

Supporting Information

Facile access to chiral chromanone-2-carboxylic acids enabled by Rhodium-catalyzed chemo- and enantioselective hydrogenation

Zhuang Nie,^{a,b, ‡} Song Liu,^{c, ‡} Tonglin Wang,^b Zhanhong Shen,^b Huifang Nie,^b Jiayue Xi,^b Dongxu Zhang,^b Xiaohui Zheng,^{*, a} Shengyong Zhang^{*, b} and Lin Yao^{*, b}

^a Key Laboratory of Resource Biology and Biotechnology in Western China, Ministry of Education, The College of Life Science, Northwest University, Xi'an 710069, PR China.

^b Department of Medicinal Chemistry and Pharmaceutical Analysis, School of Pharmacy, Fourth Military Medical University, Xi'an, 710032, PR China.

^c Chongqing Key Laboratory of Environmental Materials and Remediation Technologies, Chongqing University of Arts and Sciences, Chongqing, 402160, PR China

E-mail: zhengxh@nwu.edu.cn; syzhang@fmmu.edu.cn; yaolinlin@fmmu.edu.cn

Table of Contents

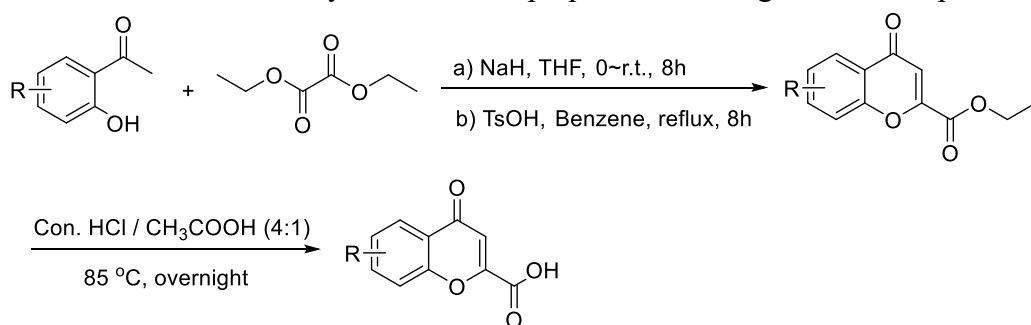
1. General Information.....	S3
2. Preparation and Characterization of Substrates.....	S3
3. Asymmetric Hydrogenation of Chromone-2-carboxylic acids.....	S11
3.1 General Procedure of Asymmetric Hydrogenation.....	S11
3.2 Ligands Screening in Asymmetric Hydrogenation.....	S11
4. Analytical Data of Hydrogenation Products.....	S13
5. Scale-up Synthesis and Transformations.....	S21
6. X-ray Analysis.....	S23
7. Computational Details.....	S25
8. NMR Spectra.....	S57
9. HPLC Spectra.....	S114
10. Reference.....	S142

1. General information

Unless otherwise noted, all experiments dealing with air- or moisture-sensitive compounds were carried out in the argon-filled glove box or using standard Schlenk techniques and oil bath were utilized as the heat source. All commercially available chemicals including solvents were used without further purification. ^1H NMR, ^{13}C NMR were recorded on a Bruker ADVANCE III (400 MHz) spectrometer with CDCl_3 , CD_3OD , DMSO-d as the solvent and tetramethylsilane (TMS) as the internal standard. Enantiomeric excesses were determined by Daicel chiral column on an Agilent 1260 Series HPLC instrument. Optical rotations were measured on a PERKIN ELMER polarimeter 343 instruments. High-Resolution Mass Spectroscopy (HRMS) was carried out on a VARIA FT-ICR MS. The absolute configuration of the hydrogenation products was determined by comparison of analytical data with the literature.

2. Preparation and characterization of substrates

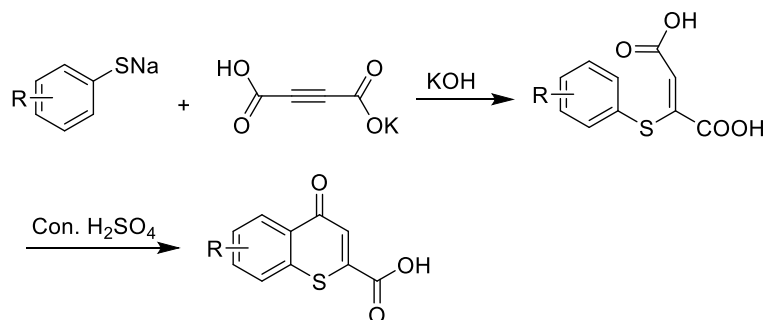
The 4-oxo-4H-chromene-2-carboxylic acids were prepared according to literature procedure.¹



Sodium hydride (60% dispersion in mineral oil, 2.07 g, 86.2 mmol) was rinsed three times with hexanes, then suspended in THF (40 mL). A mixture of 2'-hydroxyacetophenone (22.0 mmol) and diethyl oxalate (55.1 mmol) in THF (2.5 mL) was added dropwise to the above suspension at 0°C. After complete addition, the reaction mixture was stirred for a further 8h at r.t., then quenched by pouring onto ice and further acidified to pH 6 with 6 M aq HCl. The solution was extracted with ethyl acetate and the combined organic layers were washed with brine and dried over magnesium sulfate. The solvent was evaporated to yield the crude 1, 3-dione. Without further purification, a solution of the crude 1, 3-dione product (14.0 mmol) was dissolved in benzene (40 mL) and was treated by 277.5 mg TsOH, and the mixture allowed to reflux for 8 h. After completion of the reaction, the mixture was washed with saturated aq. NaHCO_3 and was extracted by EtOAc for three times, the combined organics were purified by column chromatography to afford the pure chromone-2-carboxylate.

2g of the chromone-2-carboxylate was added in a 250 mL round-bottom flask, and treated with 20 mL concentrated HCl and 80 mL glacial acetic acid. The mixture was stirred under 85°C overnight, and then was cooled to room temperature, the corresponding chromone-2-carboxylic acid was precipitated and was filtered under reduced pressure.

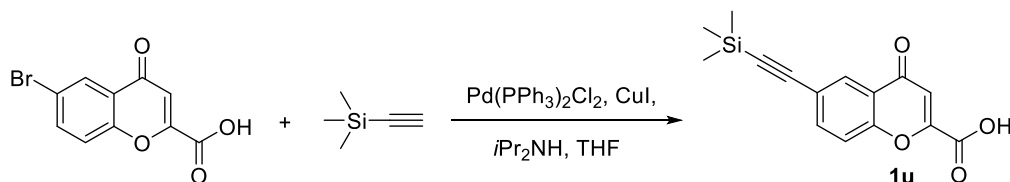
The 4-oxo-4H-thiochromene-2-carboxylic acids were prepared according to literature procedure.²



Sodium benzenethiolate (15 mmol) was dissolved in water (30 mL) containing KOH (45 mmol, 2.52g). Solid acetylene dicarboxylic acid mono potassium salt (15 mmol, 2.28g) was then added and the mixture was heated at 50°C for one hour. The cool solution was poured into water and the aqueous solution was washed with dichloromethane, adjusted to pH 2~3 with 3M HCl. The titled product was precipitated and filtered under reduce pressure, used directly in the next step.

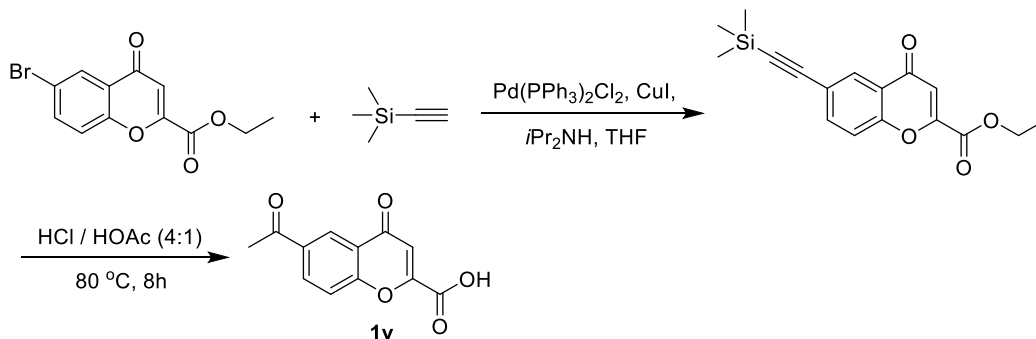
To 8 mL of concentrated sulphuric acid was slowly the above obtained 2-(phenylthio) fumaric acid with stirring. After standing for 1 hour, the solution was poured onto cold ice and the precipitated greenish sold was filtered off, washed with water until acid-free and dried. The crude solid was crystallized from ethanol to give the 4-oxo-4H-thiochromene-2-carboxylic acid.

The alkyne functionalized substrate **1u** was prepared according to literature procedure.³



In a 50 mL sealed tube, a solution of 6-bromo-4-oxo-4H-chromene-2-carboxylic acid **1m** (269 mg, 1 mmol), Pd(PPh₃)₂Cl₂ (28 mg, 0.04 mmol) and CuI (3.8 mg, 0.02 mmol) in dry THF (10 mL) was degassed and *i*Pr₂NH (0.28 mL, 2 mmol) was added. After 10 min, trimethylsilylacetylene (0.21 mL, 1.5 mmol) was added slowly and mixture was left to stir at 45°C. After completion of reaction (monitored by TLC), the reaction mixture was filtered through acelite pad. The organic layer was evaporated under reduced pressure and the resulting crude mixture was purified by silica gel column chromatography to afford the pure product as a light yellow solid.

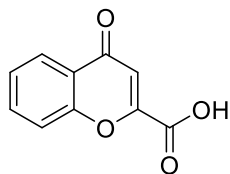
6-acetyl-4-oxo-4H-chromene-2-carboxylic acid **1v** was prepared following literature procedure.³



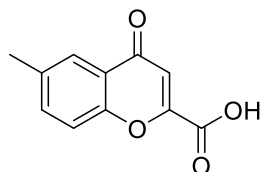
In a 250 mL sealed tube, a solution of ethyl 6-bromo-4-oxo-4H-chromene-2-carboxylate (2 g, 7 mmol), Pd(PPh₃)₂Cl₂ (196.5 mg, 0.28 mmol) and CuI (26.6 mg, 0.14 mmol) in dry THF (80 mL) was degassed and *i*Pr₂NH (1.96 mL, 14mmol) was added. After 10 min, trimethylsilylacetylene (1.48 mL, 10.5 mmol) was added slowly and mixture was left to stir at 45°C. After completion of reaction (monitored by TLC), the reaction mixture was filtered through acelite pad. The organic layer was evaporated under reduced pressure and used directly in the next step.

The aboved-obtained crude product was dissolved in a solution of concentrated hydrochloric acid and glacial acetic acid (4:1) and stirred at 80°C overnight. After completion of reaction, extracted with ethyl acetate for three times. The organic layers were collected and evaporated under reduced pressure. The obtained crude product was purified by silica gel column chromatography to afford the pure product as a white solid.

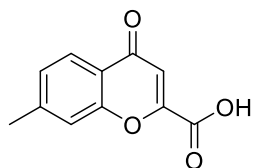
Characterization data of all the unsaturated acids was showed as followings:



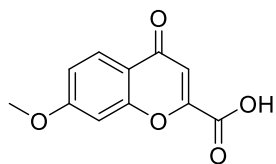
4-oxo-4H-chromene-2-carboxylic acid (1a): 89% yield, white solid. Mp:216-217°C. ¹H NMR (400 MHz, DMSO-d₆) δ 8.06 (d, *J*=7.3 Hz, 1H), 7.89 (t, *J*=7.2 Hz, 1H), 7.75 (d, *J*=8.5 Hz, 1H), 7.55 (t, *J*=7.5 Hz, 1H), 6.92 (s, 1H). ¹³C NMR (100 MHz, DMSO-d₆) δ 177.59, 161.41, 155.44, 153.27, 135.18, 126.06, 124.91, 123.72, 118.88, 113.47. HRMS (ESI): *m/z* for C₁₀H₆O₄ [M+H]⁺ calcd 191.0266, found 191.0326.



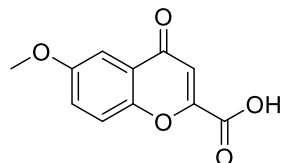
6-methyl-4-oxo-4H-chromene-2-carboxylic acid (1b): 87% yield, white solid. Mp:232-233°C. ¹H NMR (400 MHz, DMSO-d₆) δ 8.16 (s, 1H), 7.90 (d, *J*= 8.3 Hz, 1H), 7.66 (d, *J*= 8.2 Hz, 1H), 7.47 (s, 1H), 2.47 (s, 3H). ¹³C NMR (100 MHz, DMSO-d₆) δ 177.50, 161.45, 153.72, 153.10, 136.23, 135.76, 124.11, 123.44, 118.65, 113.29, 20.39. HRMS (ESI): *m/z* for C₁₁H₈O₄ [M+H]⁺ calcd 205.0423, found 205.0478.



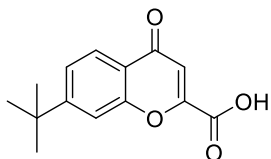
7-methyl-4-oxo-4H-chromene-2-carboxylic acid (1c): 89% yield, white solid. Mp:213-214°C. ¹H NMR (400 MHz, DMSO-d₆) δ 7.93 (d, *J*= 8.1 Hz, 1H), 7.53 (s, 1H), 7.35 (d, *J*= 8.1 Hz, 1H), 6.87 (s, 1H), 2.48 (s, 3H). ¹³C NMR (100 MHz, DMSO-d₆) δ 177.26, 161.43, 155.50, 152.99, 146.26, 127.38, 124.63, 121.51, 118.29, 113.44, 21.21. HRMS (ESI): *m/z* for C₁₁H₈O₄ [M+H]⁺ calcd 205.0423, found 205.0481.



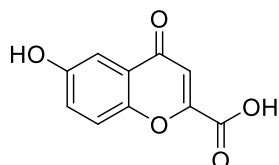
7-methoxy-4-oxo-4H-chromene-2-carboxylic acid (1d): 87% yield, white solid. Mp:215-217°C. ¹H NMR (400 MHz, DMSO-d₆) δ 7.96 (d, *J* = 8.9 Hz, 1H), 7.24 (d, *J* = 2.2 Hz, 1H), 7.12 (dd, *J* = 8.9, 2.3 Hz, 1H), 6.86 (s, 1H), 3.93 (s, 3H). ¹³C NMR (100 MHz, DMSO-d₆) δ 176.59, 164.51, 161.39, 157.38, 152.90, 126.31, 117.60, 115.52, 113.64, 100.96, 56.24. HRMS (ESI): *m/z* for C₁₁H₈O₅ [M+H]⁺ calcd 221.0372, found 221.0430.



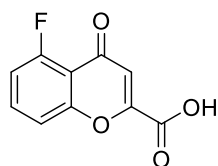
6-methoxy-4-oxo-4H-chromene-2-carboxylic acid (1e): 88% yield, white solid. Mp:212-213°C. ¹H NMR (400 MHz, DMSO-d₆) δ 7.72 (d, *J* = 9.2 Hz, 1H), 7.48 (dd, *J* = 9.2, 3.1 Hz, 1H), 7.42 (d, *J* = 3.0 Hz, 1H), 6.90 (s, 1H), 3.88 (s, 3H). ¹³C NMR (100 MHz, DMSO-d₆) δ 177.25, 161.44, 156.97, 152.97, 150.15, 124.38, 120.52, 112.52, 104.51, 55.79. HRMS (ESI): *m/z* for C₁₁H₈O₅ [M+H]⁺ calcd 221.0372, found 221.0428.



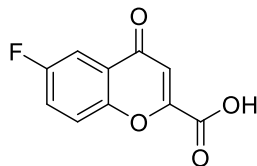
7-(tert-butyl)-4-oxo-4H-chromene-2-carboxylic acid (1f): 86% yield, white solid. Mp:204-205°C. ¹H NMR (400 MHz, DMSO-d₆) δ 7.98 (d, *J* = 8.2 Hz, 1H), 7.62 (d, *J* = 9.0 Hz, 2H), 6.89 (s, 1H), 1.36 (s, 9H). ¹³C NMR (100 MHz, DMSO-d₆) δ 177.21, 161.44, 158.89, 155.48, 153.12, 124.57, 123.78, 121.48, 114.86, 113.50, 35.22, 30.52. HRMS (ESI): *m/z* for C₁₄H₁₄O₄ [M+H]⁺ calcd 247.0892, found 247.0949.



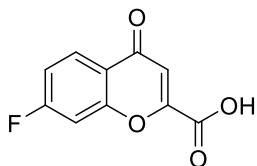
6-hydroxy-4-oxo-4H-chromene-2-carboxylic acid (1g): 75% yield, white solid. Mp:275-276°C. ¹H NMR (400 MHz, DMSO-d₆) δ 10.18 (s, 1H), 7.67-7.57 (m, 1H), 7.30 (d, *J* = 2.7 Hz, 2H), 6.84 (s, 1H). ¹³C NMR (100 MHz, DMSO-d₆) δ 177.36, 161.54, 155.32, 152.81, 149.10, 124.70, 124.14, 120.27, 112.22, 107.28. HRMS (ESI): *m/z* for C₁₀H₆O₅ [M+H]⁺ calcd 207.0215, found 207.0275.



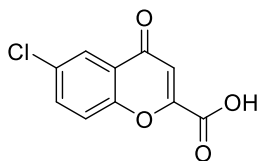
5-fluoro-4-oxo-4H-chromene-2-carboxylic acid (1h): 90% yield, white solid. Mp:207-208°C. ¹H NMR (400 MHz, DMSO-d₆) δ 7.85 (dd, *J* = 14.2, 8.3 Hz, 1H), 7.55 (d, *J* = 8.5 Hz, 1H), 7.30 (dd, *J* = 10.3, 8.9 Hz, 1H), 6.82 (s, 1H). ¹³C NMR (100 MHz, DMSO-d₆) δ 181.07, 166.37, 165.97, 163.36, 161.57, 157.47, 140.59, 120.10, 119.76, 119.29, 117.76, 117.56. ¹⁹F NMR (100 MHz, DMSO-d₆) -112.82. HRMS (ESI): *m/z* for C₁₀H₅FO₄ [M+H]⁺ calcd 209.0172, found 209.0230.



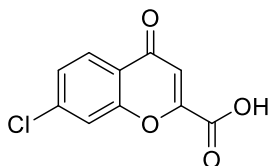
6-fluoro-4-oxo-4H-chromene-2-carboxylic acid (1i): 89% yield, white solid. Mp:196-197°C. ¹H NMR (400 MHz, DMSO-d₆) δ 7.87 (dd, *J* = 9.2, 4.3 Hz, 1H), 7.82-7.76 (m, 1H), 7.74 (dd, *J* = 8.3, 3.0 Hz, 1H), 6.93 (s, 1H). ¹³C NMR (100 MHz, DMSO-d₆) δ 177.02, 161.25, 160.43, 158.00, 153.52, 151.90, 124.91, 123.44, 123.19, 121.78, 112.61, 109.63, 109.40. ¹⁹F NMR (100 MHz, DMSO-d₆) δ -114.53. HRMS (ESI): *m/z* for C₁₀H₅FO₄ [M+H]⁺ calcd 209.0172, found 209.0230.



7-fluoro-4-oxo-4H-chromene-2-carboxylic acid (1j): 86% yield, white solid. Mp:205-206°C. ¹H NMR (400 MHz, DMSO-d₆) δ 8.12 (dd, *J* = 8.7, 6.5 Hz, 1H), 7.74 (dd, *J* = 9.6, 2.0 Hz, 1H), 7.43 (td, *J* = 8.7, 2.1 Hz, 1H), 6.92 (s, 1H). ¹³C NMR (100 MHz, DMSO-d₆) δ 176.66, 166.71, 164.19, 161.14, 156.55, 153.53, 127.79, 120.89, 114.81, 114.58, 113.65, 105.74, 105.48. ¹⁹F NMR (100 MHz, DMSO-d₆) δ -101.99. HRMS (ESI): *m/z* for C₁₀H₅FO₄ [M+H]⁺ calcd 209.0172, found 209.0231.

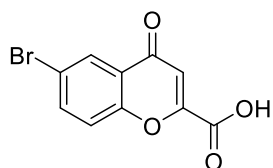


6-chloro-4-oxo-4H-chromene-2-carboxylic acid (1k): 85% yield, white solid. Mp:217-218°C. ¹H NMR (400 MHz, DMSO-d₆) δ 7.99 (d, *J* = 2.2 Hz, 1H), 7.92 (dd, *J* = 9.0, 2.5 Hz, 1H), 7.82 (d, *J* = 9.0 Hz, 1H), 6.95 (s, 1H). ¹³C NMR (100 MHz, DMSO-d₆) δ 176.58, 161.17, 154.03, 153.54, 135.00, 130.51, 124.82, 123.88, 121.41, 113.35. HRMS (ESI): *m/z* for C₁₀H₅ClO₄ [M+H]⁺ calcd 224.9876, found 224.9933.

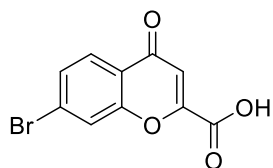


7-chloro-4-oxo-4H-chromene-2-carboxylic acid (1l): 87% yield, white solid. Mp:209-211°C. ¹H NMR (400 MHz, DMSO-d₆) δ 8.05 (d, *J* = 8.6 Hz, 1H), 7.96 (d, *J* = 1.6 Hz, 1H), 7.59 (dd, *J* = 8.6, 1.7 Hz, 1H), 6.93 (s, 1H). ¹³C NMR (100 MHz, DMSO-d₆) δ 176.89, 161.14, 155.68, 153.45, 139.43, 126.66, 122.56,

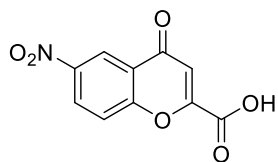
118.75, 113.75. HRMS (ESI): m/z for $C_{10}H_5ClO_4$ $[M+H]^+$ calcd 224.9876, found 224.9932.



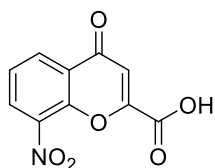
6-bromo-4-oxo-4H-chromene-2-carboxylic acid (1m): 83% yield, white solid. Mp:209-211°C. 1H NMR (400 MHz, DMSO- d_6) δ 8.11 (d, $J = 2.4$ Hz, 1H), 8.02 (dd, $J = 8.9, 2.5$ Hz, 1H), 7.73 (d, $J = 8.9$ Hz, 1H), 6.95 (s, 1H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 176.46, 171.96, 161.17, 154.43, 153.55, 137.73, 127.01, 125.21, 121.59, 118.49, 113.47, 21.02. HRMS (ESI): m/z for $C_{10}H_5BrO_4$ $[M+H]^+$ calcd 268.9371, found 268.9430.



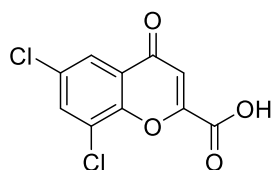
7-bromo-4-oxo-4H-chromene-2-carboxylic acid (1n): 82% yield, white solid. Mp:198-199°C. 1H NMR (400 MHz, DMSO- d_6) δ 8.08 (d, $J = 1.6$ Hz, 1H), 7.96 (d, $J = 8.5$ Hz, 1H), 7.72 (dd, $J = 8.5, 1.7$ Hz, 1H), 6.93 (s, 1H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 177.01, 161.13, 155.59, 153.31, 129.34, 128.21, 126.72, 122.83, 121.65, 113.77. HRMS (ESI): m/z for $C_{10}H_5BrO_4$ $[M+H]^+$ calcd 268.9371, found 268.9428.



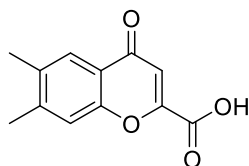
6-nitro-4-oxo-4H-chromene-2-carboxylic acid (1o): 85% yield, white solid. Mp:236-237°C. 1H NMR (400 MHz, DMSO- d_6) δ 8.70 (d, $J = 2.8$ Hz, 1H), 8.60 (dd, $J = 9.2, 2.8$ Hz, 1H), 7.99 (d, $J = 9.2$ Hz, 1H), 7.01 (s, 1H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 176.85, 160.95, 158.45, 153.93, 144.63, 129.14, 123.71, 121.20, 120.90, 113.71. HRMS (ESI): m/z for $C_{10}H_5NO_6$ $[M+H]^+$ calcd 236.0117, found 236.0183.



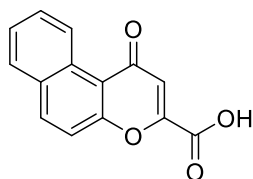
8-nitro-4-oxo-4H-chromene-2-carboxylic acid (1p): 78% yield, white solid. Mp:203-204°C. 1H NMR (400 MHz, DMSO- d_6) δ 8.54 (dd, $J = 7.9, 1.5$ Hz, 1H), 8.36 (dd, $J = 8.0, 1.5$ Hz, 1H), 7.70 (t, $J = 8.0$ Hz, 1H), 7.03 (s, 1H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 176.20, 160.77, 153.28, 147.48, 139.11, 130.60, 125.49, 125.27, 114.18. HRMS (ESI): m/z for $C_{10}H_5NO_6$ $[M+H]^+$ calcd 236.0117, found 236.0171.



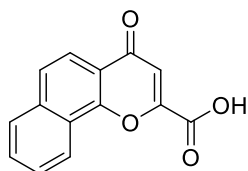
6,8-dichloro-4-oxo-4H-chromene-2-carboxylic acid (1q): 73% yield, white solid. Mp:202-203°C. ¹H NMR (400 MHz, DMSO-d₆) δ 8.26 (d, *J* = 2.0 Hz, 1H), 7.94 (d, *J* = 2.0 Hz, 1H), 6.99 (s, 1H). ¹³C NMR (100 MHz, DMSO-d₆) δ 176.22, 160.89, 153.58, 150.19, 134.49, 130.22, 125.81, 124.35, 123.09, 113.62. HRMS (ESI): *m/z* for C₁₀H₄Cl₂O₄ [M+H]⁺ calcd 258.9487, found 258.9536.



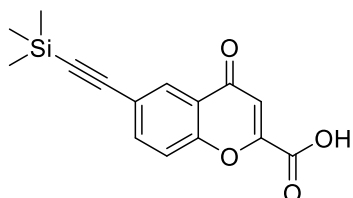
6,7-dimethyl-4-oxo-4H-chromene-2-carboxylic acid (1r): 87% yield, white solid. Mp:210-211°C. ¹H NMR (400 MHz, DMSO-d₆) δ 7.79 (s, 1H), 7.54 (s, 1H), 6.85 (s, 1H), 2.39 (s, 3H), 2.34 (s, 3H). ¹³C NMR (100 MHz, DMSO-d₆) δ 177.27, 161.51, 153.98, 152.96, 145.60, 135.27, 124.29, 121.63, 118.64, 113.32, 19.86, 18.86. HRMS (ESI): *m/z* for C₁₂H₁₀O₄ [M+H]⁺ calcd 219.0579, found 219.0635.



1-oxo-1H-benzo[f]chromene-3-carboxylic acid (1s): 84% yield, white solid. Mp:220-221°C. ¹H NMR (400 MHz, DMSO-d₆) δ 9.87 (d, *J* = 8.5 Hz, 1H), 8.40 (d, *J* = 9.2 Hz, 1H), 8.14 (d, *J* = 7.9 Hz, 1H), 7.81 (dd, *J* = 17.0, 8.7 Hz, 2H), 7.72 (t, *J* = 7.5 Hz, 1H), 7.06 (s, 1H). ¹³C NMR (100 MHz, DMSO-d₆) δ 179.27, 161.28, 157.01, 150.99, 136.72, 130.35, 129.37, 128.67, 127.00, 125.79, 118.04, 117.00, 116.49. HRMS (ESI): *m/z* for C₁₄H₈O₄ [M+H]⁺ calcd 241.0423, found 241.0480.

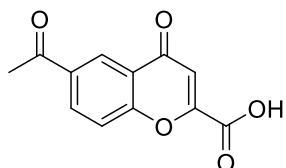


4-oxo-4H-benzo[h]chromene-2-carboxylic acid (1t): 86% yield, white solid. Mp:256-257°C. ¹H NMR (400 MHz, DMSO-d₆) δ 8.52-8.50 (m, 1H), 8.14 (dd, *J* = 6.1, 2.0 Hz, 1H), 7.98 (s, 2H), 7.92-7.78 (m, 2H), 7.07 (s, 1H). ¹³C NMR (100 MHz, DMSO-d₆) δ 177.16, 161.37, 152.69, 135.59, 130.00, 128.27, 127.90, 125.98, 123.34, 122.03, 120.25, 119.71, 114.78. HRMS (ESI): *m/z* for C₁₄H₈O₄ [M+H]⁺ calcd 241.0423, found 241.0477.

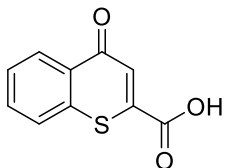


4-oxo-6-((trimethylsilyl)ethynyl)-4H-chromene-2-carboxylic acid (1u): 40% yield, light yellow solid.

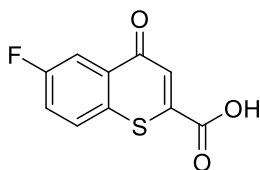
Mp: 217-218°C. ^1H NMR (400 MHz, DMSO- d_6) δ 8.01 (d, $J = 1.6$ Hz, 1H), 7.89 (dd, $J = 8.7, 1.8$ Hz, 1H), 7.74 (d, $J = 8.7$ Hz, 1H), 6.93 (s, 1H), 0.26 (s, 9H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 177.03, 161.45, 155.41, 153.74, 137.70, 128.39, 124.02, 120.11, 113.83, 103.42, 96.17, 0.00. HRMS (ESI): m/z for $\text{C}_{15}\text{H}_{14}\text{O}_4\text{Si}$ $[\text{M}+\text{H}]^+$ calcd 287.0661, found 287.0715.



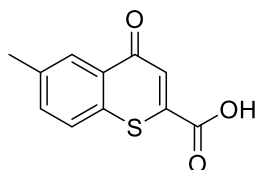
6-acetyl-4-oxo-4H-chromene-2-carboxylic acid (1v): 87% yield, white solid. Mp: 255-256°C. ^1H NMR (400 MHz, DMSO- d_6) δ 8.57 (d, $J = 1.6$ Hz, 1H), 8.35 (dd, $J = 8.8, 1.8$ Hz, 1H), 7.86 (d, $J = 8.8$ Hz, 1H), 6.98 (s, 1H), 2.69 (s, 3H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 196.49, 177.48, 161.18, 157.89, 153.59, 133.93, 125.81, 123.39, 119.65, 113.78, 26.81. HRMS (ESI): m/z for $\text{C}_{12}\text{H}_8\text{O}_5$ $[\text{M}-\text{H}]^-$ calcd 231.0372, found 231.0308.



4-oxo-4H-thiochromene-2-carboxylic acid (1w): 68% yield, light yellow solid. Mp: 225-227°C. ^1H NMR (400 MHz, DMSO- d_6) δ 8.34 (dd, $J = 8.1, 1.1$ Hz, 1H), 8.00 (d, $J = 8.1$ Hz, 1H), 7.84-7.80 (m, 1H), 7.70-7.66 (m, 1H), 7.49 (s, 1H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 180.19, 163.82, 143.30, 136.95, 132.71, 130.51, 128.55, 127.93, 127.66. HRMS (ESI): m/z for $\text{C}_{10}\text{H}_6\text{O}_3\text{S}$ $[\text{M}-\text{H}]^-$ calcd 205.0038, found 204.9982.



7-fluoro-4-oxo-4H-thiochromene-2-carboxylic acid (1x): 78% yield, light yellow solid. Mp: 228-230°C. ^1H NMR (400 MHz, DMSO- d_6) δ 8.15 (dd, $J = 8.9, 5.0$ Hz, 1H), 8.02 (dd, $J = 9.5, 2.7$ Hz, 1H), 7.79 (td, $J = 8.6, 2.8$ Hz, 1H), 7.50 (s, 1H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 179.46, 163.68, 163.02, 160.55, 143.94, 132.93, 132.53, 130.98, 126.78, 121.60, 121.36, 112.86, 112.63. HRMS (ESI): m/z for $\text{C}_{10}\text{H}_5\text{FO}_3\text{S}$ $[\text{M}+\text{H}]^+$ calcd 224.9943, found 224.9994.

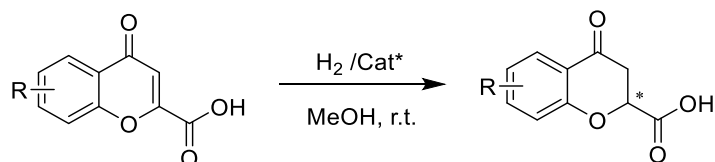


7-methyl-4-oxo-4H-thiochromene-2-carboxylic acid (1y): 78% yield, light yellow solid. Mp: 244-246°C. ^1H NMR (400 MHz, DMSO- d_6) δ 8.15 (s, 1H), 7.89 (d, $J = 8.3$ Hz, 1H), 7.65 (d, $J = 7.2$ Hz, 1H),

7.47 (s, 1H), 2.47 (s, 3H). ¹³C NMR (100 MHz, DMSO-d₆) δ 180.02, 163.85, 143.09, 138.51, 133.94, 130.37, 127.73, 127.21, 20.78. HRMS (ESI): *m/z* for C₁₁H₈O₃S [M+H]⁺ calcd 221.0194, found 221.0249.

3. Asymmetric hydrogenation of chromone-2-carboxylic acids

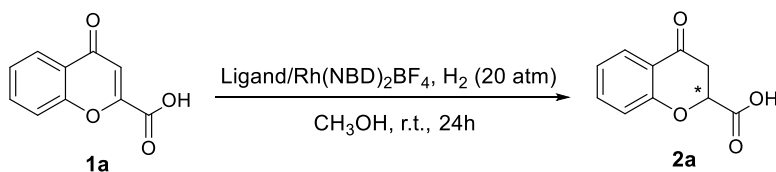
3.1 General procedure of asymmetric hydrogenation

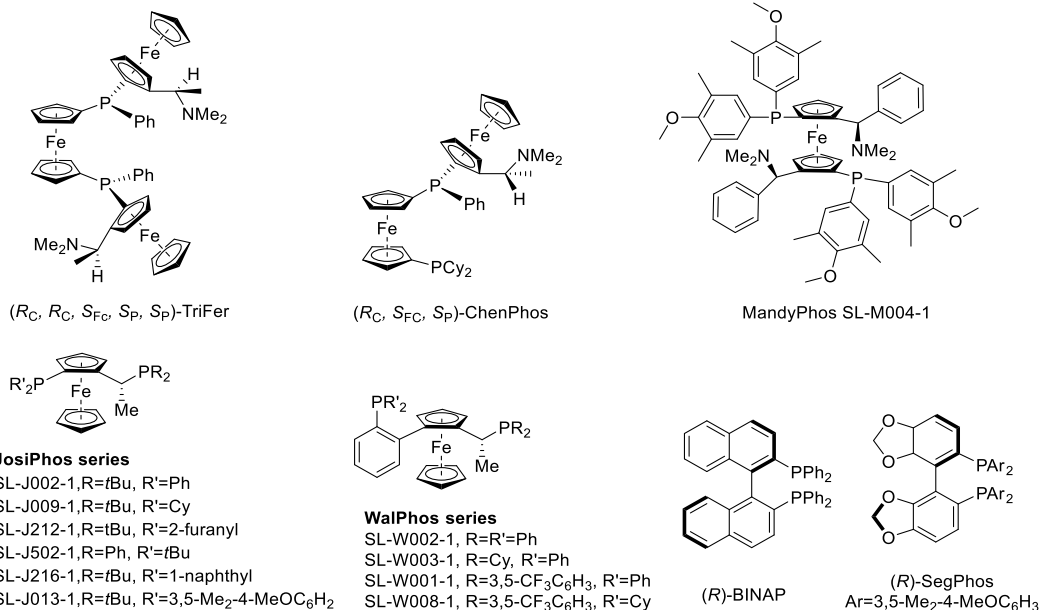


A solution of SL-J216-1 (1.41mg, 0.0022 mmol) and Rh(nbd)₂BF₄ (0.46 mg, 0.002 mmol) in MeOH (1 mL) was stirred under nitrogen atmosphere. After 30 min, the clear yellow solution was transferred into a hydrogenation tube equipped with a stir bar, and the 4-oxo-4*H*-chromene-2-carboxylic acids was added. The hydrogenation tube was then put into an autoclave. The air in the autoclave was replaced with hydrogen for three times. The autoclave was then charged with hydrogen to 20 atm, and the reaction mixture was stirred at room temperature for 20 h. After releasing the hydrogen, the reaction mixture was concentrated on a rotary evaporator. The conversion of substrate was determined by ¹H NMR analysis. The crude product was purified by flash chromatography on silica gel column to give the pure product. The product was reacted with trimethylsilyl diazomethane (1.1 eq) in THF to afford the corresponding methyl ester. After a flash chromatography on neutral Al₂O₃ column, the desired methyl ester was obtained and the *ee* values of the products were determined by chiral HPLC.

3.2 Ligands screening in asymmetric hydrogenation

Table S1 Screening of ligands and metal precursors in asymmetric hydrogenation^a

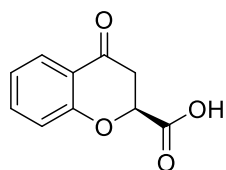




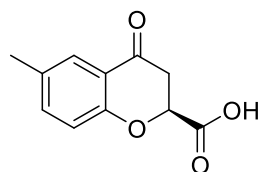
entry	ligand	metal precursor	yield (%) ^b	ee (%) ^c
1	ChenPhos	[Rh(NBD) ₂]BF ₄	63	62
2	TriFer	[Rh(NBD) ₂]BF ₄	80	85
3	SL-M004-1	[Rh(NBD) ₂]BF ₄	75	50
4	SL-J002-1	[Rh(NBD) ₂]BF ₄	92	71
5	SL-J009-1	[Rh(NBD) ₂]BF ₄	20	84
6	SL-J212-1	[Rh(NBD) ₂]BF ₄	92	85
7	SL-J502-1	[Rh(NBD) ₂]BF ₄	86	66
8	SL-J216-1	[Rh(NBD)₂]BF₄	97	99
9	SL-J013-1	[Rh(NBD) ₂]BF ₄	95	63
10	SL-W008-1	[Rh(NBD) ₂]BF ₄	90	80
11	SL-W002-1	[Rh(NBD) ₂]BF ₄	93	53
12	SL-W003-1	[Rh(NBD) ₂]BF ₄	92	33
13	SL-W001-1	[Rh(NBD) ₂]BF ₄	83	55
14	(<i>R</i>)-BINAP	[Rh(NBD) ₂]BF ₄	15	19
15	(<i>R</i>)-SegPhos	[Rh(NBD) ₂]BF ₄	20	15
16	SL-J216-1	[Rh(COD)Cl] ₂	50	99
17	SL-J216-1	[Rh(NBD)Cl] ₂	75	99
18	SL-J216-1	[Ir(COD)Cl] ₂	NR ^d	
19	SL-J216-1	Ru(PPh ₃) ₄ Cl	Trace	ND ^e

^a Reaction conditions: 0.2 mmol scale, [substrate]=0.1 mol L⁻¹, solvent=2 mL, 1.0 mol% of catalyst (M/L=1:1.1). ^b Obtained after flash column chromatography. ^c Determined by chiral HPLC analysis on a chiral stationary phase. ^d No reaction. ^e Not determined.

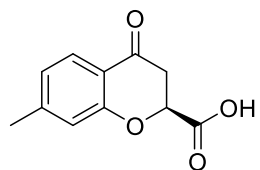
4. Analytical Data of Hydrogenation Products



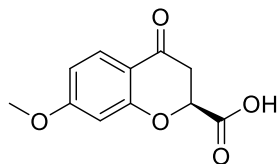
(S)-4-oxochromane-2-carboxylic acid (2a): White solid, 97% yield, 99% *ee*. Mp:154-156°C. $[\alpha]_D^{20} = +72.1$ (*c* 0.21, CH₂Cl₂). ¹H NMR (400 MHz, DMSO-*d*₆) δ 13.45 (s, 1H), 7.74 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.67-7.56 (m, 1H), 7.21-6.99 (m, 2H), 5.34 (dd, *J* = 7.4, 5.3 Hz, 1H), 3.12 (dd, *J* = 17.0, 5.2 Hz, 1H), 2.98 (dd, *J* = 17.0, 7.5 Hz, 1H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 189.84, 170.37, 160.00, 136.36, 126.09, 121.57, 120.65, 117.95, 74.50. HRMS (ESI): *m/z* for C₁₀H₈O₄ [M+H]⁺ calcd 193.0423, found 193.0493. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, *t*_R=14.80 min for major isomer, and *t*_R=21.58 min for minor isomer.



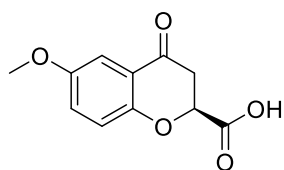
(S)-6-methyl-4-oxochromane-2-carboxylic acid (2b): White solid, 92% yield, 98% *ee*. Mp:158-160°C. $[\alpha]_D^{20} = +59.5$ (*c*=0.13 in MeOH). ¹H NMR (400 MHz, DMSO-*d*₆) δ 13.38 (s, 1H), 7.52 (s, 1H), 7.41 (d, *J* = 8.4 Hz, 1H), 7.00 (d, *J* = 8.4 Hz, 1H), 5.27 (dd, *J* = 7.3, 5.4 Hz, 1H), 3.07 (dd, *J* = 17.0, 5.2 Hz, 1H), 2.94 (dd, *J* = 17.0, 7.5 Hz, 1H), 2.27 (s, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 189.89, 170.43, 158.07, 137.20, 130.60, 125.61, 120.27, 117.78, 74.47, 19.88. HRMS (ESI): *m/z* for C₁₁H₁₀O₄ [M+H]⁺ calcd 207.0579, found 207.0641. HPLC condition: Chiralcel AS-H column (25 cm × 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, *t*_R=13.58 min for major isomer, and *t*_R=20.40 min for minor isomer.



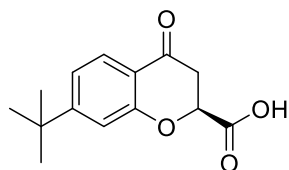
(S)-7-methyl-4-oxochromane-2-carboxylic acid (2c): White solid, 93% yield, 98% *ee*. Mp:169-170°C. $[\alpha]_D^{20} = +37.3$ (*c*=0.13 in MeOH). ¹H NMR (400 MHz, DMSO-*d*₆) δ 13.41 (s, 1H), 7.62 (d, *J* = 7.8 Hz, 1H), 6.93-6.90 (m, 2H), 5.30 (d, *J* = 4.8 Hz, 1H), 3.10-3.06 (m, 1H), 2.92 (dd, *J* = 17.0, 7.1 Hz, 1H), 2.34 (s, 3H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 189.35, 170.47, 160.02, 147.47, 126.00, 122.80, 118.44, 117.81, 74.48, 21.34. HRMS (ESI): *m/z* for C₁₁H₁₀O₄ [M+H]⁺ calcd 207.0579, found 207.0643. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, *t*_R=13.18 min for major isomer, and *t*_R=18.00 min for minor isomer.



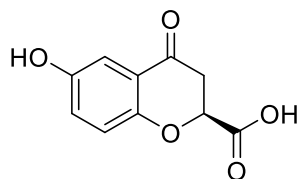
(S)-7-methoxy-4-oxochromane-2-carboxylic acid (2d): Brown solid, 93% yield, 99% *ee*. Mp:169-171°C. $[\alpha]_D^{20} = -0.7$ ($c=0.13$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.37 (s, 1H), 7.66 (d, $J = 8.6$ Hz, 1H), 6.66-6.62 (m, 2H), 5.30-5.27 (m, 1H), 3.83 (s, 3H), 3.01 (dd, $J = 17.0, 5.0$ Hz, 1H), 2.89 (dd, $J = 16.9, 7.4$ Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 188.23, 170.40, 165.71, 162.05, 127.88, 114.44, 109.97, 101.04, 74.78, 55.84. HRMS (ESI): m/z for $\text{C}_{11}\text{H}_{10}\text{O}_5$ $[\text{M}+\text{H}]^+$ calcd 223.0528, found 223.0586. HPLC condition: Chiralcel OD-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, $t_R=22.93$ min for major isomer, and $t_R=30.06$ min for minor isomer.



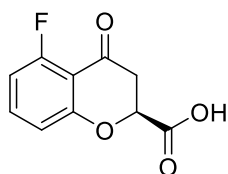
(S)-6-methoxy-4-oxochromane-2-carboxylic acid (2e): White solid, 92% yield, 97% *ee*. Mp:150-152°C. $[\alpha]_D^{20} = +37.2$ ($c=0.17$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.40 (s, 1H), 7.28-7.11 (m, 2H), 7.06 (d, $J = 8.9$ Hz, 1H), 5.27-5.24 (m, 1H), 3.75 (s, 3H), 3.07 (dd, $J = 17.1, 4.9$ Hz, 1H), 2.96 (dd, $J = 17.0, 7.6$ Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 189.81, 170.46, 154.47, 153.70, 124.62, 120.57, 119.34, 107.16, 74.55. HRMS (ESI): m/z for $\text{C}_{11}\text{H}_{10}\text{O}_5$ $[\text{M}+\text{H}]^+$ calcd 223.0528, found 223.0590. HPLC condition: Chiralcel OD-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, $t_R=15.70$ min for major isomer, and $t_R=19.40$ min for minor isomer.



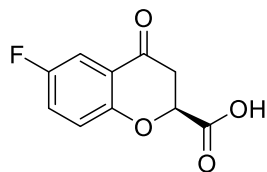
(S)-7-(tert-butyl)-4-oxochromane-2-carboxylic acid (2f): White solid, 92% yield, 98% *ee*. Mp:131-133°C. $[\alpha]_D^{20} = +16.1$ ($c=0.11$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.41 (s, 1H), 7.66 (d, $J = 8.3$ Hz, 1H), 7.14 (d, $J = 8.3$ Hz, 1H), 7.05 (d, $J = 1.2$ Hz, 1H), 5.29 (dd, $J = 7.8, 5.2$ Hz, 1H), 3.03 (dd, $J = 16.9, 5.1$ Hz, 1H), 2.93 (dd, $J = 16.9, 8.0$ Hz, 1H), 1.28 (s, 9H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 189.43, 170.37, 160.16, 159.94, 125.86, 119.16, 118.33, 114.22, 74.52, 35.06, 30.53. HRMS (ESI): m/z for $\text{C}_{14}\text{H}_{16}\text{O}_4$ $[\text{M}+\text{H}]^+$ calcd 249.1049, found 249.1117. HPLC condition: Chiralcel OD-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, $t_R=51.76$ min for major isomer, and $t_R=57.27$ min for minor isomer.



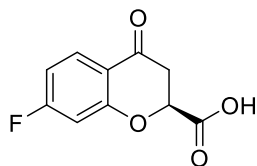
(S)-6-hydroxy-4-oxochromane-2-carboxylic acid (2g): Light brown solid, 90% yield, 98% *ee*. Mp:234-236°C. $[\alpha]_D^{20} = +67.8$ ($c=0.11$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.26 (s, 1H), 9.45 (s, 1H), 7.03 (d, $J = 11.2$ Hz, 2H), 6.95 (d, $J = 8.6$ Hz, 1H), 5.2-5.18 (m, 1H), 3.01 (dd, $J = 17.0, 4.7$ Hz, 1H), 2.91 (dd, $J = 17.0, 7.9$ Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 190.05, 170.55, 153.21, 151.66, 124.57, 120.80, 118.95, 109.72, 74.46. HRMS (ESI): m/z for $\text{C}_{10}\text{H}_8\text{O}_5$ $[\text{M}+\text{H}]^+$ calcd 209.0372, found 209.0442. HPLC condition: Chiralcel OD-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, $t_R=32.39$ min for minor isomer, and $t_R=37.42$ min for major isomer.



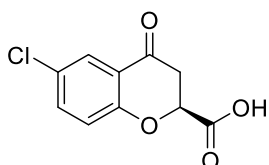
(S)-5-fluoro-4-oxochromane-2-carboxylic acid (2h): White solid, 93% yield, 98% *ee*. Mp:156-157°C. $[\alpha]_D^{20} = +54.0$ ($c=0.15$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.49 (s, 1H), 7.59 (dt, $J = 14.5, 7.3$ Hz, 1H), 6.96 (d, $J = 8.3$ Hz, 1H), 6.87 (t, $J = 9.6$ Hz, 1H), 5.36 (t, $J = 6.2$ Hz, 1H), 3.11 (dd, $J = 16.7, 5.1$ Hz, 1H), 2.94 (dd, $J = 16.8, 7.4$ Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 187.52, 170.08, 161.77, 160.84, 159.16, 136.60, 113.91, 110.67, 108.96, 108.76, 74.43. HRMS (ESI): m/z for $\text{C}_{10}\text{H}_7\text{FO}_4$ $[\text{M}+\text{H}]^+$ calcd 211.0328, found 211.0401. HPLC condition: Chiralcel OD-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, $t_R=20.86$ min for major isomer, and $t_R=22.63$ min for minor isomer.



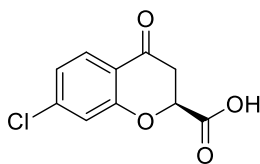
(S)-6-fluoro-4-oxochromane-2-carboxylic acid (2i): White solid, 95% yield, 99% *ee*. Mp:161-163°C. $[\alpha]_D^{20} = +62.2$ ($c=0.16$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.50 (s, 1H), 7.49 (td, $J = 8.6, 3.2$ Hz, 1H), 7.43 (dd, $J = 8.4, 3.1$ Hz, 1H), 7.19 (dd, $J = 9.0, 4.3$ Hz, 1H), 5.34 (dd, $J = 7.4, 5.3$ Hz, 1H), 3.13 (dd, $J = 17.1, 5.2$ Hz, 1H), 2.99 (dd, $J = 17.1, 7.5$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 189.31, 170.22, 157.79, 156.42, 155.41, 123.91, 123.66, 121.11, 120.17, 110.99, 110.76, 74.67. $^{19}\text{F NMR}$ (100 MHz, DMSO- d_6) δ -121.35. HRMS (ESI): m/z for $\text{C}_{10}\text{H}_7\text{FO}_4$ $[\text{M}+\text{H}]^+$ calcd 211.0328, found 211.0404. HPLC condition: Chiralcel AS-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, $t_R=14.38$ min for major isomer, and $t_R=17.74$ min for minor isomer.



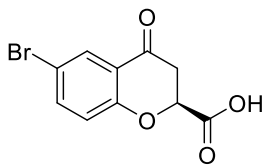
(S)-7-fluoro-4-oxochromane-2-carboxylic acid (2j): White solid, 95% yield, 99% *ee*. Mp:148-149°C. $[\alpha]_D^{20} = +50.9$ ($c=0.10$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.55 (s, 1H), 7.81 (dd, $J = 8.5, 7.0$ Hz, 1H), 7.04 (dd, $J = 10.3, 2.2$ Hz, 1H), 6.95 (td, $J = 8.6, 2.3$ Hz, 1H), 5.39 (t, $J = 6.2$ Hz, 1H), 3.13 (dd, $J = 17.1, 5.3$ Hz, 1H), 2.97 (dd, $J = 17.1, 7.2$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 188.53, 170.13, 167.97, 165.45, 161.76, 129.00, 117.95, 109.87, 109.64, 104.86, 104.61, 75.04. $^{19}\text{F NMR}$ (100 MHz, DMSO- d_6) δ -101.18. HRMS (ESI): m/z for $\text{C}_{10}\text{H}_7\text{FO}_4$ $[\text{M}+\text{H}]^+$ calcd 211.0328, found 211.0404. HPLC condition: Chiralcel AS-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, $t_R=15.83$ min for minor isomer, and $t_R=17.17$ min for major isomer.



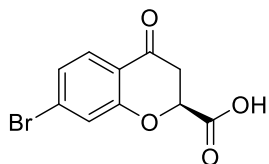
(S)-6-chloro-4-oxochromane-2-carboxylic acid (2k): White solid, 93% yield, 99% *ee*. Mp:159-160°C. $[\alpha]_D^{20} = +71.6$ ($c=0.10$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.53 (s, 1H), 7.64 (d, $J = 12.3$ Hz, 2H), 7.18 (d, $J = 8.0$ Hz, 1H), 5.37 (s, 1H), 3.15 (d, $J = 14.3$ Hz, 1H), 3.00 (dd, $J = 16.7, 6.4$ Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 188.95, 170.13, 158.71, 135.91, 125.75, 125.00, 121.65, 120.35, 74.70. HRMS (ESI): m/z for $\text{C}_{10}\text{H}_7\text{ClO}_4$ $[\text{M}+\text{H}]^+$ calcd 227.0033, found 227.0107. HPLC condition: Chiralcel AS-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, $t_R=14.86$ min for major isomer, and $t_R=20.03$ min for minor isomer.



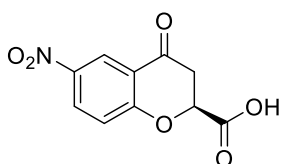
(S)-7-chloro-4-oxochromane-2-carboxylic acid (2l): White solid, 92% yield, 98% *ee*. Mp:141-142°C. $[\alpha]_D^{20} = +25.0$ ($c=0.10$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.56 (s, 1H), 7.74 (d, $J = 8.4$ Hz, 1H), 7.28 (s, 1H), 7.15 (d, $J = 8.4$ Hz, 1H), 5.40 (t, $J = 5.9$ Hz, 1H), 3.16 (dd, $J = 17.1, 5.2$ Hz, 1H), 2.98 (dd, $J = 17.1, 6.8$ Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 188.93, 170.14, 160.54, 140.51, 127.87, 122.08, 119.62, 117.80, 74.92. HRMS (ESI): m/z for $\text{C}_{10}\text{H}_7\text{ClO}_4$ $[\text{M}+\text{H}]^+$ calcd 227.0033, found 227.0106. HPLC condition: Chiralcel AS-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, $t_R=13.79$ min for minor isomer, and $t_R=15.63$ min for major isomer.



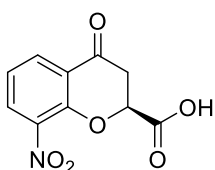
(S)-6-bromo-4-oxochromane-2-carboxylic acid (2m): Light yellow solid, 95% yield, 99% *ee*. Mp:167-168°C. $[\alpha]_D^{20} = +59.0$ ($c=0.10$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.59 (s, 1H), 7.78-7.74 (m, 2H), 7.12 (d, $J = 8.7$ Hz, 1H), 5.37 (t, $J = 6.1$ Hz, 1H), 3.15 (dd, $J = 17.0, 5.1$ Hz, 1H), 2.99 (dd, $J = 17.1, 7.2$ Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 188.85, 170.12, 159.12, 138.65, 128.03, 122.15, 120.67, 113.29, 74.69. HRMS (ESI): m/z for $\text{C}_{10}\text{H}_7\text{BrO}_4$ $[\text{M}+\text{H}]^+$ calcd 270.9528, found 270.9602. HPLC condition: Chiralcel AS-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, $t_R=15.40$ min for major isomer, and $t_R=20.18$ min for minor isomer.



(S)-7-bromo-4-oxochromane-2-carboxylic acid (2n): White solid, 93% yield, 98% *ee*. Mp:172-173°C. $[\alpha]_D^{20} = +10.4$ ($c=0.11$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.57 (s, 1H), 7.65 (d, $J = 8.4$ Hz, 1H), 7.41 (s, 1H), 7.28 (dd, $J = 8.4, 0.6$ Hz, 1H), 5.39 (t, $J = 6.1$ Hz, 1H), 3.16 (dd, $J = 16.9, 5.6$ Hz, 1H), 2.97 (dd, $J = 17.1, 6.9$ Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 189.12, 170.14, 160.42, 129.52, 127.84, 124.91, 120.73, 119.88, 74.90. HRMS (ESI): m/z for $\text{C}_{10}\text{H}_7\text{BrO}_4$ $[\text{M}+\text{H}]^+$ calcd 270.9528, found 270.9600. HPLC condition: Chiralcel AS-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, $t_R=14.33$ min for minor isomer, and $t_R=16.47$ min for major isomer.

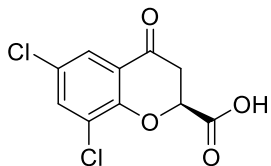


(S)-6-nitro-4-oxochromane-2-carboxylic acid (2o): Yellow solid, 87% yield, 83% *ee*. Mp:179-180°C. $[\alpha]_D^{20} = +56.5$ ($c=0.10$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.72 (s, 1H), 8.46-8.40 (m, 2H), 7.38 (d, $J = 9.1$ Hz, 1H), 5.56 (t, $J = 6.1$ Hz, 1H), 3.29 (dd, $J = 17.1, 5.5$ Hz, 1H), 3.09 (dd, $J = 17.1, 6.8$ Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 187.70, 168.88, 163.31, 140.69, 129.74, 121.00, 119.43, 118.82, 74.42. HRMS (ESI): m/z for $\text{C}_{10}\text{H}_7\text{NO}_6$ $[\text{M}-\text{H}]^-$ calcd 236.0273, found 236.0198. HPLC condition: Chiralcel OD-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, $t_R=58.00$ min for major isomer, and $t_R=67.67$ min for minor isomer.

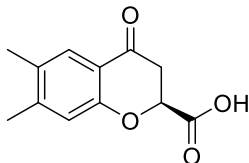


(S)-8-nitro-4-oxochromane-2-carboxylic acid (2p): Yellow solid, 89% yield, 87% *ee*. Mp:180-181°C. $[\alpha]_D^{20} = -106.2$ ($c=0.13$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.73 (s, 1H), 8.24 (d, $J = 7.9$ Hz, 1H), 8.05 (d, $J = 7.6$ Hz, 1H), 7.27 (t, $J = 7.9$ Hz, 1H), 5.60 (t, $J = 5.7$ Hz, 1H), 3.36 (dd, $J = 17.2, 5.7$ Hz, 1H), 3.07 (dd, $J = 17.2, 5.8$ Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 188.18, 169.69, 152.67, 139.40,

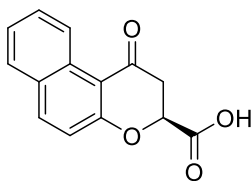
131.19, 122.88, 121.15, 75.72. HRMS (ESI): m/z for $C_{10}H_7NO_6$ $[M-H]^-$ calcd 236.0273, found 236.0191. HPLC condition: Chiralcel OD-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, t_R =38.69 min for major isomer, and t_R =49.17 min for minor isomer.



(S)-6,8-dichloro-4-oxochromane-2-carboxylic acid (2q): Light brown solid, 90% yield, 98% *ee*. Mp:174-175°C. $[\alpha]_D^{20} = +17.6$ ($c=0.11$ in MeOH). 1H NMR (400 MHz, DMSO- d_6) δ 13.70 (s, 1H), 7.96 (d, $J = 1.9$ Hz, 1H), 7.65 (d, $J = 1.9$ Hz, 1H), 5.54 (t, $J = 5.7$ Hz, 1H), 3.26 (dd, $J = 17.2, 5.4$ Hz, 1H), 3.04 (dd, $J = 17.1, 6.3$ Hz, 1H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 188.25, 169.78, 154.56, 135.23, 125.50, 124.13, 123.23, 122.61, 75.28. HRMS (ESI): m/z for $C_{10}H_6Cl_2O_4$ $[M-H]^-$ calcd 258.9643, found 258.9572. HPLC condition: Chiralcel OD-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, t_R =14.83 min for major isomer, and t_R =17.08 min for minor isomer.

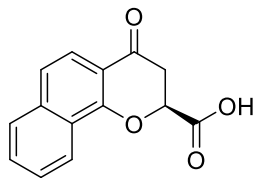


(S)-6,7-dimethyl-4-oxochromane-2-carboxylic acid (2r): White solid, 92% yield, 99% *ee*. Mp:181-182°C. $[\alpha]_D^{20} = +31.8$ ($c=0.11$ in MeOH). 1H NMR (400 MHz, DMSO- d_6) δ 13.34 (s, 1H), 7.46 (s, 1H), 6.91 (s, 1H), 5.23 (t, $J = 6.1$ Hz, 1H), 3.03 (dd, $J = 17.0, 5.2$ Hz, 1H), 2.89 (dd, $J = 17.0, 7.2$ Hz, 1H), 2.25 (s, 3H), 2.18 (s, 3H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 189.45, 170.57, 158.31, 146.51, 129.90, 125.92, 118.34, 74.45, 19.91, 18.31. HRMS (ESI): m/z for $C_{12}H_{12}O_4$ $[M+H]^+$ calcd 221.0736, found 221.0802. HPLC condition: Chiralcel OD-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, t_R =11.74 min for major isomer, and t_R =14.56 min for minor isomer.

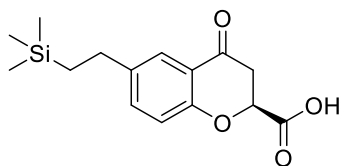


(S)-1-oxo-2,3-dihydro-1H-benzo[f]chromene-3-carboxylic acid (2s): Light yellow solid, 94% yield, 98% *ee*. Mp:158-159°C. $[\alpha]_D^{20} = +106.2$ ($c=0.13$ in MeOH). 1H NMR (400 MHz, DMSO- d_6) δ 13.48 (s, 1H), 9.32 (d, $J = 8.6$ Hz, 1H), 8.17 (d, $J = 9.0$ Hz, 1H), 7.93 (d, $J = 7.9$ Hz, 1H), 7.66 (t, $J = 7.5$ Hz, 1H), 7.48 (t, $J = 7.4$ Hz, 1H), 7.29 (d, $J = 9.0$ Hz, 1H), 5.44 (dd, $J = 7.3, 5.7$ Hz, 1H), 3.22 (dd, $J = 16.7, 5.5$ Hz, 1H), 3.06 (dd, $J = 16.7, 7.6$ Hz, 1H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 191.11, 170.30, 162.24, 137.77, 130.62, 129.57, 128.76, 124.87, 118.88, 111.92, 74.53. HRMS (ESI): m/z for $C_{14}H_{10}O_4$ $[M+H]^+$ calcd 243.0579, found 243.0650. HPLC condition: Chiralcel AS-H column (25 cm \times 0.46 cm ID), hexane/2-

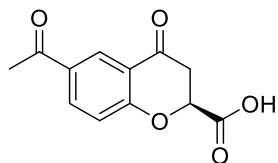
propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, t_R =16.22 min for major isomer, and t_R =20.78 min for minor isomer.



(S)-4-oxo-3,4-dihydro-2H-benzo[h]chromene-2-carboxylic acid (2t): Light yellow solid, 95% yield, 99% *ee*. Mp: 189-190°C. $[\alpha]_D^{20} = +104.5$ ($c=0.13$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.56 (s, 1H), 8.31 (d, $J = 8.2$ Hz, 1H), 7.95 (d, $J = 8.0$ Hz, 1H), 7.73 (t, $J = 7.5$ Hz, 2H), 7.65 (t, $J = 7.5$ Hz, 1H), 7.55 (d, $J = 8.7$ Hz, 1H), 5.61 (t, $J = 6.2$ Hz, 1H), 3.25 (dd, $J = 17.0, 5.5$ Hz, 1H), 3.08 (dd, $J = 17.0, 7.0$ Hz, 1H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 189.39, 170.40, 158.08, 136.93, 129.90, 127.91, 126.71, 124.16, 123.11, 121.00, 115.21, 75.34. HRMS (ESI): m/z for $\text{C}_{14}\text{H}_{10}\text{O}_4$ $[\text{M}+\text{H}]^+$ calcd 243.0579, found 243.0651. HPLC condition: Chiralcel OD-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, t_R =15.08 min for major isomer, and t_R =19.60 min for minor isomer.

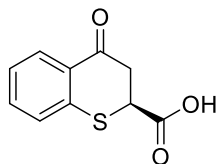


(S)-4-oxo-6-(2-(trimethylsilyl)ethyl)chromane-2-carboxylic acid (2u): White solid, 96% yield, 92% *ee*. Mp: 96-97°C. $[\alpha]_D^{20} = +59.9$ ($c=0.10$ in MeOH). $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.70 (d, $J = 2.0$ Hz, 1H), 7.37 (dd, $J = 8.5, 2.2$ Hz, 1H), 7.00 (d, $J = 8.5$ Hz, 1H), 5.10 (dd, $J = 9.4, 5.1$ Hz, 1H), 3.14-3.01 (m, 2H), 2.60-2.56 (m, 2H), 0.85-0.81 (m, 2H), -0.02 (s, 9H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 191.72, 175.02, 159.90, 141.34, 138.50, 127.17, 122.25, 119.67, 76.47, 41.13, 30.90, 20.33, 0.00. HRMS (ESI): m/z for $\text{C}_{15}\text{H}_{20}\text{O}_4\text{Si}$ $[\text{M}+\text{H}]^+$ calcd 293.1131, found 293.1165. HPLC condition: Double Chiralcel AD-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=98:1, flow rate=1.0 mL/min, 254 nm UV detector, t_R =18.25 min for major isomer, and t_R =20.27 min for minor isomer.

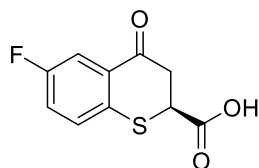


(S)-6-acetyl-4-oxochromane-2-carboxylic acid (2v): White solid, 88% yield, 98% *ee*. Mp: 204-205°C. $[\alpha]_D^{20} = +56.9$ ($c=0.10$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 8.29 (d, $J = 1.8$ Hz, 1H), 8.14 (dd, $J = 8.7, 2.0$ Hz, 1H), 7.24 (d, $J = 8.7$ Hz, 1H), 5.46 (t, $J = 6.1$ Hz, 1H), 3.22 (dd, $J = 17.0, 5.5$ Hz, 1H), 3.03 (dd, $J = 17.1, 6.9$ Hz, 1H), 2.57 (s, 3H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 196.06, 189.39, 170.08, 163.20, 135.50, 130.49, 126.95, 120.13, 118.49, 74.88, 26.49. HRMS (ESI): m/z for $\text{C}_{12}\text{H}_{10}\text{O}_5$ $[\text{M}+\text{H}]^+$ calcd

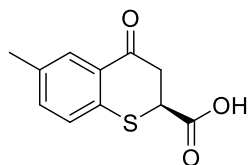
235.0528, found 235.0594. HPLC condition: Double Chiralcel AD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=97:3, flow rate=0.8 mL/min, 254 nm UV detector, t_R =53.96 min for major isomer, and t_R =58.48 min for minor isomer.



(S)-4-oxothiochromane-2-carboxylic acid (2w): Light brown solid, 75% yield, 90% *ee*. Mp:157-158°C. $[\alpha]_D^{20} = +369.5$ ($c=0.13$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.17 (s, 1H), 7.95 (d, $J = 7.7$ Hz, 1H), 7.49 (t, $J = 7.1$ Hz, 1H), 7.35 (d, $J = 7.8$ Hz, 1H), 7.25 (t, $J = 7.4$ Hz, 1H), 4.46-4.35 (m, 1H), 3.09 (qd, $J = 16.9, 5.2$ Hz, 2H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 192.07, 171.58, 138.50, 133.72, 130.03, 127.87, 127.31, 125.42, 41.24, 40.79. HRMS (ESI): m/z for $\text{C}_{10}\text{H}_8\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$ calcd 209.0194, found 209.0263. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, t_R =14.34 min for minor isomer, and t_R =16.27 min for major isomer.



(S)-7-fluoro-4-oxothiochromane-2-carboxylic acid (2x): White solid, 82% yield, 94% *ee*. Mp:175-177°C. $[\alpha]_D^{20} = +344.2$ ($c=0.10$ in MeOH). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.22 (s, 1H), 7.76-7.60 (m, 1H), 7.52-7.31 (m, 2H), 4.41 (t, $J = 5.1$ Hz, 1H), 3.22-2.97 (m, 2H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 191.36, 171.51, 161.19, 158.77, 134.05, 131.55, 129.72, 121.51, 121.28, 113.73, 113.50, 41.18, 40.46. $^{19}\text{F NMR}$ (100 MHz, DMSO- d_6) δ -116.24. HRMS (ESI): m/z for $\text{C}_{10}\text{H}_7\text{FO}_3\text{S}$ $[\text{M}+\text{H}]^+$ calcd 227.0100, found 227.0180. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, t_R =13.40 min for minor isomer, and t_R =16.39 min for major isomer.

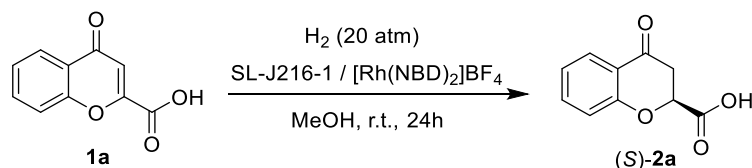


(S)-7-methyl-4-oxothiochromane-2-carboxylic acid (2y): White solid, 68% yield, 90% *ee*. Mp:184-186°C. $[\alpha]_D^{20} = +10.8$ ($c=0.49$ in CH_2Cl_2). $^1\text{H NMR}$ (400 MHz, DMSO- d_6) δ 13.13 (s, 1H), 7.77 (s, 1H), 7.33 (d, $J = 6.7$ Hz, 1H), 7.24 (d, $J = 8.0$ Hz, 1H), 4.36 (dd, $J = 5.9, 4.5$ Hz, 1H), 3.06 (qd, $J = 16.9, 5.2$ Hz, 2H), 2.29 (s, 3H). $^{13}\text{C NMR}$ (100 MHz, DMSO- d_6) δ 192.20, 171.60, 135.06, 134.87, 134.58, 129.87, 128.00, 127.27, 41.25, 40.97, 20.30. HRMS (ESI): m/z for $\text{C}_{11}\text{H}_{10}\text{O}_3\text{S}$ $[\text{M}-\text{H}]^-$ calcd 221.0351, found 221.0288. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=90:10,

flow rate=1.0 mL/min, 254 nm UV detector, t_R =12.33 min for minor isomer, and t_R =14.17 min for major isomer.

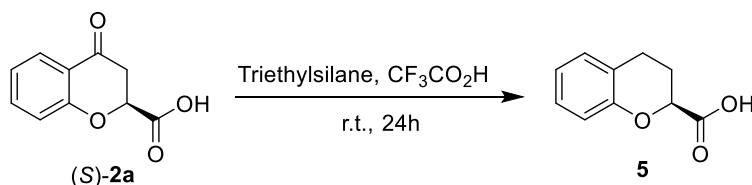
5. Scale-up Synthesis and Transformations

5.1 Scale-up synthesis of 2a



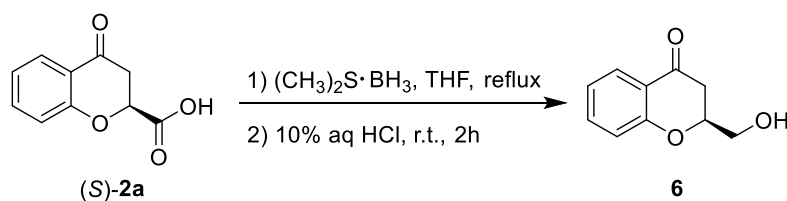
SL-J216-1 (0.70 mg, 0.0011 mmol) and Rh(NBD)₂BF₄ (0.37 mg, 0.001 mmol) were dissolved in anhydrous MeOH (20 mL) under nitrogen. The mixture was stirred for 30 min at room temperature. The substrate **1a** (1.90g, 10 mmol) was placed in a 50 mL flame-dried round bottom flask equipped with a magnetic stirrer bar. This flask was put into an autoclave. The pre-prepared solution of catalyst was added under a nitrogen atmosphere. After purging with hydrogen for three times, the hydrogen pressure was finally pressurized to 20 bar. The reaction mixture was concentrated and purified via a silica gel column chromatography (PE/EtOAc/HCOOH=5/1/0.05) to provide (*S*)-4-oxochromane-2-carboxylic acid **2a** (1.82g, 95% yield, 97% *ee*).

5.2 Synthesis of (*S*)-chromane-2-carboxylic acid (**5**)



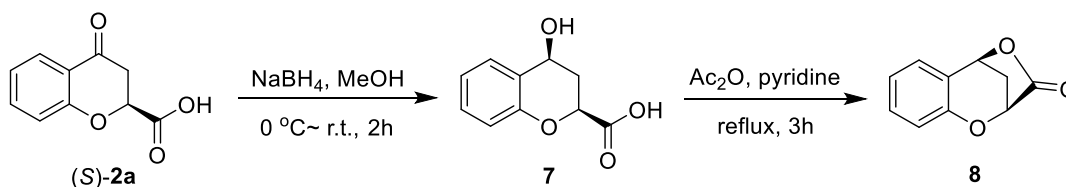
(*S*)-**2a** (500 mg, 2.60 mmol) was dissolved in 10 mL of trifluoroacetic acid. Triethyl silane (2 mL) was added slowly and the solution was stirred at room temperature. When the reaction was completed, the trifluoroacetic acid and excessive triethyl silane were removed under vacuum. To the residue, 10 mL of water and 20 mL of diethyl ether were added, the organic layer was separated and the aqueous layer was extracted with diethyl ether (2×10 mL). The combined organic layers were washed with a saturated aqueous solution of NaCl, dried over anhydrous Na₂SO₄ and concentrated in vacuo, The residue was purified via silica gel column chromatography (PE/EtOAc/HCOOH=5/1/0.05) to provide (*S*)-chromane-2-carboxylic acid **5** as a white solid (430 mg, 93% yield, 96% *ee*). Mp: 76-77 °C. $[\alpha]_D^{20} = -13.6$ (*c* 0.14, CH₂Cl₂). ¹H NMR (400 MHz, CDCl₃) δ 7.16-7.12 (m, 1H), 7.06 (d, *J* = 7.3 Hz, 1H), 6.94-6.89 (m, 2H), 4.76 (dd, *J* = 8.3, 3.5 Hz, 1H), 2.94-2.78 (m, 2H), 2.40-2.34 (m, 1H), 2.24-2.15 (m, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 174.44, 152.79, 129.58, 127.76, 121.32, 116.85, 73.37, 24.52, 23.48. HRMS (ESI): *m/z* for C₁₀H₁₀O₃ [M-H]⁻ calcd 177.0630, found 177.0560. HPLC condition: Chiralcel AS-H column (25 cm × 0.46 cm ID), hexane/2-propanol=95:5, flow rate=0.8 mL/min, 254 nm UV detector, t_R =9.27 min for major isomer, and t_R =10.36 min for minor isomer.

5.3 Synthesis of (*S*)-2-(hydroxymethyl)chroman-4-one (**6**)



To a stirred solution of (*S*)-**2a** (384 mg, 2.0 mmol) in THF (10 mL) at 0 °C, borane-methyl sulfide complex (2.0 M in THF, 1.6 mL, 3.2 mmol) was added dropwise for about 15 minutes. The solution was warmed to room temperature and then heated at reflux for 4 hours. The solution was cooled to room temperature and 10% aqueous HCl (10 mL) was added over 15 minutes and the solution was stirred at room temperature for 2 hours. The solution was then poured into EtOAc (30 mL) and washed successively with water, saturated NaHCO₃ and saturated NH₄Cl. The organic layer was separated and dried over anhydrous Na₂SO₄, and then concentrated and purified via silica gel column chromatography (PE/EtOAc=10/1) to provide (*S*)-2-(hydroxymethyl)chroman-4-one **6** as a light yellow viscous oil (310 mg, 87% yield, 96% *ee*). $[\alpha]_{\text{D}}^{20} = +43.8$ (*c* 0.60, CH₂Cl₂). ¹H NMR (400 MHz, CDCl₃) δ 7.90 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.52-7.47 (m, 1H), 7.06-7.00 (m, 2H), 4.59 (ddt, *J* = 13.4, 5.6, 2.9 Hz, 1H), 4.00 (dd, *J* = 12.2, 3.0 Hz, 1H), 3.85 (dd, *J* = 12.2, 5.3 Hz, 1H), 2.95 (dd, *J* = 16.9, 13.5 Hz, 1H), 2.64 (dd, *J* = 16.9, 2.8 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 191.91, 161.09, 136.16, 127.07, 121.68, 120.90, 117.85, 78.19, 64.56, 39.0. HRMS (ESI): *m/z* for C₁₀H₁₀O₃ [M+H]⁺ calcd 179.0630, found 179.0700. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, *t_R*=14.29 min for major isomer, and *t_R*=16.44 min for minor isomer.

5.4 Synthesis of (2*S*,5*S*)-5H-2,5-methanobenzo[*e*][1,4]dioxepin-3(2H)-one (**8**)



Step 1: Synthesis of (2*S*,4*S*)-4-hydroxychromane-2-carboxylic acid (**7**)

To a suspension of (*S*)-**2a** (500 mg, 2.60 mmol) in MeOH (10 mL) at 0 °C was added NaBH₄ (196.7 mg, 5.3 mmol) in portions and the mixture was stirred at room temperature for 2 hours. After the reaction was completed, the methanol was removed in vacuo and the residue was dissolved in EtOAc (20 mL). The resulting mixture was washed with water (50 mL × 2) and a saturated aqueous solution of NaCl (50 mL), dried over anhydrous Na₂SO₄ and concentrated in vacuo. The residue was purified by column chromatography, eluted with PE/EtOAc (100/1 to 10/1) to afford (2*S*,4*S*)-4-hydroxychromane-2-carboxylic acid **7** as a white solid. (430 mg, 93% yield, 29:1 *dr*, >99% *ee*). Mp: 128-129 °C. $[\alpha]_{\text{D}}^{20} = +119.3$ (*c* 0.13, MeOH). ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.91 (s, 1H), 7.34 (d, *J* = 7.3 Hz, 1H), 7.15 (dd, *J* = 11.2, 4.1 Hz, 1H), 6.90 (t, *J* = 7.3 Hz, 1H), 6.80 (d, *J* = 8.1 Hz, 1H), 5.44 (s, 1H), 4.82-4.75 (m,

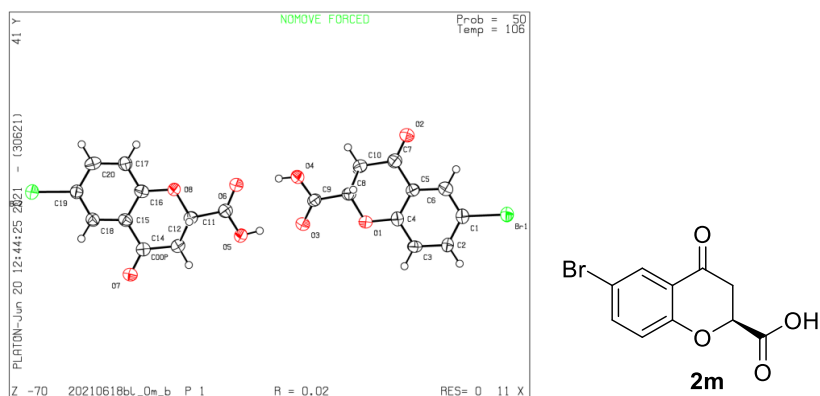
2H), 2.35-2.30 (m, 1H), 2.04-1.96 (m, 1H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 171.48, 152.85, 128.32, 126.28, 120.25, 115.85, 71.65, 62.15, 33.44. HRMS (ESI): m/z for $\text{C}_{10}\text{H}_{10}\text{O}_4$ $[\text{M}-\text{H}]^-$ calcd 193.0579, found 193.0506. HPLC condition: Chiralcel OD-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, t_{R} =18.53 min for major isomer, and t_{R} =23.74 min for minor isomer. The absolute configuration of compound **6** was assigned according to the X-ray crystal structure.

Step 2: Synthesis of (2*S*,5*S*)-5H-2,5-methanobenzo[e][1,4]dioxepin-3(2H)-one (**8**)

Mix the (2*S*,4*S*)-4-hydroxychromane-2-carboxylic acid **7** (300 mg, 1.5 mmol) with 5 mL of Ac_2O in 10 mL of pyridine. The solution was heated at 80°C for 3 hours. The reaction was concentrated under vacuum and the residue was dissolved in EtOAc (20 mL). The resulting mixture was washed with water (15 mL \times 3), dried over anhydrous Na_2SO_4 and concentrated in vacuo. The residue was purified by column chromatography (PE/EtOAc=10/1) to give (2*S*,5*S*)-5H-2,5-methanobenzo[e][1,4]dioxepin-3(2H)-one **8** as a white solid. (430 mg, 90% yield, >99:1 dr, 99% *ee*). Mp: 78-79 °C. $[\alpha]_{\text{D}}^{20} = +92.7$ (*c* 0.15, CH_2Cl_2). ^1H NMR (400 MHz, CDCl_3) δ 7.31 (td, $J = 8.2, 1.5$ Hz, 1H), 7.16 (dd, $J = 7.4, 1.1$ Hz, 1H), 6.92 (dd, $J = 14.3, 7.8$ Hz, 2H), 5.36 (d, $J = 5.0$ Hz, 1H), 4.87 (d, $J = 3.1$ Hz, 1H), 2.56 (ddd, $J = 12.8, 5.0, 3.4$ Hz, 1H), 2.44 (d, $J = 12.8$ Hz, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 171.34, 152.55, 131.64, 127.36, 123.01, 121.19, 116.78, 76.10, 72.90, 31.84. HRMS (ESI): m/z for $\text{C}_{10}\text{H}_8\text{O}_3$ $[\text{M}+\text{H}]^+$ calcd 177.0473, found 177.0550. HPLC condition: Chiralcel OD-H column (25 cm \times 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, t_{R} =16.14 min for major isomer, and t_{R} =18.49 min for minor isomer.

6. X-ray analysis

X-Ray Crystallography Data for **2m** (CCDC 2089780): A colorless crystal suitable for X-ray crystallography was obtained from *n*-hexane/DCM/THF solution at room temperature under air atmosphere.



The ORTEP drawing (50% probability for thermal ellipsoids) of **2m**

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. [CIF dictionary](#) [Interpreting this report](#)

Datablock: 20210618bl_0m_b

Bond precision:	C-C = 0.0070 Å	Wavelength=1.34139	
Cell:	a=5.0850(3)	b=10.2391(6)	c=10.6291(6)
	alpha=61.505(1)	beta=86.820(1)	gamma=79.073(1)
Temperature:	106 K		
	Calculated	Reported	
Volume	477.16(5)	477.16(5)	
Space group	P 1	P 1	
Hall group	P 1	P 1	
Moiety formula	C10 H7 Br O4	2(C10 H7 Br O4)	
Sum formula	C10 H7 Br O4	C20 H14 Br2 O8	
Mr	271.06	542.13	
Dx, g cm-3	1.887	1.887	
Z	2	1	
Mu (mm-1)	3.851	4.003	
F000	268.0	268.0	
F000'	266.69		
h, k, lmax	6, 12, 12	6, 12, 12	
Nref	3624[1812]	3534	
Tmin, Tmax	0.487, 0.619	0.024, 0.091	
Tmin'	0.428		

Correction method= # Reported T Limits: Tmin=0.024 Tmax=0.091
AbsCorr = MULTI-SCAN

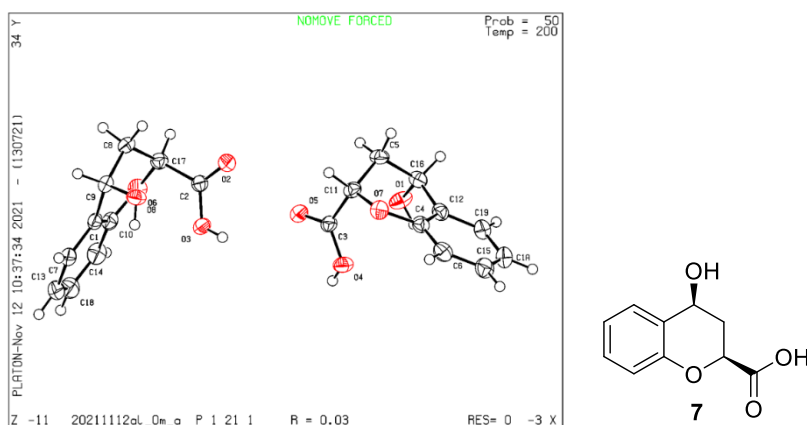
Data completeness= 1.95/0.98 Theta(max)= 54.994

R(reflections)= 0.0224(3525) wR2(reflections)= 0.0572(3534)

S = 1.056 Npar= 273

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

X-Ray Crystallography Data for **7** (CCDC 2122207): A colorless crystal suitable for X-ray crystallography was obtained from *n*-hexane/DCM/THF solution at room temperature under air atmosphere.



The ORTEP drawing (50% probability for thermal ellipsoids) of **7**

Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Gaussian 16, Revision A.03; Wallingford CT, 2016.

