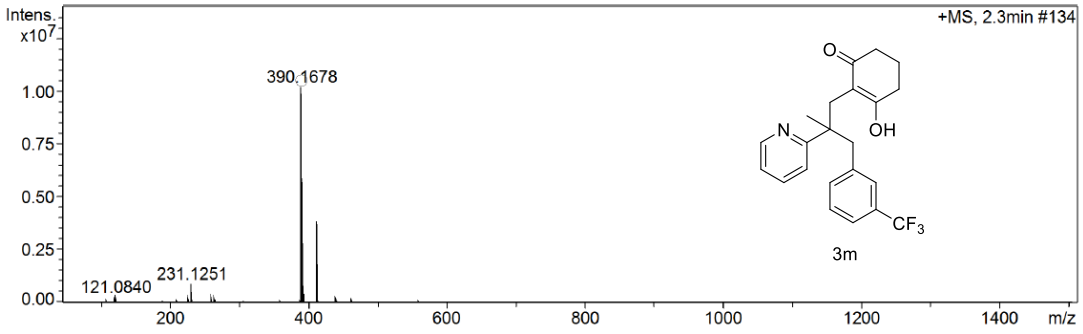
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0114 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
390.1678	1	C22H23F3NO2	390.1675	-0.6	194.2		1	100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-04-01 10:19:11

Analysis Name F:\gaofenbian(xiepengfei)\0331_RE6_01_12400.d

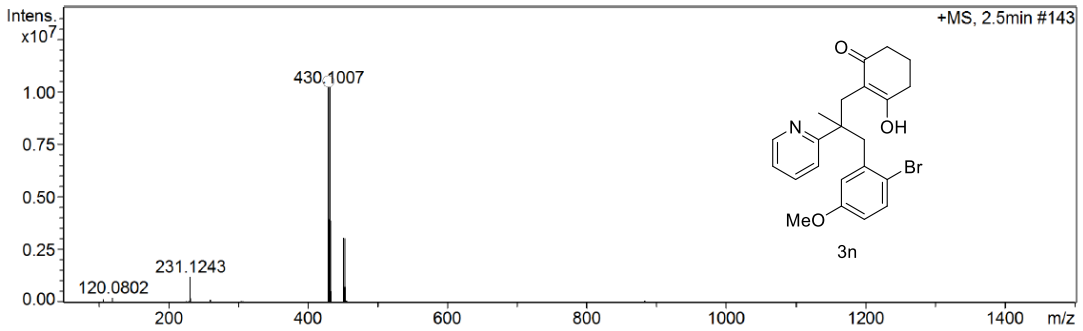
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0331 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
430.1007	1	C22H25BrNO3	430.1012	1.4	90.3		1	100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-01-17 23:21:30

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BD1_01_11134.d

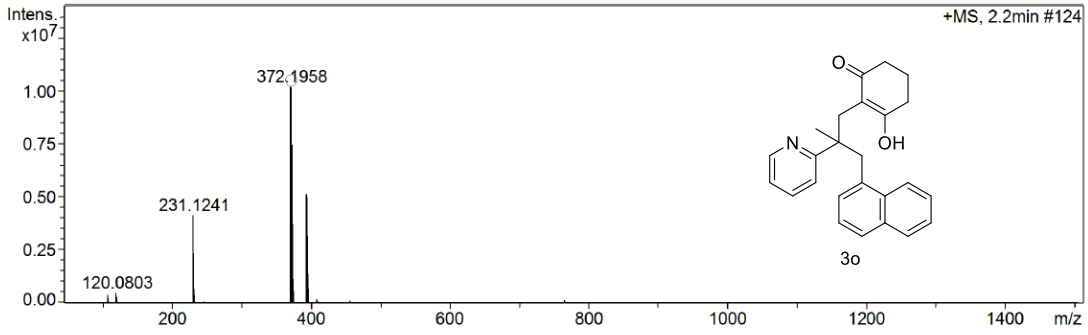
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0114 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥ Conf	N-Rule
372.1958	1	C25H26NO2	372.1958	0.0	265.5	1		100.00	14.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-01-17 23:36:11

