

Supporting Information

Ir/f-Ampha Complex Catalyzed Asymmetric Sequential Hydrogenation of Enones: A General Access to Chiral Alcohols with Two Contiguous Chiral Centers

Wendian Li, Tilong Yang, Nan Song, Ruihao Li, Jiao Long, Lin He, Xumu Zhang, Hui Lv

Table of contents

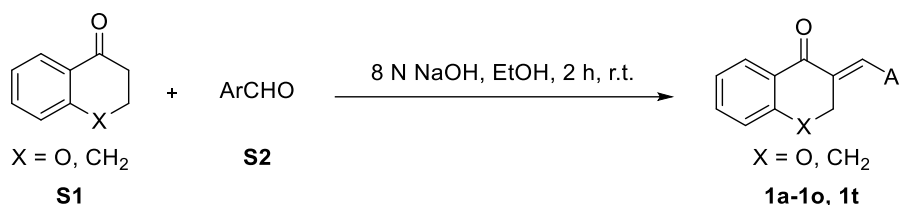
I. General Remarks	S2
II. Preparation and physical data of enones	S2
III. General procedure for asymmetric hydrogenation of enones	S21
IV Determination of absolute configuration	S40
V. Application in drug synthesis	S41
VI. Computational studies	S44
VII. NMR spectra of enones and hydrogenation product	S86
VIII. HPLC charts for hydrogenation products and derivatives	S175
IV. Reference	S265

I. General Remarks

All reactions and manipulations which are sensitive to moisture or air were performed in an argon-filled glovebox or using standard Schlenk techniques. Hydrogen gas (99.999%) was purchased from Shanghai Regulator Factory Co., Ltd. Anhydrous EtOH, ⁱPrOH, TFE, DCM, 1,4-dioxane, Hexane were purchased from J&K. DCE were freshly distilled from calcium hydride. Solvents were transferred by syringe. Melting point (m.p.) was determined by RY-1 Melting Point Apparatus. ¹H, ¹³C and spectra were recorded with a Bruker ADVANCE III (400 MHz) spectrometer with CDCl₃ as the solvent and tetramethylsilane (TMS) as the internal standard. Chemical shifts are reported in parts per million (ppm, δ scale) downfield from TMS at 0.00 ppm and referenced to the CDCl₃ at 7.26 ppm (for ¹H NMR) or 77.0 ppm (for ¹³C NMR). Data are reported as: multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constant in hertz (Hz) and signal area integration in natural numbers. ¹³C NMR and analyses were run with decoupling. Optical rotation was determined using a Perkin Elmer 343 polarimeter. HPLC analysis was conducted on an Agilent 1260 Series instrument. Column Chromatography was performed with silica gel Merck 60 (300-400 mesh).

II. Preparation and physical data of enones

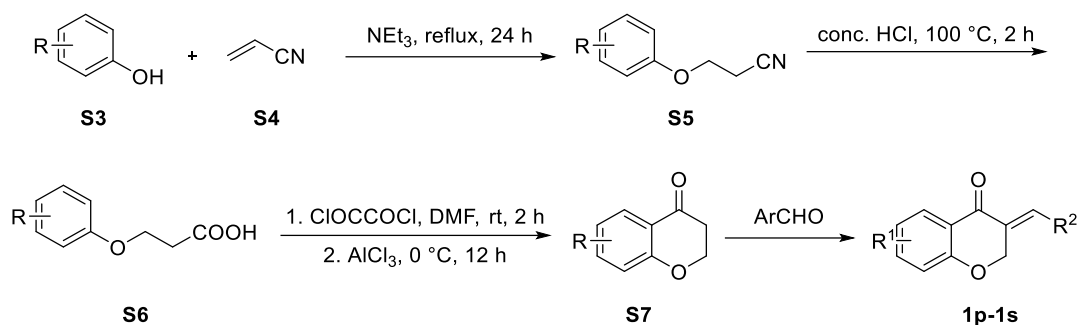
Preparation of Substrates 1a-1o and 1t



Prepared according to a previously reported procedure.^[1]

To a solution of tetralone derivatives **S1** (10 mmol) and appropriate aldehyde **S2** (10 mmol) in ethanol (4 mL) was slowly added an aqueous solution of NaOH (0.0024 mol, 8 N) at room temperature. The mixture was stirred for 2 h. The solid precipitate was collected by filtration and then washed with cold ethanol (4 mL) three times. The solid was dried in vacuo to give target substrates (**1a-1o** and **1t**).

Preparation of substrates 1p-1s

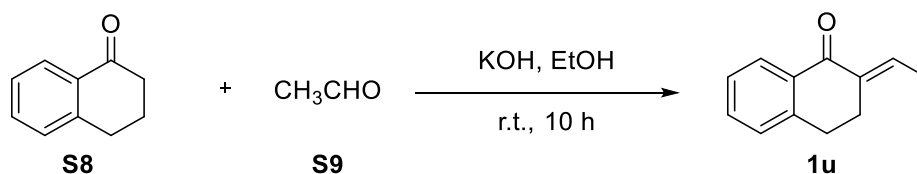


A mixture of compound **S3** (40 mmol), acrylonitrile **S4** (4.5 g, 84.8 mmol) and triethylamine (0.9 g, 8.8 mmol) was refluxed for 24 hours. After completion of the reaction, the mixture was poured into cold water (50 mL) and extracted with ethyl ether (25 mL $\times$ 3). The combined organic layer was successively washed with 10% aqueous NaOH (30 mL), 2N HCl (30 mL), and brine (30 mL). The organic layer was then dried over sodium sulfate. After the solvent is evaporated to obtain compound **S5** as a yellow solid.

A mixture of compound **S5** and concentrated HCl (40 mL) was refluxed for 2 hours. After being cooled, the mixture was filtered and the precipitate was dried overnight under vacuum to give compound **S6** as a white powder.

To the solution of **S6** in dry CH_2Cl_2 (4.5 mL/mmol) was added one drop of DMF at 0°C . Oxalyl chloride (1.5 eq) was then added dropwise under nitrogen atmosphere at 0°C . The reaction was stirred at 0°C for 1.5 hours and the mixture was concentrated at high vacuum to give the desired acid chloride, which was directly used without further purification. To the acid chloride in dry CH_2Cl_2 (4.5 mL/mmol) was added AlCl_3 (1.5 eq) slowly at 0°C . The mixture was stirred at 0°C for 1.5 hours and quenched with water followed by extraction with CH_2Cl_2 . The combined organic layer was dried over anhydrous Na_2SO_4 , filtered and concentrated. The residue was purified by column chromatography to give the desired product **S7**. **1p-1s** were prepared from **S7** and benzaldehyde using the same procedure as for **1a-1o**.

Preparation of Substrate **1u**

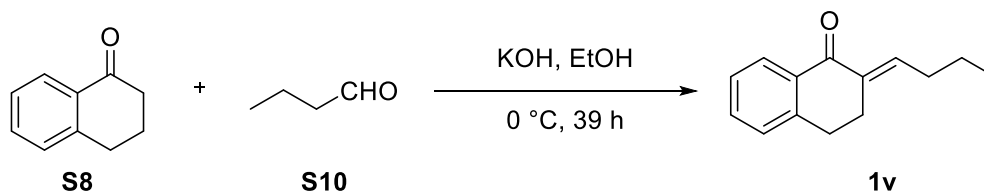


Prepared according to a previously reported procedure.^[2]

In a round bottomed flask containing a stirred mixture of potassium hydroxide (6.4 mmol) in ethanol (29 mL) were successively added 1-tetralone **S8** (5.8 mmol) and acetaldehyde **S9** (5.8 mmol). After stirring at room temperature for 10 hours, water was added and the mixture

was extracted with diethyl ether. The organic layer was dried over magnesium sulfate. After filtration and evaporation of the solvent, the residue was purified by flash-chromatography (eluant: petroleum/ethedethyl acetate 30:1) to give the desired product **1u**.

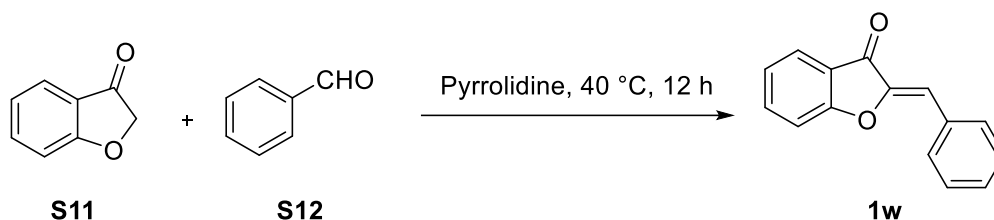
Preparation of Substrate **1v**



Prepared according to a previously reported procedure.^[2]

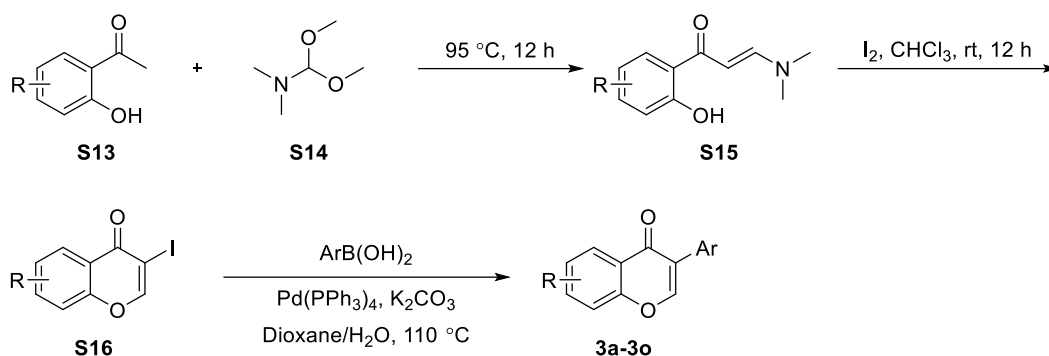
In a round bottomed flask containing a stirred mixture of potassium hydroxide (6.4 mmol) in ethanol (29 mL) were successively added 1-tetralone **S8** (5.8 mmol) and butyraldehyde **S10** (5.8 mmol). After stirring at 0 °C for 42 hours, water was added and the mixture was extracted with diethyl ether. The organic layer was dried over magnesium sulfate. After filtration and evaporation of the solvent, the residue was purified by flash-chromatography (eluant: petroleum/ethedethyl acetate 30:1) to give the desired product **1v**.

Preparation of Substrate **1w**



A mixture of 1-methyl-4-piperidone **S11** (10 mmol) and pyrrolidine (24 mmol) in CH₂Cl₂ (100 mL) was stirred about 5 min at room temperature. Then, benzaldehyde **S12** (10 mmol) was added and the mixture was stirred for 12 h at 40 °C. After completion of the reaction (TLC), the solvent was removed under vacuum. The crude product was subjected to column chromatography on silica gel using petroleum ether/ethyl acetate (PE/EA = 30:1) as the eluent to give **1w**.

Preparation of Substrates **3a-3o**



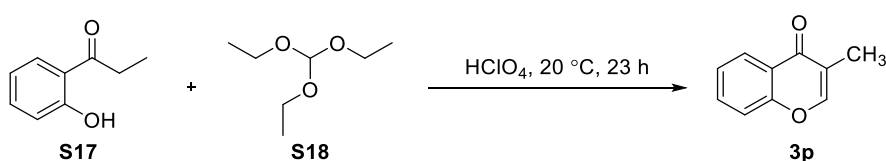
Prepared according to a previously reported procedure.^[3]

A mixture of a substituted 2-hydroxyacetophenone **S13** (20 mmol) and *N,N*-dimethylformamide dimethylacetal **S14** (30 mmol) was heated at 95 °C overnight. The reaction mixture is cooled to room temperature and excess methanol and dimethylformamide dimethyl acetal are removed in vacuo to leave a light brown solid. The solid is chromatographed over silica gel with ethyl acetate as the eluent to the desired product **S15**.

To a solution of a substituted 3-(dimethylamino)-1-(2-hydroxyphenyl)propenone **S15** (10 mmol) in CHCl_3 (30 mL) was added a chloroform solution of iodine (10 mmol) dropwise over several minutes. After complete addition of iodine, the reaction mixture is diluted with water (30 mL) and vigorously stirred for 5 min. The organic layer is then separated, dried with magnesium sulfate, and solvent removed in vacuo to give a yellow solid. This solid is chromatographed over silica gel with 5% ethyl acetate as the eluent to the desired product **S16**.

3-Iodo-4H-1-benzopyran-4-one (5 mmol) **S16**, K_2CO_3 (15 mmol, 3 eq), boronic acid (9 mmol, 1.2 eq) and $\text{Pd}(\text{PPh}_3)_4$ (0.5 mmol, 10 mol%) were taken in a round-bottom flask and 1,4-dioxane (15 mL) and H_2O (2.5 mL) were added to the mixture. The mixture was heated at 110 °C for 18-24 h until complete consumption of the substrate as indicated by TLC. It was cooled to rt and concentrated under reduced pressure. The mixture was extracted with EtOAc (2 × 50 mL) and washed with water (2 × 25 mL) and brine (1 × 25 mL), dried with anhyd. Na_2SO_4 , and concentrated under reduced pressure. The column chromatographic purification of crude mass was performed on silica gel using EtOAc- petroleum ether (25-40%) as eluting solvent to afford the isoflavones **3a-3o**.

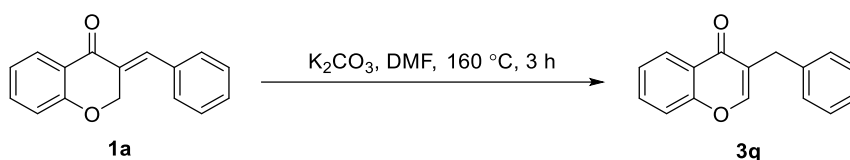
Preparation of Substrate 3p



Prepared according to a previously reported procedure.^[4]

Concentrated HClO₄ (3.1 g, 30.8 mmol, 2.64 mL, 1.7 eq) was added dropwise to a solution of 2'-hydroxypropiophenone **S17** (2.7 g, 18 mmol, 1 eq) in triethyl orthoformate **S18** (26.6 g, 180 mmol, 30 mL, 10 eq). The reaction mixture was then stirred for 23 h at room temperature. After addition of water (10 mL) and dichloromethane (10 mL) the phases were separated and the aqueous phase was extracted with dichloromethane (3 × 20 mL). The combined organic phases were dried over Na₂SO₄ and evaporated to dryness. The crude product was then purified by flash chromatography (petroleum ether/ethyl acetate 3:1) yielding the corresponding product **3p**.

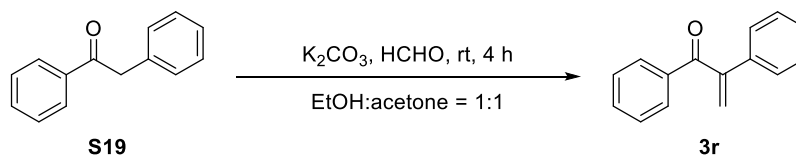
Preparation of Substrate **3q**



Prepared according to a previously reported procedure.^[5]

A mixture of *E*-3-benzylidenechromanone (**1a**) (708 mg, 3 mmol), anh. K₂CO₃ (704 mg, 5.1 mmol) and abs. DMF (36 mL) was refluxed for 3 h, then poured into brine and extracted with ethyl acetate (3 × 50 mL). After drying, the solvent was removed under reduced pressure and the residue was submitted to column chromatography (eluent: petroleum ether/ethyl acetate 15:1) to afford 340 mg (48%) of pure **3q** as brownish prisms.

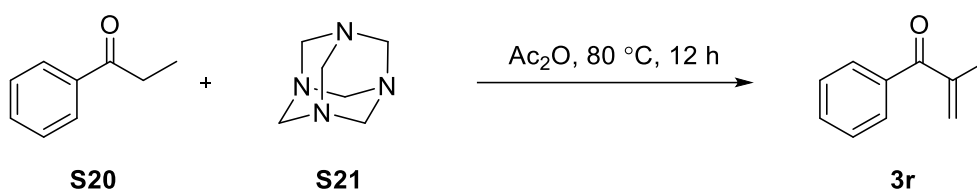
Preparation of Substrate **3r**



Prepared according to a previously reported procedure.^[6]

1,2-Diphenylethan-1-one **S19** (1.96 g, 10 mmol) and K₂CO₃ (1.48 g, 10.7 mmol) were added in 50 mL EtOH:acetone (v:v = 1:1). Then formaldehyde (1.5 mL, 18.0 mmol) was added at room temperature. After 4 h, the aqueous layer was extracted with ethyl acetate (3 × 50 mL) and the combined organic layer was dried over anhydrous Na₂SO₄, filtered and concentrated under reduced pressure. The residue was purified by chromatography (petroleum ether/ethyl acetate, v:v = 50:1) to afford product **3r**.

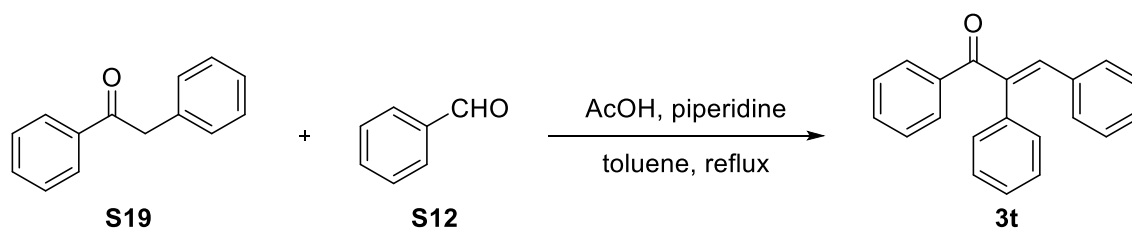
Preparation of Substrate 3s



Prepared according to a previously reported procedure.^[7]

To a mixture of the acetophenone **S20** (10 mmol) and acetic anhydride (2.24 g, 22 mmol), under an argon atmosphere, was added hexamethylenetetramine **S21** (1.96 g, 14 mmol). The reaction mixture was heated overnight at 80 °C, then allowed to cool to room temperature and quenched into a stirred mixture of dichloromethane (200 mL) and 2 M sodium hydroxide (200 mL). The organic layer was separated and washed with 1 M HCl (100 mL), brine and water. The organic phase was dried with MgSO₄, filtered and evaporated. The crude material was purified by flash chromatography (petroleum ether/ethyl acetate 20:1) and the solvent was evaporated to afford the product **3r**.

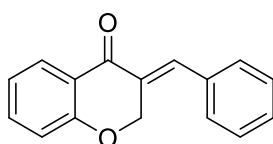
Preparation of Substrate 3t



Prepared according to a previously reported procedure.^[6]

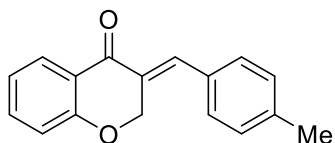
A solution of 1,2-diphenylethan-1-one **S19** (1.96 g, 10 mmol), benzaldehyde **S12** (1.06 g, 10 mmol), AcOH (0.5 mL) and piperidine (0.2 mL) in 25 mL toluene was refluxed overnight using a Dean-stark apparatus. After cooling to room temperature, the reaction was quenched by the addition of saturated aqueous NaHCO₃ solution (10 mL). The aqueous layer was extracted with ethyl acetate (3 × 50 mL) and the combined organic layer was dried over anhydrous Na₂SO₄, filtered and concentrated under reduced pressure. The residue was purified by chromatography (petroleum ether/ethyl acetate, v:v = 50:1) to afford product **3t**.

(*E*)-3-Benzylidenechroman-4-one (**1a**)



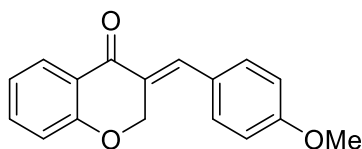
White solid, 32% yield, 0.8 g, mp 108-112 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.03 (dd, J = 7.9, 1.6 Hz, 1H), 7.89 (s, 1H), 7.54-7.38 (m, 4H), 7.35-7.28 (m, 2H), 7.12-7.04 (m, 1H), 6.97 (d, J = 8.2 Hz, 1H), 5.36 (d, J = 1.7 Hz, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.3, 161.1, 137.5, 135.9, 134.3, 130.9, 130.0, 129.5, 128.7, 127.9, 122.0, 121.9, 117.9, 67.6. HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{12}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 259.0730. Found: 259.0730.

(*E*)-3-(4-Methylbenzylidene)chroman-4-one (**1b**)



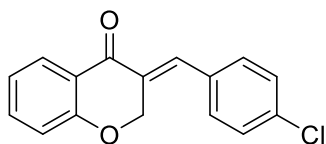
White solid, 27% yield, 0.3 g, mp 116-120 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.95 (dd, J = 7.9, 1.7 Hz, 1H), 7.79 (s, 1H), 7.41 (ddd, J = 8.4, 7.2, 1.8 Hz, 1H), 7.22-7.12 (m, 4H), 7.03-6.97 (m, 1H), 6.89 (dd, J = 8.3, 0.7 Hz, 1H), 5.30 (d, J = 1.9 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 181.3, 160.0, 138.9, 136.6, 134.8, 130.5, 129.1, 129.0, 128.5, 126.9, 121.0, 120.8, 116.8, 66.7, 20.5. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{14}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 273.0886. Found: 273.0889.

(*E*)-3-(4-Methoxybenzylidene)chroman-4-one (**1c**)



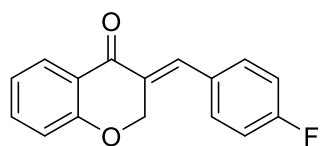
Yellow solid, 32% yield, 0.9 g, mp 142-145 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.02 (dd, J = 7.9, 1.6 Hz, 1H), 7.84 (s, 1H), 7.48 (ddd, J = 8.4, 7.2, 1.8 Hz, 1H), 7.31-7.26 (m, 2H), 7.10-7.04 (m, 1H), 7.01-6.94 (m, 3H), 5.38 (d, J = 1.8 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.2, 160.9, 160.7, 137.4, 135.7, 132.1, 128.9, 127.9, 127.0, 122.1, 121.8, 117.8, 114.2, 67.8, 55.4. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{14}\text{NaO}_3$ ($[\text{M}+\text{Na}]$): 289.0835. Found: 289.0837.

(*E*)-3-(4-Chlorobenzylidene)chroman-4-one (**1d**)



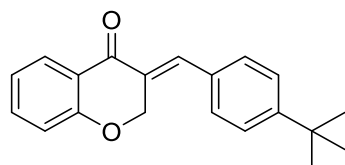
White solid, 60% yield, 1.6 g, mp 172-175 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.02 (dd, J = 7.9, 1.6 Hz, 1H), 7.81 (s, 1H), 7.50 (ddd, J = 8.8, 7.3, 1.7 Hz, 1H), 7.46-7.40 (m, 2H), 7.26-7.22 (m, 2H), 7.12-7.05 (m, 1H), 6.98 (d, J = 8.3 Hz, 1H), 5.32 (d, J = 1.8 Hz, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.0, 161.1, 136.1, 136.0, 135.6, 132.8, 131.4, 131.2, 129.1, 128.0, 122.0, 121.9, 117.9, 67.4. HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{11}\text{ClNaO}_2$ ($[\text{M}+\text{Na}]$): 293.0340. Found: 293.0343.

(*E*)-3-(4-Fluorobenzylidene)chroman-4-one (**1e**)



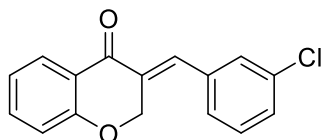
White solid, 46% yield, 1.2 g, mp 144-147 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.03 (dd, J = 7.9, 1.6 Hz, 1H), 7.83 (s, 1H), 7.50 (ddd, J = 8.4, 7.2, 1.8 Hz, 1H), 7.34-7.28 (m, 2H), 7.19-7.12 (m, 2H), 7.11-7.05 (m, 1H), 6.98 (dd, J = 8.3, 0.6 Hz, 1H), 5.33 (d, J = 1.8 Hz, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.1, 163.2 (d, J = 252.5 Hz), 161.0, 136.3, 136.0, 132.0 (d, J = 8.5 Hz), 130.7 (d, J = 2.0 Hz), 130.5 (d, J = 3.0 Hz), 127.9, 122.0, 121.9, 117.9, 116.0 (d, J = 21.2 Hz), 67.5. HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{11}\text{FNaO}_2$ ($[\text{M}+\text{Na}]$): 277.0635. Found: 277.0637.

(*E*)-3-(4-(Tert-butyl)benzylidene)chroman-4-one (**1f**)



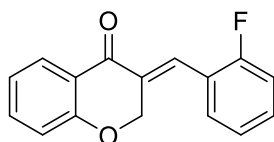
Yellow solid, 33% yield, 0.9 g, mp 144-147 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.03 (dd, J = 7.9, 1.7 Hz, 1H), 7.87 (brs, 1H), 7.51-7.44 (m, 3H), 7.30-7.24 (m, 2H), 7.10-7.04 (m, 1H), 6.97 (dd, J = 8.3, 0.7 Hz, 1H), 5.38 (d, J = 1.9 Hz, 2H), 1.35 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.3, 161.1, 153.1, 137.5, 135.8, 131.6, 130.2, 130.1, 128.0, 125.75, 122.1, 121.9, 117.9, 67.8, 34.9, 31.2. HRMS (EI) m/z Calcd. for $\text{C}_{20}\text{H}_{20}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 315.1356. Found: 315.1362.

(*E*)-3-(3-Chlorobenzylidene)chroman-4-one (**1g**)



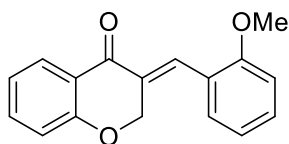
White solid, 65% yield, 1.8 g, mp 124-128 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.02 (dd, J = 7.9, 1.6 Hz, 1H), 7.81-7.77 (m, 1H), 7.51 (ddd, J = 8.5, 7.2, 1.8 Hz, 1H), 7.42-7.36 (m, 2H), 7.29 (s, 1H), 7.22-7.16 (m, 1H), 7.13-7.05 (m, 1H), 6.98 (dd, J = 8.3, 0.6 Hz, 1H), 5.31 (d, J = 1.9 Hz, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.0, 161.2, 136.1, 136.1, 135.8, 134.8, 132.1, 130.0, 129.7, 129.5, 128.0, 138.0, 122.1, 121.9, 118.0, 67.4. HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{11}\text{ClNaO}_2$ ($[\text{M}+\text{Na}]$): 293.0340. Found: 293.0342.

(*E*)-3-(2-Fluorobenzylidene)chroman-4-one (**1h**)



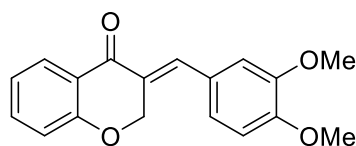
White solid, 56% yield, 1.4 g, mp 129-132 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.04 (dd, J = 7.9, 1.7 Hz, 1H), 7.87-7.84 (m, 1H), 7.50 (ddd, J = 8.5, 7.2, 1.8 Hz, 1H), 7.45-7.37 (m, 1H), 7.25-7.20 (m, 2H), 7.20-7.13 (m, 1H), 7.12-7.05 (m, 1H), 6.98 (dd, J = 8.3, 0.6 Hz, 1H), 5.20 (t, J = 1.6 Hz, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.0, 161.4, 160.5 (d, J = 252.5 Hz), 136.0, 132.8, 131.5 (d, J = 8.4 Hz), 130.9 (d, J = 2.6 Hz), 130.4 (d, J = 2.9 Hz), 128.0, 124.2 (d, J = 3.7 Hz), 122.4 (d, J = 14.4 Hz), 122.0, 121.9, 118.0, 116.1 (d, J = 21.2 Hz), 67.9 (d, J = 5.7 Hz). HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{11}\text{FNaO}_2$ ($[\text{M}+\text{Na}]$): 277.0635. Found: 277.0637.

(*E*)-3-(2-Methoxybenzylidene)chroman-4-one (**1i**)



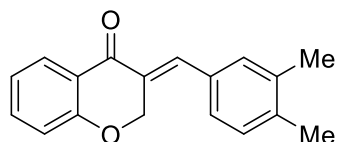
White solid, 48% yield, 1.3 g, mp 112-116 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.08-7.99 (m, 2H), 7.48 (ddd, J = 8.4, 7.2, 1.8 Hz, 1H), 7.44-7.36 (m, 1H), 7.10-7.03 (m, 2H), 7.03-6.98 (m, 1H), 6.98-6.93 (m, 2H), 5.23 (d, J = 1.8 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.5, 161.3, 158.2, 135.7, 134.0, 131.2, 130.8, 130.5, 128.0, 123.5, 122.2, 121.8, 120.3, 117.9, 110.9, 68.1, 55.5. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{14}\text{NaO}_3$ ($[\text{M}+\text{Na}]$): 289.0835. Found: 289.0837.

(*E*)-3-(3,4-Dimethoxybenzylidene)chroman-4-one (**1j**)



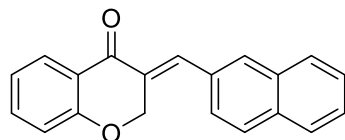
Yellow solid, 9% yield, 0.3 g, mp 121-124 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.02 (dd, J = 7.9, 1.6 Hz, 1H), 7.83 (s, 1H), 7.49 (ddd, J = 8.5, 7.2, 1.8 Hz, 1H), 7.11-7.04 (m, 1H), 6.99-6.92 (m, 2H), 6.92-6.85 (m, 2H), 5.40 (d, J = 1.8 Hz, 2H), 3.93 (d, J = 8.8 Hz, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.1, 160.9, 150.4, 148.9, 137.5, 135.7, 129.2, 127.9, 127.2, 123.6, 123.0, 121.89, 117.8, 113.2, 111.0, 67.8, 56.0, 56.0. HRMS (EI) m/z Calcd. for $\text{C}_{18}\text{H}_{16}\text{NaO}_4$ ($[\text{M}+\text{Na}]$): 319.0941. Found: 319.0945.

(*E*)-3-(3,4-Dimethylbenzylidene)chroman-4-one (**1k**)



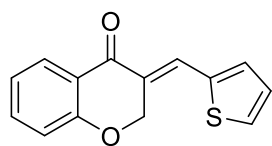
White solid, 30% yield, 0.4 g, mp 118-120 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.02 (dd, J = 7.9, 1.6 Hz, 1H), 7.84 (s, 1H), 7.48 (ddd, J = 8.4, 7.2, 1.8 Hz, 1H), 7.21 (d, J = 7.8 Hz, 1H), 7.11 (s, 1H), 7.09-7.03 (m Hz, 2H), 6.96 (dd, J = 8.3, 0.6 Hz, 1H), 5.37 (d, J = 1.8 Hz, 2H), 2.31 (s, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.4, 161.09, 138.8, 137.9, 137.1, 135.8, 132.0, 131.5, 130.0, 129.9, 127.9, 127.7, 122.1, 121.9, 117.9, 67.8, 19.89, 19.9. HRMS (EI) m/z Calcd. for $\text{C}_{18}\text{H}_{16}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 287.1043. Found: 287.1042.

(*E*)-3-(Naphthalen-2-ylmethylene)chroman-4-one (**1l**)



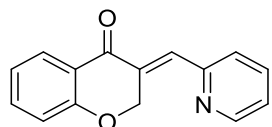
Yellow solid, 33% yield, 0.5 g, mp 135-138 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.08-8.01 (m, 2H), 7.93-7.84 (m, 3H), 7.76 (s, 1H), 7.59-7.53 (m, 2H), 7.53-7.47 (m, 1H), 7.43 (dd, J = 8.5, 1.6 Hz, 1H), 7.12-7.06 (m, 1H), 6.98 (d, J = 8.3 Hz, 1H), 5.46 (d, J = 1.8 Hz, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.3, 161.1, 137.6, 135.9, 133.4, 133.0, 131.9, 131.0, 130.1, 128.5, 128.4, 128.0, 127.8, 127.4, 127.0, 126.8, 122.0, 122.0, 118.0, 67.7. HRMS (EI) m/z Calcd. for $\text{C}_{20}\text{H}_{14}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 309.0886. Found: 309.0889.

(*E*)-3-(Thiophen-2-ylmethylene)chroman-4-one (**1m**)



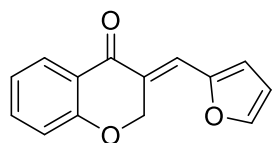
Yellow solid, 56% yield, 1.4 g, mp 132-135 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.04-7.98 (m, 2H), 7.61 (d, *J* = 5.1 Hz, 1H), 7.49 (ddd, *J* = 8.5, 7.2, 1.8 Hz, 1H), 7.35 (d, *J* = 3.4 Hz, 1H), 7.20-7.16 (m, 1H), 7.10-7.04 (m, 1H), 6.99 (dd, *J* = 8.3, 0.6 Hz, 1H), 5.47 (d, *J* = 2.0 Hz, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 181.4, 161.0, 137.6, 135.8, 134.04, 131.1, 128.8, 128.3, 127.9, 127.2, 121.9, 117.9, 67.8. HRMS (EI) *m/z* Calcd. for C₁₄H₁₀NaO₂S ([M+Na]): 265.0294. Found: 265.0299.

(*E*)-3-(Pyridin-2-ylmethylene)chroman-4-one (**1n**)



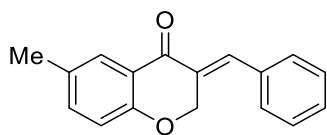
Yellow solid, 40% yield, 1.2 g, mp 144-146 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.72 (dd, *J* = 4.6, 0.8 Hz, 1H), 8.02 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.75 (td, *J* = 7.7, 1.8 Hz, 1H), 7.71 (t, *J* = 2.1 Hz, 1H), 7.54-7.47 (m, 2H), 7.29-7.22 (m, 2H), 7.10-7.03 (m, 1H), 7.00 (dd, *J* = 8.3, 0.5 Hz, 1H), 5.92 (d, *J* = 2.1 Hz, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 182.36, 161.70, 154.12, 149.68, 136.60, 136.01, 134.26, 133.37, 127.96, 127.91, 123.22, 121.80, 121.67, 118.10, 68.39. HRMS (EI) *m/z* Calcd. for C₁₅H₁₁NNaO₂ ([M+Na]): 260.0682. Found: 260.0683.

(*E*)-3-(Furan-2-ylmethylene)chroman-4-one (**1o**)



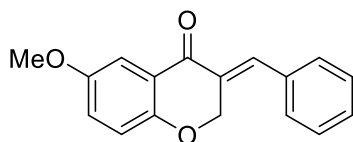
Yellow solid, 74% yield, 1.7 g, mp 127-129 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.00 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.62 (d, *J* = 1.6 Hz, 1H), 7.53-7.51 (m, 1H), 7.49 (ddd, *J* = 8.4, 7.2, 1.8 Hz, 1H), 7.09-7.03 (m, 1H), 6.99 (dd, *J* = 8.3, 0.6 Hz, 1H), 6.76 (d, *J* = 3.5 Hz, 1H), 6.55 (dd, *J* = 3.5, 1.8 Hz, 1H), 5.61 (d, *J* = 1.8 Hz, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 181.5, 161.2, 151.1, 145.4, 135.4, 127.6, 126.4, 121.7, 121.6, 121.5, 118.4, 117.6, 112.4, 67.7. HRMS (EI) *m/z* Calcd. for C₁₄H₁₀NaO₃ ([M+Na]): 249.0522. Found: 249.0526.

(*E*)-3-Benzylidene-6-methylchroman-4-one (**1p**)



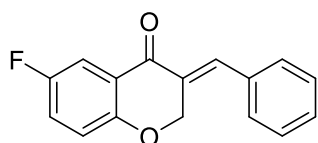
Yellow solid, 45% yield, 1.5 g, mp 152-155 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.87 (s, 1H), 7.82 (d, J = 1.5 Hz, 1H), 7.49-7.37 (m, 3H), 7.34-7.28 (m, 3H), 6.87 (d, J = 8.4 Hz, 1H), 5.32 (d, J = 1.8 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.5, 159.2, 137.4, 137.0, 134.4, 131.4, 131.1, 130.0, 129.4, 128.7, 127.5, 121.6, 117.7, 67.5, 20.5. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{14}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 273.0886. Found: 273.0887.

(*E*)-3-Benzylidene-6-methoxychroman-4-one (**1q**)



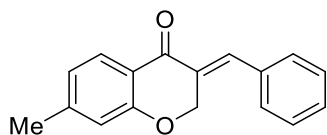
Yellow solid, 5% total yield, 0.3 g, mp 123-128 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.88 (s, 1H), 7.49-7.40 (m, 4H), 7.34-7.29 (m, 2H), 7.11 (dd, J = 9.0, 3.2 Hz, 1H), 6.91 (d, J = 9.0 Hz, 1H), 5.31 (d, J = 1.8 Hz, 2H), 3.84 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.3, 155.8, 154.5, 137.5, 134.4, 131.0, 130.0, 129.5, 128.7, 125.2, 122.0, 119.3, 108.1, 67.6, 55.8. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{14}\text{NaO}_3$ ($[\text{M}+\text{Na}]$): 289.0835. Found: 289.0841.

(*E*)-3-Benzylidene-6-fluorochroman-4-one (**1r**)



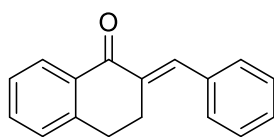
Yellow solid, 2% total yield, 0.2 g, mp 128-132 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.90 (s, 1H), 7.67 (dd, J = 8.3, 3.2 Hz, 1H), 7.51-7.39 (m, 3H), 7.35-7.28 (m, 2H), 7.21 (ddd, J = 9.0, 7.8, 3.2 Hz, 1H), 6.96 (dd, J = 9.0, 4.2 Hz, 1H), 5.34 (d, J = 1.8 Hz, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 181.6, 157.6 (d, J = 242.4 Hz), 157.3, 138.2, 134.2, 130.2, 130.0, 129.7, 128.8, 123.4 (d, J = 24.2 Hz), 122.5 (d, J = 6.7 Hz), 119.6 (d, J = 7.4 Hz), 112.9 (d, J = 23.2 Hz), 67.7. HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{11}\text{FNaO}_2$ ($[\text{M}+\text{Na}]$): 277.0635. Found: 277.0634.

(*E*)-3-Benzylidene-7-methylchroman-4-one (**1s**)



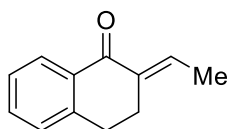
White solid, 11% total yield, 0.8 g, mp 97-99 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.92 (d, J = 8.0 Hz, 1H), 7.86 (s, 1H), 7.49-7.37 (m, 3H), 7.34-7.28 (m, 2H), 6.89 (dd, J = 8.0, 0.8 Hz, 1H), 6.77 (s, 1H), 5.33 (d, J = 1.8 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 182.0, 161.1, 147.5, 137.1, 134.5, 131.0, 130.0, 129.4, 128.7, 127.8, 123.3, 119.7, 117.9, 67.6, 22.0. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{14}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 273.0886. Found: 273.0889.

(*E*)-3-(Pyridin-2-ylmethylene)chroman-4-one (**1t**)



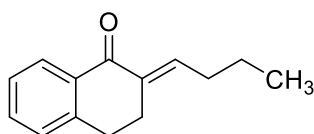
Yellow solid, 71% yield, 1.7 g, mp 111-115 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.14 (dd, J = 7.8, 1.1 Hz, 1H), 7.88 (s, 1H), 7.50 (td, J = 7.5, 1.4 Hz, 1H), 7.47-7.40 (m, 4H), 7.40-7.33 (m, 2H), 7.28-7.23 (m, 1H), 3.14 (td, J = 6.5, 1.7 Hz, 2H), 3.02-2.90 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 188.0, 143.3, 136.7, 135.9, 135.5, 133.5, 133.3, 129.9, 128.6, 128.5, 128.3, 128.2, 127.1, 28.9, 27.2. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{14}\text{NaO}$ ($[\text{M}+\text{Na}]$): 257.0937. Found: 257.0938.

(*E*)-2-Ethylidene-3,4-dihydronaphthalen-1(2*H*)-one (**1u**)^[2]



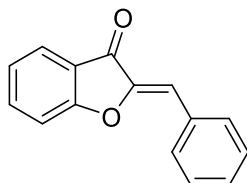
Yield oil, 30% yield, 0.3g. ^1H NMR (400 MHz, CDCl_3) δ 8.09 (dd, J = 7.8, 1.5 Hz, 1H), 7.46 (td, J = 7.5, 1.4 Hz, 1H), 7.36-7.30 (m, 1H), 7.24 (d, J = 7.6 Hz, 1H), 7.07-6.99 (m, 1H), 2.98-2.93 (t, J = 6.4 Hz, 2H), 2.79 (t, J = 6.4 Hz, 2H), 1.89 (d, J = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 187.4, 143.7, 135.9, 134.8, 133.6, 133.0, 128.2, 128.2, 126.9, 28.9, 25.2, 14.0.

(*E*)-2-Butylidene-3,4-dihydronaphthalen-1(2*H*)-one (**1v**)^[2]



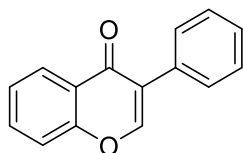
Yield oil, 30% yield, 0.3g. ^1H NMR (400 MHz, CDCl_3) δ 8.10 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.46 (td, $J = 7.4, 1.5$ Hz, 1H), 7.33 (td, $J = 7.6, 1.2$ Hz, 1H), 7.28-7.21 (m, 1H), 6.99-6.91 (m, 1H), 2.95 (t, $J = 6.0$ Hz, 2H), 2.79 (t, $J = 6.1$ Hz, 2H), 2.24 (q, $J = 7.5$ Hz, 2H), 1.54 (m, 2H), 0.97 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 187.57, 143.72, 140.02, 135.12, 133.62, 132.98, 128.20, 128.16, 126.87, 30.22, 29.11, 25.61, 22.09, 13.94.

(*Z*)-2-Benzylidenebenzofuran-3(2*H*)-one (**1w**)



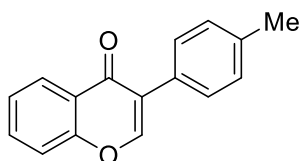
Yellow solid, 58% yield, 1.3 g, mp 116-120 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.98-7.90 (m, 2H), 7.82 (dd, $J = 7.7, 0.8$ Hz, 1H), 7.70-7.63 (m, 1H), 7.50-7.38 (m, 3H), 7.37-7.32 (m, 1H), 7.26-7.20 (m, 1H), 6.91 (s, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 184.9, 166.2, 146.9, 137.0, 132.3, 131.6, 129.9, 128.9, 124.7, 123.5, 121.6, 113.1, 113.0. HRMS (EI) m/z Calcd. for $\text{C}_{15}\text{H}_{10}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 245.0573. Found: 245.0574.

3-Phenyl-4*H*-chromen-4-one (**3a**)^[8]



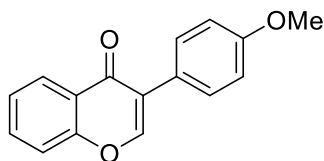
White solid. ^1H NMR (400 MHz, CDCl_3) δ 8.32 (dd, $J = 8.0, 1.7$ Hz, 1H), 8.03 (s, 1H), 7.72-7.65 (m, 1H), 7.61-7.54 (m, 2H), 7.52-7.36 (m, 5H); ^{13}C NMR (101 MHz, CDCl_3) δ 176.2, 156.2, 153.1, 133.6, 131.9, 129.0, 128.5, 128.2, 126.5, 125.4, 125.3, 124.6, 118.1.

3-(*p*-Tolyl)-4*H*-chromen-4-one (**3b**)^[8]



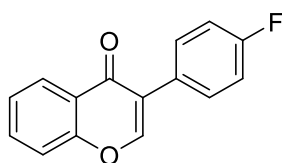
White solid. ^1H NMR (400 MHz, CDCl_3) δ 8.32 (ddd, $J = 8.0, 1.7, 0.5$ Hz, 1H), 8.01 (s, 1H), 7.71-7.65 (m, 1H), 7.50-7.40 (m, 4H), 7.29-7.22 (m, 2H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 176.4, 156.2, 152.8, 138.1, 133.5, 129.2, 128.9, 128.8, 126.5, 125.4, 125.2, 124.6, 118.0, 21.3.

3-(4-Methoxyphenyl)-4*H*-chromen-4-one (**3c**)^[9]



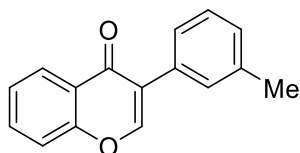
White solid. ¹H NMR (400 MHz, CDCl₃) δ 8.31 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.99 (s, 1H), 7.70-7.64 (m, 1H), 7.54-7.49 (m, 2H), 7.49-7.45 (m, 1H), 7.45-7.39 (m, 1H), 7.00-6.96 (m, 2H), 3.84 (s, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 176.5, 159.7, 156.2, 152.5, 133.5, 130.1, 126.4, 125.2, 125.0, 124.6, 124.1, 118.0, 114.0, 55.4.

3-(4-Fluorophenyl)-4*H*-chromen-4-one (**3d**)^[8]



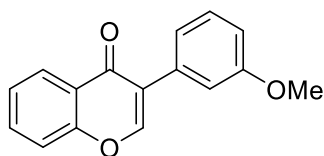
Yellow solid. ¹H NMR (400 MHz, CDCl₃) δ 8.31 (dd, *J* = 7.9, 1.7 Hz, 1H), 8.01 (s, 1H), 7.73-7.66 (m, 1H), 7.61-7.52 (m, 2H), 7.52-7.40 (m, 2H), 7.17-7.10 (m, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 176.2, 162.8 (d, *J* = 248.5), 156.2, 152.9, 133.7, 130.7 (d, *J* = 9.1), 127.8 (d, *J* = 3.0), 126.4, 125.4, 124.6, 124.5, 118.1, 115.5 (d, *J* = 21.2).

3-(*m*-Tolyl)-4*H*-chromen-4-one (**3e**)^[8]



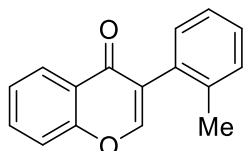
White solid. ¹H NMR (400 MHz, CDCl₃) δ 8.32 (dd, *J* = 8.0, 1.7 Hz, 1H), 8.02 (s, 1H), 7.72-7.66 (m, 1H), 7.49 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.47-7.41 (m, 1H), 7.40 (s, 1H), 7.37-7.31 (m, 2H), 7.24-7.17 (m, 1H), 2.41 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 176.4, 156.2, 153.1, 138.2, 133.6, 131.7, 129.7, 129.0, 128.5, 126.5, 126.0, 125.5, 125.3, 124.6, 118.1, 21.5.

3-(3-Methoxyphenyl)-4*H*-chromen-4-one (**3f**)^[9]



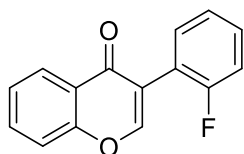
White solid. ^1H NMR (400 MHz, CDCl_3) δ 8.32 (dd, $J = 8.0, 1.7$ Hz, 1H), 8.04 (s, 1H), 7.72-7.66 (m, 1H), 7.49 (dd, $J = 8.4, 1.0$ Hz, 1H), 7.47-7.40 (m, 1H), 7.35 (t, $J = 7.9$ Hz, 1H), 7.19-7.15 (m, 1H), 7.15-7.10 (m, 1H), 6.97-6.91 (m, 1H), 3.85 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 176.2, 159.6, 156.2, 153.2, 133.7, 133.2, 129.5, 126.5, 125.3, 125.3, 124.6, 121.2, 118.1, 114.5, 114.1, 55.3.

3-(*o*-Tolyl)-4*H*-chromen-4-one (**3g**)^[10]



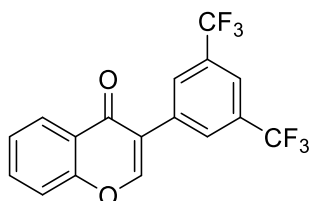
White solid. ^1H NMR (400 MHz, CDCl_3) δ 8.31 (dd, $J = 8.0, 1.7$ Hz, 1H), 7.89 (s, 1H), 7.74-7.67 (m, 1H), 7.51 (d, $J = 8.5$, 1H), 7.47-7.41 (m, 1H), 7.35-7.27 (m, 2H), 7.27-7.21 (m, 1H), 7.21-7.16 (m, 1H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 176.0, 156.5, 153.6, 138.1, 133.6, 131.6, 130.5, 130.2, 128.7, 126.6, 126.5, 125.8, 125.2, 124.4, 118.1, 20.1.

3-(2-Fluorophenyl)-4*H*-chromen-4-one (**3h**)^[11]



White solid. ^1H NMR (400 MHz, CDCl_3) δ 8.31 (dd, $J = 8.0, 1.7$ Hz, 1H), 8.06 (d, $J = 1.3$ Hz, 1H), 7.74-7.66 (m, 1H), 7.53-7.47 (m, 2H), 7.47-7.41 (m, 1H), 7.42-7.34 (m, 1H), 7.22 (td, $J = 7.5, 1.3$ Hz, 1H), 7.20-7.13 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 175.6, 160.3 (d, $J = 242.4$), 156.2, 154.5 (d, $J = 3.0$), 133.8, 132.0 (d, $J = 3.0$), 130.2 (d, $J = 9.1$), 126.4, 125.4, 124.5, 124.1 (d, $J = 4.0$), 120.3, 119.5 (d, $J = 15.2$), 118.1, 115.9 (d, $J = 23.2$).

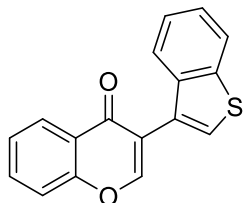
3-(3,5-Bis(trifluoromethyl)phenyl)-4*H*-chromen-4-one (**3i**)



White solid. ^1H NMR (400 MHz, CDCl_3) δ 8.32 (dd, $J = 8.0, 1.7$, 1H), 8.14 (s, 1H), 8.07 (brs, 2H), 7.90 (brs, 1H), 7.78-7.72 (m, 1H), 7.54 (dd, $J = 8.4, 1.3$ Hz, 1H), 7.52-7.46 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 175.5, 156.2, 153.8, 134.3, 134.0, 131.9 (q, $J = 33.3$), 129.1

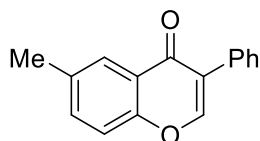
(m), 126.4, 125.9, 124.3, 123.3 (q, $J = 273.7$), 123.1, 122.0 (q, $J = 4.0$), 118.2. HRMS (EI) m/z Calcd. for $C_{17}H_9F_6O_2$ ($[M+H]$): 359.0501. Found: 359.0495.

3-(Benzo[b]thiophen-3-yl)-4H-chromen-4-one (**3j**)



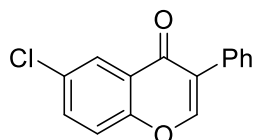
Yellow solid. 1H NMR (400 MHz, $CDCl_3$) δ 8.34 (dd, $J = 8.0, 1.5$ Hz, 1H), 8.16 (s, 1H), 7.94-7.87 (m, 1H), 7.78-7.69 (m, 2H), 7.64 (s, 1H), 7.56-7.51 (m, 1H), 7.51-7.42 (m, 1H), 7.41-7.35 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.1, 156.3, 153.9, 140.1, 138.1, 133.9, 127.2, 126.7, 126.5, 125.5, 124.5, 124.4, 124.4, 122.9, 120.7, 118.2. HRMS (EI) m/z Calcd. for $C_{17}H_{11}O_2S$ ($[M+H]$): 279.0474. Found: 279.0473.

6-Methyl-3-phenyl-4H-chromen-4-one (**3k**)^[12]



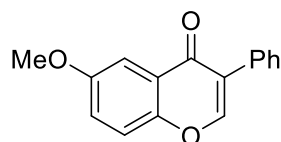
Yellow solid. 1H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, $J = 1.3$ Hz, 1H), 8.00 (s, 1H), 7.59-7.54 (m, 2H), 7.49 (dd, $J = 8.6, 2.3$ Hz, 1H), 7.47-7.41 (m, 2H), 7.41-7.35 (m, 2H), 2.48 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.3, 154.5, 153.0, 135.2, 134.9, 132.1, 129.0, 128.5, 128.1, 125.7, 125.2, 124.3, 117.8, 21.0.

6-Chloro-3-phenyl-4H-chromen-4-one (**3l**)^[8]



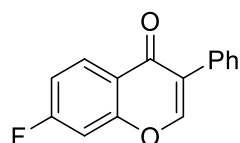
Yellow solid. 1H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, $J = 2.6$ Hz, 1H), 8.02 (s, 1H), 7.63 (dd, $J = 8.9, 2.6$ Hz, 1H), 7.58-7.53 (m, 2H), 7.48-7.37 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.1, 154.6, 153.2, 133.9, 131.4, 131.3, 128.9, 128.6, 128.5, 125.8, 125.5, 125.5, 119.8.

6-Methoxy-3-phenyl-4H-chromen-4-one (**3m**)^[10]



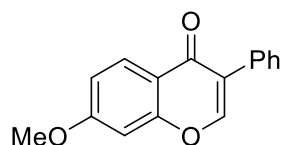
Yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 8.02 (s, 1H), 7.68 (d, $J = 3.1$ Hz, 1H), 7.60-7.55 (m, 2H), 7.48-7.36 (m, 4H), 7.28 (dd, $J = 9.1, 3.1$ Hz, 1H), 3.92 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 176.0, 157.0, 152.9, 151.1, 132.0, 129.0, 128.5, 128.1, 125.2, 124.6, 123.8, 119.5, 105.4, 56.0.

7-Fluoro-3-phenyl-4H-chromen-4-one (**3n**)^[11]



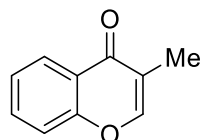
White solid. ^1H NMR (400 MHz, CDCl_3) δ 8.33 (dd, $J = 9.6, 6.3$ Hz, 1H), 8.00 (s, 1H), 7.59-7.52 (m, 2H), 7.48-7.37 (m, 3H), 7.20-7.13 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 175.4, 165.6 (d, $J = 9.1$), 157.2 (d, $J = 13.1$), 153.1, 131.4, 129.1, 129.0, 128.8 (d, $J = 38.4$), 128.4, 125.6, 121.5 (d, $J = 3.0$), 114.1 (d, $J = 22.2$), 104.7 (d, $J = 25.2$).

7-Methoxy-3-phenyl-4H-chromen-4-one (**3o**)^[8]



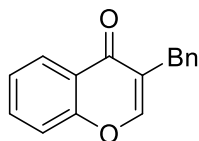
White solid. ^1H NMR (400 MHz, CDCl_3) δ 8.22 (d, $J = 8.9$ Hz, 1H), 7.95 (s, 1H), 7.59-7.54 (m, 2H), 7.47-7.41 (m, 2H), 7.41-7.35 (m, 1H), 7.00 (dd, $J = 8.9, 2.4$ Hz, 1H), 6.86 (d, $J = 2.4$ Hz, 1H), 3.92 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 175.7, 164.0, 158.0, 152.6, 131.9, 128.99, 128.5, 128.1, 127.8, 125.3, 118.4, 114.7, 100.1, 55.9.

3-Methyl-4H-chromen-4-one (**3p**)^[4]



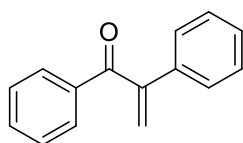
White solid. ^1H NMR (400 MHz, CDCl_3) δ 8.24 (dd, $J = 8.0, 1.7$ Hz, 1H), 7.80 (m, 1H), 7.67-7.60 (m, 1H), 7.44-7.40 (m, 1H), 7.40-7.35 (m, 1H), 2.04 (d, $J = 1.2$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 178.3, 156.7, 151.7, 133.3, 125.8, 124.8, 123.6, 120.7, 118.0, 11.3.

3-Benzyl-4H-chromen-4-one (**3q**)^[5]



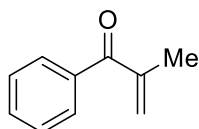
Yellow solid. ¹H NMR (400 MHz, CDCl₃) δ 8.23 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.67-7.61 (m, 1H), 7.61-7.59 (m, 1H), 7.43-7.35 (m, 2H), 7.33-7.28 (m, 4H), 7.25-7.20 (m, 1H), 3.82 (d, *J* = 0.9 Hz, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 177.5, 156.5, 153.1, 138.6, 133.4, 129.1, 128.6, 126.5, 126.0, 125.0, 124.7, 123.9, 118.0, 31.7.

1,2-Diphenylprop-2-en-1-one (**3r**)^[6]



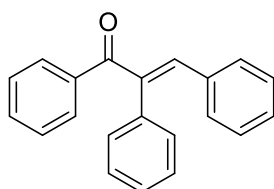
Yellow solid. ¹H NMR (400 MHz, CDCl₃) δ 7.93-7.91 (m, 1H), 7.90-7.89 (m, 1H), 7.58-7.52 (m, 1H), 7.46-7.40 (m, 4H), 7.38-7.29 (m, 3H), 6.07 (s, 1H), 5.64 (s, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 197.6, 148.3, 137.1, 137.0, 133.1, 130.0, 128.6, 128.5, 128.4, 127.1, 121.0.

2-Methyl-1-phenylprop-2-en-1-one (**3s**)^[7]



Colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.77-7.70 (m, 2H), 7.56-7.50 (m, 1H), 7.46-7.40 (m, 2H), 5.91 (m, 1H), 5.64-5.61 (m, 1H), 2.08 (dd, *J* = 1.5, 0.9 Hz, 3H); ¹³C NMR (101 MHz, CDCl₃) δ 198.4, 143.8, 137.7, 132.0, 129.4, 128.2, 127.1, 18.7.

(*E*)-1,2,3-Triphenylprop-2-en-1-one (**3t**)^[6]



White solid. ¹H NMR (400 MHz, CDCl₃) δ 7.89-7.83 (m, 2H), 7.57-7.50 (m, 1H), 7.48-7.41 (m, 2H), 7.39- 7.31 (m, 3H), 7.31-7.26 (m, 2H), 7.25-7.14 (m, 4H), 7.12-7.05 (m, 2H); ¹³C

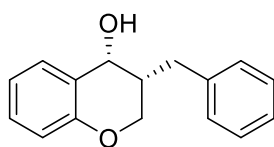
NMR (101 MHz, CDCl₃) δ 197.6, 140.8, 140.2, 138.2, 136.5, 134.8, 132.2, 130.4, 129.8, 129.7, 129.0, 128.8, 128.3, 128.3, 127.9.

III. General procedure for asymmetric hydrogenation of enones

To a 4.0 mL vial was added the catalyst precursor [Ir(COD)Cl]₂ (3.4 mg, 5.0×10⁻³ mmol), ligand **L3** (7.5 mg, 1.0×10⁻² mmol) and anhydrous ⁱPrOH (2.0 mL) under argon atmosphere. The mixture was stirred at 25 °C for 30 min, giving orange solution in the argon-filled glovebox. The resulting solution (100 μ L) transferred by syringe into a 5.0 mL vial charged with different substrates (0.5 mmol) and NaOH (0.025 mmol, 1 mg) in 2.0 mL anhydrous *n*-hexane. The vials were transferred to an autoclave, which was then charged with 50 atm of H₂ and stirred at room temperature for 12-24 h. The hydrogen gas was released slowly in a well-ventilated hood and the solution was concentrated and passed through a short column of silica gel to give target product. The product was analyzed by chiral HPLC for ee values. The dr value and yield was determined by ¹H NMR analysis.

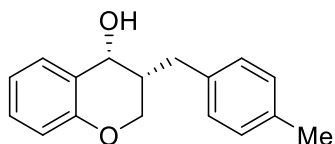
The racemic products were prepared by reduction of corresponding enones or α -substituted ketones with NaBH₄.

(3*R*,4*R*)-3-Benzylchroman-4-ol (**2a**)



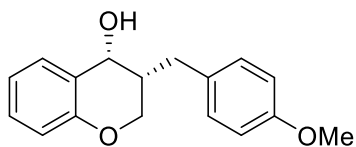
White solid, >99% yield, 119.8 mg; mp 120-122 °C, 99% ee; >20:1 dr; [α]_D²⁵ = +161.1 (*c* = 1.00, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; *t*_R (*S*, *S*) = 12.44 min (minor), *t*_R (*R*, *R*) = 14.92 min (major). ¹H NMR (400 MHz, CDCl₃) δ 7.36-7.30 (m, 2H), 7.30-7.23 (m, 3H), 7.23-7.17 (m, 2H), 6.89 (t, *J* = 7.4 Hz, 1H), 6.86-6.82 (m, 1H), 4.51 (s, 1H), 4.12-4.09 (m, 1H), 4.09-4.06 (m, 1H), 2.89 (dd, *J* = 13.6, 8.4 Hz, 1H), 2.68 (dd, *J* = 13.6, 7.3 Hz, 1H), 2.41-2.26 (m, 1H), 1.72 (d, *J* = 8.5 Hz, 1H); ¹³C NMR (101 MHz, CDCl₃) δ 154.3, 139.2, 130.2, 123.0, 129.1, 128.6, 126.4, 124.2, 120.5, 116.9, 65.0, 65.0, 40.0, 32.8. HRMS (EI) *m/z* Calcd. for C₁₆H₁₆NaO₂ ([*M*+Na]): 263.1043. Found: 263.1053.

(3*R*,4*R*)-3-(4-Methylbenzyl)chroman-4-ol (**2b**)



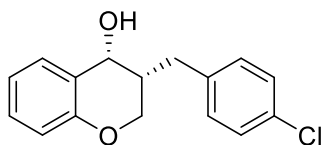
Yellow solid, >99% yield, 126.5 mg; mp 109-112 °C, 99% ee; >20:1 dr; $[\alpha]_D^{25} = +137.4$ (c = 1.00, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_R (S, S) = 10.45 min (minor), t_R (R, R) = 11.47 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.23-7.18 (m, 2H), 7.18-7.11 (m, 4H), 6.92-6.86 (m, 1H), 6.86-6.81 (m, 1H), 4.51 (s, 1H), 4.10-4.08 (m, 1H), 4.07 (s, 1H), 2.84 (dd, $J = 13.7, 8.5$ Hz, 1H), 2.64 (dd, $J = 13.7, 7.2$ Hz, 1H), 2.38-2.25 (m, 4H), 1.73-1.66 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.4, 136.0, 135.9, 130.2, 129.9, 129.3, 129.0, 124.2, 120.5, 116.9, 65.0, 64.9, 40.0, 32.4, 21.0. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{18}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 277.1199. Found: 277.1190.

(3R,4R)-3-(4-Methoxybenzyl)chroman-4-ol (2c)



Yellow solid, >99% yield, 134.6 mg; mp 129-131 °C, >99% ee; >20:1 dr; $[\alpha]_D^{25} = +111.4$ (c = 1.00, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_R (S, S) = 15.87 min (minor), t_R (R, R) = 18.46 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.24-7.16 (m, 4H), 6.92-6.81 (m, 4H), 4.50 (s, 1H), 4.10-4.08 (m, 1H), 4.07 (s, 1H), 3.80 (s, 3H), 2.82 (dd, $J = 13.8, 8.5$ Hz, 1H), 2.62 (dd, $J = 13.8, 7.2$ Hz, 1H), 2.35-2.22 (m, 1H), 1.79-1.65 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 158.1, 154.4, 131.1, 130.2, 130.0, 123.0, 124.2, 120.5, 116.9, 114.0, 65.0, 64.9, 55.3, 40.1, 31.9. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{18}\text{NaO}_3$ ($[\text{M}+\text{Na}]$): 293.1148. Found: 293.1145.

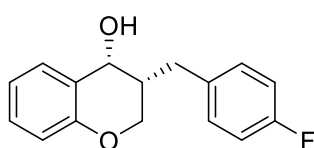
(3R,4R)-3-(4-Chlorobenzyl)chroman-4-ol (2d)



White solid, >99% yield, 136.5 mg; mp 110-112 °C, >99% ee; >20:1 dr; $[\alpha]_D^{25} = +113.3$ (c = 1.00, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H

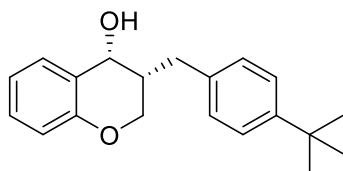
column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_R (*S, S*) = 12.68 min (minor), t_R (*R, R*) = 13.64 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.32-7.27 (m, 2H), 7.24-7.17 (m, 4H), 6.90 (td, J = 7.5, 1.1 Hz, 1H), 6.84 (d, J = 8.0 Hz, 1H), 4.48 (s, 1H), 4.12-4.04 (m, 2H), 2.86 (dd, J = 13.7, 8.6 Hz, 1H), 2.64 (dd, J = 13.7, 7.1 Hz, 1H), 2.36-2.19 (m, 1H), 1.68 (s, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.3, 137.6, 132.1, 130.5, 130.1, 130.0, 128.7, 124.1, 120.7, 117.0, 64.9, 64.7, 40.0, 32.2. HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{14}\text{ClO}_2$ ($[\text{M}-\text{H}]$): 273.0688. Found: 273.0711.

(3*R*,4*R*)-3-(4-Fluorobenzyl)chroman-4-ol (**2e**)



White solid, >99% yield, 128.4 mg; mp 132-137 °C, 99% ee; >20:1 dr; $[\alpha]_{\text{D}}^{25}$ = +91.0 (c = 1.00, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_R (*S, S*) = 11.92 min (minor), t_R (*R, R*) = 12.74 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.29-7.17 (m, 4H), 7.06-6.96 (m, 2H), 6.92-6.87 (m, 1H), 6.84 (d, J = 8.3 Hz, 1H), 4.48 (t, J = 3.5 Hz, 1H), 4.12-4.03 (m, 2H), 2.86 (dd, J = 13.7, 8.6 Hz, 1H), 2.64 (dd, J = 13.7, 7.2 Hz, 1H), 2.34-2.20 (m, 1H), 1.70 (d, J = 4.5 Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 161.6 (d, J = 245.4 Hz), 154.3, 134.8 (d, J = 3.2 Hz), 130.5 (d, J = 8.1 Hz), 130.1, 130.0, 124.1, 120.6, 117.0, 115.5 (d, J = 21.2 Hz), 64.9, 65.0, 40.1, 32.0. HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{15}\text{FNaO}_2$ ($[\text{M}+\text{Na}]$): 281.0948. Found: 281.0924.

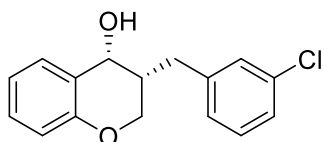
(3*R*,4*R*)-3-(4-(Tert-butyl)benzyl)chroman-4-ol (**2f**)



Yellow solid, >99% yield, 147.4 mg; mp 32-34 °C. >99% ee; >20:1 dr; $[\alpha]_{\text{D}}^{25}$ = +104.0 (c = 1.00, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95:5; flow rate = 0.4 mL/min; UV detection at 210 nm; t_R (*S, S*) = 26.84 min (major), t_R (*R, R*) = 35.14 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.37-7.32 (m, 2H), 7.23-7.16 (m, 4H), 6.87 (ddd, J = 21.7, 10.9, 4.5 Hz, 1H), 6.86-8.82 (m, 1H), 4.52 (s, 1H), 4.11-4.06 (m, 2H), 2.85 (dd, J = 13.7, 8.3 Hz, 1H), 2.64 (dd, J = 13.7, 7.4 Hz, 1H), 2.39-2.24

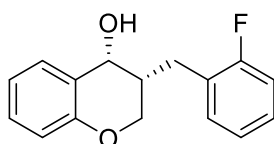
(m, 1H), 1.71 (d, $J = 4.1$ Hz, 1H), 1.32 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.4, 149.2, 136.0, 130.2, 130.0, 128.8, 125.5, 124.2, 120.5, 117.0, 65.0, 40.0, 34.5, 32.3, 31.4. HRMS (EI) m/z Calcd. for $\text{C}_{20}\text{H}_{24}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 313.1669. Found: 313.1668.

(3*R*,4*R*)-3-(3-Chlorobenzyl)chroman-4-ol (2g)



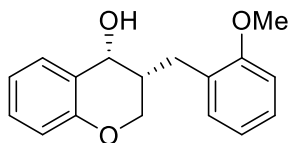
White solid, >99% yield, 134.8 mg; mp 62-66 °C, 99% ee; >20:1 dr; $[\alpha]_{\text{D}}^{25} = +110.7$ ($c=1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_{R} (S, S) = 12.34 min (minor), t_{R} (R, R) = 12.97 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.29-7.26 (m, 1H), 7.25-7.18 (m, 4H), 7.18-7.13 (m, 1H), 6.90 (td, $J = 7.5, 1.1$ Hz, 1H), 6.87-6.81 (m, 1H), 4.49 (t, $J = 3.3$ Hz, 1H), 4.16-4.02 (m, 2H), 2.87 (dd, $J = 13.6, 8.5$ Hz, 1H), 2.64 (dd, $J = 13.6, 7.2$ Hz, 1H), 2.37-2.23 (m, 1H), 1.74-1.66 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.3, 141.3, 134.4, 130.1, 129.8, 129.3, 127.4, 126.6, 124.0, 120.7, 117.0, 64.8, 62.7, 39.9, 32.5. HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{14}\text{ClO}_2$ ($[\text{M}-\text{H}]$): 273.0688. Found: 273.0685.

(3*R*,4*R*)-3-(2-Fluorobenzyl)chroman-4-ol (2h)



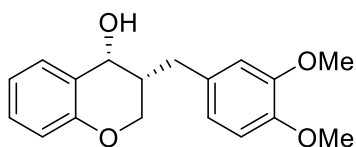
White solid, >99% yield, 128.1 mg; mp 119-121 °C, 99% ee; >20:1 dr; $[\alpha]_{\text{D}}^{25} = +135.2$ ($c = 1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_{R} (S, S) = 10.06 min (minor), t_{R} (R, R) = 10.87 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.29 (td, $J = 7.6, 1.6$ Hz, 1H), 7.25-7.18 (m, 3H), 7.11 (td, $J = 7.4, 0.8$ Hz, 1H), 7.08-7.02 (m, 1H), 6.89 (td, $J = 7.5, 1.1$ Hz, 1H), 6.87-6.82 (m, 1H), 4.51 (t, $J = 3.2$ Hz, 1H), 4.17-4.04 (m, 2H), 2.91 (dd, $J = 13.6, 8.1$ Hz, 1H), 2.74 (dd, $J = 13.7, 7.3$ Hz, 1H), 2.44-2.30 (m, 1H), 1.89-1.75 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 161.4 (d, $J = 245.4$ Hz), 154.3, 131.6 (d, $J = 4.8$ Hz), 130.2, 130.0, 128.3 (d, $J = 8.2$ Hz), 126.1 (d, $J = 15.8$ Hz), 124.2 (d, $J = 4.0$ Hz), 124.0, 120.6, 117.0, 115.5 (d, $J = 22.2$ Hz), 65.1, 64.8, 38.9, 26.6 (d, $J = 2.1$ Hz). HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{15}\text{FNaO}_2$ ($[\text{M}+\text{Na}]$): 281.0948. Found: 281.0955.

(3*R*,4*R*)-3-(2-Methoxybenzyl)chroman-4-ol (**2i**)



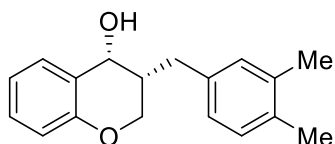
White solid, 99% yield, 133.0 mg; mp 172-175 °C, 98% ee; >20:1 dr; $[\alpha]_{\text{D}}^{25} = +50.8$ ($c = 1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_{R} (S, S) = 13.32 min (minor), t_{R} (R, R) = 27.24 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.28-7.15 (m, 4H), 6.99-6.90 (m, 2H), 6.89-6.80 (m, 2H), 4.36 (s, 1H), 4.23-4.06 (m, 2H), 3.88 (s, 3H), 2.91 (dd, $J = 13.4, 9.9$ Hz, 1H), 2.83 (d, $J = 3.0$ Hz, 1H), 2.61 (dd, $J = 13.4, 5.8$ Hz, 1H), 2.39-2.26 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 157.2, 154.5, 131.2, 130.8, 129.7, 127.87, 127.2, 123.7, 121.2, 120.4, 116.8, 110.6, 65.4, 64.6, 55.6, 39.9, 27.1. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{18}\text{NaO}_3$ ($[\text{M}+\text{Na}]$): 293.1148. Found: 293.1148.

(3*R*,4*R*)-3-(3,4-Dimethoxybenzyl)chroman-4-ol (**2j**)



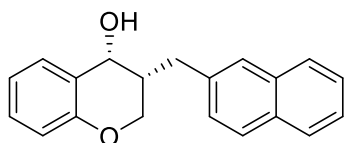
Yellow solid, >99% yield, 149.5 mg; mp 100-108 °C, >99% ee; >20:1 dr; $[\alpha]_{\text{D}}^{25} = +99.2$ ($c = 1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_{R} (S, S) = 31.97 min (minor), t_{R} (R, R) = 35.25 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.25-7.18 (m, 2H), 6.90 (td, $J = 7.5, 1.1$ Hz, 1H), 6.87-6.78 (m, 4H), 4.52 (s, 1H), 4.15-4.04 (m, 2H), 3.88 (s, 6H), 2.83 (dd, $J = 13.7, 8.5$ Hz, 1H), 2.64 (dd, $J = 13.7, 7.2$ Hz, 1H), 2.38-2.23 (m, 1H), 1.71 (s, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.4, 149.0, 147.5, 131.6, 130.2, 130.0, 124.2, 121.0, 120.6, 116.9, 112.2, 111.3, 65.0, 64.9, 56.0, 55.9, 40.1, 32.5. HRMS (EI) m/z Calcd. for $\text{C}_{18}\text{H}_{20}\text{NaO}_4$ ($[\text{M}+\text{Na}]$): 323.1254. Found: 323.1255.

(3*R*,4*R*)-3-(3,4-Dimethylbenzyl)chroman-4-ol (**2k**)



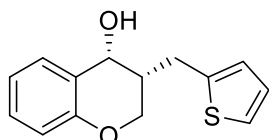
White solid, >99% yield, 133.0 mg; mp 108-110 °C. >99% ee; >20:1 dr; $[\alpha]_D^{25} = +28.9$ ($c = 1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_R (*S, S*) = 11.74 min (major), t_R (*R, R*) = 16.39 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.24-7.17 (m, 2H), 7.12-7.06 (m, 1H), 7.04 (s, 1H), 7.03-6.98 (m, 1H), 6.92-6.86 (m, 1H), 6.86-6.82 (m, 1H), 4.53 (t, $J = 3.6$ Hz, 1H), 4.12-4.05 (m, 2H), 2.81 (dd, $J = 13.7, 8.4$ Hz, 1H), 2.62 (dd, $J = 13.7, 7.2$ Hz, 1H), 2.37-2.28 (m, 1H), 2.26 (s, 6H), 1.75-1.65 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.4, 136.7, 136.5, 134.5, 130.4, 130.2, 129.9, 129.8, 126.5, 124.2, 120.5, 116.9, 65.1, 65.0, 40.0, 32.3, 19.8, 19.4. HRMS (EI) m/z Calcd. for $\text{C}_{18}\text{H}_{20}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 291.1356. Found: 291.1359.

(3*R*,4*R*)-3-(Naphthalen-2-ylmethyl)chroman-4-ol (**2l**)



Yellow solid, >99% yield, 144.5 mg; mp 135-138 °C, >99% ee; >20:1 dr; $[\alpha]_D^{25} = +98.9$ ($c = 1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak AS-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_R (*S, S*) = 14.15 min (minor), t_R (*R, R*) = 20.77 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.86-7.78 (m, 3H), 7.73 (s, 1H), 7.51-7.42 (m, 2H), 7.42-7.38 (m, 1H), 7.24-7.14 (m, 2H), 6.91-6.82 (m, 2H), 4.52 (s, 1H), 4.22-4.07 (m, 2H), 3.04 (dd, $J = 13.7, 8.6$ Hz, 1H), 2.84 (dd, $J = 13.7, 7.1$ Hz, 1H), 2.52-2.37 (m, 1H), 1.80-1.70 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.4, 136.7, 133.6, 132.2, 130.2, 130.0, 128.3, 127.7, 127.6, 127.5, 127.5, 126.1, 125.5, 124.2, 120.58, 117.0, 65.1, 64.9, 39.9, 33.0. HRMS (EI) m/z Calcd. for $\text{C}_{20}\text{H}_{18}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 313.1199. Found: 313.1207.

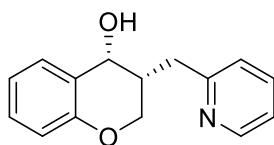
(3*R*,4*R*)-3-(Thiophen-2-ylmethyl)chroman-4-ol (**2m**)



Yellow solid, >99% yield, 122.6 mg; mp 115-118 °C, >99% ee; >20:1 dr; $[\alpha]_D^{25} = +129.4$ ($c = 1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_R (*S, S*)

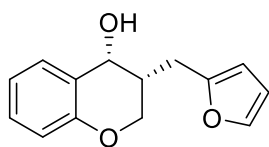
=13.24 min (minor), $t_R(R, R) = 14.71$ min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.24-7.16 (m, 3H), 6.98-6.95 (m, 1H), 6.94-6.88 (m, 2H), 6.85 (d, $J = 8.0$ Hz, 1H), 4.61 (s, 1H), 4.18-4.02 (m, 2H), 3.13 (dd, $J = 14.8, 8.3$ Hz, 1H), 2.90 (dd, $J = 14.8, 7.3$ Hz, 1H), 2.41-2.30 (m, 1H), 1.80-1.70 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.3, 141.6, 130.2, 130.0, 127.0, 125.7, 124.0, 123.8, 120.7, 117.0, 64.8, 64.8, 40.5, 27.1. HRMS (EI) m/z Calcd. for $\text{C}_{20}\text{H}_{13}\text{O}_2\text{S}$ ($[\text{M}-\text{H}]$): 245.0642. Found: 245.0642.

(3*R*,4*R*)-3-(Pyridin-2-ylmethyl)chroman-4-ol (2n)



Yellow solid, >99% yield, 119.9 mg; mp 110-112 °C >99% ee; >20:1 dr; $[\alpha]_D^{25} = +147.2$ ($c = 1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; $t_R(S, S) = 34.88$ min (minor), $t_R(R, R) = 37.07$ min (major). ^1H NMR (400 MHz, CDCl_3) δ 8.58-8.50 (m, 1H), 7.67 (td, $J = 7.7, 1.8$ Hz, 1H), 7.30 (dd, $J = 7.6, 1.5$ Hz, 1H), 7.28-7.14 (m, 3H), 6.90 (td, $J = 7.5, 1.0$ Hz, 1H), 6.83 (d, $J = 8.2$ Hz, 1H), 4.43 (d, $J = 3.6$ Hz, 1H), 4.14-4.09 (m, 2H), 3.00 (dd, $J = 13.4, 10.8$ Hz, 1H), 2.84 (dd, $J = 13.4, 5.1$ Hz, 1H), 2.47-2.34 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 159.2, 154.5, 148.8, 137.3, 131.0, 129.3, 123.9, 123.7, 121.8, 120.6, 116.58, 65.9, 63.9, 39.8, 35.3. HRMS (EI) m/z Calcd. for $\text{C}_{15}\text{H}_{15}\text{NO}_2$ ($[\text{M}-\text{H}]$): 240.1030 Found: 240.1033.

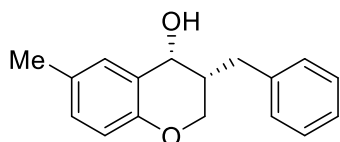
(3*R*,4*R*)-3-(Furan-2-ylmethyl)chroman-4-ol (2o)



Yellow solid, >99% yield, 114.9 mg; mp 68-70 °C. >99% ee; >20:1 dr; $[\alpha]_D^{25} = +142.9$ ($c = 1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; $t_R(S, S) = 11.29$ min (minor), $t_R(R, R) = 11.91$ min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.35 (dd, $J = 1.8, 0.7$ Hz, 1H), 7.27-7.18 (m, 3H), 6.91 (td, $J = 7.4, 1.1$ Hz, 1H), 6.85 (d, $J = 8.3$ Hz, 1H), 6.33 (dd, $J = 3.1, 1.9$ Hz, 1H), 6.12 (dd, $J = 3.1, 0.6$ Hz, 1H), 4.58 (s, 1H), 4.14-4.02 (m, 2H), 2.92 (dd, $J = 15.1, 8.1$ Hz, 1H), 2.72 (dd, $J = 15.1, 7.4$ Hz, 1H), 2.48-2.38 (m, 1H), 1.90 (d, $J = 4.0$ Hz,

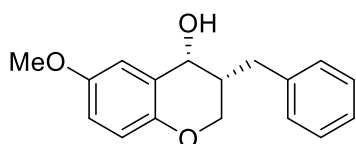
1H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.3, 153.2, 141.5, 130.3, 130.0, 123.9, 120.6, 117.0, 110.4, 106.6, 65.2, 64.8, 37.9, 25.5. HRMS (EI) m/z Calcd. for $\text{C}_{14}\text{H}_{14}\text{NaO}_3$ ($[\text{M}+\text{Na}]$): 253.0835. Found: 253.0838.

(3*R*,4*R*)-3-Benzyl-6-methylchroman-4-ol (2p)



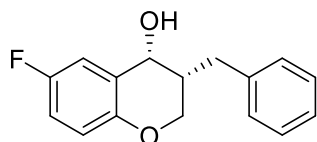
Yellow solid, >99% yield, 126.1 mg; mp 147-150 °C, >99% ee; >20:1 dr; $[\alpha]_{\text{D}}^{25} = +83.9$ ($c = 1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_{R} (*S*, *S*) = 10.76 min (minor), t_{R} (*R*, *R*) = 13.00 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.36-7.20 (m, 5H), 7.04-6.98 (m, 2H), 6.77-6.72 (m, 1H), 4.47 (s, 1H), 4.11-4.00 (m, 2H), 2.88 (dd, $J = 13.6, 8.4$ Hz, 1H), 2.67 (dd, $J = 13.6, 7.3$ Hz, 1H), 2.37-2.28 (m, 1H), 2.25 (s, 3H), 1.67 (s, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 152.1, 139.2, 130.7, 130.3, 129.8, 129.1, 128.6, 126.3, 123.8, 116.7, 65.0, 65.0, 40.2, 32.9, 20.4. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{18}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 277.1199. Found: 277.1181.

(3*R*,4*R*)-3-Benzyl-6-methoxychroman-4-ol (2q)



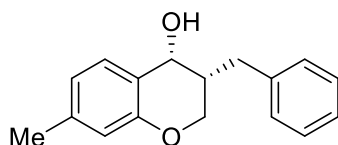
Yellow solid, >99% yield, 132.1 mg; mp 157-159 °C, >99% ee; >20:1 dr; $[\alpha]_{\text{D}}^{25} = +55.8$ ($c = 1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_{R} (*S*, *S*) = 18.10 min (minor), t_{R} (*R*, *R*) = 22.30 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.36-7.30 (m, 2H), 7.30-7.21 (m, 3H), 6.82-6.73 (m, 3H), 4.49 (t, $J = 3.6$ Hz, 1H), 4.07-4.02 (m, 2H), 3.74 (s, 3H), 2.88 (dd, $J = 13.6, 8.5$ Hz, 1H), 2.67 (dd, $J = 13.6, 7.3$ Hz, 1H), 2.41-2.25 (m, 1H), 1.71 (d, $J = 4.8$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 153.5, 148.3, 139.2, 129.1, 128.6, 126.4, 124.3, 117.7, 116.7, 113.8, 65.3, 65.0, 55.8, 40.2, 32.7. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{18}\text{NaO}_3$ ($[\text{M}+\text{Na}]$): 293.1148. Found: 293.1153.

(3*R*,4*R*)-3-Benzyl-6-fluorochroman-4-ol (2r)



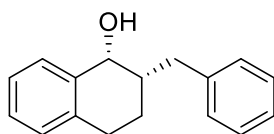
Yellow solid, >99% yield, 128.4 mg; mp 104-107 °C, 99% ee; >20:1 dr; $[\alpha]_D^{25} = +116.5$ ($c = 1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_R (S, S) = 12.70 min (minor), t_R (R, R) = 15.23 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.37-7.30 (m, 2H), 7.29-7.22 (m, 3H), 6.95-6.88 (m, 2H), 6.81-6.76 (m, 1H), 4.49 (t, $J = 3.5$ Hz, 1H), 4.10-4.02 (m, 2H), 2.87 (dd, $J = 13.7, 8.3$ Hz, 1H), 2.67 (dd, $J = 13.7, 7.4$ Hz, 1H), 2.36-2.26 (m, 1H), 1.80-1.74 (s, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 156.7 (d, $J = 239.4$ Hz), 150.3, 139.0, 129.1, 128.7, 126.5, 124.8 (d, $J = 6.6$ Hz), 118.0 (d, $J = 7.8$ Hz), 116.9 (d, $J = 23.2$ Hz), 115.7 (d, $J = 22.2$ Hz), 65.1, 64.9, 39.9, 32.6. HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{15}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 281.0948. Found: 281.0936.

(3R,4R)-3-Benzyl-7-methylchroman-4-ol (**2s**)



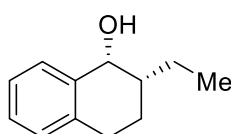
Yellow solid, >99% yield, 126.4 mg; mp 150-152 °C, 97% ee; >20:1 dr; $[\alpha]_D^{25} = +125.0$ ($c = 1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_R (S, S) = 17.41 min (minor), t_R (R, R) = 22.17 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.38-7.20 (m, 5H), 7.09 (d, $J = 7.7$ Hz, 1H), 6.71 (d, $J = 7.8$ Hz, 1H), 6.66 (s, 1H), 4.48 (s, 1H), 4.16-3.99 (m, 2H), 2.88 (dd, $J = 13.6, 8.4$ Hz, 1H), 2.67 (dd, $J = 13.6, 7.3$ Hz, 1H), 2.38-2.24 (m, 4H), 1.63 (s, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.2, 140.2, 139.3, 129.9, 129.2, 128.6, 126.3, 121.6, 121.4, 117.2, 65.0, 64.7, 40.2, 32.9, 21.3. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{18}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 277.1199. Found: 277.1166.

(1R,2S)-2-Benzyl-1,2,3,4-tetrahydronaphthalen-1-ol (**2t**)^[13]



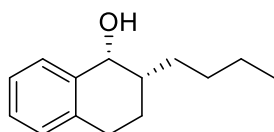
Yellow oil, >99% yield, 119.0 mg; 92% ee; >20:1 dr; $[\alpha]_{\text{D}}^{25} = +67.4$ ($c = 1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; $t_{\text{R}}(\text{S}, \text{S}) = 10.60$ min (minor), $t_{\text{R}}(\text{R}, \text{R}) = 11.66$ min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.35-7.09 (m, 9H), 4.51 (s, 1H), 2.95 (dd, $J = 13.5, 7.8$ Hz, 1H), 2.92-2.83 (m, 1H), 2.80-2.68 (m, 2H), 2.09-1.96 (m, 1H), 1.90-1.76 (m, 1H), 1.75-1.65 (m, 1H), 1.59 (s, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 140.7, 138.5, 137.0, 130.1, 129.3, 129.2, 128.4, 128.1, 126.2, 126.0, 69.4, 41.76, 38.2, 29.2, 22.6. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{18}\text{NaO}$ ($[\text{M}+\text{Na}]$): 261.1250. Found: 261.1270.

(1*R*,2*R*)-2-Ethyl-1,2,3,4-tetrahydronaphthalen-1-ol (**2u**)^[14]



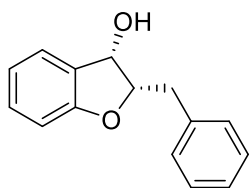
Yellow oil, 90% yield, 79 mg, >99% ee; 10:1 dr; $[\alpha]_{\text{D}}^{20} = +91.6$ ($c = 1.00$, CHCl_3). The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 90:10; flow rate = 0.3 mL/min; UV detection at 210 nm; $t_{\text{R}}(\text{R}, \text{R}) = 21.50$ min (major), $t_{\text{R}}(\text{S}, \text{S}) = 22.67$ min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.36-7.32 (m, 1H), 7.20 (m, 2H), 7.12 (m, 1H), 4.65 (s, 1H), 2.91-2.70 (m, 2H), 1.76-1.67 (m, 2H), 1.67-1.56 (m, 2H), 1.50-1.39 (m, 2H), 1.04 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 138.7, 137.2, 130.1, 129.1, 127.9, 126.1, 69.7, 41.4, 29.3, 24.4, 22.8, 11.7. HRMS (EI) m/z Calcd. for $\text{C}_{12}\text{H}_{16}\text{NaO}$ ($[\text{M}+\text{Na}]$): 199.1077. Found: 199.1099.

(1*R*,2*R*)-2-Butyl-1,2,3,4-tetrahydronaphthalen-1-ol (**2v**)^[15]



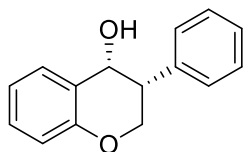
Colorless oil, 80% yield, 32.6 mg, 86% ee; 8:1 dr; $[\alpha]_{\text{D}}^{20} = +44.5$ ($c=1.00$, CHCl_3). The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 98:2; flow rate = 0.5 mL/min; UV detection at 210 nm; $t_{\text{R}}(\text{R}, \text{R}) = 42.47$ min (major), $t_{\text{R}}(\text{S}, \text{S}) = 46.42$ min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.35-7.33 (m, 1H), 7.24-7.17 (m, 2H), 7.15-7.11 (m, 1H), 4.64 (s, 1H), 2.89-2.72 (m, 2H), 1.81-1.62 (m, 4H), 1.38-1.32 (m, 6H), 0.94 (t, $J = 7.1$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 138.7, 137.1, 130.0, 129.1, 127.9, 126.1, 70.1, 39.5, 31.3, 29.3, 29.2, 23.0, 14.1.

(2*S*,3*S*)-2-Benzyl-2,3-dihydrobenzofuran-3-ol (**2w**)^[16]



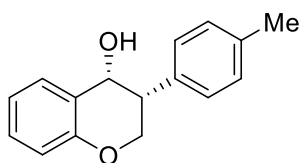
Yellow solid, >99% yield, 113.0 mg; mp 106-109 °C, 93% ee; >20:1 dr; $[\alpha]_D^{25} = -6.4$ ($c = 1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 0.8 mL/min; UV detection at 210 nm; t_R (*R, R*) = 17.86 min (minor), t_R (*S, S*) = 22.02 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.44-7.38 (m, 3H), 7.38-7.32 (m, 2H), 7.30-7.22 (m, 2H), 6.93 (td, $J = 7.4, 0.8$ Hz, 1H), 6.87 (d, $J = 8.1$ Hz, 1H), 5.03 (d, $J = 3.5$ Hz, 1H), 4.67-4.60 (m, 1H), 3.30 (dd, $J = 14.1, 6.9$ Hz, 1H), 3.20 (dd, $J = 14.1, 7.5$ Hz, 1H), 1.65 (s, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 159.8, 138.0, 130.9, 129.4, 129.1, 128.6, 126.6, 125.8, 121.18, 110.78, 87.8, 72.3, 34.5. HRMS (EI) m/z Calcd. for $\text{C}_{15}\text{H}_{14}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 249.0886. Found: 249.0888.

(3*R*,4*R*)-3-Phenylchroman-4-ol (**4a**)^[17]



Colorless oil, 99% yield, 45 mg, 99% ee; >20:1 dr; $[\alpha]_D^{20} = +192.5$ ($c = 1.00$, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak IC-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R (*R, R*) = 10.06 min (major), t_R (*S, S*) = 15.10 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.42-7.35 (m, 2H), 7.34-7.22 (m, 5H), 6.98-6.89 (m, 2H), 4.81 (s, 1H), 4.61 (dd, $J = 11.7, 10.5$ Hz, 1H), 4.34 (ddd, $J = 10.5, 3.6, 1.3$ Hz, 1H), 3.34 (dt, $J = 11.8, 3.3$ Hz, 1H), 1.79 (d, $J = 3.5$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.3, 137.8, 130.6, 130.0, 128.9, 128.4, 127.5, 123.6, 120.7, 117.0, 67.2, 64.1, 44.2.

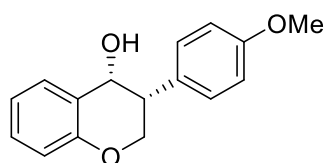
(3*R*,4*R*)-3-(*p*-Tolyl)chroman-4-ol (**4b**)



Colorless oil, 99% yield, 47.6 mg, >99% ee; >20:1 dr; $[\alpha]_D^{20} = +166.7$ ($c = 1.00$, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak IC-H column, hexane:

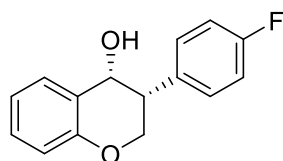
isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R (*R, R*) = 11.47 min (major), t_R (*S, S*) = 17.20 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.30 (dd, J = 7.6, 1.6 Hz, 1H), 7.28-7.22 (m, 1H), 7.21-7.15 (m, 4H), 6.97-6.88 (m, 2H), 4.78 (t, J = 2.7 Hz, 1H), 4.59 (dd, J = 11.7, 10.5 Hz, 1H), 4.32 (ddd, J = 10.4, 3.6, 1.3 Hz, 1H), 3.31 (dt, J = 11.8, 3.4 Hz, 1H), 2.35 (s, 3H), 1.77 (d, J = 3.6 Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.3, 137.2, 134.6, 130.6, 130.0, 129.6, 128.2, 123.7, 120.6, 116.9, 67.2, 64.2, 43.8, 21.1. HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{15}\text{O}_2$ ($[\text{M}-\text{H}]$): 239.1066. Found: 239.1056.

(3*R*,4*R*)-3-(4-Methoxyphenyl)chroman-4-ol (**4c**)



Colorless oil, 99% yield, 51 mg, 96% ee; >20:1 dr; $[\alpha]_{\text{D}}^{20}$ = +201.8 (c = 1.00, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak IC-H column, hexane: isopropanol = 90:10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R (*R, R*) = 12.94 min (major), t_R (*S, S*) = 17.35 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.30 (dd, J = 7.6, 1.7 Hz, 1H), 7.25 (m, 1H), 7.22-7.19 (m, 2H), 6.98-6.88 (m, 4H), 4.77 (t, J = 2.7 Hz, 1H), 4.56 (dd, J = 11.7, 10.5 Hz, 1H), 4.31 (ddd, J = 10.5, 3.6, 1.4 Hz, 1H), 3.81 (s, 3H), 3.29 (dt, J = 11.7, 3.4 Hz, 1H), 1.78 (d, J = 3.7 Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 159.0, 154.2, 130.6, 130.0, 129.6, 129.4, 123.7, 120.6, 116.9, 114.3, 67.2, 64.3, 55.3, 43.4. HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{16}\text{NaO}_3$ ($[\text{M}+\text{Na}]$): 279.0991. Found: 279.0984.

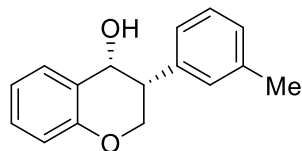
(3*R*,4*R*)-3-(4-Fluorophenyl)chroman-4-ol (**4d**)



Yellow oil, 99% yield, 48.5 mg, >99% ee; >20:1 dr; $[\alpha]_{\text{D}}^{20}$ = +196.9 (c = 1.00, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak IC-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R (*R, R*) = 8.92 min (major), t_R (*S, S*) = 12.62 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.32-7.23 (m, 4H), 7.11-7.03 (m, 2H), 6.95 (td, J = 7.4, 1.2 Hz, 1H), 6.91 (d, J = 8.2 Hz, 1H), 4.78 (s, 1H), 4.56 (t, J = 11.1 Hz, 1H), 4.30 (ddd, J = 10.5, 3.6, 1.3 Hz, 1H), 3.31 (dt, J = 11.7, 3.4 Hz, 1H), 1.77 (d, J = 3.5 Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 162.2 (d, J = 246.4 Hz), 154.1, 133.5 (d, J = 4.0 Hz), 130.4,

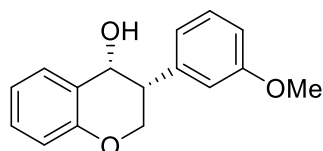
130.1, 130.0 (d, $J = 8.1$ Hz), 123.6, 120.8, 117.0, 115.7 (d, $J = 21.2$ Hz), 67.1, 64.2, 43.5. HRMS (EI) m/z Calcd. for $C_{15}H_{14}FO_2$ ($[M+H]$): 245.0972. Found: 245.0994.

(3*R*,4*R*)-3-(*m*-Tolyl)chroman-4-ol (**4e**)



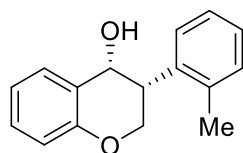
Yellow oil, 99% yield, 47.7 mg, 99% ee; >20:1 dr; $[\alpha]_D^{20} = +188.2$ ($c = 1.00$, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak IC-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R (*R, R*) = 9.93 min (major), t_R (*S, S*) = 14.24 min (minor). 1H NMR (400 MHz, $CHCl_3$) δ 7.32-7.22 (m, 3H), 7.15-7.06 (m, 3H), 6.98-6.89 (m, 2H), 4.80 (s, 1H), 4.61 (dd, $J = 11.9, 10.4$ Hz, 1H), 4.34 (ddd, $J = 10.4, 3.6, 1.4$ Hz, 1H), 3.31 (dt, $J = 11.9, 3.4$ Hz, 1H), 2.37 (s, 3H), 1.77 (d, $J = 3.4$ Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.3, 138.6, 137.6, 130.7, 130.0, 129.1, 128.8, 128.3, 125.3, 123.6, 120.64, 117.0, 67.2, 64.0, 44.1, 21.5. HRMS (EI) m/z Calcd. for $C_{16}H_{15}O_2$ ($[M-H]$): 239.1066. Found: 279.1081.

(3*R*,4*R*)-3-(3-Methoxyphenyl)chroman-4-ol (**4f**)



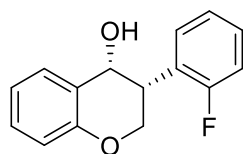
Colorless oil, 99% yield, 51.0 mg, 99% ee; >20:1 dr; $[\alpha]_D^{20} = +116.8$ ($c = 1.00$, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak IB-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R (*R, R*) = 19.99 min (major), t_R (*S, S*) = 36.81 min (minor). 1H NMR (400 MHz, $CDCl_3$) δ 7.33-7.28 (m, 2H), 7.28-7.22 (m, 1H), 6.95 (td, $J = 7.4, 1.2$ Hz, 1H), 6.91 (m, 1H), 6.89-6.83 (m, 3H), 4.83-4.79 (m, 1H), 4.59 (dd, $J = 11.8, 10.4$ Hz, 1H), 4.34 (ddd, $J = 10.4, 3.6, 1.4$ Hz, 1H), 3.81 (s, 3H), 3.32 (dt, $J = 11.7, 3.3$ Hz, 1H), 1.81 (d, $J = 3.6$ Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9, 154.3, 139.3, 130.6, 130.0, 129.9, 123.6, 120.7, 120.6, 116.9, 114.5, 112.5, 67.1, 64.0, 55.3, 44.2. HRMS (EI) m/z Calcd. for $C_{16}H_{15}O_3$ ($[M-H]$): 255.1016. Found: 255.1010.

(3*R*,4*R*)-3-(*o*-Tolyl)chroman-4-ol (**4g**)



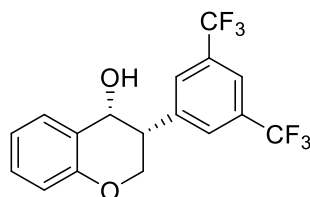
Yellow oil, 99% yield, 47.6 mg, 95% ee; >20:1 dr; $[\alpha]_D^{20} = +258.7$ ($c = 1.00$, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak IC-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R (R, R) = 10.16 min (major), t_R (S, S) = 17.69 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.32-7.28 (m, 1H), 7.28-7.18 (m, 4H), 7.17-7.12 (m, 1H), 6.99-6.91 (m, 2H), 4.79-4.75 (m, 1H), 4.66 (dd, $J = 11.9, 10.4$ Hz, 1H), 4.25 (ddd, $J = 10.3, 3.3, 1.5$ Hz, 1H), 3.56 (dt, $J = 12.0, 3.1$ Hz, 1H), 2.37 (s, 3H), 1.78 (d, $J = 3.2$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.4, 136.6, 135.7, 131.0, 131.0, 130.0, 127.5, 127.3, 126.3, 123.8, 120.7, 117.1, 65.2, 64.3, 40.3, 19.7. HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{16}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 263.1042. Found: 263.1055.

(3R,4R)-3-(2-Fluorophenyl)chroman-4-ol (4h)



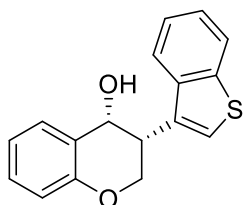
Yellow oil, 99% yield, 48.6 mg, 98% ee; >20:1 dr; $[\alpha]_D^{20} = +199.4$ ($c = 1.00$, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak IC-H column, hexane: isopropanol = 90:10; flow rate = 0.5 mL/min; UV detection at 210 nm; t_R (R, R) = 11.53 min (major), t_R (S, S) = 14.11 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.34-7.23 (m, 4H), 7.19-7.07 (m, 2H), 6.96 (td, $J = 7.4, 1.2$ Hz, 1H), 6.92 (dd, $J = 8.2, 1.1$ Hz, 1H), 4.87 (s, 1H), 4.62 (ddd, $J = 11.9, 10.4, 1.5$ Hz, 1H), 4.31 (ddd, $J = 10.4, 3.5, 1.4$ Hz, 1H), 3.70 (dt, $J = 12.0, 3.3$ Hz, 1H), 1.78 (d, $J = 3.8$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 160.88 (d, $J = 247.5$), 154.2, 130.6, 130.1, 129.1 (d, $J = 4.0$), 128.9 (d, $J = 8.1$), 124.9 (d, $J = 14.1$), 124.3 (d, $J = 4.0$), 123.7, 120.77, 117.1, 115.6 (d, $J = 22.2$), 66.0, 63.6 (d, $J = 1.3$), 37.1 (d, $J = 2.1$). HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{14}\text{O}_2$ ($[\text{M}+\text{H}]$): 245.0972. Found: 245.0982.

(3R,4R)-3-(3,5-Bis(trifluoromethyl)phenyl)chroman-4-ol (4i)



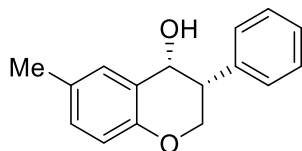
Yellow oil, 99% yield, 72.0 mg, >99% ee; >20:1 dr; $[\alpha]_{\text{D}}^{20} = +103.8$ ($c = 1.00$, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak IC-H column, hexane: isopropanol = 95:5; flow rate = 0.5 mL/min; UV detection at 210 nm; t_{R} (*R, R*) = 8.34 min (major), t_{R} (*S, S*) = 8.97 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.83 (s, 1H), 7.80 (s, 2H), 7.32-7.26 (m, 2H), 6.98 (td, $J = 7.5, 1.0$ Hz, 1H), 6.94 (d, $J = 8.2$ Hz, 1H), 4.86 (s, 1H), 4.60 (dd, $J = 11.7, 10.6$ Hz, 1H), 4.32 (ddd, $J = 10.5, 3.6, 1.3$ Hz, 1H), 3.42 (dt, $J = 11.8, 3.3$ Hz, 1H), 1.86 (s, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 153.8, 140.7, 131.8 (q, $J = 33.3$ Hz), 130.5, 130.0, 129.0, 123.5, 123.3 (q, $J = 273.7$ Hz), 121.4, 121.1, 117.2, 66.5, 63.7, 44.0. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{12}\text{NaF}_6\text{O}_2$ ($[\text{M}+\text{Na}]$): 385.0634. Found: 385.0636.

(3*R*,4*R*)-3-(Benzo[*b*]thiophen-3-yl)chroman-4-ol (**4j**)



Yellow oil, 99% yield, 56.1 mg, 96% ee; >20:1 dr; $[\alpha]_{\text{D}}^{20} = +221.7$ ($c = 1.00$, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak IB-H column, hexane: isopropanol = 95:5; flow rate = 0.5 mL/min; UV detection at 210 nm; t_{R} (*R, R*) = 36.48 min (major), t_{R} (*S, S*) = 46.26 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.94-7.89 (m, 1H), 7.82-7.77 (m, 1H), 7.44-7.37 (m, 2H), 7.34 (brs, 1H), 7.34-7.26 (m, 2H), 7.00-6.92 (m, 2H), 4.94 (t, $J = 3.8$ Hz, 1H), 4.64 (dd, $J = 11.3, 10.6$ Hz, 1H), 4.39 (ddd, $J = 10.4, 3.5, 1.3$ Hz, 1H), 3.82 (dt, $J = 11.5, 3.2$ Hz, 1H), 1.85 (d, $J = 3.8$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 153.2, 139.1, 137.4, 130.6, 129.6, 129.1, 123.8, 123.3, 122.5, 122.3, 122.1, 120.2, 119.8, 116.0, 64.3, 63.0, 37.4. HRMS (EI) m/z Calcd. for $\text{C}_{17}\text{H}_{14}\text{NaF}_6\text{O}_2\text{S}$ ($[\text{M}+\text{Na}]$): 305.0607. Found: 305.0603.

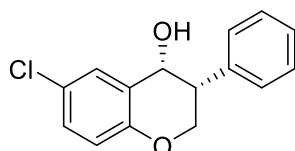
(3*R*,4*R*)-6-Methyl-3-phenylchroman-4-ol (**4k**)



Yellow oil, 99% yield, 47.7 mg, 99% ee; >20:1 dr; $[\alpha]_{\text{D}}^{20} = +179.0$ ($c = 1.00$, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_{R} (*R, R*) = 14.89 min (major), t_{R} (*S, S*) = 24.11 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.41-7.35 (m, 2H), 7.34

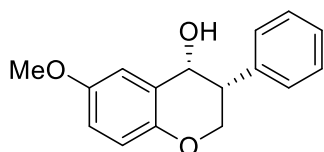
-7.30 (m, 1H), 7.29-7.26 (m, 2H), 7.12-7.03 (m, 2H), 6.81 (d, $J = 8.3$ Hz, 1H), 4.76 (s, 1H), 4.58 (dd, $J = 11.7, 10.4$ Hz, 1H), 4.31 (ddd, $J = 10.4, 3.5, 1.4$ Hz, 1H), 3.32 (dt, $J = 11.8, 3.3$ Hz, 1H), 2.29 (s, 3H), 1.76 (d, $J = 3.6$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 152.0, 137.9, 130.8, 129.9, 128.9, 128.4, 127.5, 123.2, 116.7, 67.2, 64.1, 44.4, 20.5. HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{15}\text{O}_2$ ($[\text{M}-\text{H}]$): 239.1066. Found: 239.1064.

(3*R*,4*R*)-6-Chloro-3-phenylchroman-4-ol (**4l**)



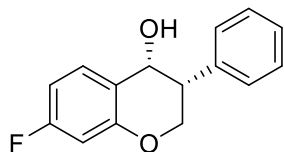
Colorless oil, 99% yield, 51.7 mg, >99% ee; >20:1 dr; $[\alpha]_{\text{D}}^{20} = +175.4$ ($c = 1.00$, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_{R} (*R, R*) = 18.52 min (major), t_{R} (*S, S*) = 31.99 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.42-7.36 (m, 2H), 7.35-7.30 (m, 1H), 7.30-7.23 (m, 3H), 7.20 (dd, $J = 8.8, 2.6$ Hz, 1H), 6.85 (d, $J = 8.8$ Hz, 1H), 4.76 (t, $J = 3.9$ Hz, 1H), 4.58 (dd, $J = 11.5, 10.6$ Hz, 1H), 4.34 (ddd, $J = 10.5, 3.6, 1.3$ Hz, 1H), 3.31 (dt, $J = 11.5, 3.4$ Hz, 1H), 1.82 (d, $J = 3.9$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 152.9, 137.1, 130.13, 130.0, 129.0, 128.4, 127.7, 125.3, 124.9, 118.4, 66.8, 64.3, 44.0. HRMS (EI) m/z Calcd. for $\text{C}_{15}\text{H}_{13}\text{NaClO}_2$ ($[\text{M}+\text{Na}]$): 283.0496. Found: 283.0504.

(3*R*,4*R*)-6-Methoxy-3-phenylchroman-4-ol (**4m**)



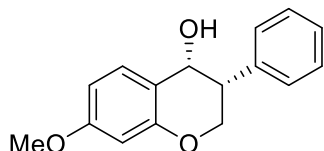
Yellow oil, 99% yield, 50.8 mg, 96% ee; >20:1 dr; $[\alpha]_{\text{D}}^{20} = +208.3$ ($c = 1.00$, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak IB-H column, hexane: isopropanol = 90:10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_{R} (*R, R*) = 10.89 min (major), t_{R} (*S, S*) = 14.91 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.41-7.36 (m, 2H), 7.35-7.30 (m, 1H), 7.30-7.24 (m, 2H), 6.86-6.83 (m, 3H), 4.82-4.76 (m, 1H), 4.55 (dd, $J = 11.4, 10.6$ Hz, 1H), 4.31 (ddd, $J = 10.5, 3.5, 1.3$ Hz, 1H), 3.77 (s, 3H), 3.33 (dt, $J = 11.4, 3.4$ Hz, 1H), 1.78 (d, $J = 4.0$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 153.6, 148.2, 137.0, 128.9, 128.4, 127.5, 123.8, 117.7, 116.8, 114.3, 67.3, 64.2, 55.8, 44.4. HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{15}\text{O}_3$ ($[\text{M}-\text{H}]$): 255.1016. Found: 255.1010.

(3*R*,4*R*)-7-Fluoro-3-phenylchroman-4-ol (**4n**)



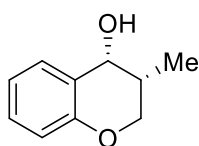
Yellow oil, 99% yield, 48.2 mg, 97% ee; >20:1 dr; $[\alpha]_D^{20} = +183.9$ ($c = 1.00$, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R (*R, R*) = 16.26 min (major), t_R (*S, S*) = 27.53 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.42-7.36 (m, 2H), 7.35-7.30 (m, 1H), 7.30-7.22 (m, 3H), 6.70-6.64 (m, 1H), 6.64-6.60 (m, 1H), 4.80-4.76 (m, 1H), 4.61 (dd, $J = 11.9, 10.4$ Hz, 1H), 4.35 (ddd, $J = 10.5, 3.6, 1.4$ Hz, 1H), 3.32 (dt, $J = 11.8, 3.4$ Hz, 1H), 1.77 (d, $J = 3.5$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 163.6 (d, $J = 247.5$ Hz), 155.5 (d, $J = 13.1$ Hz), 137.4, 131.8 (d, $J = 10.1$ Hz), 129.0, 128.3, 127.7, 119.7 (d, $J = 3.0$ Hz), 108.1 (d, $J = 22.2$ Hz), 103.9 (d, $J = 25.3$ Hz), 66.7, 64.1, 44.0. HRMS (EI) m/z Calcd. for $\text{C}_{15}\text{H}_{14}\text{FO}_2$ ($[\text{M}+\text{H}]$): 245.0972. Found: 245.0971.

(3*R*,4*R*)-7-Methoxy-3-phenylchroman-4-ol (**4o**)^[17]



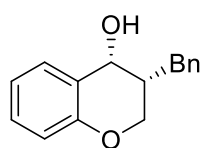
Colorless oil, 99% yield, 50.8 mg, 97% ee; >20:1 dr; $[\alpha]_D^{20} = +136.2$ ($c = 1.00$, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak IB-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R (*R, R*) = 16.88 min (major), t_R (*S, S*) = 25.21 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.41-7.36 (m, 2H), 7.34-7.26 (m, 3H), 7.20 (d, $J = 8.5$ Hz, 1H), 6.54 (dd, $J = 8.4, 2.5$ Hz, 1H), 6.45 (d, $J = 2.5$ Hz, 1H), 4.77 (s, 1H), 4.61 (dd, $J = 11.9, 10.4$ Hz, 1H), 4.33 (ddd, $J = 10.4, 3.6, 1.3$ Hz, 1H), 3.79 (s, 3H), 3.32 (dt, $J = 11.9, 3.3$ Hz, 1H), 1.70 (d, $J = 3.3$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 161.1, 155.3, 137.9, 131.3, 128.9, 128.4, 127.5, 116.2, 108.0, 101.2, 66.8, 64.1, 55.4, 44.4.

(3*R*,4*R*)-3-Methylchroman-4-ol (**4p**)^[18]



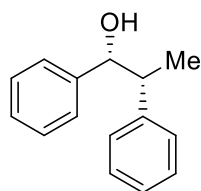
Colorless oil, 85% yield, 28.0 mg, 99% ee; 11:1 dr; $[\alpha]_D^{20} = +110.3$ ($c = 1.00$, CHCl_3). The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R (R, R) = 11.23 min (major), t_R (S, S) = 13.20 min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.27 (dd, $J = 7.6, 1.6$ Hz, 1H), 7.21 (ddd, $J = 8.9, 7.4, 1.7$ Hz, 1H), 6.91 (td, $J = 7.4, 1.1$ Hz, 1H), 6.84 (dd, $J = 8.2$ Hz, 1.0 Hz, 1H), 4.56 (s, 1H), 4.07-3.93 (m, 2H), 2.22-2.10 (m, 1H), 1.71 (s, 1H), 1.09 (d, $J = 7.0$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 154.2, 130.1, 129.8, 124.4, 120.5, 116.9, 66.9, 66.5, 32.7, 11.7.

(3*R*,4*R*)-3-Benzylchroman-4-ol (**4q**)



White solid, >99% yield, 47.8 mg; mp 120-122 °C, 99% ee; >20:1 dr; $[\alpha]_D^{25} = +163.4$ ($c = 1.00$, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_R (S, S) = 13.28 min (minor), t_R (R, R) = 16.13 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.36-7.30 (m, 2H), 7.29-7.23 (m, 3H), 7.23-7.17 (m, 2H), 6.89 (td, $J = 7.4, 1.2$ Hz, 1H), 6.88-6.82 (m, 1H), 4.51 (t, $J = 4.6$ Hz, 1H), 4.15-4.03 (m, 2H), 2.89 (dd, $J = 13.6, 8.4$ Hz, 1H), 2.68 (dd, $J = 13.6, 7.3$ Hz, 1H), 2.38-2.28 (m, 1H), 1.69 (d, $J = 4.6$ Hz, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 153.3, 138.1, 129.1, 128.9, 128.1, 127.5, 125.3, 123.1, 119.5, 115.9, 63.9, 63.9, 39.0, 31.8. HRMS (EI) m/z Calcd. for $\text{C}_{16}\text{H}_{16}\text{NaO}_2$ ($[\text{M}+\text{Na}]$): 263.1043. Found: 263.1053.

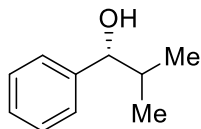
(1*R*,2*R*)-1,2-Diphenylpropan-1-ol (**4r**)^[19]



White solid, >99% yield, 42.0 mg, 98% ee; >20:1 dr; $[\alpha]_D^{20} = +51.2$ ($c = 1.00$, CHCl_3). The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; t_R (S, S) = 15.44 min (minor), t_R (R, R) = 17.37 min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.39-7.32 (m, 6H), 7.32-7.24 (m, 4H), 4.66 (dd, $J = 8.7, 2.3$ Hz, 1H), 3.06-2.97 (m, 1H), 1.84 (d, $J = 2.4$ Hz, 1H), 1.07

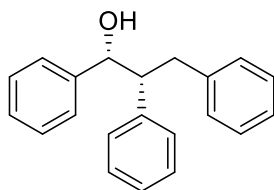
(d, $J = 7.1$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 143.4, 142.5, 128.7, 128.3, 128.1, 127.8, 127.0, 126.9, 79.7, 48.2, 18.4.

(*R*)-2-Methyl-1-phenylpropan-1-ol (**4s**)^[20]



Colorless oil, >99% yield, 29.8 mg, 98% ee; $[\alpha]_{\text{D}}^{20} = +21.9$ ($c = 1.00$, CH_2Cl_2). The enantiomeric excess was determined by HPLC on Chiralpak IC-H column, hexane: isopropanol = 95:5; flow rate = 1.0 mL/min; UV detection at 210 nm; $t_{\text{R}}(\text{R}) = 5.28$ min (major), $t_{\text{R}}(\text{S}) = 5.82$ min (minor). ^1H NMR (400 MHz, CDCl_3) δ 7.35-7.22 (m, 5H), 4.33 (d, $J = 6.9$ Hz, 1H), 1.99-1.89 (m, 2H), 0.99 (d, $J = 6.7$ Hz, 3H), 0.79 (d, $J = 6.8$ Hz, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 143.7, 128.2, 127.4, 126.6, 80.1, 35.3, 19.0, 18.3.

(1*R*,2*R*)-1,2,3-Triphenylpropan-1-ol (**4t**)^[21]



white solid, 86% yield, 50.0 mg, mp 80-81 °C, >99% ee; >20:1 dr; $[\alpha]_{\text{D}}^{20} = +3.2$ ($c = 1.00$, CHCl_3). The enantiomeric excess was determined by HPLC on Chiralpak IC-H column, hexane: isopropanol = 98:2; flow rate = 0.5 mL/min; UV detection at 210 nm; $t_{\text{R}}(\text{S,S}) = 24.10$ min (minor), $t_{\text{R}}(\text{R,R}) = 27.18$ min (major). ^1H NMR (400 MHz, CDCl_3) δ 7.36-7.31 (m, 2H), 7.31-7.24 (m, 4H), 7.23-7.17 (m, 2H), 7.14-7.06 (m, 5H), 6.91-6.85 (m, 2H), 4.86 (d, $J = 7.4$ Hz, 1H), 3.21-3.12 (m, 1H), 2.95-2.79 (m, 2H), 1.85 (s, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 142.8, 140.3, 140.1, 129.2, 129.1, 128.5, 128.2, 127.9, 127.1, 127.0, 125.9, 77.4, 56.3, 38.8.

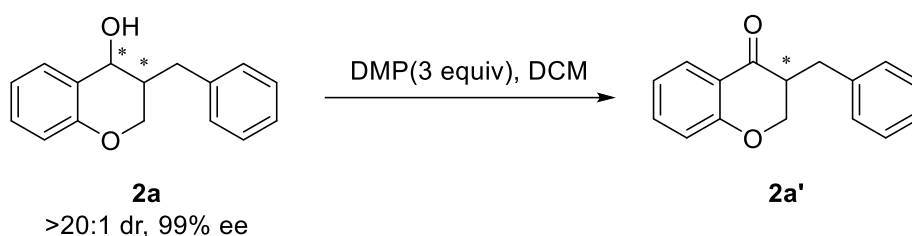
Procedure for asymmetric hydrogenation of **1a on gram-scale with low catalyst loading (S/C = 20 000)**

To a 4.0 mL vial was added the catalyst precursor $[\text{Ir}(\text{COD})\text{Cl}]_2$ (3.4 mg, 5.0×10^{-3} mmol), ligand **L3** (7.5 mg, 1×10^{-2} mmol) and anhydrous *i*PrOH (2.0 mL) under argon atmosphere. The mixture was stirred at 25 °C for 30 min, giving orange solution in the argon-filled glovebox. The resulting solution (50 μL) transferred by syringe into a 100 mL vial charged with **1a** (1.2 g, 5 mmol) and NaOH (10 mg, 0.25 mmol) in 16 mL anhydrous *n*-hexane. The vials were

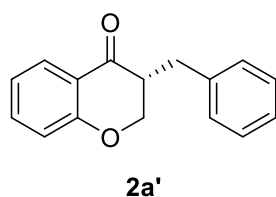
transferred to an autoclave, which was then charged with 80 atm of H₂ and stirred at room temperature for 96 h. The hydrogen gas was released slowly in a well-ventilated hood and the solution was concentrated, the crude material was purified by flash column chromatography (SiO₂, EtOAc/hexane, 20:1) to give **2a** as a white solid.

IV Determination of absolute configuration

The relative configuration of product **2a** was determined by comparison of the ¹H and ¹³C NMR spectra with the literature data.^[22] The absolute configuration of the product **2a** was assigned by comparison of the optical rotation and retention time of HPLC with the literature data for oxidation product **2a'**,^[23] which was prepared from product **2a**.



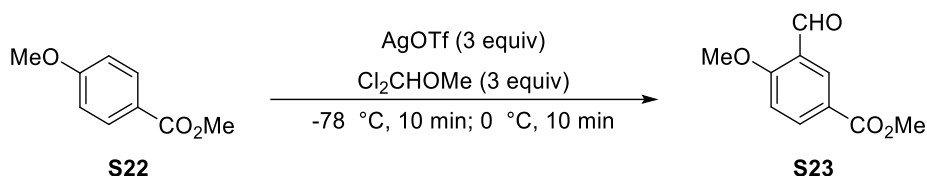
To a stirred solution of **2a** (0.208 mmol) in CH₂Cl₂ (5 mL) was added Dess-Martin periodinane (0.624 mmol, 3 equiv.) at 0 °C. The reaction mixture was stirred for 1 h at 0 °C, and quenched with saturated aqueous NaHCO₃. The organic materials were extracted with CH₂Cl₂. The combined organic layer was washed with saturated aqueous NaHCO₃, and dried over Na₂SO₄. After evaporation of solvents, the residue was purified by preparative thin layer chromatography (hexane/ethyl acetate = 4/1 as eluent) to afford the oxidation product **2a'**.