7.2 Computational Methods

All density functional theory (DFT) calculations were conducted using the GAUSSIAN 16 series of programs. Density functional B3-LYP⁴ with a standard 6-31G(d) basis set (LanL08⁵ basis set for Rh and Fe) was used for geometry optimizations. Harmonic frequency calculations were performed for all stationary points to confirm them as local minima or transition structures, and to derive thermochemical corrections for the enthalpies and free energies. All minima had zero imaginary frequency and all transition states had only one imaginary frequency. The DFT method M06 functional⁶ with larger basis set 6-311+G(d) (LanL08 basis set for Rh and Fe) was used to calculate single point energies with methanol as solvent with a continuum solvation model (SMD⁷). The energies reported in this study are M06-calculated Gibbs free energies in methanol solvent. In order to evaluate accurately the entropy of the multi-component system, the solution-translational entropy correction has been recalculated with THERMO program.⁸ The optimized structures were displayed using CYLview.⁹

7.3 Calculated Gibbs energy profiles

The calculated Gibbs energy profiles for the enantioselective hydrogenation using JosiPhos SL-J216-1 as ligand were given in Figure S1, where the active catalyst Rh(I) species **CP1** was set as the relative zero point. As shown in Figure S1, the oxidation of H₂ onto the Rh(I) center in **CP1** occurred via transition state **TS1** to give Rh(III) hydride species **CP2**. The free energy barrier of **TS1** is only 6.2 kcal/mol. The coordination of the carboxylic acid anion, which is generated by ionization of chromone-2-carboxylic acid in MeOH, to the Rh(III) center in **CP2** generate the carboxyl-Rh(III) intermediate **CP3** with 3.5 kcal/mol exergonic. The subsequent protonation of carbonyl in intermediate **CP3** by the protonated methanol gives aromatic oxonium ion intermediate **CP4**. The following 1,4-migration of hydride from Rh(III) center to carbonyl cation with a *Re*-face occurs via transition state **TS2** with a free energy barrier of 5.2 kcal/mol to give the cationic Rh(III) intermediate **CP5**. In **TS2**, the MeOH has a secondary interaction with JosiPhos SL-J216-1, that is, a hydrogen-bonding interaction of MeOH with naphthalene unit. The O-H reductive elimination occurs via transition state **TS3** with an overall activation free energy of 24.1 kcal/mol, where the active catalyst Rh(I) **CP1** and enol intermediate **CP6** was generated. The isomerization of enol intermediate **CP6** would give the **2a** product with *S* configuration. As seen in Figure S1, the calculated results show that the 1,4-migration of hydride from Rh(III) center to carbonyl cation with a *Si*-face in **CP4'** occurs via transition state **TS2'** with a free energy barrier of 8.4 kcal/mol to give the cationic Rh(III) intermediate **CP5'**. The free energy of **TS2'** is 1.6 kcal/mol higher than that of **TS2**. The following O-H bond reductive elimination generates the enol intermediate **CP6'** with *R* configuration via transition state **TS3'**. The hydrogen-bonding interaction of MeOH with naphthalene unit leads to the relative free energy of **TS2** is 1.6 kcal/mol lower than that of **TS2'**. The free energy of **TS3'** is also 1.3

kcal/mol higher than that of **TS3**. The calculated results indicated that the generation of enantiomer (*R*)-**2a** is demonstrated to be kinetically unfavorable, which is consistent with the experiment observation.

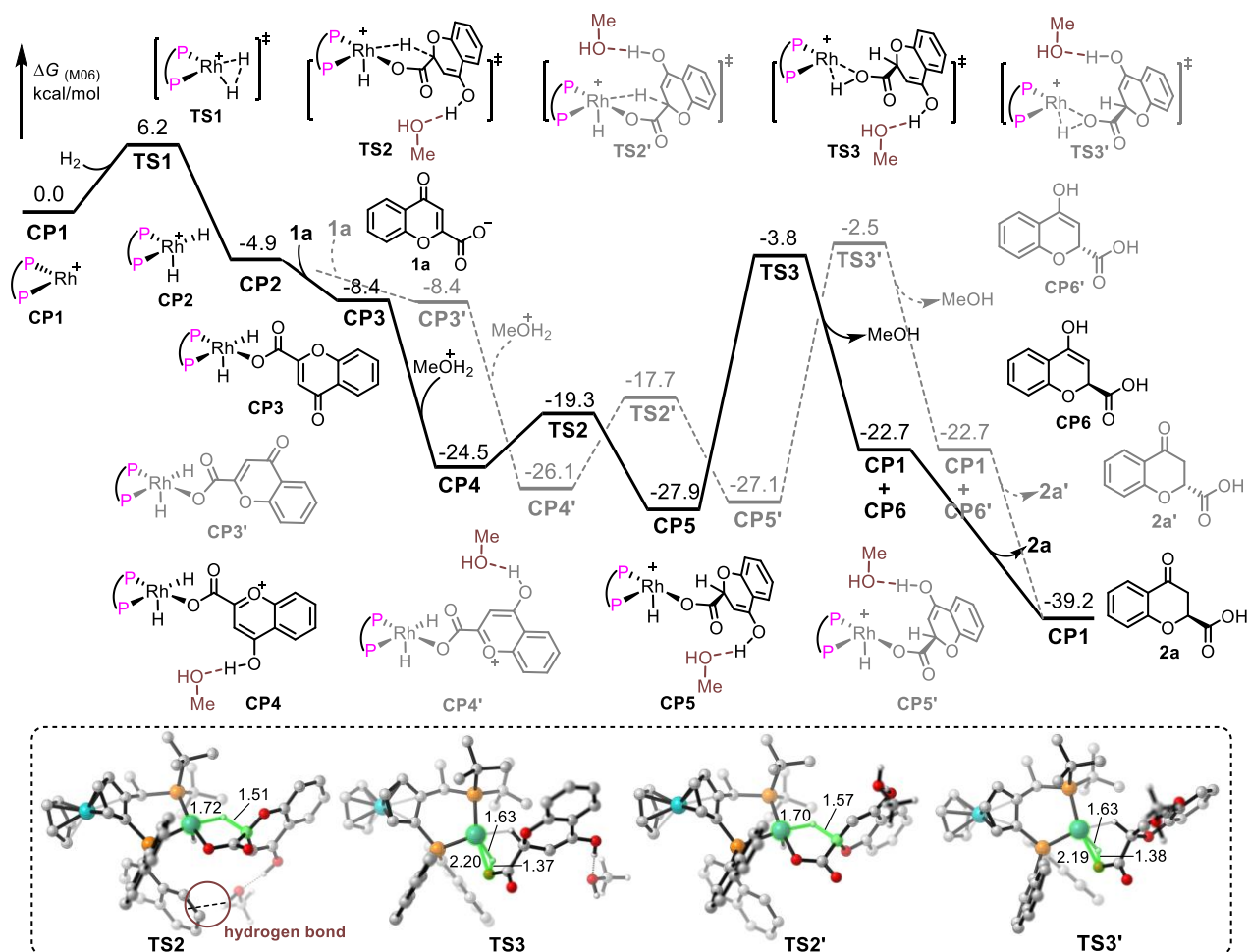


Figure S1 Calculated Gibbs energy profiles for the highly chemo- and enantioselective hydrogenation of chromone-2-carboxylic acids.

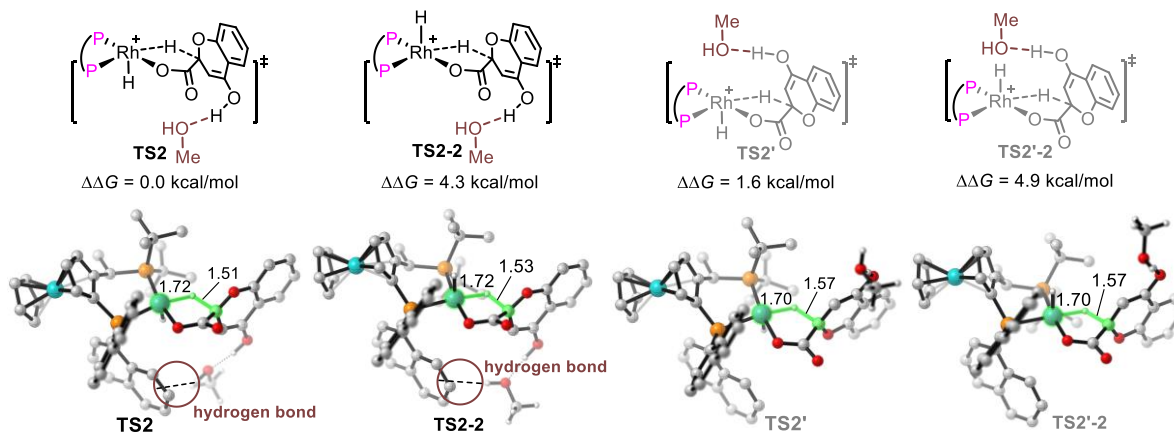


Figure S2 Transition states **TS2** and **TS2'** with different configurations.

We also calculated the transition states for the axial H migrates to carbonyl cation in **CP4** and **CP4'**. The calculated results were shown in Figure S2. The free energy of **TS2-2** is 4.3 kcal/mol higher than that of **TS2**. The free energy of **TS2'-2** is 3.3 kcal/mol higher than that of **TS2'**. Thus, the calculated results indicated that the axial H migrates to carbonyl cation in **CP4** and **CP4'** are unfavorable.

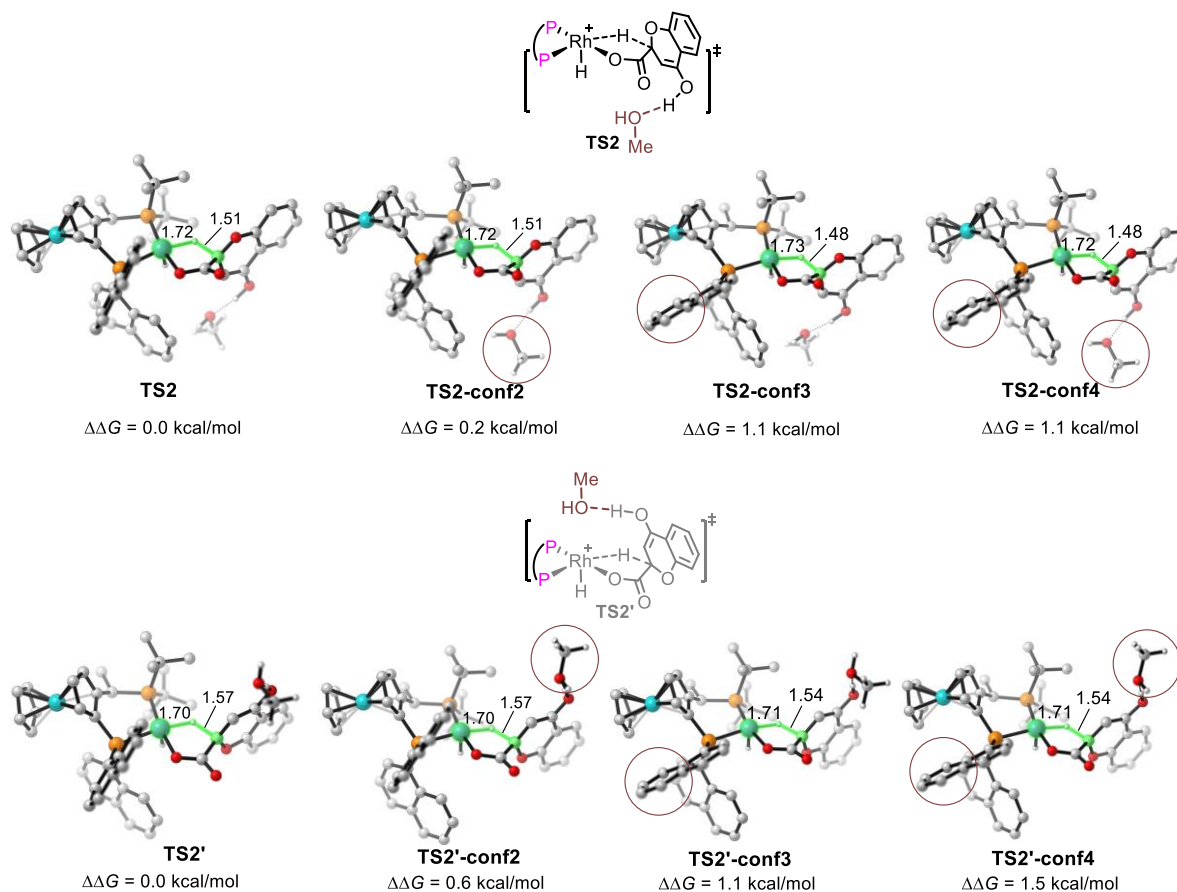


Figure S3 Conformational search on key transition states **TS2** and **TS2'**.

We performed the conformation search for **TS2** and **TS2'**. We've got four conformations for both transition states. The orientation of the methyl groups in methanol and the naphthalene ring is different in these different conformations.

7.4 B3-LYP and M06 absolute calculation energies, enthalpies, and free energies

Geometry	$E_{(\text{elec-B3-LYP})}^a$	$H_{(\text{corr-B3-LYP})}^b$	$G_{(\text{corr-B3-LYP})}^c$	$E_{(\text{solv-M06})}^d$	IF ^e
CP1	-2466.280242	0.777517	0.678802	-2465.491497	-
H ₂	-1.175482	0.01345	0.010522	-1.168172793	-
TS1	-2467.451743	0.792905	0.691803	-2466.652235	-832.3
CP2	-2467.462809	0.795427	0.694219	-2466.672425	-
1a	-685.0172818	0.140521	0.103822	-684.903934	-

CP3	-3152.658178	0.940215	0.817248	-3151.601044	-
MeO ⁺ H ₂	-116.013629	0.068852	0.052479	-116.100148	-
CP4	-3268.792851	1.010699	0.877251	-3267.734375	-
TS2	-3268.766668	1.007730	0.853069	-3267.724611	-647.7
CP5	-3268.770904	1.011180	0.877354	-3267.739918	-
TS3	-3268.730199	1.009103	0.874899	-3267.699017	-1214.7
MeOH	-115.712205	0.055710	0.040105	-115.687418	-
CP6	-686.742125	0.177317	0.139085	-686.533316	-
2a	-686.770004	0.177735	0.139094	-686.559631	-
CP3'	-3152.658448	0.940212	0.817098	-3151.600973	-
CP4'	-3268.793489	1.010980	0.876659	-3267.736388	-
TS2'	-3268.766822	1.007949	0.875092	-3267.721438	-621.4
CP5'	-3268.770569	1.011219	0.877889	-3267.739134	-
TS3'	-3268.730684	1.009255	0.875464	-3267.697577	-1207.6
CP6'	-686.742125	0.177317	0.139085	-686.533316	-
2a'	-686.770004	0.177735	0.139094	-686.559631	-
TS2-2	-3268.760891	1.008084	0.875841	-3267.717753	-653.1
TS2'-2	-3268.763427	1.008256	0.874917	-3267.716127	-616.5
TS2-conf2	-3268.766809	1.007824	0.875909	-3267.724398	-638.3
TS2-conf3	-3268.765910	1.007922	0.876070	-3267.723095	-610.4
TS2-conf4	-3268.766157	1.007972	0.875987	-3267.723063	-603.8
TS2'-conf2	-3268.766656	1.008049	0.875246	-3267.720707	-621.3
TS2'-conf3	-3268.765074	1.008066	0.874964	-3267.719628	-611.4
TS2'-conf4	-3268.764885	1.008065	0.874715	-3267.718690	-613.4

^aThe electronic energy calculated by B3-LYP in gas phase. ^bThe thermal correction to enthalpy calculated by B3-LYP in gas phase. ^cThe thermal correction to Gibbs free energy calculated by B3-LYP in gas phase. ^dThe electronic energy calculated by M06 in methanol solvent. ^eThe B3-LYP calculated imaginary frequencies for the transition states.

7.5 B3-LYP geometries for all the optimized compounds and transition states

CP1				C	1.97357300	0.67924600	-0.92050600
Fe	3.25980700	-0.95353300	-0.81309500	C	3.89601000	-1.75516400	1.01309200

C	2.86168700	0.65508900	-2.04189900	H	-1.79716500	4.86127500	-0.64474600
H	3.60054100	1.40808500	-2.27774700	H	-2.04266800	4.44524900	-2.33864300
C	1.19440000	-0.55216400	-0.96492600	P	-0.39009200	-0.84245200	-0.09996200
C	5.32353900	-0.90212900	-0.58591700	C	-1.39953900	-1.86054200	-1.28284600
H	5.97276600	-0.23124300	-1.13307300	C	-2.50171500	-1.35464300	-2.05855400
C	1.65816700	-1.30355100	-2.10369500	C	-1.03469900	-3.19417700	-1.40896500
H	1.27961000	-2.26623000	-2.41504500	C	-3.02569400	-0.03642500	-1.95048000
C	4.02700600	-2.72747800	-0.02638800	C	-3.14522700	-2.24740600	-2.98802300
H	3.54580100	-3.69578800	-0.06882300	C	-1.67522700	-4.06114500	-2.32016000
C	4.69614200	-0.62973000	0.66707100	H	-0.23835300	-3.60031600	-0.79387900
H	4.80044100	0.27662400	1.24876000	C	-4.09237200	0.38121200	-2.71699800
C	2.66868000	-0.55907200	-2.76164100	H	-2.58273200	0.64466800	-1.22474300
H	3.22829400	-0.87867900	-3.63062100	C	-4.23486800	-1.77986800	-3.77224200
C	4.91246700	-2.19937000	-1.01136200	C	-2.70213400	-3.58986200	-3.10295000
H	5.19261000	-2.68206700	-1.93835200	H	-1.35247300	-5.09537400	-2.39208200
H	3.28623100	-1.84461000	1.90108100	C	-4.70134800	-0.49255400	-3.64682200
C	1.86165800	1.81086200	0.08223900	H	-4.47221400	1.39311700	-2.60380800
H	1.90714300	1.36849900	1.08234800	H	-4.70050700	-2.46948600	-4.47144900
C	3.01249600	2.82666100	-0.02771800	H	-3.20215300	-4.24555700	-3.81102600
H	2.91286100	3.62870800	0.70777900	H	-5.53753000	-0.14935400	-4.24859700
H	3.96393100	2.31868100	0.16146200	C	-0.25397400	-1.93842500	1.37839600
H	3.07509800	3.28856400	-1.01410200	C	-1.23856300	-1.73269800	2.40226100
P	0.10188200	2.51738300	0.12110600	C	0.74941700	-2.86718900	1.57059700
C	-0.31034800	3.46391000	-1.49782800	C	-2.34287300	-0.83391100	2.25793500
C	-0.05456500	3.63597200	1.68305900	C	-1.10511300	-2.43621400	3.64245400
C	0.29518700	5.12633600	1.53386900	C	0.84895300	-3.59708200	2.78029800
H	0.16090800	5.62004400	2.50508600	H	1.48898800	-3.02273700	0.79434600
H	1.33643600	5.27935300	1.23430300	C	-3.22803800	-0.61040000	3.29849500
H	-0.34841700	5.64318600	0.81764200	H	-2.67767900	-0.51157500	1.24320000
C	0.80425400	3.03249300	2.81737900	C	-2.02935600	-2.17592300	4.69127000
H	0.59676900	1.96701300	2.96666000	C	-0.04592400	-3.37142300	3.79975600
H	1.87627100	3.16108100	2.64293200	H	1.64824800	-4.32202700	2.90320500
H	0.56502400	3.55201000	3.75359300	C	-3.05744700	-1.27192800	4.53474400
C	-1.54495800	3.49381900	2.09147500	H	-4.07784100	0.04987700	3.15073000
H	-1.72181400	4.01099900	3.04364000	H	-1.91200100	-2.71285100	5.62899500
H	-2.23778000	3.90436600	1.35474300	H	0.04470000	-3.90571200	4.74164800
H	-1.82969500	2.43725800	2.30645100	H	-3.75499800	-1.08878000	5.34607100
C	0.67082400	4.60347500	-1.84862400	Rh	-1.33102700	0.92865600	0.87029900
H	0.27455100	5.14036700	-2.71968800				
H	0.79994800	5.33367100	-1.04827200	H₂			
H	1.65479200	4.22311700	-2.13169900	H	0.00000000	0.00000000	0.37139400
C	-0.30452300	2.45224400	-2.66521000	H	0.00000000	0.00000000	-0.37139400
H	-0.59422900	2.98266200	-3.58118800				
H	0.68362100	2.01899300	-2.83559300	TS1			
H	-1.01908700	1.63974900	-2.51700400	Fe	0.15009800	-3.47516200	0.27452300
C	-1.73715000	4.04098100	-1.36597200	C	1.13287300	-1.76674200	-0.50607300
H	-2.46469600	3.27258000	-1.08263500	C	0.63481100	-3.94563500	2.25314100

C	1.28769600	-2.90193200	-1.36242800	H	4.19585900	2.17003000	-2.97175700
H	2.22316100	-3.37782900	-1.62310700	H	3.17744100	1.81433600	-4.36413600
C	-0.28667400	-1.52957700	-0.36715300	P	-0.96966200	0.06080900	0.14244000
C	0.25666600	-5.52192800	0.60939700	C	-2.75479600	0.00594000	-0.30583000
H	0.42017600	-6.24928500	-0.17478500	C	-3.25693200	0.53214800	-1.54468200
C	-0.97618000	-2.50971800	-1.16638500	C	-3.62235700	-0.59144900	0.59607800
H	-2.04889700	-2.58893000	-1.27310200	C	-2.44938700	1.18930400	-2.51236800
C	-0.77692300	-4.05634900	2.05884300	C	-4.66214600	0.39794300	-1.81985300
H	-1.54505500	-3.50320900	2.58207500	C	-5.00074400	-0.71908500	0.31467200
C	1.27117100	-4.85649800	1.35856300	H	-3.24619400	-0.96682200	1.54310800
H	2.33756400	-5.00440300	1.25015200	C	-2.99030500	1.67906400	-3.68149600
C	-0.00312700	-3.34248300	-1.78117700	H	-1.38887100	1.31511000	-2.31643800
H	-0.20761900	-4.19947700	-2.40911700	C	-5.18587200	0.90966800	-3.03786000
C	-1.00907500	-5.02583400	1.04172900	C	-5.50548200	-0.23724900	-0.87095300
H	-1.97435300	-5.31335100	0.64651400	H	-5.65341900	-1.19471800	1.04041800
H	1.13756900	-3.29272000	2.95472200	C	-4.37125600	1.53591800	-3.95267200
C	2.23018200	-0.91841800	0.09311200	H	-2.35103100	2.18103800	-4.40242200
H	1.90153600	-0.60806400	1.09148500	H	-6.24950300	0.79859900	-3.23183300
C	3.52449100	-1.73804100	0.27279100	H	-6.56492900	-0.33004500	-1.09552700
H	4.24701100	-1.23331300	0.91290000	H	-4.78388800	1.92421700	-4.87896000
H	3.26124600	-2.68227100	0.75983000	C	-0.95857700	0.40883000	1.94965100
H	4.01617000	-1.97722400	-0.67176400	C	-1.09663000	1.80124300	2.29557300
P	2.37340600	0.82681900	-0.76482100	C	-0.68567900	-0.52144400	2.93259200
C	2.66713200	0.60481100	-2.65592100	C	-1.36073900	2.83399500	1.33391500
C	3.89307800	1.67957900	0.09152700	C	-0.92332300	2.18739700	3.66377600
C	5.25638900	1.10335300	-0.35880600	C	-0.54851900	-0.13402900	4.28803200
H	6.03620000	1.52806100	0.28526000	H	-0.55578900	-1.55948900	2.65477400
H	5.33130700	0.01899400	-0.28463100	C	-1.41496400	4.16587100	1.71348600
H	5.49941000	1.39254100	-1.38491100	H	-1.70922300	2.58493500	0.32199300
C	3.71160500	1.50985400	1.61822700	C	-0.99957200	3.56340300	4.01269600
H	2.73563100	1.88484800	1.94680100	C	-0.66074100	1.18934800	4.64308100
H	3.82005700	0.47772200	1.95980200	H	-0.34297100	-0.88815200	5.04203100
H	4.48118300	2.10110700	2.12917100	C	-1.22651600	4.53538400	3.06205500
C	3.93920900	3.20322400	-0.18154500	H	-1.62882000	4.92568200	0.96781900
H	4.88762800	3.58409900	0.21634000	H	-0.87115000	3.83947000	5.05616000
H	3.90353100	3.46169400	-1.24101000	H	-0.53953800	1.49450500	5.67898200
H	3.13615800	3.73659500	0.33043700	H	-1.27719000	5.58108800	3.34868100
C	3.66311900	-0.52495200	-2.99246000	Rh	0.45411800	1.98755000	-0.24878300
H	3.81178600	-0.53964000	-4.07937400	H	1.28328000	3.33867100	-0.04828500
H	4.64400900	-0.38594800	-2.53321600	H	0.97953700	3.10497500	-1.23042900
H	3.27585700	-1.50612200	-2.70930800				
C	1.30875800	0.27607100	-3.31189900	CP2			
H	1.46885600	0.12971800	-4.38762300	Fe	0.51530500	-3.32785500	0.20237600
H	0.85589200	-0.63648100	-2.91824300	C	1.43251000	-1.47793400	-0.29479000
H	0.60158400	1.09957300	-3.18495200	C	0.81406500	-3.95767700	2.17507900
C	3.17448500	1.92521400	-3.27289800	C	1.86515600	-2.53976200	-1.15263600
H	2.52386200	2.77275100	-3.03407200	H	2.87828600	-2.90572800	-1.25087600

C	-0.00649700	-1.38463800	-0.41617300	P	-0.96963700	0.09363100	0.04419500
C	0.59386700	-5.39281100	0.38164100	C	-2.64590600	-0.19444800	-0.66667200
H	0.83036200	-6.05555000	-0.44031000	C	-2.97157500	0.22365800	-2.00316900
C	-0.42544700	-2.37495700	-1.37265300	C	-3.61906900	-0.77879100	0.12762300
H	-1.44591300	-2.55553000	-1.68023800	C	-2.04251300	0.80485900	-2.91161400
C	-0.57292700	-4.04225100	1.84282300	C	-4.32121200	0.04418800	-2.46507100
H	-1.38146500	-3.51791700	2.33316300	C	-4.93734900	-0.97187500	-0.34345600
C	1.53415000	-4.79500200	1.27157700	H	-3.37637300	-1.08152900	1.14155600
H	2.60668300	-4.93709500	1.25009800	C	-2.41760100	1.21488700	-4.17302900
C	0.72738700	-3.07223300	-1.82980900	H	-0.99508300	0.88979100	-2.62408600
H	0.73301700	-3.90282700	-2.52308600	C	-4.67781600	0.47503500	-3.77175900
C	-0.70767300	-4.92534900	0.73349600	C	-5.28041500	-0.56002500	-1.60955300
H	-1.63131700	-5.17478300	0.22830800	H	-5.67520600	-1.43266800	0.30621100
H	1.24687200	-3.37205700	2.97584400	C	-3.75287100	1.05478100	-4.60927600
C	2.29810600	-0.53883200	0.51211600	H	-1.68189200	1.65413800	-4.84067100
H	1.71950200	-0.23155700	1.39008000	H	-5.70457300	0.33540100	-4.09965200
C	3.58102100	-1.22020500	1.02813800	H	-6.29586100	-0.68906200	-1.97491900
H	4.09420200	-0.61601700	1.77701500	H	-4.03987400	1.38112800	-5.60412500
H	3.29180000	-2.16105000	1.50731200	C	-1.22165600	0.24437500	1.85960400
H	4.29408500	-1.45696700	0.23709200	C	-1.89961900	1.40309100	2.38349100
P	2.48879300	1.18009100	-0.36067400	C	-0.66176700	-0.67349700	2.72874300
C	3.33950500	0.99647900	-2.07643500	C	-2.49443300	2.40990000	1.57310500
C	3.46354400	2.29587300	0.86684900	C	-1.98292900	1.55619900	3.80952000
C	4.97883200	1.98292000	0.85903500	C	-0.75022500	-0.51319300	4.13240800
H	5.45263600	2.57675500	1.64973800	H	-0.14503600	-1.53496300	2.32545000
H	5.21200800	0.93556000	1.05751900	C	-3.12132300	3.50343500	2.13288600
H	5.45492700	2.26714100	-0.08253100	H	-2.47725800	2.31616300	0.49199600
C	2.89007900	2.06549000	2.28418500	C	-2.64342300	2.69030400	4.35370800
H	1.80731900	2.22526400	2.32249500	C	-1.39894300	0.57727300	4.65874200
H	3.10864200	1.07109700	2.68191600	H	-0.30502000	-1.25783800	4.78610400
H	3.35088400	2.79260100	2.96292000	C	-3.19980400	3.64787800	3.53683900
C	3.27649400	3.79045000	0.52395900	H	-3.56657300	4.25634600	1.48890700
H	3.87350600	4.37496200	1.23455400	H	-2.70007700	2.78757900	5.43479000
H	3.61801800	4.04461400	-0.48100900	H	-1.47317900	0.70990000	5.73499500
H	2.23499200	4.10408000	0.61752600	H	-3.70110000	4.51069700	3.96490600
C	4.48529800	-0.03515100	-2.08095700	Rh	0.41672300	1.91712200	-0.83642700
H	4.94166800	-0.03900200	-3.07851500	H	0.40798300	2.63082200	0.50484100
H	5.27446200	0.20583000	-1.36377700	H	1.25640200	3.16725800	-1.35333300
H	4.12795400	-1.04810800	-1.88642000				
C	2.23473300	0.53709700	-3.05804700	1a			
H	2.67229500	0.42252800	-4.05789200	C	-2.98629500	-1.61414700	-0.00005500
H	1.78654800	-0.41958100	-2.78086400	C	-1.61665400	-1.83851900	-0.00007400
H	1.44494800	1.29794000	-3.15018600	C	-0.74103200	-0.74072300	-0.00002500
C	3.88182300	2.35179600	-2.57688700	C	-1.23245700	0.57403700	0.00004500
H	3.11343400	3.12926300	-2.58159600	C	-2.62243800	0.77419100	0.00006500
H	4.73810400	2.70569000	-1.99808600	C	-3.49682200	-0.30316800	0.00001500
H	4.22500600	2.21717000	-3.61000900	H	-3.66776600	-2.46204100	-0.00009500

H	-1.19490000	-2.83885400	-0.00012800
C	-0.28121600	1.71715000	0.00009900
H	-2.97250300	1.80251800	0.00012000
H	-4.57187100	-0.13927000	0.00003100
C	1.10634200	1.30687700	0.00009200
C	1.49880100	0.00330200	-0.00000100
H	1.89686500	2.04700200	0.00017000
O	-0.68099000	2.89047500	0.00020400
O	0.58804900	-1.01815600	-0.00004900
C	2.98911300	-0.47209200	-0.00004500
O	3.14342400	-1.70955900	-0.00028600
O	3.80028100	0.48089000	0.00003000

CP3

Fe	3.64224500	-1.24226300	-2.08570300
C	2.64113600	0.53589100	-1.44628600
C	4.63253300	-2.77833500	-1.06777300
C	2.92079700	0.53763400	-2.85061400
H	3.54145900	1.25449400	-3.37119500
C	1.83035000	-0.62461500	-1.16532000
C	5.68019700	-1.29193500	-2.49310000
H	6.24767100	-0.44973000	-2.86708300
C	1.60754800	-1.30325200	-2.41458700
H	1.03880400	-2.21268900	-2.53996700
C	4.34049900	-3.17218200	-2.40563000
H	3.70724700	-3.99874900	-2.69971100
C	5.45928500	-1.61374900	-1.12020700
H	5.85007800	-1.06724300	-0.27166000
C	2.26158800	-0.57677200	-3.44864600
H	2.30128500	-0.85495500	-4.49370300
C	4.98954000	-2.25553000	-3.28719300
H	4.93216300	-2.26419600	-4.36783000
H	4.26516800	-3.26100700	-0.17290700
C	3.03081500	1.59787600	-0.44792500
H	3.18729100	1.09745600	0.51268900
C	4.36472500	2.27084500	-0.82514400
H	4.74921600	2.89720800	-0.01959400
H	5.10545000	1.48569900	-1.01398800
H	4.30007800	2.88602200	-1.72405900
P	1.50754300	2.69836300	0.02667100
C	0.93689600	3.70819700	-1.51827500
C	2.21891400	3.88319500	1.39498500
C	3.07601200	5.04710000	0.84750100
H	3.51641200	5.58299100	1.69841900
H	3.89894700	4.72525400	0.20695800
H	2.47549300	5.77156500	0.29095500
C	3.07287000	3.04053100	2.37105700

H	2.52299600	2.17292700	2.74880800
H	4.01210300	2.69180000	1.93336900
H	3.33267900	3.66635600	3.23430900
C	1.07581800	4.50624400	2.22962200
H	1.52372600	5.19729100	2.95649100
H	0.36626400	5.07538600	1.62526000
H	0.51570800	3.74708700	2.77689200
C	2.07869000	4.31394600	-2.36032900
H	1.63348000	4.93681600	-3.14756200
H	2.75795100	4.94893600	-1.78795000
H	2.66443600	3.53936800	-2.86234500
C	0.12628700	2.75639200	-2.42873500
H	-0.20064700	3.32462500	-3.31068300
H	0.72196800	1.91284500	-2.78513500
H	-0.76342700	2.37077300	-1.92866900
C	-0.01602700	4.83627000	-1.06649500
H	-0.82887100	4.45325700	-0.44308000
H	0.49812300	5.63524100	-0.52467700
H	-0.46530200	5.28743200	-1.96085500
P	0.79135300	-0.83660600	0.33458300
C	-0.02843900	-2.48186800	0.01041300
C	-1.15876300	-2.60623900	-0.87181000
C	0.46391000	-3.61653900	0.63492200
C	-1.72380500	-1.51079000	-1.57905500
C	-1.74624400	-3.90444500	-1.06876400
C	-0.12024200	-4.88918800	0.43754800
H	1.31689400	-3.54095600	1.29943100
C	-2.80823900	-1.67744600	-2.41342100
H	-1.31498700	-0.51689200	-1.44794900
C	-2.86038000	-4.04266300	-1.94015100
C	-1.20439800	-5.02955900	-0.39422800
H	0.29557700	-5.75037300	0.95329900
C	-3.38467700	-2.95520800	-2.60004600
H	-3.22733500	-0.81196800	-2.91790100
H	-3.29319200	-5.03150900	-2.07278600
H	-1.66317500	-6.00333000	-0.54894700
H	-4.24038400	-3.07394300	-3.25907700
C	1.86121900	-1.21241900	1.80415400
C	1.25680300	-1.37870100	3.10304900
C	3.23715200	-1.26192300	1.68877100
C	-0.14633200	-1.32042900	3.33128500
C	2.11194300	-1.62301100	4.23231200
C	4.07351300	-1.48183600	2.81057100
H	3.68846200	-1.13953500	0.71315700
C	-0.67044200	-1.50208500	4.59344000
H	-0.82493600	-1.10121400	2.51502200
C	1.53666100	-1.81233800	5.51755900

C	3.52127400	-1.66589400	4.05385600	H	-7.33047000	-0.40433200	0.19232700
H	5.15175500	-1.51248800	2.67600700	C	-3.03780000	-1.41461300	1.92006100
C	0.17385400	-1.75703600	5.69831400	H	-2.59525100	-2.35351200	2.21835900
H	-1.74525100	-1.44142100	4.73816700	C	-5.42094400	-3.15504500	0.40018000
H	2.19969100	-1.99971700	6.35907600	H	-5.00665600	-4.03908100	0.86642000
H	4.15224300	-1.84512200	4.92131200	C	-5.79376100	-1.42475400	-1.08313700
H	-0.25478600	-1.90126800	6.68631600	H	-5.73821300	-0.78208700	-1.95237200
Rh	-0.23831000	1.41412600	0.79439300	C	-4.10242700	-0.74472700	2.58154600
H	0.56751100	1.40011300	2.10421300	H	-4.63257000	-1.10189200	3.45448900
H	-0.78125100	2.80184300	1.28791900	C	-6.41529500	-2.29824200	0.96092700
C	-8.04585300	0.89213800	-2.44813600	H	-6.88414900	-2.41706400	1.92884500
C	-6.68933600	1.07721600	-2.21715700	H	-4.29262700	-3.03166200	-1.52666200
C	-6.16058900	0.71702100	-0.97170800	C	-3.39783300	1.68712900	-0.23192300
C	-6.97089300	0.17886700	0.03894000	H	-3.13652000	1.27161500	-1.21068900
C	-8.34030500	0.00173800	-0.22067900	C	-4.74939800	2.41109100	-0.39250200
C	-8.87684200	0.35273600	-1.45025600	H	-4.75580600	3.07817300	-1.25490800
H	-8.46567100	1.16965400	-3.41116200	H	-5.52759400	1.65793700	-0.55587300
H	-6.02880900	1.49484800	-2.97014800	H	-5.03234400	2.99520100	0.48489500
C	-6.38000800	-0.18774600	1.34799500	P	-1.80674900	2.73660100	0.08821900
H	-8.94948000	-0.41594900	0.57483300	C	-1.85646900	3.50393000	1.85369400
H	-9.93635100	0.21394400	-1.64499800	C	-1.84296900	4.08623500	-1.29337200
C	-4.94492900	0.07258600	1.43398500	C	-2.85686400	5.22053500	-1.01942600
C	-4.25259700	0.59199400	0.39377600	H	-2.89014000	5.87798100	-1.89731100
H	-4.41808000	-0.15569100	2.35165400	H	-3.87318200	4.86760800	-0.83988700
O	-7.04285600	-0.66428800	2.26912700	H	-2.55819400	5.83862500	-0.16874600
O	-4.81793900	0.91809100	-0.79658500	C	-2.18781100	3.38829200	-2.63004600
C	-2.77681500	0.87694600	0.42958400	H	-1.52106200	2.54251100	-2.83142400
O	-2.21436900	1.41010700	-0.56169600	H	-3.22023800	3.03292900	-2.67941300
O	-2.14262600	0.55806200	1.48553400	H	-2.05688400	4.11085800	-3.44490400
MeO⁺H₂				C	-0.45040200	4.73253900	-1.47240500
C	0.79778400	0.00000000	0.01886300	H	-0.53313200	5.50716600	-2.24576400
H	1.10567200	0.90114000	-0.50713900	H	-0.08139200	5.21163400	-0.56367200
H	1.10567300	-0.90113500	-0.50714800	H	0.29565900	4.00431900	-1.79532000
H	1.06602700	-0.00000500	1.07457500	C	-3.25041000	3.97501900	2.30871100
O	-0.72021400	0.00000000	-0.09108700	H	-3.16004300	4.42789400	3.30447900
H	-1.15118200	-0.80339900	0.27761500	H	-3.67868200	4.73136400	1.64522500
H	-1.15118200	0.80339900	0.27761500	H	-3.95459100	3.14452500	2.39632200
CP4				C	-1.35778700	2.39239100	2.80943500
Fe	-4.65970700	-1.23741900	0.66043500	H	-1.36606700	2.77800500	3.83753400
C	-3.49658200	0.53568200	0.73984700	H	-1.98705300	1.49941000	2.78669400
C	-5.03909700	-2.61790300	-0.86309300	H	-0.31717500	2.10945200	2.59315400
C	-4.39991500	0.43978700	1.84675000	C	-0.86614500	4.68335100	1.96321900
H	-5.19943000	1.13210300	2.07265200	H	0.14133600	4.40433000	1.64260100
C	-2.64853700	-0.63613700	0.77072200	H	-1.18784700	5.56079700	1.39639700
C	-6.64619900	-1.22959500	0.04492100	H	-0.80763700	4.98354400	3.01713700
				P	-1.02317100	-0.80307600	-0.05624200
				C	-0.42935100	-2.41700600	0.65192800

C	0.32674800	-2.48397400	1.87308100
C	-0.77749300	-3.59137500	0.00345600
C	0.71809000	-1.34294500	2.62442100
C	0.70682200	-3.77706200	2.37783000
C	-0.40058900	-4.85757700	0.50596000
H	-1.35244500	-3.55049200	-0.91589400
C	1.44580200	-1.45961700	3.78838700
H	0.45253400	-0.35429100	2.27187000
C	1.45193500	-3.86483500	3.58518200
C	0.32800000	-4.94666400	1.66832600
H	-0.69156400	-5.75421700	-0.03367100
C	1.81580200	-2.73376100	4.27898800
H	1.74169200	-0.56139000	4.32169600
H	1.72704900	-4.85053800	3.95240800
H	0.62215200	-5.91586800	2.06352700
H	2.38400400	-2.81562000	5.20126900
C	-1.20879100	-1.18895600	-1.86082100
C	-0.05423200	-1.54001500	-2.65365700
C	-2.43322500	-1.04710400	-2.48503100
C	1.24978500	-1.71352000	-2.11270300
C	-0.22905800	-1.76835300	-4.06262700
C	-2.58818600	-1.23630000	-3.88086200
H	-3.30609600	-0.80692300	-1.89052600
C	2.30026300	-2.14322300	-2.90087500
H	1.43358300	-1.50934400	-1.06551900
C	0.87787300	-2.18419200	-4.85013700
C	-1.51117900	-1.59358900	-4.65257300
H	-3.56938900	-1.11190700	-4.33048700
C	2.11715300	-2.38883400	-4.28374900
H	3.26854700	-2.33080300	-2.44094300
H	0.72055600	-2.36448200	-5.91053100
H	-1.62354600	-1.75879600	-5.72096300
H	2.94237200	-2.75614700	-4.88893000
Rh	0.08543000	1.42608700	0.09400900
H	0.11561000	1.54679300	-1.42106000
H	0.80133400	2.82936600	0.05010400
C	8.60200800	0.22319800	2.58926200
C	7.24253000	0.44545200	2.74276200
C	6.43179000	0.41197100	1.60468700
C	6.96417300	0.15869200	0.32055700
C	8.35428900	-0.06587100	0.19541900
C	9.15907800	-0.03287000	1.31810600
H	9.24699100	0.24746400	3.46217100
H	6.79236600	0.64515800	3.70886100
C	6.05045900	0.14900700	-0.78592100
H	8.76594300	-0.26064300	-0.78850700
H	10.22658700	-0.20394900	1.22494300

C	4.69073000	0.39200000	-0.53027600
C	4.25963400	0.61681500	0.75538300
H	3.95421600	0.41266800	-1.32117700
O	6.51985500	-0.09281500	-1.98515900
O	5.09743900	0.63336400	1.78927600
C	2.79789200	0.90791600	1.08813400
O	2.52037300	1.42920500	2.16563800
O	2.04027000	0.56373500	0.11486100
C	4.65354200	0.82909600	-4.96315600
H	3.74157400	1.39815900	-5.17013500
H	5.49144400	1.52104500	-4.86302000
H	4.85543100	0.13666400	-5.78798100
O	4.54222000	0.13154200	-3.71270500
H	3.78147700	-0.47713000	-3.73611800
H	5.78719400	-0.06605600	-2.68018800

TS2

Fe	4.54124000	-1.21973200	-0.50384300
C	2.54192700	-1.89038500	-0.27384600
C	5.48858900	0.16542300	-1.75485000
C	3.47003400	-2.75564800	0.38602200
H	3.63448300	-3.80026300	0.15859100
C	2.70519700	-0.56903400	0.29194700
C	5.83590000	-2.11492200	-1.86453500
H	5.78225800	-3.15175600	-2.16960400
C	3.72672900	-0.65649900	1.30516000
H	4.08123800	0.16479300	1.91046000
C	6.34754000	-0.19988500	-0.67932300
H	6.74155800	0.46900200	0.07425300
C	5.16797600	-1.01878700	-2.48802400
H	4.53951300	-1.07937400	-3.36722200
C	4.18053200	-2.00191900	1.36750800
H	4.97040000	-2.37518000	2.00571500
C	6.56395300	-1.60894700	-0.74764000
H	7.14731700	-2.19675300	-0.05129300
H	5.13049900	1.16429600	-1.96313600
C	1.50378300	-2.27774400	-1.29767800
H	1.40702700	-1.43987900	-1.99649600
C	1.93460000	-3.50494100	-2.12345900
H	1.29405700	-3.65839900	-2.99262600
H	2.95094300	-3.33035000	-2.49246700
H	1.94586600	-4.43137100	-1.54755700
P	-0.26161900	-2.24243400	-0.52270100
C	-0.41037300	-3.56736500	0.86908600
C	-1.44566200	-2.61418900	-1.99922400
C	-1.49895100	-4.10446100	-2.40268000
H	-2.11558400	-4.19824000	-3.30532500

H	-0.52059600	-4.52940300	-2.63320000	C	-1.21783900	4.27090600	-1.06450400
H	-1.96499300	-4.72416100	-1.63243500	H	-0.37055100	2.85662700	0.27127600
C	-0.97725900	-1.76940200	-3.20746000	C	-0.43166400	4.27098000	-3.34890900
H	-0.86842700	-0.70945600	-2.95223900	C	1.30879400	2.67208100	-4.06123800
H	-0.03528500	-2.11951300	-3.63729500	H	2.82949700	1.24720800	-4.54550600
H	-1.73640400	-1.83893700	-3.99585900	C	-1.25370800	4.80193400	-2.37737100
C	-2.88020900	-2.15655000	-1.65578800	H	-1.85198300	4.69624600	-0.29130400
H	-3.52759500	-2.38186500	-2.51274200	H	-0.43667200	4.67638600	-4.35767800
H	-3.29713400	-2.66982300	-0.78714000	H	1.25982100	3.09345900	-5.06200400
H	-2.93041200	-1.08091800	-1.47316800	H	-1.90418600	5.64194400	-2.60744300
C	0.29812300	-4.90011800	0.56053600	Rh	-0.69105100	-0.20323400	0.54222600
H	0.10082500	-5.60072300	1.38192900	H	-1.08115300	0.31110600	-0.83061300
H	-0.05899200	-5.36854600	-0.36002500	H	-2.37054800	-0.53878000	0.74707500
H	1.38199800	-4.77887100	0.49555900	C	-7.38803300	-2.22553000	1.65685400
C	0.22554300	-2.94702100	2.13540400	C	-6.15649000	-1.80095200	2.14410900
H	0.16674100	-3.67330400	2.95629900	C	-5.44967900	-0.83450600	1.42851400
H	1.27684800	-2.68348200	1.99947200	C	-5.95526800	-0.28530900	0.23596000
H	-0.32453300	-2.05455000	2.46498700	C	-7.20181600	-0.73217600	-0.23841200
C	-1.89524600	-3.84467700	1.18904500	C	-7.91071400	-1.69503500	0.46619300
H	-2.45118600	-2.92632200	1.40122100	H	-7.95001500	-2.97314300	2.20840400
H	-2.40711800	-4.38745200	0.39086500	H	-5.73928000	-2.18807400	3.06757700
H	-1.94112000	-4.47288400	2.08749400	C	-5.15576900	0.72408700	-0.43026900
P	1.45895000	0.75734500	0.20125800	H	-7.59279500	-0.30752000	-1.15628600
C	2.05687600	2.02083500	1.40191200	H	-8.87380800	-2.03541100	0.09934600
C	1.93473200	1.83546300	2.82319700	C	-3.93552400	1.06214500	0.09868900
C	2.65192900	3.17183700	0.90763200	C	-3.42691100	0.40531900	1.26526900
C	1.38444800	0.67562600	3.43034000	H	-3.29791600	1.80243400	-0.36919300
C	2.41687700	2.87495000	3.69020100	O	-5.67223900	1.27500800	-1.52368500
C	3.13093500	4.18288100	1.77004000	O	-4.25266100	-0.42182500	1.95893100
H	2.75457600	3.31500000	-0.16239900	C	-2.50710600	1.25117100	2.19098200
C	1.29461900	0.55138200	4.79890500	O	-2.99684000	1.75972000	3.17473300
H	1.03272300	-0.13651400	2.80374800	O	-1.28544900	1.37619000	1.74764200
C	2.30500400	2.72061900	5.09864300	C	-4.19898100	2.98161800	-4.26579800
C	3.00648600	4.03905200	3.13144800	H	-3.34436800	2.98422600	-4.95161000
H	3.58966600	5.07137700	1.34684500	H	-4.92770200	2.24556800	-4.61048100
C	1.75434200	1.58584600	5.64639100	H	-4.66891200	3.97281500	-4.26109100
H	0.86325700	-0.34640700	5.23241000	O	-3.79707200	2.57878400	-2.95055700
H	2.66817200	3.52143500	5.73743900	H	-3.11872100	3.19552700	-2.62440500
H	3.36293400	4.81607500	3.80279200	H	-5.00177300	1.85911100	-1.97390900
H	1.67234500	1.47952800	6.72383200				
C	1.43265400	1.59398900	-1.44689300	CP5			
C	0.50409800	2.66576600	-1.72019200	Fe	4.50530300	-1.45785400	-0.14160600
C	2.23477200	1.11394700	-2.46520300	C	2.46162500	-1.85361600	-0.55633700
C	-0.36508900	3.23239600	-0.74499400	C	5.86457300	0.01377600	-0.75163900
C	0.45946200	3.20388900	-3.05269200	C	3.10825100	-2.97846100	0.04311100
C	2.17790000	1.64888700	-3.77481100	H	3.23029500	-3.95384300	-0.40827900
H	2.93201600	0.31318400	-2.25411200	C	2.58836900	-0.74218100	0.36011800

C	6.03341500	-2.21415900	-1.33407300	C	1.91352700	1.61617400	1.90105700
H	5.97377200	-3.14134800	-1.88884200	C	1.44366100	1.11487100	3.16480200
C	3.30526000	-1.21519600	1.51821300	C	2.66996400	2.77765000	1.85660800
H	3.56572800	-0.62126500	2.38182100	C	0.69878400	-0.08400600	3.32245300
C	6.37380100	-0.69605000	0.37276000	C	1.76062600	1.86008700	4.35101900
H	6.61010000	-0.27043400	1.33895200	C	2.98526700	3.49449900	3.03180900
C	5.65007200	-0.92413300	-1.80831400	H	3.02728800	3.15881700	0.90669300
H	5.27424800	-0.70107600	-2.79847300	C	0.27447200	-0.51365600	4.56036200
C	3.60637100	-2.59057800	1.32358600	H	0.46861300	-0.68925000	2.45079900
H	4.16984900	-3.21724800	2.00201500	C	1.30412700	1.39516000	5.61412500
C	6.48036400	-2.07305300	0.01264200	C	2.53057100	3.04858600	4.24994900
H	6.80687200	-2.87590400	0.66038500	H	3.57866900	4.40075100	2.95988700
H	5.65889600	1.07482700	-0.78670100	C	0.57376900	0.23498100	5.72202800
C	1.66529000	-1.82205700	-1.83627600	H	-0.29564100	-1.43431800	4.64608100
H	1.80660200	-0.83259300	-2.28335100	H	1.54729800	1.97805900	6.49854600
C	2.15883200	-2.85256900	-2.86788100	H	2.75677900	3.60110400	5.15820600
H	1.70118500	-2.69954700	-3.84633300	H	0.22914800	-0.10975500	6.69217800
H	3.24027600	-2.72560600	-2.98791900	C	2.01770700	1.89730200	-1.04953900
H	1.97757800	-3.88597000	-2.56999400	C	1.31015900	3.13651800	-1.26777900
P	-0.20922500	-1.71615400	-1.42354300	C	3.01169900	1.50896900	-1.93141000
C	-0.79652300	-3.32546400	-0.54020500	C	0.27049400	3.62237500	-0.42717800
C	-1.08547500	-1.46623400	-3.12208500	C	1.68763700	3.93714400	-2.40205900
C	-1.20960200	-2.75517400	-3.96384800	C	3.36642100	2.30242900	-3.04636300
H	-1.64224500	-2.49370700	-4.93760700	H	3.53980600	0.58080600	-1.75810500
H	-0.25050900	-3.24018300	-4.15597700	C	-0.35458600	4.82367100	-0.69348900
H	-1.87576400	-3.49005300	-3.50562200	H	-0.05331400	3.05457000	0.43736800
C	-0.28097800	-0.41356600	-3.91979900	C	1.02382300	5.17010200	-2.64174900
H	-0.11471700	0.50508400	-3.34665300	C	2.71758900	3.49193900	-3.27300900
H	0.68785800	-0.78678300	-4.26269600	H	4.15547300	1.96739600	-3.71343100
H	-0.85524000	-0.14100700	-4.81339100	C	0.02226900	5.60880100	-1.80653800
C	-2.50191000	-0.89028600	-2.89580900	H	-1.14309700	5.16821900	-0.03052800
H	-2.97284200	-0.73713900	-3.87493600	H	1.32729100	5.76275500	-3.50094200
H	-3.15069200	-1.55550200	-2.32299400	H	2.98418400	4.11284500	-4.12452800
H	-2.47370800	0.07748100	-2.38732500	H	-0.47594600	6.55477900	-1.99748400
C	-0.16068500	-4.61793800	-1.08701000	Rh	-0.65455400	0.06318000	0.07580400
H	-0.61760500	-5.47556100	-0.57710100	H	-0.73830900	0.95925200	-1.14543000
H	-0.32446000	-4.75146500	-2.15944800	H	-2.53790500	-0.09545800	0.06240000
H	0.91259800	-4.66066400	-0.88739300	C	-6.02654800	-3.34523700	2.21161100
C	-0.42102000	-3.17475200	0.95282900	C	-4.91551000	-2.51615500	2.35035400
H	-0.72863200	-4.08168200	1.48911100	C	-4.79919300	-1.39377800	1.52990800
H	0.65166700	-3.04395300	1.11205900	C	-5.78911100	-1.07985500	0.58275900
H	-0.95551100	-2.33587000	1.41855800	C	-6.90188100	-1.92666600	0.46171900
C	-2.33284900	-3.45070800	-0.61595000	C	-7.01783600	-3.05640700	1.26474000
H	-2.84319000	-2.55230300	-0.25994900	H	-6.12181100	-4.21990200	2.84843000
H	-2.69298400	-3.68196300	-1.62081400	H	-4.14433600	-2.71469300	3.08759600
H	-2.64421800	-4.27536500	0.03687900	C	-5.63080400	0.15315700	-0.18112200
P	1.55494400	0.75623200	0.31834300	H	-7.66941100	-1.67506200	-0.26176500

H	-7.88134600	-3.70658300	1.16525400
C	-4.48334400	0.87287400	-0.06652300
C	-3.38160300	0.40692400	0.78601600
H	-4.34404900	1.80457000	-0.60440900
O	-6.68291100	0.50198700	-0.93350000
O	-3.69825100	-0.59630500	1.71796200
C	-2.61246000	1.53660200	1.54309600
O	-3.23396100	2.34388000	2.19920800
O	-1.30800700	1.49990900	1.39695600
C	-6.88277800	3.51215700	-3.06469500
H	-6.51944500	4.51747700	-3.30578400
H	-6.56333300	2.82214200	-3.84758500
H	-7.97820500	3.51813800	-3.01795000
O	-6.30132800	3.03815500	-1.84112900
H	-6.57143600	3.62627600	-1.11770200
H	-6.53981000	1.39774800	-1.33511900

TS3

Fe	4.50499300	-1.51698600	-0.14433900
C	2.46174400	-1.90482400	-0.56082600
C	5.84830800	-0.04218200	-0.77829700
C	3.10503500	-3.03683100	0.02827300
H	3.22203200	-4.00958800	-0.43040500
C	2.59222700	-0.80149300	0.36333100
C	6.04474900	-2.27917000	-1.31650500
H	5.99709100	-3.21754600	-1.85328500
C	3.30388800	-1.28531600	1.51882400
H	3.56487300	-0.69905300	2.38780000
C	6.36219000	-0.72426600	0.36152800
H	6.59058700	-0.27747500	1.32002200
C	5.64845600	-1.00284200	-1.81697800
H	5.27358600	-0.80329500	-2.81252100
C	3.60362200	-2.65984100	1.31207400
H	4.16510900	-3.29335100	1.98580600
C	6.48607100	-2.10656600	0.02845200
H	6.81949400	-2.89285100	0.69278000
H	5.63067300	1.01548300	-0.83573800
C	1.65137600	-1.85188400	-1.82997000
H	1.80120100	-0.86230100	-2.27127300
C	2.10995000	-2.87620800	-2.88281800
H	1.61358400	-2.72292000	-3.84256800
H	3.18532700	-2.74136600	-3.04347600
H	1.94814500	-3.91174400	-2.58243800
P	-0.20912500	-1.70872900	-1.38344400
C	-0.83060600	-3.34402200	-0.56763700
C	-1.10600300	-1.34178800	-3.04775400
C	-1.30643100	-2.57806500	-3.94931300

H	-1.75518500	-2.24861800	-4.89496500
H	-0.37235100	-3.08773500	-4.19561700
H	-1.98779300	-3.31081100	-3.51024000
C	-0.27311500	-0.28326800	-3.80667100
H	-0.05658500	0.59203400	-3.18514700
H	0.67034800	-0.67994700	-4.19234000
H	-0.85370800	0.06105800	-4.67116000
C	-2.48365000	-0.71251400	-2.74699400
H	-2.97456700	-0.47521600	-3.69934400
H	-3.15066200	-1.37637300	-2.19322400
H	-2.38090100	0.21867000	-2.18200300
C	-0.26001700	-4.62521600	-1.20706900
H	-0.74491700	-5.49266500	-0.74168000
H	-0.44449300	-4.68660300	-2.28264800
H	0.81322500	-4.72517400	-1.02845100
C	-0.40149100	-3.29586900	0.91797000
H	-0.73665700	-4.21666200	1.41268000
H	0.68096500	-3.22524400	1.04481000
H	-0.86991100	-2.45475000	1.44475600
C	-2.37234500	-3.41246800	-0.60065400
H	-2.84036300	-2.52989600	-0.15691900
H	-2.77397800	-3.55144900	-1.60693300
H	-2.69023400	-4.27611100	-0.00366300
P	1.55516500	0.69640400	0.32469000
C	1.97797000	1.58217100	1.88399900
C	1.49335500	1.15671200	3.17121500
C	2.82006900	2.68102200	1.79402500
C	0.66470000	0.02156100	3.38114000
C	1.88516500	1.91485700	4.32820300
C	3.20845300	3.40870300	2.94016400
H	3.19069000	3.00369200	0.82747800
C	0.22930500	-0.33132200	4.63986800
H	0.36594300	-0.58447800	2.53056900
C	1.41667100	1.52737400	5.61280300
C	2.74127400	3.03715200	4.17835000
H	3.86782800	4.26421400	2.83032700
C	0.60298300	0.43013000	5.77091600
H	-0.40865500	-1.20164800	4.76461800
H	1.71825800	2.11909500	6.47310200
H	3.02417400	3.59820000	5.06529400
H	0.24888000	0.14543100	6.75700300
C	2.02028200	1.81894500	-1.06601200
C	1.35187200	3.07993700	-1.28422300
C	2.97043200	1.38695800	-1.97608300
C	0.39690300	3.64416800	-0.39432200
C	1.68644600	3.82991000	-2.46553600
C	3.29574900	2.13734500	-3.12930900

H	3.48894700	0.45438600	-1.79722200
C	-0.20608600	4.85539100	-0.66548700
H	0.14006500	3.13997700	0.52805000
C	1.04641800	5.07418300	-2.71272800
C	2.65894200	3.32967600	-3.37177000
H	4.04962100	1.76363300	-3.81625800
C	0.11481800	5.57955900	-1.83561500
H	-0.92691700	5.25927400	0.03969800
H	1.31567400	5.62430200	-3.61073700
H	2.89574400	3.91355300	-4.25753100
H	-0.36388600	6.53426300	-2.03261300
Rh	-0.62147900	-0.02888200	0.19678500
H	-1.23200100	1.45468200	-0.07847100
H	-2.58001200	-0.27710600	0.26978400
C	-6.56977700	-3.16621600	2.05005600
C	-5.38379200	-2.47071700	2.27948700
C	-5.09102200	-1.35355100	1.49860000
C	-5.97321200	-0.91496800	0.49745300
C	-7.16289800	-1.62714500	0.28439700
C	-7.45830100	-2.75014500	1.05113700
H	-6.80276500	-4.03633300	2.65687900
H	-4.68901100	-2.76892900	3.05787200
C	-5.61794500	0.29510300	-0.23837700
H	-7.84635100	-1.27983500	-0.48248500
H	-8.38070000	-3.29635500	0.88054600
C	-4.40296000	0.86920000	-0.04823100
C	-3.42163200	0.27367000	0.88989100
H	-4.11591700	1.77054000	-0.58037600
O	-6.56812300	0.76528900	-1.05970100
O	-3.92524500	-0.68479700	1.78198400
C	-2.68285400	1.35538600	1.72411400
O	-3.16631600	1.84544300	2.70935100
O	-1.47174100	1.70668700	1.24402300
C	-6.21204600	3.62133800	-3.33518900
H	-5.76768800	4.59118400	-3.58584900
H	-5.81466900	2.86324300	-4.01226800
H	-7.30057200	3.67322400	-3.45562600
O	-5.84266200	3.21689000	-2.00823400
H	-6.19356800	3.86523100	-1.37688300
H	-6.28766800	1.62765400	-1.45950400
MeOH			
C	0.66187300	-0.01961000	0.00001300
H	1.07903000	0.99111000	-0.00026700
H	1.03683500	-0.54351100	0.89331200
H	1.03683900	-0.54400600	-0.89299400
O	-0.74854900	0.12244600	-0.00002800

H	-1.13555400	-0.76550200	0.00009600
CP6			
H	-1.46180700	-0.20096600	1.59737800
C	3.03075600	-1.64740300	-0.00418500
C	1.65450200	-1.87790700	-0.01187800
C	0.77777800	-0.79426700	0.01057900
C	1.26762200	0.52625000	0.02414800
C	2.65215800	0.73759200	0.02938900
C	3.53274700	-0.34291500	0.02234500
H	3.71268000	-2.49335300	-0.01290200
H	1.24411200	-2.88226400	-0.03376000
C	0.28027700	1.60578500	-0.03361100
H	3.02495000	1.75637700	0.03198300
H	4.60470100	-0.16934500	0.03087400
C	-1.02448100	1.33950000	0.14328900
C	-1.43736800	-0.06594300	0.49740600
H	-1.80467900	2.09156500	0.08926700
O	0.80080000	2.83812600	-0.30110300
O	-0.56455800	-1.06070900	-0.04319700
C	-2.86744400	-0.34450200	0.03632900
O	-3.05822500	-1.60106500	-0.39989800
O	-3.75230700	0.48008200	0.11100300
H	0.08072700	3.48911500	-0.28992100
H	-4.00564600	-1.65974100	-0.63023200
2a			
H	-1.27527700	0.10841500	1.42287300
C	3.00983100	-1.66402600	-0.02001900
C	1.63523400	-1.86073600	-0.10053000
C	0.78050000	-0.75296800	-0.07440600
C	1.30470700	0.55136800	0.01626800
C	2.69704100	0.72249700	0.10665400
C	3.54863500	-0.37250400	0.09171700
H	3.67091100	-2.52644700	-0.03593400
H	1.20323200	-2.85353900	-0.17274800
C	0.40466200	1.72599300	-0.05770300
H	3.07479100	1.73815300	0.17384300
H	4.62341100	-0.23381300	0.15894300
C	-1.06324600	1.39071300	-0.29828100
C	-1.40773500	0.04119200	0.32942900
H	-1.23454500	1.34484600	-1.38297900
O	0.80048200	2.87790100	0.02100100
O	-0.56070500	-1.00291300	-0.15468300
C	-2.86462000	-0.34301600	0.09393800
O	-3.05796500	-1.67119700	0.01354800
O	-3.75840200	0.47167700	0.03472300

H	-4.01977900	-1.79418400	-0.10516200
H	-1.70007500	2.18175200	0.10204500

CP3'

Fe	3.87988500	-1.46752700	-1.60356300
C	2.89531400	0.38411900	-1.18436100
C	4.60230000	-3.01989900	-0.40077700
C	3.39752900	0.31907300	-2.52382400
H	4.13560800	0.98147300	-2.95568500
C	1.98140900	-0.71924000	-1.00810700
C	5.95084300	-1.63619600	-1.66765600
H	6.61832500	-0.83693700	-1.96238800
C	1.92432400	-1.43061500	-2.25771900
H	1.32962800	-2.31126400	-2.44970500
C	4.51100200	-3.44069700	-1.75899800
H	3.88877600	-4.24231800	-2.13442100
C	5.49074100	-1.90189000	-0.34295000
H	5.76698200	-1.34868400	0.54533600
C	2.77853600	-0.77918800	-3.19068300
H	2.96961800	-1.09737600	-4.20720300
C	5.34612400	-2.58767900	-2.54233300
H	5.46577600	-2.62795000	-3.61713900
H	4.06773600	-3.45457200	0.43232800
C	3.18368000	1.45942200	-0.16570200
H	3.15726500	0.98770100	0.82156400
C	4.59718400	2.04622900	-0.34538700
H	4.88962300	2.67489300	0.49620400
H	5.31053700	1.21622300	-0.39950300
H	4.70757300	2.63622700	-1.25663300
P	1.67290500	2.65771900	0.02828600
C	1.40852900	3.63193400	-1.61898300
C	2.23265600	3.85811100	1.45288200
C	3.23214500	4.95039900	1.00902100
H	3.56544200	5.49804100	1.90022200
H	4.12440200	4.55826300	0.51789400
H	2.76949500	5.68119200	0.34029200
C	2.87191800	3.01098500	2.57800400
H	2.21663100	2.19298100	2.89311500
H	3.84355500	2.59058500	2.30490100
H	3.03401800	3.65720500	3.45008700
C	1.01311800	4.57575900	2.07646300
H	1.38325600	5.27386400	2.83946300
H	0.43948100	5.15350300	1.34875600
H	0.33221900	3.87148100	2.55606700
C	2.69976800	4.14342400	-2.29045200
H	2.41796700	4.75717200	-3.15632500
H	3.31764900	4.76427500	-1.63862400

H	3.31057100	3.32041800	-2.67089000
C	0.69612200	2.68649000	-2.61419500
H	0.54542500	3.23272400	-3.55565800
H	1.28946500	1.79810800	-2.84233400
H	-0.28225300	2.37094200	-2.24880200
C	0.46321600	4.82502900	-1.35891500
H	-0.45683400	4.51027700	-0.85841400
H	0.93249600	5.61790800	-0.76950200
H	0.18409300	5.26171800	-2.32666300
P	0.70053100	-0.81562800	0.30577300
C	-0.17205100	-2.41036200	-0.11452300
C	-1.13557300	-2.48919100	-1.18114500
C	0.11469800	-3.55142500	0.61742300
C	-1.48098700	-1.38603700	-2.00824400
C	-1.77339700	-3.75079100	-1.44787200
C	-0.52067100	-4.78664700	0.35239400
H	0.84161100	-3.51052200	1.42034200
C	-2.40331300	-1.51272700	-3.02470300
H	-1.03208600	-0.41733100	-1.82789500
C	-2.71847600	-3.84713900	-2.50489900
C	-1.44705300	-4.88343300	-0.65722400
H	-0.26862000	-5.65408600	0.95622700
C	-3.02986800	-2.75433900	-3.28045300
H	-2.65533500	-0.64502600	-3.62707700
H	-3.19250500	-4.80862400	-2.68834300
H	-1.94222000	-5.82850800	-0.86787700
H	-3.75673500	-2.83960700	-4.08344300
C	1.49228700	-1.21196200	1.93735200
C	0.67967200	-1.30000400	3.12561600
C	2.86283900	-1.34758900	2.04599800
C	-0.73463800	-1.14577400	3.12442100
C	1.32649800	-1.56165600	4.38236600
C	3.49404800	-1.58418400	3.29173600
H	3.47019800	-1.28129700	1.15322100
C	-1.46300400	-1.25264300	4.29006300
H	-1.25942000	-0.90947000	2.20602300
C	0.54318500	-1.67390700	5.56238800
C	2.74035900	-1.69695900	4.43357200
H	4.57567900	-1.68439200	3.33277300
C	-0.82411400	-1.52596600	5.52114800
H	-2.54014400	-1.11645100	4.25819400
H	1.05019800	-1.87612700	6.50309700
H	3.21227900	-1.88822800	5.39453100
H	-1.41234600	-1.61062700	6.43091600
Rh	-0.24531800	1.50075200	0.54933700
H	0.34735700	1.48079000	1.96789900
H	-0.77258800	2.93091100	0.92514700

C	-8.23092300	-0.65530700	1.48717400
C	-6.86356600	-0.42500400	1.55546200
C	-6.22167700	0.16061800	0.45777400
C	-6.92957100	0.51521700	-0.70039900
C	-8.31257200	0.27075700	-0.74374200
C	-8.96100600	-0.30809800	0.33656200
H	-8.73831800	-1.10855500	2.33436400
H	-6.27899900	-0.68370400	2.43226100
C	-6.21916100	1.13303900	-1.84481100
H	-8.84159900	0.55254300	-1.64879000
H	-10.03045500	-0.49394100	0.29775200
C	-4.78868800	1.31536600	-1.61335700
C	-4.20091300	0.93500300	-0.45491900
H	-4.17731400	1.76442400	-2.38561000
O	-6.78739600	1.45651200	-2.88808300
O	-4.87339800	0.36674300	0.57654700
C	-2.73235600	1.10678400	-0.18155300
O	-2.27896800	0.77593300	0.95724400
O	-1.99914100	1.57868300	-1.09221900

CP4'

Fe	-4.24739700	-0.65213700	2.00592500
C	-3.17431200	0.87809200	0.97727200
C	-5.08450700	-2.48145800	1.42661200
C	-3.65110300	1.31271200	2.25543600
H	-4.34756700	2.12152900	2.43051600
C	-2.32793500	-0.27191700	1.19807200
C	-6.32479600	-0.65837900	2.11443400
H	-6.94014700	0.23170700	2.10440500
C	-2.28365600	-0.50671400	2.61785700
H	-1.73751300	-1.30088300	3.10560200
C	-4.99623100	-2.40029900	2.84614600
H	-4.42181700	-3.05765600	3.48531600
C	-5.90391800	-1.40260400	0.97199500
H	-6.16588400	-1.18557800	-0.05546200
C	-3.08243000	0.47849100	3.26329200
H	-3.27495100	0.54347100	4.32609100
C	-5.76466900	-1.27534600	3.27206000
H	-5.87124900	-0.92746000	4.29112700
H	-4.59706500	-3.21995500	0.80528200
C	-3.41633000	1.54111700	-0.35731000
H	-3.42683000	0.75000200	-1.11377700
C	-4.79138800	2.23436800	-0.41601500
H	-5.06317200	2.51511800	-1.43422000
H	-5.54729300	1.52673400	-0.05873800
H	-4.85459200	3.12807100	0.20670500
P	-1.84479400	2.50774900	-0.94462900

C	-1.46997900	3.95058500	0.27769600
C	-2.31088700	3.15647500	-2.70311300
C	-3.25966900	4.37649300	-2.68416100
H	-3.54994000	4.60692500	-3.71697800
H	-4.17806800	4.20942600	-2.11929300
H	-2.77245300	5.26896100	-2.28278600
C	-2.97730300	1.99465700	-3.47633700
H	-2.35908600	1.09067000	-3.46959700
H	-3.96956100	1.73718900	-3.09654900
H	-3.10163800	2.29877000	-4.52288000
C	-1.04339800	3.55671100	-3.49235800
H	-1.35993400	3.93603900	-4.47258000
H	-0.46751100	4.34491500	-3.00325200
H	-0.37920500	2.70586700	-3.65306000
C	-2.71919200	4.68143100	0.80621300
H	-2.39358400	5.51630400	1.44031000
H	-3.33860900	5.10032000	0.00895100
H	-3.33926900	4.03105900	1.42714100
C	-0.71410000	3.32100300	1.47267600
H	-0.49063500	4.11176800	2.20182400
H	-1.30301400	2.55776700	1.98698700
H	0.24676500	2.88902800	1.16695500
C	-0.52567200	4.98252800	-0.37573600
H	0.37406000	4.51311500	-0.78271600
H	-1.01138300	5.56043700	-1.16640100
H	-0.21033700	5.69477600	0.39772300
P	-1.08154700	-0.87604300	-0.00047600
C	-0.24481200	-2.25403500	0.92625200
C	0.75102300	-1.99410800	1.93217100
C	-0.58649800	-3.56564400	0.64002600
C	1.15591000	-0.68746400	2.31859500
C	1.36378400	-3.10794200	2.60465600
C	0.02206400	-4.65589800	1.30437300
H	-1.33805400	-3.77559600	-0.11272300
C	2.10924100	-0.48659800	3.29350200
H	0.71144100	0.17491100	1.83670700
C	2.34103400	-2.86769700	3.60862500
C	0.97874600	-4.43167000	2.26441700
H	-0.27612000	-5.66838300	1.04784900
C	2.70900600	-1.58643800	3.95032300
H	2.39691600	0.52785700	3.55396100
H	2.78867600	-3.72281600	4.10940200
H	1.45052800	-5.26348800	2.78180300
H	3.45182600	-1.41814800	4.72535100
C	-1.90255500	-1.74781200	-1.41308200
C	-1.11207200	-2.23681600	-2.51548900
C	-3.27872300	-1.86705900	-1.46144100

C	0.30715400	-2.14767800	-2.57047100	C	-5.65041900	-2.02483900	-0.24054900
C	-1.78928700	-2.85529100	-3.62246600	C	-3.03466700	-1.16460400	-2.80237100
C	-3.93772700	-2.46571600	-2.56234100	H	-3.12970800	-1.97692000	-3.51042900
H	-3.86800600	-1.49944000	-0.63170700	C	-2.58535300	0.04366500	-0.87437900
C	1.00877100	-2.63843700	-3.65133600	C	-6.43374600	-0.86784900	-2.07719900
H	0.85582000	-1.67021800	-1.76684600	H	-6.72946100	-0.62262800	-3.08874000
C	-1.03232800	-3.35717700	-4.71509100	C	-3.27988600	0.89949400	-1.80222900
C	-3.20703200	-2.95368400	-3.61733100	H	-3.55468500	1.92834200	-1.62162400
H	-5.02169600	-2.54123200	-2.56082400	C	-5.89446800	-0.67404500	0.15698300
C	0.33940300	-3.25379300	-4.73361900	H	-5.72557300	-0.25599100	1.13974600
H	2.09114100	-2.54410400	-3.67252800	C	-5.98635900	-2.14328600	-1.62224500
H	-1.56251100	-3.82414500	-5.54141200	H	-5.89577500	-3.03644800	-2.22645600
H	-3.70117700	-3.42116200	-4.46538300	C	-3.53783000	0.15825900	-2.98829100
H	0.90679700	-3.63802800	-5.57655400	H	-4.07729500	0.51675000	-3.85495900
Rh	0.02908900	1.16958500	-0.89574800	C	-6.37482000	0.04014000	-0.97749800
H	-0.32487500	0.72512800	-2.30419100	H	-6.62188300	1.09305100	-1.00711900
H	0.68529200	2.40736300	-1.62534800	H	-5.28329900	-2.82312800	0.39143300
C	7.16194400	-2.97210900	-1.55467400	C	-1.65561300	-2.40355400	-0.92845500
C	5.88567000	-2.43724900	-1.47947800	H	-1.83441700	-2.39998400	0.15191200
C	5.71221600	-1.22954100	-0.79732600	C	-2.15330900	-3.76142500	-1.45872300
C	6.79374600	-0.55641800	-0.19032300	H	-3.24229700	-3.79408500	-1.34604600
C	8.08463200	-1.12556400	-0.28376900	H	-1.92502400	-3.92652900	-2.51259900
C	8.26156600	-2.31816700	-0.95856200	H	-1.74200400	-4.59700200	-0.89103300
H	7.31651800	-3.90886100	-2.08113700	P	0.23546000	-2.02221100	-0.93200300
H	5.02587900	-2.92179600	-1.92875900	C	0.87752100	-1.88128800	-2.74412600
C	6.51148000	0.67427800	0.49212600	C	1.02952000	-3.51449800	-0.00228100
H	8.91830600	-0.61129300	0.18069100	C	1.13936000	-4.80021200	-0.85152600
H	9.25104400	-2.75752600	-1.03215900	H	0.18733500	-5.12741800	-1.27284100
C	5.18362000	1.13461800	0.52921900	H	1.85450200	-4.69477500	-1.67147900
C	4.19381100	0.41528700	-0.10057500	H	1.50627400	-5.61052100	-0.20916300
H	4.90021200	2.04634600	1.04023000	C	0.17239000	-3.79788200	1.25394800
O	7.51435500	1.30582000	1.05195400	H	0.70172700	-4.52710600	1.87909900
O	4.44737200	-0.72248000	-0.74426600	H	0.01890900	-2.89872500	1.86059800
C	2.74012800	0.87065300	-0.10861100	H	-0.80514800	-4.22685500	1.01904300
O	1.98247400	0.23221100	-0.90040400	C	2.44467000	-3.14054200	0.49031400
O	2.46319600	1.81233700	0.64986400	H	2.86603300	-4.00574500	1.01760600
C	7.19148500	4.80229800	1.64472100	H	3.12812500	-2.88864300	-0.32313600
H	6.54298900	5.61986200	1.97331800	H	2.42147500	-2.30032500	1.18714300
H	7.14424800	4.72300700	0.55784800	C	0.26046100	-2.89345100	-3.72826400
H	8.22497200	4.99528500	1.95169900	H	0.74247100	-2.77174000	-4.70690900
O	6.71473300	3.54562700	2.16674800	H	0.40819100	-3.93130300	-3.41927900
H	7.22649700	2.16354900	1.50094700	H	-0.80822900	-2.71973300	-3.87360300
H	6.73267300	3.57458800	3.13664900	C	0.52886300	-0.45126000	-3.21967400
				H	0.87794800	-0.32224800	-4.25263900
				H	-0.54422000	-0.24793500	-3.20396500
TS2'				H	1.04116500	0.30801100	-2.61246600
Fe	-4.48323900	-0.72368400	-1.38888400	C	2.41466200	-2.01729200	-2.77999800
C	-2.42647700	-1.24482700	-1.51004100				

H	2.75848300	-1.77096800	-3.79286700
H	2.90686200	-1.32866100	-2.08666200
H	2.75537900	-3.03253100	-2.56391300
P	-1.57278700	0.62488700	0.52910500
C	-1.96426800	2.42230500	0.65167700
C	-1.46403100	3.37167700	-0.30635800
C	-2.75721500	2.86025900	1.70037800
C	-0.68427500	3.02148100	-1.44157900
C	-1.78977200	4.75923200	-0.12754600
C	-3.07694100	4.22709400	1.86310600
H	-3.14076900	2.14969700	2.42400600
C	-0.24036800	3.97198300	-2.33417300
H	-0.44675500	1.97808400	-1.62259400
C	-1.30981200	5.71800600	-1.06056400
C	-2.59515200	5.15598400	0.97248000
H	-3.69813200	4.53269600	2.69955500
C	-0.55007200	5.33840100	-2.14225500
H	0.34962700	3.67009100	-3.19538300
H	-1.56186600	6.76355800	-0.90349800
H	-2.82759200	6.21071800	1.09496700
H	-0.19280700	6.08033800	-2.85022400
C	-2.09624100	-0.13506600	2.12520500
C	-1.40305200	0.17284200	3.35268300
C	-3.09971900	-1.08734200	2.12621300
C	-0.35349700	1.12791500	3.45627100
C	-1.80219400	-0.51979000	4.54830400
C	-3.47782800	-1.76711100	3.30775400
H	-3.61461500	-1.31241200	1.20159600
C	0.26317000	1.37905000	4.66472400
H	-0.01750800	1.67367300	2.58243000
C	-1.14779300	-0.23139500	5.77602400
C	-2.84277600	-1.48550800	4.49271300
H	-4.27424700	-2.50500900	3.26999400
C	-0.13499100	0.69796500	5.83766600
H	1.06154200	2.11419100	4.71088200
H	-1.46693000	-0.76173300	6.66969700
H	-3.12729700	-1.99835400	5.40804600
H	0.35671100	0.91150100	6.78227700
Rh	0.69997900	0.05018800	0.05576400
H	0.77311600	-0.68007400	1.38176300
H	2.37955500	-0.17999500	-0.07244100
C	6.61797100	-2.33585200	2.33055300
C	5.47377300	-1.55063800	2.41825700
C	5.14220500	-0.72871800	1.34076100
C	5.93953800	-0.67205900	0.18448700
C	7.09505900	-1.47285000	0.12032700
C	7.42709400	-2.30117800	1.18263400

H	6.88760900	-2.97919100	3.16265800
H	4.84034600	-1.55328900	3.29887100
C	5.54124500	0.25150600	-0.85918500
H	7.71567000	-1.42339100	-0.76733700
H	8.31855300	-2.91806600	1.13062800
C	4.36294600	0.94818000	-0.72487900
C	3.53573500	0.76560300	0.42536800
H	4.03603000	1.64986000	-1.48418800
O	6.37673900	0.37946900	-1.88444100
O	4.02019500	0.04898000	1.47335500
C	2.67386500	1.96486800	0.91806000
O	1.39019400	1.86741800	0.78237600
O	3.30666900	2.89878700	1.37193600
C	6.20534200	3.68465700	-2.96320500
H	5.73991400	4.53893400	-3.46537900
H	6.01390900	3.75513600	-1.89130900
H	7.28665200	3.69274500	-3.14058700
O	5.60623200	2.45081600	-3.40449700
H	6.07664700	1.10290800	-2.50339100
H	5.74694500	2.35939500	-4.36021200

CP5'

Fe	-4.43323500	-0.24220300	-1.61236300
C	-2.39537800	-0.79984100	-1.81584600
C	-5.89637900	-0.53584500	-0.14323100
C	-2.95314200	-0.36914700	-3.05929700
H	-3.04783000	-0.97091400	-3.95317900
C	-2.53134400	0.29327900	-0.87805100
C	-5.97407500	-1.48886400	-2.24485900
H	-5.89133700	-2.19762500	-3.05836100
C	-3.16618700	1.38434400	-1.57503600
H	-3.41327600	2.34449600	-1.14679300
C	-6.31268800	0.46698200	-1.06427700
H	-6.52471200	1.50059100	-0.82508400
C	-5.68296400	-1.74651000	-0.87198600
H	-5.36673100	-2.69626700	-0.46049700
C	-3.40660000	0.97686900	-2.91535000
H	-3.90401100	1.56403400	-3.67582700
C	-6.36293600	-0.12206700	-2.36339800
H	-6.61488800	0.38864000	-3.28343200
H	-5.74941800	-0.39411000	0.91867500
C	-1.67308500	-2.09224200	-1.53110000
H	-1.89633700	-2.36862300	-0.49531400
C	-2.16219600	-3.25199200	-2.41747200
H	-1.76842100	-4.21281800	-2.08321600
H	-3.25412600	-3.30198800	-2.34539700
H	-1.90472200	-3.13154300	-3.47048500

P	0.21338200	-1.75958600	-1.36773700	C	-3.18358000	-1.55488400	1.70608400
C	0.94760000	-1.18229400	-3.05388800	C	-0.43134400	0.13367400	3.66121400
C	0.96914100	-3.43429200	-0.78748500	C	-1.96461000	-1.69183000	4.22993500
C	1.12495000	-4.47926100	-1.91399900	C	-3.62677500	-2.50536200	2.65396300
H	1.47847500	-5.41783500	-1.46939300	H	-3.66798400	-1.51046800	0.73983500
H	0.19058600	-4.69939200	-2.43419700	C	0.14601700	0.02928400	4.91048900
H	1.86658000	-4.18029100	-2.65895600	H	-0.04656300	0.88182500	2.97806400
C	0.05369000	-4.00806700	0.31936600	C	-1.35001000	-1.76555500	5.50866300
H	-0.13286600	-3.28475100	1.12066800	C	-3.02864800	-2.56887800	3.88928300
H	-0.90917700	-4.35993000	-0.06091400	H	-4.44151200	-3.17702500	2.39921300
H	0.55599200	-4.87160400	0.77139800	C	-0.31401500	-0.92506100	5.84585600
C	2.35663400	-3.18870000	-0.15377100	H	0.96325200	0.69469600	5.17320100
H	2.75547700	-4.15140500	0.18927300	H	-1.71754800	-2.50284500	6.21777100
H	3.08136100	-2.77046600	-0.85492200	H	-3.36173500	-3.29438400	4.62710200
H	2.30134900	-2.52695300	0.71422500	H	0.14881300	-0.99065100	6.82608000
C	0.38197300	-1.92061500	-4.28244200	Rh	0.65042700	0.00265700	0.14565700
H	0.92017500	-1.57923900	-5.17589200	H	0.62094100	-1.04389700	1.24235200
H	0.50540700	-3.00475400	-4.22195600	H	2.53108600	-0.11454000	0.08496800
H	-0.67581200	-1.69655900	-4.44026400	C	6.66128000	-2.90600800	1.60683800
C	0.62495200	0.32438700	-3.18838800	C	5.48862600	-2.22366500	1.92312100
H	1.02505500	0.68989800	-4.14294800	C	5.12567600	-1.11128400	1.16366800
H	-0.44671200	0.53469800	-3.17494600	C	5.92782800	-0.66422200	0.09957700
H	1.10991300	0.91160300	-2.39650600	C	7.10721200	-1.36391900	-0.19994400
C	2.48556200	-1.32204300	-3.04335000	C	7.46936700	-2.48205800	0.54361000
H	2.94904100	-0.81767800	-2.18943500	H	6.94865700	-3.77244200	2.19532600
H	2.81904500	-2.36203400	-3.05606800	H	4.85609700	-2.52763700	2.75074400
H	2.87826800	-0.84723100	-3.95131800	C	5.51004200	0.54517500	-0.60022900
P	-1.57245000	0.46009300	0.66112400	H	7.72967100	-1.00951800	-1.01412100
C	-1.88387400	2.18021100	1.22762000	H	8.38255600	-3.01887400	0.30652900
C	-1.34131500	3.32146100	0.54012800	C	4.30275600	1.10332600	-0.31590200
C	-2.67289200	2.36416400	2.35294300	C	3.40487200	0.49612000	0.68044700
C	-0.55723300	3.24372000	-0.64164800	H	3.96931700	2.01000500	-0.81058900
C	-1.62435200	4.62836900	1.06388300	O	6.39373000	1.03847900	-1.47842900
C	-2.95157900	3.65541700	2.85284800	O	3.97942700	-0.45390800	1.53083100
H	-3.08500400	1.50789000	2.87457800	C	2.61871900	1.53249500	1.54508400
C	-0.06979700	4.37339800	-1.26108200	O	1.32118300	1.54275100	1.33675400
H	-0.35027900	2.27340600	-1.08205000	O	3.22548100	2.25540900	2.30413000
C	-1.10098000	5.77535300	0.40776700	C	6.06007700	4.15202300	-3.41355000
C	-2.42945600	4.76131400	2.22581200	H	5.58642800	5.12856800	-3.56478500
H	-3.57155100	3.76139700	3.73769000	H	7.15030200	4.26784700	-3.41668300
C	-0.33812700	5.65630000	-0.73030500	H	5.77031700	3.48657100	-4.22863600
H	0.52344500	4.27912300	-2.16649600	O	5.59411800	3.53987300	-2.20134600
H	-1.32102800	6.75475200	0.82429300	H	6.08812900	1.91846800	-1.81886700
H	-2.62837900	5.75820600	2.61048300	H	5.84305000	4.10476700	-1.45200000
H	0.05353600	6.54036700	-1.22436300				
C	-2.15438800	-0.67302400	1.98837500	TS3'			
C	-1.50051400	-0.72118200	3.27463300	Fe	-4.42662300	-0.07631800	-1.68488200