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BD3_01_11136.d

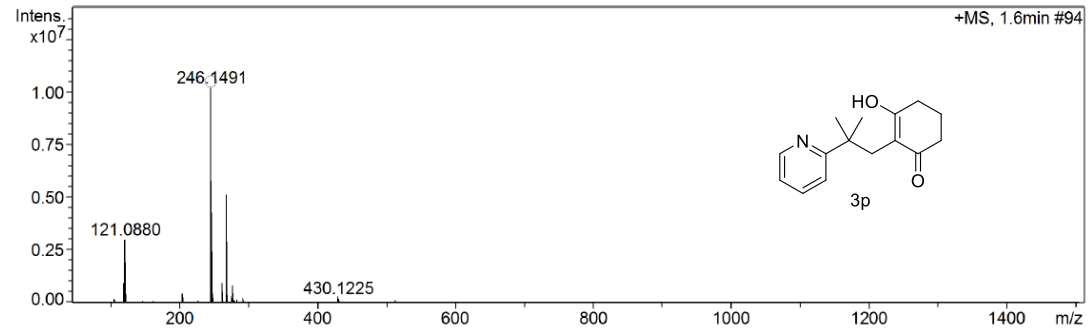
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0114 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥ Conf	N-Rule
246.1491	1	C15H20NO2	246.1489	-1.0	146.1	1		100.00	7.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-01-17 22:28:11

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BC2_01_11127.d

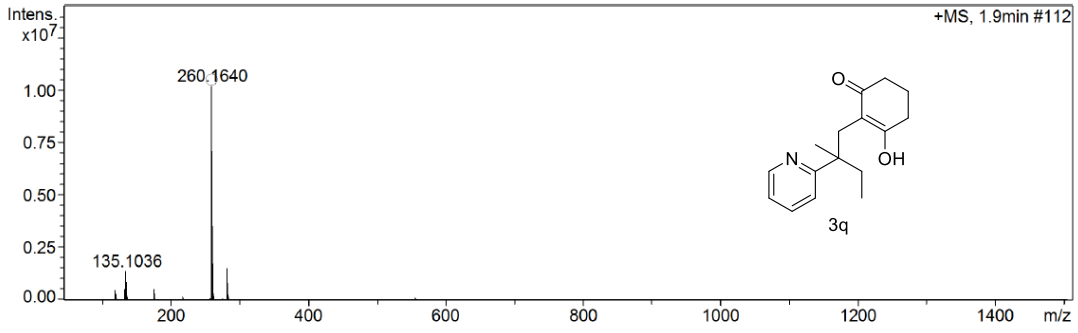
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0114 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
260.1640	1	C16H22NO2	260.1645	1.9	62.0	1	100.00	7.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-01-18 0:05:52

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BD7_01_11140.d

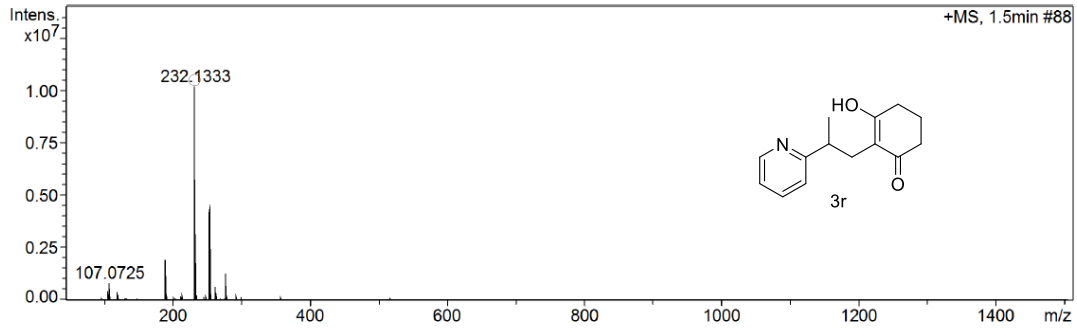
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0114 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
232.1333	1	C14H18NO2	232.1332	-0.5	88.5	1	100.00	7.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-01-17 23:28:52