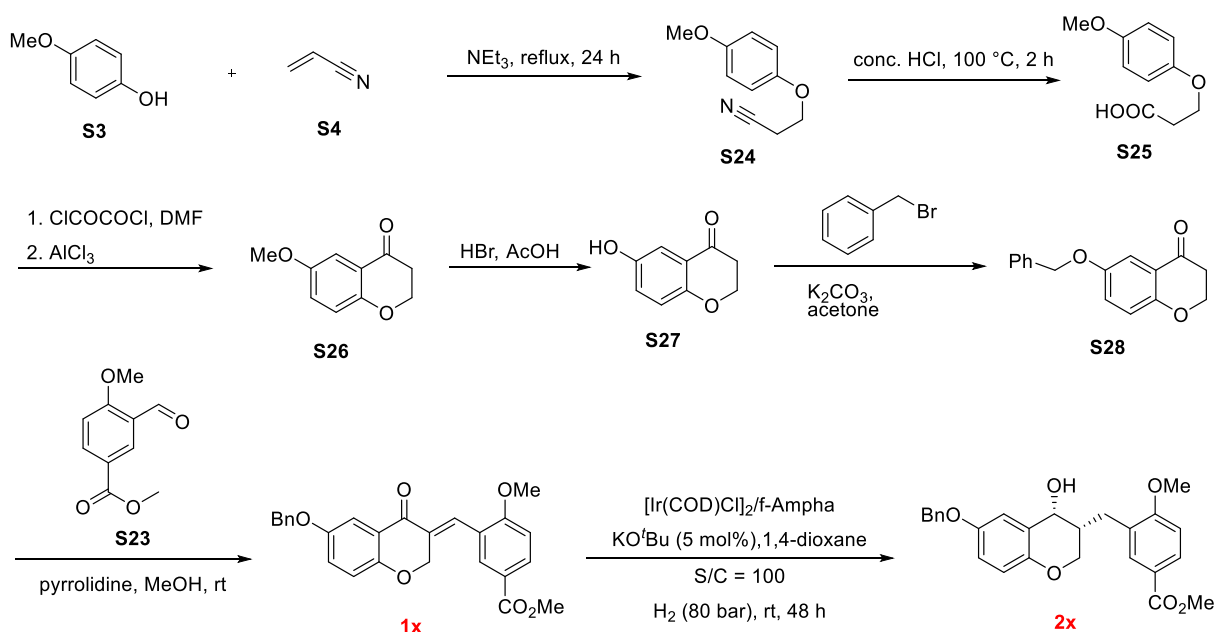
White solid, 97% yield, 48.6 mg; 95% ee; >20:1 dr; $[\alpha]_D^{25} = -9.0$ (c = 1.00, MeOH). {lit. $[\alpha]_D^{25} = -10.5$ (c = 1.00, MeOH, 98% ee for (R)-isomer)}^[23]; The enantiomeric excess was determined by HPLC on Chiralpak OD-H column, hexane: isopropanol = 95:5; flow rate = 1 mL/min; UV detection at 210 nm; t_R (R) = 7.90 min (major). t_R (S) = 8.66 min (minor). ¹H NMR (400 MHz, CDCl₃) δ 7.94 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.52-7.44 (m, 1H), 7.37-7.29 (m, 2H), 7.29-7.20 (m, 3H), 7.09-7.00 (m, 1H), 6.97 (dd, *J* = 8.4, 0.5 Hz, 1H), 4.37 (dd, *J* = 11.5, 4.3 Hz, 1H), 4.18 (dd, *J* = 11.5, 8.4 Hz, 1H), 3.29 (dd, *J* = 13.9, 4.4 Hz, 1H), 2.98-2.89 (m, 1H),

2.71 (dd, $J = 13.9, 10.5$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 193.9, 161.6, 138.3, 136.0, 129.1, 128.7, 127.5, 126.7, 121.5, 120.5, 117.8, 69.4, 47.7, 32.4.

V. Application in drug synthesis



The compound **S23** was prepared according to the literature procedure.^[24] To a suspension of substrate **S22** (3.2 mmol) and AgOTf (9.6 mmol, 3.0 eq) in dry CH_2Cl_2 (1.5 mL/ mmol) was added a solution of Cl_2CHOMe (3.00 mmol, 3.0 equiv.) in dry CH_2Cl_2 (0.5 mL/mmol) at -78 $^\circ\text{C}$ under an argon atmosphere. After being stirred for 10 min, then The reaction was stirred at 0 $^\circ\text{C}$ for another 10 min. the reaction mixture was quenched with saturated aqueous NaHCO_3 . After being stirred at room temperature for 30 min, the reaction mixture was filtered through a pad of celite. The organic layer was separated and the aqueous layer was extracted twice with EtOAc. The combined organic layers were washed with brine, dried with MgSO_4 , and filtered. The filtrate was concentrated in vacuo, and the resulting residue was purified by flash column chromatography on silica gel (eluted with hexane/EtOAc = 50/1-1/4) to afford the desired benzaldehyde derivative **S23** with 0.9 g and 97% yield.



The compound **S26** was prepared according to the preparation of Substrates **1p-1s**.

The compound **S27** was prepared according to the literature procedure^[25]: A mixture of 4.38 g (24.6 mmol) of compound **S26** in 30 mL 48% HBr aqueous solution and 30 mL acetic acid was heated to reflux under N₂. After 4 hours, the reaction mixture was cooled to room temperature and 86 mL H₂O was added. The suspension was kept at 0° C overnight. The mixture was filtered, and the precipitate washed two times with H₂O, two times with hexanes and then dried under vacuum to give 1.5 g of the target product as a dark purple/black solid.

The compound **S28** was prepared according to the literature procedure^[25]: A mixture of 1.49 g (9.08 mmol) of compound **S27**, 1.69 g (12.22 mmol) of K₂CO₃, and 1.59 g (9.33 mmol) of benzyl bromide in 9 mL acetone was heated to reflux under N₂. After 20 hours, the reaction mixture was cooled to room temperature, diluted with 1.5 L ethyl acetate, and filtered through celite (trademark). The filtrate was concentrated to obtain compound **S28** with 2.2 g and 95% yield.

The compound **1x** was prepared according to the literature procedure^[25]: 1.6 g (8 mmol) of **S23** was added to a room temperature suspension of 2.0 g (8 mmol) of **S28** and 0.57 g (8 mmol) of pyrrolidine in 350 mL CH₃OH. After stirring 20 hours at room temperature, the reaction mixture was filtered, washed two times with CH₃OH and the precipitate dried under vacuum to give 3.2 g of the compound **1x** as a yellow powder (94 % yield). mp 172-174 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.09 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.96 (s, 1H), 7.75 (d, *J* = 1.9 Hz, 1H), 7.55 (d, *J* = 3.1 Hz, 1H), 7.49-7.43 (m, 2H), 7.43-7.37 (m, 2H), 7.36-7.31 (m, 1H), 7.17 (dd, *J* = 9.0, 3.2 Hz, 1H), 6.98 (d, *J* = 8.7 Hz, 1H), 6.91 (d, *J* = 9.0 Hz, 1H), 5.20 (d, *J* = 1.8 Hz, 2H), 5.09 (s, 2H), 3.93 (s, 3H), 3.91 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 182.1, 166.4, 161.7, 156.2, 153.6, 136.7, 133.0, 132.6, 131.8, 131.8, 128.6, 128.1, 127.7, 125.7, 123.5, 122.3, 122.0, 119.3, 110.5, 109.6, 70.6, 67.9, 55.9, 52.2.

The synthesis of **2x**: To a 4.0 mL vial was added the catalyst precursor [Ir(COD)Cl]₂ (3.4 mg, 5.0×10⁻³ mmol), ligand **L3** (7.5 mg, 1.0×10⁻² mmol) and anhydrous ⁱPrOH (1.0 mL) under argon atmosphere. The mixture was stirred for 30 min at 25 °C giving orange solution in the argon-filled glovebox. The resulting solution (200 μL) transferred by syringe into a 5.0 mL vial charged with compound **1x** (0.2 mmol) and KO^tBu (0.02 mmol, 2.2 mg) in 2.0 mL anhydrous 1,4-Dioxane. The vials were transferred to an autoclave, which was then charged with 80 atm of H₂ and stirred at room temperature for 28 h. The hydrogen gas was released slowly in a well-ventilated hood and the solution was concentrated, The crude material was purified by flash column chromatography (SiO₂, EtOAc/hexane, 20:1) to give the **2x** (76 mg, 88 % yield, 19:1

dr) as a White solid. mp 52-54 °C. >99% ee. $[\alpha]_{\text{D}}^{25} = +61.8$ (c=0.25, MeOH). The enantiomeric excess was determined by HPLC on Chiralpak AD-H column, hexane: isopropanol = 80:20; flow rate = 1 mL/min; UV detection at 210 nm; $t_{\text{R}}(\text{S}, \text{S}) = 28.25$ min (minor), $t_{\text{R}}(\text{R}, \text{R}) = 35.77$ min (major). ^1H NMR (400 MHz, CDCl_3) δ 8.00-7.88 (m, 2H), 7.43-7.33 (m, 4H), 7.33 -7.28 (m, 1H), 6.92 (d, $J = 8.6$ Hz, 1H), 6.88-6.81 (m, 2H), 6.76 (d, $J = 8.8$ Hz, 1H), 5.02-4.91 (m, 2H), 4.36 (s, 1H), 4.14-4.00 (m, 2H), 3.91 (s, 3H), 3.89 (s, 3H), 2.90 (dd, $J = 13.5, 9.1$ Hz, 1H), 2.67 (dd, $J = 13.5, 6.3$ Hz, 1H), 2.45 (s, 1H), 2.40-2.30 (m, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 166.9, 161.1, 152.6, 148.6, 137.2, 132.6, 130.2, 128.6, 127.9, 127.5, 127.5, 124.1, 122.8, 117.7, 117.6, 115.4, 110.1, 70.7, 65.2, 65.1, 55.8, 52.0, 39.2, 27.2. HRMS (EI) m/z Calcd. for $\text{C}_{26}\text{H}_{26}\text{NaO}_6$ ($[\text{M}+\text{Na}]$): 457.1622. Found: 457.1621.

VI. Computational studies

DFT calculations were performed using the Gaussian 16 package.^[26] All the structures are optimized using the B3LYP-D3(BJ) functional^[27] with the basis set SDD for Ir and Fe,^[28] 6-31+G* for Na and O, and 6-31G* for other main group atoms.^[29] Polarization functions ($\zeta_f = 0.938$) and ($\zeta_f = 2.462$) were added for Ir and Fe respectively.^[30] Geometric structures of all species were optimized at T = 298.15 K. H₂ was optimized at hydrogen pressure of 50 bar. An entropy correction of -2.6 kcal/mol was made for two-to-one transformations. Frequency calculations were performed to verify the optimized structures as local minima or transition states. Transition state structures were confirmed to connect appropriate reactants or products by intrinsic reaction coordinate (IRC) calculations.^[31] Solvent effects were considered using the SMD mode^[32] at the B3LYP-D3(BJ)/6-311++G** level with SDD for Ir and Fe.

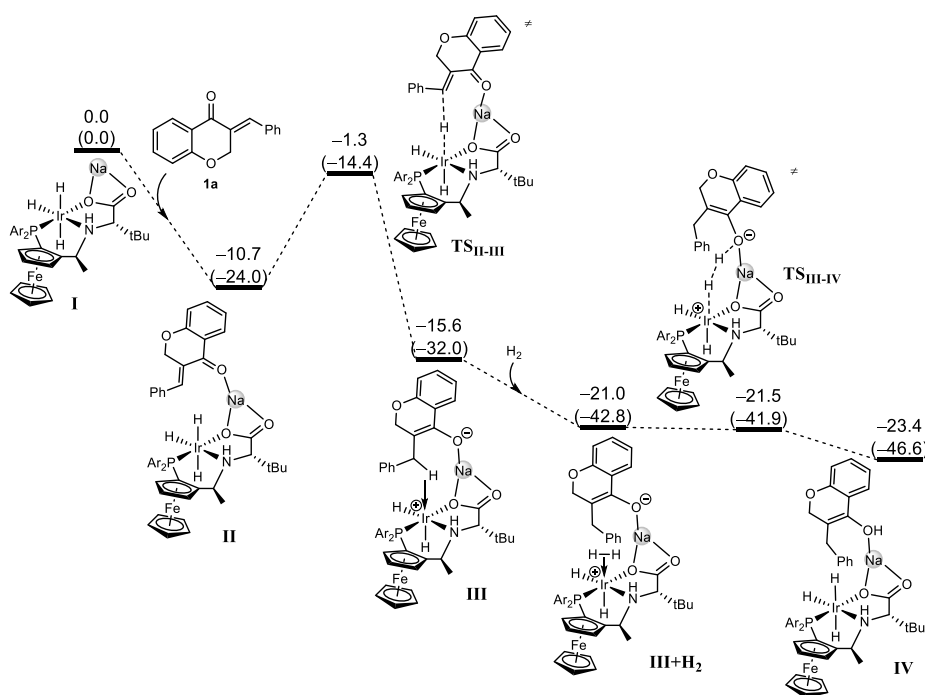


Figure S1. Energy profile for the 1,4-addition of **1a**. The relative Gibbs free energies and electronic energies (in parentheses) are given in kcal/mol.

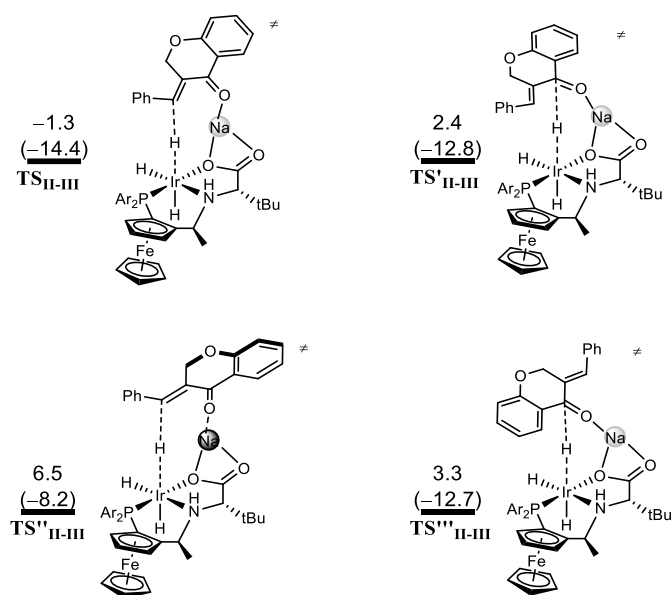


Figure S2. Transition states and relative Gibbs free energies and electronic energies (in parentheses) in kcal/mol calculated for the hydride transfer to the enone **1a**.

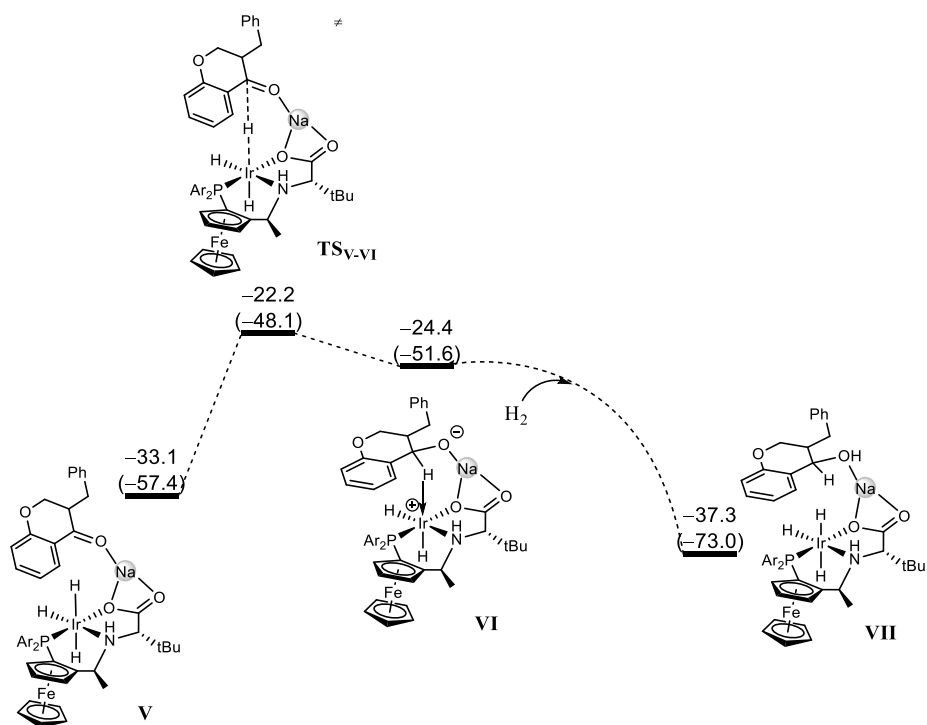


Figure S3. Energy profile for the hydrogenation of **2a'**. The relative Gibbs free energies and electronic energies (in parentheses) are given in kcal/mol. We could not locate the transition state from VI to VII, even the intermediate of H₂ coordination to **VI**. Because H₂ activation between Ir(III) and the enolate anion is barrierless.

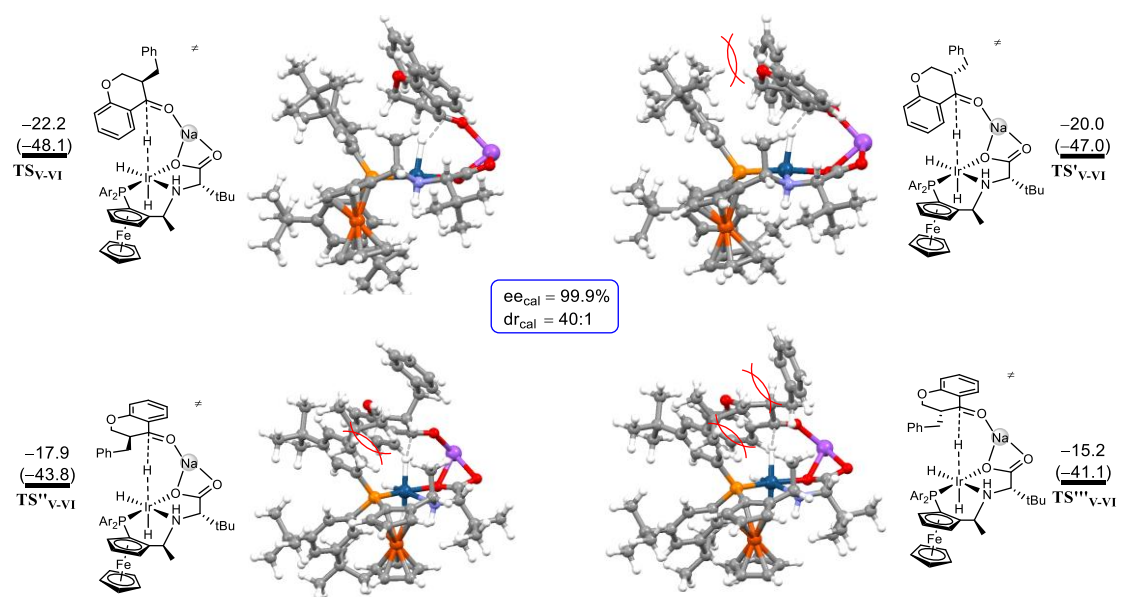
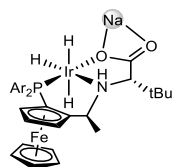


Figure S4. The structures of the transition stats for DKR of **2a'**.

DFT-calculated Cartesian Coordinates

I



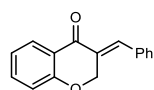
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H	-4.44886300	-2.34930300	0.44332600
C	-1.45585000	-0.52179800	2.26432100
C	-0.24189800	0.00139200	1.68257500
C	0.49757100	0.63681300	2.73637900
H	1.42733900	1.17130900	2.61047700
C	-0.23773400	0.51025600	3.94705300
H	0.03707000	0.93275900	4.90459500
C	-1.43917500	-0.19739200	3.65609800
H	-2.23138700	-0.42811300	4.35710400
C	1.20940600	1.39535000	-0.37334700
C	2.46531500	1.58179900	0.21323400
H	2.89478800	0.78133700	0.80566700
C	3.18131900	2.76706500	0.02344600
C	2.60350600	3.76310600	-0.77815400
H	3.14458300	4.68587300	-0.93406100
C	1.35978900	3.59335400	-1.40150400
C	0.67436500	2.38973000	-1.19109900
H	-0.28244200	2.19550300	-1.66254200
C	1.61729900	-1.37254700	0.01951000
C	1.85278800	-2.14260300	1.15670900
H	1.21909900	-2.00833100	2.02544100
C	2.89877000	-3.07509200	1.19257800
C	3.70770600	-3.20140100	0.05777800
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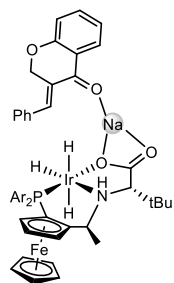
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II



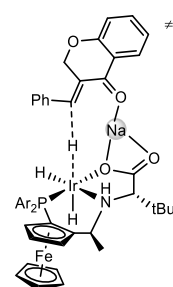
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H	-0.13351100	-1.85780100	2.21752800	C	3.48999000	-1.25672700	4.90632300
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C	-3.07604000	-6.35003300	-0.56992500	H	4.79271900	-1.43691800	-4.25822000
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H	-4.65638900	-3.72198100	1.06235600	C	0.73953000	3.91963400	4.12798400
H	-5.38270900	-5.17583900	0.37168400	C	1.16405200	1.64177700	5.10683200
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H	0.56889300	-1.98626500	0.06647700	H	1.08607400	4.69139300	3.43114200
Na	1.47189500	-2.89646900	-1.89025700	H	-0.27495900	3.63006900	3.83144200
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C	7.80418100	0.05139600	-3.70605800	H	1.77670900	0.73701300	5.07361300
C	7.89312100	-0.11057500	-2.32991300	H	1.19153800	2.04351700	6.12667500
C	6.86724000	-0.77163500	-1.64468900	H	0.12875500	1.35627600	4.89697700
C	5.73572000	-1.24725600	-2.34597000	H	3.03580100	3.47473700	5.62555800
C	5.67655300	-1.07607700	-3.74280400	H	3.80422800	2.32461500	4.51481900
O	7.01173100	-0.90915300	-0.30132800	H	3.46459400	3.98794100	3.99325600
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C	4.71107500	-1.71640200	-0.13978900	C	5.20326100	2.06520500	0.03588600
C	4.56932700	-1.75765000	-1.61109600	C	3.66463600	1.83488400	-1.91753100
O	3.53263200	-2.11597500	-2.19327000	C	3.74925000	3.99615500	-0.66606200
C	3.62803100	-1.54193900	0.64812000	H	5.39800900	2.52032900	1.01247400
C	3.60259100	-1.39468100	2.10680300	H	5.28394300	0.98180700	0.14522700
C	2.61215200	-2.09306600	2.81660900	H	5.99605100	2.39162100	-0.64734700

H	2.75086600	2.17795400	-2.41436900
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H	4.52292300	4.35180600	-1.35766700
H	2.77181000	4.30216900	-1.05458700
H	3.89879800	4.49704500	0.29632200
C	-1.50191400	5.60508500	-0.40695400
C	-2.17972300	5.69117100	0.97844100
C	0.02217800	5.80230900	-0.24014000
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H	-3.26081400	5.53160000	0.89317800
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H	-5.14691300	2.04637500	-3.41918100
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TS_{II-III}



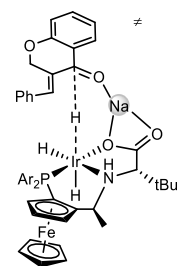
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C	-3.15874600	-1.75297500	2.84179300
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H	-2.15809800	2.78183200	0.44879100
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H	-3.99247200	3.33809100	-3.37878400
C	-2.77401900	1.58247300	-3.19825100
C	-1.97070200	0.83965000	-2.32318900
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C	0.01840900	1.52532400	1.13687100
C	-0.21412800	1.63898600	2.50738600
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C	1.01197300	3.69641800	2.54517700
H	1.37599300	4.56388900	3.08372700
C	1.26169300	3.61662300	1.16344700
C	0.77584100	2.50203800	0.47432600

H	0.94043700	2.39855200	-0.59137900	H	-1.38269600	-3.21773000	0.10787500
C	-4.18040200	-3.05844500	-0.38805300	H	1.76578000	-1.08301300	0.28130800
H	-3.70539100	-4.02825300	-0.38383900	Na	3.53979900	-3.61746300	-1.89432900
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H	-5.86930800	-3.32503300	1.06350500	C	5.50713600	2.52996800	-4.36364200
C	-5.64557900	-1.33409300	0.05641700	C	5.04539900	2.84607100	-3.09091200
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C	-4.67526100	-0.85843100	-0.87711300	C	5.06833400	0.47632500	-2.51033000
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C	1.50156000	-4.17070400	-0.37717900	C	4.27438500	-0.18695700	-0.25688600
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C	0.27104800	-2.23148100	2.83492200	O	4.65114100	-1.79353500	-1.99230200
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O	1.45484400	-3.25663700	-1.28197000	H	5.67543400	3.32741200	-5.08213100
C	-0.58811100	-5.57554500	0.04616200	H	4.84898100	3.87056100	-2.79338400
C	0.23913500	-6.87337800	0.08828800	H	5.70069300	-0.85556300	-4.05790200
H	-0.40146000	-7.72095100	-0.18296500	H	4.18035900	1.58965900	0.99365400
H	1.08649700	-6.84359300	-0.59848200	H	5.77080200	1.26294300	0.28604000
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C	-1.08829500	-5.34165400	-1.39213100	H	4.18061000	-2.94716200	2.35616800
H	-1.75383000	-6.15848500	-1.69343900	H	4.00668000	-2.84656500	4.82370900
H	-1.63818300	-4.40161800	-1.50595900	H	3.15800300	-0.77946400	5.92714600
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H	1.21191600	6.33083800	1.82158700
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C	-4.65268200	4.20253100	0.36220400
C	-2.62505100	5.46182100	-0.44398300
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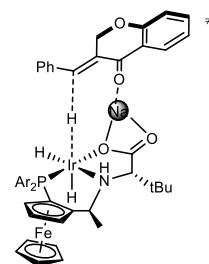
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H	-2.49852600	0.77151300	2.72007500
C	-1.54715000	-0.72941900	4.06951400
H	-2.09656700	-0.60438600	4.99326200
C	-0.54369100	-1.70653200	3.81462500
H	-0.17460100	-2.44341300	4.51667400
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C	-3.13951500	1.53299400	0.29029400
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C	-3.15710800	-0.28972200	-1.28817400	H	2.22997300	-6.56336300	-1.07576100
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H	-6.74301100	3.35568000	-0.74456100
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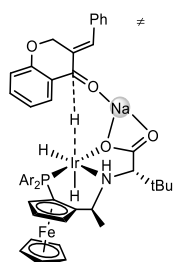
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H	-2.74724700	-0.48375400	2.63928500	H	3.55092700	0.15493700	1.40492800
C	-1.13217200	-1.29176500	3.94249700	H	2.48301900	0.58143300	2.75166500
H	-1.65273300	-1.49462900	4.86921600	Ir	0.80208400	-0.68739100	-1.22532300
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C	-2.59998400	-0.73763900	-0.45224300	H	0.13612400	-2.16320400	-1.57870700
C	-3.75158800	-0.32313900	0.23851700	C	1.90944800	-1.23944800	1.74486700
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H	-0.23624000	1.76223900	2.16825400	H	1.55374500	-4.44595700	-0.57547800
C	-1.34035100	3.58168100	1.82082800	H	2.87844300	-4.56570600	-1.73354800
C	-2.24777600	4.20318200	0.95665500	C	3.23609300	-4.15233600	1.70598100
H	-2.62166800	5.18530200	1.21065400	H	3.92040000	-3.60230600	2.36257100
C	-2.68848800	3.59822400	-0.23190200	H	2.21430900	-3.92448400	2.01496300
C	-2.20358700	2.32480900	-0.53554300	H	3.40103200	-5.22127600	1.88300100
H	-2.53795900	1.81431000	-1.43040300	H	1.30287100	-2.64817800	0.42783400
C	-0.47904700	-4.54322200	1.69087900	H	1.53515600	0.89459400	-1.06353100
H	0.51913400	-4.90497500	1.49936700	Na	4.19798500	-0.63336000	-3.60824600
C	-1.17608400	-4.64135900	2.93173400	C	7.32032900	-0.30521200	0.96125200
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C	-2.46974200	-4.06662100	2.75047300	C	6.60156500	1.72880200	2.08014000
H	-3.22538400	-3.95136300	3.51661500	C	5.75057300	2.00665200	1.00950900
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C	6.48915400	-0.01015800	-0.11578800	H	-4.13209300	6.06040300	0.07015300
O	5.02131300	3.15848900	1.03644100	H	-2.84948800	6.23070600	-1.14362800
C	3.72456200	3.11905200	0.40995500	C	-0.84584600	4.23108800	3.12114800
C	3.66947900	2.32373500	-0.87279400	C	-1.28318700	3.35627500	4.31758400
C	4.76315700	1.45512600	-1.19985700	C	0.69555500	4.32769800	3.09691500
O	4.91778600	0.91542600	-2.32828400	C	-1.41137500	5.64597400	3.32363900
C	2.54432900	2.26560300	-1.68677200	H	-2.37530300	3.27562400	4.35720100
C	1.50151200	3.29281000	-1.81599500	H	-0.87622200	2.34243000	4.24797400
C	1.03589200	3.56965600	-3.11422600	H	-0.93711100	3.79620100	5.26072900
C	0.20490500	4.65800200	-3.36275300	H	1.03451700	4.97396600	2.27936500
C	-0.19751200	5.48216300	-2.30952700	H	1.06760600	4.75170800	4.03706300
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C	1.03370200	4.09094700	-0.75970900	H	-1.02123300	6.07030900	4.25519200
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H	8.03468200	0.35120200	2.88978800	H	-2.50464500	5.63998100	3.39392600
H	6.63413700	2.41669300	2.91864600	C	-6.26527900	-0.49383900	0.73138300
H	6.41385300	-0.67340100	-0.97129600	C	-6.83277500	-1.75140300	1.42573200
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H	2.68499200	1.67868200	-2.58572300	H	-7.08893700	-2.53313500	0.70374000
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C	-5.12907200	3.64224800	-0.70217300	H	-7.58152800	-0.65390900	-1.02182900
C	-3.82232900	5.77162100	-0.93954900	C	-4.02468700	-3.27289700	-2.93600100
H	-2.52917000	4.25614800	-2.92240600	C	-3.58524500	-2.59581800	-4.25292700
H	-3.62717600	2.87221300	-2.83267900	C	-3.06567800	-4.44172700	-2.61914500
H	-4.26950500	4.46749700	-3.21833200	C	-5.43905000	-3.84340900	-3.12631000
H	-5.34439000	3.84875300	0.35256500	H	-4.25541600	-1.76626000	-4.50564100
H	-5.94111900	4.06456000	-1.30724800	H	-2.56871200	-2.19698900	-4.17753200
H	-5.12762300	2.55563700	-0.84006600	H	-3.60683000	-3.31791800	-5.07821000
H	-4.55244700	6.19846400	-1.63592200	H	-3.33054800	-4.91917600	-1.66912600

H	-3.11628000	-5.19886100	-3.41081800
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H	-5.43488800	-4.57505100	-3.94154600
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TS''''_{II-III}



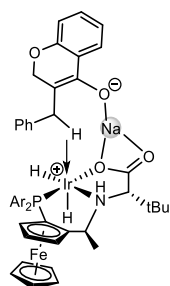
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C	0.51139900	-1.22499900	2.30907700
C	-0.71081500	-0.71594000	1.72992300
C	-1.71138000	-0.75822700	2.75959600
H	-2.74724700	-0.48375400	2.63928500
C	-1.13217200	-1.29176500	3.94249700
H	-1.65273300	-1.49462900	4.86921600
C	0.23156400	-1.58592900	3.66281600
H	0.94453500	-2.03073900	4.34544100
C	-2.59998400	-0.73763900	-0.45224300
C	-3.75158800	-0.32313900	0.23851700
H	-3.66373100	0.45095400	0.98797600
C	-4.99706900	-0.88086200	-0.04199600
C	-5.07375300	-1.84571700	-1.06533200
H	-6.03835800	-2.28509700	-1.28871300
C	-3.95760600	-2.24235400	-1.80204100
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H	-1.81537000	-1.94854500	-2.01052900
C	-1.34079500	1.65305700	0.33670500
C	-0.90060200	2.29197000	1.49480400

H	-0.23624000	1.76223900	2.16825400
C	-1.34035100	3.58168100	1.82082800
C	-2.24777600	4.20318200	0.95665500
H	-2.62166800	5.18530200	1.21065400
C	-2.68848800	3.59822400	-0.23190200
C	-2.20358700	2.32480900	-0.53554300
H	-2.53795900	1.81431000	-1.43040300
C	-0.47904700	-4.54322200	1.69087900
H	0.51913400	-4.90497500	1.49936700
C	-1.17608400	-4.64135900	2.93173400
H	-0.78332900	-5.05244300	3.85239200
C	-2.46974200	-4.06662100	2.75047300
H	-3.22538400	-3.95136300	3.51661500
C	-2.56811100	-3.60712000	1.40297700
H	-3.40517000	-3.08205300	0.96627900
C	-1.33390800	-3.89711500	0.74883800
H	-1.07341400	-3.62172200	-0.26332500
C	3.49310100	-1.97903000	-1.56420000
O	4.59342300	-2.26089600	-2.09037400
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H	3.55092700	0.15493700	1.40492800
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Ir	0.80208400	-0.68739100	-1.22532300
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H	1.94285900	0.80321300	1.05912800
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C	1.90944800	-1.23944800	1.74486700
H	2.51109000	-1.85711400	2.41945300
O	2.57999100	-1.36439000	-2.22962000
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C	4.99589400	-4.20960600	-0.01996900
H	5.16506400	-5.24137600	0.31191800
H	5.27326300	-4.12167300	-1.06863500
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H	2.73122700	-5.75892500	-0.43205800

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C	3.23609300	-4.15233600	1.70598100	H	1.29398000	3.84820200	0.26073400
H	3.92040000	-3.60230600	2.36257100	C	-3.76636700	4.24312700	-1.11634700
H	2.21430900	-3.92448400	2.01496300	C	-3.52705700	3.93864700	-2.60948700
H	3.40103200	-5.22127600	1.88300100	C	-5.12907200	3.64224800	-0.70217300
H	1.30287100	-2.64817800	0.42783400	C	-3.82232900	5.77162100	-0.93954900
H	1.53515600	0.89459400	-1.06353100	H	-2.52917000	4.25614800	-2.92240600
Na	4.19798500	-0.63336000	-3.60824600	H	-3.62717600	2.87221300	-2.83267900
C	7.32032900	-0.30521200	0.96125200	H	-4.26950500	4.46749700	-3.21833200
C	7.38102400	0.57282900	2.05060300	H	-5.34439000	3.84875300	0.35256500
C	6.60156500	1.72880200	2.08014000	H	-5.94111900	4.06456000	-1.30724800
C	5.75057300	2.00665200	1.00950900	H	-5.12762300	2.55563700	-0.84006600
C	5.70033100	1.14961700	-0.10362100	H	-4.55244700	6.19846400	-1.63592200
C	6.48915400	-0.01015800	-0.11578800	H	-4.13209300	6.06040300	0.07015300
O	5.02131300	3.15848900	1.03644100	H	-2.84948800	6.23070600	-1.14362800
C	3.72456200	3.11905200	0.40995500	C	-0.84584600	4.23108800	3.12114800
C	3.66947900	2.32373500	-0.87279400	C	-1.28318700	3.35627500	4.31758400
C	4.76315700	1.45512600	-1.19985700	C	0.69555500	4.32769800	3.09691500
O	4.91778600	0.91542600	-2.32828400	C	-1.41137500	5.64597400	3.32363900
C	2.54432900	2.26560300	-1.68677200	H	-2.37530300	3.27562400	4.35720100
C	1.50151200	3.29281000	-1.81599500	H	-0.87622200	2.34243000	4.24797400
C	1.03589200	3.56965600	-3.11422600	H	-0.93711100	3.79620100	5.26072900
C	0.20490500	4.65800200	-3.36275300	H	1.03451700	4.97396600	2.27936500
C	-0.19751200	5.48216300	-2.30952700	H	1.06760600	4.75170800	4.03706300
C	0.20044600	5.17842000	-1.00719400	H	1.16205500	3.34590000	2.96600600
C	1.03370200	4.09094700	-0.75970900	H	-1.02123300	6.07030900	4.25519200
H	7.92048300	-1.21007100	0.95413800	H	-1.12457900	6.31794300	2.50663300
H	8.03468200	0.35120200	2.88978800	H	-2.50464500	5.63998100	3.39392600
H	6.63413700	2.41669300	2.91864600	C	-6.26527900	-0.49383900	0.73138300
H	6.41385300	-0.67340100	-0.97129600	C	-6.83277500	-1.75140300	1.42573200
H	3.47935200	4.16855700	0.22799300	C	-5.98978100	0.56579500	1.81174800
H	3.01344400	2.74004400	1.15784200	C	-7.31677600	0.07267300	-0.24706400
H	2.68499200	1.67868200	-2.58572300	H	-7.08893700	-2.53313500	0.70374000
H	1.35932900	2.93544000	-3.93503000	H	-6.10049400	-2.16948900	2.12634600
H	-0.12330400	4.86735100	-4.37710100	H	-7.74072600	-1.50176900	1.98775600

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H	-5.28018500	0.20180700	2.56393000
H	-8.23438300	0.33930200	0.29086400
H	-6.93997400	0.97236700	-0.74535400
H	-7.58152800	-0.65390900	-1.02182900
C	-4.02468700	-3.27289700	-2.93600100
C	-3.58524500	-2.59581800	-4.25292700
C	-3.06567800	-4.44172700	-2.61914500
C	-5.43905000	-3.84340900	-3.12631000
H	-4.25541600	-1.76626000	-4.50564100
H	-2.56871200	-2.19698900	-4.17753200
H	-3.60683000	-3.31791800	-5.07821000
H	-3.33054800	-4.91917600	-1.66912600
H	-3.11628000	-5.19886100	-3.41081800
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III



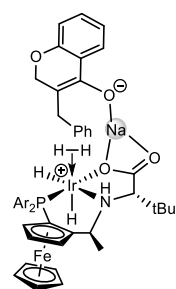
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H	-3.40668500	1.22371000	2.03560200

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H	-4.46230500	-0.50572000	3.79704100
C	-2.88024200	-1.90965800	3.06460900
H	-3.07810300	-2.81811800	3.61912200
C	-2.06874700	1.36777700	-0.72022400
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C	-3.57757000	3.27746200	-0.80630900
C	-3.91575600	2.90403800	-2.11604600
H	-4.63986700	3.49726300	-2.65612700
C	-3.32896200	1.80486500	-2.75577600
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H	-1.90027600	0.20327700	-2.50093700
C	0.07674100	1.55180700	1.12756000
C	0.30403700	1.44367800	2.50164300
H	-0.10769300	0.59994500	3.03902900
C	1.03968200	2.42272900	3.18037000
C	1.50947900	3.51495700	2.44124800
H	2.05046900	4.29847300	2.96025300
C	1.30558000	3.64923100	1.05972300
C	0.59450500	2.63686900	0.40869800
H	0.42257000	2.68971000	-0.65883700
C	-4.36757300	-2.91536000	-0.07369000
H	-3.91683600	-3.88632300	-0.21678300
C	-5.39541200	-2.60416800	0.86592100
H	-5.82900100	-3.28677300	1.58470900
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C	-4.89110300	-0.67833100	-0.30982100
H	-4.85843100	0.35378200	-0.62934000
C	-4.05385700	-1.72579400	-0.79625600
H	-3.29238400	-1.62350400	-1.55432100
C	1.26332200	-4.02865200	-0.99126900
O	2.21918300	-4.81268400	-1.12627700
C	0.49452000	-2.39042800	2.55907500
H	1.29241300	-3.12808600	2.44399000

H	0.29989300	-2.26477200	3.62848300	C	3.46264600	-1.46970700	1.43251100
Ir	0.15192300	-1.30975300	-0.84901800	C	3.97112100	-2.76344800	1.60884600
H	0.64920100	-0.22882400	-1.90715900	C	4.41904300	-3.19694500	2.85784100
H	0.86149700	-1.44276400	2.16630100	C	4.36293000	-2.33867600	3.95659200
H	-1.12103400	-1.53182200	-1.72498700	C	3.86142700	-1.04545300	3.79155000
C	-0.79346100	-2.80457800	1.85279300	C	3.41544600	-0.61406800	2.54169400
H	-1.15656400	-3.73250800	2.31103300	H	7.44382000	1.34852600	-4.99911300
O	1.13908900	-2.98132900	-1.74354700	H	6.96474600	3.69455500	-4.31236600
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C	-1.45917400	-5.11080800	-1.70781200	H	4.00936700	-3.43785200	0.75694100
H	-2.14805000	-5.91210400	-1.99656600	H	4.80849700	-4.20538000	2.97090900
H	-2.04201700	-4.18461800	-1.64564000	H	4.70800200	-2.67122700	4.93165600
H	-0.73329500	-4.97940400	-2.51628400	H	3.81587400	-0.37222700	4.64275500
C	-1.81427800	-5.74059800	0.71123000	H	3.00596100	0.38531800	2.43162000
H	-1.33649500	-6.04014300	1.65125400	C	1.29107300	2.35396000	4.69283300
H	-2.45341700	-4.87785900	0.91854900	C	0.47156700	3.46728300	5.38135200
H	-2.46689300	-6.56185100	0.39503100	C	0.87171700	0.99734600	5.28640400
H	-1.50959600	-3.13386200	-0.00004300	C	2.79127000	2.57003600	4.98773400
H	1.90998700	-0.66821500	0.16091300	H	0.75344600	4.45792700	5.00919400
Na	3.25455700	-3.21638600	-2.59543700	H	-0.59999200	3.33109400	5.19595900
C	6.75505900	1.54873200	-4.18278600	H	0.63679900	3.45215400	6.46541000
C	6.48548700	2.86521100	-3.79854000	H	1.39842200	0.16600600	4.80624000
C	5.60669900	3.12405800	-2.74601000	H	1.10952800	0.97458300	6.35552200
C	5.00462800	2.05953300	-2.07508800	H	-0.20586100	0.82500800	5.18688900
C	5.24598100	0.72734900	-2.46023700	H	2.98105900	2.48015900	6.06365000
C	6.13029500	0.49372000	-3.51866300	H	3.40716700	1.83001900	4.46742200
O	4.12386900	2.35448100	-1.06793600	H	3.13159900	3.56172200	4.67490800
C	3.99297800	1.32191100	-0.06663200	C	1.80675000	4.90449700	0.33136400
C	3.81403200	-0.04428300	-0.65559300	C	3.30452300	5.13535100	0.62658700
C	4.49439500	-0.38012500	-1.80801900	C	1.63085800	4.79364400	-1.19271200
O	4.50854900	-1.54567000	-2.38142900	C	0.99062300	6.11394300	0.84000300
C	2.98219400	-1.04906600	0.05959500	H	3.49924200	5.25906600	1.69717700

H	3.90251000	4.30054900	0.25296700
H	3.64123200	6.05058700	0.12502500
H	0.57506000	4.70678800	-1.47545400
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H	2.17926900	3.93474300	-1.59112200
H	1.32621600	7.03276000	0.34459500
H	-0.07652000	5.98283600	0.62898600
H	1.10607600	6.25226300	1.92078800
C	-4.17557300	4.50747400	-0.10968700
C	-4.89227200	4.06259700	1.18437700
C	-3.03449700	5.48588500	0.24678600
C	-5.19223000	5.24690900	-0.99429600
H	-5.69385200	3.34936700	0.96007500
H	-4.20042500	3.58474900	1.88602900
H	-5.33559700	4.92674500	1.69290300
H	-2.50895900	5.81454400	-0.65660100
H	-3.43422700	6.37265000	0.75272500
H	-2.29751700	5.02355300	0.91094900
H	-5.58992300	6.11230600	-0.45342500
H	-4.73297800	5.61568600	-1.91789700
H	-6.03879400	4.60535800	-1.26367700
C	-3.65288600	1.41416100	-4.20396200
C	-2.37121900	1.55199100	-5.05550500
C	-4.13855300	-0.05152100	-4.24516800
C	-4.74707900	2.30184500	-4.81874000
H	-2.00975300	2.58618200	-5.04958600
H	-1.56598500	0.91393300	-4.67746600
H	-2.57188300	1.26455500	-6.09447700
H	-5.02586400	-0.19066600	-3.61748300
H	-4.39581300	-0.33626200	-5.27199800
H	-3.36655300	-0.74361200	-3.89411500
H	-4.95036500	1.97690900	-5.84465900
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H	-4.44241300	3.35338800	-4.86005700

III+H₂



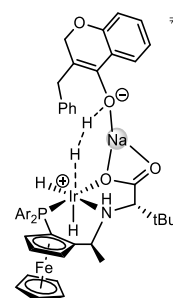
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H	0.78564800	-4.67719300	0.76253900
C	-1.56139600	-1.86580200	2.26875100
C	-1.85363700	-0.53967000	1.76426000
C	-2.83528700	0.03807700	2.63799300
H	-3.30189400	1.00170200	2.50404500
C	-3.15201300	-0.90160900	3.65498700
H	-3.89750700	-0.77295400	4.42845000
C	-2.37453100	-2.07079200	3.42572600
H	-2.40532500	-2.98334400	4.00742200
C	-2.51011500	1.18036400	-0.47372800
C	-3.09097900	2.26428200	0.19369900
H	-2.65385900	2.60627400	1.12512500
C	-4.20411600	2.92292100	-0.33626300
C	-4.70514300	2.47843000	-1.56972500
H	-5.56640700	2.97702100	-1.99103400
C	-4.11600200	1.42697600	-2.28357900
C	-3.00694500	0.78692600	-1.71598500
H	-2.50953600	-0.02349200	-2.23400100
C	-0.07901700	1.57043200	0.98821000
C	0.51777400	1.41978000	2.24550300
H	0.26031000	0.55958200	2.84981500
C	1.42744900	2.36942800	2.71431600
C	1.70387500	3.47728000	1.89691100
H	2.40712200	4.21864100	2.25392600
C	1.11023800	3.66223000	0.64410000
C	0.21813100	2.67957300	0.19696200

H	-0.25118600	2.77418000	-0.77516000	H	-1.46709600	-3.16727000	0.11127700
C	-4.18681500	-2.04334100	-0.17232000	H	5.37112400	-0.05075600	2.20169900
H	-3.55981900	-1.90662700	-1.04100900	Na	3.53308500	-2.38160400	-1.72190900
C	-4.30081300	-3.23406500	0.60605100	C	3.98078100	2.90311600	-3.97762700
H	-3.81072400	-4.17519700	0.40687000	C	4.58857700	4.07309600	-3.51726300
C	-5.18470400	-2.96967500	1.69431400	C	5.03598800	4.16009400	-2.19688500
H	-5.44988100	-3.66252400	2.48188200	C	4.88145700	3.06833700	-1.34413300
C	-5.62476900	-1.61702800	1.58046000	C	4.27776600	1.87763100	-1.79050900
H	-6.27203000	-1.10060100	2.27705900	C	3.82731400	1.81693300	-3.11380200
C	-5.00824500	-1.04314400	0.42885400	O	5.26288000	3.21619500	-0.03559500
H	-5.10064000	-0.01926400	0.09570300	C	5.65335000	2.00394800	0.63406300
C	1.40954100	-3.80372200	-1.06217700	C	4.75109800	0.83350400	0.35296800
O	2.47683700	-4.44098000	-1.07161900	C	4.12091000	0.73493000	-0.85668500
C	0.86938700	-2.46539100	2.39879800	O	3.42289700	-0.29881800	-1.25689400
H	1.64592700	-3.16489400	2.07456400	C	4.74769000	-0.31210000	1.33297800
H	0.83530200	-2.47378000	3.49259200	C	5.24849300	-1.63495800	0.76912800
Ir	-0.00638100	-1.23917900	-0.90693900	C	6.22273800	-1.67333100	-0.24021500
H	0.25307000	-0.12266900	-2.01131100	C	6.64923100	-2.88955300	-0.77954700
H	1.15470000	-1.46422500	2.07227300	C	6.10773600	-4.09610500	-0.31940300
H	-1.30366800	-1.63933200	-1.74012700	C	5.14537500	-4.07144800	0.69216400
C	-0.50517000	-2.85885200	1.84879900	C	4.72676900	-2.85134400	1.23034400
H	-0.78158700	-3.82193900	2.30172100	H	3.62351300	2.83882600	-5.00166400
O	1.21128700	-2.77576100	-1.82164500	H	4.71235700	4.92423400	-4.18146700
C	-0.62992200	-5.33284100	-0.71966000	H	5.49924400	5.06363500	-1.81317500
C	0.23500700	-6.47509100	-1.28318100	H	3.33734300	0.90298100	-3.43404100
H	-0.41440500	-7.30260700	-1.59111500	H	5.65541700	2.26519000	1.69682400
H	0.81698900	-6.15622200	-2.15118500	H	6.70679200	1.80142900	0.35154700
H	0.93971000	-6.85003000	-0.53409200	H	3.73925200	-0.48386700	1.73885000
C	-1.50449700	-4.76837700	-1.85490200	H	6.61184600	-0.73591600	-0.62622200
H	-2.07444000	-5.58243100	-2.31645900	H	7.40278700	-2.89569200	-1.56337600
H	-2.22989400	-4.02506500	-1.50758300	H	6.42612600	-5.04137600	-0.74916700
H	-0.89399300	-4.28919500	-2.62534000	H	4.69769400	-4.99763100	1.03896500
C	-1.51369000	-5.91399400	0.40092700	H	3.96380900	-2.83781800	2.00533000
H	-0.90262500	-6.42924200	1.15131500	C	2.09615800	2.25559900	4.09069800
H	-2.09598400	-5.14569600	0.91888500	C	1.60256800	3.41476400	4.98371900
H	-2.22089400	-6.64155900	-0.01287400	C	1.76456600	0.92578400	4.78917100

C	3.62890300	2.34213500	3.93417100
H	1.84735500	4.38797000	4.54606500
H	0.51525900	3.36918100	5.11414400
H	2.06975700	3.36221300	5.97461200
H	2.09421400	0.06688900	4.19340000
H	2.27854400	0.87884600	5.75549800
H	0.69068800	0.81976300	4.98032700
H	4.11474500	2.26775700	4.91457700
H	3.99549900	1.52807600	3.30318600
H	3.94168600	3.28477000	3.47556300
C	1.35525100	4.91612300	-0.20496100
C	2.63339900	5.65765300	0.22588500
C	1.47950800	4.54342400	-1.69685500
C	0.14291600	5.85685700	-0.02058000
H	2.53837100	6.08081800	1.23267200
H	3.50535000	4.99809800	0.20787300
H	2.82051700	6.49198700	-0.45886500
H	0.53348900	4.17338100	-2.10592300
H	1.76122100	5.42725200	-2.27927700
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H	0.27305000	6.76980500	-0.61462600
H	-0.78437200	5.37039800	-0.34277000
H	0.02482700	6.14617600	1.03037100
C	-4.82041200	4.09682300	0.43752400
C	-5.25745900	3.60937500	1.83683200
C	-3.76309300	5.21212400	0.59030700
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H	-5.99066300	2.79858100	1.75551100
H	-4.40760500	3.23974600	2.42015200
H	-5.71527500	4.42971800	2.40193600
H	-3.44115800	5.57878500	-0.39048900
H	-4.17778400	6.05750700	1.15210400
H	-2.87351900	4.85967100	1.12144700
H	-6.45481900	5.51402300	0.31991800
H	-5.79636000	5.08054100	-1.26232400
H	-6.84585000	3.94248700	-0.39201500

C	-4.62670100	0.96202400	-3.65381000
C	-3.51796500	1.19627000	-4.70381000
C	-4.96218900	-0.54452800	-3.59335800
C	-5.88861600	1.72005700	-4.09648300
H	-3.26581500	2.26033900	-4.77210300
H	-2.60341900	0.65020800	-4.45125900
H	-3.85231200	0.85873600	-5.69206800
H	-5.71912700	-0.74905500	-2.82794600
H	-5.35039400	-0.88482000	-4.56042600
H	-4.07803800	-1.14661800	-3.36152500
H	-6.21815700	1.34685400	-5.07198900
H	-6.71493400	1.58001400	-3.39011500
H	-5.70250800	2.79480100	-4.19992100
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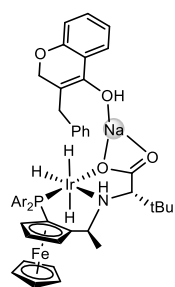
TS_{III+H2-IV}



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C	0.38665600	-4.22607300	-0.07282000
H	0.89303100	-4.66118900	0.79239400
C	-1.50436100	-1.88274200	2.27923000
C	-1.82005000	-0.56480900	1.76777200
C	-2.81221100	-0.00062100	2.63857300
H	-3.29654300	0.95342000	2.49977100
C	-3.11298400	-0.94073000	3.66016100
H	-3.86122400	-0.82158900	4.43254800
C	-2.31449600	-2.09685500	3.43681400
H	-2.32934600	-3.00724800	4.02253600

C	-2.50807200	1.13093400	-0.47796100	H	-1.24891800	-1.67387000	-1.74322400
C	-3.11559000	2.20240300	0.18586600	C	-0.43080100	-2.85997300	1.86564200
H	-2.68911200	2.55583100	1.11796800	H	-0.69070100	-3.82436000	2.32620100
C	-4.24300900	2.83372400	-0.34732600	O	1.29061900	-2.76676000	-1.79999800
C	-4.73036400	2.37643700	-1.58163500	C	-0.50760300	-5.35082000	-0.68806500
H	-5.60228000	2.85390900	-2.00558500	C	0.37859100	-6.48081000	-1.24320200
C	-4.11472600	1.33820400	-2.29235700	H	-0.25549600	-7.32139000	-1.54787000
C	-2.99276400	0.72469700	-1.72079700	H	0.95687300	-6.15666900	-2.11173900
H	-2.47517800	-0.07601200	-2.23451000	H	1.08808600	-6.83917000	-0.49048100
C	-0.09027600	1.57632600	0.98500400	C	-1.39002000	-4.80918200	-1.82825900
C	0.50469000	1.44385500	2.24477100	H	-1.94339900	-5.63639300	-2.28674800
H	0.27133800	0.57525800	2.84673200	H	-2.12941600	-4.07732400	-1.48674800
C	1.38240600	2.42050600	2.71919600	H	-0.78683300	-4.32219100	-2.59952500
C	1.62900400	3.53700400	1.90426200	C	-1.38288400	-5.94148200	0.43418300
H	2.30450400	4.30146200	2.26688200	H	-0.76410400	-6.44133700	1.18869300
C	1.03721000	3.70365100	0.64760700	H	-1.97951900	-5.18061500	0.94655700
C	0.17832700	2.69404000	0.19547500	H	-2.07621000	-6.68396400	0.02328900
H	-0.28869500	2.77383300	-0.77887000	H	-1.38504600	-3.19460200	0.12828700
C	-4.11955300	-2.11945300	-0.16302200	H	5.39703100	0.11042800	2.18125300
H	-3.48951200	-1.97542700	-1.02843500	Na	3.60159100	-2.36037700	-1.72000700
C	-4.21516100	-3.30798000	0.62120800	C	3.73609000	2.85680000	-4.02347400
H	-3.70714100	-4.24097500	0.42893000	C	4.35041600	4.04527700	-3.62366400
C	-5.10747700	-3.05392900	1.70513400	C	4.84055200	4.18072100	-2.32250200
H	-5.36287900	-3.74734000	2.49546400	C	4.72209600	3.11826000	-1.42883000
C	-5.57113100	-1.70988900	1.58278400	C	4.11804700	1.90768500	-1.81619600
H	-6.22988500	-1.20143900	2.27448600	C	3.62224100	1.79815700	-3.12000000
C	-4.96100600	-1.13119000	0.43012700	O	5.13624100	3.31795700	-0.13727200
H	-5.07040600	-0.11083000	0.09146100	C	5.53845000	2.14595000	0.58970000
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O	2.58164800	-4.40801000	-1.04099700	C	4.02395200	0.79475600	-0.84520700
C	0.93640400	-2.43799500	2.41311500	O	3.35524400	-0.28430200	-1.20601900
H	1.72091300	-3.13825400	2.10983000	C	4.75259100	-0.19095000	1.34154300
H	0.89661900	-2.42006700	3.50667700	C	5.28587500	-1.49810700	0.77335700
Ir	0.03791600	-1.24298300	-0.89987500	C	6.26214100	-1.50612800	-0.23494900
H	0.29710000	-0.11979200	-1.99716900	C	6.71839300	-2.70823200	-0.78149200
H	1.21221000	-1.44422300	2.05778400	C	6.20554500	-3.93035600	-0.32881100

C	5.24230100	-3.93519600	0.68234600	H	2.07197100	3.85503400	-1.88968500
C	4.79382500	-2.72882200	1.22790600	H	0.13773500	6.82201900	-0.53973400
H	3.34354700	2.75589700	-5.03136000	H	-0.89992300	5.41065800	-0.25227200
H	4.44393700	4.87461800	-4.31946400	H	-0.04993300	6.17311200	1.10357900
H	5.30633800	5.10092200	-1.98441900	C	-4.89101800	3.99147600	0.42503200
H	3.13035300	0.87044700	-3.39397700	C	-5.32481700	3.49070800	1.82066000
H	5.50971300	2.45090300	1.64043100	C	-3.86160900	5.13114300	0.58689600
H	6.60159800	1.94998500	0.34219400	C	-6.12998900	4.55370300	-0.29071600
H	3.76742900	-0.39203900	1.78602500	H	-6.03798300	2.66290500	1.73304600
H	6.63185700	-0.55860500	-0.61539600	H	-4.46984400	3.13963800	2.40792600
H	7.47330300	-2.69146700	-1.56378900	H	-5.80529400	4.29860000	2.38500500
H	6.54720000	-4.86508900	-0.76367300	H	-3.54183400	5.50706600	-0.39113800
H	4.81507600	-4.87356700	1.02149000	H	-4.29969600	5.96559200	1.14734300
H	4.02806500	-2.73838300	1.99971200	H	-2.96778100	4.79860200	1.12364800
C	2.04484200	2.32620000	4.10031400	H	-6.55671800	5.37133400	0.30013900
C	1.51778600	3.47496600	4.98767000	H	-5.87995100	4.95453100	-1.27907400
C	1.74093500	0.99059700	4.80043100	H	-6.90794900	3.79210800	-0.41551100
C	3.57616600	2.44967800	3.95473500	C	-4.61103000	0.85847500	-3.66268800
H	1.74272700	4.45312500	4.55043300	C	-3.50466900	1.11409200	-4.71018400
H	0.43093900	3.40382500	5.10961800	C	-4.91310200	-0.65498800	-3.59856000
H	1.97831300	3.43488500	5.98228900	C	-5.88805700	1.58713500	-4.11126000
H	2.09386800	0.13792800	4.20909200	H	-3.27627100	2.18338700	-4.78112400
H	2.24980000	0.95837900	5.77011300	H	-2.57901200	0.58948700	-4.45280600
H	0.66869700	0.85978200	4.98477800	H	-3.82833000	0.76599800	-5.69839600
H	4.05658600	2.39671100	4.93920400	H	-5.66804700	-0.87362500	-2.83507800
H	3.96844800	1.63835800	3.33524400	H	-5.29018800	-1.00705100	-4.56588200
H	3.86833800	3.39590700	3.48967800	H	-4.01660300	-1.23618100	-3.36113300
C	1.24524000	4.96974600	-0.19362700	H	-6.20612900	1.20446200	-5.08694700
C	2.53289900	5.71457700	0.20387400	H	-6.71328000	1.43034100	-3.40712300
C	1.31952500	4.62071000	-1.69440100	H	-5.72562900	2.66557700	-4.21647600
C	0.03409600	5.89972900	0.04517800	H	1.97250300	-0.53060600	-0.49011100
H	2.46717200	6.12952700	1.21625800	H	1.45582900	-0.80560900	0.15343500
H	3.40710400	5.05975900	0.15475900				
H	2.69435700	6.55612900	-0.47875500	IV			
H	0.35906100	4.26134900	-2.07846300				
H	1.58507300	5.51325900	-2.27119900				



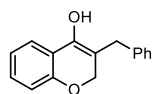
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C	0.16760000	-4.40911500	-0.05126000
H	0.62209000	-4.89042100	0.81785700
C	-1.48719000	-1.89277400	2.30476000
C	-1.66185700	-0.54540600	1.80297700
C	-2.58823400	0.11180800	2.68137900
H	-2.97222600	1.11112400	2.55261300
C	-2.98278500	-0.79695900	3.69962300
H	-3.71254300	-0.60473900	4.47513700
C	-2.30933700	-2.02813300	3.46658200
H	-2.41639000	-2.93601400	4.04674200
C	-2.21079300	1.18558600	-0.45578000
C	-2.78433000	2.27487800	0.21086800
H	-2.37329500	2.58947800	1.16317000
C	-3.86606500	2.96959000	-0.33906300
C	-4.33735700	2.56612200	-1.59842400
H	-5.17308600	3.09359700	-2.03606900
C	-3.75212100	1.51294900	-2.31086300
C	-2.68191800	0.83079900	-1.71867300
H	-2.19817800	0.00073900	-2.22011900
C	0.21041000	1.46121800	1.02346800
C	0.82832600	1.24776500	2.25947400
H	0.64766400	0.31523900	2.77801000
C	1.64355000	2.22821100	2.83298500
C	1.79845900	3.43808300	2.14078700
H	2.38314300	4.22775400	2.60039200
C	1.21078300	3.67822700	0.89181200
C	0.42937700	2.65778900	0.33417400

H	-0.04412500	2.79951100	-0.62848400
C	-4.08663000	-1.87027000	-0.12986100
H	-3.42137500	-1.78524700	-0.97782100
C	-4.29939000	-3.04157300	0.65780100
H	-3.87383700	-4.01752700	0.47606800
C	-5.17582500	-2.70314900	1.73222800
H	-5.50155000	-3.36724200	2.52200700
C	-5.51275700	-1.32246100	1.60102500
H	-6.12942700	-0.75287100	2.28400000
C	-4.84079700	-0.80774000	0.45216200
H	-4.85233300	0.21720900	0.11052500
C	1.33028600	-4.04314300	-0.98929800
O	2.40884900	-4.66393100	-0.90773500
C	0.87267900	-2.71682200	2.42808400
H	1.55354400	-3.54241200	2.19615100
H	0.82193300	-2.60934900	3.51626200
Ir	0.06587300	-1.41938400	-0.87747000
H	0.43998000	-0.32135400	-1.97437700
H	1.28085100	-1.80736300	1.98488500
H	-1.27472000	-1.73534800	-1.80453800
C	-0.53389800	-2.98392000	1.88220400
H	-0.90189100	-3.91271200	2.34390000
O	1.15008900	-3.07588700	-1.82443200
C	-0.79568100	-5.45664100	-0.69440200
C	0.02698600	-6.62858000	-1.26030600
H	-0.65012700	-7.42484100	-1.59033800
H	0.63286600	-6.32167800	-2.11721800
H	0.70510100	-7.04285800	-0.50683600
C	-1.63296400	-4.84285200	-1.83118200
H	-2.23232600	-5.62814500	-2.30623500
H	-2.32592000	-4.07106300	-1.48194600
H	-0.99531600	-4.37731900	-2.58685500
C	-1.71770600	-6.00644600	0.41084900
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H	-2.26776200	-5.21356000	0.92770200
H	-2.45490400	-6.69529500	-0.01683600

H	-1.52131600	-3.24396400	0.14469700	C	3.80364500	2.37869700	4.13373300
H	5.21429600	0.36772900	1.85281100	H	1.72012700	4.04435000	4.90428300
Na	3.38151900	-2.61698200	-1.70461800	H	0.54453200	2.77762800	5.28878400
C	2.61702300	2.93822100	-4.09854400	H	2.05940300	2.89336200	6.21042200
C	3.45247600	4.04677200	-3.93693800	H	2.59920700	-0.12041900	4.03656600
C	4.33859800	4.11567000	-2.85940600	H	2.67466300	0.50647500	5.69172500
C	4.38016700	3.06897200	-1.94260100	H	1.10989300	0.32729300	4.89008000
C	3.56898800	1.93193500	-2.10814100	H	4.26689700	2.26441800	5.12081100
C	2.68208300	1.88126800	-3.19025500	H	4.31688100	1.70680400	3.43854100
O	5.27190900	3.13897800	-0.90176600	H	3.98146200	3.40577800	3.80102700
C	4.89391300	2.42175500	0.28675100	C	1.33402700	5.06026300	0.22959700
C	4.37682600	1.03194000	0.00879300	C	2.78679000	5.57677600	0.25931500
C	3.71886800	0.83752900	-1.14912200	C	0.86322700	5.03675800	-1.23535400
O	3.17906200	-0.37150200	-1.51106700	C	0.44498200	6.04437000	1.02306500
C	4.53490900	-0.01953100	1.08043200	H	3.17937400	5.65495900	1.27827600
C	5.06655200	-1.35918800	0.60294900	H	3.45179700	4.93050100	-0.31604600
C	6.05267400	-1.43883900	-0.39192400	H	2.82975500	6.57883700	-0.18323600
C	6.51837300	-2.67893200	-0.83674600	H	-0.20663200	4.81433600	-1.31477300
C	6.00681700	-3.86292100	-0.29028600	H	1.02759000	6.02009600	-1.68967100
C	5.03353600	-3.79365200	0.71011200	H	1.41487400	4.29866400	-1.82505700
C	4.57177500	-2.54973300	1.15266900	H	0.49427100	7.04676300	0.58041300
H	1.91949600	2.89567700	-4.92954100	H	-0.59960800	5.71877600	1.01541400
H	3.40763300	4.87078500	-4.64334700	H	0.76815000	6.11751500	2.06749100
H	4.98649800	4.97325900	-2.71023100	C	-4.50395400	4.12077400	0.45205200
H	2.04993100	1.00612300	-3.29912700	C	-5.07840700	3.56280900	1.77339800
H	4.14605800	3.01562800	0.83324500	C	-3.43110100	5.18309700	0.77076900
H	5.80414400	2.38635200	0.89106500	C	-5.64532900	4.80320700	-0.31952600
H	3.57272100	-0.18116100	1.58311000	H	-5.82991800	2.79023100	1.57460000
H	6.42882700	-0.52323500	-0.83912600	H	-4.29500600	3.11719600	2.39540300
H	7.27999800	-2.72145900	-1.61109300	H	-5.55305000	4.36218400	2.35514100
H	6.35637900	-4.82774300	-0.64551700	H	-2.99430100	5.58441500	-0.15043000
H	4.60489400	-4.70400900	1.11580600	H	-3.87005500	6.01566300	1.33336200
H	3.79257300	-2.50183900	1.90792400	H	-2.61778500	4.76656800	1.37249500
C	2.29872500	2.04463900	4.20954900	H	-6.05859000	5.62071900	0.28125500
C	1.61498000	2.99903500	5.21324200	H	-5.29520300	5.22907100	-1.26625900
C	2.15762500	0.60380000	4.73073800	H	-6.46224000	4.10662000	-0.53791700

C	-4.23237000	1.07514300	-3.70028800
C	-3.07839900	1.26602200	-4.70950700
C	-4.62722000	-0.41776400	-3.65544600
C	-5.44598700	1.88478200	-4.18380000
H	-2.78057300	2.31936200	-4.76449000
H	-2.19835000	0.68075400	-4.42482900
H	-3.39079500	0.94488900	-5.71057300
H	-5.42060600	-0.59129500	-2.91972600
H	-4.99144100	-0.74303400	-4.63729500
H	-3.77586200	-1.05138400	-3.38836500
H	-5.75238900	1.53281900	-5.17482500
H	-6.30356500	1.77079800	-3.51075700
H	-5.21512800	2.95273800	-4.26846200
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H	1.49136400	-1.17918000	0.03567900

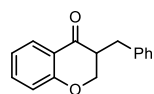
2a'-1



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C	2.16533800	-0.95081200	-0.25069000
C	2.22195700	0.43475700	0.01123500
C	3.44337300	0.98974800	0.41612700
O	0.99596600	-1.53921800	-0.63931300
C	0.09295900	-0.68724600	-1.36763200
C	-0.09438000	0.65876000	-0.71814200
C	0.97051400	1.18845200	-0.09181700
O	0.90677500	2.44800400	0.46519300
C	-1.43438000	1.33209600	-0.83696000
C	-2.55649300	0.51552900	-0.21658500
C	-2.43060200	0.02051100	1.08815700
C	-3.45711700	-0.72132500	1.66988100
C	-4.62736200	-0.98361900	0.95305400
C	-4.76052900	-0.49968600	-0.34819900

C	-3.72908000	0.24256700	-0.92762700
H	5.51084700	0.63540600	0.89925700
H	5.35714100	-1.81759400	0.50136400
H	3.19780000	-2.82285800	-0.25191400
H	3.52194100	2.06250200	0.57504700
H	-0.85076600	-1.23444700	-1.39595500
H	0.46908600	-0.59234700	-2.40073200
H	-1.37678300	2.31632900	-0.36069400
H	-1.67214900	1.51184500	-1.89567000
H	-1.51525200	0.21385800	1.64117700
H	-3.34333000	-1.09830100	2.68261600
H	-5.42655000	-1.56429300	1.40502900
H	-5.66442100	-0.70258200	-0.91616200
H	-3.83590200	0.61595000	-1.94355900
H	1.55335300	2.50952200	1.18551500

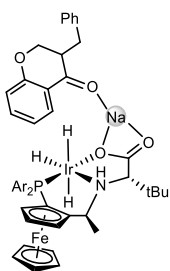
2a'



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C	-2.32290000	-0.96702900	0.08702700
C	-2.39839300	0.43623900	-0.02110400
C	-3.66069800	1.05547500	0.00581900
O	-1.13878700	-1.64009900	0.05325000
C	-0.04381500	-0.92647000	-0.53962800
C	0.13534900	0.46199700	0.06637300
C	-1.16604600	1.24887100	-0.08335900
O	-1.17983400	2.46880900	-0.20141200
C	1.34250500	1.20686700	-0.53054900
C	2.65477800	0.52889800	-0.21162300
C	3.32247300	-0.24495700	-1.16805300
C	4.51494800	-0.90021700	-0.85476400
C	5.05792600	-0.78962300	0.42533200
C	4.40271000	-0.01795200	1.38785500

C	3.21259700	0.63452100	1.06983900
H	-5.78709200	0.78944500	0.17530500
H	-5.62224000	-1.68497200	0.39821600
H	-3.39902700	-2.80555300	0.32848400
H	-3.69337000	2.13689600	-0.07746000
H	0.83528300	-1.54971600	-0.37694500
H	-0.22690500	-0.84637300	-1.62171800
H	0.29421500	0.33508100	1.14912700
H	1.32825700	2.22989900	-0.14394000
H	1.21030600	1.28523300	-1.61671300
H	2.90608100	-0.33002800	-2.16921000
H	5.01950800	-1.49397700	-1.61195700
H	5.98631600	-1.29701800	0.67130400
H	4.82197600	0.07920700	2.38547900
H	2.71019500	1.23962500	1.82135300

V



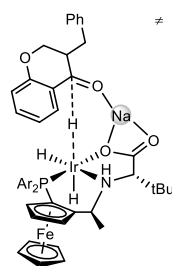
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C	-1.44974500	-4.16834000	-0.11530100
H	-0.83318600	-4.70962300	0.60596800
C	-1.59530900	-1.22760300	2.31863800
C	-1.49236900	0.09239700	1.74266800
C	-1.93032500	1.02966600	2.73852400
H	-2.01683000	2.09653200	2.59444400
C	-2.29964400	0.30893800	3.90789300
H	-2.71776700	0.73373800	4.81102700
C	-2.09977700	-1.07721300	3.64698900
H	-2.31748200	-1.89325000	4.32441500
C	-1.90510700	1.93809900	-0.43543600

C	-1.68976700	3.18400500	0.17443500
H	-0.90406000	3.27657800	0.91243500
C	-2.44565600	4.29681000	-0.18676500
C	-3.43355700	4.13069500	-1.17621800
H	-4.02653000	4.99120700	-1.46182400
C	-3.65439400	2.90974000	-1.81672800
C	-2.86317200	1.81322500	-1.43503800
H	-2.97153400	0.84577100	-1.91300000
C	0.69353400	1.30969500	0.38245400
C	1.26648400	1.38371300	1.65130300
H	0.78000200	0.88214800	2.47937500
C	2.45055200	2.10445900	1.86891500
C	3.02000500	2.77996700	0.78346100
H	3.92025000	3.35715400	0.93854700
C	2.45890300	2.73353700	-0.50362400
C	1.30808600	1.96396100	-0.69039900
H	0.84653800	1.89606800	-1.67066100
C	-4.97708500	-1.44045400	1.49615700
H	-4.94095100	-2.50155700	1.30000000
C	-5.39279400	-0.83305800	2.71891400
H	-5.69222400	-1.35300000	3.61941000
C	-5.30559000	0.58181500	2.55413200
H	-5.51388900	1.32262100	3.31507300
C	-4.82867100	0.84711700	1.23501000
H	-4.60410200	1.81863200	0.81806200
C	-4.62265500	-0.40442300	0.58125600
H	-4.20093200	-0.54800700	-0.40396100
C	-0.68932900	-4.24602500	-1.46083600
O	-0.03206600	-5.25709900	-1.71997500
C	0.41183600	-2.64194000	1.87001800
H	0.78086200	-3.59475200	1.48286300
H	0.70902700	-2.55986600	2.92047900
Ir	-0.91190400	-1.32910200	-1.20314400
H	-0.53611400	-0.41667800	-2.48695300
H	0.88249800	-1.84482500	1.29464200
H	-2.51814500	-1.16550800	-1.63868500

C	-1.11101700	-2.54433700	1.76507600	C	6.75927200	1.08529800	-1.83169500
H	-1.54716200	-3.33204200	2.39477300	H	2.37439900	-6.50300400	0.11840500
O	-0.81441800	-3.23214700	-2.26476900	H	3.16311300	-5.92301500	2.41582300
C	-2.82847100	-4.90354900	-0.19372500	H	3.98268500	-3.62444300	2.91531300
C	-2.63169900	-6.34770500	-0.69014000	H	2.52451200	-4.81620200	-1.68532600
H	-3.58767500	-6.88219500	-0.63593600	H	4.18235500	0.25820300	0.67761400
H	-2.27434000	-6.38077700	-1.72093900	H	2.64314700	-0.56170800	0.34271800
H	-1.90296300	-6.88398500	-0.07293500	H	6.06567200	-1.96601100	-0.58653100
C	-3.78950000	-4.17513800	-1.15192600	H	6.55242500	-0.33508600	1.24332400
H	-4.74155500	-4.71608600	-1.20203500	H	7.63619000	1.80313000	1.87036100
H	-4.00867300	-3.14848500	-0.84177200	H	8.16320600	3.49356700	0.12189200
H	-3.36836000	-4.11377800	-2.15918900	H	7.61054000	3.01637200	-2.25598000
C	-3.43862300	-4.97878400	1.22001400	H	6.51963700	0.88123400	-2.87253000
H	-2.80029800	-5.56720800	1.89008900	C	3.01850200	3.54411000	-1.68118100
H	-3.58138700	-3.99492300	1.67605300	C	3.39310700	2.59402800	-2.83825900
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Na	0.97709800	-2.25150000	-3.10944700	H	2.53874600	1.98878600	-3.15880600
C	2.77820500	-5.51898900	0.32888300	H	3.74294600	3.16763100	-3.70520300
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C	3.72657200	-2.94432900	0.90010400	H	1.02397000	4.00818700	-2.48885500
C	3.35203400	-3.28345500	-0.42194400	H	4.62929400	4.90766000	-2.16869600
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C	3.73150100	-0.66017300	0.31209800	C	3.04744000	2.15403000	3.28175900
C	4.18538700	-1.00142500	-1.09667900	C	2.04913500	2.87730000	4.21338300
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O	3.16978800	-2.50926300	-2.66834900	C	4.38977000	2.90308500	3.32258700
C	5.72955800	-1.14417100	-1.22772700	H	1.86266200	3.89911600	3.86369800
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H	-1.32810400	4.99562400	2.32130700
H	-1.61731500	7.66461500	-0.27131900
H	-0.87631900	6.32861700	-1.17900400
H	-2.57216800	6.75461400	-1.45401500
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C	-3.97962000	2.31122200	-4.22611100
C	-5.68401000	1.60402100	-2.51244400
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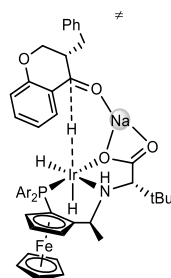
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C	-1.61640200	3.22575300	0.15751600
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C	-2.32919100	4.32049700	-0.32580100
C	-3.05724300	4.15907200	-1.51983500
H	-3.61714000	5.00457400	-1.90073100
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C	1.09253100	1.16889300	2.23358900
H	0.50581500	0.48859600	2.83854900
C	2.22033500	1.79588500	2.78636800
C	2.92641500	2.69068800	1.98224600
H	3.78381900	3.20512200	2.39640000
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C	1.47492900	2.27214700	0.11548900
H	1.17444600	2.42684500	-0.91343800

C	-5.06211300	-1.36538500	0.69411000	H	1.25815900	-1.66621600	-0.75488800
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H	-6.18158900	-1.30340400	2.63544000	C	3.36376700	-4.70420800	2.34023900
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H	-5.92068700	1.37403600	2.42286600	C	3.60342400	-2.60280900	1.16833100
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H	-4.53201200	1.90048900	0.16299100	C	2.44393300	-4.44115900	0.12684700
C	-4.52581700	-0.31807900	-0.11298000	O	4.14184800	-1.34854800	1.17898400
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O	-0.17644900	-5.25745600	-1.95391500	C	2.66671000	-2.27819900	-1.16655400
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C	-1.27796200	-2.48844800	1.77062600	C	5.28722200	0.95986100	-3.00692200
H	-1.79105500	-3.27881400	2.32903300	H	2.30683200	-6.25986000	1.26924200
O	-0.49458100	-3.08367500	-2.19571300	H	3.54341400	-5.31112300	3.22353000
C	-2.68315900	-4.91426600	-0.21082800	H	4.38619500	-2.96490700	3.12831900
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H	-3.38178700	-6.95261000	-0.42888900	H	4.15008300	0.48348600	0.32382600
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C	-3.55795900	-4.35698100	-1.35067100	H	7.02320300	-0.31627000	-0.38800200
H	-4.54051700	-4.84188700	-1.34513600	H	8.35979100	1.73468800	-0.78441700
H	-3.71993200	-3.27618800	-1.26908000	H	7.73487900	3.29390300	-2.61921600
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H	-3.68948600	-3.77207300	1.39961200	C	3.00232900	3.94073400	-1.66354900
H	-4.37762200	-5.36005900	1.06128200	C	3.06746700	5.37836300	0.38611000
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C	2.62546800	1.46031300	4.22658300
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C	-3.81598900	2.78143700	-3.56018400

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H	-2.09340100	3.32208400	-4.79576100
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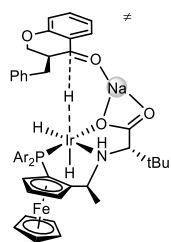


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H	0.91213100	-3.30397800	4.49048700
C	2.18586700	-1.83595100	3.37834700
H	3.10909600	-1.82807400	3.94378100
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H	-2.55944800	-2.13294700	1.27132800	H	3.84529100	-0.17758900	2.20713400
C	-3.01942300	-3.72136700	-0.09845500	O	2.94315600	0.87066800	-2.30017800
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H	-3.20922500	-5.16663500	-1.67460500	C	6.84400900	0.42445100	-0.71291200
C	-1.59215500	-3.82324300	-2.09423800	H	7.71182600	-0.24601200	-0.72165700
C	-0.88293700	-2.70996500	-1.61330600	H	6.78179200	0.93761600	-1.67199600
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C	-1.51808200	0.27515500	1.06119600	C	5.35255400	-1.42878600	-1.52846900
C	-1.31660600	0.80908000	2.33174700	H	6.17934500	-2.14755900	-1.54655500
H	-0.37879600	0.62518900	2.84099900	H	4.42254300	-1.99477500	-1.40178600
C	-2.30908900	1.57463100	2.96313800	H	5.30427200	-0.94611200	-2.50980700
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H	-4.31118600	2.31175300	2.77099600	H	6.02528500	-0.40340700	1.73351500
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C	3.03702600	-4.76137500	1.80039800	C	3.83910800	4.63474500	1.11507600
H	3.75487700	-4.97598800	2.58104000	C	3.10762700	5.04155500	2.23725400
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O	4.83709000	2.00367600	-2.17433000	C	1.05513700	3.50711200	-1.23745000
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H	3.09269000	2.15294000	1.82836700	C	-1.22615000	3.00723600	-2.23989900
H	2.20679000	1.40048700	3.16129200	C	-2.61856400	3.49331500	-2.58413800
Ir	1.29729700	0.18558300	-1.11243200	C	-3.10402800	4.76456300	-2.25310000
H	0.18460000	0.32004000	-2.24190500	C	-4.38689200	5.16787700	-2.63406200
H	1.44333900	1.58921200	1.56292300	C	-5.21185100	4.30756300	-3.35660700
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C	-3.46257000	2.63953200	-3.31187900	H	-2.95486500	3.39870800	5.86978200
H	4.92209900	4.71746600	1.10310600	H	-3.40427200	3.85070900	4.21912700
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H	1.13229300	5.27123100	3.09233000	C	-4.22579100	-4.26847700	0.67588000
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H	-5.37378400	2.35233800	-4.25548200	H	-5.35275200	-3.91258100	2.49303700
H	-3.10115200	1.64879500	-3.58013900	H	-3.62867300	-3.56046000	2.66671300
C	-5.16530100	1.33197600	0.39824600	H	-6.36426800	-4.53923000	0.32484400
C	-5.29404800	0.53233700	-0.90859500	H	-5.68190100	-3.10256300	-0.46523200
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H	-4.60184700	0.89316700	-1.67298500	C	-1.39142400	-3.37429000	-4.54991300
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H	-6.30834700	0.64297900	-1.30763700	C	-2.02579100	-5.67452100	-3.79637600
H	-6.23041400	1.35062000	2.32802400	H	-2.44255300	-3.07014400	-4.60992200
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H	-6.42783200	2.94925900	-0.34676800	H	0.47848600	-5.57113200	-2.59506200
H	-5.39990200	3.42271600	1.01730700	H	0.59519100	-5.30132600	-4.34715900
H	-4.69625700	3.22049100	-0.59629900	H	0.94880000	-3.98373800	-3.22065900
C	-2.03498100	2.14662100	4.35986800	H	-1.69616800	-6.07858400	-4.75963300
C	-1.80745700	0.97617700	5.34234700	H	-1.91165000	-6.46592000	-3.04676700
C	-0.77214100	3.03349800	4.31082300	H	-3.09156400	-5.43581300	-3.88508100
C	-3.20262500	3.00028800	4.87990300	H	-0.50126000	4.87235600	-1.43340000
H	-2.69614100	0.33719400	5.39939400	H	-1.27186500	1.96077800	-1.92040600
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H	-1.59503900	1.35863700	6.34797900				
H	-0.89966000	3.84995400	3.59479200				
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TS''V-VI



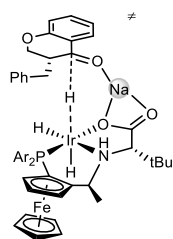
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C	0.95527300	-1.35867500	-2.55823500
C	1.22745800	-0.09294400	-1.91644500
C	1.84381900	0.75515100	-2.89732300
H	2.20837200	1.75503500	-2.71946600
C	1.96896700	0.03026200	-4.11374500
H	2.44537000	0.38446400	-5.01840300
C	1.43141900	-1.27087700	-3.90201400
H	1.40174600	-2.07675400	-4.62442400
C	2.22289100	1.41382800	0.33900400
C	2.44576600	2.66220100	-0.25163700
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C	3.54931100	3.44355600	0.10158700
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H	5.28672800	3.53310900	1.35661000
C	4.21115500	1.71198500	1.70999400
C	3.09151400	0.96057100	1.33080900
H	2.87107800	0.00982500	1.80068700
C	-0.46547700	1.64281900	-0.48696200
C	-1.21357700	1.65309300	-1.66145100
H	-1.01294900	0.90893100	-2.42272000
C	-2.22085500	2.60821100	-1.87213700
C	-2.42176800	3.56998500	-0.88132000
H	-3.18303800	4.32555500	-1.02837200
C	-1.68544700	3.58706400	0.31866400
C	-0.71495300	2.60282000	0.50606200
H	-0.13769700	2.56582000	1.42129600

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H	4.87437800	-2.39483500	-4.08335700
C	4.98974600	-0.48156400	-2.91942400
H	5.32224400	0.23323300	-3.66078500
C	4.65168900	-0.18555600	-1.56461000
H	4.67732000	0.78799600	-1.09594800
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H	3.81940300	-1.48612400	0.05506500
C	-0.29387300	-4.35699800	1.14497300
O	-0.91184300	-5.37864600	1.52297400
C	-1.33993100	-2.20802100	-2.03382000
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C	-2.92973500	-1.41833600	1.67840500	C	-3.68834000	1.15518500	-3.30714700
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H	-1.24777000	-0.45529700	5.94624100	H	-4.87045400	3.44909200	-2.36274100
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C	-1.18352400	4.43597500	2.66705200	H	5.91115500	4.95676100	-0.29607300
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H	2.64874400	-0.46357600	1.77777200
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H	-1.13764100	0.87823800	-2.40337300
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C	3.64680900	-2.27746700	-0.96113700
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C	3.43608700	-3.35304300	-1.87447300
H	2.94604700	-4.28890100	-1.65285100
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O	-2.19743000	-4.87234800	1.76712500
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H	-2.73094100	-2.61134500	-1.66482900
H	-2.22443100	-1.60946100	-3.03692500
Ir	-0.06507400	-1.41375300	1.03115100
H	0.23051500	-0.52268300	2.30217700
H	-1.98640500	-1.03380200	-1.36760600
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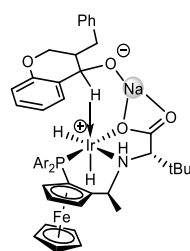


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H	-2.22443100	-1.60946100	-3.03692500
Ir	-0.06507400	-1.41375300	1.03115100
H	0.23051500	-0.52268300	2.30217700
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C	-0.58122600	-2.55199200	-1.99666800

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C	-2.32907300	1.97892400	3.04271700	H	-0.03920800	4.40056900	2.53800200
C	-2.11784300	0.61117300	3.27435700	H	-0.06296800	7.37514800	0.28604800
C	-1.30065100	0.23625400	4.34637100	H	0.81290400	6.16650400	-0.67307200
O	-3.11037400	2.44644200	2.02171200	H	-0.84127400	6.62060400	-1.11359800
C	-3.39564300	1.49913700	0.97481700	C	-2.75484500	2.85861100	-3.31603800
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C	-2.85141900	-0.43441300	2.46679800	C	-3.80826600	1.74615900	-3.13309400
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C	4.69714300	3.44471400	-2.44021900
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C	6.04645700	4.21504000	-0.48463900
H	5.35578300	2.58693500	-2.61858100
H	3.70641000	3.19748600	-2.83570000
H	5.08077200	4.29662300	-3.01414900
H	3.62192600	5.24296900	0.34286700
H	4.01973500	5.85567900	-1.27580800
H	2.66263000	4.73879000	-1.05438400
H	6.37172500	5.08485100	-1.06565200
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H	6.78173400	3.41752900	-0.63975000
C	5.13096000	0.17281100	2.71206700
C	4.33411300	0.34125500	4.02504100
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H	4.21454400	1.40180700	4.27330900
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VI



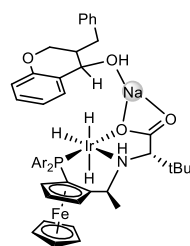
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H	-2.26234200	3.22420300	-4.80913800
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VII



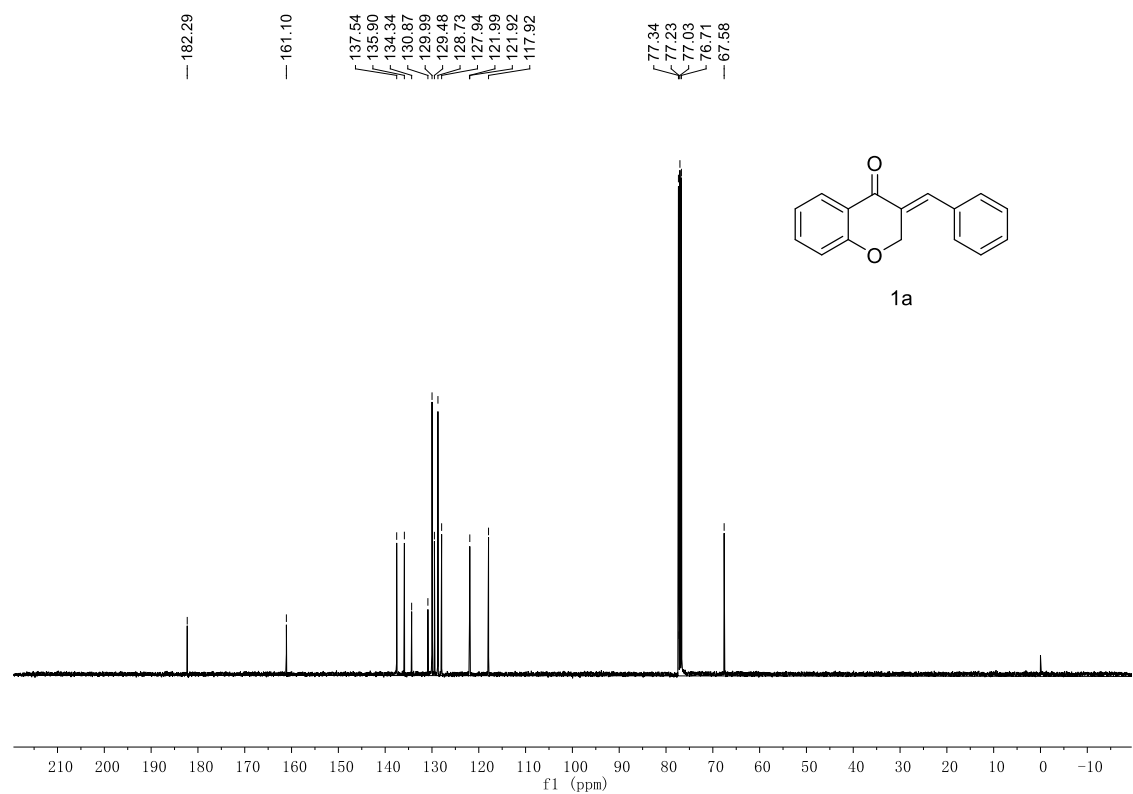
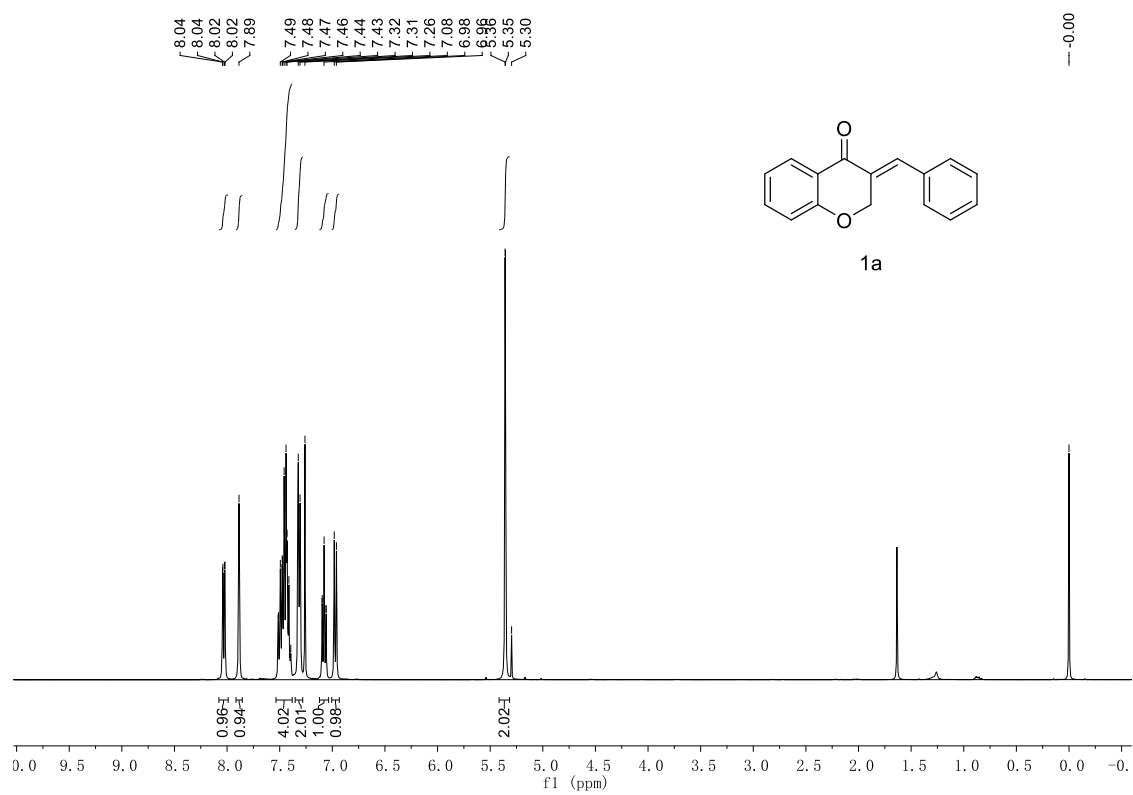
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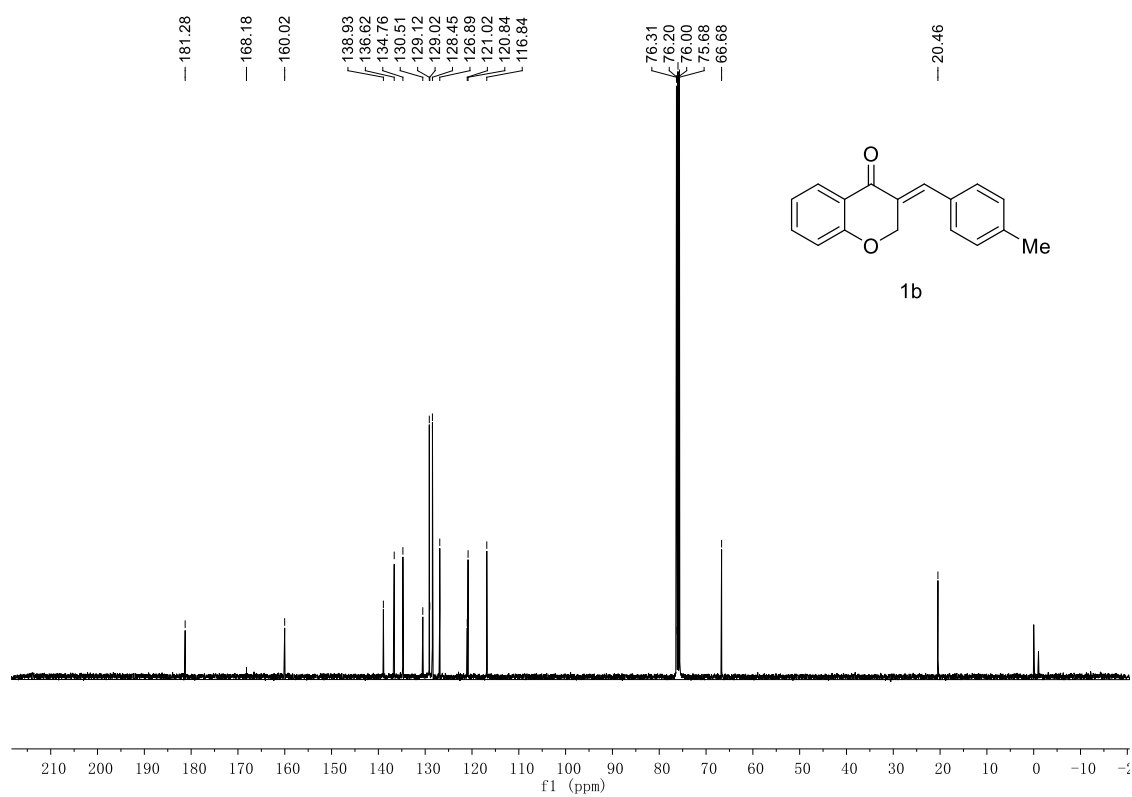
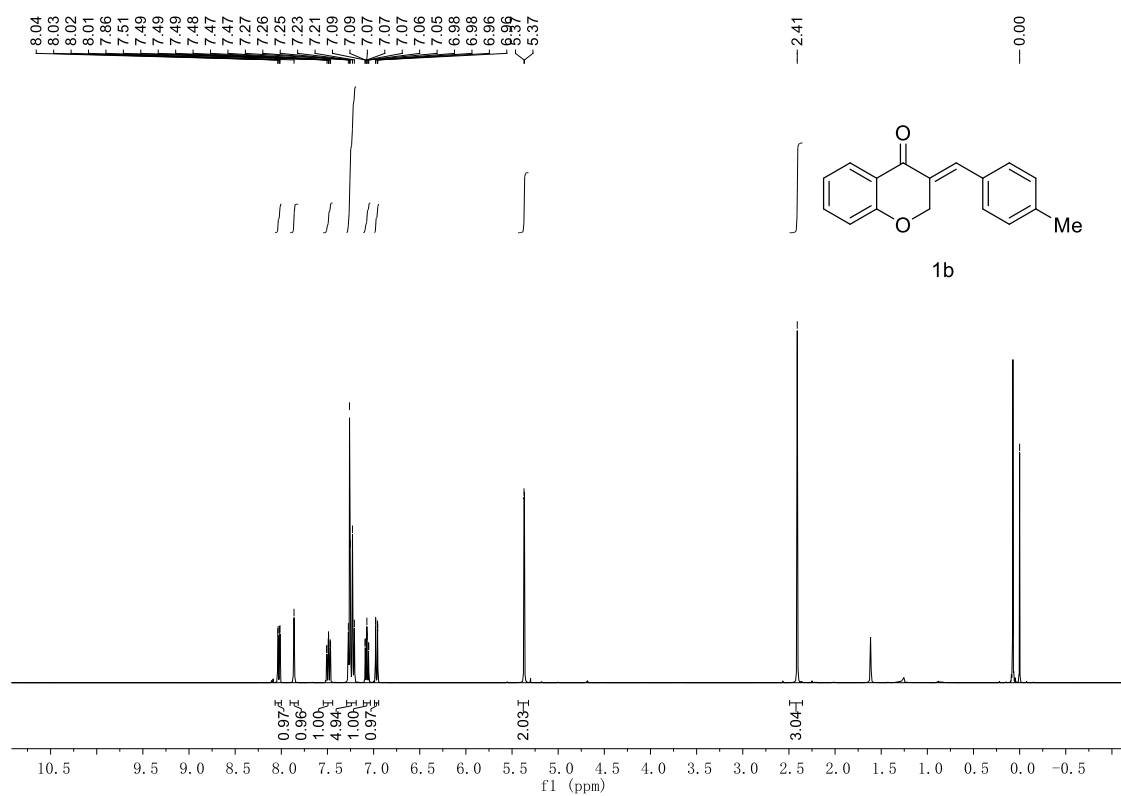
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VII. NMR spectra of enones and hydrogenation product

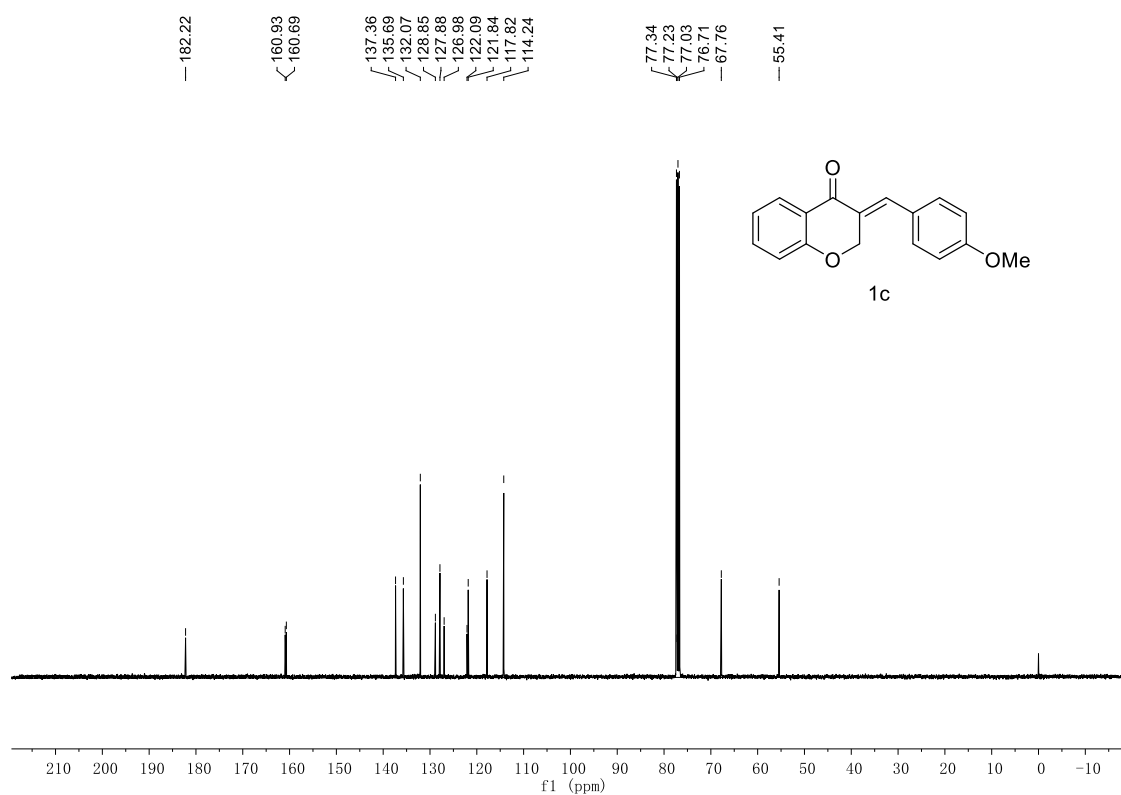
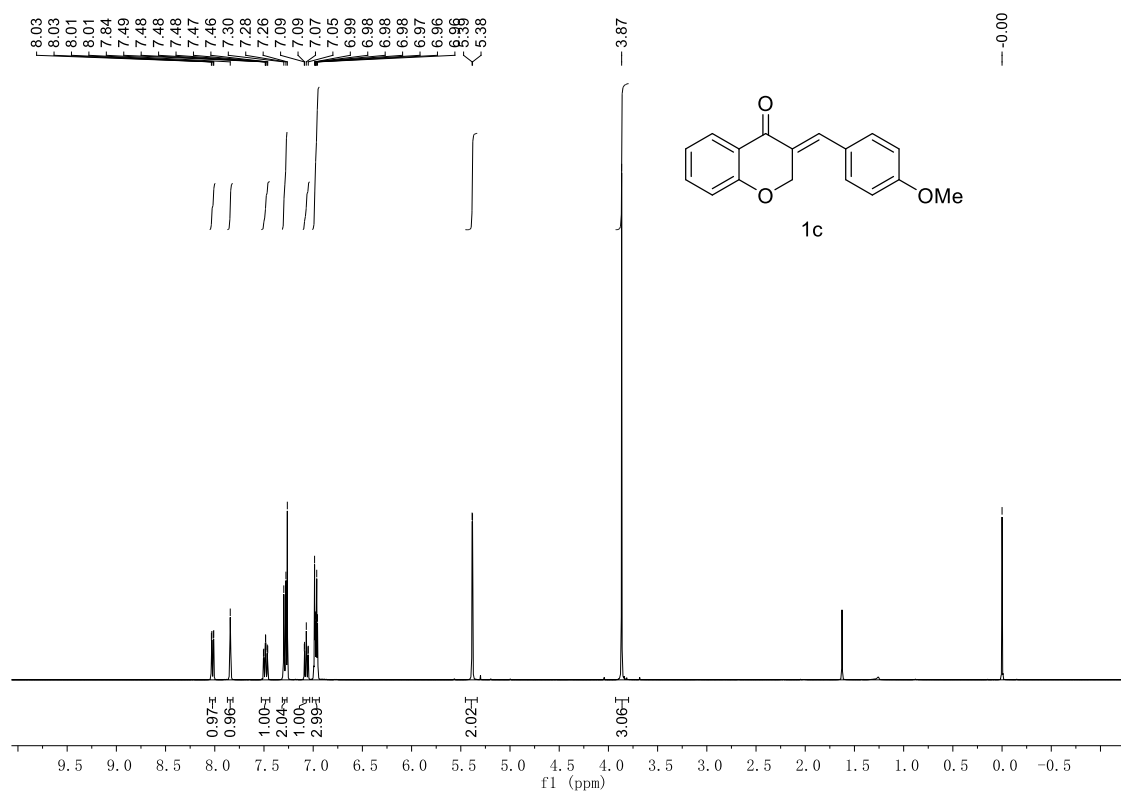
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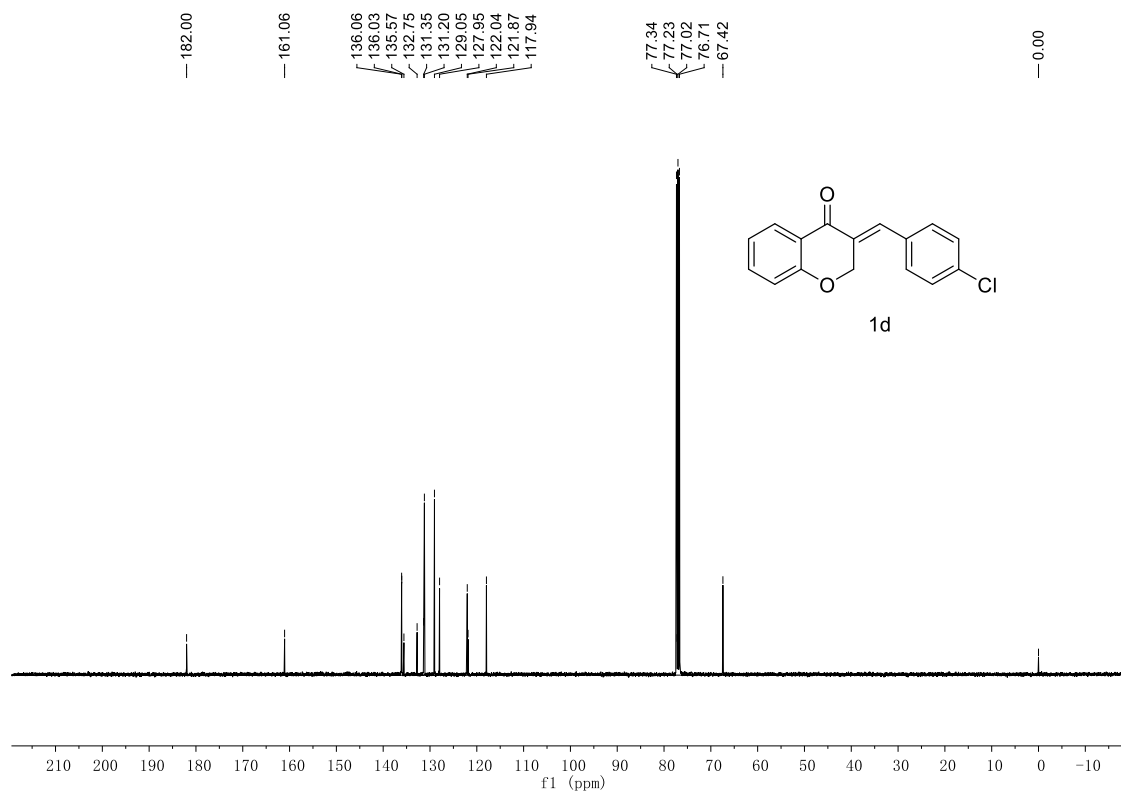
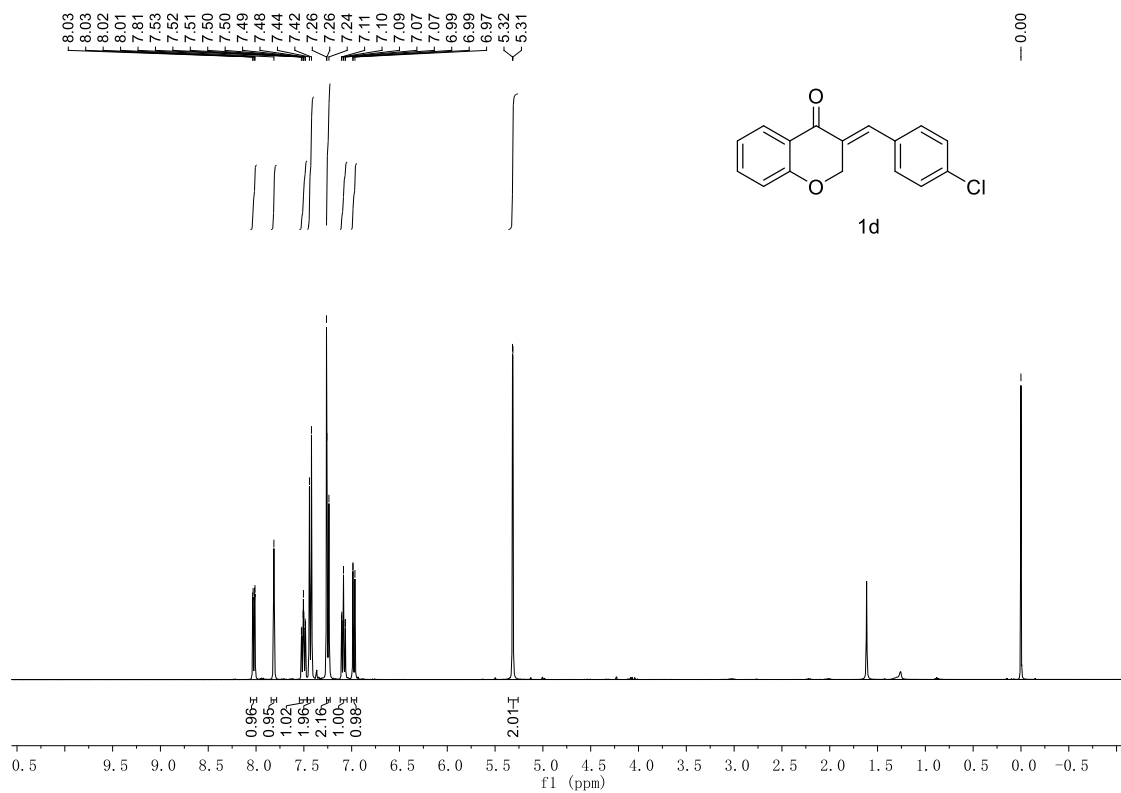
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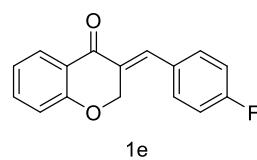
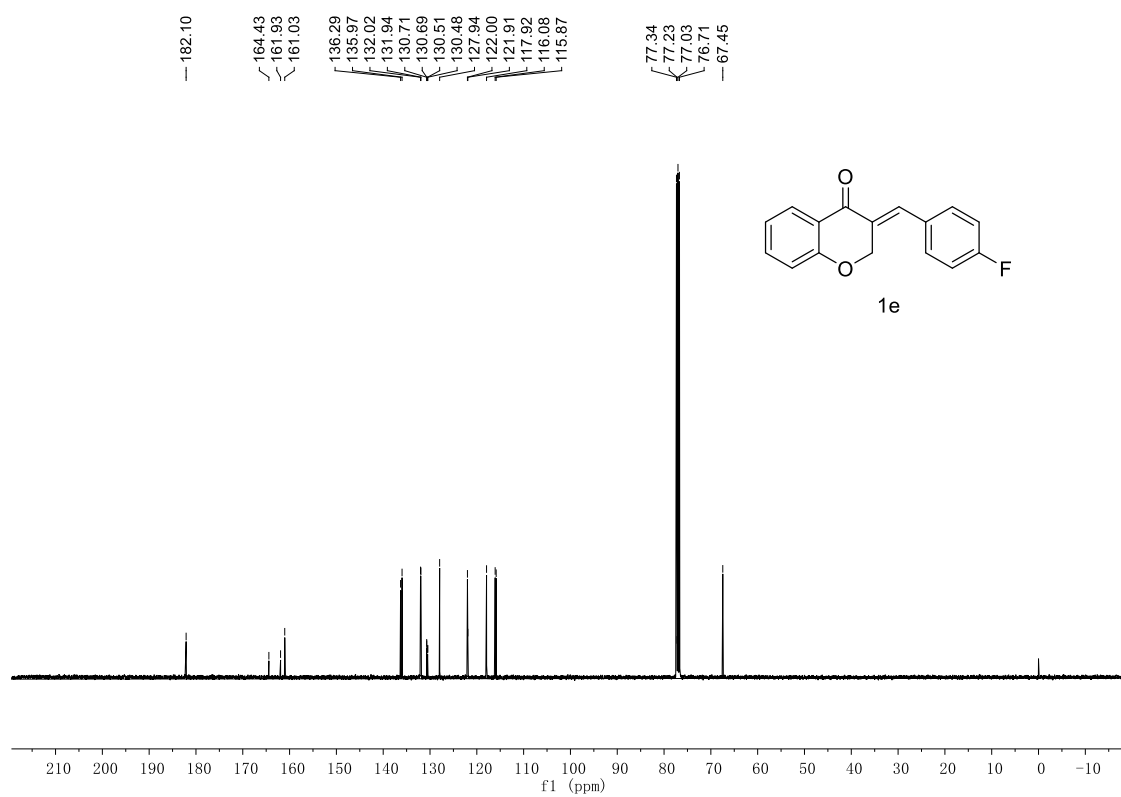
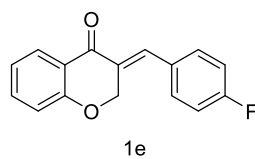
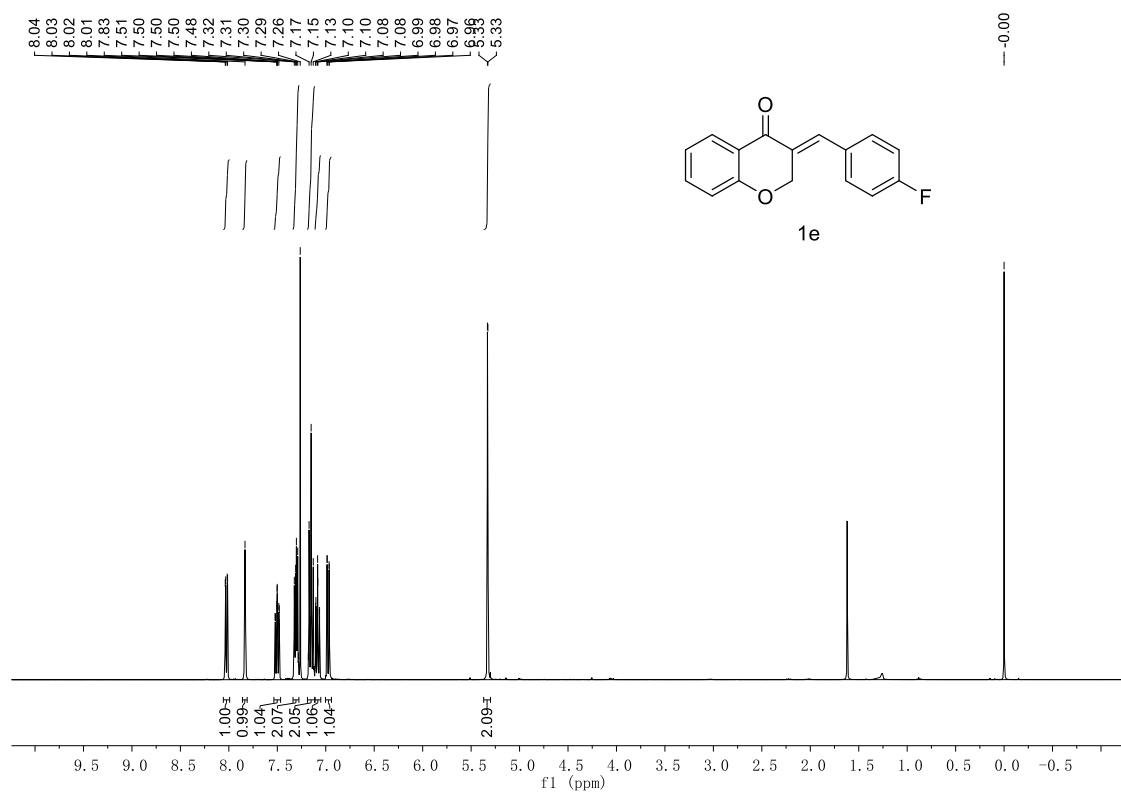
¹H and ¹³C-NMR of 1c



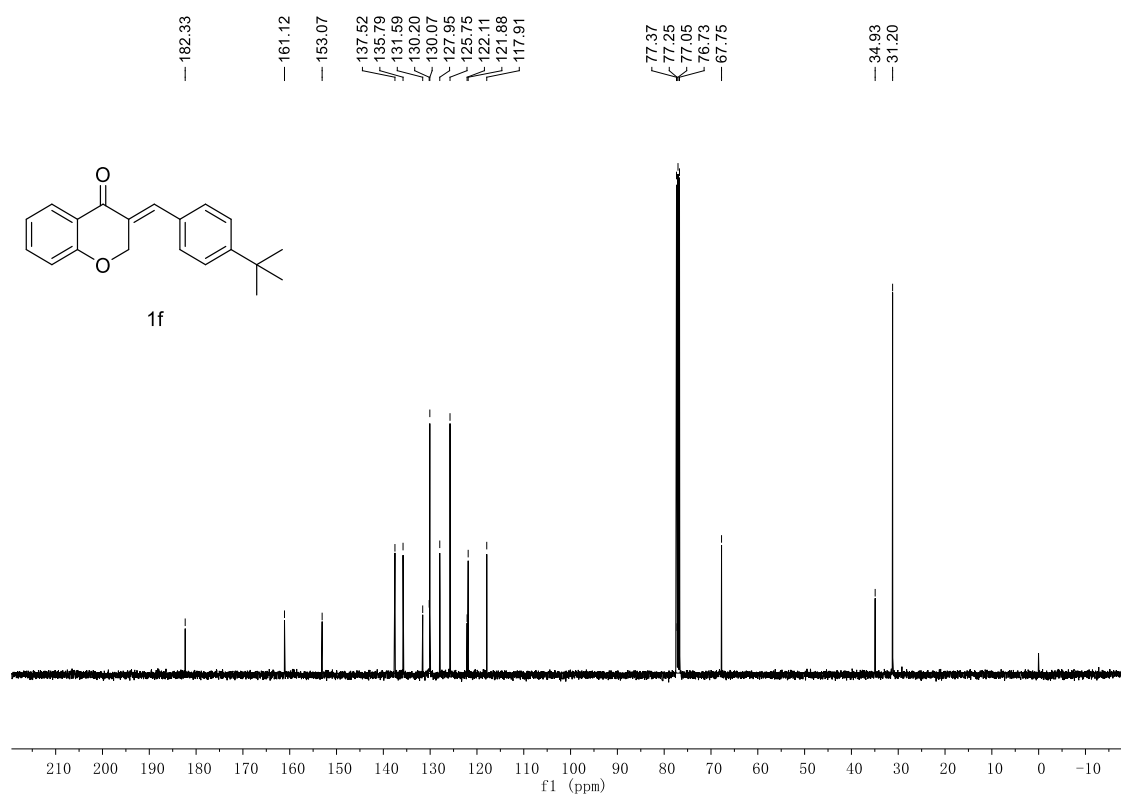
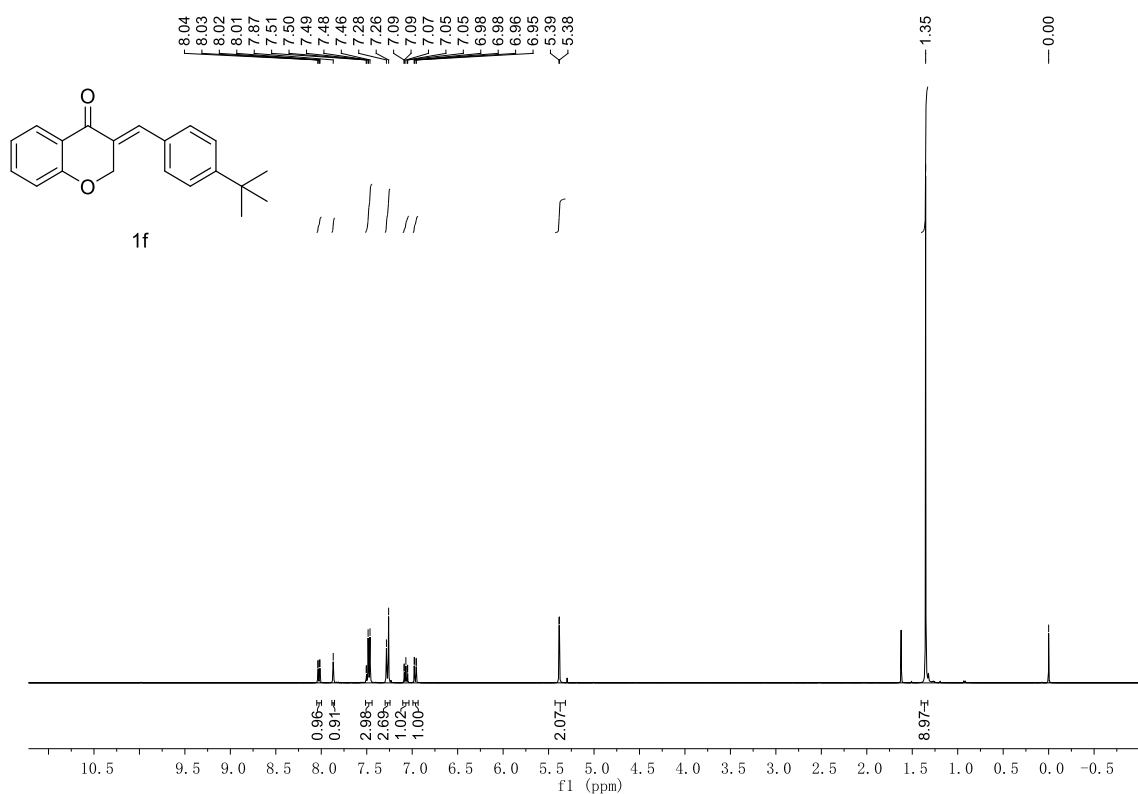
¹H and ¹³C-NMR of 1d