C	-2.40162100	-0.67257900	-1.89999500	C	2.50537800	-1.23165900	-3.05340200
C	-5.89369800	-0.44589000	-0.23855300	H	2.94605900	-0.71645200	-2.19430100
C	-2.93603900	-0.16660500	-3.12469200	H	2.84032200	-2.27132600	-3.04274800
H	-3.03355000	-0.71788100	-4.05009000	H	2.92319400	-0.76755800	-3.95558200
C	-2.52188100	0.37233600	-0.90843200	P	-1.57097300	0.42325700	0.64527100
C	-6.00456500	-1.22011500	-2.41122000	C	-1.91899600	2.09285900	1.34294000
H	-5.94444400	-1.86197800	-3.28031600	C	-1.34458700	3.29495900	0.79687000
C	-3.11883700	1.51457000	-1.55280500	C	-2.79110200	2.17445500	2.41857100
H	-3.34632100	2.45755400	-1.07767300	C	-0.47730700	3.32924800	-0.32848200
C	-6.28215300	0.64132100	-1.07245300	C	-1.68402600	4.54936600	1.41117700
H	-6.46302200	1.65753400	-0.74829100	C	-3.12411500	3.41451100	3.00665000
C	-5.71892200	-1.59821700	-1.06519400	H	-3.22965400	1.27310300	2.83169500
H	-5.43090000	-2.58763900	-0.73428100	C	0.03660000	4.51481900	-0.80706400
C	-3.35749900	1.18192900	-2.91453000	H	-0.21476700	2.40038600	-0.82624100
H	-3.83245700	1.82000000	-3.64789500	C	-1.13241700	5.75441200	0.89796800
C	-6.35308200	0.16264900	-2.41519800	C	-2.57339800	4.57473900	2.51740300
H	-6.59140000	0.75452600	-3.28906300	H	-3.80875700	3.43806000	3.84890300
H	-5.73941200	-0.39709200	0.83062000	C	-0.28792800	5.74334100	-0.18730300
C	-1.69752100	-1.98376500	-1.66544200	H	0.69663400	4.50608500	-1.67012100
H	-1.94102700	-2.30605200	-0.64889200	H	-1.39654900	6.69100100	1.38194200
C	-2.17635700	-3.10344300	-2.60611400	H	-2.81455700	5.53312700	2.96991800
H	-1.76278000	-4.07364200	-2.32590900	H	0.12646000	6.67080500	-0.57085400
H	-3.26668100	-3.17468500	-2.52499700	C	-2.19126200	-0.80899500	1.87215100
H	-1.93424700	-2.92502900	-3.65413900	C	-1.59141300	-0.95568000	3.17731700
P	0.18176200	-1.66545000	-1.44260300	C	-3.19275500	-1.68223500	1.48153900
C	0.96842400	-1.09347500	-3.10977100	C	-0.59487500	-0.08856500	3.70349000
C	0.91208100	-3.33862200	-0.83208600	C	-2.04234300	-2.03670900	4.01296300
C	1.11497700	-4.39058500	-1.94265900	C	-3.63656700	-2.73172500	2.31809400
H	1.46930400	-5.31936300	-1.47807600	H	-3.65617500	-1.55545400	0.51219700
H	0.19747900	-4.63028700	-2.48474200	C	-0.05541000	-0.29462900	4.95686300
H	1.87185700	-4.08928800	-2.67113500	H	-0.25592000	0.76790700	3.13562400
C	-0.04448800	-3.90403600	0.24285500	C	-1.46630700	-2.21805500	5.29916500
H	-0.25626400	-3.17297400	1.03013500	C	-3.06396000	-2.90982500	3.55375200
H	-0.99302100	-4.25647900	-0.17243700	H	-4.42771900	-3.39221400	1.97501200
H	0.43891200	-4.76691800	0.71660600	C	-0.48735600	-1.37075100	5.76423900
C	2.26816100	-3.07131300	-0.14531800	H	0.70353500	0.38829100	5.32750900
H	2.65092300	-4.01804900	0.25564400	H	-1.82163000	-3.04175300	5.91296600
H	3.02531100	-2.68208300	-0.82902800	H	-3.38949700	-3.71846100	4.20311900
H	2.16668600	-2.37231300	0.68948700	H	-0.05525000	-1.51831400	6.74947300
C	0.44395800	-1.84483300	-4.34949600	Rh	0.62259500	0.07398300	0.06844000
H	1.02384100	-1.52363500	-5.22408600	H	1.12209400	-0.05225400	1.61215000
H	0.54750700	-2.92979500	-4.26962900	H	2.62547000	0.05415600	-0.08902100
H	-0.60245500	-1.60693700	-4.55510800	C	6.36965300	-3.10396700	1.68006100
C	0.64251500	0.41023200	-3.26945200	C	5.23411500	-2.33405600	1.92856600
H	1.07922500	0.76941900	-4.21040300	C	5.01551300	-1.18414300	1.17129600
H	-0.43075000	0.60987200	-3.30264500	C	5.92697700	-0.78066700	0.18158400
H	1.08007900	1.00567600	-2.45775400	C	7.06464700	-1.56782600	-0.05041500

C	7.28240300	-2.72742100	0.68777200
H	6.54285300	-4.00191800	2.26604700
H	4.52085700	-2.60329000	2.70083500
C	5.67110000	0.48484100	-0.50404900
H	7.77230500	-1.24715700	-0.80692800
H	8.16491500	-3.33143500	0.50161900
C	4.50231400	1.14102100	-0.29387800
C	3.46032200	0.55967700	0.57488500
H	4.29660200	2.09924200	-0.75778100
O	6.66980400	0.92453000	-1.28344000
O	3.89520400	-0.44390700	1.46997000
C	2.70140500	1.60981200	1.43302800
O	1.42177900	1.29043000	1.70068100
O	3.21817300	2.62830000	1.81575900
C	6.67830200	4.07209800	-3.21259900
H	6.27029800	5.07457600	-3.38458300
H	7.77268600	4.12332000	-3.16843500
H	6.38553300	3.42304400	-4.03975200
O	6.12475500	3.49138700	-2.02264500
H	6.46548300	1.83235300	-1.62545900
H	6.37229900	4.04157100	-1.26222300

CP6'

H	1.46180700	-0.20096600	1.59737800
C	-3.03075600	-1.64740300	-0.00418500
C	-1.65450200	-1.87790700	-0.01187800
C	-0.77777800	-0.79426700	0.01057900
C	-1.26762200	0.52625000	0.02414800
C	-2.65215800	0.73759200	0.02938900
C	-3.53274700	-0.34291500	0.02234500
H	-3.71268000	-2.49335300	-0.01290200
H	-1.24411200	-2.88226400	-0.03376000
C	-0.28027700	1.60578500	-0.03361100
H	-3.02495000	1.75637700	0.03198300
H	-4.60470100	-0.16934500	0.03087400
C	1.02448100	1.33950000	0.14328900
C	1.43736800	-0.06594300	0.49740600
H	1.80467900	2.09156500	0.08926700
O	-0.80080000	2.83812600	-0.30110300
O	0.56455800	-1.06070900	-0.04319700
C	2.86744400	-0.34450200	0.03632900
O	3.05822500	-1.60106500	-0.39989800
O	3.75230700	0.48008200	0.11100300
H	-0.08072700	3.48911500	-0.28992100
H	4.00564600	-1.65974100	-0.63023200

2a'

H	1.27527700	0.10841500	1.42287300
C	-3.00983100	-1.66402600	-0.02001900
C	-1.63523400	-1.86073600	-0.10053000
C	-0.78050000	-0.75296800	-0.07440600
C	-1.30470700	0.55136800	0.01626800
C	-2.69704100	0.72249700	0.10665400
C	-3.54863500	-0.37250400	0.09171700
H	-3.67091100	-2.52644700	-0.03593400
H	-1.20323200	-2.85353900	-0.17274800
C	-0.40466200	1.72599300	-0.05770300
H	-3.07479100	1.73815300	0.17384300
H	-4.62341100	-0.23381300	0.15894300
C	1.06324600	1.39071300	-0.29828100
C	1.40773500	0.04119200	0.32942900
H	1.23454500	1.34484600	-1.38297900
O	-0.80048200	2.87790100	0.02100100
O	0.56070500	-1.00291300	-0.15468300
C	2.86462000	-0.34301600	0.09393800
O	3.05796500	-1.67119700	0.01354800
O	3.75840200	0.47167700	0.03472300
H	4.01977900	-1.79418400	-0.10516200
H	1.70007500	2.18175200	0.10204500

TS2-2

Fe	4.56305800	-1.31989000	-0.05280200
C	2.52965200	-1.91826500	0.06474100
C	5.65112400	-0.12574500	-1.38272900
C	3.36346500	-2.71488100	0.90933100
H	3.51194800	-3.78346300	0.82888200
C	2.68658200	-0.54153100	0.47758500
C	5.96675100	-2.40086100	-1.14303900
H	5.92344200	-3.46965500	-1.30636300
C	3.60327700	-0.52274300	1.58845000
H	3.92619000	0.35936600	2.12177100
C	6.39486900	-0.34227400	-0.18734000
H	6.72537800	0.42295200	0.50234600
C	5.38300600	-1.39872100	-1.97457600
H	4.84334900	-1.57781300	-2.89563300
C	4.00470900	-1.86013800	1.85553900
H	4.71926800	-2.16848800	2.60710700
C	6.59233000	-1.74799400	-0.04033900
H	7.09464600	-2.23611000	0.78435700
H	5.33559700	0.83685700	-1.76156700
C	1.57411700	-2.39055300	-1.00207900
H	1.55832500	-1.61866600	-1.77623600
C	2.04561200	-3.68543500	-1.68712600
H	1.38277100	-3.98691000	-2.49979700

H	3.03658500	-3.50330700	-2.11681700	C	1.53879400	1.26826300	-1.68498100
H	2.13595400	-4.52744800	-1.00062500	C	0.56241800	2.19226000	-2.21563400
P	-0.25277000	-2.24752200	-0.40663600	C	2.43649100	0.66399400	-2.54613400
C	-0.64158800	-3.62515100	0.89200200	C	-0.36943100	2.90890400	-1.41243800
C	-1.30096000	-2.50585300	-2.01875400	C	0.54616200	2.42852800	-3.63495400
C	-1.50913400	-3.97068800	-2.45606000	C	2.41635000	0.91111800	-3.93991400
H	-2.06065100	-3.97177600	-3.40493900	H	3.17562000	-0.01649400	-2.14265000
H	-0.57358800	-4.50732400	-2.62814500	C	-1.26680900	3.79471900	-1.97785600
H	-2.10444000	-4.54237200	-1.74016400	H	-0.37664900	2.78936100	-0.33531900
C	-0.61331800	-1.73745300	-3.17036500	C	-0.39664300	3.33815700	-4.18386100
H	-0.39551600	-0.69682600	-2.90676300	C	1.48448400	1.76676100	-4.47343300
H	0.31480000	-2.21002700	-3.50327400	H	3.14283400	0.41946200	-4.58054000
H	-1.29226100	-1.72130800	-4.03179900	C	-1.28603100	4.01398600	-3.37625700
C	-2.68868300	-1.86261300	-1.80901300	H	-1.93959400	4.35160600	-1.33065400
H	-3.28163100	-1.99711300	-2.72273400	H	-0.38741500	3.50910800	-5.25721400
H	-3.24765000	-2.30733000	-0.98305800	H	1.45713600	1.95959000	-5.54271800
H	-2.61289200	-0.78741900	-1.61959800	H	-1.97129600	4.73993100	-3.80690800
C	-0.09970400	-5.01856300	0.50120600	Rh	-0.69136500	-0.08639800	0.45570000
H	-0.51425100	-5.75688700	1.19862900	H	-2.31855400	-0.47344700	0.83551700
H	-0.37351700	-5.33312800	-0.50671900	H	-0.29223400	-0.68287000	1.78274000
H	0.98751300	-5.06768900	0.59718500	C	-7.05666400	-2.36207500	2.24794500
C	-0.00082100	-3.24746800	2.24824200	C	-5.87112700	-1.73067600	2.60794300
H	-0.11787700	-4.09792600	2.93188200	C	-5.28587100	-0.83997800	1.70769700
H	1.06727800	-3.03027800	2.16977900	C	-5.87142100	-0.56680400	0.45698500
H	-0.49770600	-2.39001800	2.71079500	C	-7.07124900	-1.21806900	0.11533800
C	-2.16730100	-3.71612300	1.10946700	C	-7.65590400	-2.11026400	1.00257000
H	-2.60381100	-2.74508200	1.36052600	H	-7.52292000	-3.05492000	2.94186300
H	-2.69766800	-4.12705800	0.24656500	H	-5.39679000	-1.90194100	3.56831700
H	-2.35482000	-4.39019700	1.95458700	C	-5.21227000	0.40245600	-0.39501100
P	1.49579400	0.77985800	0.10013100	H	-7.52532500	-1.00417100	-0.84582700
C	2.08522600	2.25943700	1.02991000	H	-8.58196200	-2.61011500	0.73707000
C	1.93958500	2.39682300	2.45622400	C	-4.01729300	0.94297900	0.01409600
C	2.70534700	3.26674000	0.30379300	C	-3.40414600	0.52575900	1.23821500
C	1.35167300	1.41621300	3.29887500	H	-3.49722800	1.67978100	-0.58628800
C	2.43618300	3.59529300	3.07724700	O	-5.82118400	0.71378400	-1.53357700
C	3.19333700	4.43595700	0.92700100	O	-4.13020500	-0.21972000	2.11076800
H	2.82527200	3.16919400	-0.76932600	C	-2.48177000	1.56879700	1.92326200
C	1.24592400	1.60620900	4.65922800	O	-2.92958100	2.21729200	2.84284600
H	0.97140000	0.50046500	2.86454200	O	-1.32127000	1.69071500	1.33988100
C	2.30889800	3.76233700	4.48278200	C	-5.15470600	3.90113500	-2.93986300
C	3.05461000	4.59691400	2.28475900	H	-5.03754400	4.35855700	-3.92879000
H	3.67225000	5.20138800	0.32387500	H	-6.21414600	3.70513400	-2.76600900
C	1.72563100	2.79140100	5.26226200	H	-4.78989400	4.58906700	-2.16773100
H	0.78295000	0.83988600	5.27430400	O	-4.48848200	2.63276700	-2.87809900
H	2.68590400	4.67804200	4.93077100	H	-3.53330500	2.75993600	-3.00410400
H	3.42085200	5.49585200	2.77404200	H	-5.28582800	1.37560800	-2.05047300
H	1.63143700	2.93042600	6.33504100				

TS2'-2

Fe	-4.23513700	-0.18904000	-1.91924200	H	-0.02604100	0.05692700	-3.51996600
C	-2.18876100	-0.75830900	-1.89718600	H	1.50358200	0.59554700	-2.80118200
C	-5.85301800	-0.48117800	-0.62271400	C	2.82010700	-1.72293600	-2.63334400
C	-2.60134300	-0.31000700	-3.19070400	H	3.16565800	-1.05046700	-1.84311900
H	-2.59964200	-0.89974200	-4.09780900	H	3.12705800	-2.74162400	-2.38381600
C	-2.42557500	0.32307500	-0.96762700	H	3.34344700	-1.44551500	-3.55717600
C	-5.70290200	-1.42359000	-2.72561500	P	-1.60094700	0.46085900	0.65284000
H	-5.53486500	-2.12940100	-3.52839100	C	-2.09090600	2.10939500	1.32889200
C	-2.96926900	1.42622900	-1.71581800	C	-1.58411200	3.35498900	0.81161000
H	-3.25766800	2.38264400	-1.30478600	C	-2.98239400	2.12615300	2.39174000
C	-6.15841100	0.52896300	-1.57922100	C	-0.69891800	3.46098300	-0.29485500
H	-6.38863000	1.56291300	-1.35903600	C	-2.01570300	4.57767600	1.43348900
C	-5.56843800	-1.68977000	-1.33030400	C	-3.40139200	3.33425300	2.99158100
H	-5.30526500	-2.64334600	-0.89118800	H	-3.37416300	1.19591300	2.78632000
C	-3.06075100	1.03712700	-3.08099900	C	-0.26027000	4.68434600	-0.75290800
H	-3.46759000	1.63653100	-3.88466400	H	-0.36276100	2.56084500	-0.79330800
C	-6.06827300	-0.05361800	-2.87896900	C	-1.53905900	5.82301400	0.94202700
H	-6.21318600	0.46328100	-3.81844500	C	-2.92123400	4.53372300	2.52553900
H	-5.82647300	-0.34487200	0.44978900	H	-4.09877600	3.30154500	3.82315700
C	-1.52608700	-2.06389500	-1.53498200	C	-0.67887400	5.88177100	-0.12916300
H	-1.84158600	-2.30354000	-0.51595600	H	0.41357600	4.72849400	-1.60440400
C	-1.98765400	-3.23469500	-2.41998700	H	-1.87510900	6.73379500	1.43085200
H	-1.51300700	-4.17659600	-2.13905800	H	-3.23127200	5.46920400	2.98410800
H	-3.06880100	-3.35527800	-2.29254200	H	-0.32488100	6.84004900	-0.49780800
H	-1.80055800	-3.07013800	-3.48152700	C	-2.25798700	-0.77784400	1.85596700
P	0.35417100	-1.81097100	-1.20856900	C	-1.61856000	-0.96122400	3.13686700
C	1.30149200	-1.59387200	-2.87819000	C	-3.30822700	-1.60215000	1.49346400
C	0.91722200	-3.43258000	-0.30385100	C	-0.55241300	-0.14902100	3.61542800
C	1.21472500	-4.63965600	-1.21706900	C	-2.09499400	-2.01643700	3.99067500
H	1.47448600	-5.49614300	-0.58185100	C	-3.77300400	-2.63186100	2.34489200
H	0.35721800	-4.94024200	-1.82396300	H	-3.78470000	-1.45502700	0.53322500
H	2.06266800	-4.46761600	-1.88401900	C	0.02258300	-0.38171000	4.84841800
C	-0.18516600	-3.83912800	0.70010700	H	-0.18106600	0.68020500	3.02409300
H	-0.47601900	-3.01706900	1.36167300	C	-1.48127600	-2.22389600	5.25515000
H	-1.08378800	-4.22418800	0.20979500	C	-3.17428100	-2.83636300	3.56445700
H	0.20439200	-4.64451000	1.33468900	H	-4.60419000	-3.25515000	2.02733700
C	2.18942300	-3.11480400	0.51421500	C	-0.44066900	-1.42849200	5.67769500
H	2.49209900	-4.01948300	1.05699200	H	0.83307300	0.25819000	5.18545200
H	3.03099700	-2.80537800	-0.10873400	H	-1.85591400	-3.02529500	5.88692600
H	2.01462200	-2.32860100	1.25686500	H	-3.52073200	-3.62718800	4.22498800
C	0.87895900	-2.59814900	-3.97370500	H	0.01835400	-1.59559800	6.64768600
H	1.58536800	-2.51586500	-4.80915300	Rh	0.71887500	-0.01230300	0.26775200
H	0.88412400	-3.63804200	-3.64386800	H	2.40017600	-0.07424400	0.04303300
H	-0.11147100	-2.36635800	-4.37173400	H	0.70227700	0.85216100	-0.97090000
C	1.03844500	-0.17212500	-3.42584100	C	6.95520600	-2.54781200	1.27151400
H	1.48494400	-0.09947500	-4.42601300	C	5.76899900	-1.96348400	1.70158700
				C	5.29363300	-0.83863300	1.02651100

C	5.98892900	-0.28420700	-0.06223400	H	1.48479000	-3.72367500	-2.91344300
C	7.18909300	-0.89077400	-0.47706300	H	3.11850500	-3.34340200	-2.37579300
C	7.66409000	-2.01573400	0.18164200	H	2.11202700	-4.44186000	-1.42956100
H	7.33654200	-3.42275800	1.78921700	P	-0.17408900	-2.27328900	-0.53204300
H	5.21179500	-2.34979000	2.54829600	C	-0.33658200	-3.56479100	0.88943600
C	5.44010900	0.91231100	-0.66947800	C	-1.30638500	-2.70569800	-2.03243300
H	7.73036200	-0.45950400	-1.31165100	C	-1.31788900	-4.20619700	-2.40019600
H	8.58997600	-2.48154000	-0.14040000	H	-1.90870300	-4.33496500	-3.31569000
C	4.22970400	1.39389600	-0.22933600	H	-0.32520900	-4.61527200	-2.59551700
C	3.51551700	0.72453400	0.81035800	H	-1.79055000	-4.81725300	-1.62708000
H	3.78380600	2.28064100	-0.66588900	C	-0.81921800	-1.88126000	-3.24721200
O	6.17648100	1.48186800	-1.61759000	H	0.14250300	-2.22138100	-3.63965700
O	4.13426800	-0.27478300	1.49422700	H	-1.55217900	-1.98634800	-4.05617700
C	2.60949100	1.56569000	1.75661100	H	-0.73922200	-0.81333600	-3.01545800
O	1.32881100	1.46309800	1.59042500	C	-2.75946000	-2.27036000	-1.74265600
O	3.20298300	2.25234200	2.56470800	H	-3.37592200	-2.52584100	-2.61376700
C	5.16922300	4.29237300	-3.69700500	H	-3.19274200	-2.77368800	-0.87621100
H	4.54066200	5.17721200	-3.84321800	H	-2.83576900	-1.19249900	-1.58303000
H	4.79011900	3.47897700	-4.31774700	C	0.41056100	-4.88827100	0.63808600
H	6.20072500	4.51852100	-3.99015200	H	1.49282200	-4.74368900	0.60152600
O	5.09399800	3.83590300	-2.33551100	H	0.20459600	-5.57139000	1.47199900
H	5.76849800	2.33830700	-1.92587000	H	0.09164400	-5.38897400	-0.27951700
H	5.42887800	4.53534600	-1.75143700	C	0.24659600	-2.89681100	2.15705200

TS2-conf2

Fe	4.60382500	-1.14651700	-0.39368100	H	1.29736600	-2.61912800	2.04774500
C	2.61205700	-1.85499900	-0.20861300	H	-0.32882900	-2.00482200	2.44242600
C	6.38790700	-0.08437600	-0.54126300	C	-1.82368100	-3.86876500	1.17211200
C	3.53707600	-2.68114000	0.50380000	H	-2.40596400	-2.95906700	1.34674000
H	3.73100900	-3.72766600	0.31108100	H	-2.29942200	-4.44105400	0.37217600
C	2.72908600	-0.51548400	0.32452900	H	-1.88210000	-4.47755500	2.08314000
C	5.29370100	-0.99197300	-2.36121400	P	1.45948100	0.78035400	0.15370800
H	4.69801700	-1.09738300	-3.25880200	C	1.99781800	2.09968600	1.32158300
C	3.71911500	-0.55234100	1.37145000	C	1.84470100	1.96229100	2.74536400
H	4.03692200	0.29294800	1.96397600	C	2.57590100	3.24721300	0.79989700
C	6.64318100	-1.48849000	-0.55617300	C	1.30862400	0.81103300	3.38118300
H	7.21723500	-2.03780800	0.17829400	C	2.27910900	3.04441900	3.58506300
C	5.55777600	0.22317200	-1.65679400	C	3.00789000	4.30063500	1.63599500
H	5.18145200	1.20482900	-1.90991300	H	2.70147200	3.35394500	-0.27197000
C	4.19924400	-1.88528300	1.48587600	C	1.18813200	0.73395400	4.75086800
H	4.97594500	-2.22333000	2.15891700	H	0.99352400	-0.03242400	2.77672000
C	5.96766900	-2.04926200	-1.67985200	C	2.13631000	2.93797900	4.99514500
H	5.95182800	-3.09631700	-1.95257400	C	2.85326400	4.20252000	2.99838600
H	6.73795600	0.61850900	0.20300400	H	3.45483000	5.18487600	1.19177500
C	1.61446900	-2.29266900	-1.25250800	C	1.60072000	1.80978200	5.57068200
H	1.52194900	-1.47659200	-1.97700900	H	0.76885300	-0.15849400	5.20664300
C	2.09614700	-3.53181700	-2.03095700	H	2.46364500	3.77027800	5.61272500
				H	3.17358200	5.01199800	3.64929700

H	1.49482300	1.74010500	6.64903500
C	1.46057300	1.55185200	-1.52559100
C	0.51009200	2.58401600	-1.86722700
C	2.30428200	1.05536800	-2.50149800
C	-0.39792700	3.16685100	-0.93858600
C	0.48531600	3.06432800	-3.22241600
C	2.26678600	1.53292300	-3.83388600
H	3.01845800	0.28537500	-2.23900200
C	-1.26634000	4.16974200	-1.32329400
H	-0.41877100	2.83472100	0.09265600
C	-0.42549900	4.09222300	-3.58621100
C	1.37529000	2.51539700	-4.18596600
H	2.95017700	1.11920500	-4.56989700
C	-1.28237800	4.64314500	-2.65789100
H	-1.92519600	4.61437700	-0.58190300
H	-0.42028100	4.45007000	-4.61254200
H	1.33910400	2.89168600	-5.20500700
H	-1.94526400	5.45696900	-2.94092300
Rh	-0.67859000	-0.21994600	0.47179500
H	-1.05475600	0.25810000	-0.91785300
H	-2.34552700	-0.59874700	0.63941700
C	-7.17437200	-2.64336500	1.55564900
C	-5.99142400	-2.10560900	2.05138400
C	-5.36254300	-1.09067300	1.32998600
C	-5.90019700	-0.60237400	0.12498600
C	-7.09772900	-1.16191900	-0.35656400
C	-7.72684800	-2.17587000	0.35200600
H	-7.67506300	-3.43098100	2.11057200
H	-5.55354600	-2.44286400	2.98479500
C	-5.19265800	0.47588700	-0.53733800
H	-7.51474300	-0.78283500	-1.28292000
H	-8.65152500	-2.60445700	-0.02115300
C	-4.00497300	0.91662800	-0.00803500
C	-3.44605800	0.30310400	1.15802900
H	-3.43978800	1.71425100	-0.47467700
O	-5.75552400	0.97913300	-1.63012100
O	-4.21170300	-0.56892900	1.86637500
C	-2.56509300	1.20931000	2.06311500
O	-3.08356800	1.72436400	3.02926900
O	-1.34657800	1.37148100	1.62522200
C	-5.09611000	4.32982000	-2.43596800
H	-4.80455300	4.84132900	-1.51068700
H	-4.92699800	4.99144900	-3.29306900
H	-6.15853700	4.08523400	-2.38465600
O	-4.39763200	3.08867100	-2.60018600
H	-3.44040800	3.25694500	-2.62585300
H	-5.19616800	1.71010600	-2.01252600

TS2-conf3

Fe	-4.17616100	-1.86879800	0.39727700
C	-2.12853300	-2.30678300	0.12041600
C	-5.16831200	-0.63301900	1.76716600
C	-2.96588400	-3.28383600	-0.50579400
H	-3.00364100	-4.33627400	-0.25981400
C	-2.45410200	-1.02175800	-0.46163900
C	-5.38181700	-2.93004400	1.71481300
H	-5.26055300	-3.98154200	1.93991100
C	-3.47993600	-1.24590600	-1.44951100
H	-3.94019200	-0.48094400	-2.05773600
C	-6.03085800	-0.96699400	0.68379700
H	-6.47557000	-0.26702600	-0.01068600
C	-4.76088300	-1.84479900	2.40340000
H	-4.10508300	-1.92931100	3.26046400
C	-3.78140900	-2.63352200	-1.47828500
H	-4.53895400	-3.10485400	-2.09022300
C	-6.16617100	-2.38733700	0.65402200
H	-6.73255100	-2.95667600	-0.07109400
H	-4.86876300	0.36602200	2.05012000
C	-1.03253900	-2.57343200	1.12265100
H	-1.02549400	-1.74303100	1.83643500
C	-1.29167500	-3.86185900	1.92766700
H	-0.63412700	-3.94182700	2.79374300
H	-2.32110800	-3.83387100	2.30025400
H	-1.17786200	-4.77081100	1.33486900
P	0.69840900	-2.31699400	0.32349800
C	0.96113800	-3.55605000	-1.12838000
C	1.94685600	-2.59929400	1.76558900
C	2.16874400	-4.08806000	2.11376300
H	2.80915600	-4.14570800	3.00275400
H	1.24733500	-4.62574900	2.34245600
H	2.68465600	-4.62452200	1.31323200
C	1.41394300	-1.84574700	3.00705000
H	0.52361400	-2.30646300	3.44215200
H	2.19172200	-1.85564100	3.78013400
H	1.18753100	-0.79683700	2.78512700
C	3.31670900	-1.97799900	1.41708200
H	4.00276900	-2.16873400	2.25200100
H	3.76689800	-2.40712600	0.51990000
H	3.24770200	-0.89624200	1.28352600
C	0.41112800	-4.97202200	-0.87215300
H	0.84596900	-5.44149700	0.01416600
H	-0.67706500	-4.97631400	-0.77478600
H	0.66005200	-5.60584300	-1.73287100
C	0.23097100	-2.94920200	-2.35164200

H	0.37299800	-3.61028400	-3.21616300
H	-0.84301700	-2.83373700	-2.19263200
H	0.65084000	-1.97214000	-2.63671600
C	2.46065100	-3.65421600	-1.48387400
H	2.91026400	-2.67318300	-1.66524900
H	3.04412600	-4.17006600	-0.71734400
H	2.55662800	-4.23637600	-2.40887900
P	-1.37355100	0.44755400	-0.44956000
C	-2.10799600	1.53522000	-1.74885200
C	-3.32190900	2.29783800	-1.58093900
C	-1.45916900	1.54253700	-2.97461900
C	-4.09233400	2.33614800	-0.38692300
C	-3.79980200	3.06449400	-2.70121600
C	-1.94722000	2.29159100	-4.06898400
H	-0.53036600	1.00212700	-3.09898200
C	-5.24362000	3.09012600	-0.29508400
H	-3.76877300	1.76656300	0.47287400
C	-4.98899500	3.83151700	-2.57246900
C	-3.08926800	3.04082600	-3.93079700
H	-1.40200600	2.27600800	-5.00757900
C	-5.70036900	3.84999500	-1.39538100
H	-5.80377100	3.10354600	0.63604500
H	-5.32787100	4.40554300	-3.43105100
H	-3.46941200	3.62857000	-4.76252800
H	-6.60695500	4.44147900	-1.30913000
C	-1.40183800	1.33444200	1.17433400
C	-0.68815600	2.57605500	1.34266000
C	-2.01349400	0.74716800	2.26759000
C	0.00734900	3.24081000	0.29283400
C	-0.66659100	3.17731000	2.64862700
C	-1.97906200	1.34508900	3.54972100
H	-2.55829000	-0.18041200	2.13758400
C	0.67066100	4.43060400	0.51500200
H	0.03506300	2.81415200	-0.70215000
C	0.02095000	4.40672700	2.84245200
C	-1.32458600	2.53842500	3.73401500
H	-2.47978000	0.85716500	4.38111900
C	0.67619400	5.02763000	1.79972900
H	1.18124600	4.91926300	-0.31005300
H	0.00515000	4.85862200	3.83131300
H	-1.29936500	3.01048900	4.71282900
H	1.17305400	5.98206800	1.95354200
Rh	0.90033800	-0.25066300	-0.73483400
H	1.17998900	0.33530300	0.63738700
H	2.62383200	-0.36769200	-0.85124600
C	7.88666700	-1.43755700	-1.34341400
C	6.63667100	-1.23249900	-1.91802700

C	5.76490500	-0.32304100	-1.31943400
C	6.12293600	0.38395200	-0.15700300
C	7.39129200	0.15815800	0.40727900
C	8.26462500	-0.74603000	-0.18113100
H	8.57629800	-2.13812000	-1.80446000
H	6.32887300	-1.74602100	-2.82260700
C	5.15463800	1.31642600	0.38663700
H	7.66857800	0.70480800	1.30169400
H	9.24405800	-0.91542200	0.25474200
C	3.93052000	1.43615100	-0.22120600
C	3.58477800	0.63303200	-1.35765400
H	3.17180200	2.11086000	0.15635300
O	5.52927200	2.01958000	1.45043800
O	4.55413600	-0.12665500	-1.93625000
C	2.63703400	1.28985500	-2.39935700
O	3.11195100	1.75619400	-3.41029400
O	1.38767700	1.31645400	-2.01532000
C	3.60878900	3.45658800	4.04161100
H	2.69202300	3.30992000	4.62368900
H	4.37812700	2.77779100	4.41466500
H	3.95791900	4.48962300	4.16033700
O	3.39885900	3.12320100	2.66432200
H	2.69768600	3.69344200	2.30328200
H	4.76187000	2.54066500	1.81457600

TS2-conf4

Fe	-4.25120000	-1.80178000	0.31992700
C	-2.21010200	-2.28049000	0.06618900
C	-6.08672500	-0.86130100	0.60577700
C	-3.05845400	-3.21634300	-0.60651900
H	-3.12612800	-4.27480700	-0.39524500
C	-2.49364800	-0.97005900	-0.47999800
C	-4.87255700	-1.83338400	2.31493400
H	-4.23535100	-1.96568000	3.17994000
C	-3.50568900	-1.13726700	-1.49293200
H	-3.93607600	-0.34221000	-2.08418300
C	-6.25852800	-2.27555900	0.52246300
H	-6.82592700	-2.80342000	-0.23262600
C	-5.23613300	-0.58932300	1.71565900
H	-4.91615000	0.39052800	2.04027400
C	-3.83970600	-2.51551600	-1.57202600
H	-4.59674300	-2.94844000	-2.21230800
C	-5.50852400	-2.87647000	1.57675000
H	-5.41882100	-3.93817400	1.76588200
H	-6.50000300	-0.12534400	-0.07067700
C	-1.14112100	-2.60494700	1.08022400
H	-1.12944700	-1.79830700	1.82040900

C	-1.44569000	-3.91185300	1.83815400	H	-3.33752000	3.84403600	-4.62970600
H	-0.80923600	-4.03311600	2.71506900	H	-6.51332100	4.60424600	-1.19882000
H	-2.48219400	-3.87277200	2.18946700	C	-1.41168300	1.29611400	1.25775500
H	-1.33826700	-4.80413100	1.21953900	C	-0.66786400	2.51059000	1.48371500
P	0.61098100	-2.36398800	0.32512200	C	-2.04950700	0.68093100	2.32028500
C	0.87320700	-3.56171400	-1.16109500	C	0.04484900	3.20573300	0.46597700
C	1.82125000	-2.72332800	1.78241400	C	-0.63631500	3.05193900	2.81567500
C	2.00031300	-4.22748000	2.08738900	C	-2.00546900	1.21983000	3.62816100
H	2.62009900	-4.32814100	2.98708600	H	-2.62023100	-0.22360000	2.14660400
H	1.06205500	-4.74983800	2.28016800	C	0.72773700	4.37282300	0.74207100
H	2.52056100	-4.75109800	1.28115600	H	0.06614200	2.82320300	-0.54694200
C	1.28060200	-1.99638300	3.03636000	C	0.07823600	4.25444300	3.06661700
H	0.37018900	-2.44806000	3.43800300	C	-1.31563000	2.38257700	3.86931200
H	2.04109700	-2.04972100	3.82464300	H	-2.52522400	0.71020200	4.43445500
H	1.08384300	-0.93579000	2.84354700	C	0.74290200	4.91035600	2.05250100
C	3.21317700	-2.12633000	1.48235900	H	1.24414800	4.89042100	-0.06171000
H	3.87566300	-2.35785500	2.32586600	H	0.07720500	4.65700300	4.07634700
H	3.67262700	-2.54049600	0.58288100	H	-1.27909900	2.80789100	4.86884400
H	3.17360600	-1.03973000	1.37866800	H	1.25294800	5.84983000	2.25031900
C	0.28133700	-4.97012500	-0.96296100	Rh	0.88437500	-0.27166800	-0.66771000
H	-0.80837700	-4.94857000	-0.88806700	H	1.15885500	0.27239600	0.72293400
H	0.53208100	-5.58205400	-1.83885300	H	2.59916700	-0.43341500	-0.74672500
H	0.68501700	-5.47943000	-0.08393000	C	7.71973000	-1.89132300	-1.18127700
C	0.18481300	-2.89666900	-2.37831200	C	6.50693600	-1.57163600	-1.78265700
H	0.32624800	-3.53394600	-3.26063200	C	5.70230900	-0.59715900	-1.19216700
H	-0.88861700	-2.75649100	-2.23639400	C	6.09273100	0.06441000	-0.01347000
H	0.63685300	-1.92333200	-2.62448100	C	7.32348400	-0.27573300	0.57647100
C	2.37669100	-3.68872400	-1.48905300	C	8.12799800	-1.24776100	-0.00175700
H	2.85506100	-2.71514100	-1.63229700	H	8.35665400	-2.64483000	-1.63461300
H	2.93053800	-4.24201500	-0.72665000	H	6.17808300	-2.04670700	-2.70075100
H	2.47679100	-4.24591800	-2.42891500	C	5.20451800	1.08457000	0.50938300
P	-1.37978600	0.47184500	-0.39829400	H	7.62678800	0.23731800	1.48229900
C	-2.06757800	1.62234500	-1.66854400	H	9.07794900	-1.50674500	0.45482600
C	-3.26796000	2.40431400	-1.49333300	C	4.00274700	1.30641700	-0.11580800
C	-1.39701100	1.65983100	-2.88206300	C	3.60659600	0.52630900	-1.25113500
C	-4.05479200	2.42002900	-0.30957200	H	3.30821300	2.05578900	0.24429100
C	-3.71264900	3.21755000	-2.59422200	O	5.62692400	1.75634000	1.57468100
C	-1.85191700	2.45596500	-3.95741800	O	4.52705300	-0.29092300	-1.83239400
H	-0.47645100	1.10599400	-3.00967400	C	2.69043400	1.23697700	-2.28463900
C	-5.19200200	3.19405700	-0.20961900	O	3.18897600	1.69801700	-3.28713700
H	-3.75435700	1.81760800	0.53617900	O	1.44207700	1.31040100	-1.90426300
C	-4.88851200	4.00357100	-2.45779200	C	4.52418000	5.05947300	1.88312400
C	-2.98230700	3.22147200	-3.81239900	H	4.15232900	5.42169500	0.91720500
H	-1.29119900	2.46207800	-4.88696700	H	4.30162100	5.79537700	2.66419300
C	-5.61728800	3.99779600	-1.29124500	H	5.60611800	4.93025900	1.81939500
H	-5.76521600	3.18951000	0.71360400	O	3.97755200	3.77671600	2.21472500
H	-5.20278500	4.61227900	-3.30172600	H	3.00774500	3.83805000	2.25315600

H	4.95769000	2.44142700	1.85097400	H	1.00238200	0.17631000	-4.19601900
TS2'-conf2				H	-0.45022200	0.10738000	-3.18951700
Fe	-4.42258800	-0.63611800	-1.54684000	H	1.10464700	0.62719600	-2.49283400
C	-2.35184200	-1.09833800	-1.66309800	C	2.53547500	-1.63840400	-2.87206200
C	-5.88238400	-2.05465400	-1.97728900	H	2.90028400	-1.27631800	-3.84192500
C	-2.92646800	-0.88856000	-2.95623700	H	2.99257800	-1.01954900	-2.09407500
H	-2.98291200	-1.61964400	-3.75158800	H	2.89391800	-2.66411800	-2.75756000
C	-2.55745700	0.10885200	-0.89510000	P	-1.59267700	0.55167500	0.59043400
C	-6.34397900	0.03702300	-1.11377200	C	-2.02584400	2.31667200	0.89977500
H	-6.61693400	1.08116200	-1.03753400	C	-1.52652300	3.37490700	0.06300400
C	-3.24709000	1.04724300	-1.74320800	C	-2.85012600	2.62138000	1.97127500
H	-3.55119400	2.04384400	-1.45863800	C	-0.71363100	3.16650600	-1.08374600
C	-5.58868600	-2.07904600	-0.58116900	C	-1.88842100	4.72765800	0.38301900
H	-5.21936900	-2.93261700	-0.02755900	C	-3.20404300	3.95557100	2.27399300
C	-6.34887900	-0.74767900	-2.30601500	H	-3.23260400	1.82852800	2.60433400
H	-6.62205000	-0.40099700	-3.29394800	C	-0.27371100	4.21733700	-1.85796800
C	-3.45540100	0.43633300	-3.01061600	H	-0.44614300	2.15414800	-1.36910200
H	-3.98006600	0.87702700	-3.84797500	C	-1.41167100	5.79187900	-0.42953400
C	-5.87795600	-0.78494600	-0.04842200	C	-2.72559600	4.98558800	1.50049800
H	-5.74817900	-0.47228800	0.97851200	H	-3.84918200	4.15548800	3.12413700
H	-5.75244800	-2.87500500	-2.67096000	C	-0.62045800	5.54795100	-1.52765500
C	-1.57160200	-2.29862100	-1.18788000	H	0.34206300	4.02319100	-2.73207200
H	-1.77761600	-2.41370700	-0.11847700	H	-1.69163600	6.80866300	-0.16658300
C	-2.02679300	-3.60028200	-1.87389500	H	-2.98497400	6.01568000	1.73099100
H	-3.11737300	-3.66432100	-1.79596500	H	-0.26615000	6.36969300	-2.14291100
H	-1.76765400	-3.64679600	-2.93250300	C	-2.13894700	-0.38977400	2.07838700
H	-1.61284500	-4.48444500	-1.38765300	C	-1.48011100	-0.21026300	3.34945200
P	0.31011500	-1.88531800	-1.09811800	C	-3.12596100	-1.35038400	1.94871300
C	0.99523300	-1.53754700	-2.86597400	C	-0.45038200	0.74307000	3.58471200
C	1.11228800	-3.45363900	-0.31263300	C	-1.89478600	-1.03753900	4.45044900
C	1.27074500	-4.63784300	-1.29186000	C	-3.51982600	-2.16275400	3.03775500
H	1.63990600	-5.50560100	-0.73100000	H	-3.61534800	-1.47833600	0.99227300
H	0.33632000	-4.93564500	-1.77051900	C	0.13367900	0.86708700	4.82859800
H	2.00272000	-4.43056200	-2.07679500	H	-0.10438600	1.38823700	2.78568200
C	0.22983600	-3.88696200	0.88189100	C	-1.27403200	-0.87818600	5.71851000
H	-0.73197400	-4.30614700	0.57525400	C	-2.91710800	-2.00598200	4.26205300
H	0.75866600	-4.66946500	1.43936600	H	-4.30259800	-2.90308600	2.89853600
H	0.04148700	-3.06162500	1.57716100	C	-0.27934100	0.05343100	5.90824000
C	2.50632200	-3.10877500	0.25573600	H	0.91753100	1.60450500	4.97607900
H	2.93169100	-4.01740300	0.70026500	H	-1.60440000	-1.50951100	6.53951200
H	3.20505100	-2.76015400	-0.50747400	H	-3.21391100	-2.62170400	5.10738900
H	2.44827400	-2.34757900	1.03635500	H	0.18659400	0.16755600	6.88268100
C	0.42738000	-2.44878200	-3.97092700	Rh	0.70376200	0.07797900	0.11747300
H	0.59093600	-3.51093600	-3.77215900	H	0.76244300	-0.78777800	1.36008100
H	-0.64088700	-2.28175800	-4.12709800	H	2.39227300	-0.10059200	0.01214000
H	0.93186200	-2.21162200	-4.91655400	C	6.62404500	-2.41811000	2.26994300
C	0.62730100	-0.07137900	-3.19427400	C	5.45896600	-1.67308600	2.41462200

C	5.13231800	-0.74339800	1.42693300	H	-2.45872700	-4.20357000	1.40916300
C	5.95476800	-0.54023700	0.30525000	H	-1.08171900	-4.87677700	0.53445400
C	7.13085500	-1.30334000	0.18235900	H	-0.88670000	-4.31330400	2.19485100
C	7.45852100	-2.23759000	1.15430700	P	0.71568000	-2.15566900	0.36861200
H	6.89014100	-3.14423100	3.03213100	C	1.35577100	-3.09456100	-1.18753800
H	4.80537400	-1.78804800	3.27271000	C	1.69464500	-2.62424400	1.96089500
C	5.55816700	0.48531900	-0.63911300	C	1.99195900	-4.13450900	2.09195600
H	7.77061700	-1.14142200	-0.67789400	H	1.10028900	-4.76115600	2.04069600
H	8.36599400	-2.82496800	1.05716500	H	2.69564600	-4.48376100	1.33174900
C	4.36110800	1.13766900	-0.45818200	H	2.46004900	-4.31330000	3.06806200
C	3.51116600	0.80829100	0.64201900	C	0.86790300	-2.14736500	3.17857600
H	4.03635300	1.91472400	-1.14126700	H	1.48435200	-2.25061300	4.07972600
O	6.41449600	0.74416400	-1.62189200	H	0.58436300	-1.09234700	3.09561500
O	3.98846700	-0.01061500	1.61581800	H	-0.03837300	-2.73604800	3.34101700
C	2.60800200	1.92480400	1.24319500	C	3.03671200	-1.86328200	2.00417800
O	1.33161600	1.82076300	1.05256400	H	3.56896100	-2.15271000	2.91902500
O	3.20460300	2.80973500	1.82554700	H	3.68837600	-2.09554300	1.15931600
C	5.86671100	3.05818700	-4.38872000	H	2.88410000	-0.78292500	2.03243300
H	6.93874800	3.15991000	-4.59224700	C	0.89386300	-4.55981300	-1.29500700
H	5.49697100	2.14751600	-4.86270700	H	1.35290400	-5.00996200	-2.18476600
H	5.32890200	3.91944300	-4.79914500	H	1.19496200	-5.16167200	-0.43347600
O	5.60600200	2.92077900	-2.98131500	H	-0.18852400	-4.63829400	-1.41758500
H	6.11038800	1.52021400	-2.16935700	C	0.81854800	-2.30914500	-2.40902000
H	5.92994300	3.71367000	-2.52415800	H	1.17783900	-2.78667400	-3.33001600
TS2'-conf3				H	-0.27218300	-2.28218800	-2.45127700
Fe	-4.10806600	-2.03929000	-0.46340400	H	1.19559700	-1.27452100	-2.42471500
C	-2.00912700	-2.27500600	-0.38413800	C	2.89751900	-3.05049200	-1.24661100
C	-5.06830500	-2.49935700	1.33492200	H	3.21577600	-3.44769200	-2.21910500
C	-2.60461500	-3.14398500	-1.35347300	H	3.28778800	-2.03199900	-1.16085300
H	-2.57904500	-4.22513800	-1.33581300	H	3.36798200	-3.66875600	-0.47817700
C	-2.34841900	-0.91786900	-0.75214400	P	-1.45705800	0.57732400	-0.19938300
C	-6.04807700	-2.71015500	-0.74465200	C	-2.07122900	1.88160600	-1.35741800
H	-6.40412400	-3.13158800	-1.67547300	C	-3.36600000	2.51291600	-1.26929000
C	-3.13712400	-0.98405100	-1.95618500	C	-1.22899300	2.19783900	-2.41234600
H	-3.55139100	-0.13461200	-2.47958700	C	-4.32625600	2.24553000	-0.25568400
C	-5.46385200	-1.19965800	0.89569700	C	-3.72296300	3.47201800	-2.28145300
H	-5.32228200	-0.27552100	1.43737700	C	-1.59652200	3.13461100	-3.40418100
C	-5.43281100	-3.43415800	0.31966100	H	-0.24435900	1.75343900	-2.46844500
H	-5.25223100	-4.50095900	0.33995500	C	-5.54680700	2.88706900	-0.23109800
C	-3.28123000	-2.34881600	-2.32566600	H	-4.09294100	1.53112800	0.52083300
H	-3.85470000	-2.72161600	-3.16397400	C	-4.98853200	4.11578700	-2.22589900
C	-6.06340500	-1.32779200	-0.39006500	C	-2.81574000	3.76160200	-3.33481100
H	-6.43340600	-0.51451300	-0.99976800	H	-0.90112700	3.35965400	-4.20703500
H	-4.58416000	-2.73779400	2.27322200	C	-5.88661200	3.83447300	-1.22297900
C	-1.09788000	-2.67308600	0.74970300	H	-6.25310300	2.66611700	0.56464800
H	-1.30106500	-1.99883000	1.58760800	H	-5.23336400	4.83955900	-2.99910100
C	-1.38042100	-4.10471500	1.24514200	H	-3.10691600	4.49100600	-4.08647300

H	-6.84980400	4.33495300	-1.19000200
C	-1.88257700	1.04363600	1.53465800
C	-1.36837900	2.26279200	2.10503700
C	-2.62301800	0.17703700	2.32062100
C	-0.56451100	3.19662700	1.39357900
C	-1.68328900	2.55493800	3.47782500
C	-2.91074700	0.46745700	3.67463900
H	-3.02249200	-0.73020400	1.88398500
C	-0.11378500	4.35203400	1.99678600
H	-0.27961800	3.00570100	0.36601900
C	-1.20764400	3.75856000	4.06378700
C	-2.45646000	1.63632100	4.23650300
H	-3.50002300	-0.23340700	4.25930900
C	-0.44053300	4.64292500	3.34108300
H	0.49982900	5.04499700	1.42837500
H	-1.46242900	3.96598900	5.10004500
H	-2.68040000	1.87464800	5.27321800
H	-0.08324300	5.56058200	3.79925900
Rh	0.90520100	0.09029400	-0.25307000
H	0.97616800	0.45564200	1.21705300
H	2.61030700	0.02500500	-0.20479000
C	6.62446400	0.80464300	3.26252700
C	5.43693500	1.24645900	2.68954800
C	5.20649800	0.98103500	1.33948900
C	6.14540800	0.29111100	0.55326600
C	7.34165700	-0.14273400	1.15407100
C	7.57543200	0.10788900	2.49857500
H	6.81652500	1.00580700	4.31211300
H	4.69328700	1.79527000	3.25748800
C	5.83881100	0.11134700	-0.85202800
H	8.07068500	-0.66691900	0.54636900
H	8.49873600	-0.22789800	2.95976600
C	4.62014600	0.52996500	-1.33280800
C	3.65719200	1.12868600	-0.46246500
H	4.36662300	0.42610500	-2.38186600
O	6.79374500	-0.43116900	-1.59958300
O	4.03449900	1.45258800	0.80442000
C	2.70178100	2.21070800	-1.04604100
O	1.43161600	1.95794400	-1.00160200
O	3.24609600	3.19744500	-1.50216000
C	6.58498300	1.04938500	-4.74366700
H	6.13623300	1.21946500	-5.72764300
H	6.25714000	1.83646300	-4.06272000
H	7.67759400	1.07006100	-4.82431900
O	6.11964100	-0.19423300	-4.18407600
H	6.54227800	-0.41977000	-2.56579400
H	6.37947400	-0.91941400	-4.77409100

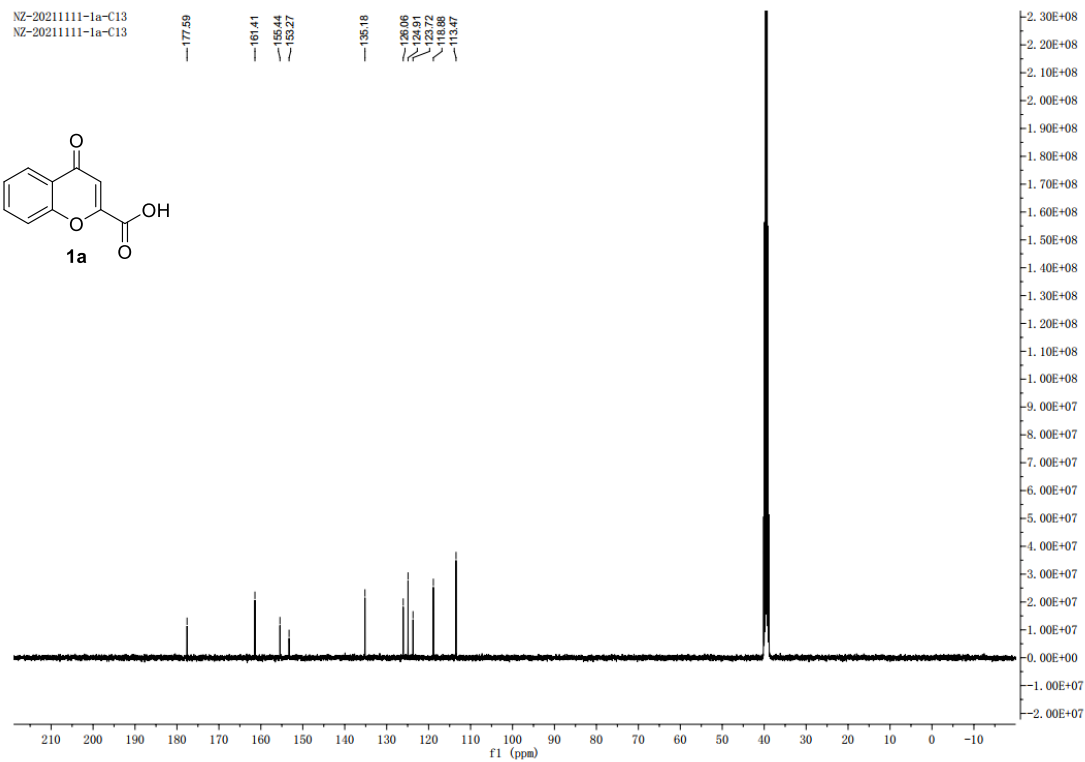
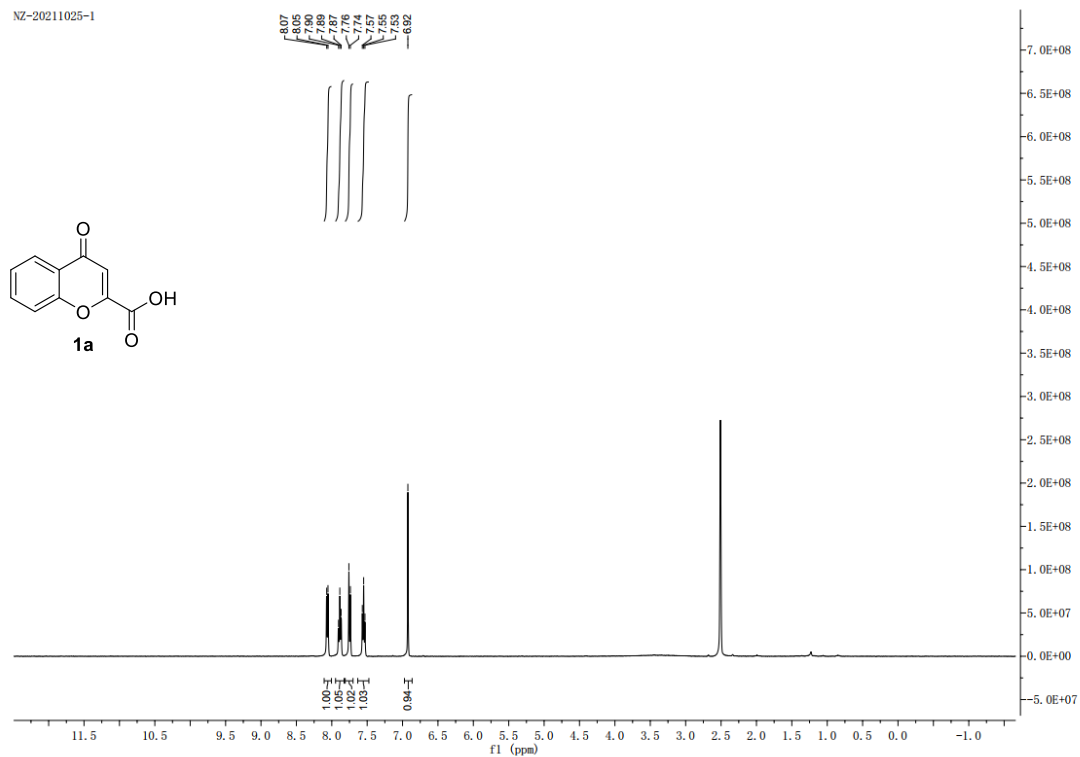
TS2'-conf4

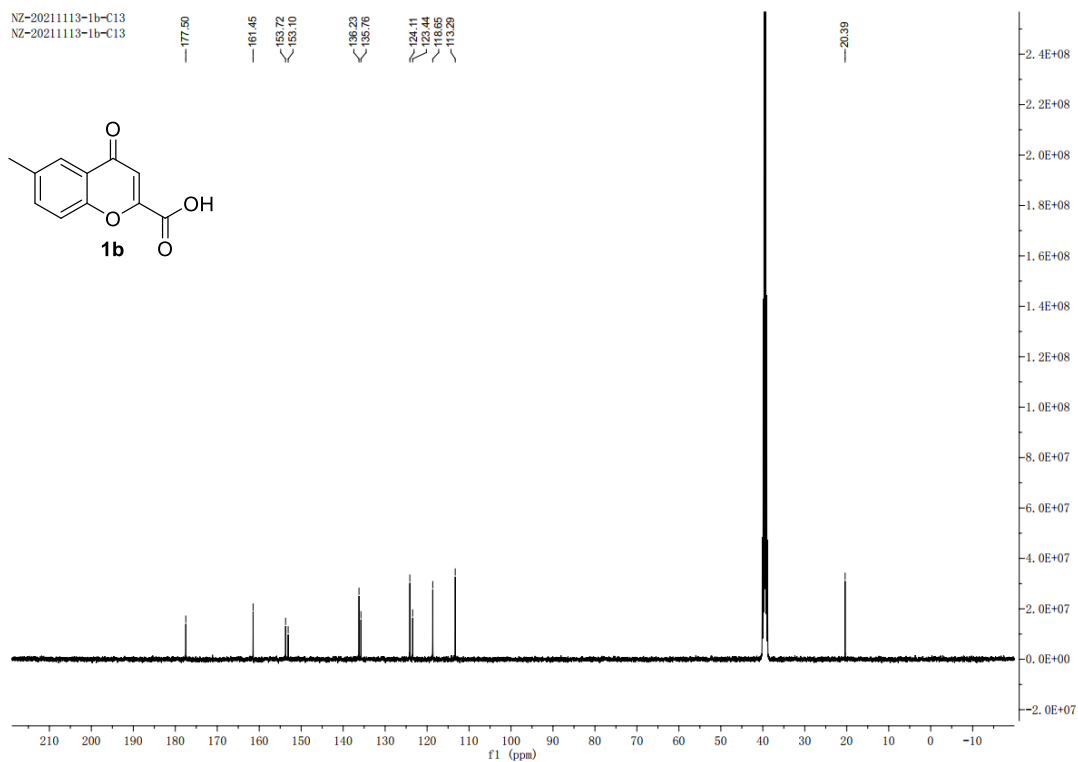
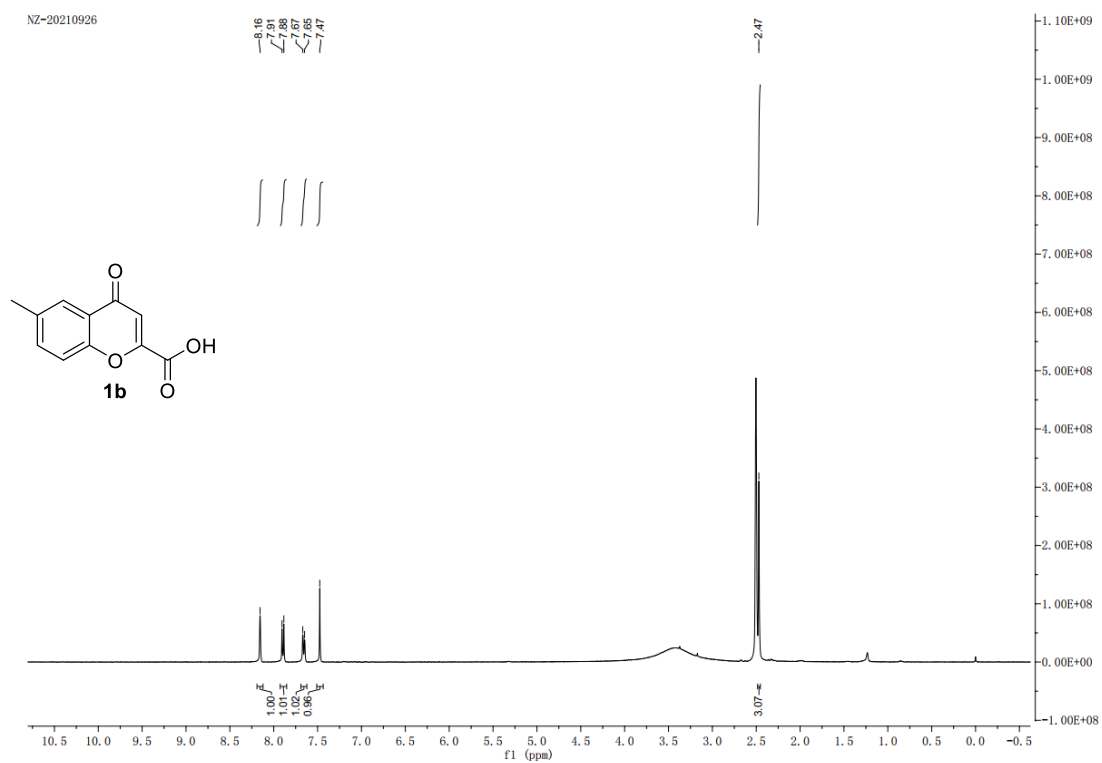
Fe	4.02338600	-2.18811100	0.18971400
C	1.91712000	-2.33099600	0.07270300
C	5.30491700	-3.51789400	-0.76032800
C	2.47207300	-3.34335900	0.91910600
H	2.40641400	-4.41073300	0.75712600
C	2.30394700	-1.04876800	0.61920900
C	6.00310300	-1.54360900	0.21585800
H	6.39584600	-0.82856200	0.92616500
C	3.07958400	-1.30468300	1.80623200
H	3.52083700	-0.54901900	2.43970300
C	4.98247800	-2.44849600	-1.64910000
H	4.49887500	-2.54740400	-2.61240000
C	5.93609200	-2.95848900	0.39043600
H	6.26893500	-3.50791000	1.26116800
C	3.16975100	-2.71101100	1.99087100
H	3.72210500	-3.21350100	2.77383800
C	5.41958100	-1.23076900	-1.04538600
H	5.31579000	-0.24057900	-1.46529600
H	5.08697000	-4.56613000	-0.91770800
C	1.00012600	-2.54008400	-1.10618500
H	1.23486400	-1.76895600	-1.84646600
C	1.23140200	-3.90327200	-1.78630900
H	2.30694500	-4.02556800	-1.95234600
H	0.89036600	-4.74975200	-1.18856300
H	0.74339200	-3.96148900	-2.75977200
P	-0.79553600	-2.00962500	-0.66402100
C	-1.47946800	-3.12071700	0.75434400
C	-1.78063000	-2.22757000	-2.30575700
C	-2.13133800	-3.69560100	-2.63502100
H	-2.59798000	-3.72752000	-3.62752700
H	-1.26317800	-4.35582400	-2.66381100
H	-2.85314200	-4.11532000	-1.92933900
C	-0.92877600	-1.62553500	-3.44850200
H	-0.04308600	-2.22046200	-3.68503600
H	-1.54231400	-1.58715600	-4.35670700
H	-0.60829100	-0.60151500	-3.22719200
C	-3.09415200	-1.41855000	-2.25166000
H	-3.62884900	-1.56431600	-3.19869200
H	-3.76087800	-1.73696400	-1.44756300
H	-2.90326300	-0.35016400	-2.13527800
C	-1.07357200	-4.60403300	0.66937400
H	-1.39333800	-5.07632200	-0.26329700
H	0.00447600	-4.73913100	0.78031300
H	-1.55347300	-5.14868400	1.49284400
C	-0.92106800	-2.52310600	2.06900700
H	-1.30243900	-3.10419600	2.91887700

H	0.16960000	-2.54159800	2.11512100	C	-6.14456700	0.60540200	-0.47990200
H	-1.26040100	-1.48645600	2.22031500	C	-7.36108400	0.28071900	-1.10835000
C	-3.01864300	-3.02624800	0.81655600	C	-7.60427200	0.69620300	-2.40963100
H	-3.35794000	-3.53751300	1.72671600	H	-6.84146500	1.78112500	-4.11616300
H	-3.36937700	-1.99121800	0.86765600	H	-4.68127900	2.37691800	-3.01049600
H	-3.50690700	-3.51783900	-0.02838200	C	-5.82577100	0.25129000	0.88908900
P	1.47337700	0.53973300	0.26761000	H	-8.09808900	-0.29064700	-0.55527300
C	2.12595400	1.65344000	1.59168800	H	-8.54338700	0.44473400	-2.89208700
C	3.44553800	2.23779600	1.59427600	C	-4.58992300	0.57617000	1.39711100
C	1.28640800	1.86086000	2.67543200	C	-3.61914100	1.24447200	0.58729700
C	4.40403300	2.06976700	0.55784400	H	-4.32813500	0.34363700	2.42337300
C	3.83065100	3.03769400	2.72726700	O	-6.78769200	-0.35049500	1.58071300
C	1.68129800	2.64128300	3.78510200	O	-4.00211400	1.72595400	-0.62671500
H	0.28411700	1.45390800	2.66746800	C	-2.62436800	2.22247200	1.27908500
C	5.64934800	2.65854800	0.62471400	O	-1.36625500	1.91531100	1.22659400
H	4.15002200	1.47626000	-0.30880900	O	-3.13019400	3.18573400	1.82070800
C	5.12142900	3.63078200	2.76400500	C	-6.44016100	-1.66155200	4.97603600
C	2.92540200	3.22109000	3.80581500	H	-7.52115500	-1.67995000	5.15515800
H	0.98749300	2.78589700	4.60761600	H	-6.15361900	-2.55694500	4.42208200
C	6.01722400	3.44979400	1.73625200	H	-5.90660100	-1.64567000	5.93228200
H	6.35375700	2.51778800	-0.19068900	O	-6.05780400	-0.53875300	4.16305500
H	5.38742200	4.23399600	3.62830200	H	-6.52257800	-0.47454900	2.53412400
H	3.23812200	3.83105300	4.64958900	H	-6.30536400	0.27965800	4.62292300
H	6.99991100	3.91038900	1.77476000				
C	1.93193800	1.21589300	-1.38715000				
C	1.47081700	2.51965200	-1.79155600				
C	2.64513900	0.43295000	-2.27894200				
C	0.69759900	3.38137200	-0.96466500				
C	1.80926800	2.97945400	-3.11181600				
C	2.95603000	0.88950600	-3.58101100				
H	3.00556100	-0.53924400	-1.96553500				
C	0.29756500	4.62393900	-1.40959000				
H	0.39593700	3.06604200	0.02678400				
C	1.38620400	4.26850400	-3.53330900				
C	2.55271200	2.14000900	-3.98347900				
H	3.52271300	0.24988400	-4.25186900				
C	0.64763100	5.07833100	-2.70169000				
H	-0.29409000	5.25845000	-0.75604700				
H	1.65810800	4.60208100	-4.53159200				
H	2.79504900	2.50519200	-4.97828500				
H	0.33038700	6.06234900	-3.03445500				
Rh	-0.90579300	0.14029500	0.24682200				
H	-0.94825700	0.69569500	-1.16369900				
H	-2.61231800	0.14940000	0.18514600				
C	-6.64216600	1.45089500	-3.10117100				
C	-5.43424300	1.78642600	-2.49950800				
C	-5.19490900	1.35602200	-1.19424500				

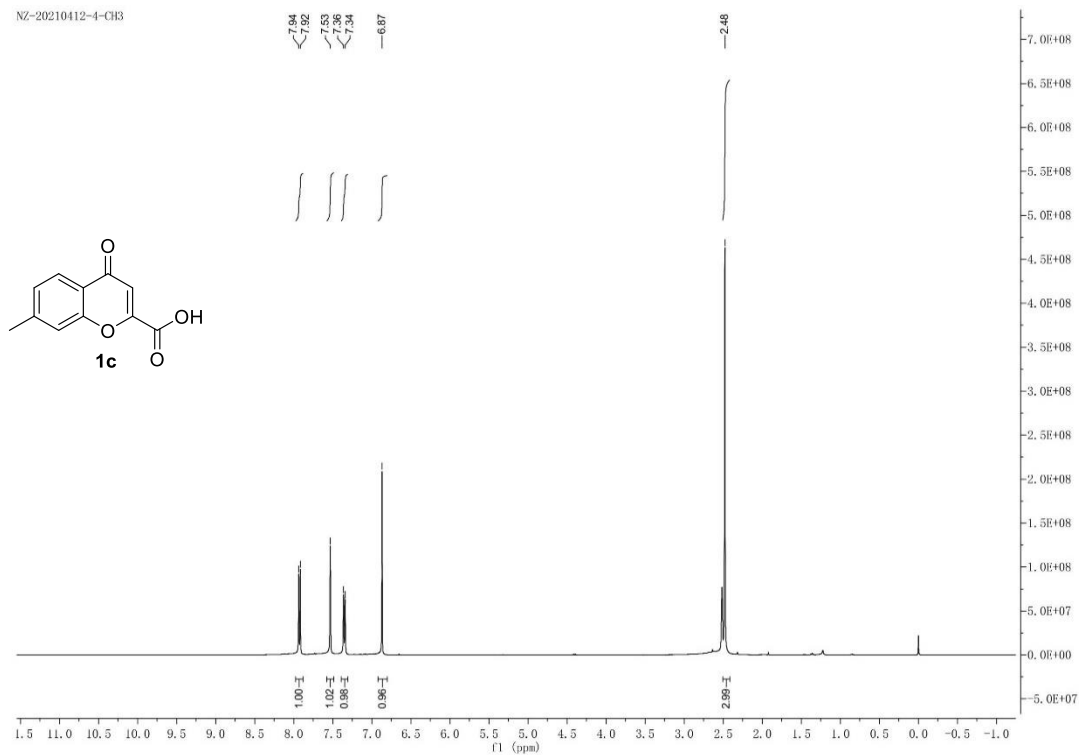
8. NMR Spectra

8.1 NMR Spectra of the substrates

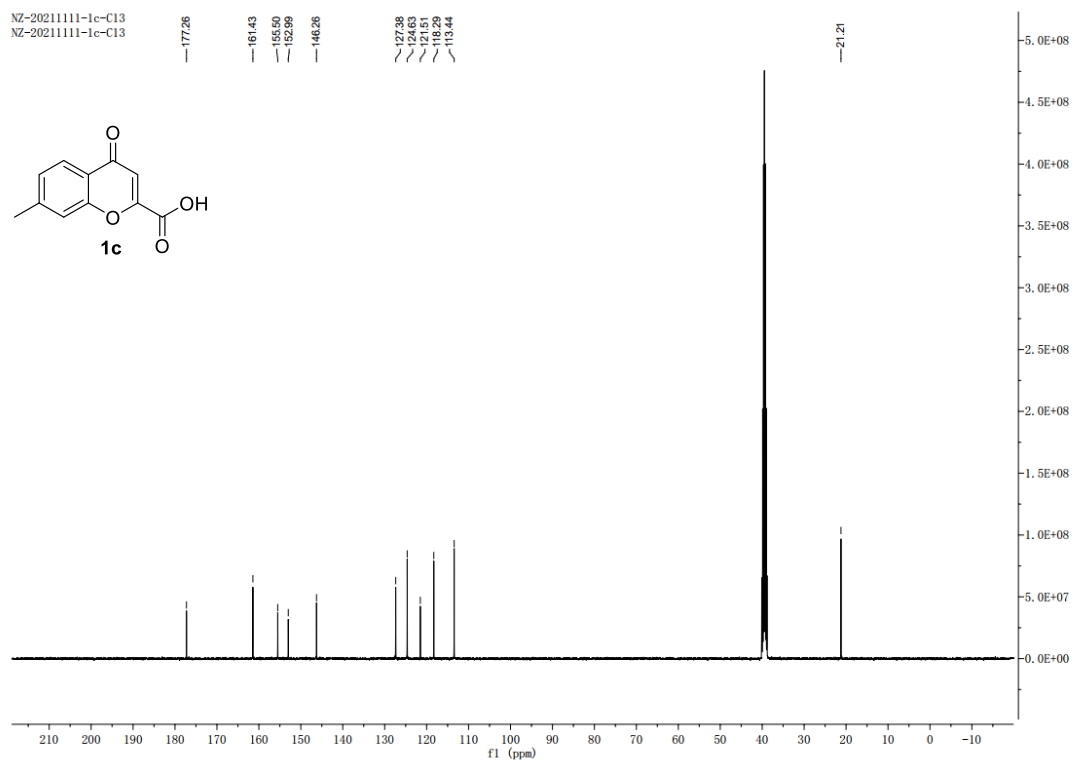




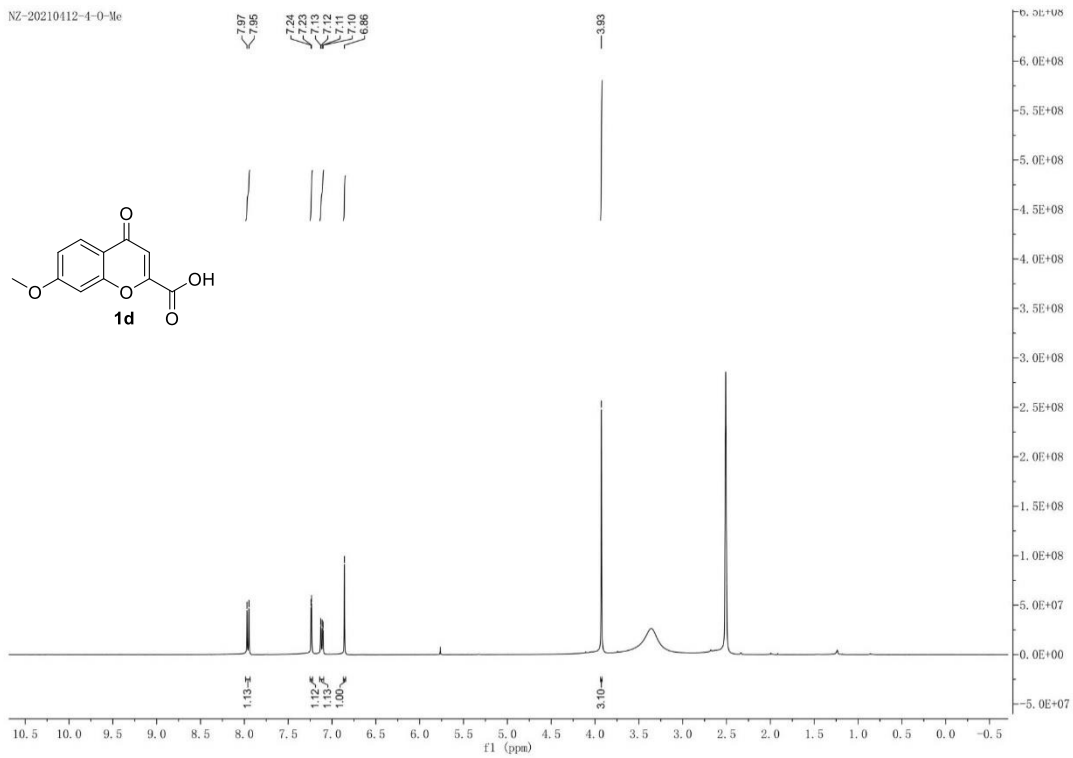
NZ-20210412-4-CH3



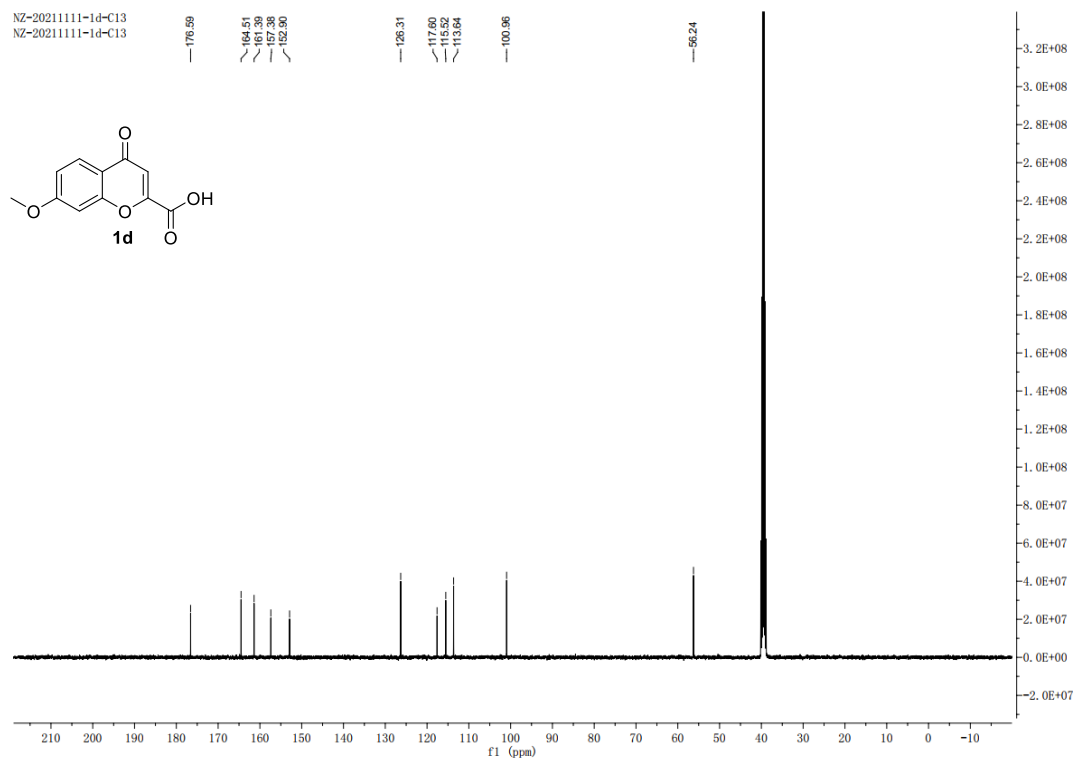
NZ-20211111-1c-C13
NZ-20211111-1c-C13

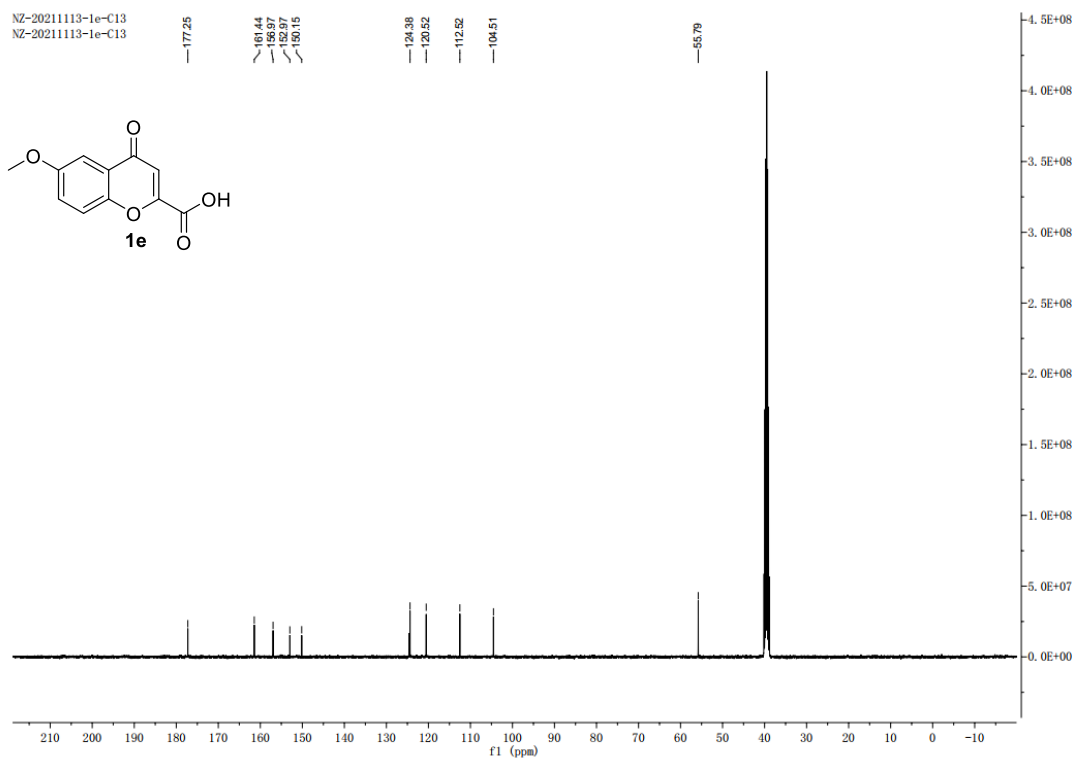
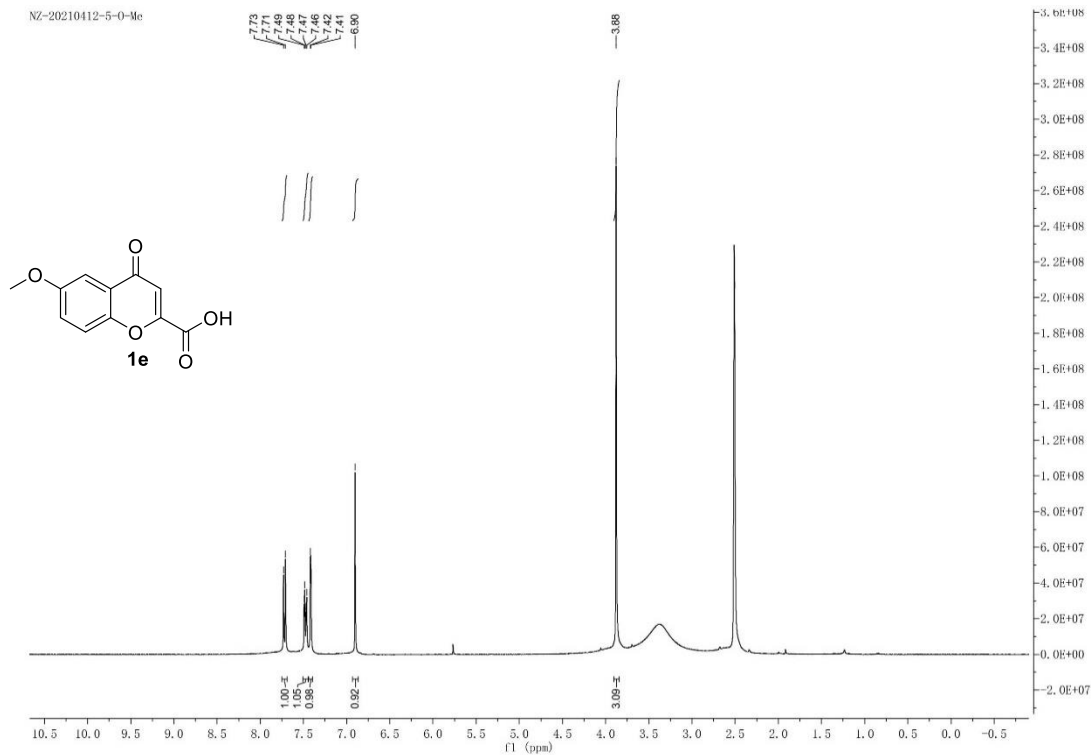