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BD2_01_11135.d

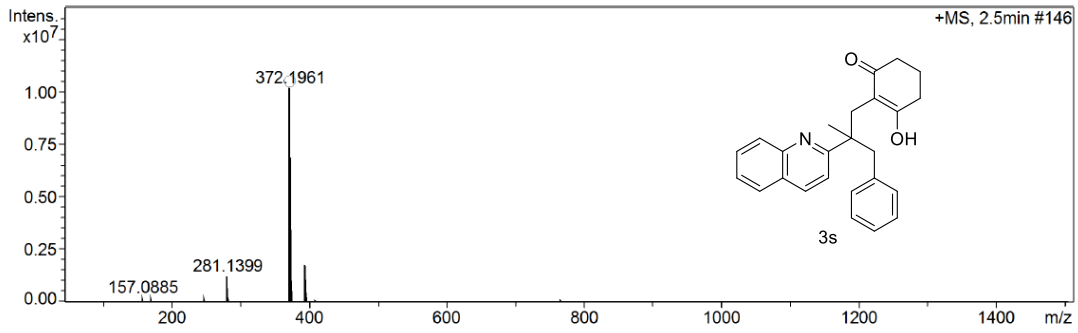
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0114 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
372.1961	1	C25H26NO2	372.1958	-0.8	231.4	1	100.00	14.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-01-17 22:58:23

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BC6_01_11131.d

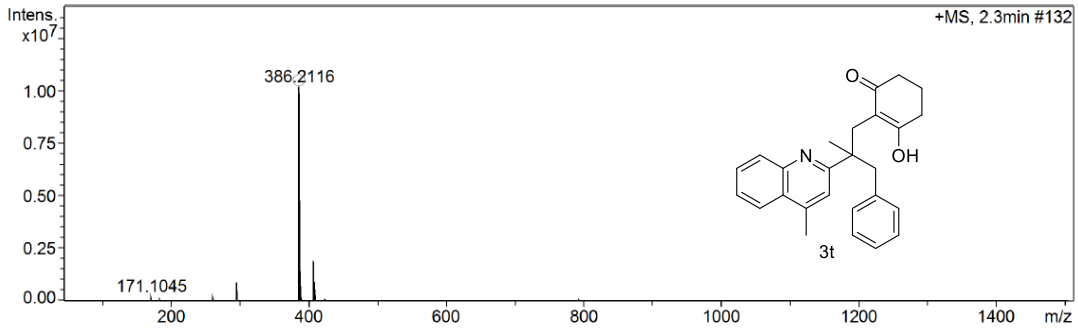
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0114 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
386.2116	1	C26H28NO2	386.2115	-0.4	368.5	1	100.00	14.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-04-01 10:04:14

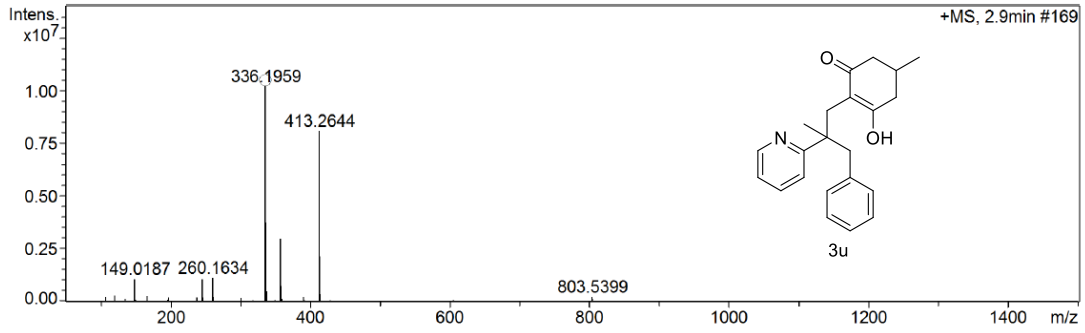
Analysis Name F:\gaofenbian(xiepengfei)\0331_RE4_01_12398.d