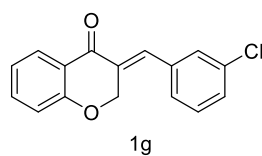
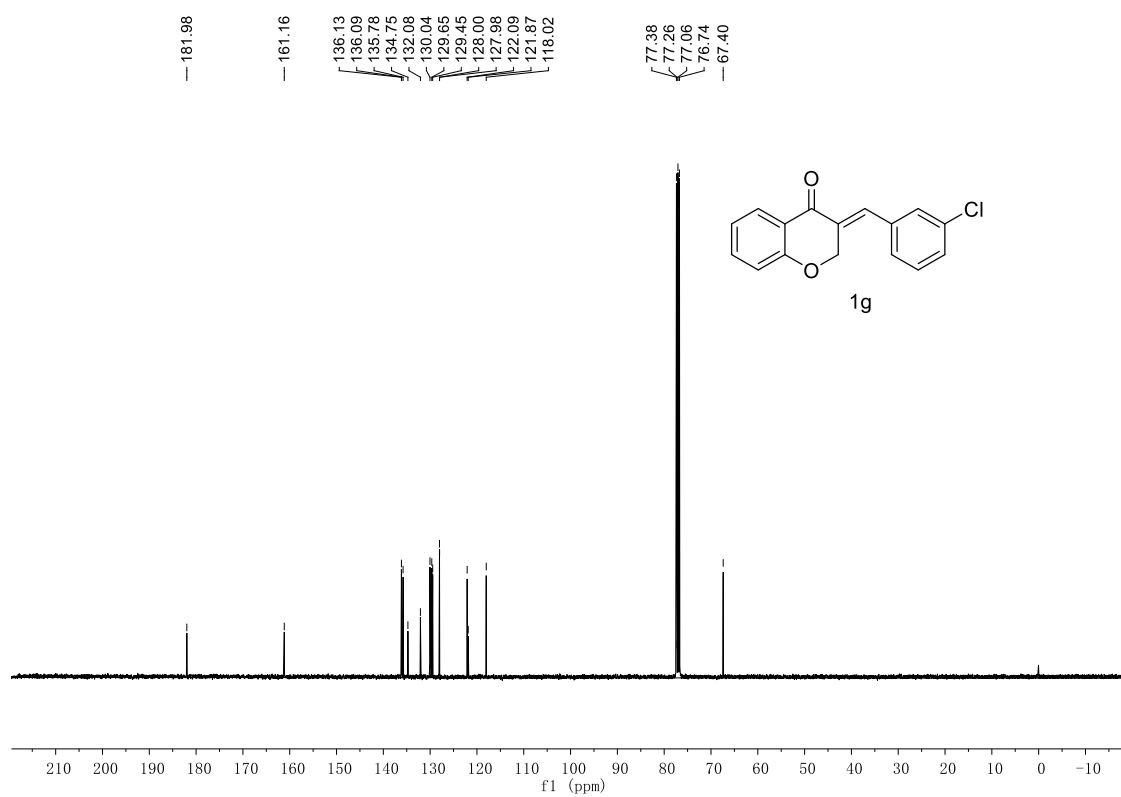
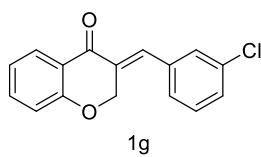
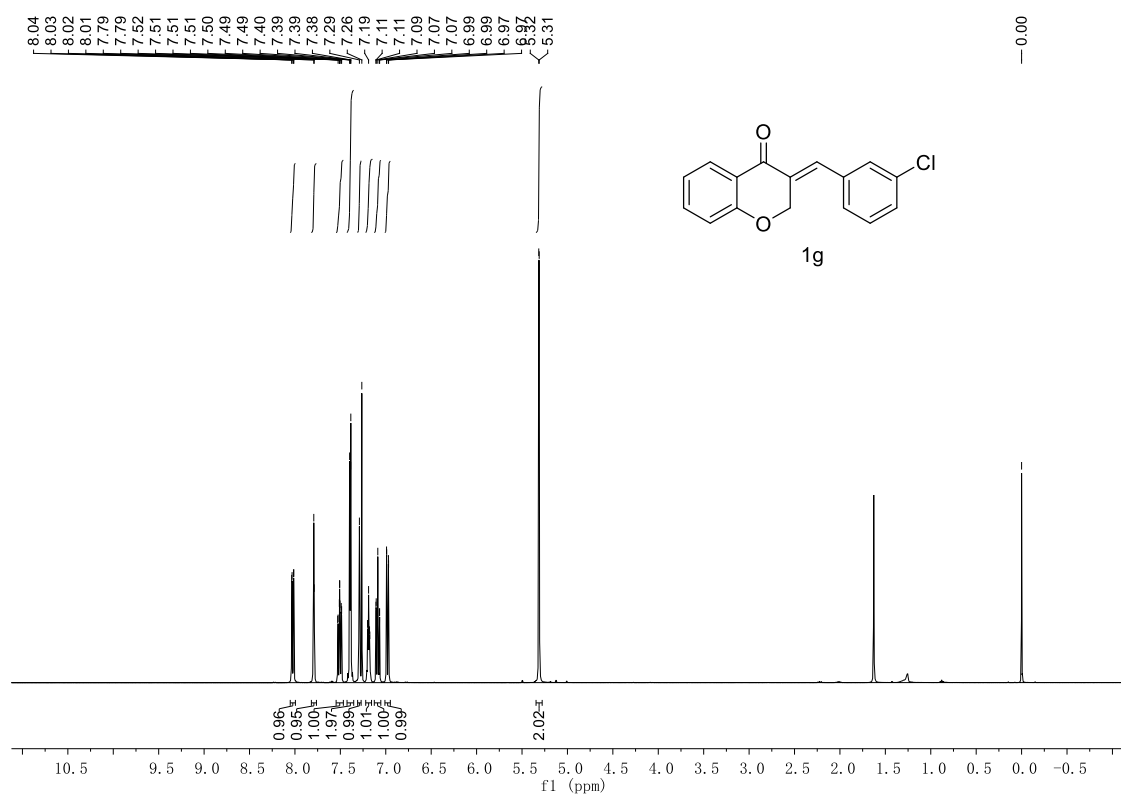
¹H and ¹³C-NMR of 1e



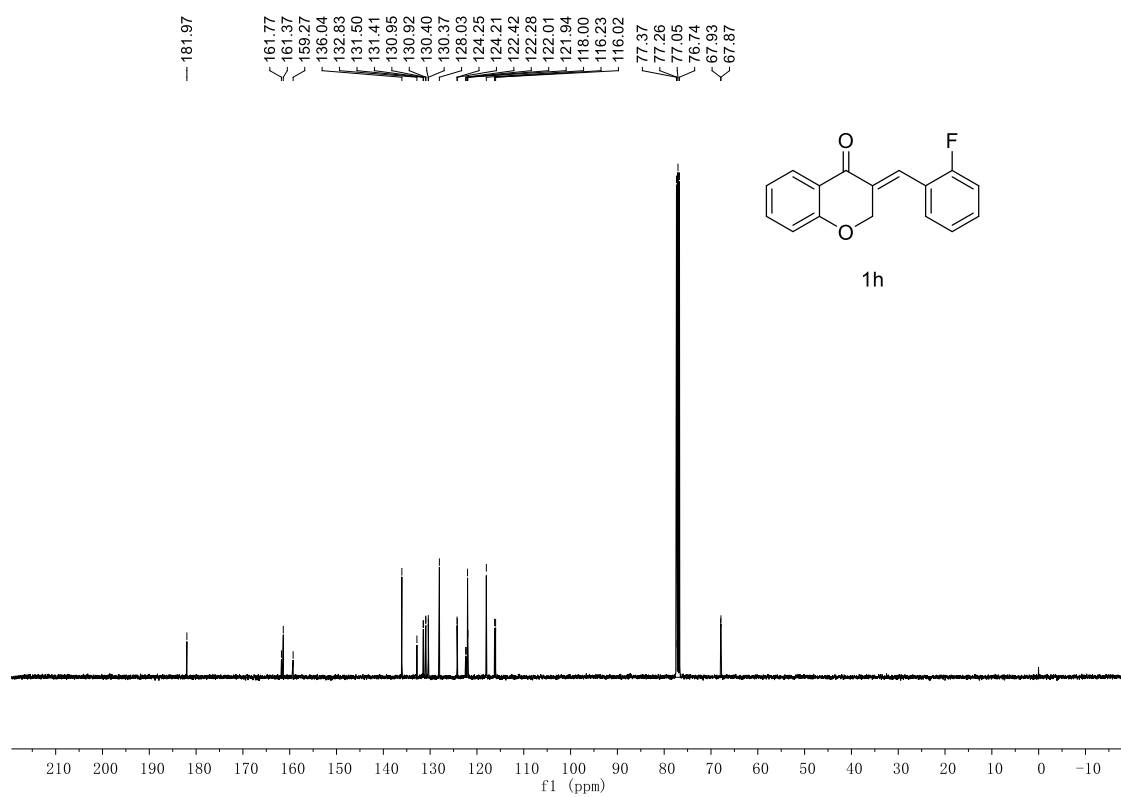
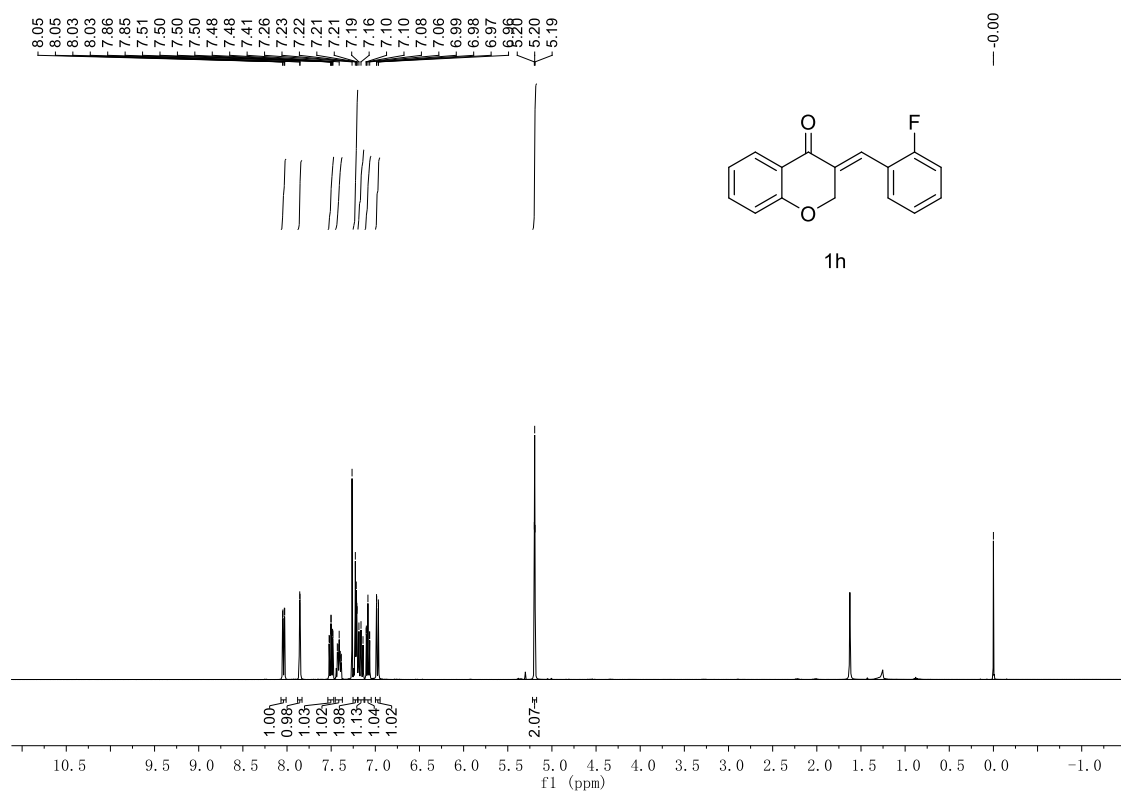
¹H and ¹³C-NMR of 1f



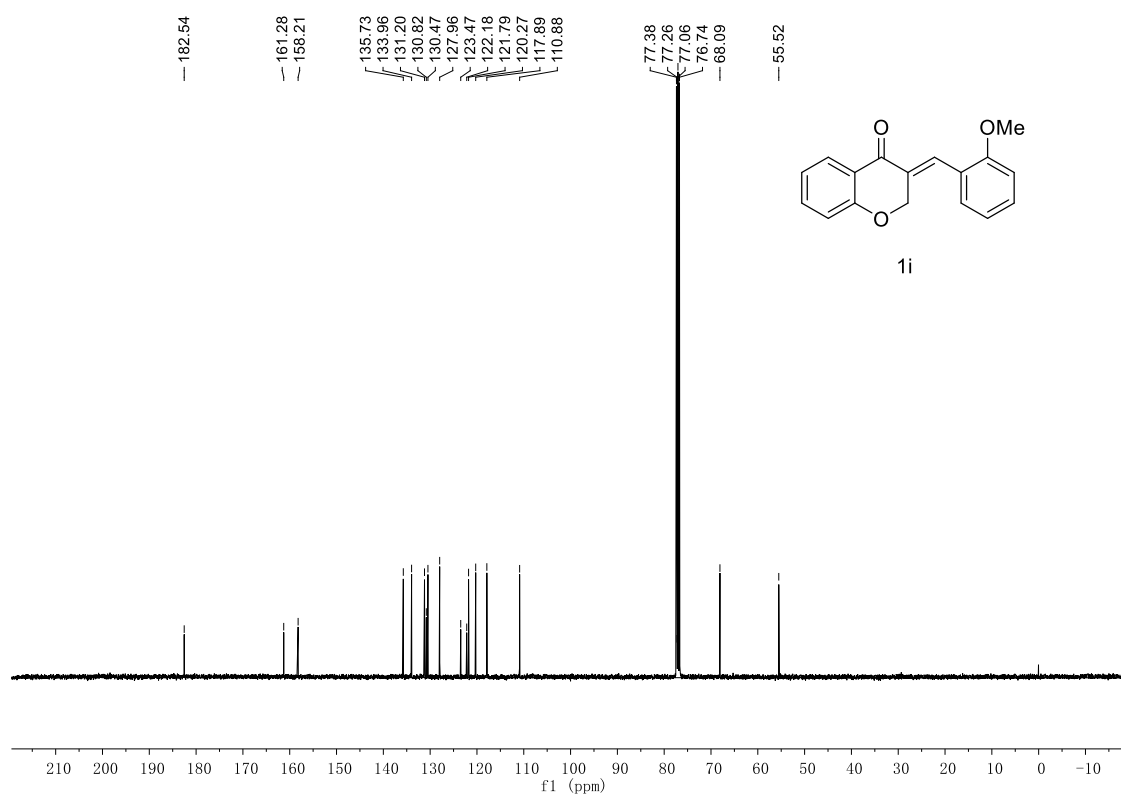
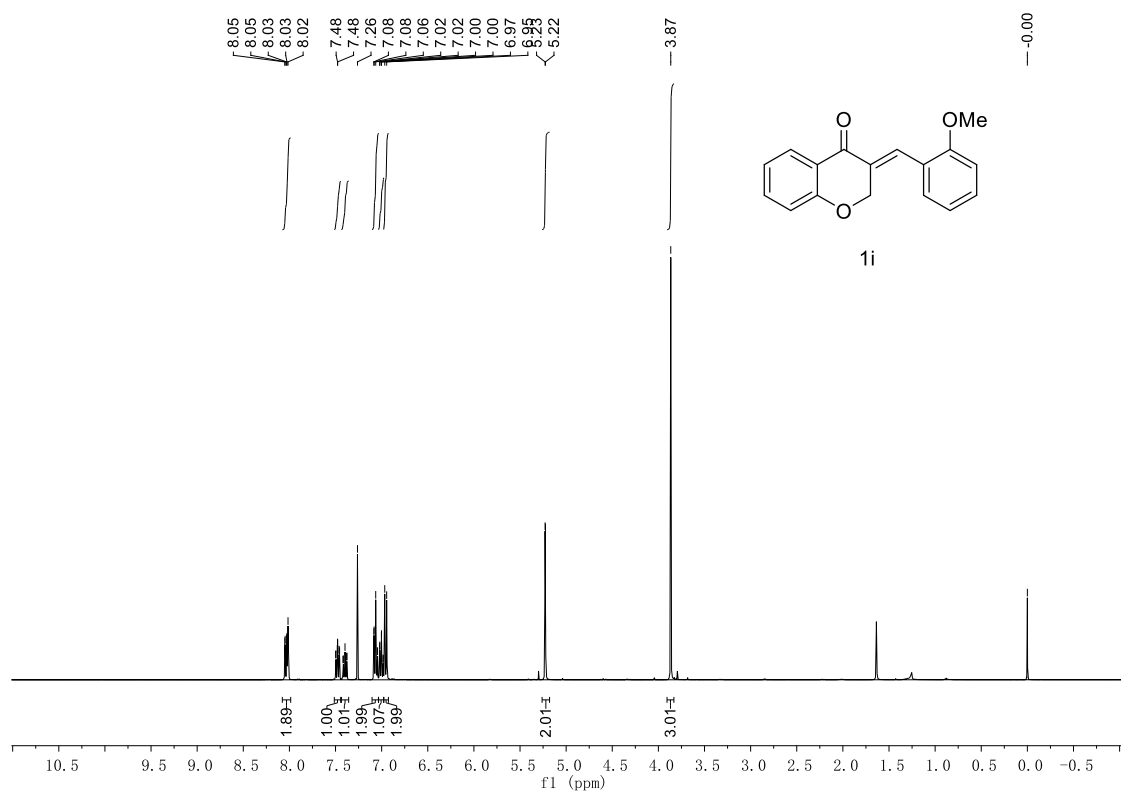
¹H and ¹³C-NMR of 1g



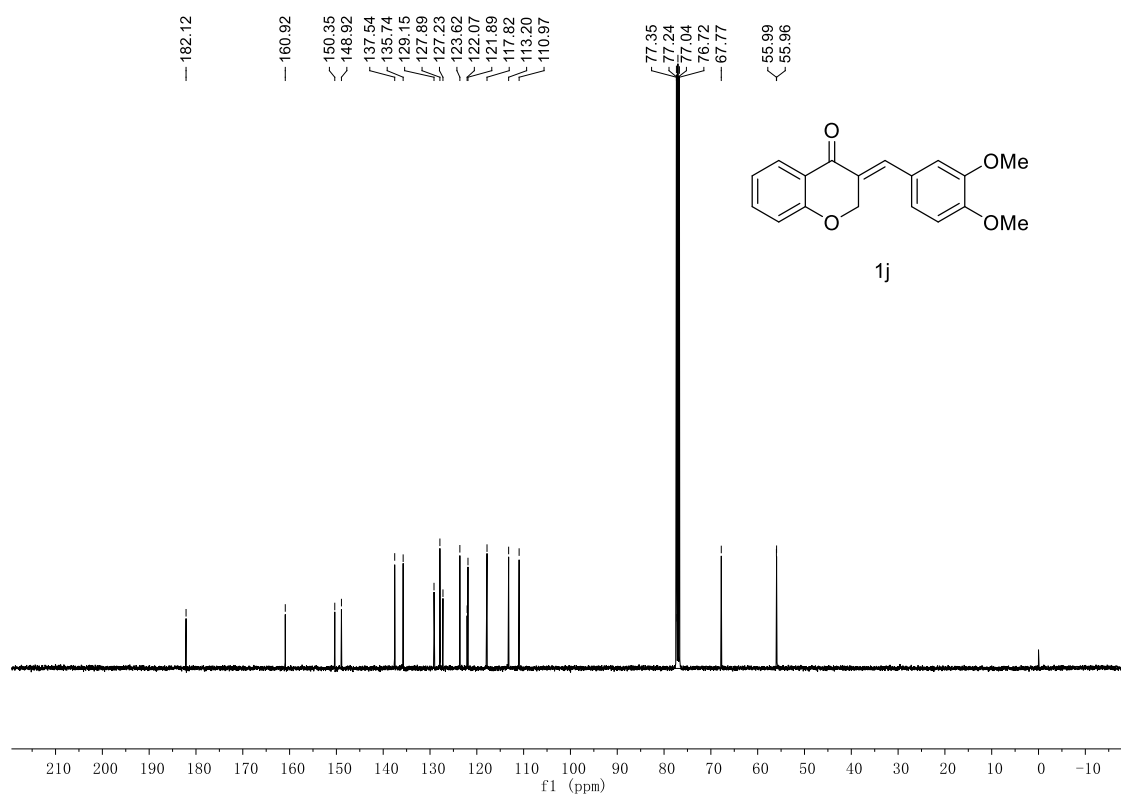
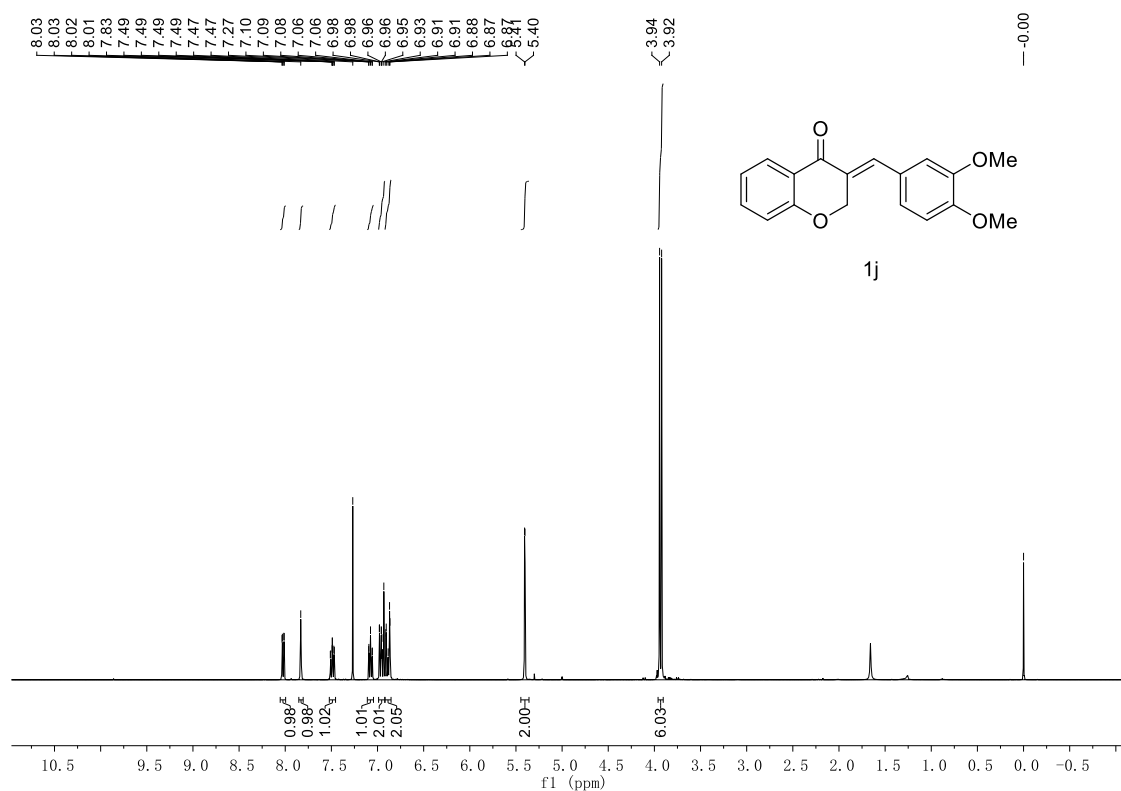
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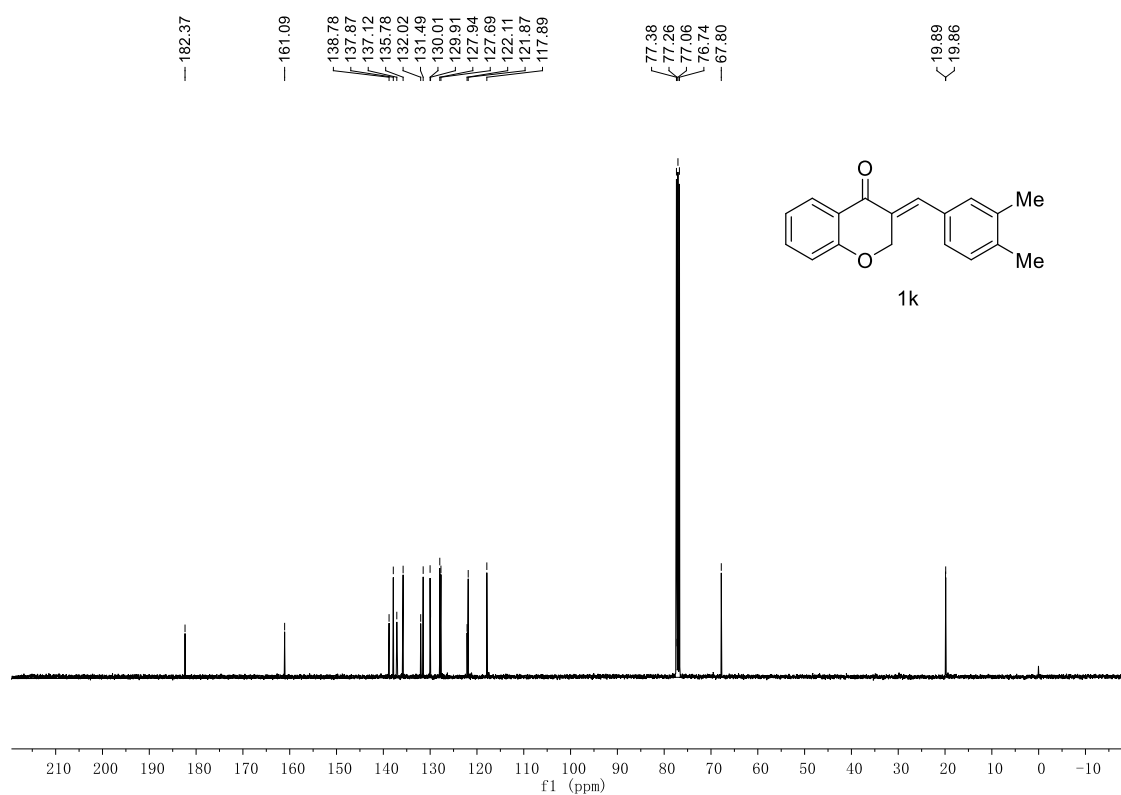
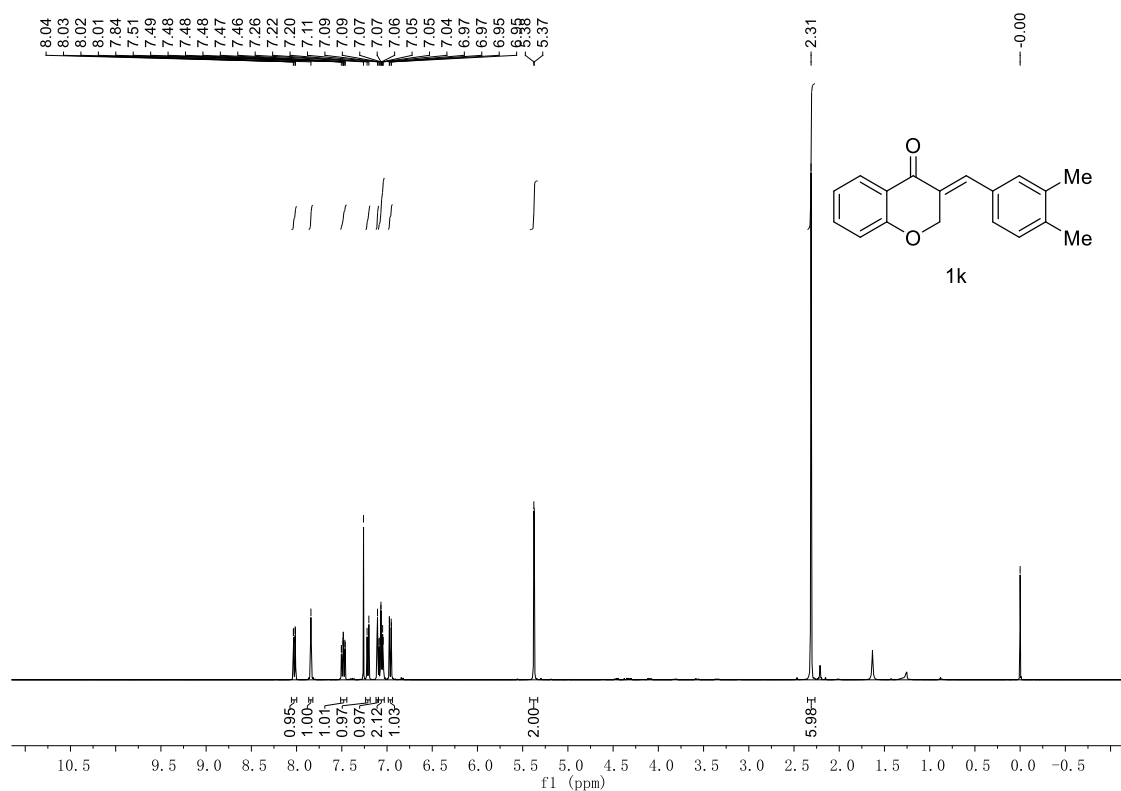
¹H and ¹³C-NMR of 1i



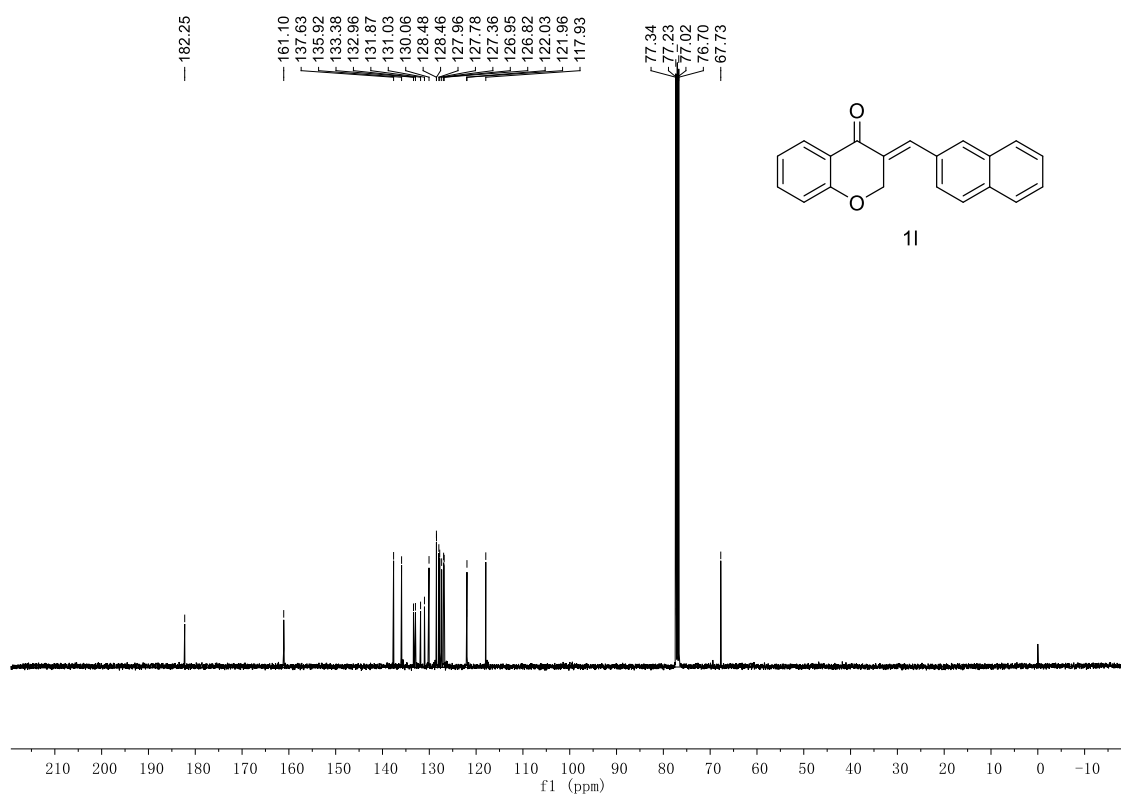
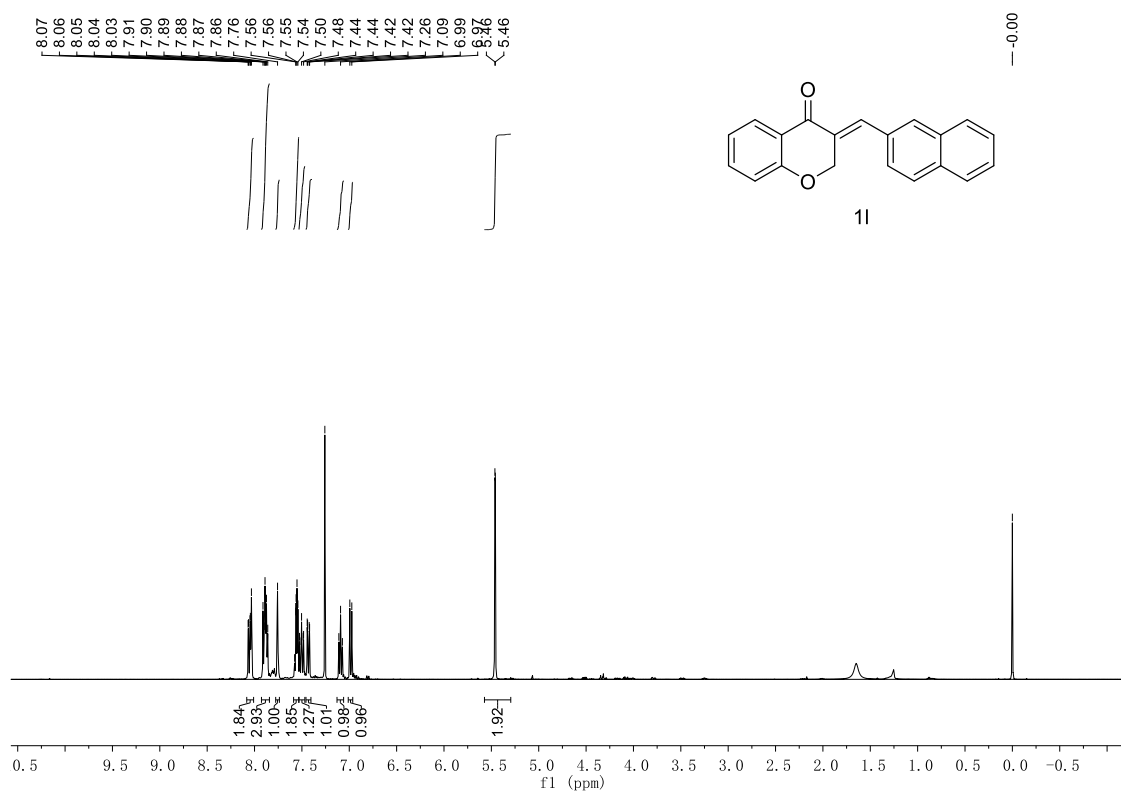
¹H and ¹³C-NMR of 1j



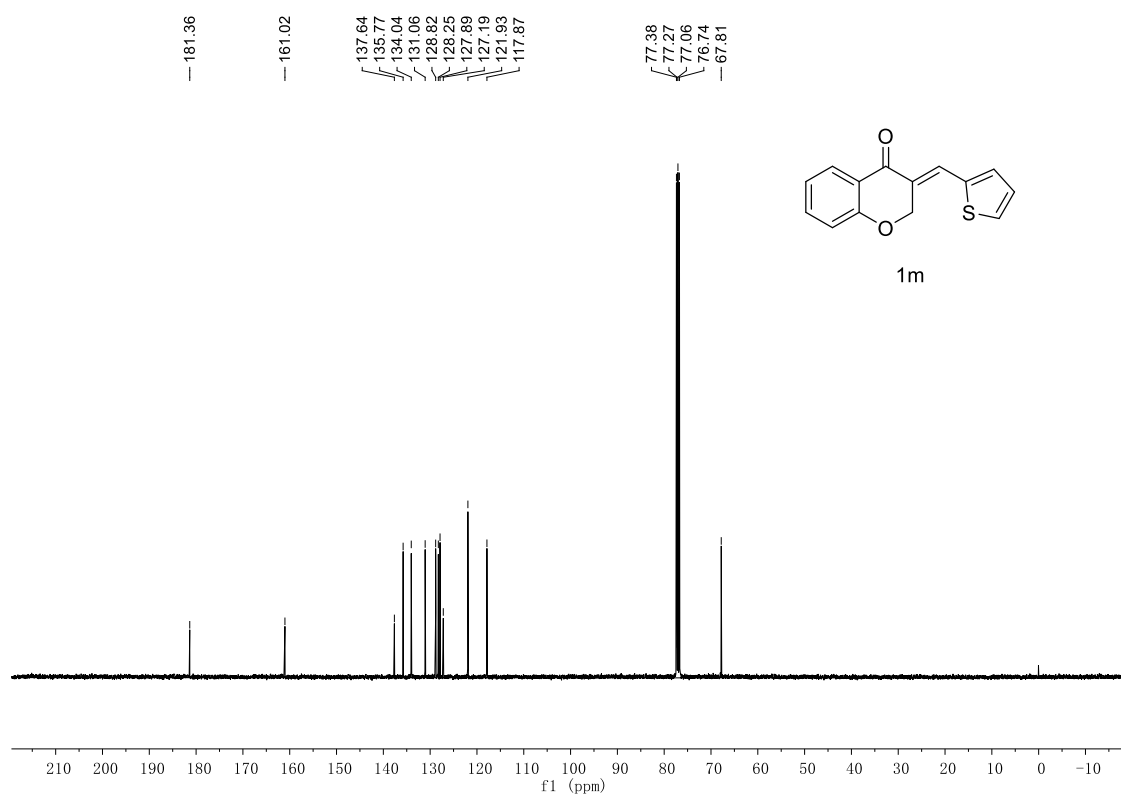
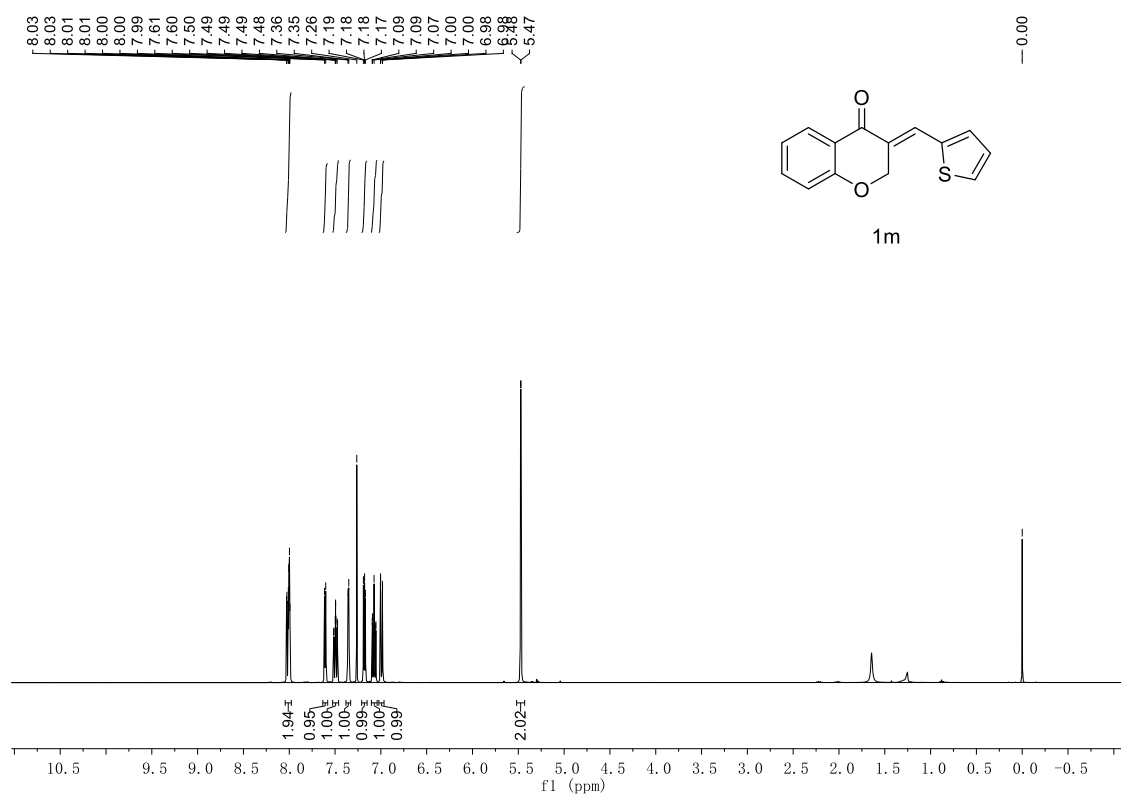
¹H and ¹³C-NMR of 1k



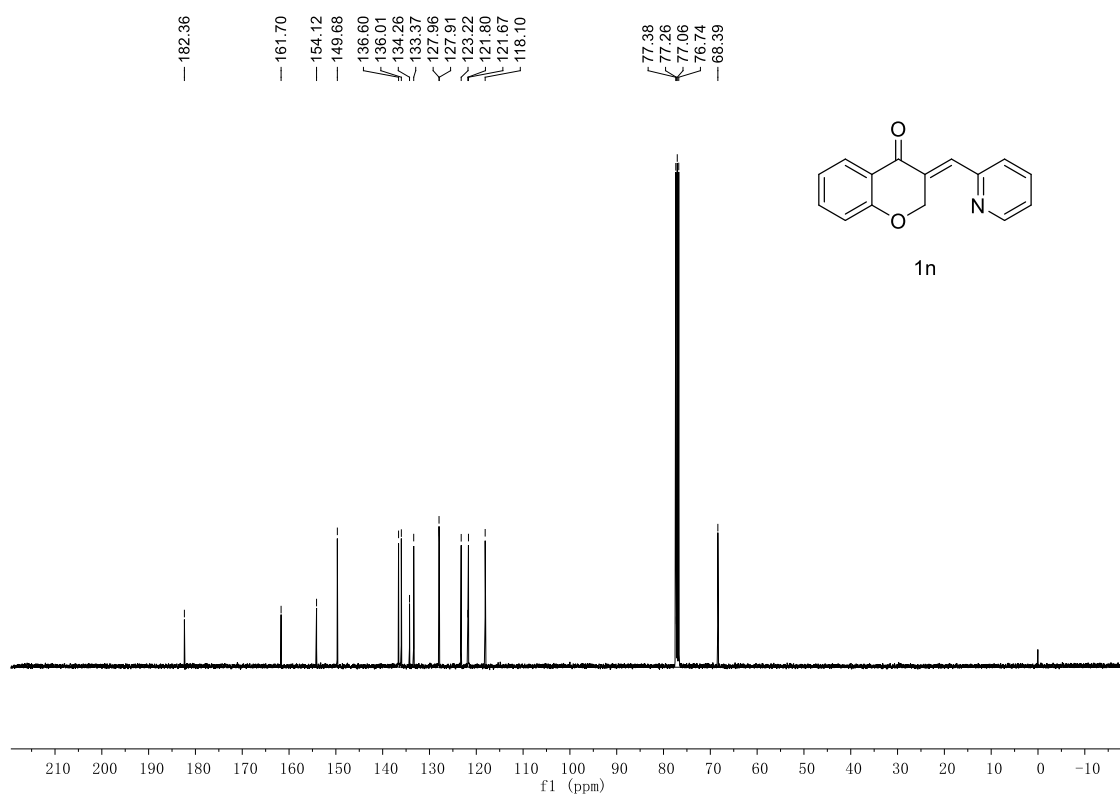
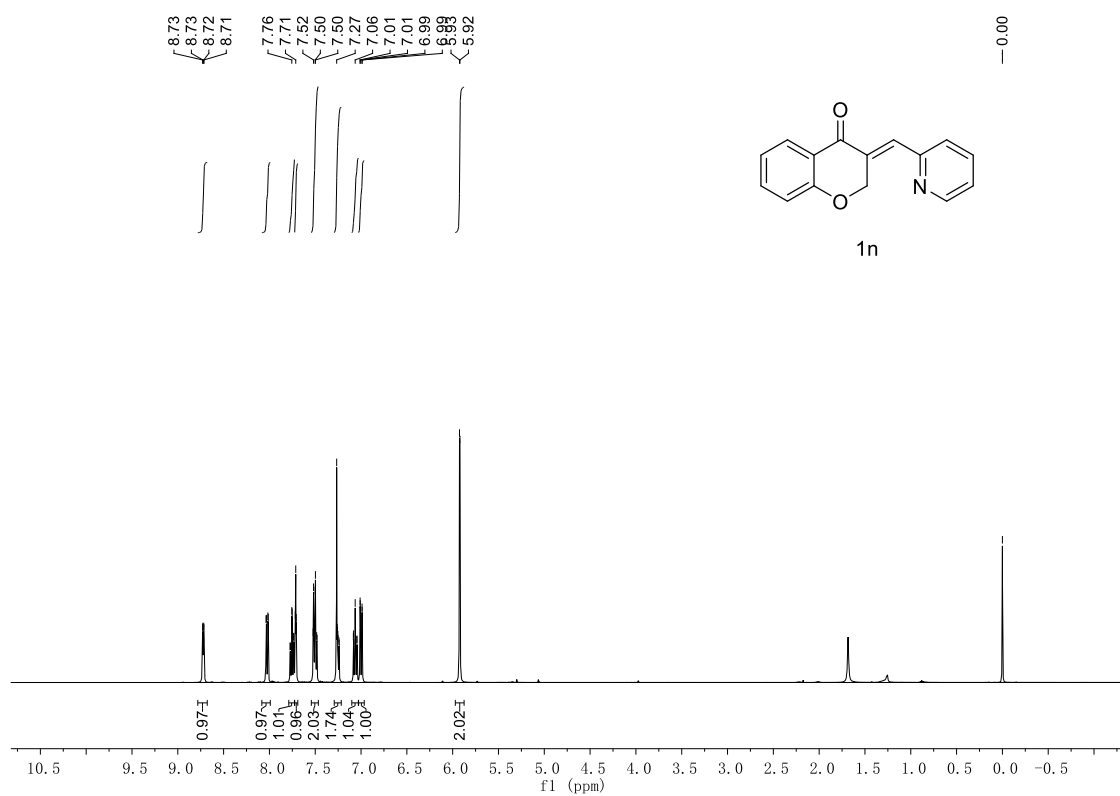
^1H and ^{13}C -NMR of 11



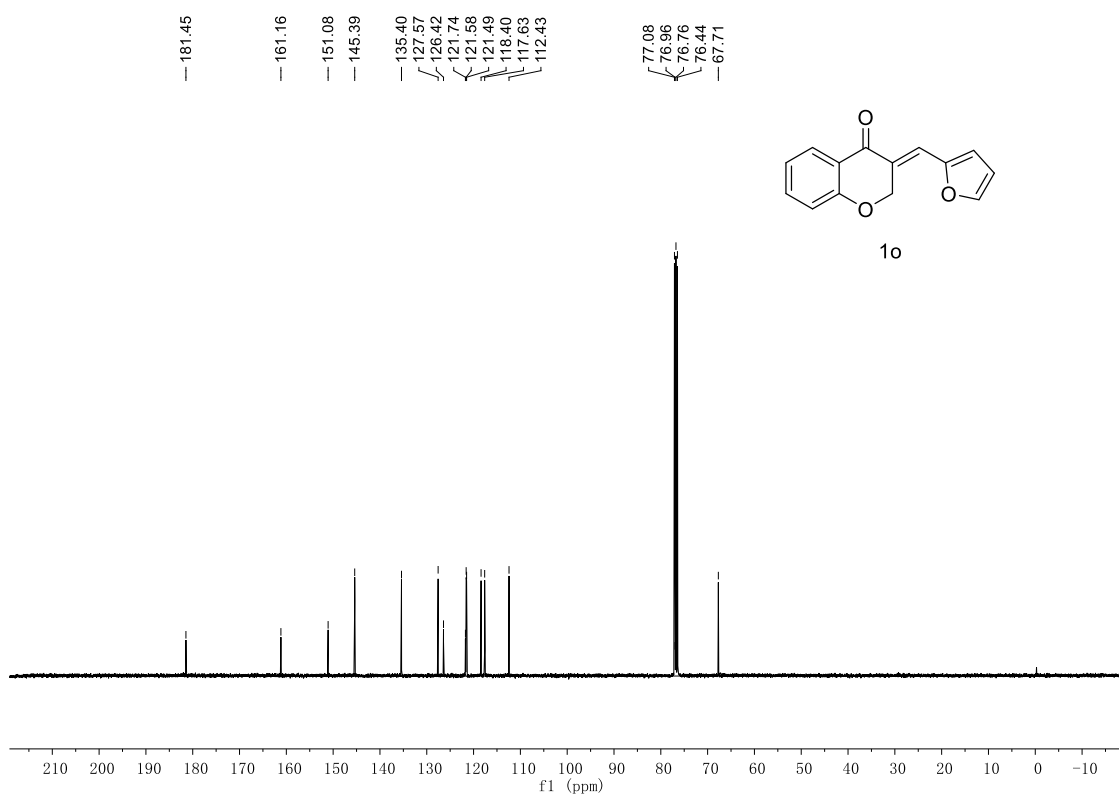
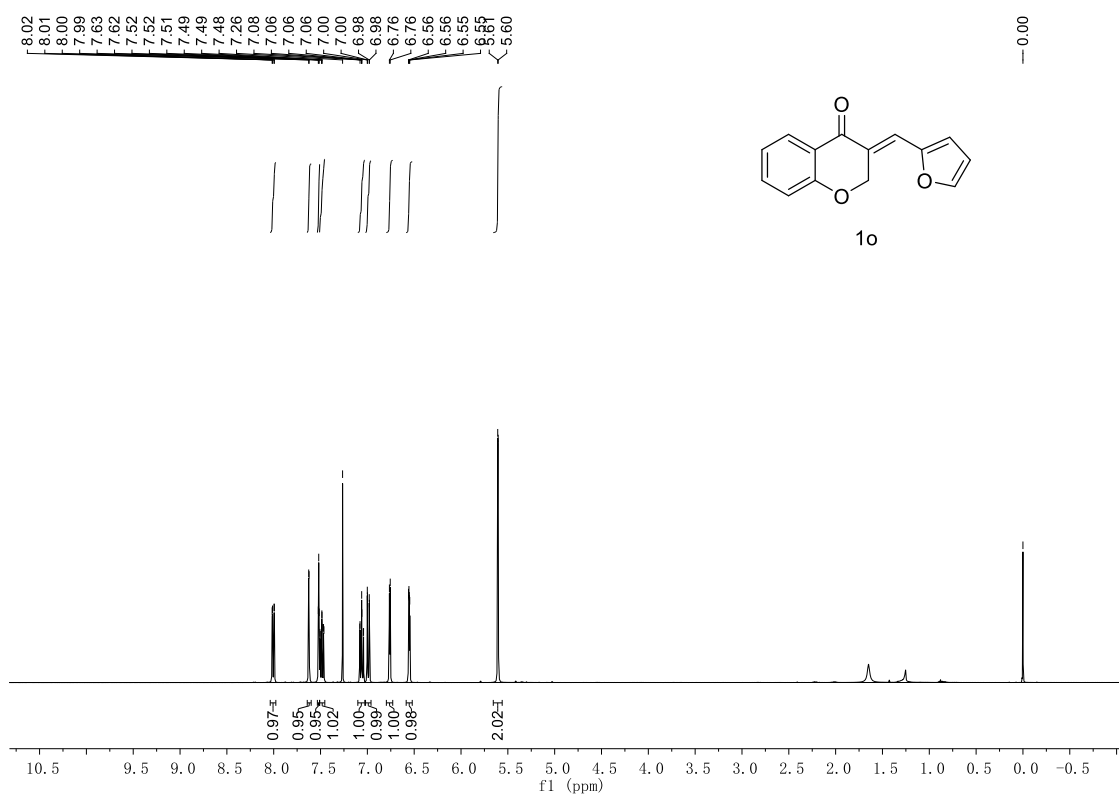
¹H and ¹³C-NMR of 1m



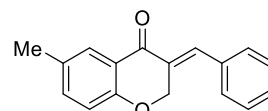
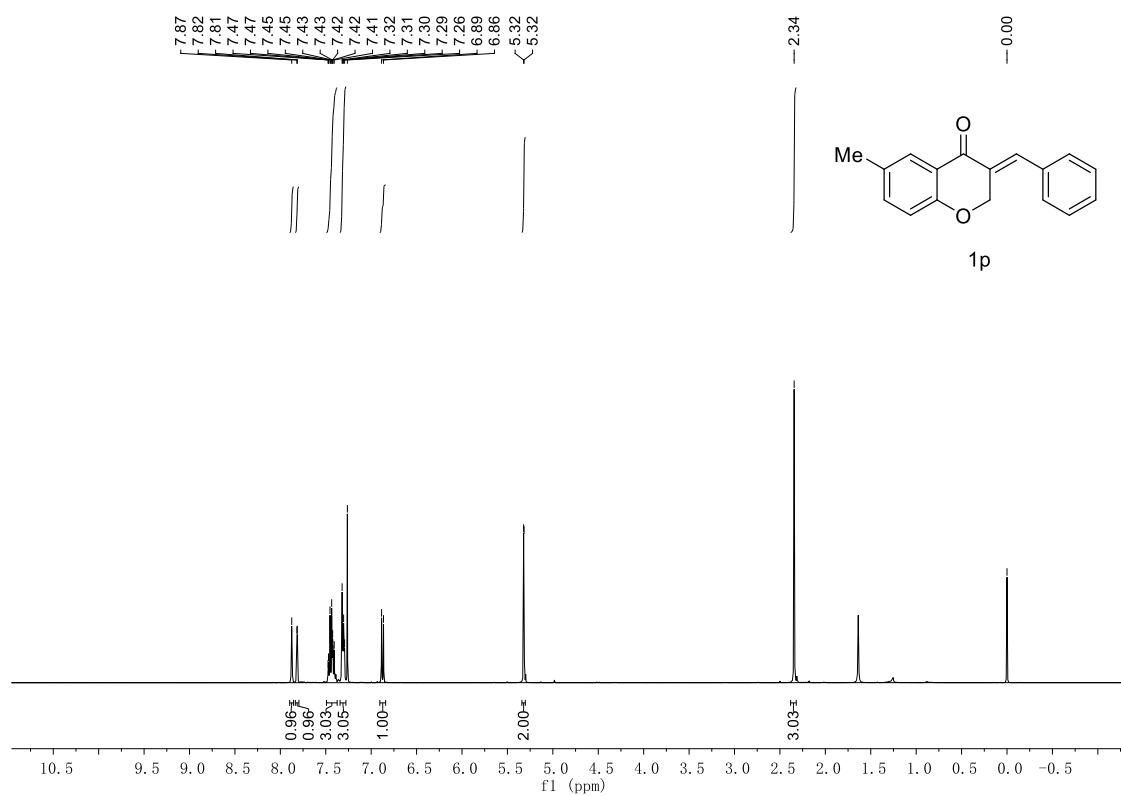
¹H and ¹³C-NMR of 1n



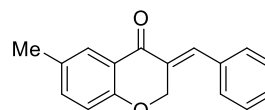
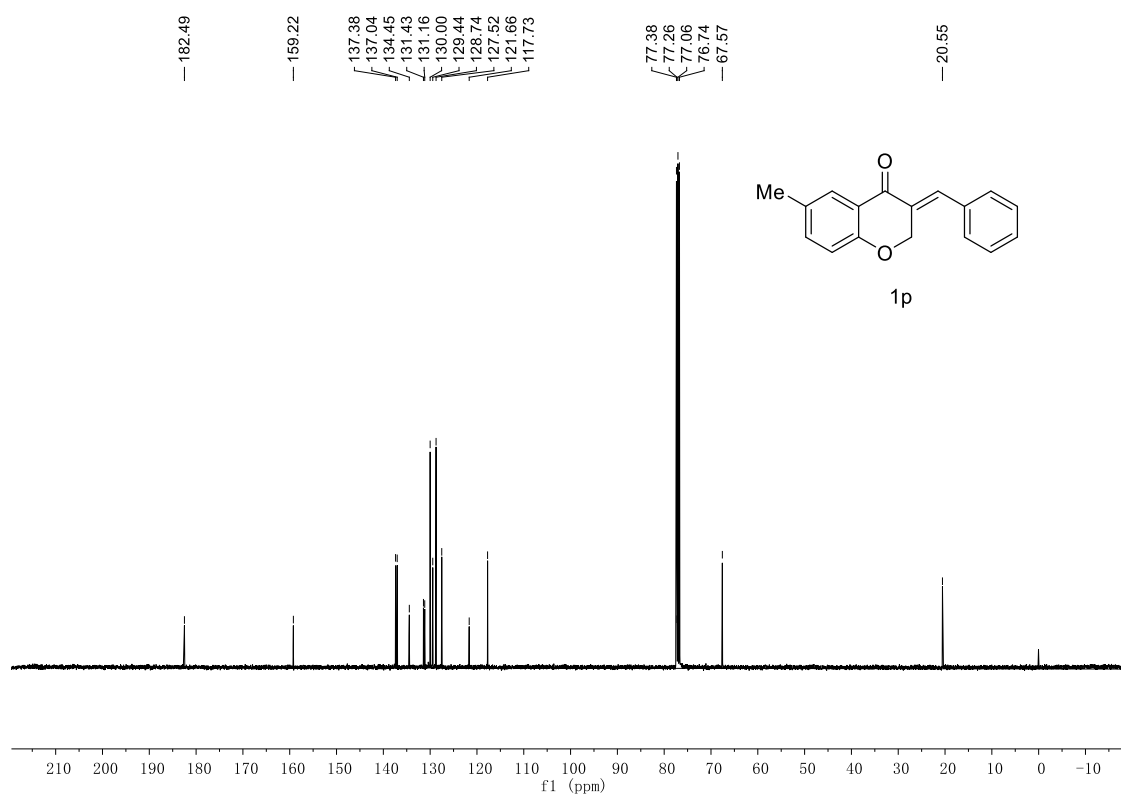
¹H and ¹³C-NMR of 1o



¹H and ¹³C-NMR of 1p

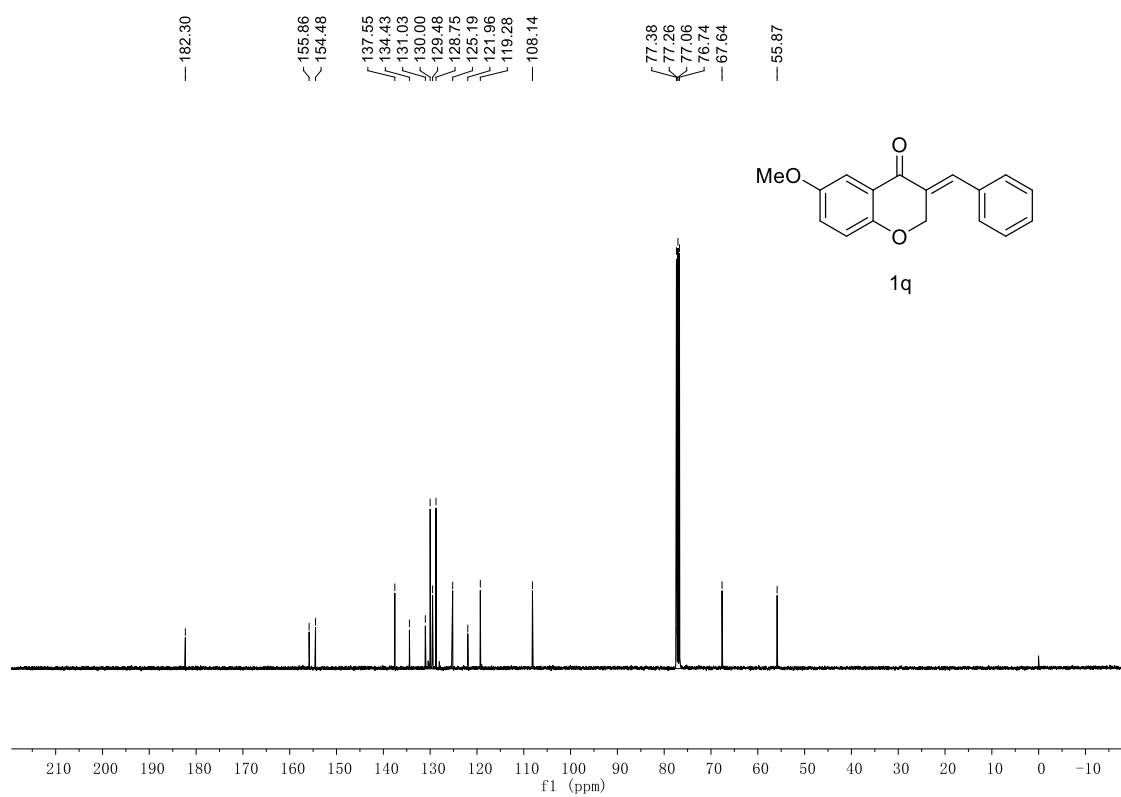
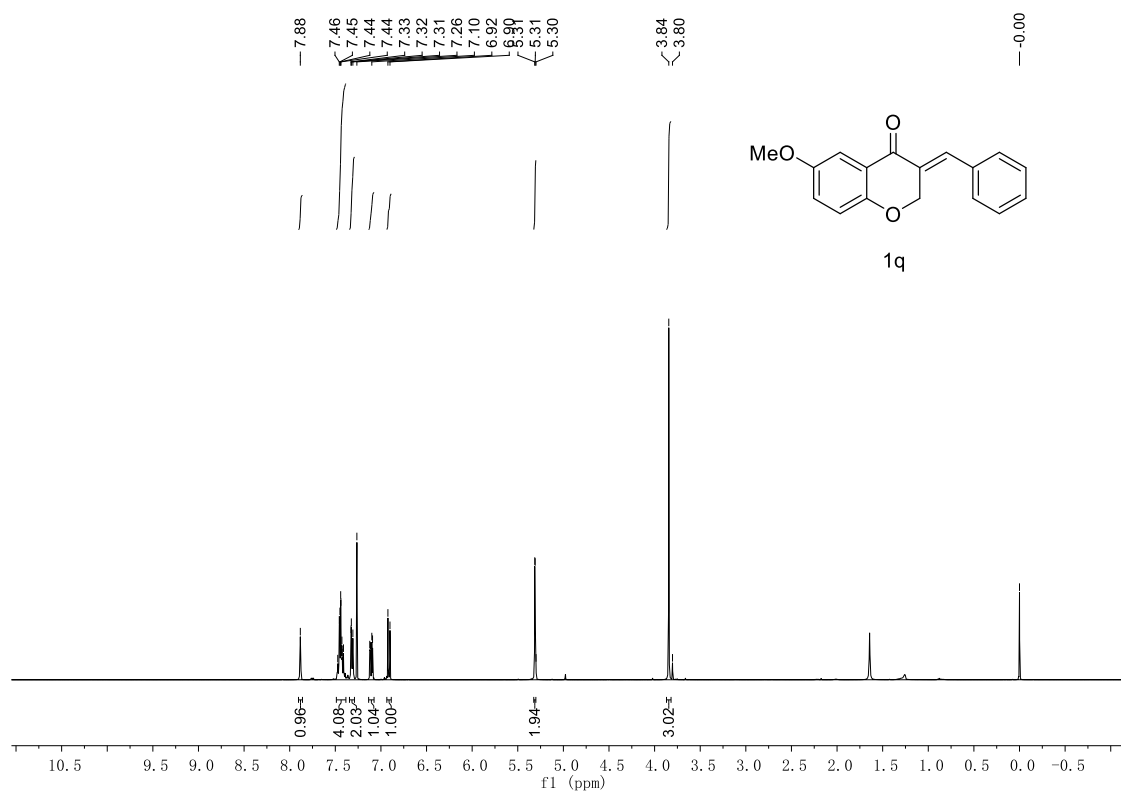


1p

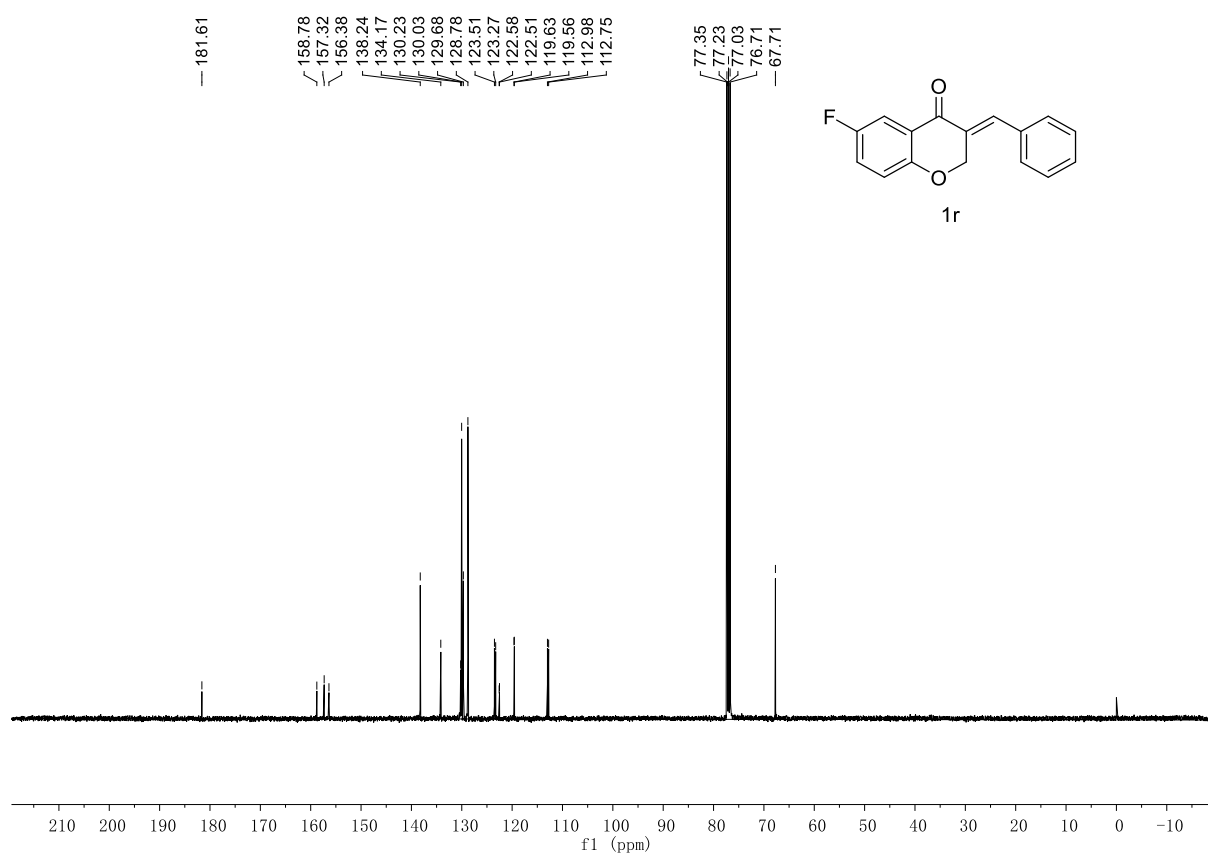
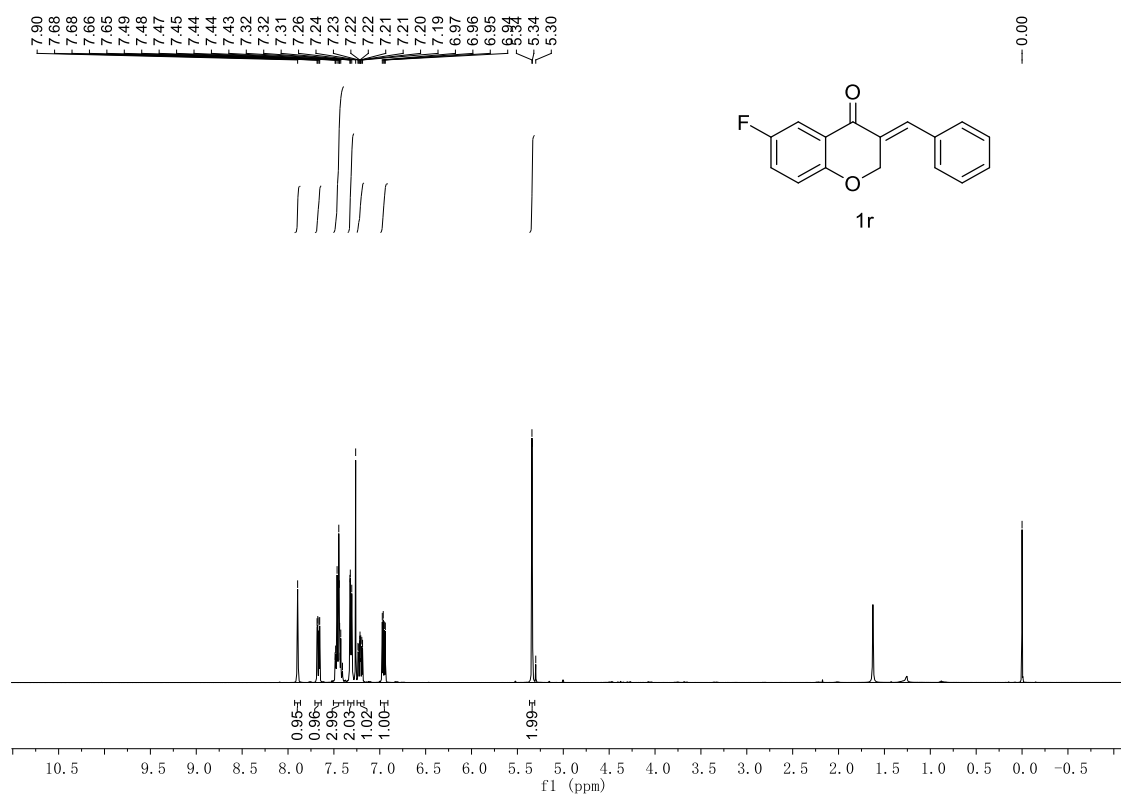


1p

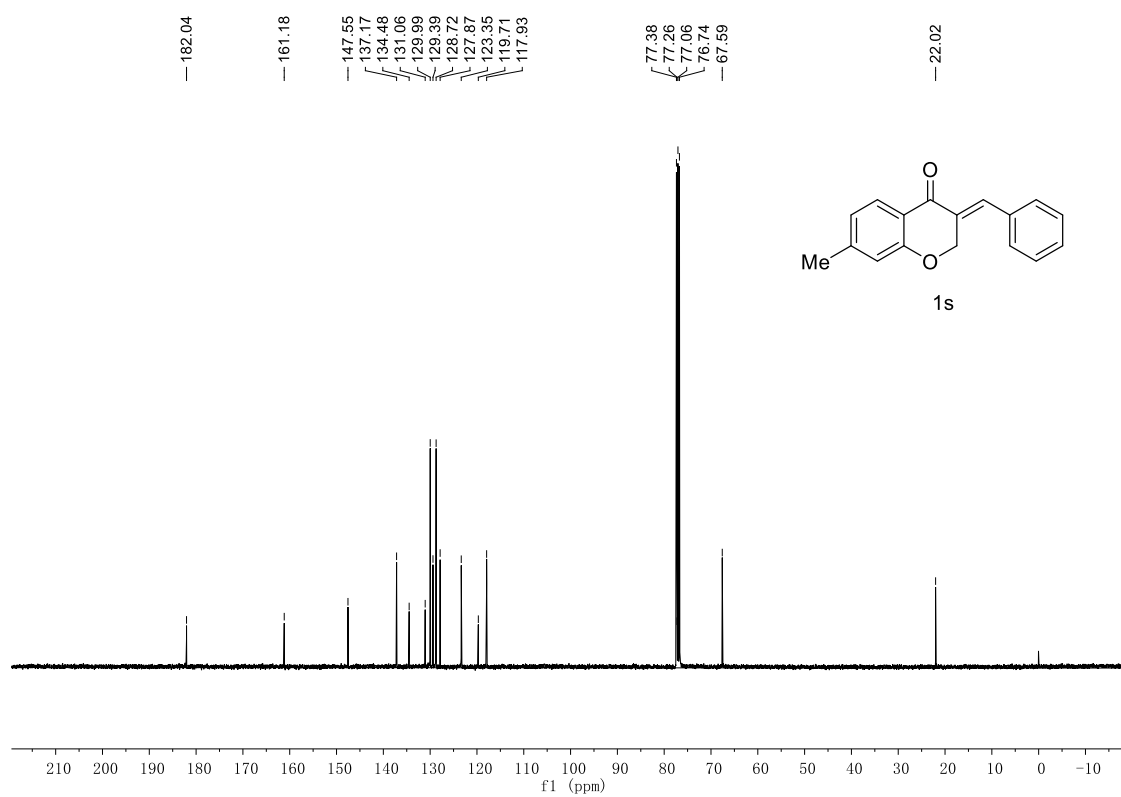
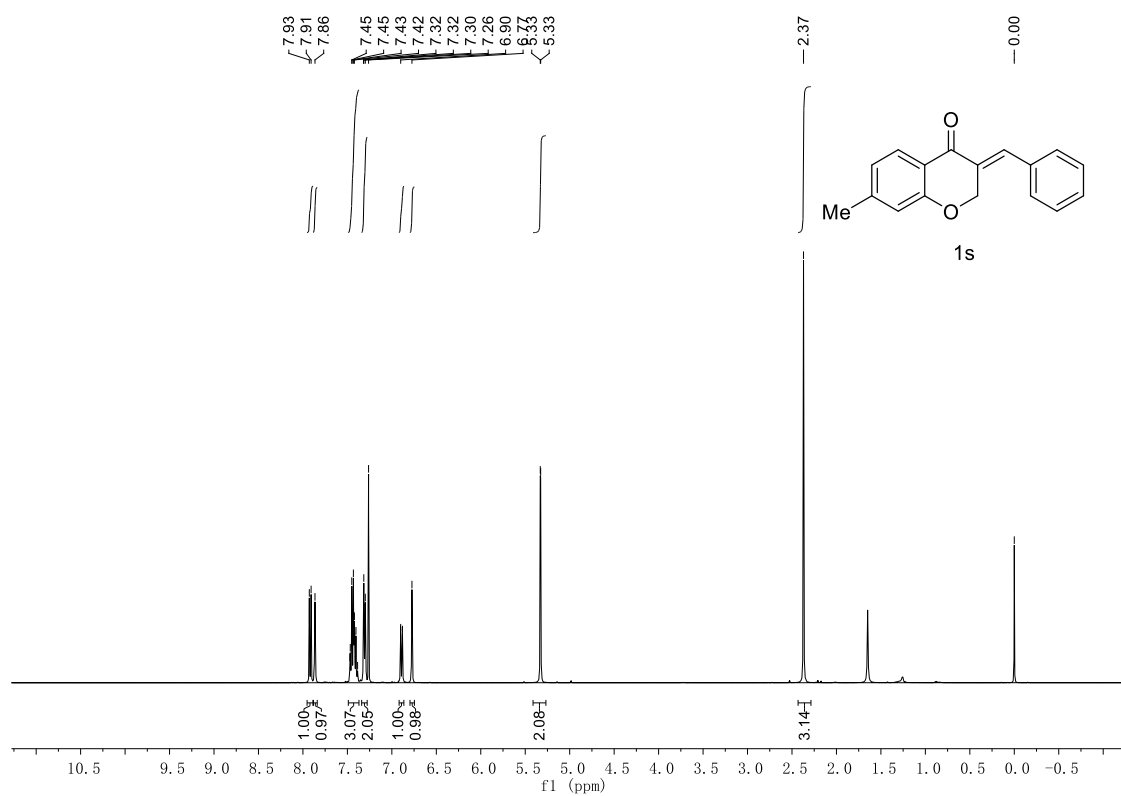
¹H and ¹³C-NMR of 1q



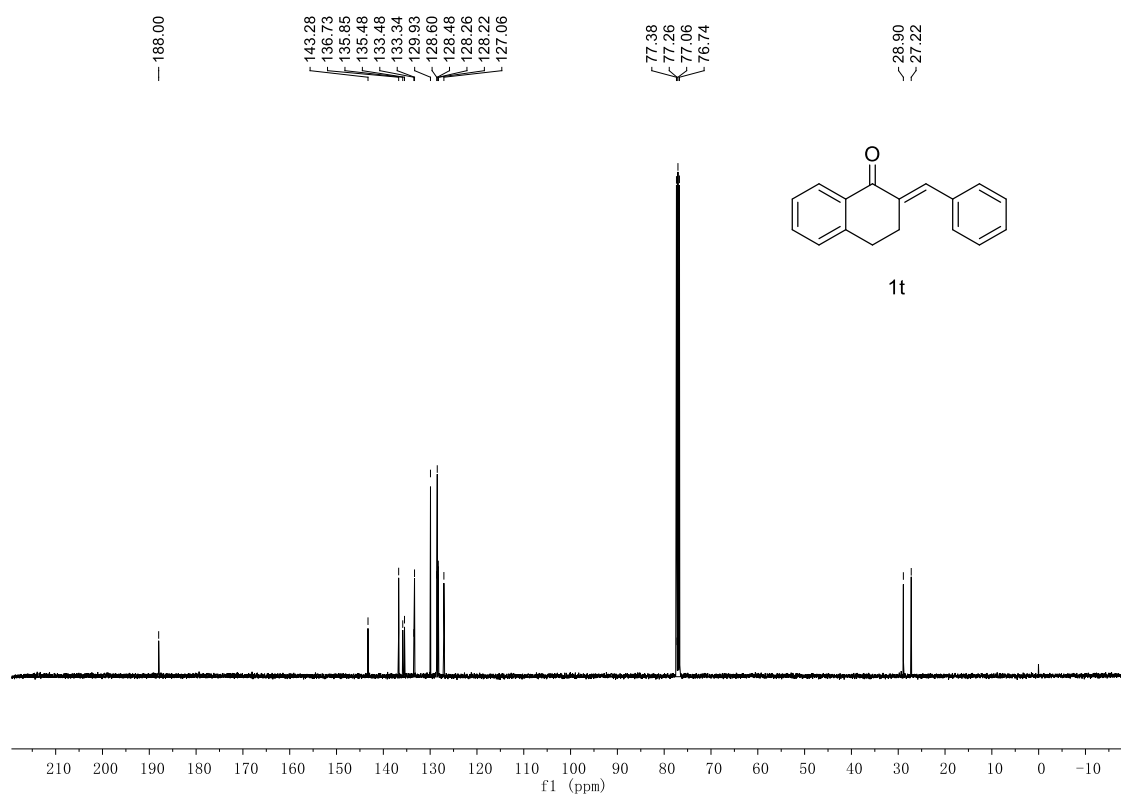
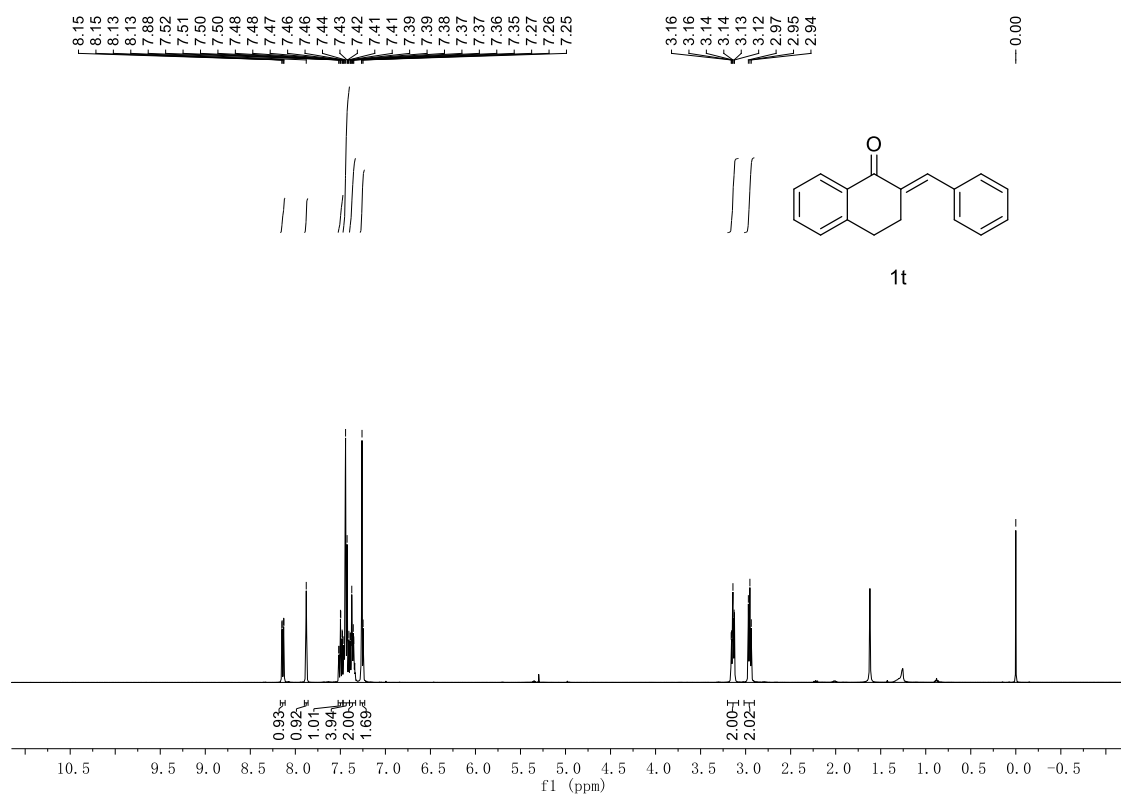
¹H and ¹³C-NMR of 1r



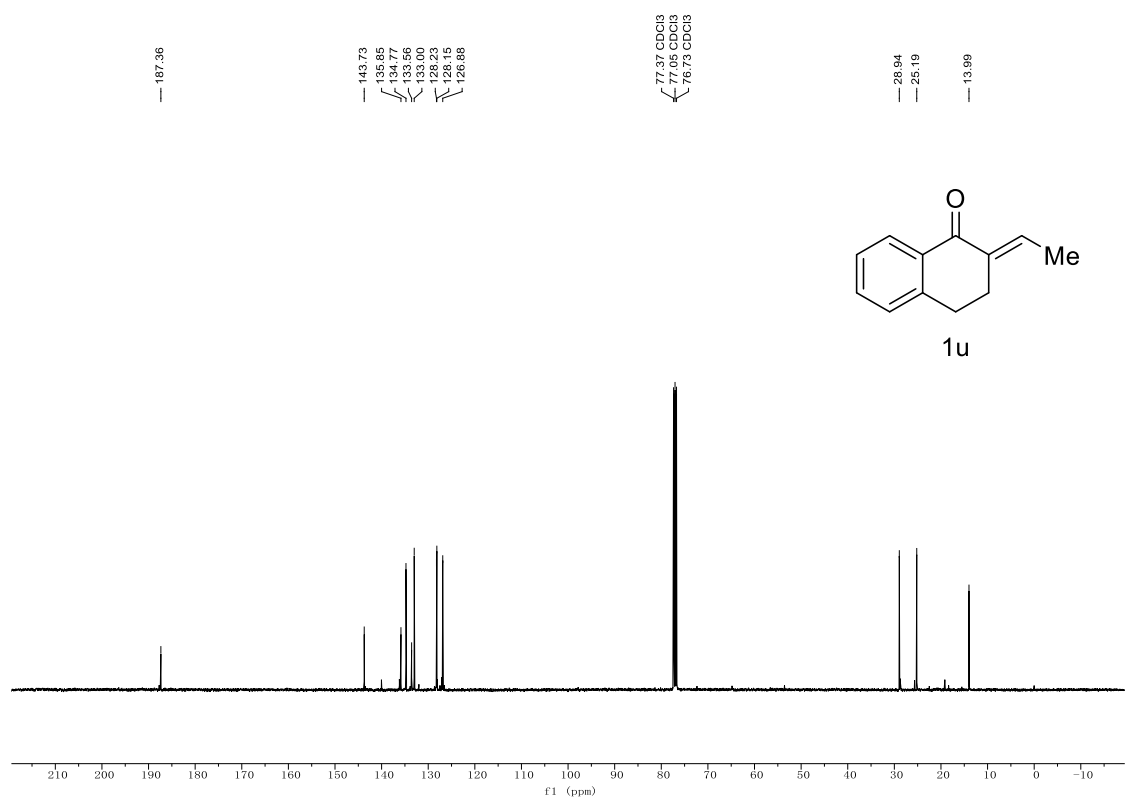
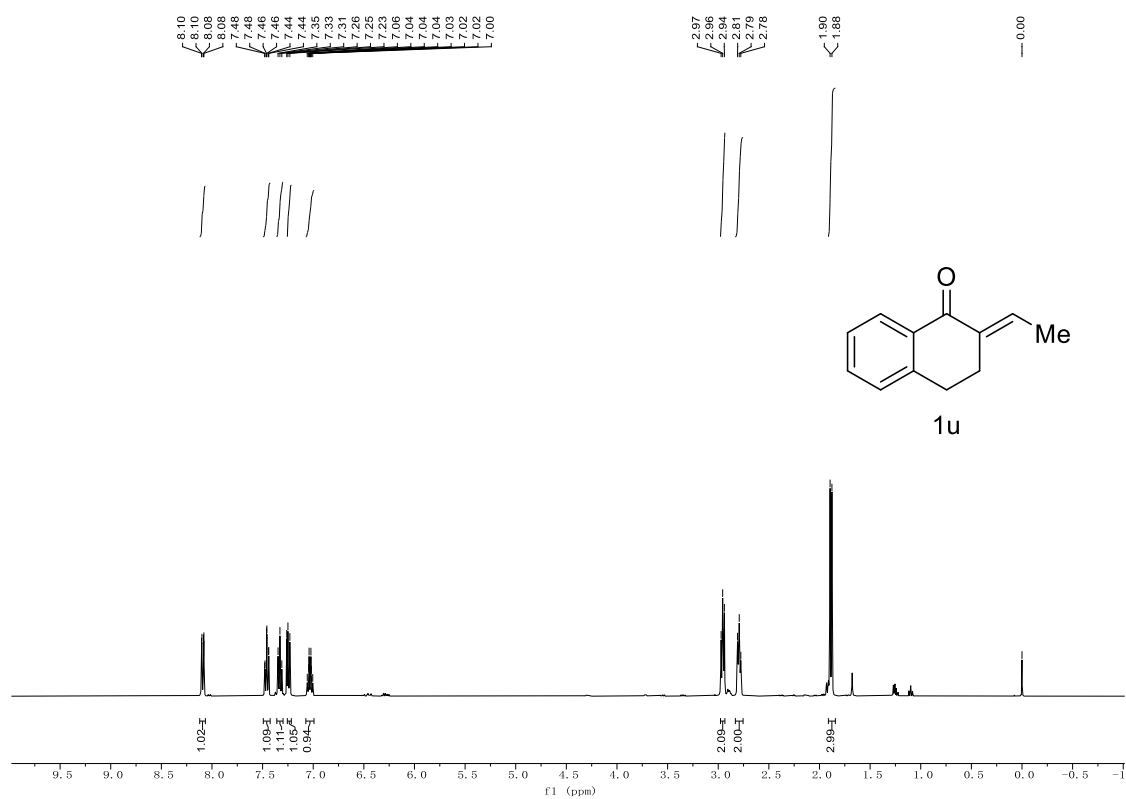
¹H and ¹³C-NMR of 1s



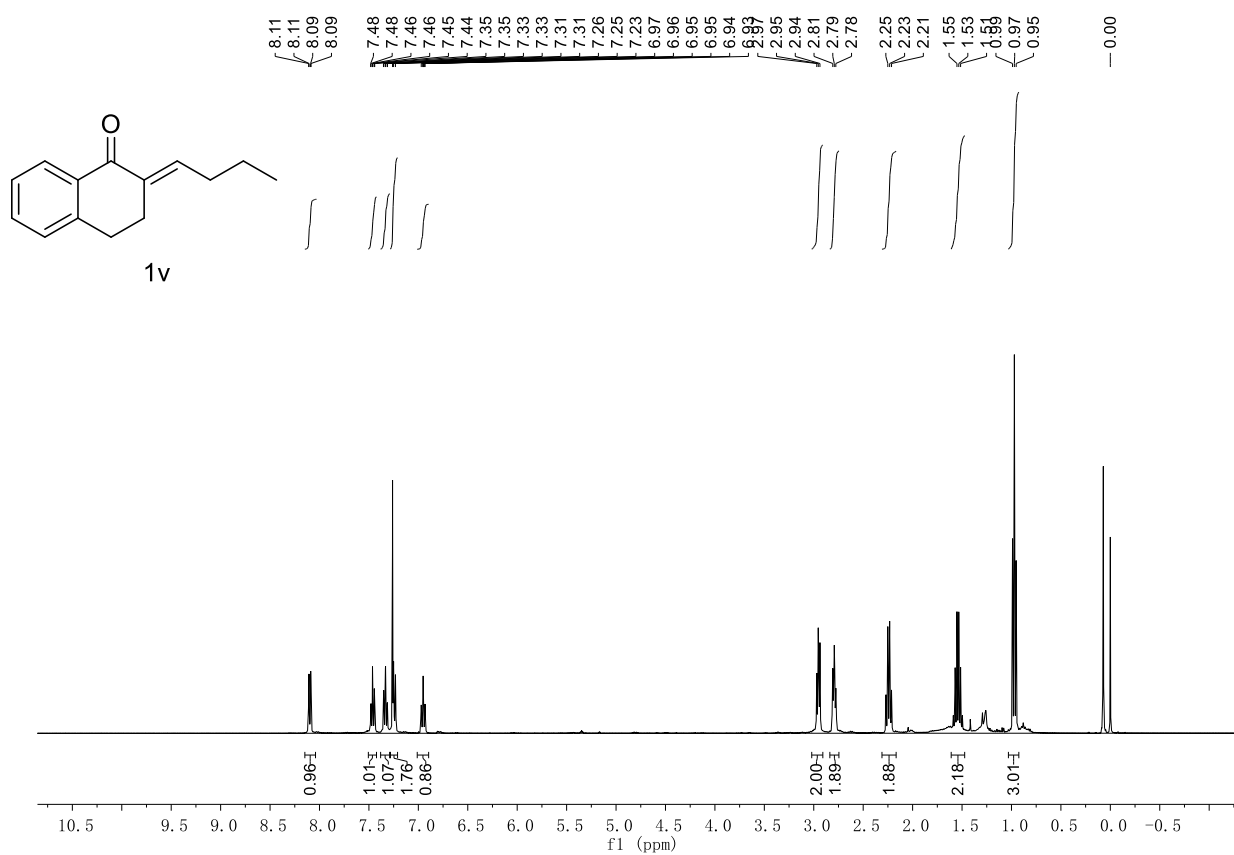
^1H and ^{13}C -NMR of 1t



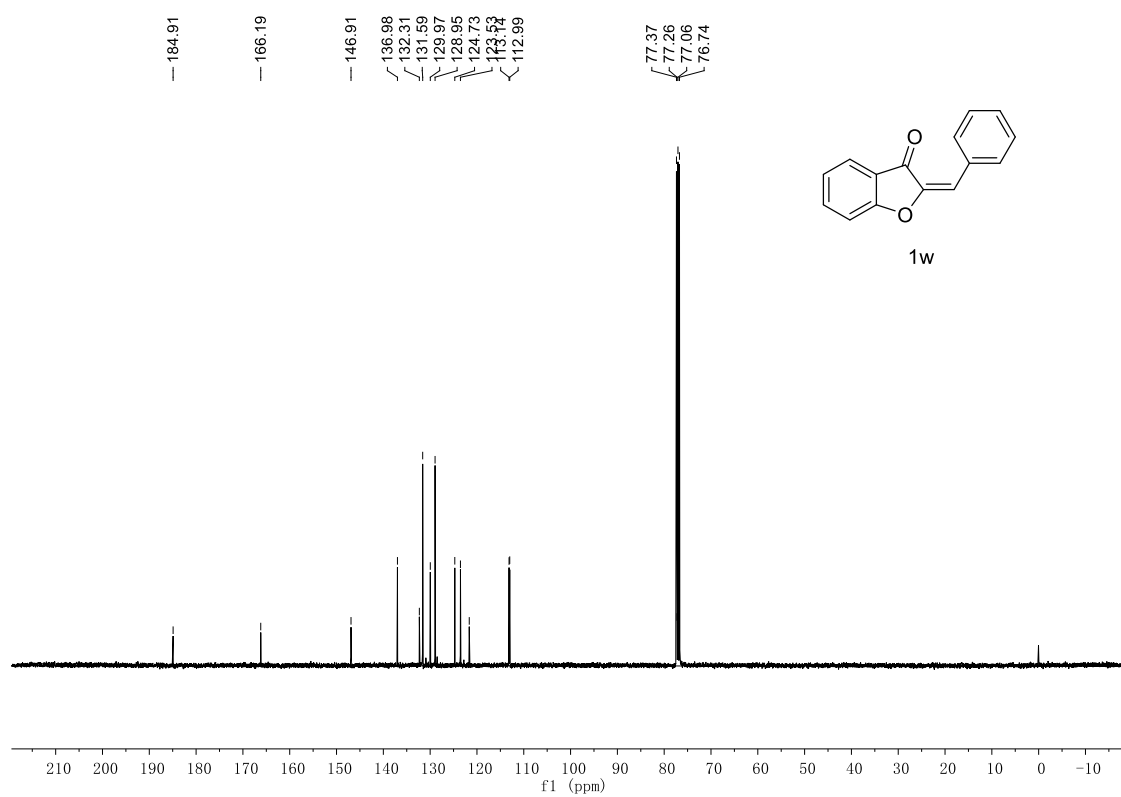
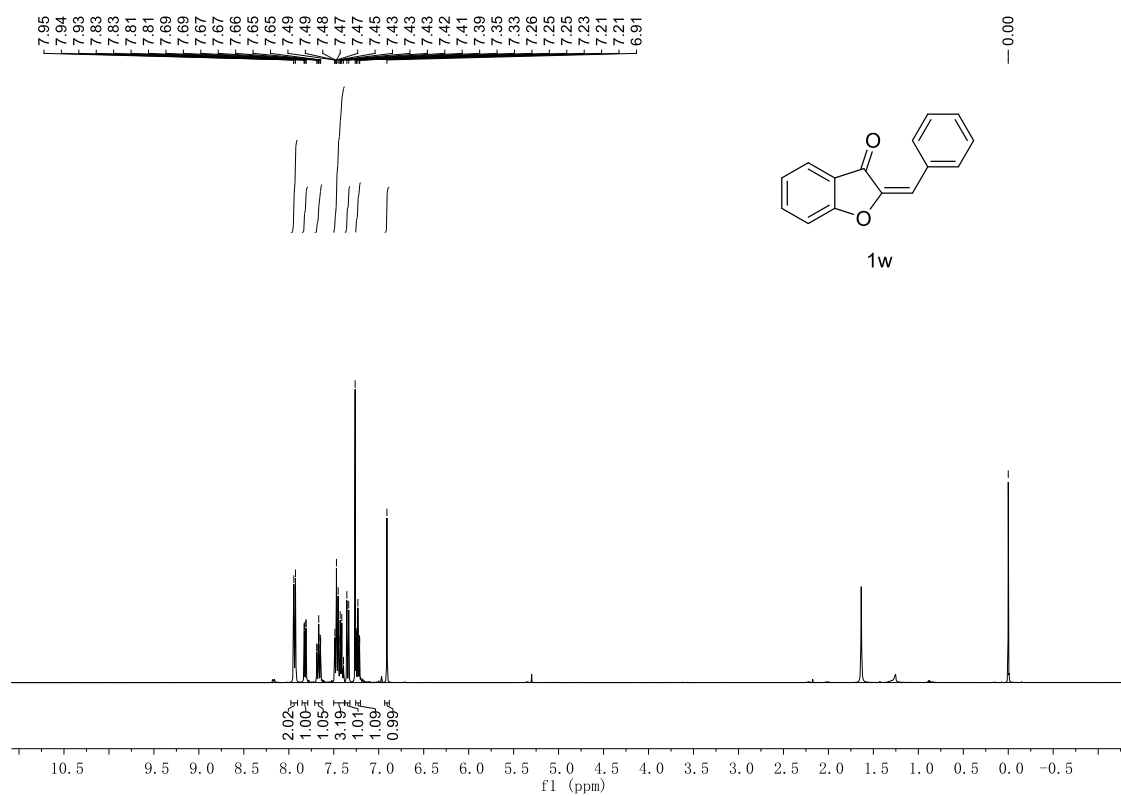
¹H and ¹³C-NMR of 1u



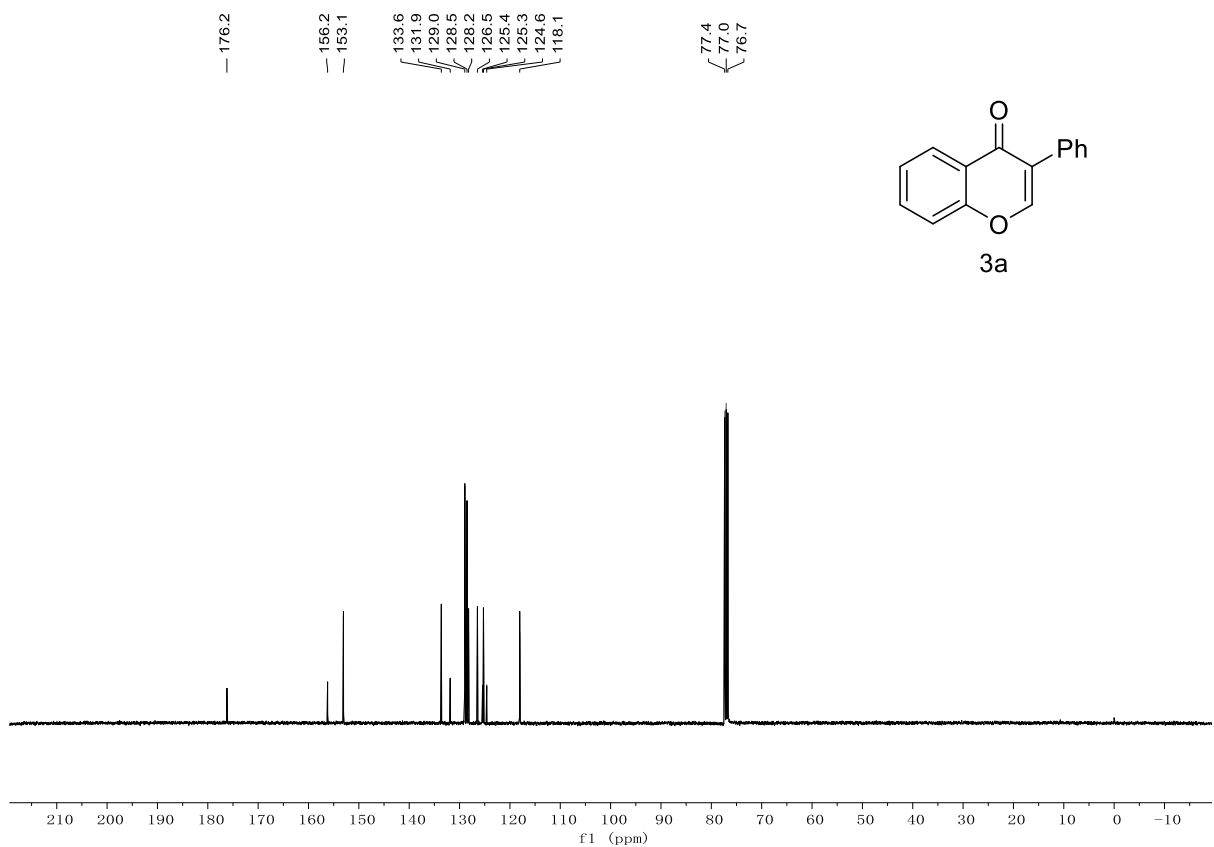
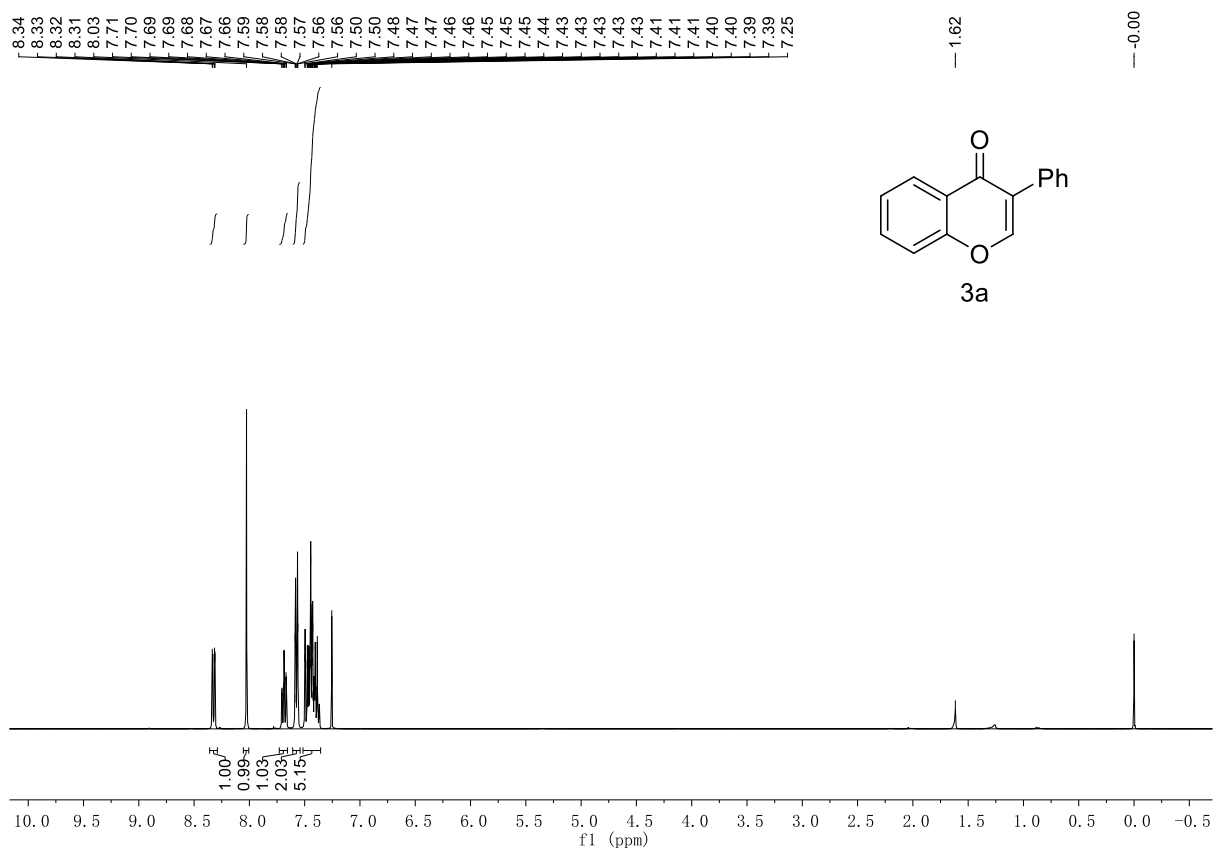
¹H and ¹³C-NMR of 1v



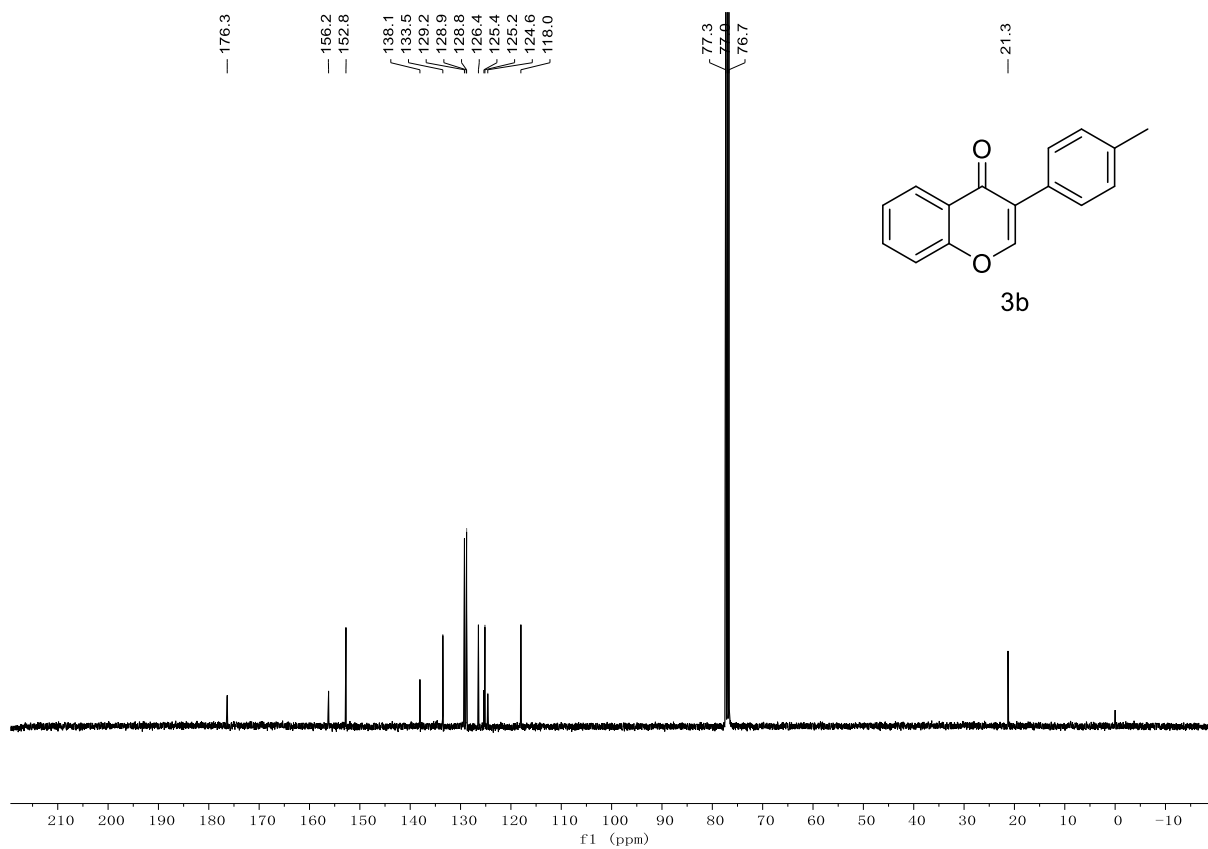
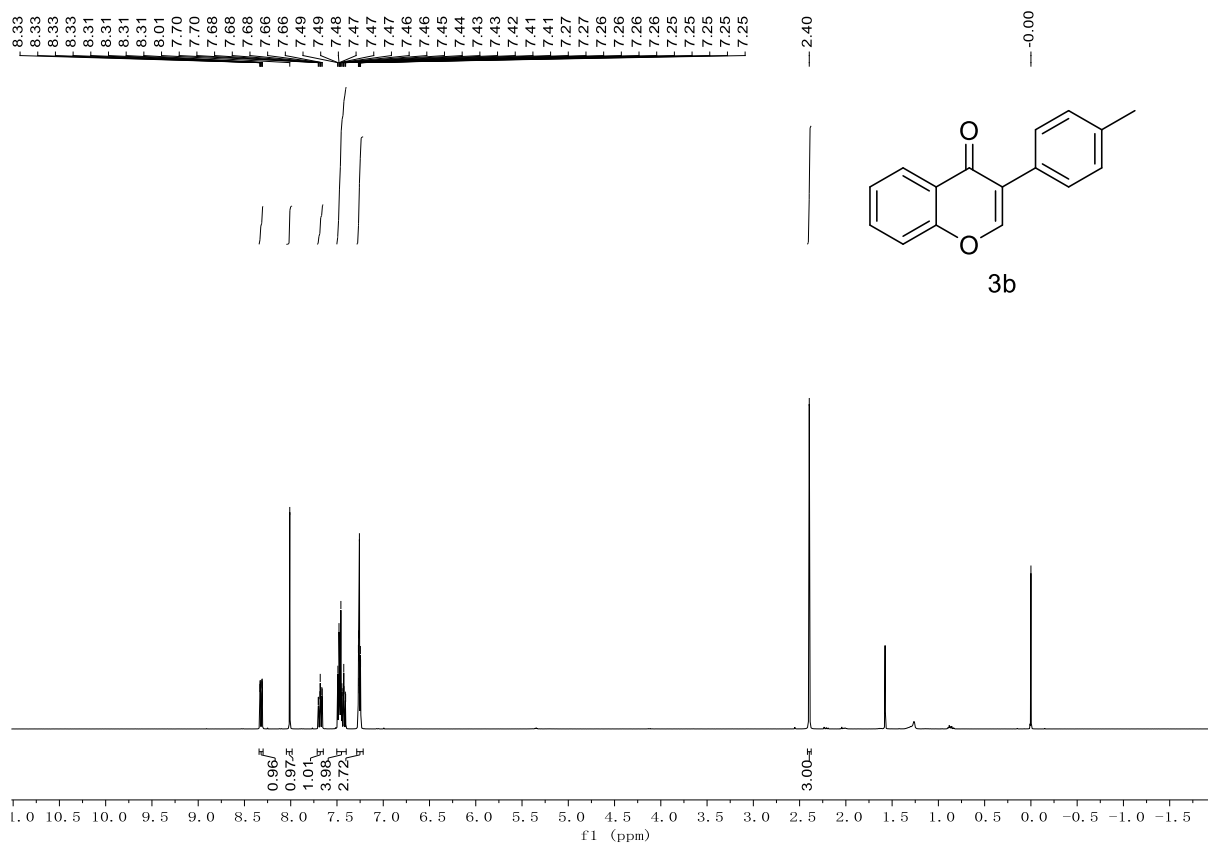
¹H and ¹³C-NMR of 1w



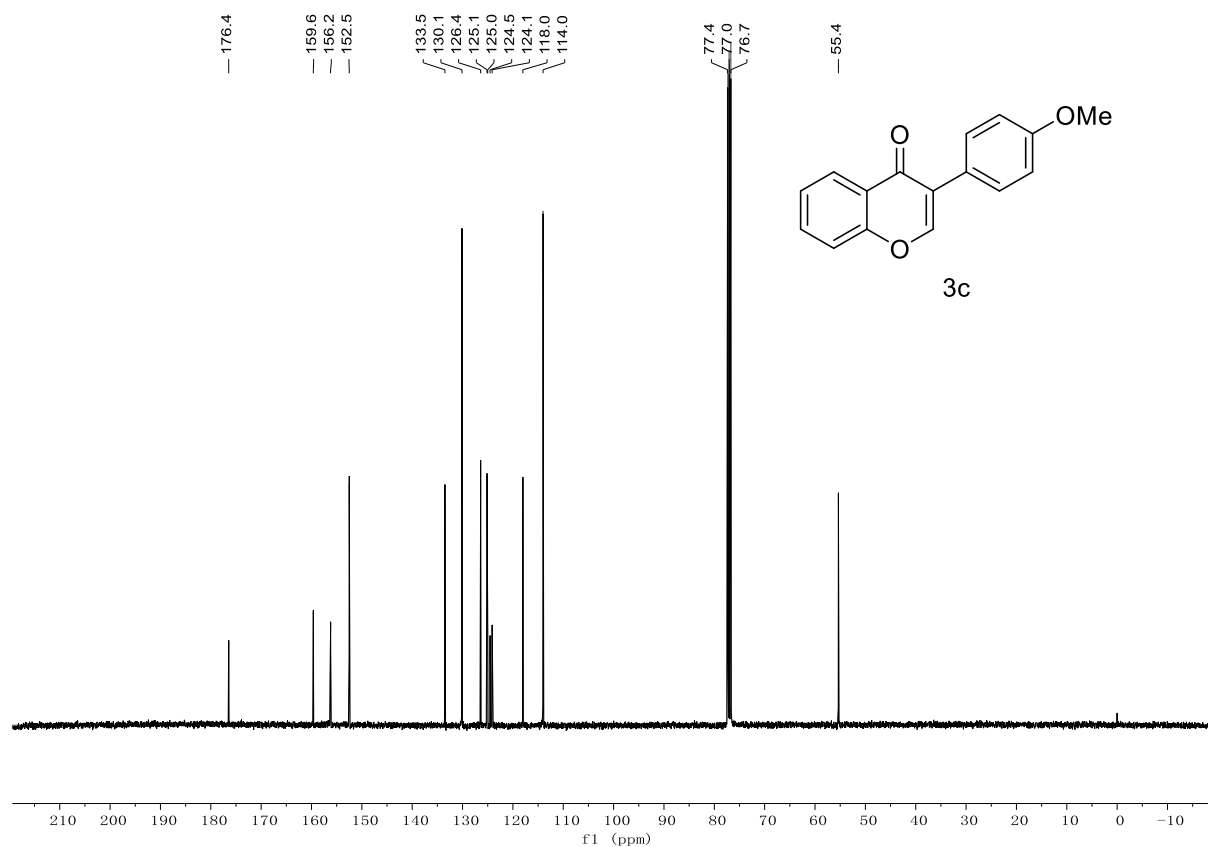
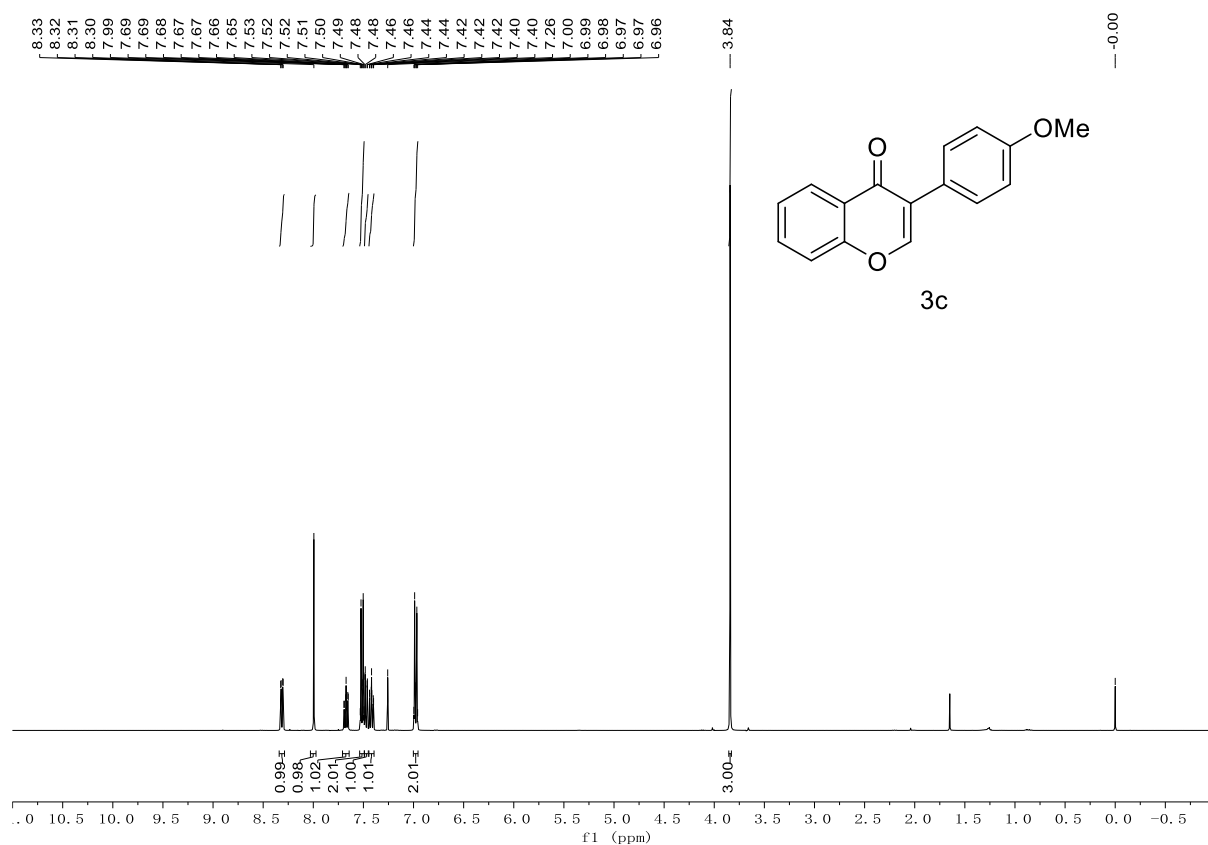
¹H and ¹³C-NMR of 3a



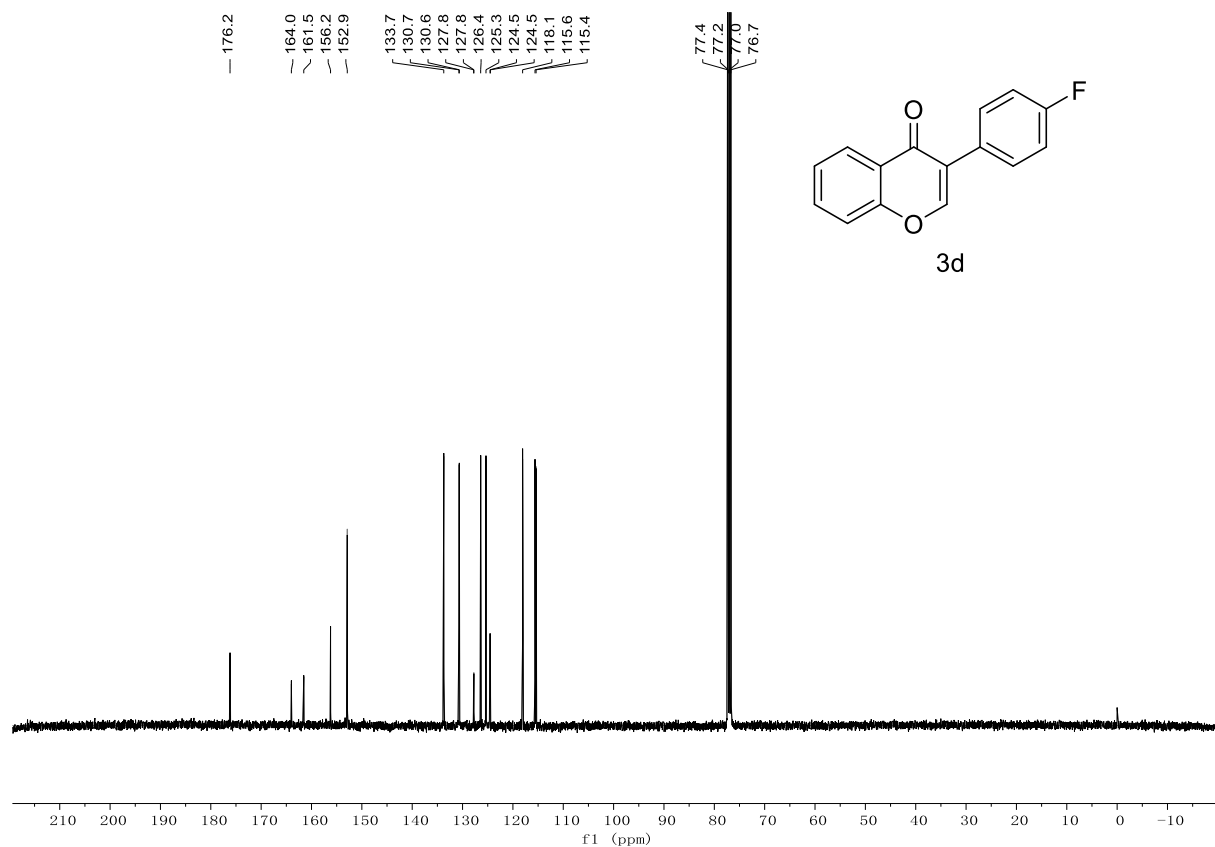
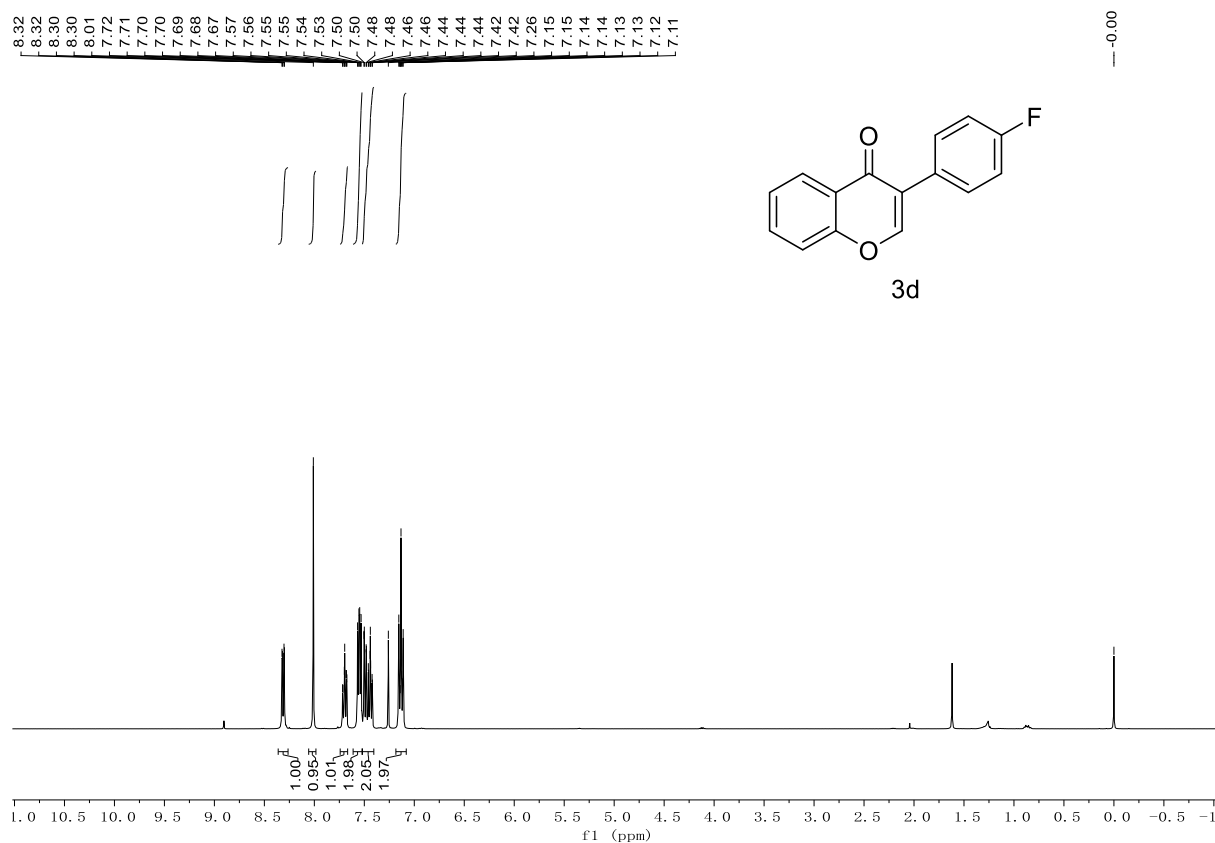
¹H and ¹³C-NMR of 3b