NZ-20210412-4-O-Me

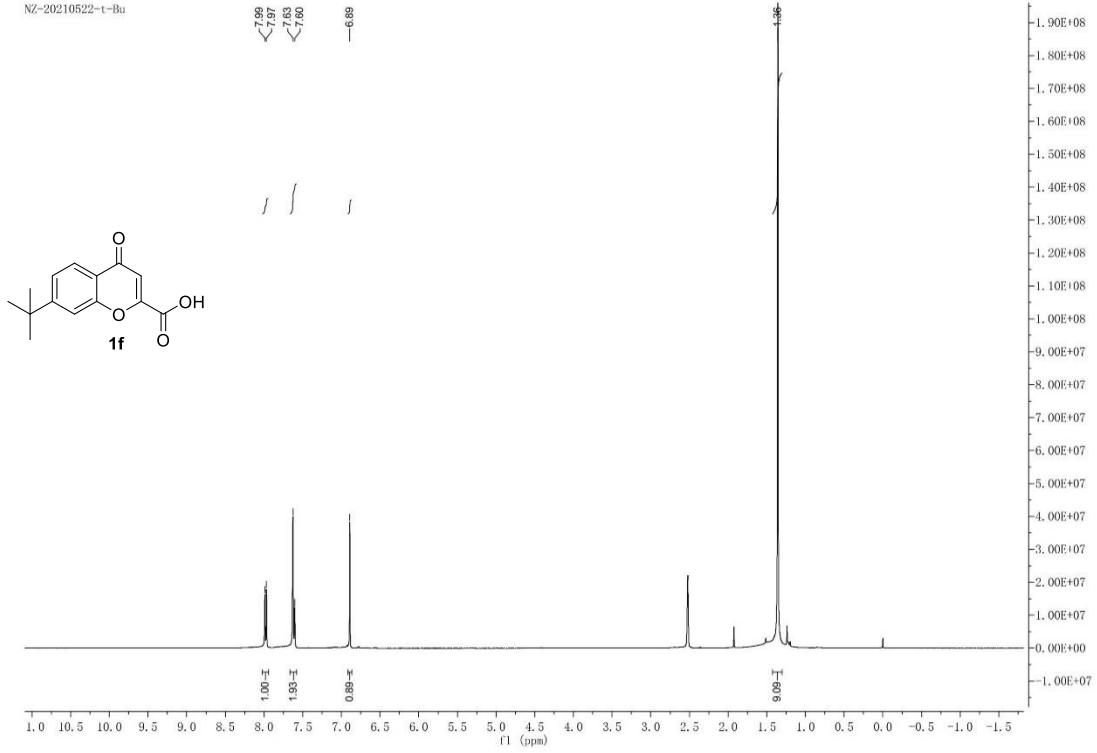


NZ-20211111-1d-C13
NZ-20211111-1d-C13

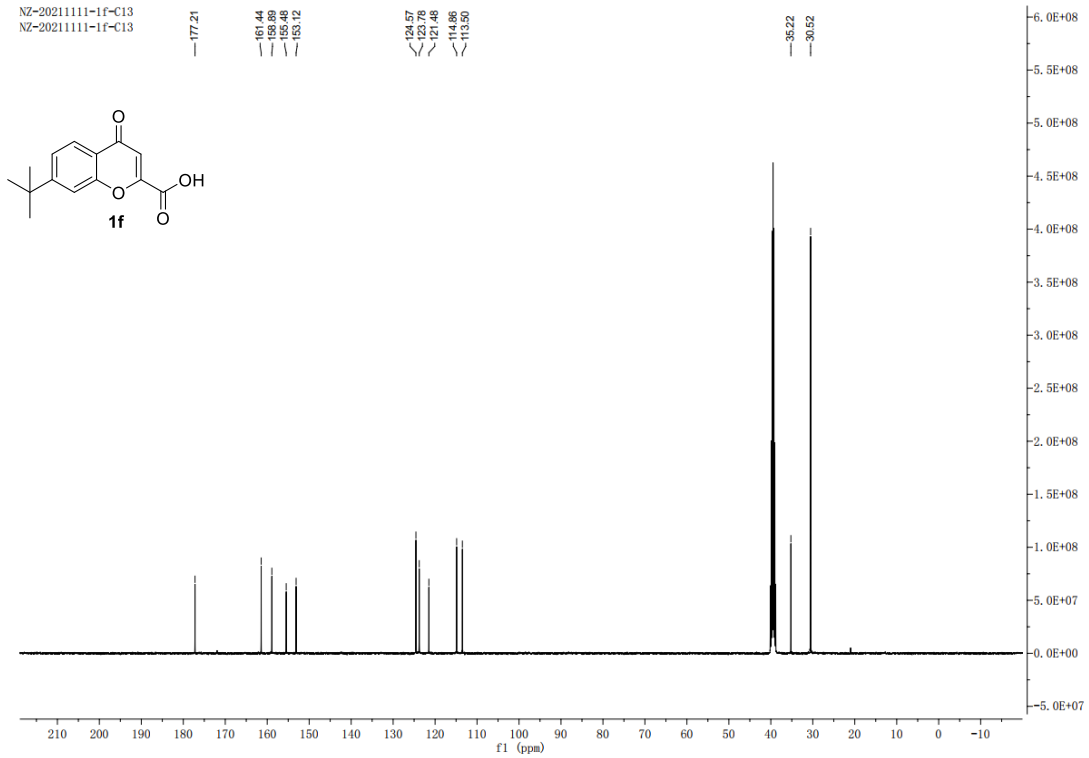




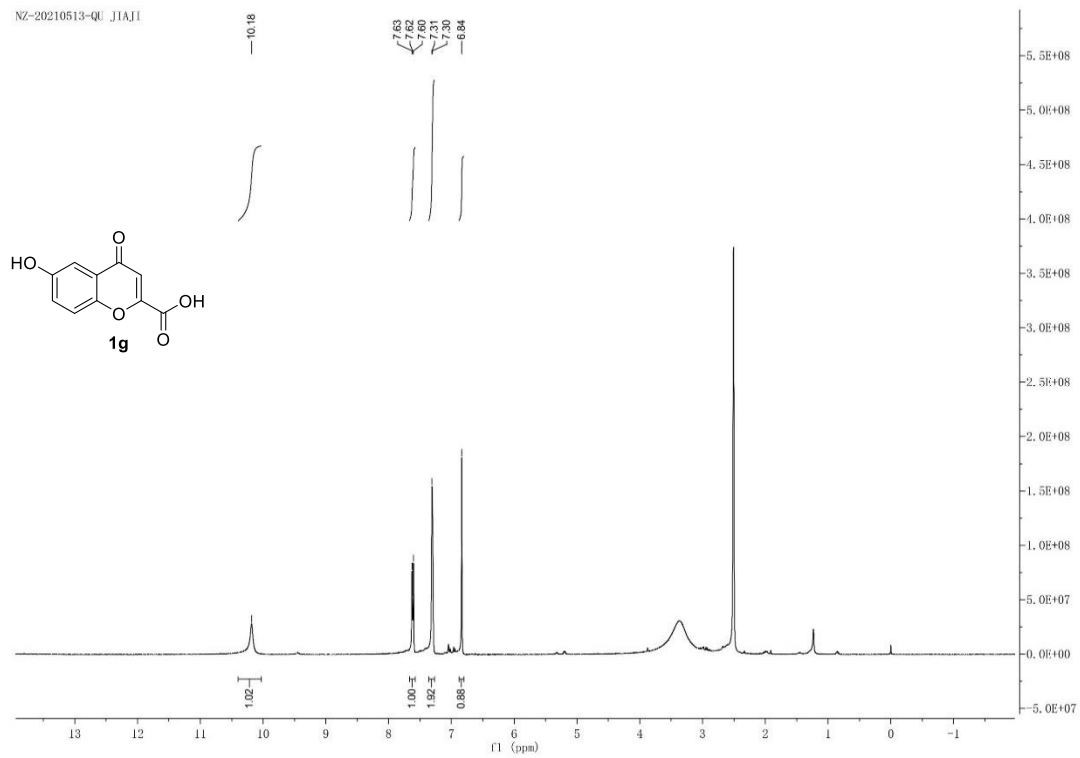
NZ-20210522-t-Bu



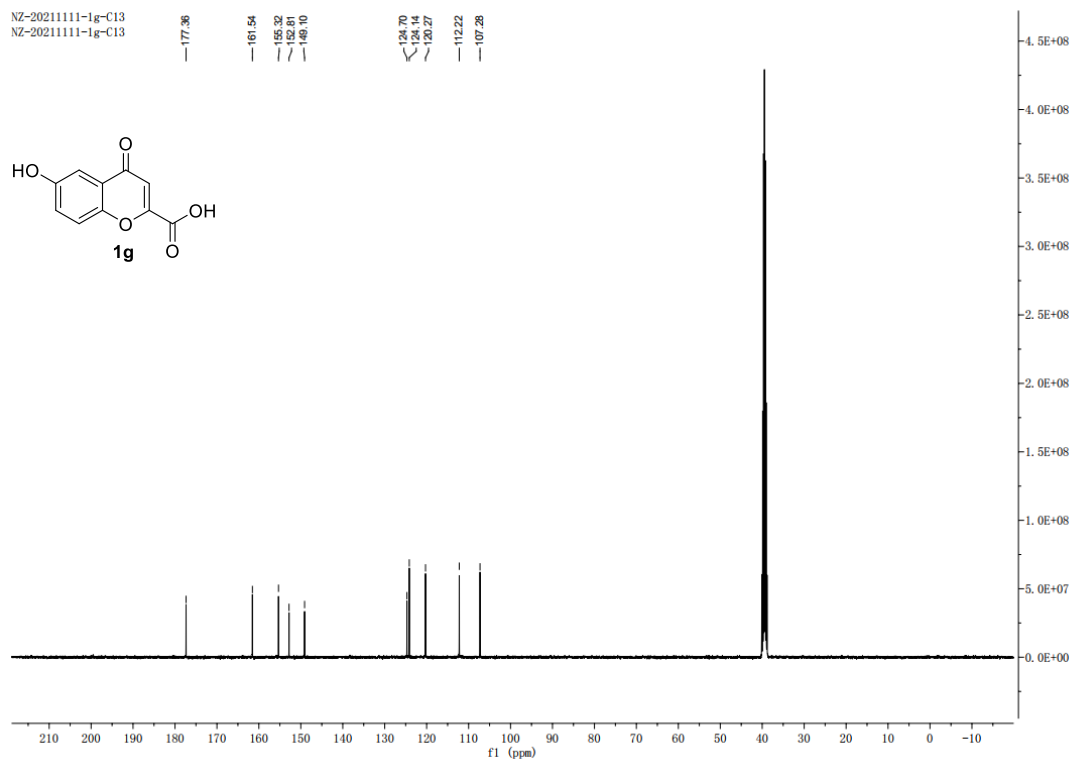
NZ-20211111-1f-C13
NZ-20211111-1f-C13



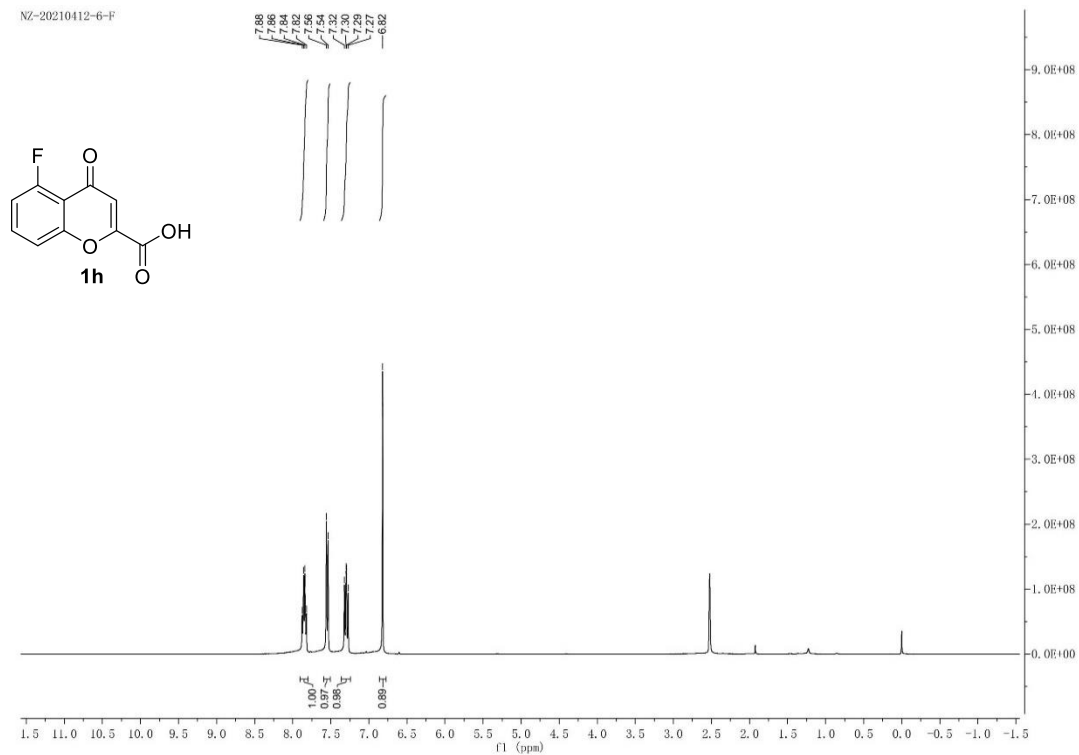
NZ-20210513-QU JIAJI



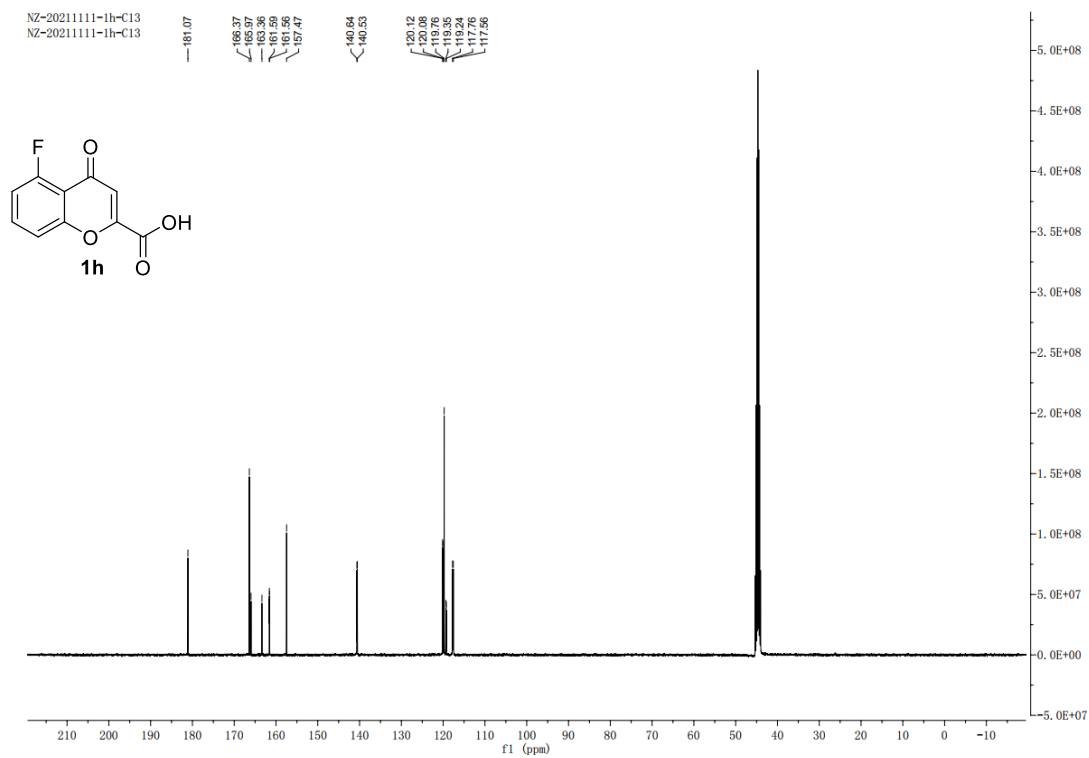
NZ-20211111-1g-C13
NZ-20211111-1g-C13



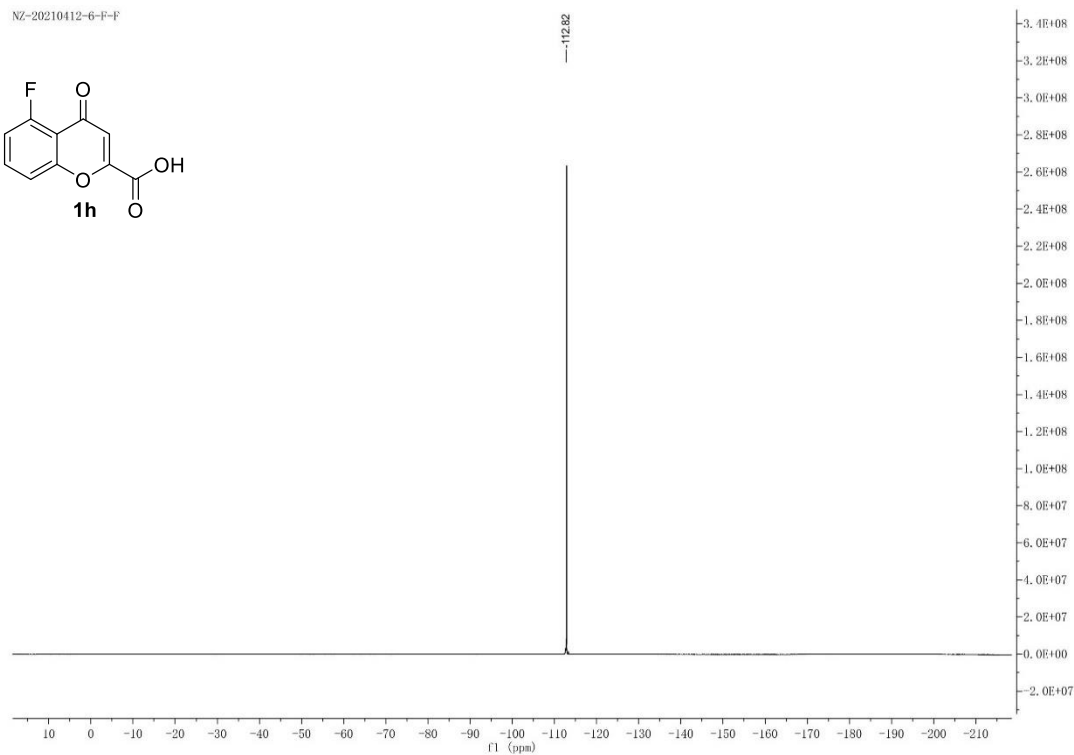
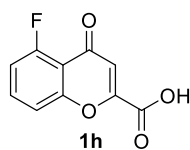
NZ-20210412-6-F



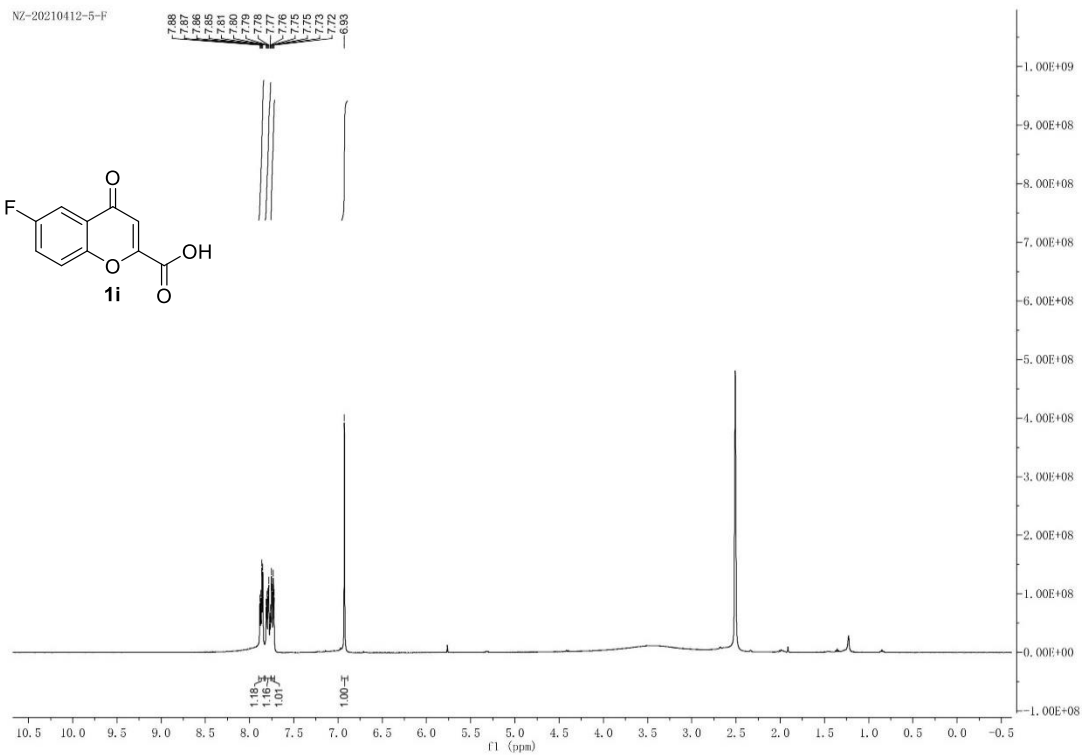
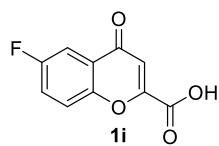
NZ-20211111-1h-C13
NZ-20211111-1h-C13

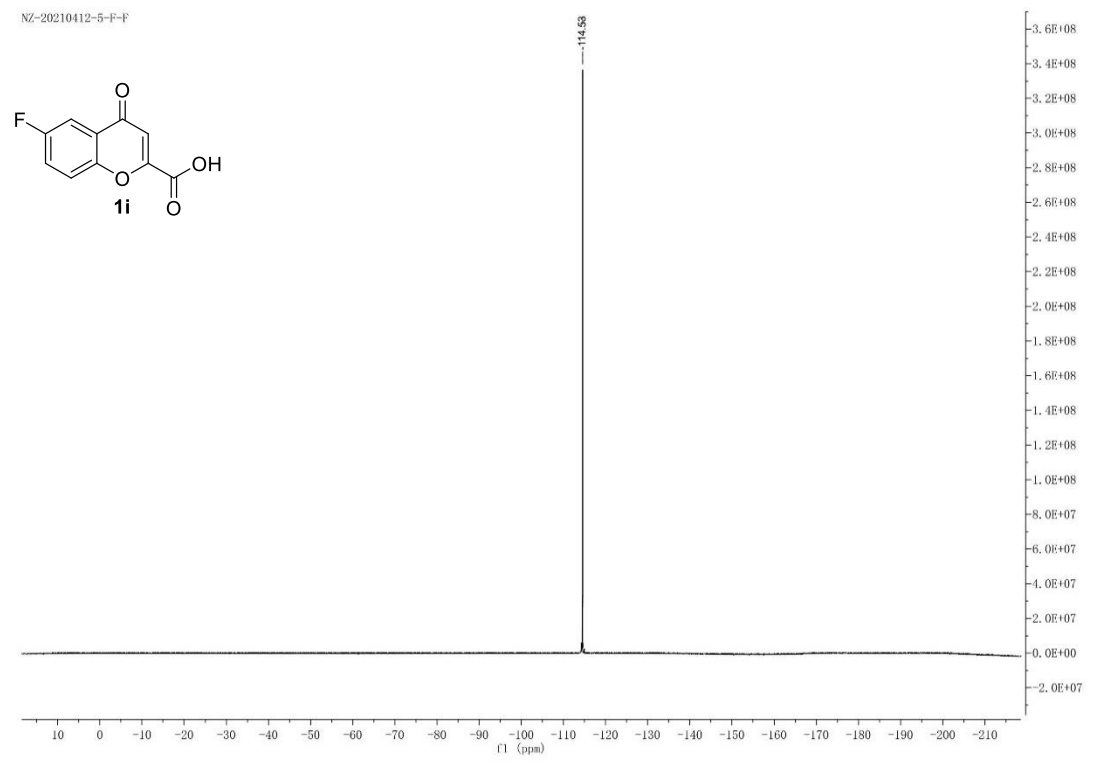
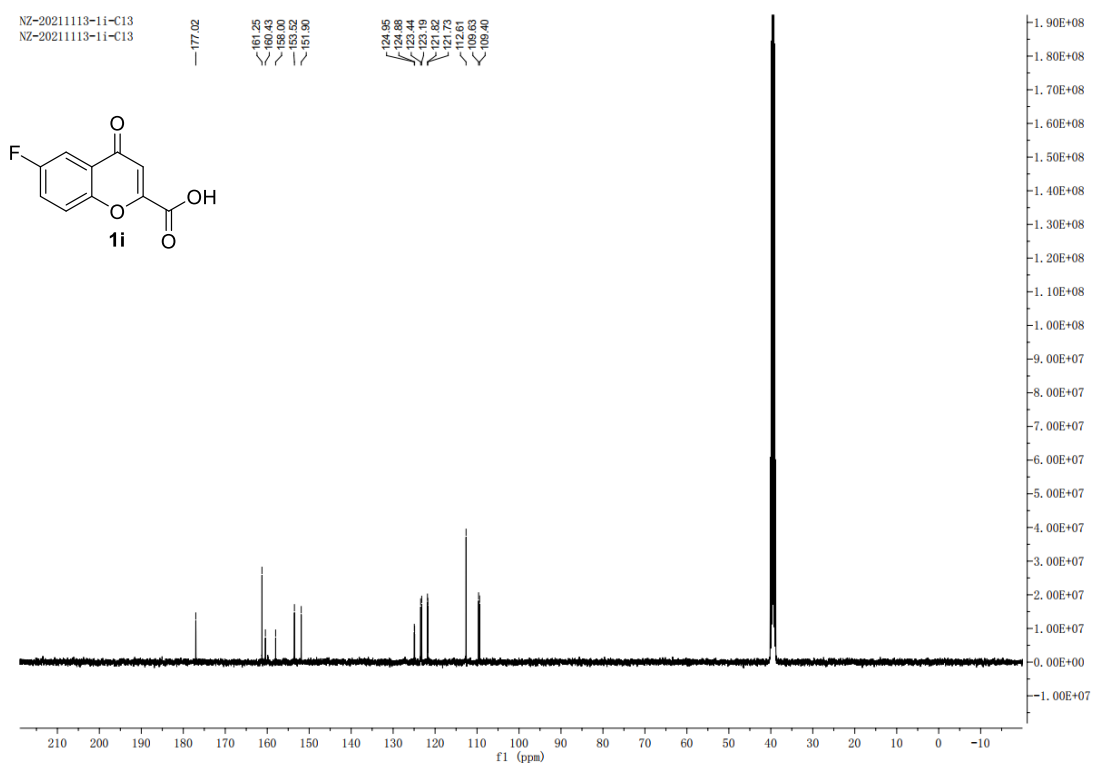


NZ-20210412-6-F-F

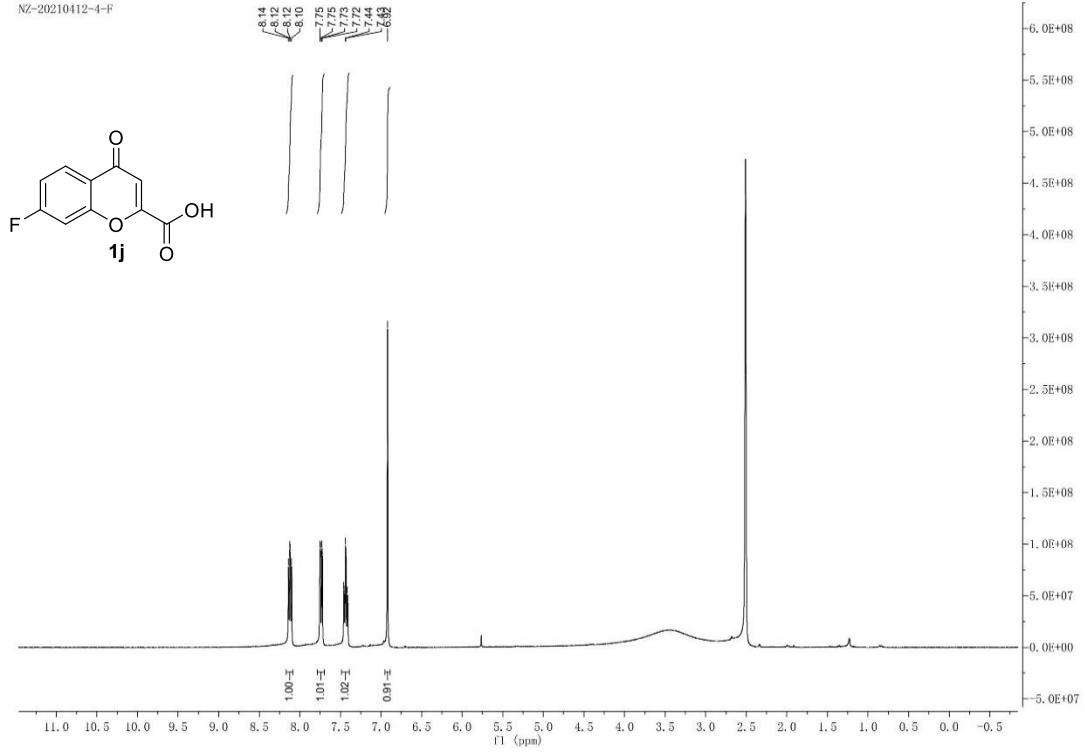


NZ-20210412-5-F

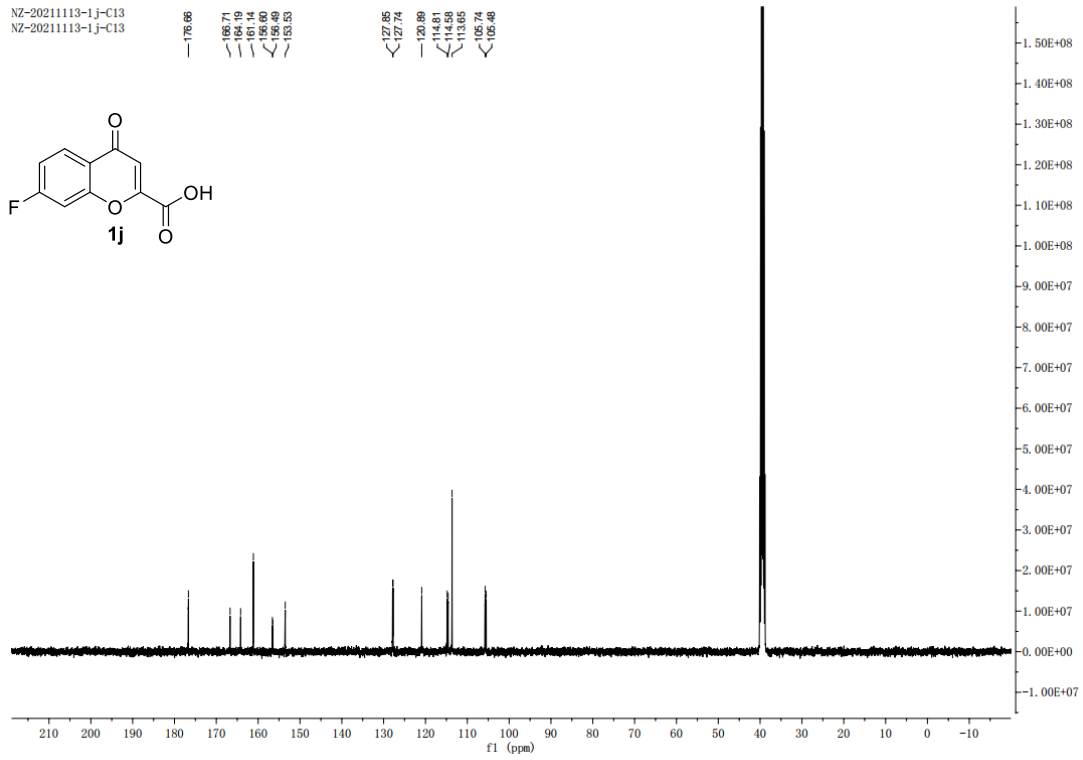




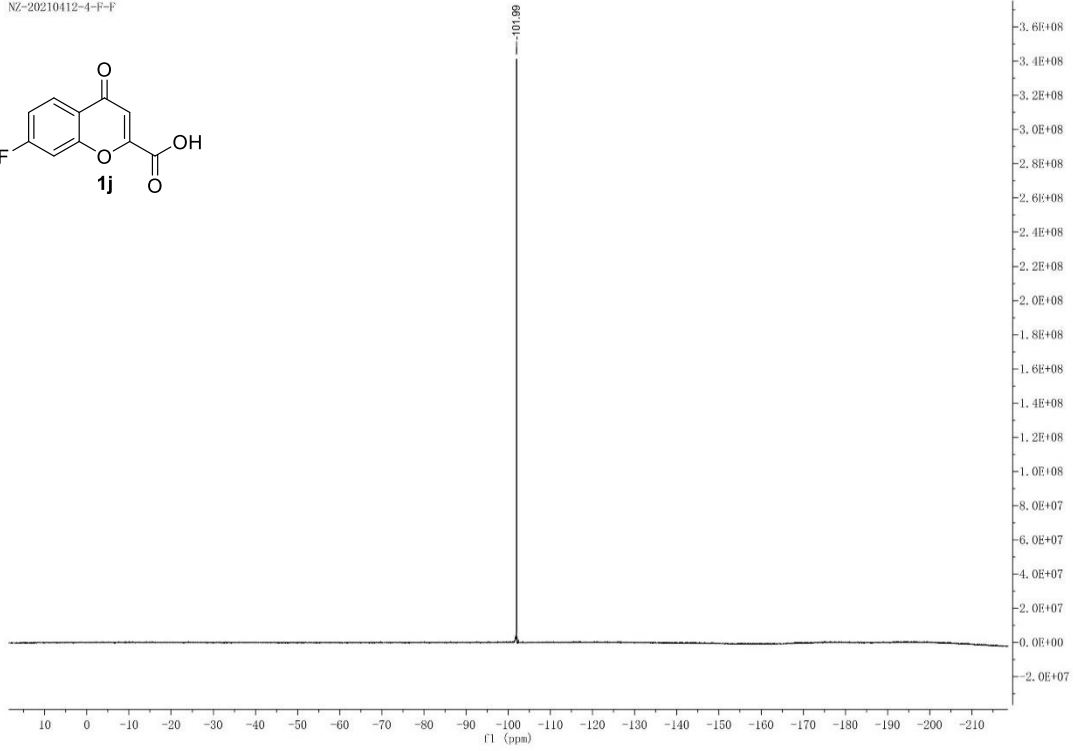
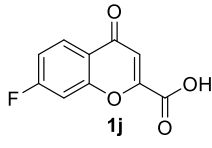
NZ-20210412-4-F



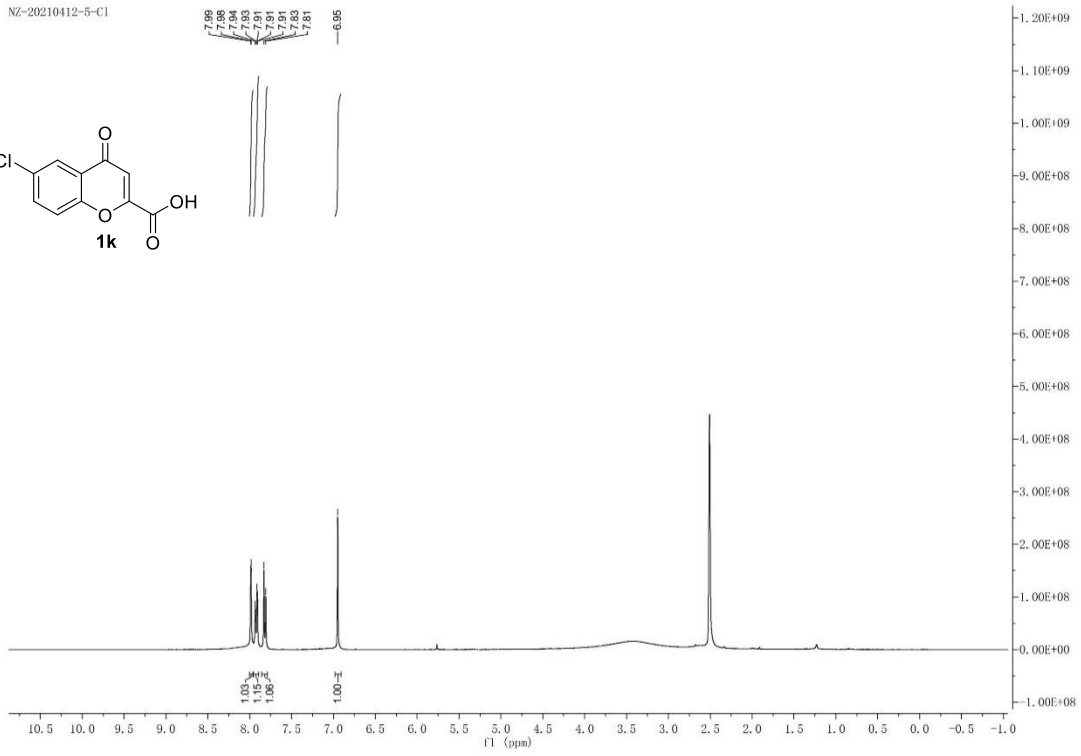
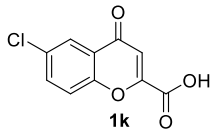
NZ-20211113-1j-C13
NZ-20211113-1j-C13

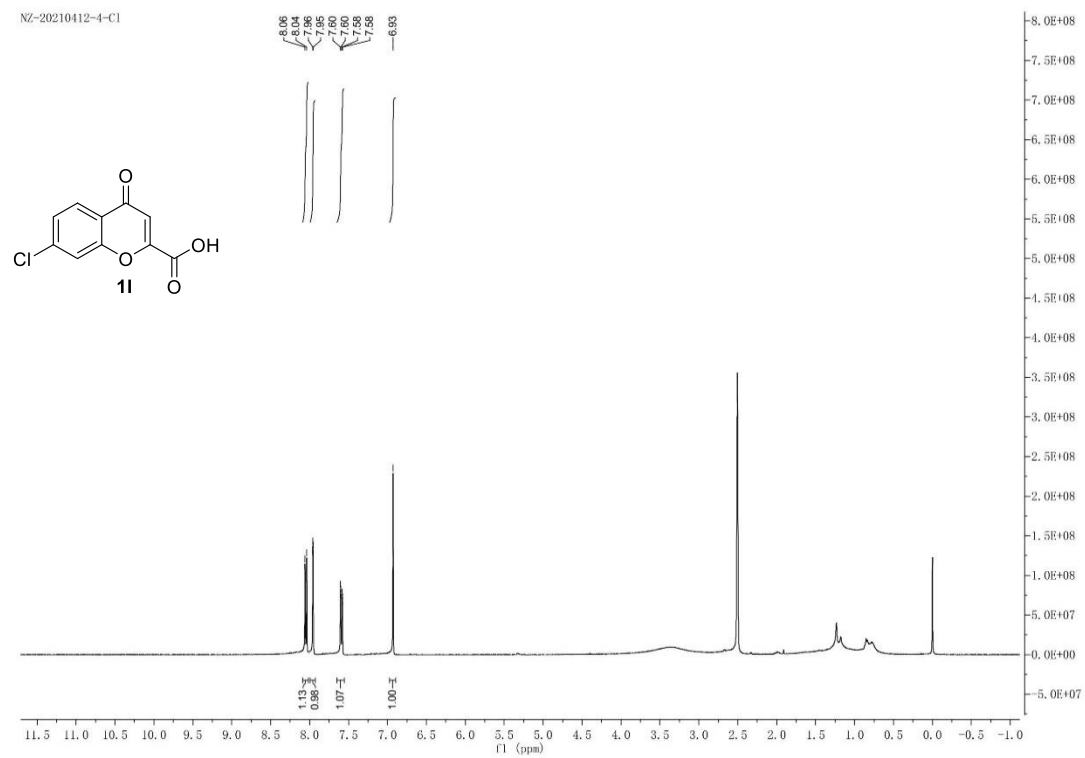
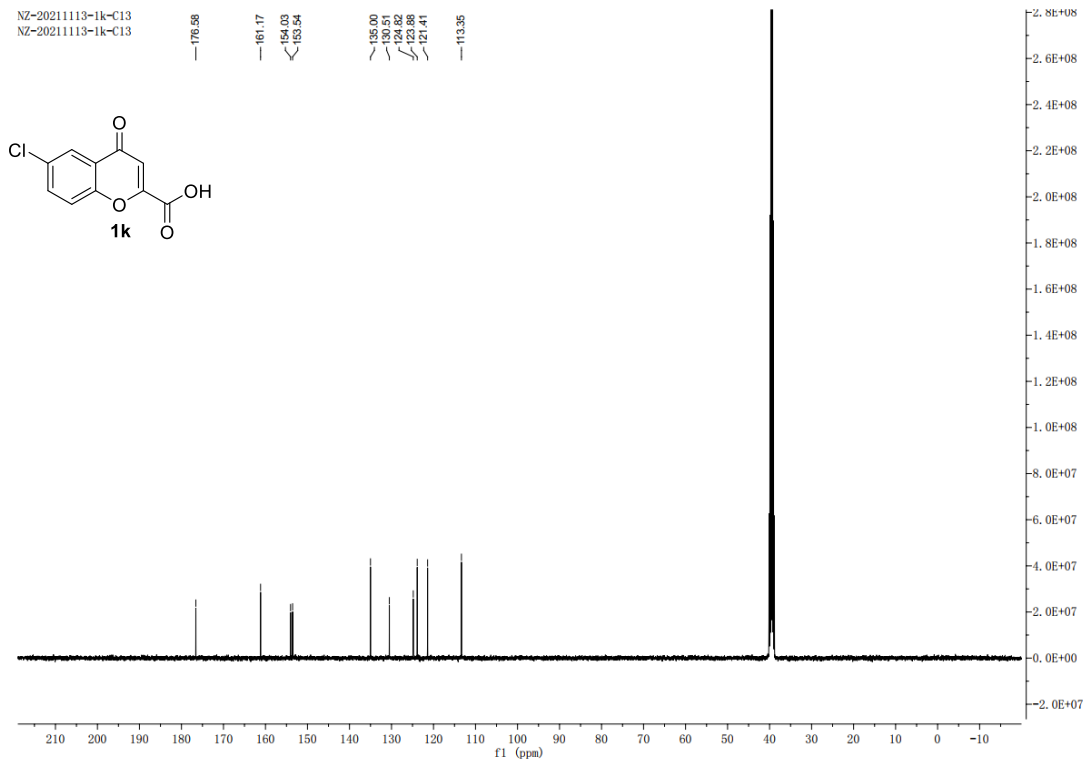


NZ-20210412-4-F-F

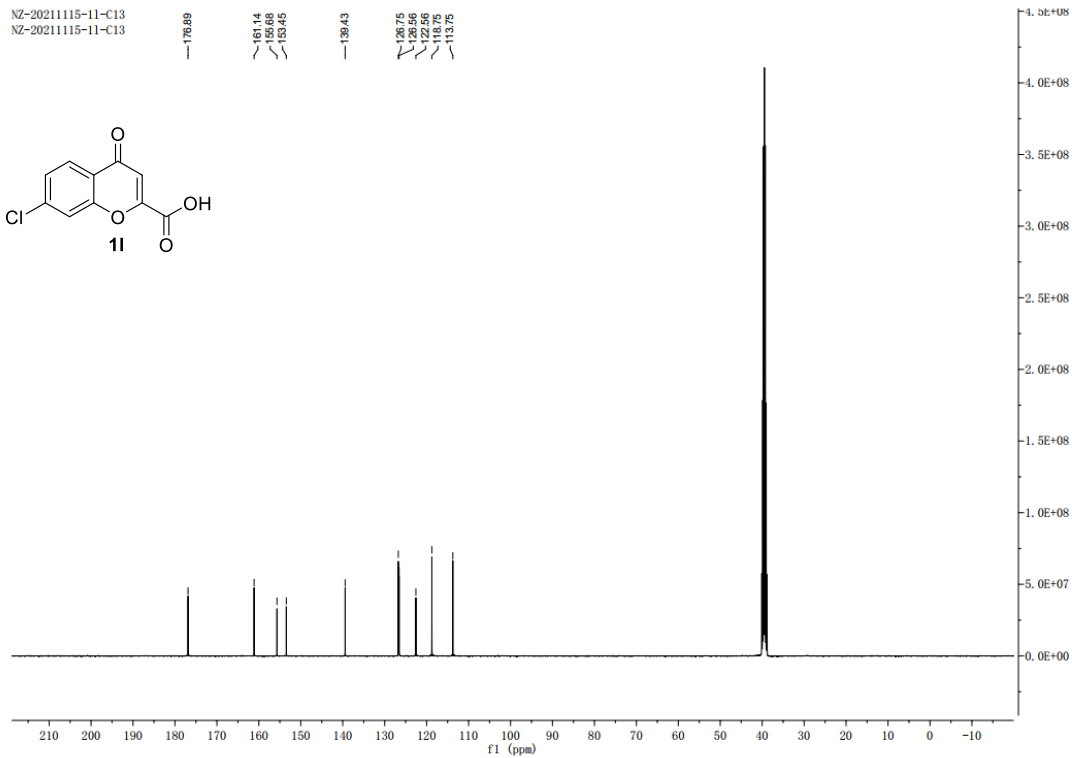
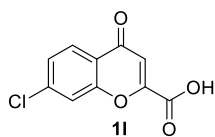


NZ-20210412-5-Cl

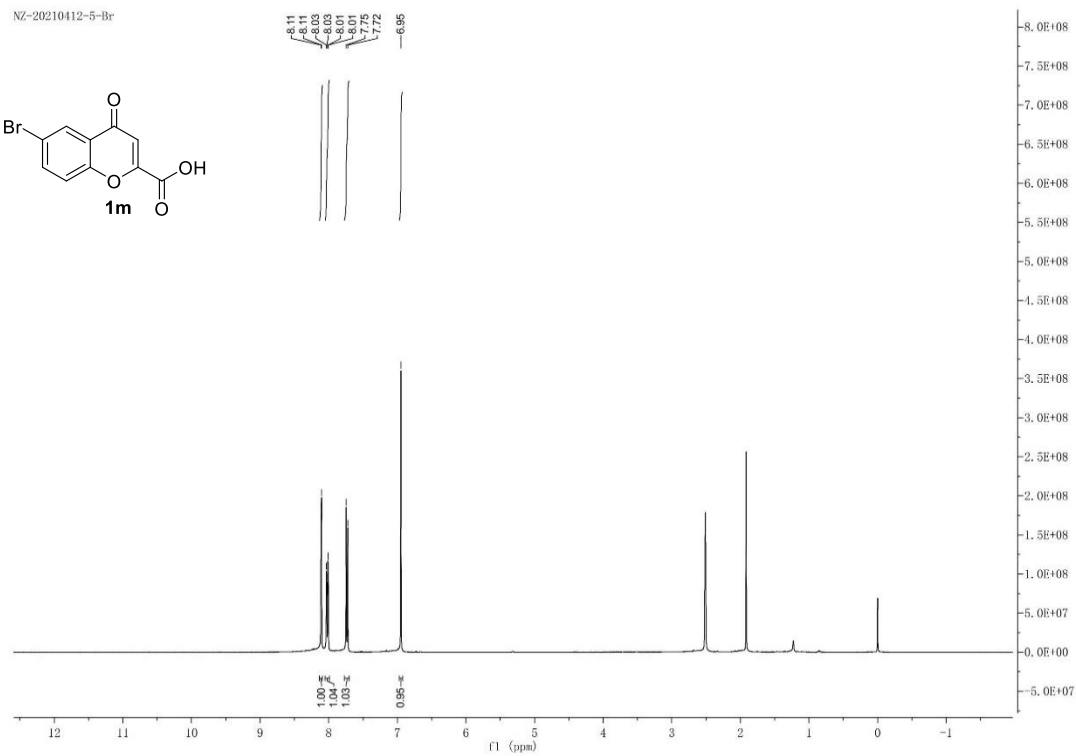
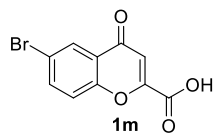




NZ-20211115-11-C13
NZ-20211115-11-C13

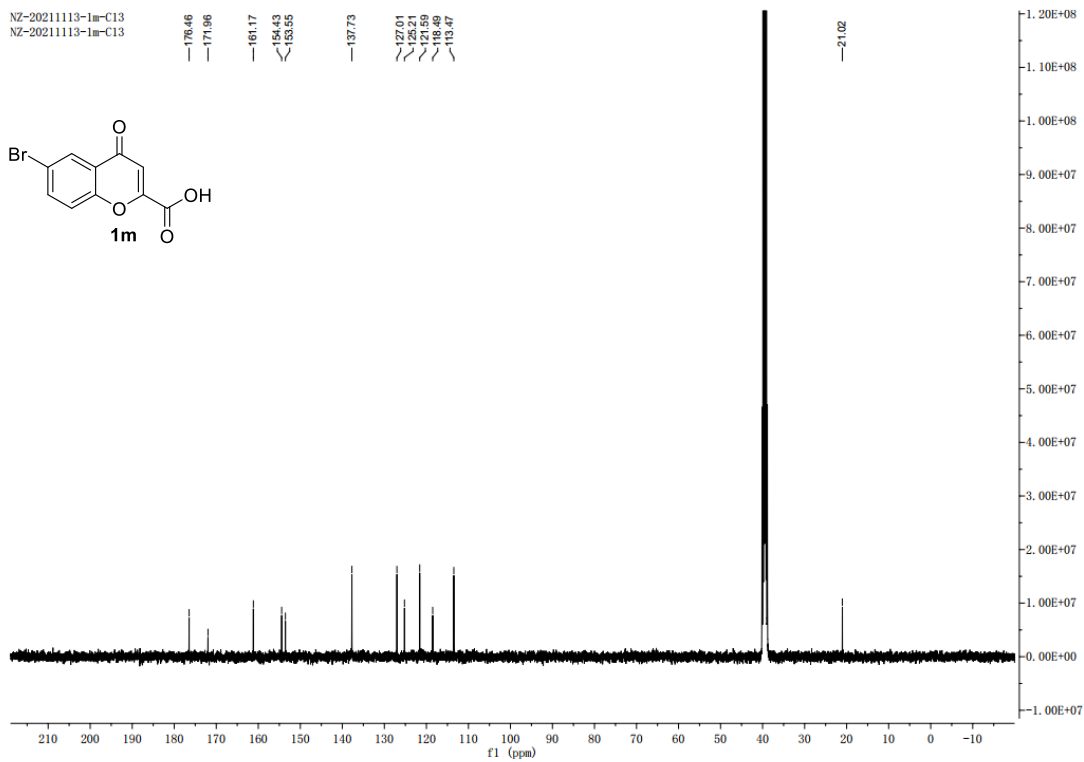
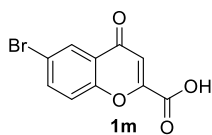


NZ-20210412-5-Br



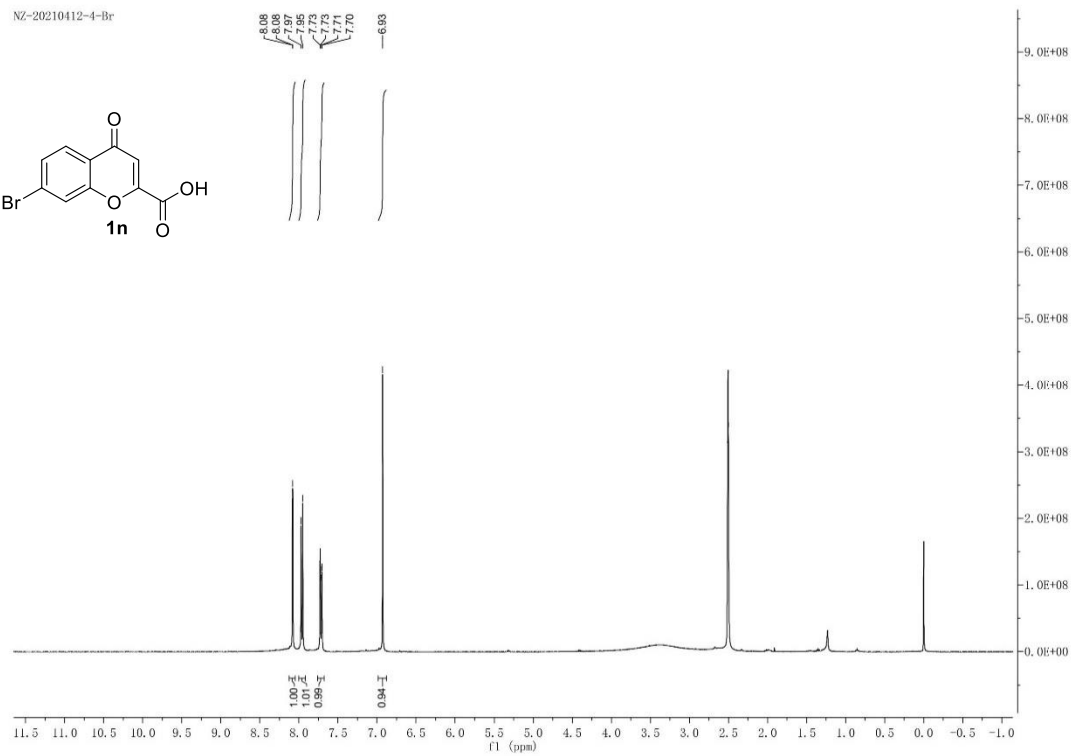
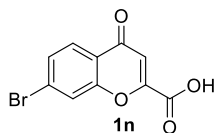
NZ-20211113-1m-C13
NZ-20211113-1m-C13

176.46
171.96
161.17
154.43
153.55
137.73
127.01
125.21
121.99
119.47

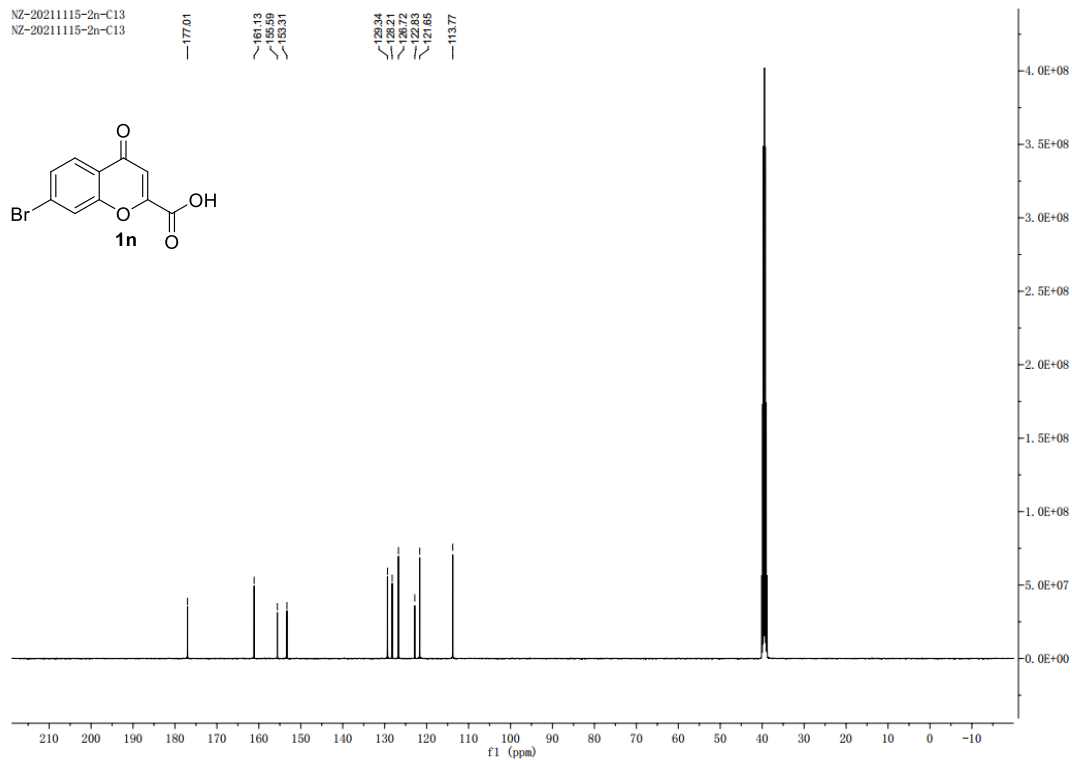
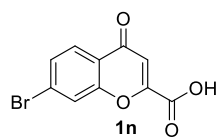


NZ-20210412-4-Br

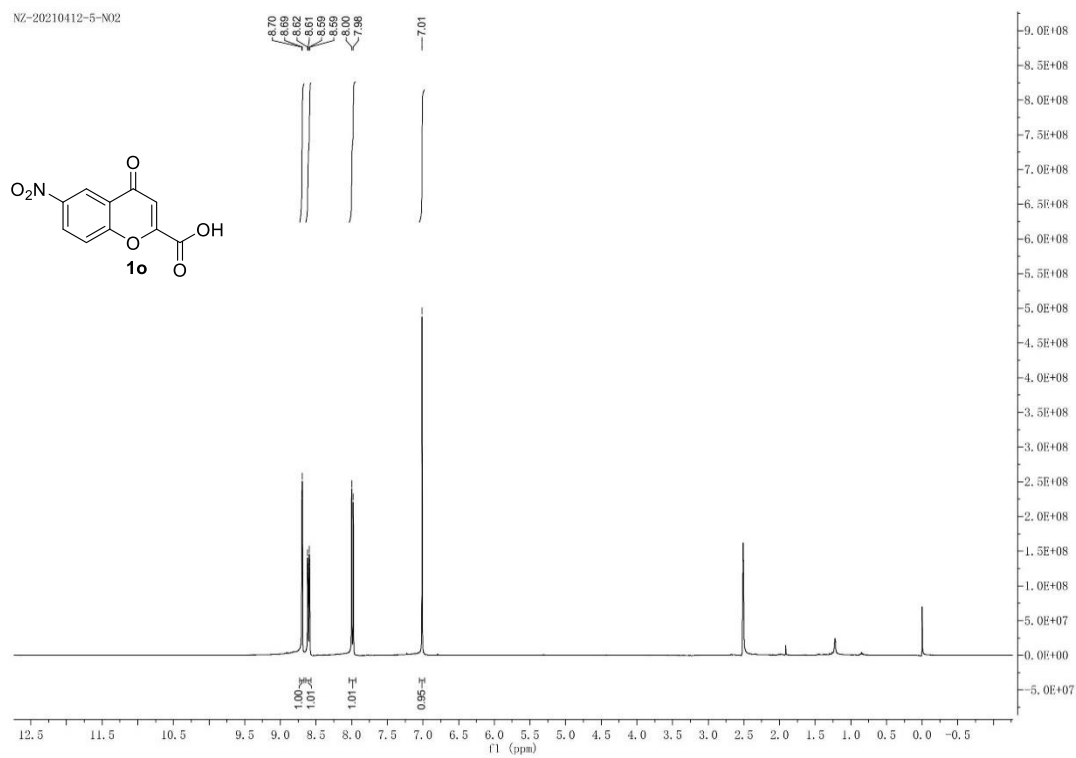
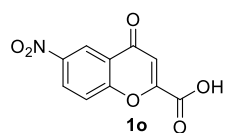
8.08
7.97
7.95
7.73
7.71
7.70
6.93



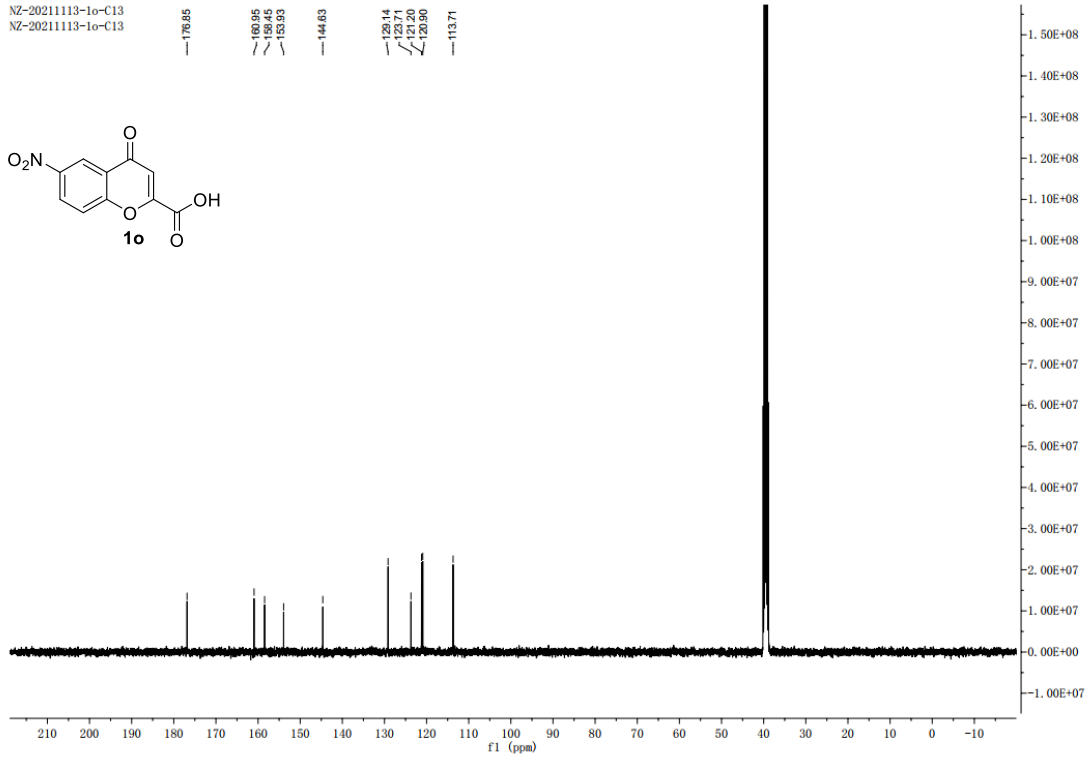
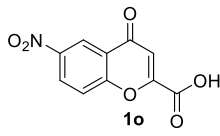
NZ-20211115-2n-C13
NZ-20211115-2n-C13



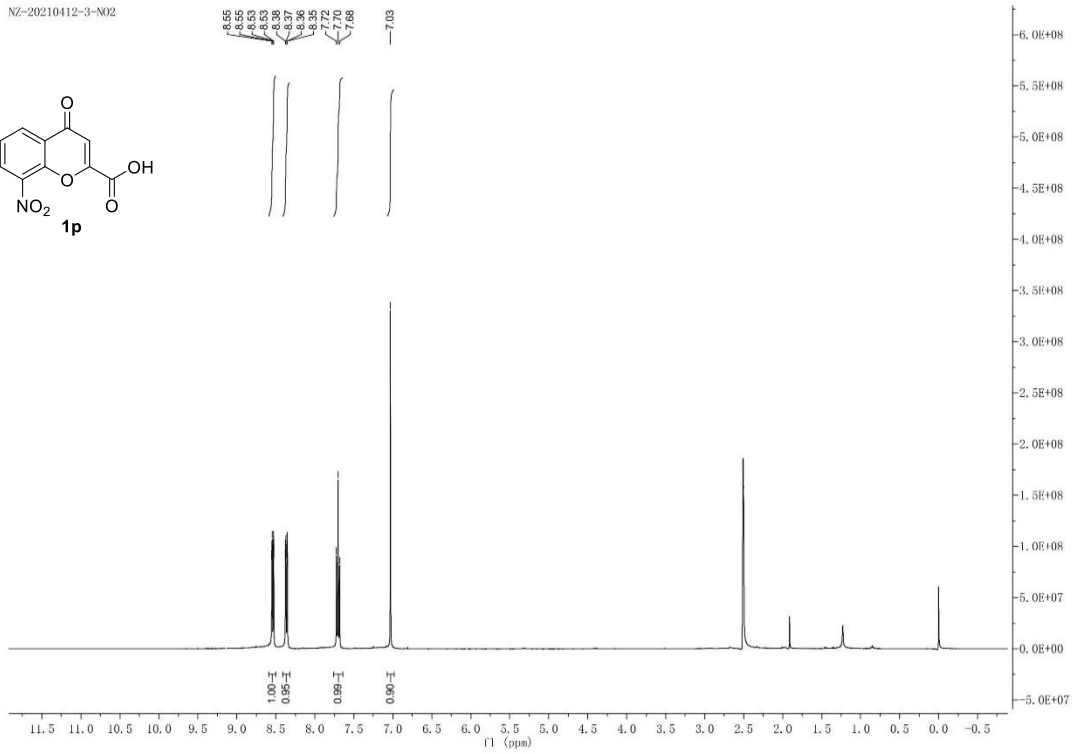
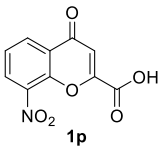
NZ-20210412-5-N02



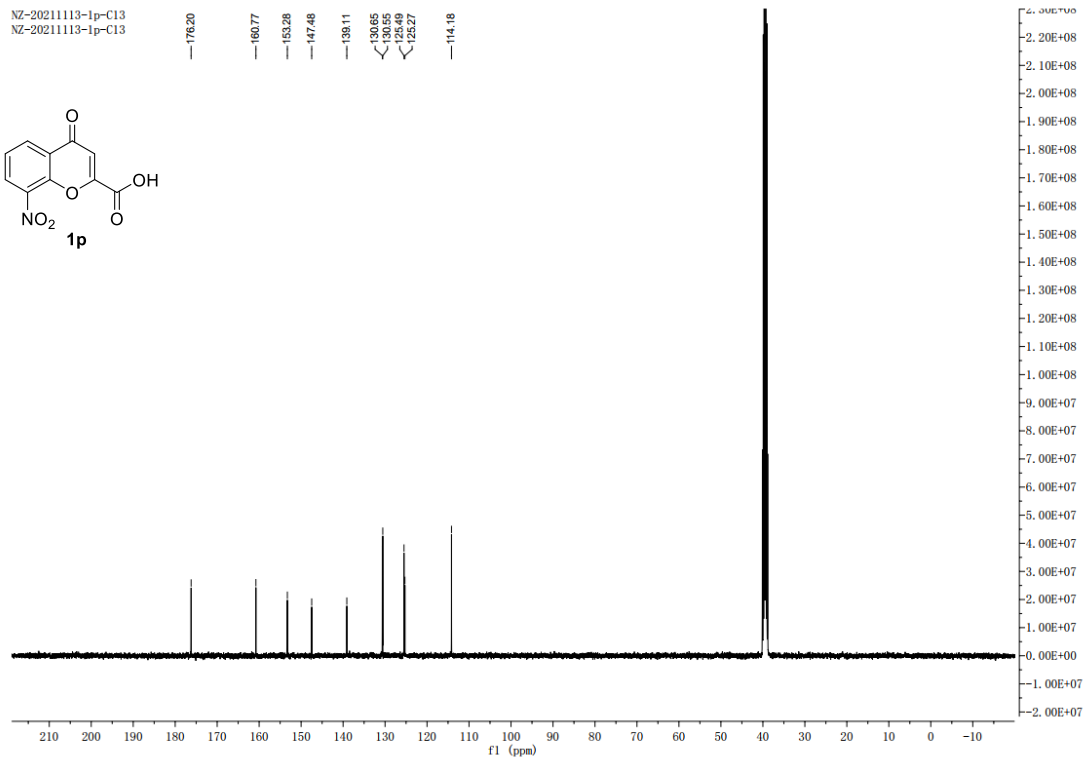
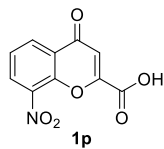
NZ-20211113-1o-C13
NZ-20211113-1o-C13



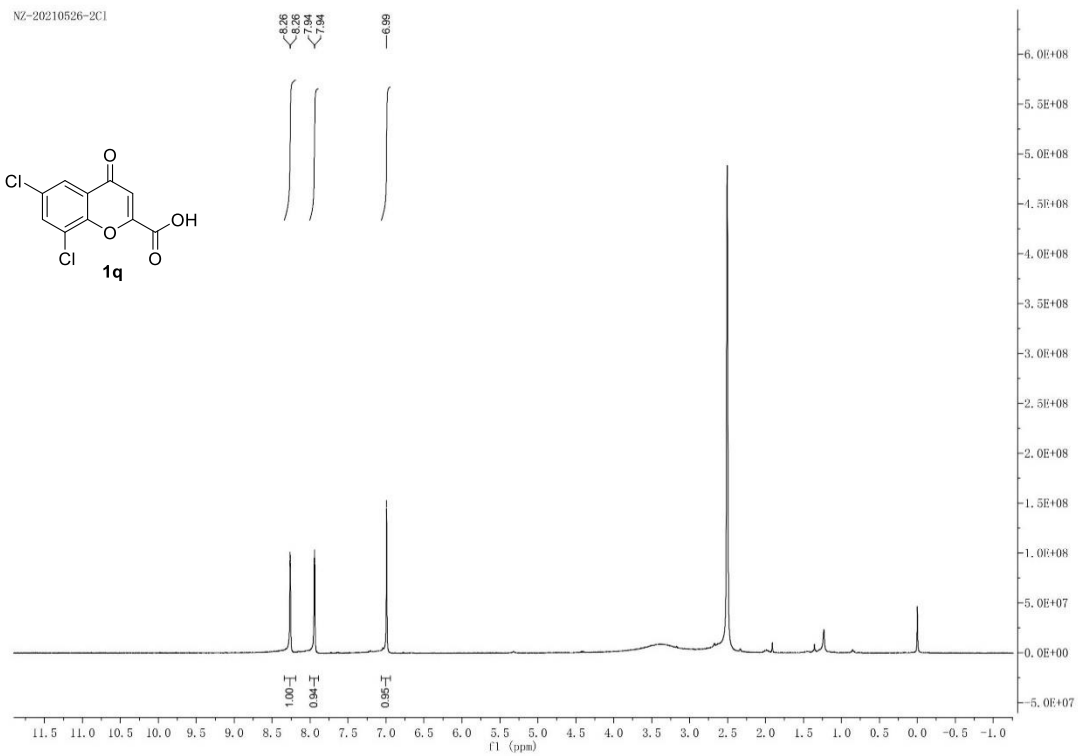
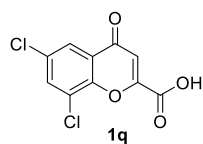
NZ-20210412-3-N02

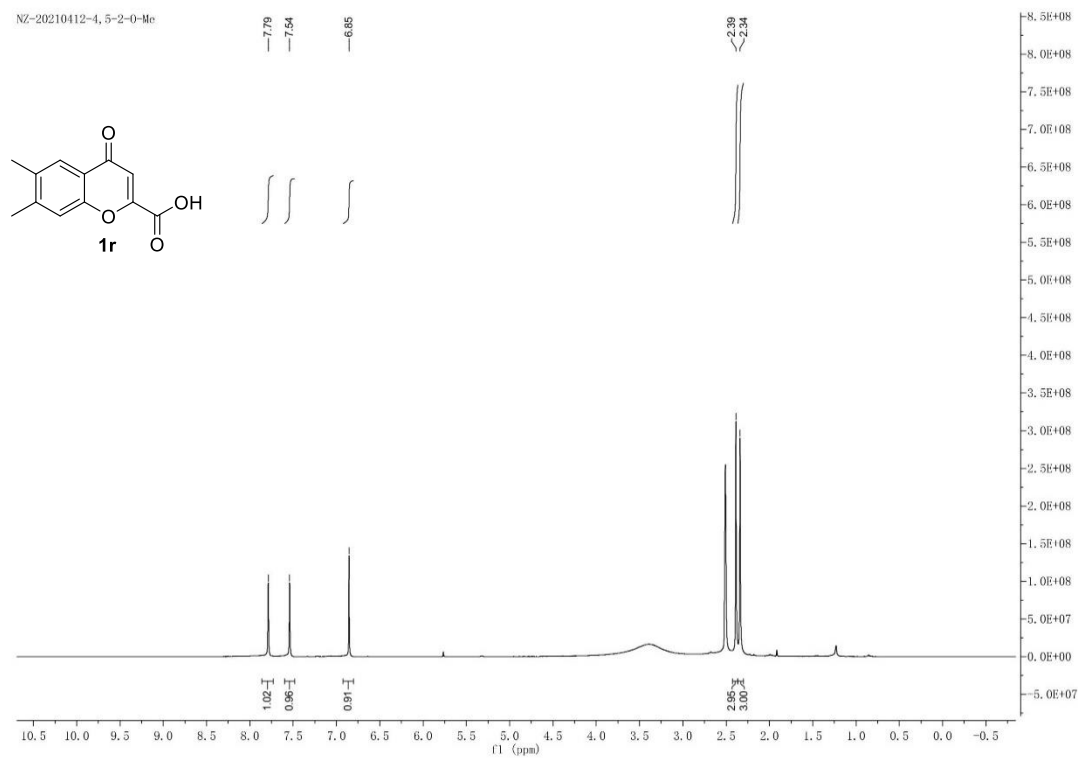
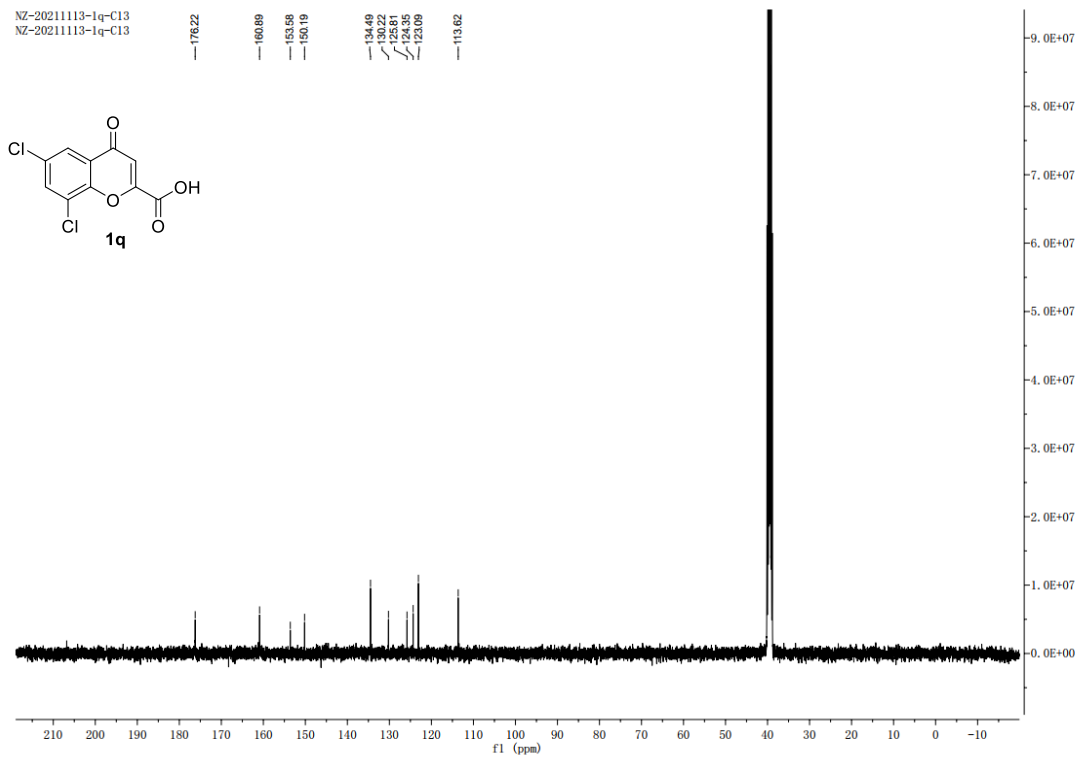


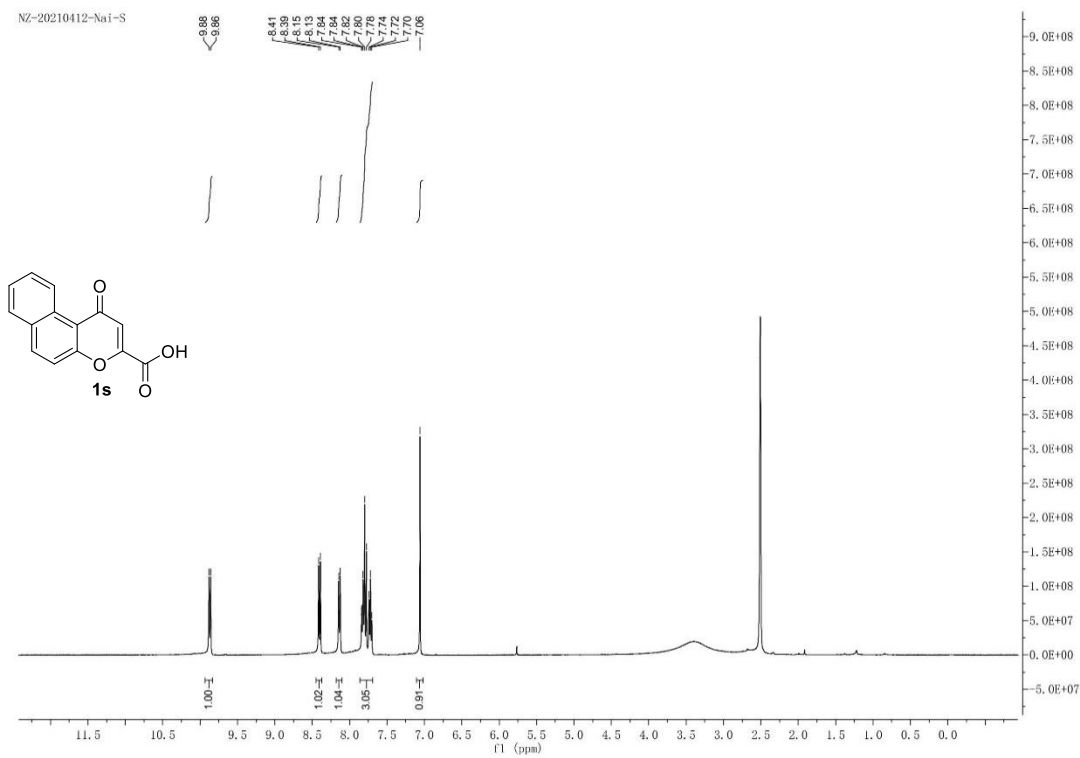
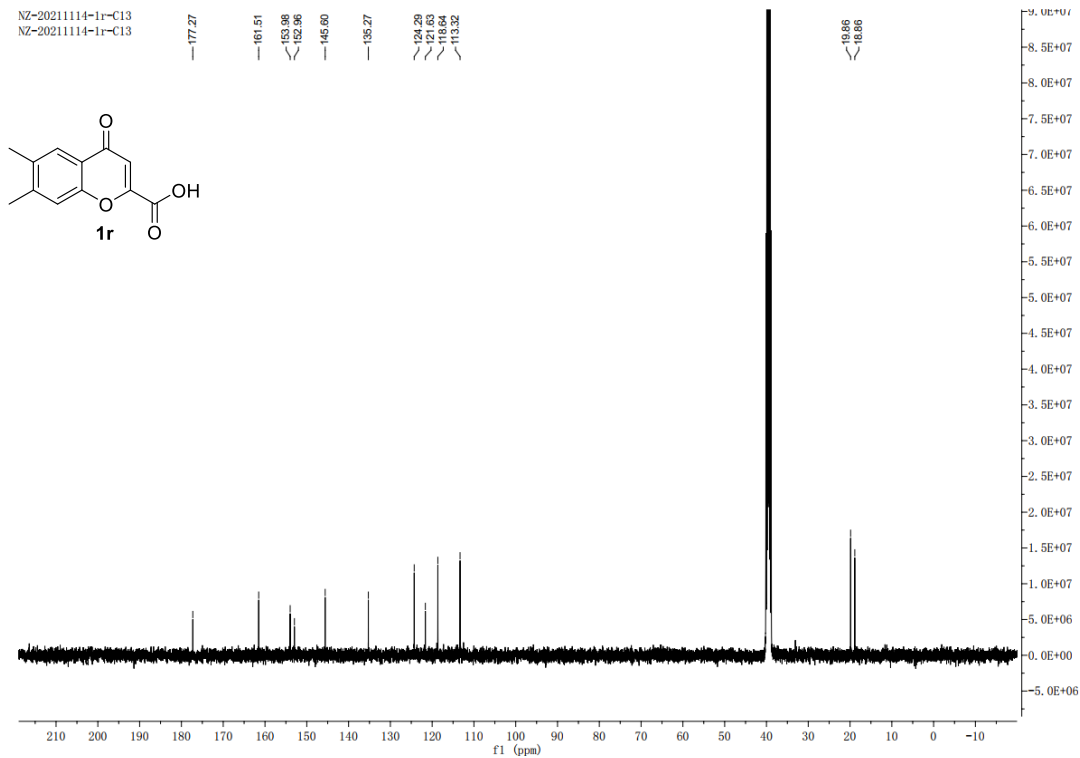
NZ-20211113-1p-C13
NZ-20211113-1p-C13



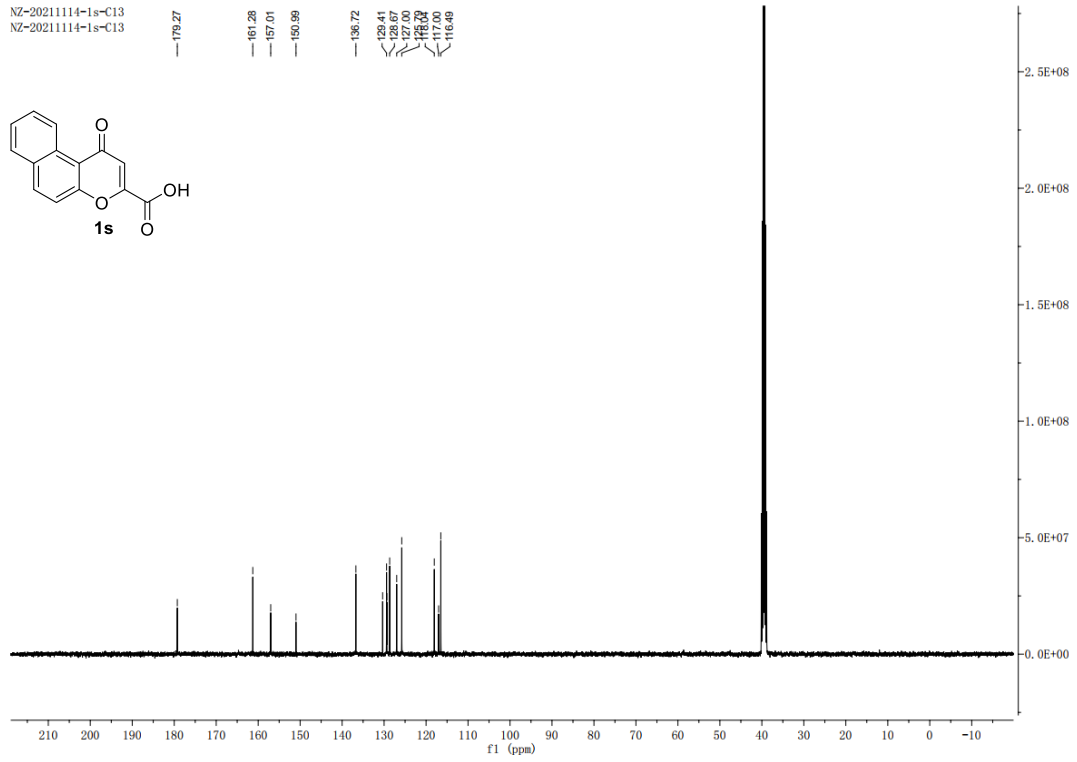
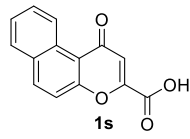
NZ-20210526-2Cl



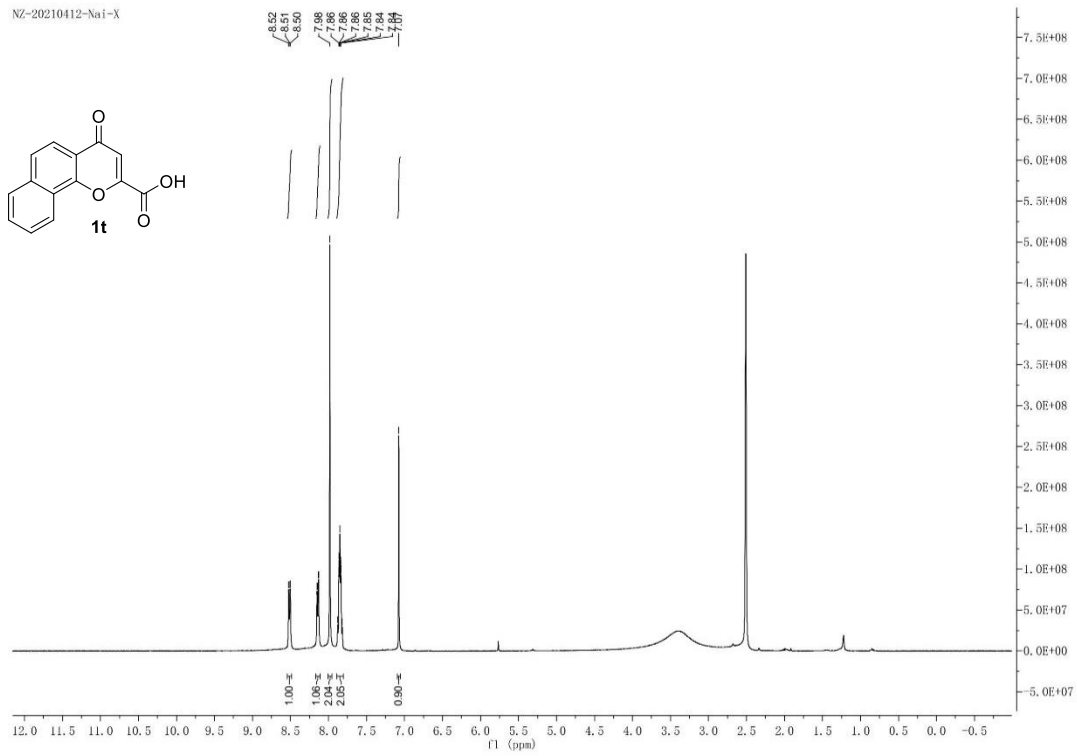
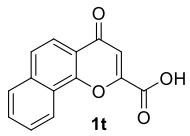




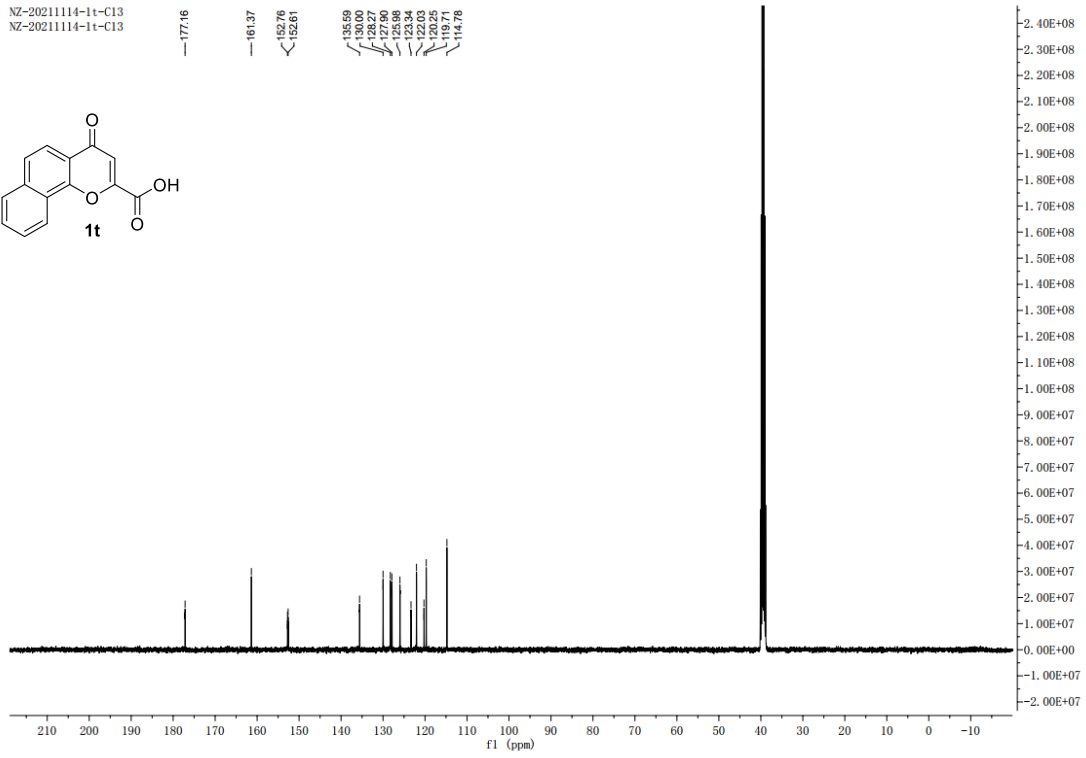
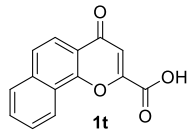
NZ-20211114-1s-C13
NZ-20211114-1s-C13