Method	LC_NO UV_P50-1500_6MIN.m	Operator	Demo User
Sample Name	0331	Instrumen compact	8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
336.1959	1	C22H26NO2	336.1958	-0.1	71.1	1	100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-04-01 9:39:34

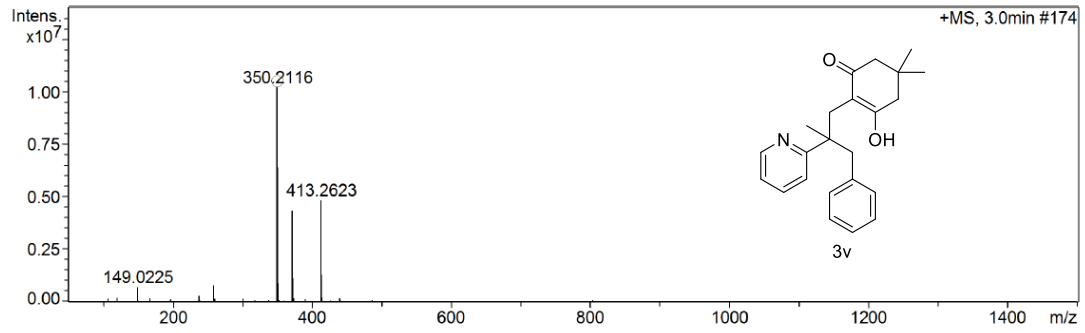
Analysis Name F:\gaofenbian(xiepengfei)\0331_RE1_01_12395.d

Method	LC_NO UV_P50-1500_6MIN.m	Operator	Demo User
Sample Name	0331	Instrumen compact	8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥	Conf	N-Rule
350.2116	1	C23H28NO2	350.2115	-0.4	215.9	1	100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-04-01 9:31:42

Analysis Name F:\gaofenbian(xiepengfei)\0331_RD8_01_12394.d

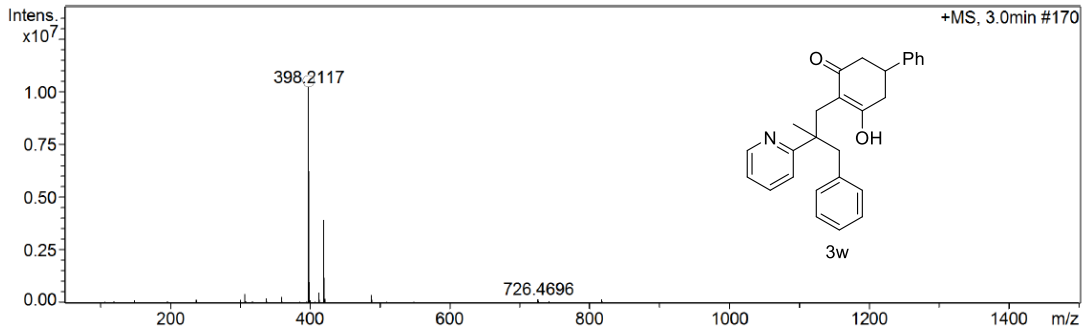
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0331 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
398.2117	1	C27H28NO2	398.2115	-0.6	182.7		1	100.00	15.0	even		ok
	1	C27H28NO2	398.2115	-0.6	182.7		1	100.00	15.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-04-01 10:27:04