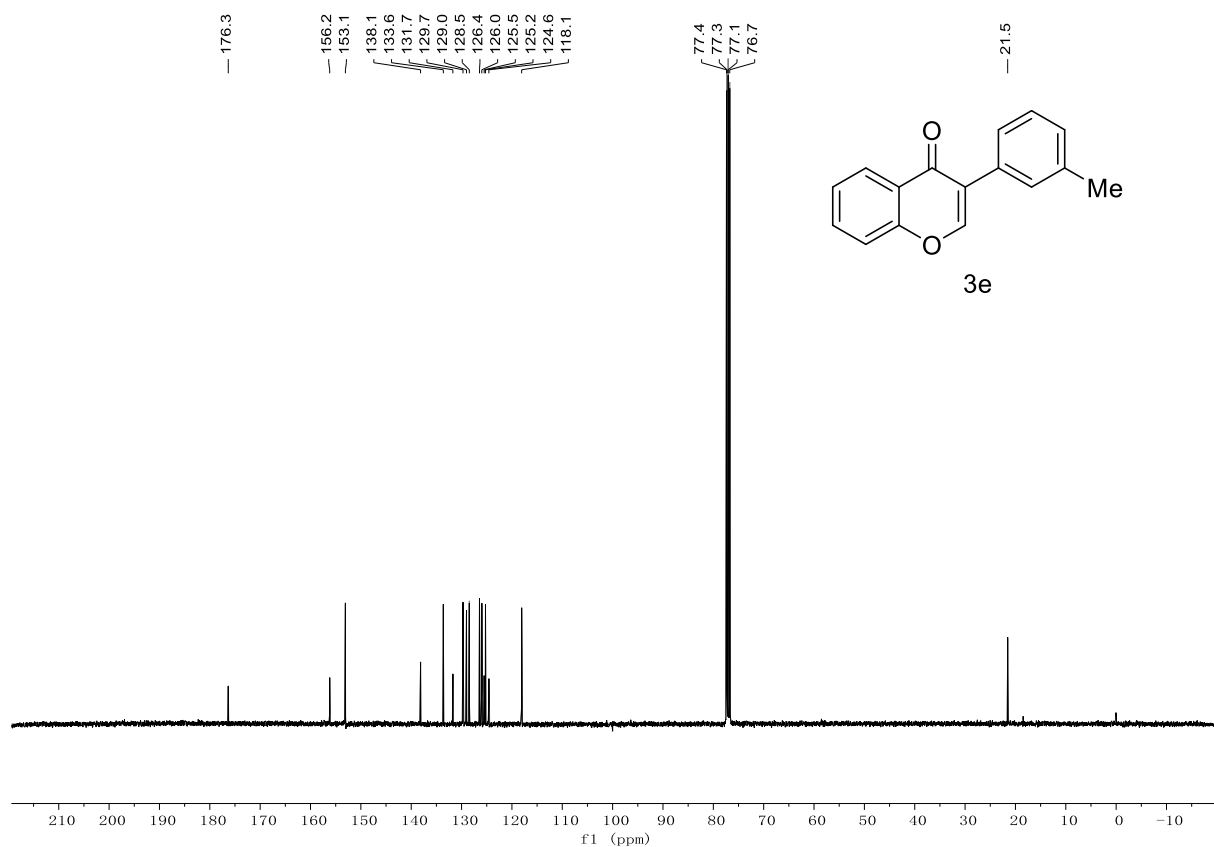
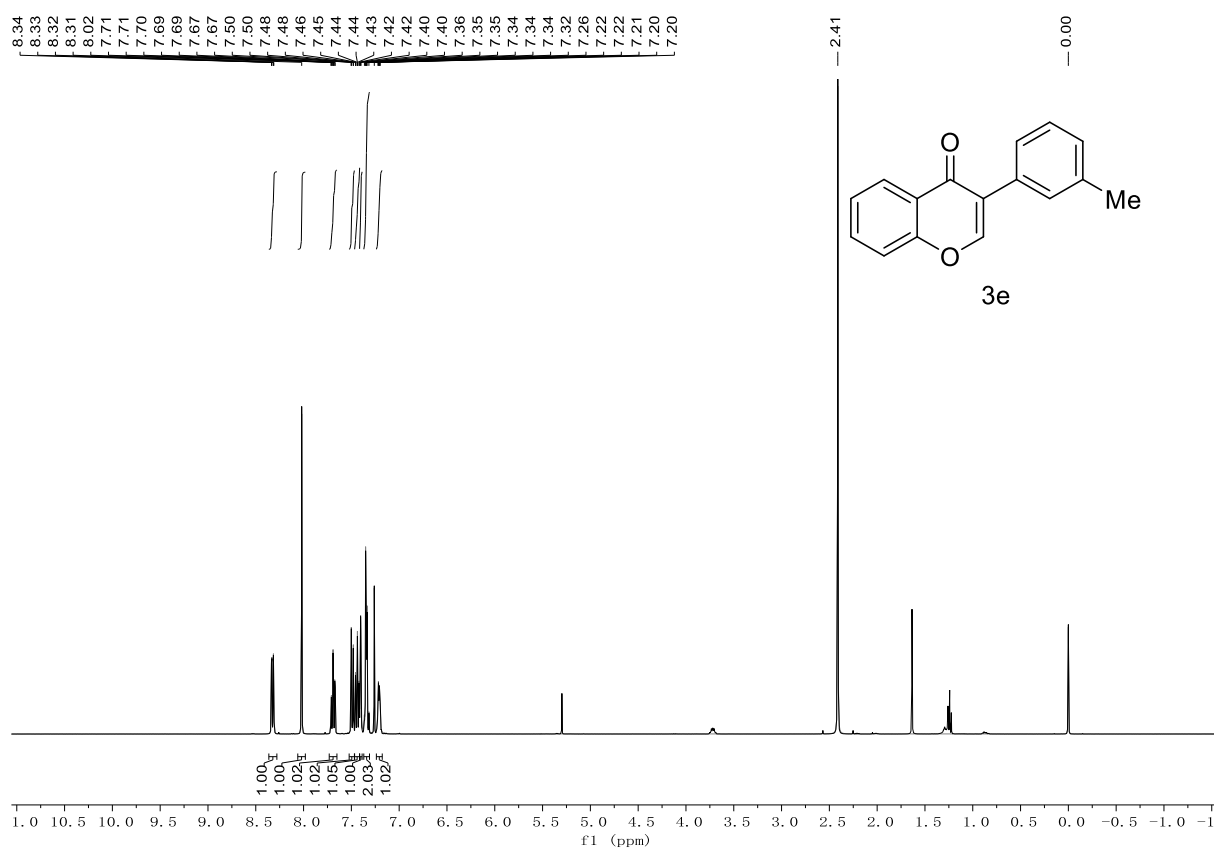
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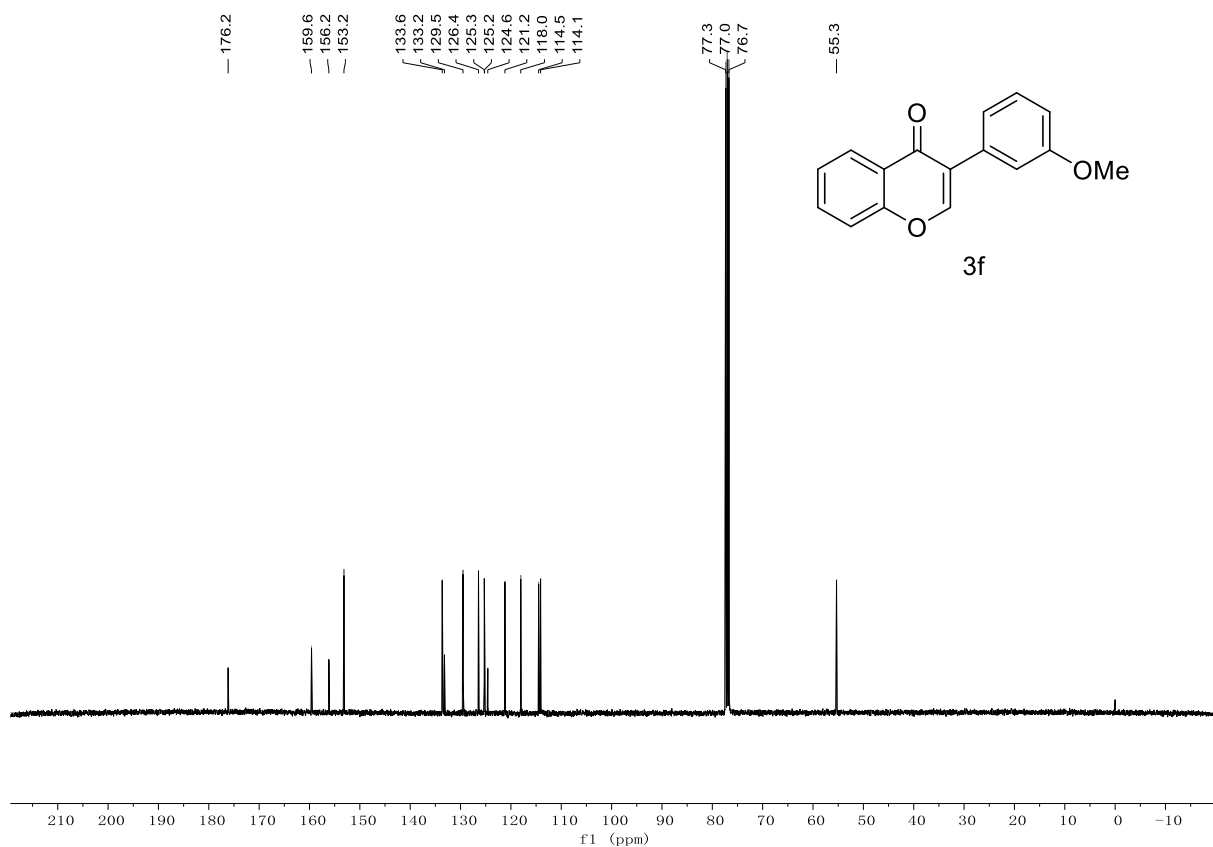
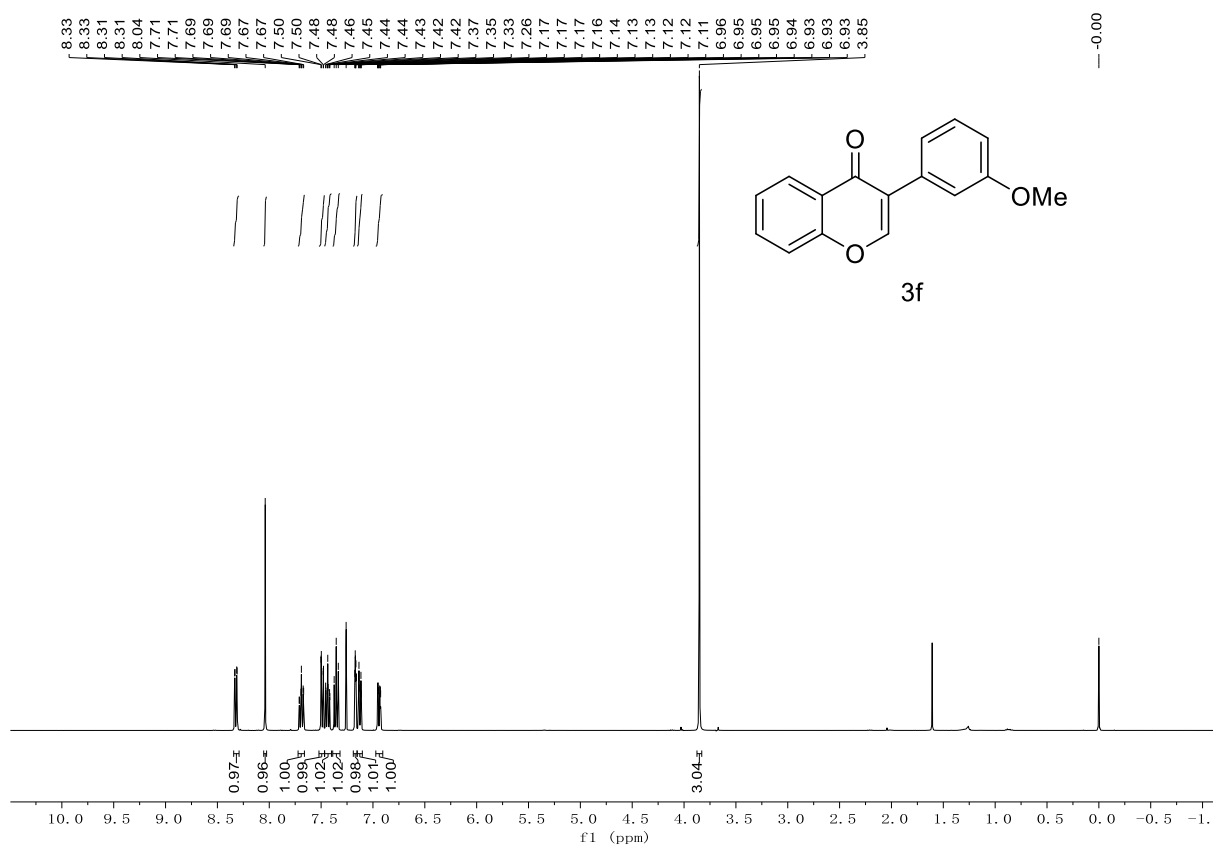
¹H and ¹³C-NMR of 3d



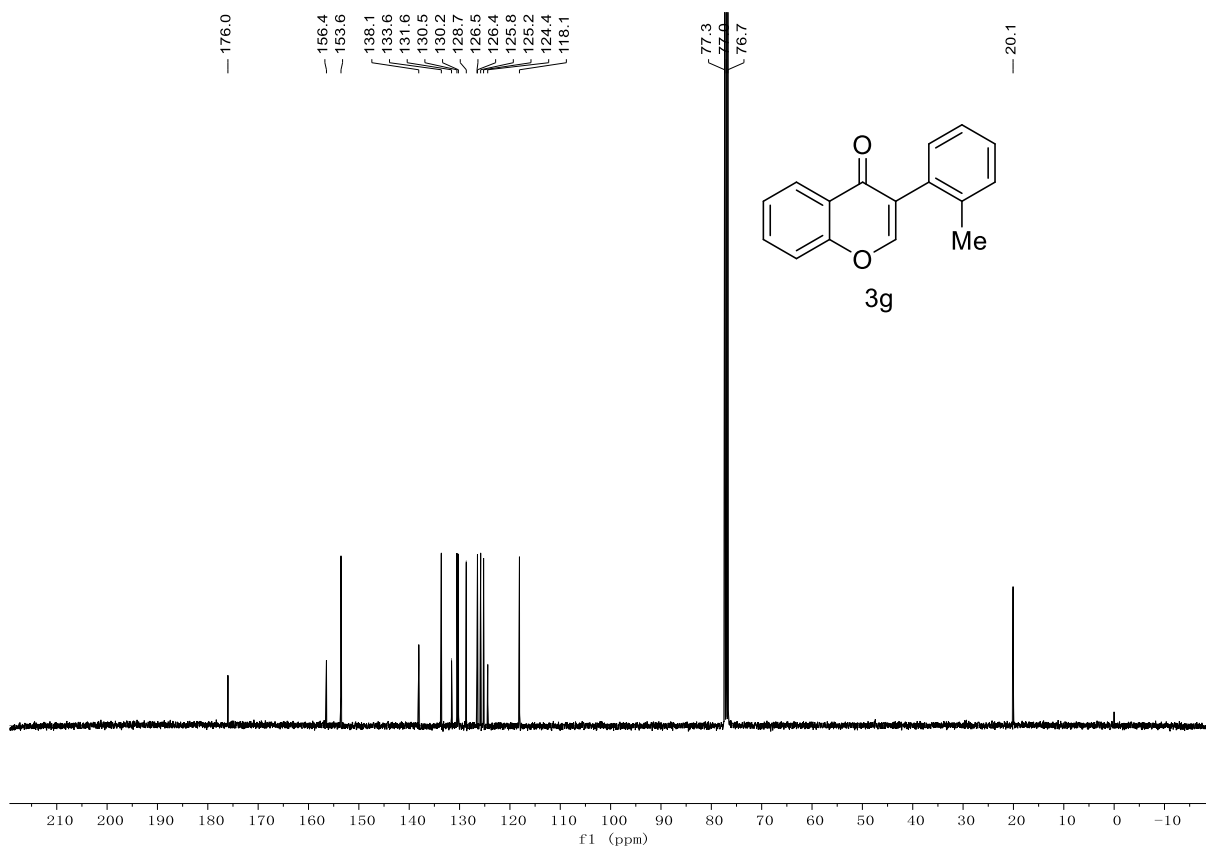
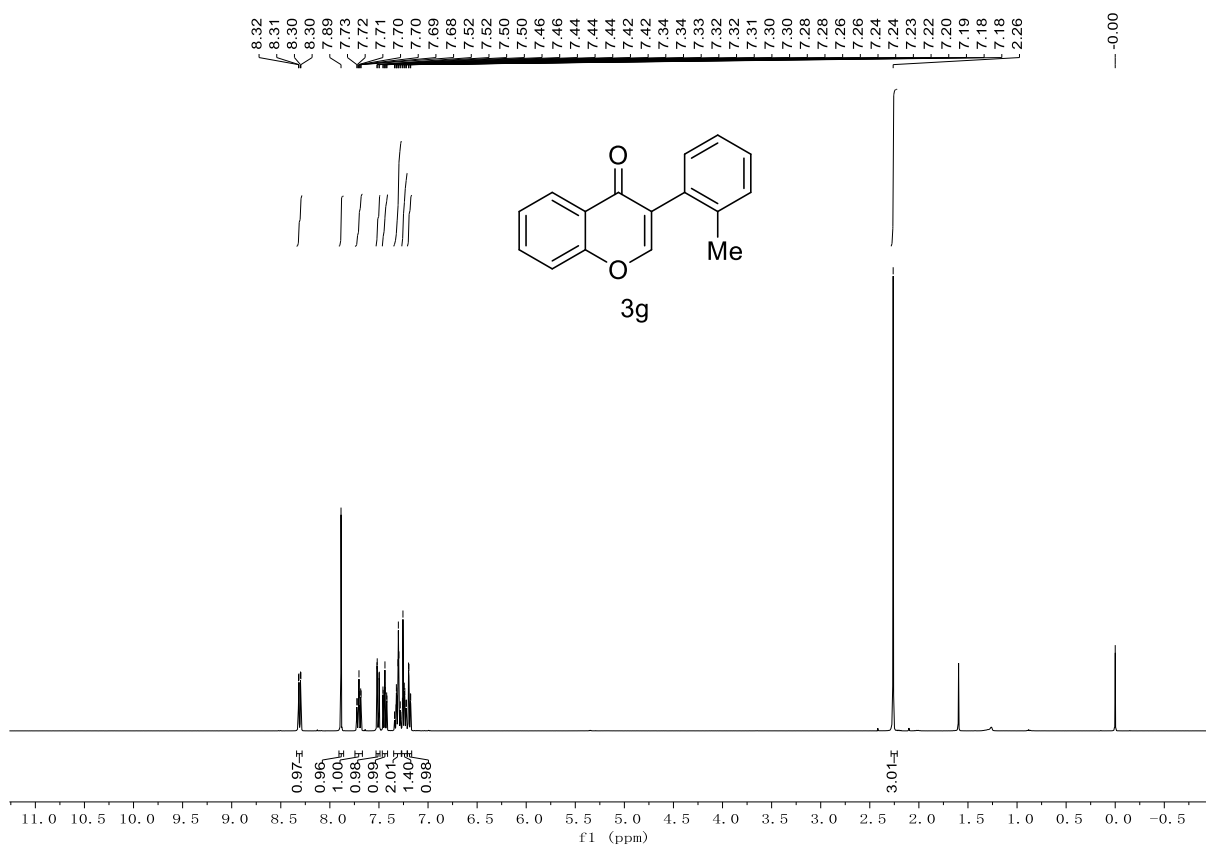
¹H and ¹³C-NMR of 3e



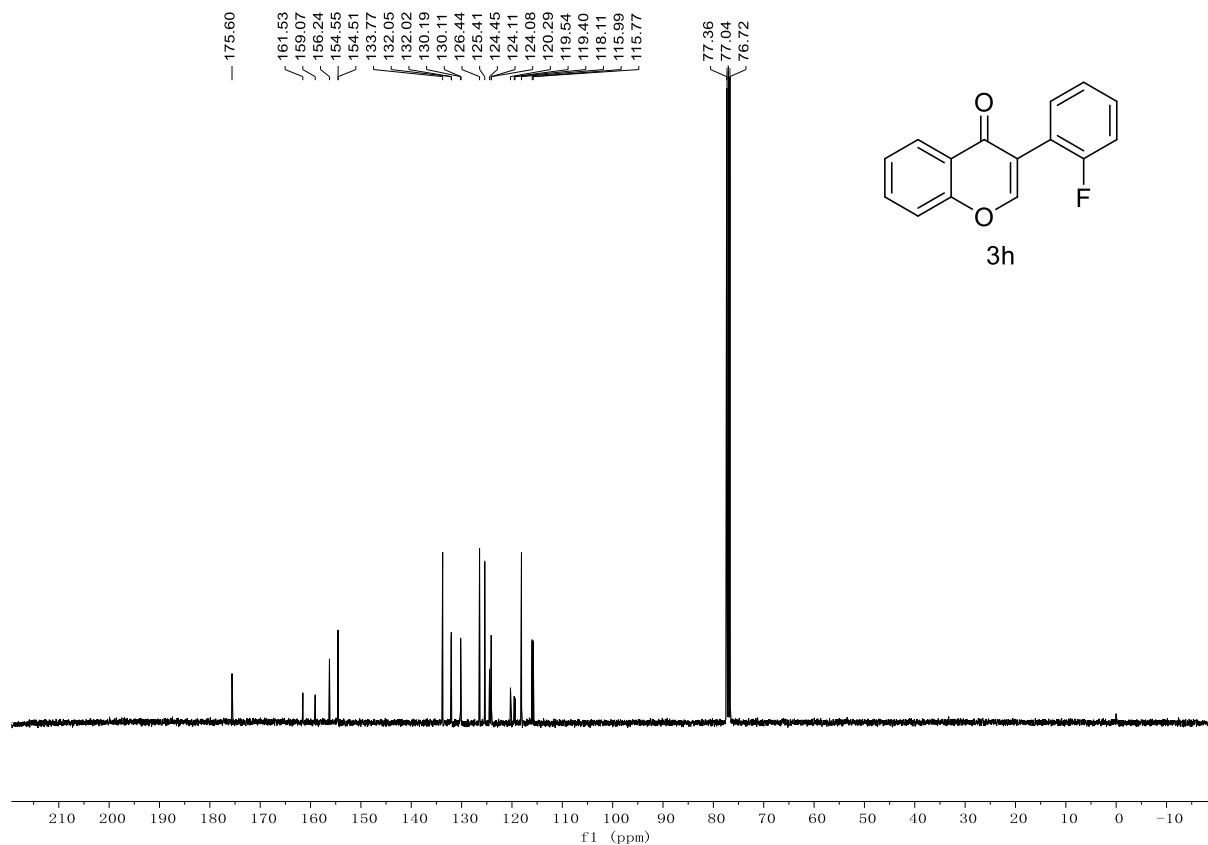
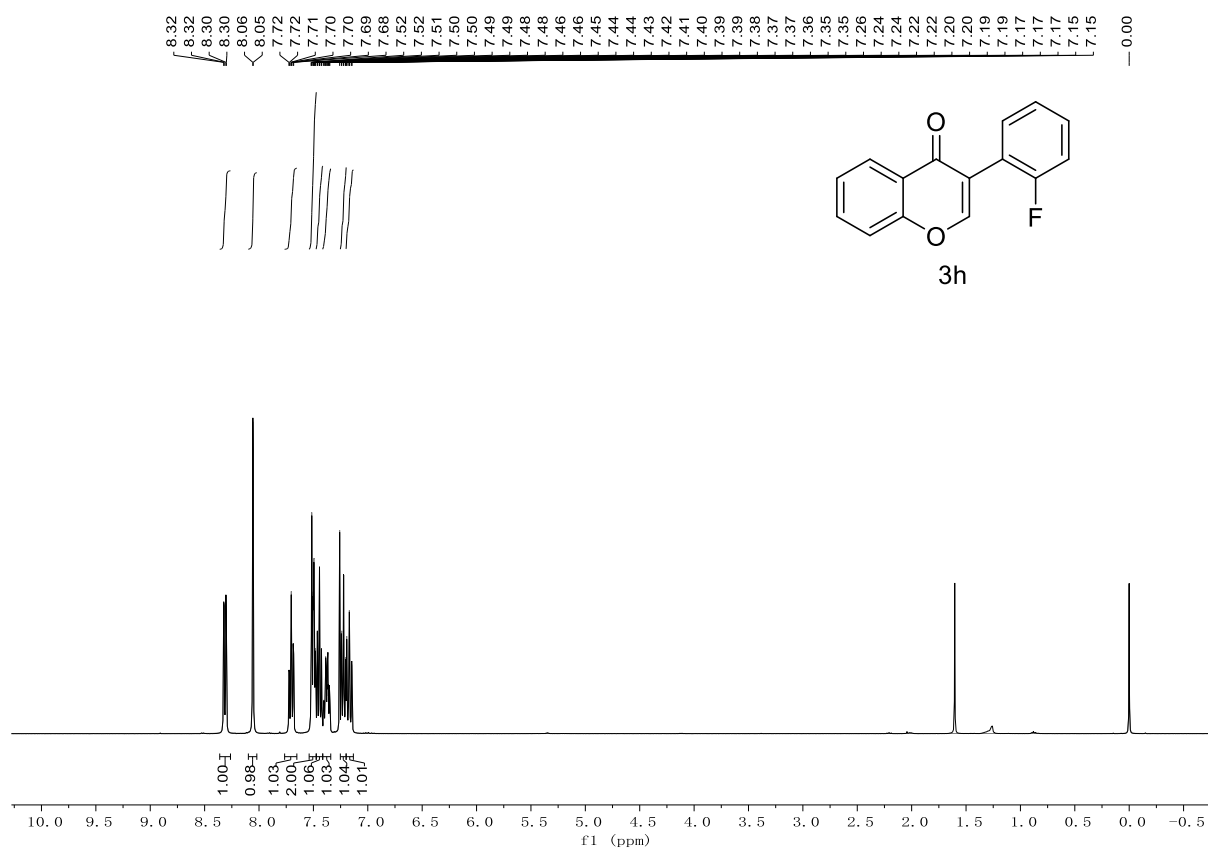
¹H and ¹³C-NMR of 3f



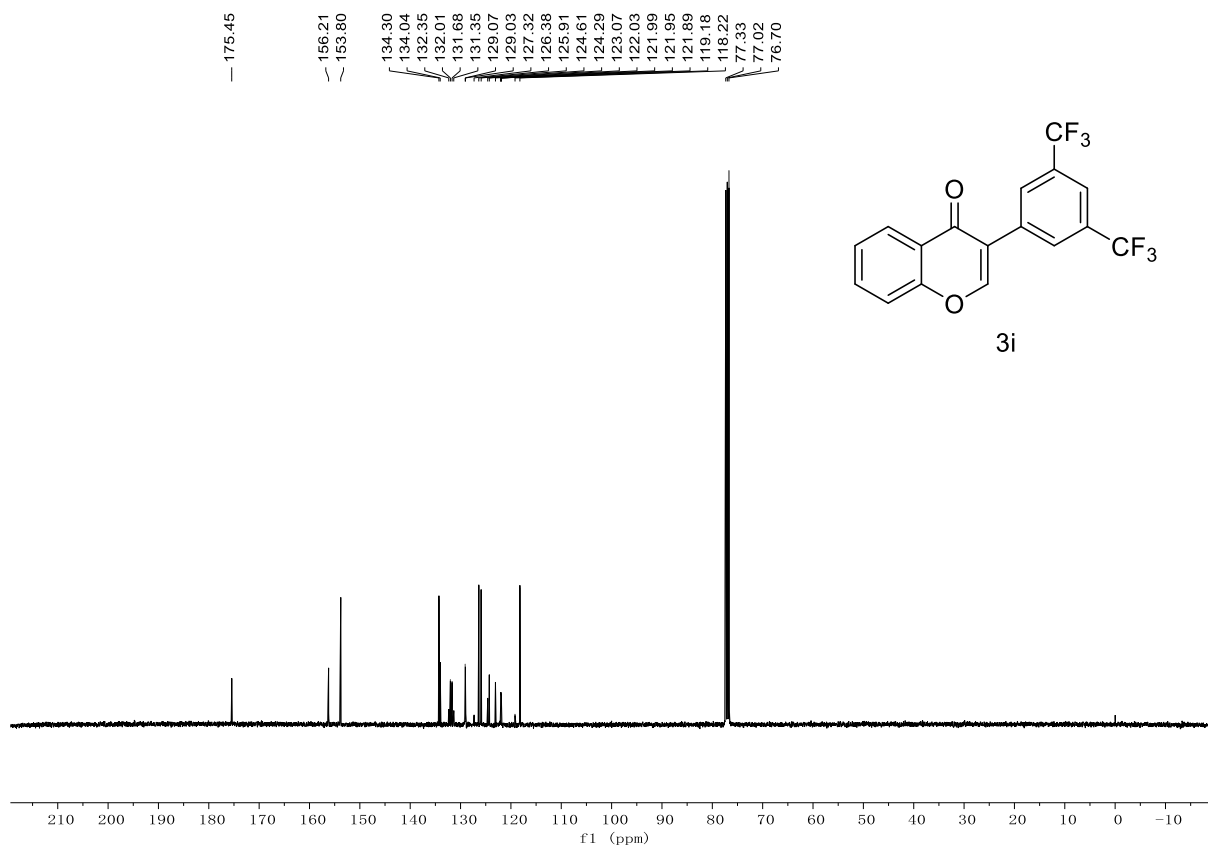
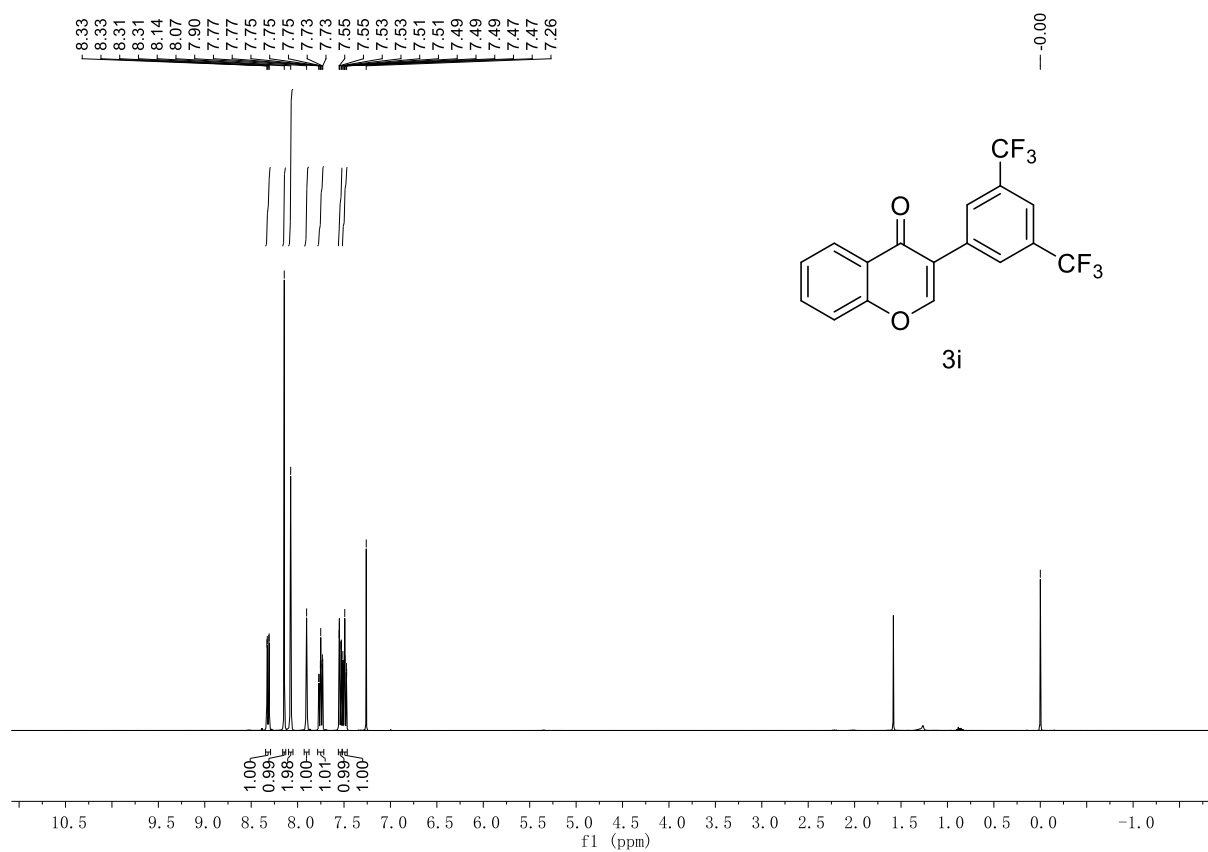
¹H and ¹³C-NMR of 3g



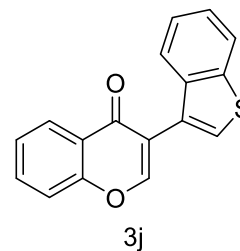
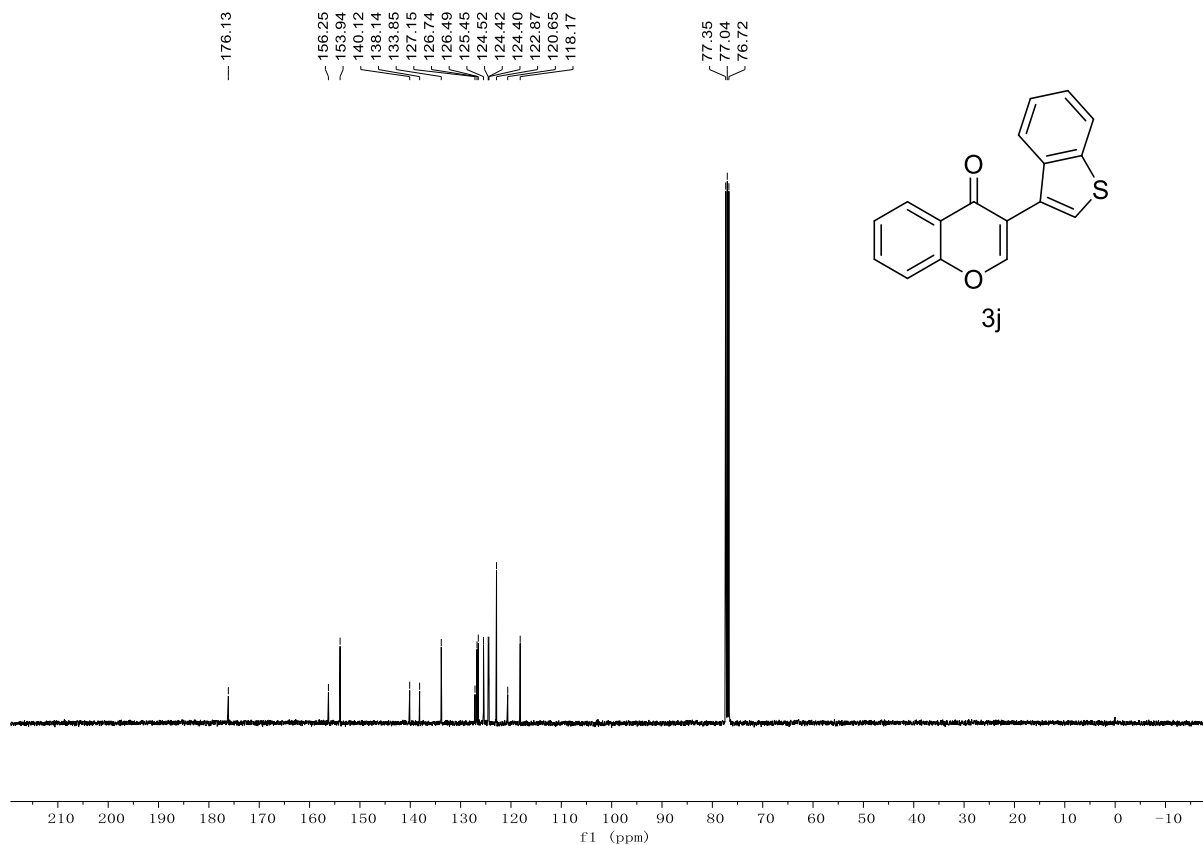
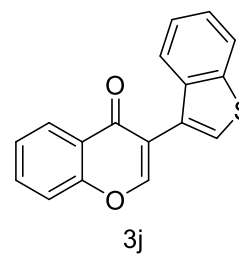
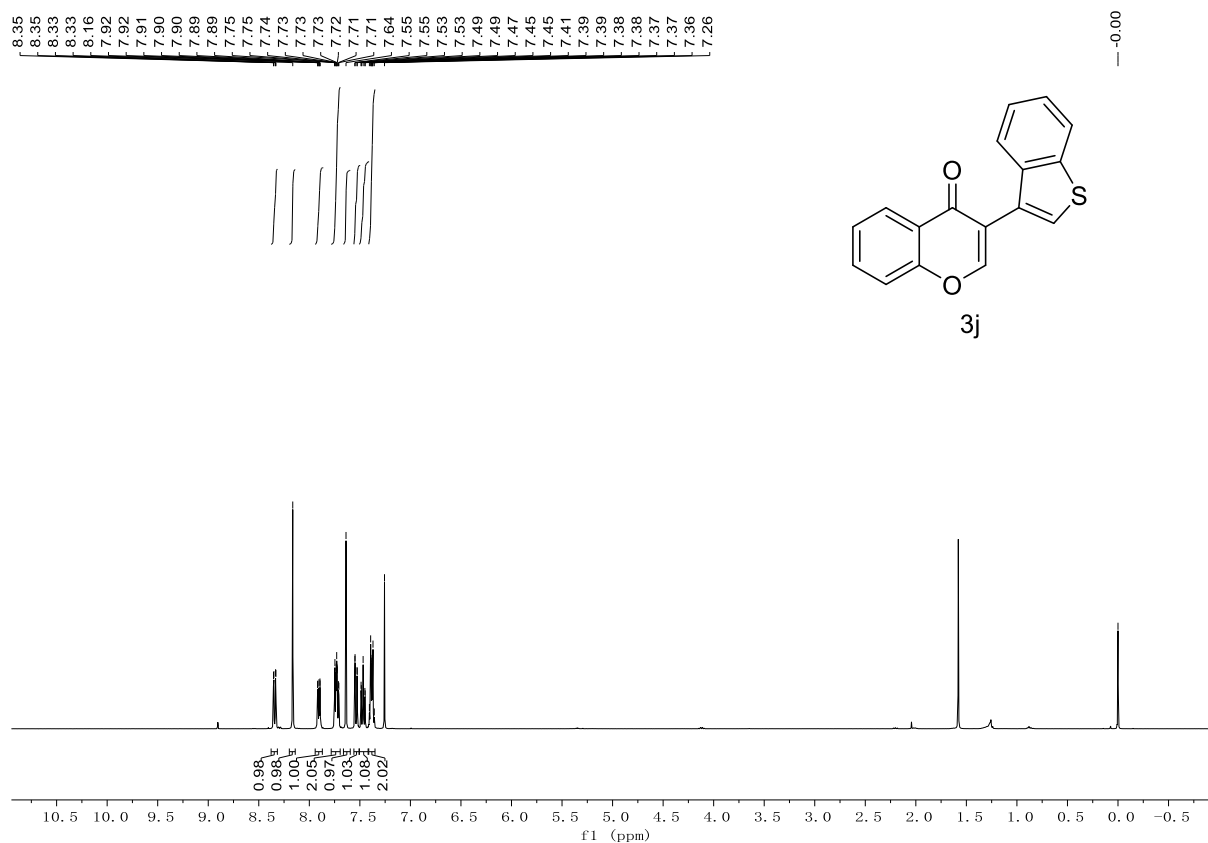
¹H and ¹³C-NMR of 3h



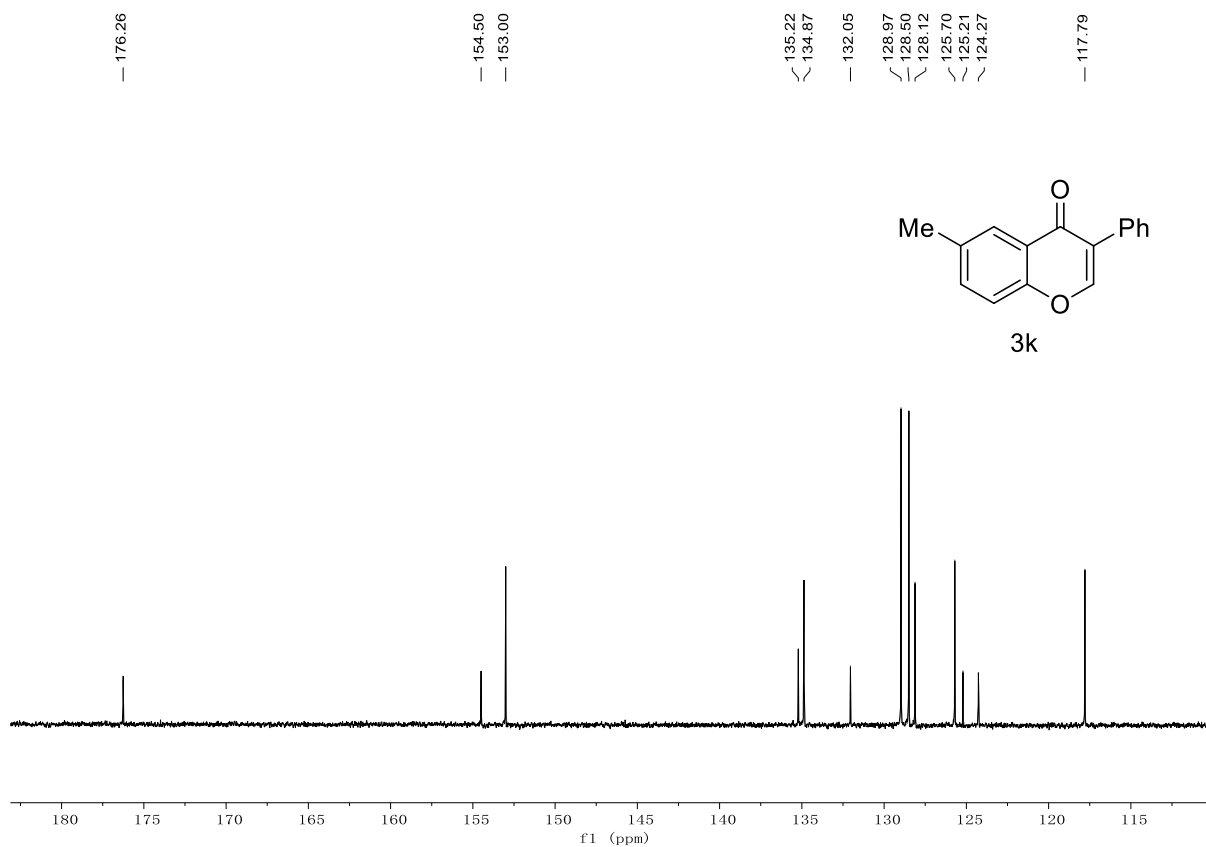
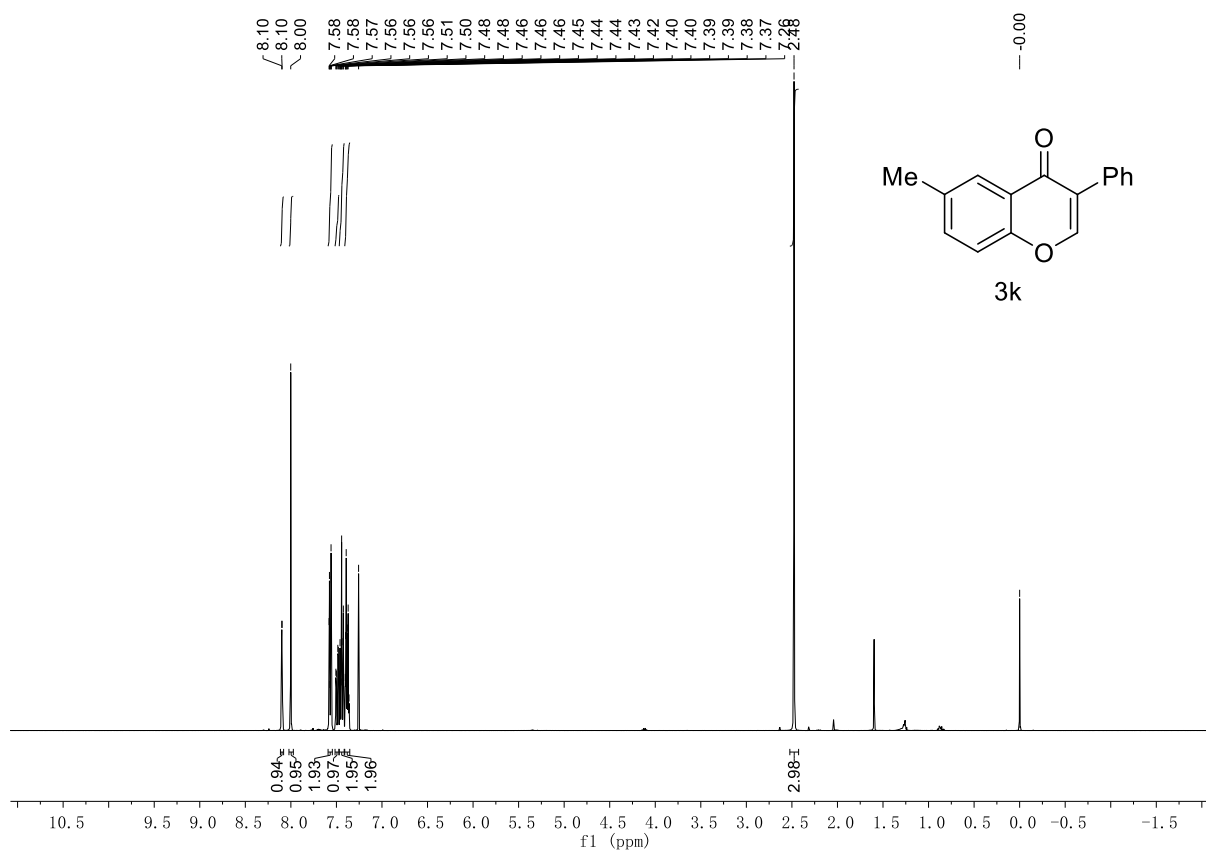
¹H and ¹³C-NMR of 3i



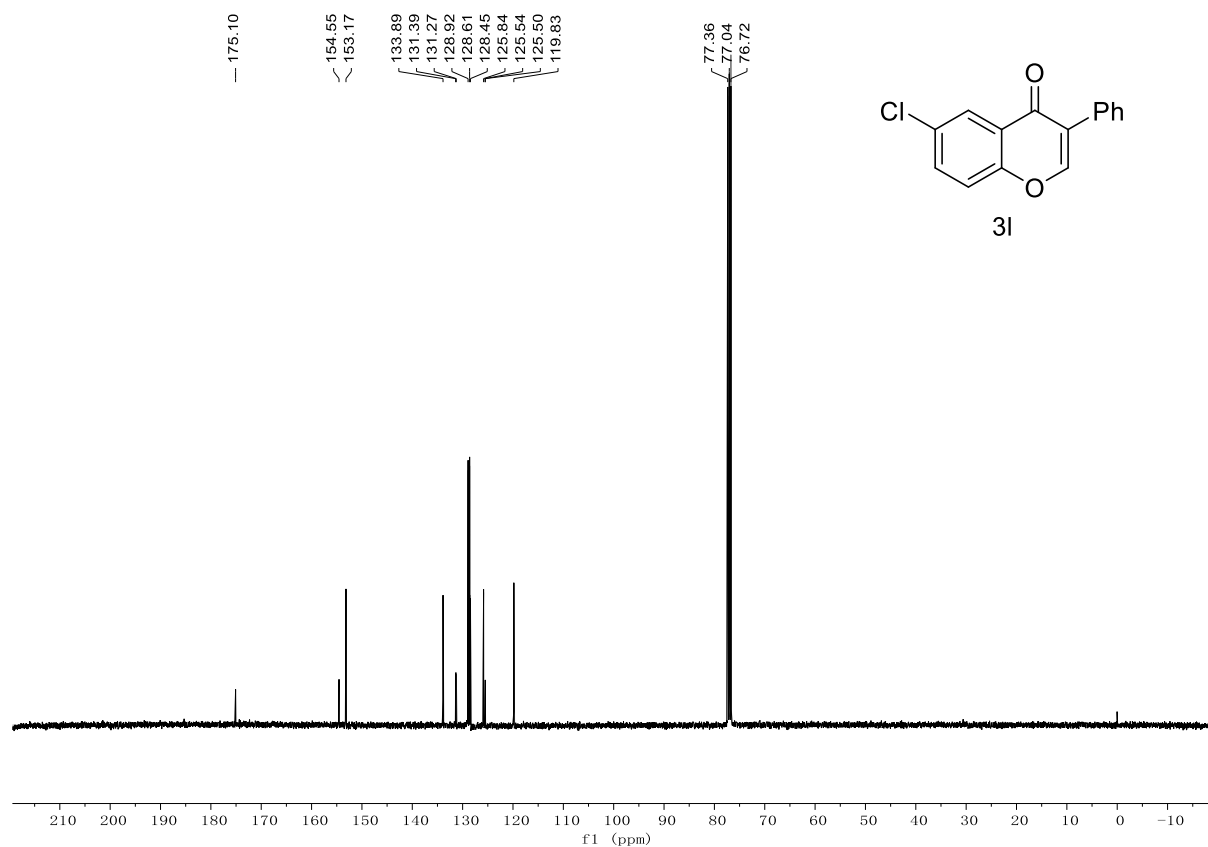
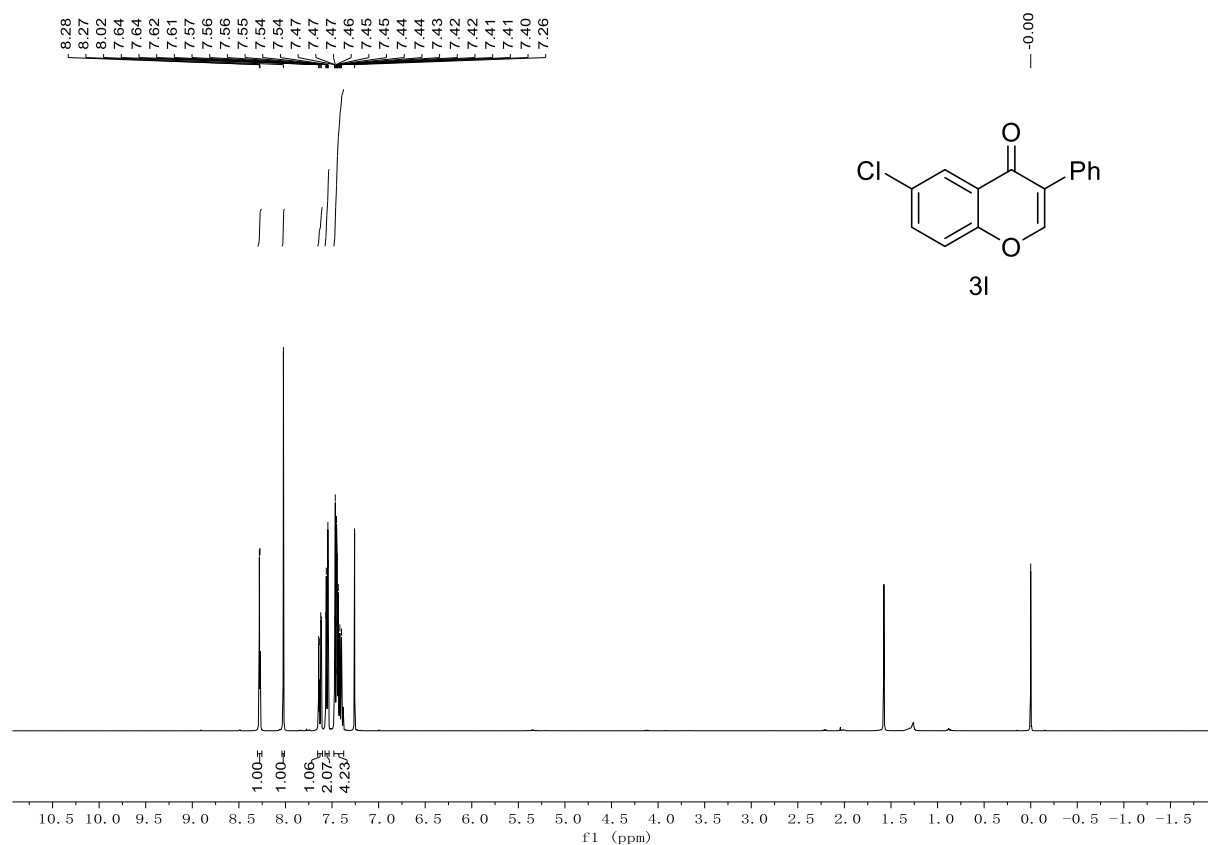
¹H and ¹³C-NMR of 3j



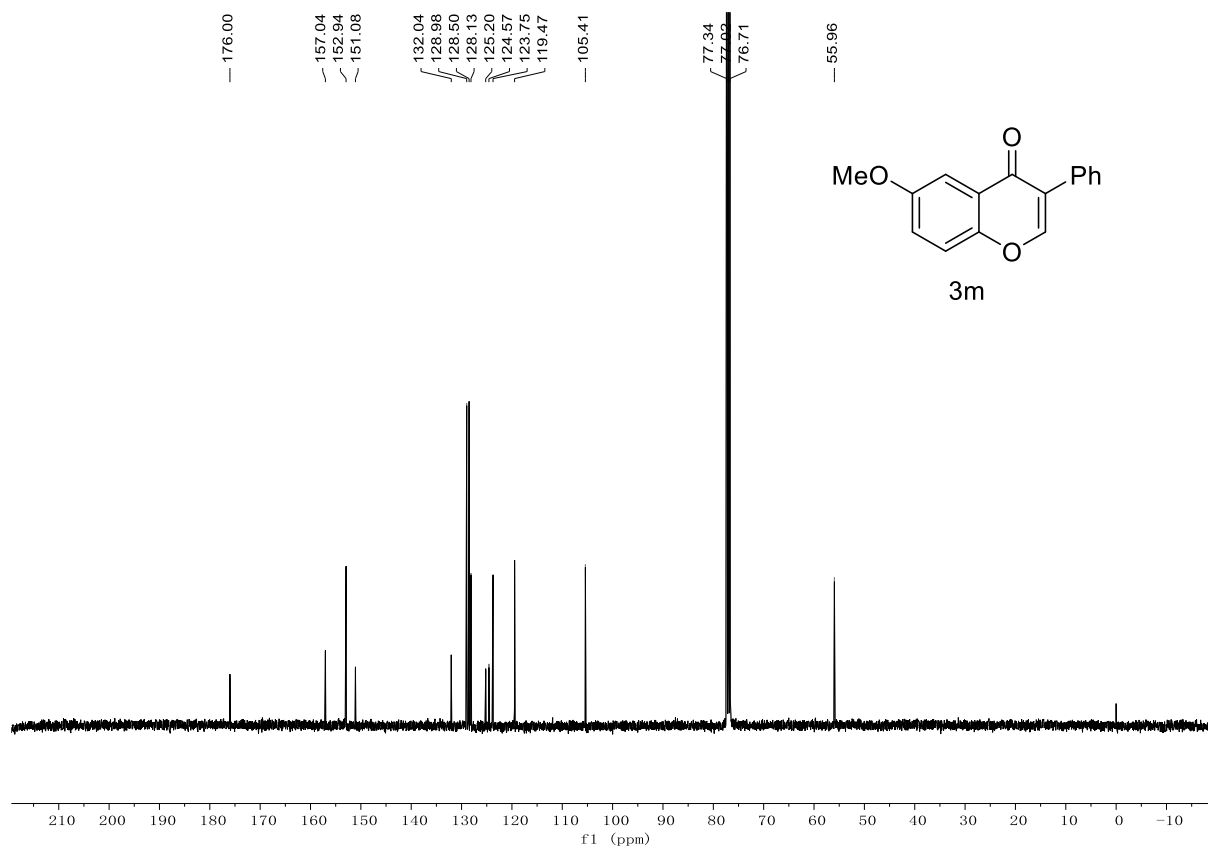
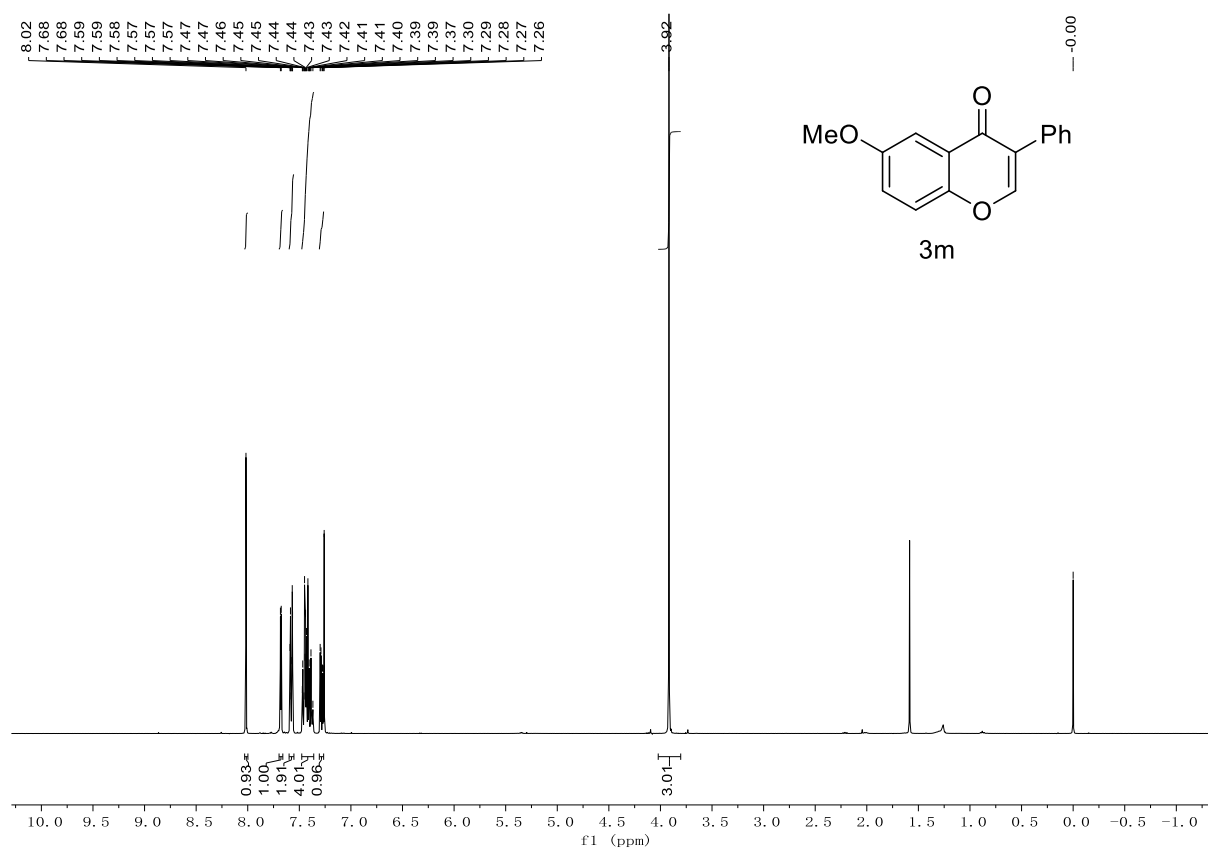
¹H and ¹³C-NMR of 3k



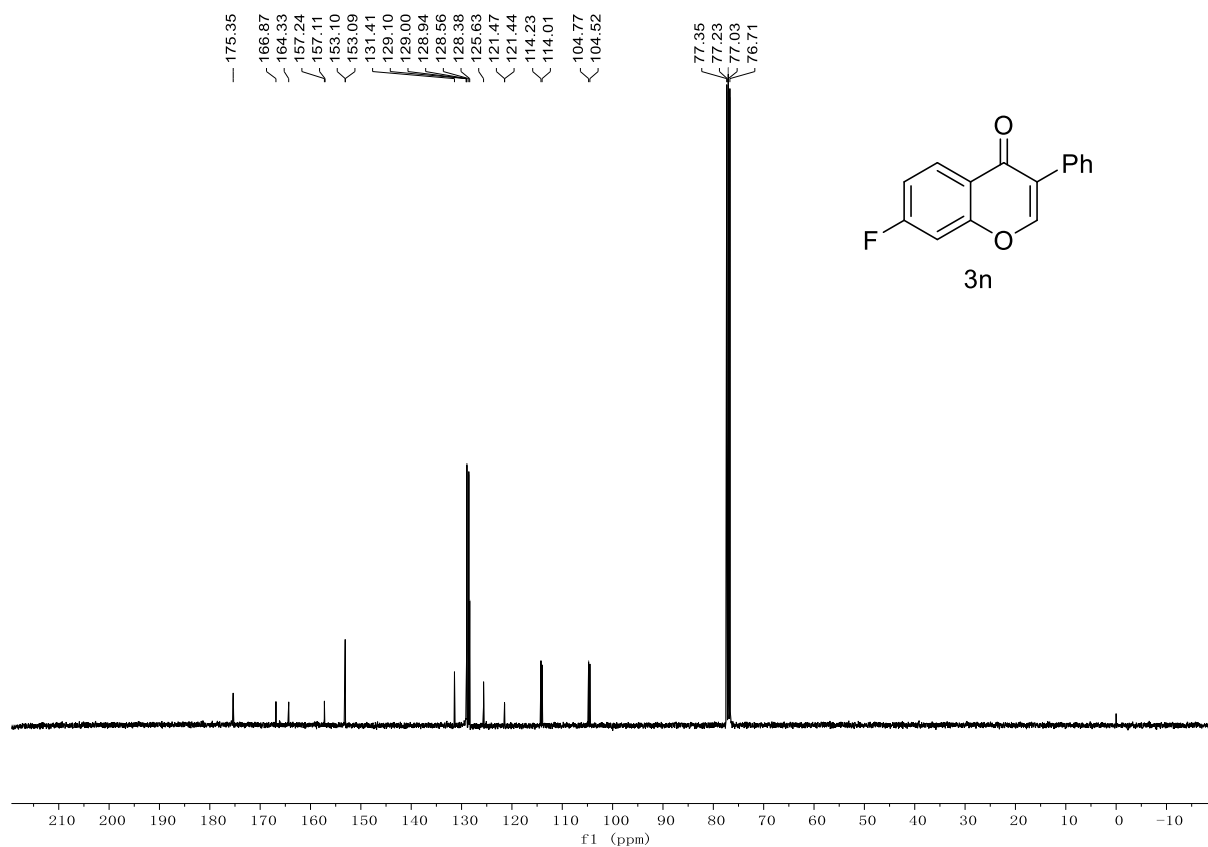
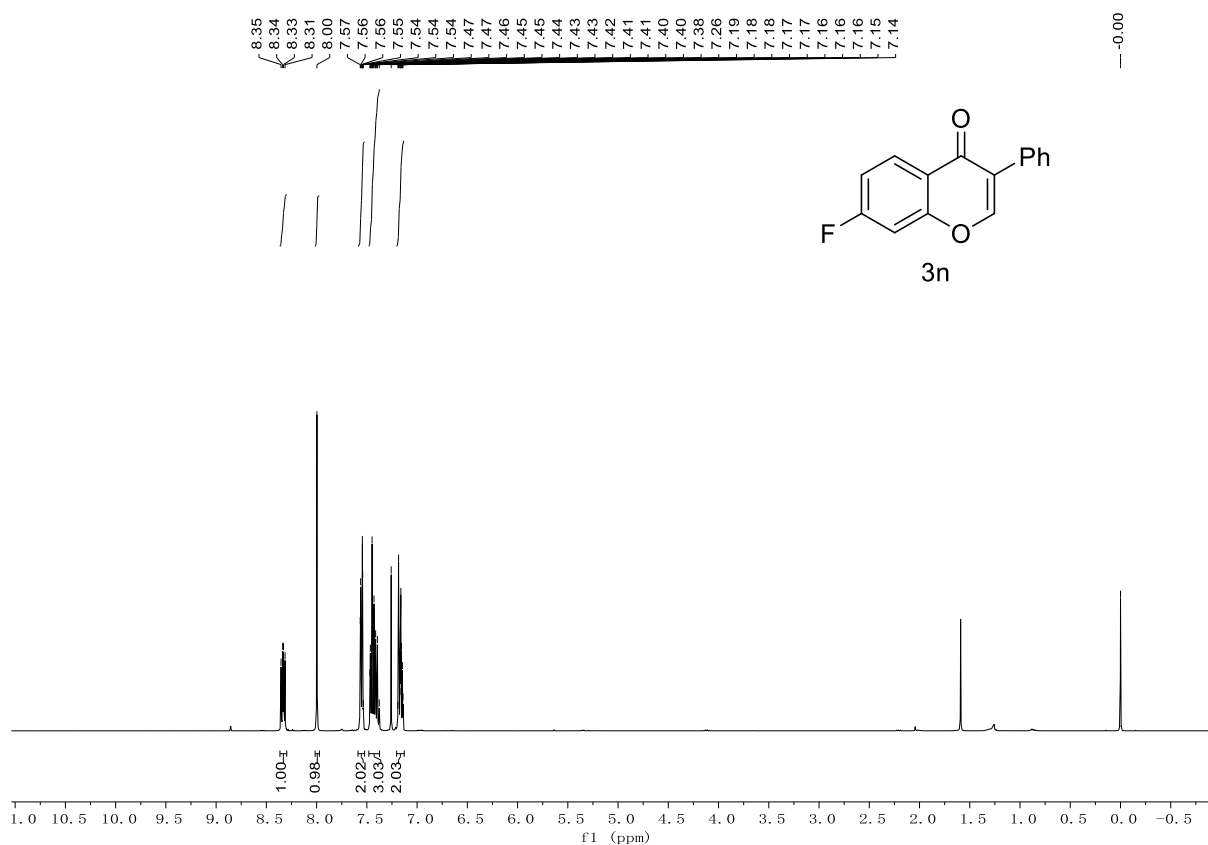
¹H and ¹³C-NMR of 3l



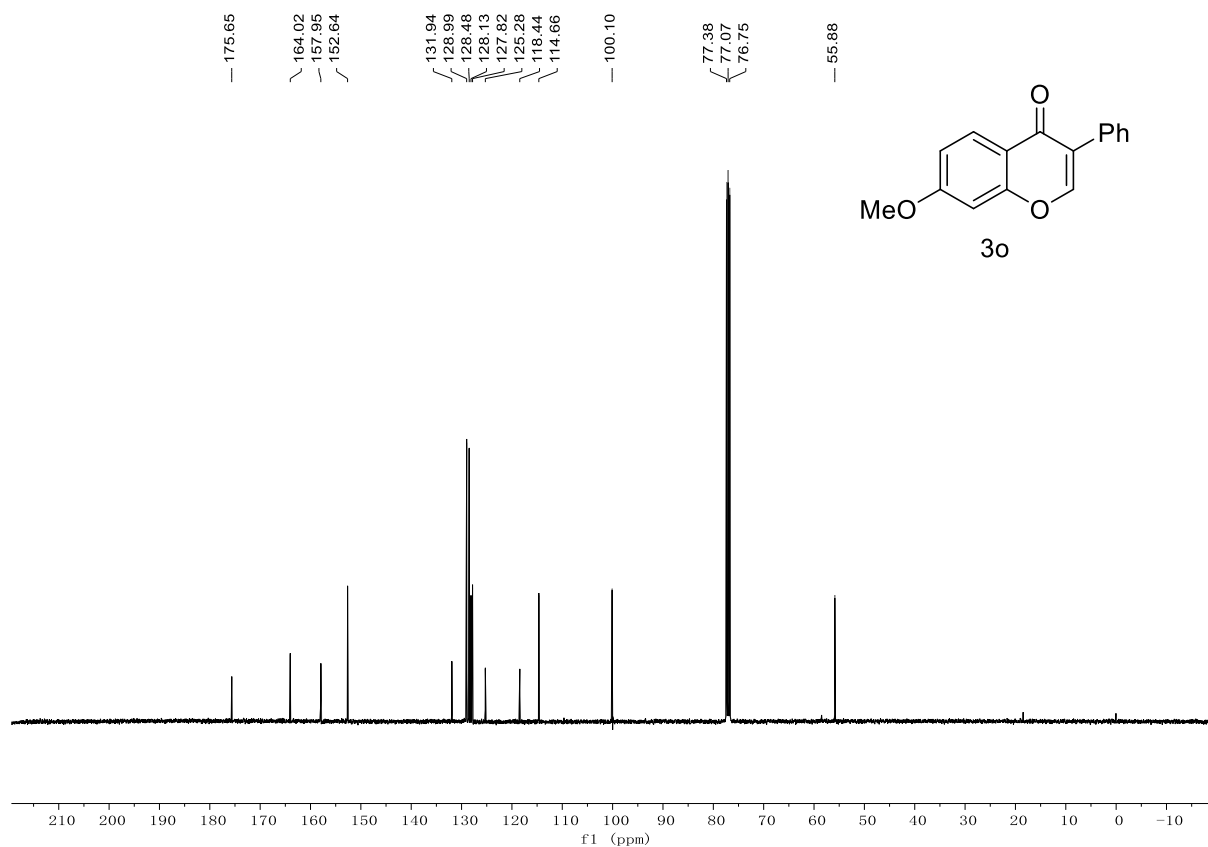
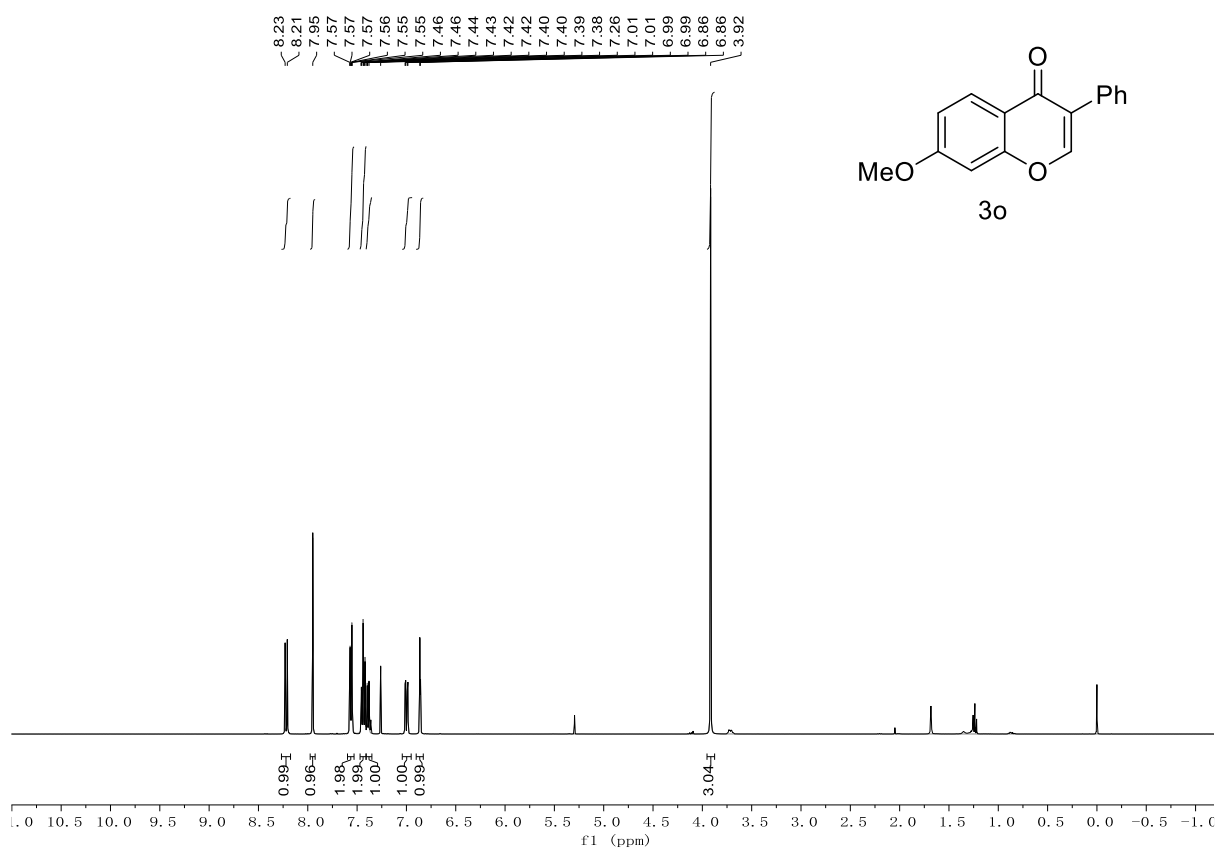
¹H and ¹³C-NMR of 3m



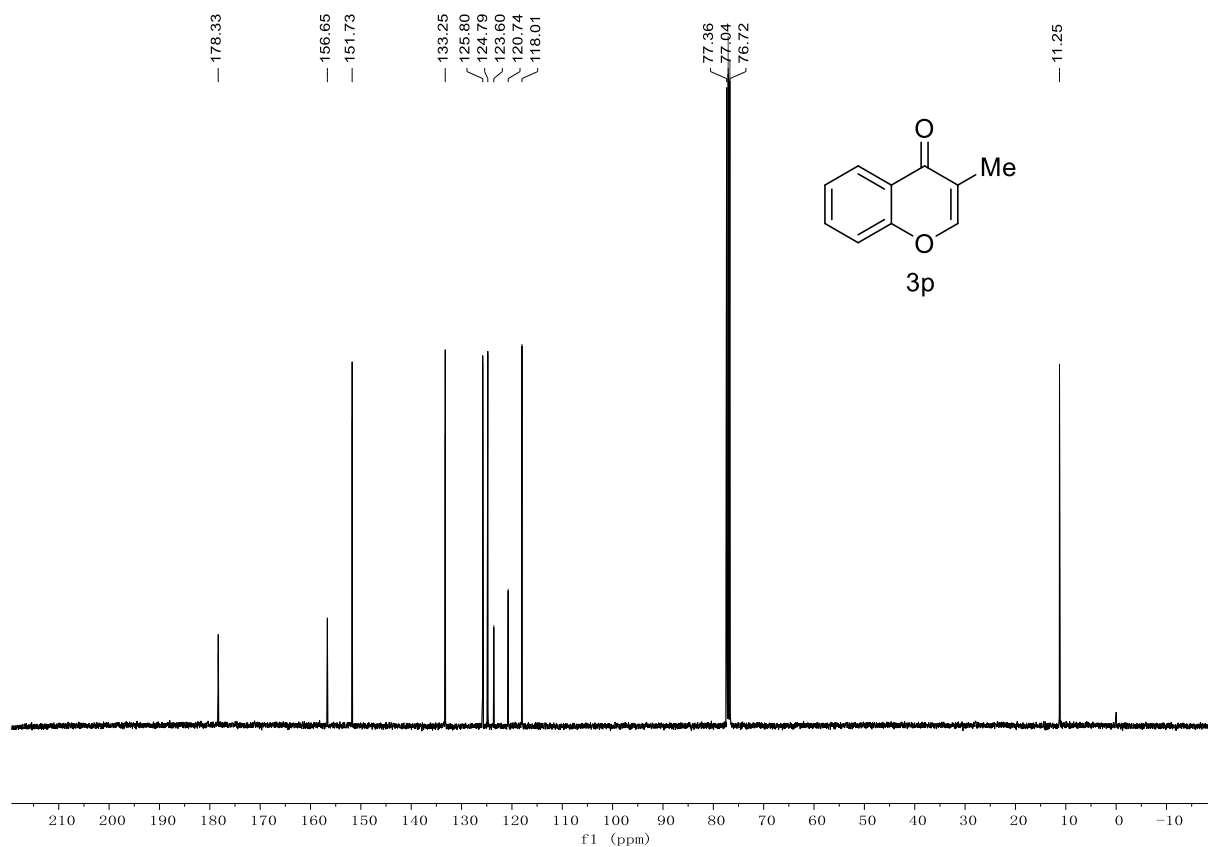
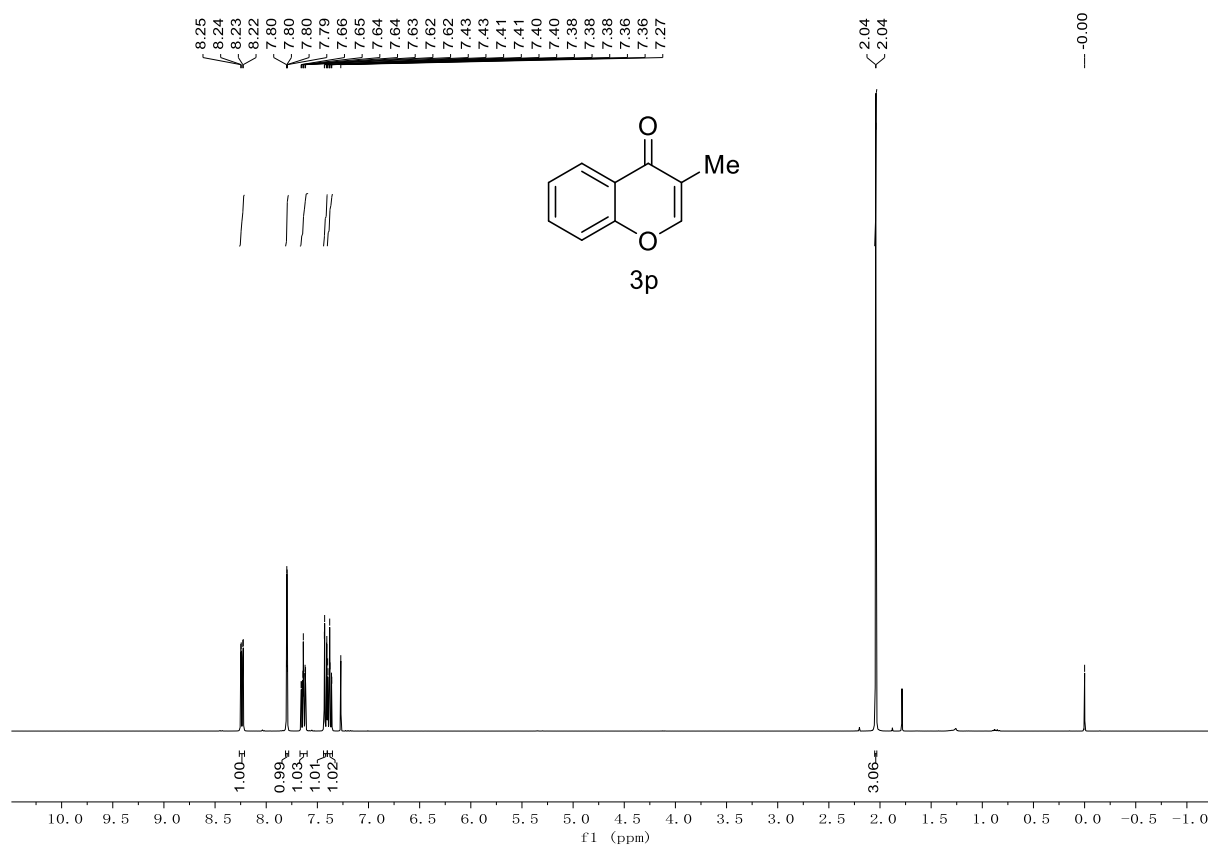
¹H and ¹³C-NMR of 3n



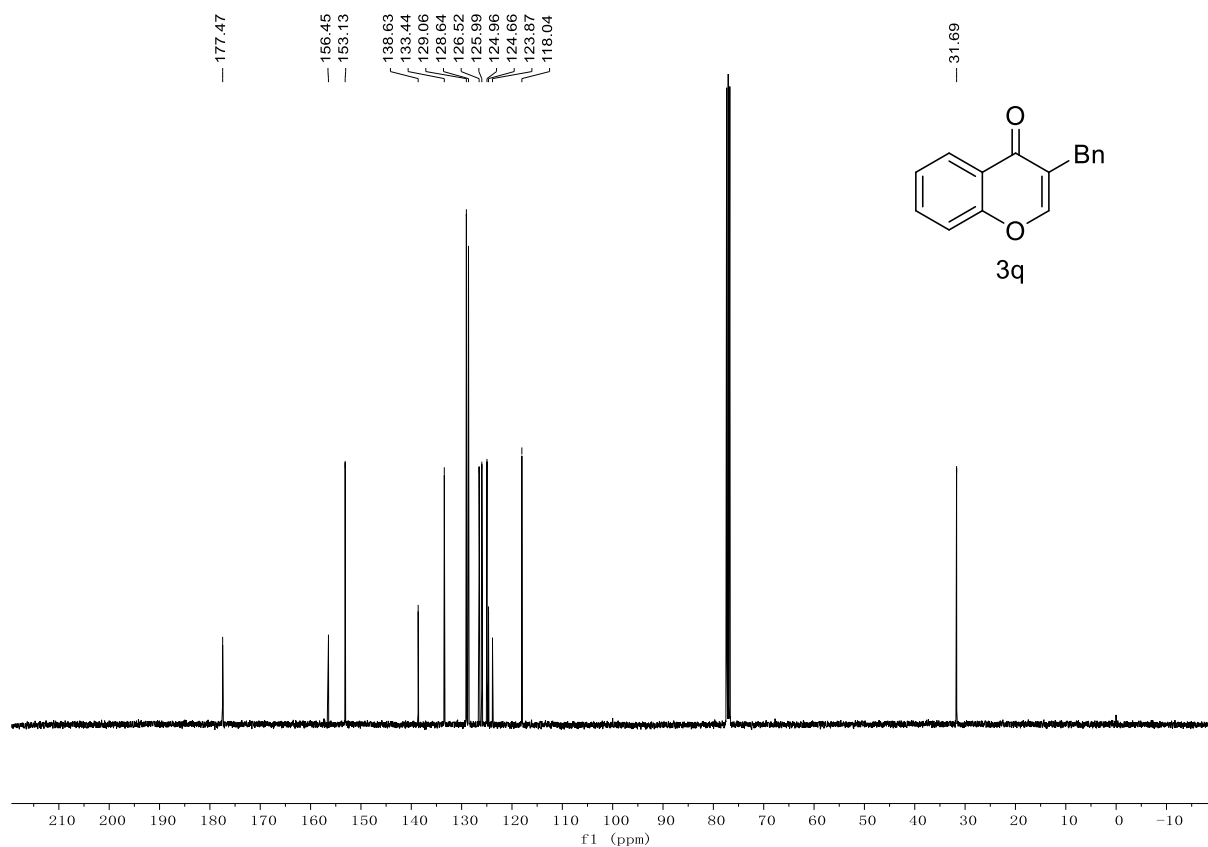
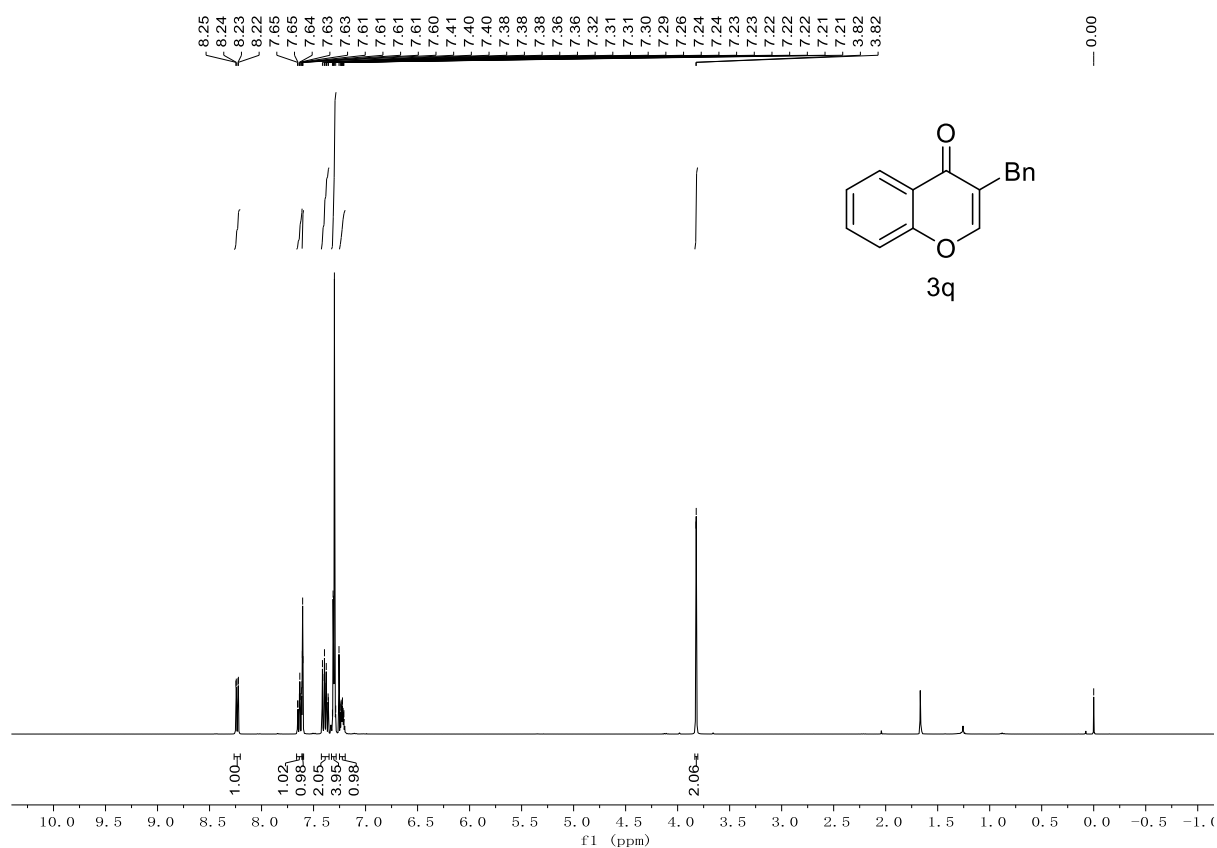
^1H and ^{13}C -NMR of 3o



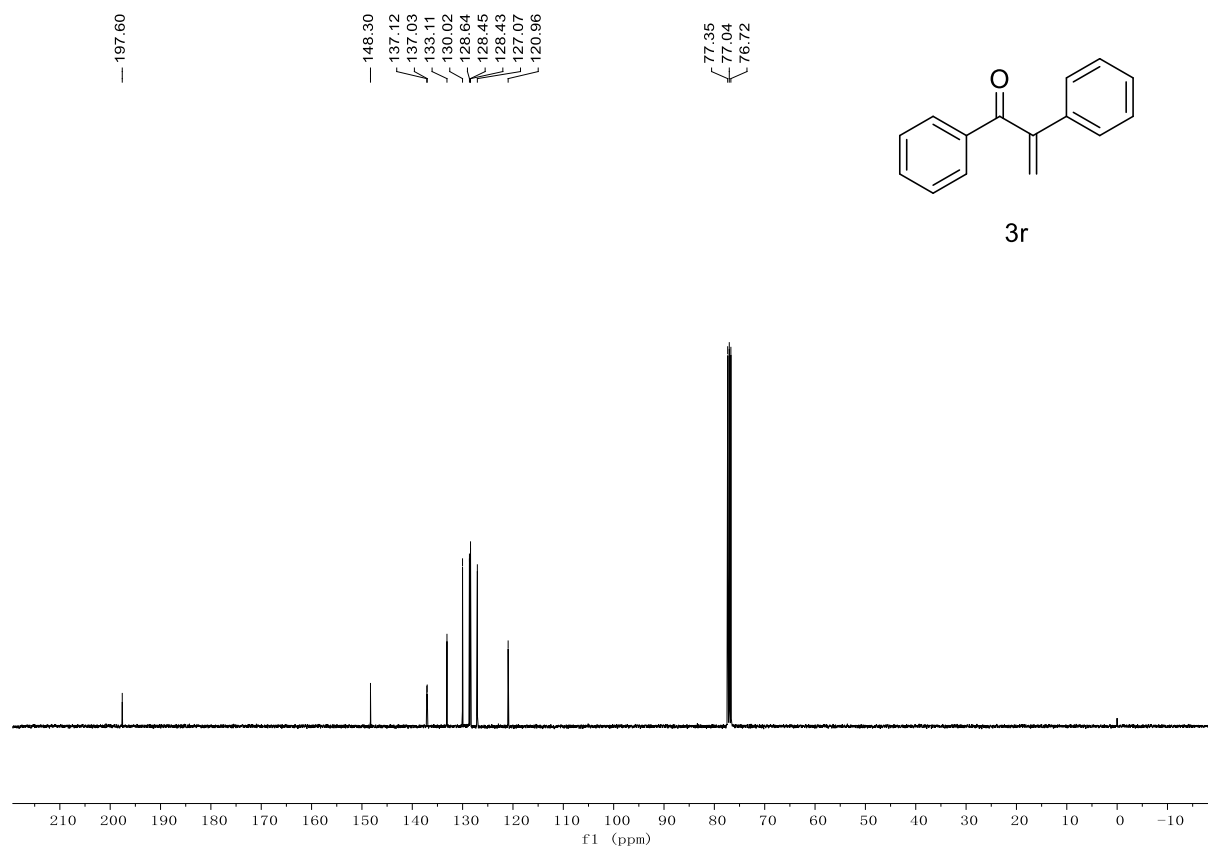
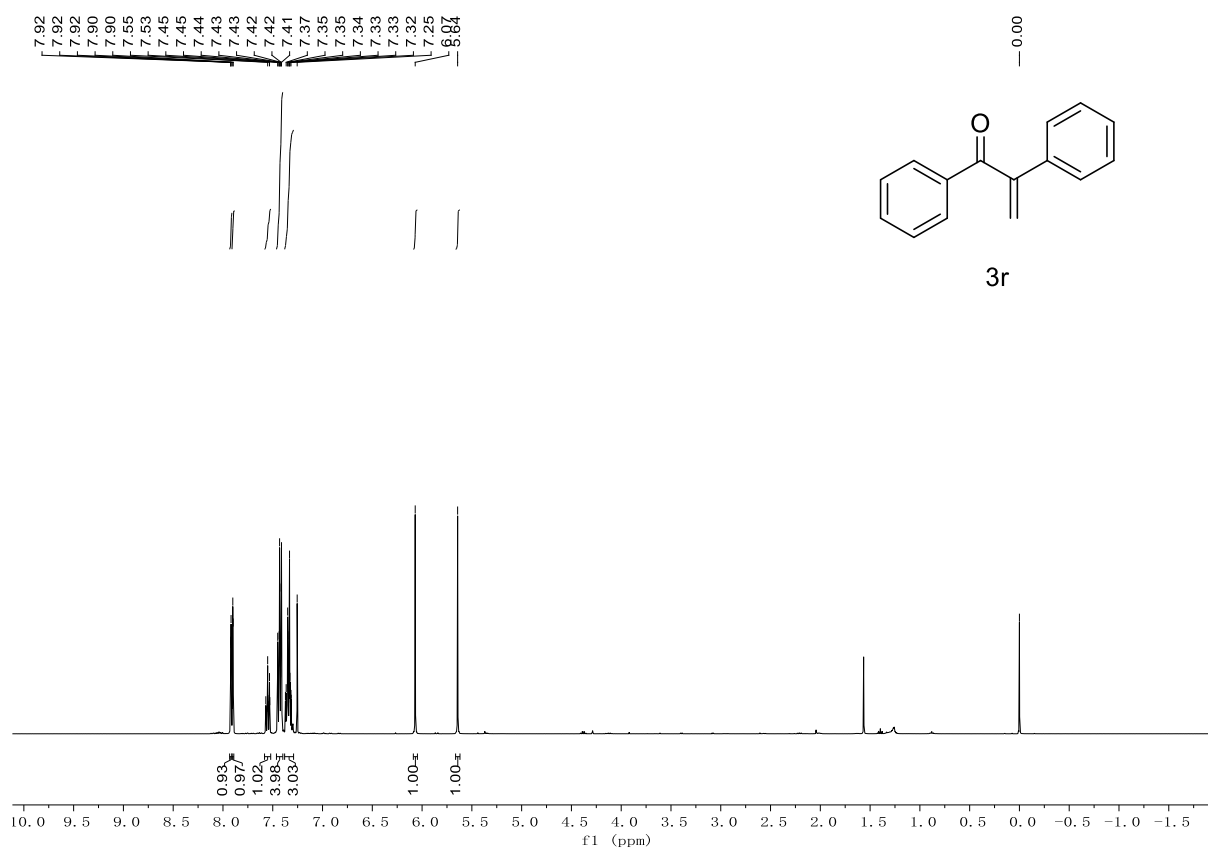
¹H and ¹³C-NMR of 3p



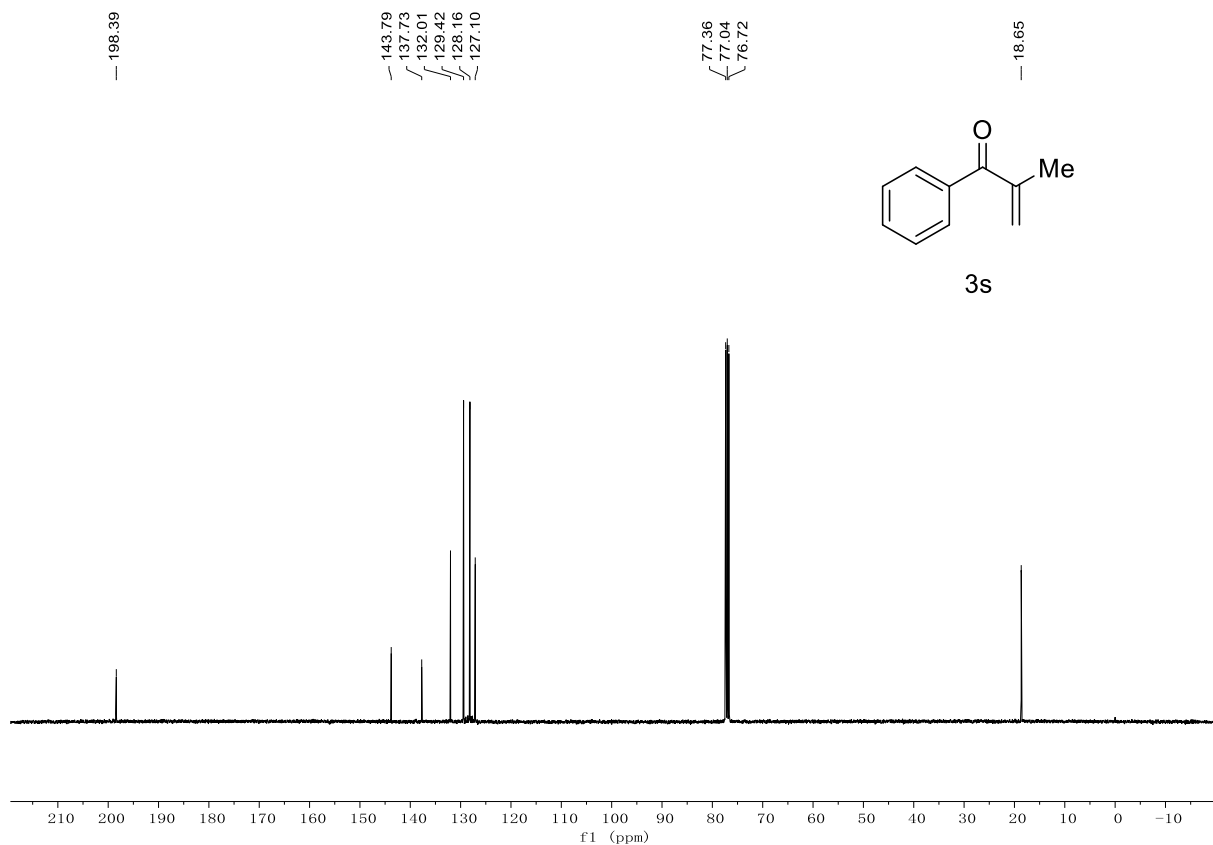
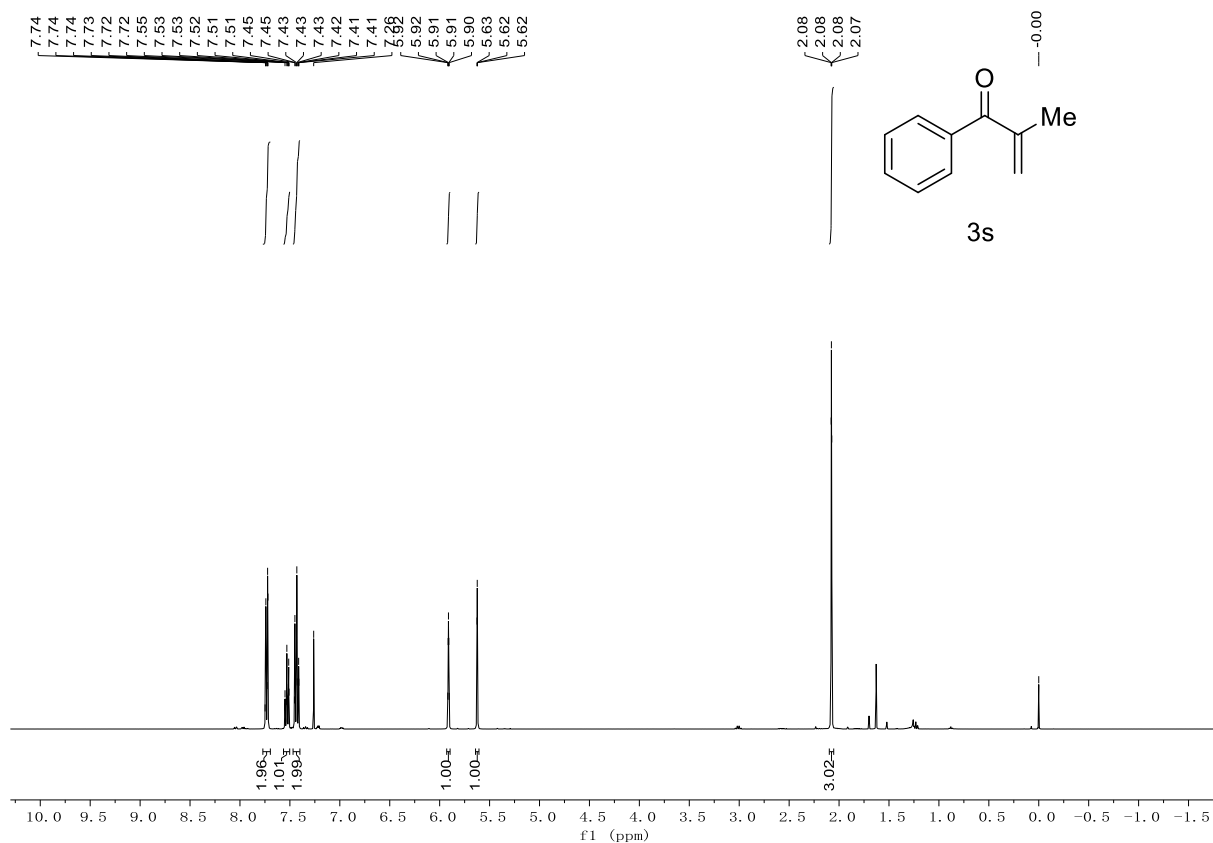
¹H and ¹³C-NMR of 3q



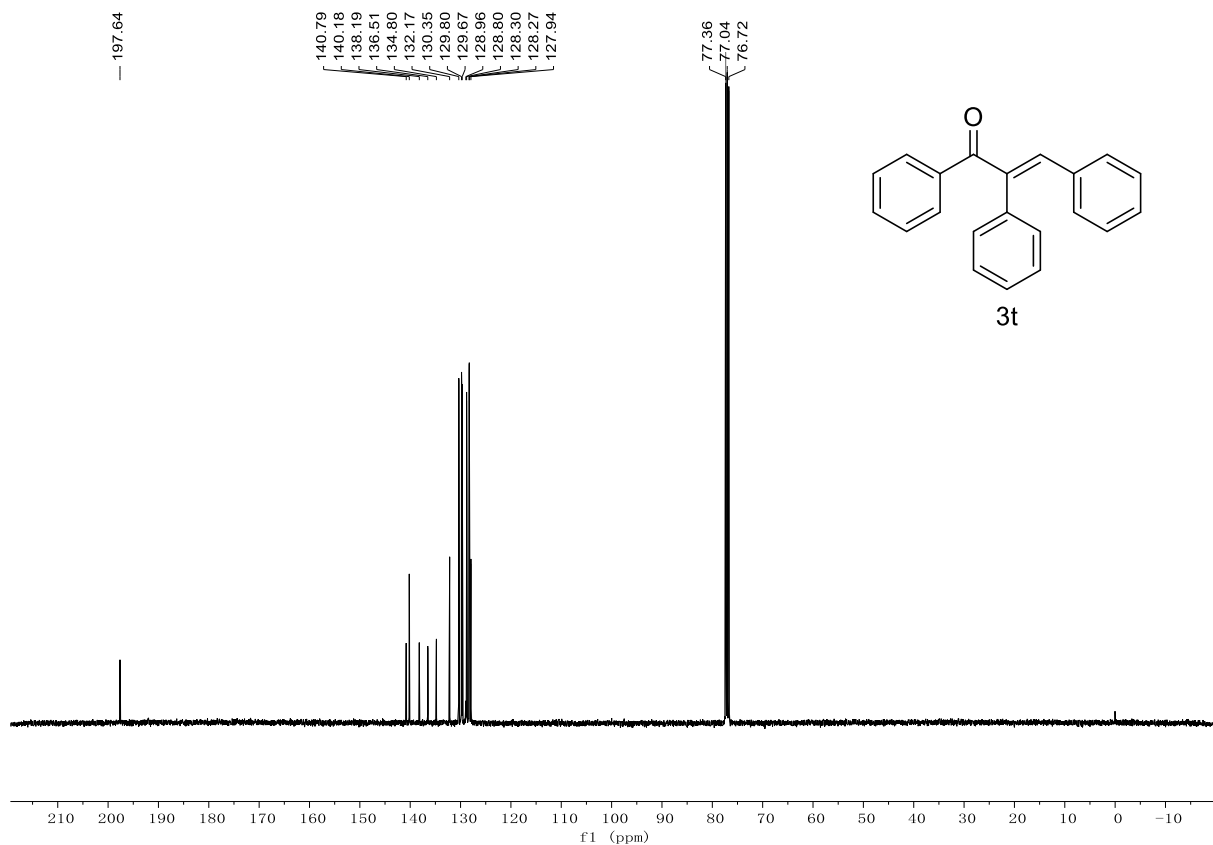
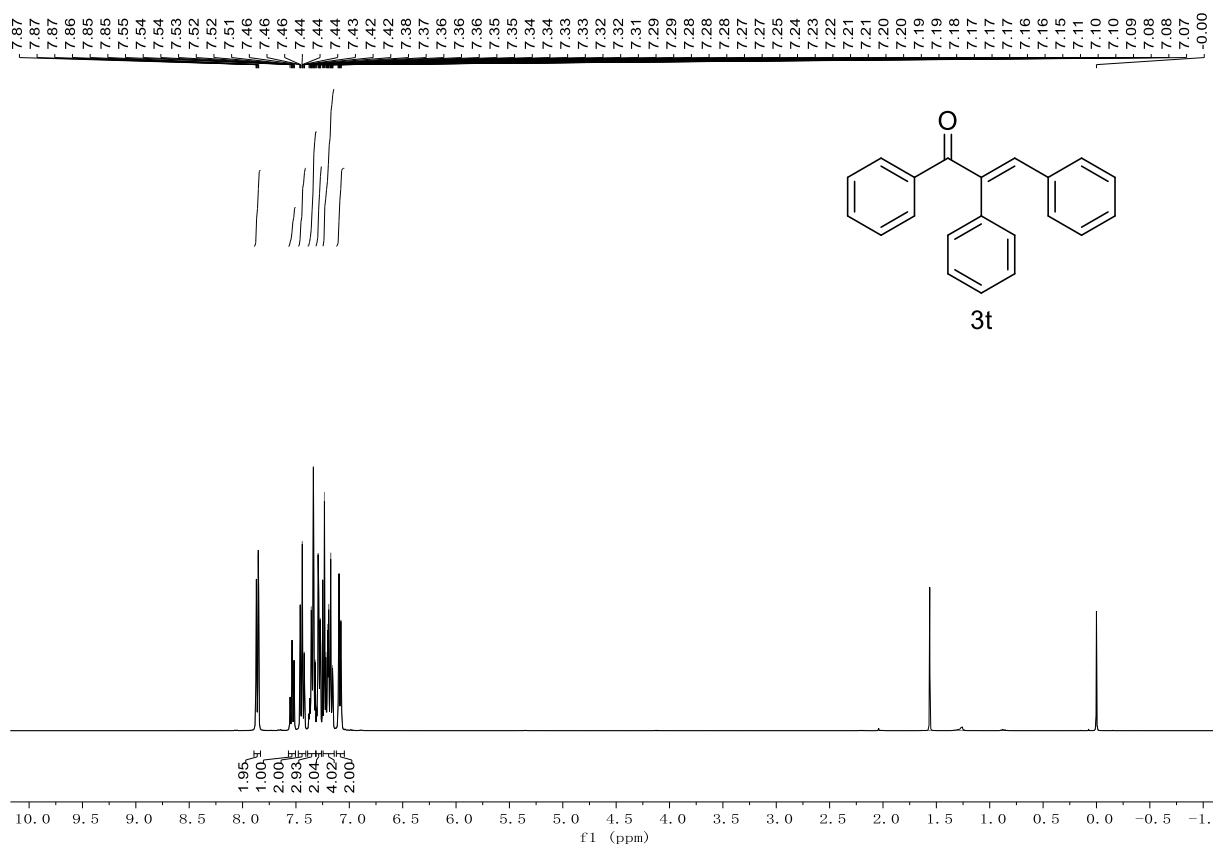
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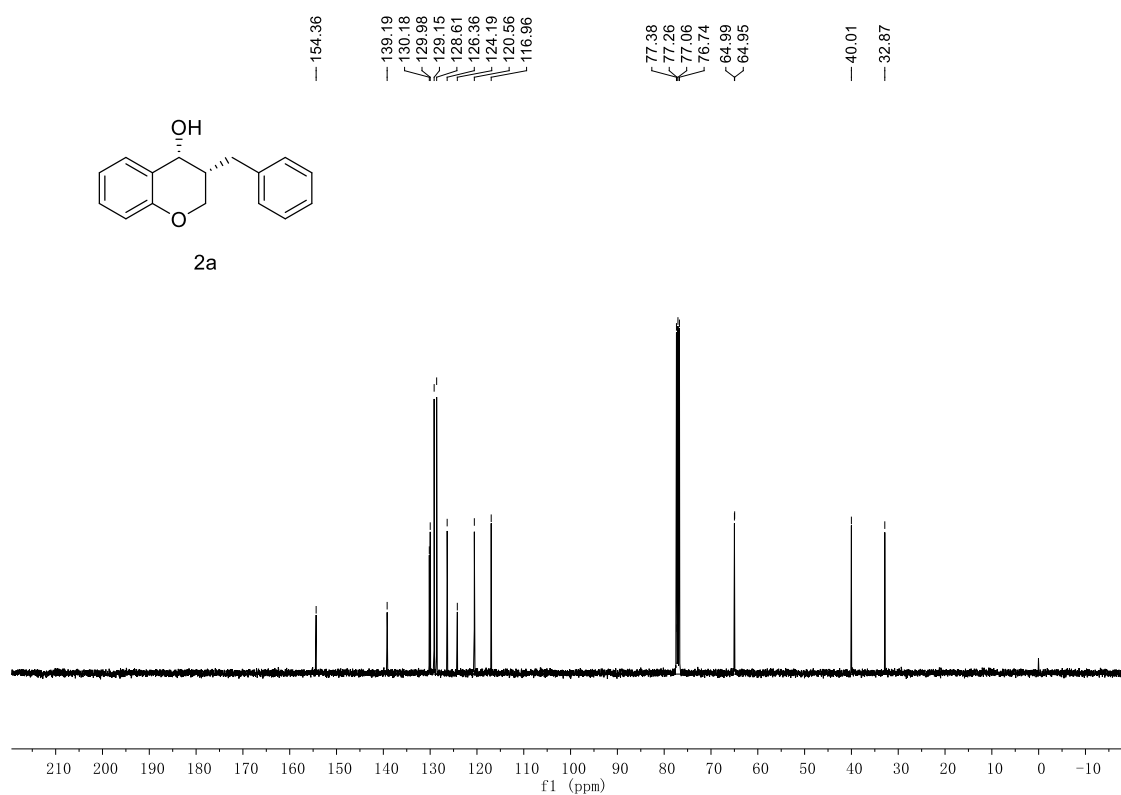
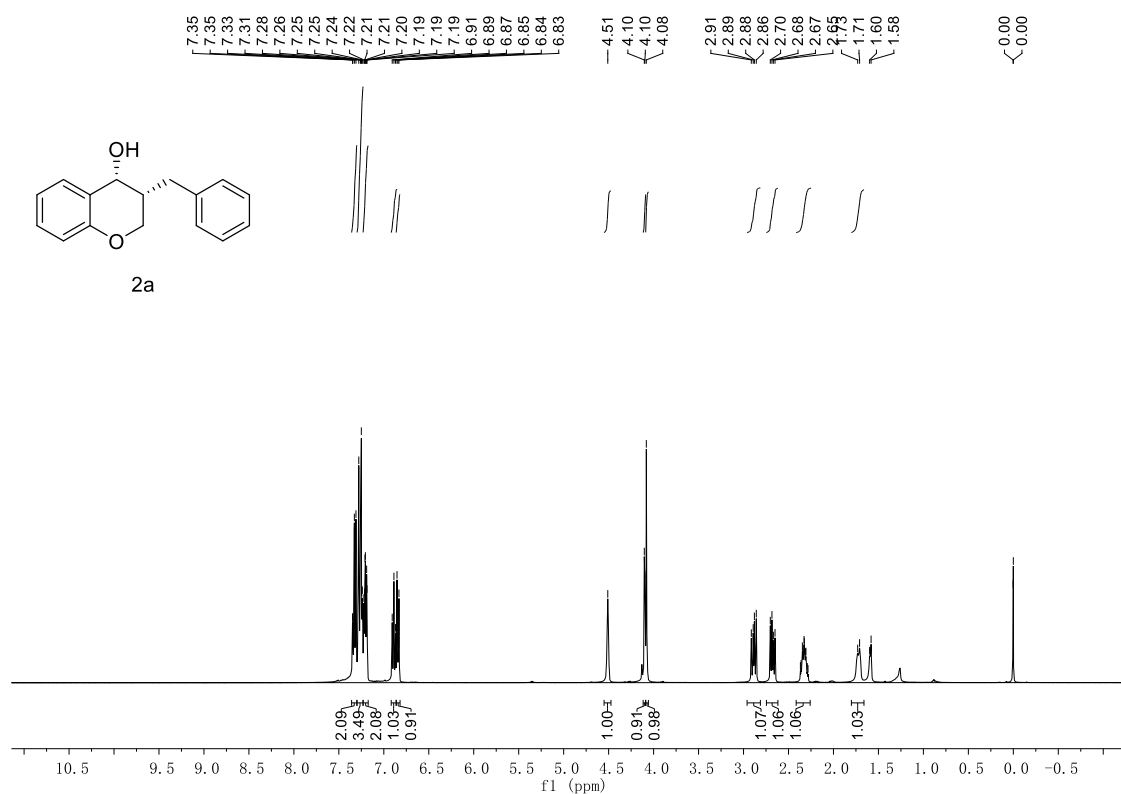
¹H and ¹³C-NMR of 3s



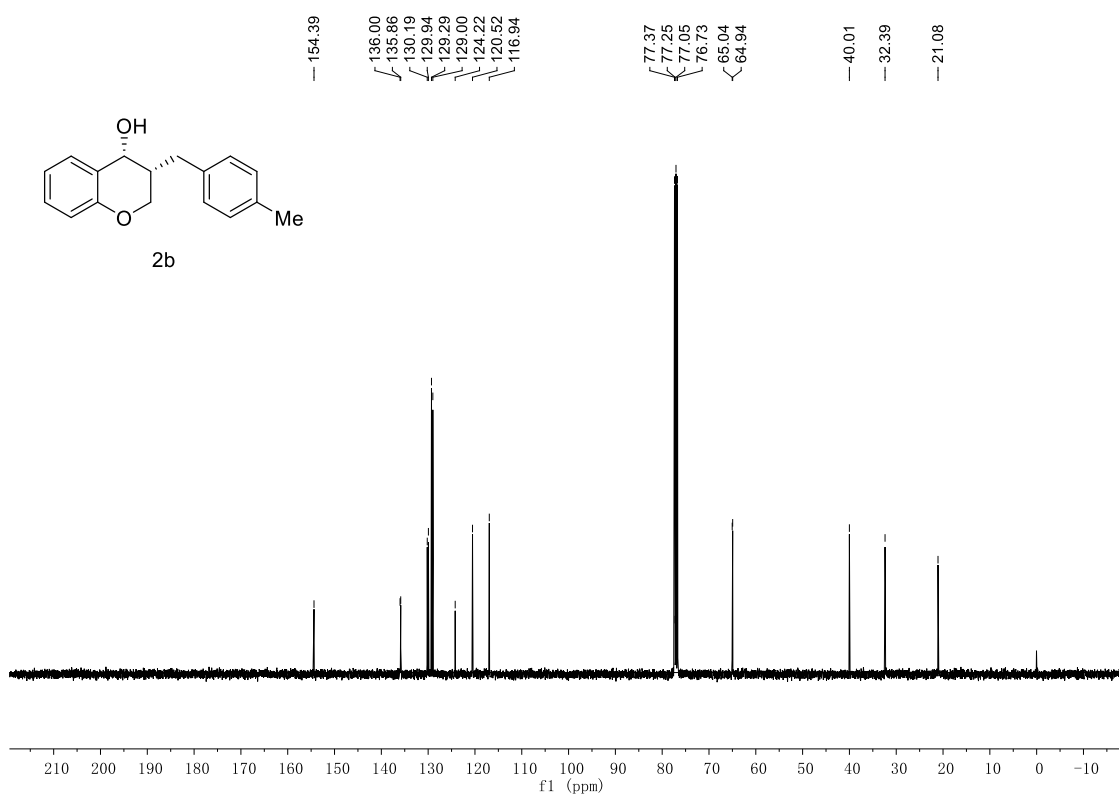
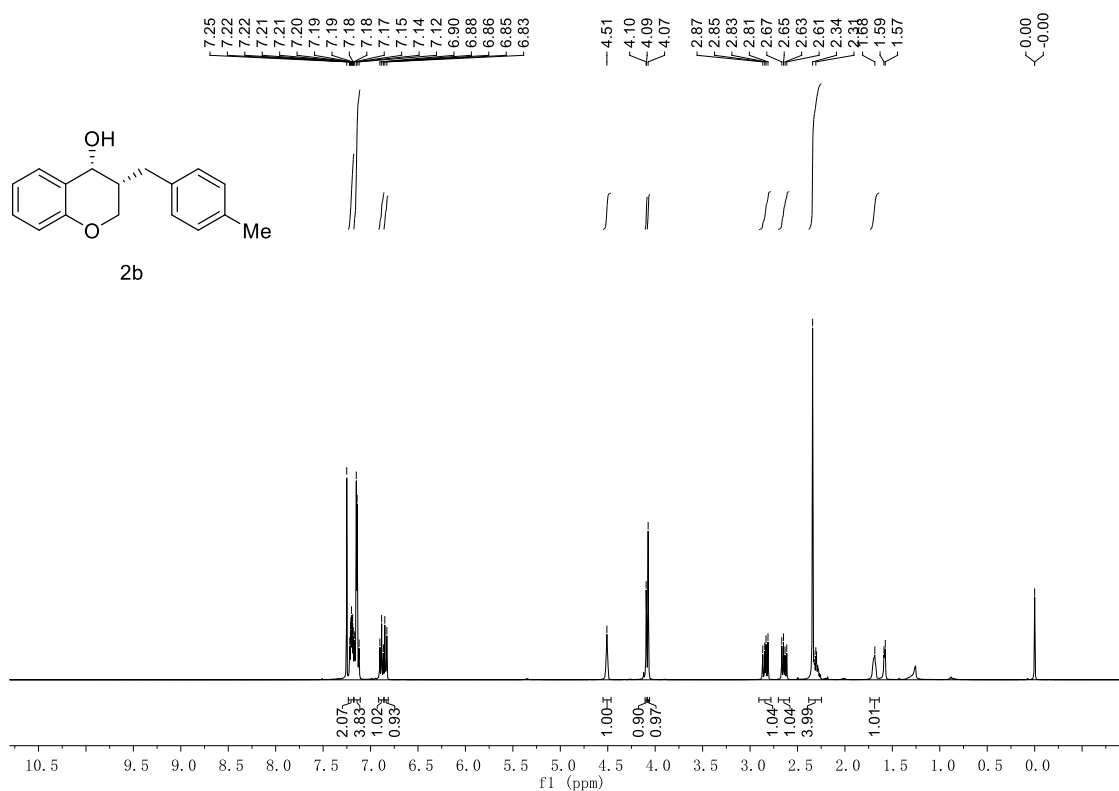
¹H and ¹³C-NMR of 3t



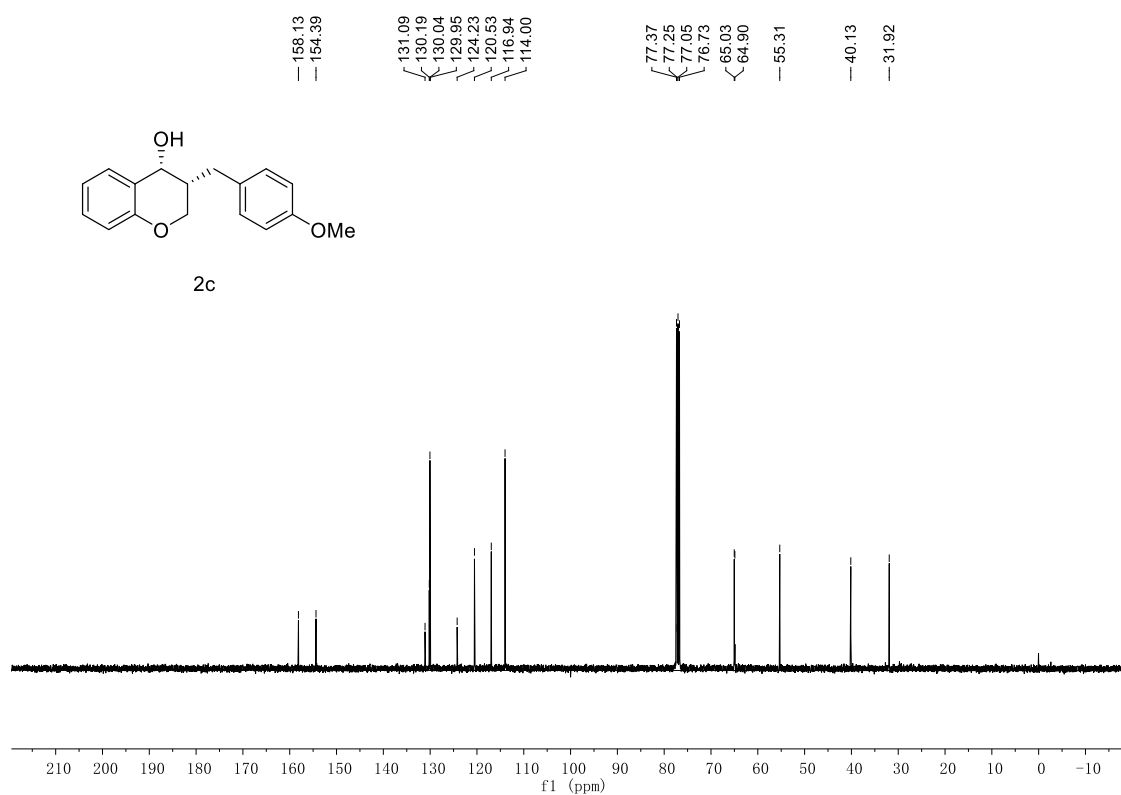
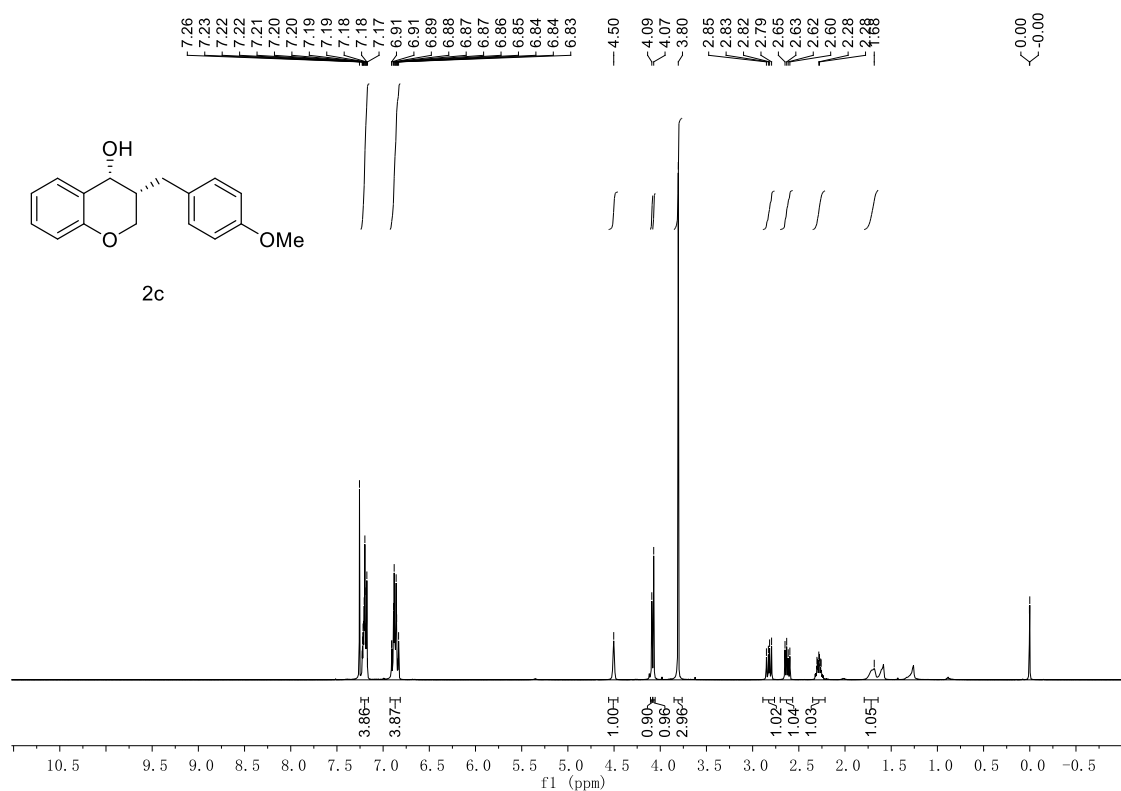
^1H and ^{13}C -NMR of 2a