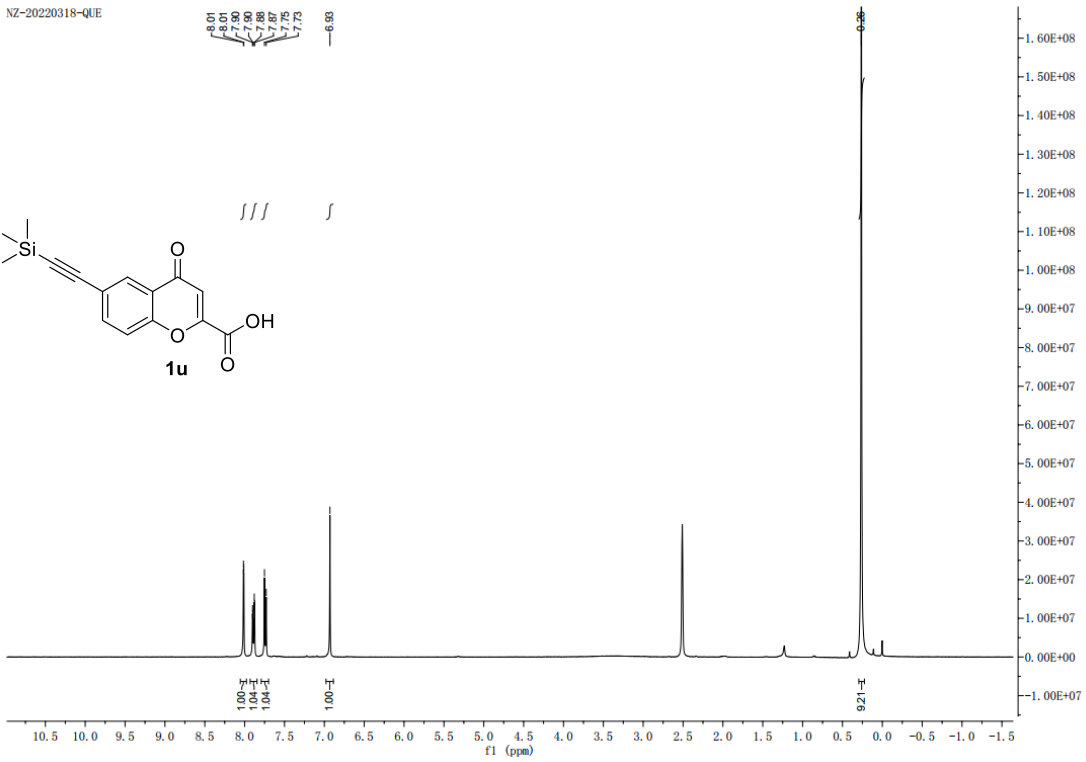
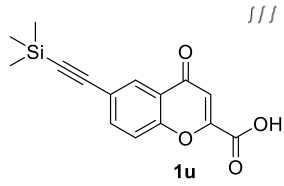
NZ-20210412-Nai-X

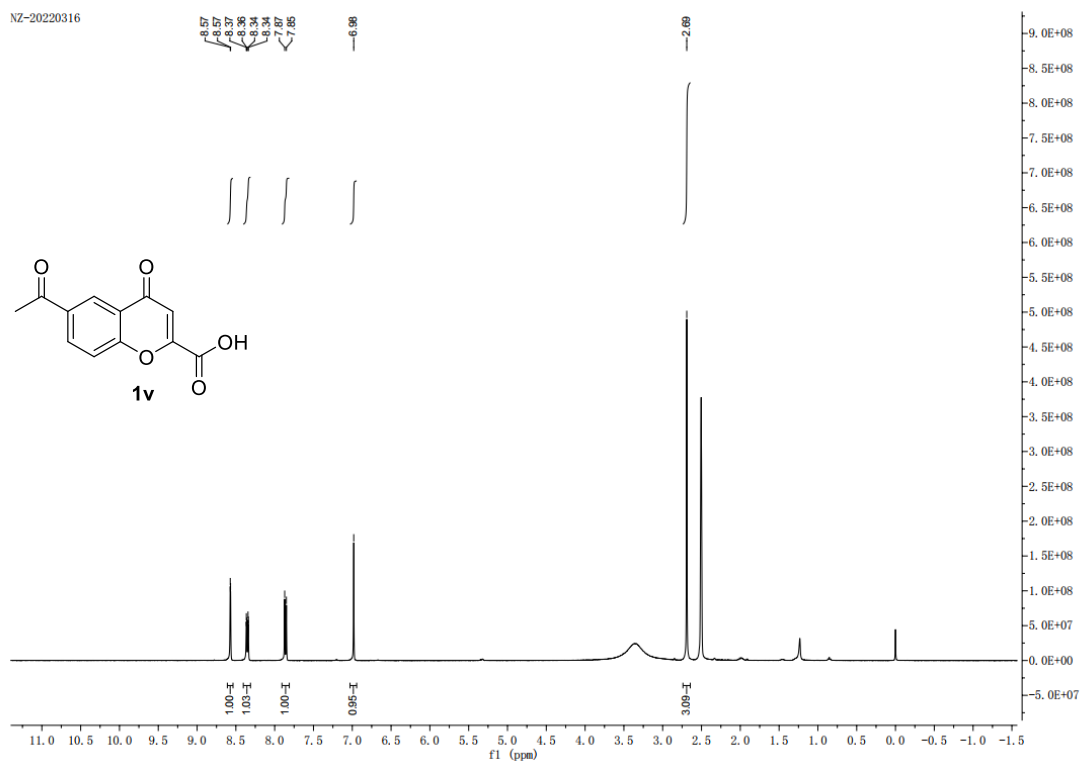
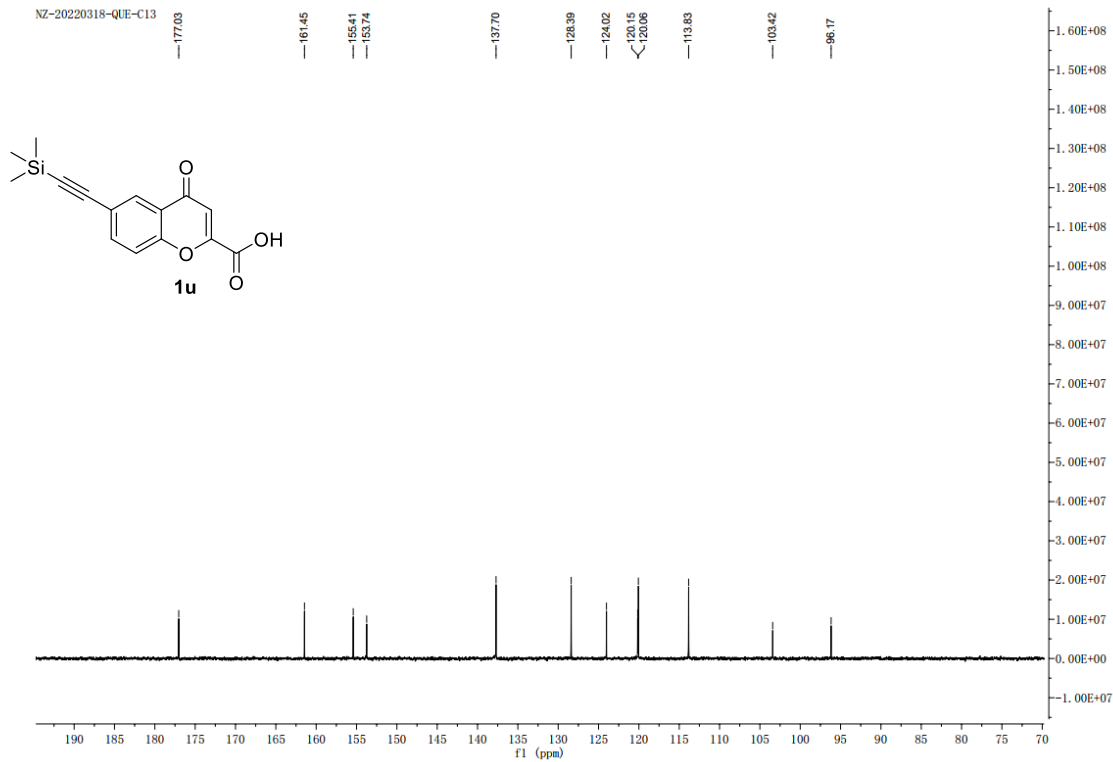


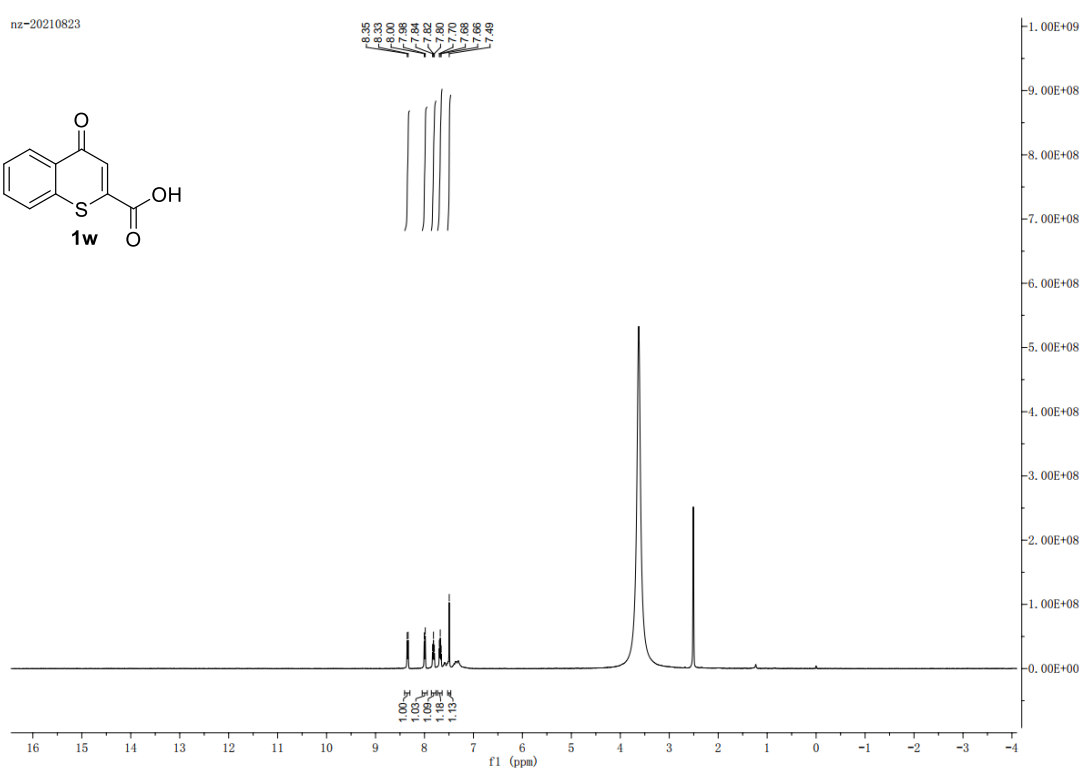
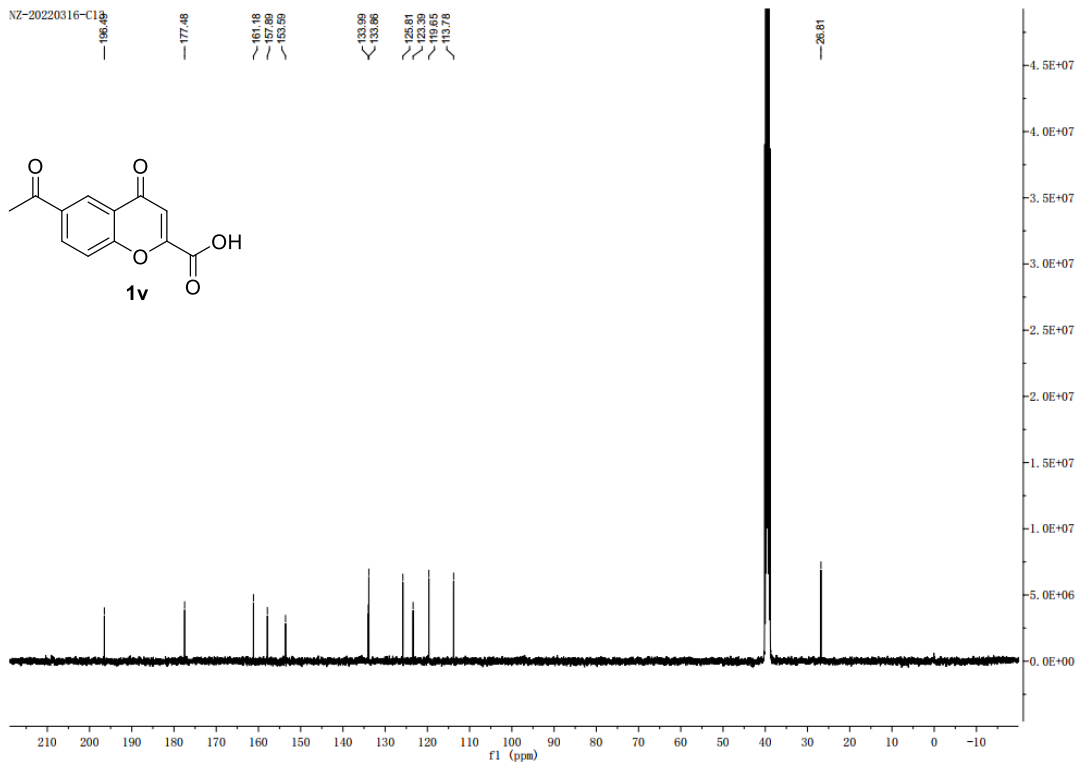
NZ-20211114-1t-C13
NZ-20211114-1t-C13

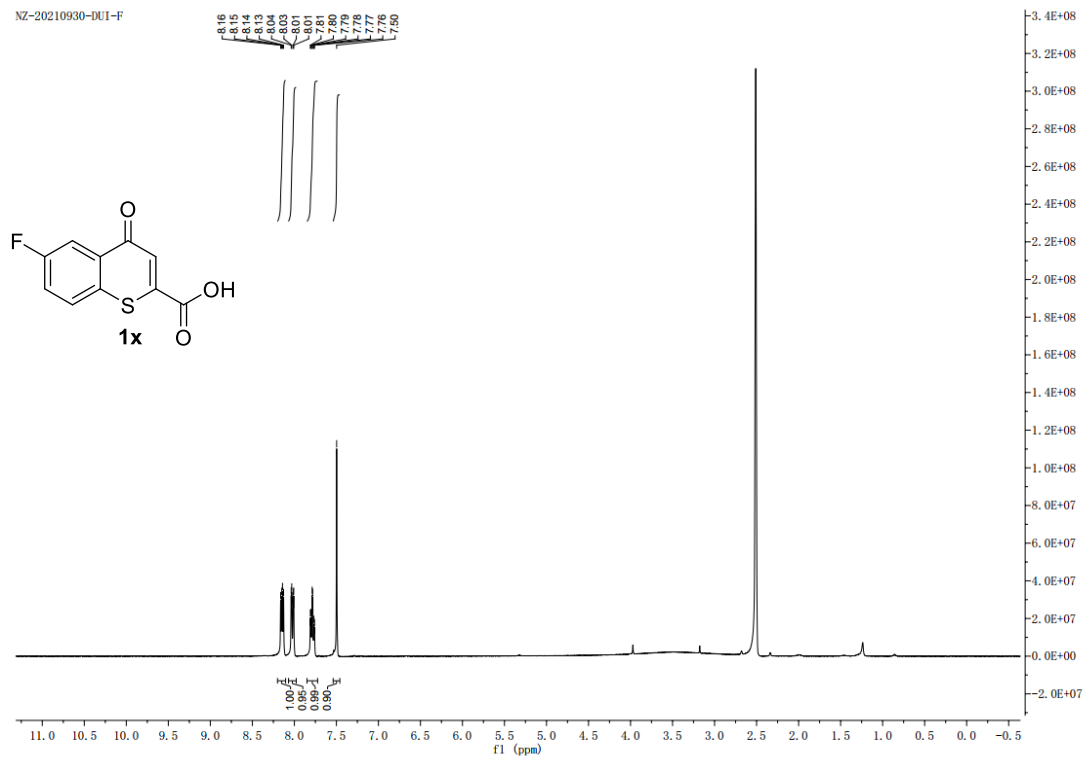
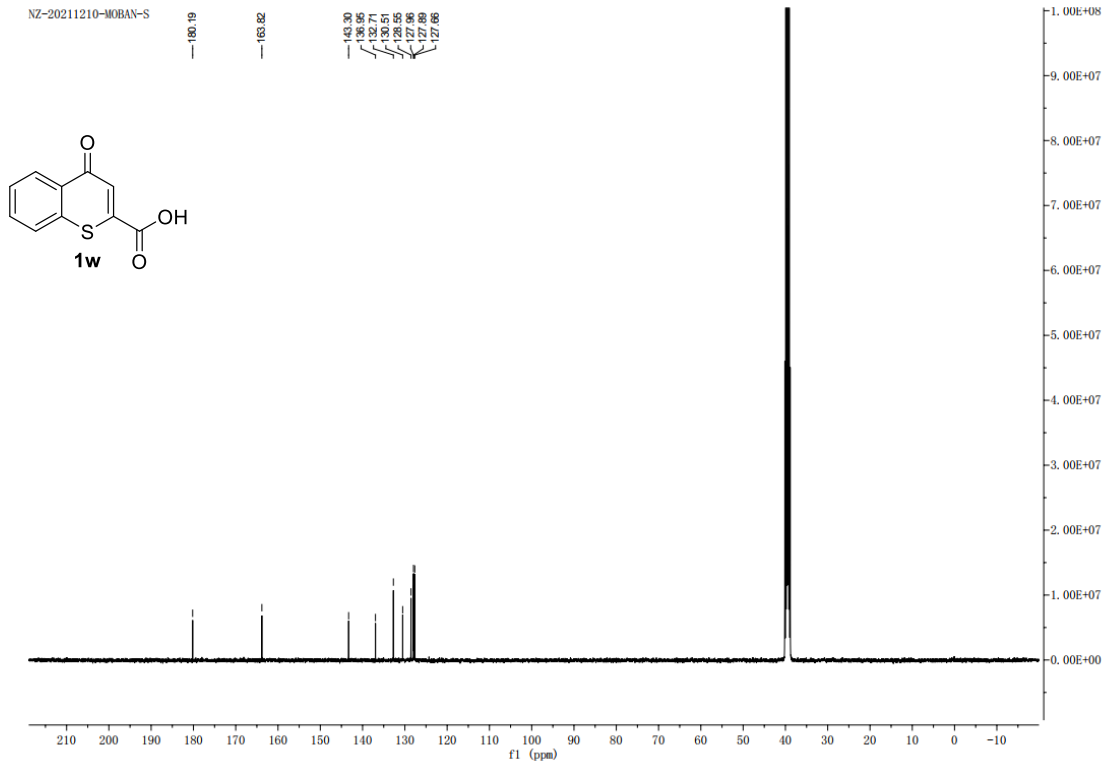


NZ-20220318-QUE

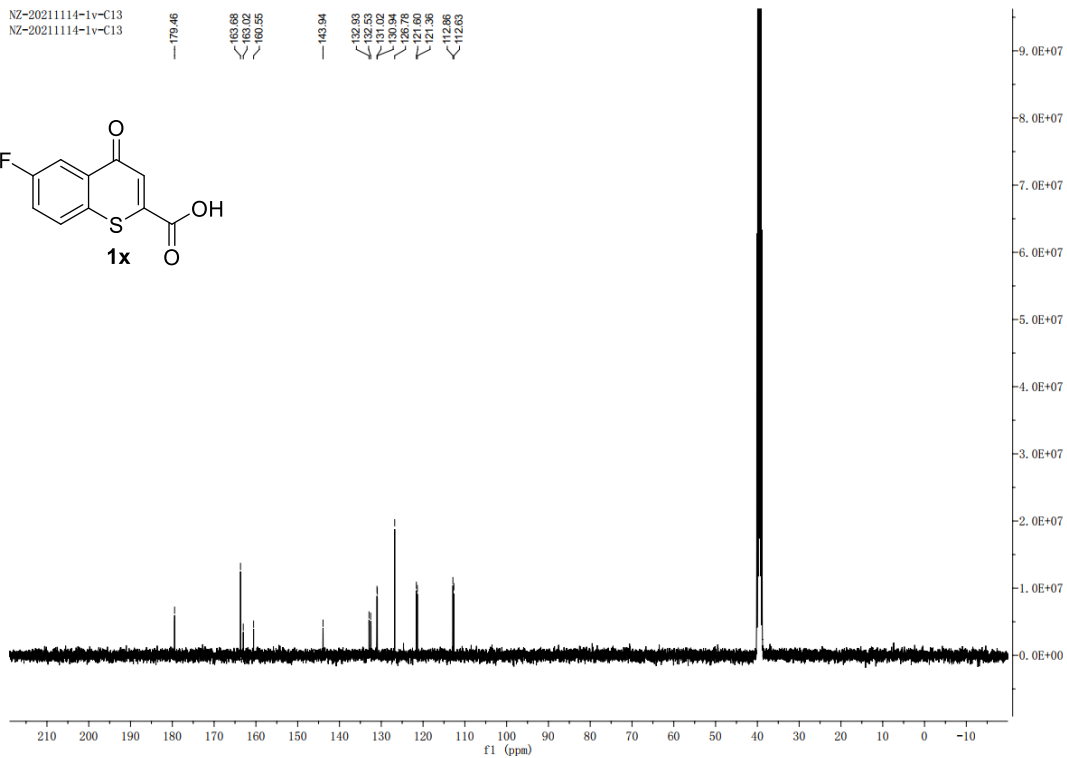
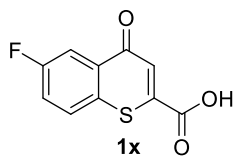




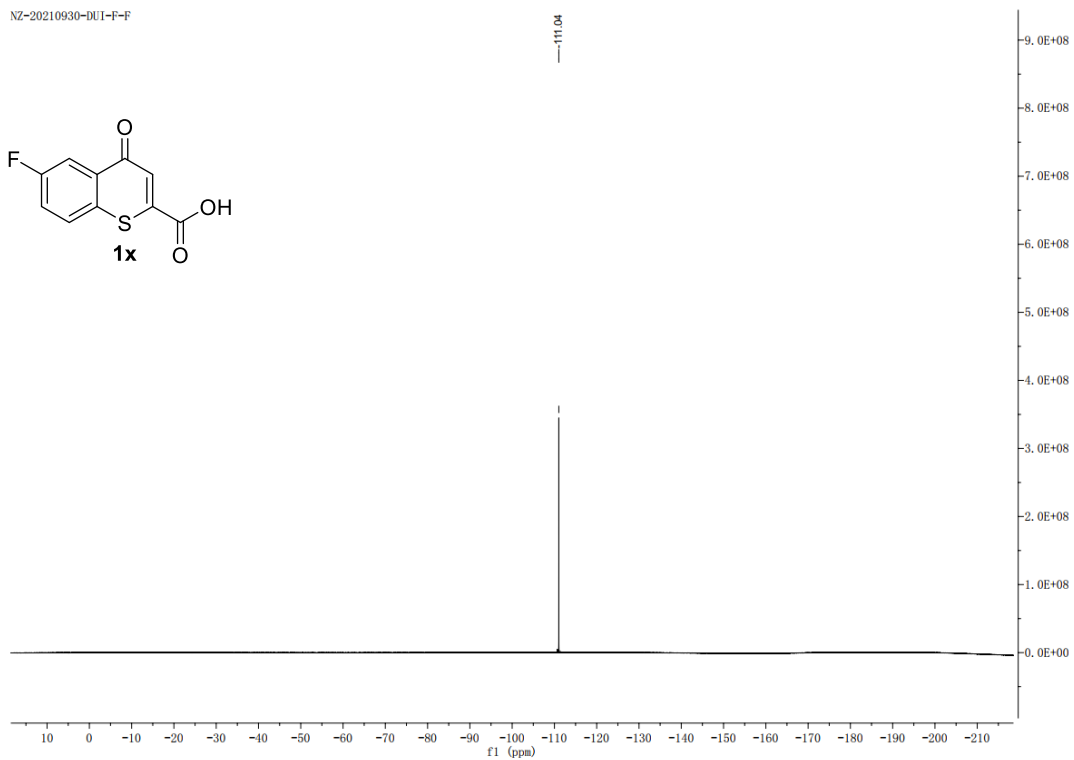
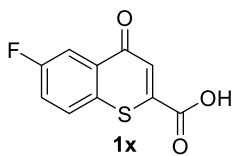




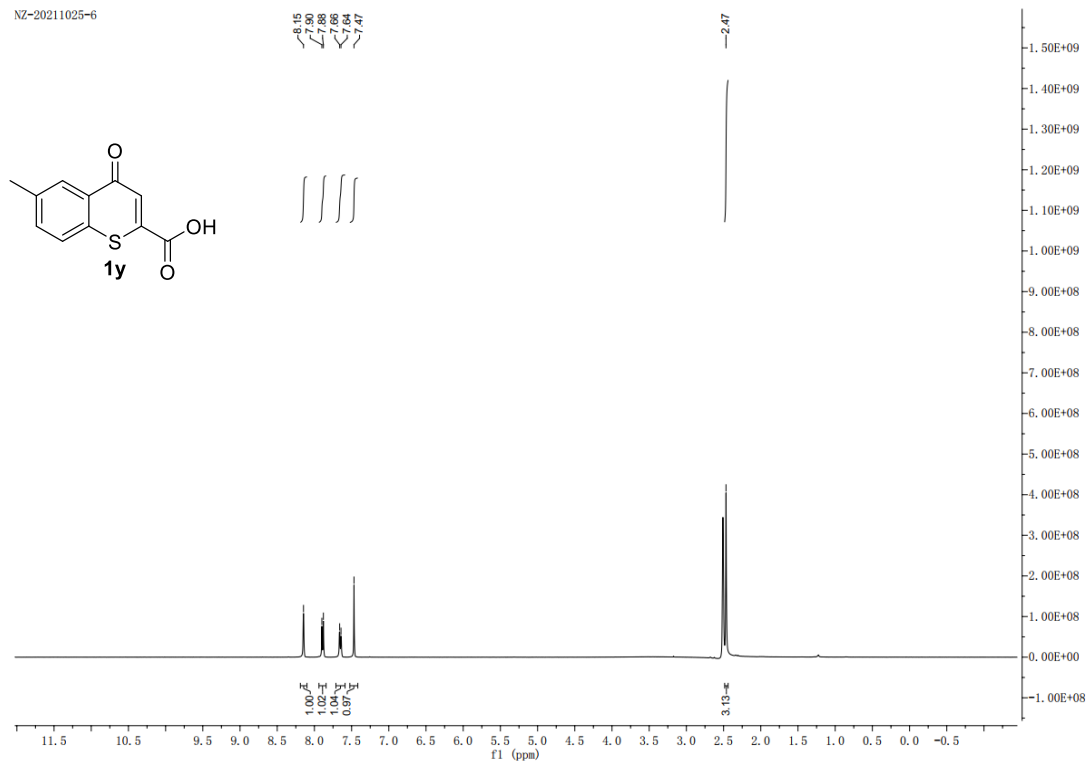
NZ-20211114-1v-C13
NZ-20211114-1v-C13



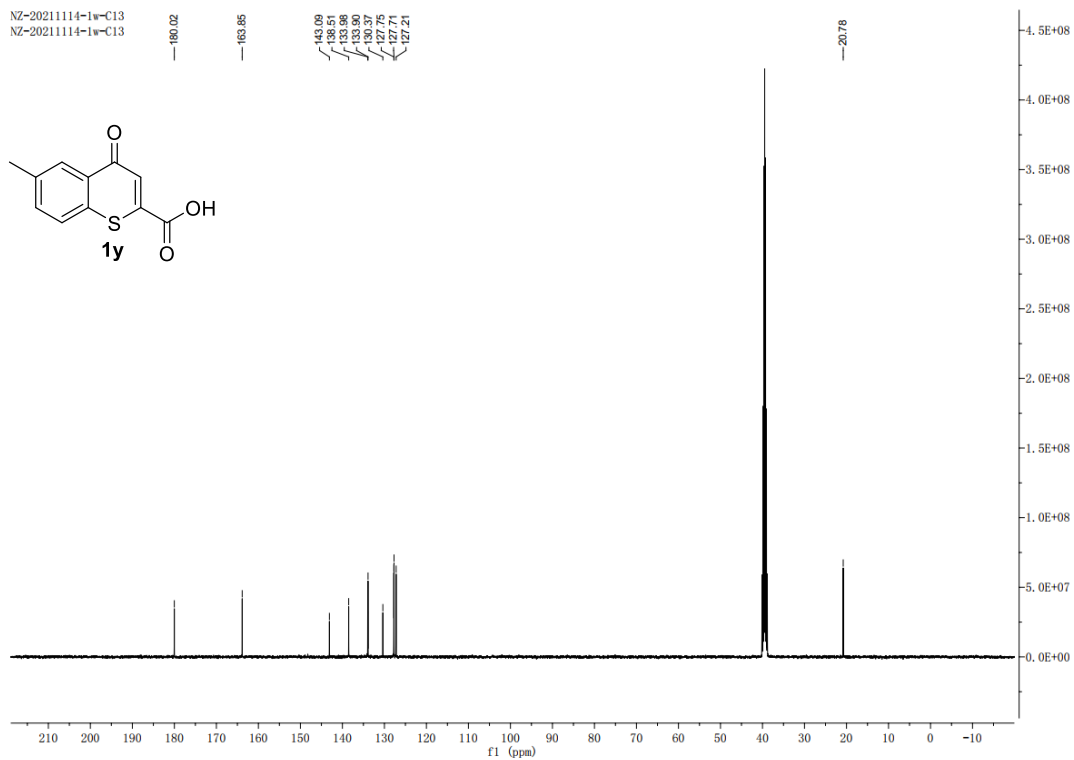
NZ-20210930-DUI-F-F



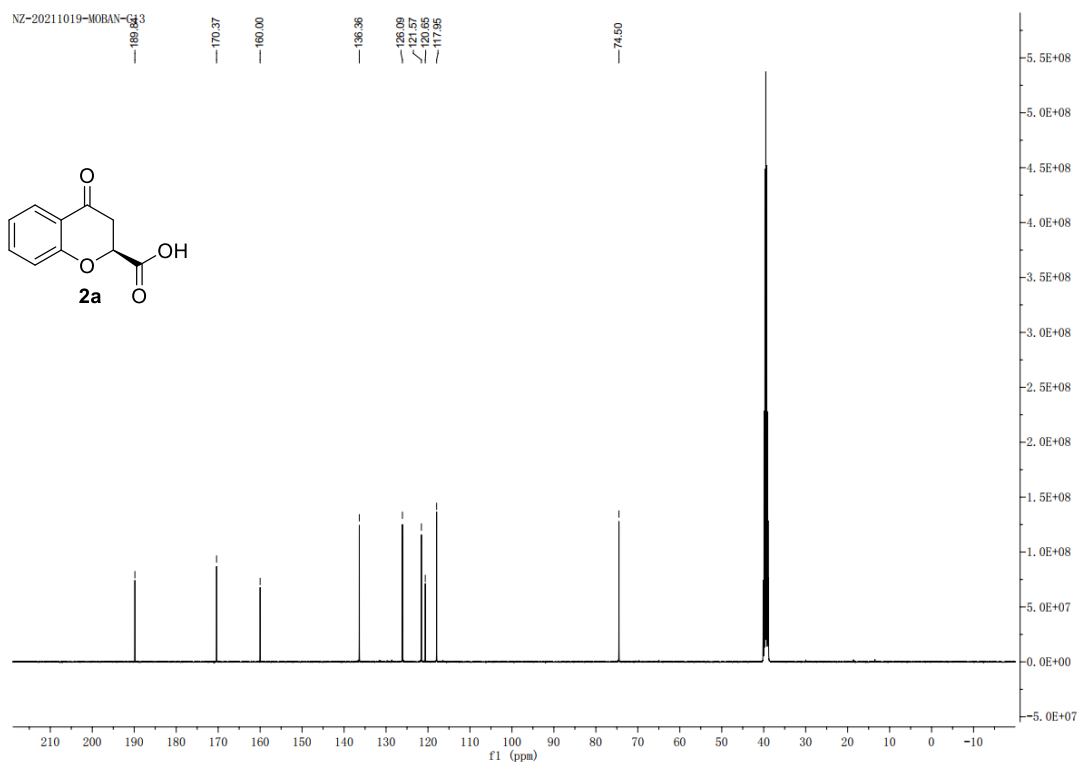
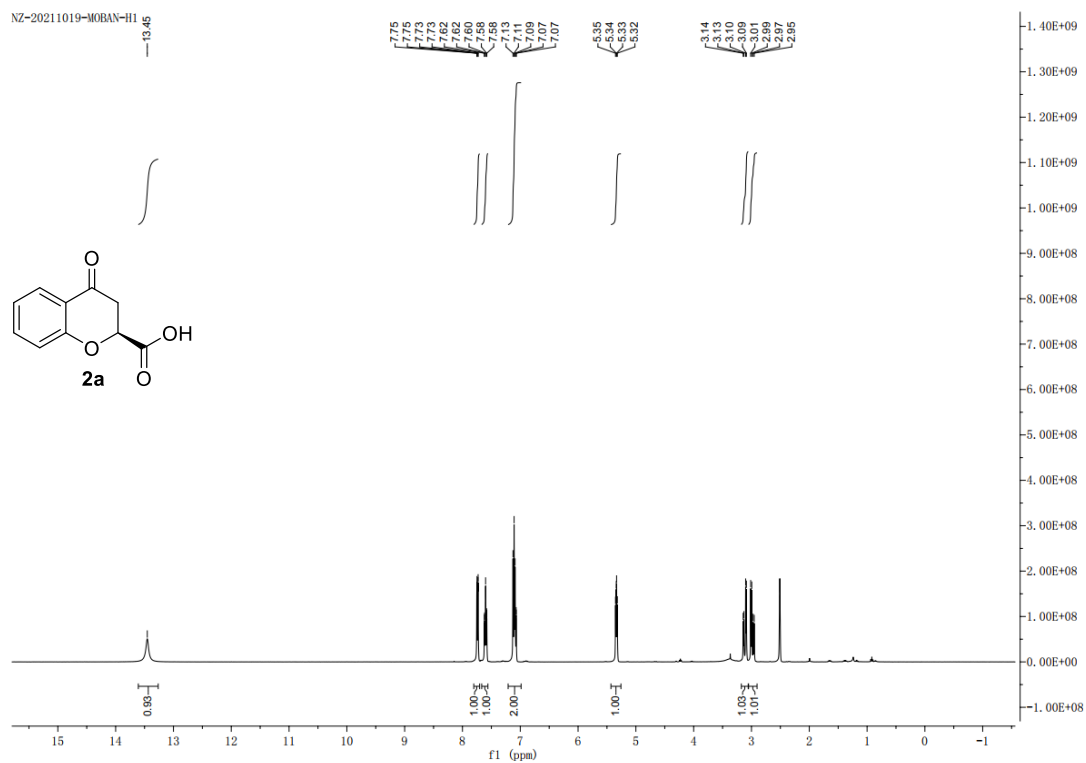
NZ-20211025-6

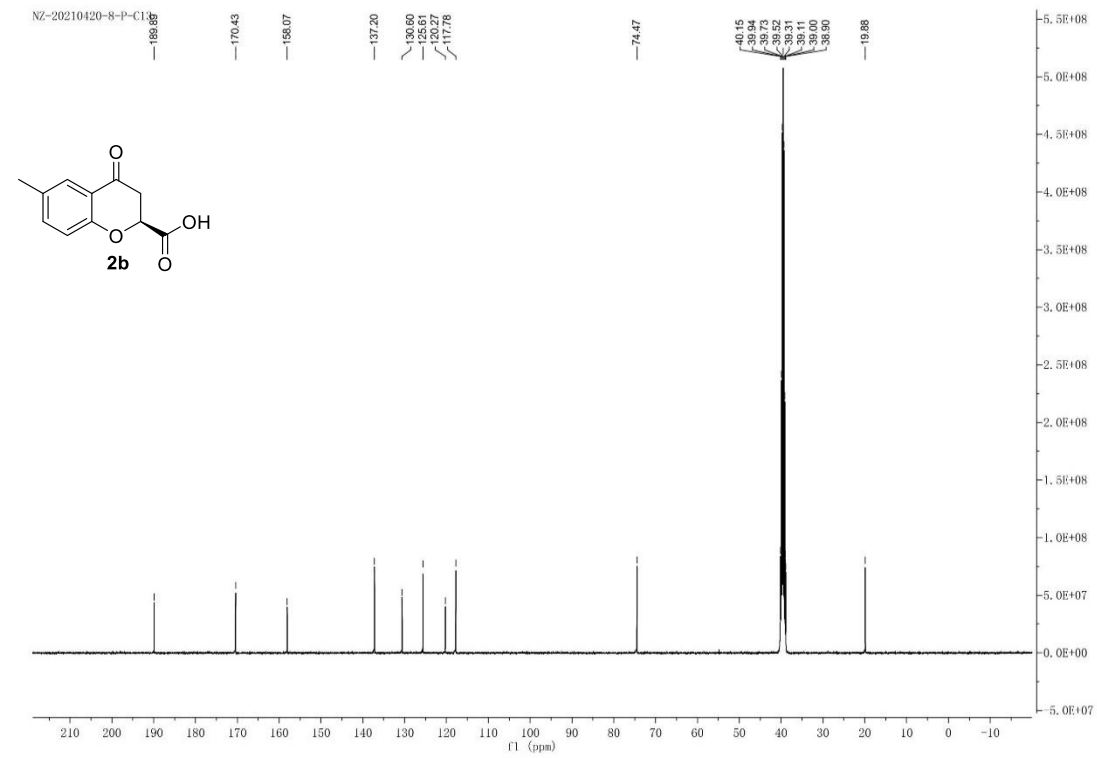
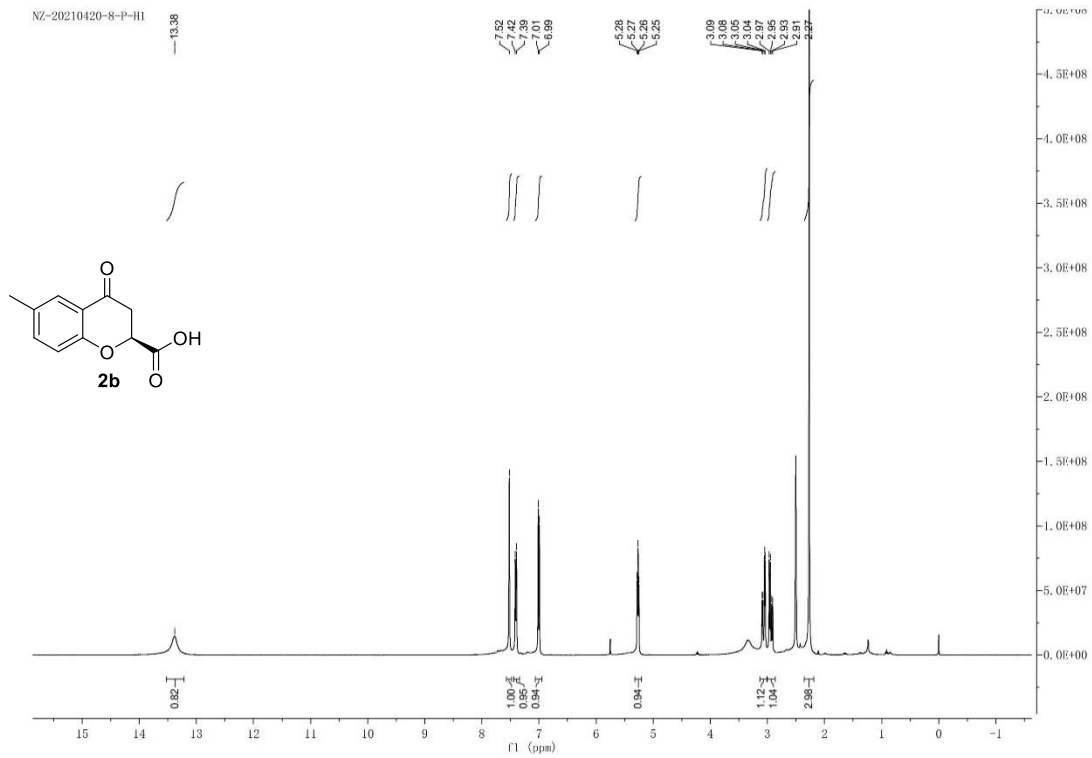


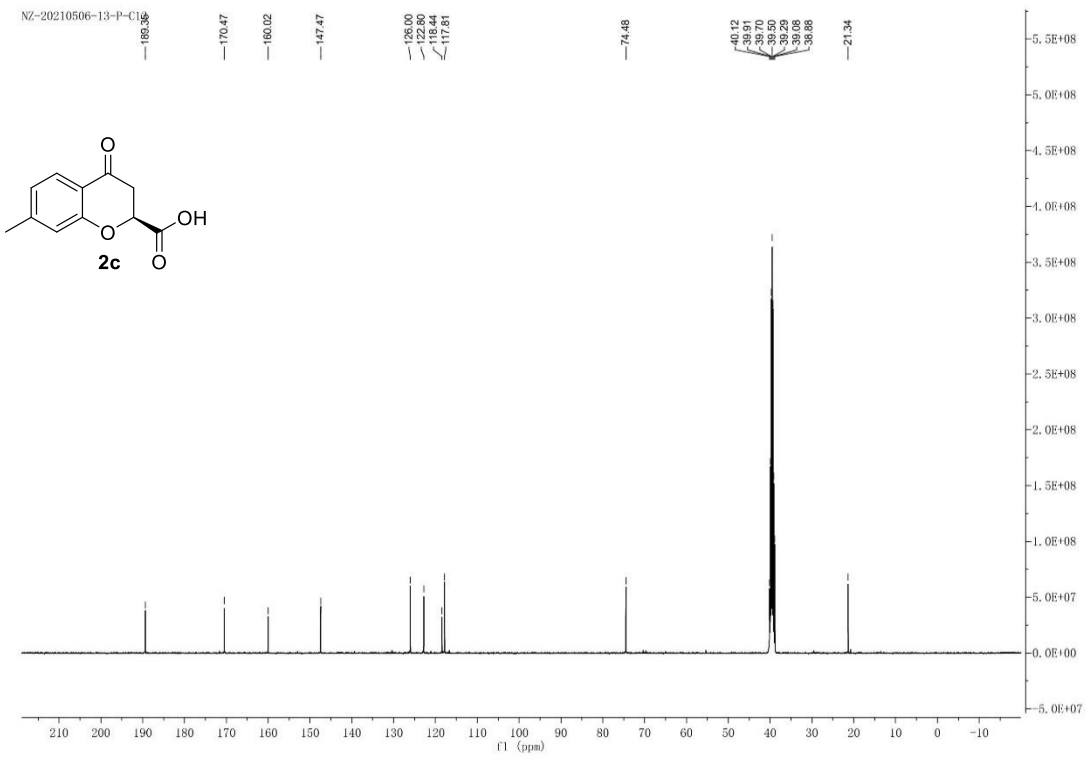
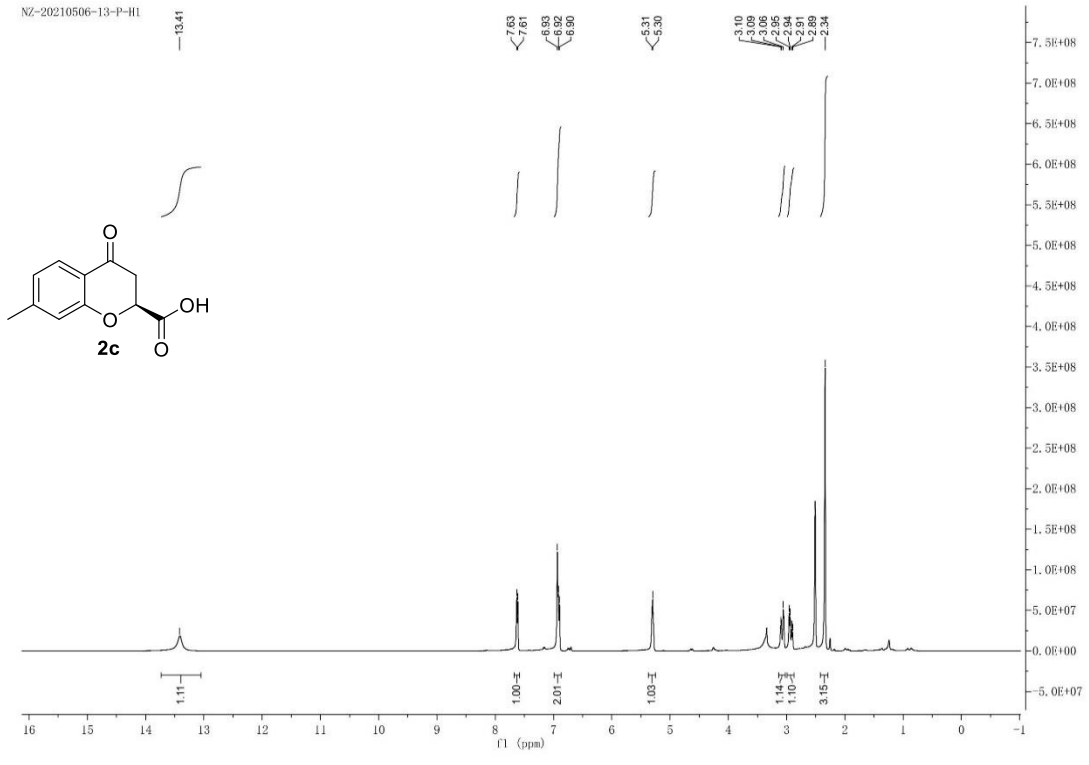
NZ-20211114-1w-C13
NZ-20211114-1w-C13

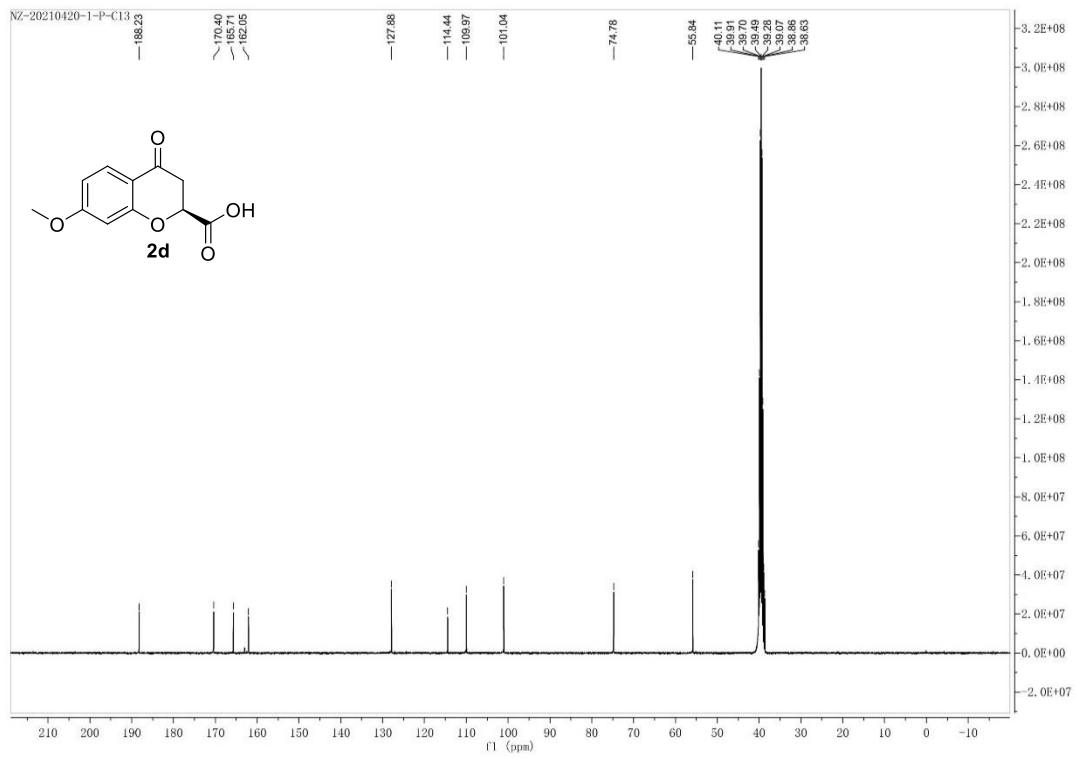
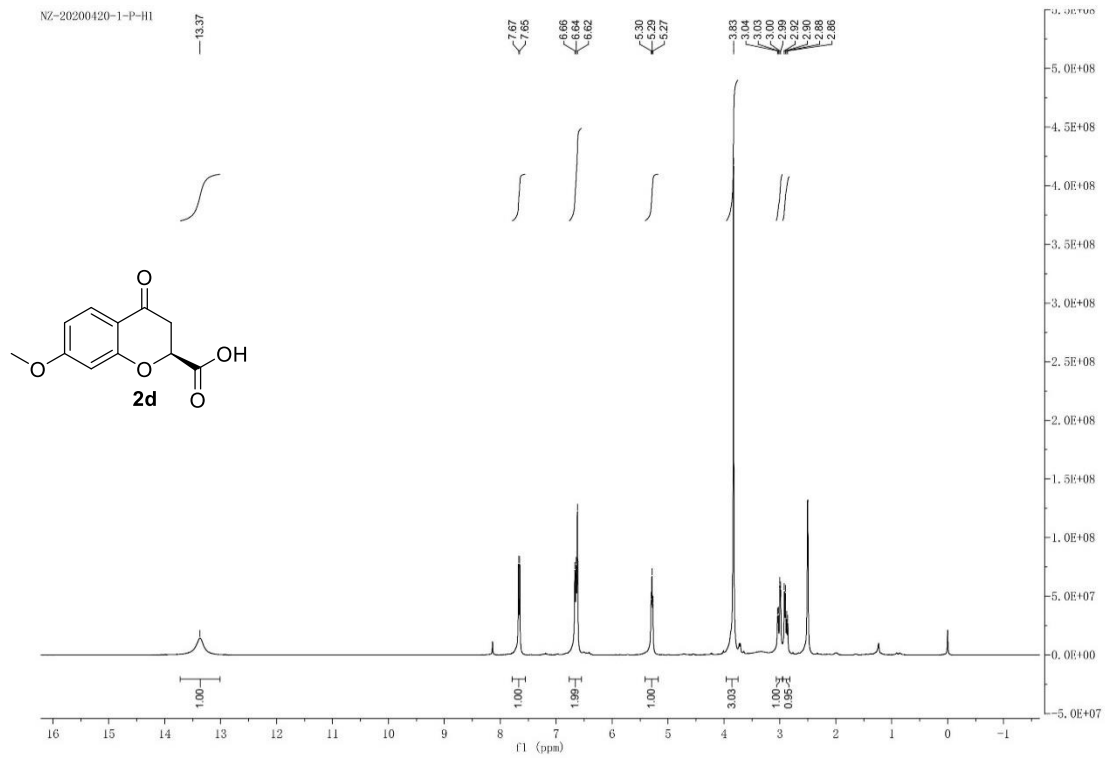


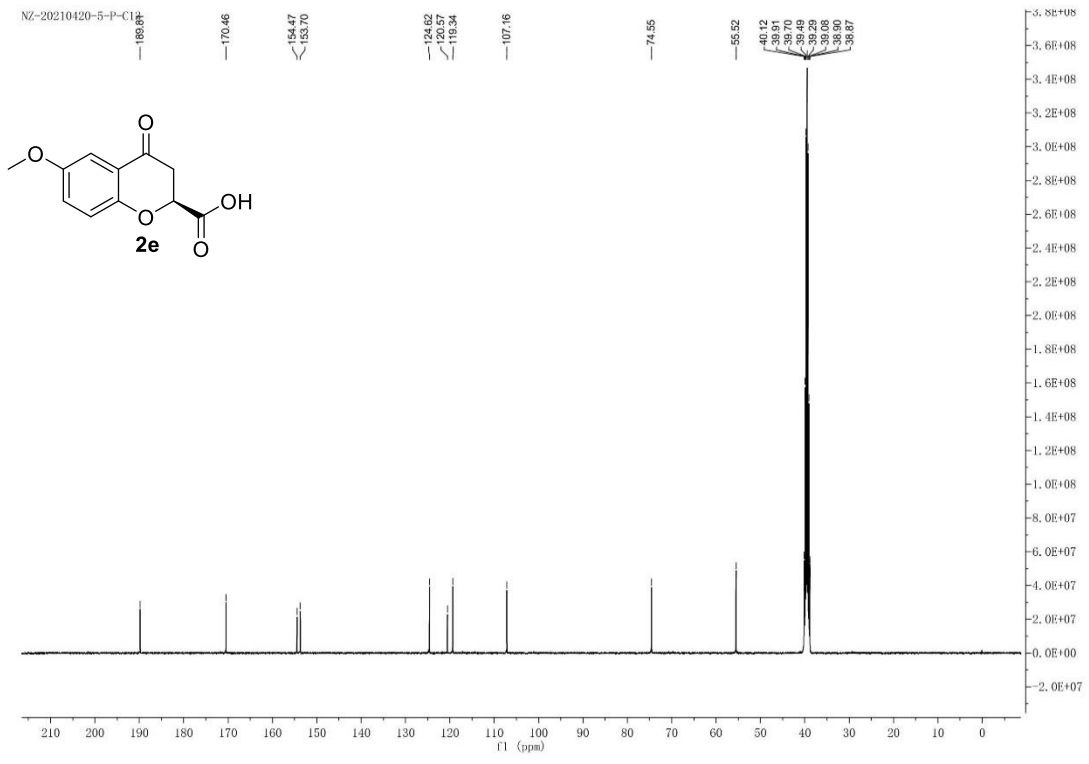
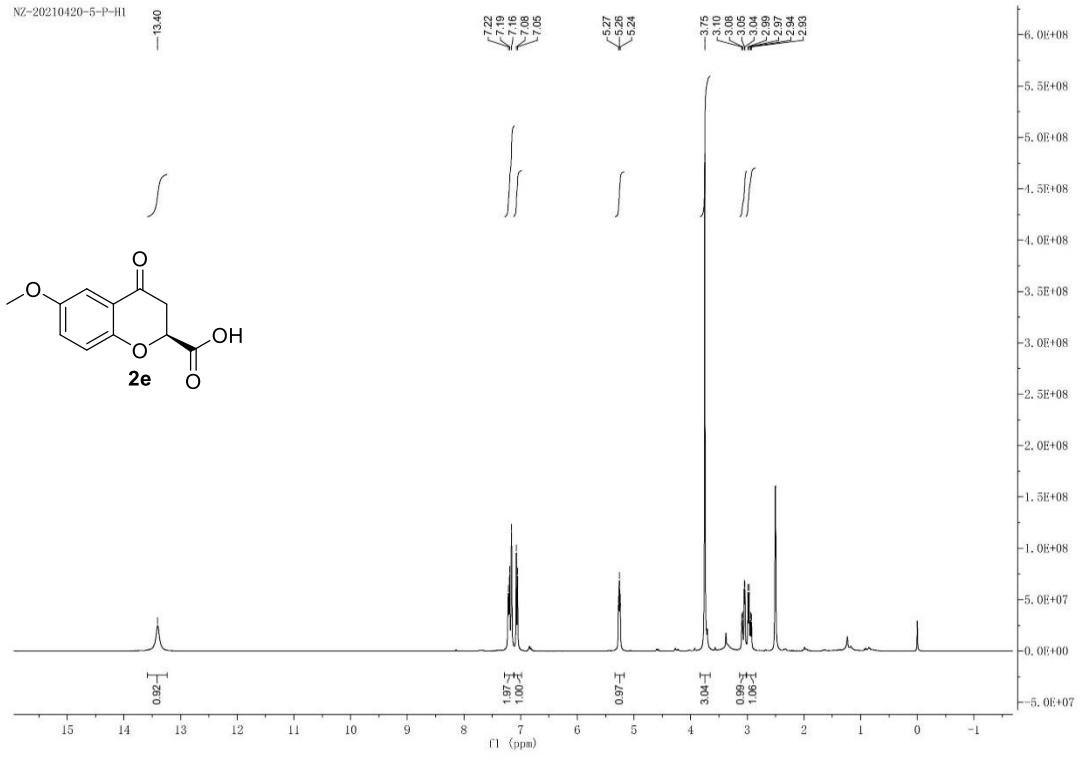
8.2 NMR Spectra of the chiral products



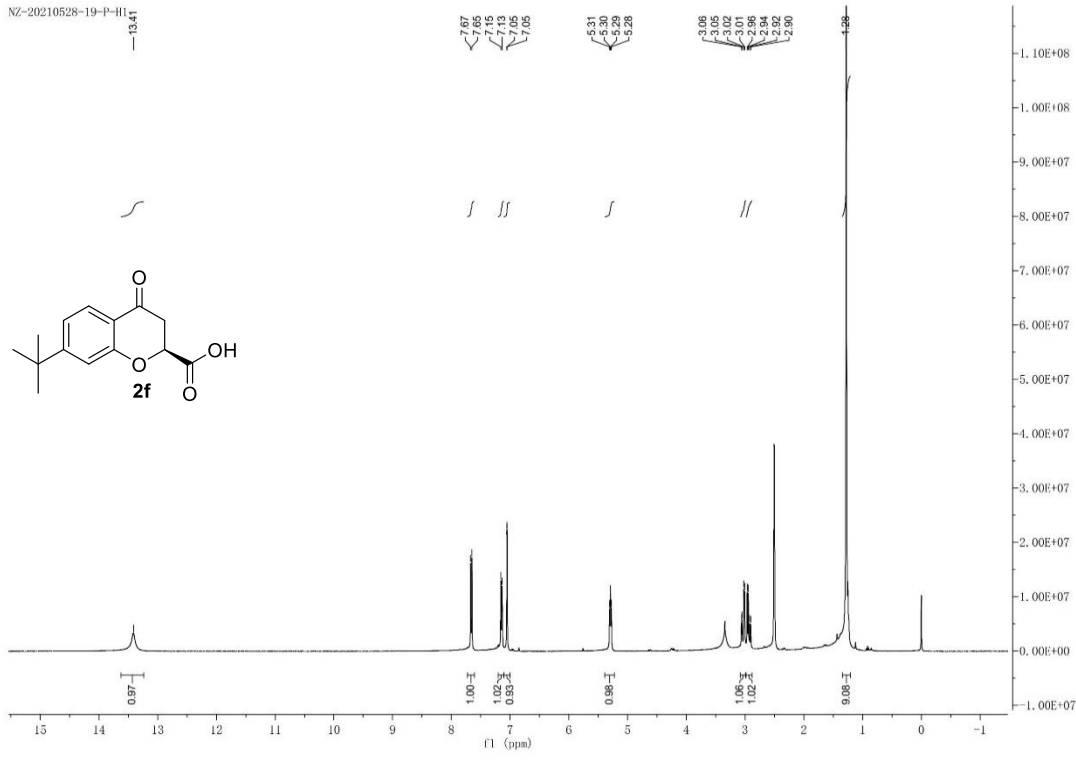
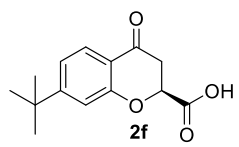




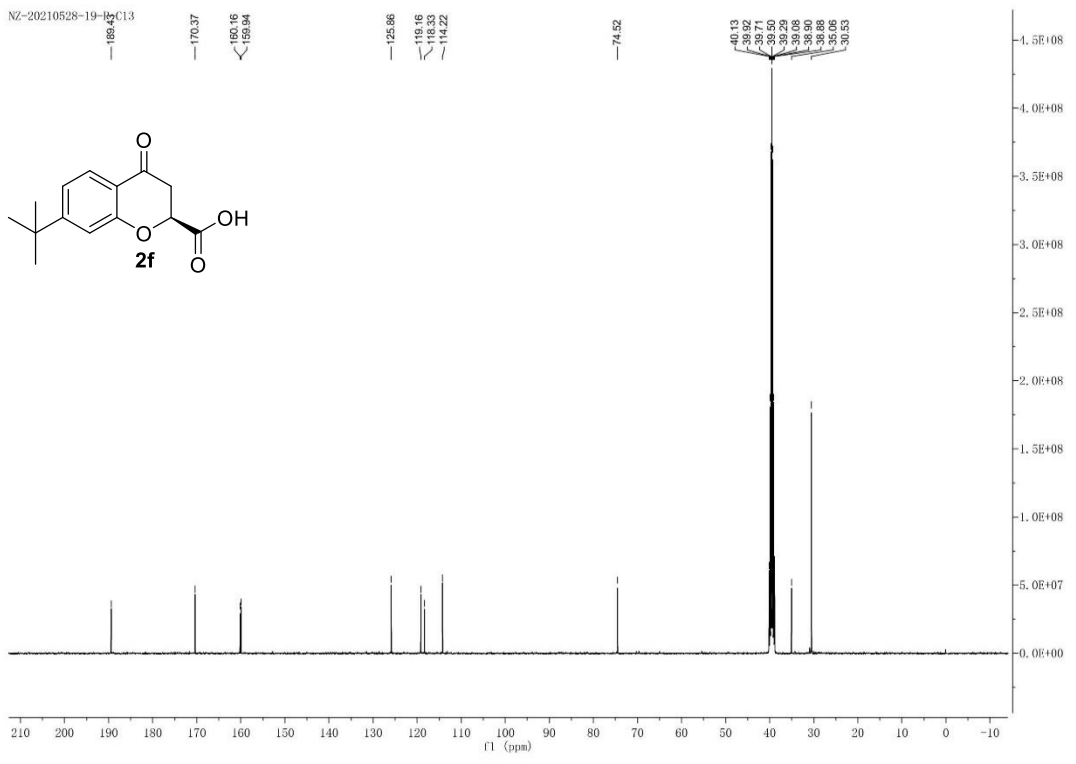
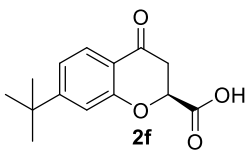




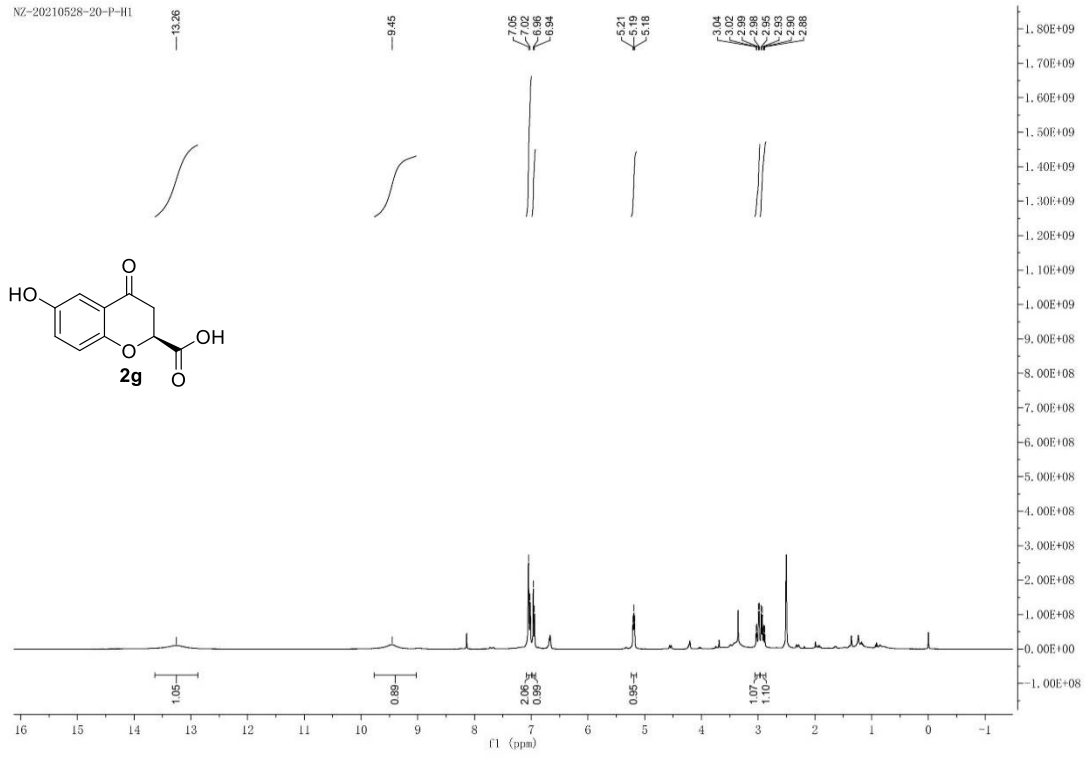
NZ-20210528-19-P-H1
-13.41



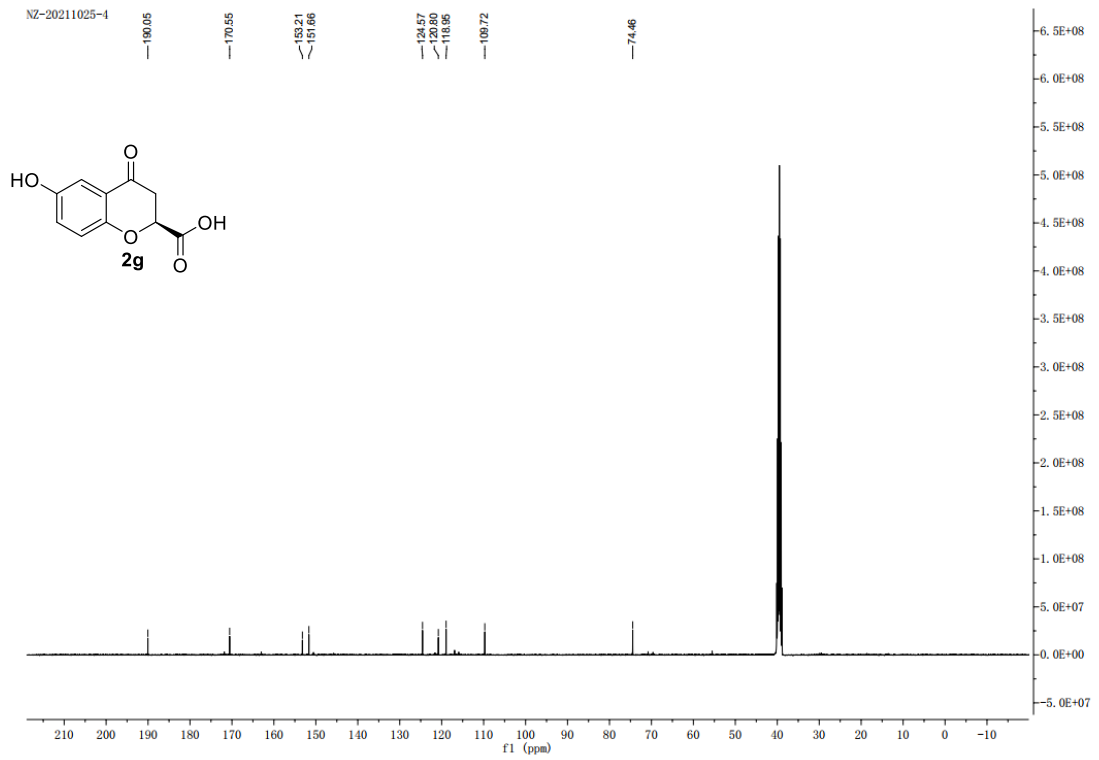
NZ-20210528-19-C13
-189.45

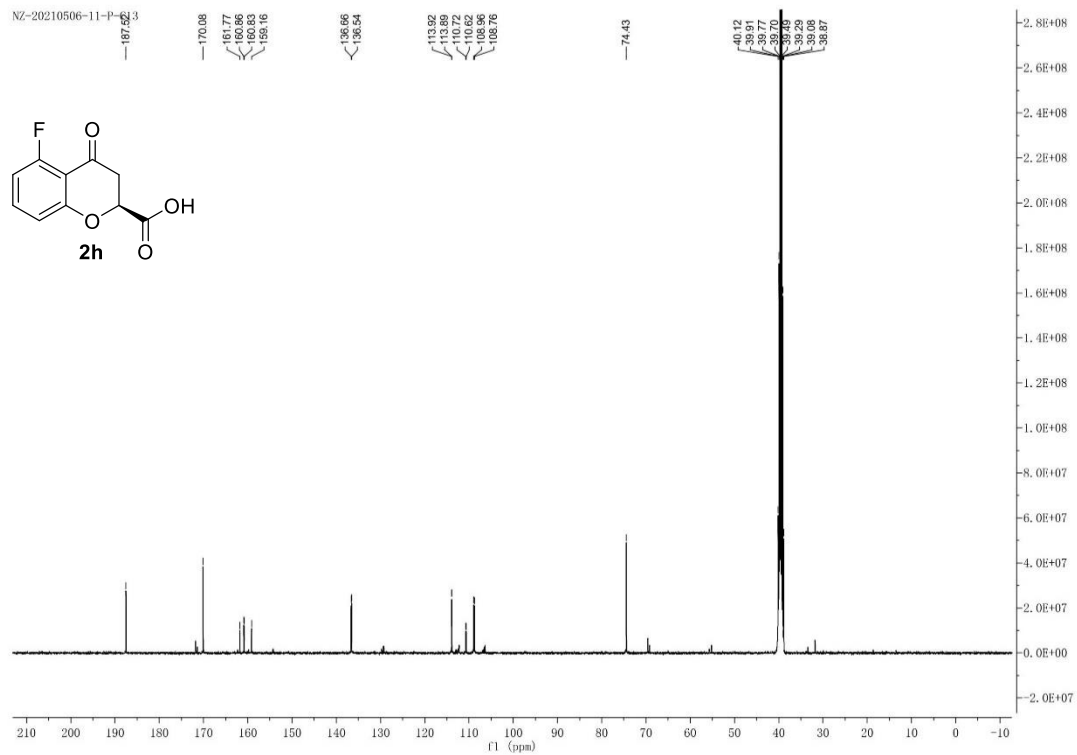
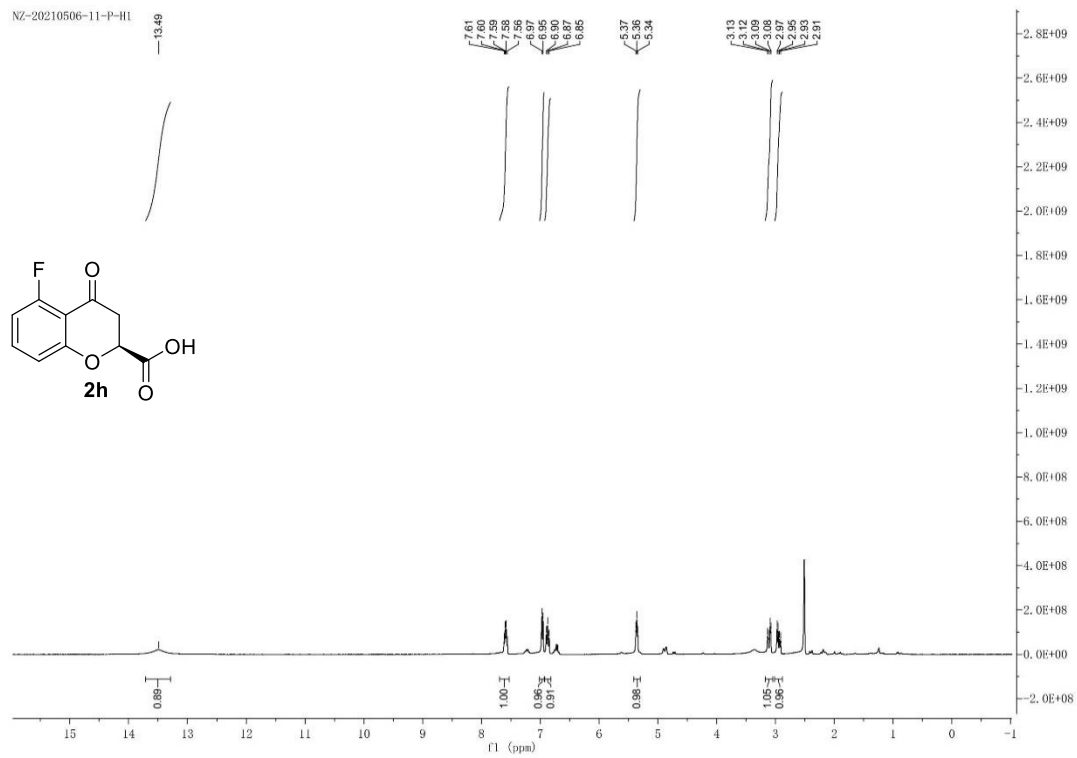


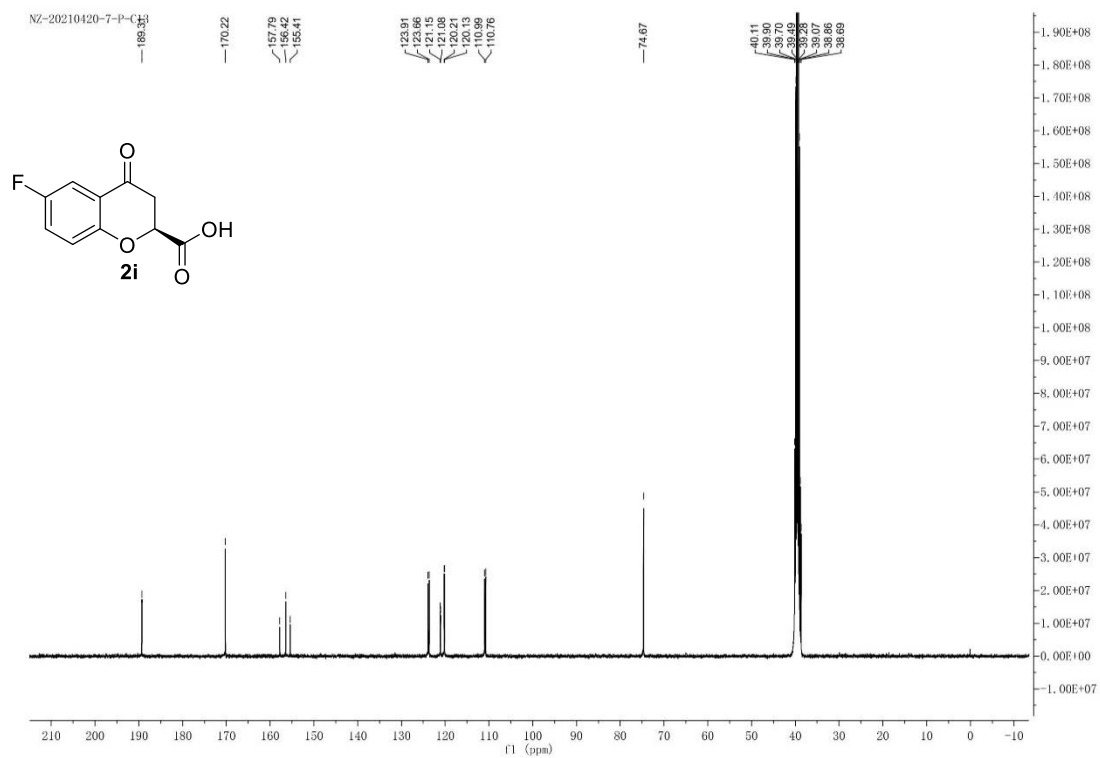
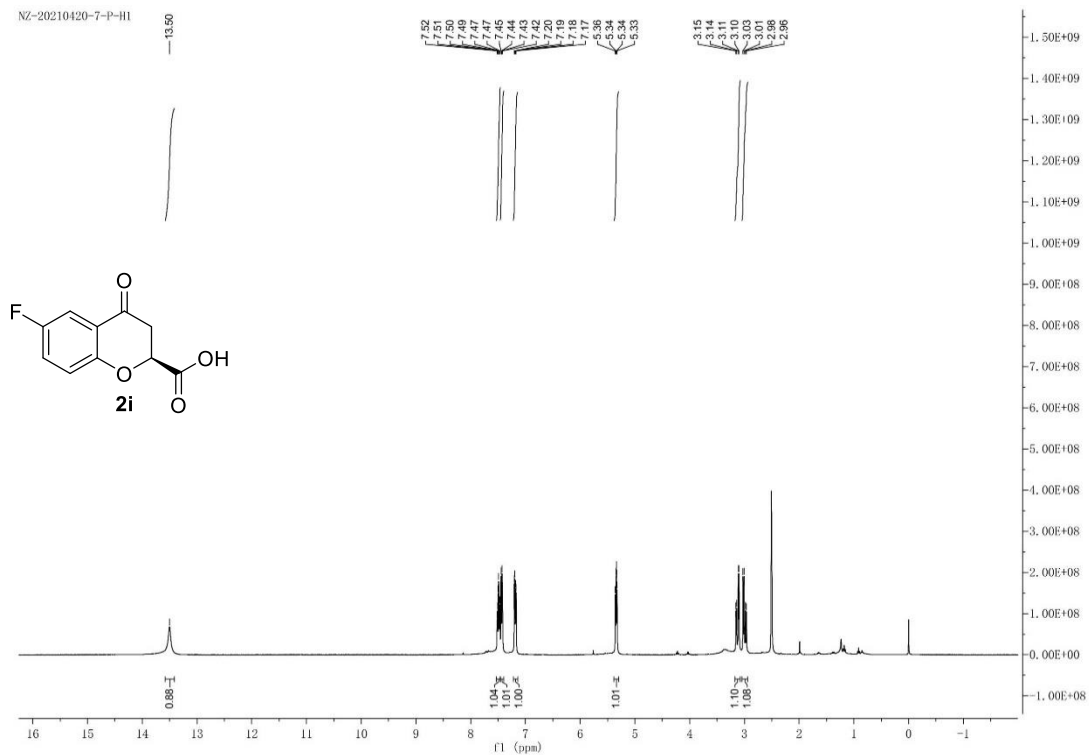
NZ-20210528-20-P-H1

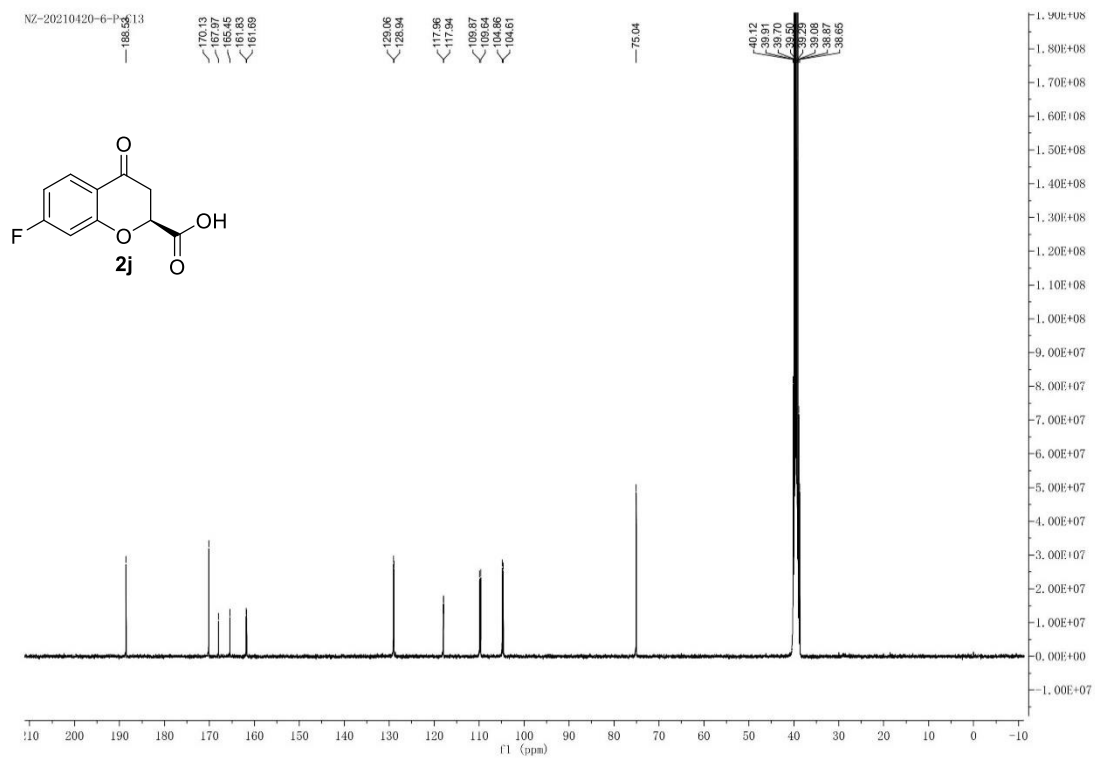
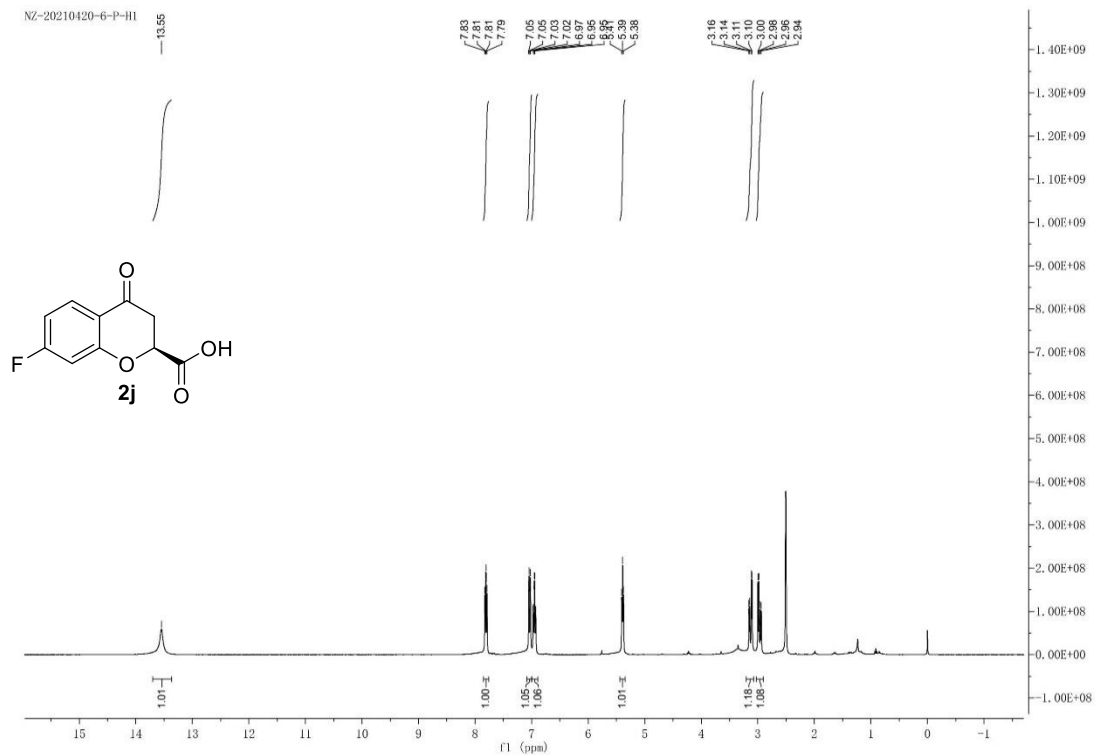