Analysis Name F:\gaofenbian(xiepengfei)\0331_RE7_01_12401.d

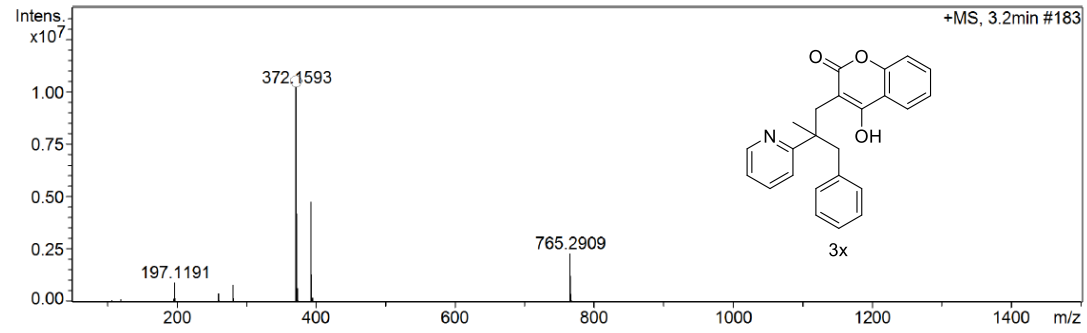
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0331 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
372.1593	1	C24H22NO3	372.1594	0.4	85.3		1	100.00	15.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-04-01 9:16:42

Analysis Name F:\gaofenbian(xiepengfei)\0331_RD6_01_12392.d

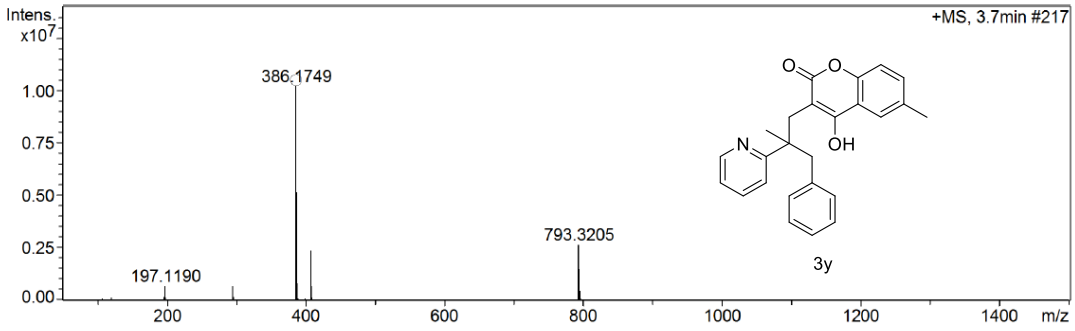
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0331 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
386.1749	1	C25H24NO3	386.1751	0.5	132.5	1		100.00	15.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-04-01 9:24:04

Analysis Name F:\gaofenbian(xiepengfei)\0331_RD7_01_12393.d

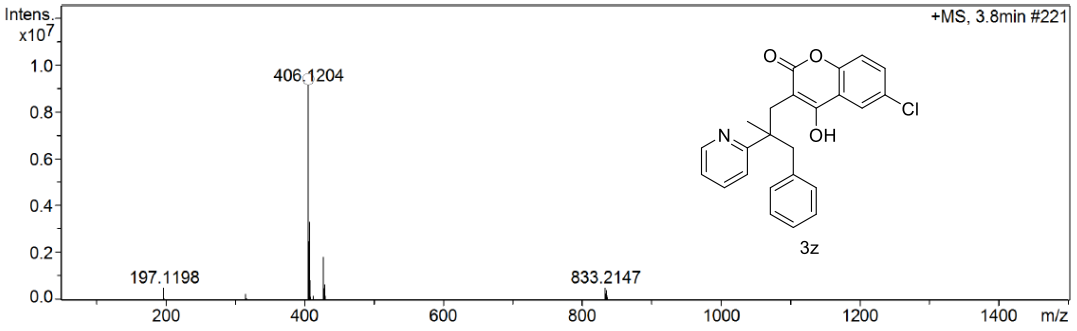
Method LC_NO UV_P50-1500_6MIN.m — Operator Demo User