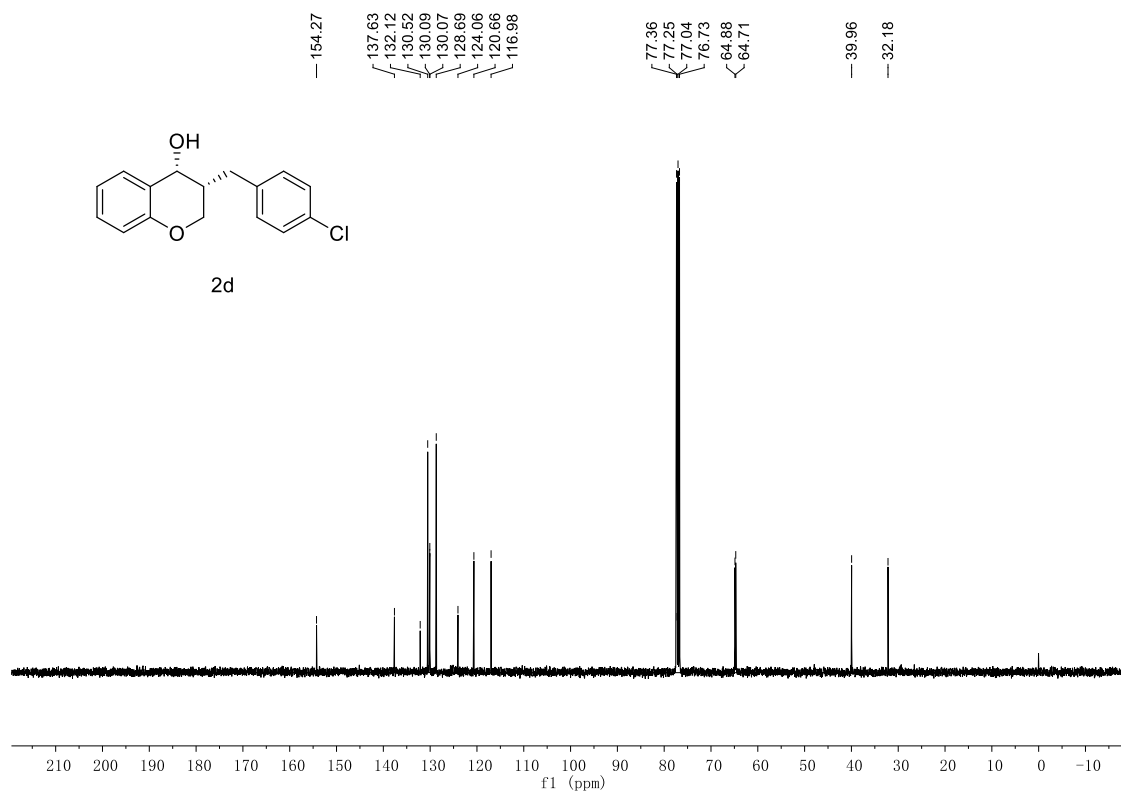
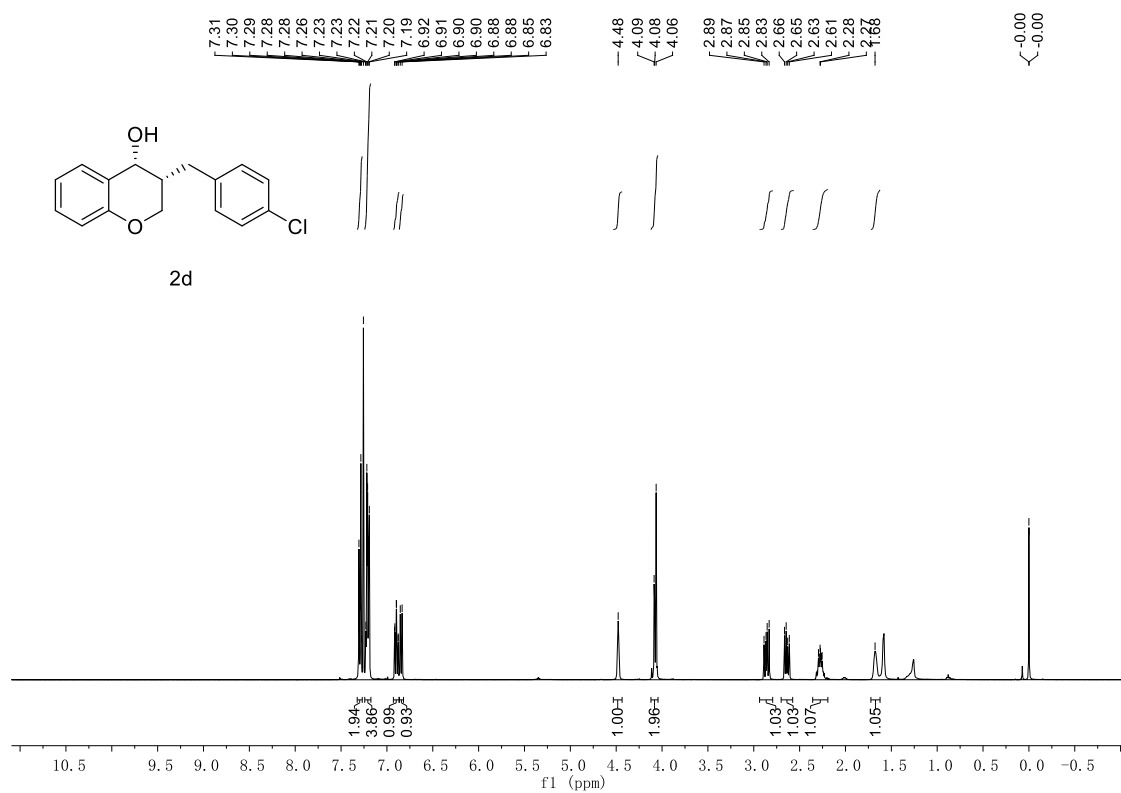
¹H and ¹³C-NMR of 2b



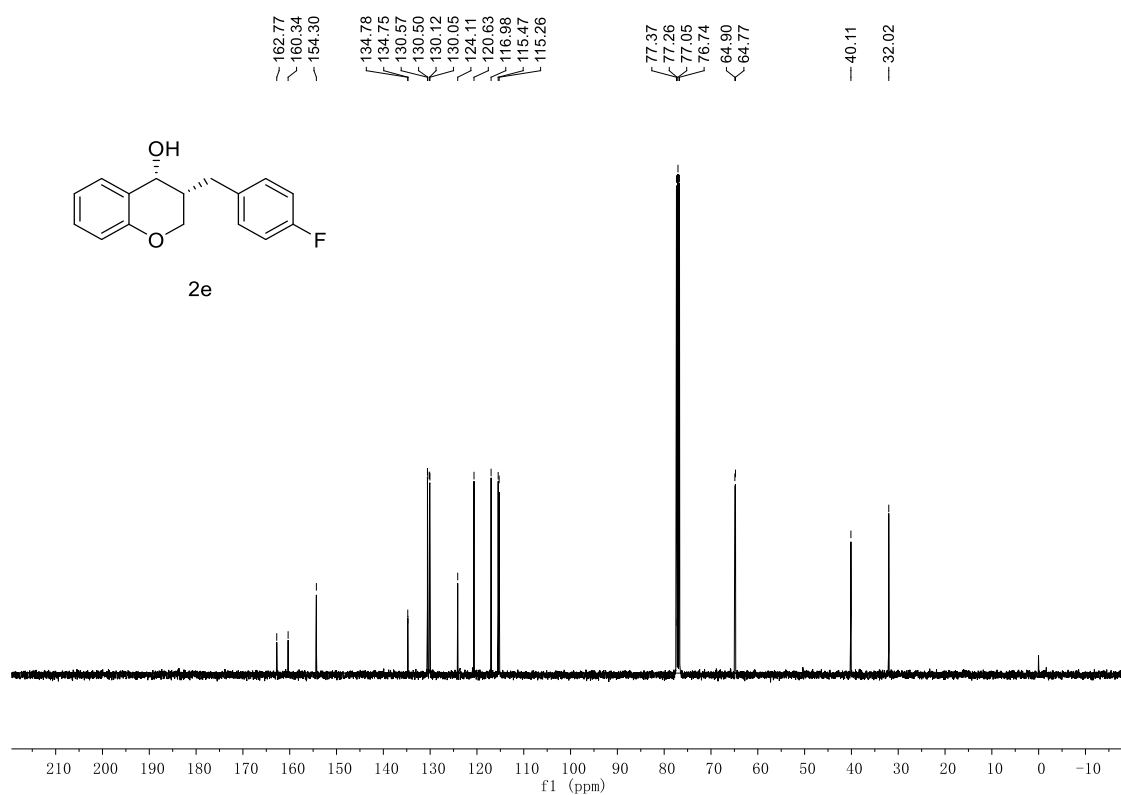
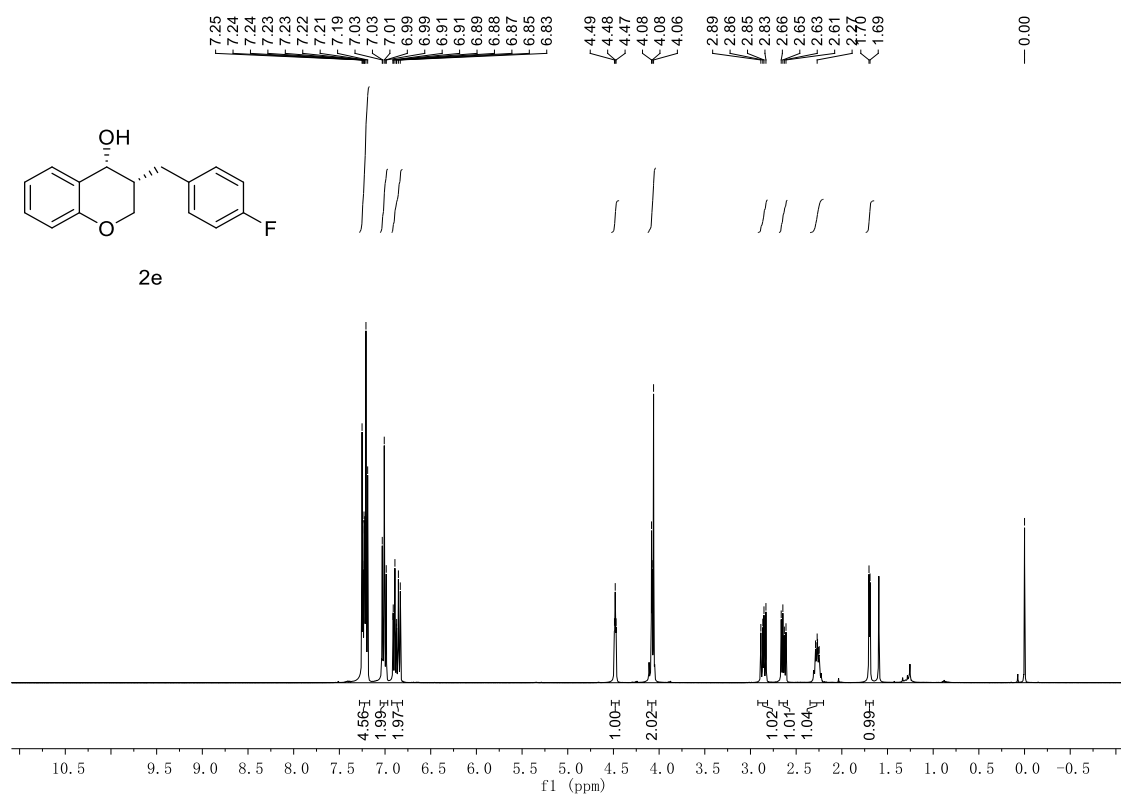
¹H and ¹³C-NMR of 2c



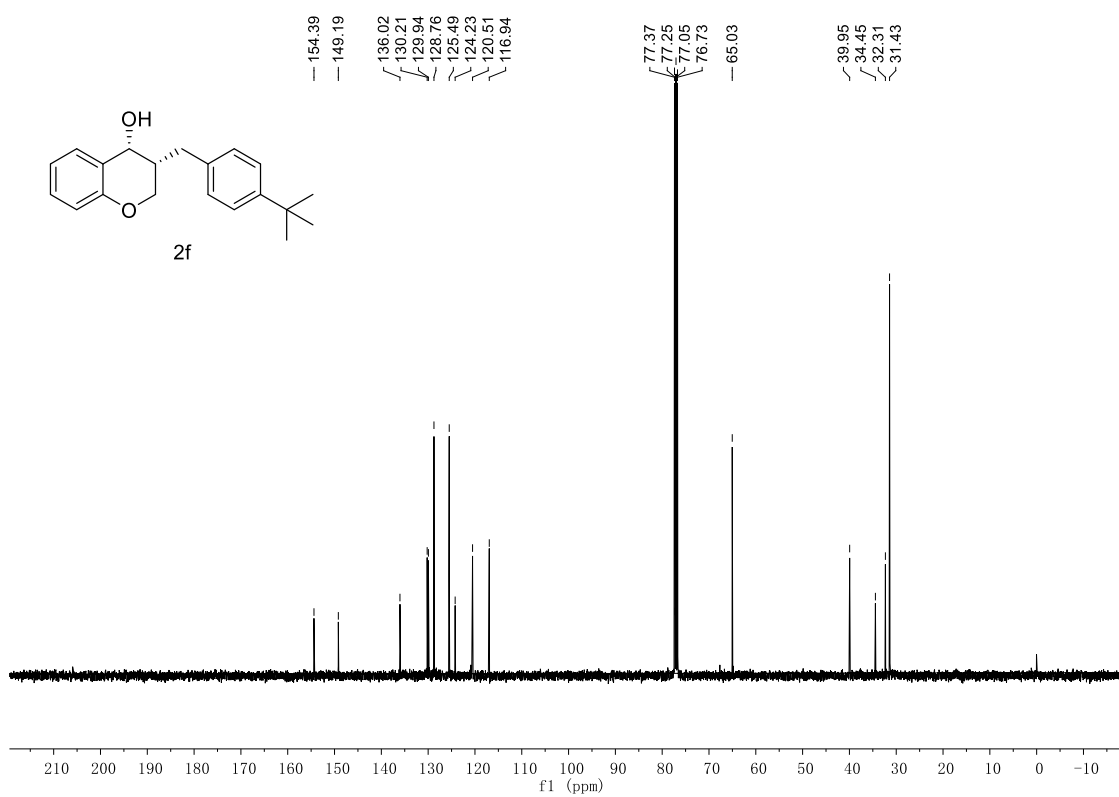
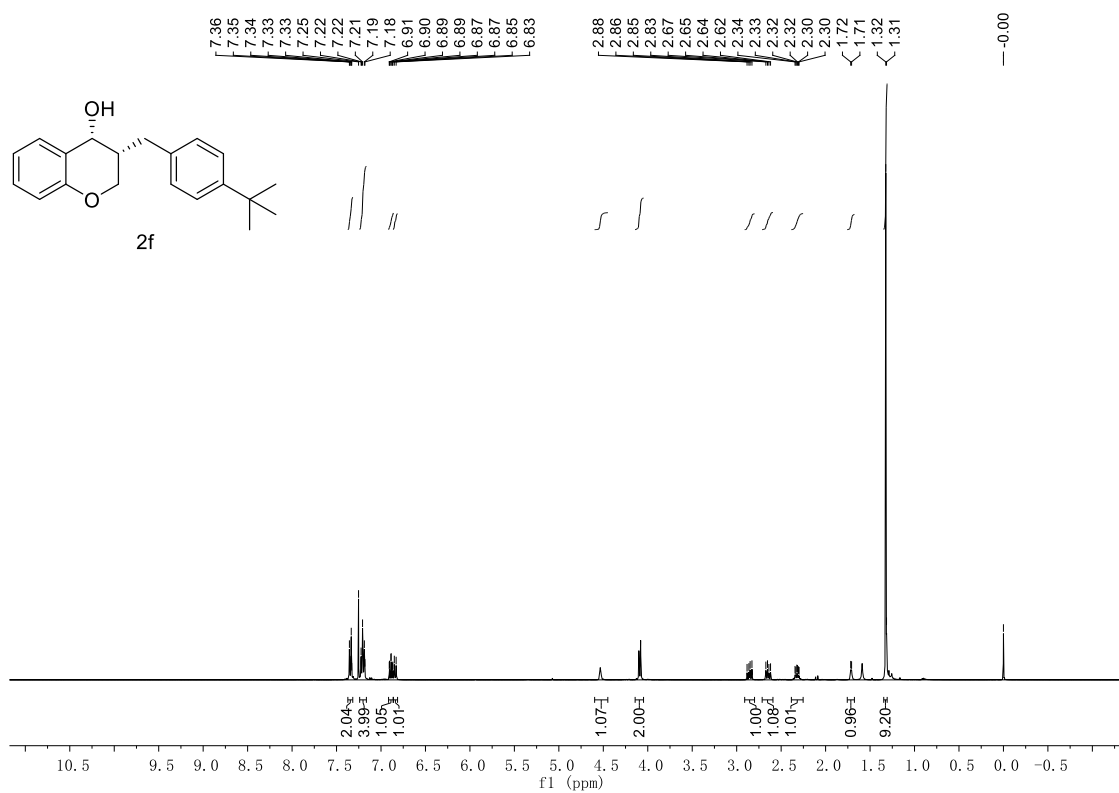
¹H and ¹³C-NMR of 2d



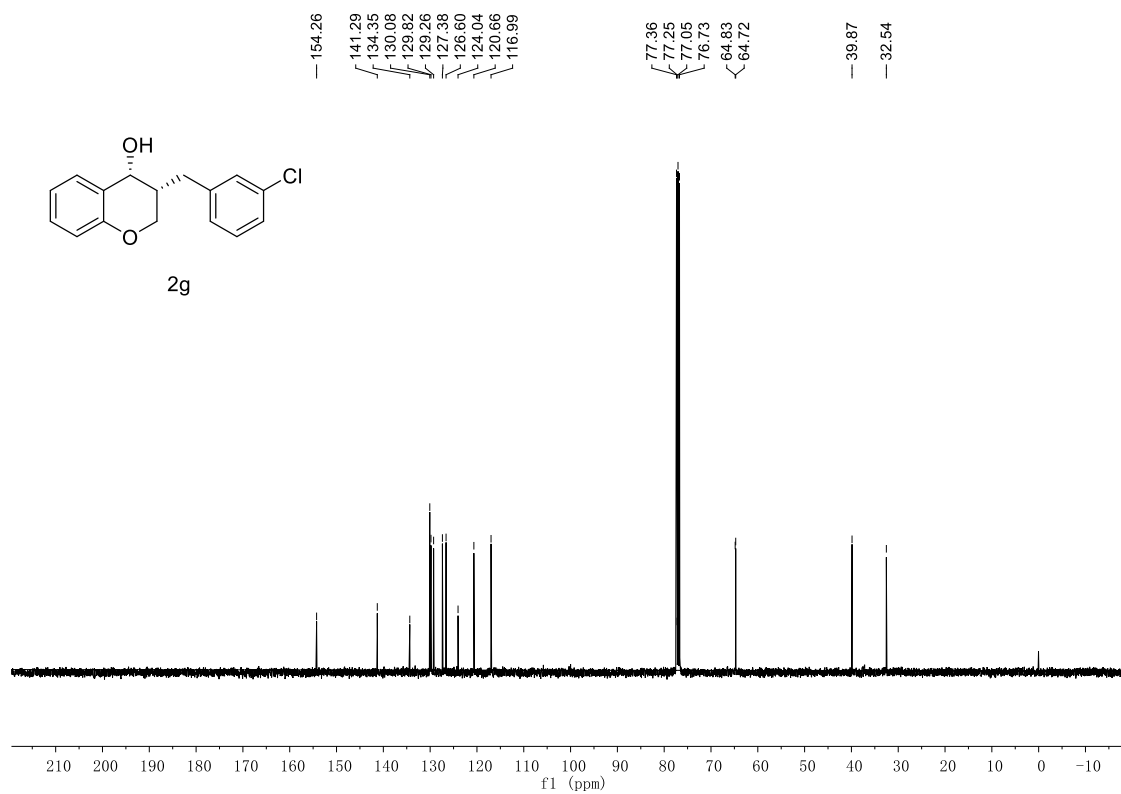
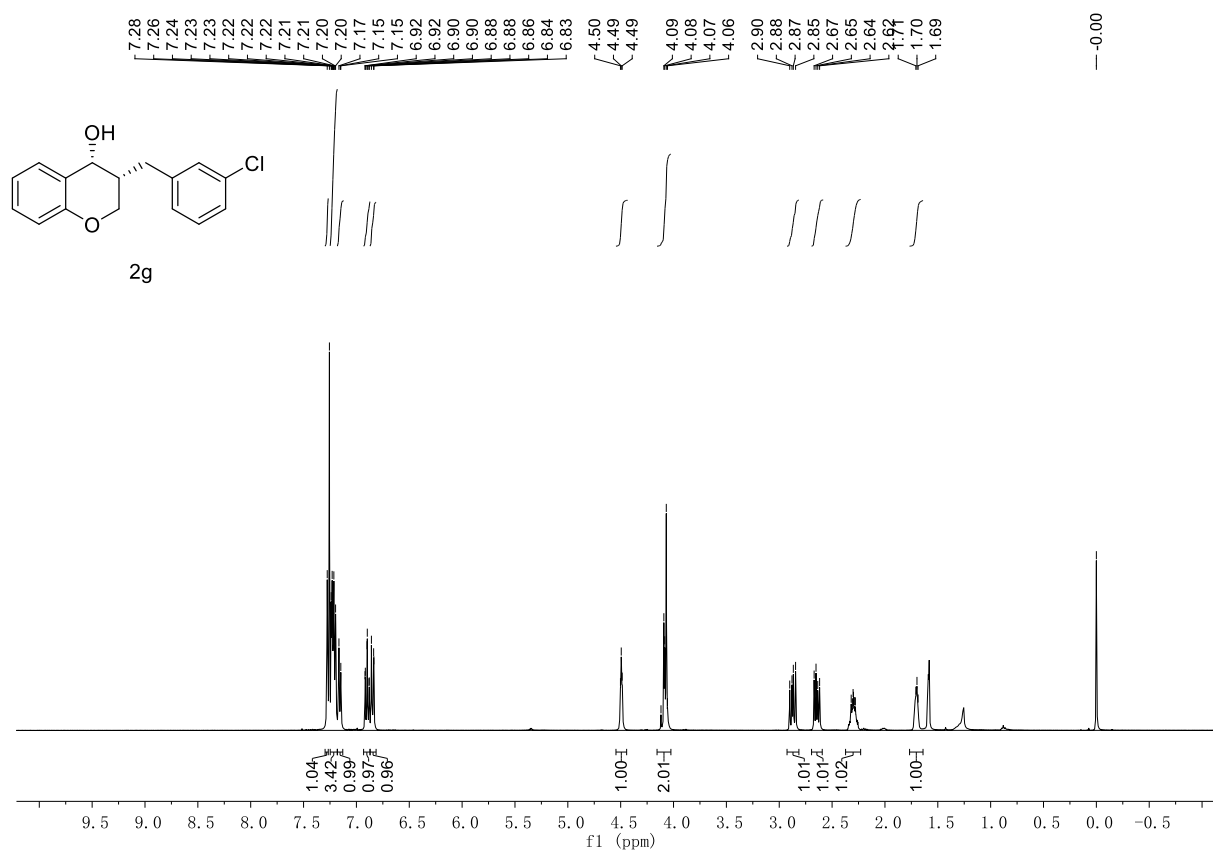
¹H and ¹³C-NMR of 2e



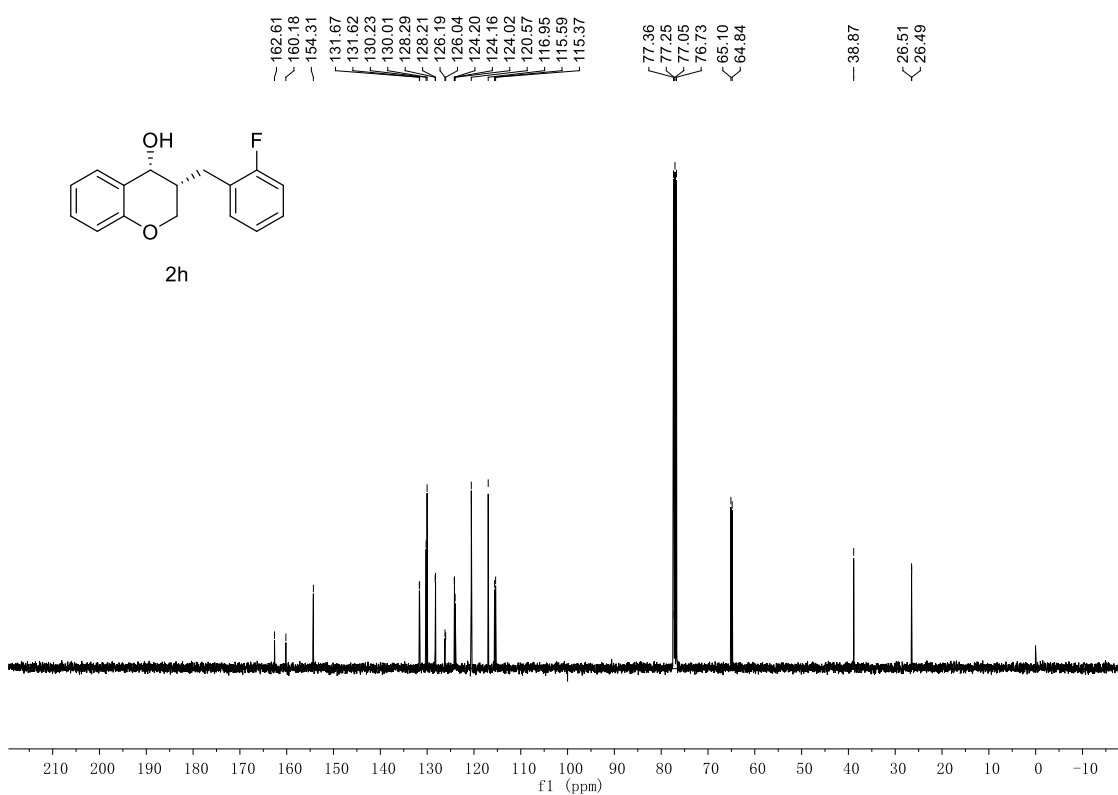
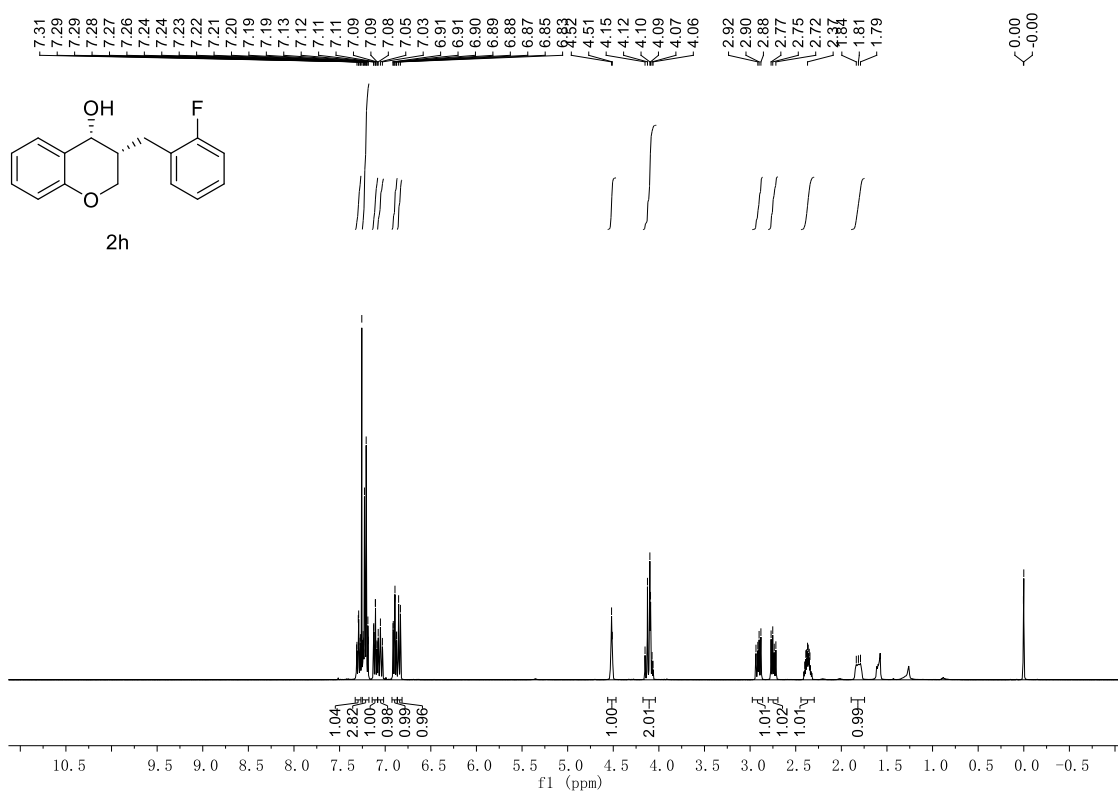
^1H and ^{13}C -NMR of 2f



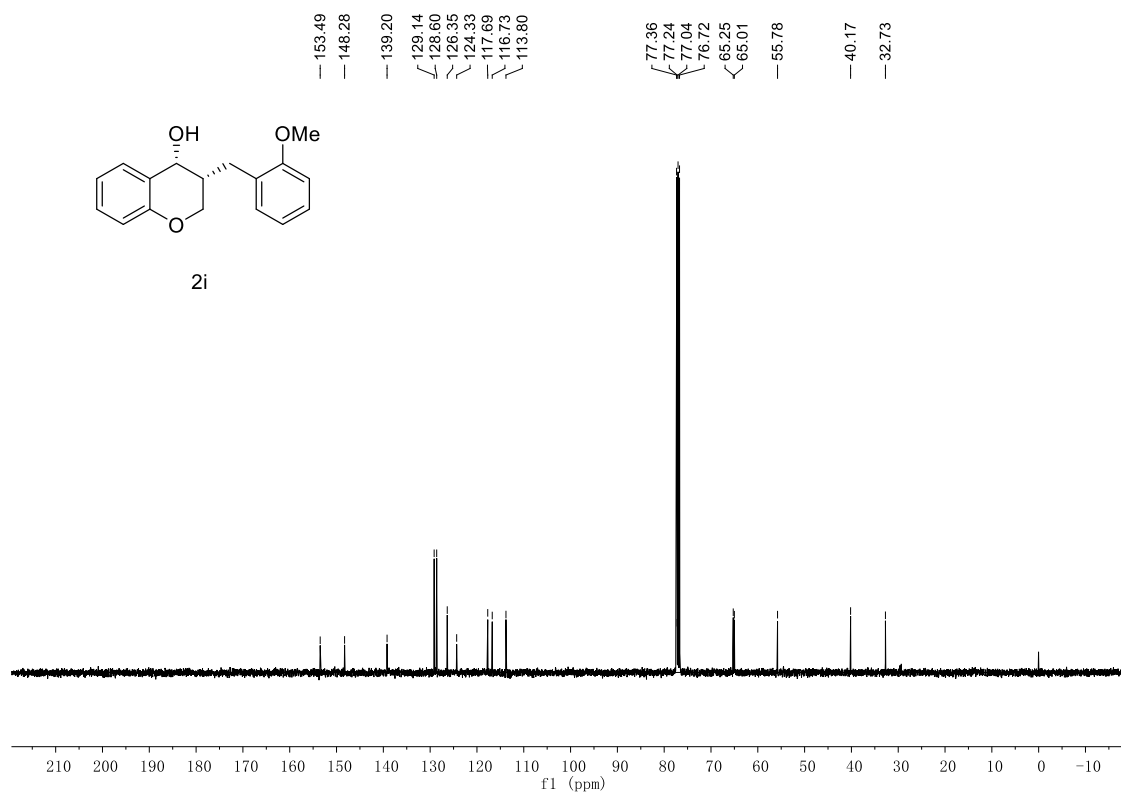
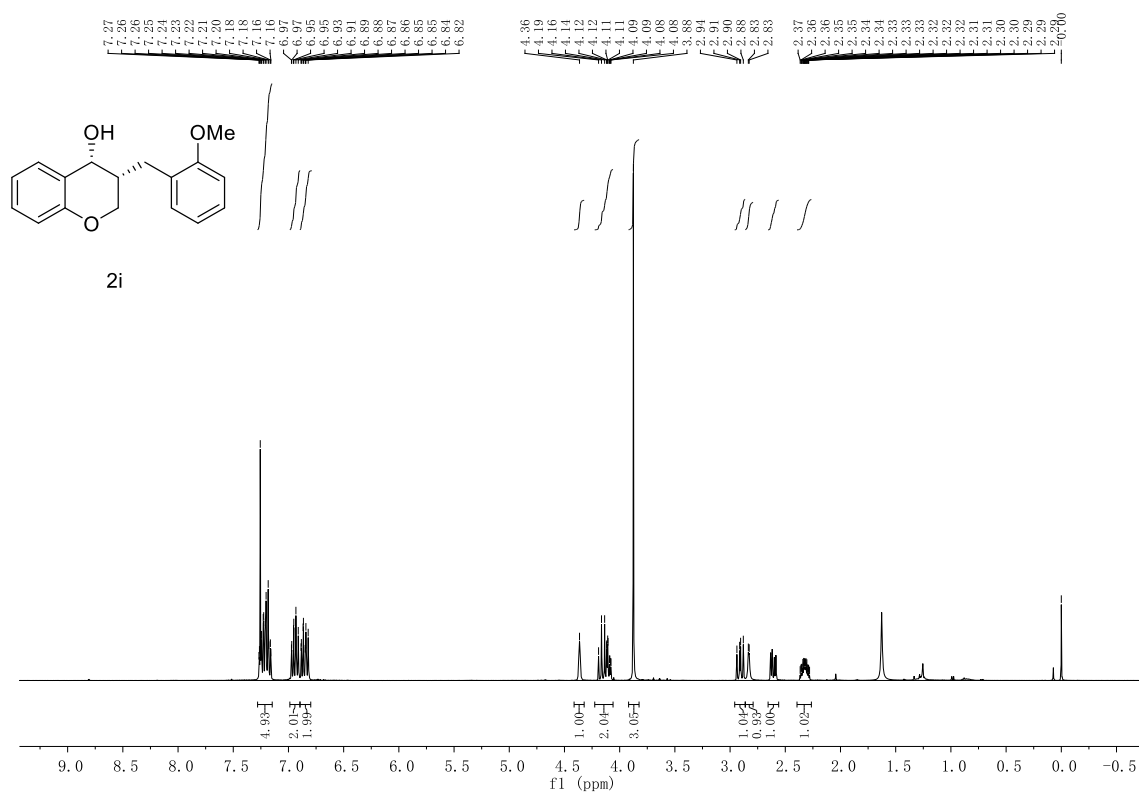
¹H and ¹³C-NMR of 2g



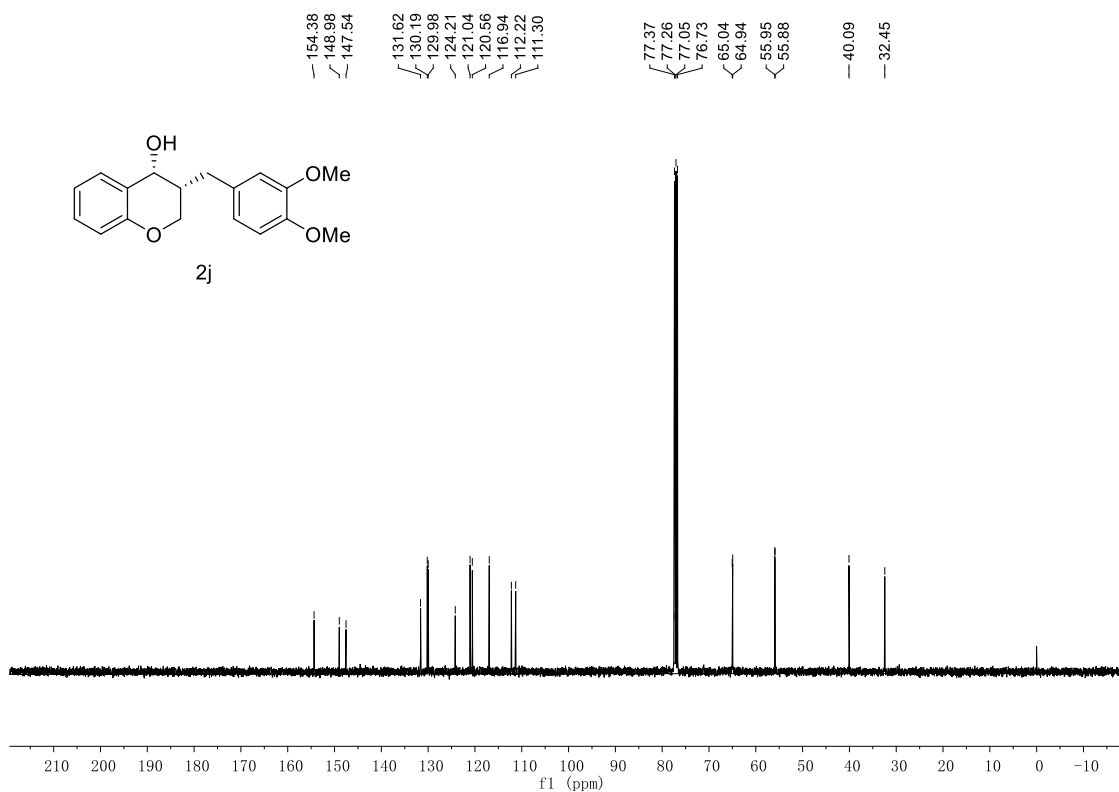
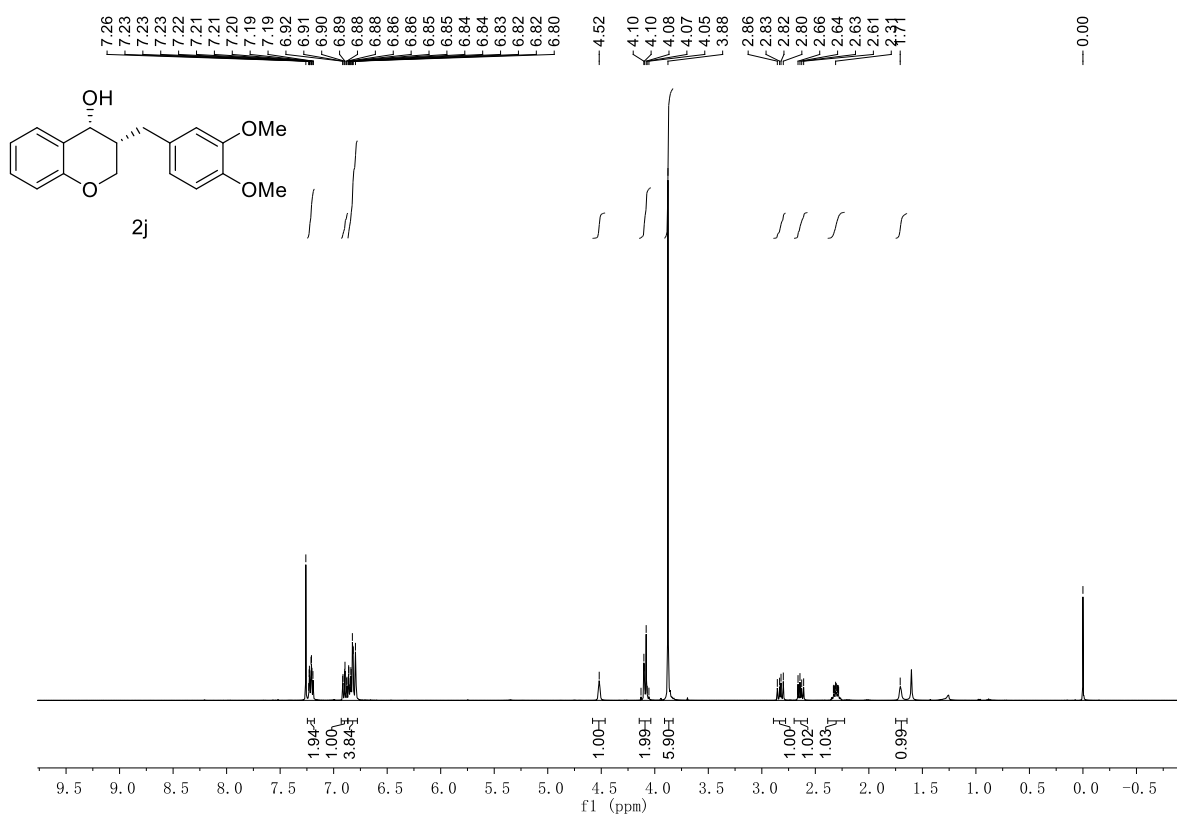
¹H and ¹³C-NMR of 2h



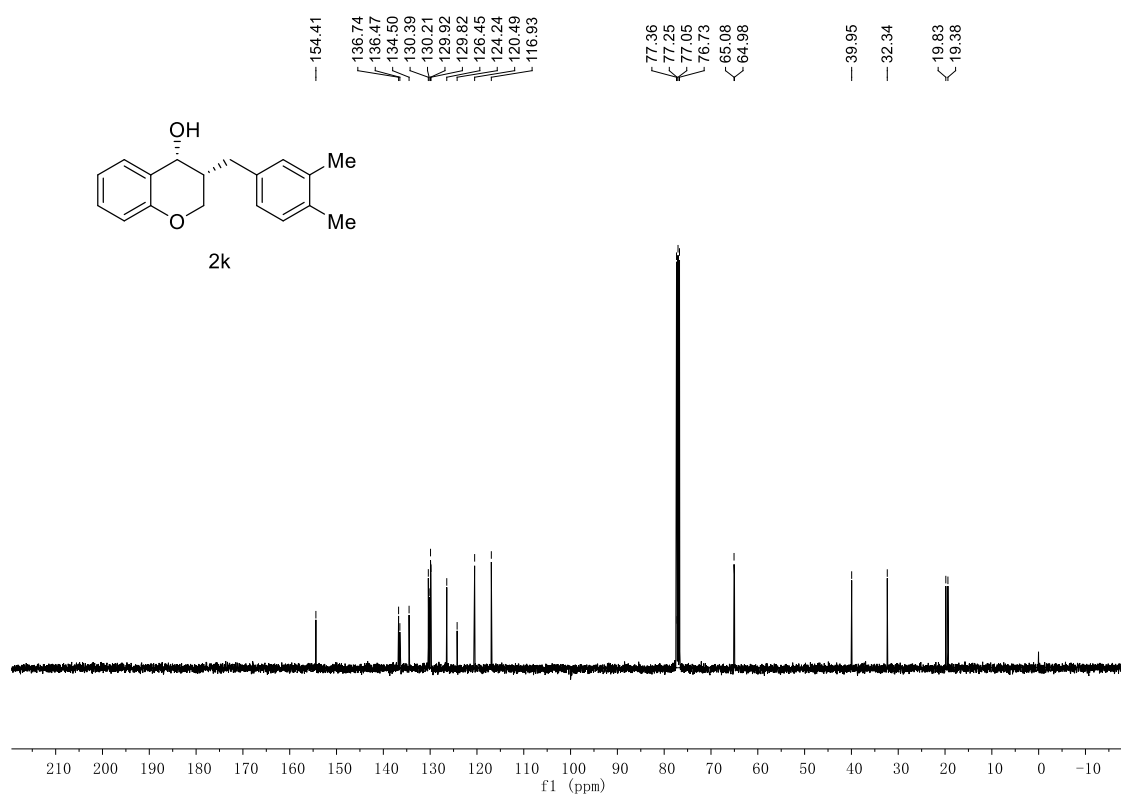
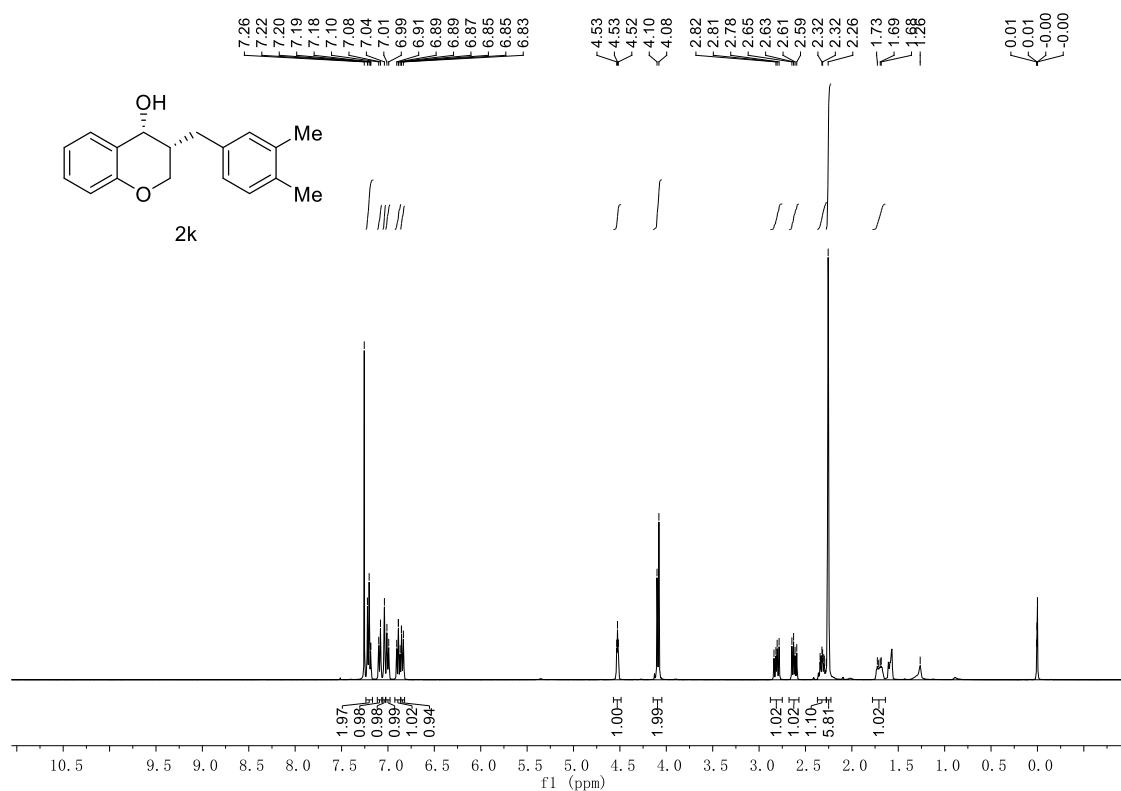
^1H and ^{13}C -NMR of 2i



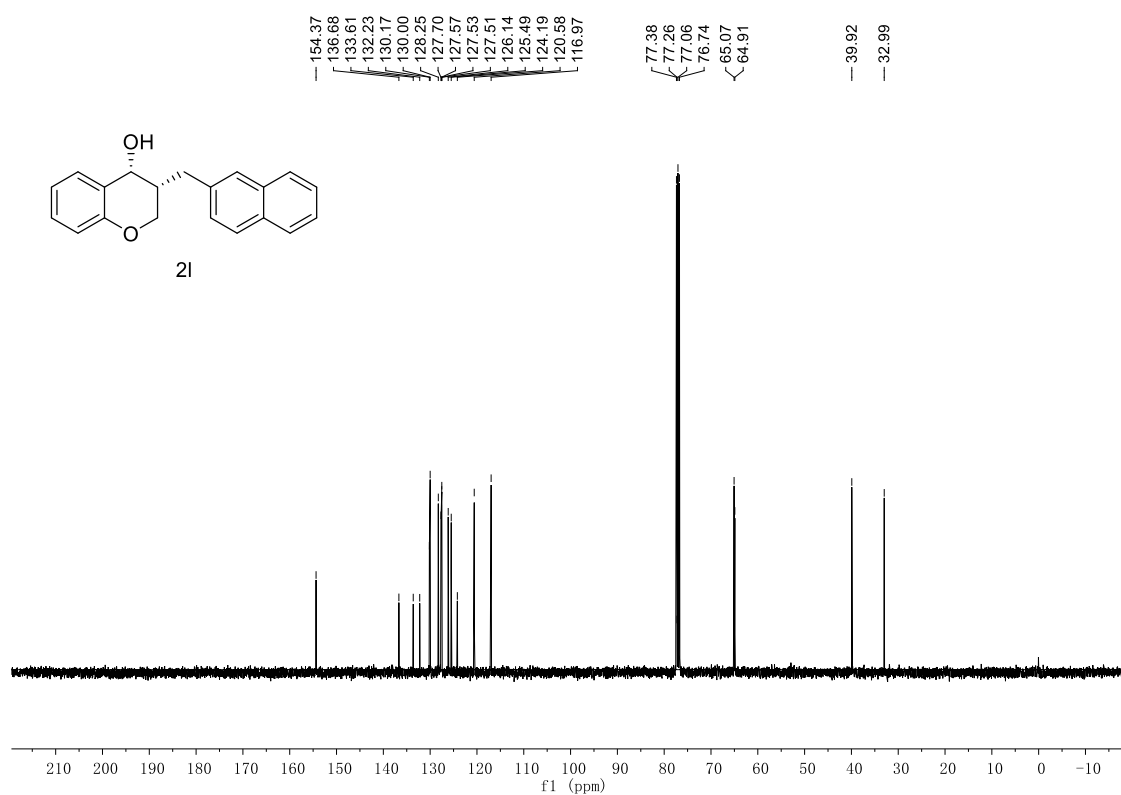
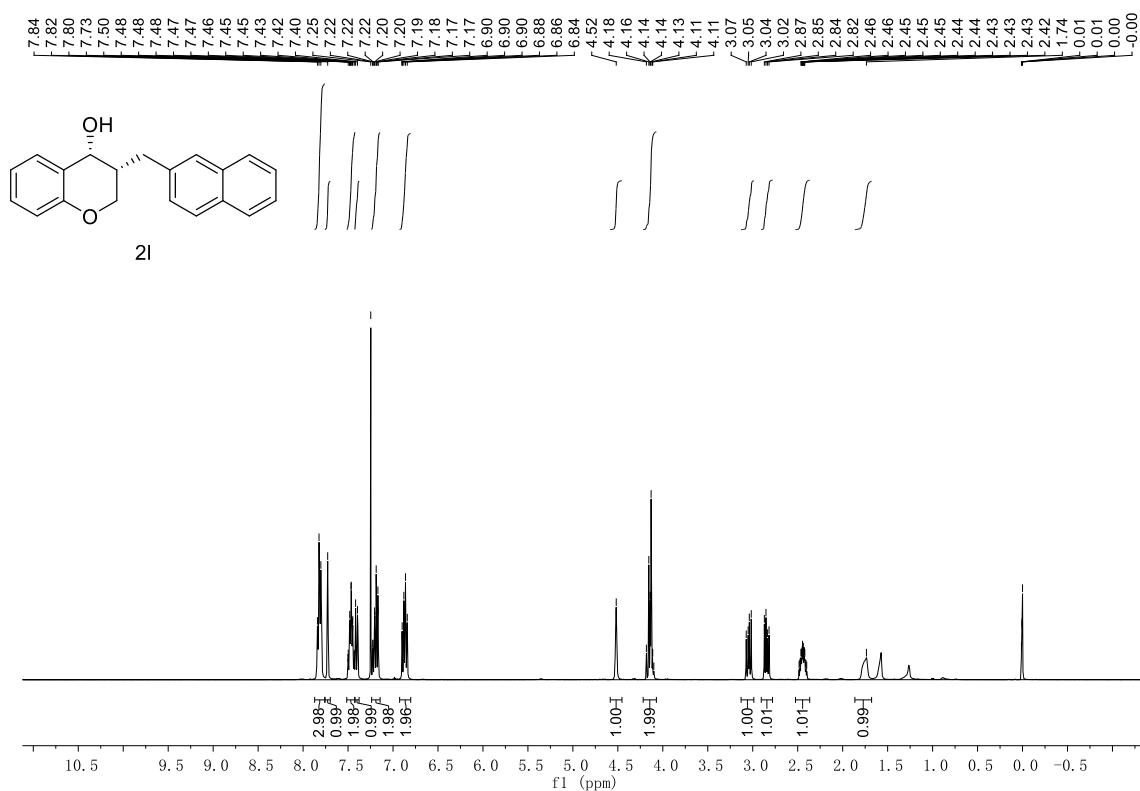
¹H and ¹³C-NMR of 2j



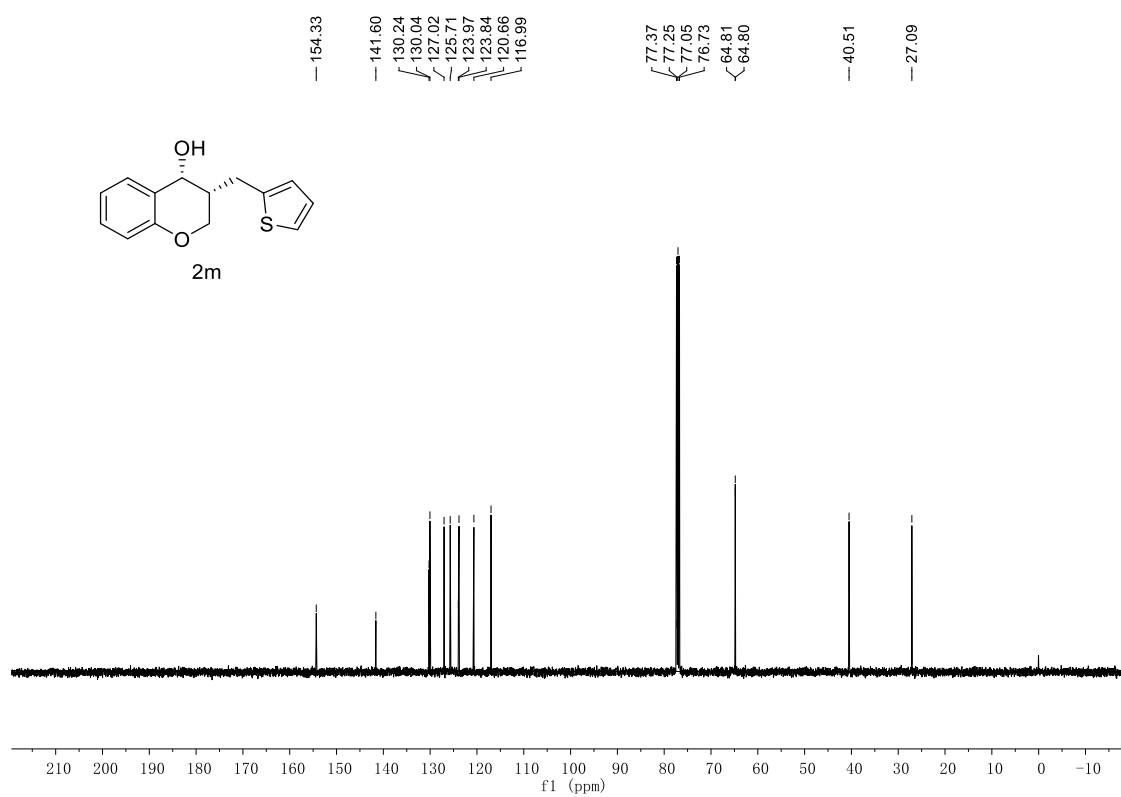
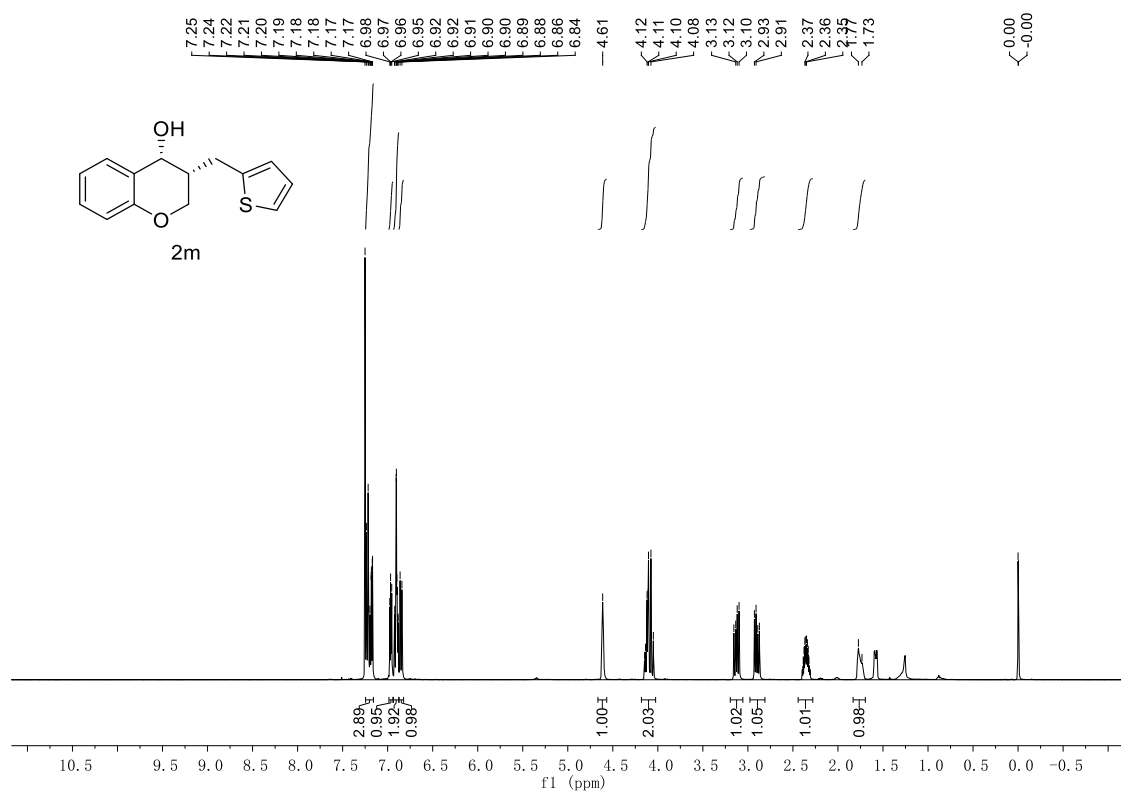
¹H and ¹³C-NMR of 2k



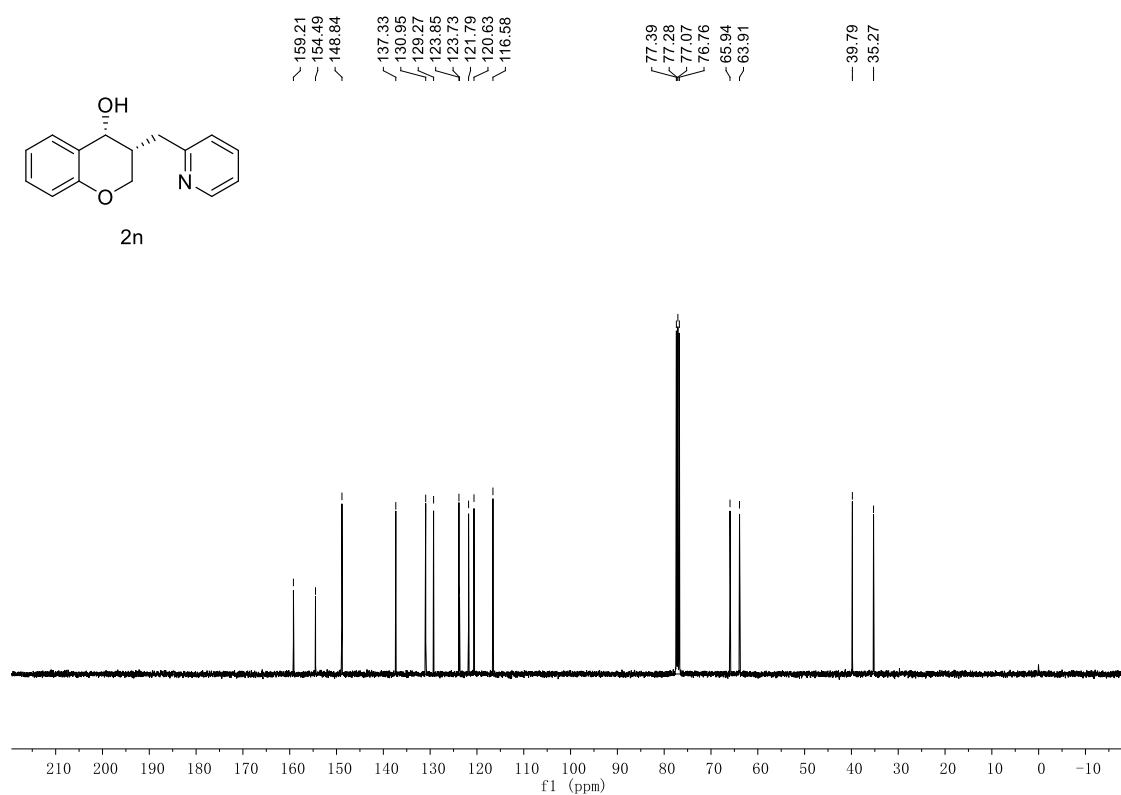
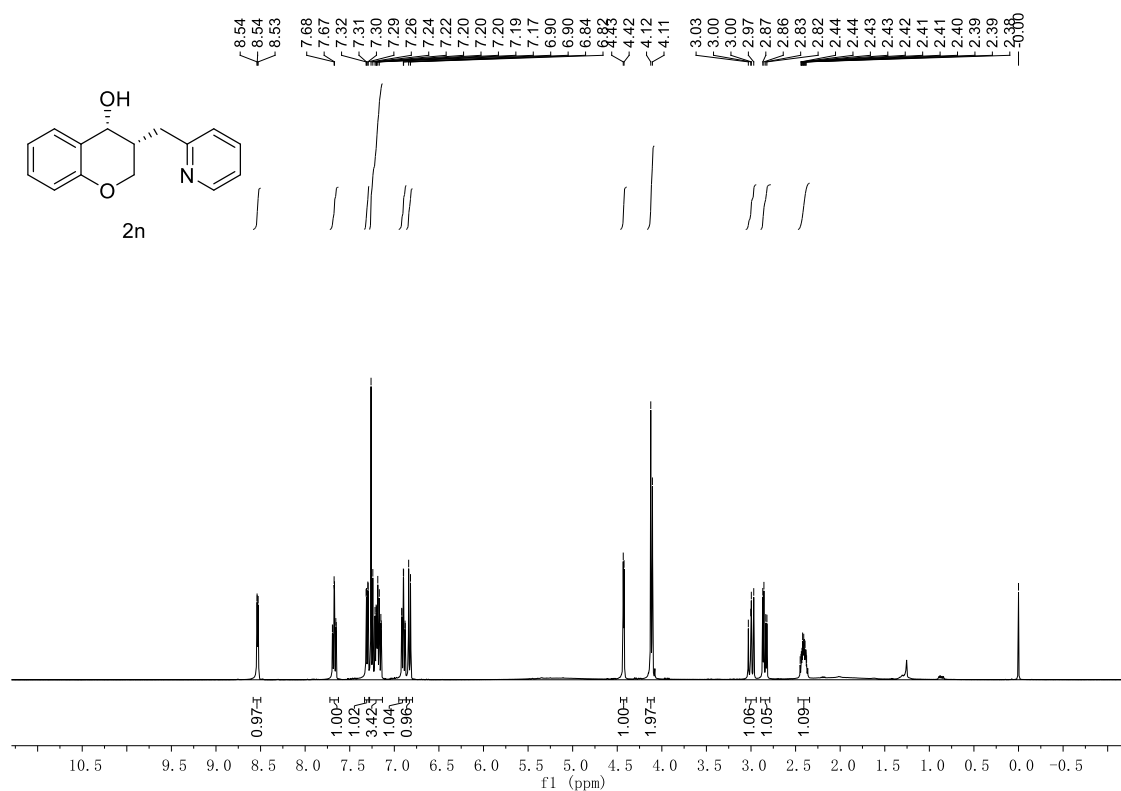
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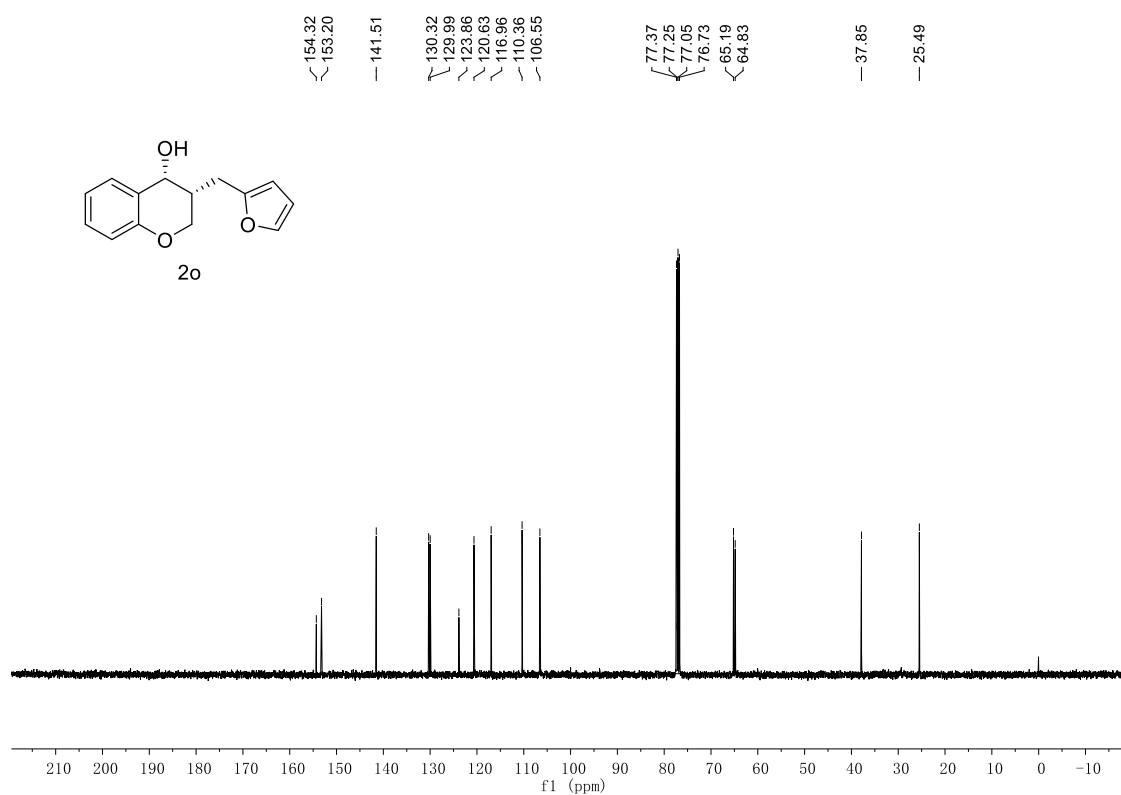
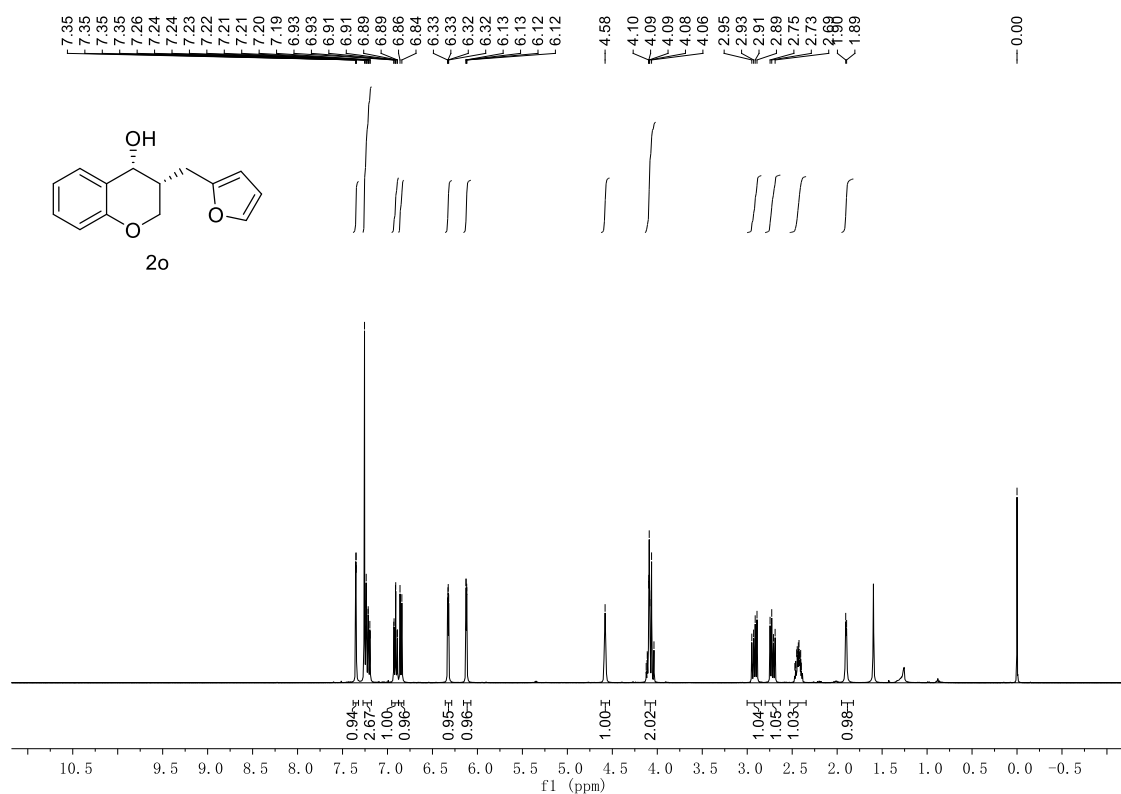
¹H and ¹³C-NMR of 2m



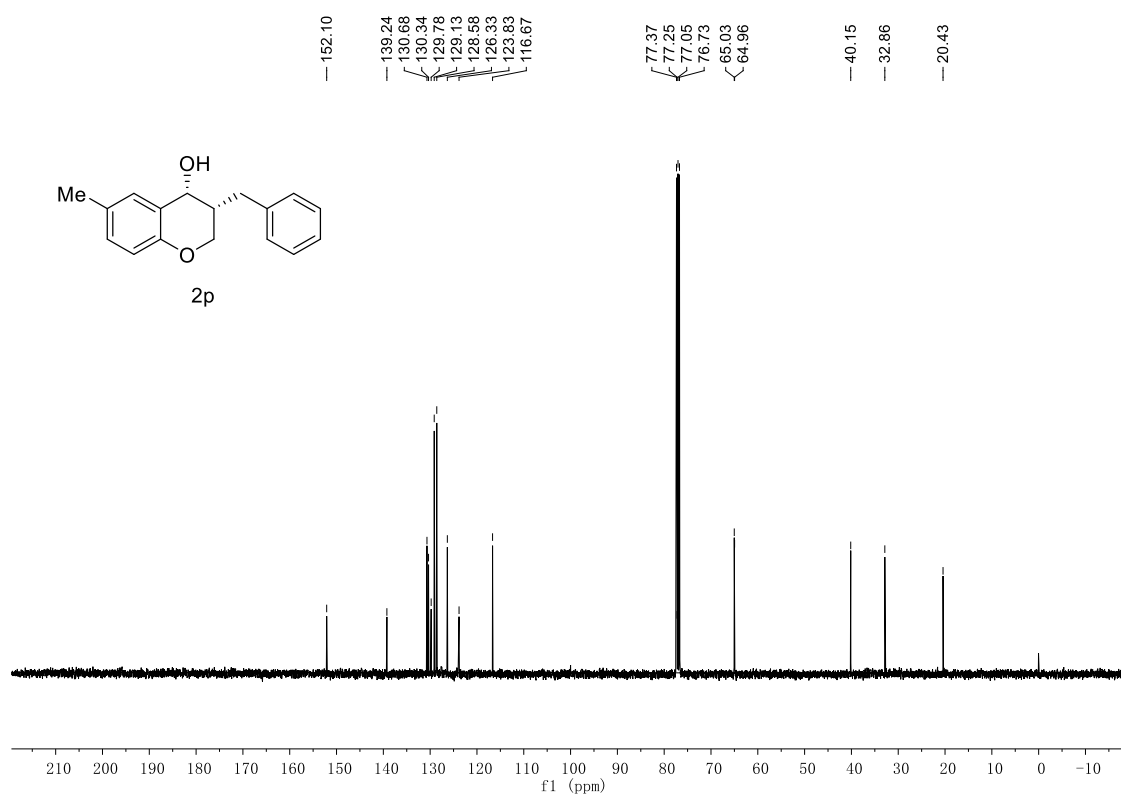
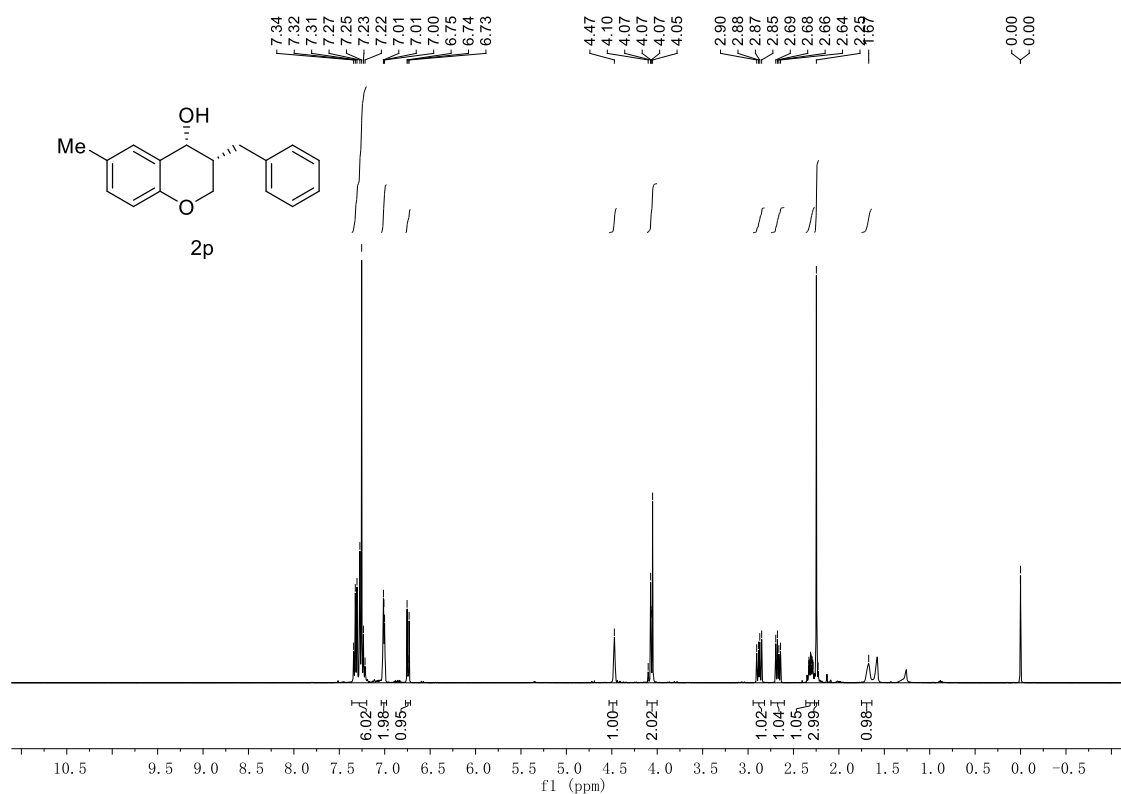
¹H and ¹³C-NMR of 2n



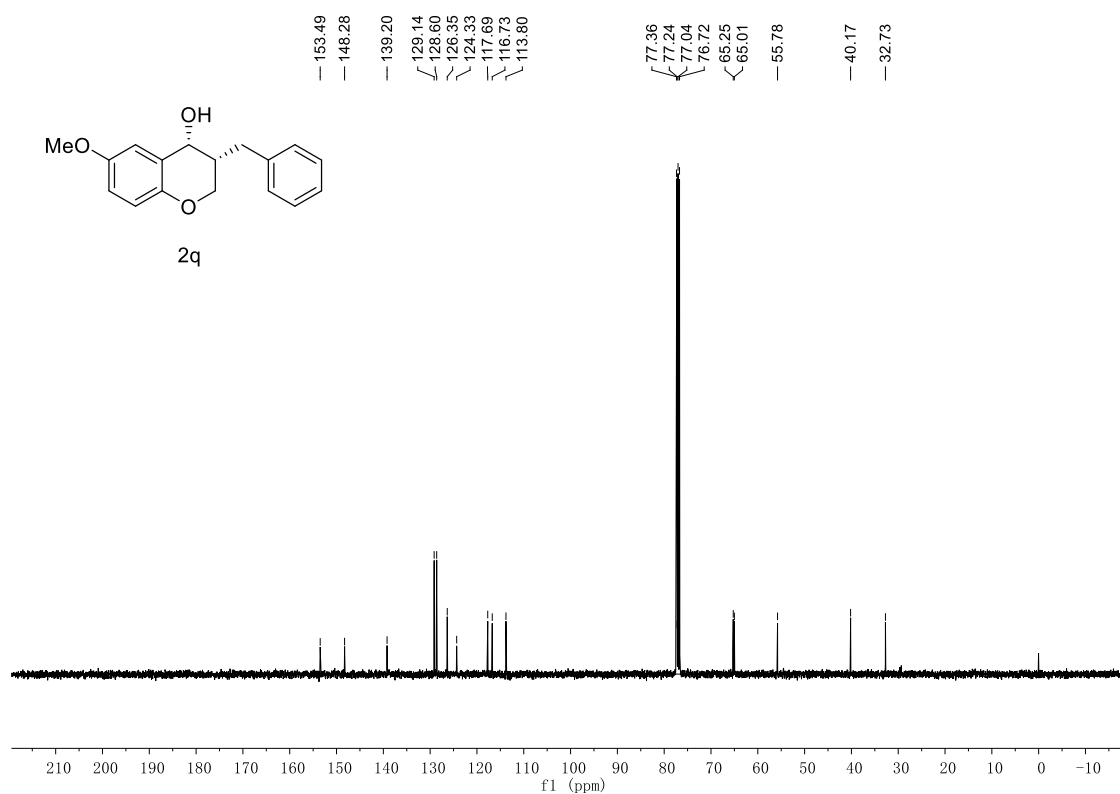
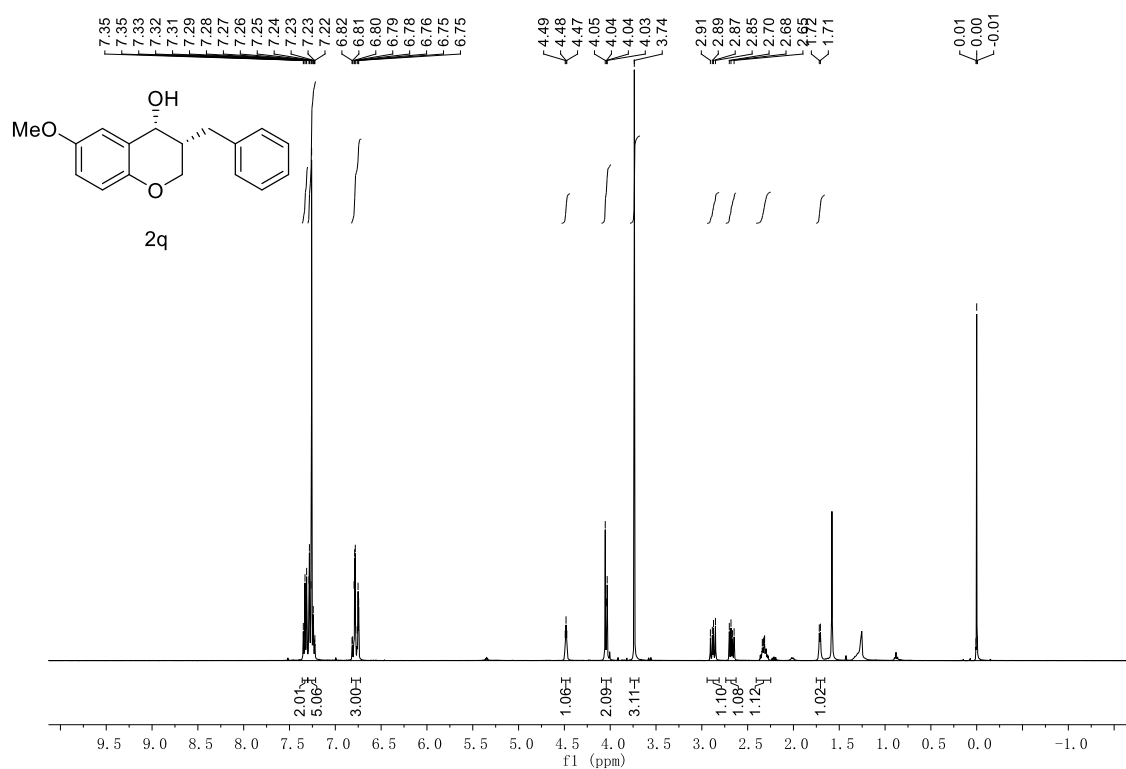
¹H and ¹³C-NMR of 2o



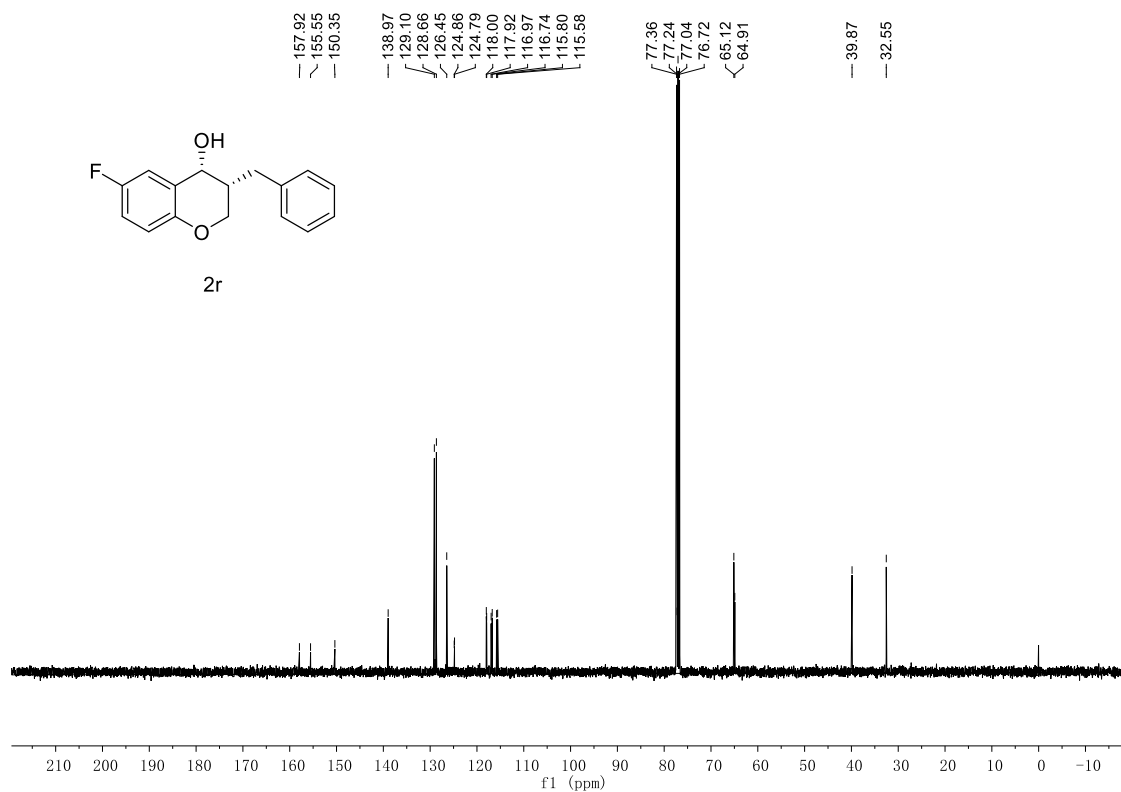
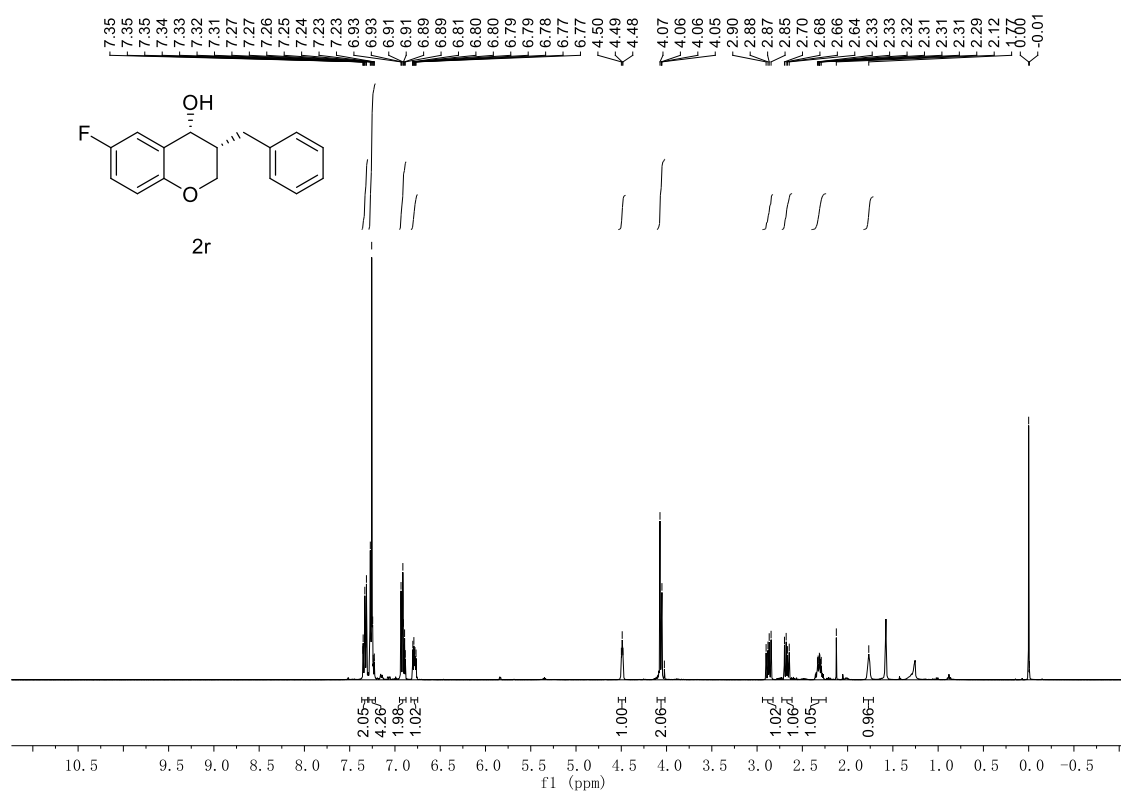
¹H and ¹³C-NMR of 2p



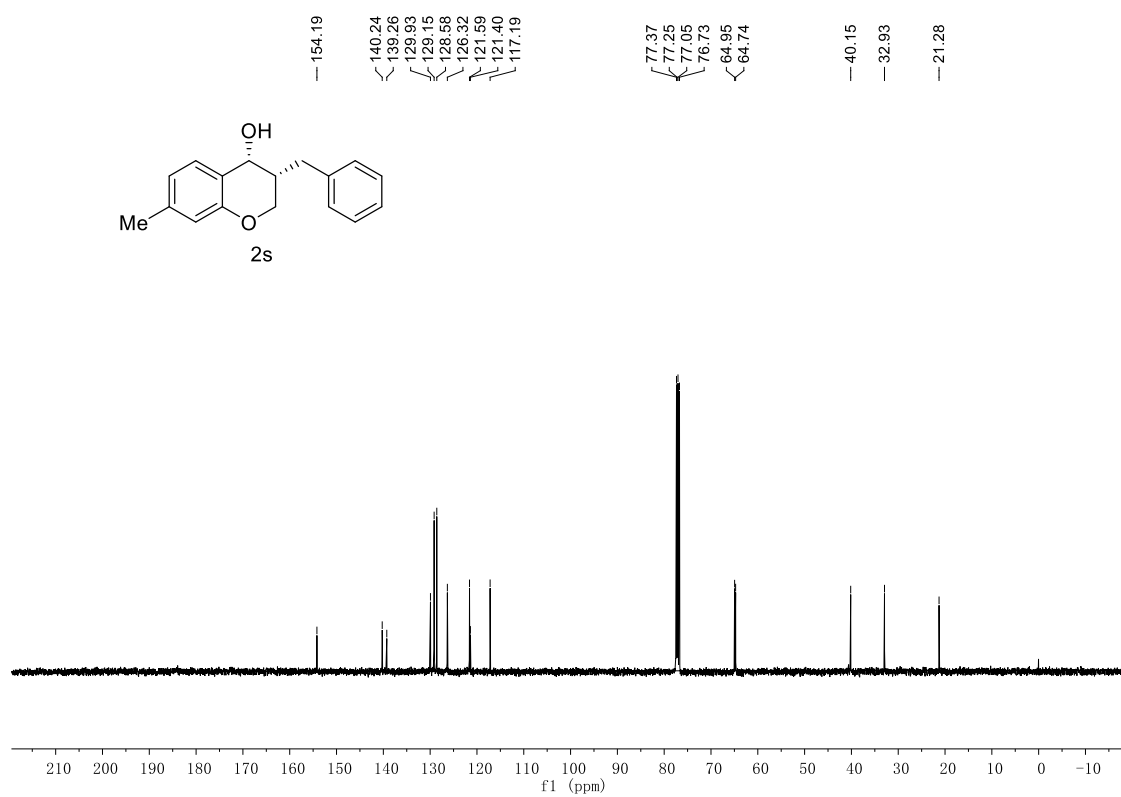
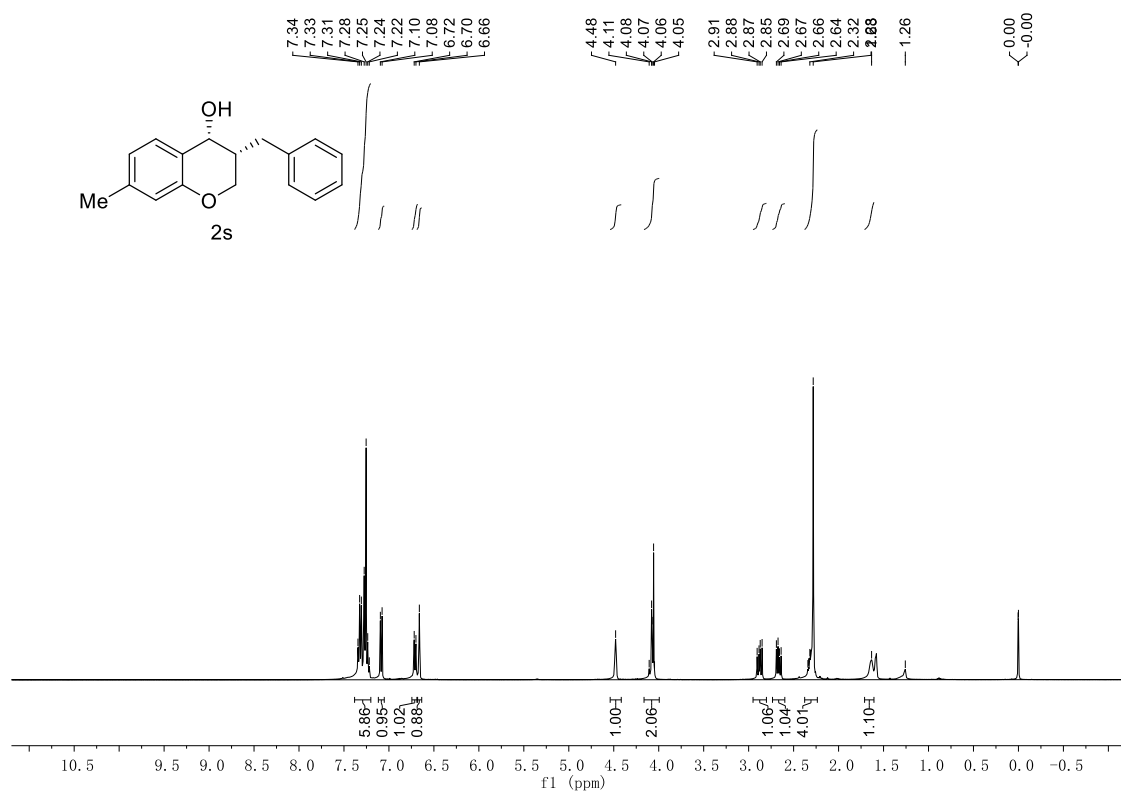
¹H and ¹³C-NMR of 2q



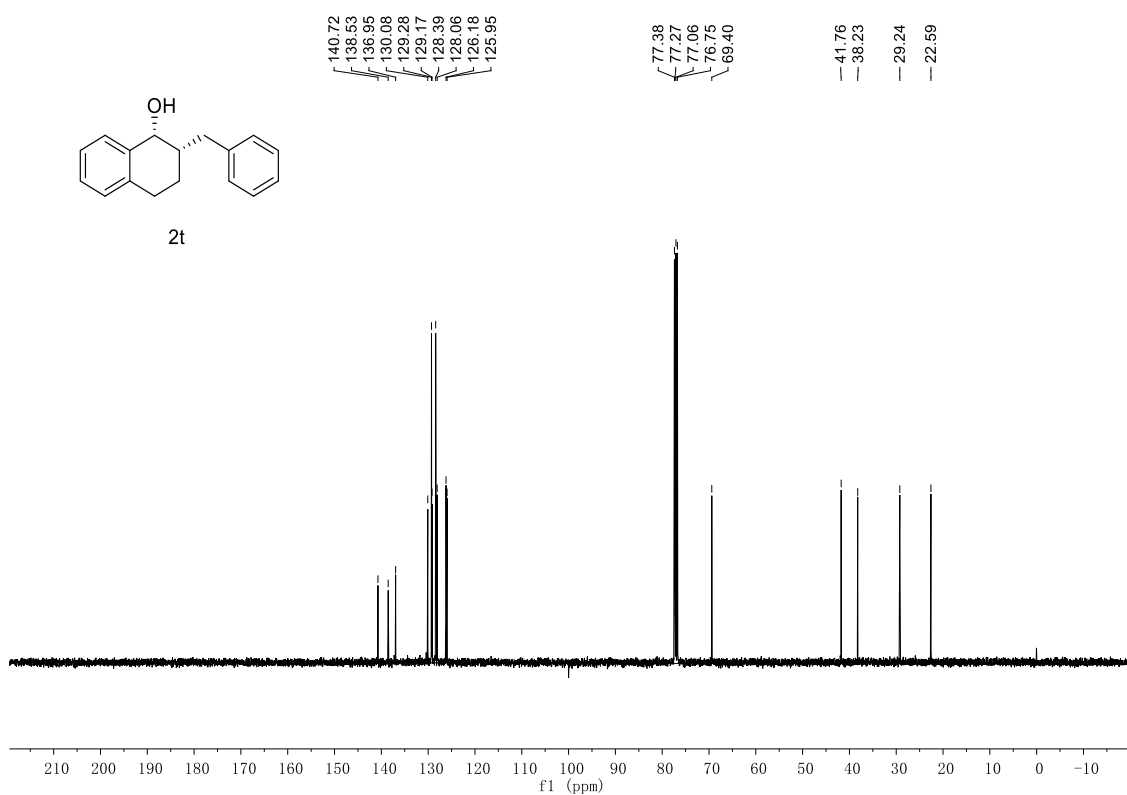
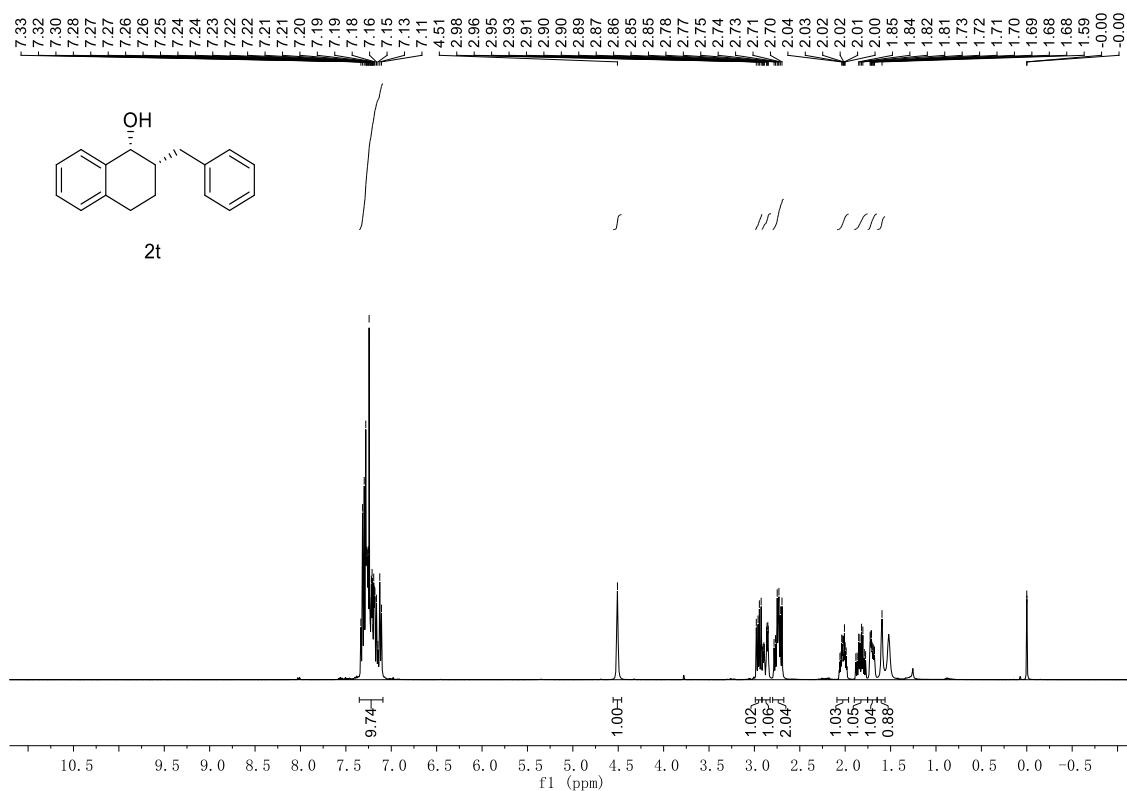
^1H and ^{13}C -NMR of 2r



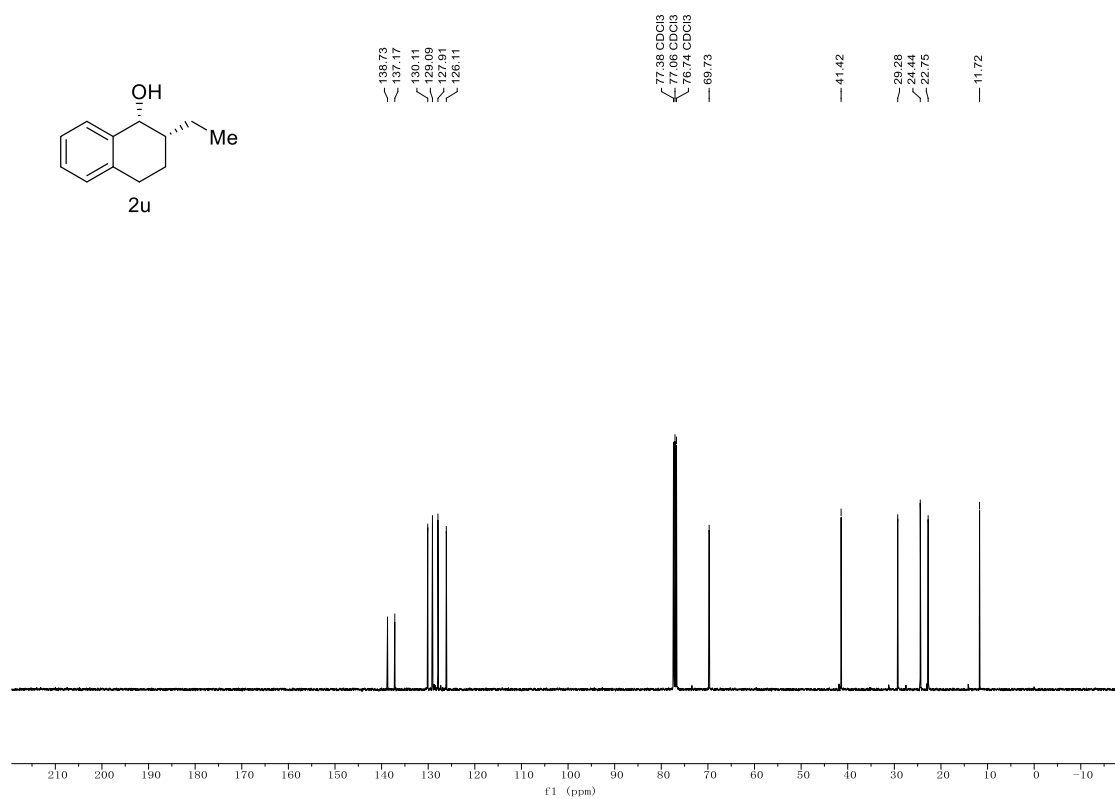
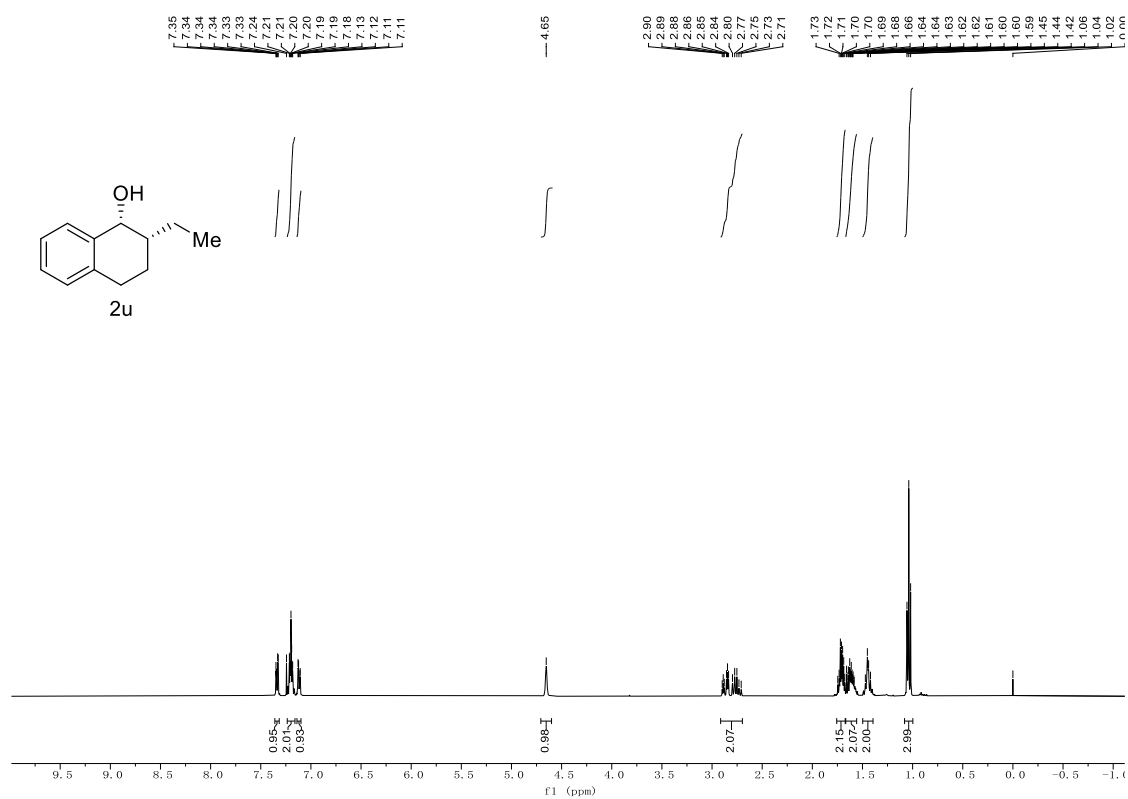
¹H and ¹³C-NMR of 2s



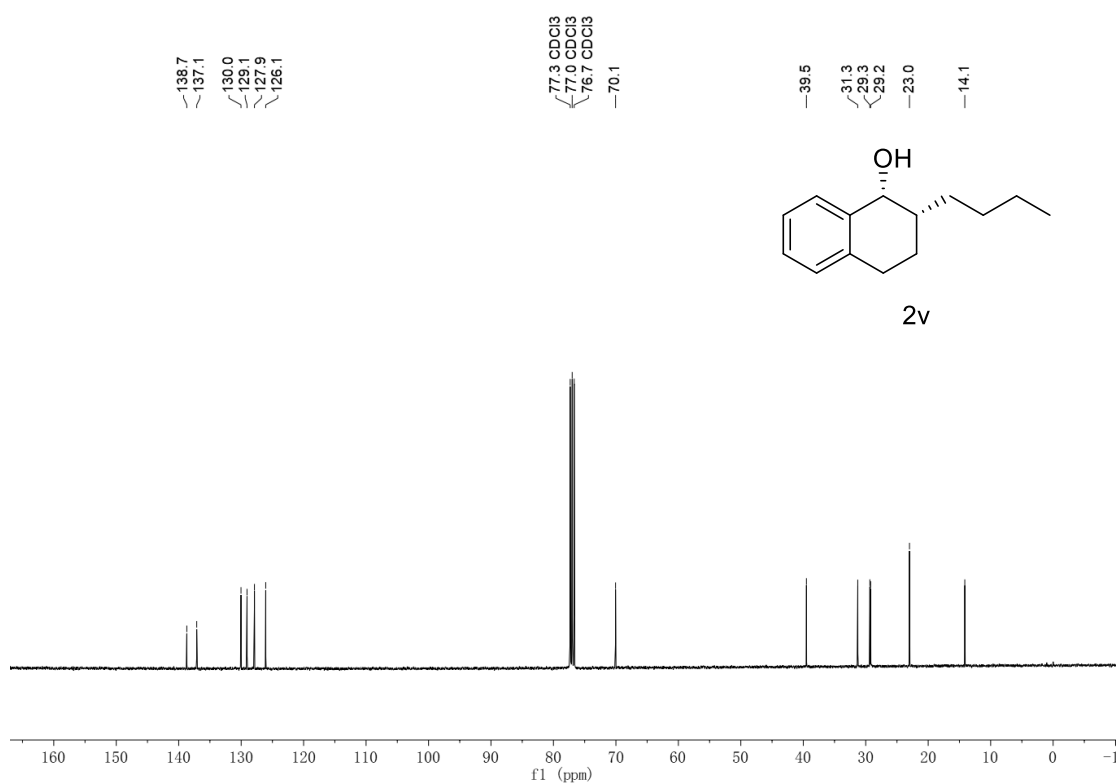
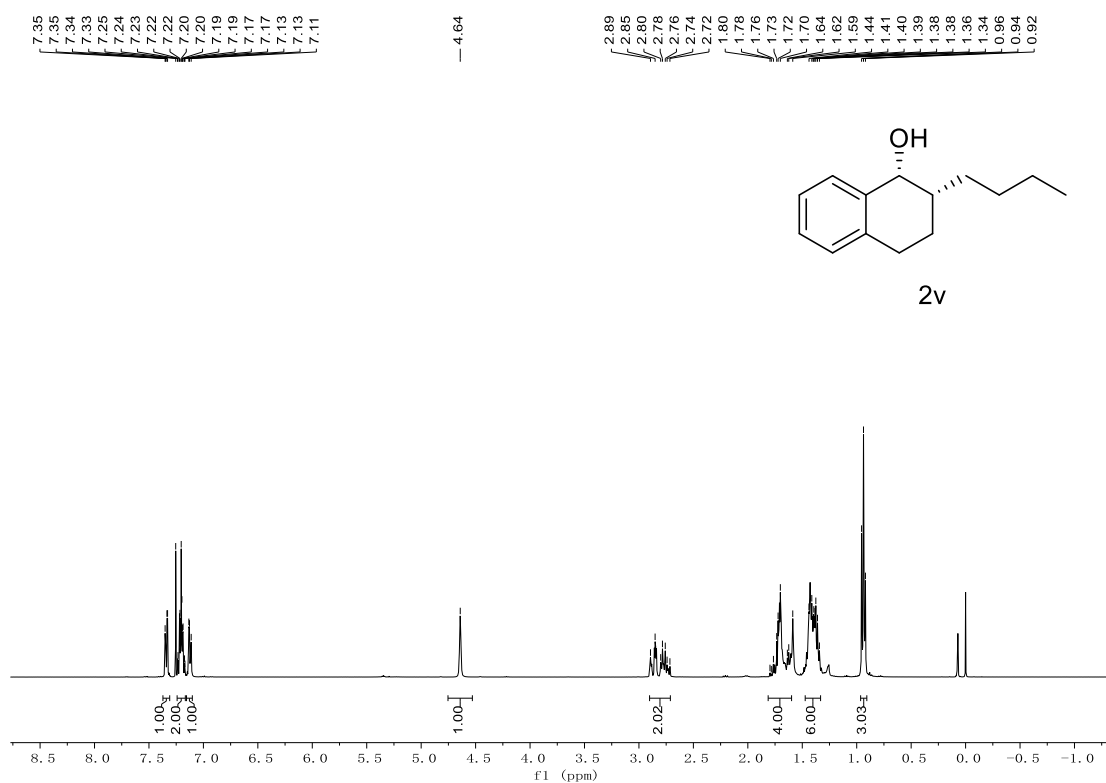
¹H and ¹³C-NMR of 2t



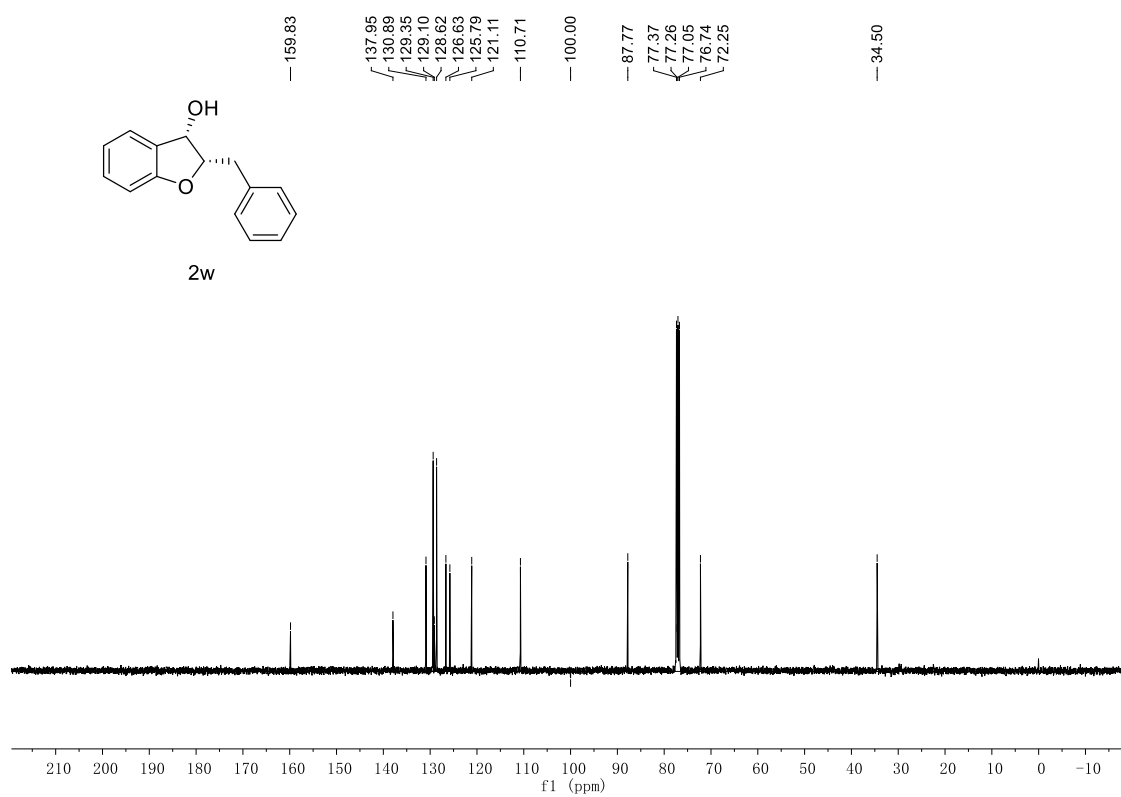
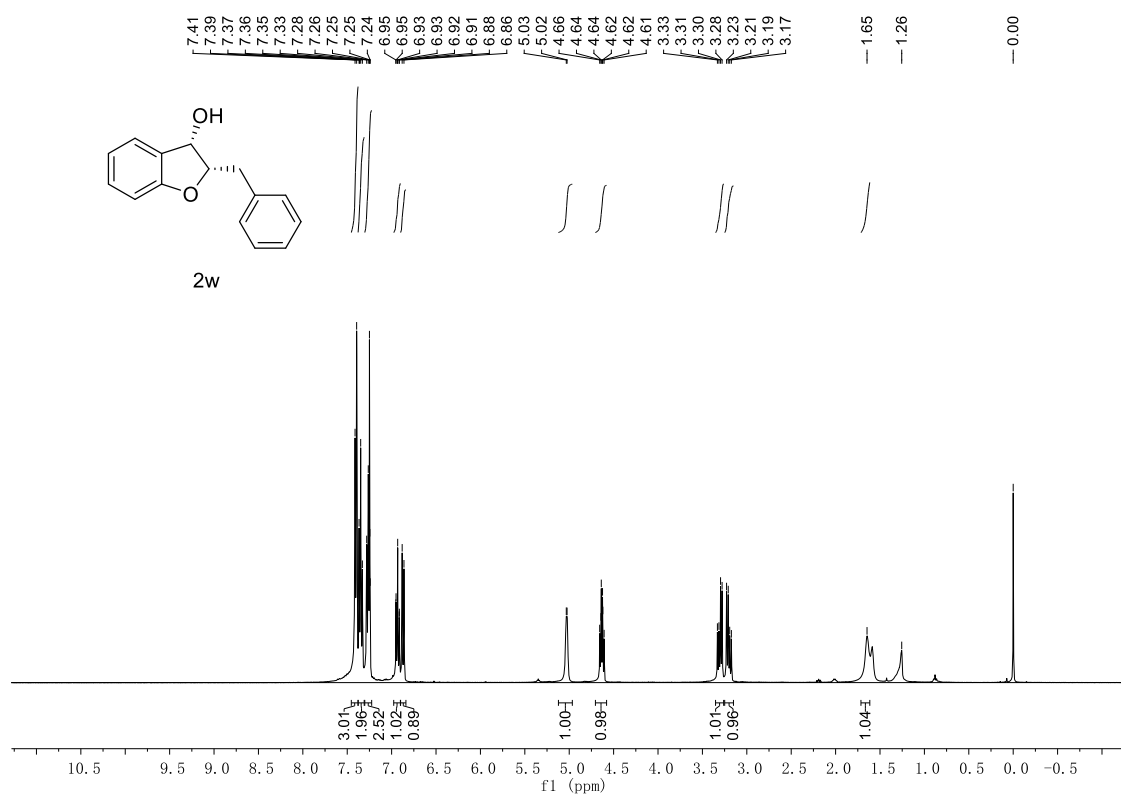
¹H and ¹³C-NMR of 2u



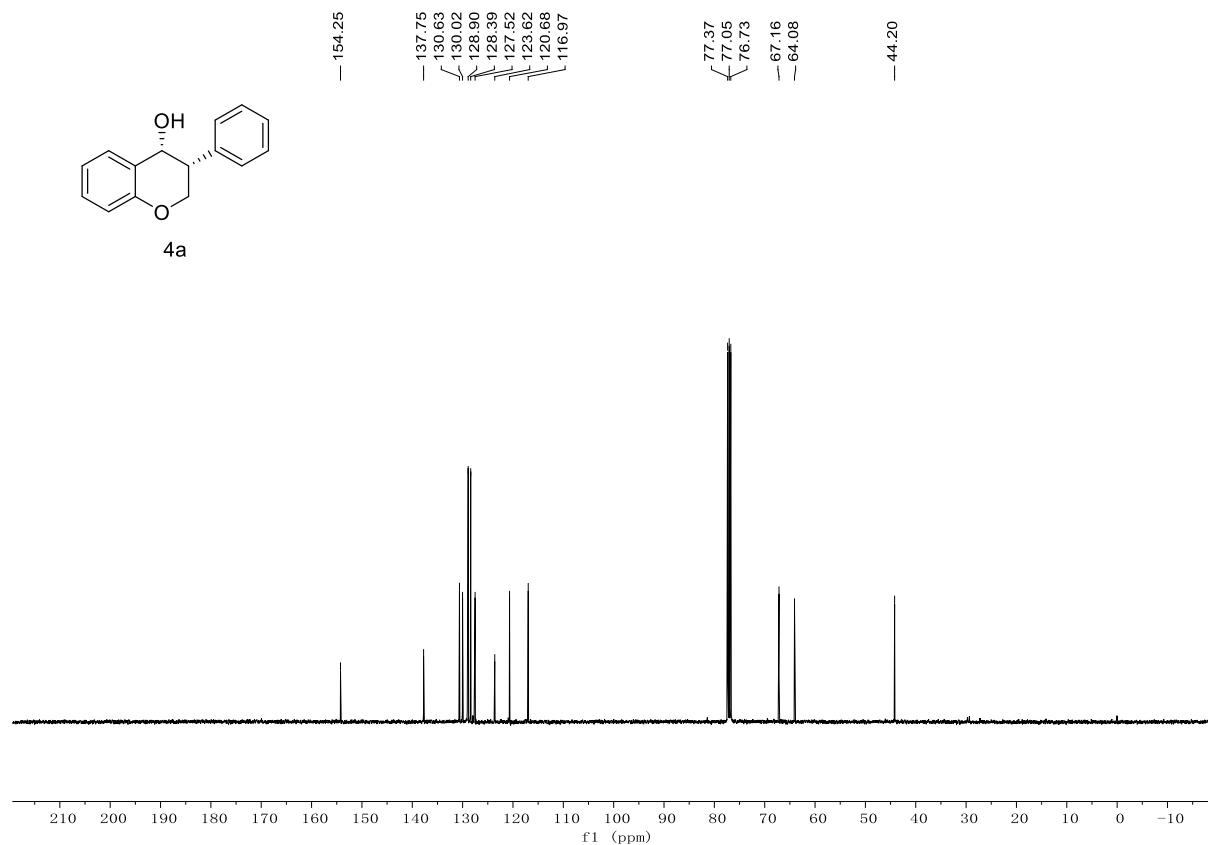
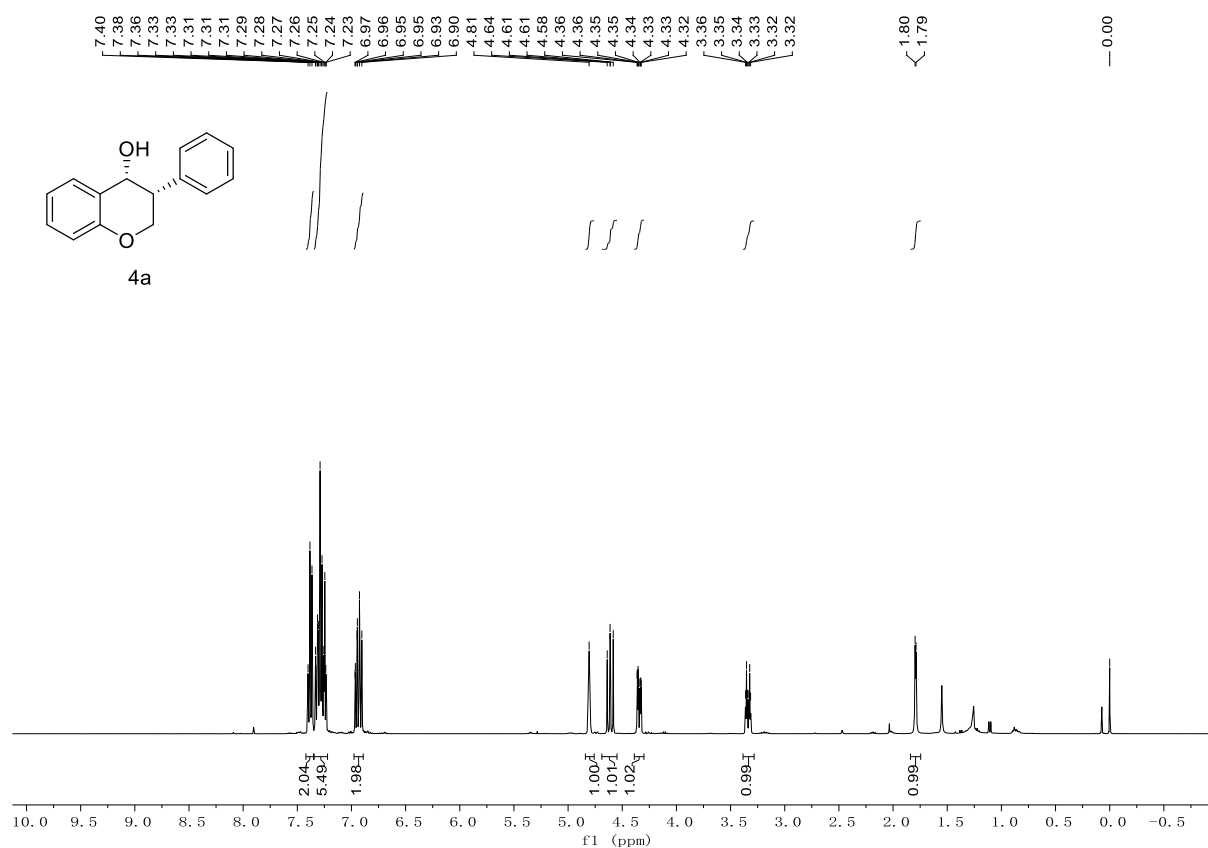
¹H and ¹³C-NMR of 2v