NZ-20211025-1

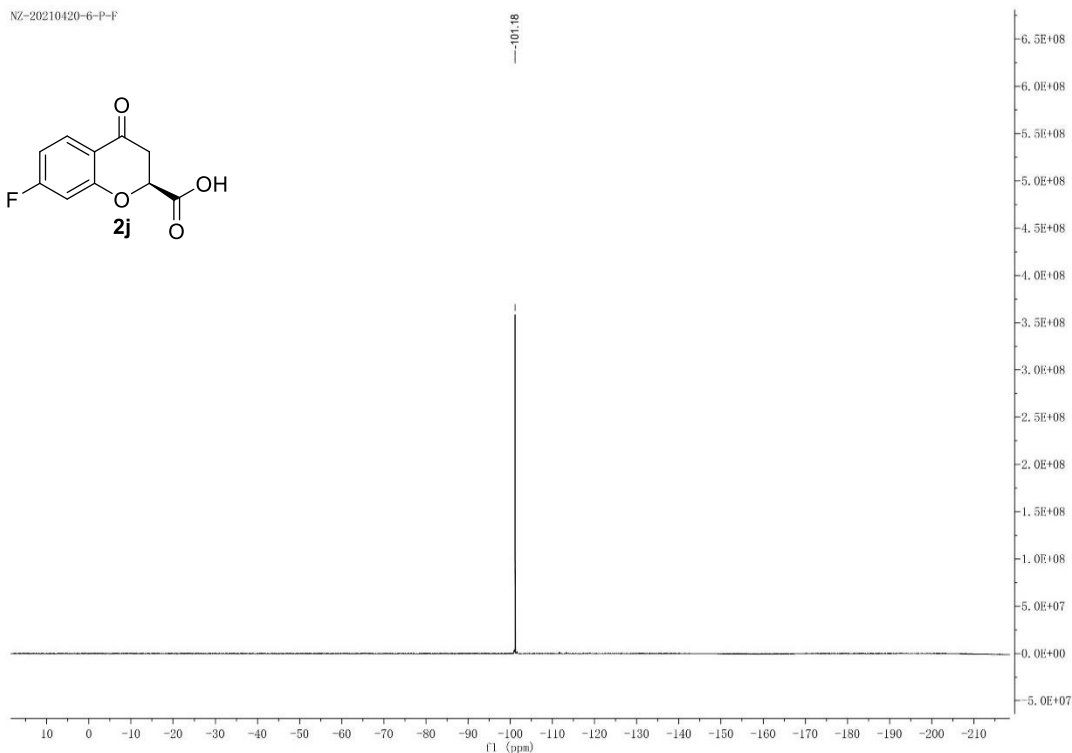
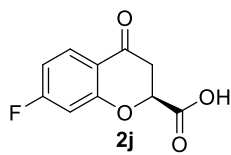




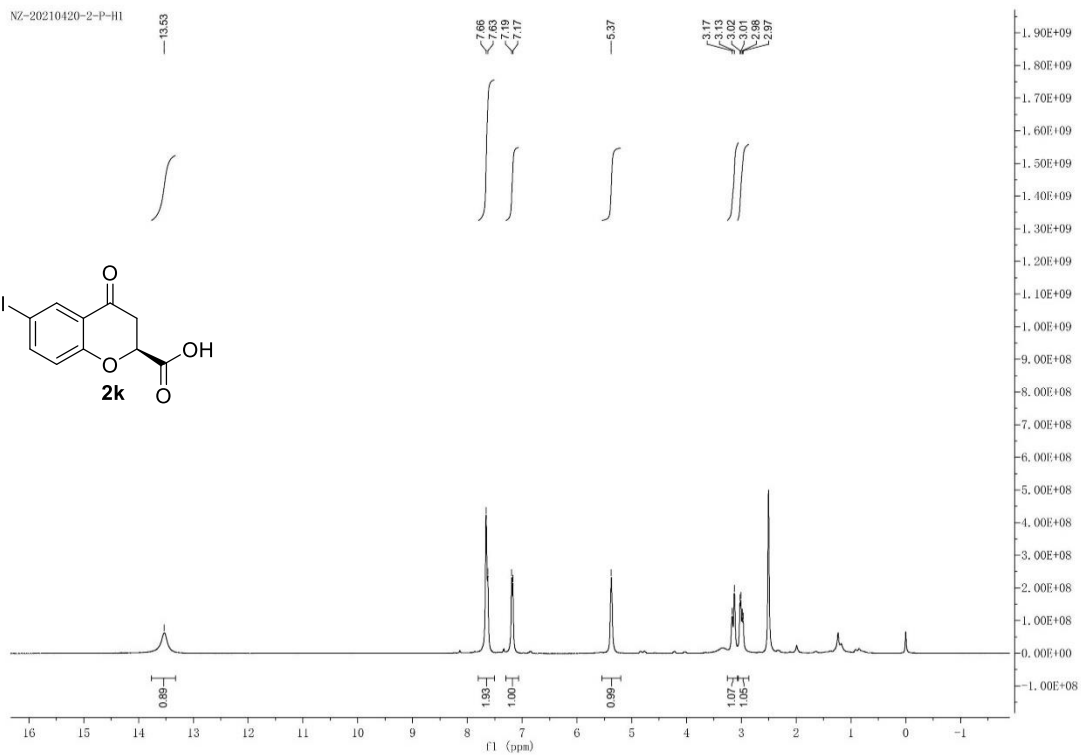
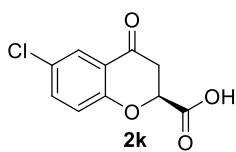


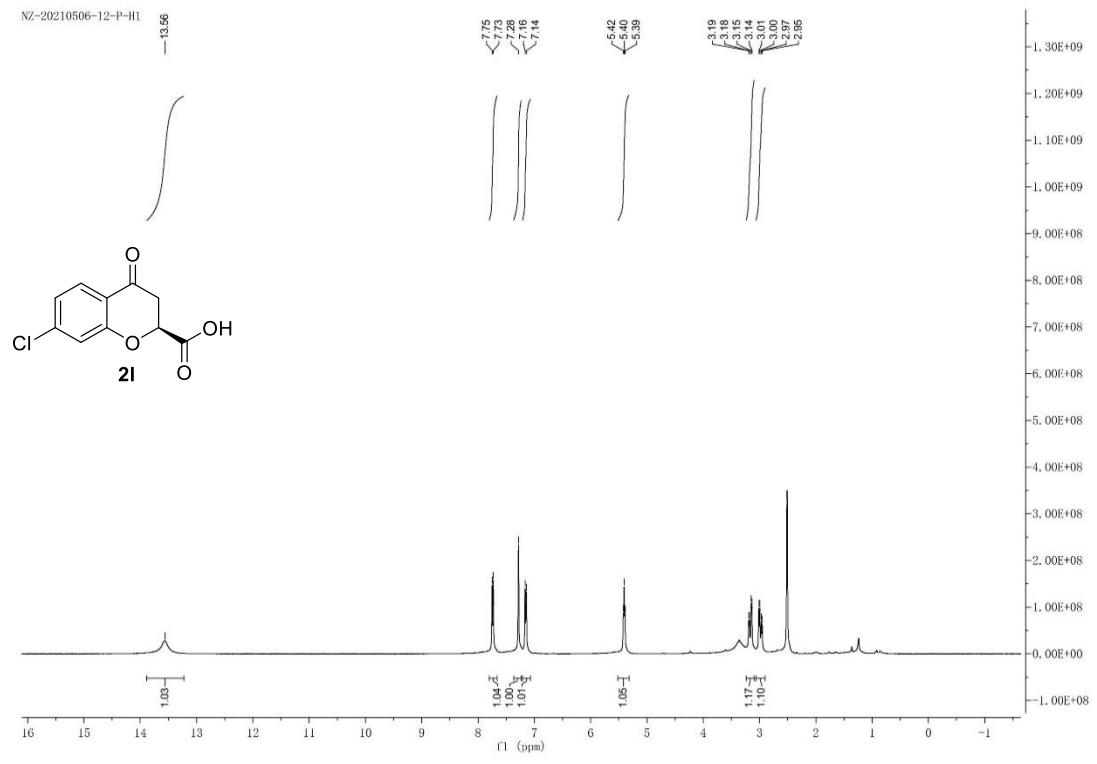
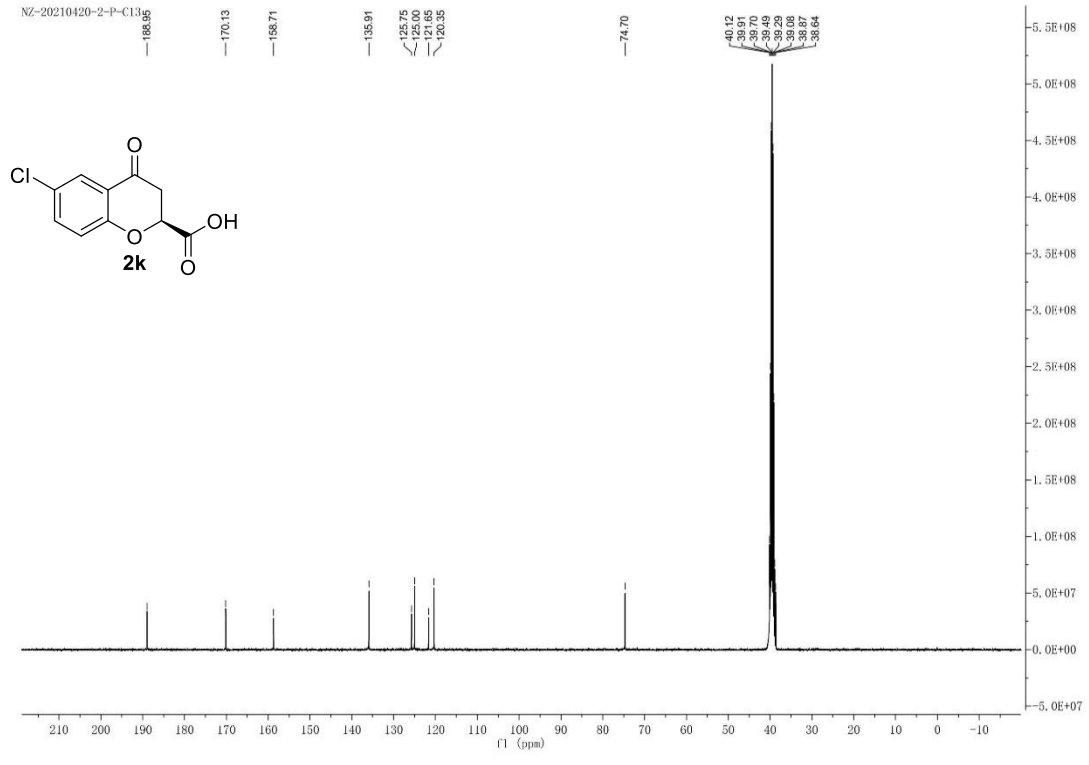


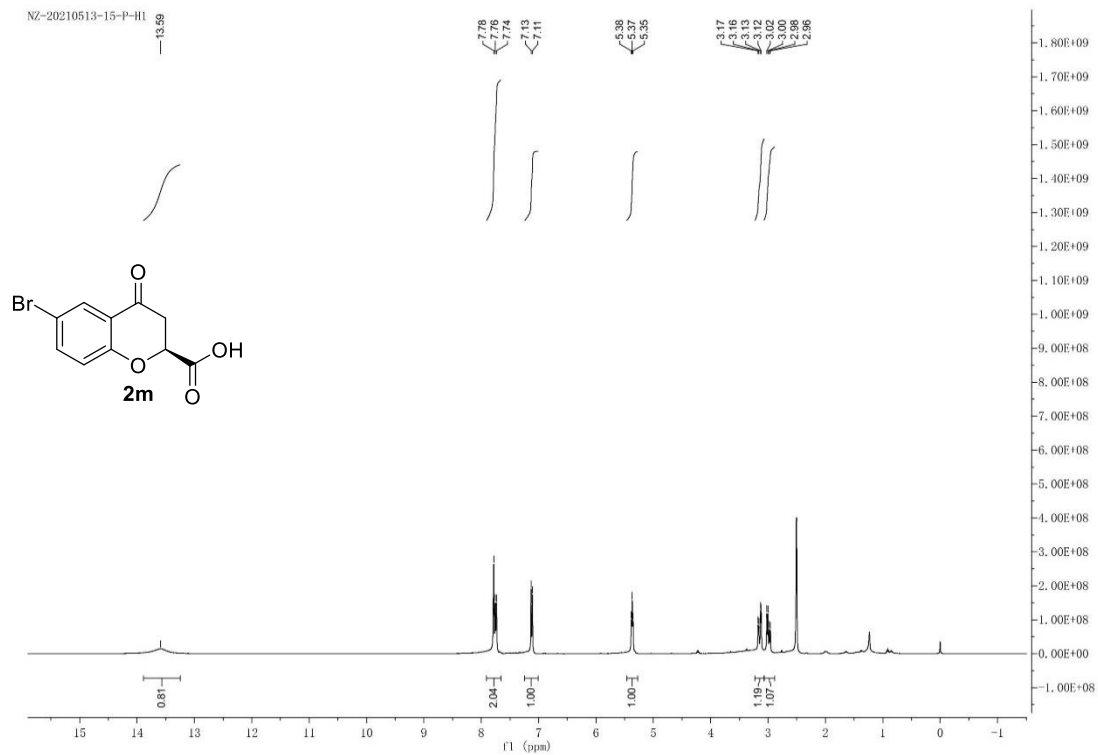
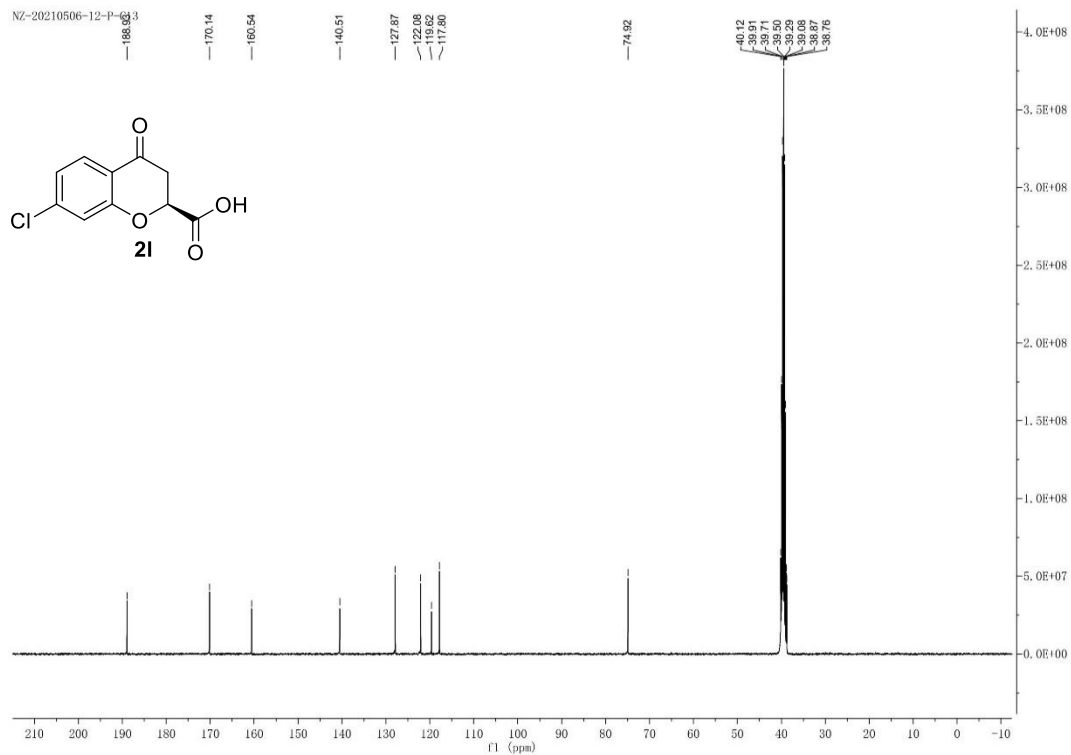
NZ-20210420-6-P-F

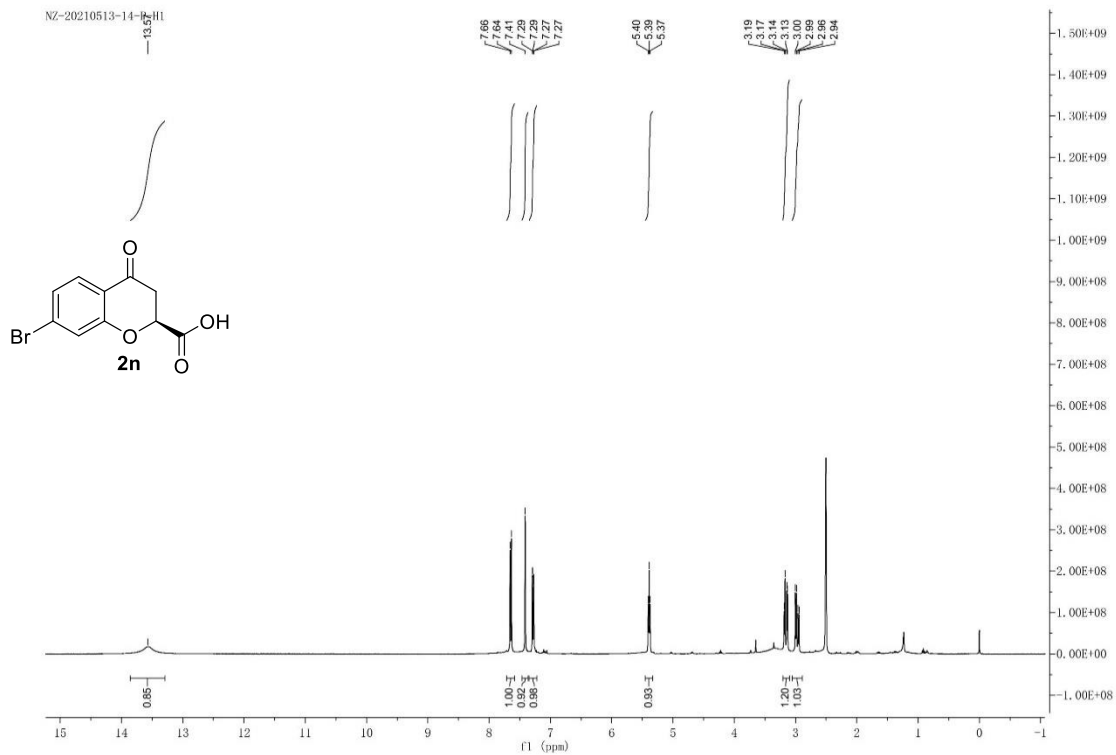
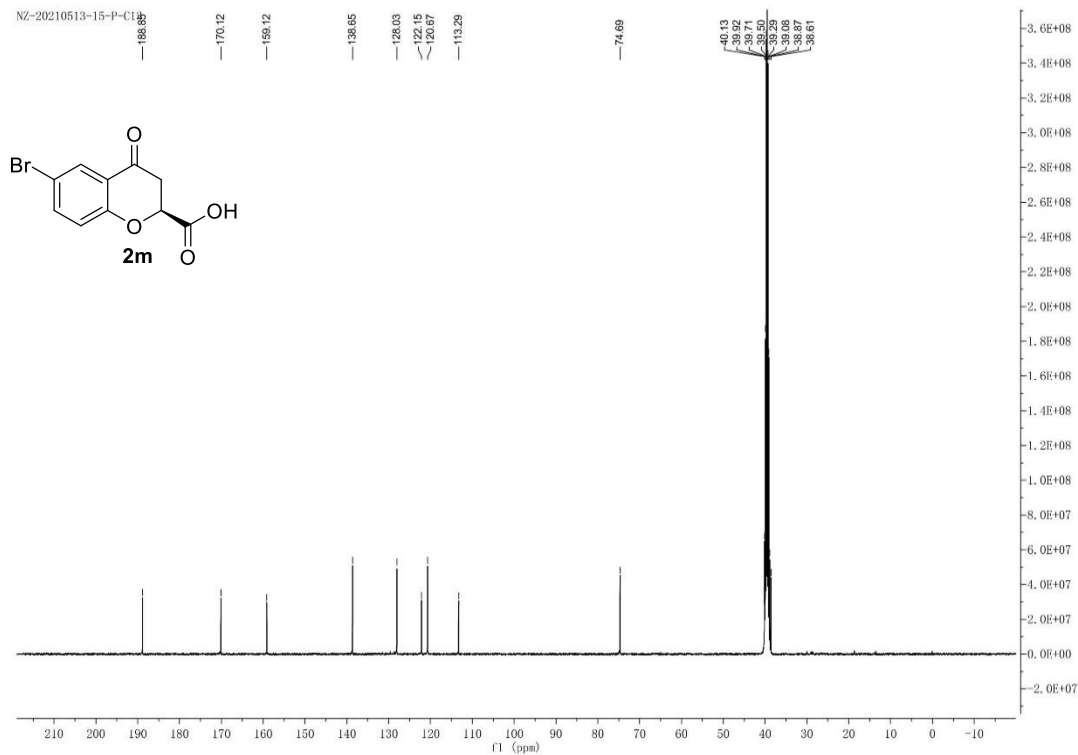


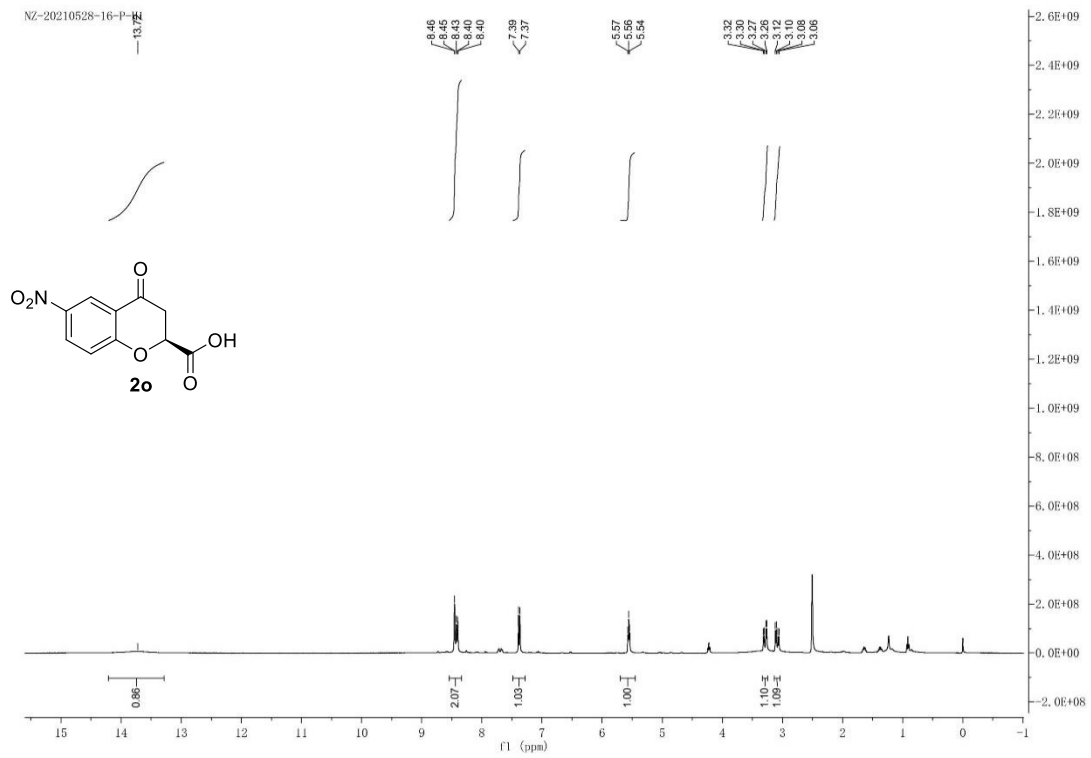
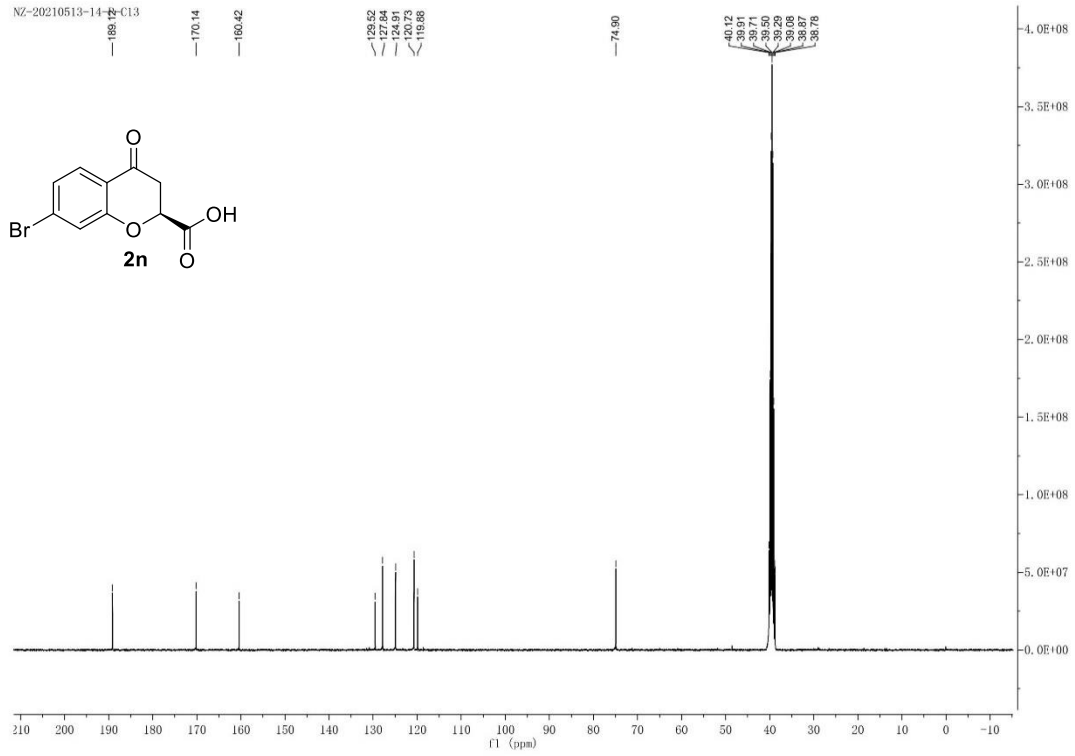
NZ-20210420-2-P-HI

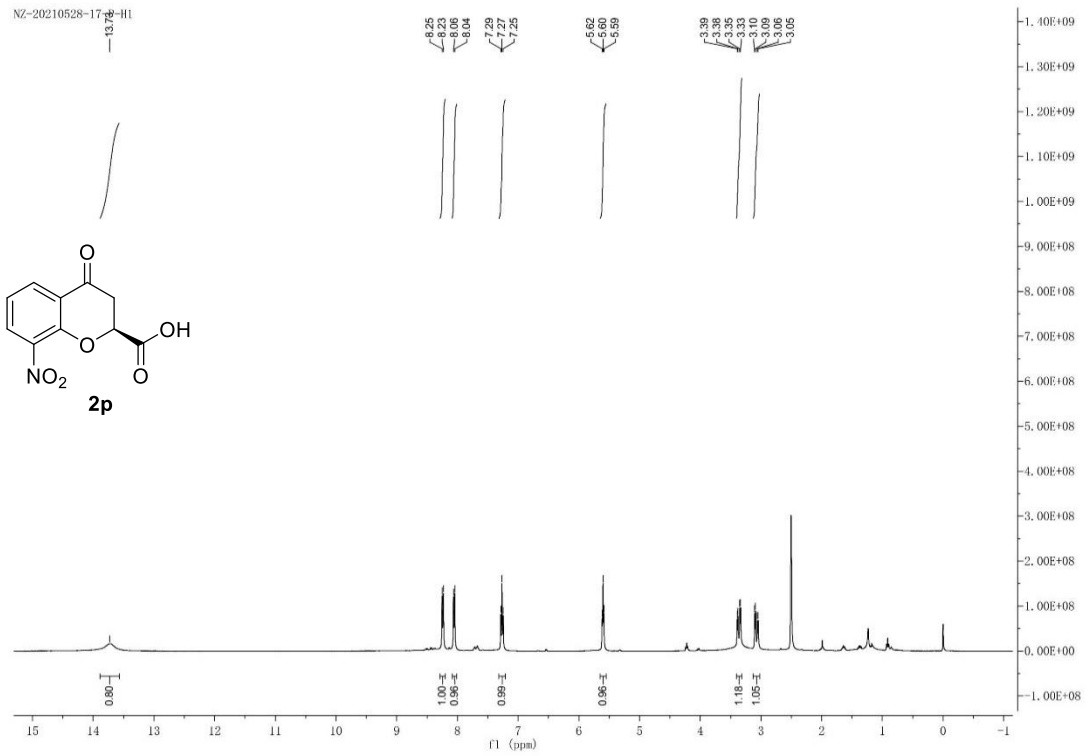
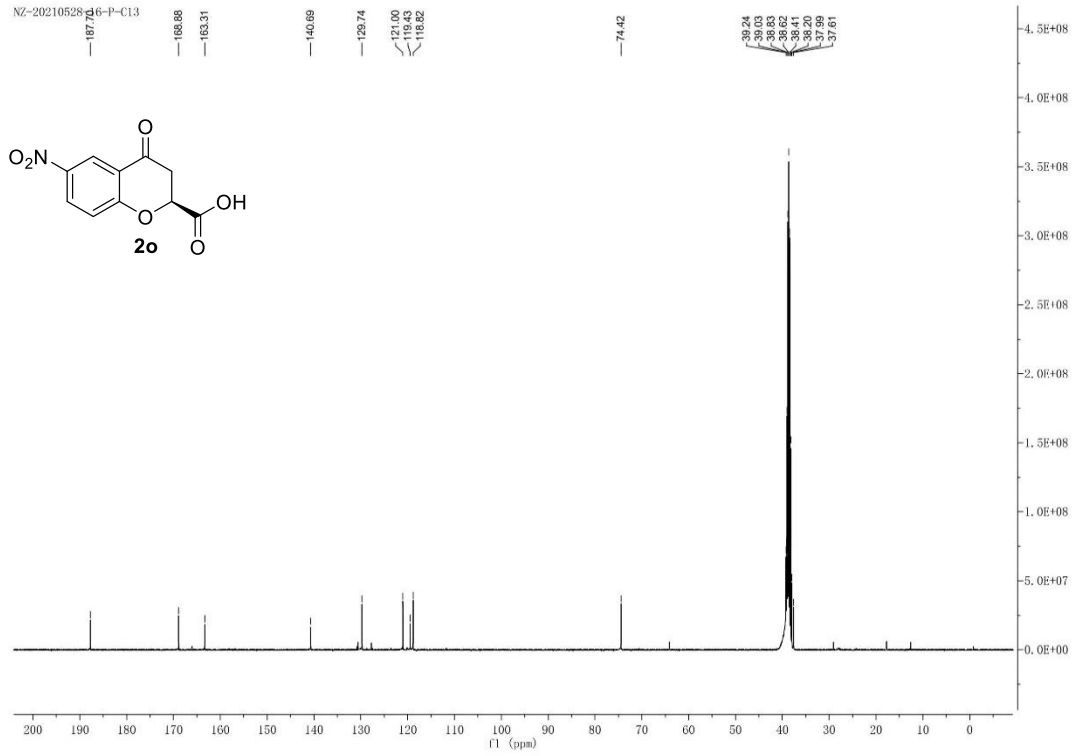


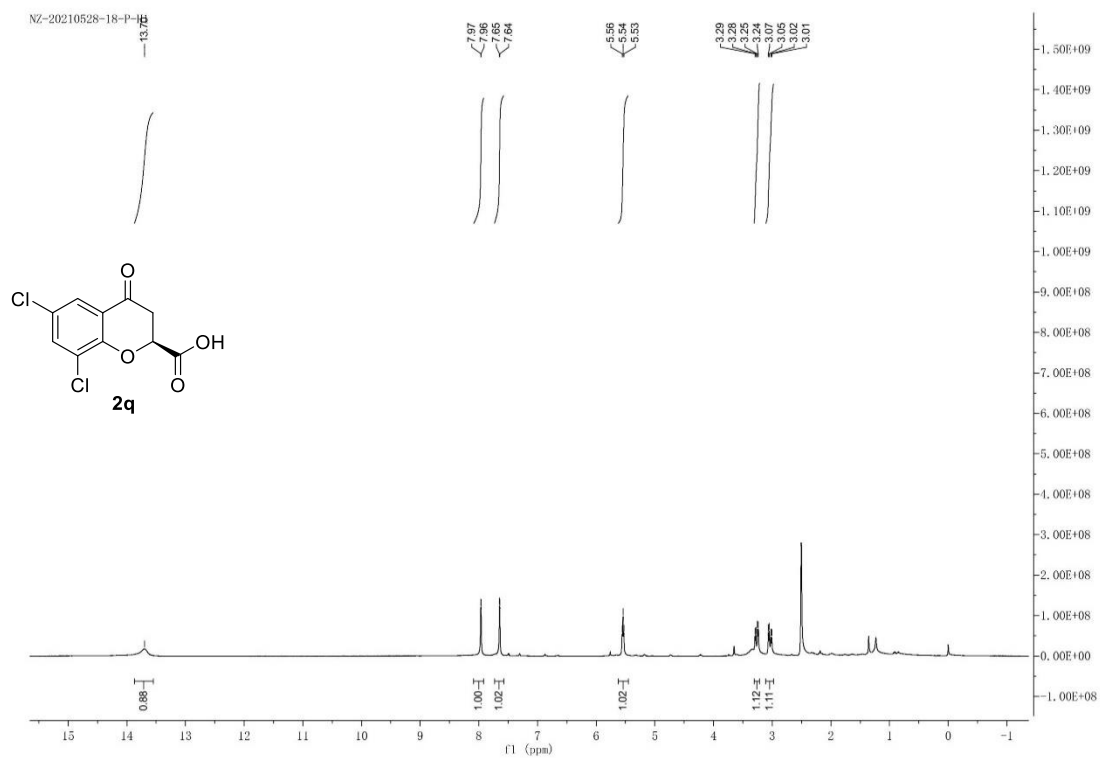
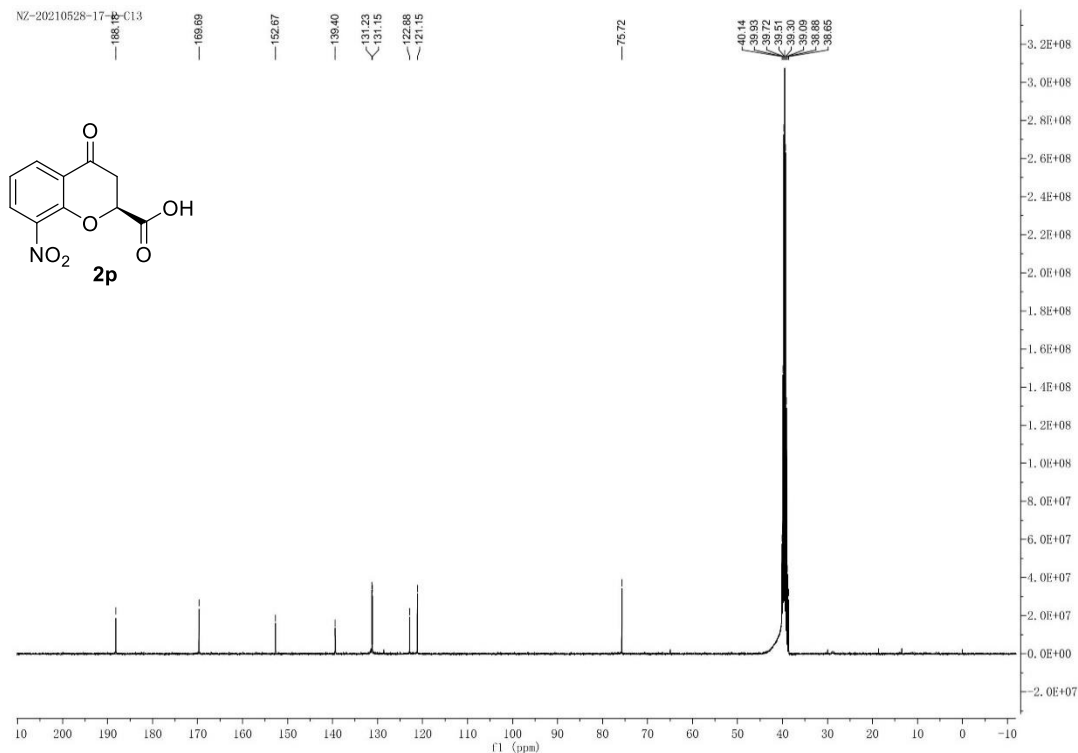


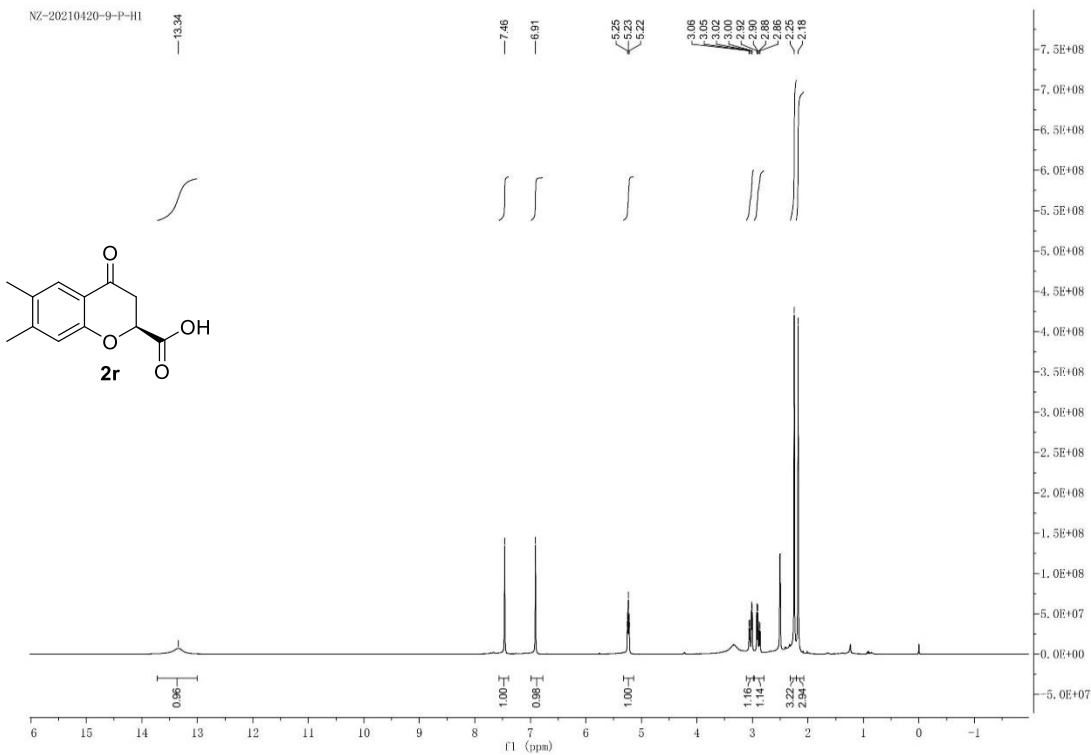
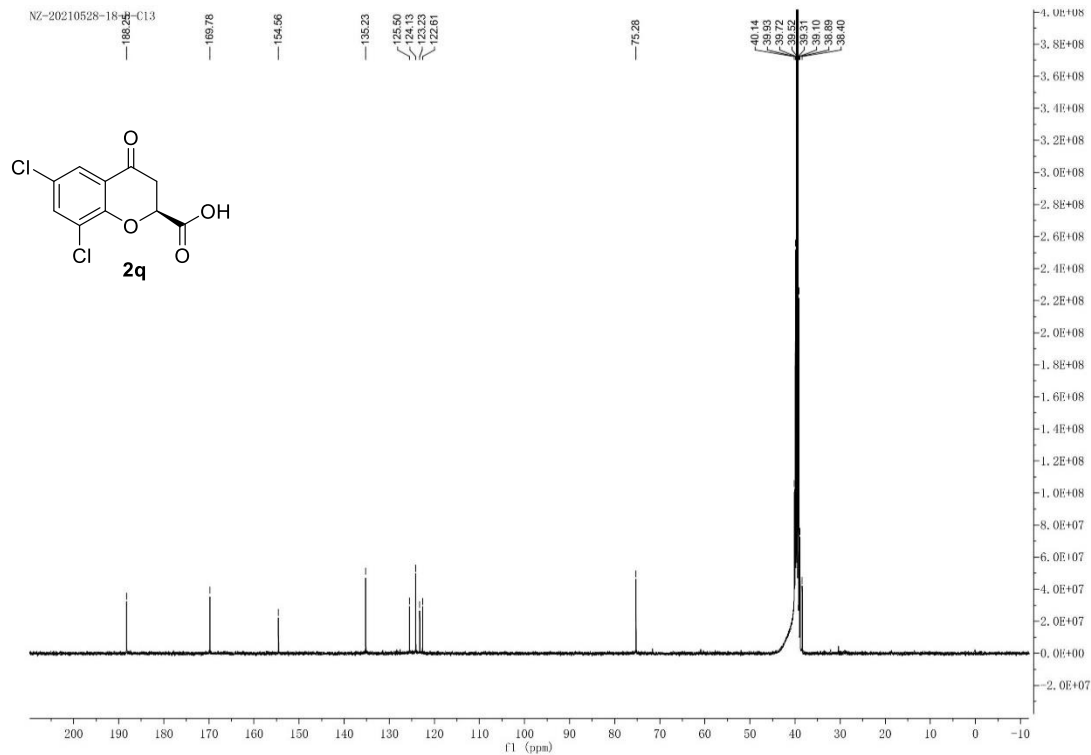


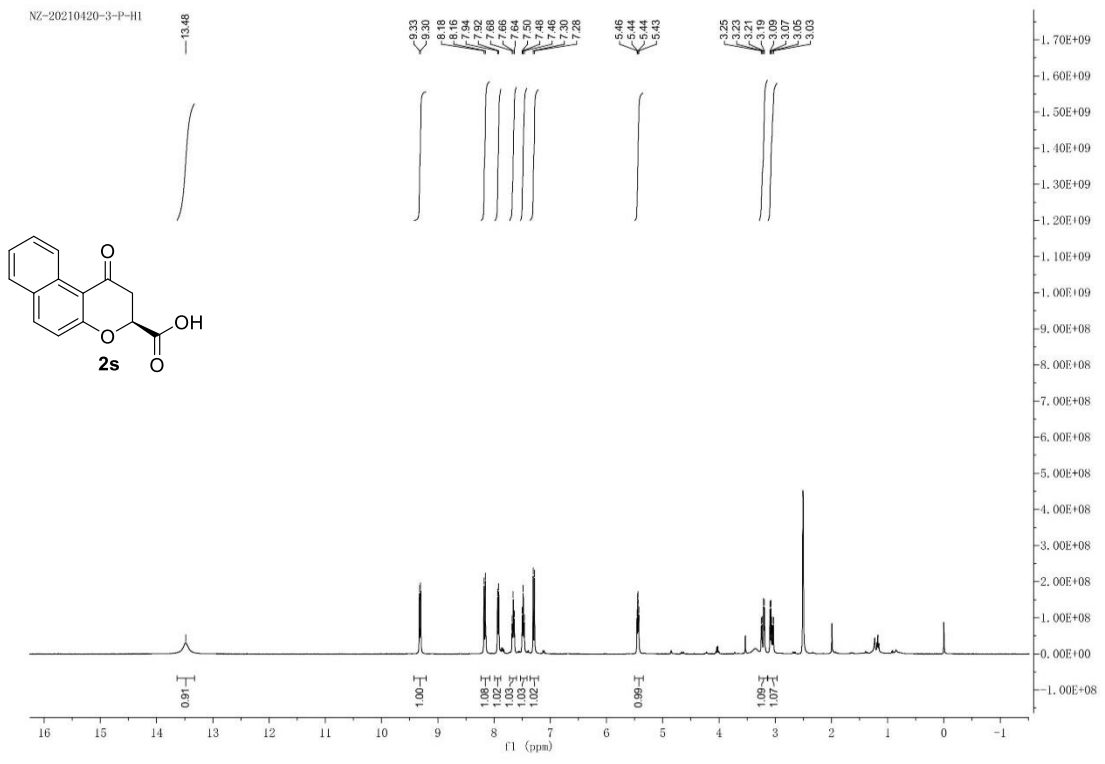
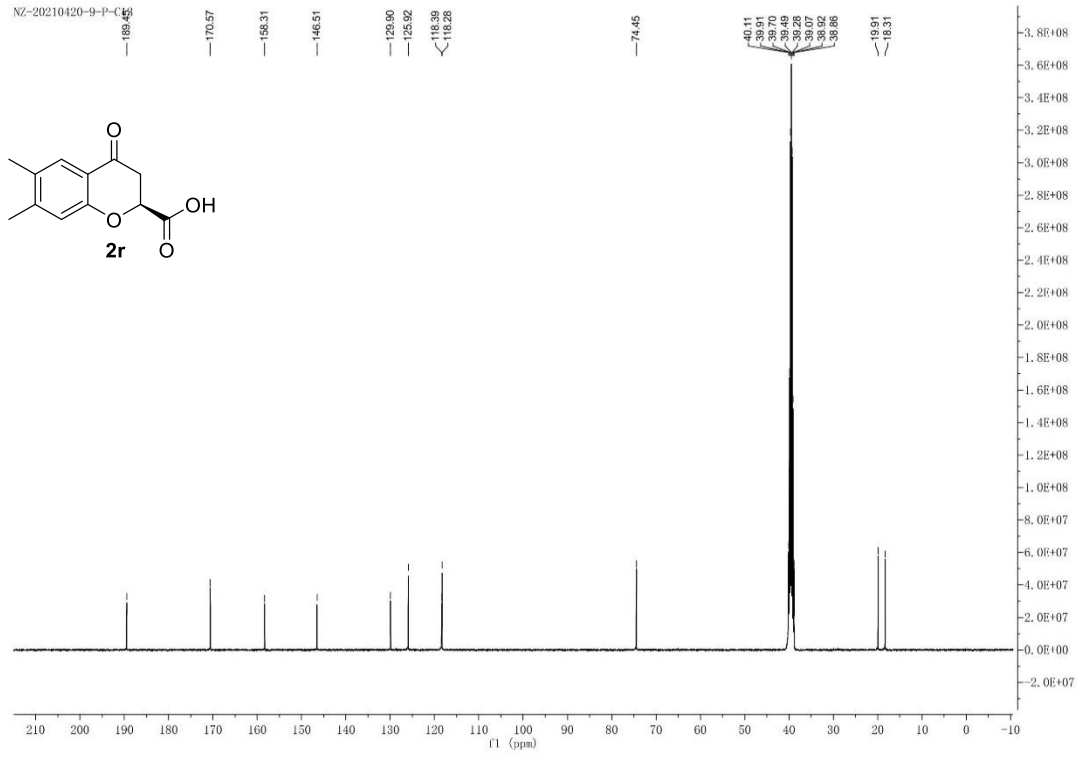


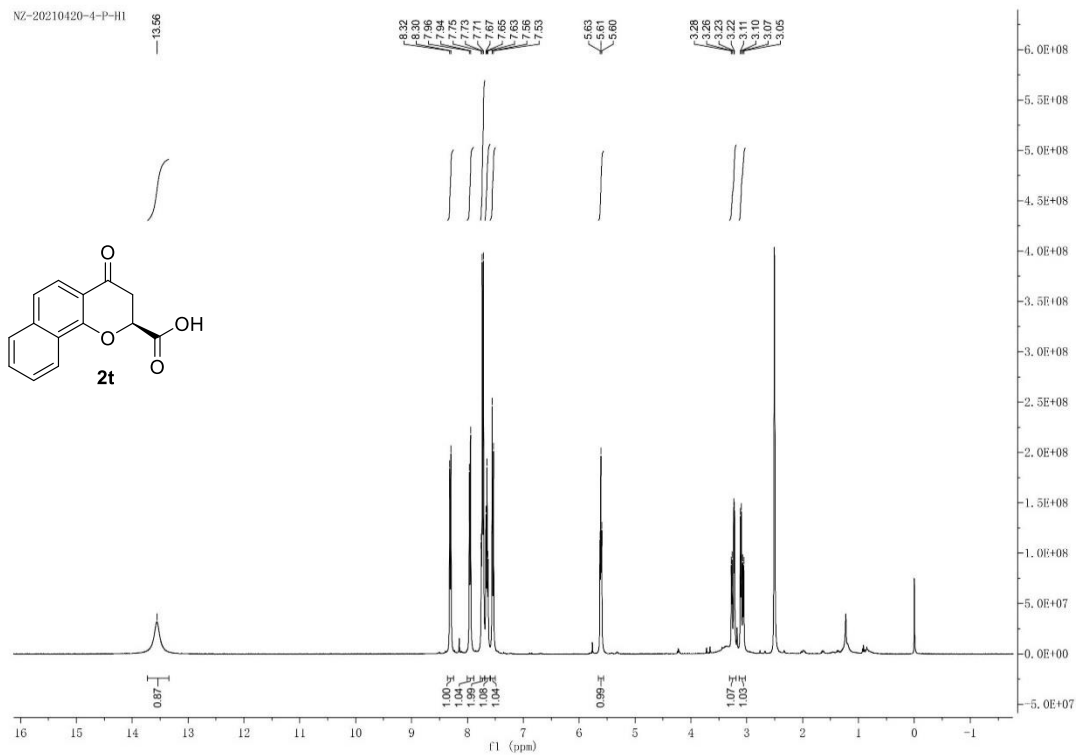
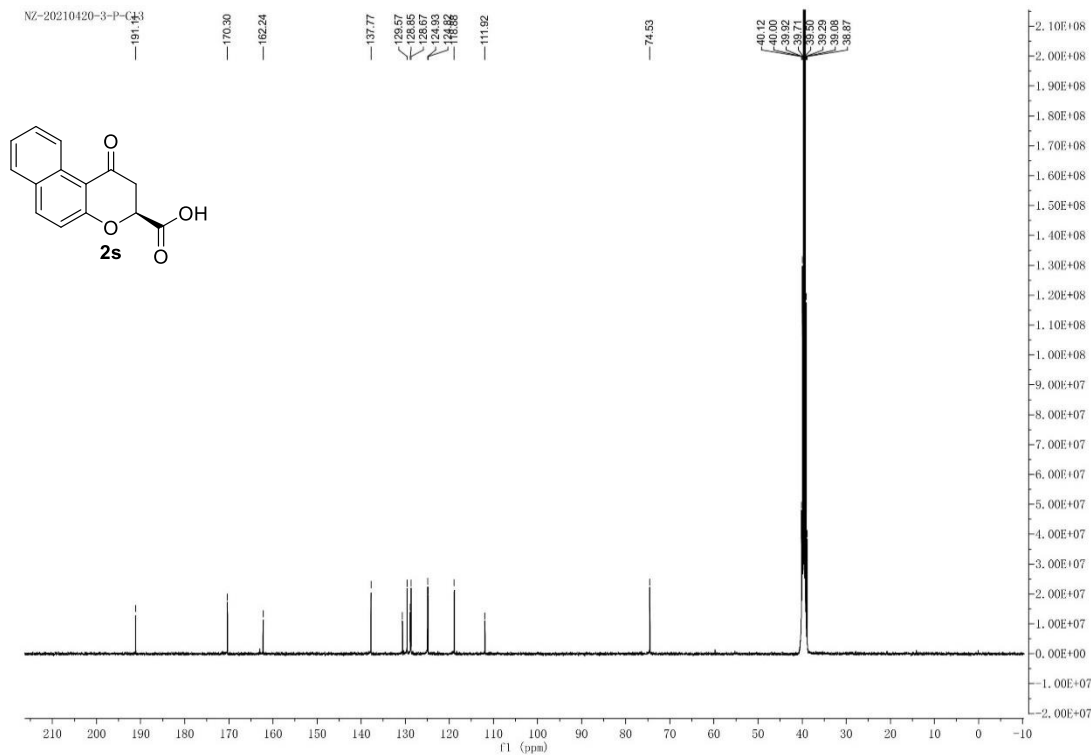


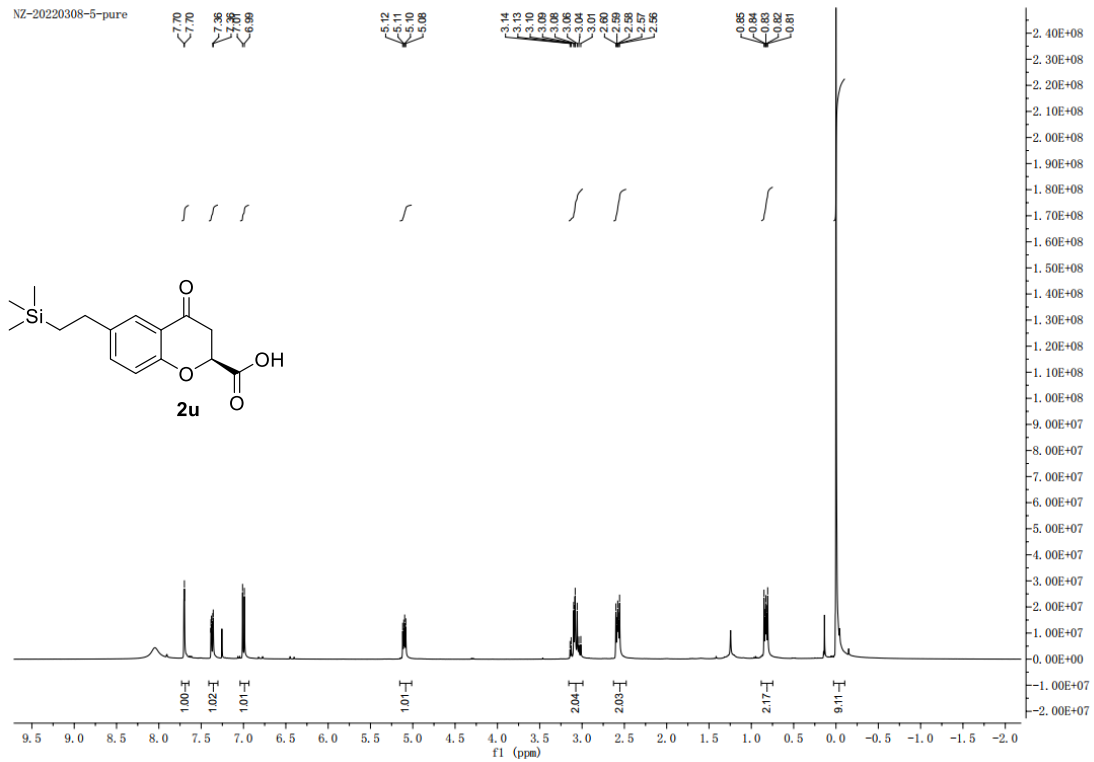
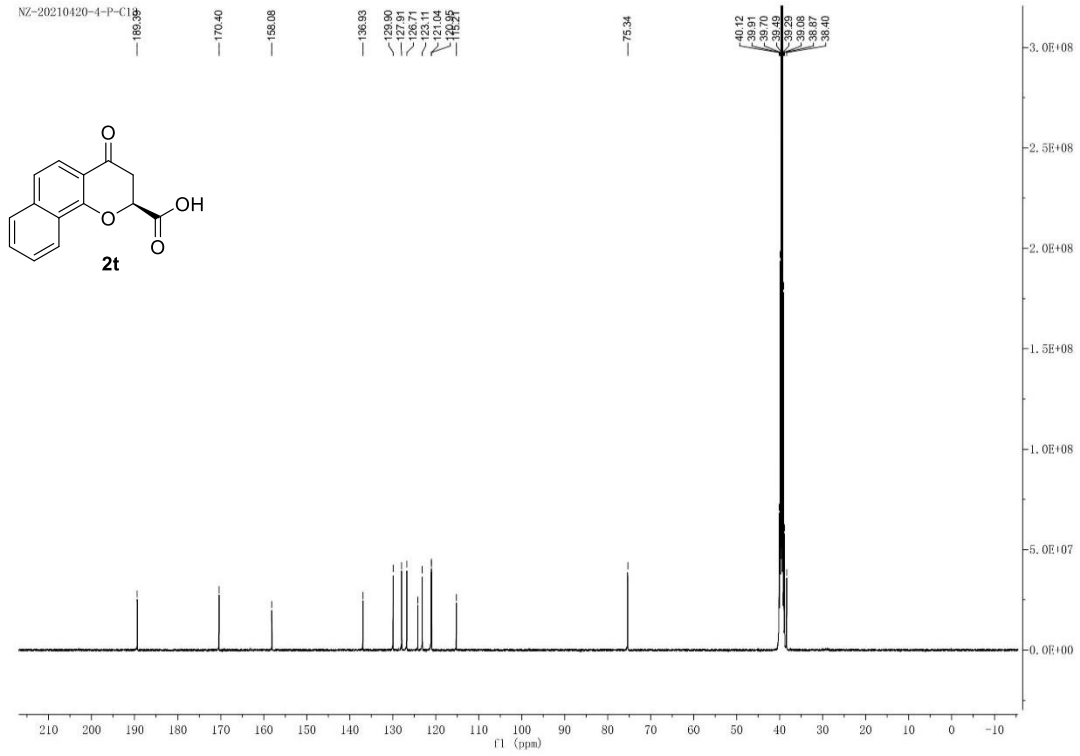


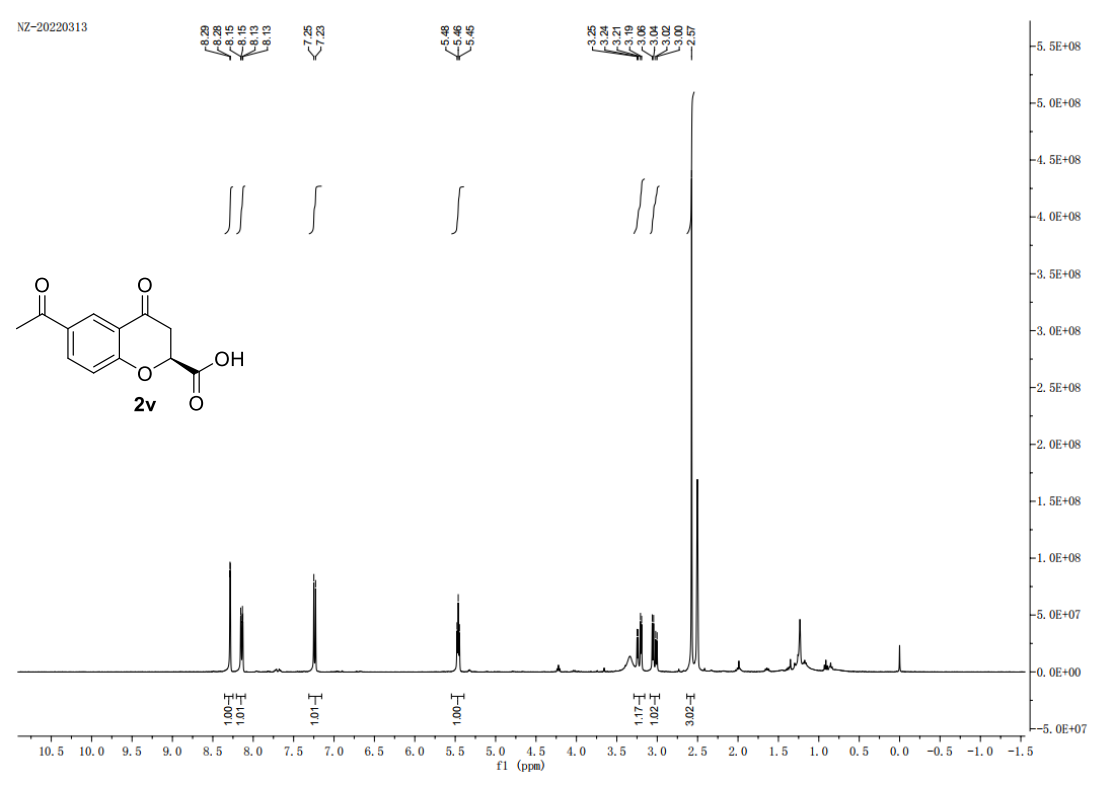
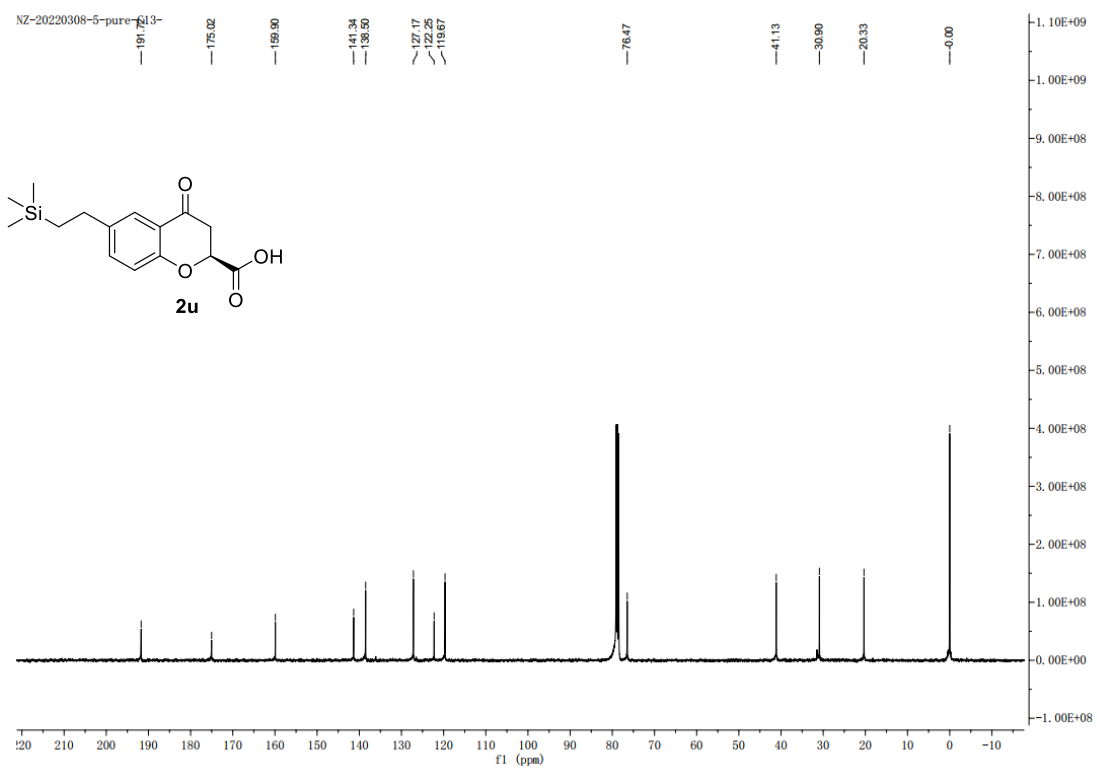


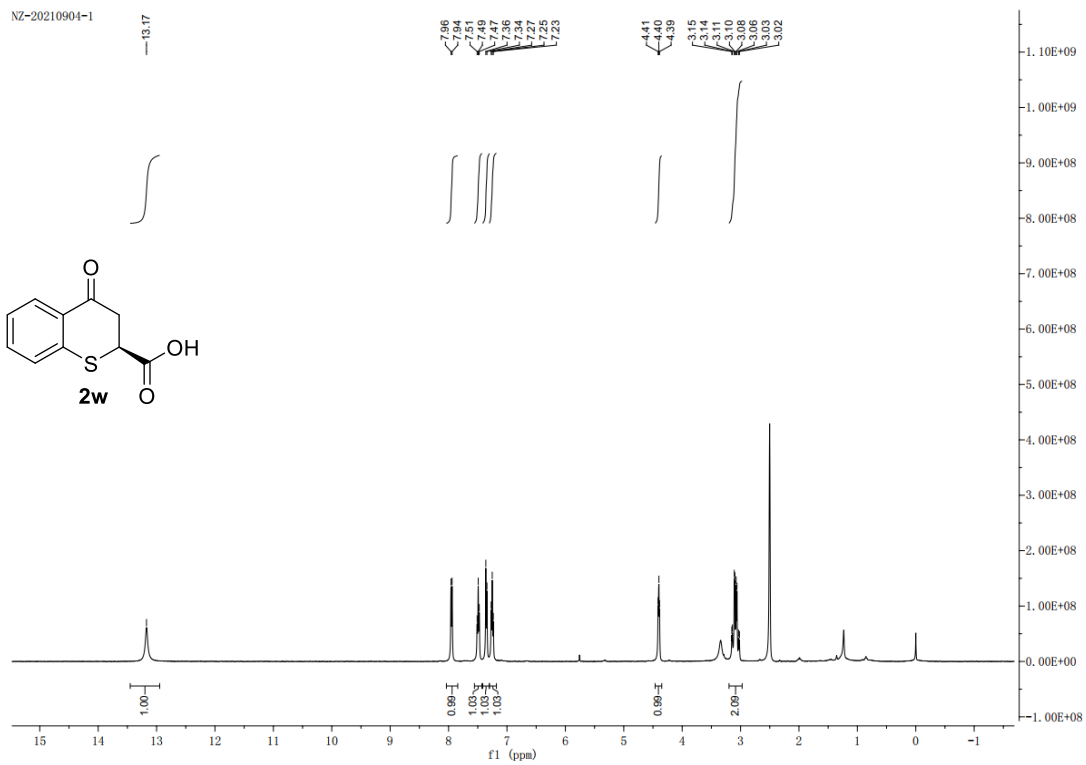
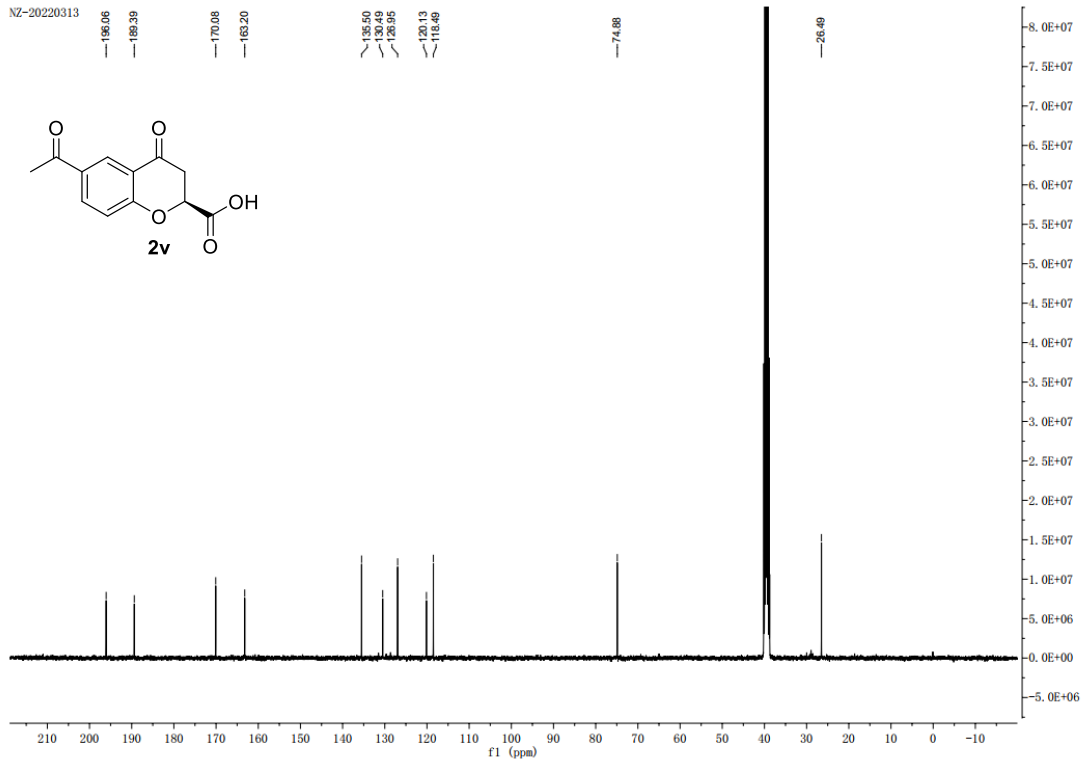


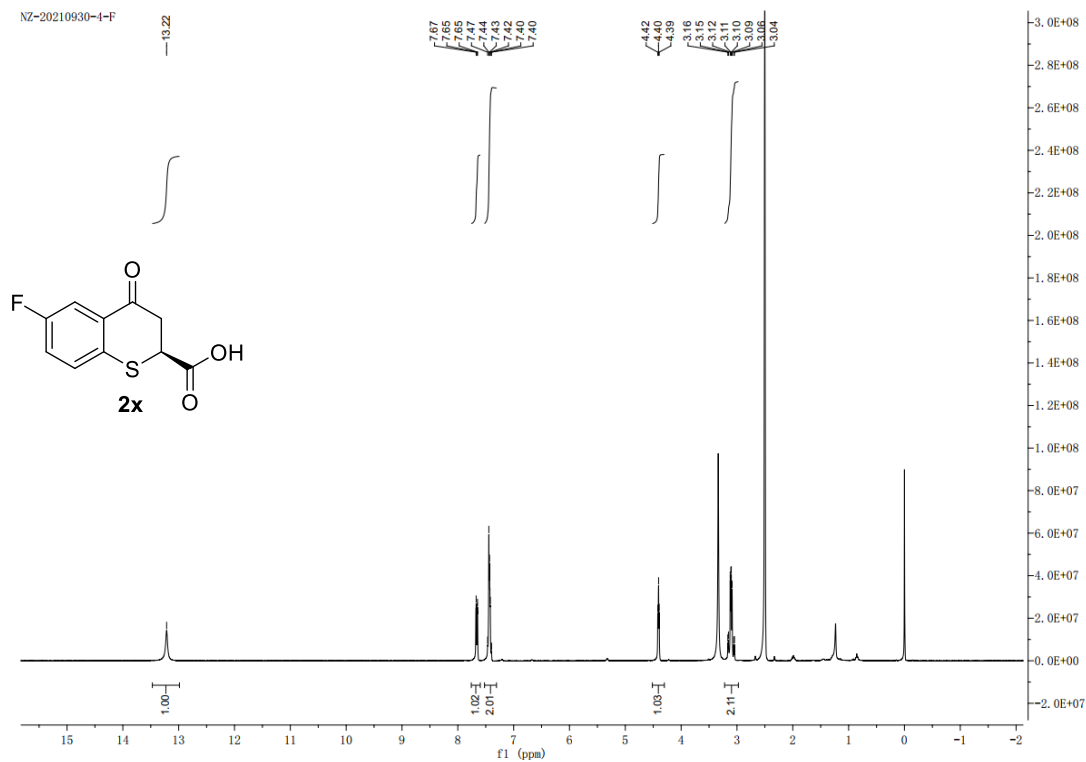
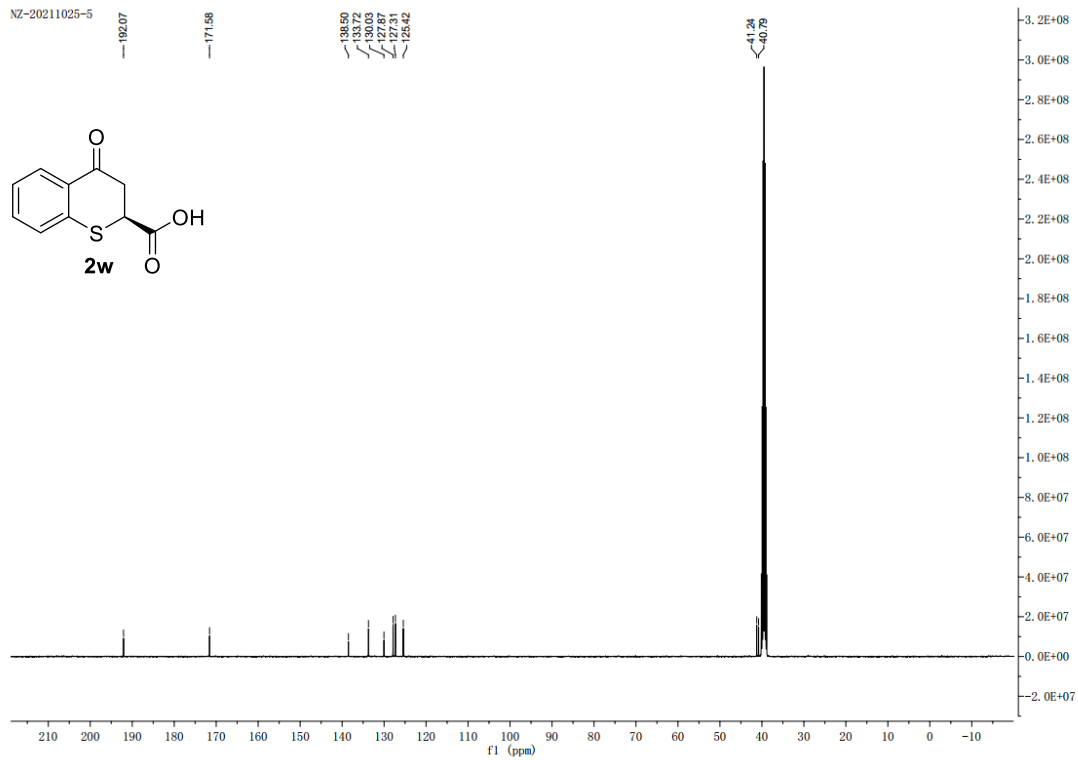


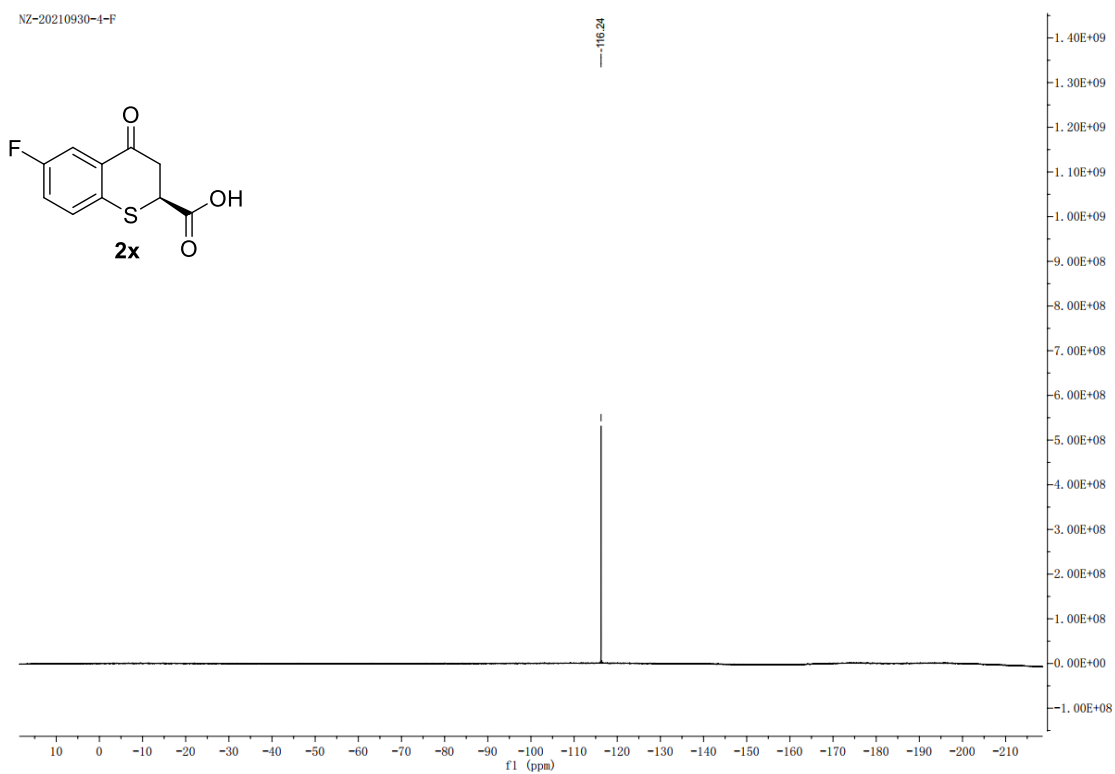
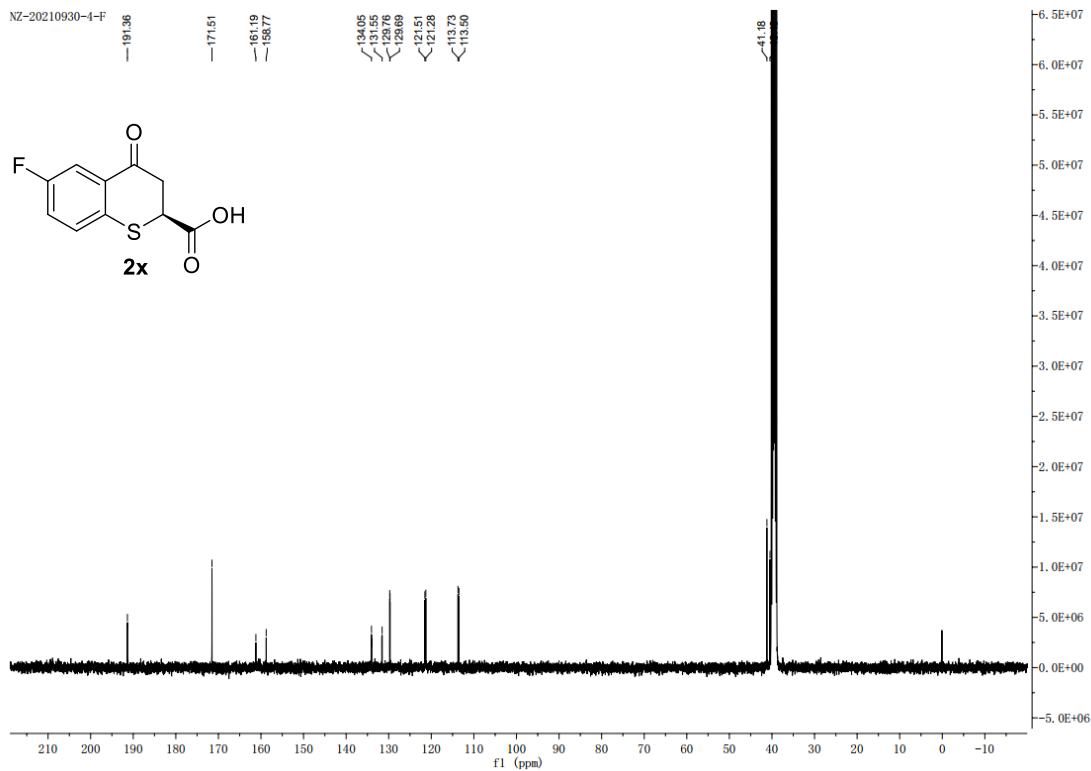


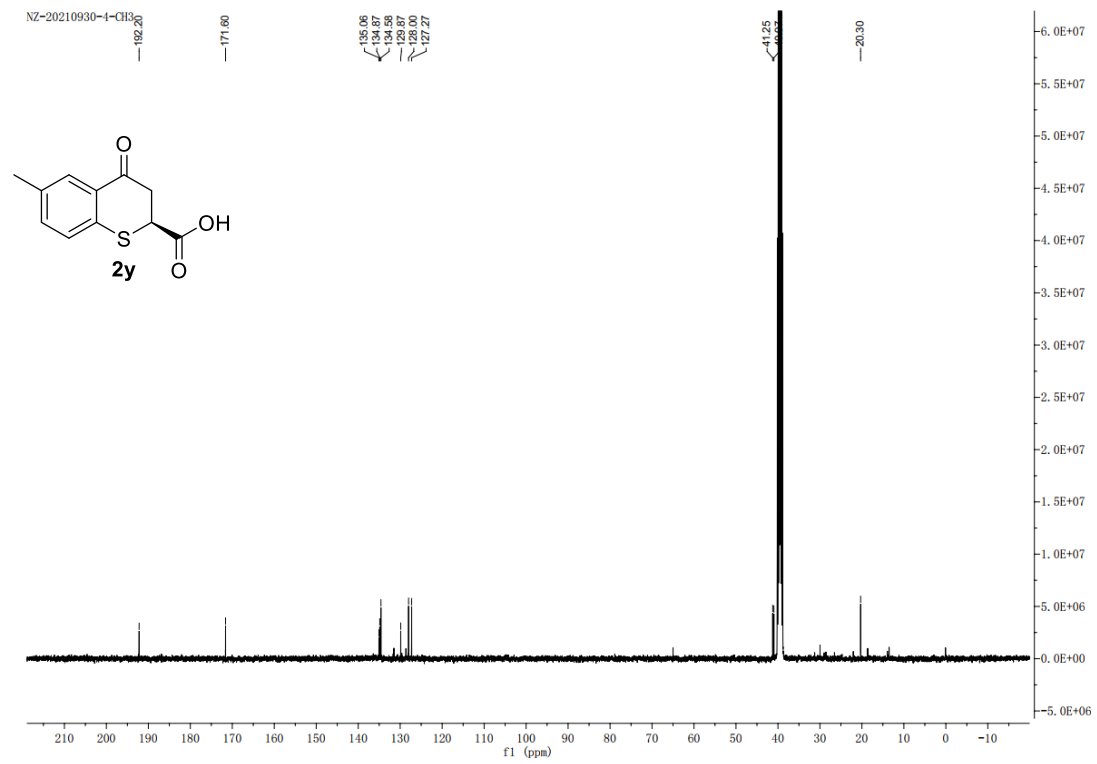
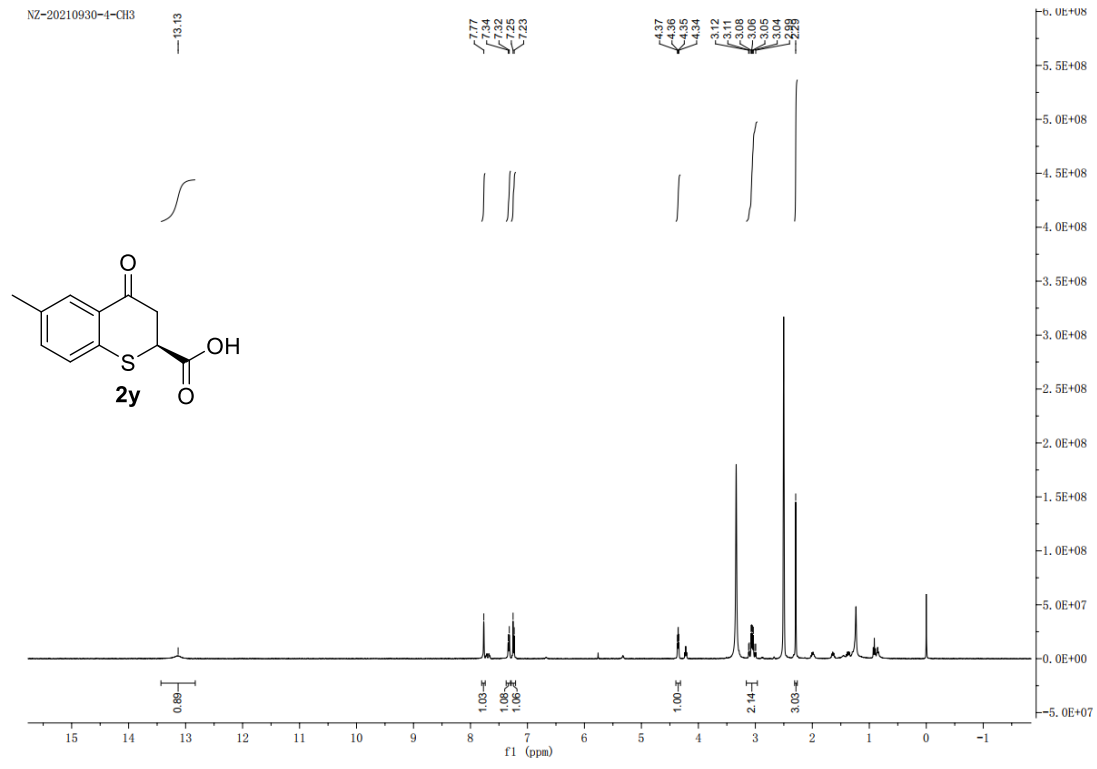


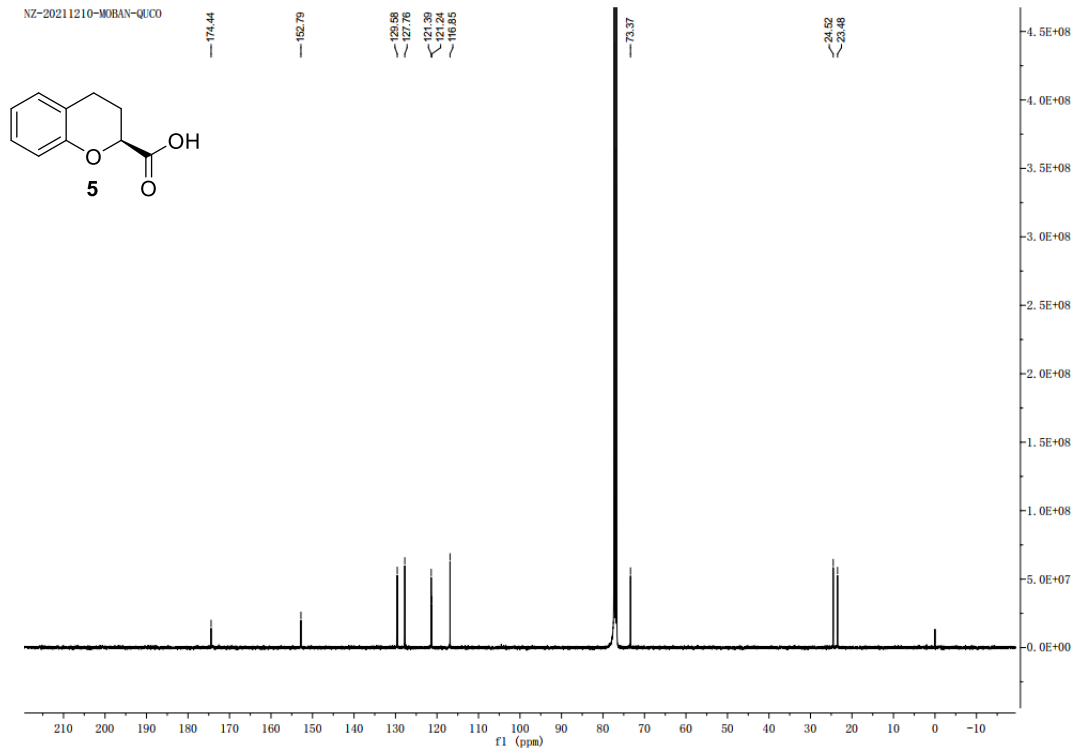
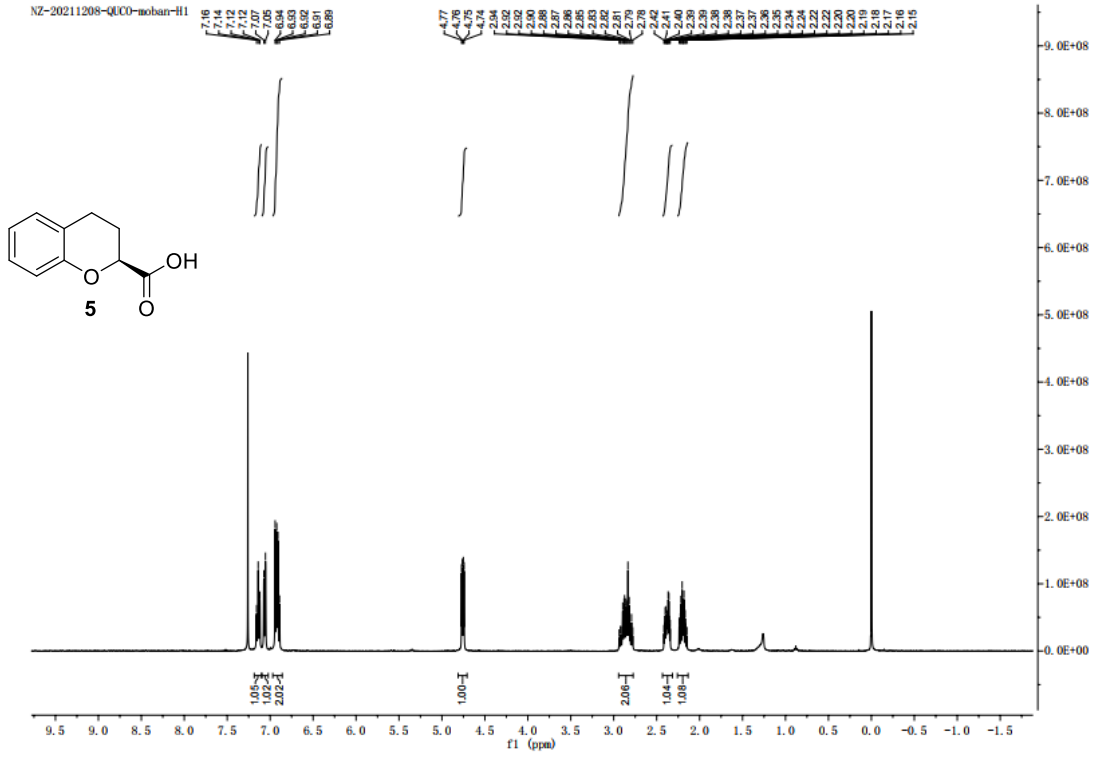