Sample Name 0331 — Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
406.1204	1	C24H21ClNO3	406.1204	0.1	4.3	1		100.00	15.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-04-01 9:55:50

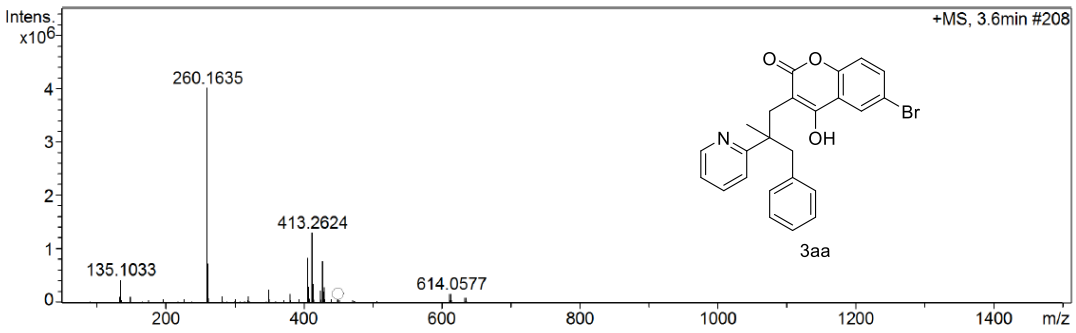
Analysis Name F:\gaofenbian(xiepengfei)\0331_RE3_01_12397.d

Method	LC_NO UV_P50-1500_6MIN.m	Operator	Demo User
Sample Name	0331	Instrumen	compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
450.0700	1	C24H21BrNO3	450.0699	-0.2	76.9	1	100.00	15.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info — Acquisition D 2022-04-01 9:08:33

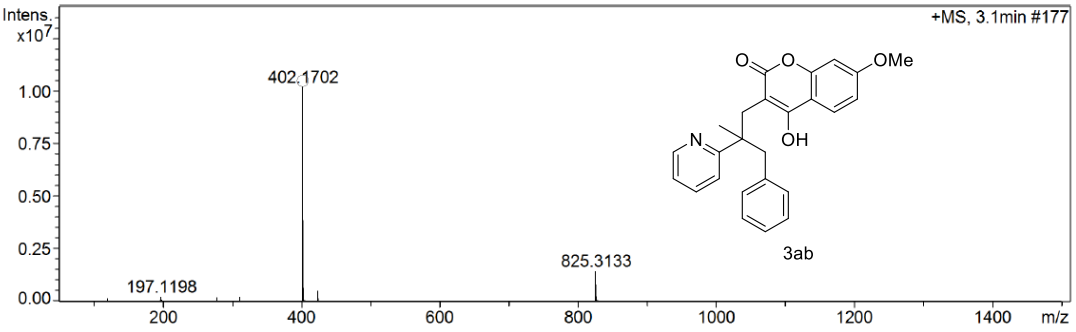
Analysis Name F:\gaofenbian(xiepengfei)\0331_RD5_01_12391.d

Method	LC_NO UV_P50-1500_6MIN.m	Operator	Demo User
Sample Name	0331	Instrumen	compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
402.1702	1	C25H24NO4	402.1700	-0.6	59.0	1	100.00	15.0	even	ok

Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2022-01-18 0:27:57

Analysis Name F:\gaofenbian(xiepengfei)\GHX MS\0114_BE2_01_11143.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