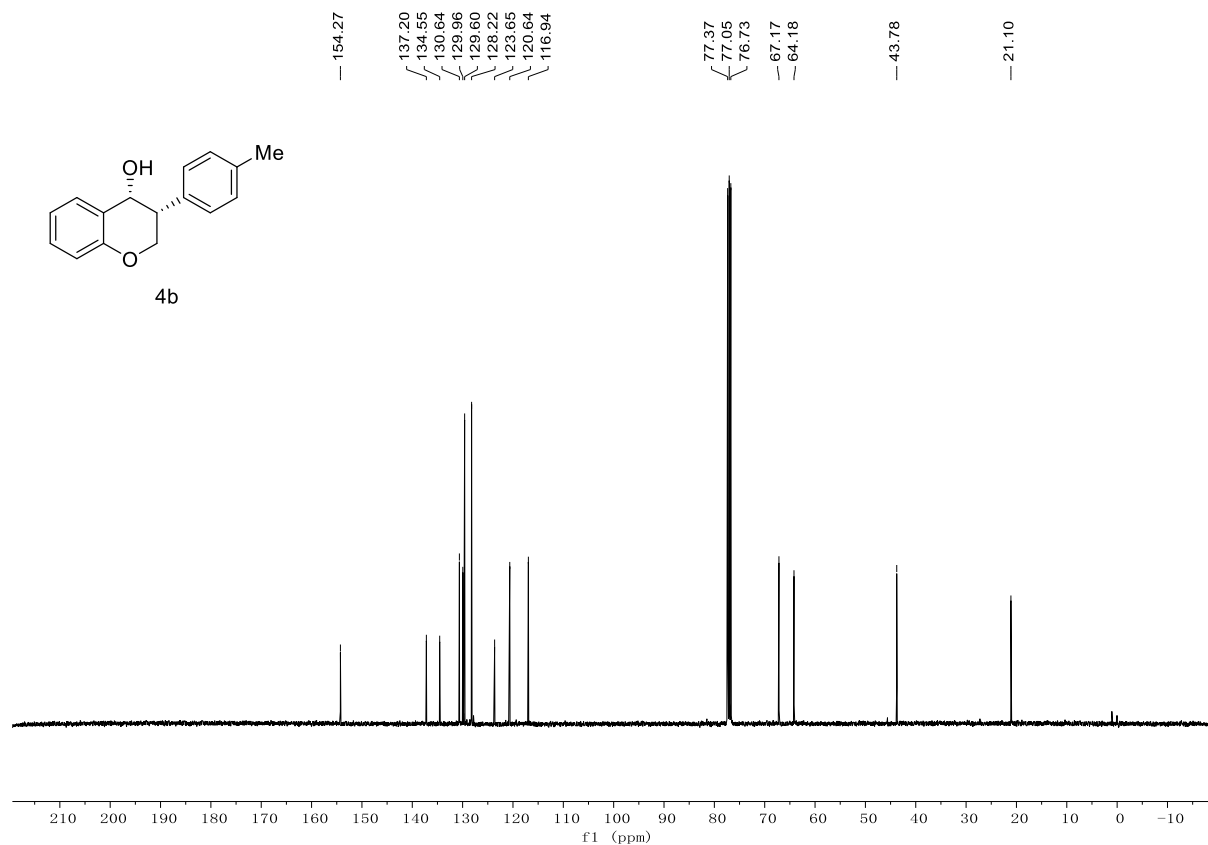
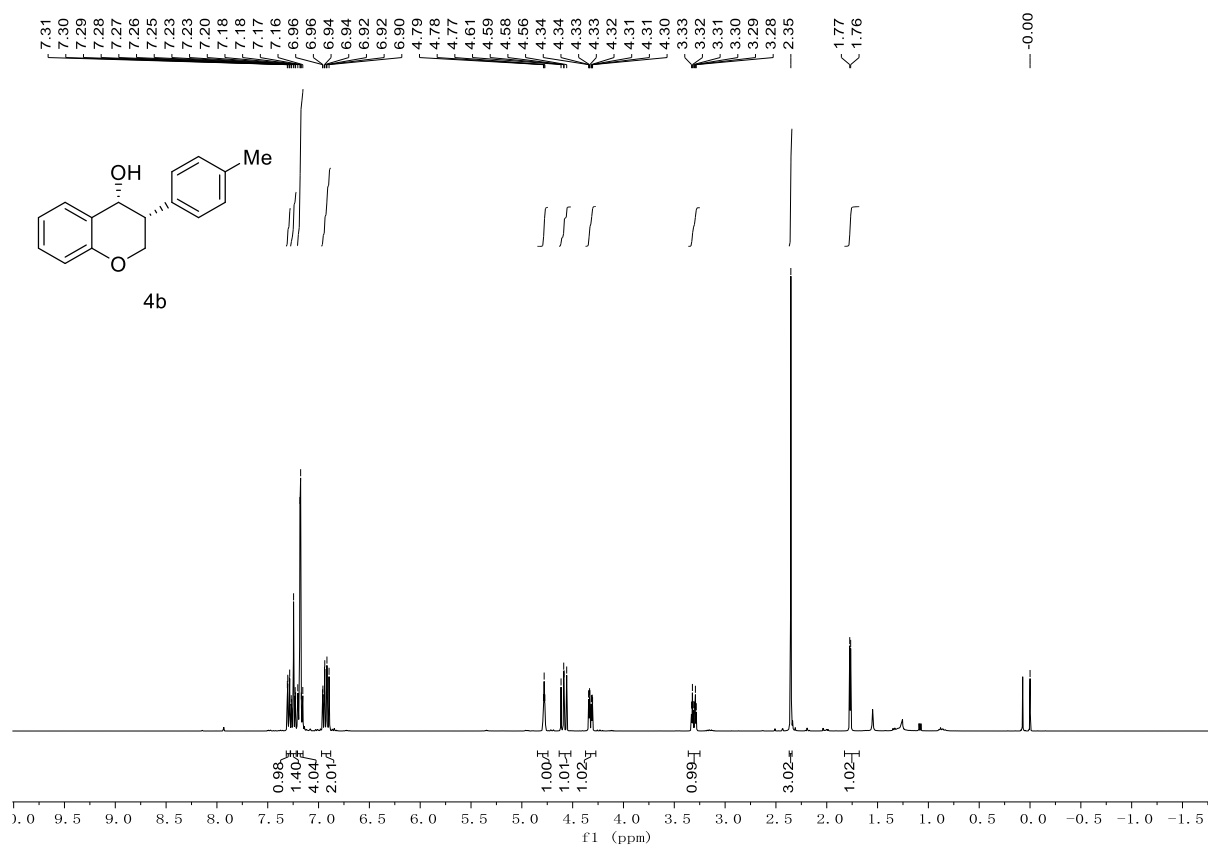
¹H and ¹³C-NMR of 2w



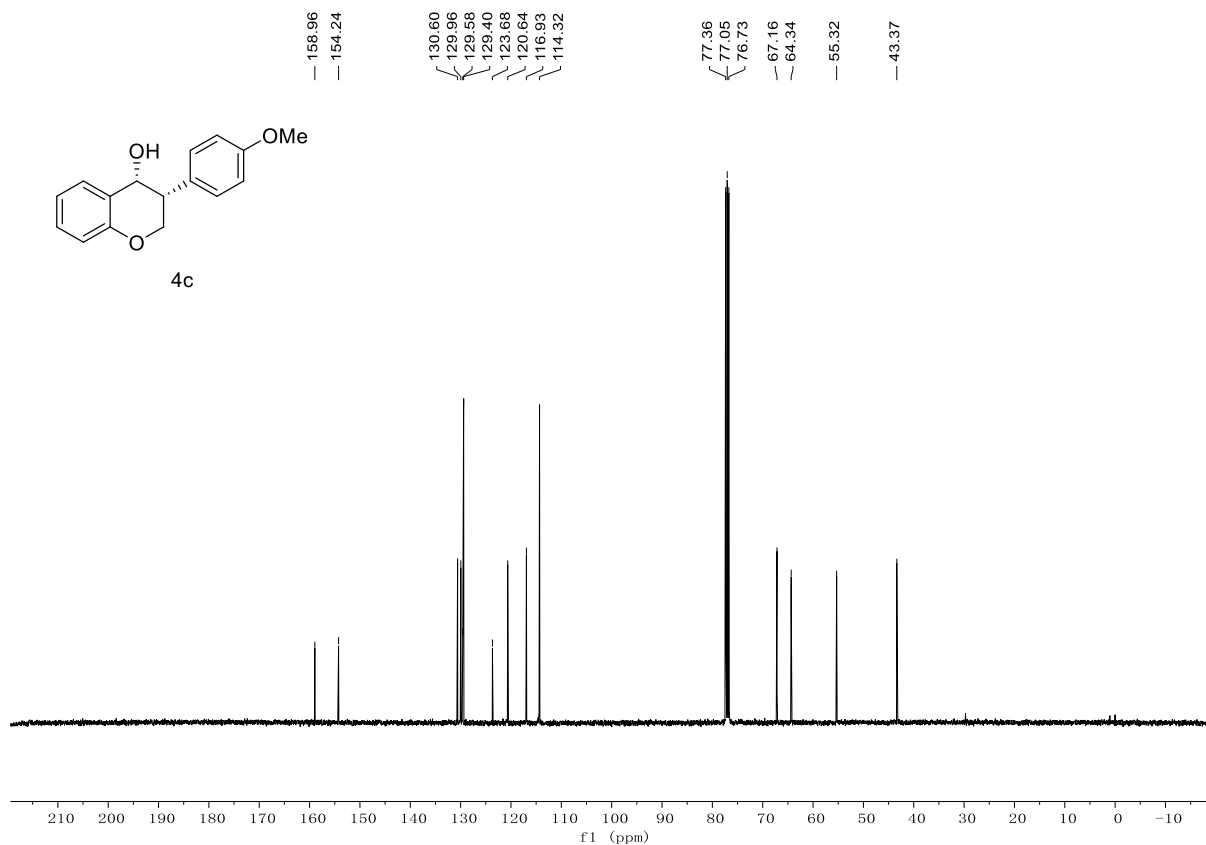
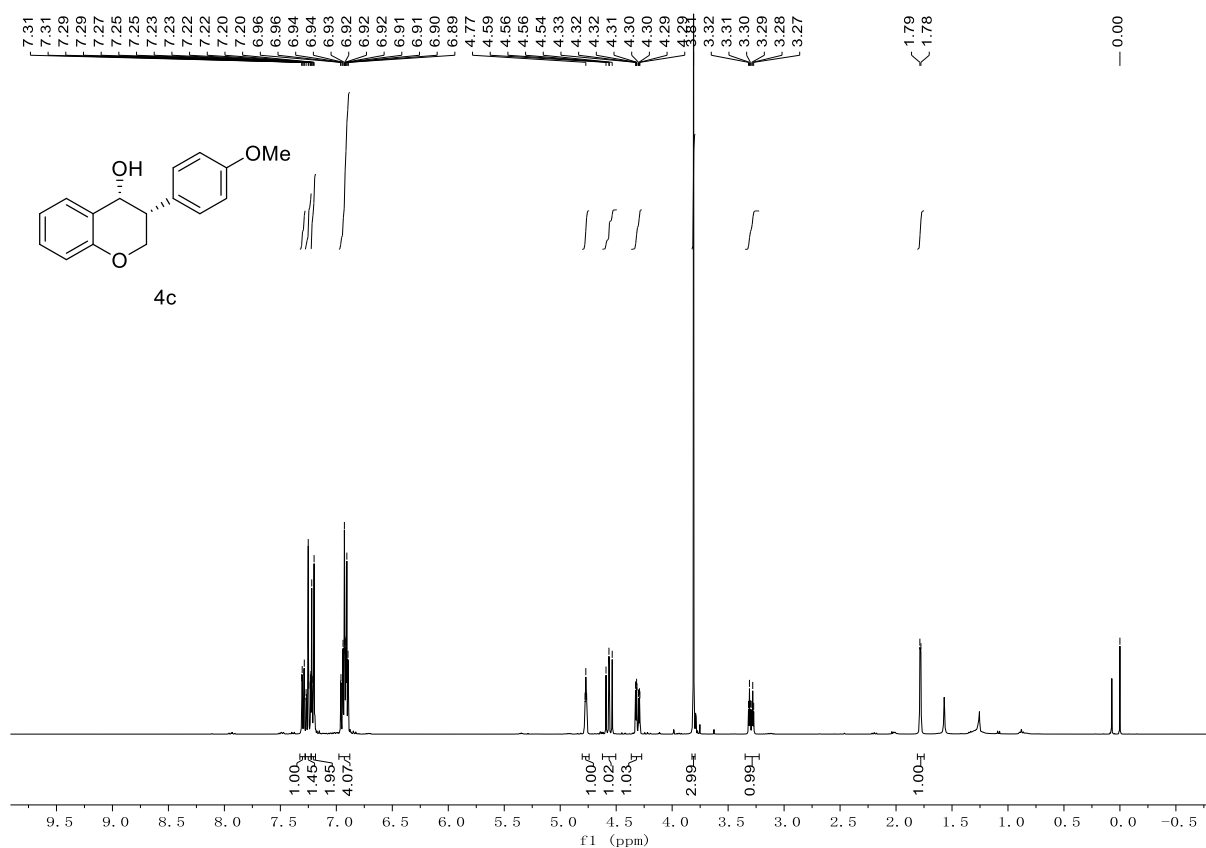
¹H and ¹³C-NMR of 4a



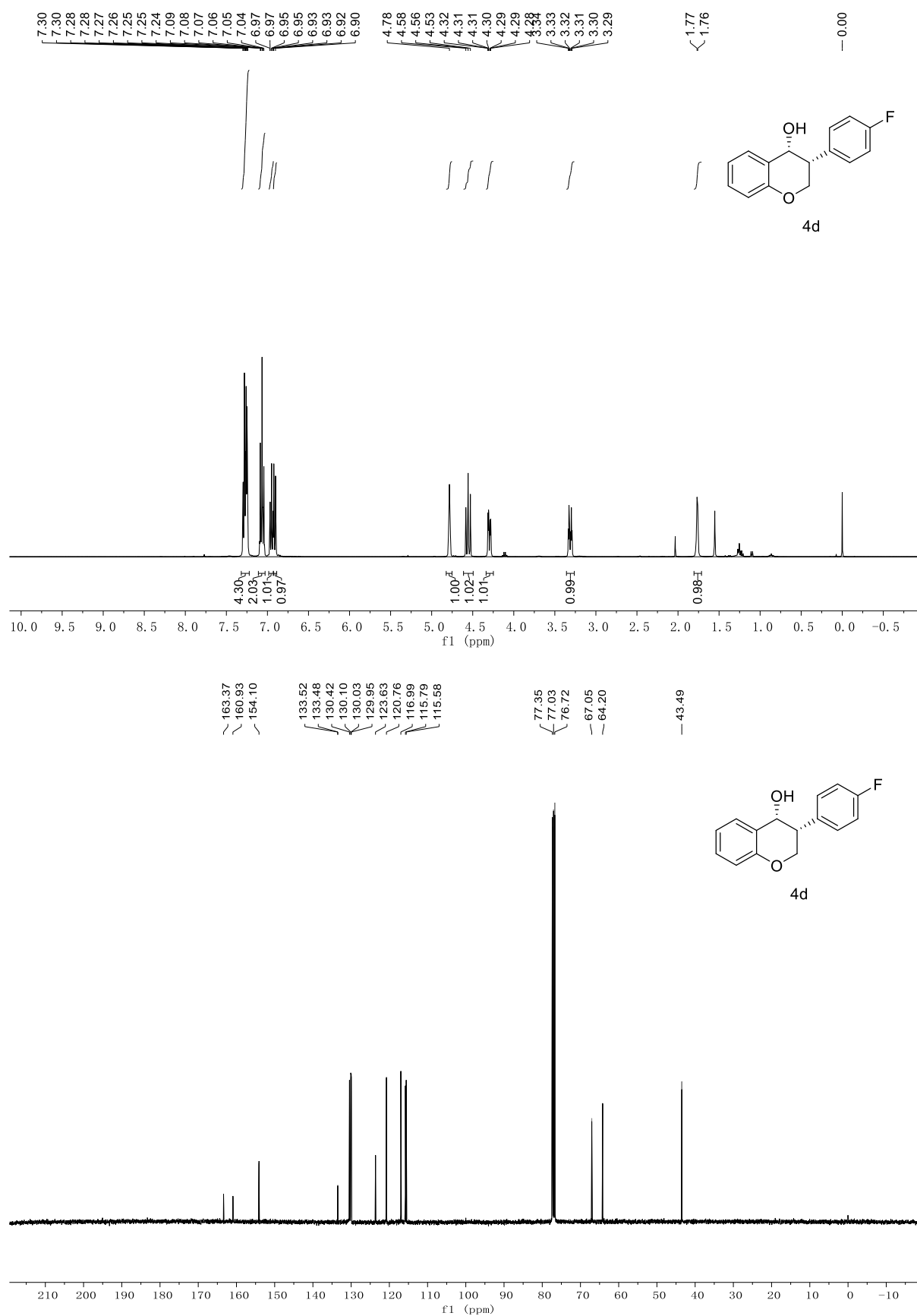
¹H and ¹³C-NMR of 4b



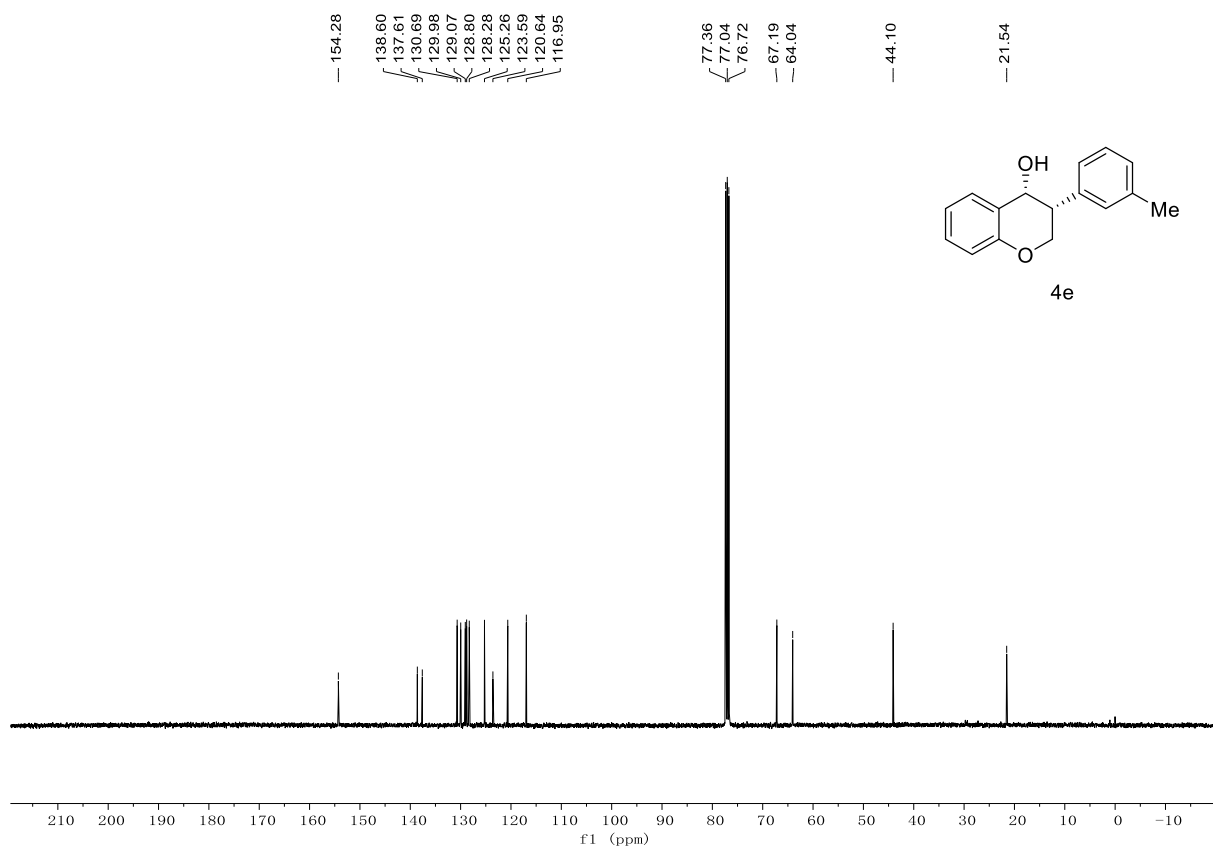
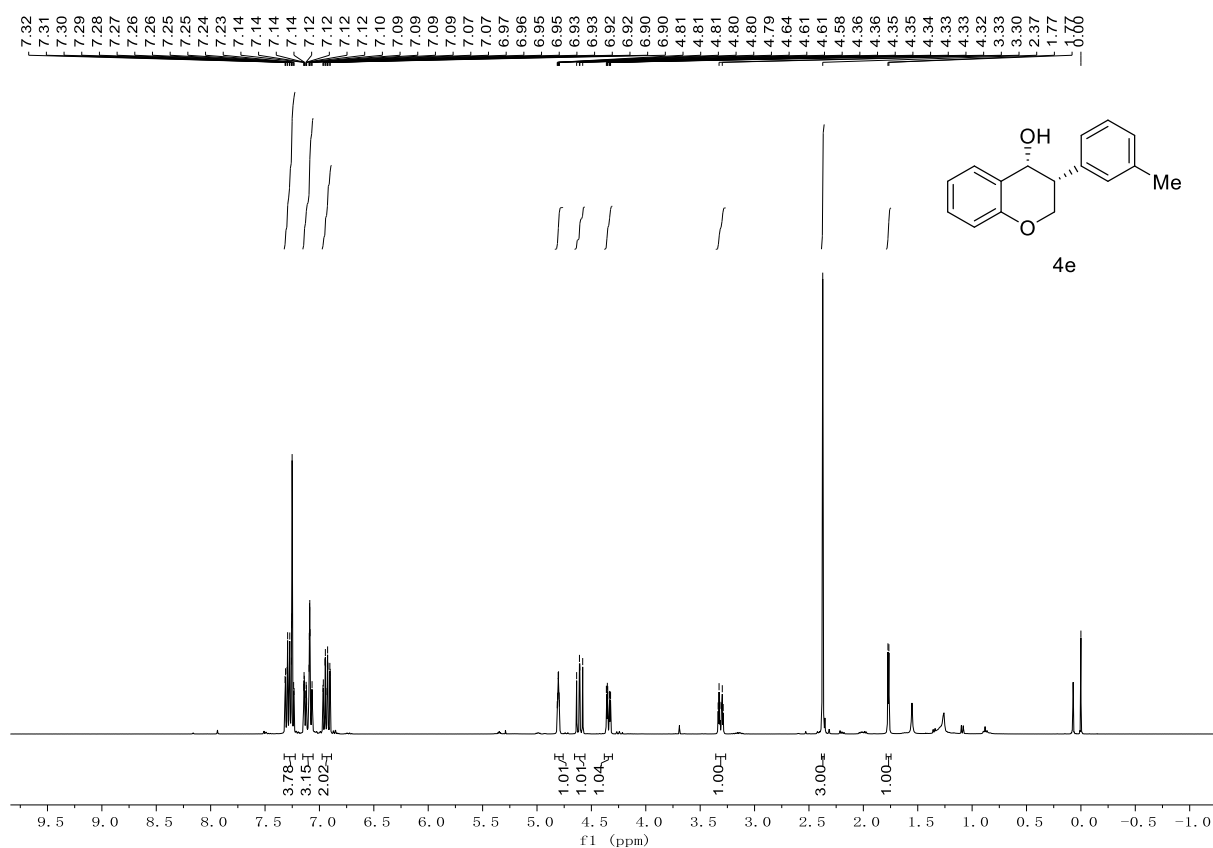
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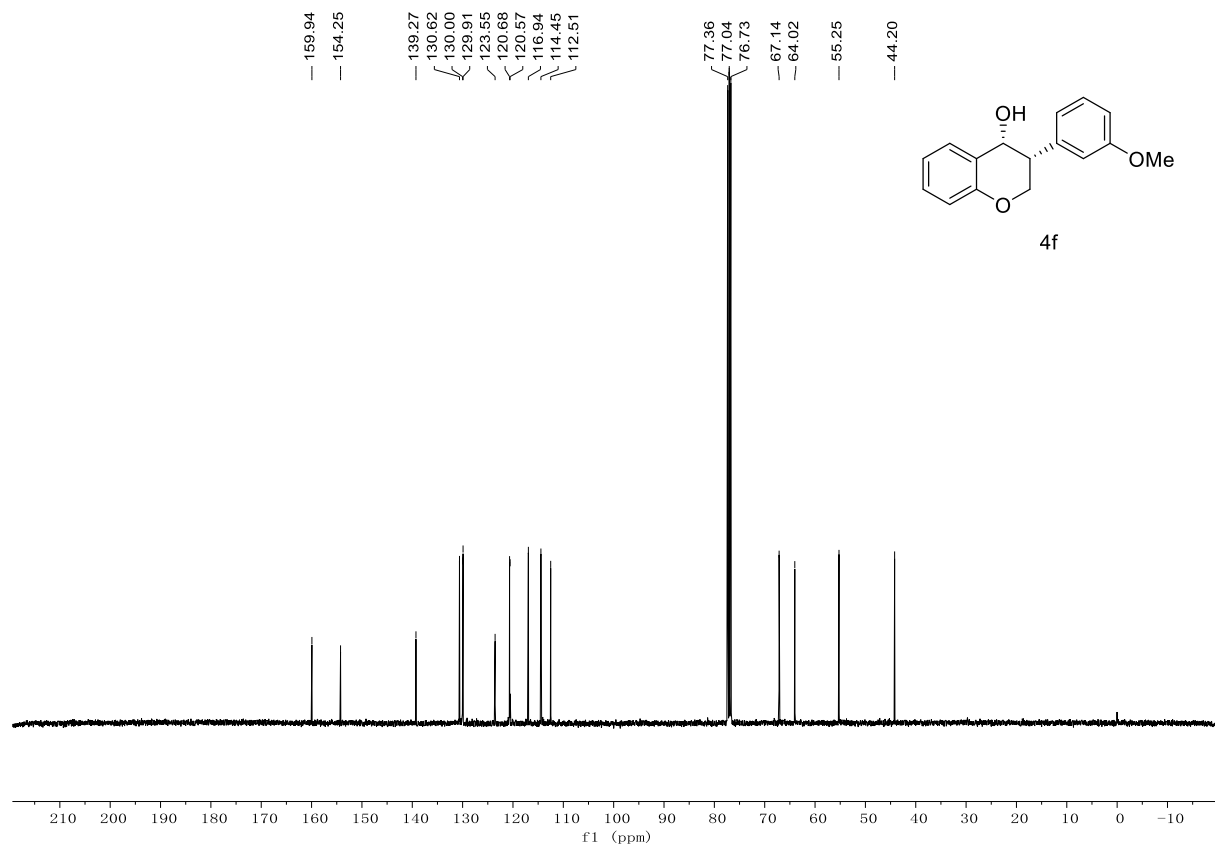
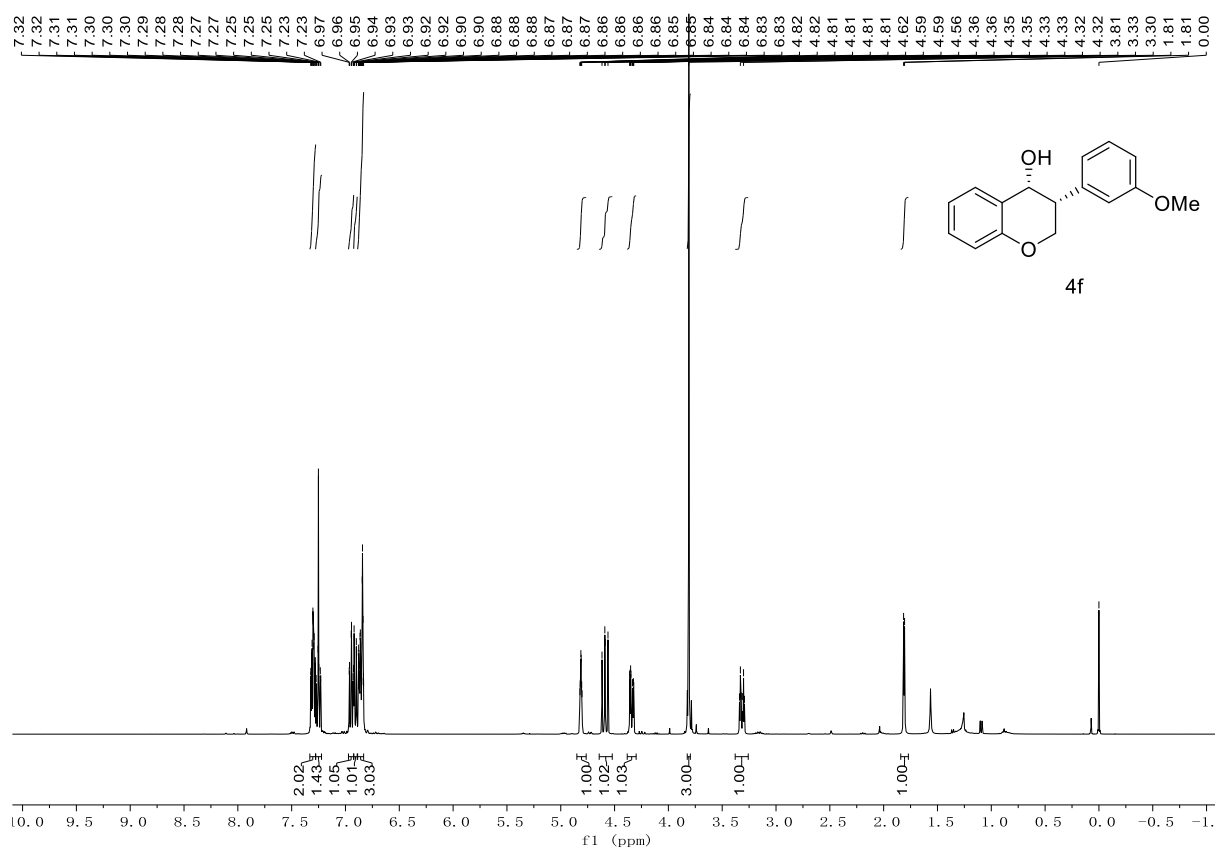
¹H and ¹³C-NMR of 4d



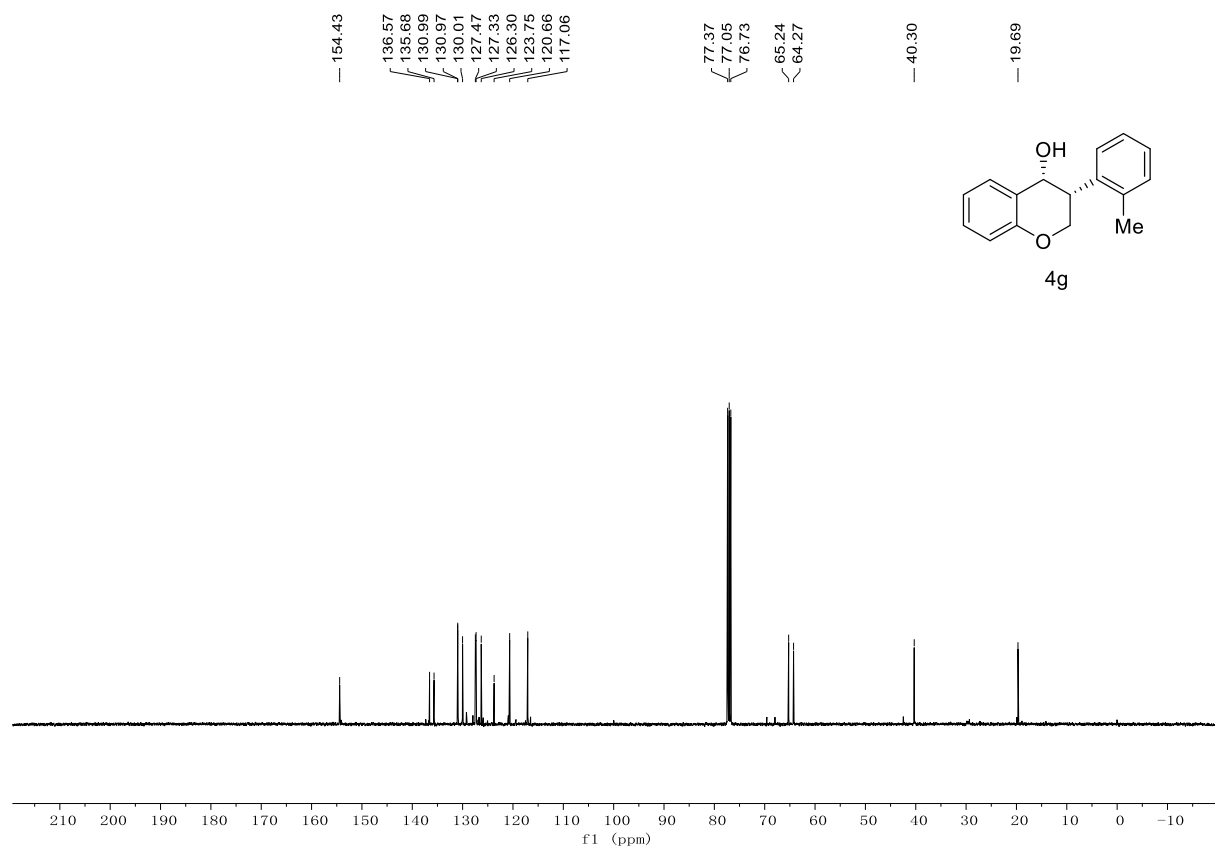
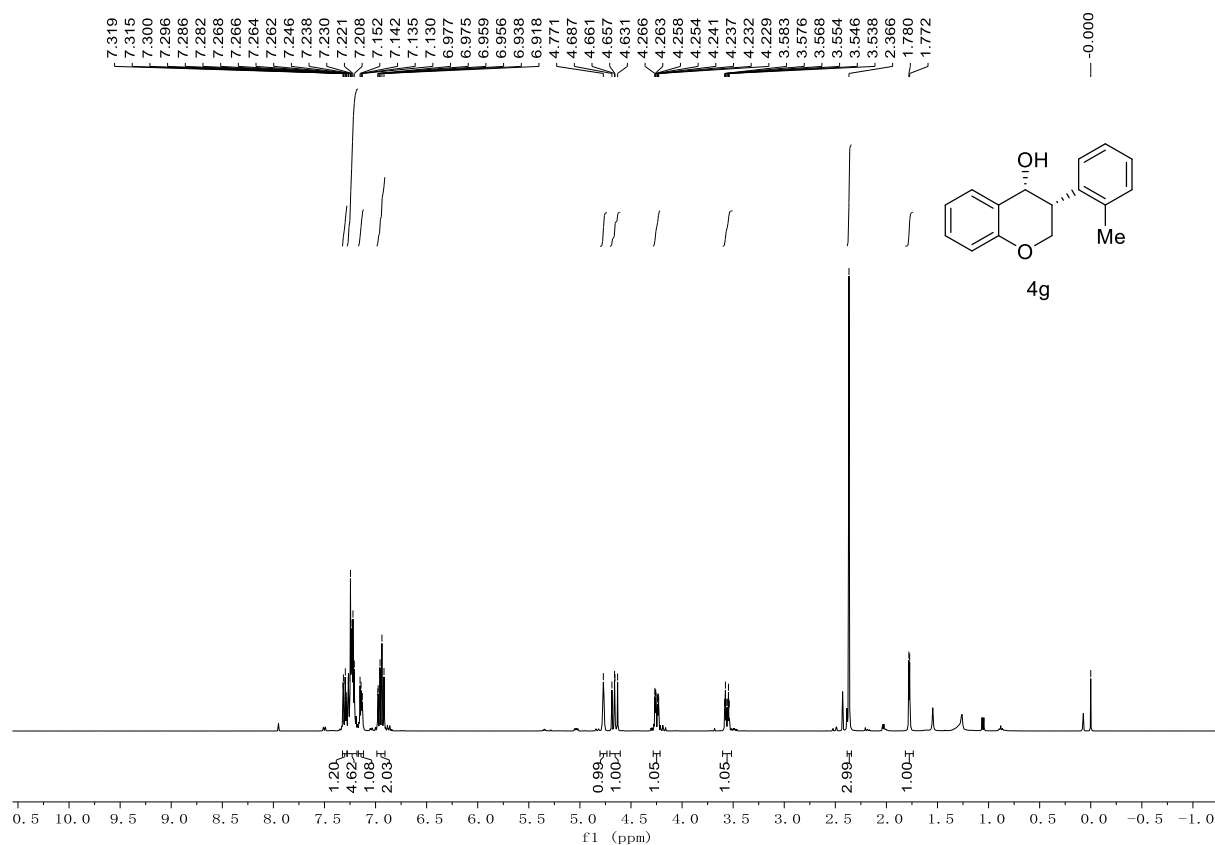
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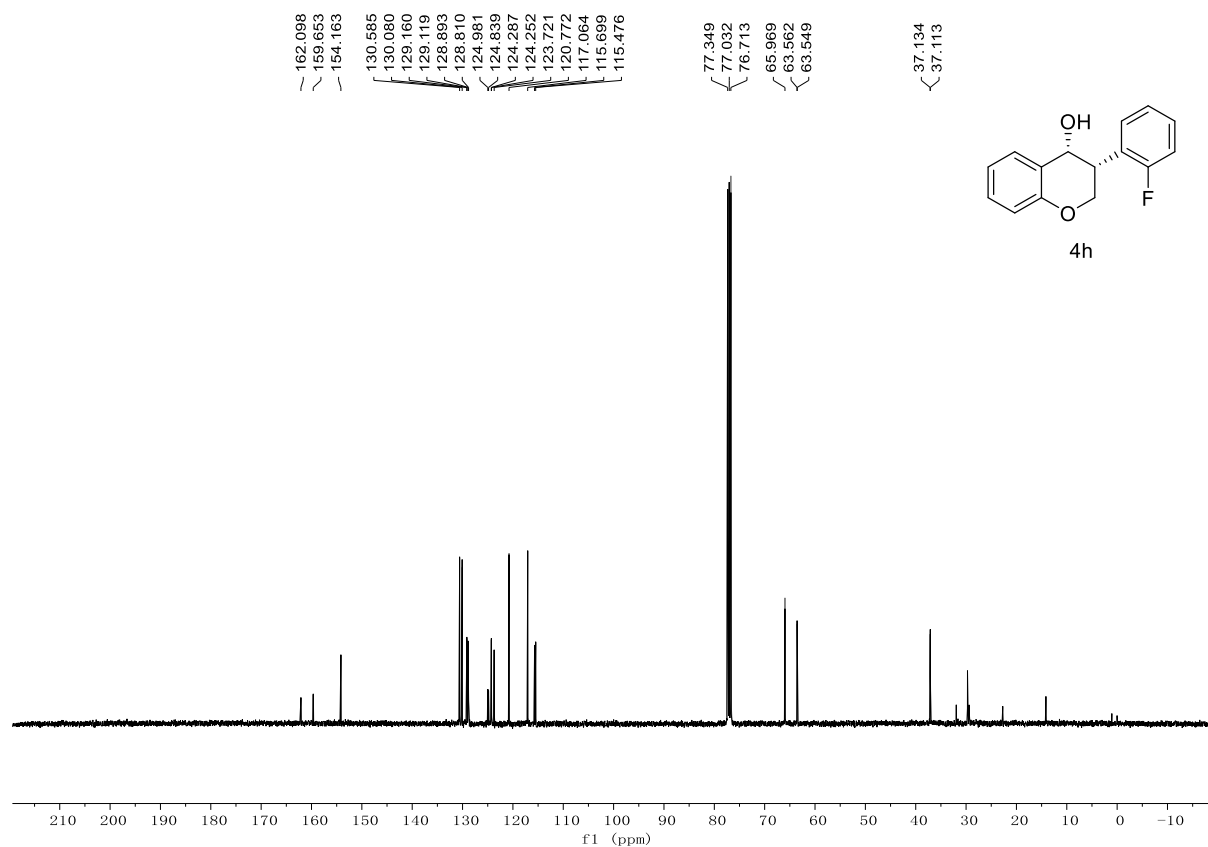
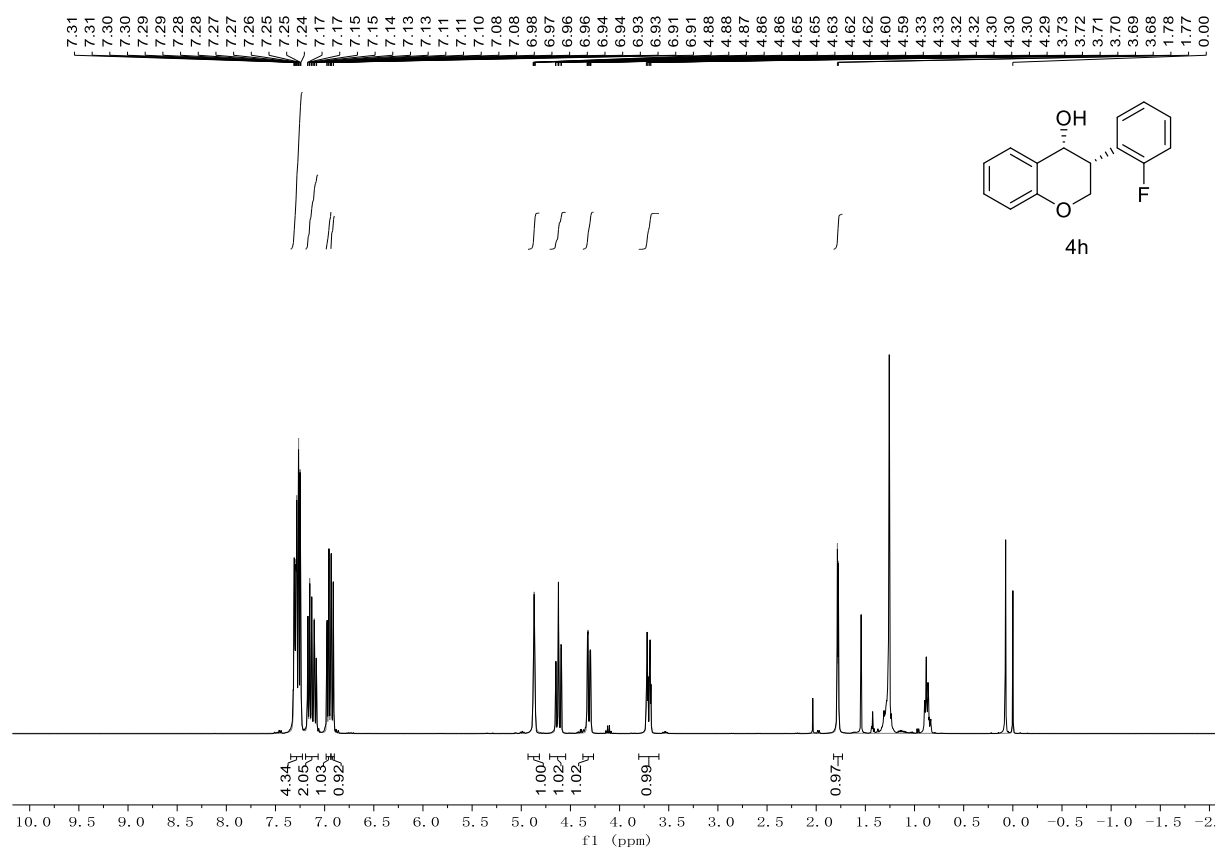
¹H and ¹³C-NMR of 4f



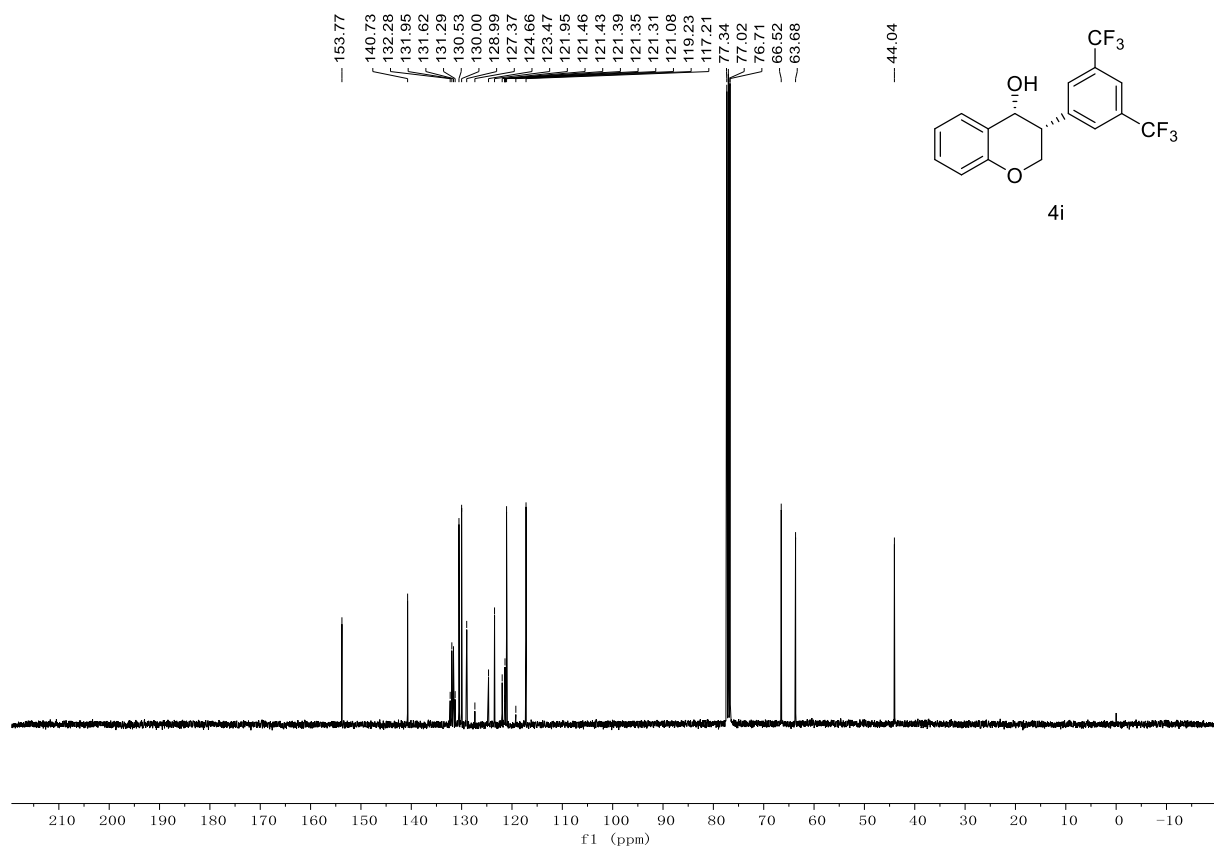
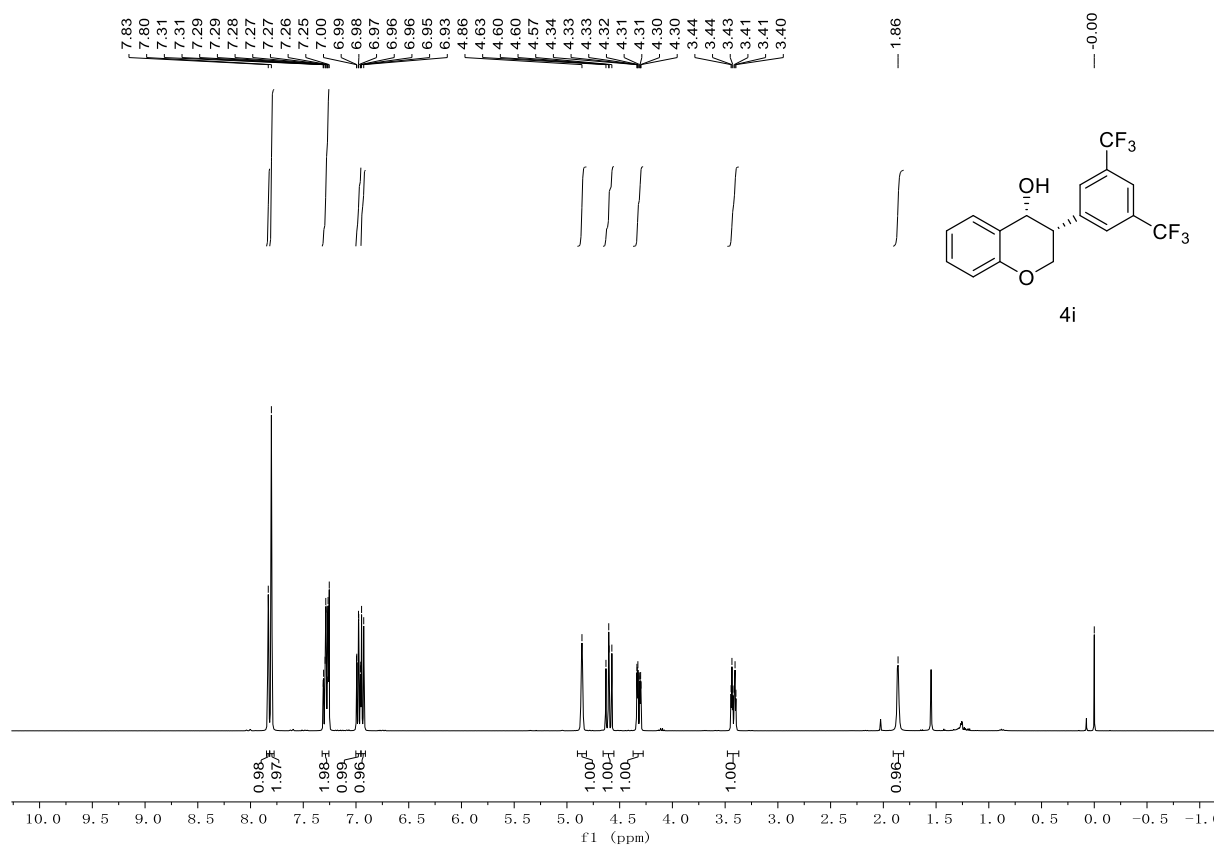
¹H and ¹³C-NMR of 4g



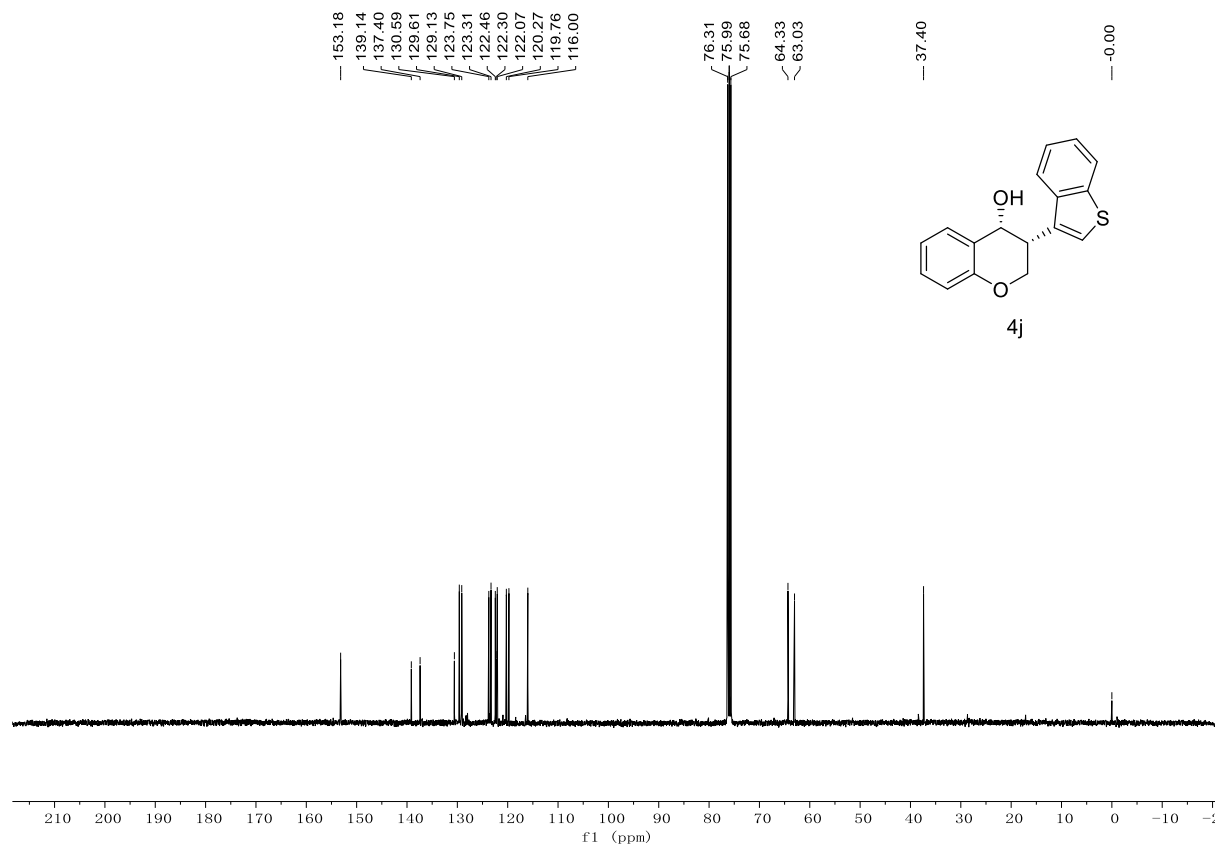
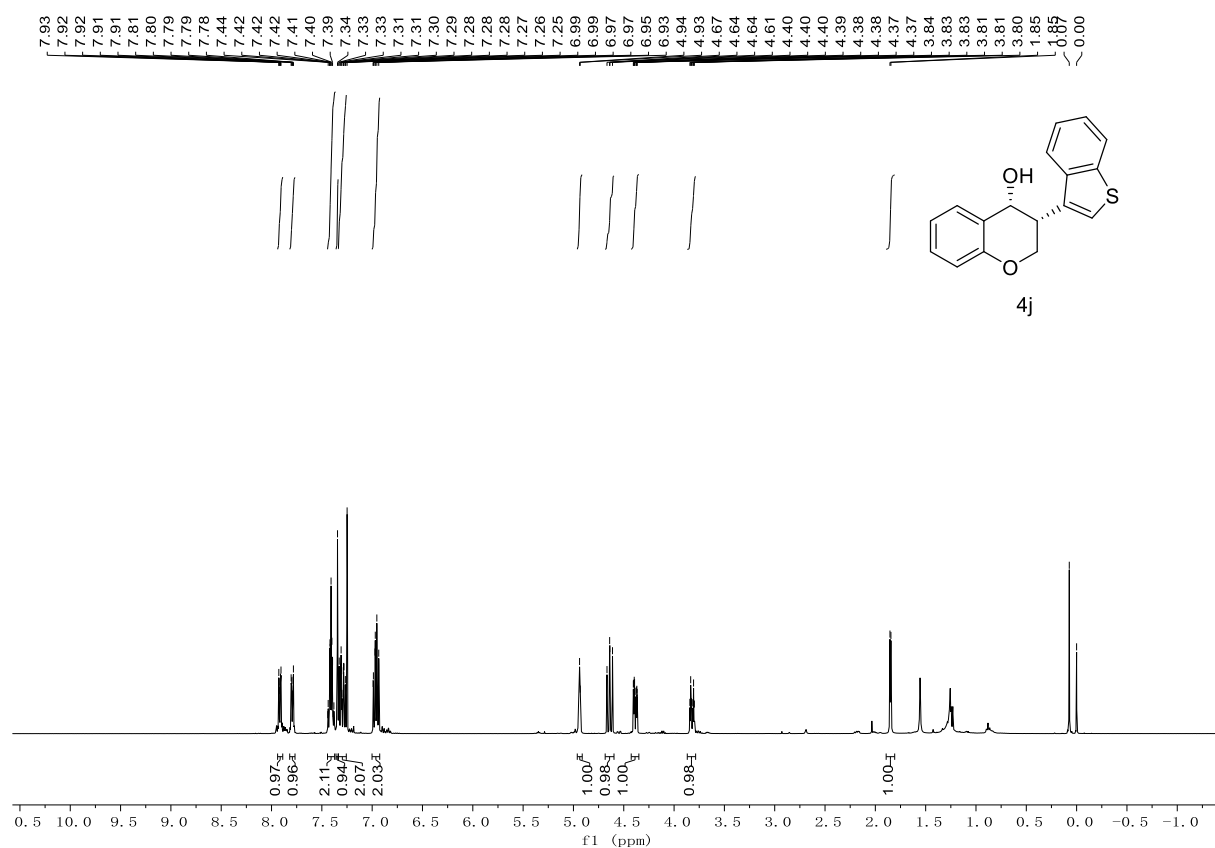
¹H and ¹³C-NMR of 4h



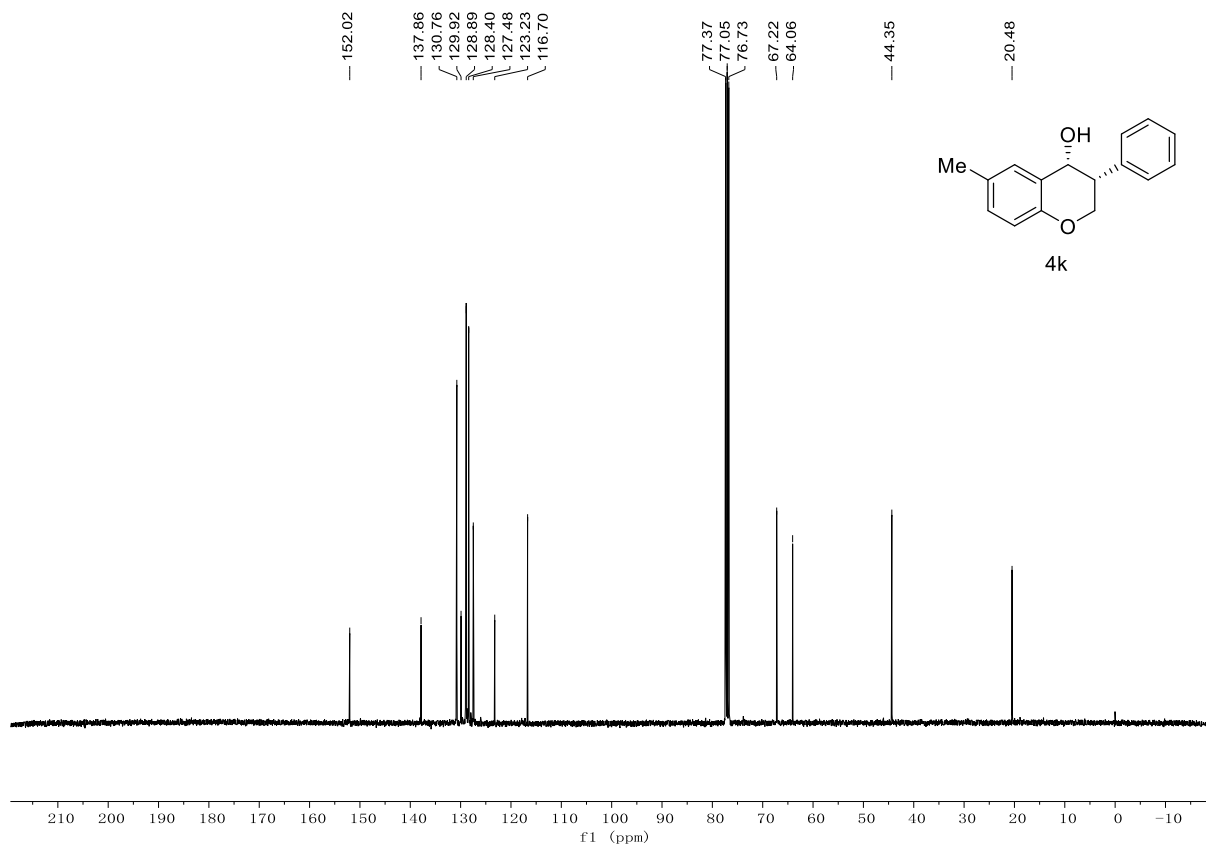
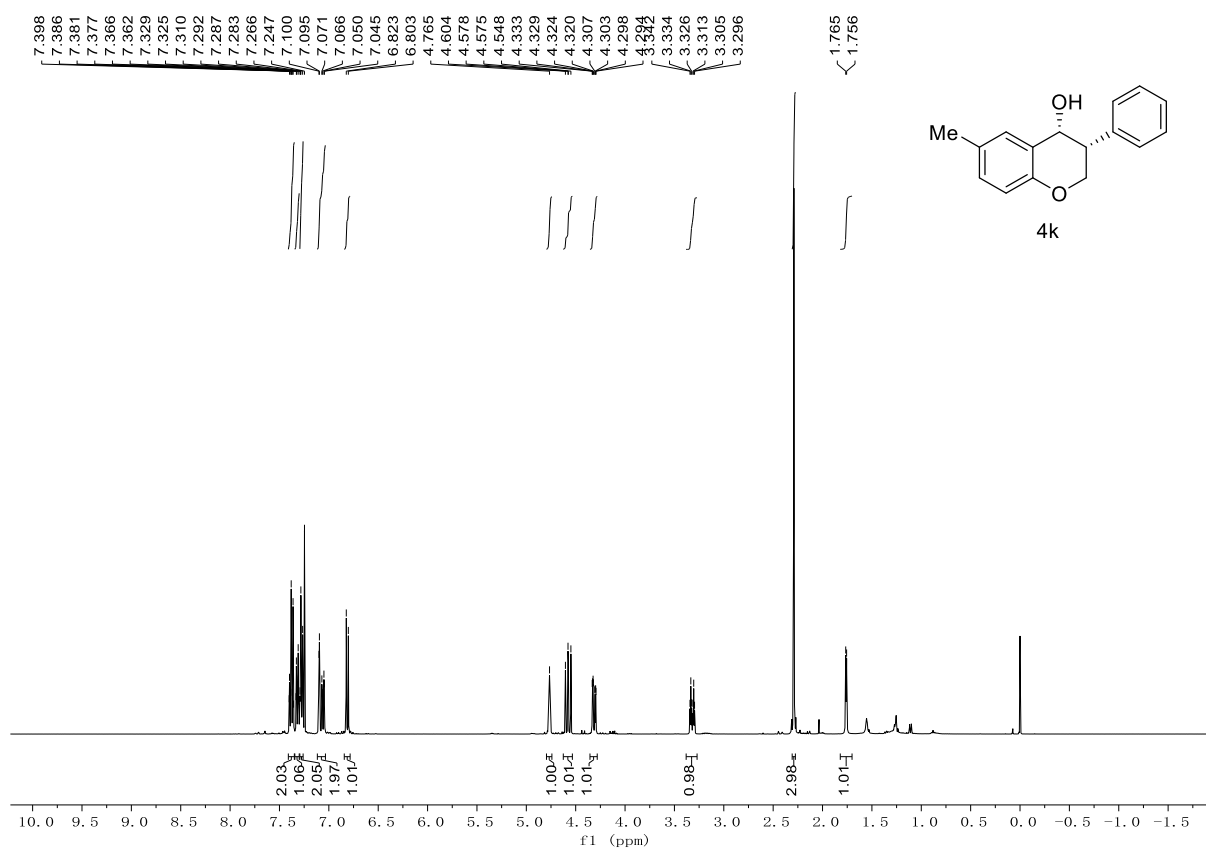
¹H and ¹³C-NMR of 4i



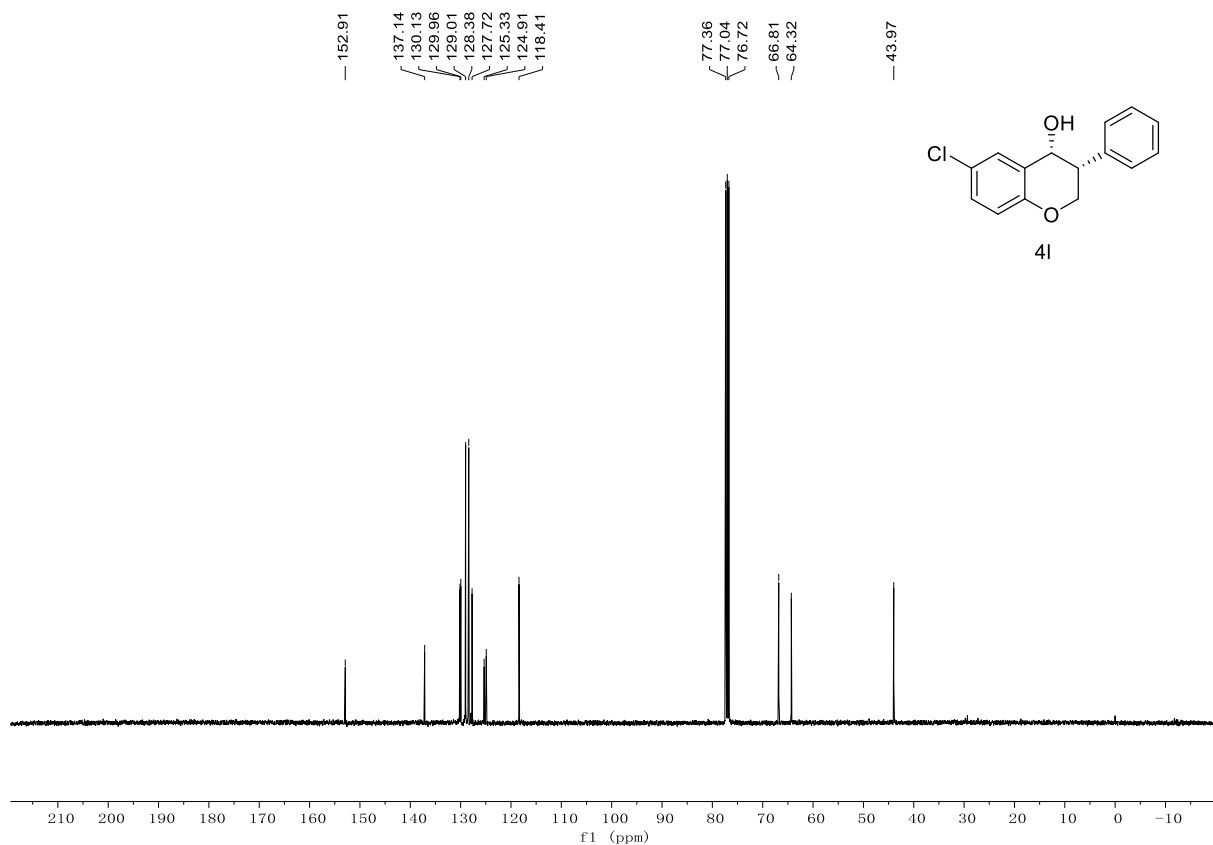
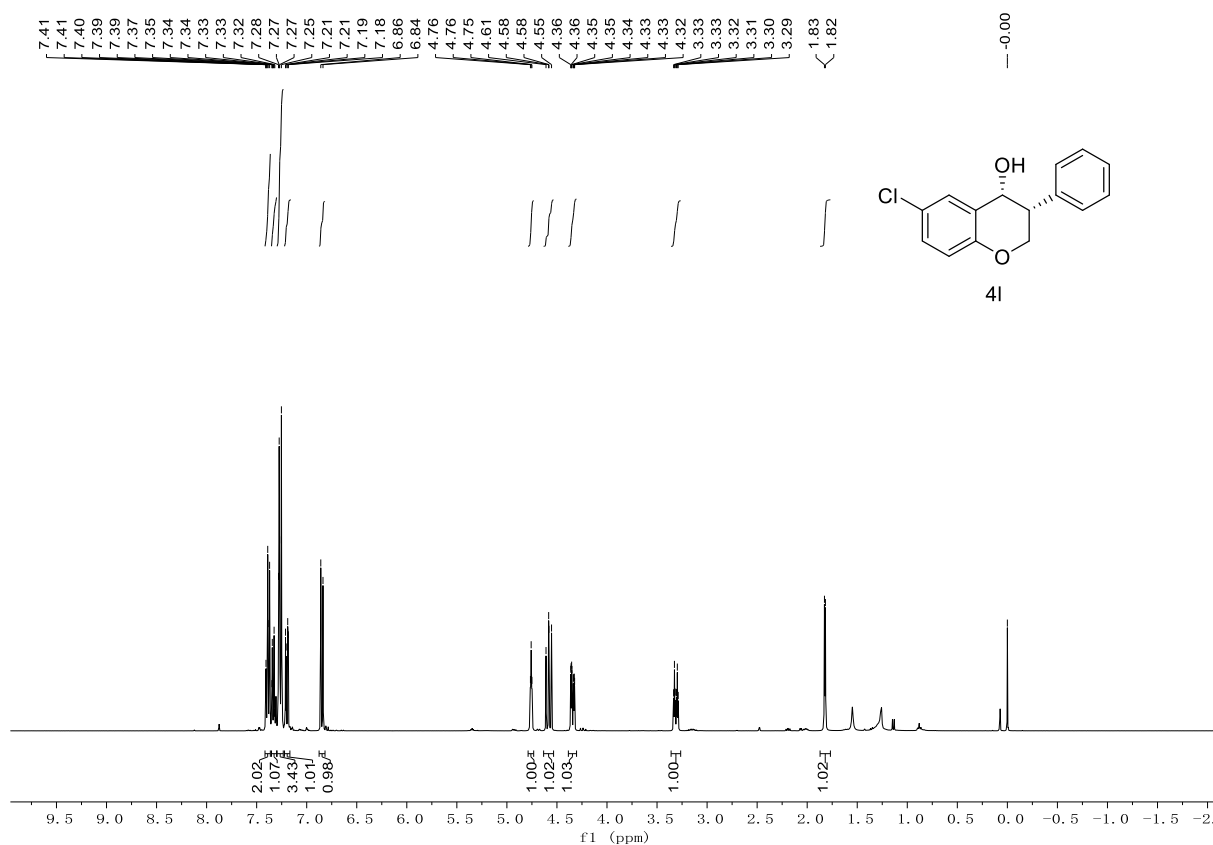
¹H and ¹³C-NMR of 4j



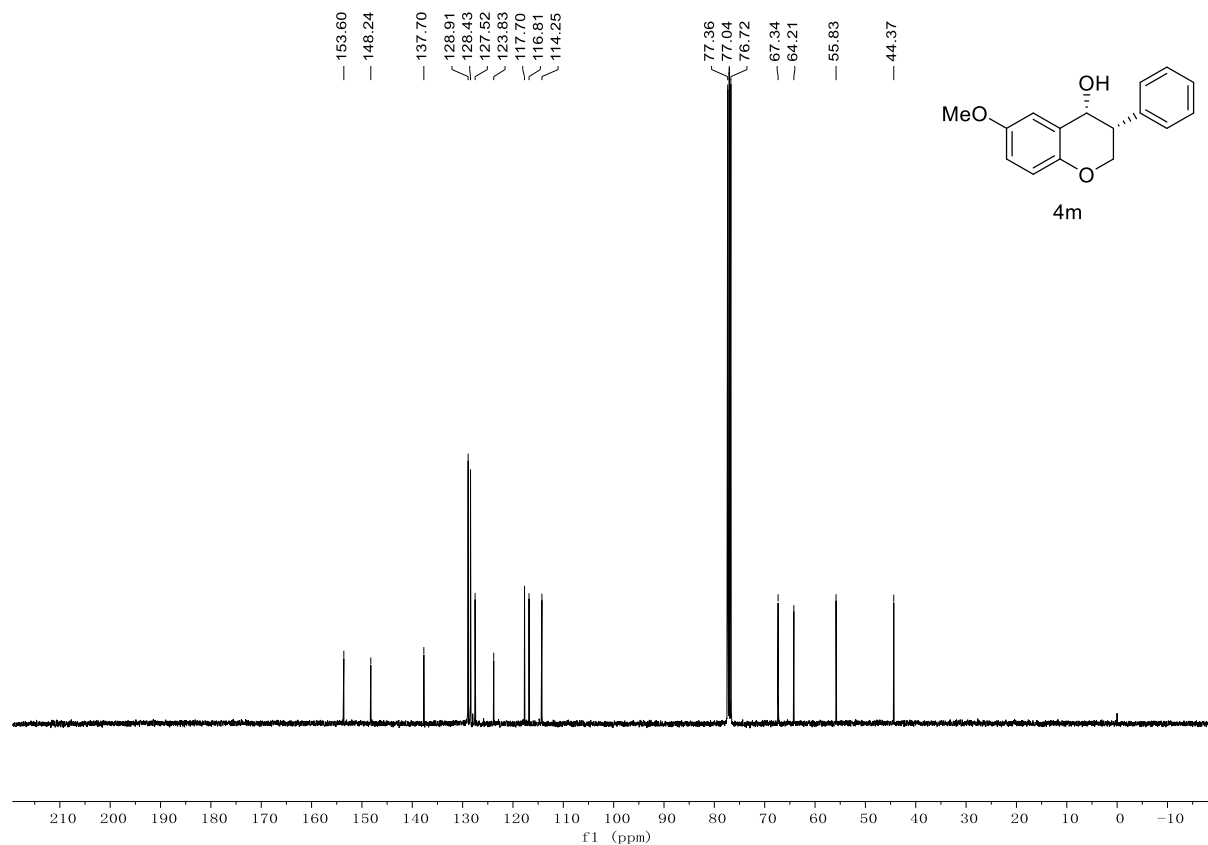
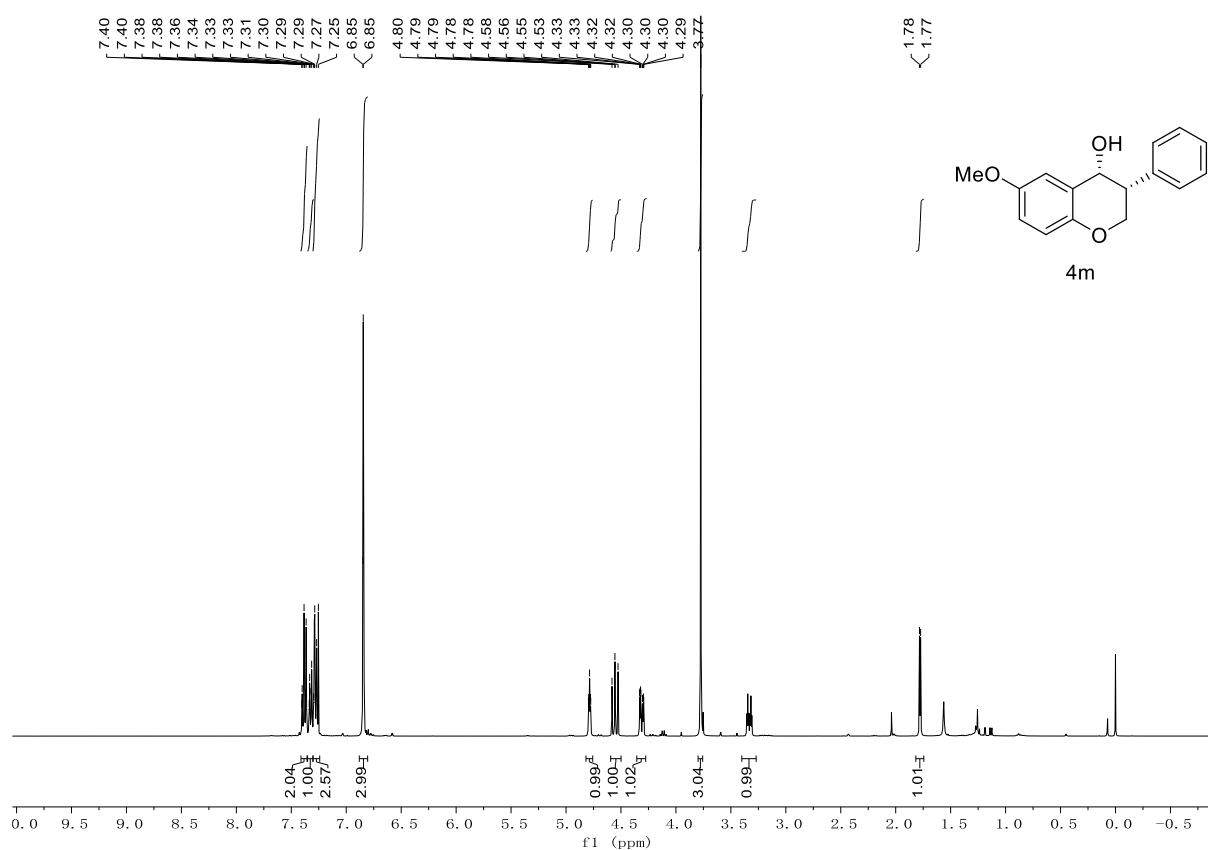
¹H and ¹³C-NMR of 4k



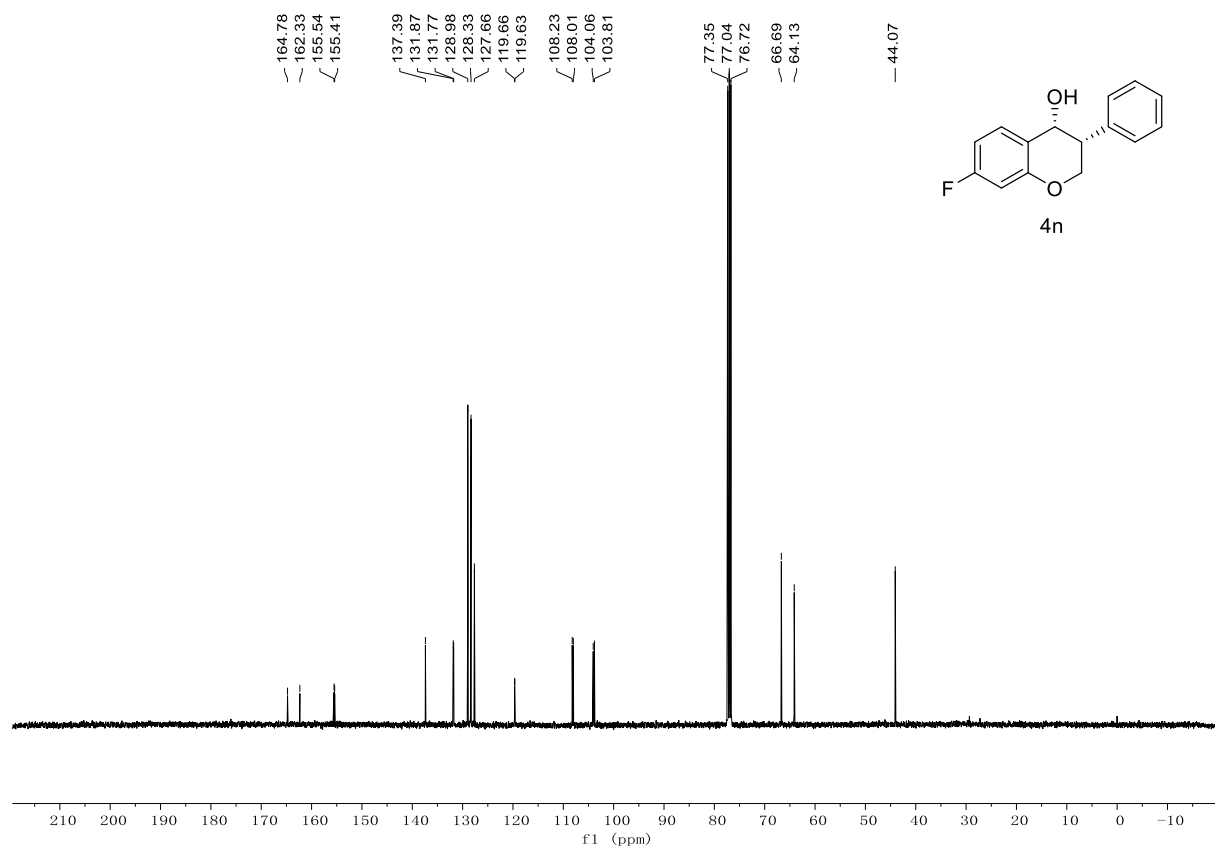
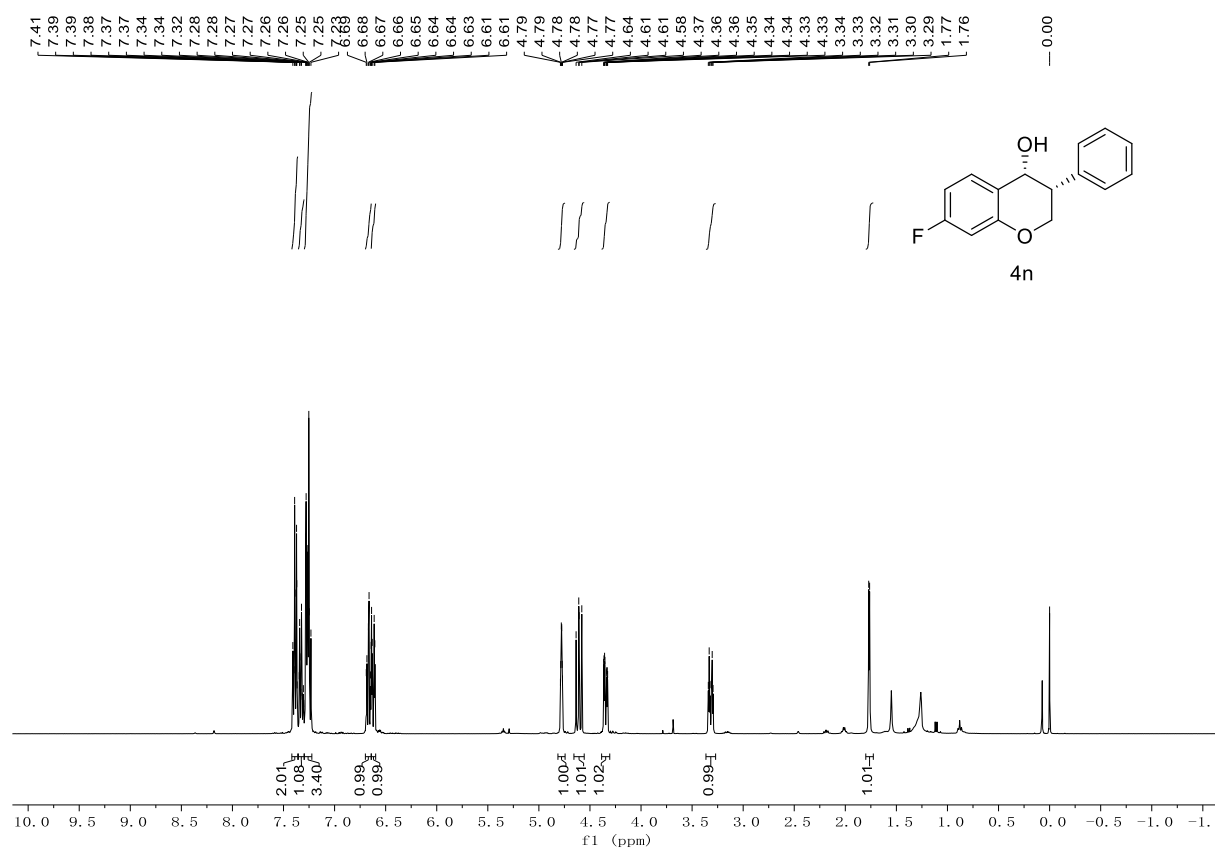
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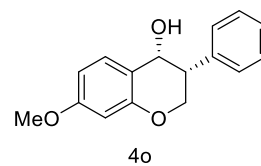
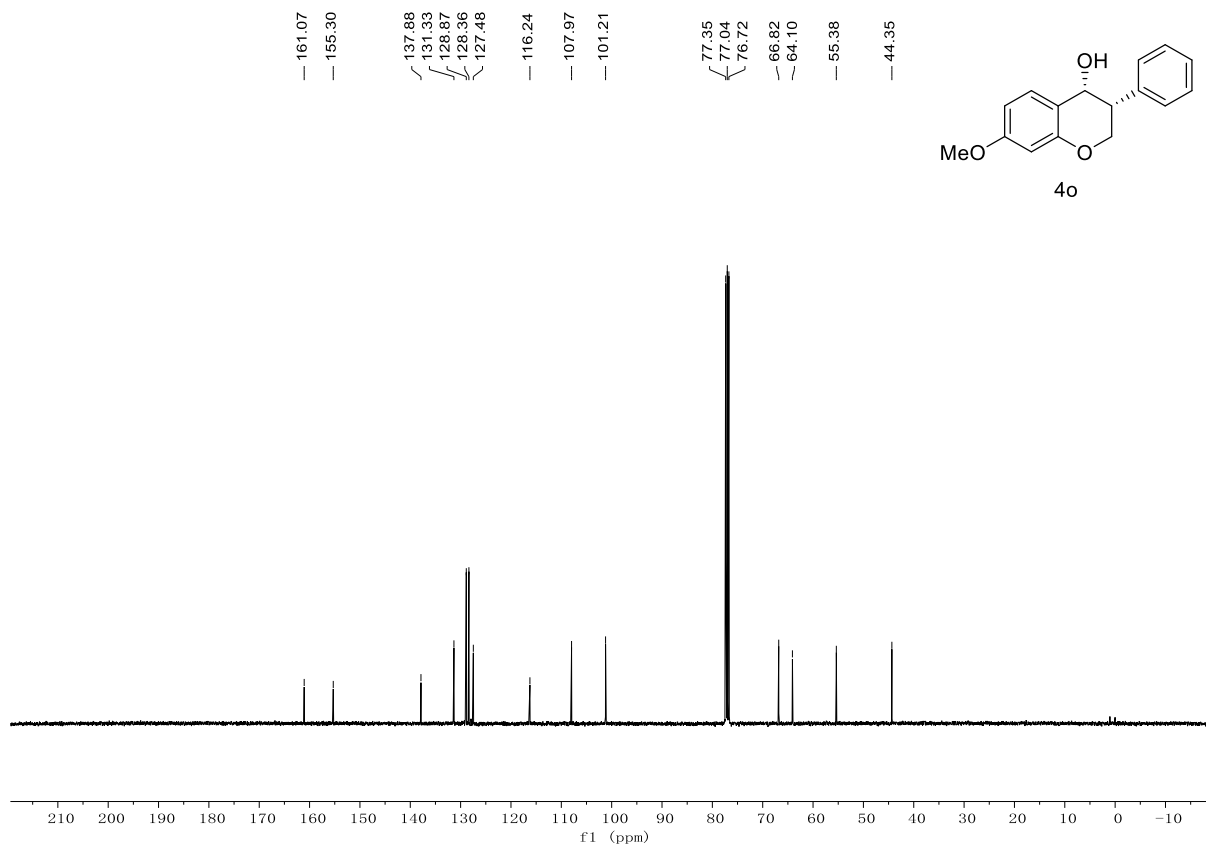
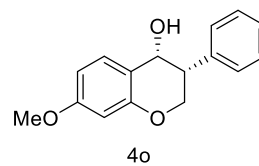
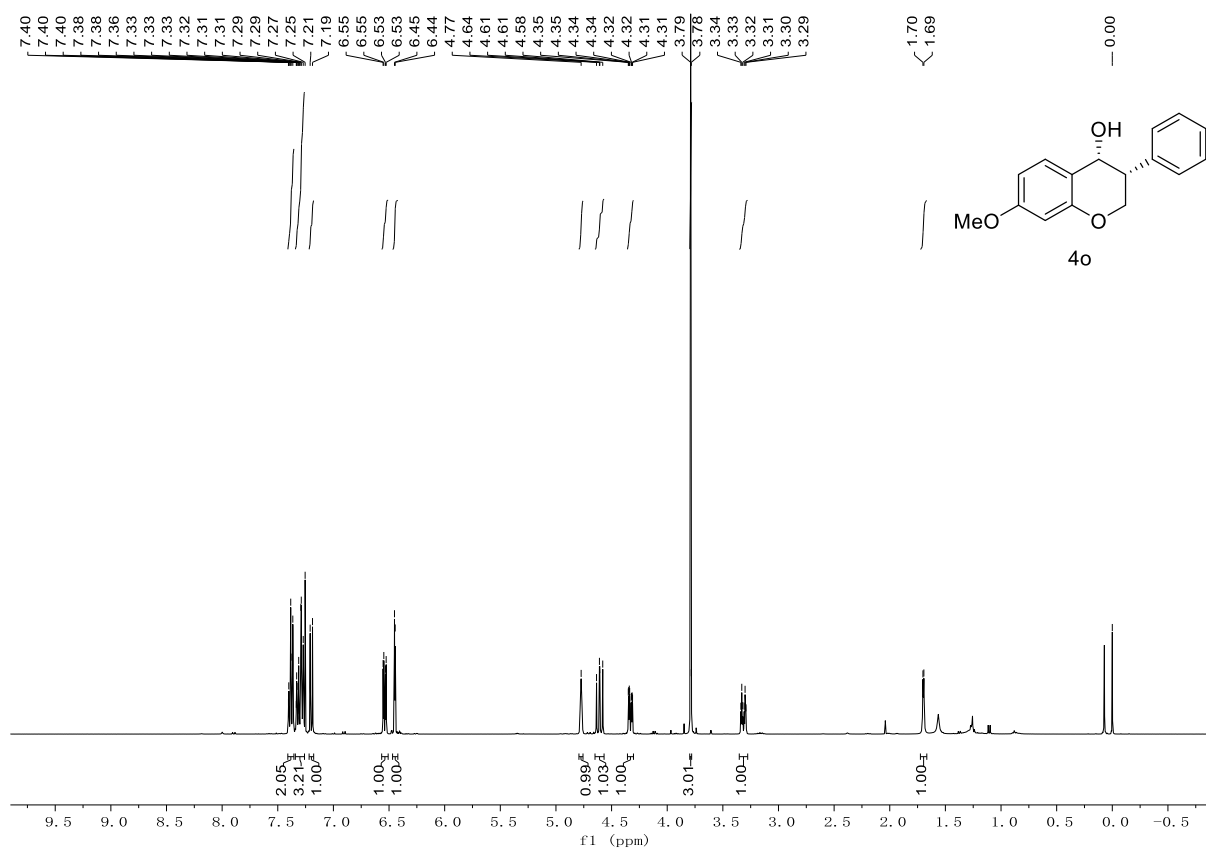
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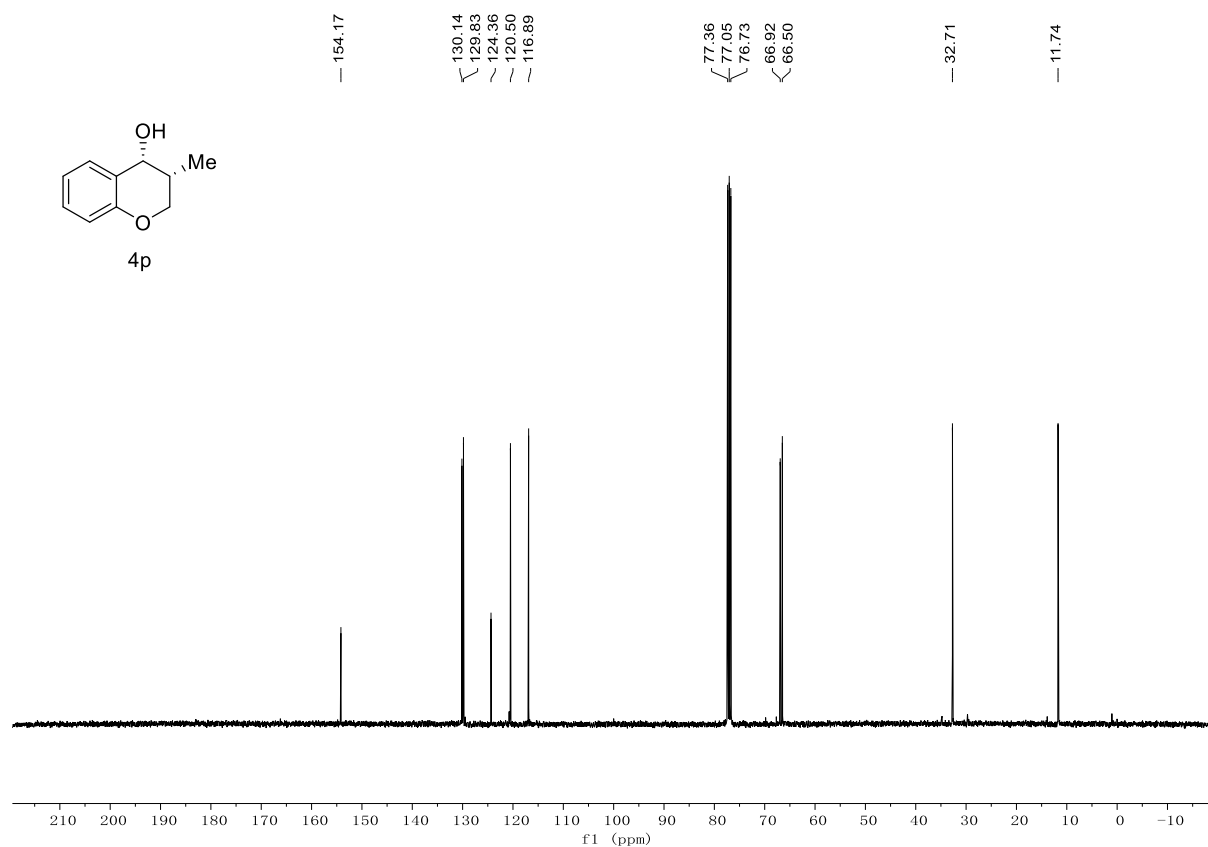
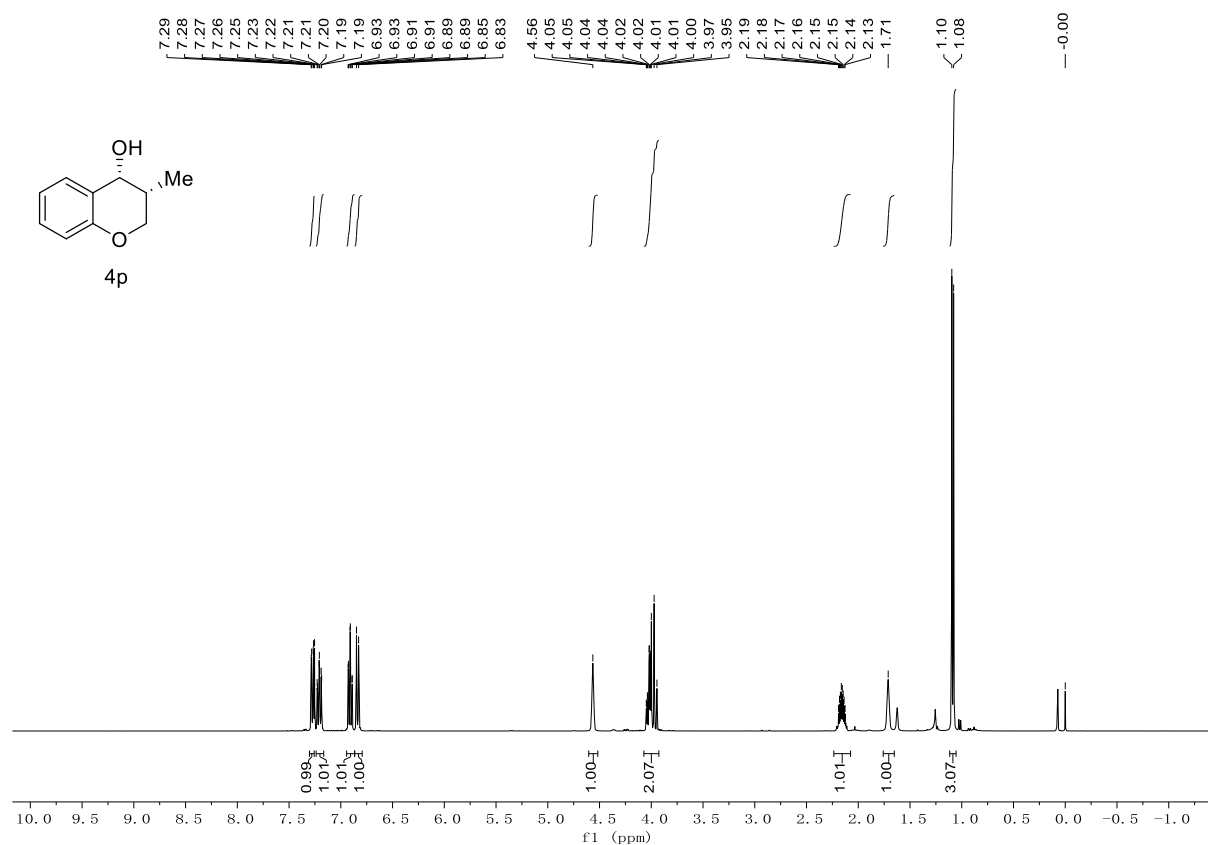
¹H and ¹³C-NMR of 4n



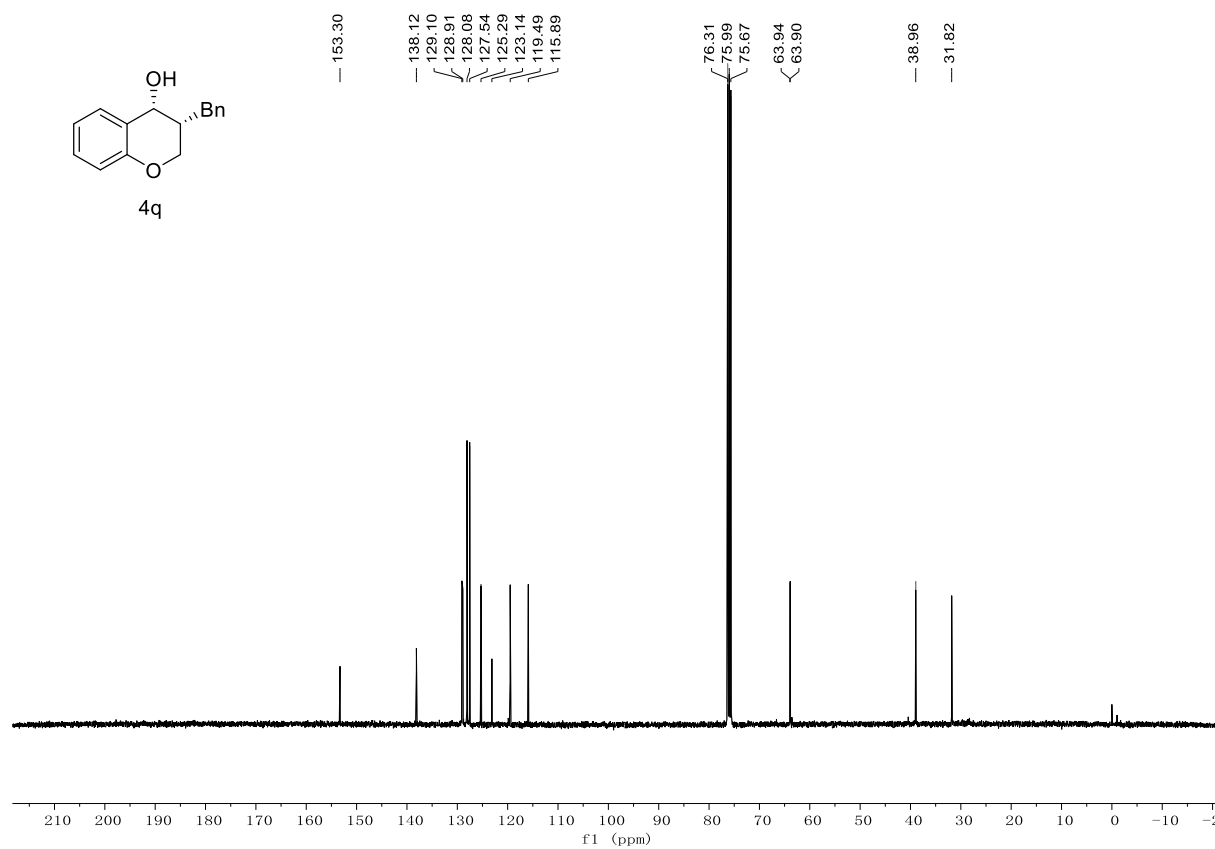
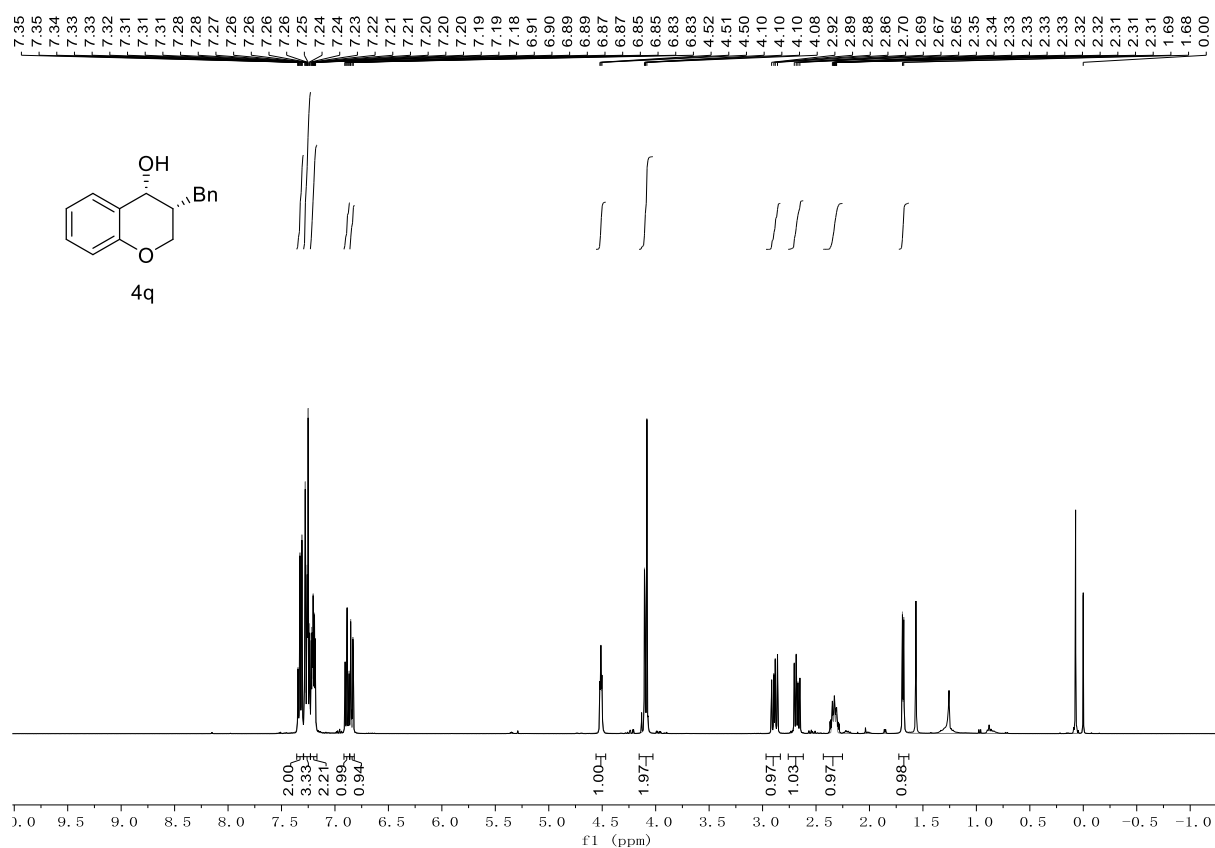
¹H and ¹³C-NMR of 4o



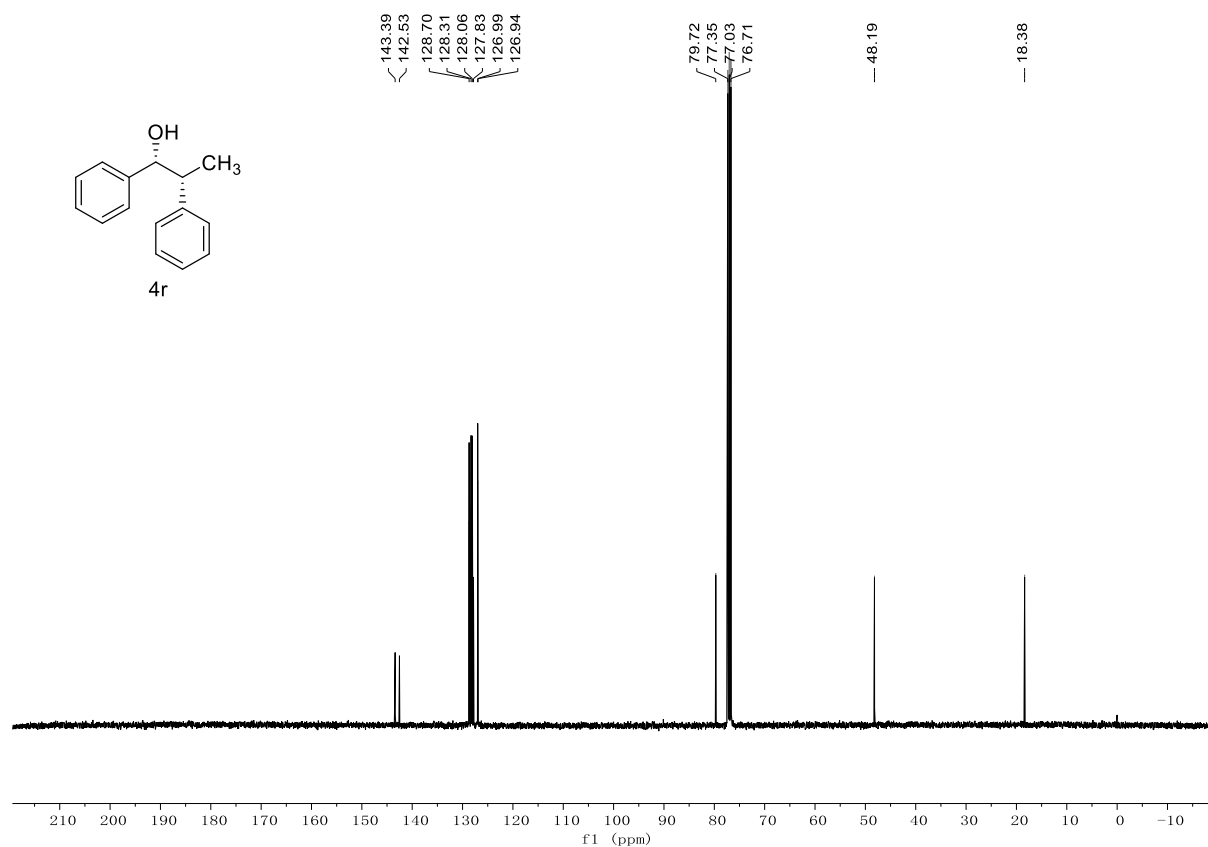
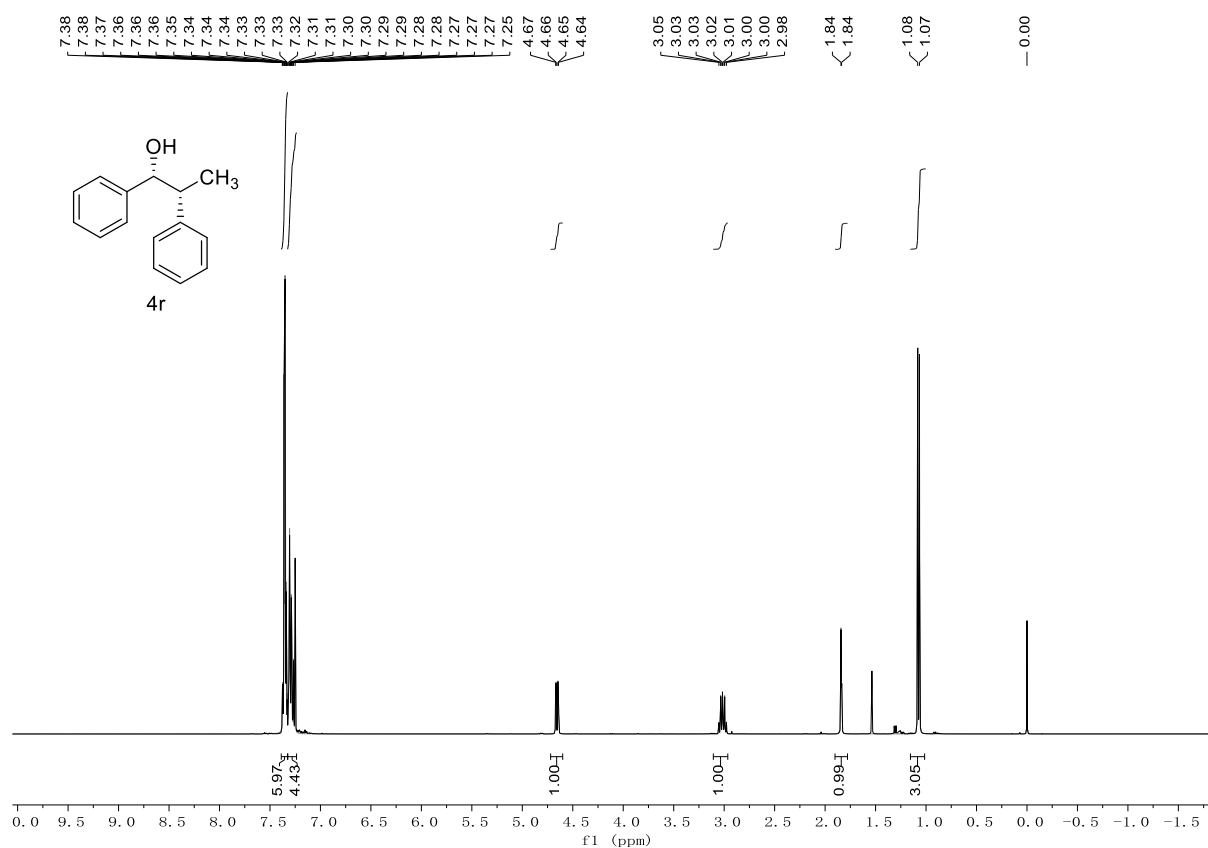
¹H and ¹³C-NMR of 4p



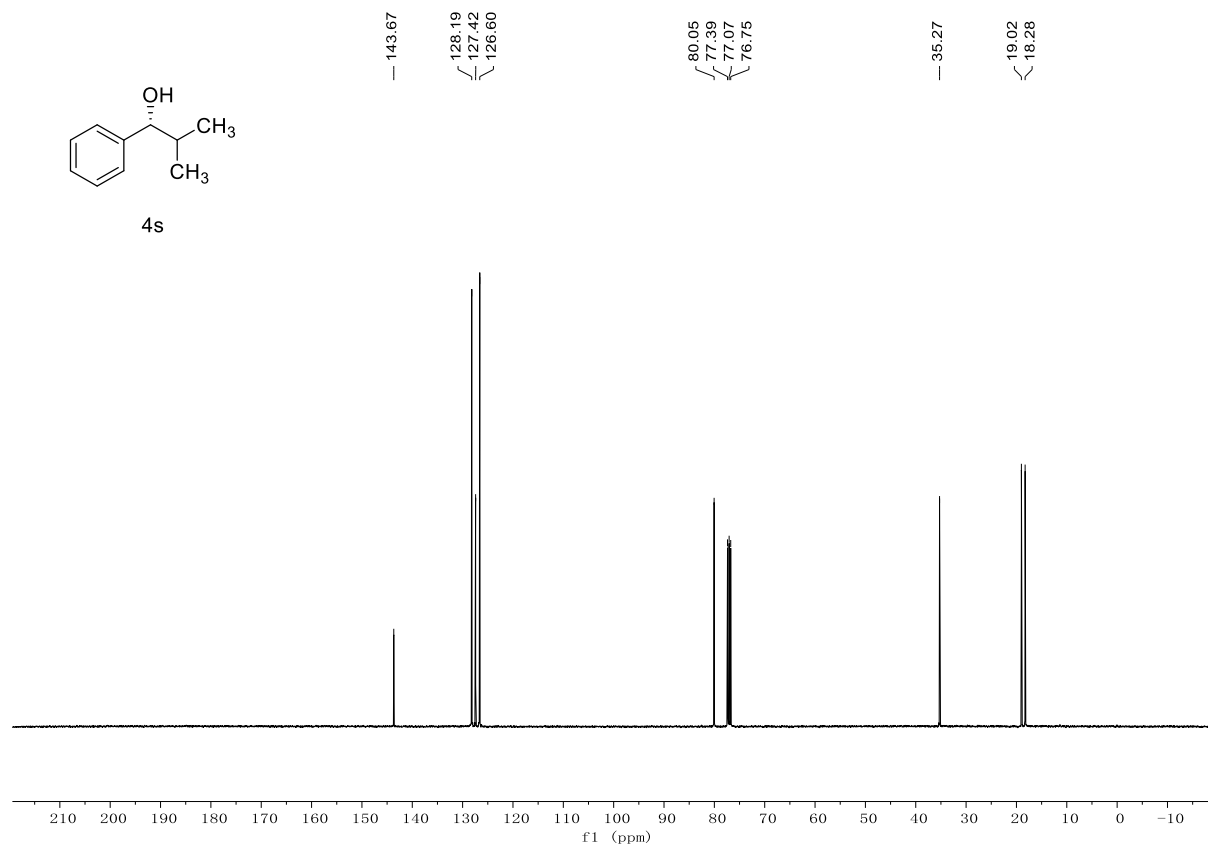
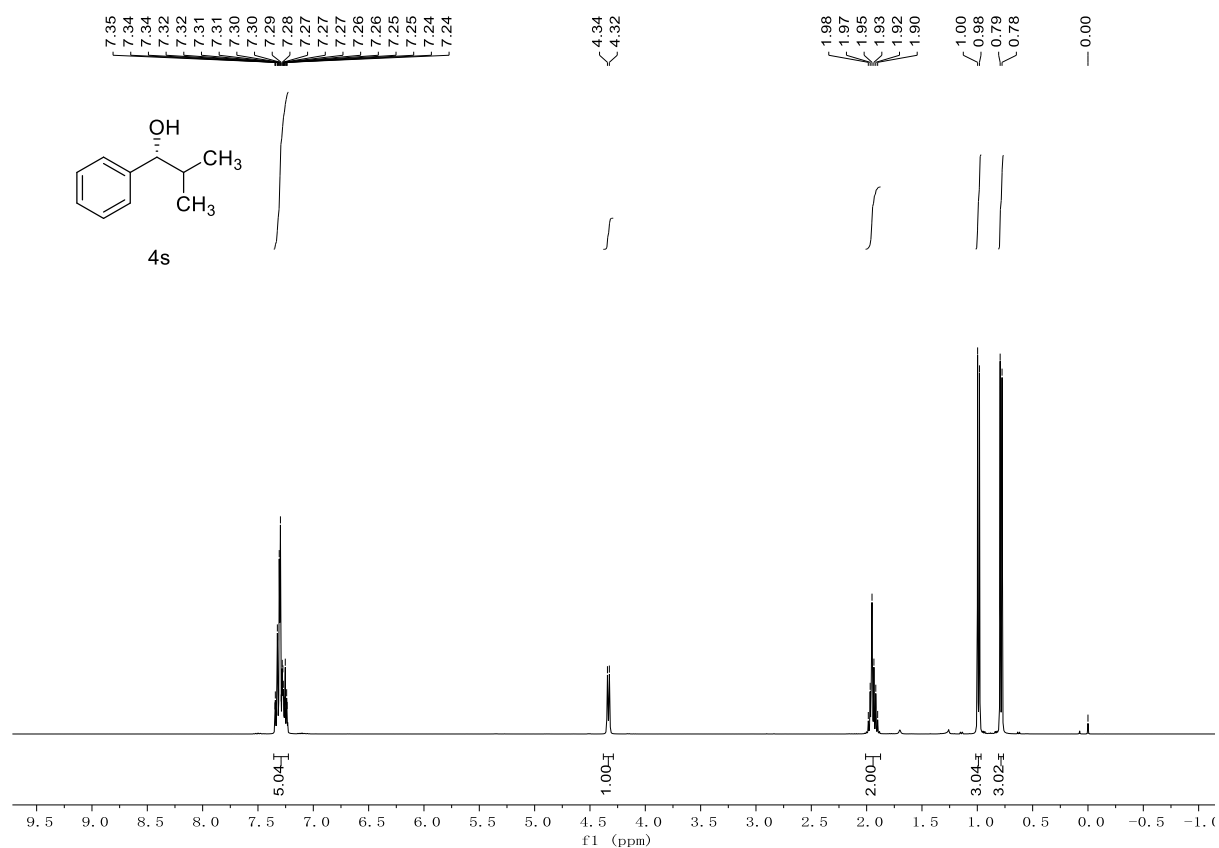
¹H and ¹³C-NMR of 4q