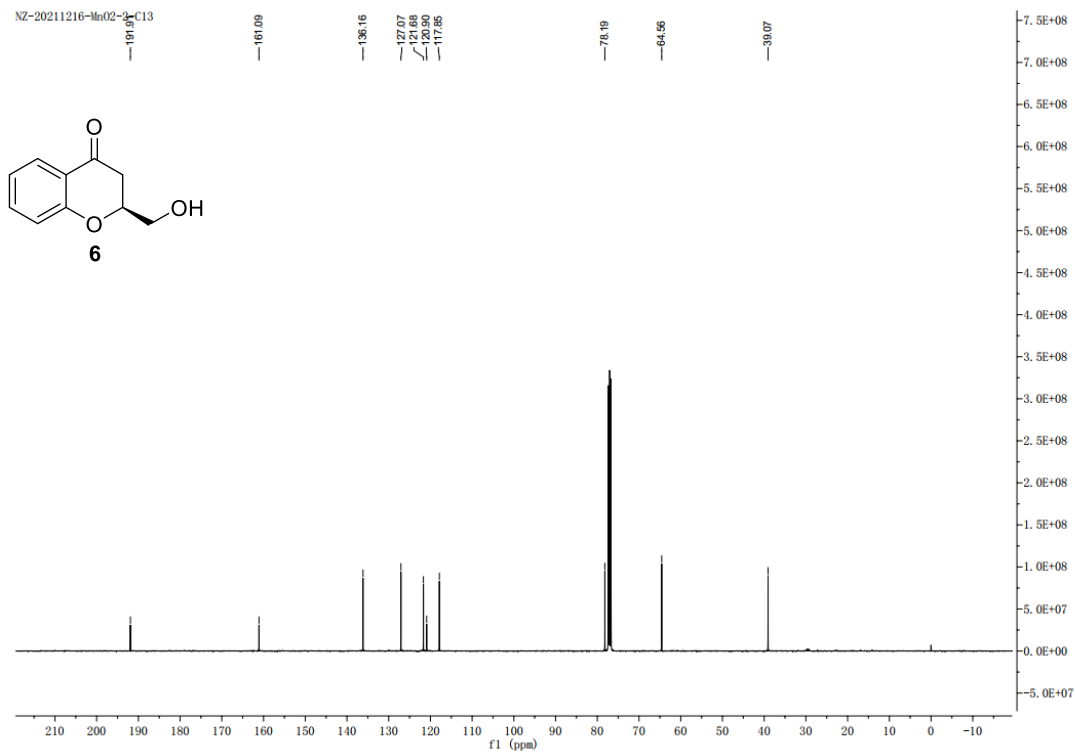
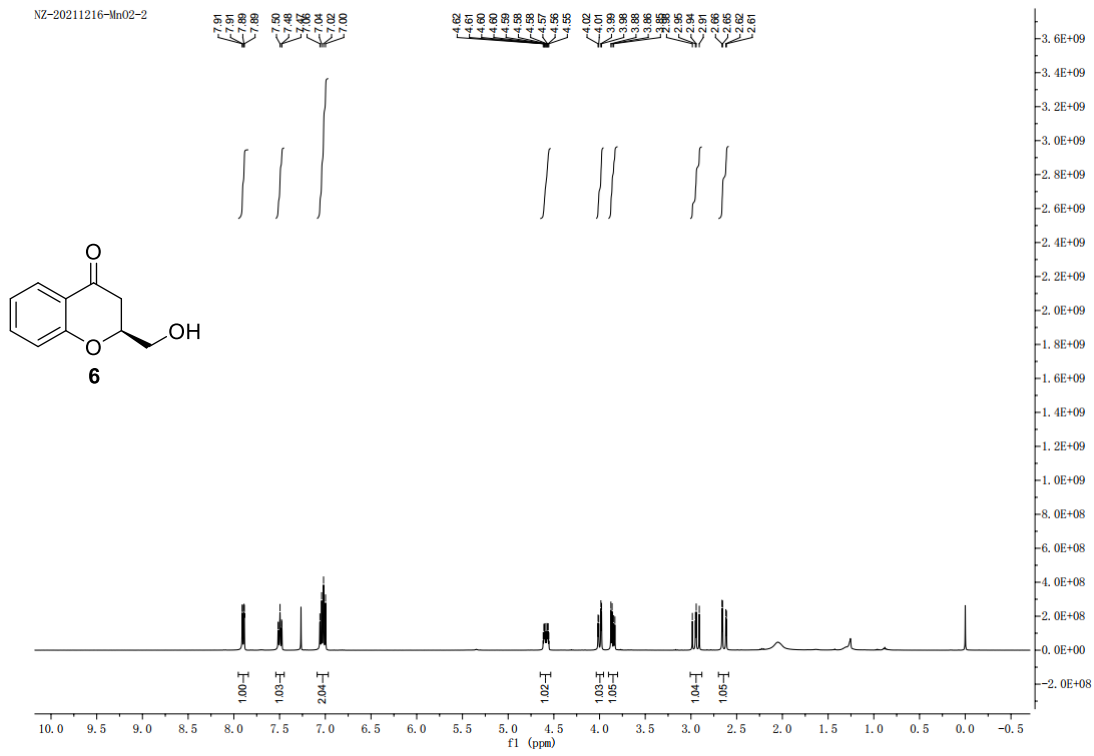




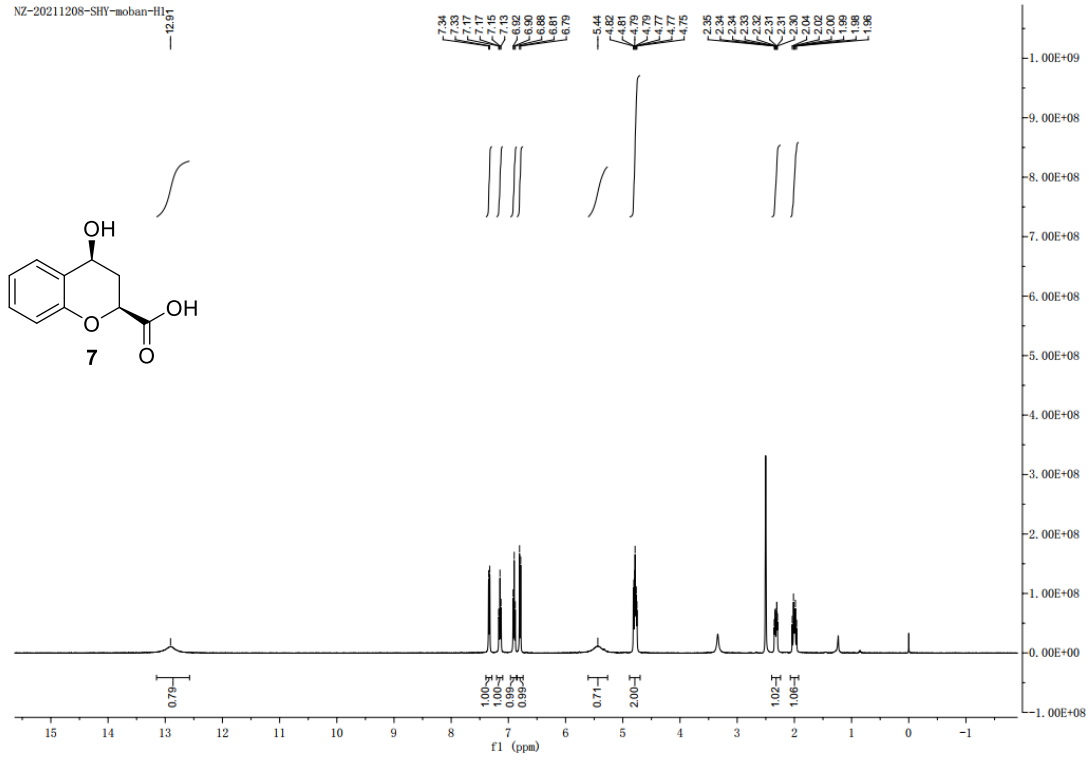




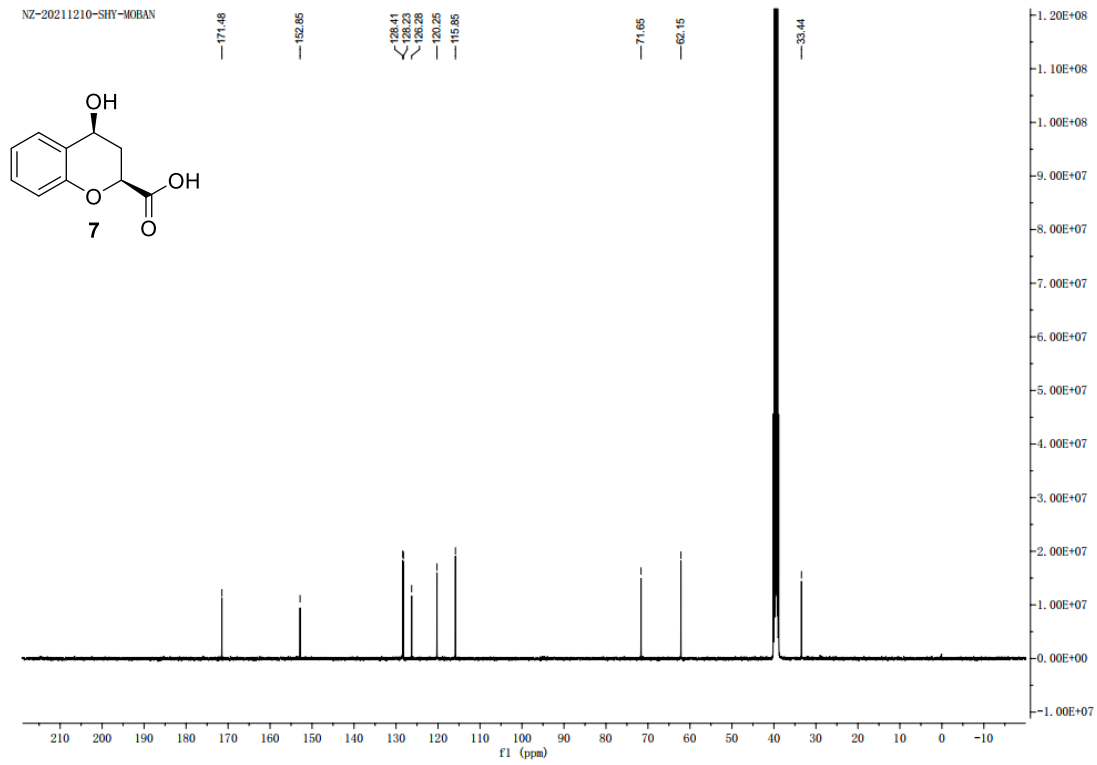


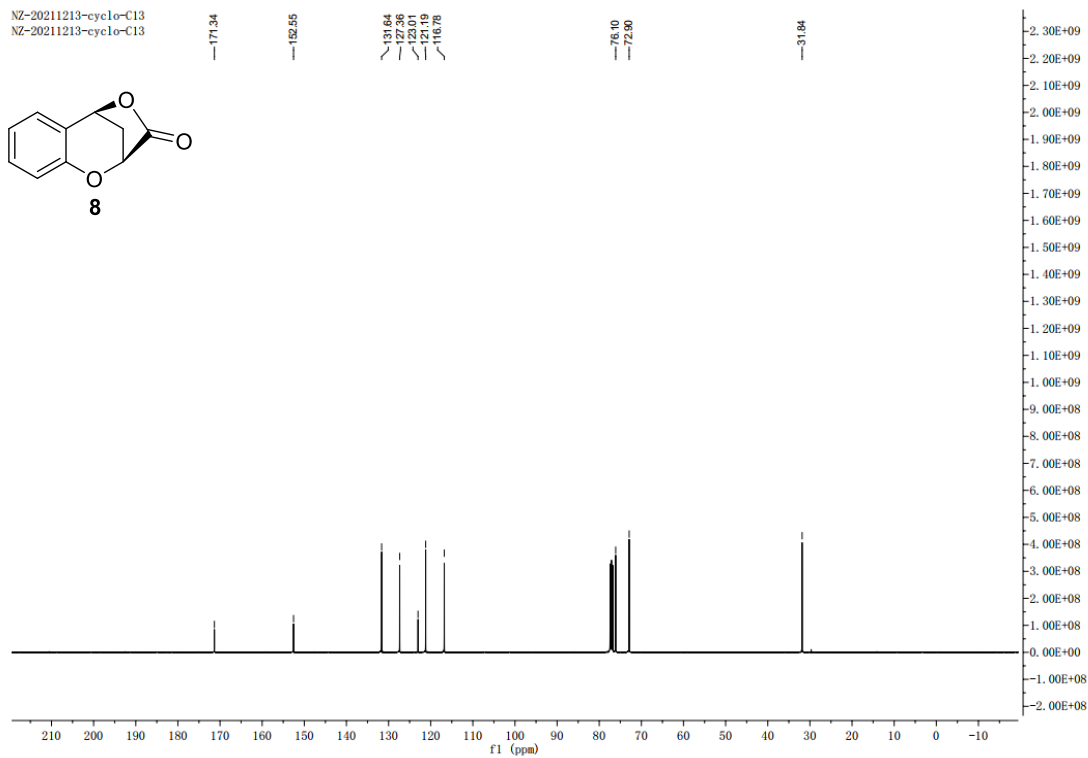
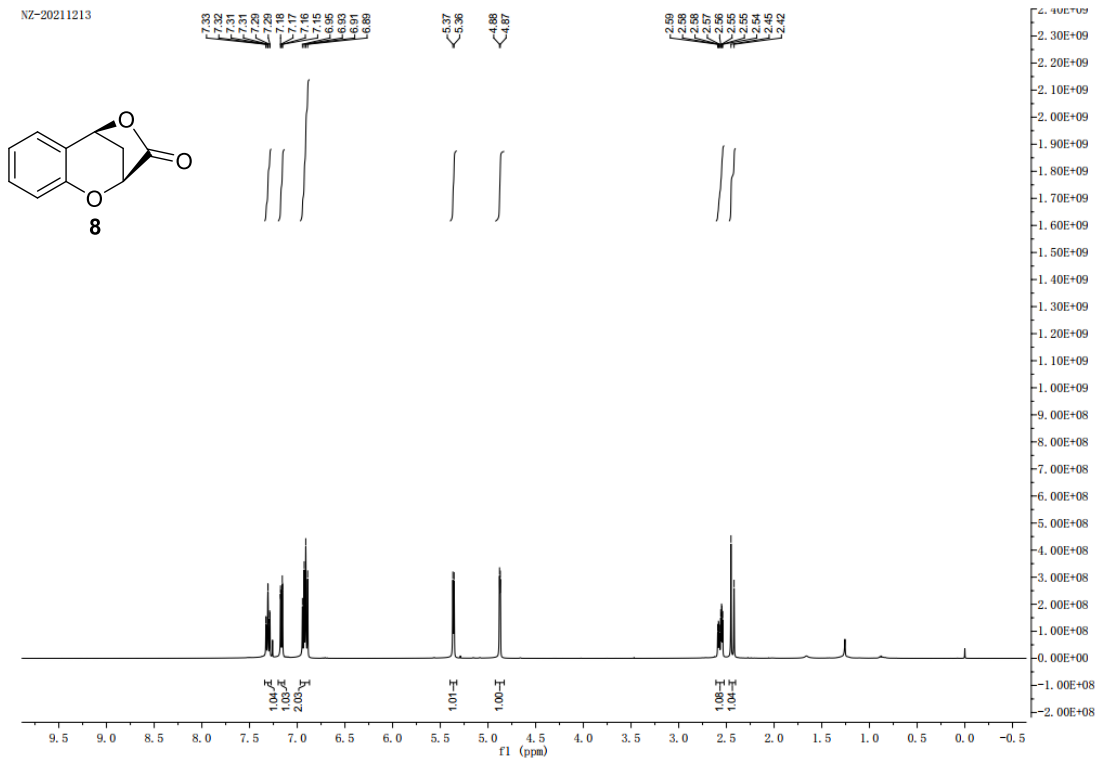


NZ-20211208-SHY-moban-H1

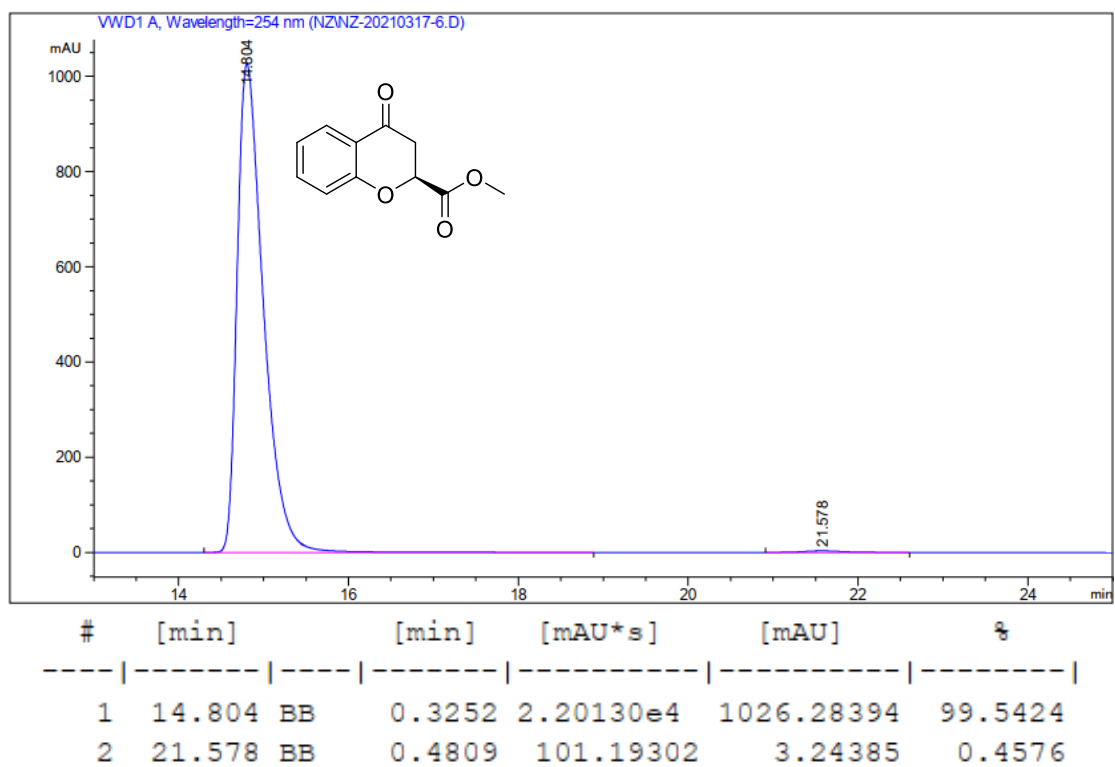
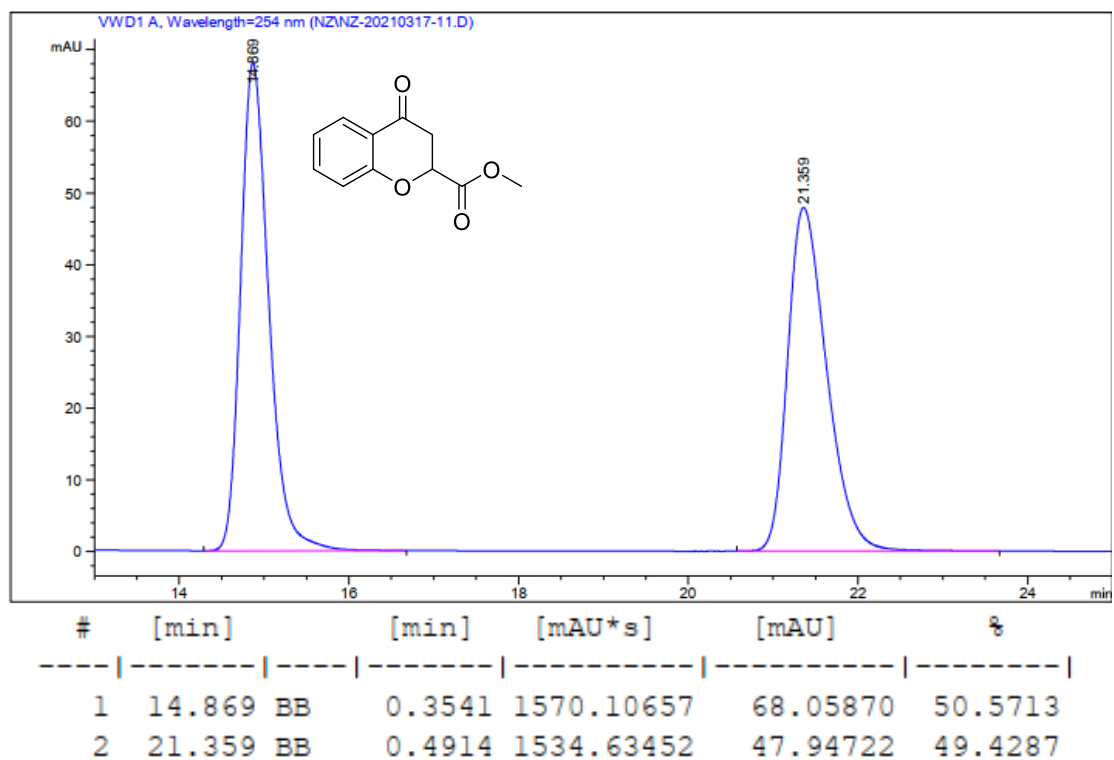


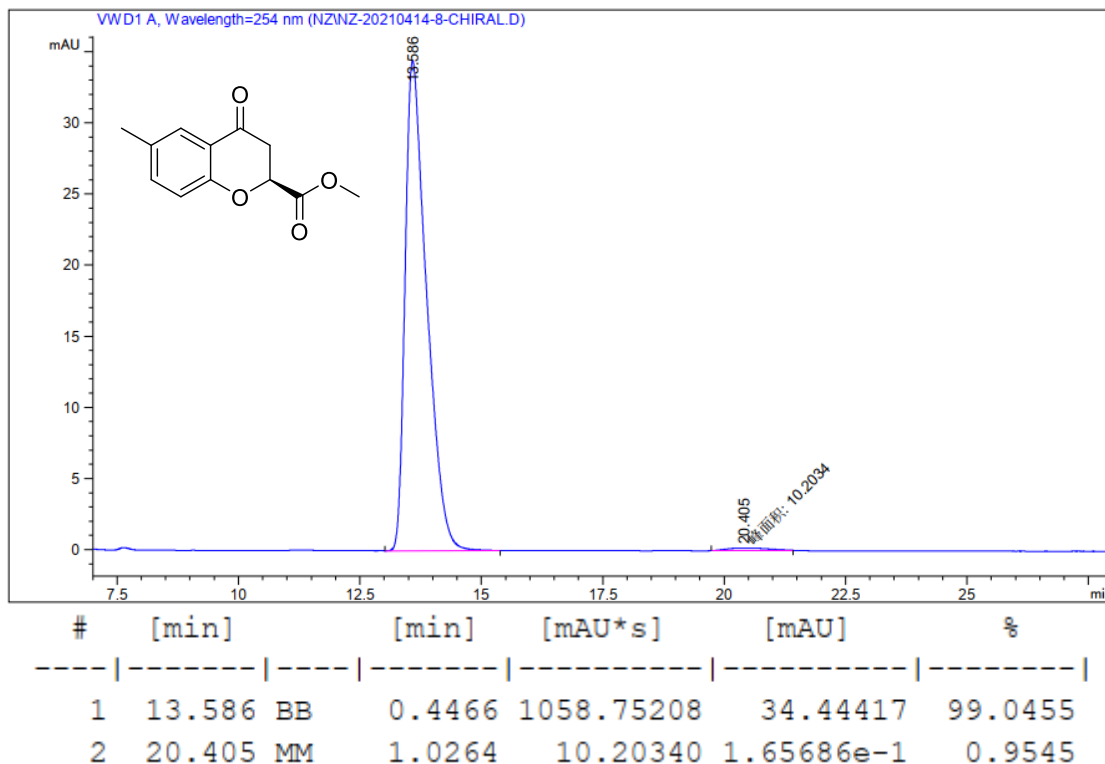
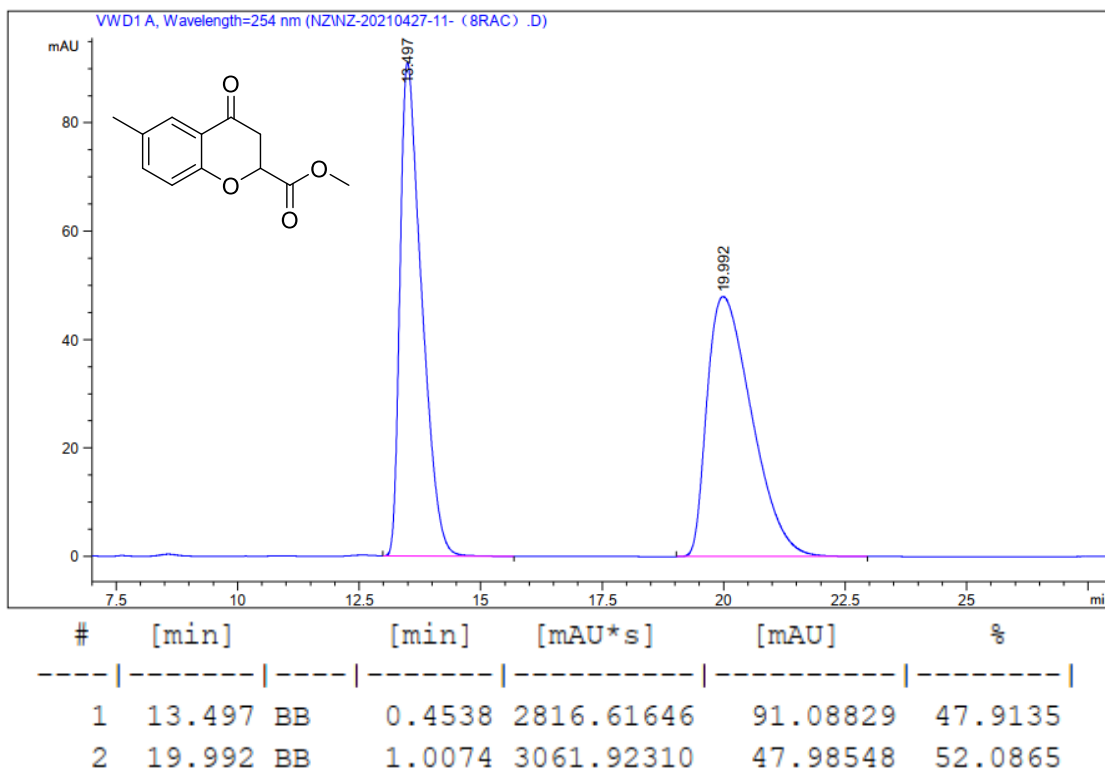
NZ-20211210-SHY-MOBAN

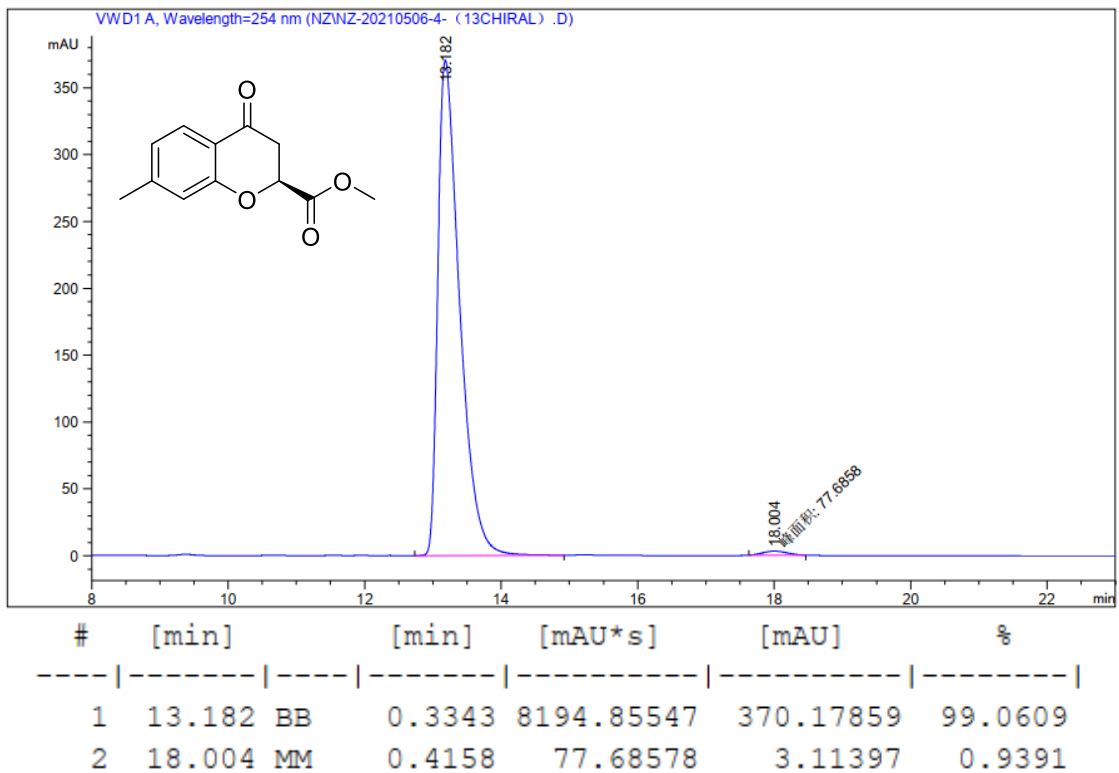
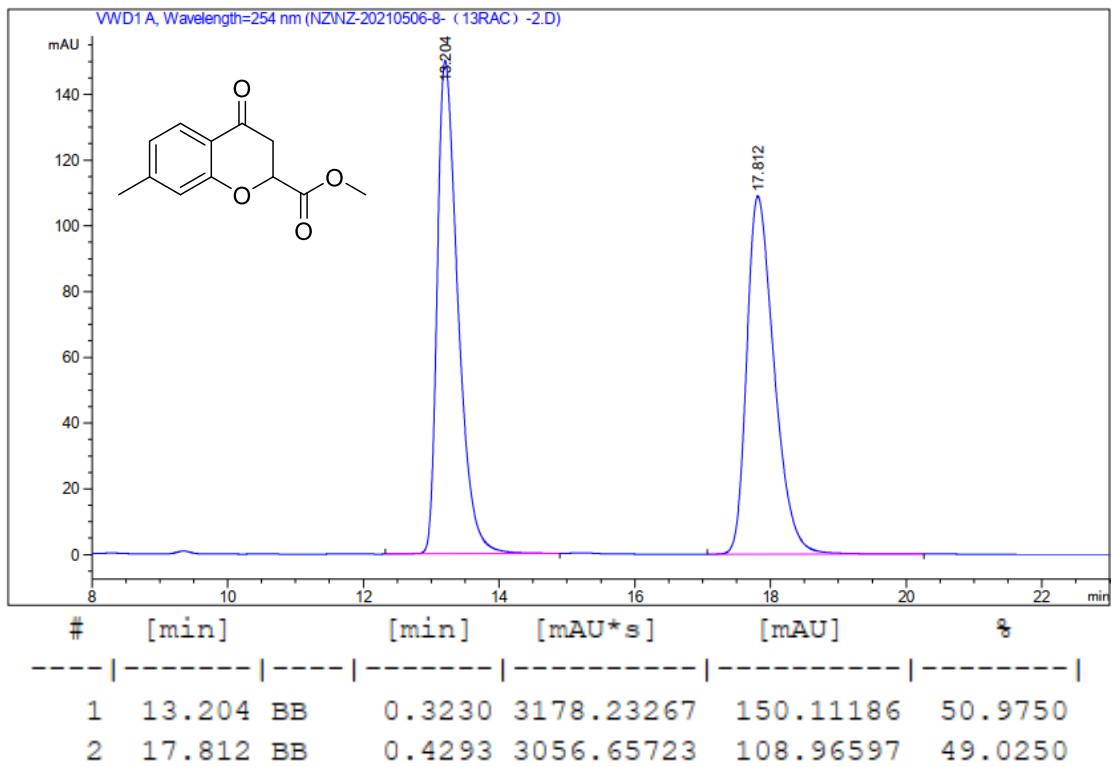


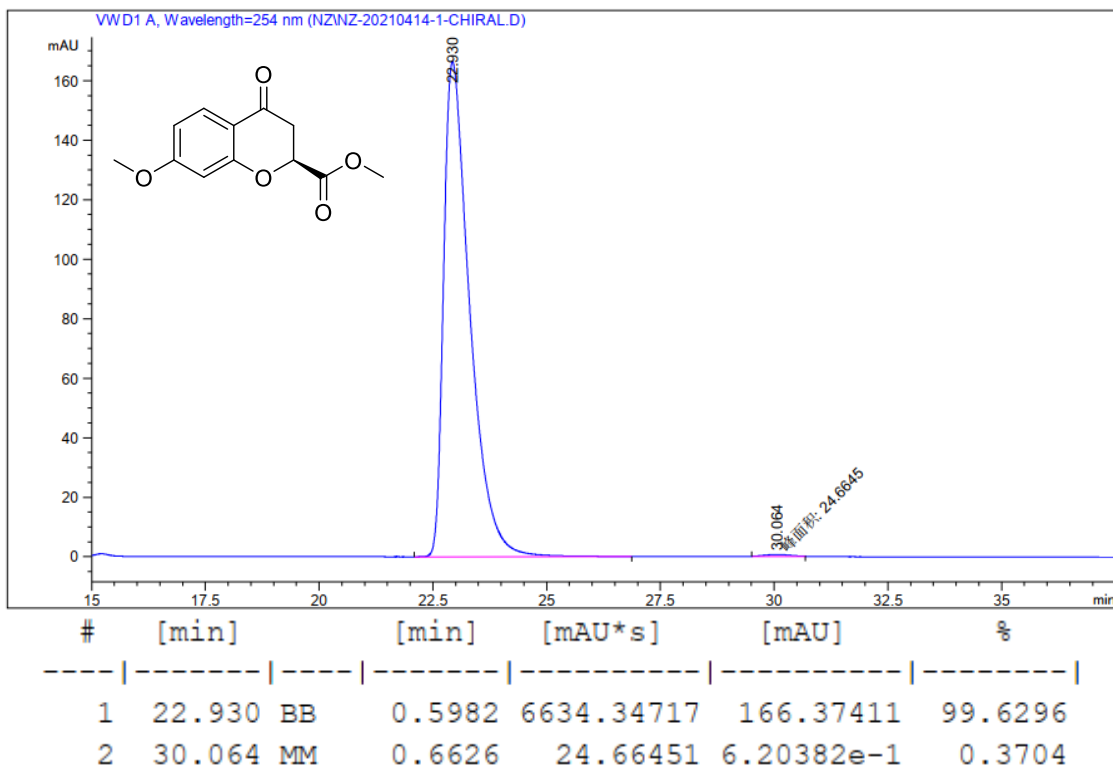
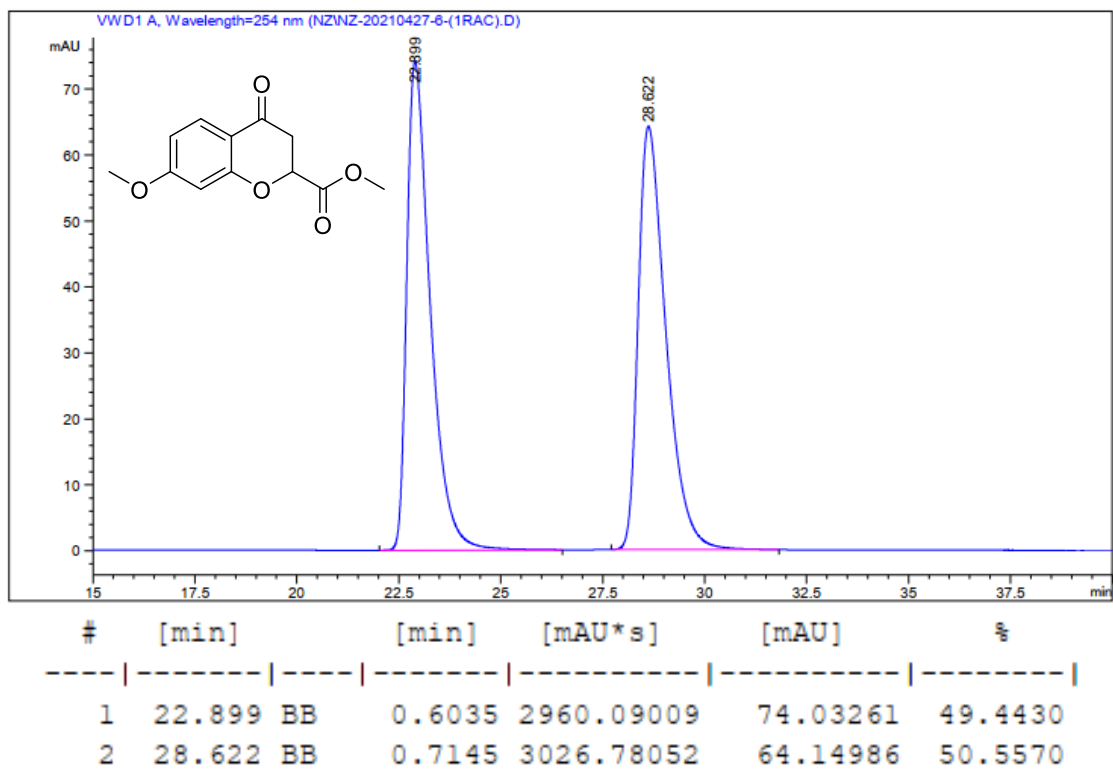


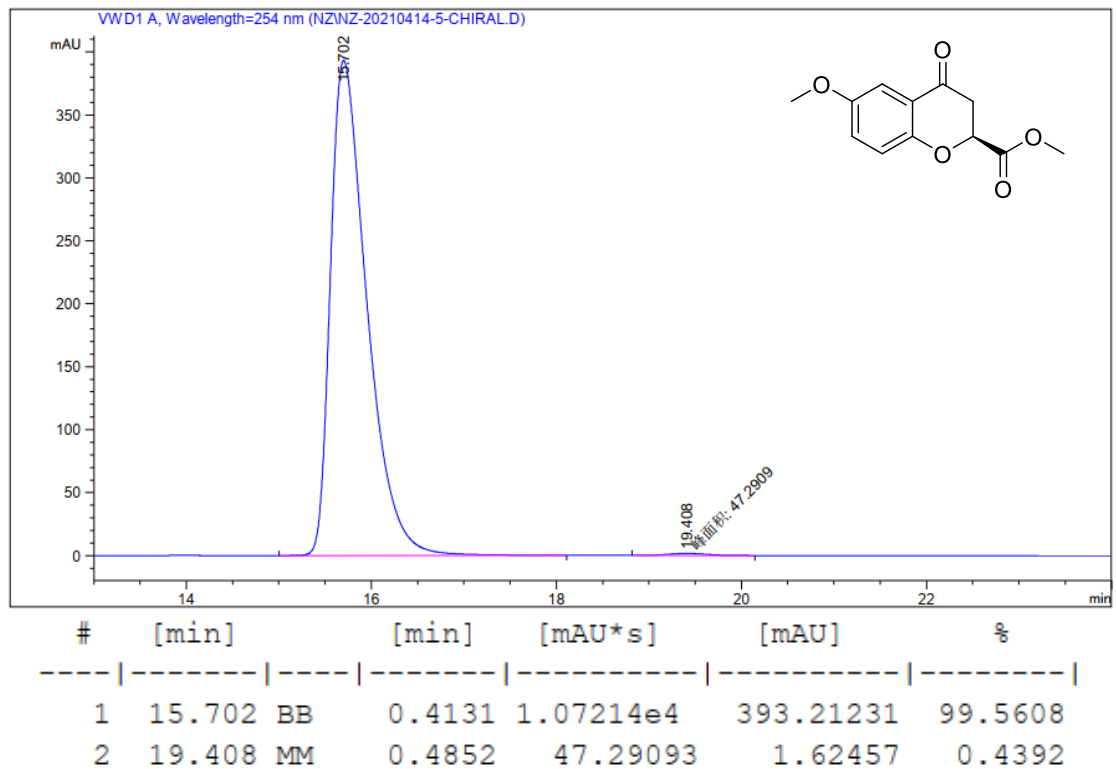
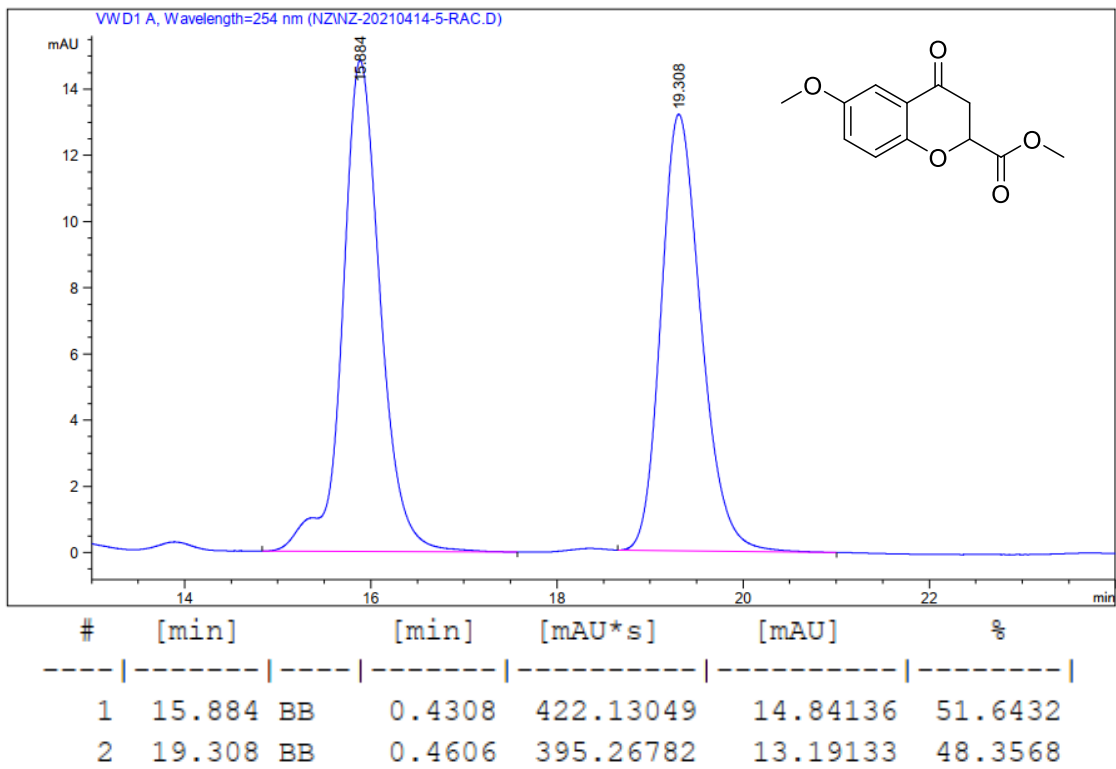
9. HPLC spectra

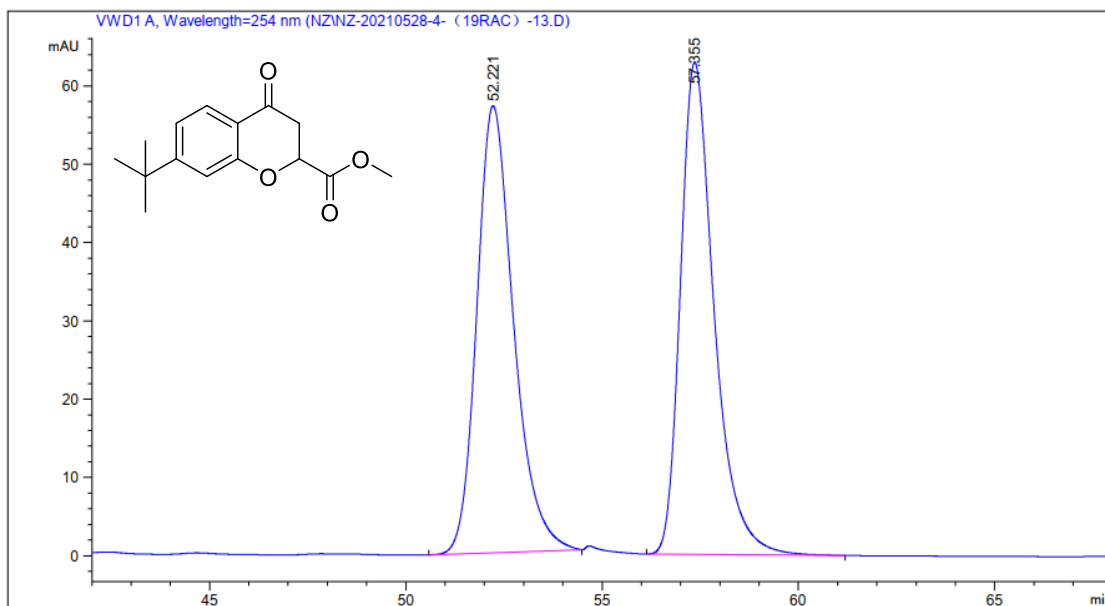




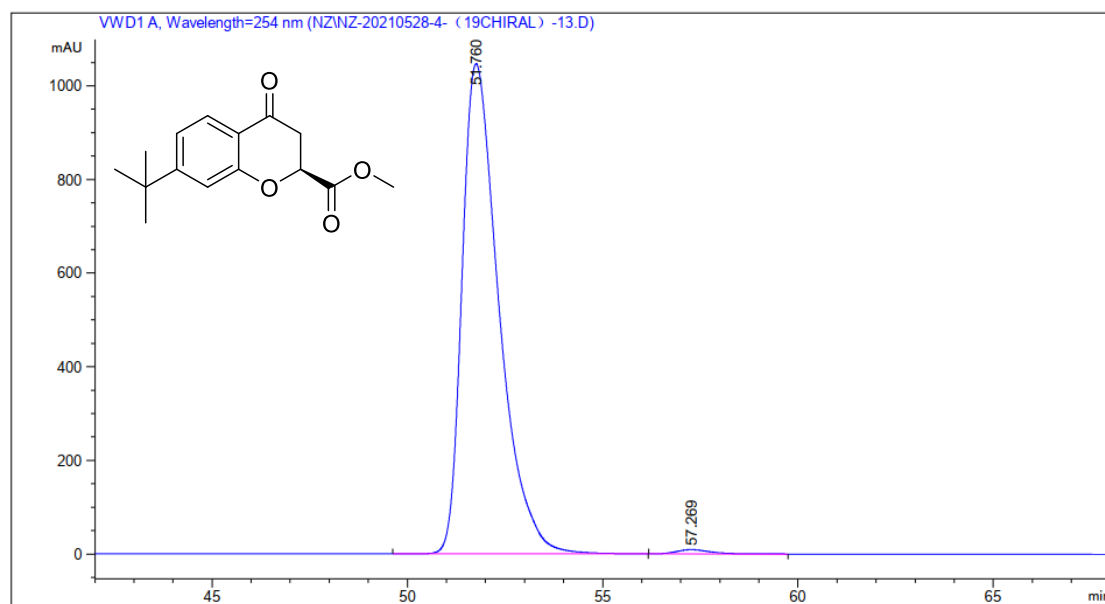




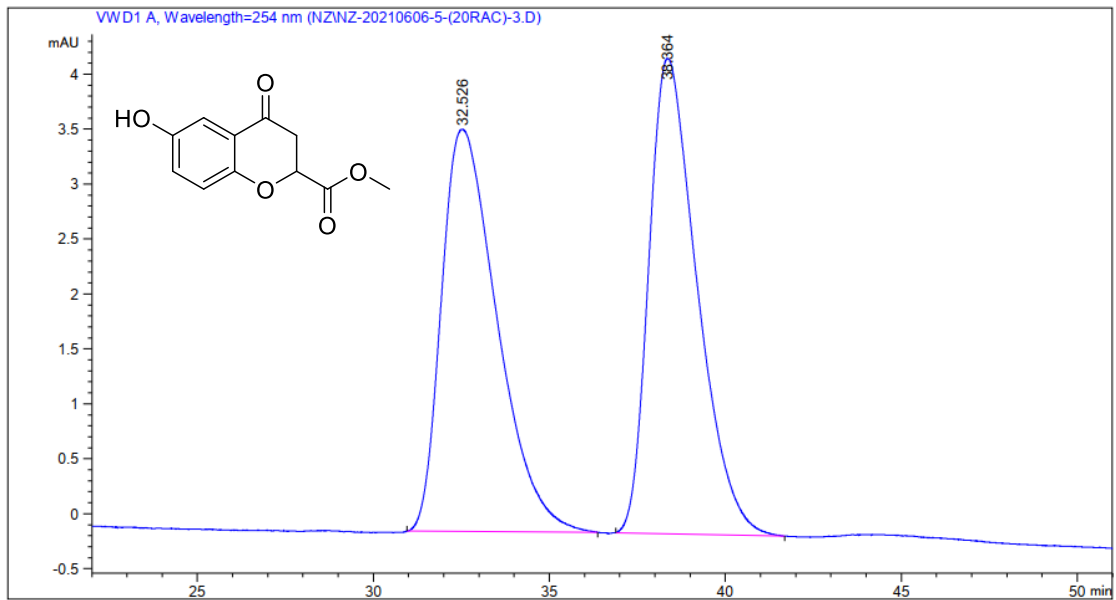




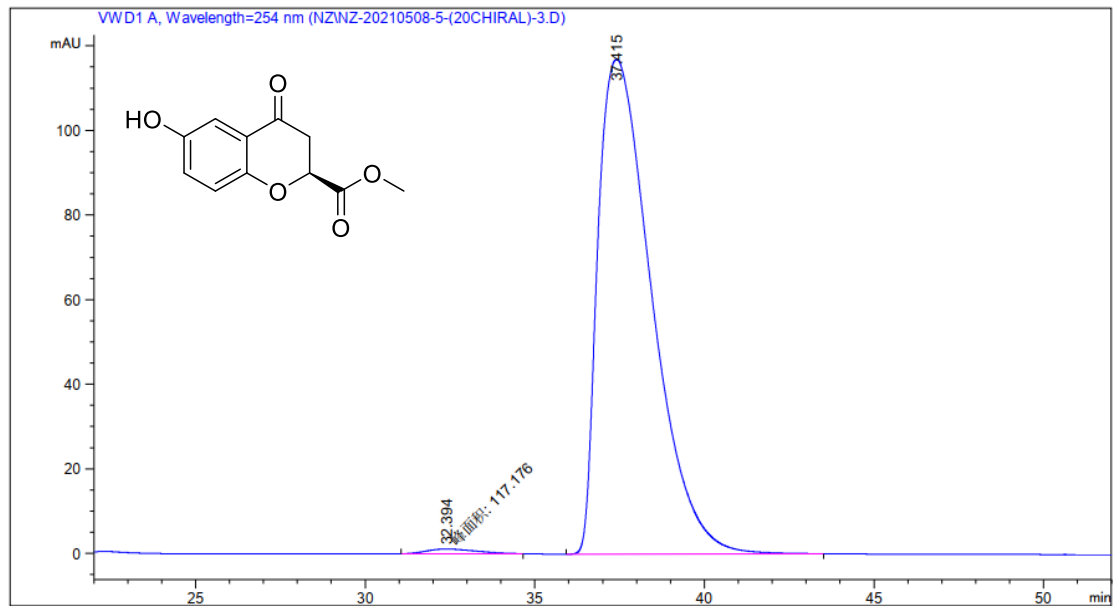
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	52.221	BB	0.9821	3713.38062	57.07147	49.7561
2	57.355	BB	0.9012	3749.77930	62.84079	50.2439



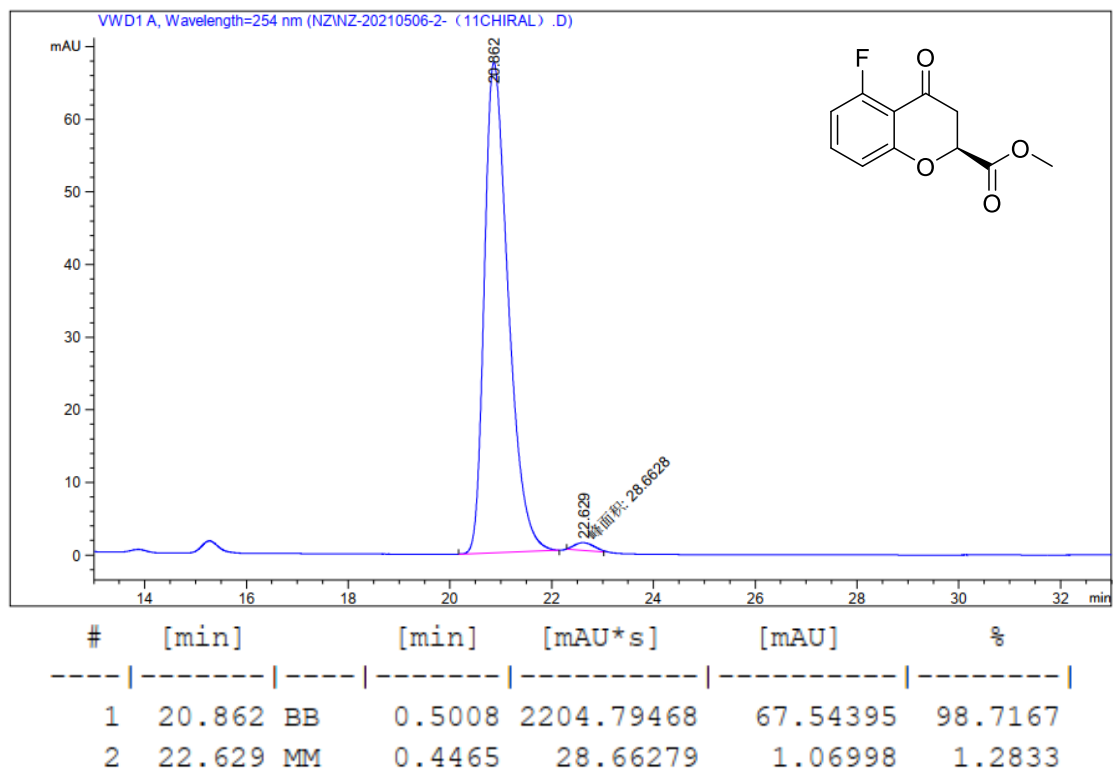
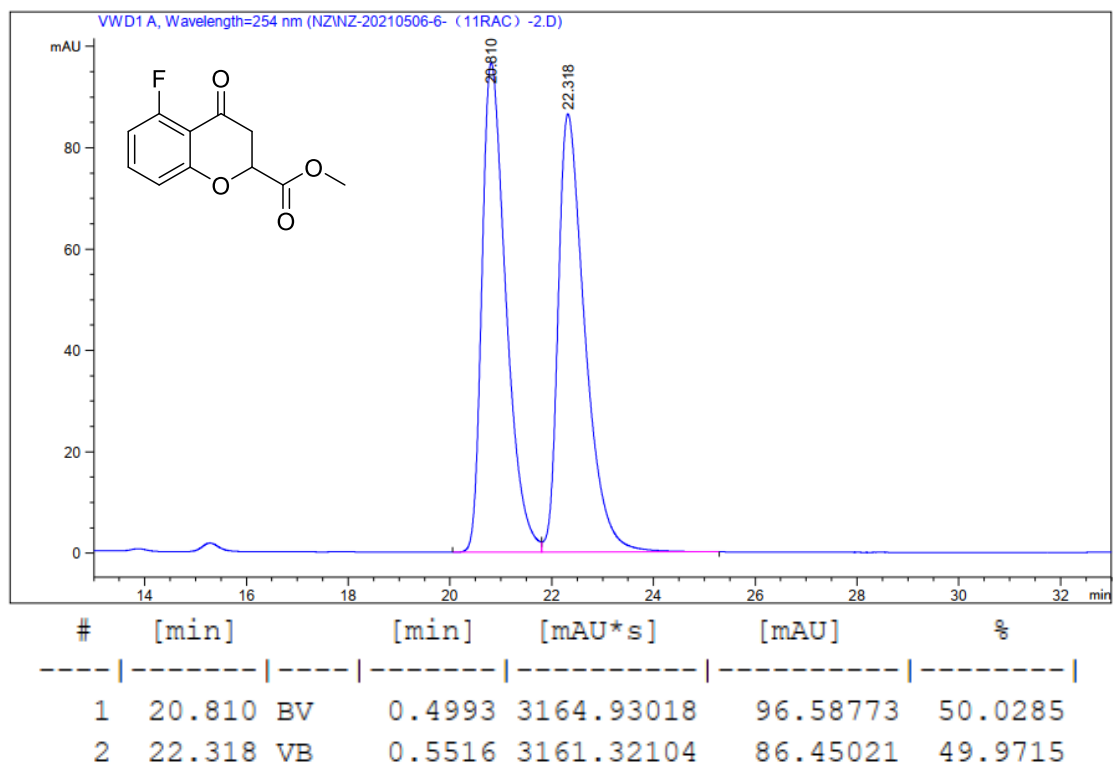
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	51.760	BB	0.9980	6.86516e4	1047.04053	99.2298
2	57.269	BB	0.8782	532.82947	9.00704	0.7702

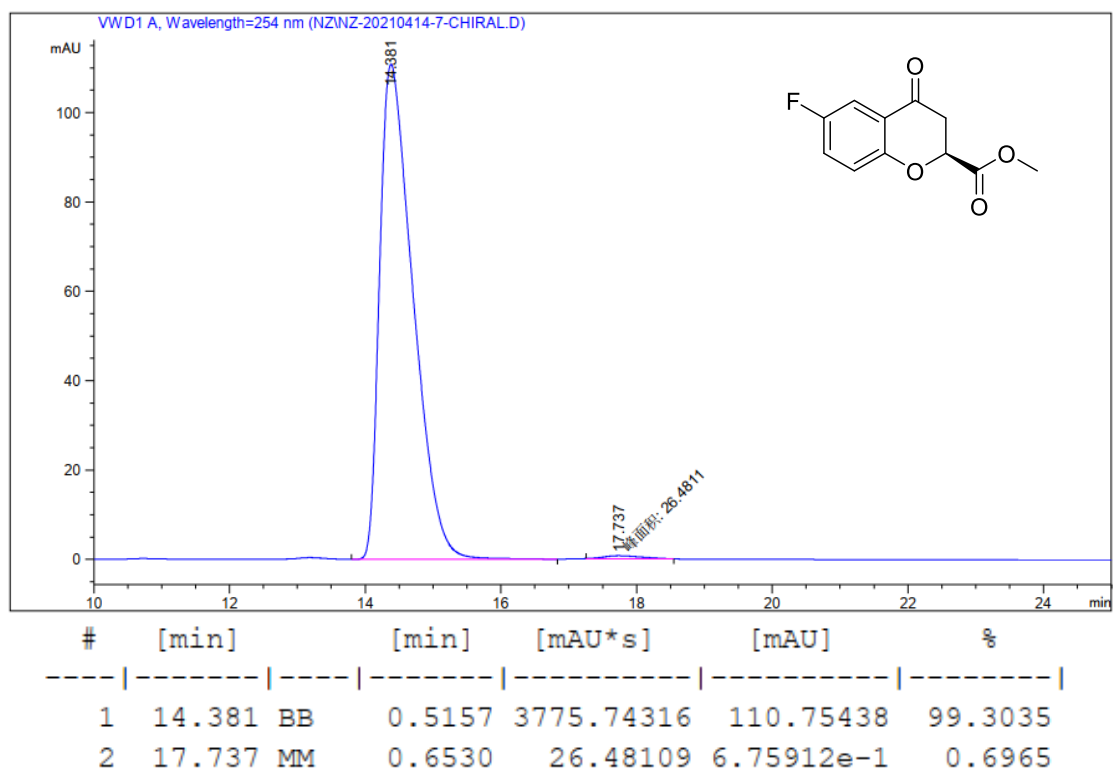
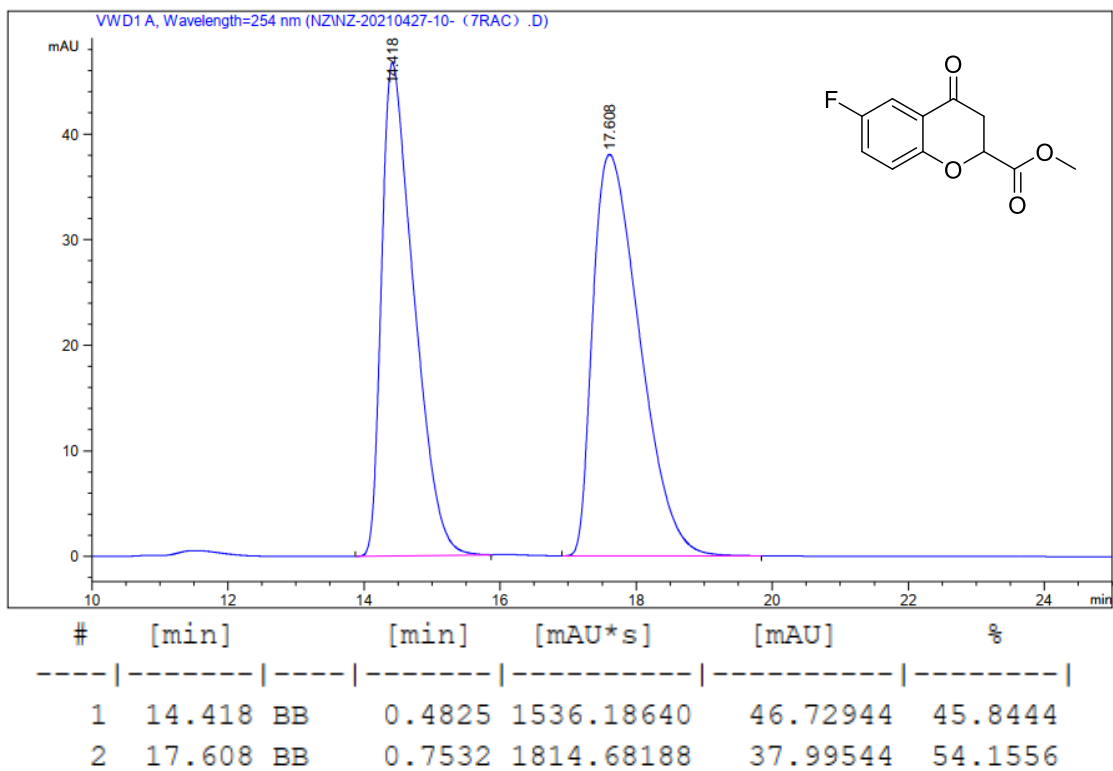


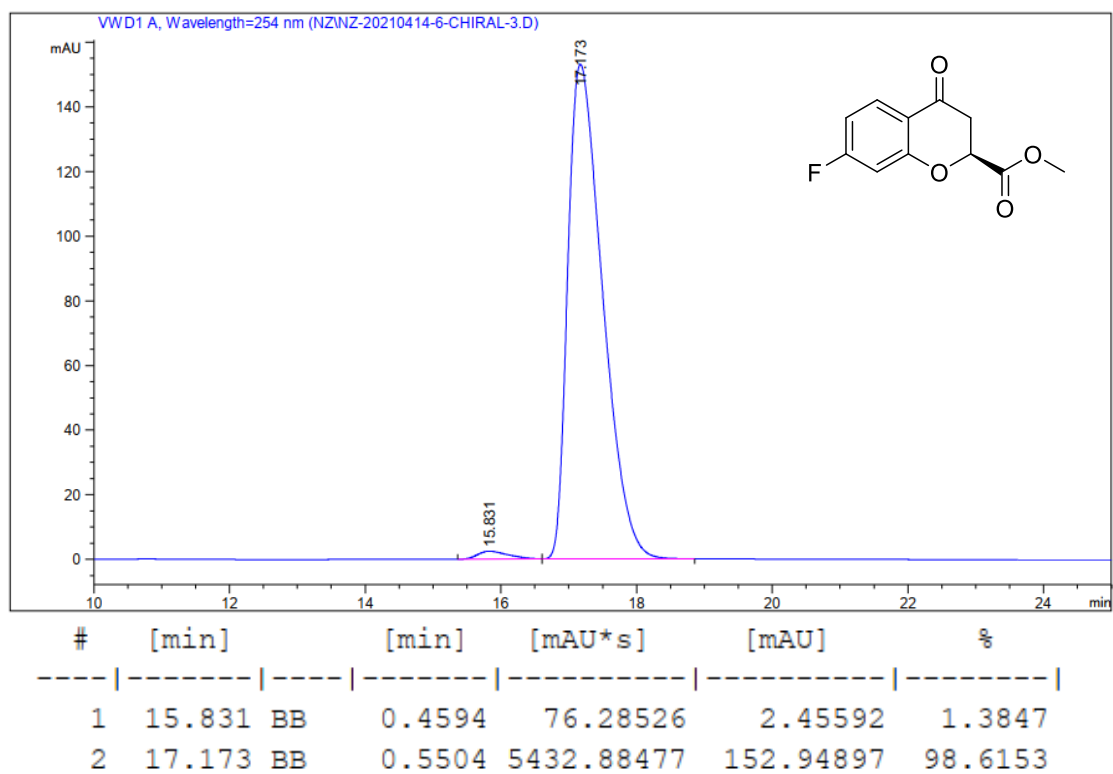
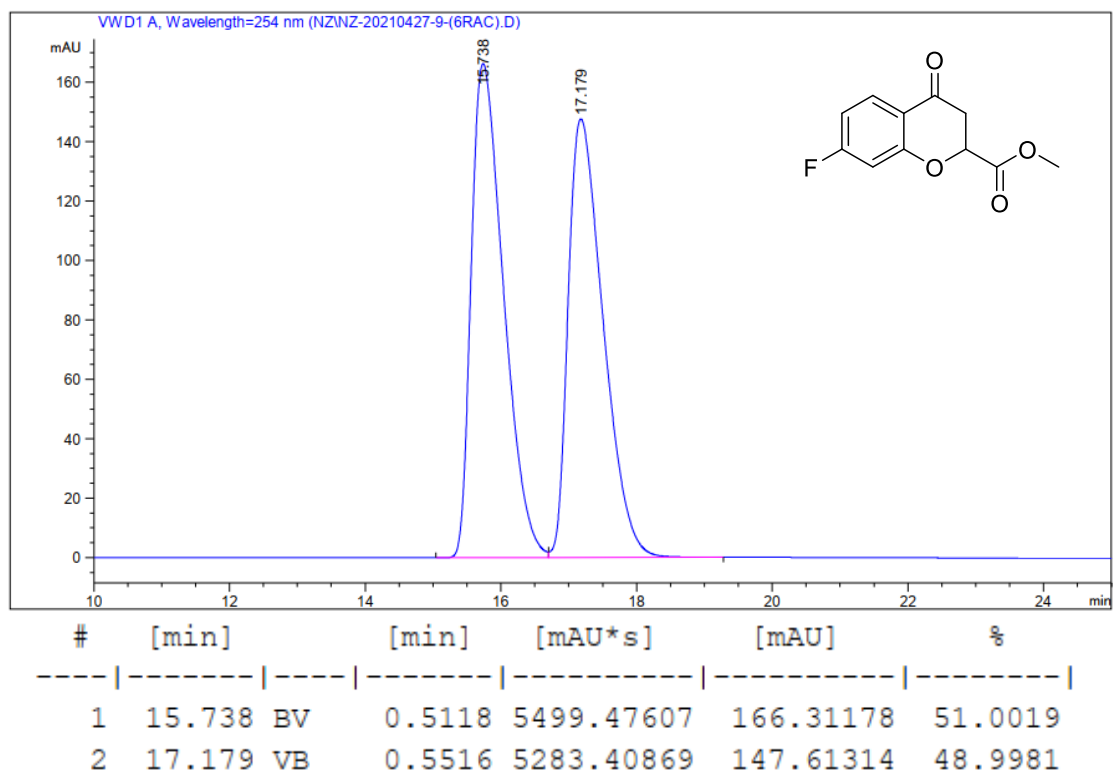
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	32.526	BB	1.2894	401.59351	3.65931	49.4285
2	38.364	BB	1.1446	410.87961	4.32415	50.5715

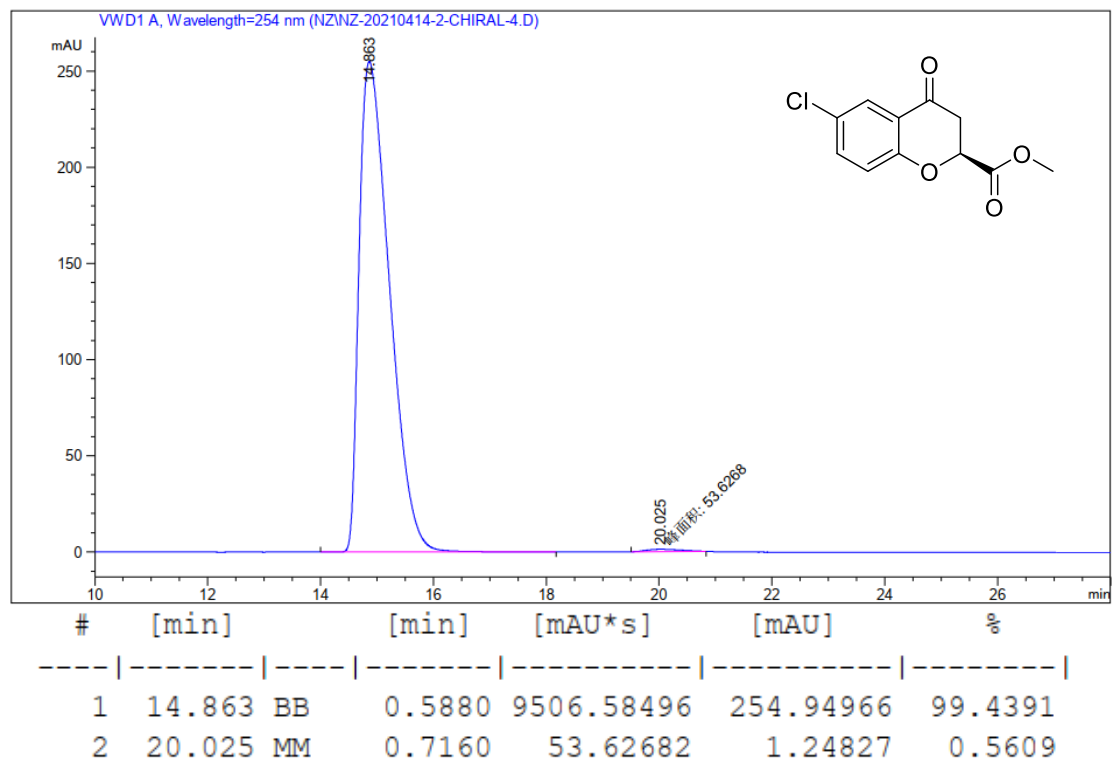
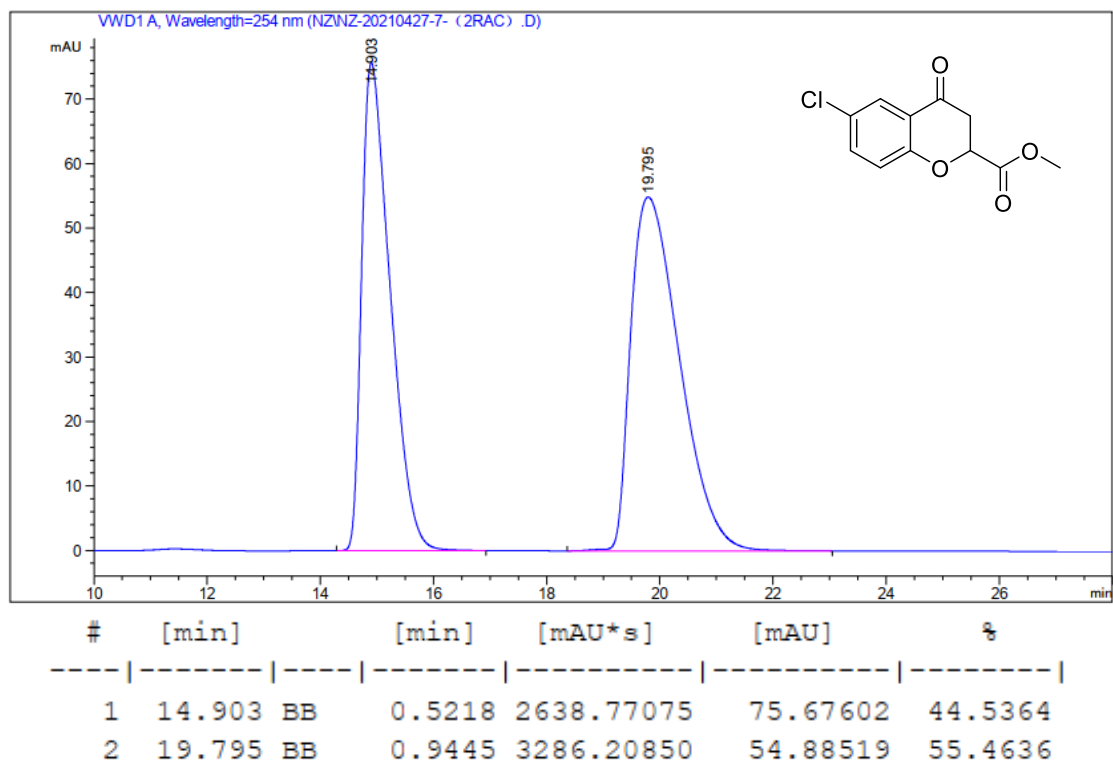


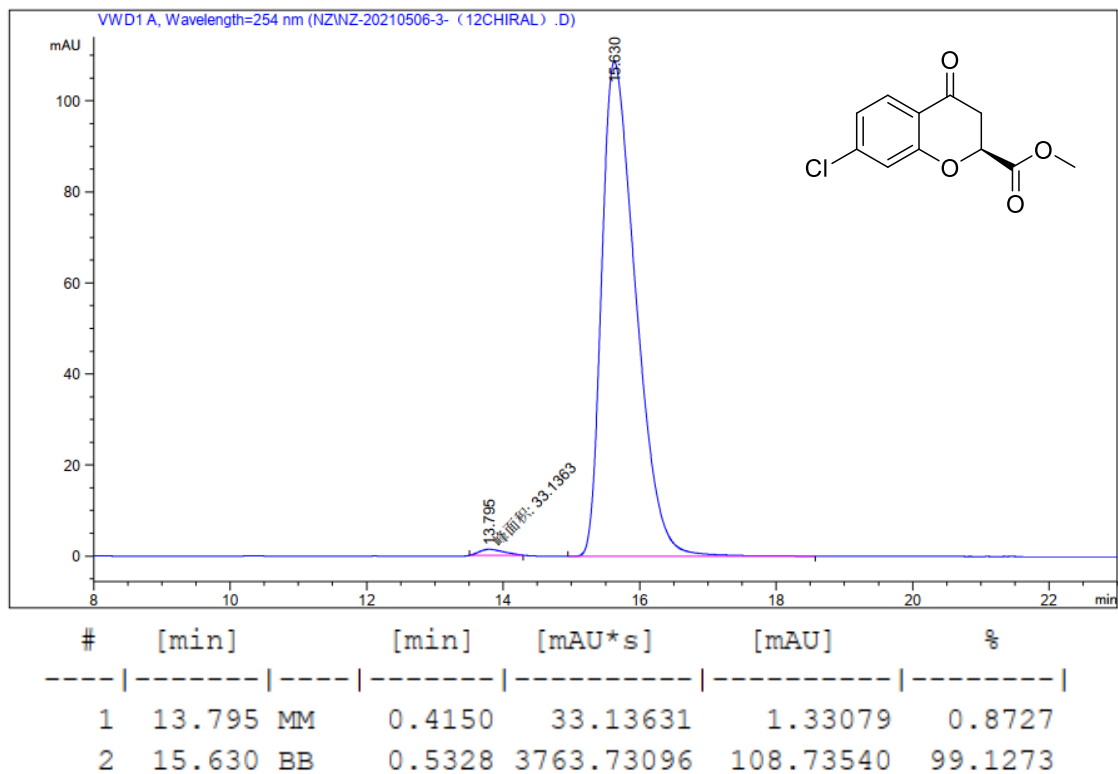
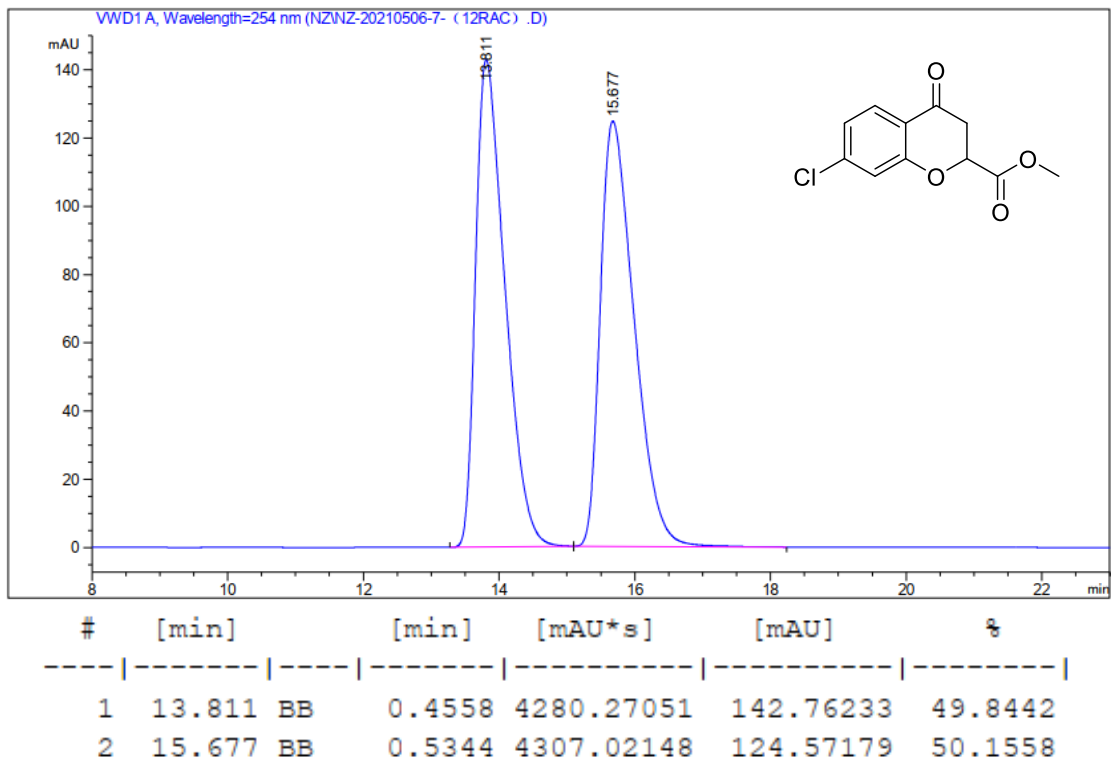
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	32.394	MM	1.7091	117.17614	1.14268	0.9043
2	37.415	BB	1.7030	1.28400e4	116.93877	99.0957

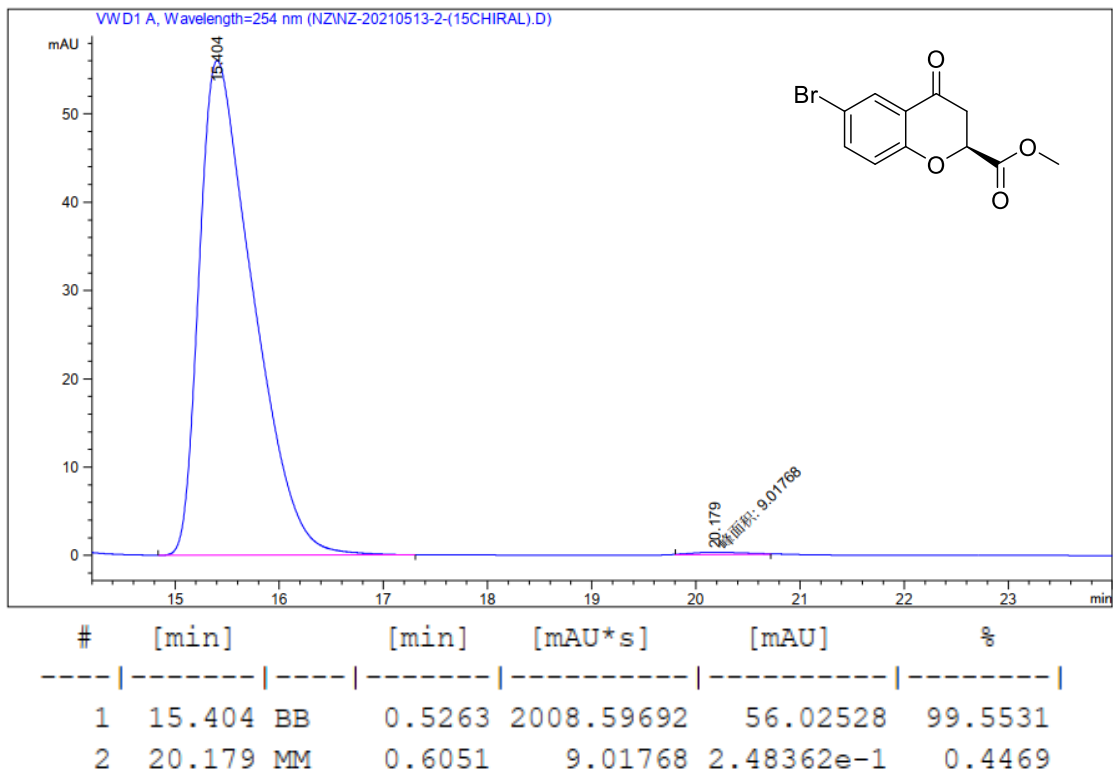
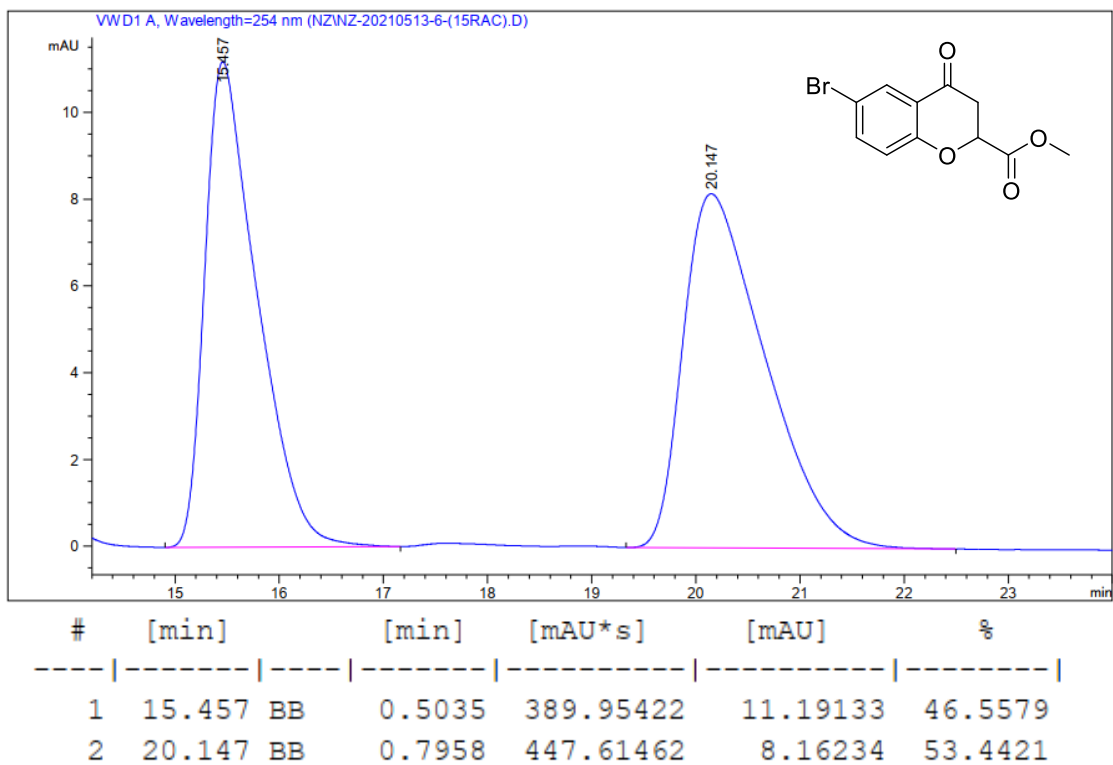