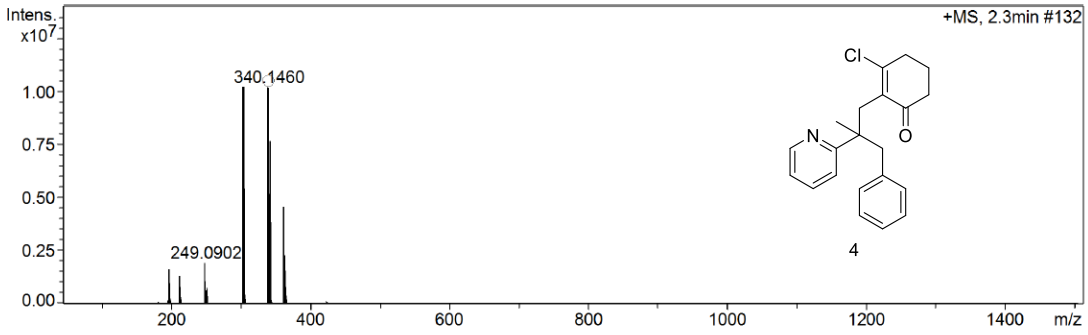
Sample Name 0114

Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
340.1460	1	C21H23ClNO	340.1463	0.7	221.3	1		100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2022-04-06 9:45:50

Analysis Name g:\Desktop\aa\0404_GD3_01_12544.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

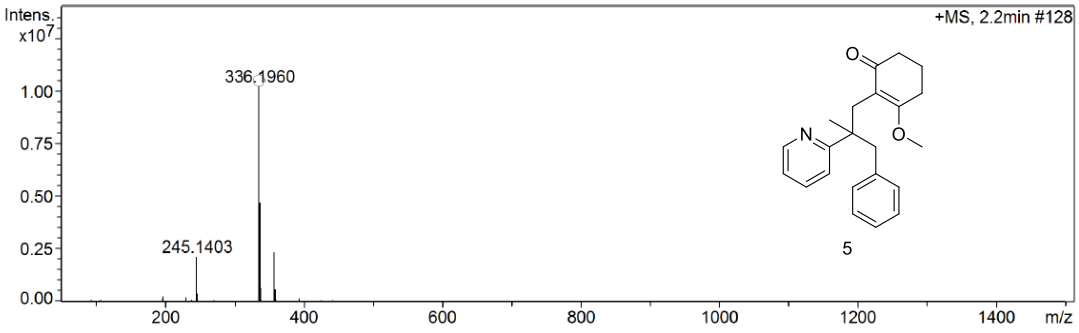
Sample Name 0404

Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e¡¥	Conf	N-Rule
336.1960	1	C22H26NO2	336.1958	-0.5	125.9	1		100.00	11.0	even		ok

Mass Spectrum SmartFormula Report

Analysis Info

Acquisition D 2022-04-06 9:53:43

Analysis Name g:\Desktop\aa\0404_GD4_01_12545.d

Method LC_NO UV_P50-1500_6MIN.m

Operator Demo User

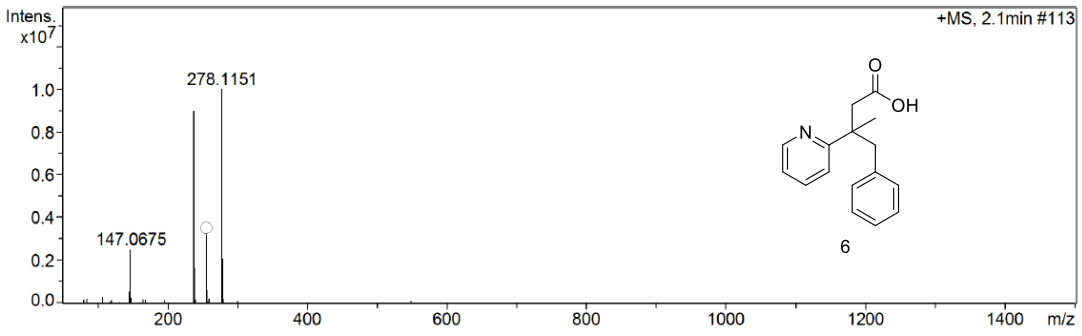
Sample Name 0404

Instrumen compact 8255754.2017 6

Comment

Acquisition Paramet

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Charging	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¡¥ Conf	N-Rule
256.1328	1	C16H18NO2	256.1332	1.7	1.3	1	100.00	9.0	even	ok