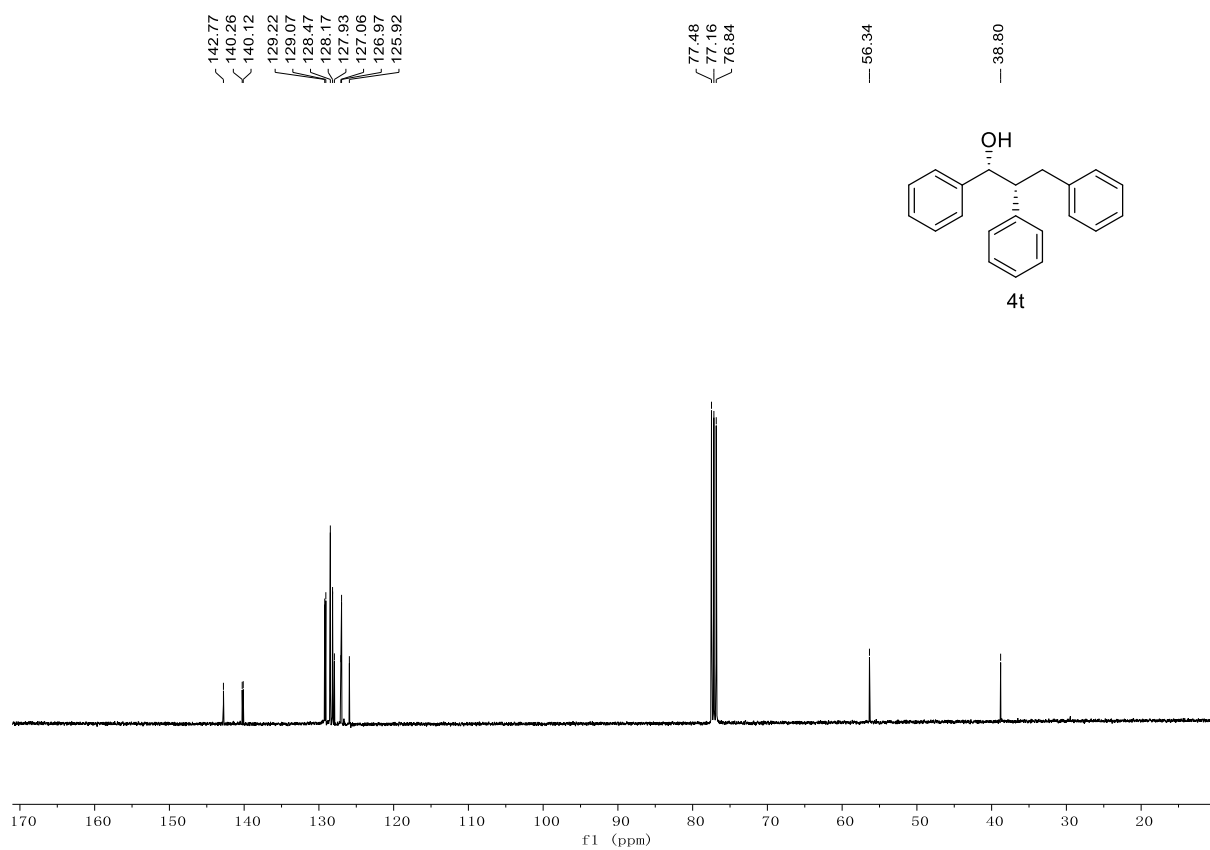
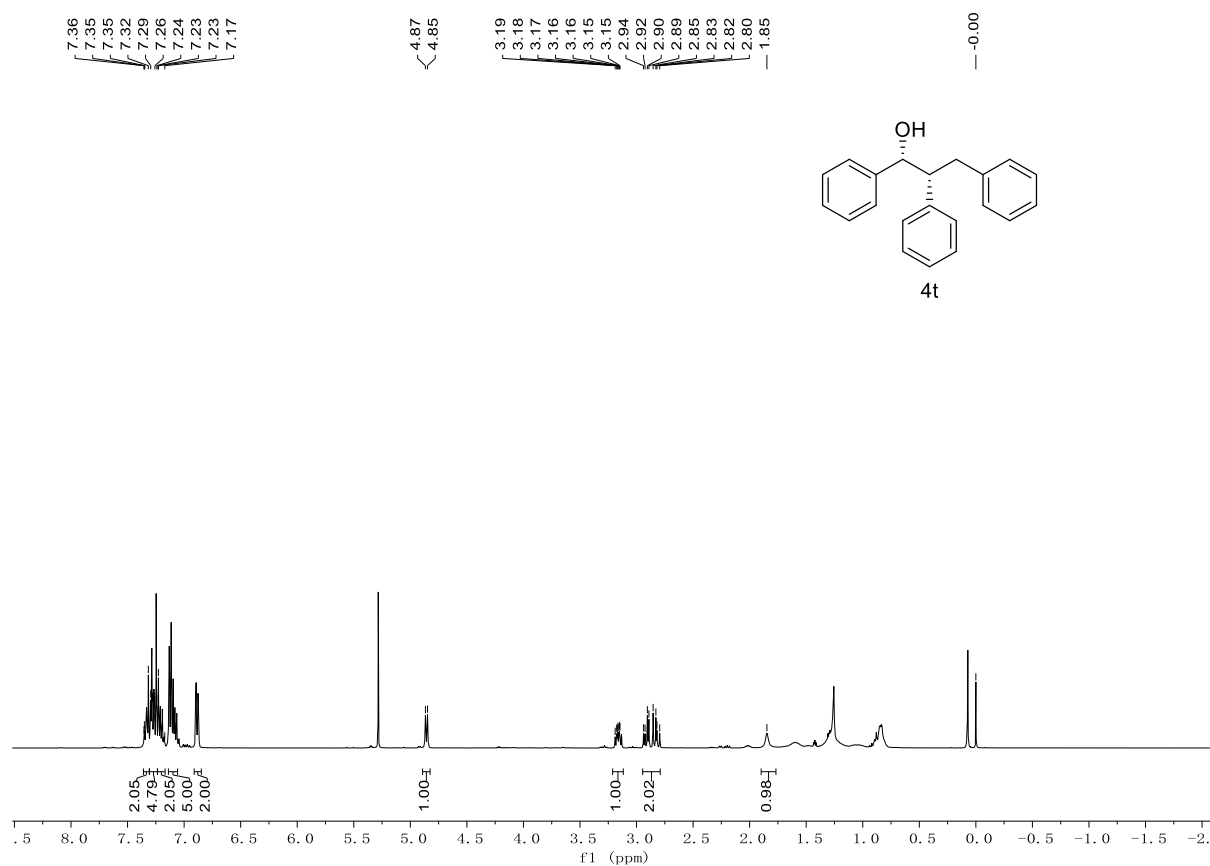
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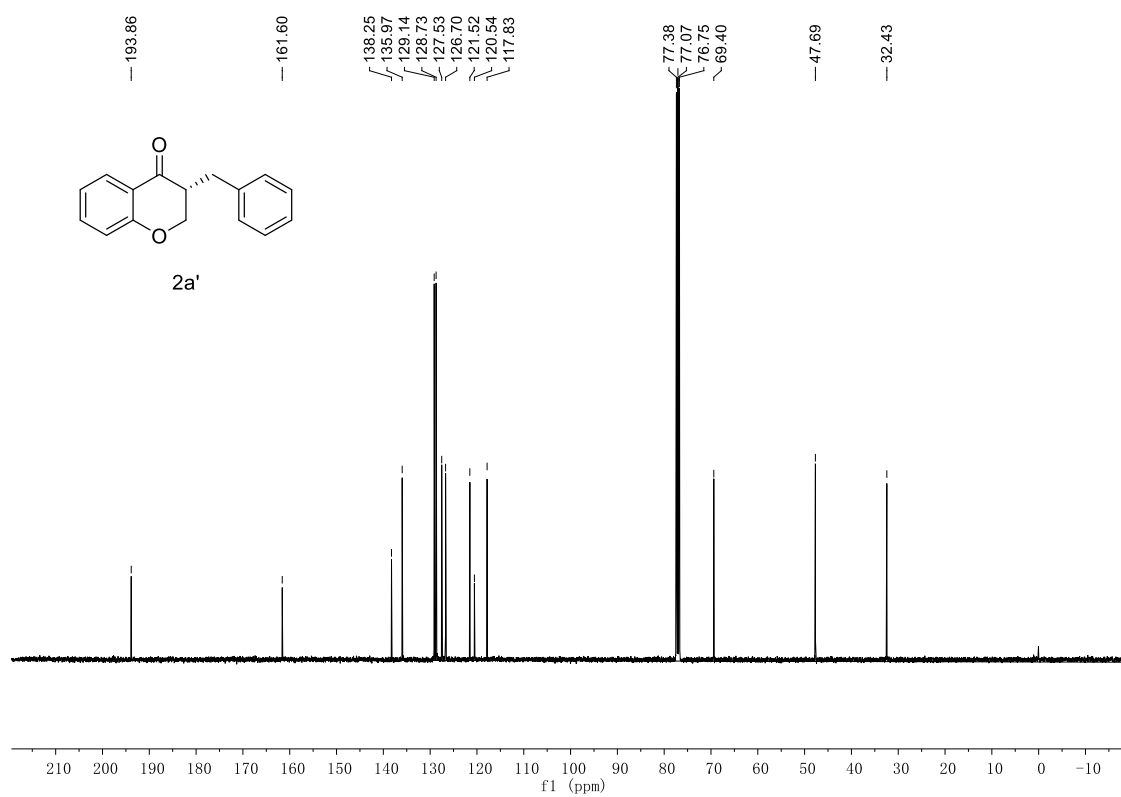
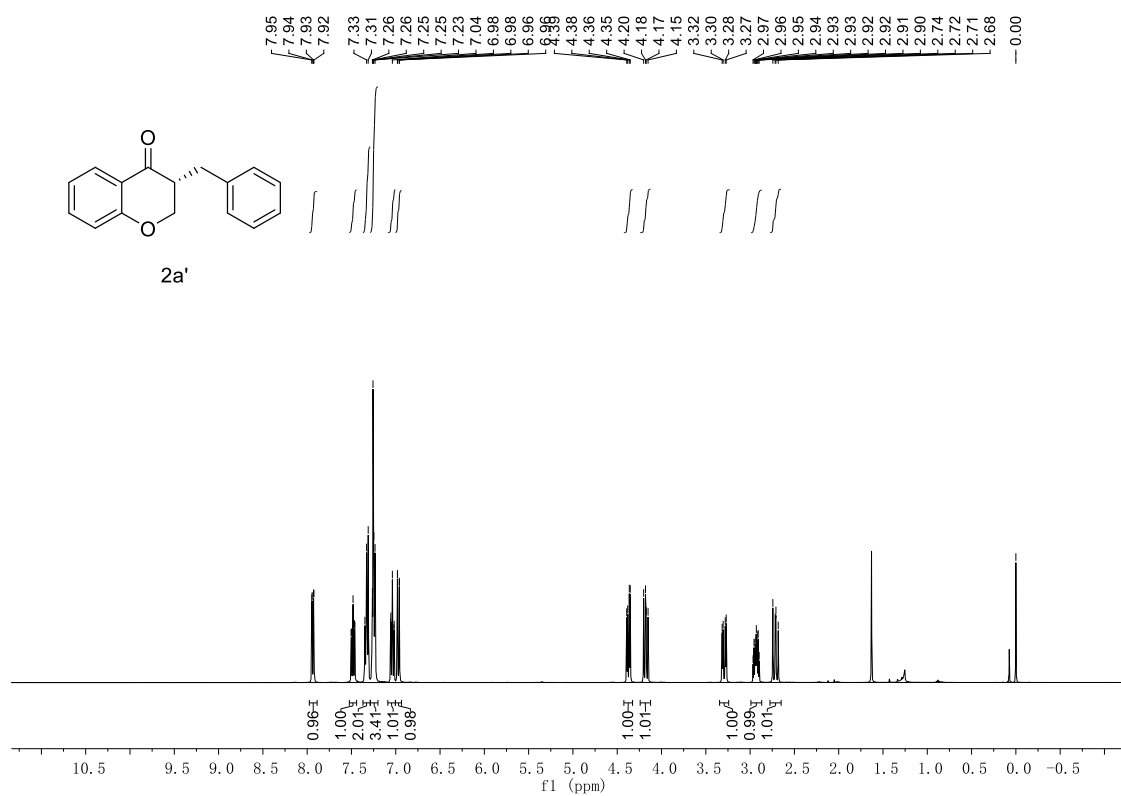
¹H and ¹³C-NMR of 4s



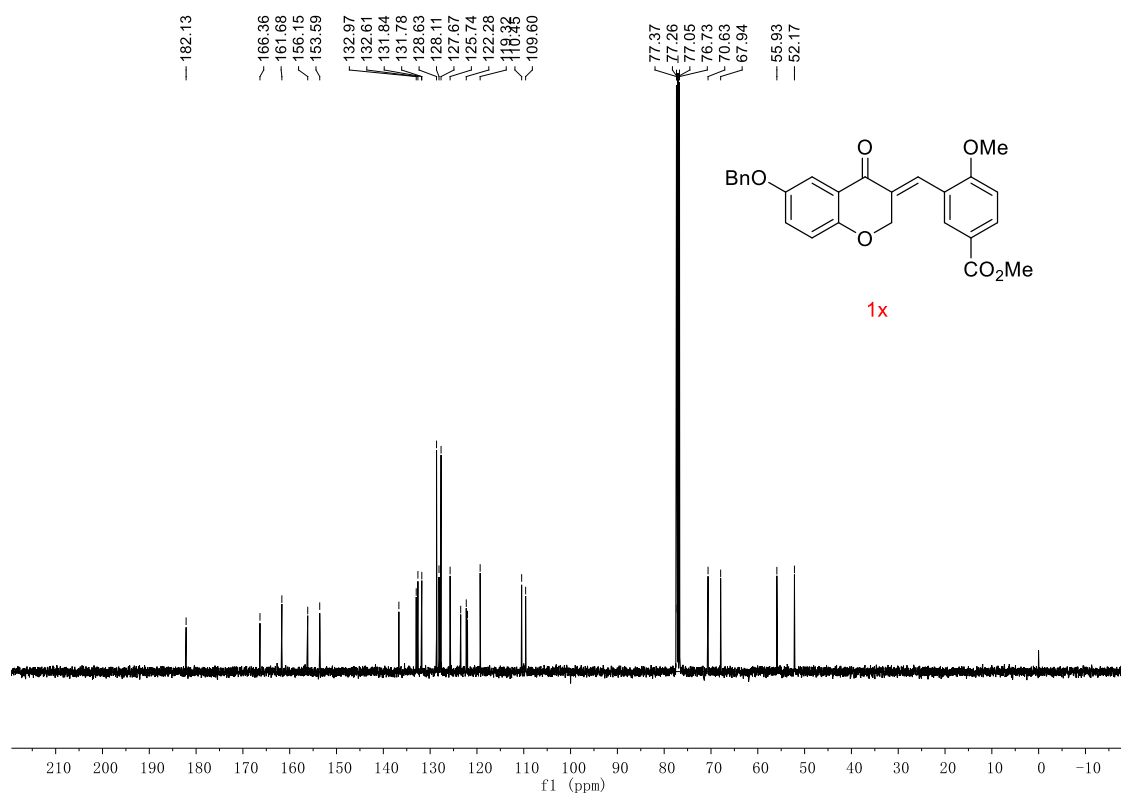
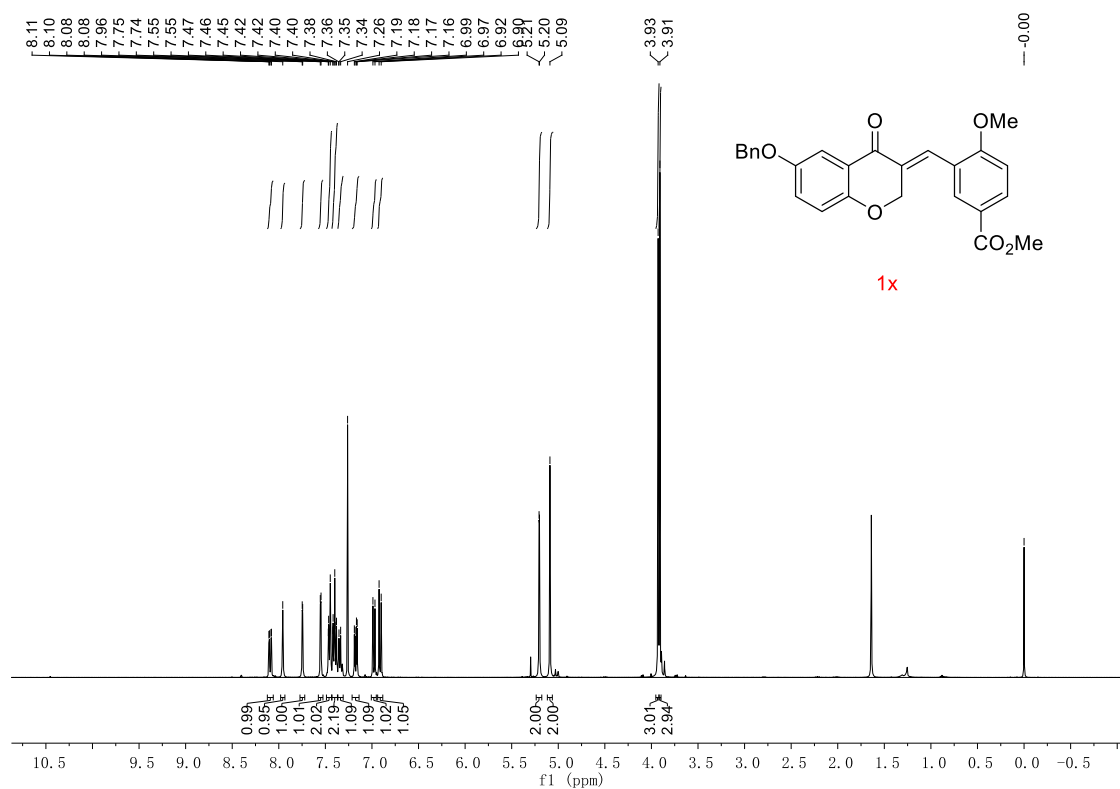
^1H and ^{13}C -NMR of 4t



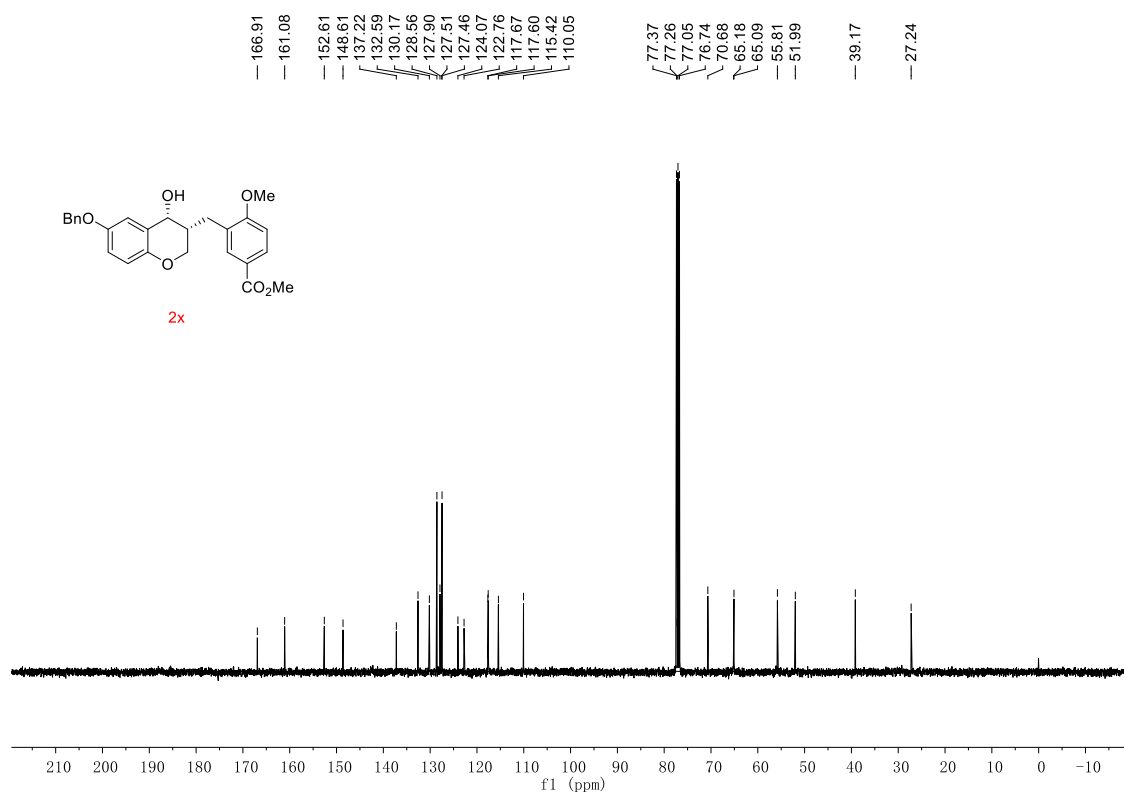
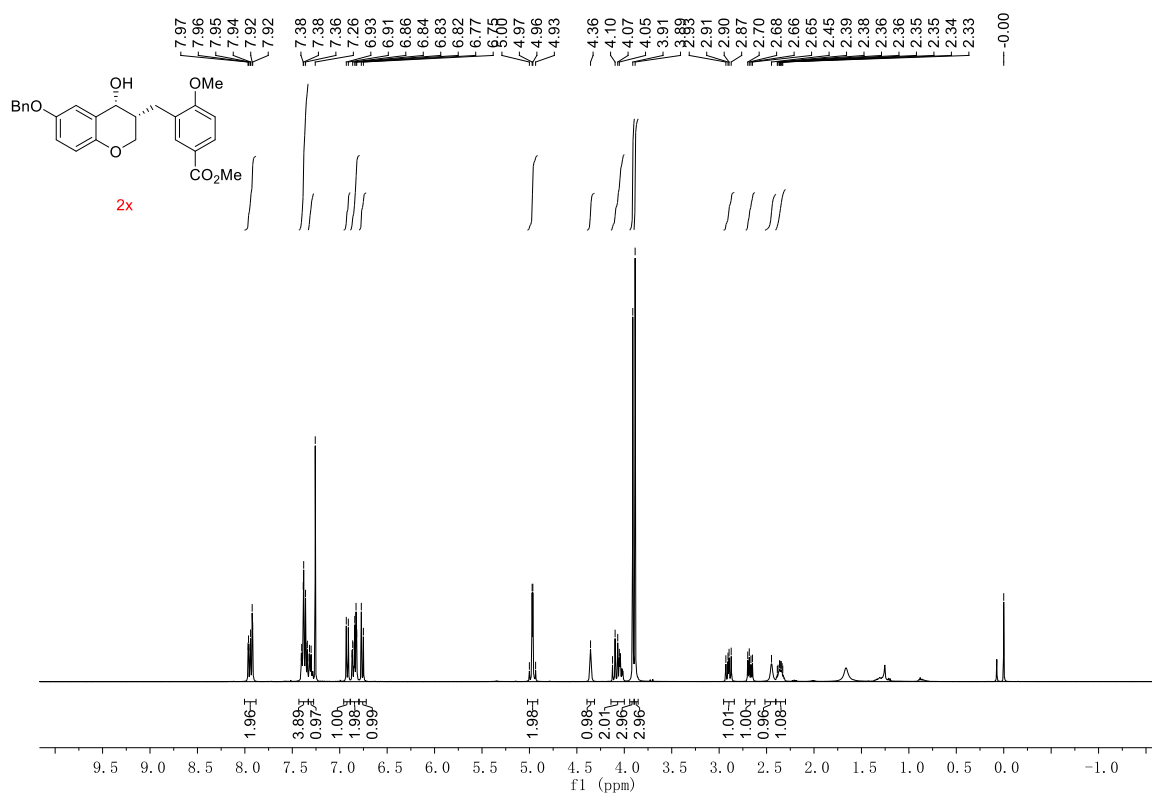
¹H and ¹³C-NMR of 2a'



¹H and ¹³C-NMR of 1x



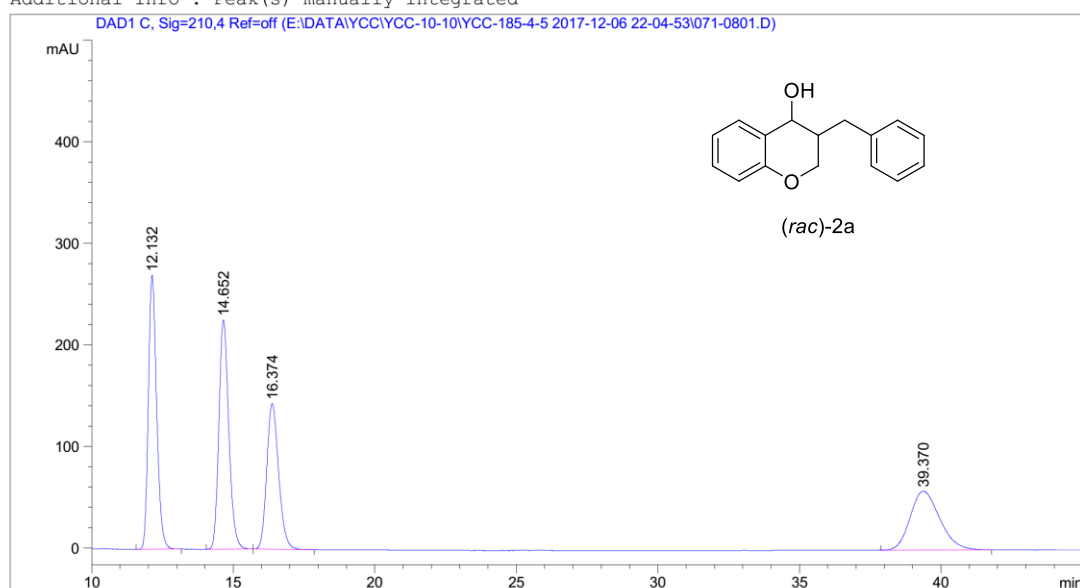
¹H and ¹³C-NMR of 2x



VIII. HPLC charts for hydrogenation products and derivatives

Data File E:\DATA\YCC\YCC-10-10\YCC-185-4-5 2017-12-06 22-04-53\071-0801.D
Sample Name: LWD-3-63-1-RAC

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Acq. Operator   : SYSTEM                      Seq. Line :    8
Acq. Instrument : 1260HPLC-DAD                Location  : Vial 71
Injection Date  : 12/7/2017 1:22:21 AM        Inj       :    1
                                           Inj Volume: 3.000 µl
Acq. Method     : E:\DATA\YCC\YCC-10-10\YCC-185-4-5 2017-12-06 22-04-53\DAD-OD(1-2)-95-5-3UL-
                                           1ML-60MIN.M
Last changed    : 12/6/2017 10:38:05 PM by SYSTEM
Analysis Method : E:\DATA\YCC\YCC-10-10\YCC-185-4-5 2017-12-06 22-04-53\DAD-OD(1-2)-95-5-3UL-
                                           1ML-60MIN.M (Sequence Method)
Last changed    : 7/27/2018 9:31:57 AM by SYSTEM
                                           (modified after loading)
Additional Info  : Peak(s) manually integrated
=====
```



Area Percent Report

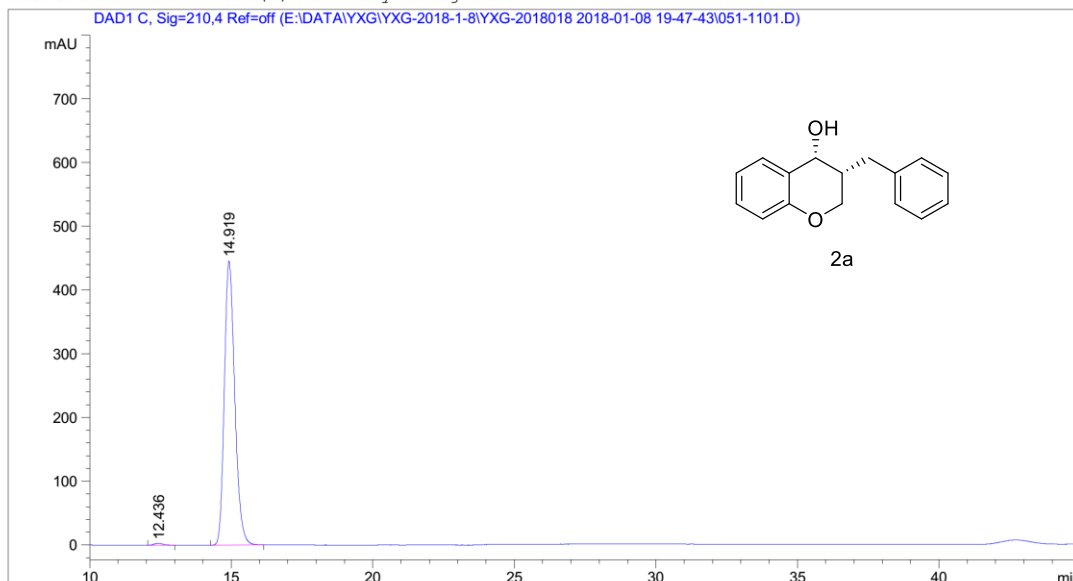
```
=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs
=====
```

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.132	BB	0.3128	5470.74756	269.58752	28.2879
2	14.652	BB	0.3754	5479.71826	225.54536	28.3343
3	16.374	BB	0.4509	4191.28711	143.43248	21.6721
4	39.370	BB	0.9739	4197.80078	57.89387	21.7058

Data File E:\DATA\YXG\YXG-2018-1-8\YXG-2018018 2018-01-08 19-47-43\051-1101.D
Sample Name: LWD-3-89-1

```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   11
Acq. Instrument : 1260HPLC-DAD                Location  : Vial 51
Injection Date  : 1/9/2018 1:20:13 AM          Inj       :    1
                                           Inj Volume: 3.000 µl
Acq. Method     : E:\DATA\YXG\YXG-2018-1-8\YXG-2018018 2018-01-08 19-47-43\DAD-OD(1-2)-95-5-
                                           3UL-1ML-60MIN.M
Last changed    : 1/8/2018 10:01:28 PM by SYSTEM
Analysis Method : E:\DATA\YXG\YXG-2018-1-8\YXG-2018018 2018-01-08 19-47-43\DAD-OD(1-2)-95-5-
                                           3UL-1ML-60MIN.M (Sequence Method)
Last changed    : 7/27/2018 9:48:28 AM by SYSTEM
                                           (modified after loading)
Additional Info  : Peak(s) manually integrated
=====
```



Area Percent Report

```
=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs
=====
```

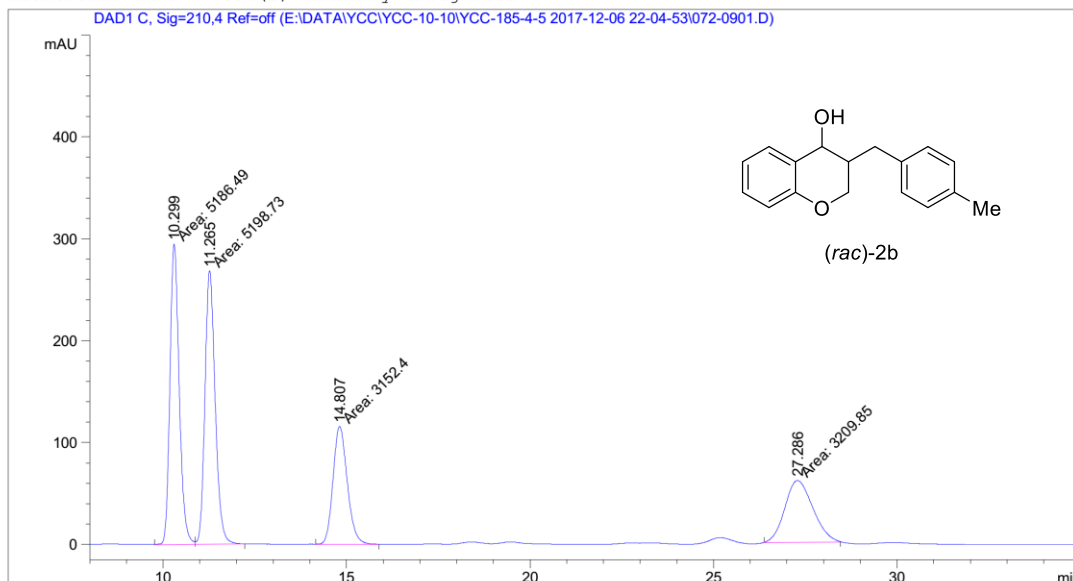
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.436	BB	0.2903	64.16340	3.03893	0.5602
2	14.919	BB	0.3923	1.13886e4	445.42419	99.4398
Totals :				1.14528e4	448.46312	

=====

Acq. Operator	: SYSTEM	Seq. Line	: 9
Acq. Instrument	: 1260HPLC-DAD	Location	: Vial 72
Injection Date	: 12/7/2017 2:23:14 AM	Inj	: 1
		Inj Volume	: 3.000 µl
Acq. Method	: E:\DATA\YCC\YCC-10-10\YCC-185-4-5 2017-12-06 22-04-53\DAD-OD(1-2)-95-5-3UL-1ML-60MIN.M		
Last changed	: 12/6/2017 10:38:05 PM by SYSTEM		
Analysis Method	: E:\DATA\YCC\YCC-10-10\YCC-185-4-5 2017-12-06 22-04-53\DAD-OD(1-2)-95-5-3UL-1ML-60MIN.M (Sequence Method)		
Last changed	: 7/27/2018 9:36:47 AM by SYSTEM (modified after loading)		

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

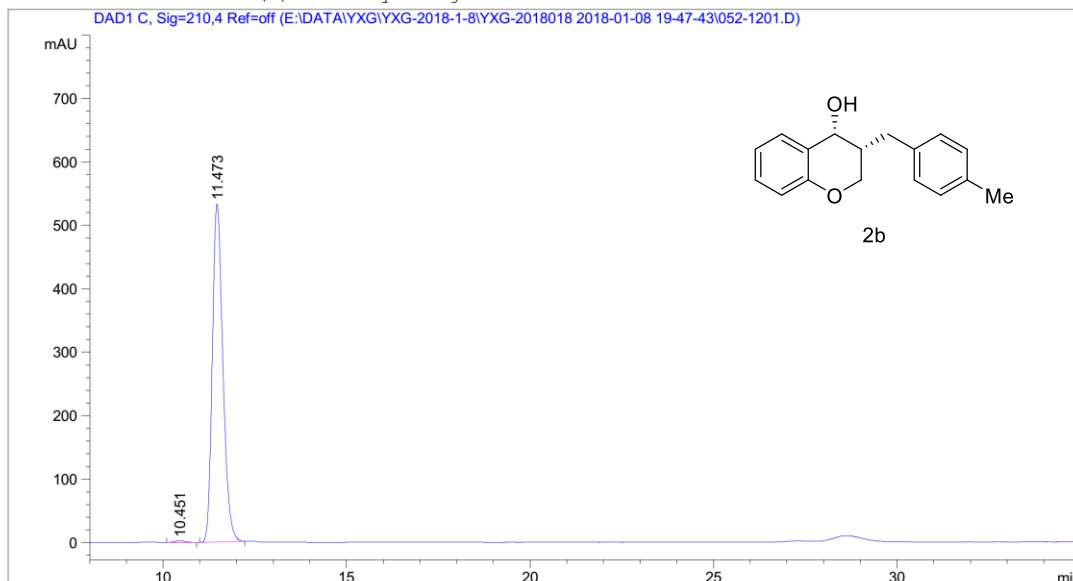
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.299	MF	0.2932	5186.49023	294.83160	30.9688
2	11.265	FM	0.3230	5198.72705	268.27664	31.0419
3	14.807	MM	0.4529	3152.39868	116.00610	18.8231
4	27.286	MM	0.8832	3209.84521	60.57419	19.1662

Data File E:\DATA\YXG\YXG-2018-1-8\YXG-2018018 2018-01-08 19-47-43\052-1201.D
Sample Name: LWD-3-89-2

```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   12
Acq. Instrument : 1260HPLC-DAD                Location  : Vial 52
Injection Date  : 1/9/2018 2:21:09 AM          Inj       :    1
                                           Inj Volume: 3.000 µl
Acq. Method     : E:\DATA\YXG\YXG-2018-1-8\YXG-2018018 2018-01-08 19-47-43\
DAD-OD(1-2)-95-5-3UL-1ML-60MIN.M
Last changed    : 1/8/2018 10:01:28 PM by SYSTEM
Analysis Method : E:\DATA\YXG\YXG-2018-1-8\YXG-2018018 2018-01-08 19-47-43\
DAD-OD(1-2)-95-5-3UL-1ML-60MIN.M (Sequence Method)
Last changed    : 7/27/2018 9:51:22 AM by SYSTEM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
DAD1 C, Sig=210,4 Ref=off (E:\DATA\YXG\YXG-2018-1-8\YXG-2018018 2018-01-08 19-47-43\052-1201.D)
```



Area Percent Report

```
=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs
```

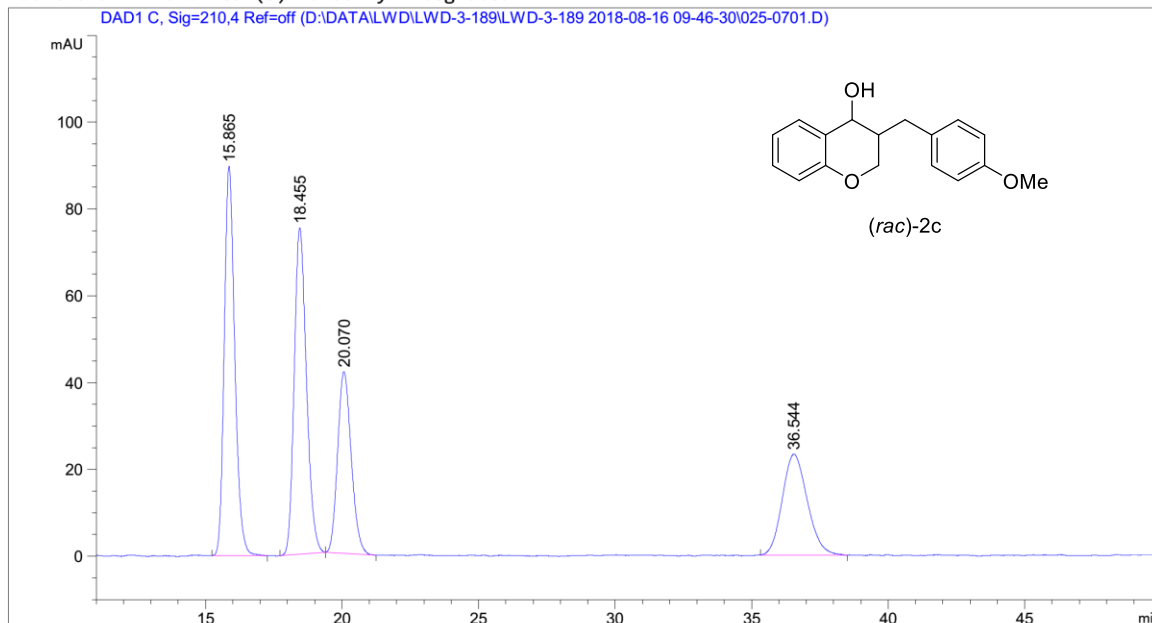
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.451	BB	0.2444	49.99823	2.79935	0.4676
2	11.473	BB	0.3090	1.06433e4	532.92218	99.5324
Totals :				1.06933e4	535.72153	

Sample Name: LWD-3-189-3-RAC

```

=====
Acq. Operator   :                               Seq. Line :    7
Acq. Instrument : Instrument 2                   Location  : Vial 25
Injection Date  : 8/16/2018 1:53:34 PM           Inj       :    1
                                                Inj Volume : 3.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-
                  3UL-ALL-50MIN.M
Last changed    : 8/16/2018 9:43:15 AM
Analysis Method : D:\METHOD\ZXH\DAD-OJ(1-6)-99-1-0.5ML-1UL-220NM-10MIN.M
Last changed    : 6/16/2020 8:31:12 PM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
  
```



```

=====
                          Area Percent Report
=====
  
```

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

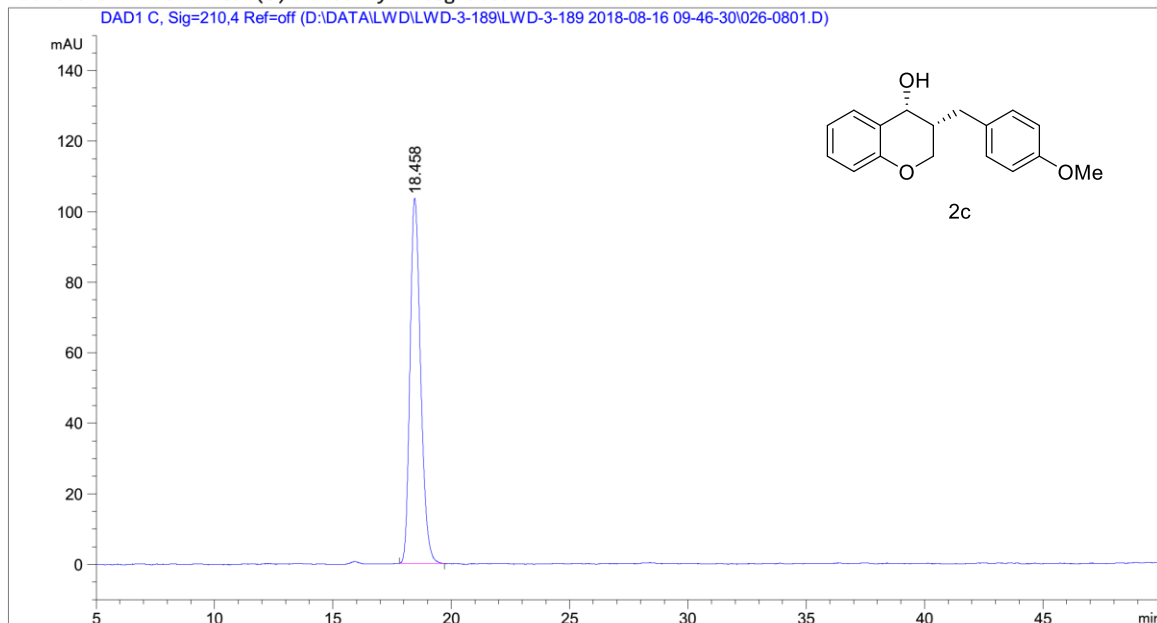
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.865	BB	0.4064	2401.82007	89.68475	31.3015
2	18.455	BB	0.4792	2340.66846	75.19595	30.5046
3	20.070	BB	0.5301	1450.59705	41.87537	18.9048
4	36.544	BB	0.7957	1480.08142	23.28203	19.2891

Totals : 7673.16699 230.03810

Sample Name: LWD-3-189-3-EE

```
=====
Acq. Operator   :                               Seq. Line :    8
Acq. Instrument : Instrument 2                   Location  : Vial 26
Injection Date  : 8/16/2018 2:44:34 PM           Inj       :    1
                                                Inj Volume: 1.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-
                  1UL-ALL-50MIN.M
Last changed    : 8/16/2018 11:20:59 AM
Analysis Method : D:\METHOD\ZXH\DAD-OJ(1-6)-99-1-0.5ML-1UL-220NM-10MIN.M
Last changed    : 6/16/2020 8:32:47 PM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
DAD1 C, Sig=210,4 Ref=off (D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\026-0801.D)
```



```
=====
Area Percent Report
=====
```

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.458	BB	0.4858	3230.73218	103.59892	100.0000

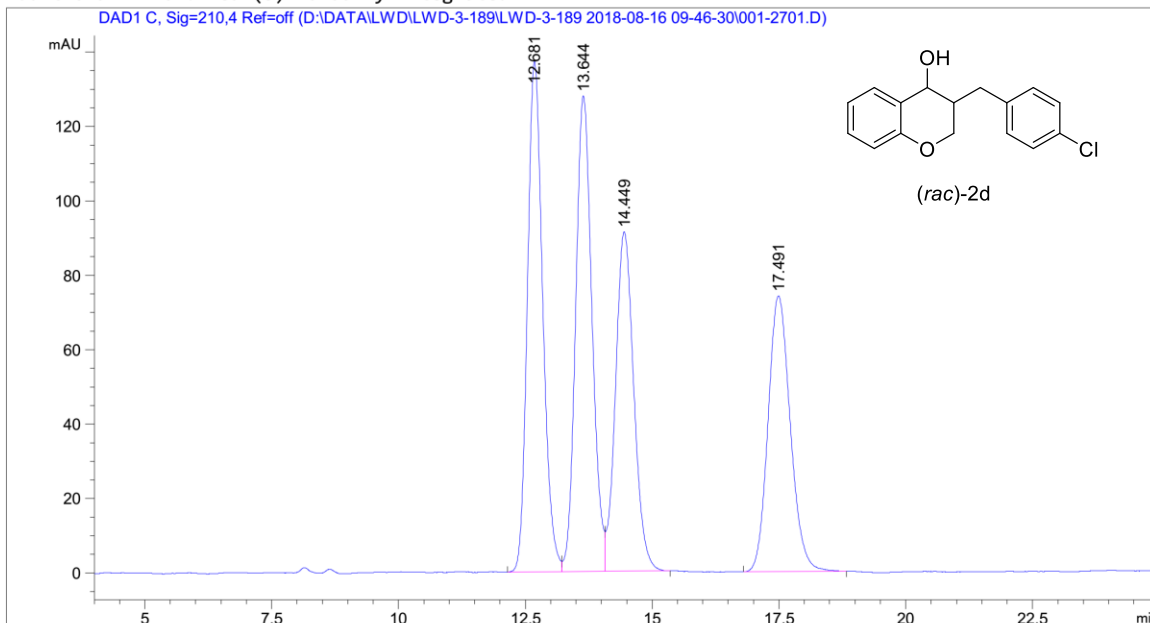
Totals : 3230.73218 103.59892

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\001-2701.D
Sample Name: LWD-3-89-4-RAC

=====

Acq. Operator	:		Seq. Line	:	27
Acq. Instrument	:	Instrument 2	Location	:	Vial 1
Injection Date	:	8/17/2018 1:33:24 AM	Inj	:	1
			Inj Volume	:	3.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-3UL-ALL-25MIN.M			
Last changed	:	8/16/2018 8:31:25 PM			
Analysis Method	:	D:\METHOD\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\001-2701.D			
Last changed	:	8/17/2018 9:21:10 AM			
	:	(modified after loading)			

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

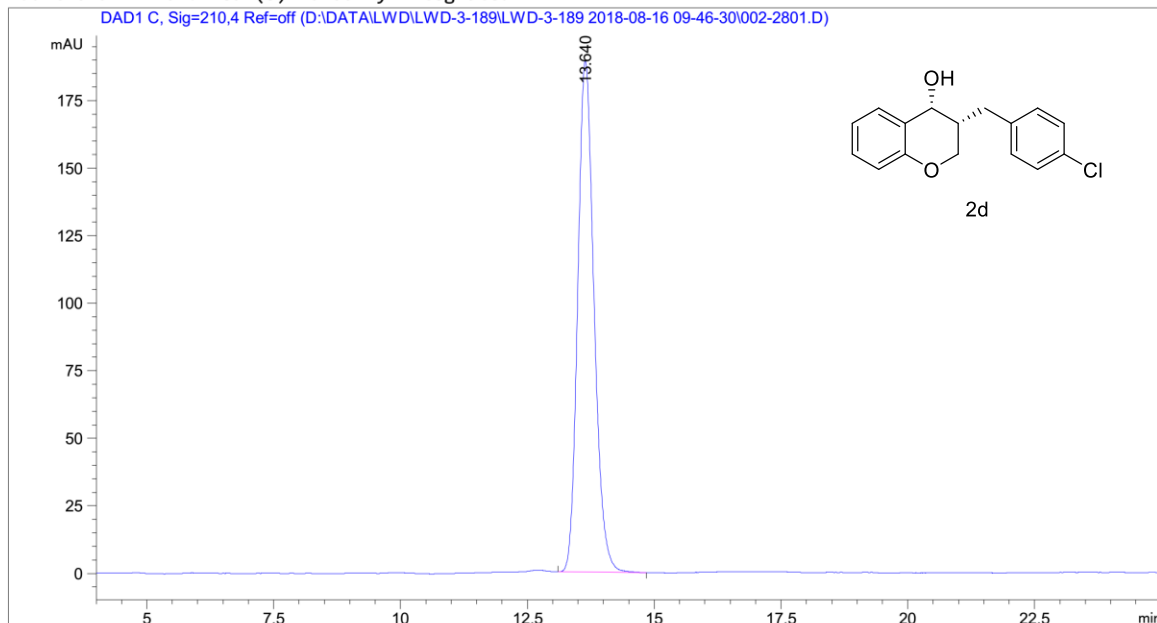
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.681	BV	0.3252	2886.75928	137.36119	28.0147
2	13.644	VV	0.3457	2869.42822	127.93890	27.8465
3	14.449	VB	0.3844	2287.50684	91.26032	22.1992
4	17.491	BB	0.4656	2260.74805	74.16558	21.9395

Totals : 1.03044e4 430.72599

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\002-2801.D
Sample Name: LWD-3-89-4-EE

```
=====
Acq. Operator   :                               Seq. Line :   28
Acq. Instrument : Instrument 2                   Location  : Vial 2
Injection Date  : 8/17/2018 1:59:22 AM           Inj       :    1
                                                Inj Volume: 1.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-
                  1UL-ALL-25MIN.M
Last changed    : 8/16/2018 8:31:59 PM
Analysis Method : D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/17/2018 9:21:49 AM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
DAD1 C, Sig=210,4 Ref=off (D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\002-2801.D)
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

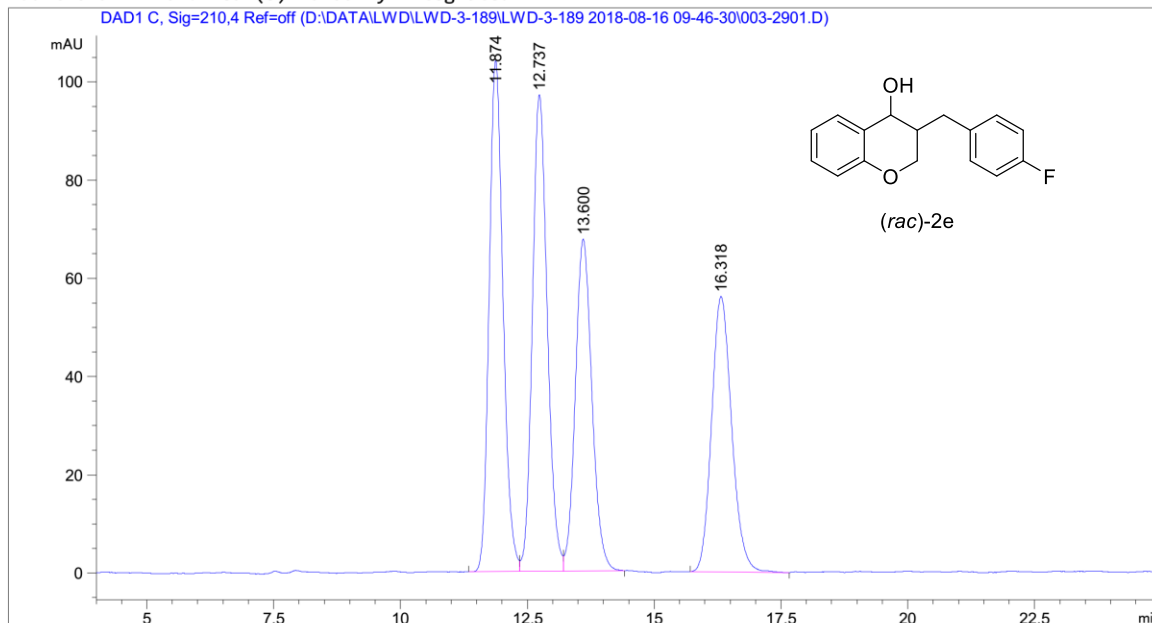
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.640	BB	0.3424	4222.12842	189.19876	100.0000

Totals : 4222.12842 189.19876

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\003-2901.D
Sample Name: LWD-3-89-5-RAC

```
=====
Acq. Operator   :                               Seq. Line :   29
Acq. Instrument : Instrument 2                   Location  : Vial 3
Injection Date  : 8/17/2018 2:25:20 AM          Inj       :    1
                                                Inj Volume: 3.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-
                  3UL-ALL-25MIN.M
Last changed    : 8/16/2018 8:31:25 PM
Analysis Method : D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/17/2018 9:23:47 AM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
DAD1 C, Sig=210,4 Ref=off (D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\003-2901.D)
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=210,4 Ref=off

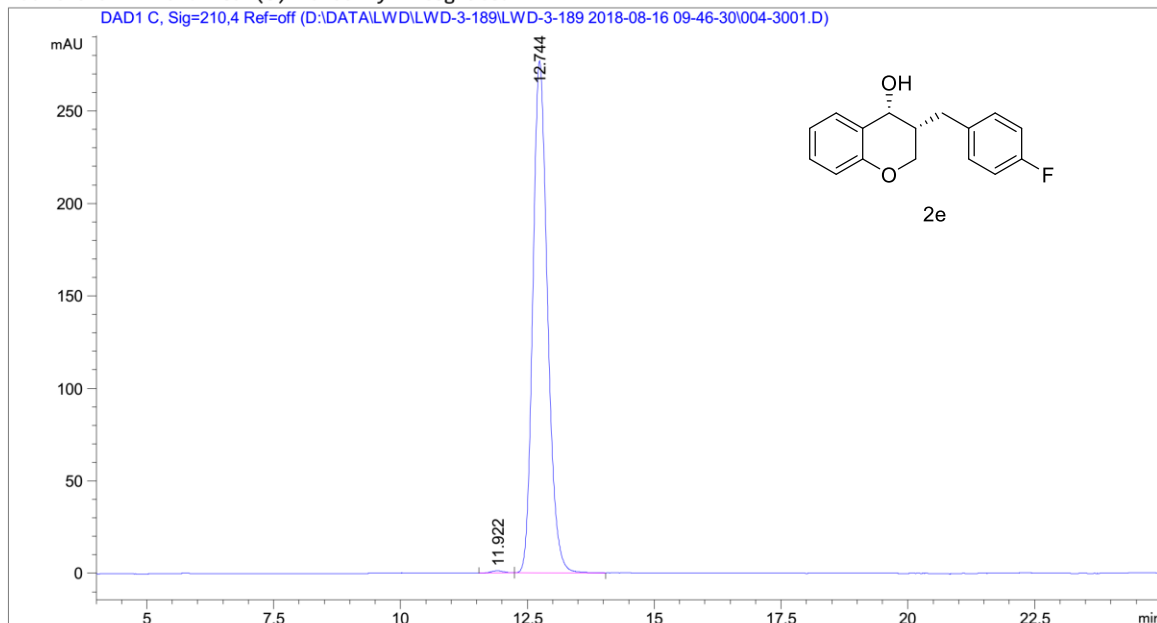
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.874	BV	0.2919	1977.30127	103.95918	28.0715
2	12.737	VV	0.3161	1980.18604	97.02351	28.1125
3	13.600	VB	0.3518	1538.59961	67.52583	21.8433
4	16.318	BB	0.4259	1547.70764	56.09602	21.9726

Totals : 7043.79456 324.60453

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\004-3001.D
Sample Name: LWD-3-89-5-EE

=====

Acq. Operator	:		Seq. Line	:	30
Acq. Instrument	:	Instrument 2	Location	:	Vial 4
Injection Date	:	8/17/2018 2:51:20 AM	Inj	:	1
			Inj Volume	:	1.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-1UL-ALL-25MIN.M			
Last changed	:	8/16/2018 8:31:59 PM			
Analysis Method	:	D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M			
Last changed	:	8/17/2018 9:24:45 AM			
		(modified after loading)			
Additional Info : Peak(s) manually integrated					



=====
Area Percent Report
=====

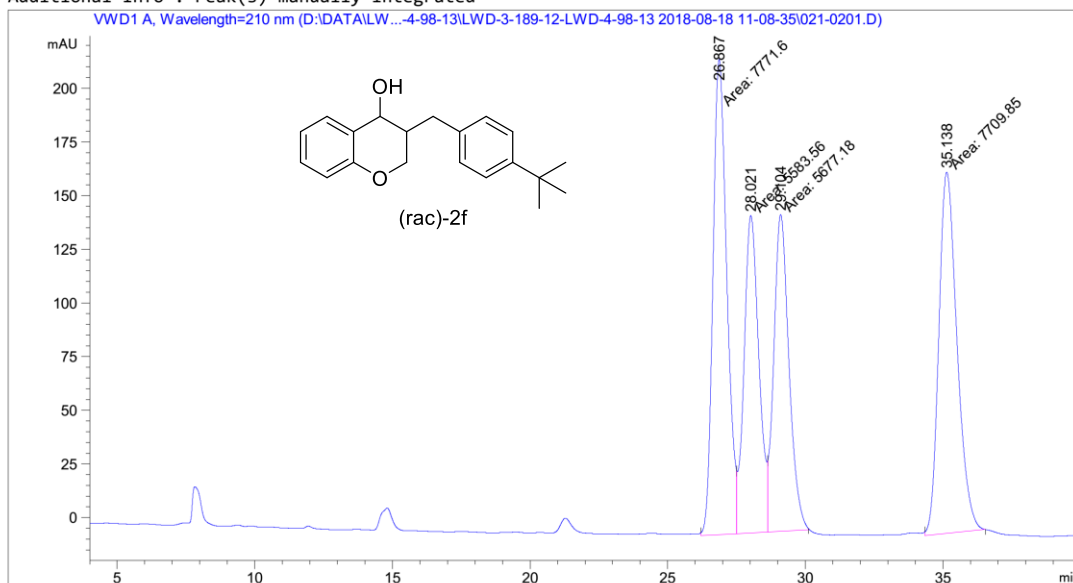
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.922	BB	0.2330	20.02549	1.15061	0.3577
2	12.744	BB	0.3092	5578.69580	276.72086	99.6423

Totals : 5598.72129 277.87146

```
=====
Acq. Operator   :                               Seq. Line :    2
Acq. Instrument : Instrument 1                   Location  : Vial 21
Injection Date  : 8/18/2018 11:52:12 AM          Inj       :    1
                                                Inj Volume: 3.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189-12-LWD-4-98-13\LWD-3-189-12-LWD-4-98-13 2018-08-18 11
                  -08-35\VWD-AD(1-2)-95-5-0.4ML-3UL-210NM-40MIN.M
Last changed    : 8/18/2018 10:35:23 AM
Analysis Method : D:\METHOD\LWD\VWD-AD(1-2)-95-5-1ML-1UL-210NM-10MIN.M
Last changed    : 8/18/2018 3:35:15 PM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
```



Area Percent Report

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

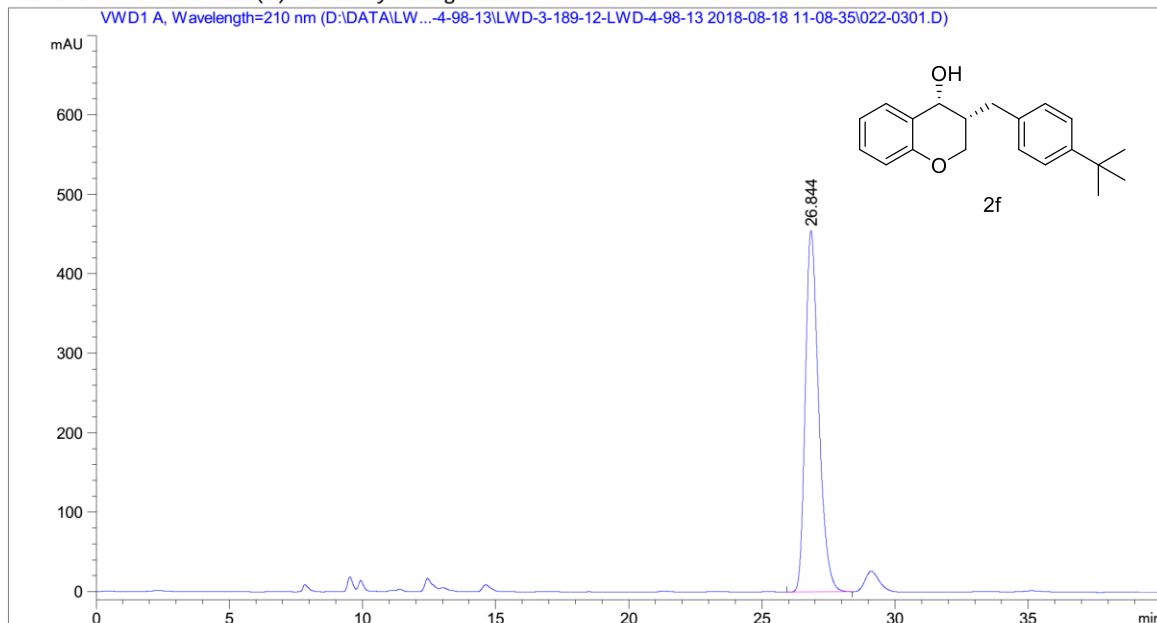
Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.867	MF	0.5852	7771.59521	221.34901	29.0612
2	28.021	MF	0.6298	5583.55957	147.74948	20.8792
3	29.104	FM	0.6415	5677.17871	147.49840	21.2293
4	35.138	MM	0.7637	7709.84619	168.25645	28.8303

Totals : 2.67422e4 684.85335

Data File D:\DATA\LW...LWD-4-98-13\LWD-3-189-12-LWD-4-98-13 2018-08-18 11-08-35\022-0301.D
Sample Name: LWD-4-98-13-EE

```
=====
Acq. Operator   :                               Seq. Line :    3
Acq. Instrument : Instrument 1                   Location  : Vial 22
Injection Date  : 8/18/2018 12:33:03 PM          Inj       :    1
                                                Inj Volume : 1.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189-12-LWD-4-98-13\LWD-3-189-12-LWD-4-98-13 2018-08-18 11
                  -08-35\VWD-AD(1-2)-95-5-0.4ML-1UL-210NM-40MIN.M
Last changed    : 8/18/2018 10:34:57 AM
Analysis Method : D:\METHOD\LSL\VWD-IB(1-6)-97-3-0.3ML-3UL-220-60MIN.M
Last changed    : 6/16/2020 8:19:08 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
VWD1 A, Wavelength=210 nm (D:\DATA\LW...4-98-13\LWD-3-189-12-LWD-4-98-13 2018-08-18 11-08-35\022-0301.D)
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: VWD1 A, Wavelength=210 nm

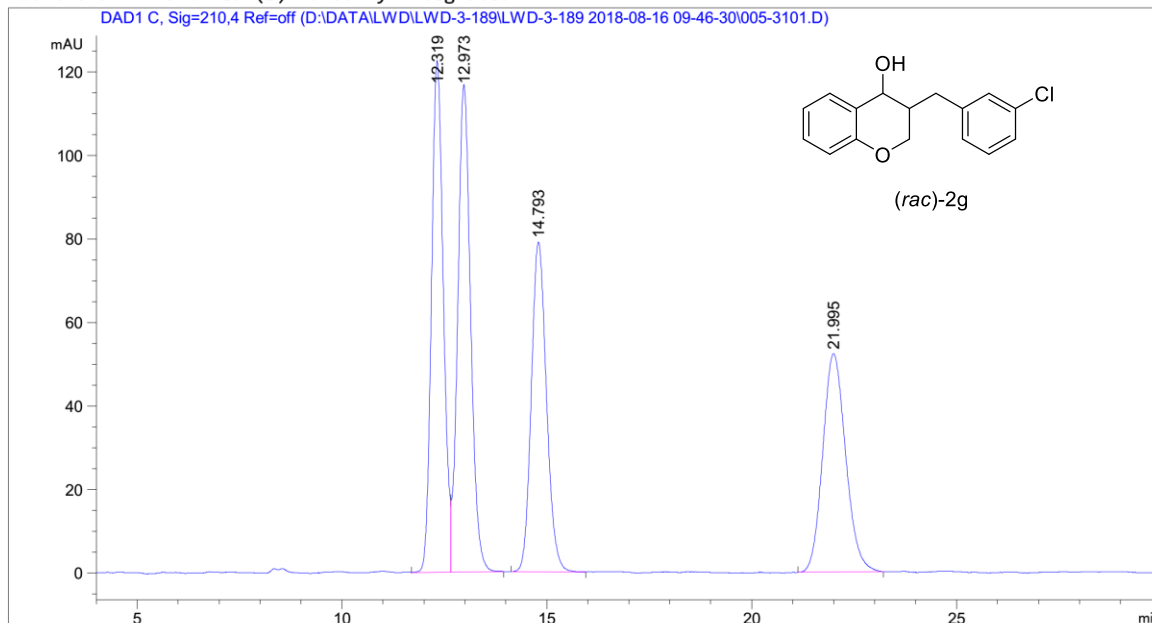
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	26.844	BB	0.5339	1.58910e4	454.54175	100.0000

Totals : 1.58910e4 454.54175

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\005-3101.D
Sample Name: LWD-3-89-6-RAC

=====

Acq. Operator	:		Seq. Line	:	31
Acq. Instrument	:	Instrument 2	Location	:	Vial 5
Injection Date	:	8/17/2018 3:17:21 AM	Inj	:	1
			Inj Volume	:	3.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-3UL-ALL-30MIN.M			
Last changed	:	8/16/2018 8:35:08 PM			
Analysis Method	:	D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M			
Last changed	:	8/17/2018 9:26:29 AM			
		(modified after loading)			
Additional Info : Peak(s) manually integrated					



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

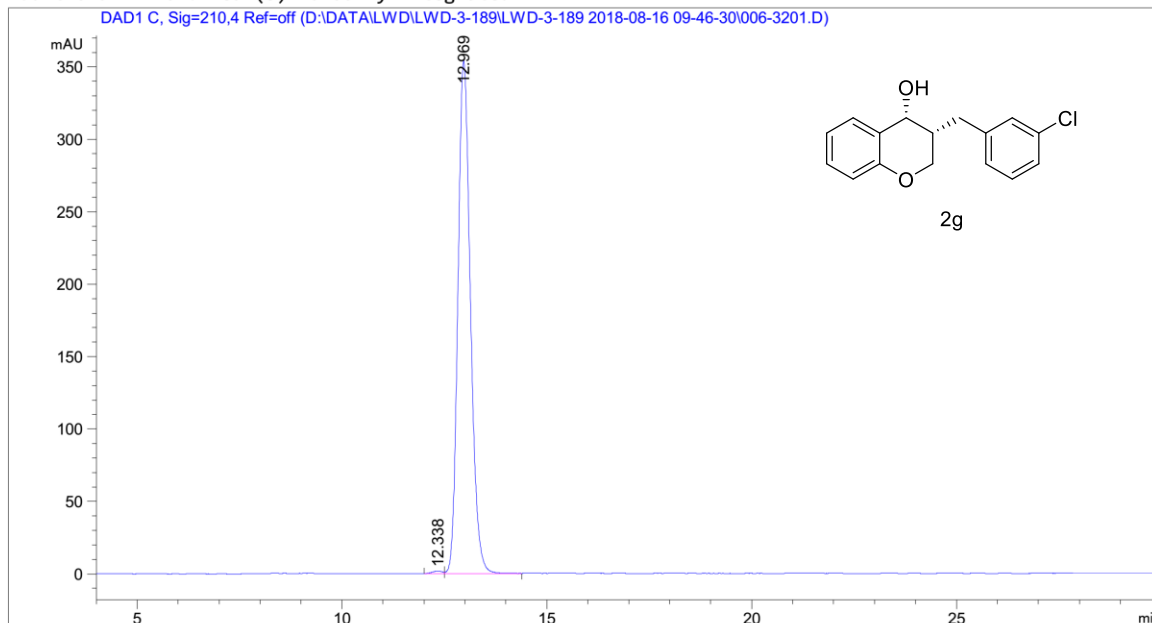
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.319	BV	0.3103	2460.51685	122.50787	27.1184
2	12.973	VB	0.3341	2544.44434	116.80338	28.0434
3	14.793	BB	0.3941	2031.87805	78.99819	22.3942
4	21.995	BB	0.5940	2036.38672	52.33509	22.4439

Totals : 9073.22595 370.64452

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\006-3201.D
Sample Name: LWD-3-89-6-EE

```
=====
Acq. Operator   :                               Seq. Line :   32
Acq. Instrument : Instrument 2                   Location  : Vial 6
Injection Date  : 8/17/2018 3:48:21 AM           Inj       :    1
                                                Inj Volume: 1.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-
                  1UL-ALL-30MIN.M
Last changed    : 8/16/2018 8:35:37 PM
Analysis Method : D:\METHOD\LWD\LWD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/17/2018 9:27:17 AM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=210,4 Ref=off

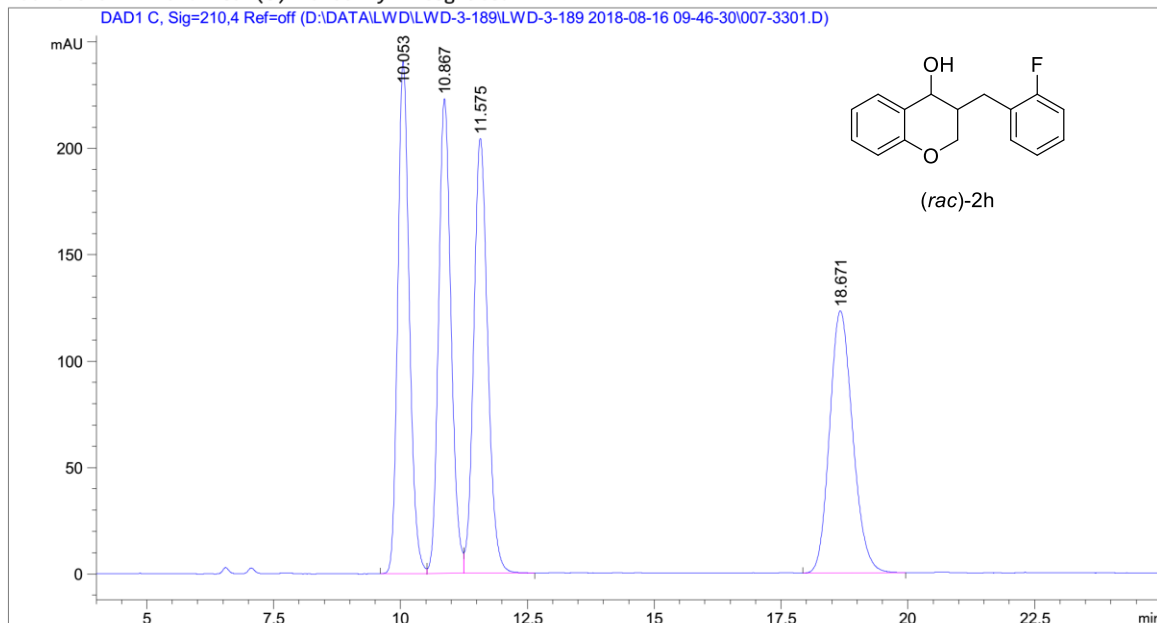
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.338	BV	0.2163	28.47222	1.70995	0.3776
2	12.969	VB	0.3277	7512.15430	353.84998	99.6224

Totals : 7540.62651 355.55992

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\007-3301.D
Sample Name: LWD-3-89-7-RAC

=====

Acq. Operator	:		Seq. Line	:	33
Acq. Instrument	:	Instrument 2	Location	:	Vial 7
Injection Date	:	8/17/2018 4:19:20 AM	Inj	:	1
			Inj Volume	:	3.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-3UL-ALL-25MIN.M			
Last changed	:	8/16/2018 8:31:25 PM			
Analysis Method	:	D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M			
Last changed	:	8/17/2018 9:27:58 AM			
		(modified after loading)			
Additional Info : Peak(s) manually integrated					



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

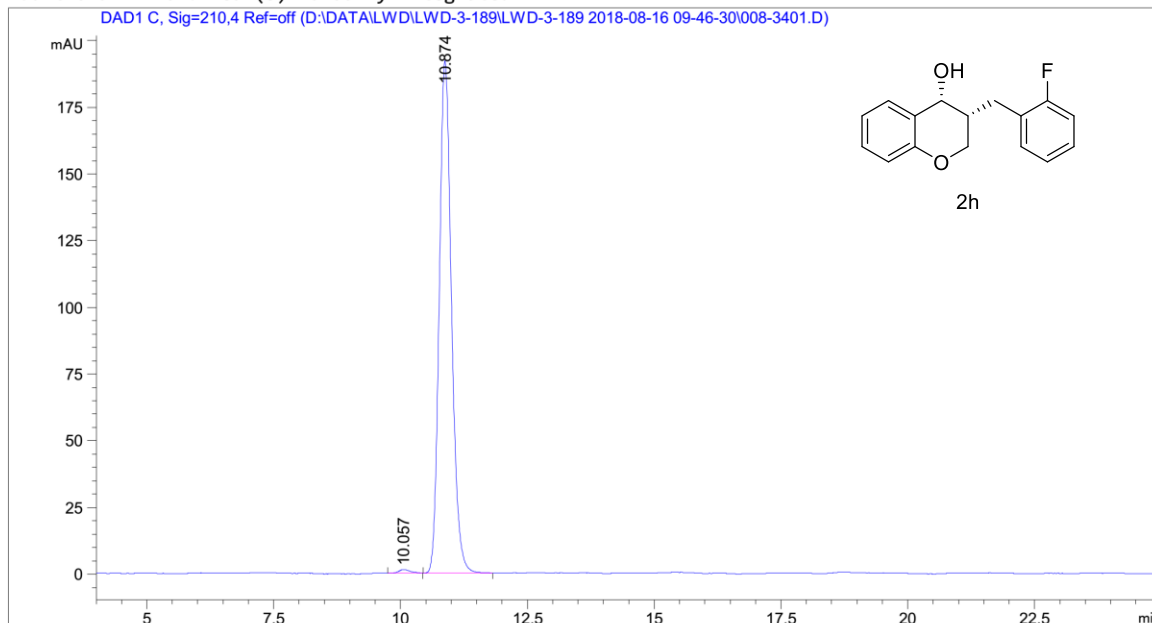
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.053	BV	0.2451	3825.17505	241.06880	24.6990
2	10.867	VV	0.2634	3815.69019	223.22298	24.6378
3	11.575	VB	0.2962	3929.52832	204.45416	25.3728
4	18.671	BB	0.4927	3916.76416	123.27117	25.2904

Totals : 1.54872e4 792.01711

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\008-3401.D
Sample Name: LWD-3-89-7-EE

```
=====
Acq. Operator   :                               Seq. Line :   34
Acq. Instrument : Instrument 2                   Location  : Vial 8
Injection Date  : 8/17/2018 4:45:18 AM           Inj       :    1
                                                Inj Volume: 1.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-
                  1UL-ALL-25MIN.M
Last changed    : 8/16/2018 8:31:59 PM
Analysis Method : D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/17/2018 9:28:53 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

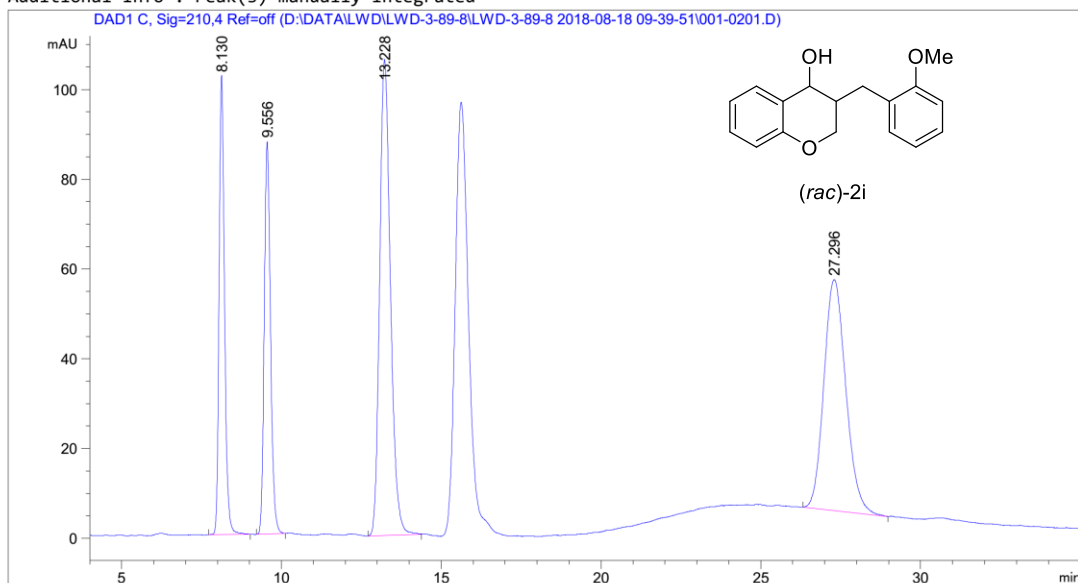
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.057	BB	0.2063	21.71116	1.35928	0.6709
2	10.874	BB	0.2573	3214.42261	191.99089	99.3291

Totals : 3236.13377 193.35017

Data File D:\DATA\LWD\LWD-3-89-8\LWD-3-89-8 2018-08-18 09-39-51\001-0201.D
Sample Name: LWD-3-89-8-RAC

```
=====
Acq. Operator   :                               Seq. Line :    2
Acq. Instrument : Instrument 2                   Location  : Vial 1
Injection Date  : 8/18/2018 10:00:50 AM          Inj       :    1
                                                Inj Volume: 3.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-89-8\LWD-3-89-8 2018-08-18 09-39-51\DAD-OD(1-2)-95-5-1ML-
                  3UL-ALL-35MIN.M
Last changed    : 8/16/2018 9:44:17 AM
Analysis Method : D:\METHOD\LWD\LWD-3-89-8\LWD-3-89-8 2018-08-18 09-39-51\97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/18/2018 11:13:52 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Area Percent Report

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.130	BB	0.1801	1211.78320	102.38054	16.5264
2	9.556	BB	0.2087	1188.78333	87.37602	16.2127
3	13.228	BB	0.3588	2478.68750	106.01793	33.8046
4	27.296	BB	0.7124	2453.15161	51.43679	33.4563

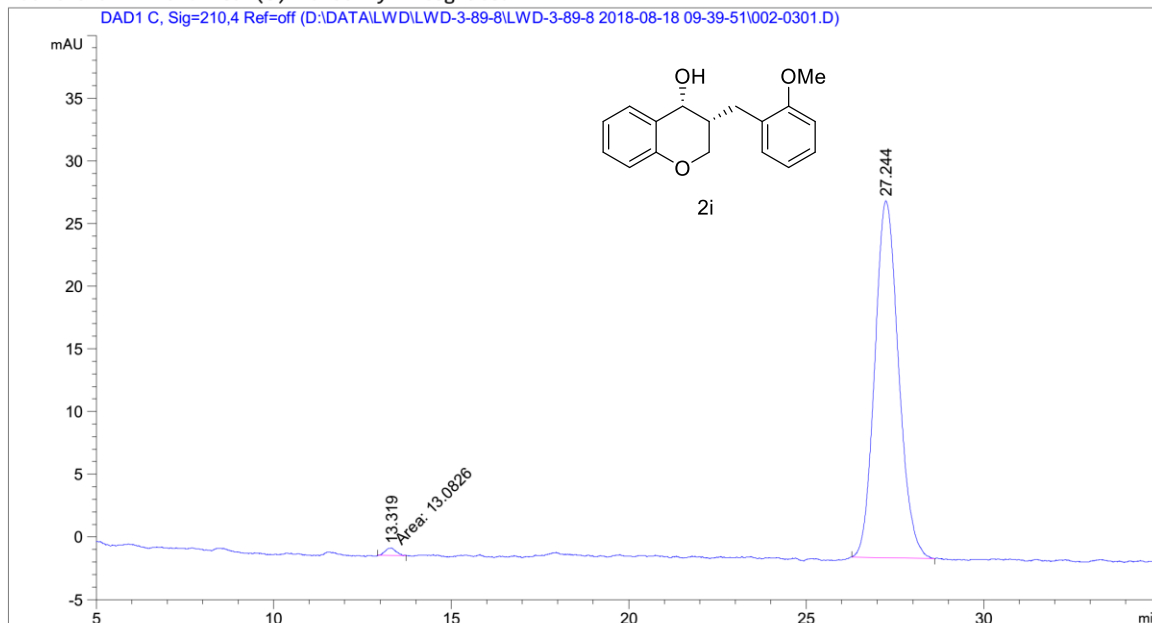
Totals : 7332.40564 347.21128

Instrument 2 8/18/2018 11:13:55 AM

Page 1 of 2

Sample Name: LWD-3-89-8-EE

```
=====
Acq. Operator   :                               Seq. Line :    3
Acq. Instrument : Instrument 2                   Location  : Vial 2
Injection Date  : 8/18/2018 10:36:49 AM          Inj       :    1
                                                Inj Volume: 1.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-89-8\LWD-3-89-8 2018-08-18 09-39-51\DAD-OD(1-2)-95-5-1ML-
                  1UL-ALL-35MIN.M
Last changed    : 8/16/2018 11:23:38 AM
Analysis Method : D:\METHOD\LSL\VWD-IB(1-6)-97-3-0.3ML-3UL-220-60MIN.M
Last changed    : 6/16/2020 8:21:58 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
DAD1 C, Sig=210,4 Ref=off (D:\DATA\LWD\LWD-3-89-8\LWD-3-89-8 2018-08-18 09-39-51\002-0301.D)
```



```
=====
                          Area Percent Report
=====
```

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

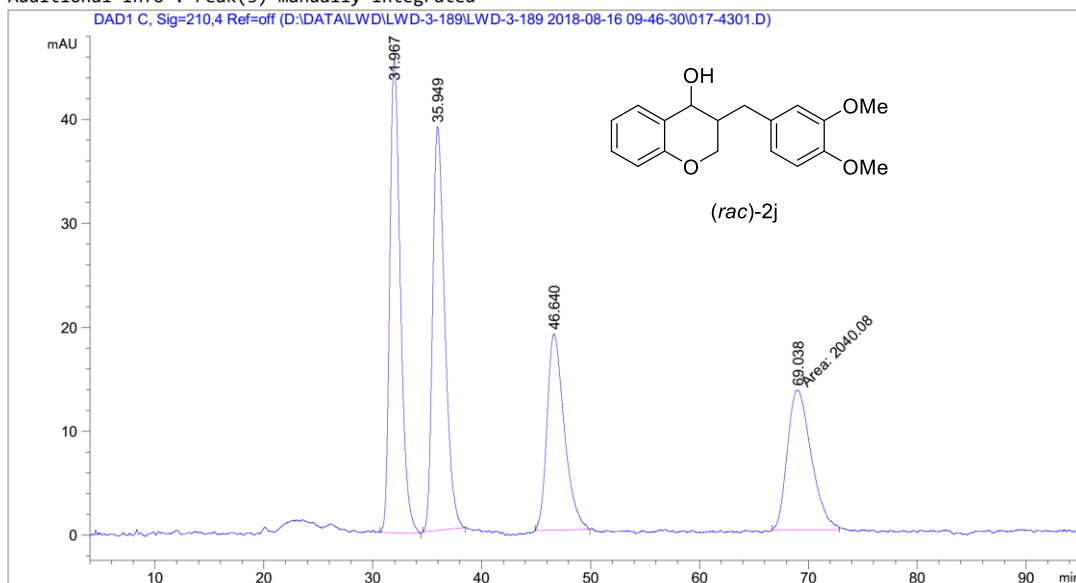
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.319	MM	0.3561	13.08259	6.12347e-1	0.9777
2	27.244	BB	0.6851	1325.05298	28.46449	99.0223

Totals : 1338.13557 29.07683

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\017-4301.D
Sample Name: LWD-3-115-2-RAC

```
=====
Acq. Operator   :                               Seq. Line :   43
Acq. Instrument : Instrument 2                   Location  : Vial 17
Injection Date  : 8/17/2018 10:49:26 AM          Inj       :    1
                                                Inj Volume: 3.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\
DAD-OD(1-2)-95-5-1ML-3UL-ALL-95MIN.M
Last changed    : 8/16/2018 8:53:33 PM
Analysis Method : D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/17/2018 3:31:24 PM
                (modified after loading)
Additional Info  : Peak(s) manually integrated
```



Area Percent Report

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	31.967	BB	0.9717	3072.13232	45.50124	30.1453
2	35.949	BB	0.9279	3001.54224	38.82710	29.4526
3	46.640	BB	1.2953	2077.33569	18.88595	20.3838
4	69.038	MM	2.5312	2040.08081	13.43263	20.0183

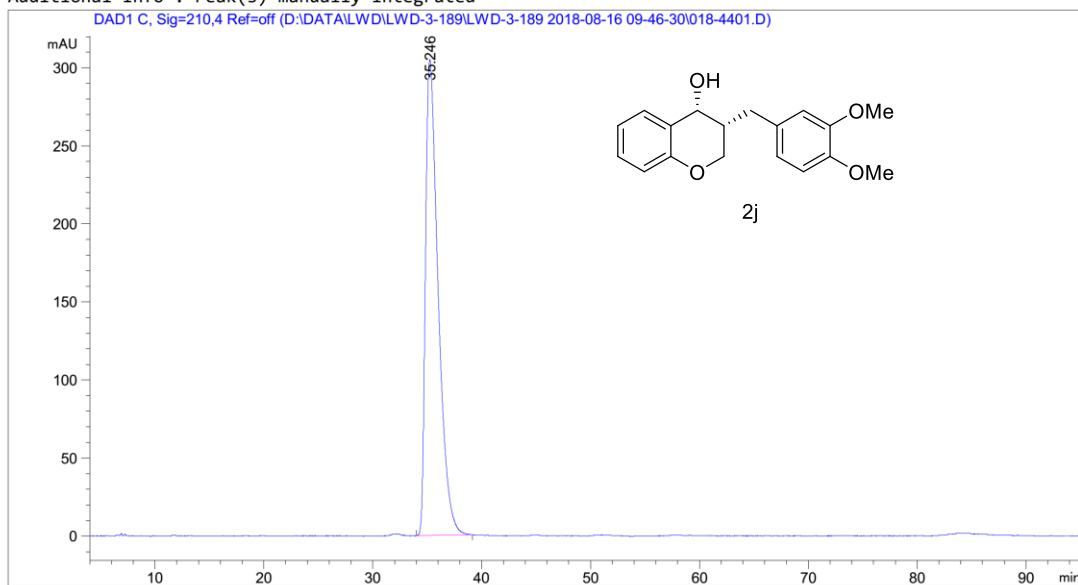
Totals : 1.01911e4 116.64692

Instrument 2 8/17/2018 3:31:29 PM

Page 1 of 2

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\018-4401.D
Sample Name: LWD-3-115-2-EE

```
=====
Acq. Operator   :                               Seq. Line :   44
Acq. Instrument : Instrument 2                  Location  : Vial 18
Injection Date  : 8/17/2018 12:25:25 PM         Inj       :    1
                                                Inj Volume: 1.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-
                  1UL-ALL-95MIN.M
Last changed    : 8/16/2018 8:54:13 PM
Analysis Method : D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/17/2018 3:32:29 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
=====
```



Area Percent Report

```
=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
=====
```

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	35.246	BB	1.1998	2.46171e4	304.93997	100.0000

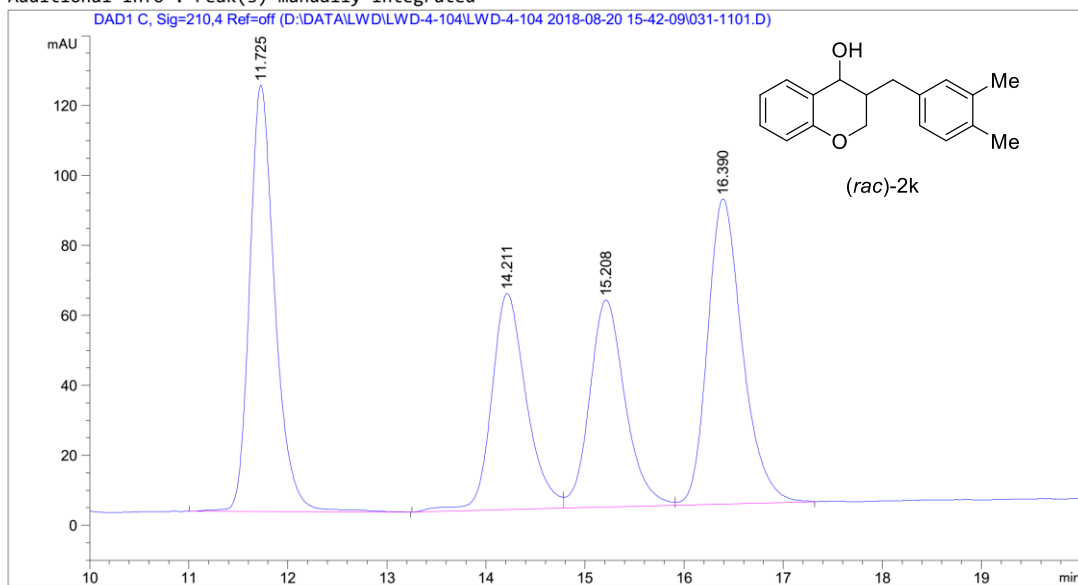
Totals : 2.46171e4 304.93997

Data File D:\DATA\LWD\LWD-4-104\LWD-4-104 2018-08-20 15-42-09\031-1101.D
Sample Name: LWD-3-113-6-RAC

=====

Acq. Operator	:		Seq. Line	:	11
Acq. Instrument	:	Instrument 2	Location	:	Vial 31
Injection Date	:	8/20/2018 10:05:09 PM	Inj	:	1
			Inj Volume	:	5.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-4-104\LWD-4-104 2018-08-20 15-42-09\DAD-AD(1-6)-95-5-1ML-5UL-ALL-20MIN.M			
Last changed	:	8/20/2018 8:15:42 PM			
Analysis Method	:	D:\METHOD\LG\DAD-IA(1-2)-80-20-1ML-2UL-ALL-10MIN.M			
Last changed	:	12/11/2018 9:52:09 AM			
		(modified after loading)			

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.725	BB	0.2695	2168.51489	121.91917	29.8056
2	14.211	BV	0.3663	1506.76208	61.82644	20.7100
3	15.208	VV	0.3814	1470.22156	59.26291	20.2078
4	16.390	VB	0.3708	2130.02246	87.24282	29.2766

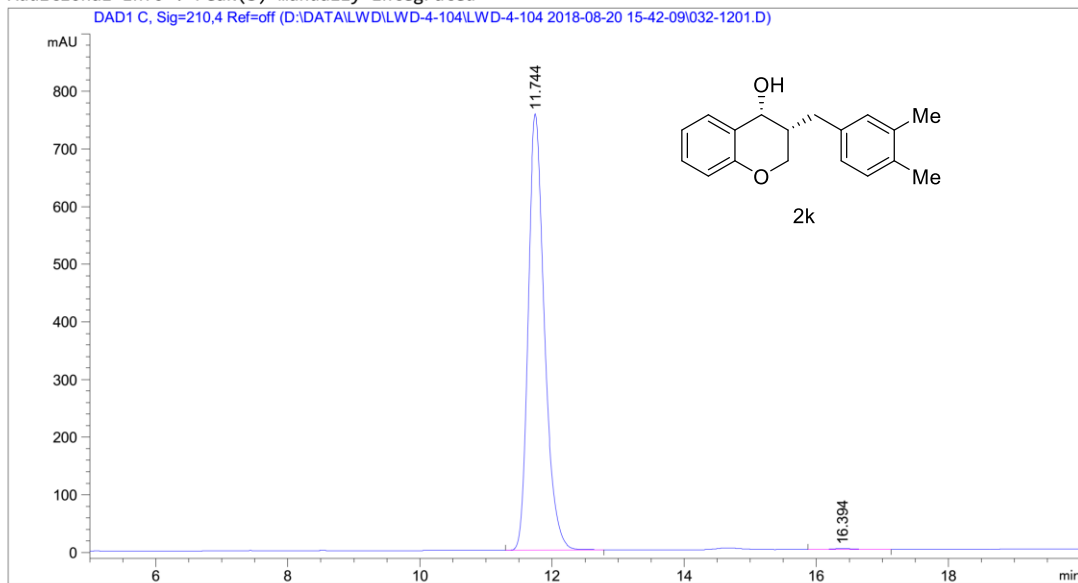
Totals : 7275.52100 330.25135

Instrument 2 12/11/2018 9:52:13 AM

Page 1 of 2

Data File D:\DATA\LWD\LWD-4-104\LWD-4-104 2018-08-20 15-42-09\032-1201.D
Sample Name: LWD-3-113-6-EE

```
=====
Acq. Operator   :                               Seq. Line :   12
Acq. Instrument : Instrument 2                   Location  : Vial 32
Injection Date  : 8/20/2018 10:26:10 PM          Inj       :    1
                                                Inj Volume: 2.000 µl
Acq. Method     : D:\DATA\LWD\LWD-4-104\LWD-4-104 2018-08-20 15-42-09\DAD-AD(1-6)-95-5-1ML-
                  2UL-ALL-20MIN.M
Last changed    : 8/20/2018 8:16:41 PM
Analysis Method : D:\METHOD\LG\DAD-IA(1-2)-80-20-1ML-2UL-ALL-10MIN.M
Last changed    : 12/11/2018 9:53:15 AM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

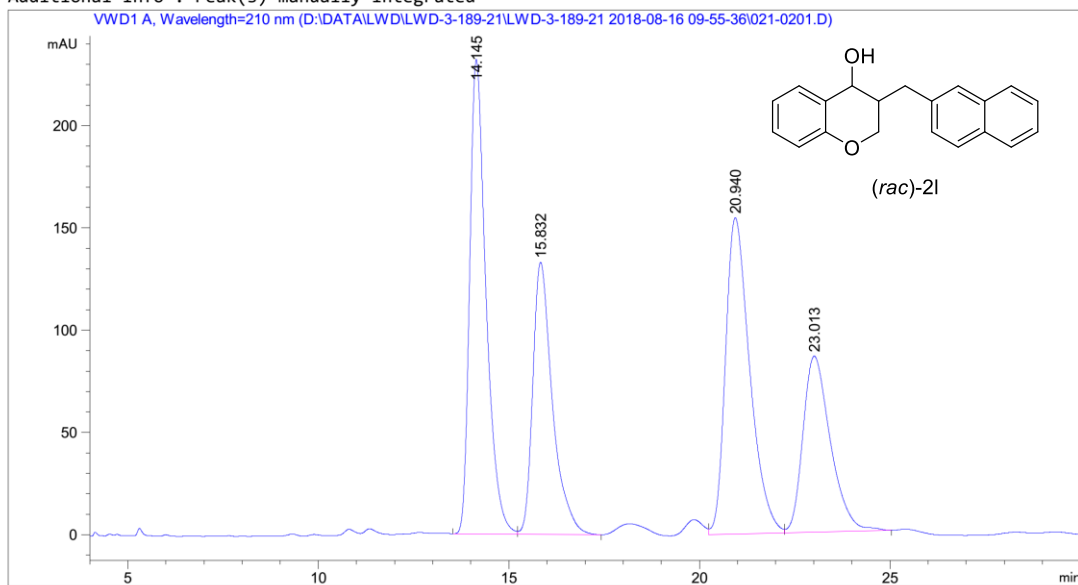
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.744	BB	0.2588	1.28971e4	756.83026	99.6767
2	16.394	BB	0.3110	41.82529	1.71203	0.3233

Totals : 1.29389e4 758.54229

Data File D:\DATA\LWD\LWD-3-189-21\LWD-3-189-21 2018-08-16 09:55-36\021-0201.D
Sample Name: LWD-3-189-21-RAC

```
=====
Acq. Operator   :                               Seq. Line :    2
Acq. Instrument : Instrument 1                   Location  : Vial 21
Injection Date  : 8/16/2018 10:12:19 AM          Inj       :    1
                                                Inj Volume: 3.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189-21\LWD-3-189-21 2018-08-16 09:55-36\VWD-AS(1-6)-95-5-
                  1ML-3UL-210NM-30MIN.M
Last changed    : 8/16/2018 9:54:17 AM
Analysis Method : D:\METHOD\LWD\VWD-AD(1-2)-98-2-1ML-3UL-210NM-60MIN.M
Last changed    : 8/17/2018 9:38:46 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
=====
```



Area Percent Report

```
=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
=====
```

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.145	BV	0.4469	6896.69531	231.93311	30.1734
2	15.832	VB	0.5359	4765.39600	133.02962	20.8488
3	20.940	VV	0.6735	6866.52197	154.80162	30.0414
4	23.013	VB	0.7610	4328.27881	86.17262	18.9364

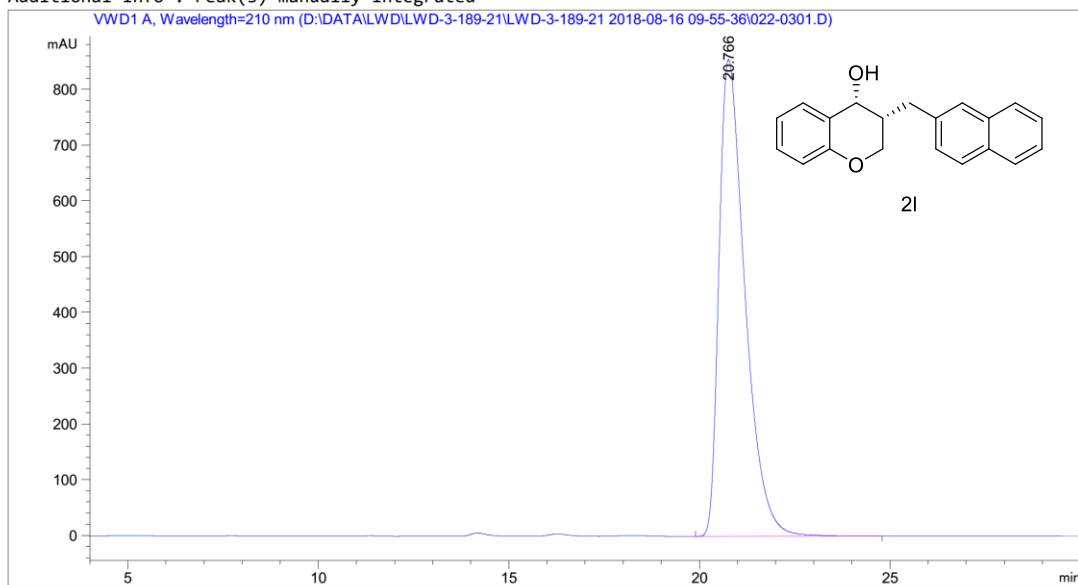
Totals : 2.28569e4 605.93696

Instrument 1 8/17/2018 9:38:49 AM

Page 1 of 2

Data File D:\DATA\LWD\LWD-3-189-21\LWD-3-189-21 2018-08-16 09-55-36\022-0301.D
Sample Name: LWD-3-189-21-EE

```
=====
Acq. Operator   :                               Seq. Line :    3
Acq. Instrument : Instrument 1                   Location  : Vial 22
Injection Date  : 8/16/2018 10:43:09 AM          Inj       :    1
                                                Inj Volume: 3.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189-21\LWD-3-189-21 2018-08-16 09-55-36\VWD-AS(1-6)-95-5-
                  1ML-3UL-210NM-30MIN.M
Last changed    : 8/16/2018 9:54:17 AM
Analysis Method : D:\METHOD\LWD\VWD-AD(1-2)-98-2-1ML-3UL-210NM-60MIN.M
Last changed    : 8/17/2018 9:40:04 AM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
=====
```



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

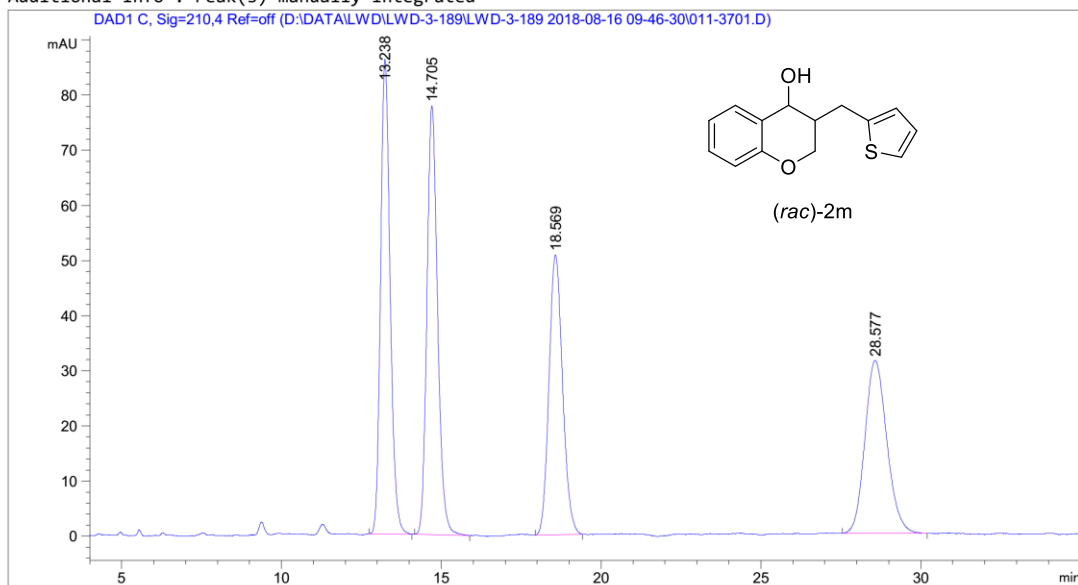
Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.766	BB	0.7255	4.04923e4	855.04865	100.0000

Totals : 4.04923e4 855.04865

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\011-3701.D
Sample Name: LWD-3-113-1-RAC

```
=====
Acq. Operator   :                               Seq. Line :   37
Acq. Instrument : Instrument 2                   Location  : Vial 11
Injection Date  : 8/17/2018 6:23:27 AM           Inj       :    1
                                                Inj Volume: 3.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\
DAD-OD(1-2)-95-5-1ML-3UL-ALL-35MIN.M
Last changed    : 8/16/2018 9:44:17 AM
Analysis Method : D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/17/2018 9:31:09 AM
                (modified after loading)
Additional Info  : Peak(s) manually integrated
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.238	BB	0.3196	1781.92883	86.05817	27.0936
2	14.705	BB	0.3576	1796.73987	77.76508	27.3188
3	18.569	BB	0.4523	1499.78674	50.82487	22.8037
4	28.577	BB	0.7152	1498.47693	31.37714	22.7838

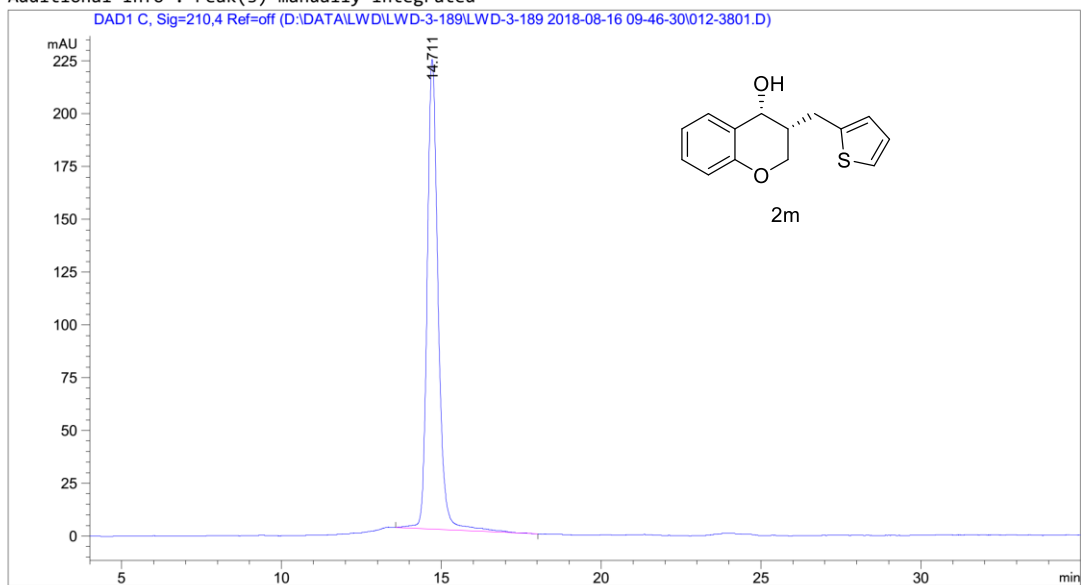
Totals : 6576.93237 246.02526

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\012-3801.D
Sample Name: LWD-3-113-1-EE

=====

Acq. Operator	:		Seq. Line	:	38
Acq. Instrument	:	Instrument 2	Location	:	Vial 12
Injection Date	:	8/17/2018 6:59:24 AM	Inj	:	1
			Inj Volume	:	1.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-1UL-ALL-35MIN.M			
Last changed	:	8/16/2018 11:23:38 AM			
Analysis Method	:	D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M			
Last changed	:	8/17/2018 9:32:10 AM			
		(modified after loading)			

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

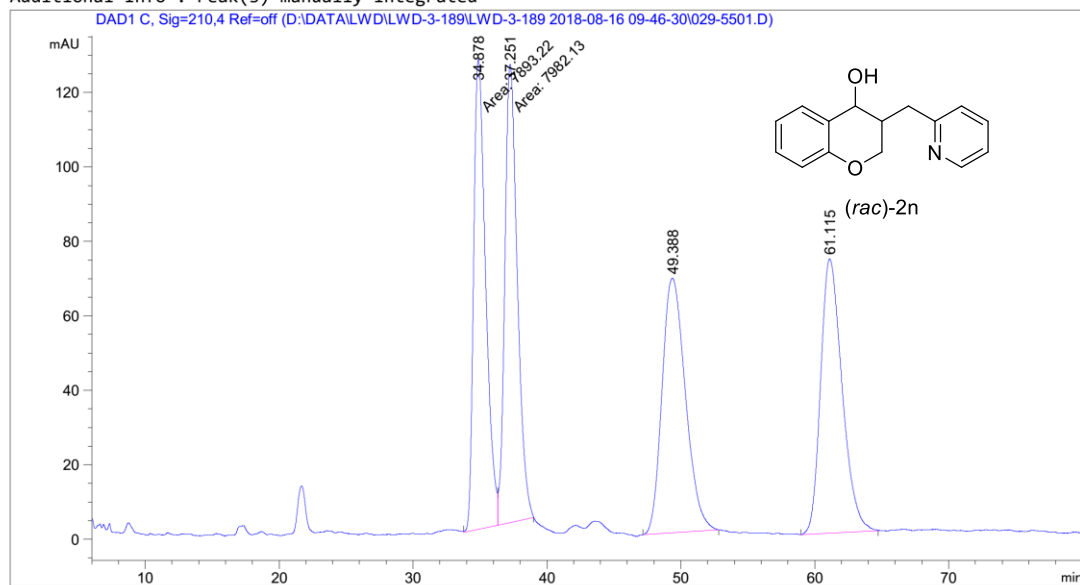
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.711	BB	0.3651	5319.56396	222.34158	100.0000

Totals : 5319.56396 222.34158

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\029-5501.D
Sample Name: LWD-3-176-3-RAC

```
=====
Acq. Operator   :                               Seq. Line :   55
Acq. Instrument : Instrument 2                  Location  : Vial 29
Injection Date  : 8/18/2018 12:11:33 AM         Inj       :    1
                                           Inj Volume: 10.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-97-3-0.8ML-
                  10UL-ALL-80MIN.M
Last changed    : 8/16/2018 9:06:17 PM
Analysis Method : D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/18/2018 9:23:28 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

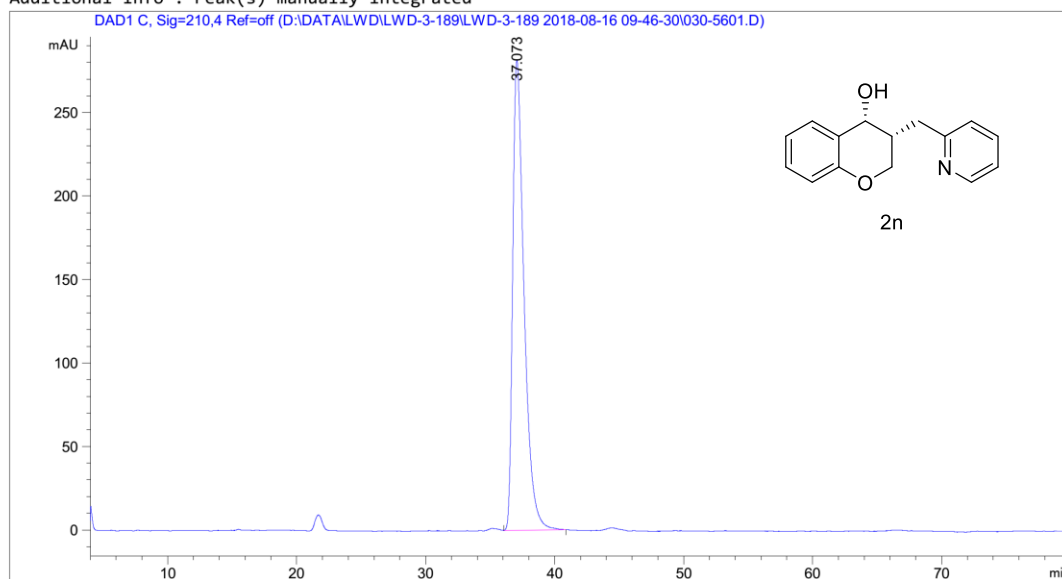
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	34.878	MF	1.0423	7893.22314	126.21693	24.3571
2	37.251	FM	1.0804	7982.13281	123.13682	24.6315
3	49.388	BB	1.4397	8313.06738	68.40965	25.6527
4	61.115	BB	1.4638	8217.76660	73.64771	25.3586

Totals : 3.24062e4 391.41111

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\030-5601.D
Sample Name: LWD-3-176-3-EE

```
=====
Acq. Operator   :                               Seq. Line :   56
Acq. Instrument : Instrument 2                   Location  : Vial 30
Injection Date  : 8/18/2018 1:32:41 AM           Inj       :    1
                                                Inj Volume: 1.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-97-3-0.8ML-
                                                1UL-ALL-80MIN.M
Last changed    : 8/16/2018 9:06:45 PM
Analysis Method : D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/18/2018 9:02:41 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Area Percent Report

```
=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	37.073	BB	0.8958	1.71783e4	281.54138	100.0000

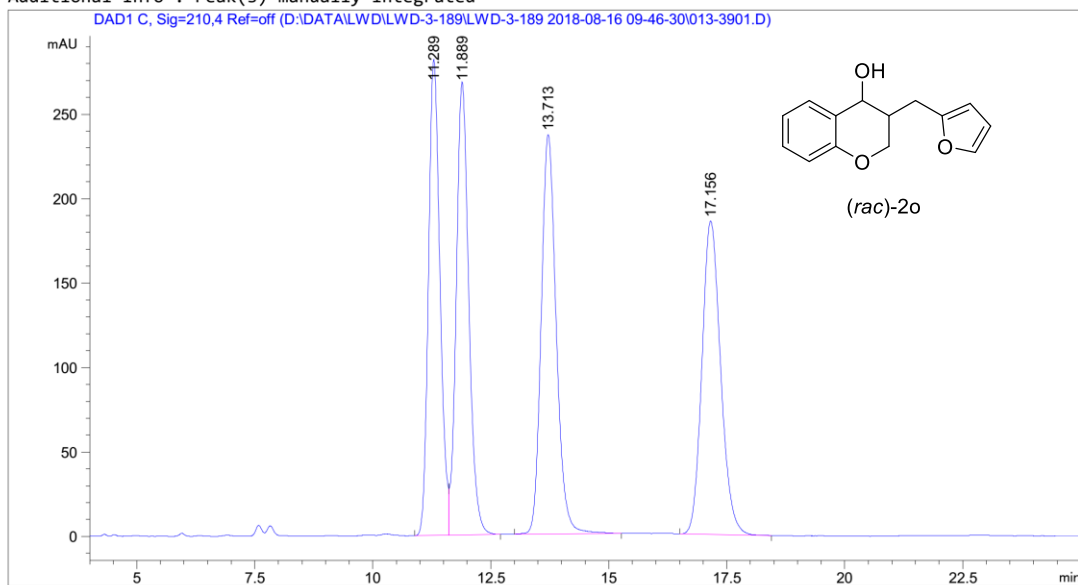
Totals : 1.71783e4 281.54138

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\013-3901.D
Sample Name: LWD-3-113-2-RAC

=====

Acq. Operator	:		Seq. Line	:	39
Acq. Instrument	:	Instrument 2	Location	:	Vial 13
Injection Date	:	8/17/2018 7:35:25 AM	Inj	:	1
			Inj Volume	:	3.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-3UL-ALL-25MIN.M			
Last changed	:	8/16/2018 8:31:25 PM			
Analysis Method	:	D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M			
Last changed	:	8/17/2018 9:34:51 AM			
		(modified after loading)			

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.289	BV	0.2619	4781.29688	281.82632	23.8316
2	11.889	VB	0.2813	4948.68945	268.18326	24.6660
3	13.713	BB	0.3395	5218.85400	236.44759	26.0126
4	17.156	BB	0.4274	5113.98486	185.65912	25.4899

Totals : 2.00628e4 972.11629

Instrument 2 8/17/2018 9:34:55 AM

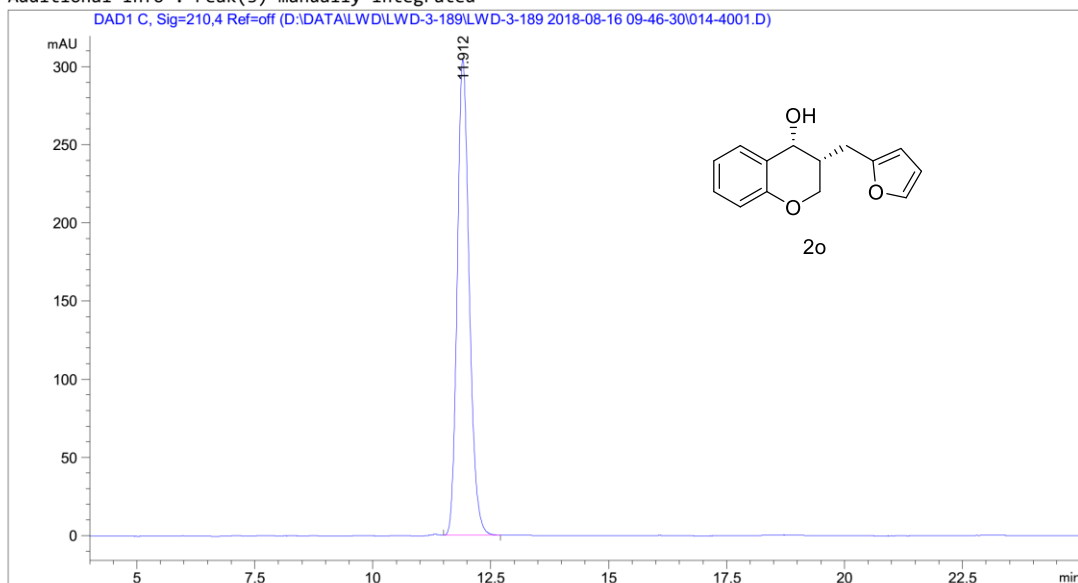
Page 1 of 2

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\014-4001.D
Sample Name: LWD-3-113-2-EE

=====

Acq. Operator	:		Seq. Line	:	40
Acq. Instrument	:	Instrument 2	Location	:	Vial 14
Injection Date	:	8/17/2018 8:01:25 AM	Inj	:	1
			Inj Volume	:	1.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-1UL-ALL-25MIN.M			
Last changed	:	8/16/2018 8:31:59 PM			
Analysis Method	:	D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M			
Last changed	:	8/17/2018 9:36:23 AM			
		(modified after loading)			

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.912	BB	0.2732	5405.20313	304.32196	100.0000

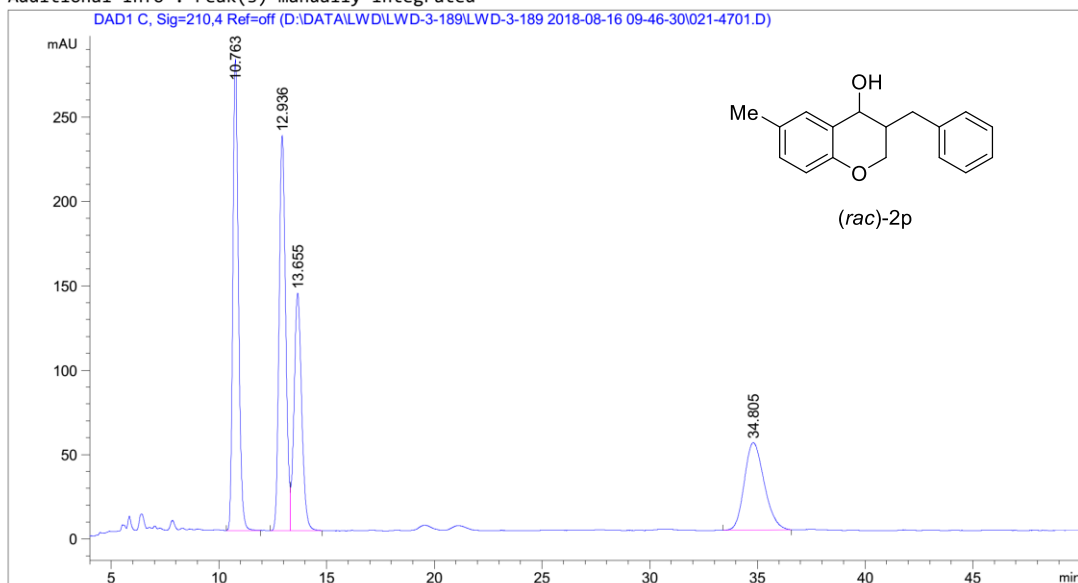
Totals : 5405.20313 304.32196

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\021-4701.D
Sample Name: LWD-3-176-5-RAC

=====

Acq. Operator	:		Seq. Line	:	47
Acq. Instrument	:	Instrument 2	Location	:	Vial 21
Injection Date	:	8/17/2018 3:23:34 PM	Inj	:	1
			Inj Volume	:	3.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-3UL-ALL-50MIN.M			
Last changed	:	8/16/2018 9:43:15 AM			
Analysis Method	:	D:\METHOD\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\021-4701.D			
Last changed	:	8/17/2018 5:10:06 PM			
	:	(modified after loading)			

Additional Info : Peak(s) manually integrated



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.763	BB	0.2788	5042.55859	279.13034	30.0341
2	12.936	BV	0.3282	4977.77734	234.00815	29.6483
3	13.655	VB	0.3744	3452.58105	140.63708	20.5640
4	34.805	BB	0.9308	3316.52222	51.81445	19.7536

Totals : 1.67894e4 705.59002

Instrument 2 8/17/2018 5:10:11 PM

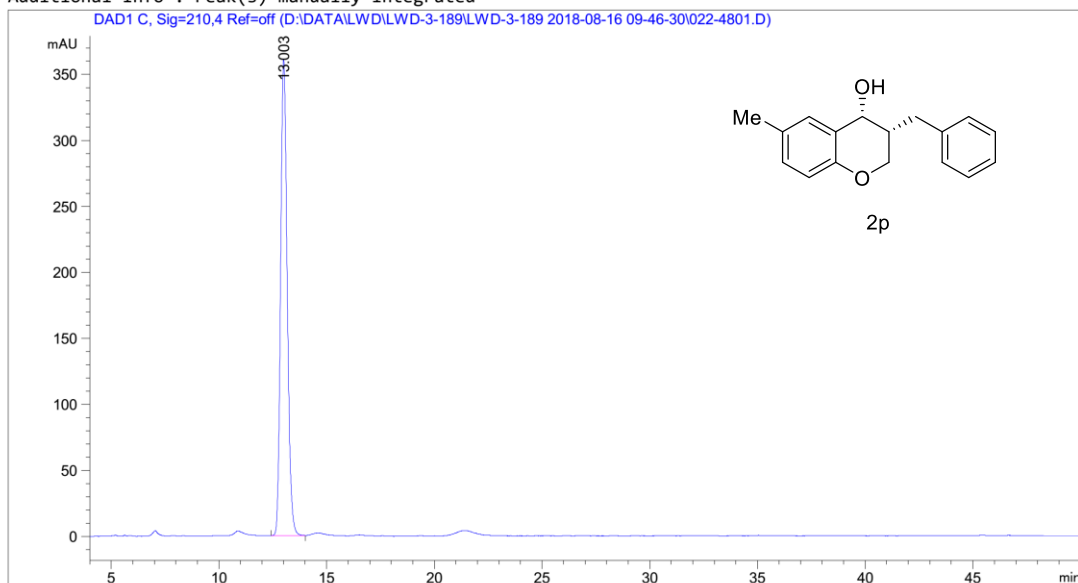
Page 1 of 2

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\022-4801.D
Sample Name: LWD-3-176-5-EE

=====

Acq. Operator	:		Seq. Line	:	48
Acq. Instrument	:	Instrument 2	Location	:	Vial 22
Injection Date	:	8/17/2018 4:14:30 PM	Inj	:	1
			Inj Volume	:	1.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-1UL-ALL-50MIN.M			
Last changed	:	8/16/2018 11:20:59 AM			
Analysis Method	:	D:\METHOD\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\97-3-0.8ML-1UL-ALL-80MIN.M			
Last changed	:	8/17/2018 5:11:41 PM			
		(modified after loading)			

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

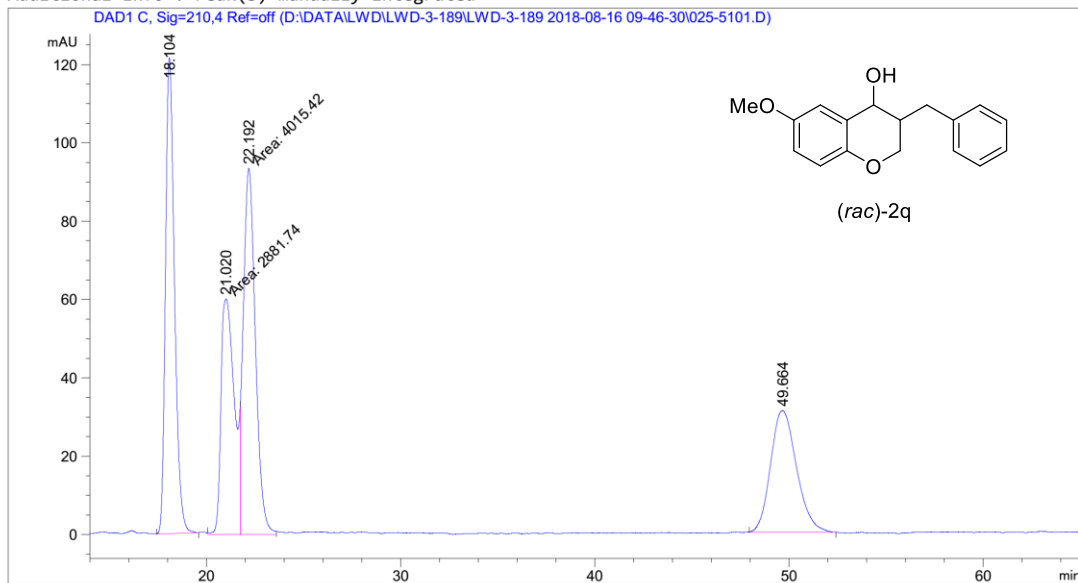
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.003	BB	0.3286	7684.91162	360.65469	100.0000

Totals : 7684.91162 360.65469

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\025-5101.D
Sample Name: LWD-3-176-7-RAC

```
=====
Acq. Operator   :                               Seq. Line :   51
Acq. Instrument : Instrument 2                   Location  : Vial 25
Injection Date  : 8/17/2018 7:17:29 PM           Inj       :    1
                                                Inj Volume: 3.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-
                                                3UL-ALL-65MIN.M
Last changed    : 8/16/2018 8:59:30 PM
Analysis Method : D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/17/2018 10:11:16 PM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
DAD1 C, Sig=210,4 Ref=off (D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\025-5101.D)
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.104	BB	0.4908	3903.32056	121.49027	28.5186
2	21.020	MF	0.7996	2881.74097	60.06852	21.0547
3	22.192	FM	0.7163	4015.41528	93.42863	29.3375
4	49.664	BB	1.0981	2886.47388	31.06365	21.0892

Totals : 1.36870e4 306.05107

Instrument 2 8/17/2018 10:11:18 PM

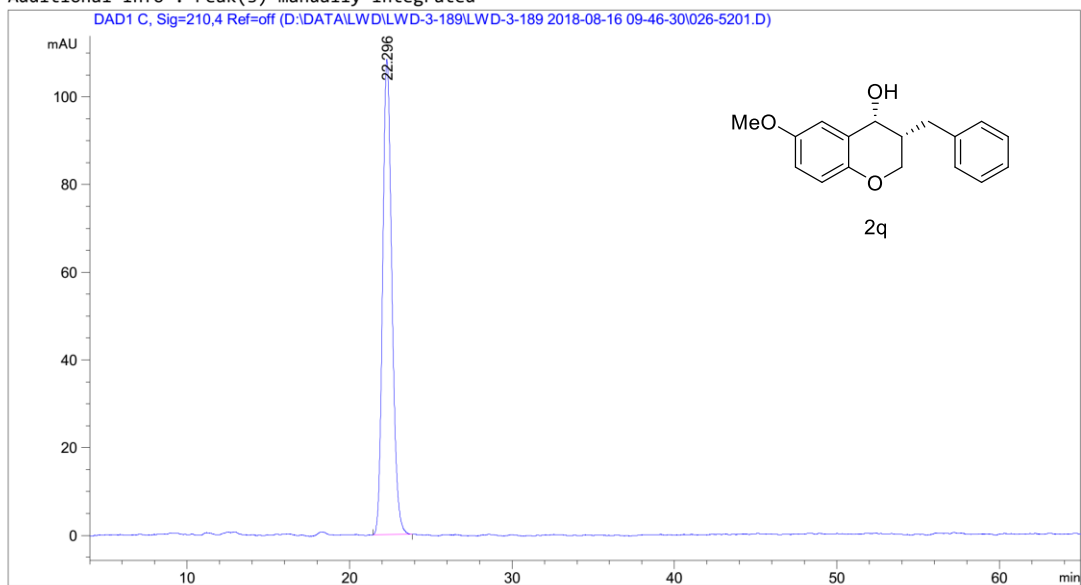
Page 1 of 2

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\026-5201.D
Sample Name: LWD-3-176-7-EE

=====

Acq. Operator	:		Seq. Line	:	52
Acq. Instrument	:	Instrument 2	Location	:	Vial 26
Injection Date	:	8/17/2018 8:23:30 PM	Inj	:	1
			Inj Volume	:	1.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-1UL-ALL-65MIN.M			
Last changed	:	8/16/2018 8:59:56 PM			
Analysis Method	:	D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M			
Last changed	:	8/17/2018 10:11:53 PM			
		(modified after loading)			

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

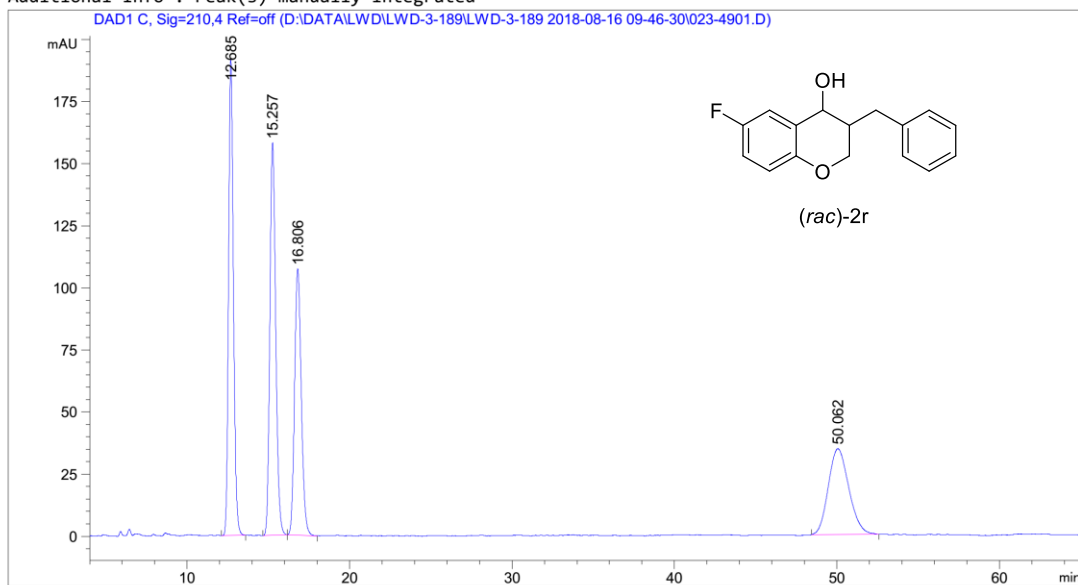
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.296	BB	0.6150	4299.39746	108.33426	100.0000

Totals : 4299.39746 108.33426

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\023-4901.D
Sample Name: LWD-3-176-6-RAC