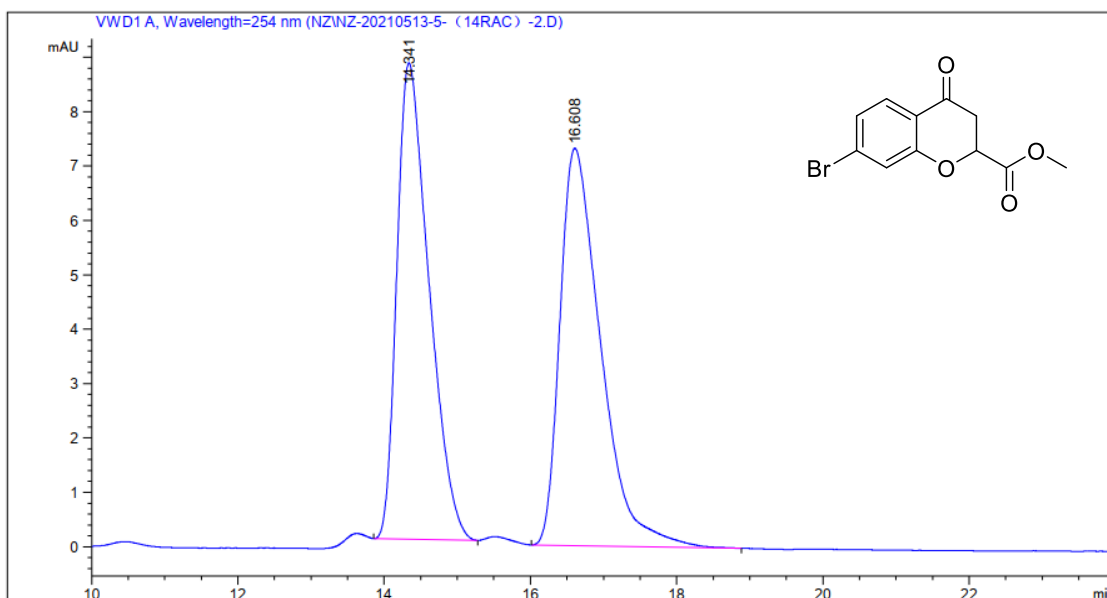




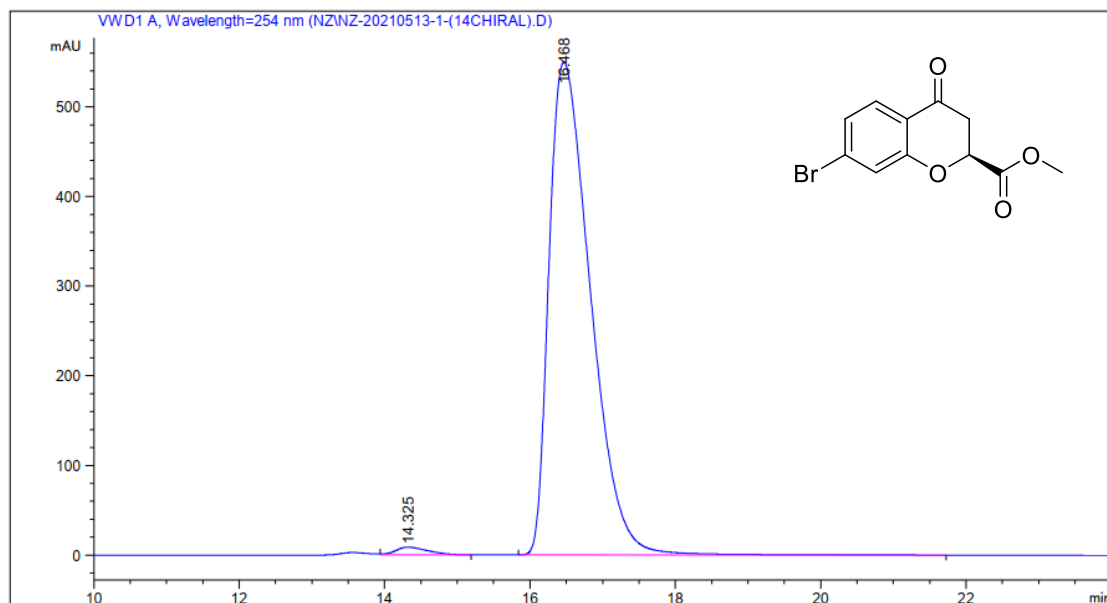




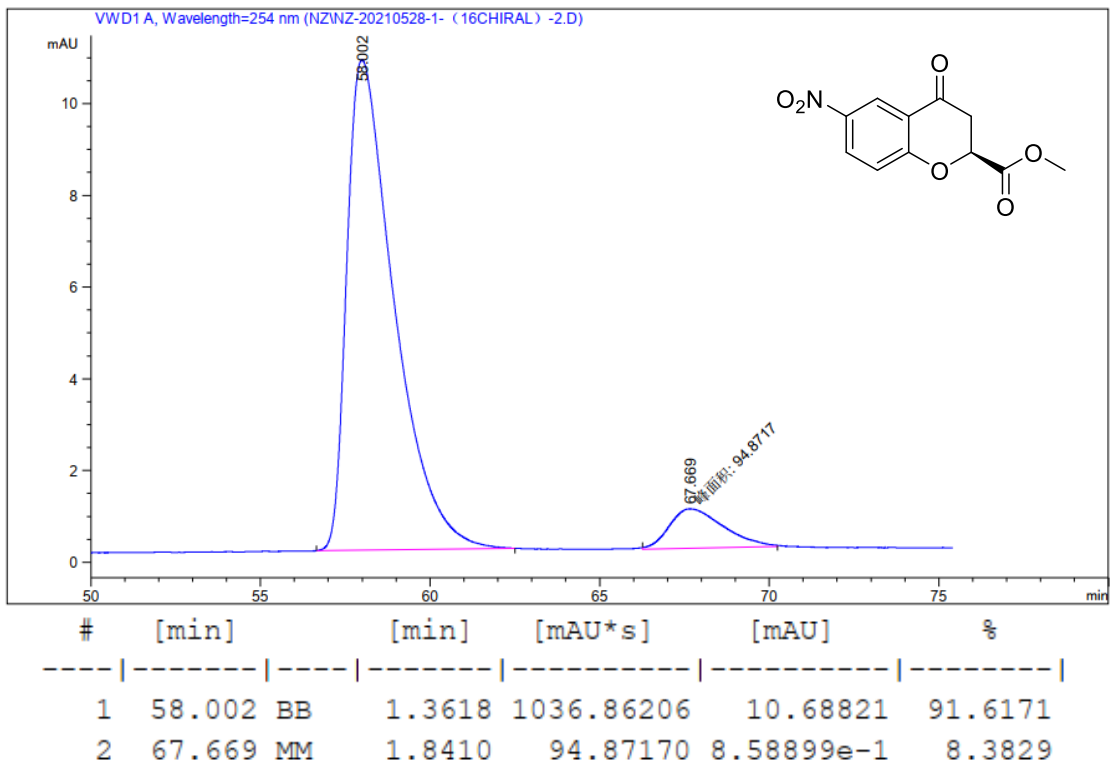
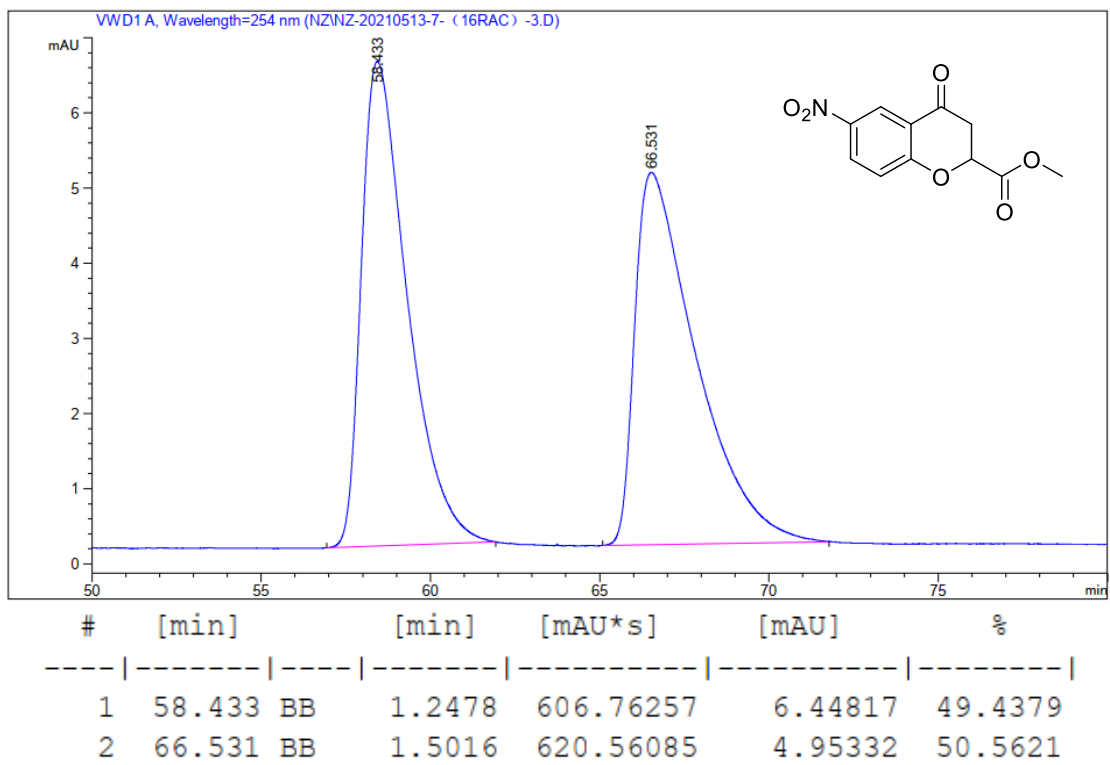


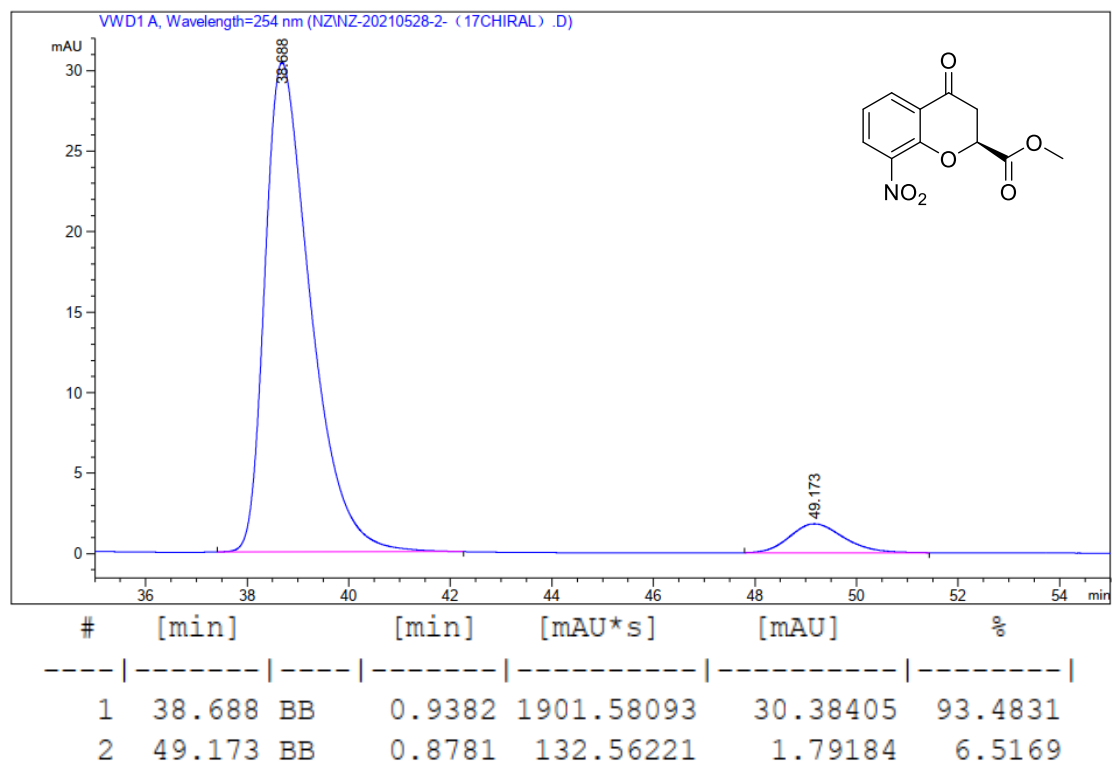
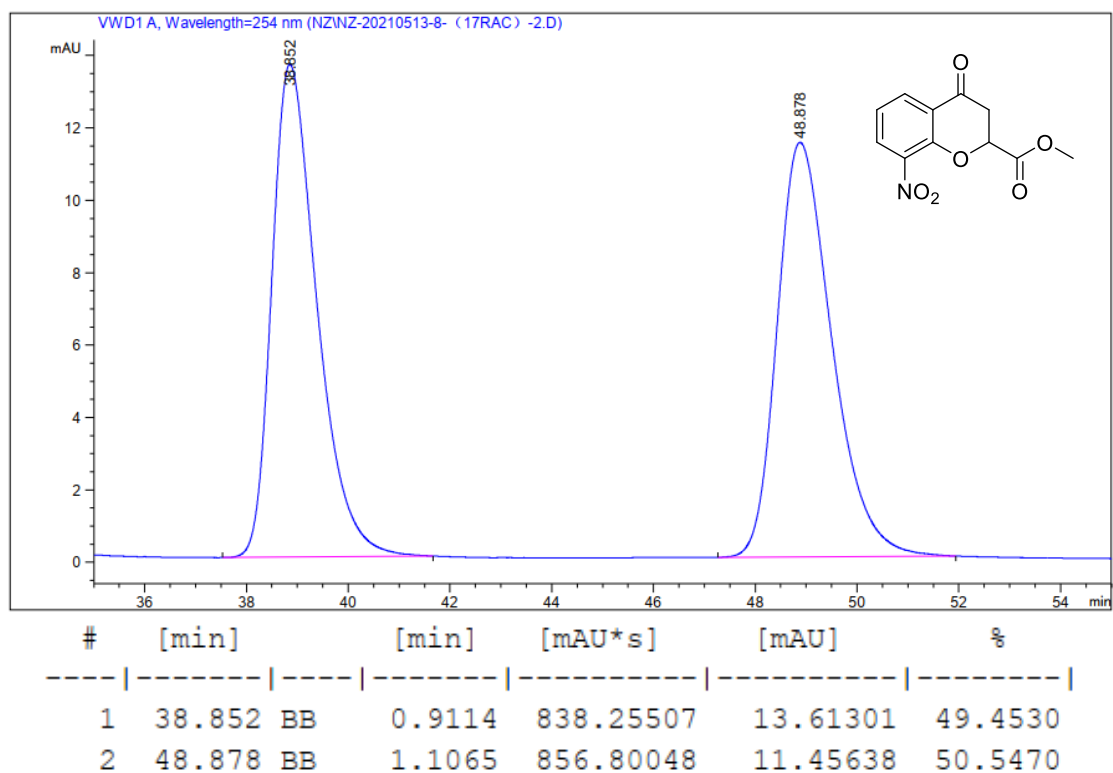


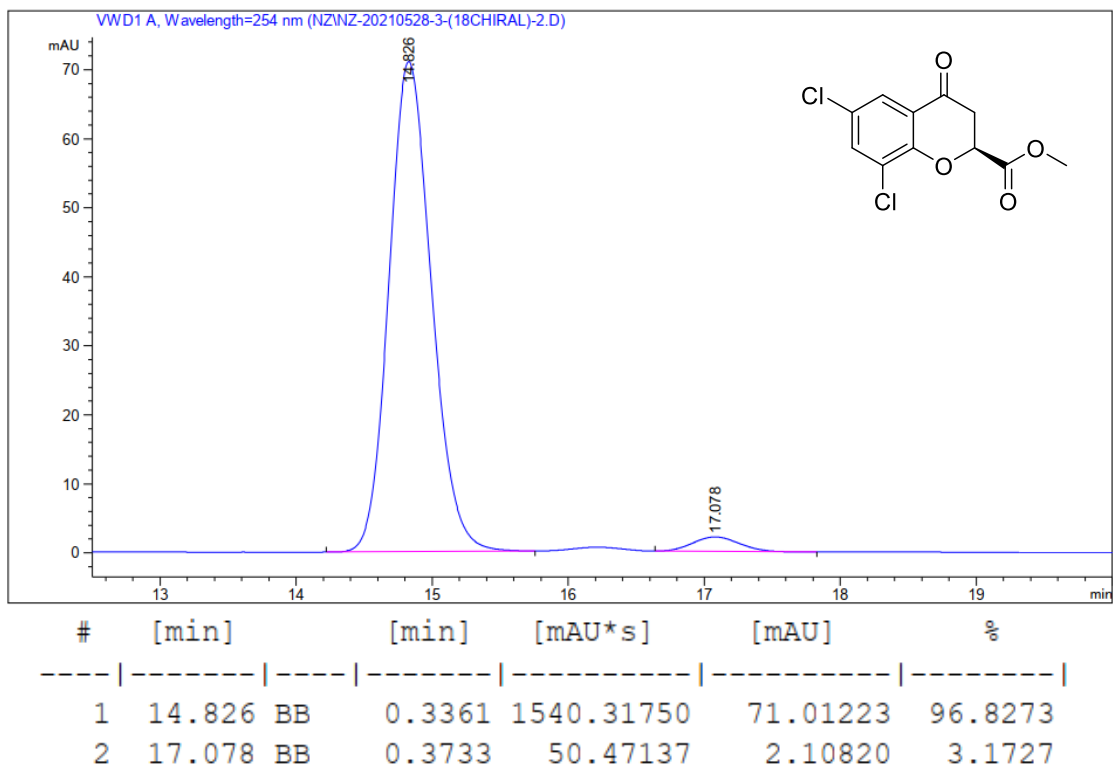
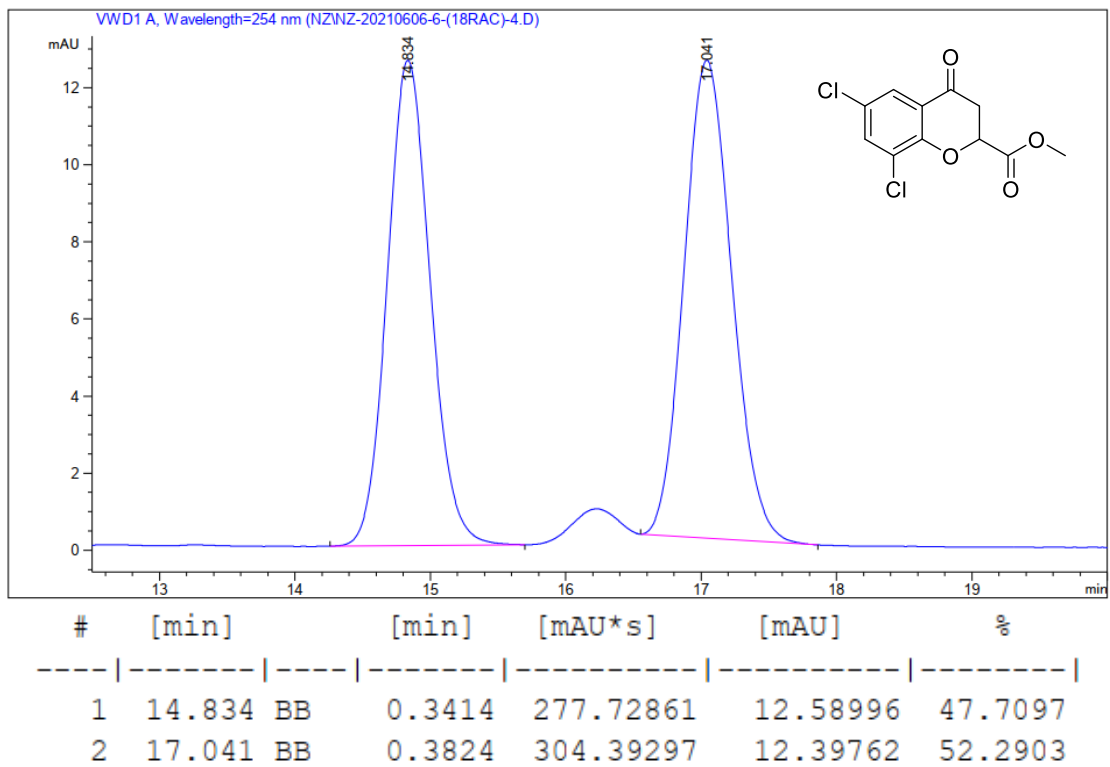
#	[min]		[min]	[mAU*s]	[mAU]	%
1	14.341	BB	0.4536	266.96771	8.75865	48.6324
2	16.608	BB	0.5662	281.98279	7.30722	51.3676

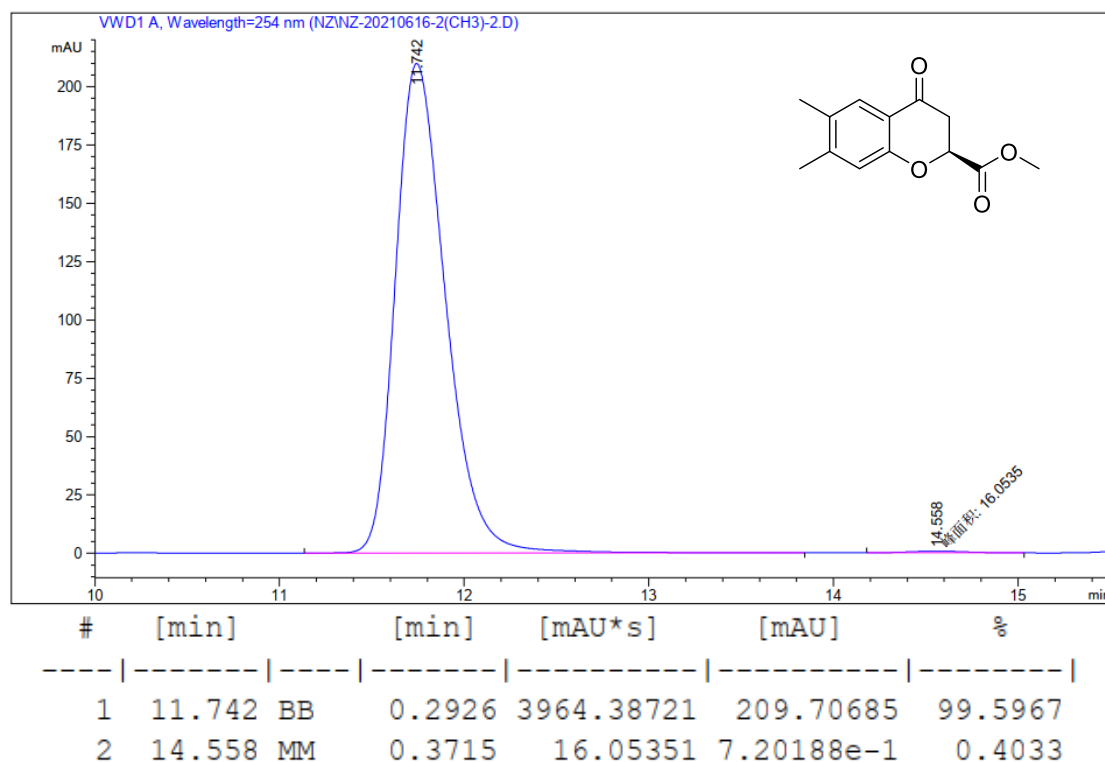
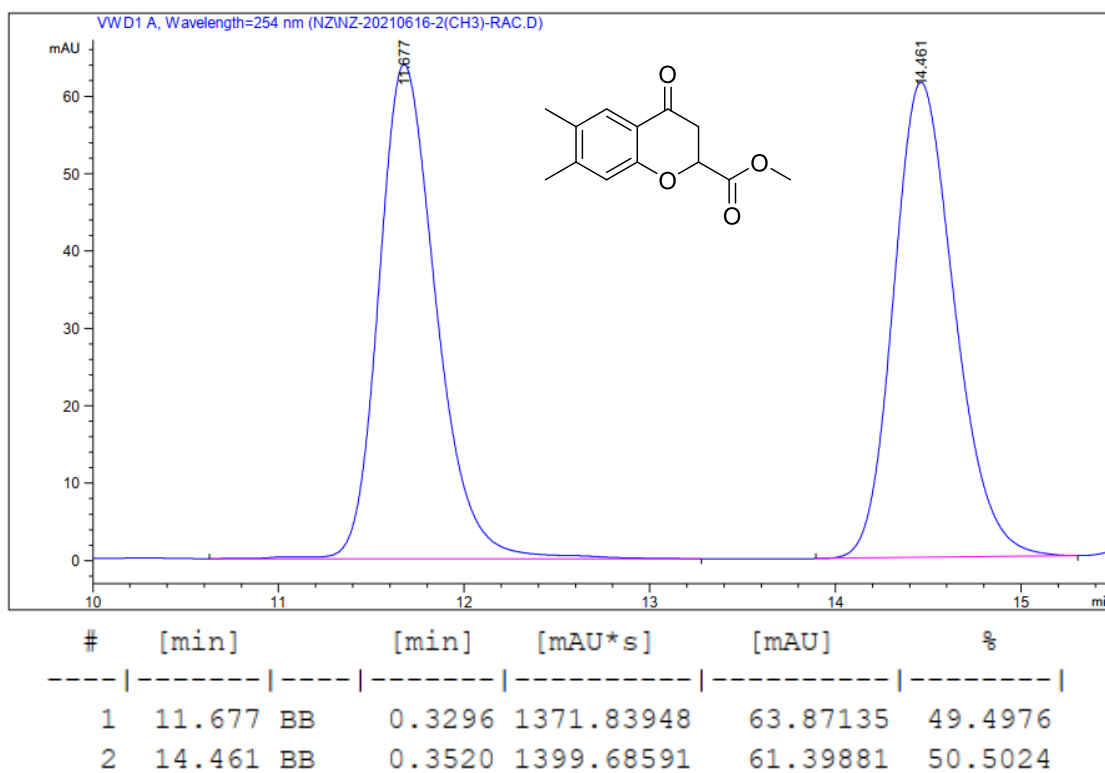


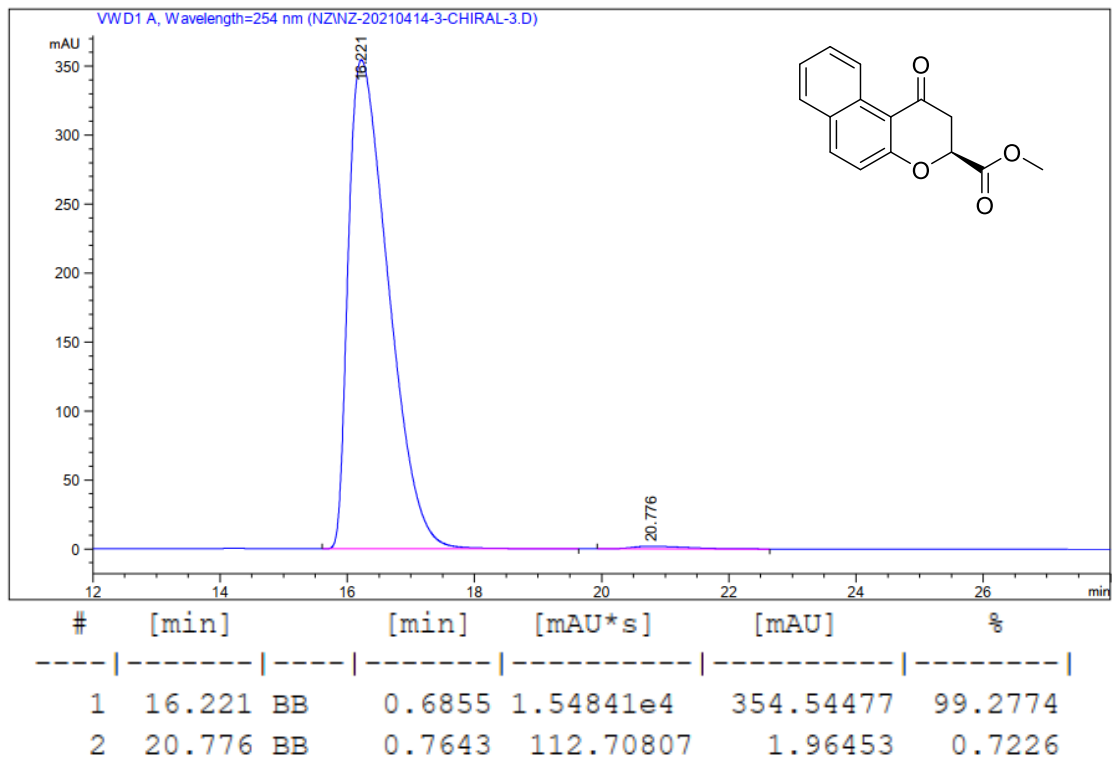
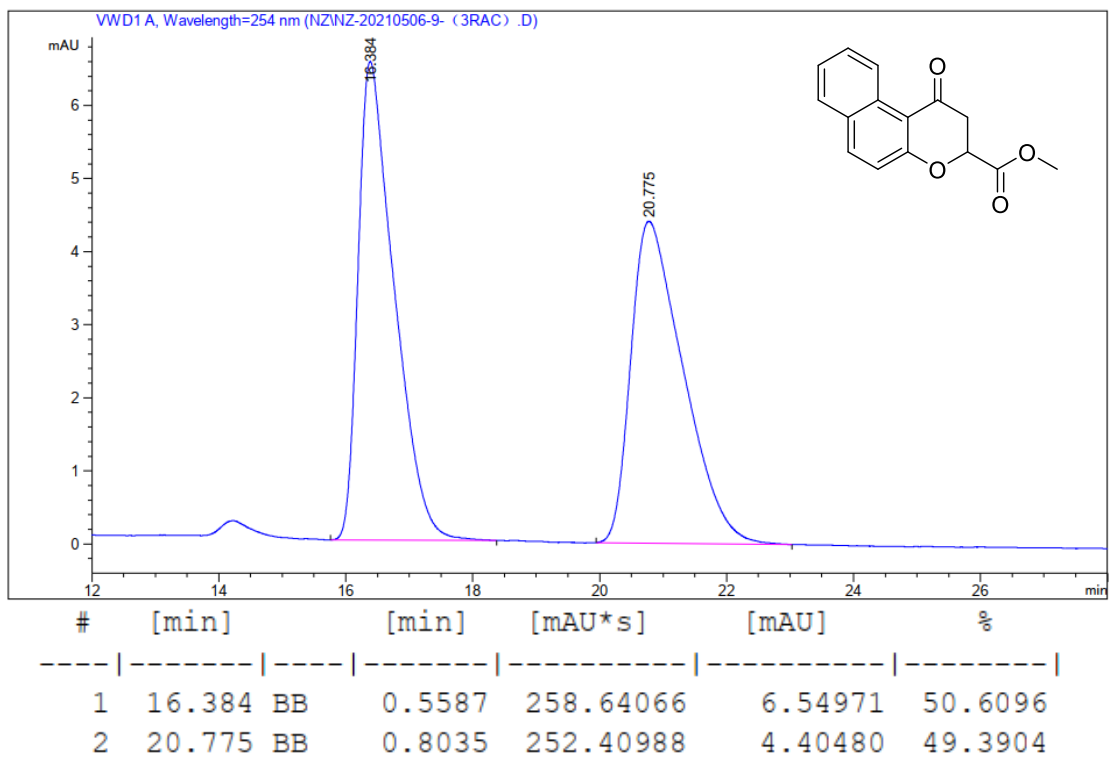
#	[min]		[min]	[mAU*s]	[mAU]	%
1	14.325	VB	0.4508	271.33249	8.79790	1.2326
2	16.468	BB	0.6165	2.17425e4	549.69641	98.7674

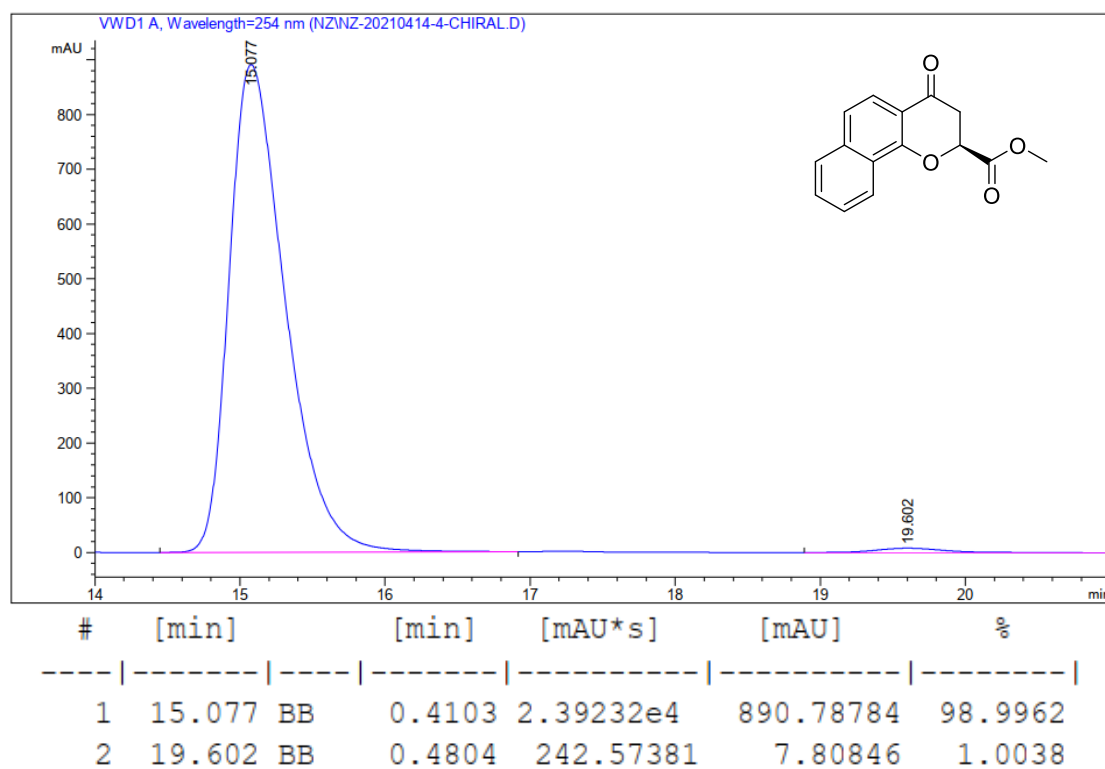
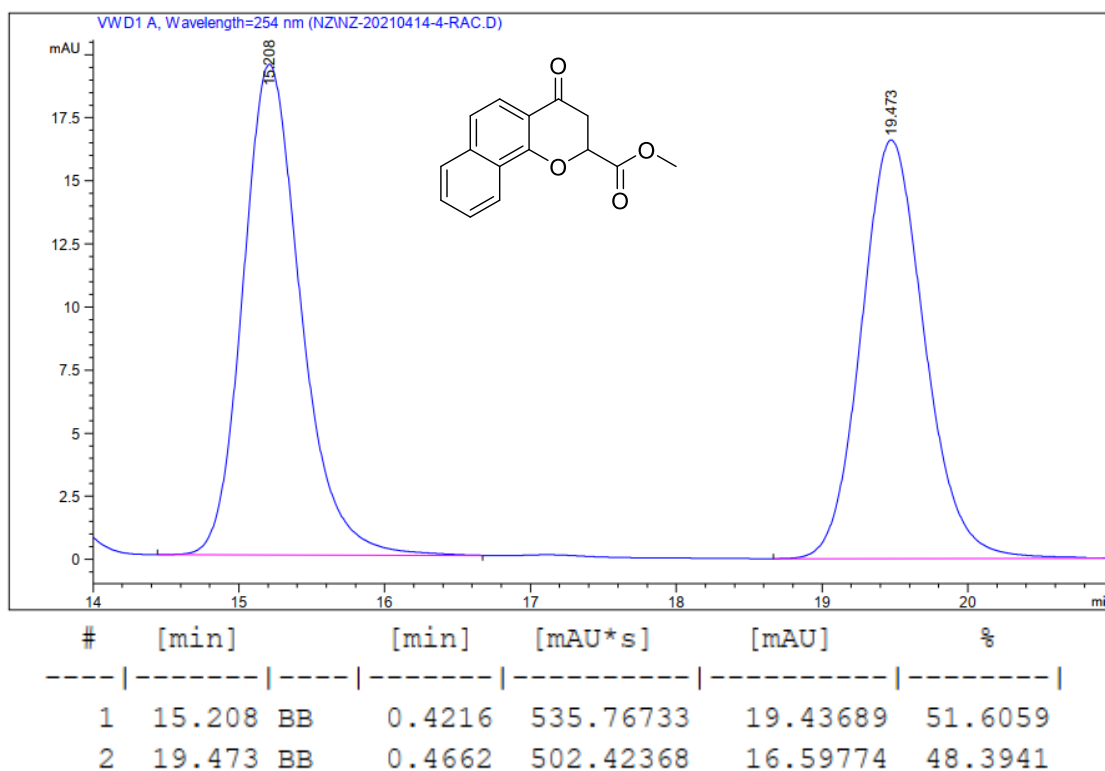


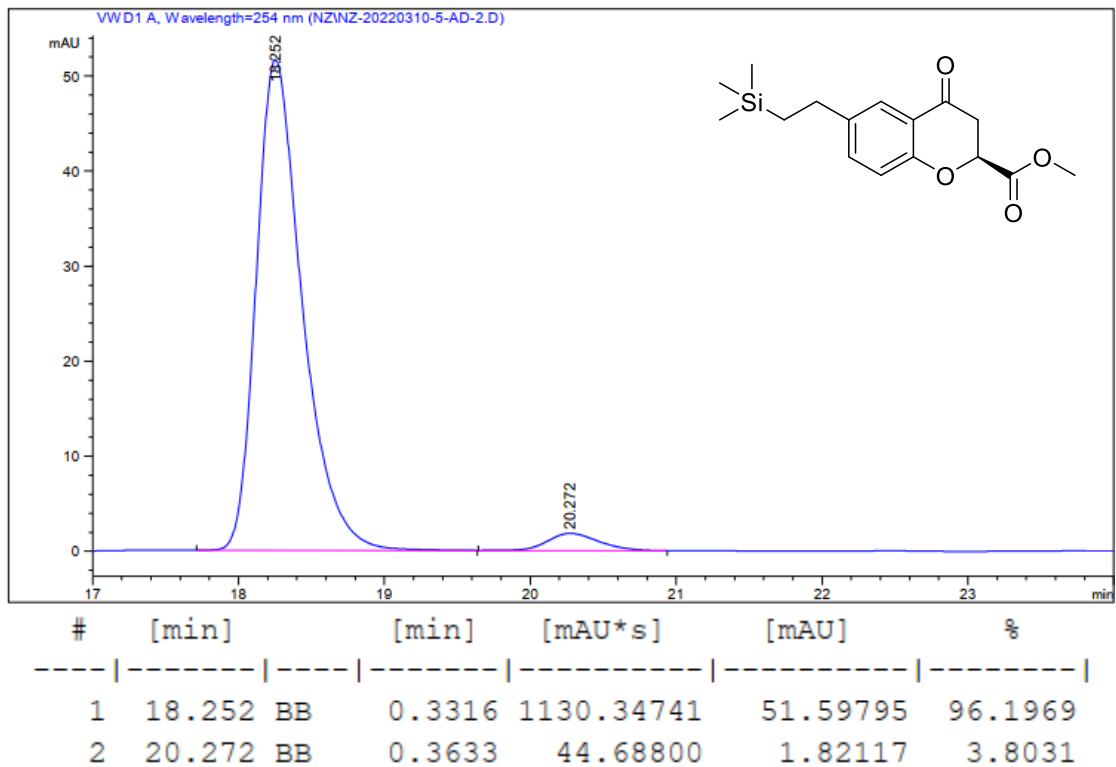
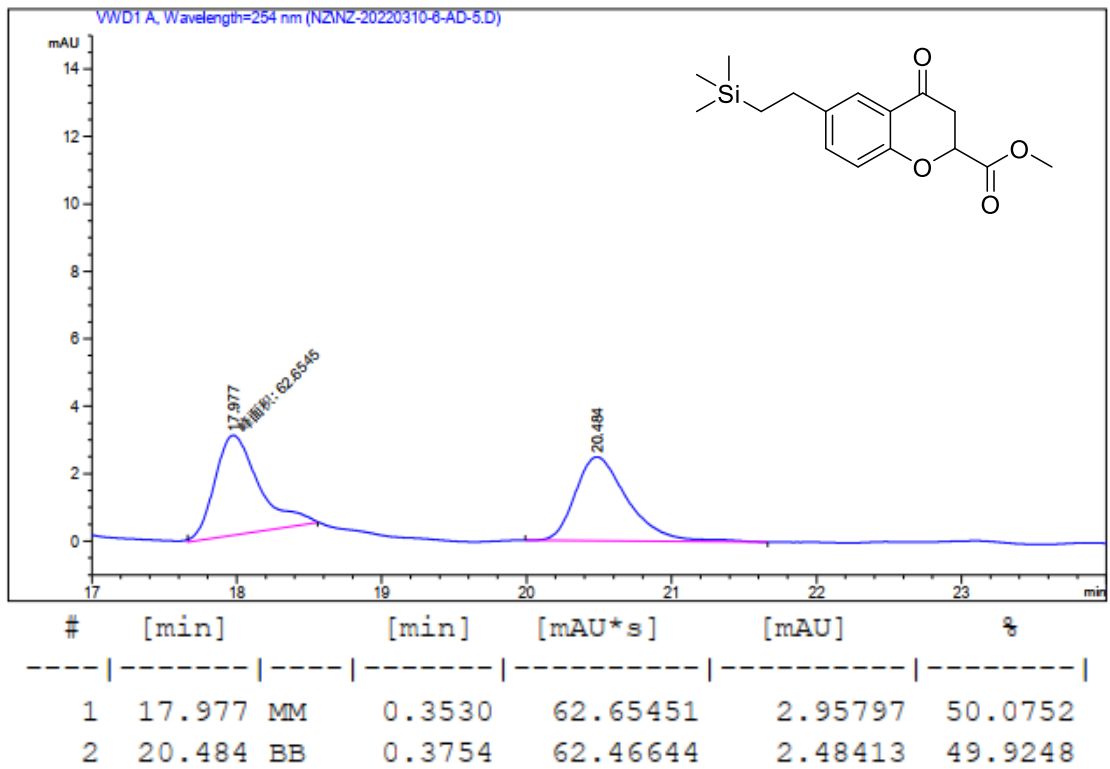


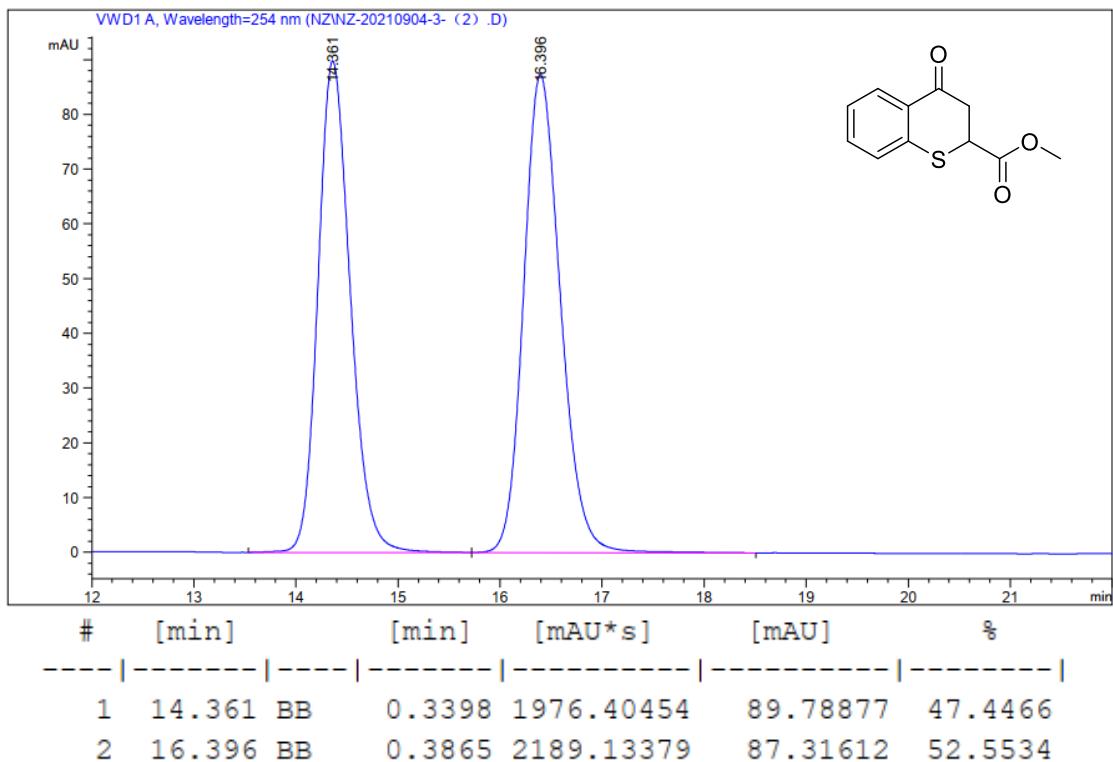
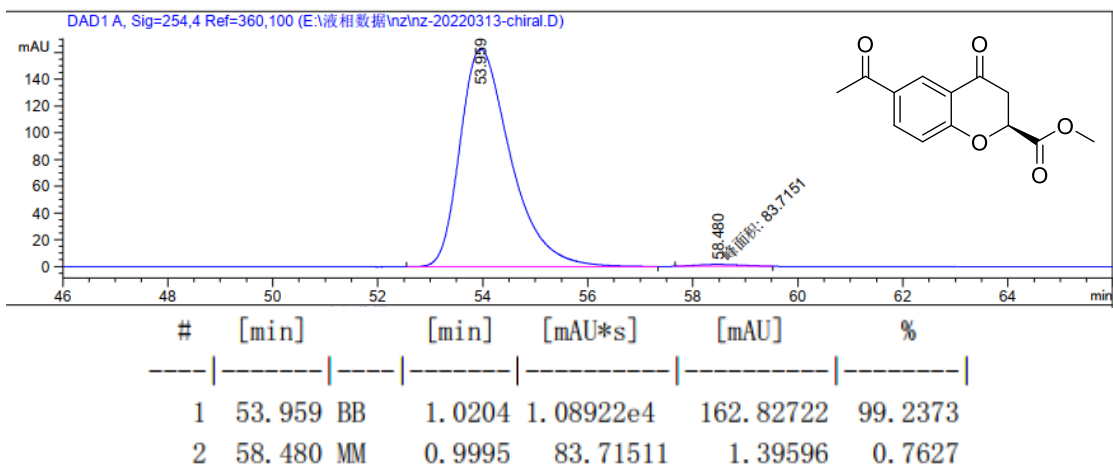
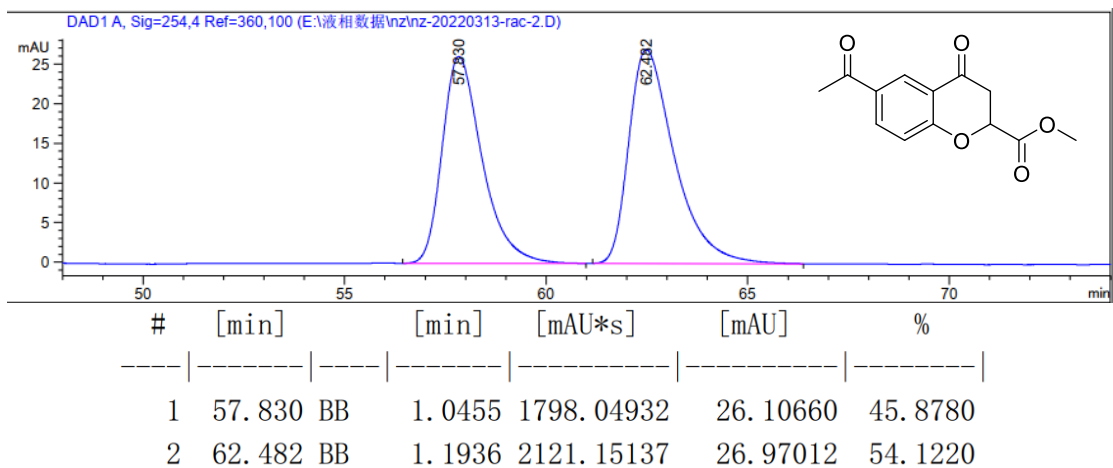


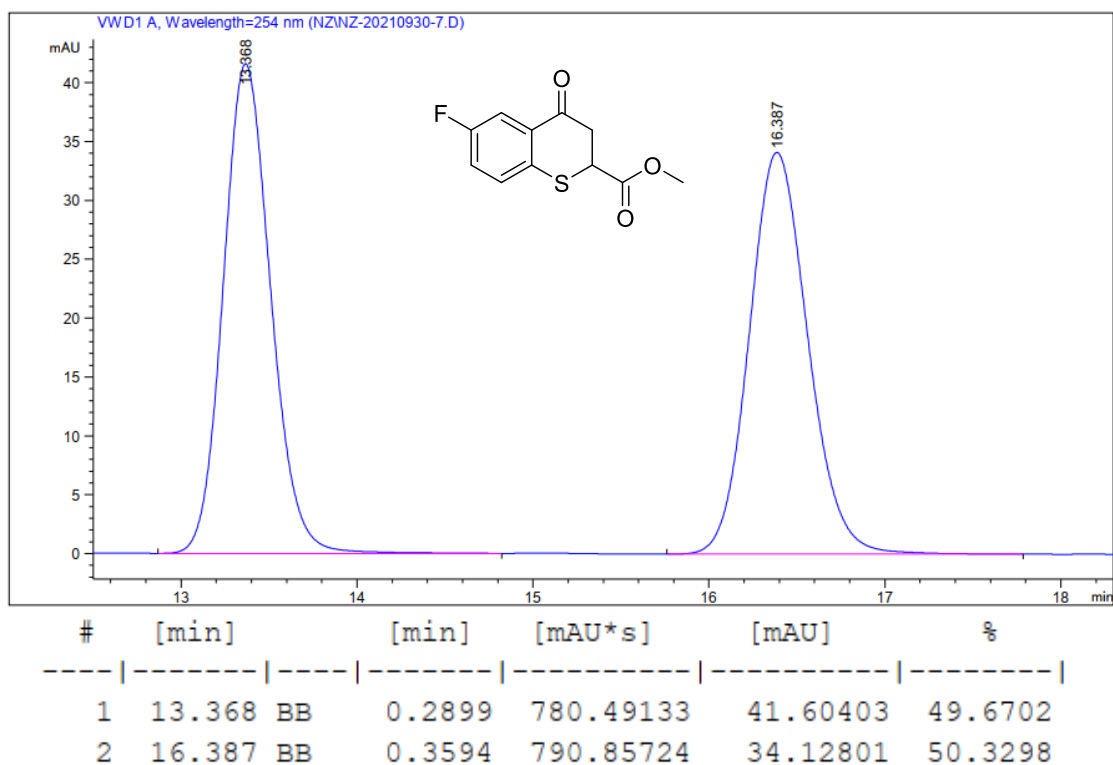
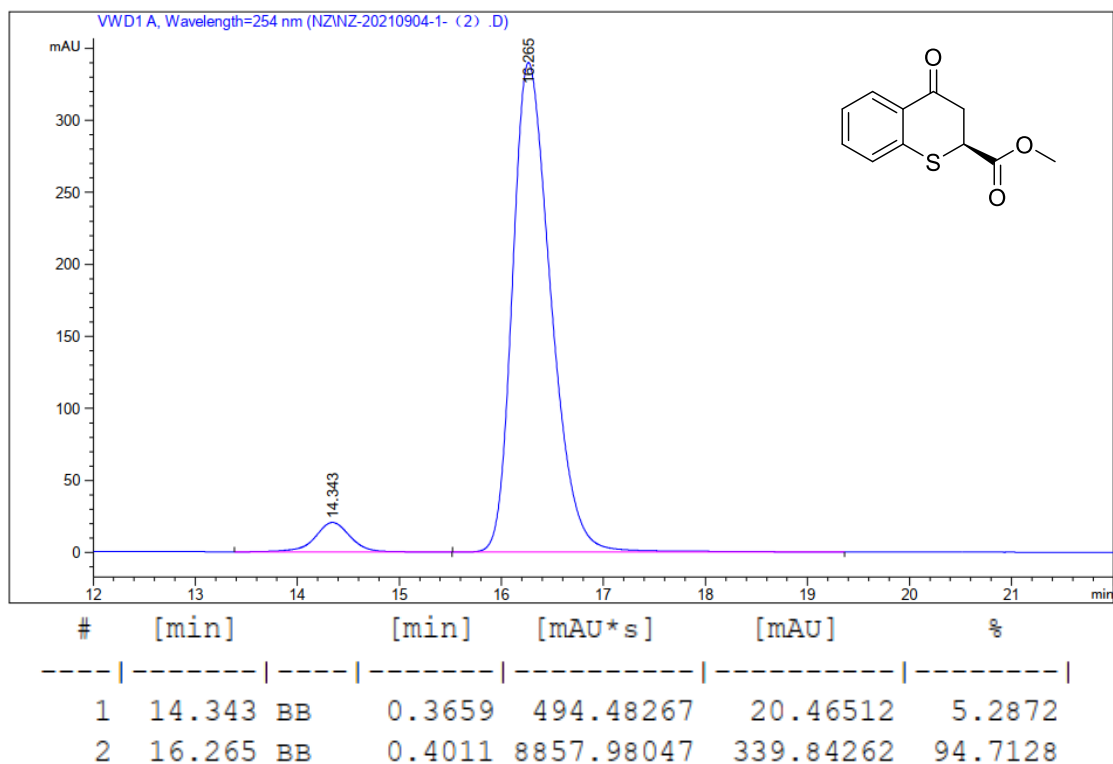


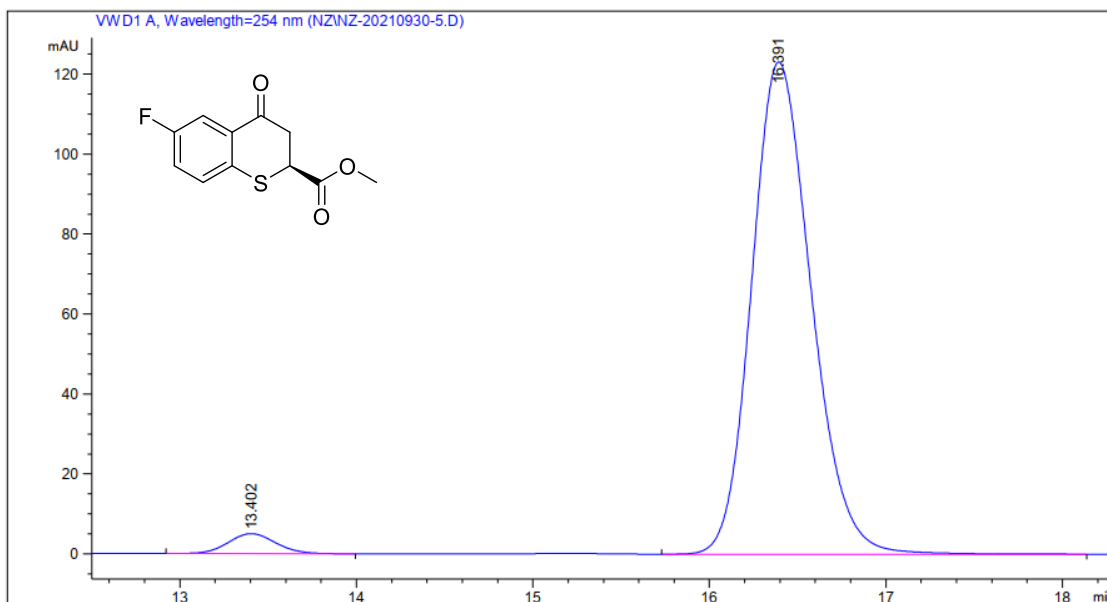




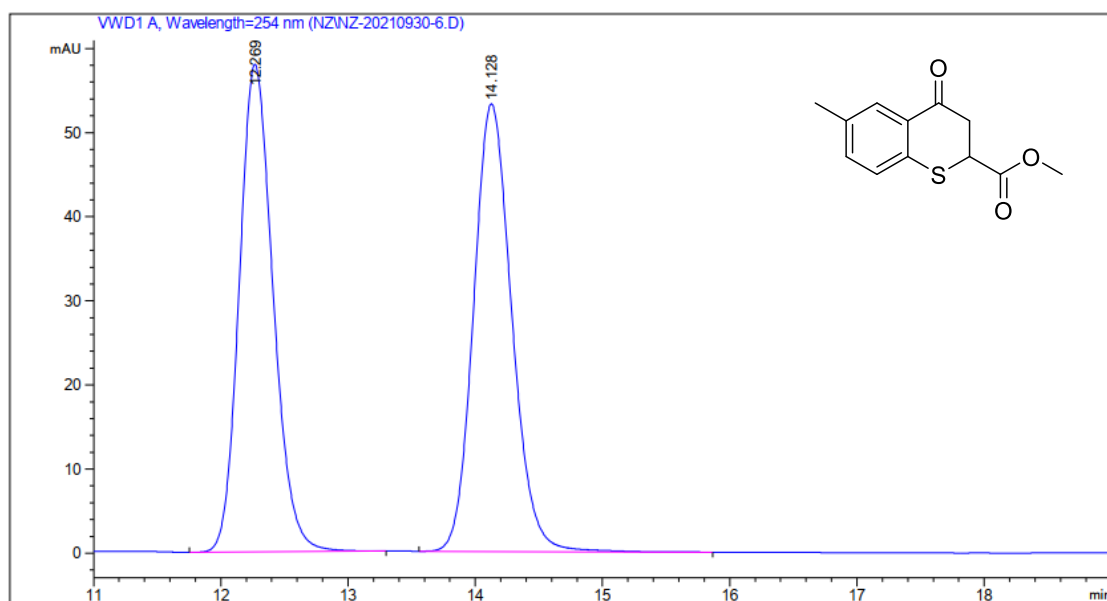




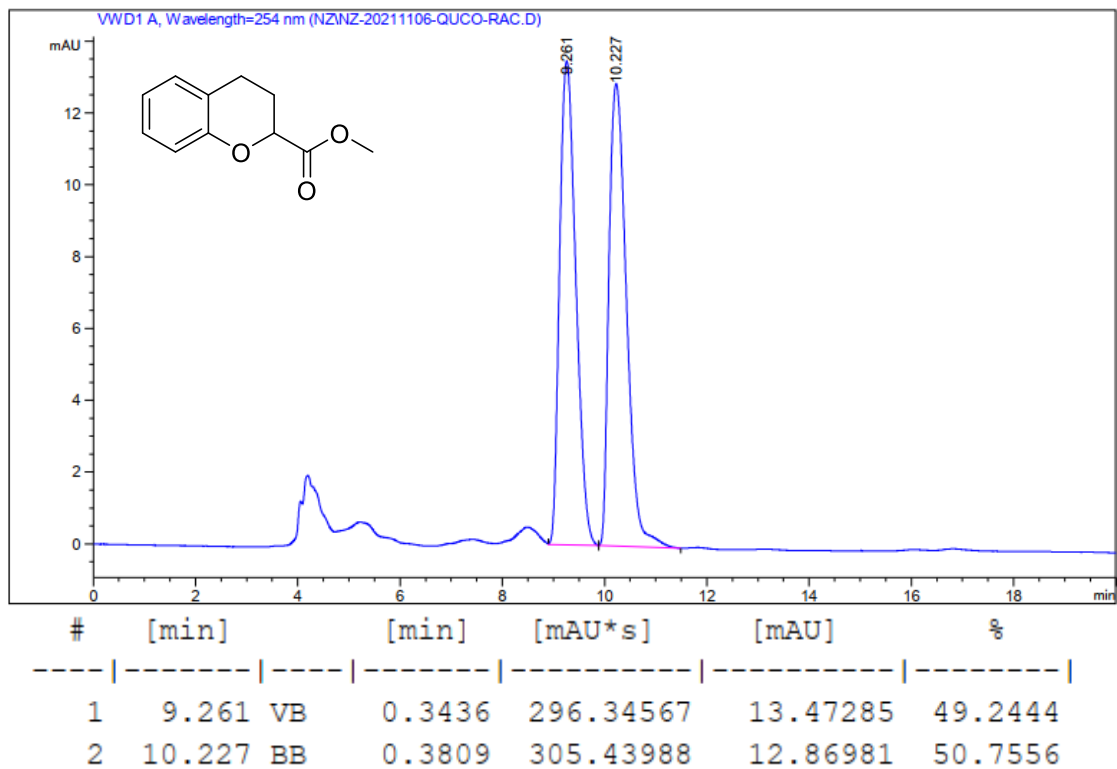
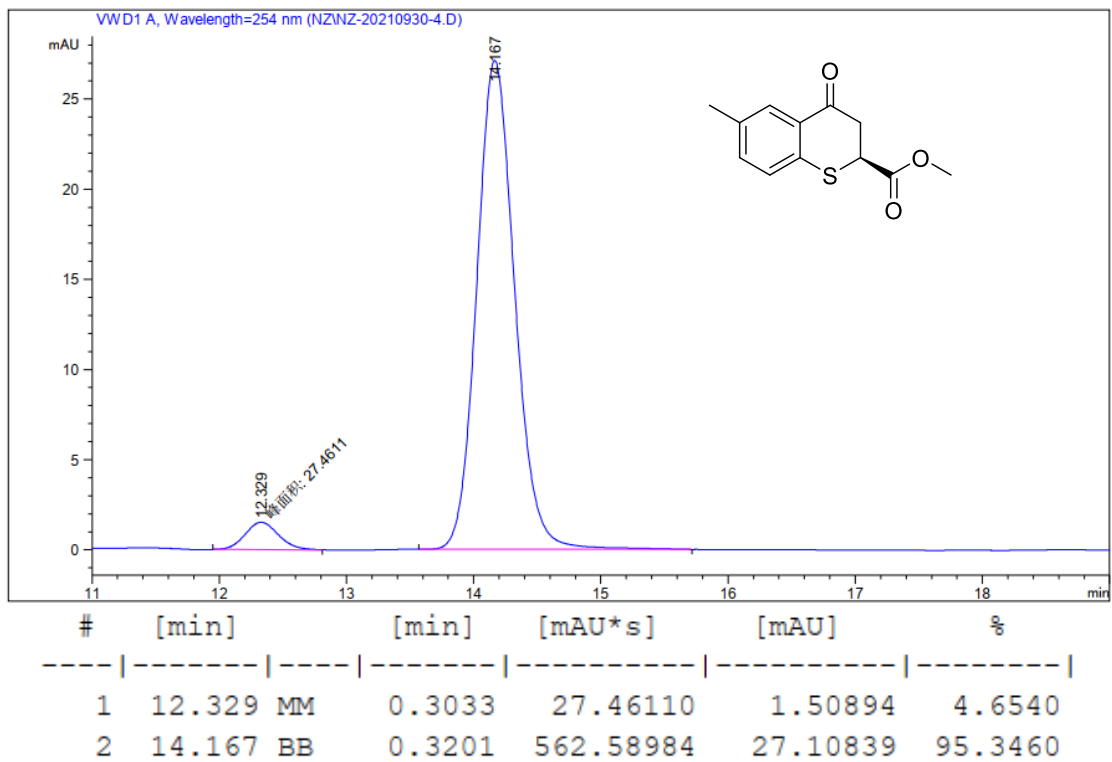


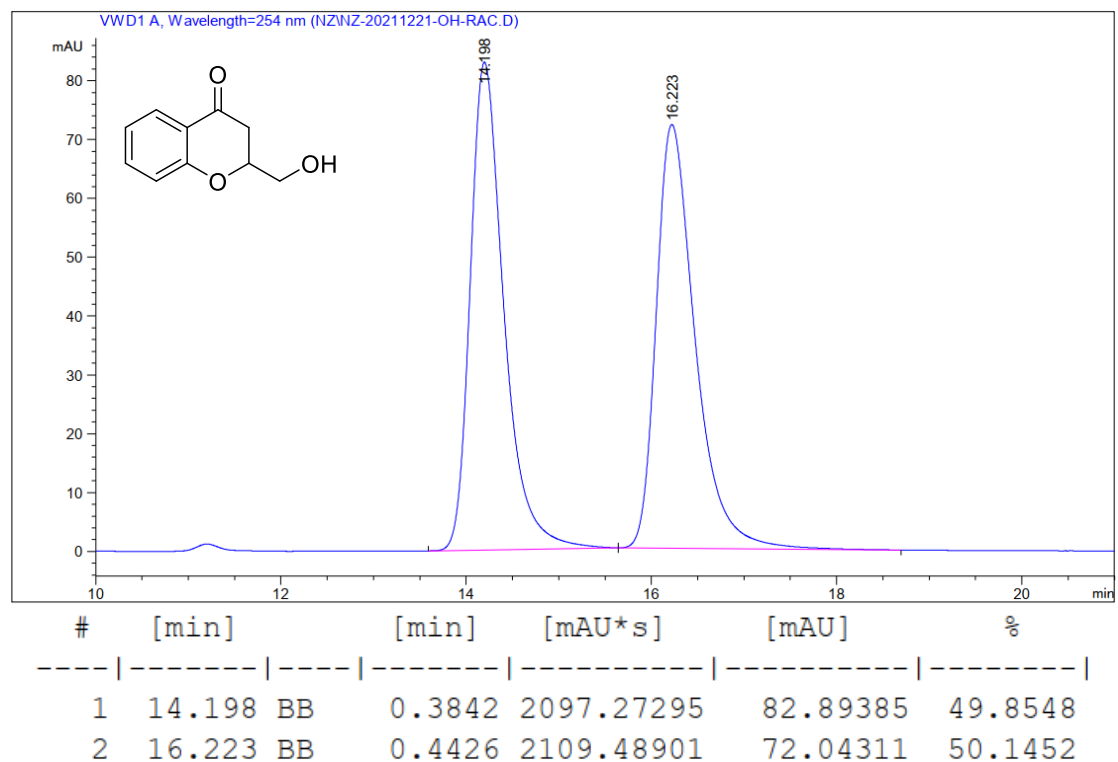
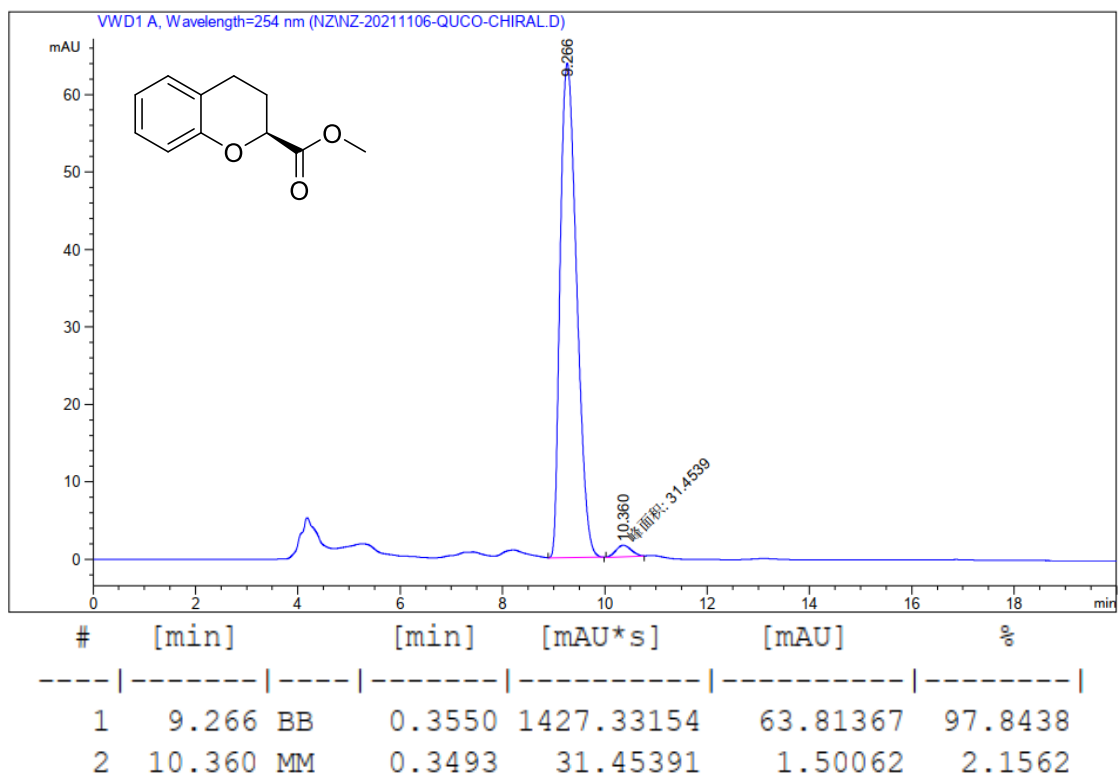


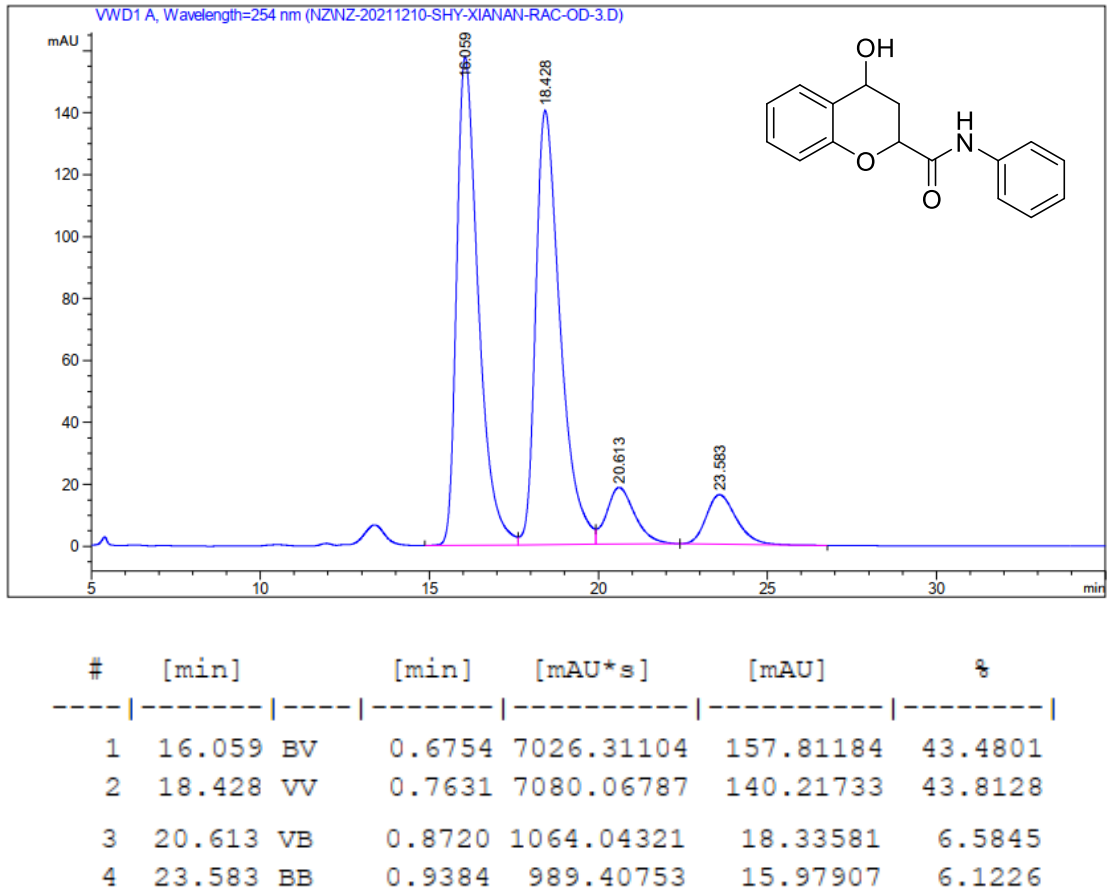
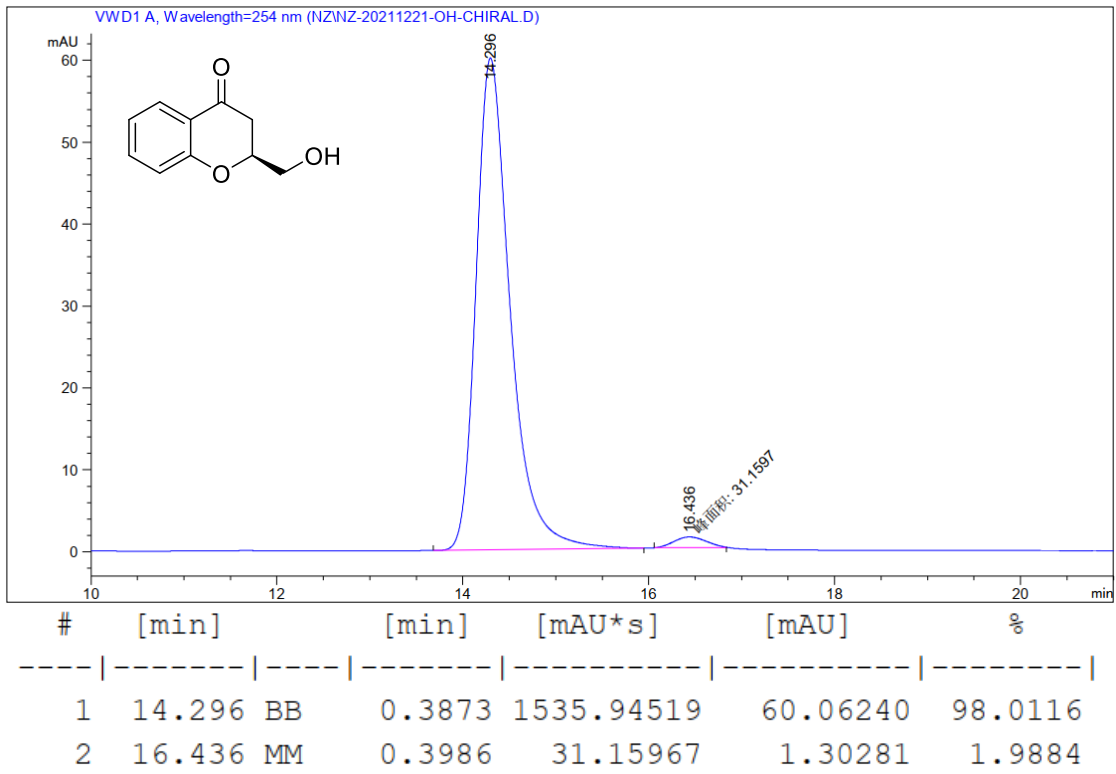
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	13.402	BB	0.2898	92.99834	4.98139	3.1209
2	16.391	BB	0.3637	2886.88770	123.05432	96.8791

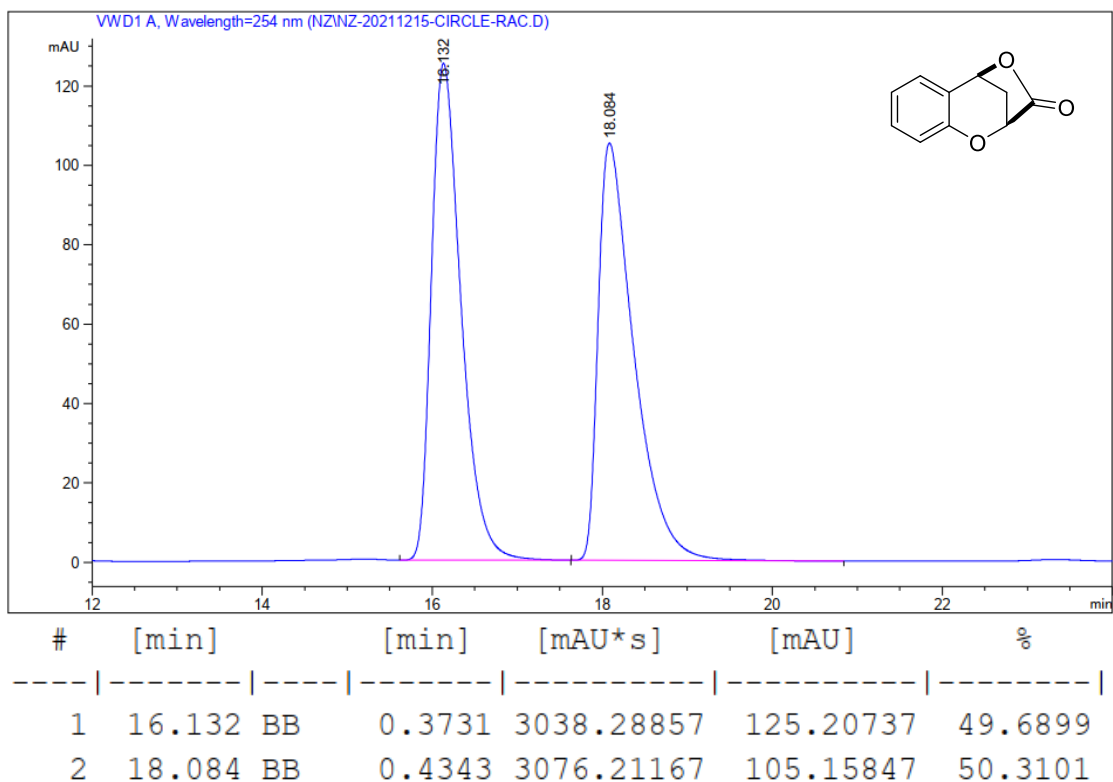
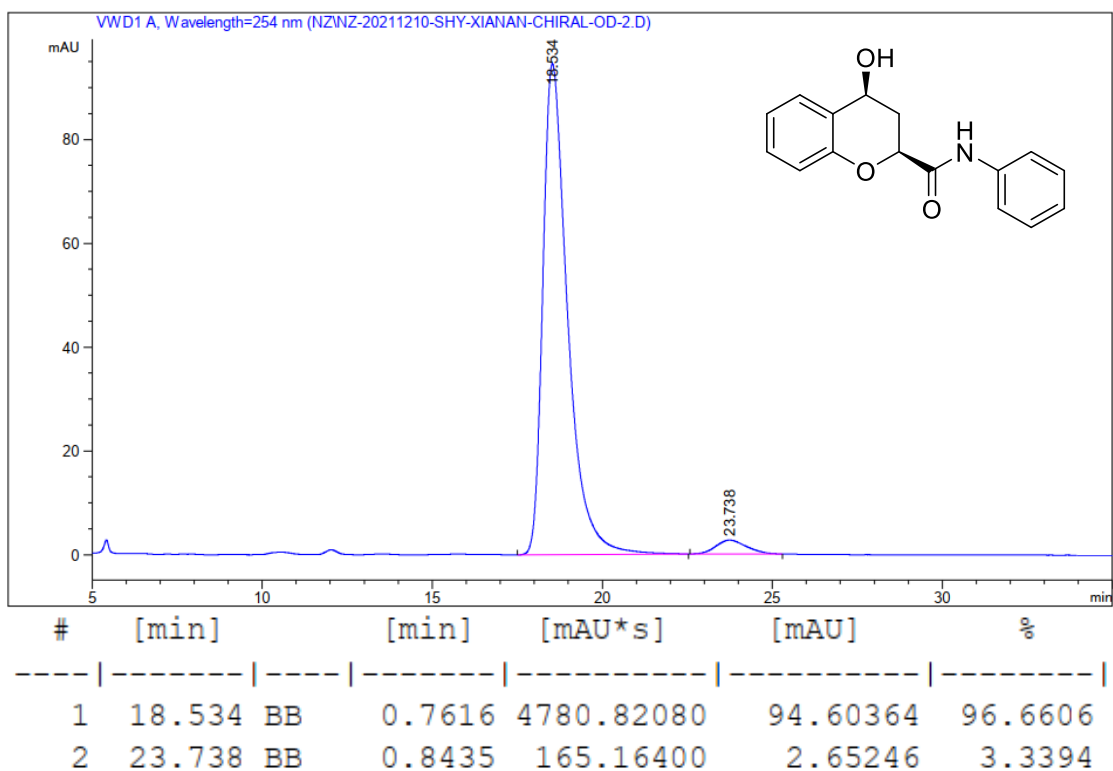


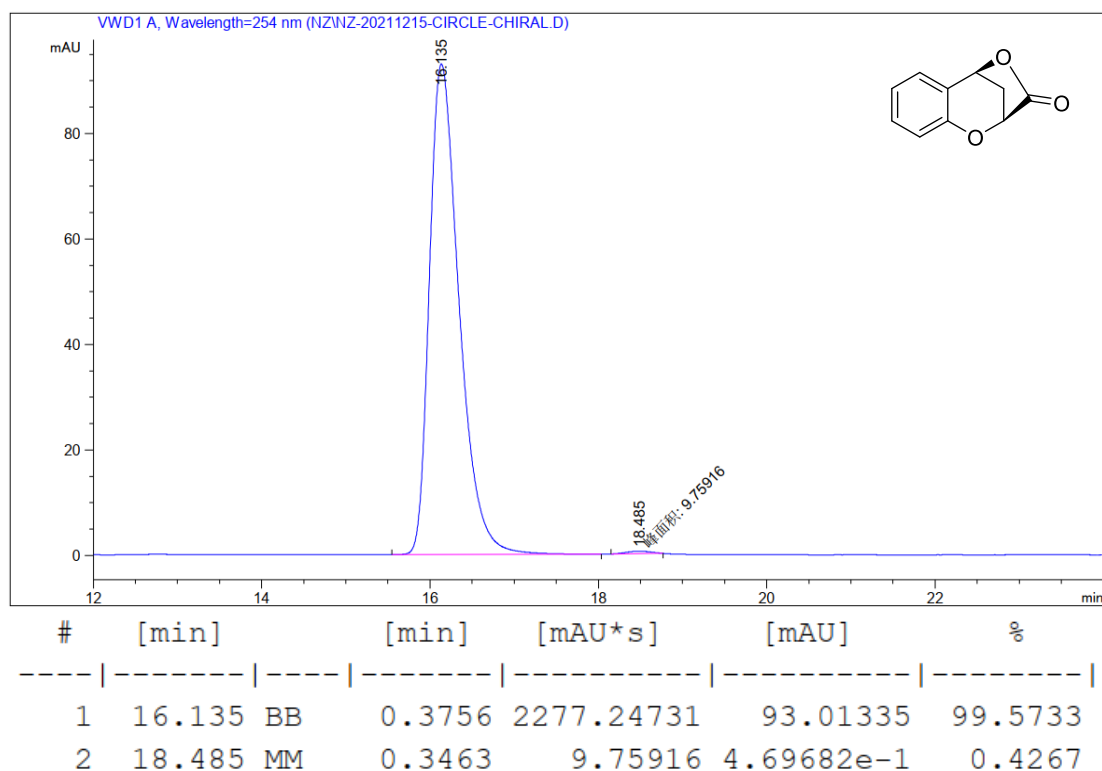
#	[min]	[min]	[mAU*s]	[mAU]	%	
1	12.269	BB	0.2853	1069.34460	57.94813	49.1108
2	14.128	BB	0.3230	1108.06982	53.20356	50.8892











10. Reference

1. Cagide, F.; Oliveira, C.; Reis, J.; Borges, F. *Molecules*, **2019**, *24*, 4214.
2. Anderson, J.; Liepa, A. *Aust. J. Chem.*, **1987**, *40*, 1179.
3. Akram, M. O.; Bera, S.; a Patil, N. T. *Chem. Commun.*, **2016**, *52*, 12306.
4. a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648-5652; b) Lee, C., Yang, W. & Parr, R. G. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1988**, *37*, 785-789.
5. a) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299-310; b) Wadt, W. R.; Hay, P. J. *J. Chem. Phys.* **1985**, *82*, 284-298; c) Roy, L. E.; Hay, P. J.; Martin, R. L. *J. Chem. Theory Comput.* **2008**, *4*, 1029-1031; d) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 270-283.
6. Zhao, Y. & Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215-241.
7. a) Cossi, M., Barone, V., Cammi, R. & Tomasi, J. *Chem. Phys. Lett.* **1996**, *255*, 327-335; b) Cancès, E., Mennucci, B. & Tomasi, J. *J. Chem. Phys.* **1997**, *107*, 3032-3041; c) Barone, V., Cossi, M. & Tomasi, J. *J. Comput. Chem.* **1998**, *19*, 404-417; d) Marenich, A. V., Cramer, C. J. & Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378-6396.
8. Fang, D.-C. THERMO; Beijing Normal University, Beijing, People's Republic of China, **2013**.
9. Legault, C. Y.; CYLView, 1.0b; Université de Sherbrooke, Canada, (**2009**). <http://www.cylview.org> (Date of access: 1/10/2017).