```
=====
Acq. Operator   :                               Seq. Line :   49
Acq. Instrument : Instrument 2                   Location  : Vial 23
Injection Date  : 8/17/2018 5:05:31 PM           Inj       :    1
                                                Inj Volume: 3.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\
DAD-OD(1-2)-95-5-1ML-3UL-ALL-65MIN.M
Last changed    : 8/16/2018 8:59:30 PM
Analysis Method : D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/17/2018 7:24:41 PM
                (modified after loading)
Additional Info  : Peak(s) manually integrated
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.685	BB	0.3211	3991.95093	191.60632	28.3920
2	15.257	BB	0.3872	3968.84009	157.90181	28.2277
3	16.806	BB	0.4447	3076.16479	107.22281	21.8787
4	50.062	BB	1.0429	3023.15820	34.54823	21.5017

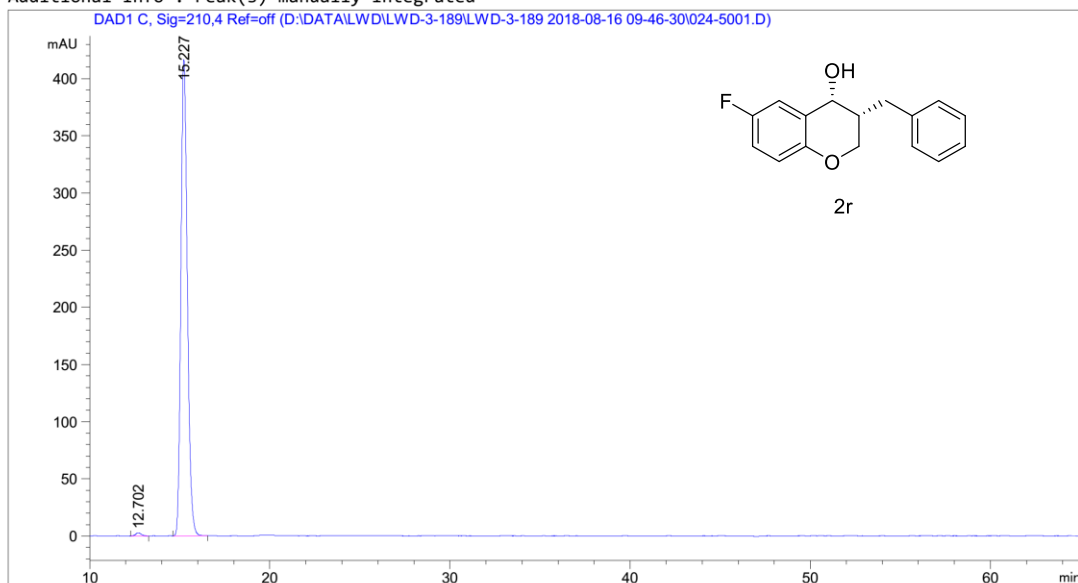
Totals : 1.40601e4 491.27917

Instrument 2 8/17/2018 7:24:43 PM

Page 1 of 2

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\024-5001.D
Sample Name: LWD-3-176-6-EE

```
=====
Acq. Operator   :                               Seq. Line :   50
Acq. Instrument : Instrument 2                   Location  : Vial 24
Injection Date  : 8/17/2018 6:11:29 PM           Inj       :    1
                                                Inj Volume: 1.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-
                                                1UL-ALL-65MIN.M
Last changed    : 8/16/2018 8:59:56 PM
Analysis Method : D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/17/2018 7:26:21 PM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

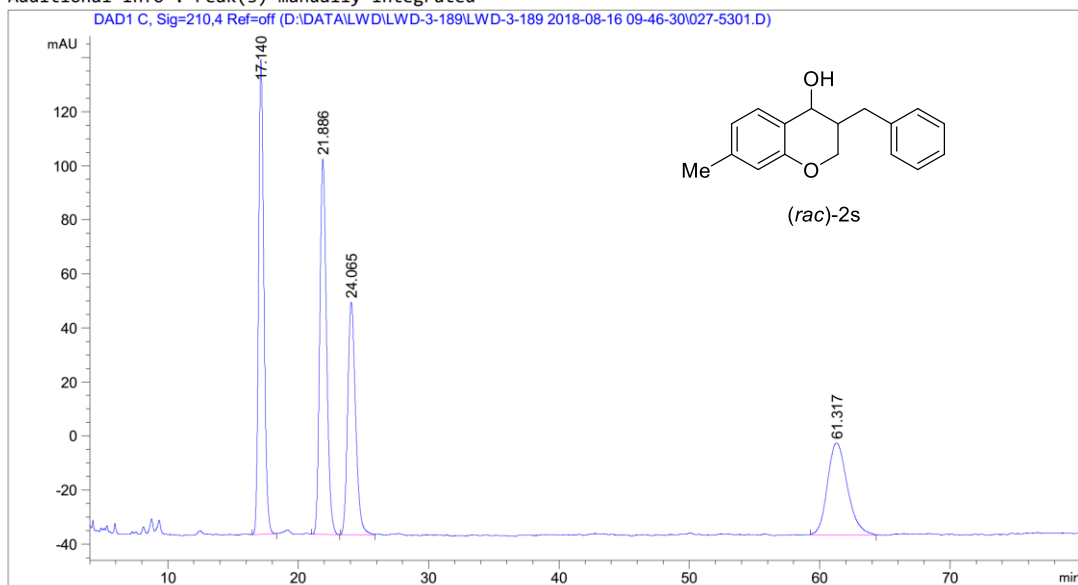
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.702	BB	0.3027	60.94179	2.79111	0.5841
2	15.227	BB	0.3846	1.03726e4	416.47278	99.4159

Totals : 1.04336e4 419.26389

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\027-5301.D
Sample Name: LWD-3-176-4-RAC

```
=====
Acq. Operator   :                               Seq. Line :   53
Acq. Instrument : Instrument 2                   Location  : Vial 27
Injection Date  : 8/17/2018 9:29:28 PM           Inj       :    1
                                                Inj Volume: 2.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-97-3-1ML-
                                                2UL-ALL-80MIN.M
Last changed    : 8/16/2018 9:02:21 PM
Analysis Method : D:\METHOD\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\027-5301.D
Last changed    : 8/18/2018 8:57:03 AM
                (modified after loading)
Additional Info : Peak(s) manually integrated
```



Area Percent Report

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.140	BB	0.4382	5000.33057	175.63075	29.0382
2	21.886	BB	0.5563	5004.27197	138.91711	29.0611
3	24.065	BB	0.6420	3610.64722	85.97623	20.9680
4	61.317	BB	1.2491	3604.56665	33.99368	20.9327

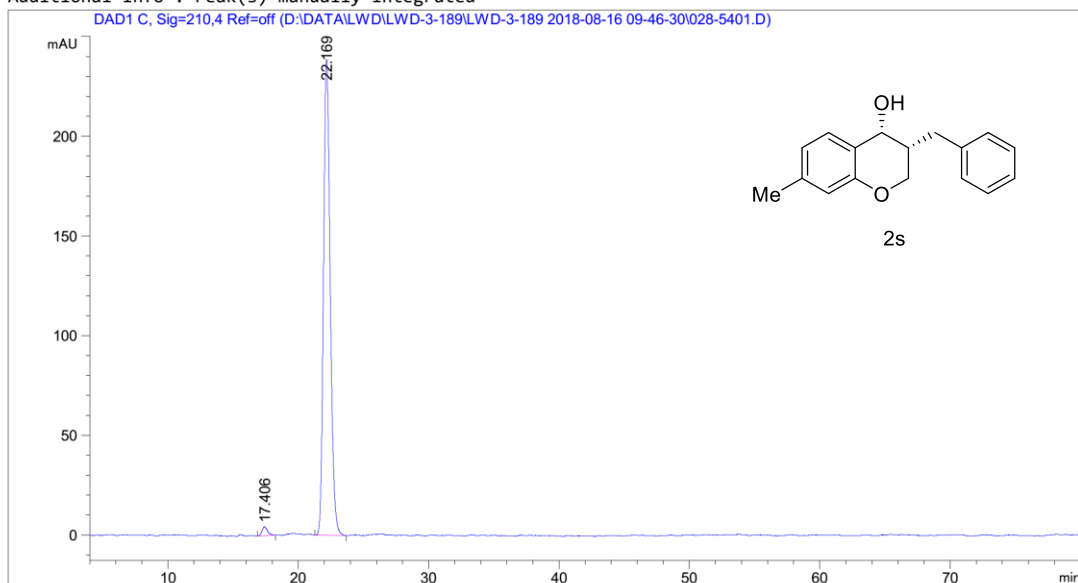
Totals : 1.72198e4 434.51778

Instrument 2 8/18/2018 8:57:10 AM

Page 1 of 2

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\028-5401.D
Sample Name: LWD-3-176-4-EE

```
=====
Acq. Operator   :                               Seq. Line :   54
Acq. Instrument : Instrument 2                   Location  : Vial 28
Injection Date  : 8/17/2018 10:50:28 PM          Inj       :    1
                                                Inj Volume: 1.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-97-3-1ML-
                  1UL-ALL-80MIN.M
Last changed    : 8/16/2018 9:02:52 PM
Analysis Method : D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/18/2018 8:59:10 AM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

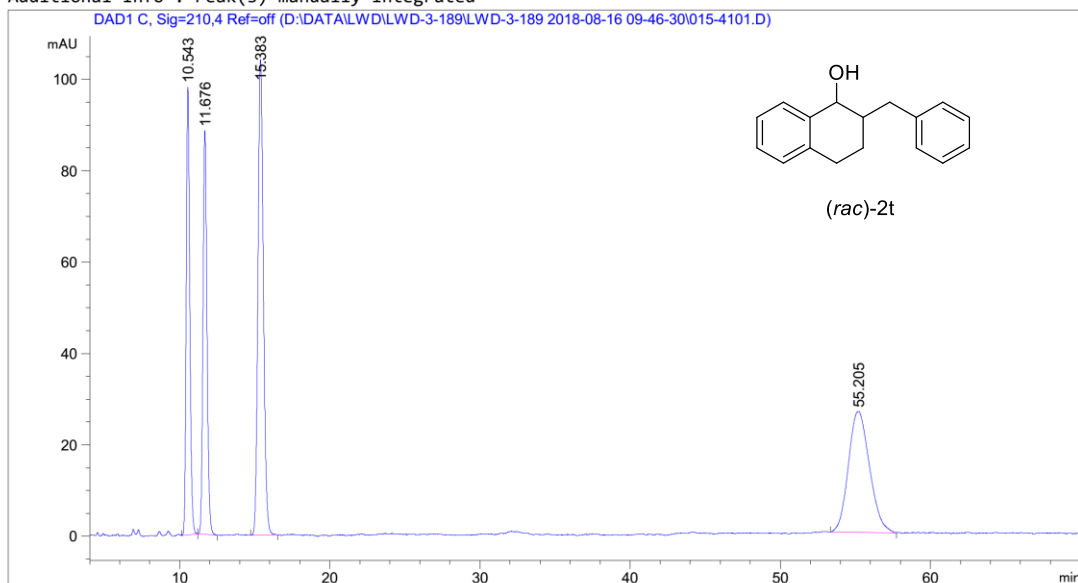
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.406	BB	0.3777	131.24475	4.50790	1.5225
2	22.169	BB	0.5470	8489.13770	238.62573	98.4775

Totals : 8620.38245 243.13363

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\015-4101.D
Sample Name: LWD-3-113-3-RAC

```
=====
Acq. Operator   :                               Seq. Line :   41
Acq. Instrument : Instrument 2                   Location  : Vial 15
Injection Date  : 8/17/2018 8:27:25 AM           Inj       :    1
                                                Inj Volume: 3.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\
DAD-OD(1-2)-95-5-1ML-3UL-ALL-70MIN.M
Last changed    : 8/16/2018 8:43:07 PM
Analysis Method : D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/17/2018 11:03:20 AM
                (modified after loading)
Additional Info  : Peak(s) manually integrated
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.543	BB	0.2545	1618.92737	98.13342	19.1970
2	11.676	BB	0.2845	1624.93506	88.39839	19.2682
3	15.383	BB	0.3857	2603.46802	104.11540	30.8715
4	55.205	BB	1.1522	2585.91626	26.50550	30.6634

Totals : 8433.24670 317.15272

Instrument 2 8/17/2018 11:03:24 AM

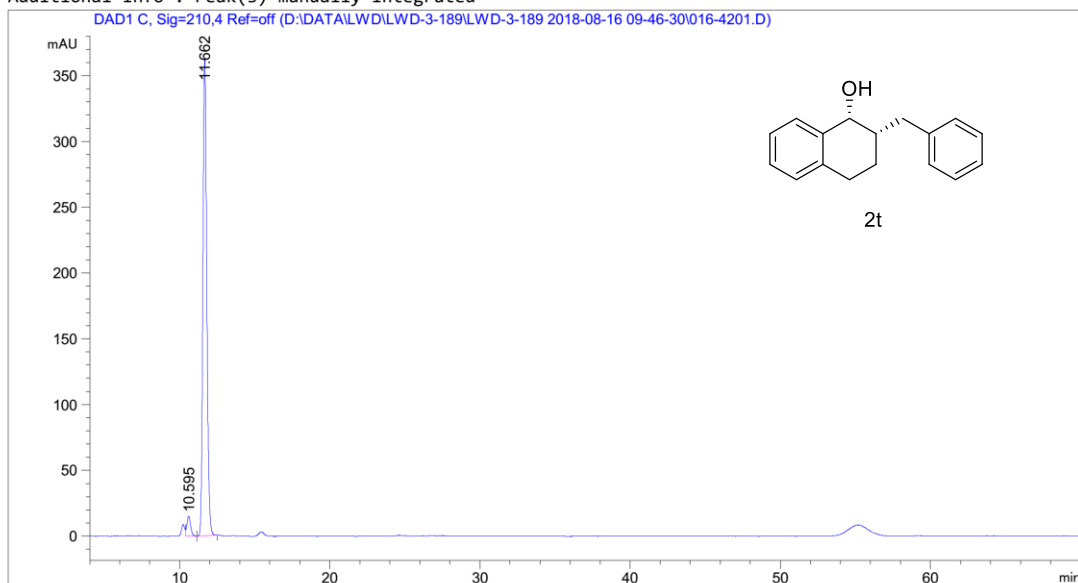
Page 1 of 2

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\016-4201.D
Sample Name: LWD-3-113-3-EE

=====

Acq. Operator	:		Seq. Line	:	42
Acq. Instrument	:	Instrument 2	Location	:	Vial 16
Injection Date	:	8/17/2018 9:38:25 AM	Inj	:	1
			Inj Volume	:	1.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-1ML-1UL-ALL-70MIN.M			
Last changed	:	8/16/2018 8:43:33 PM			
Analysis Method	:	D:\METHOD\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\016-4201.D			
Last changed	:	8/17/2018 11:04:53 AM			
	:	(modified after loading)			

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=210,4 Ref=off

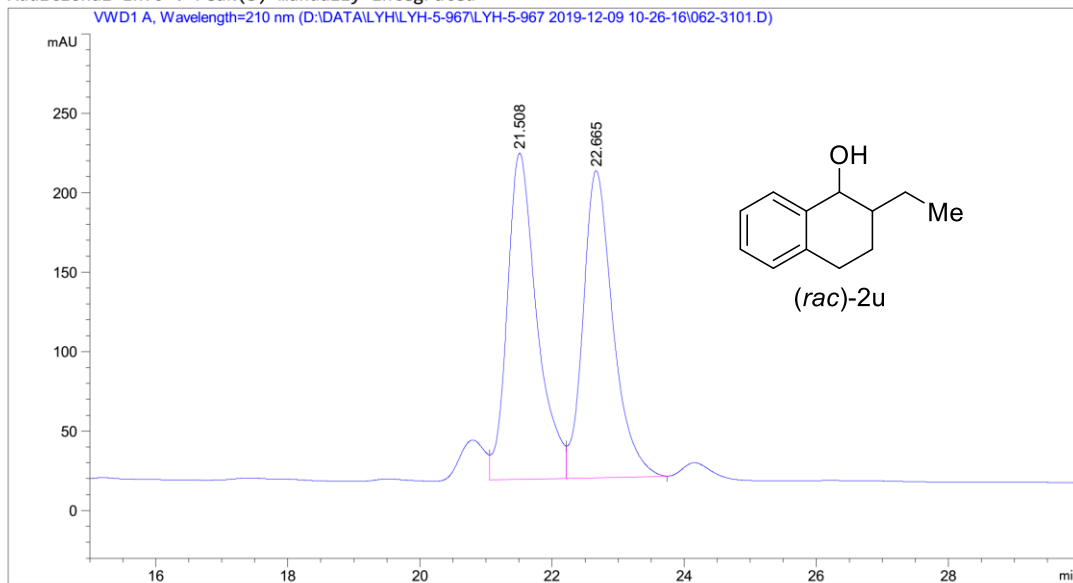
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.595	VB	0.2587	258.90076	15.20095	3.8273
2	11.662	BB	0.2777	6505.61768	361.96060	96.1727

Totals : 6764.51843 377.16155

Data File D:\DATA\LYH\LYH-5-967\LYH-5-967 2019-12-09 10-26-16\062-3101.D
Sample Name: LWD-6-110-2-DIAN1

=====

Acq. Operator	:		Seq. Line	:	31
Acq. Instrument	:	Instrument 1	Location	:	Vial 62
Injection Date	:	12/9/2019 9:53:48 PM	Inj	:	1
			Inj Volume	:	2.000 µl
Acq. Method	:	D:\DATA\LYH\LYH-5-967\LYH-5-967 2019-12-09 10-26-16\VWD-AD(1-2)-90-10-0.3ML-1UL-210NM-30MIN.M			
Last changed	:	12/9/2019 8:58:55 PM			
Analysis Method	:	D:\METHOD\LWD\VWD-AD(1-2)-90-10-0.3ML-1UL-210NM-30MIN.M			
Last changed	:	12/10/2019 8:52:00 AM			
		(modified after loading)			
Additional Info : Peak(s) manually integrated					



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

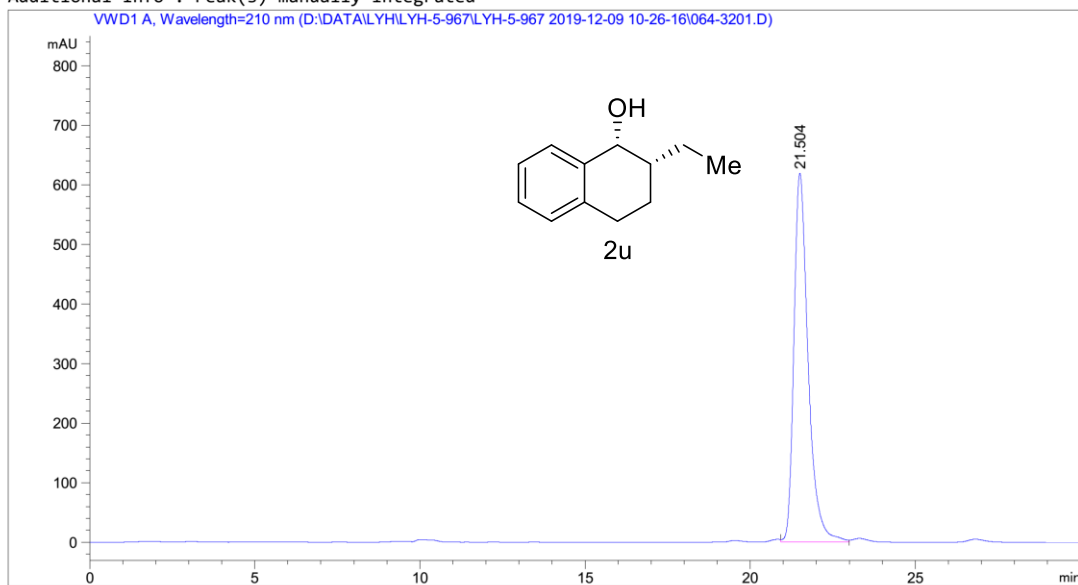
Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.508	VV	0.4673	6409.29297	205.23256	51.3639
2	22.665	VB	0.4736	6068.91553	193.12845	48.6361

Totals : 1.24782e4 398.36101

Data File D:\DATA\LYH\LYH-5-967\LYH-5-967 2019-12-09 10-26-16\064-3201.D
Sample Name: LWD-6-118-1

```
=====
Acq. Operator   :                               Seq. Line :   32
Acq. Instrument : Instrument 1                   Location  : Vial 64
Injection Date  : 12/9/2019 10:24:37 PM          Inj       :    1
                                                Inj Volume: 2.000 µl
Acq. Method     : D:\DATA\LYH\LYH-5-967\LYH-5-967 2019-12-09 10-26-16\VWD-AD(1-2)-90-10-0.3ML
                  -1UL-210NM-30MIN.M
Last changed    : 12/9/2019 8:58:55 PM
Analysis Method : D:\METHOD\LWD\VWD-AD(1-2)-90-10-0.3ML-1UL-210NM-30MIN.M
Last changed    : 12/10/2019 8:54:10 AM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
=====
```



=====
Area Percent Report
=====

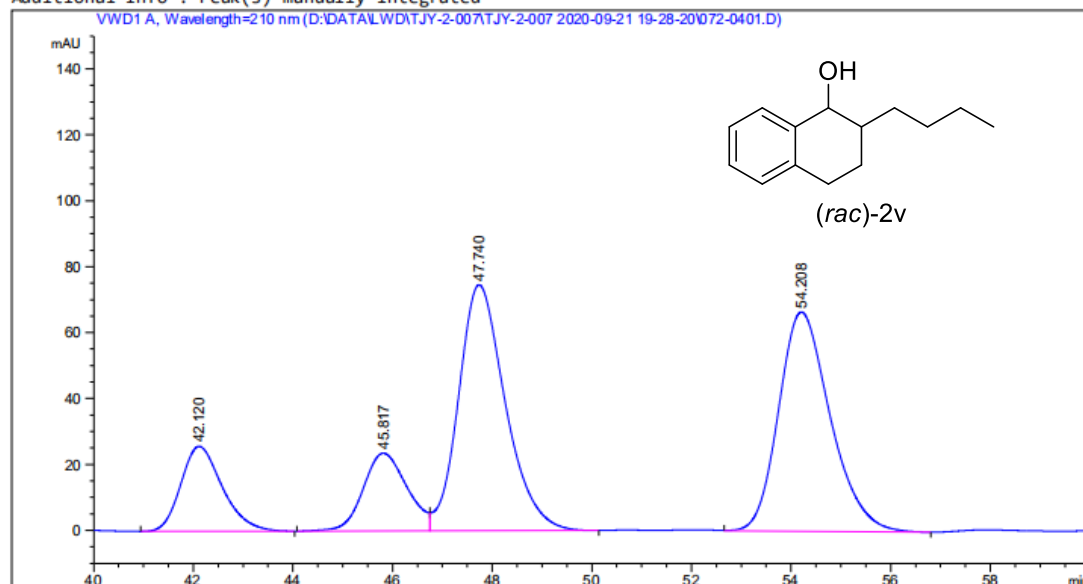
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.504	VV	0.4549	1.85533e4	618.62714	100.0000

Totals : 1.85533e4 618.62714

Acq. Operator : Seq. Line : 4
 Acq. Instrument : Instrument 1 Location : Vial 72
 Injection Date : 9/21/2020 9:17:53 PM Inj : 1
 Inj Volume : 3.000 µl
 Acq. Method : D:\DATA\LWD\TJY-2-007\TJY-2-007 2020-09-21 19-28-20\Wd-AD(1-2)-98-2-0.5ML-3UL-210NM-80MIN.M
 Last changed : 9/21/2020 7:32:20 PM
 Analysis Method : D:\METHOD\LWD\Wd-AD(1-2)-98-2-0.5ML-3UL-210NM-80MIN.M
 Last changed : 9/22/2020 11:03:10 AM
 (modified after loading)
 Additional Info : Peak(s) manually integrated



Area Percent Report

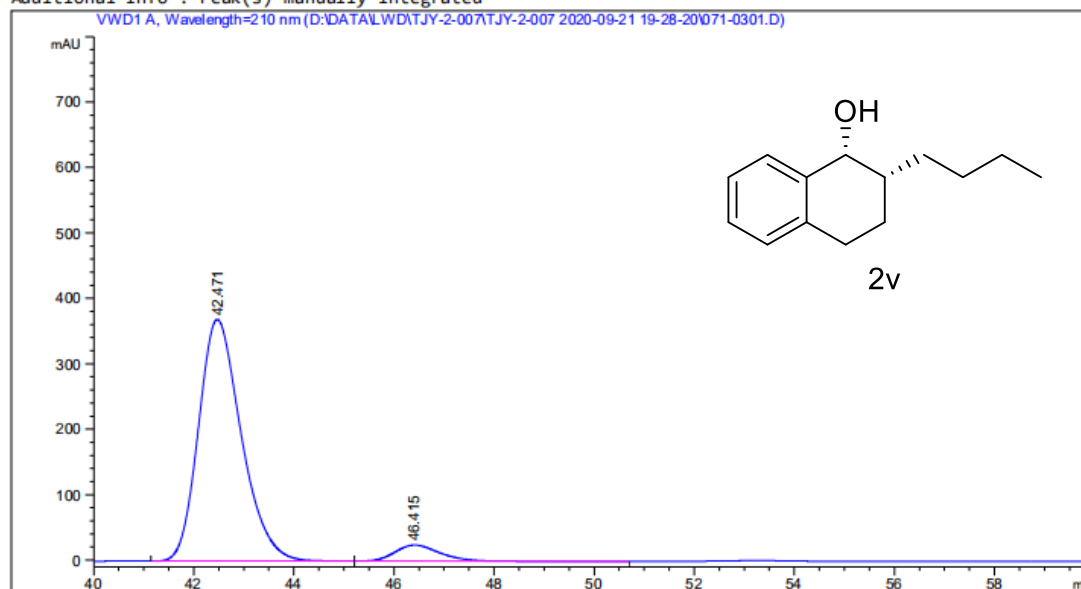
Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: Wd1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	42.120	BB	0.8837	1492.80615	25.77412	11.8415
2	45.817	BV	0.9390	1446.75659	23.60618	11.4763
3	47.740	VB	0.9931	4869.16016	74.64176	38.6241
4	54.208	VB	1.1047	4797.80322	66.57867	38.0581

Acq. Operator : Seq. Line : 3
 Acq. Instrument : Instrument 1 Location : Vial 71
 Injection Date : 9/21/2020 7:57:04 PM Inj : 1
 Inj Volume : 3.000 µl
 Acq. Method : D:\DATA\LWD\TJY-2-007\TJY-2-007 2020-09-21 19-28-20\VWD-AD(1-2)-98-2-0.5ML-3UL-210NM-80MIN.M
 Last changed : 9/21/2020 7:32:20 PM
 Analysis Method : D:\METHOD\LWD\VWD-AD(1-2)-98-2-0.5ML-3UL-210NM-60MIN.M
 Last changed : 9/24/2020 9:06:45 AM
 (modified after loading)

Additional Info : Peak(s) manually integrated



Area Percent Report

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=210 nm

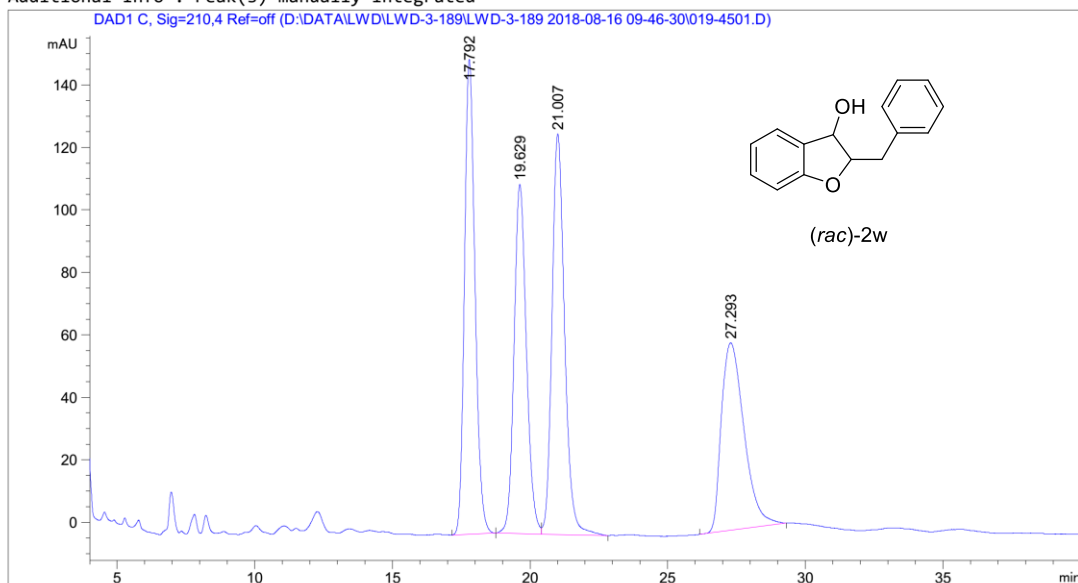
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	42.471	BB	0.9048	2.18616e4	369.23816	93.3530
2	46.415	BB	0.9538	1556.60498	24.64851	6.6470

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\019-4501.D
Sample Name: LWD-3-118-2-RAC

=====

Acq. Operator	:		Seq. Line	:	45
Acq. Instrument	:	Instrument 2	Location	:	Vial 19
Injection Date	:	8/17/2018 2:01:26 PM	Inj	:	1
			Inj Volume	:	5.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-0.8ML-5UL-ALL-40MIN.M			
Last changed	:	8/16/2018 8:56:08 PM			
Analysis Method	:	D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M			
Last changed	:	8/17/2018 3:33:24 PM			
		(modified after loading)			

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

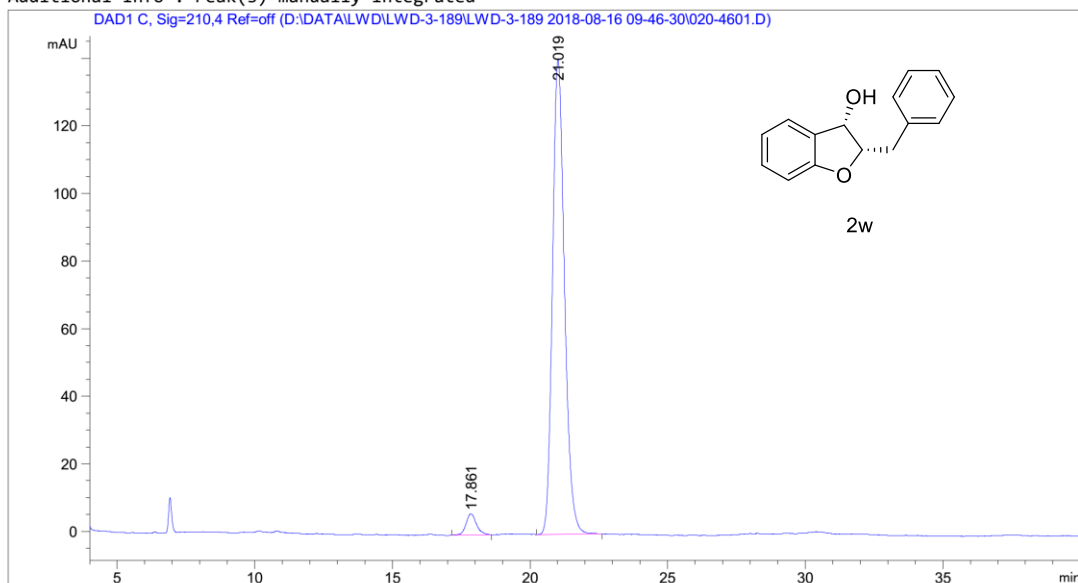
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.792	BB	0.4071	4025.33838	151.91904	26.8361
2	19.629	BV	0.4765	3470.39746	111.68341	23.1364
3	21.007	VB	0.4871	4078.22510	128.20007	27.1887
4	27.293	BB	0.8586	3425.73730	59.95417	22.8387

Totals : 1.49997e4 451.75669

Data File D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\020-4601.D
Sample Name: LWD-3-118-2-EE

```
=====
Acq. Operator   :                               Seq. Line :   46
Acq. Instrument : Instrument 2                   Location  : Vial 20
Injection Date  : 8/17/2018 2:42:29 PM           Inj       :    1
                                                Inj Volume: 1.000 µl
Acq. Method     : D:\DATA\LWD\LWD-3-189\LWD-3-189 2018-08-16 09-46-30\DAD-OD(1-2)-95-5-0.8ML-
                  1UL-ALL-40MIN.M
Last changed    : 8/16/2018 8:56:41 PM
Analysis Method : D:\METHOD\LWD\DAD-OD(1-2)-97-3-0.8ML-1UL-ALL-80MIN.M
Last changed    : 8/17/2018 3:34:50 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Area Percent Report

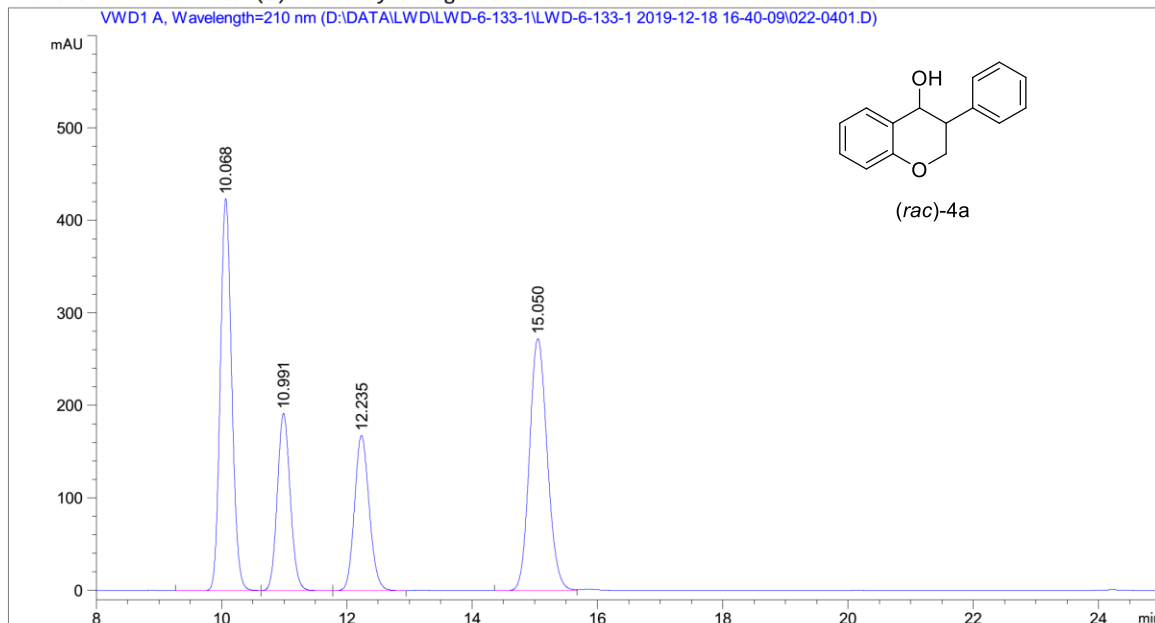
```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.861	BB	0.3850	165.14426	6.27488	3.7346
2	21.019	BB	0.4653	4256.80518	140.56371	96.2654

Totals : 4421.94943 146.83859

VWD1 A, Wavelength=210 nm (D:\DATA\LWD\LWD-6-133-1\LWD-6-133-1 2019-12-18 16-40-09\022-0401.D)



```
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: VWD1 A, Wavelength=210 nm

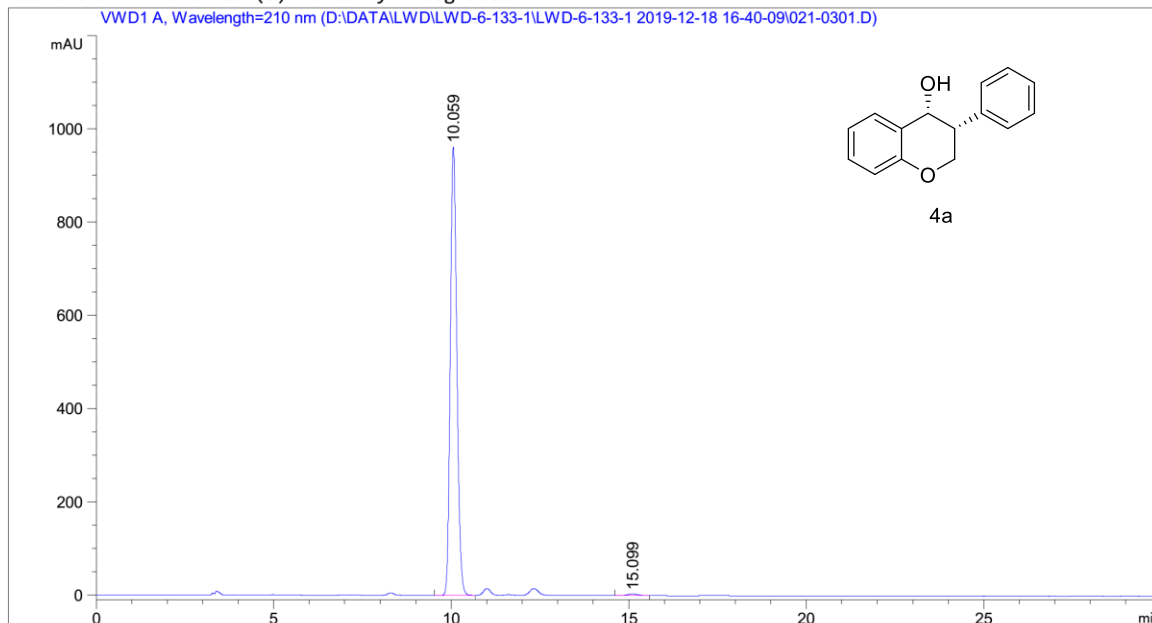
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.068	BB	0.1959	5370.57617	423.68130	33.0362
2	10.991	BB	0.2222	2743.30005	191.40637	16.8749
3	12.235	BB	0.2527	2741.24854	167.73990	16.8623
4	15.050	BV	0.3060	5401.53174	272.85406	33.2266

Totals : 1.62567e4 1055.68164

Sample Name: LWD-6-133-1

```
=====
Acq. Operator   :                               Seq. Line :    3
Acq. Instrument : Instrument 1                   Location  : Vial 21
Injection Date  : 12/18/2019 5:12:38 PM          Inj       :    1
                                                Inj Volume: 2.000 µl

Acq. Method     : D:\DATA\LWD\LWD-6-133-1\LWD-6-133-1 2019-12-18 16-40-09\VWD-IC(1-2)-95-5-
                  1ML-2UL-210NM-30MIN.M
Last changed    : 12/18/2019 4:38:02 PM
Analysis Method : D:\METHOD\LSL\DAD-OJ(1-6)-99-1-0.5ML-5UL-ALL-60MIN.M
Last changed    : 12/30/2020 9:15:47 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
=====
```



```
=====
Area Percent Report
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```

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.059	BV	0.1996	1.23387e4	961.94116	99.3882
2	15.099	BB	0.3238	75.95415	3.60568	0.6118

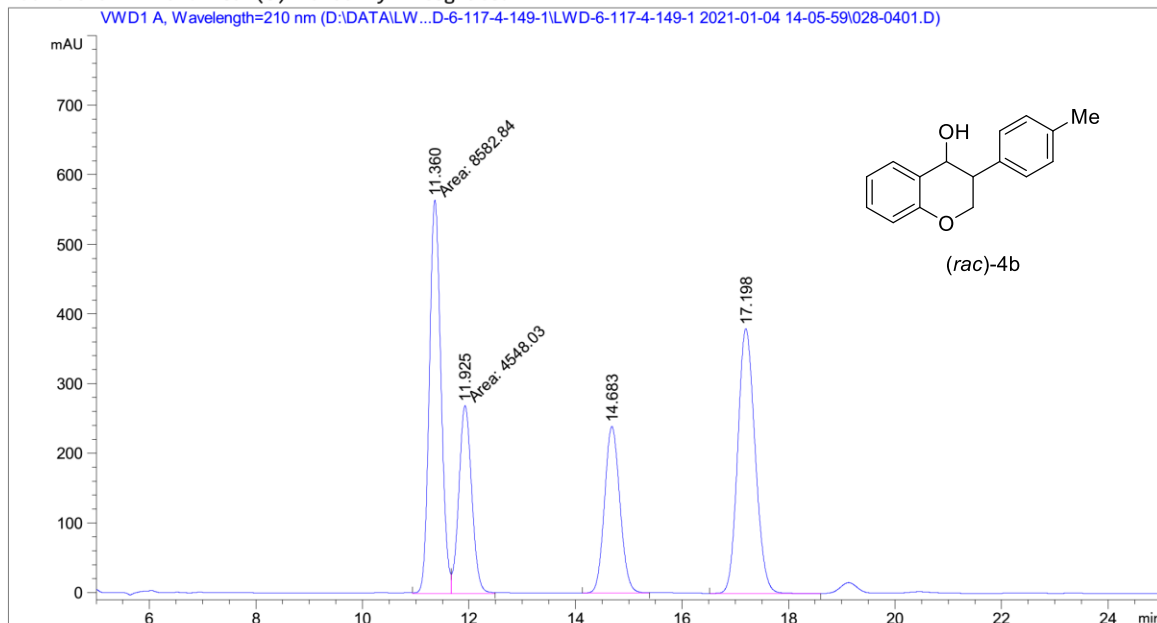
Totals : 1.24147e4 965.54684

Sample Name: LWD-6-238-1-RAC

```

=====
Acq. Operator   :                               Seq. Line :    4
Acq. Instrument : Instrument 1                   Location  : Vial 28
Injection Date  : 1/4/2021 2:59:25 PM           Inj       :    1
                                                Inj Volume: 5.000 µl

Acq. Method     : D:\DATA\LWD\LWD-6-117-4-149-1\LWD-6-117-4-149-1 2021-01-04 14-05-59\VWD-IC(
                  1-6)-95-5--1ML-5UL-210-25MIN.M
Last changed    : 12/31/2020 3:40:07 PM
Analysis Method : D:\METHOD\LWD\VWD-IC(1-6)-95-5--0.5ML-1UL-210-10MIN.M
Last changed    : 1/4/2021 3:37:08 PM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
  
```



```

=====
                        Area Percent Report
=====
  
```

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

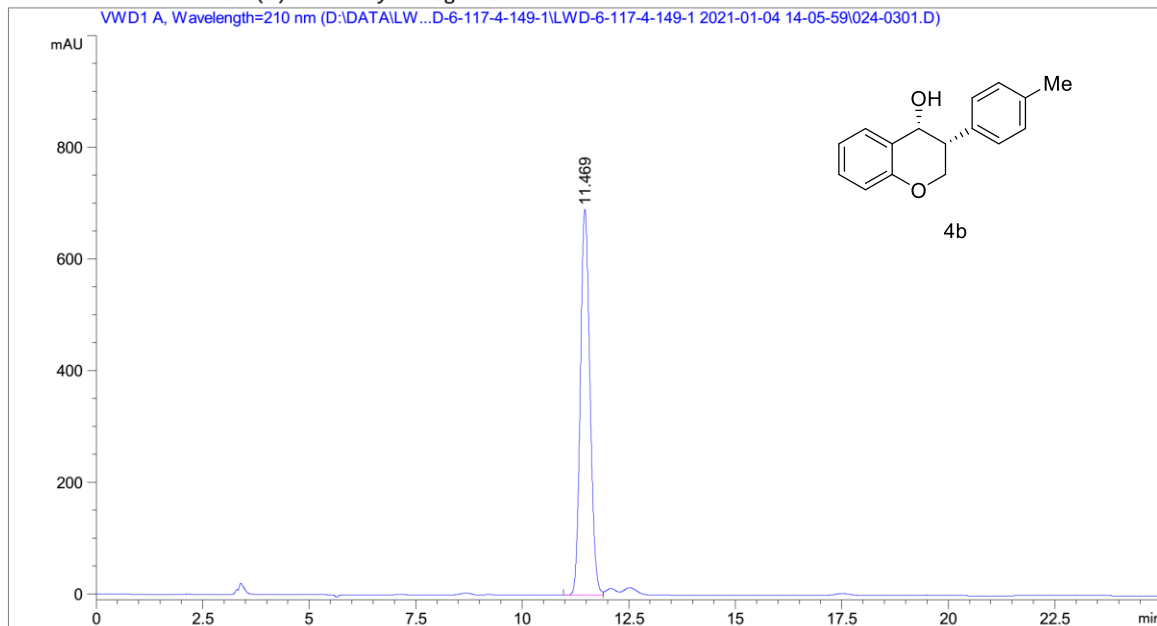
Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.360	MF	0.2532	8582.84082	564.85565	32.3158
2	11.925	FM	0.2809	4548.02637	269.82861	17.1241
3	14.683	VV	0.3131	4821.59766	239.27100	18.1541
4	17.198	BB	0.3523	8606.79102	379.92047	32.4060

Totals : 2.65593e4 1453.87573

Sample Name: LWD-6-149-1

```
=====
Acq. Operator   :                               Seq. Line :    3
Acq. Instrument : Instrument 1                   Location  : Vial 24
Injection Date  : 1/4/2021 2:33:35 PM            Inj       :    1
                                                Inj Volume: 5.000 µl
Acq. Method     : D:\DATA\LWD\LWD-6-117-4-149-1\LWD-6-117-4-149-1 2021-01-04 14-05-59\VWD-IC(
                  1-6)-95-5--1ML-5UL-210-25MIN.M
Last changed    : 12/31/2020 3:40:07 PM
Analysis Method : D:\METHOD\LWD\VWD-IC(1-6)-95-5--0.5ML-1UL-210-10MIN.M
Last changed    : 1/4/2021 3:38:25 PM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
=====
```



```
=====
                          Area Percent Report
=====
```

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: VWD1 A, Wavelength=210 nm

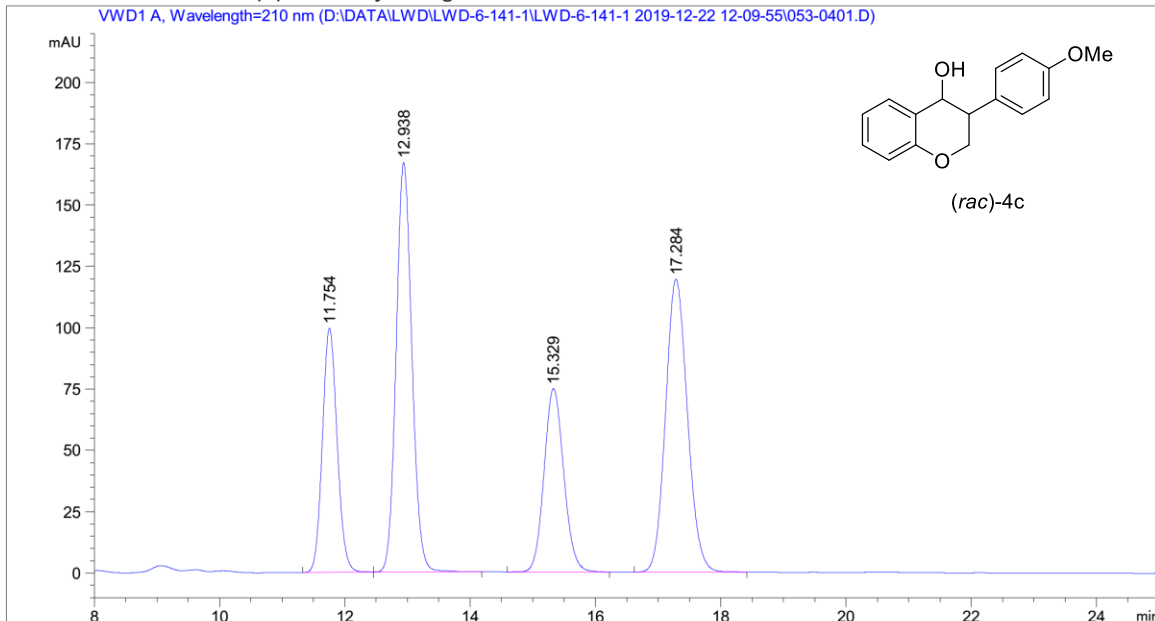
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.469	BV	0.2450	1.08309e4	690.41827	100.0000

```
Totals :                      1.08309e4  690.41827
```

Data File D:\DATA\LWD\LWD-6-141-1\LWD-6-141-1 2019-12-22 12-09-55\053-0401.D
Sample Name: LWD-6-141-1-RAC

=====

Acq. Operator	:		Seq. Line	:	4
Acq. Instrument	:	Instrument 1	Location	:	Vial 53
Injection Date	:	12/22/2019 2:05:48 PM	Inj	:	1
			Inj Volume	:	2.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-6-141-1\LWD-6-141-1 2019-12-22 12-09-55\VWD-IC(1-2)-90-10-1ML-2UL-210NM-60MIN.M			
Last changed	:	12/21/2019 7:30:34 PM			
Analysis Method	:	D:\METHOD\LSL\DAD-OJ(1-6)-99-1-0.5ML-5UL-ALL-60MIN.M			
Last changed	:	12/30/2020 9:03:36 AM			
		(modified after loading)			
Additional Info : Peak(s) manually integrated					



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

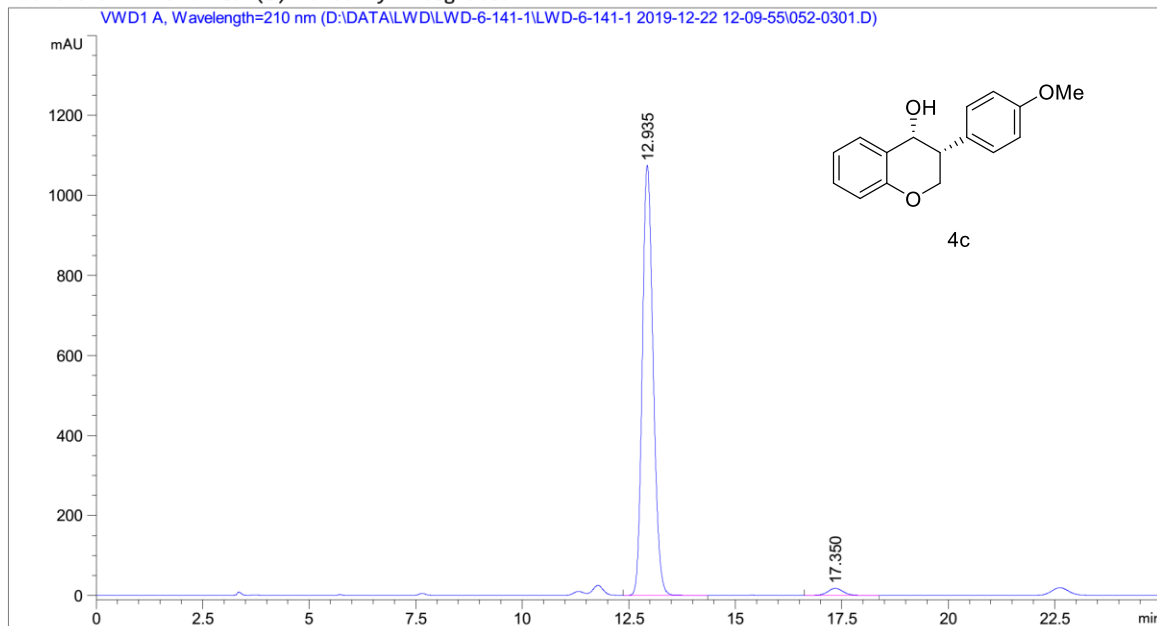
Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.754	BB	0.2524	1623.97180	99.52227	17.9126
2	12.938	BB	0.2703	2908.48389	166.89293	32.0810
3	15.329	BB	0.3392	1633.34399	74.68367	18.0160
4	17.284	BB	0.3764	2900.26465	119.41504	31.9903

Totals : 9066.06433 460.51391

Sample Name: LWD-6-141-1-EE

```
=====
Acq. Operator   :                               Seq. Line :    3
Acq. Instrument : Instrument 1                   Location  : Vial 52
Injection Date  : 12/22/2019 1:04:58 PM          Inj       :    1
                                                Inj Volume : 2.000 µl
Acq. Method     : D:\DATA\LWD\LWD-6-141-1\LWD-6-141-1 2019-12-22 12-09-55\VWD-IC(1-2)-90-10-
                  1ML-2UL-210NM-60MIN.M
Last changed    : 12/21/2019 7:30:34 PM
Analysis Method : D:\METHOD\LSL\DAD-OJ(1-6)-99-1-0.5ML-5UL-ALL-60MIN.M
Last changed    : 12/30/2020 9:06:05 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
=====
```



```
=====
Area Percent Report
=====
```

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.935	BB	0.2757	1.90471e4	1075.22815	97.7275
2	17.350	BB	0.3823	442.90363	17.73792	2.2725

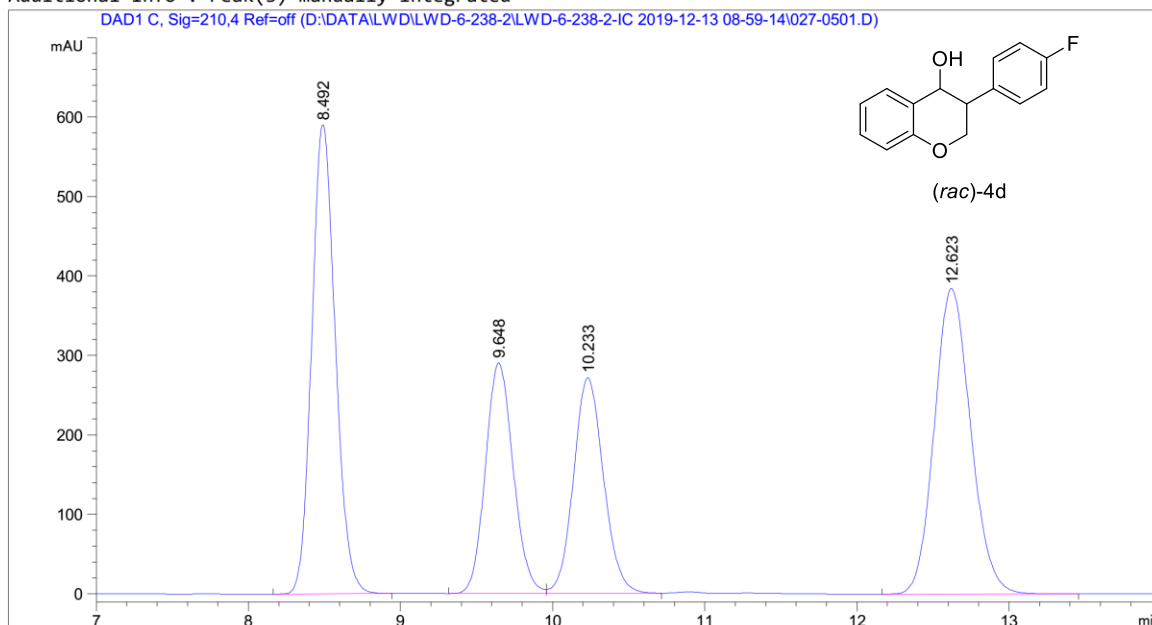
Totals : 1.94900e4 1092.96607

Data File D:\DATA\LWD\LWD-6-238-2\LWD-6-238-2-IC 2019-12-13 08-59-14\027-0501.D
Sample Name: LWD-6-238-3

=====

Acq. Operator	:		Seq. Line	:	5
Acq. Instrument	:	Instrument 2	Location	:	Vial 27
Injection Date	:	12/13/2019 10:29:30 AM	Inj	:	1
			Inj Volume	:	2.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-6-238-2\LWD-6-238-2-IC 2019-12-13 08-59-14\DAD-IC(1-6)-95-5 -1ML-2UL-ALL-40MIN.M			
Last changed	:	12/13/2019 10:42:22 AM (modified after loading)			
Analysis Method	:	D:\METHOD\ZXH\DAD-OD(1-2)-98-2-1.0ML-1UL-220NM-80MIN.M			
Last changed	:	12/18/2019 9:13:10 AM (modified after loading)			

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

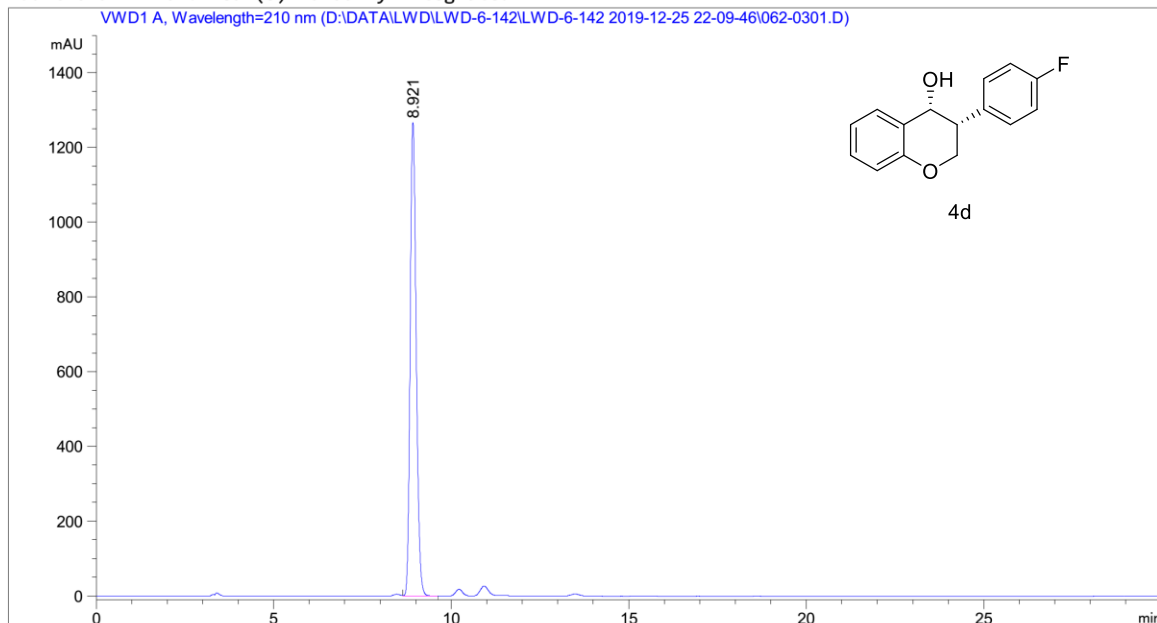
Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.492	BB	0.1656	6353.20557	590.30145	31.5473
2	9.648	BV	0.1980	3682.42773	290.25793	18.2854
3	10.233	VB	0.2116	3714.69189	271.58087	18.4456
4	12.623	BB	0.2578	6388.34912	384.61862	31.7218

Data File D:\DATA\LWD\LWD-6-142\LWD-6-142 2019-12-25 22-09-46\062-0301.D
Sample Name: LWD-6-142-1

```
=====
Acq. Operator   :                               Seq. Line :    3
Acq. Instrument : Instrument 1                   Location  : Vial 62
Injection Date  : 12/25/2019 11:03:04 PM         Inj       :    1
                                                Inj Volume: 2.000 µl
Acq. Method     : D:\DATA\LWD\LWD-6-142\LWD-6-142 2019-12-25 22-09-46\VWD-IC(1-2)-95-5-1ML-
                  2UL-210NM-40MIN.M
Last changed    : 12/18/2019 9:03:42 PM
Analysis Method : D:\METHOD\LSL\DAD-OJ(1-6)-99-1-0.5ML-5UL-ALL-60MIN.M
Last changed    : 12/30/2020 9:18:35 AM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
=====
```



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.921	VB	0.1840	1.49987e4	1267.61719	100.0000

Totals : 1.49987e4 1267.61719

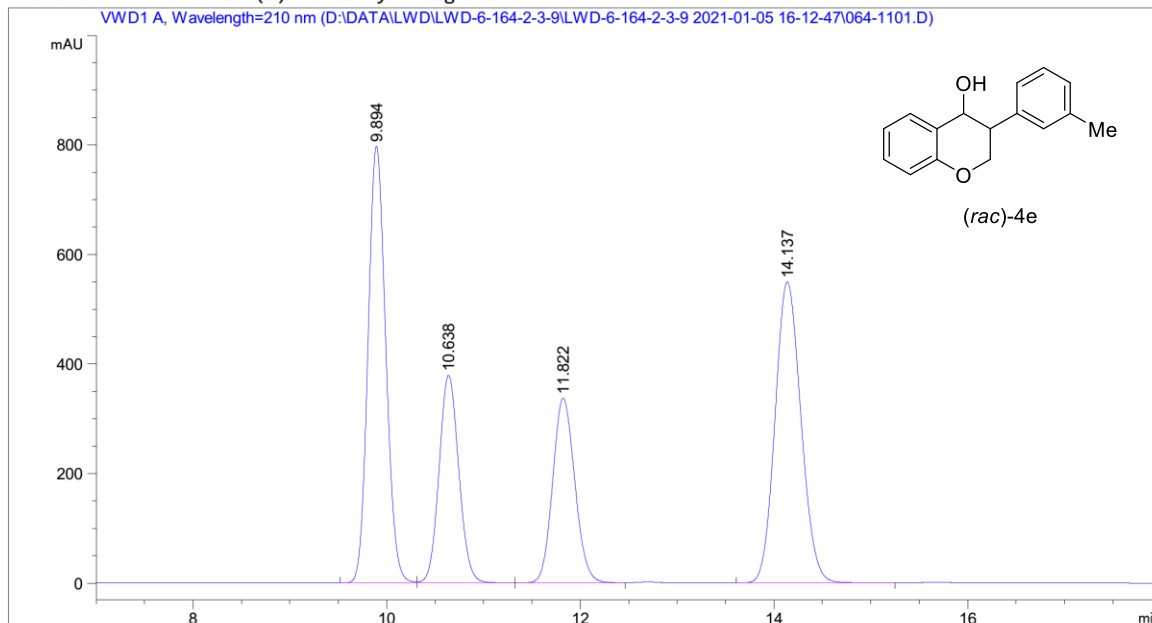
Sample Name: LWD-6-238-18-RAC

```

=====
Acq. Operator   :                               Seq. Line :   11
Acq. Instrument : Instrument 1                   Location  : Vial 64
Injection Date  : 1/5/2021 8:41:08 PM           Inj       :    1
                                                Inj Volume: 3.000 µl

Acq. Method     : D:\DATA\LWD\LWD-6-164-2-3-9\LWD-6-164-2-3-9 2021-01-05 16-12-47\VWD-IC(1-6)
                  -95-5--1ML-3UL-210-30MIN.M

Last changed    : 1/5/2021 4:11:37 PM
Analysis Method : D:\METHOD\LWD\VWD-IC(1-6)-95-5--1ML-3UL-210-40MIN.M
Last changed    : 1/5/2021 9:12:59 PM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
  
```



```

=====
                        Area Percent Report
=====
  
```

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.894	BV	0.1982	1.01206e4	796.88885	32.5840
2	10.638	VB	0.2212	5361.64551	378.71051	17.2622
3	11.822	BV	0.2475	5358.87891	337.06647	17.2533
4	14.137	BV	0.2891	1.02189e4	549.18060	32.9005

Totals : 3.10600e4 2061.84644

WVD1 A, Wavelength=210 nm (D:\DATA\LWD\LWD-6-164-2-3-9\LWD-6-164-2-3-9 2021-01-05 16-12-47\061-1001.D)

Chemical structure of 4e: CC1=CC=C(C=C1)[C@H]2C=CC(=C2)O[C@@H]3C=CC=CC=C3

Retention Time (min)	Intensity (mAU)
9.932	~380
14.236	~20

```
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.932	BV	0.1992	4771.45068	373.22333	99.3336
2	14.236	VB	0.4166	32.00837	1.08985	0.6664

Totals :	4803.45906	374.31318
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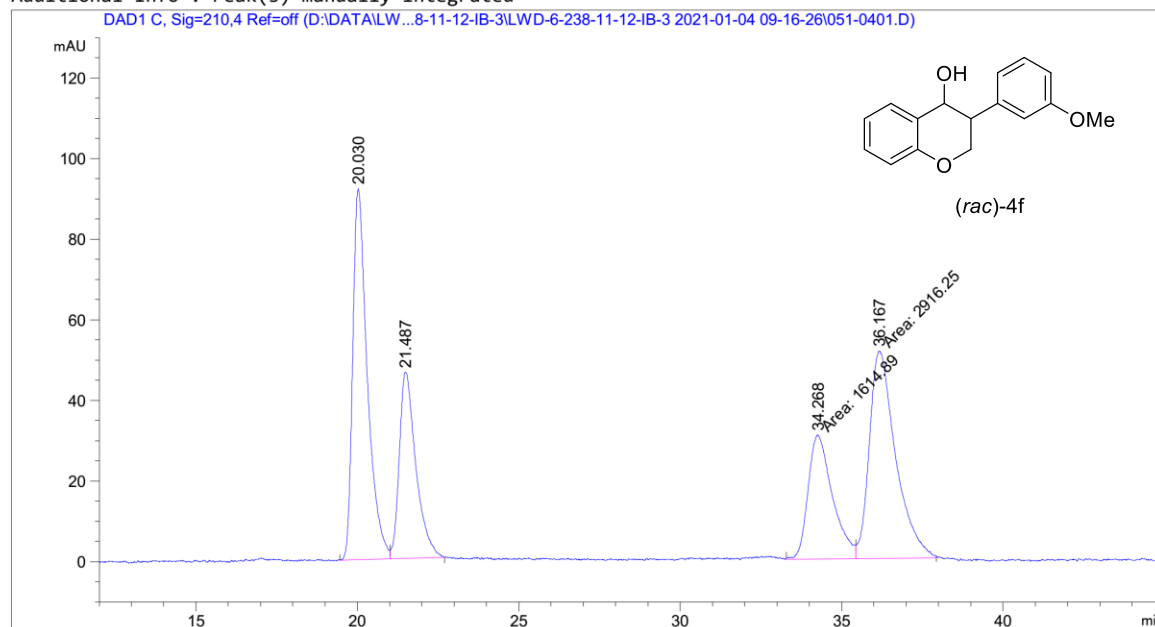
Sample Name: LWD-6-238-11

```

=====
Acq. Operator   :                               Seq. Line :    4
Acq. Instrument : Instrument 2                   Location  : Vial 51
Injection Date  : 1/4/2021 10:33:48 AM           Inj       :    1
                                                Inj Volume : 3.000 µl

Acq. Method     : D:\DATA\LWD\LWD-6-238-11-12-IB-3\LWD-6-238-11-12-IB-3 2021-01-04 09-16-26
                  \DAD-IB(1-6)-95-5-1ML-3UL-ALL-60MIN.M
Last changed    : 1/4/2021 11:16:56 AM
                  (modified after loading)
Analysis Method : D:\METHOD\LWD\DAD-IB(1-6)-95-5-1ML-3UL-ALL-60MIN.M
Last changed    : 1/4/2021 11:21:48 AM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated

```



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                        Area Percent Report
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```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

Signal 1: DAD1 C, Sig=210,4 Ref=off

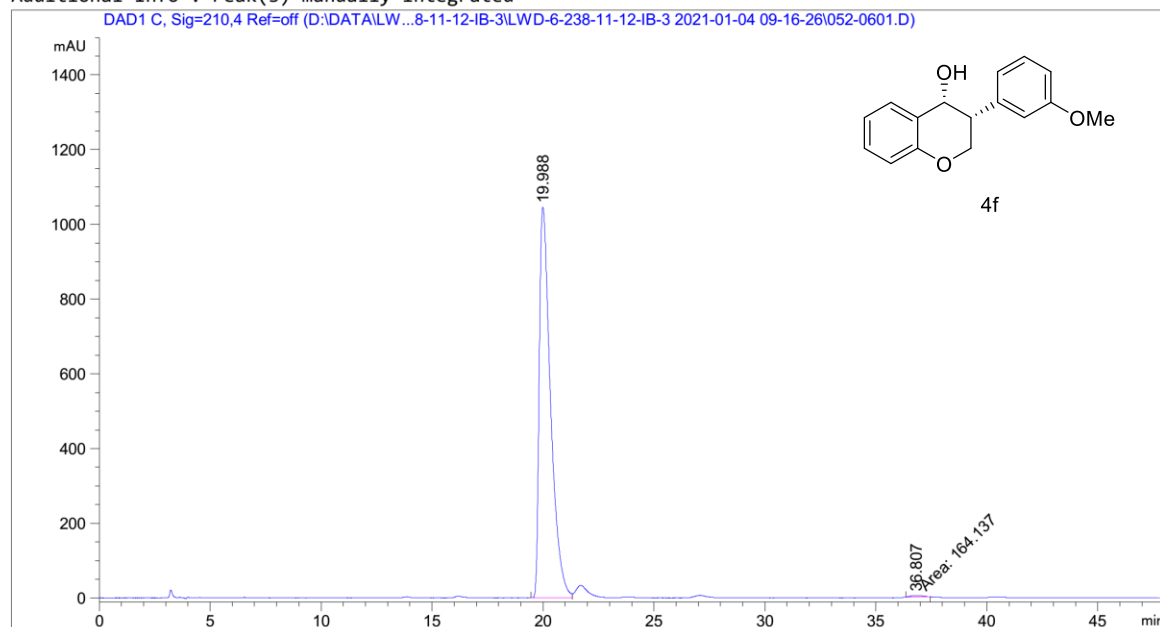
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.030	BV	0.4455	2898.64941	92.00972	31.9165
2	21.487	VB	0.4608	1652.19043	46.24879	18.1920
3	34.268	MF	0.8762	1614.88525	30.71714	17.7812
4	36.167	FM	0.9435	2916.24951	51.51293	32.1103

Sample Name: LWD-6-149-4

```

=====
Acq. Operator   :                               Seq. Line :    6
Acq. Instrument : Instrument 2                   Location  : Vial 52
Injection Date  : 1/4/2021 11:56:48 AM          Inj       :    1
                                                Inj Volume: 3.000 µl

Acq. Method     : D:\DATA\LWD\LWD-6-238-11-12-IB-3\LWD-6-238-11-12-IB-3 2021-01-04 09-16-26
                  \DAD-IB(1-6)-95-5-1ML-3UL-ALL-60MIN.M
Last changed    : 1/4/2021 12:44:51 PM
                  (modified after loading)
Analysis Method : D:\METHOD\LWD\DAD-IB(1-6)-95-5-1ML-3UL-ALL-60MIN.M
Last changed    : 1/4/2021 12:46:00 PM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
  
```



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                        Area Percent Report
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```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

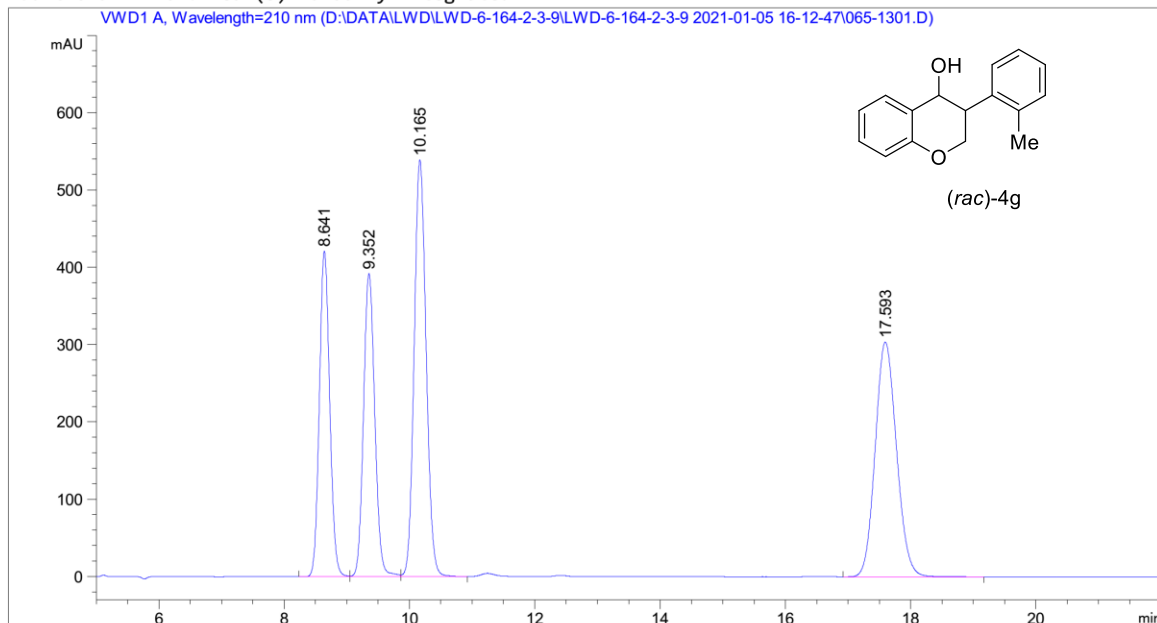
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.988	BV	0.5000	3.70890e4	1045.09094	99.5594
2	36.807	MM	0.6851	164.13708	3.99314	0.4406

Totals : 3.72531e4 1049.08408

Sample Name: LWD-6-238-9-RAC

```
=====
Acq. Operator   :                               Seq. Line :   13
Acq. Instrument : Instrument 1                   Location  : Vial 65
Injection Date  : 1/5/2021 9:42:47 PM             Inj       :    1
                                                Inj Volume : 3.000 µl
Acq. Method     : D:\DATA\LWD\LWD-6-164-2-3-9\LWD-6-164-2-3-9 2021-01-05 16-12-47\VWD-IC(1-6)
                                                -95-5--1ML-3UL-210-30MIN.M
Last changed    : 1/5/2021 4:11:37 PM
Analysis Method : D:\METHOD\LCZ\VWD-OD(1-2)-98-2--1ML-5UL-220-80MIN.M
Last changed    : 1/6/2021 9:25:47 AM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
VWD1 A, Wavelength=210 nm (D:\DATA\LWD\LWD-6-164-2-3-9\LWD-6-164-2-3-9 2021-01-05 16-12-47\065-1301.D)
```



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                          Area Percent Report
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```

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.641	BV	0.1781	4840.77100	421.00116	20.1223
2	9.352	VV	0.1935	4893.10547	392.22614	20.3398
3	10.165	VB	0.2058	7151.54590	539.13275	29.7278
4	17.593	BB	0.3676	7171.37793	303.62662	29.8102

Totals : 2.40568e4 1655.98666

WVD1 A, Wavelength=210 nm (D:\DATA\LWD\LWD-6-164-2-3-9\LWD-6-164-2-3-9 2021-01-05 16-12-47\062-1201.D)

Chromatogram showing a major peak at 10.164 minutes and a minor peak at 17.689 minutes. The y-axis is mAU (0-300) and the x-axis is time (0-30 minutes). The chemical structure of 4g is shown as an inset.

Cc1ccc(cc1)[C@H]2COC(=O)c3ccccc32

4g

```
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: VWD1 A, Wavelength=210 nm

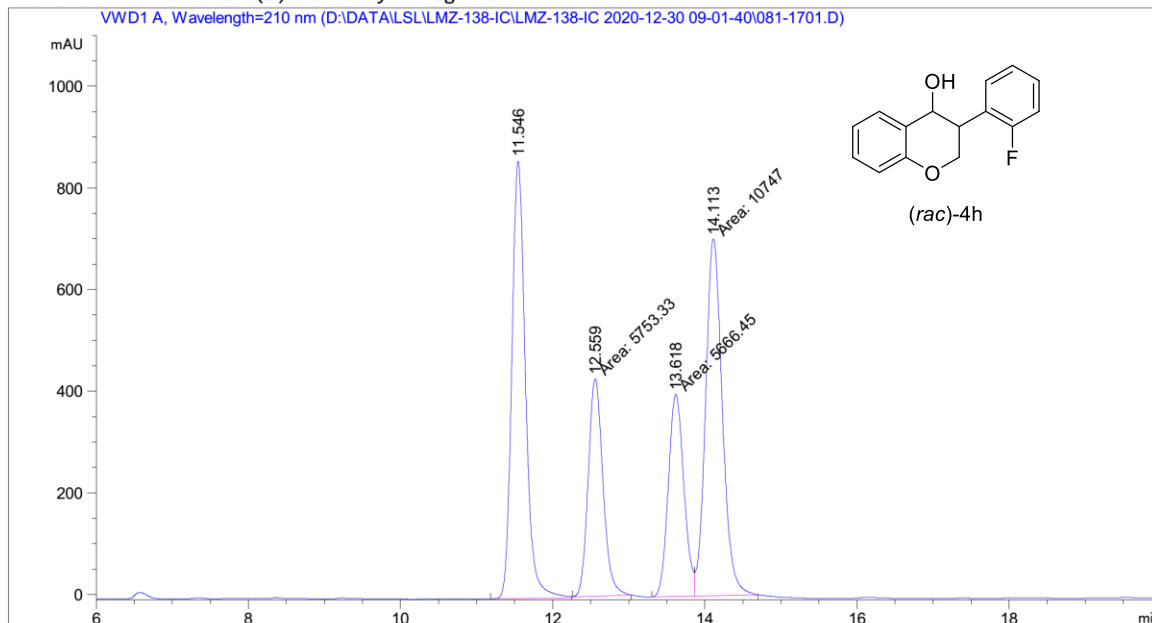
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.164	VB	0.2074	4054.71411	302.43280	97.6082
2	17.689	BB	0.3819	99.35859	3.95759	2.3918

Totals :	4154.07270	306.39039
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Sample Name: LWD-6-238-19

```

=====
Acq. Operator   :                               Seq. Line :   17
Acq. Instrument : Instrument 1                   Location  : Vial 81
Injection Date  : 12/30/2020 7:13:21 PM          Inj       :    1
                                                Inj Volume: 2.000 µl
Acq. Method     : D:\DATA\LSL\LMZ-138-IC\LMZ-138-IC 2020-12-30 09-01-40\VWD-IC(1-6)-90-10--0.
                                                5ML-2UL-210-60MIN.M
Last changed    : 12/30/2020 2:24:25 PM
Analysis Method : D:\METHOD\LSL\DAD-OJ(1-6)-99-1-0.5ML-5UL-ALL-60MIN.M
Last changed    : 12/31/2020 1:19:26 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
  
```



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 Area Percent Report
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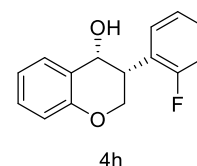
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.546	BV	0.1914	1.07218e4	860.32983	32.6004
2	12.559	MM	0.2240	5753.32813	428.05359	17.4934
3	13.618	MF	0.2373	5666.45068	398.06229	17.2292
4	14.113	FM	0.2552	1.07470e4	701.84137	32.6769

Totals : 3.28886e4 2388.28708

VWD1 A, Wavelength=210 nm (D:\DATA\SL\LMZ-138-IC\LMZ-138-IC 2020-12-30 09-01-40\082-1801.D)



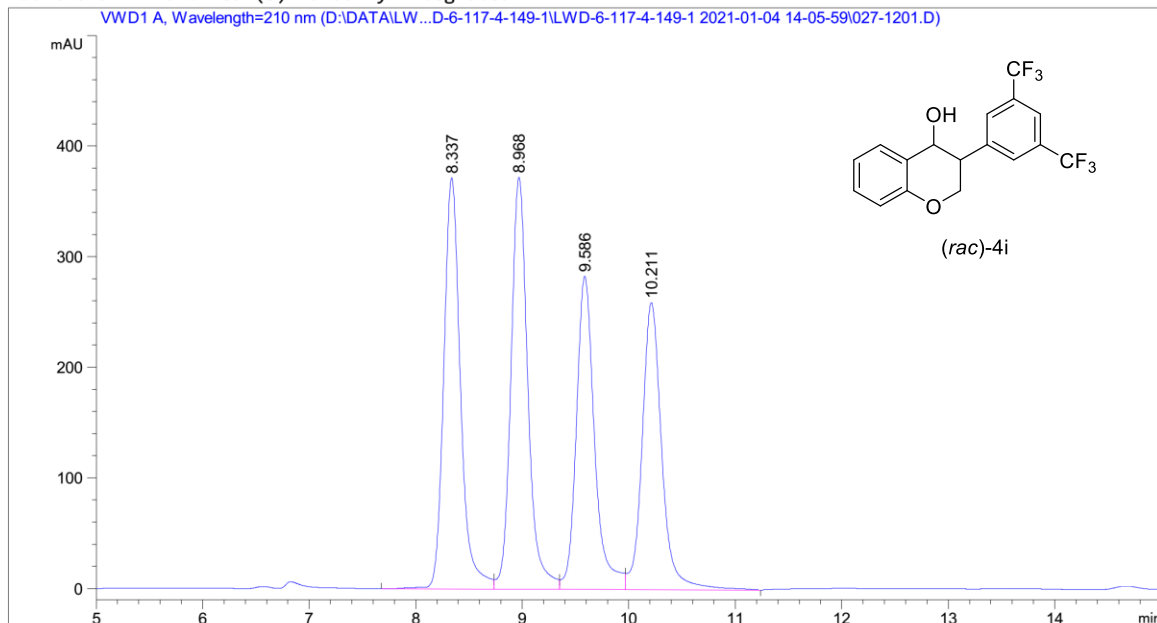
```
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.532	BV	0.1932	1.23423e4	978.45062	99.0067
2	14.107	VB	0.2374	123.82002	7.92111	0.9933

Page 1 of 2

Sample Name: LWD-6-238-4-RAC

```
=====
Acq. Operator   :                               Seq. Line :   12
Acq. Instrument : Instrument 1                   Location  : Vial 27
Injection Date  : 1/4/2021 6:26:12 PM             Inj       :    1
                                                Inj Volume : 1.000 µl
Acq. Method     : D:\DATA\LWD\LWD-6-117-4-149-1\LWD-6-117-4-149-1 2021-01-04 14-05-59\VWD-IC(
                  1-6)-95-5--0.5ML-1UL-210-25MIN.M
Last changed    : 12/31/2020 4:26:33 PM
Analysis Method : D:\METHOD\LWD\VWD-IC(1-6)-95-5--0.5ML-1UL-210-10MIN.M
Last changed    : 1/4/2021 6:55:27 PM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
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Area Percent Report
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Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

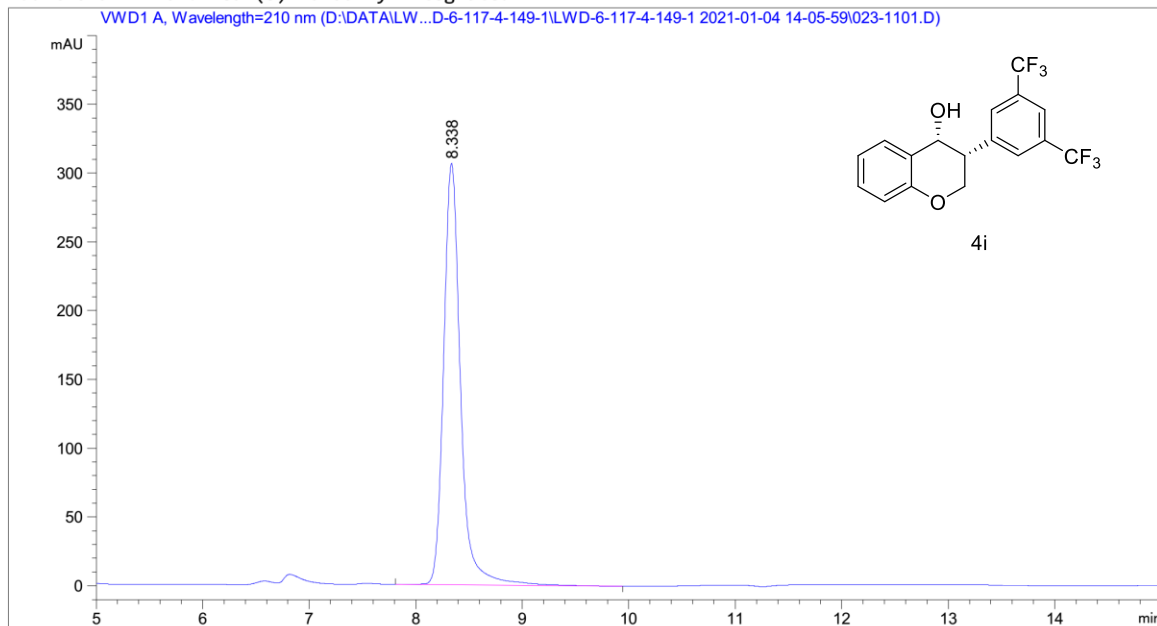
Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.337	BV	0.1673	4055.16455	371.71115	27.2967
2	8.968	VV	0.1686	4102.79590	372.29910	27.6173
3	9.586	VV	0.1811	3374.65723	283.00702	22.7159
4	10.211	VB	0.1954	3323.28735	259.49707	22.3701

Totals : 1.48559e4 1286.51434

Sample Name: LWD-6-117-4

```
=====
Acq. Operator   :                               Seq. Line :   11
Acq. Instrument : Instrument 1                   Location  : Vial 23
Injection Date  : 1/4/2021 6:00:26 PM             Inj       :    1
                                                Inj Volume: 1.000 µl
Acq. Method     : D:\DATA\LWD\LWD-6-117-4-149-1\LWD-6-117-4-149-1 2021-01-04 14-05-59\VWD-IC(
                  1-6)-95-5--0.5ML-1UL-210-25MIN.M
Last changed    : 12/31/2020 4:26:33 PM
Analysis Method : D:\METHOD\LWD\VWD-IC(1-6)-95-5--0.5ML-1UL-210-10MIN.M
Last changed    : 1/4/2021 6:56:30 PM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
=====
```



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Area Percent Report
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```

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.338	BB	0.1687	3376.16040	306.10257	100.0000

Totals : 3376.16040 306.10257

Sample Name: LWD-6-171-4

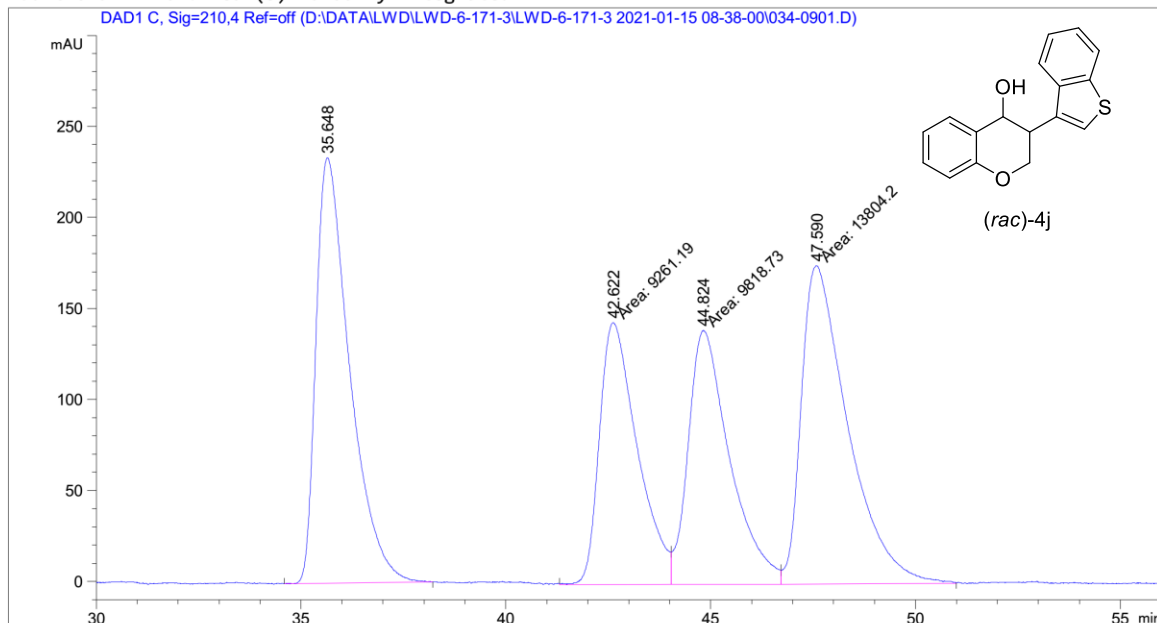
=====

Acq. Operator : Seq. Line : 9
Acq. Instrument : Instrument 2 Location : Vial 34
Injection Date : 1/15/2021 12:18:33 PM Inj : 1
Inj Volume : 3.000 µl

Acq. Method : D:\DATA\LWD\LWD-6-171-3\LWD-6-171-3 2021-01-15 08-38-00\DAD-IB(1-2)-95-5-0.
5ML-3UL-ALL-60MIN.M

Last changed : 1/15/2021 9:55:11 AM
Analysis Method : D:\METHOD\LWD\DAD-IB(1-2)-95-5-0.5ML-3UL-ALL-60MIN.M
Last changed : 1/15/2021 3:19:22 PM
(modified after loading)

Additional Info : Peak(s) manually integrated



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Area Percent Report

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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	35.648	BB	0.8394	1.33767e4	233.83585	28.9158
2	42.622	MF	1.0725	9261.18555	143.91989	20.0195
3	44.824	MF	1.1730	9818.72852	139.51012	21.2248
4	47.590	FM	1.3156	1.38042e4	174.87128	29.8399

Totals : 4.62607e4 692.13713

Data File D:\DATA\LWD\LWD-6-172-2-IB\LWD-6-172-2-IB 2021-01-17 10-11-03\074-0401.D
Sample Name: LWD-6-172-2

=====

Acq. Operator	:		Seq. Line	:	4
Acq. Instrument	:	Instrument 2	Location	:	Vial 74
Injection Date	:	1/17/2021 10:45:56 AM	Inj	:	1
			Inj Volume	:	3.000 µl

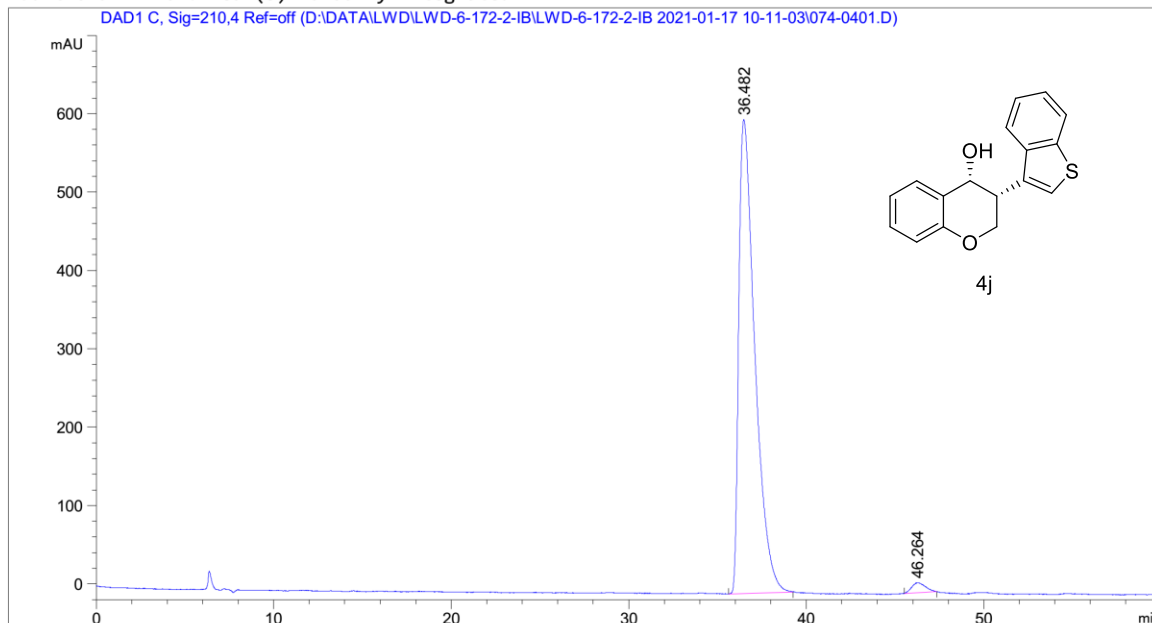
Acq. Method : D:\DATA\LWD\LWD-6-172-2-IB\LWD-6-172-2-IB 2021-01-17 10-11-03\DAD-IB(1-2)-95-5-0.5ML-3UL-ALL-60MIN.M

Last changed : 1/15/2021 9:55:11 AM

Analysis Method : D:\METHOD\LSL\DAD-OJ(1-6)-100-0-0.5ML-5UL-ALL-120MIN.M

Last changed : 1/17/2021 11:50:35 AM
(modified after loading)

Additional Info : Peak(s) manually integrated



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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	36.482	BB	0.7375	3.79268e4	604.89648	98.2258
2	46.264	BV	0.6311	685.05054	12.78541	1.7742

Totals : 3.86119e4 617.68189

VWD1 A, Wavelength=210 nm (D:\DATA\GY\TK-1-231-2\TK-1-231-2 2021-01-06 09-04-53\033-1501.D)

The chromatogram displays two distinct peaks. The first peak is at 14.980 minutes with a maximum absorbance of approximately 325 mAU. The second peak is at 23.921 minutes with a maximum absorbance of approximately 185 mAU. The baseline is stable and near zero throughout the run.

Retention Time (min)	Approximate mAU
14.980	325
23.921	185

Cc1ccc2c(c1)OC(c3ccccc3)CO2
(rac)-4k

```
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.980	BB	0.4105	8609.57129	321.47183	49.8713
2	23.921	BB	0.7190	8654.01172	184.22775	50.1287

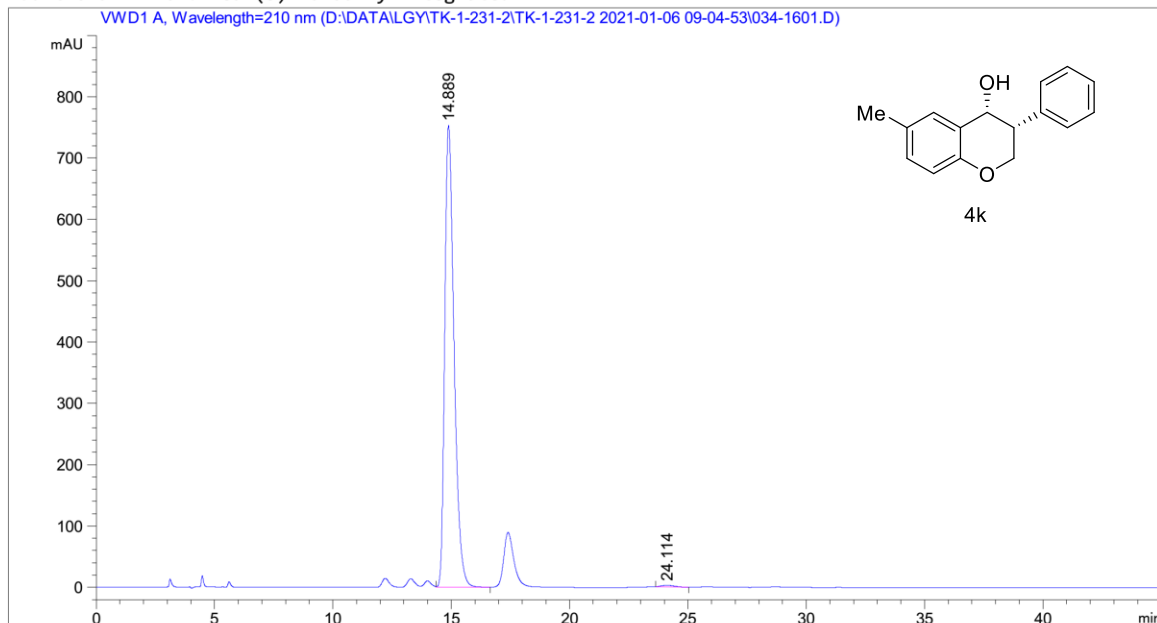
Page 1 of 2

Data File D:\DATA\LGY\TK-1-231-2\TK-1-231-2 2021-01-06 09-04-53\034-1601.D
Sample Name: LWD-6-149-10-009555

=====

Acq. Operator	:		Seq. Line	:	16
Acq. Instrument	:	Instrument 1	Location	:	Vial 34
Injection Date	:	1/6/2021 5:33:37 PM	Inj	:	1
			Inj Volume	:	2.000 µl
Acq. Method	:	D:\DATA\LGY\TK-1-231-2\TK-1-231-2 2021-01-06 09-04-53\VWD-OD(1-2)-95-5--1ML-2UL-210-45MIN.M			
Last changed	:	1/6/2021 9:44:21 AM			
Analysis Method	:	D:\METHOD\TK\VWD-OD(1-2)-97-3--0.75ML-5UL-254-10MIN.M			
Last changed	:	1/6/2021 6:54:44 PM			
		(modified after loading)			

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=210 nm

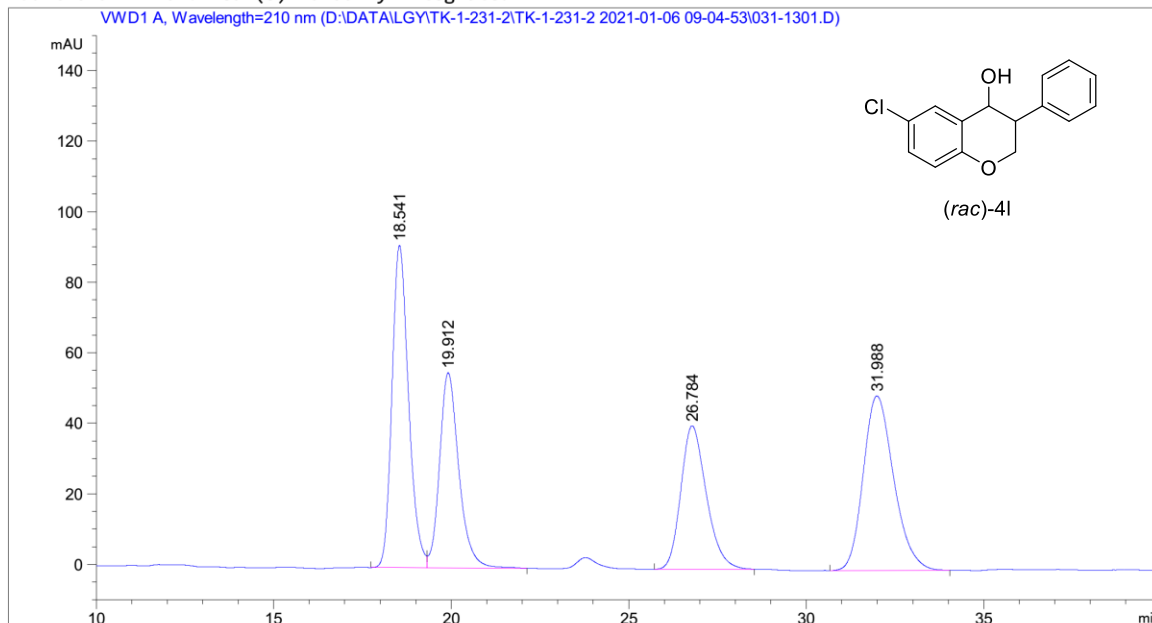
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.889	VB	0.4198	2.06305e4	752.60175	99.4894
2	24.114	BB	0.5175	105.88883	2.83658	0.5106

Totals : 2.07364e4 755.43832

Data File D:\DATA\LGY\TK-1-231-2\TK-1-231-2 2021-01-06 09-04-53\031-1301.D
Sample Name: LWD-6-238-13-RAC-OD

=====

Acq. Operator	:		Seq. Line	:	13
Acq. Instrument	:	Instrument 1	Location	:	Vial 31
Injection Date	:	1/6/2021 3:16:14 PM	Inj	:	1
			Inj Volume	:	2.000 µl
Acq. Method	:	D:\DATA\LGY\TK-1-231-2\TK-1-231-2 2021-01-06 09-04-53\VWD-OD(1-2)-95-5--1ML-2UL-210-45MIN.M			
Last changed	:	1/6/2021 9:44:21 AM			
Analysis Method	:	D:\METHOD\LWD\VWD-OD(1-2)-95-5--1ML-2UL-210-45MIN.M			
Last changed	:	1/6/2021 5:47:17 PM			
		(modified after loading)			
Additional Info : Peak(s) manually integrated					



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Area Percent Report
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Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

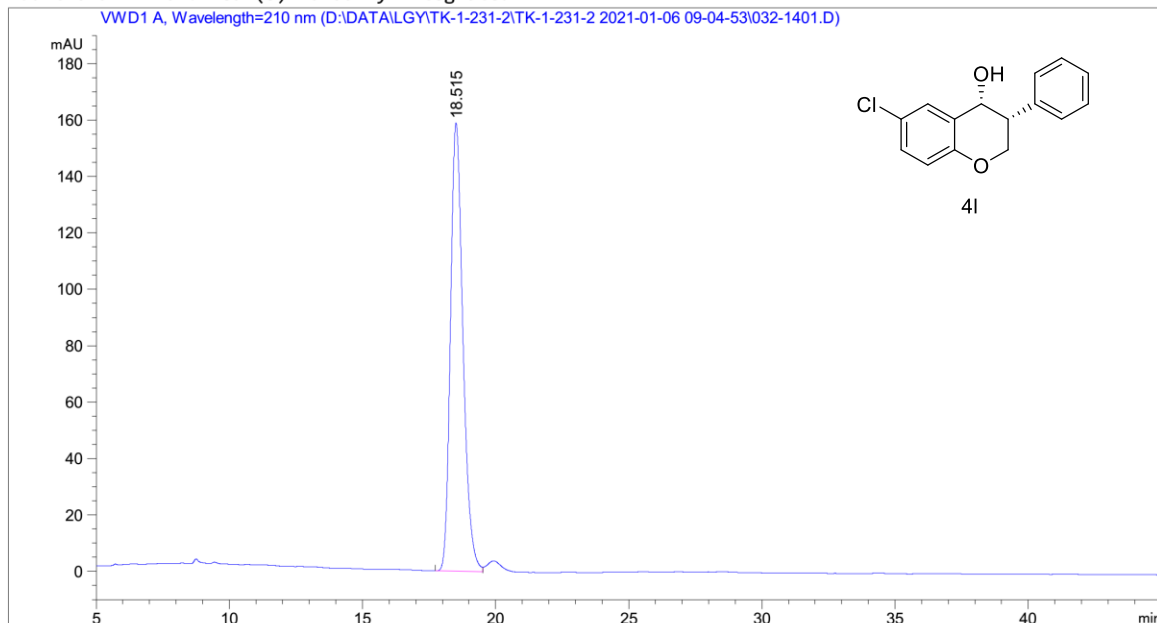
Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.541	BV	0.4990	2969.23389	91.40263	29.5607
2	19.912	VB	0.5747	2091.02563	55.35147	20.8175
3	26.784	BB	0.7610	2028.52393	40.66510	20.1953
4	31.988	BB	0.9118	2955.76465	49.48739	29.4266

Totals : 1.00445e4 236.90659

Sample Name: LWD-6-164-9

```
=====
Acq. Operator   :                               Seq. Line :   14
Acq. Instrument : Instrument 1                   Location  : Vial 32
Injection Date  : 1/6/2021 4:02:00 PM             Inj       :    1
                                                Inj Volume: 2.000 µl
Acq. Method     : D:\DATA\LGY\TK-1-231-2\TK-1-231-2 2021-01-06 09-04-53\VWD-OD(1-2)-95-5--1ML
                  -2UL-210-45MIN.M
Last changed    : 1/6/2021 9:44:21 AM
Analysis Method : D:\METHOD\LWD\VWD-OD(1-2)-95-5--1ML-2UL-210-45MIN.M
Last changed    : 1/6/2021 5:48:27 PM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
VWD1 A, Wavelength=210 nm (D:\DATA\LGY\TK-1-231-2\TK-1-231-2 2021-01-06 09-04-53\032-1401.D)
```



```
=====
Area Percent Report
=====
```

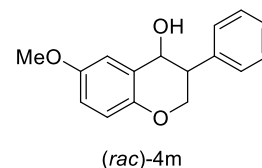
```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.515	BV	0.5012	5177.97266	158.88605	100.0000

```
Totals :                      5177.97266  158.88605
```

Additional Info : Peak(s) manually integrated

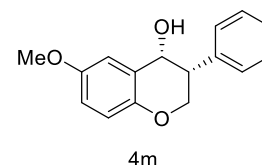


```
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.887	BV	0.2751	1.21088e4	656.65869	49.8601
2	14.680	BV	0.3939	1.21767e4	458.44376	50.1399

Page 1 of 2

Additional Info : Peak(s) manually integrated



```
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.885	BB	0.2694	7095.53418	391.65707	98.1687
2	14.913	BB	0.3032	132.36275	5.53064	1.8313

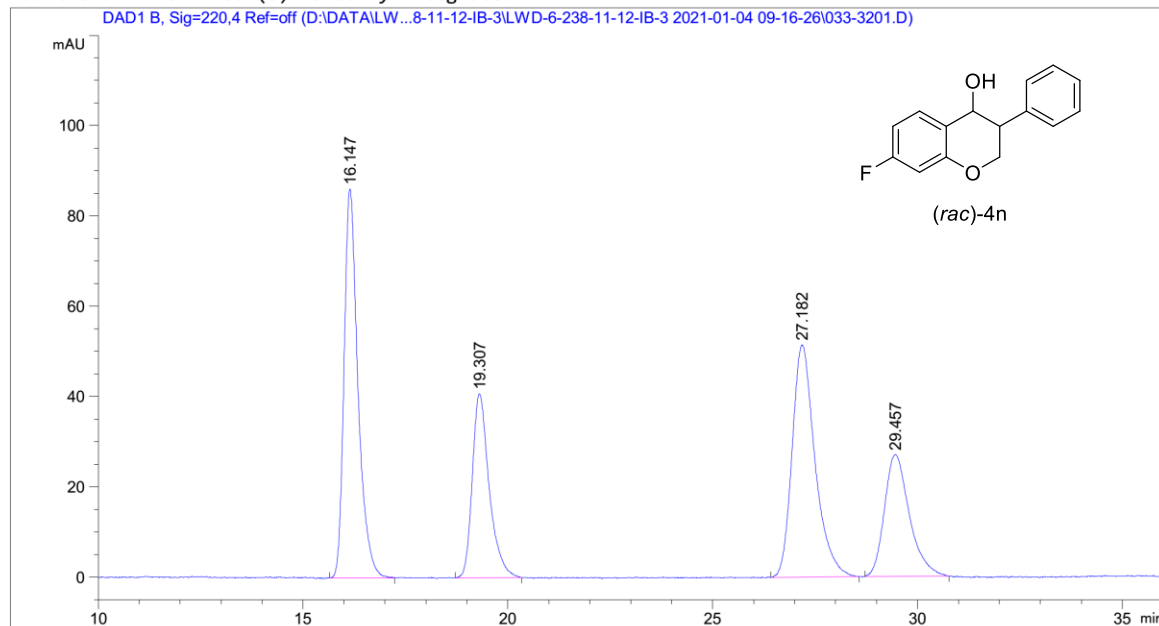
Totals :	7227.89693	397.18771
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Sample Name: LWD-6-238-20

```

=====
Acq. Operator   :                               Seq. Line :   32
Acq. Instrument : Instrument 2                  Location  : Vial 33
Injection Date  : 1/4/2021 11:50:09 PM          Inj       :    1
                                                Inj Volume : 2.000 µl

Acq. Method     : D:\DATA\LWD\LWD-6-238-11-12-IB-3\LWD-6-238-11-12-IB-3 2021-01-04 09-16-26
                  \DAD-AD(1-2)-95-5-1ML-2UL-ALL-60MIN.M
Last changed    : 1/4/2021 9:39:12 PM
Analysis Method : D:\METHOD\LWD\DAD-AD(1-2)-95-5-1ML-5UL-ALL-60MIN.M
Last changed    : 1/5/2021 8:24:57 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
  
```



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                        Area Percent Report
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```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 B, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.147	BB	0.3563	2025.76831	86.17216	31.9332
2	19.307	BB	0.4131	1170.46936	40.75436	18.4507
3	27.182	BB	0.5327	2005.71643	51.46304	31.6171
4	29.457	BB	0.5396	1141.82410	26.98804	17.9991

Totals : 6343.77820 205.37761

Data File D:\DATA\LWD\LWD-6-164\LWD-6-164 2021-01-05 14-39-14\034-0501.D
Sample Name: LWD-6-164-3

=====

Acq. Operator	:		Seq. Line	:	5
Acq. Instrument	:	Instrument 2	Location	:	Vial 34
Injection Date	:	1/5/2021 3:54:27 PM	Inj	:	1
			Inj Volume	:	3.000 µl

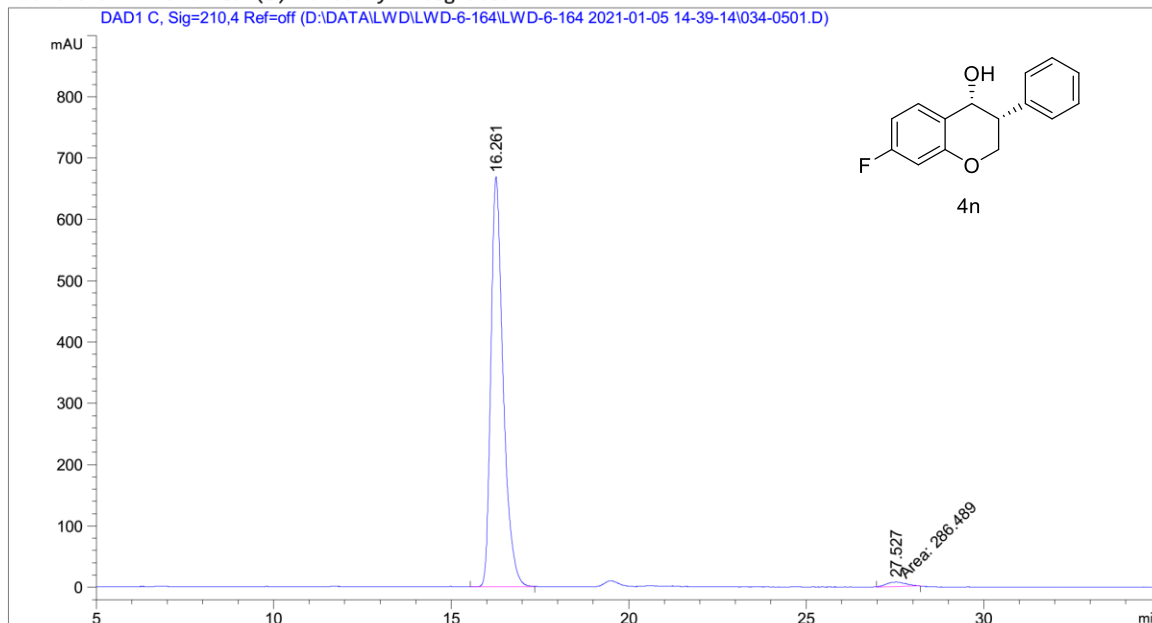
Acq. Method : D:\DATA\LWD\LWD-6-164\LWD-6-164 2021-01-05 14-39-14\DAD-AD(1-2)-95-5-1ML-3UL-ALL-35MIN.M

Last changed : 11/15/2018 8:24:06 PM

Analysis Method : D:\METHOD\LWD\DAD-IB(1-6)-80-20-1ML-3UL-ALL-10MIN.M

Last changed : 1/5/2021 4:30:44 PM
(modified after loading)

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

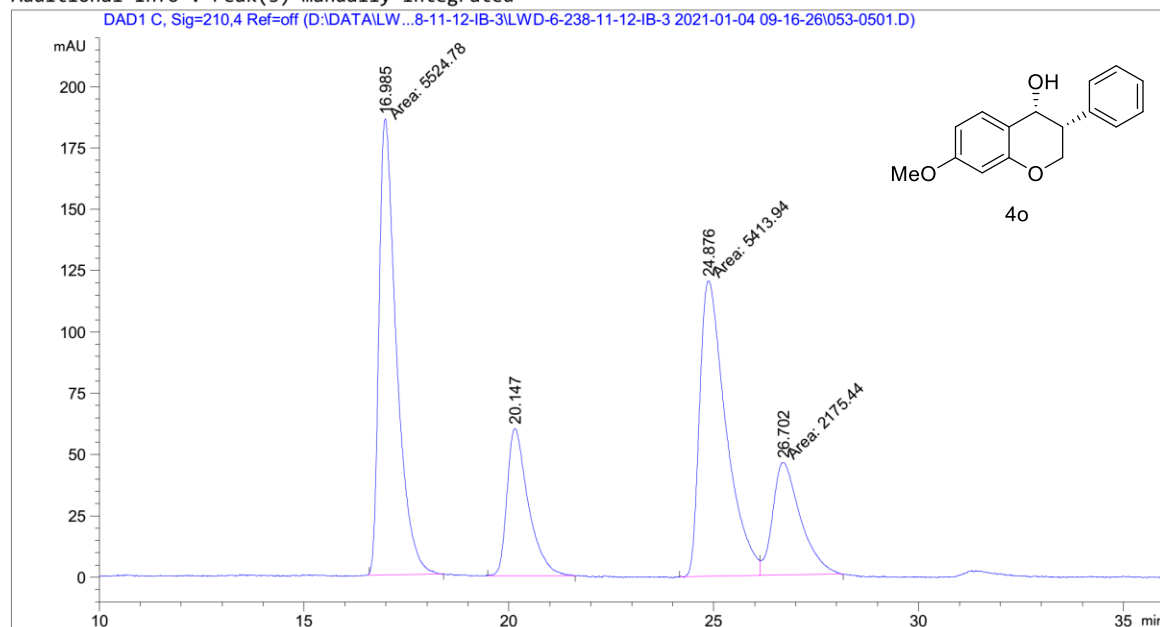
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.261	BB	0.3590	1.60957e4	668.33484	98.2512
2	27.527	MM	0.6363	286.48865	7.50443	1.7488

Totals : 1.63822e4 675.83927

```
=====
Acq. Operator   :                               Seq. Line :    5
Acq. Instrument : Instrument 2                   Location  : Vial 53
Injection Date  : 1/4/2021 11:19:48 AM          Inj       :    1
                                                Inj Volume: 3.000 µl

Acq. Method     : D:\DATA\LWD\LWD-6-238-11-12-IB-3\LWD-6-238-11-12-IB-3 2021-01-04 09-16-26
                  \DAD-IB(1-6)-95-5-1ML-3UL-ALL-60MIN.M
Last changed    : 1/4/2021 11:54:35 AM
                  (modified after loading)
Analysis Method : D:\METHOD\LWD\DAD-IB(1-6)-95-5-1ML-3UL-ALL-60MIN.M
Last changed    : 1/4/2021 11:58:39 AM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
=====
```



Area Percent Report

```
=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
=====
```

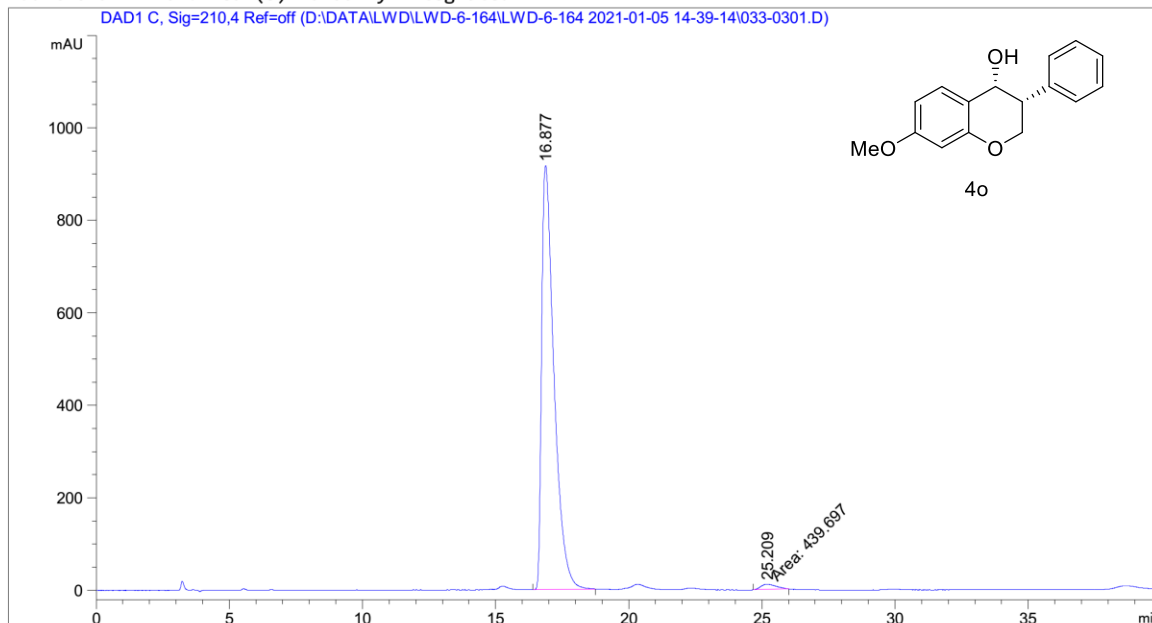
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.985	MM	0.4951	5524.77734	185.98650	36.1532
2	20.147	BB	0.4977	2167.40356	59.96283	14.1831
3	24.876	MF	0.7488	5413.94238	120.50600	35.4279
4	26.702	FM	0.7911	2175.44067	45.83366	14.2357

Data File D:\DATA\LWD\LWD-6-164\LWD-6-164 2021-01-05 14-39-14\033-0301.D
Sample Name: LWD-6-164-1

=====

Acq. Operator	:		Seq. Line	:	3
Acq. Instrument	:	Instrument 2	Location	:	Vial 33
Injection Date	:	1/5/2021 3:02:22 PM	Inj	:	1
			Inj Volume	:	3.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-6-164\LWD-6-164 2021-01-05 14-39-14\DAD-IB(1-6)-95-5-1ML-3UL-ALL-40MIN.M			
Last changed	:	1/5/2021 2:37:35 PM			
Analysis Method	:	D:\METHOD\LWD\DAD-IB(1-6)-80-20-1ML-3UL-ALL-10MIN.M			
Last changed	:	1/5/2021 4:04:56 PM			
		(modified after loading)			
Additional Info : Peak(s) manually integrated					



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=210,4 Ref=off

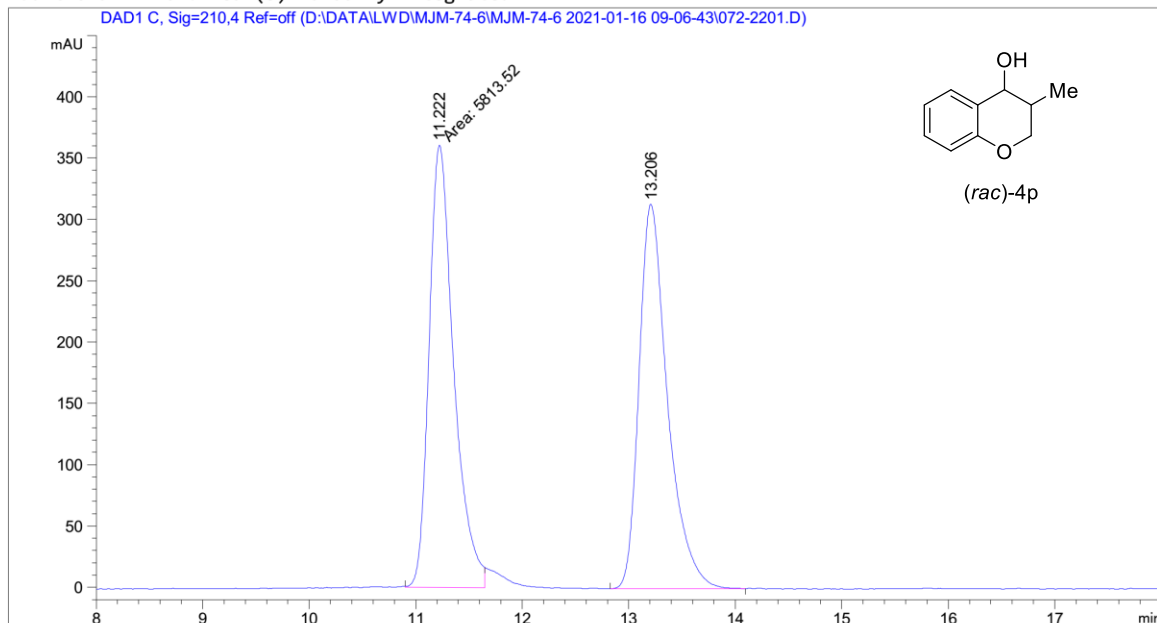
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.877	BV	0.4644	2.95906e4	917.06512	98.5358
2	25.209	MM	0.6544	439.69656	11.19787	1.4642

Totals : 3.00303e4 928.26299

Data File D:\DATA\LWD\MJM-74-6\MJM-74-6 2021-01-16 09-06-43\072-2201.D
Sample Name: LWD-6-171-10-DIAN1

=====

Acq. Operator	:		Seq. Line	:	22
Acq. Instrument	:	Instrument 2	Location	:	Vial 72
Injection Date	:	1/16/2021 9:30:45 PM	Inj	:	1
			Inj Volume	:	2.000 µl
Acq. Method	:	D:\DATA\LWD\MJM-74-6\MJM-74-6 2021-01-16 09-06-43\DAD-AD(1-2)-95-5-1ML-2UL-ALL-60MIN.M			
Last changed	:	1/4/2021 9:39:12 PM			
Analysis Method	:	D:\METHOD\LSL\DAD-OJ(1-6)-100-0-0.5ML-5UL-ALL-120MIN.M			
Last changed	:	1/17/2021 9:59:15 AM			
		(modified after loading)			
Additional Info : Peak(s) manually integrated					



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=210,4 Ref=off

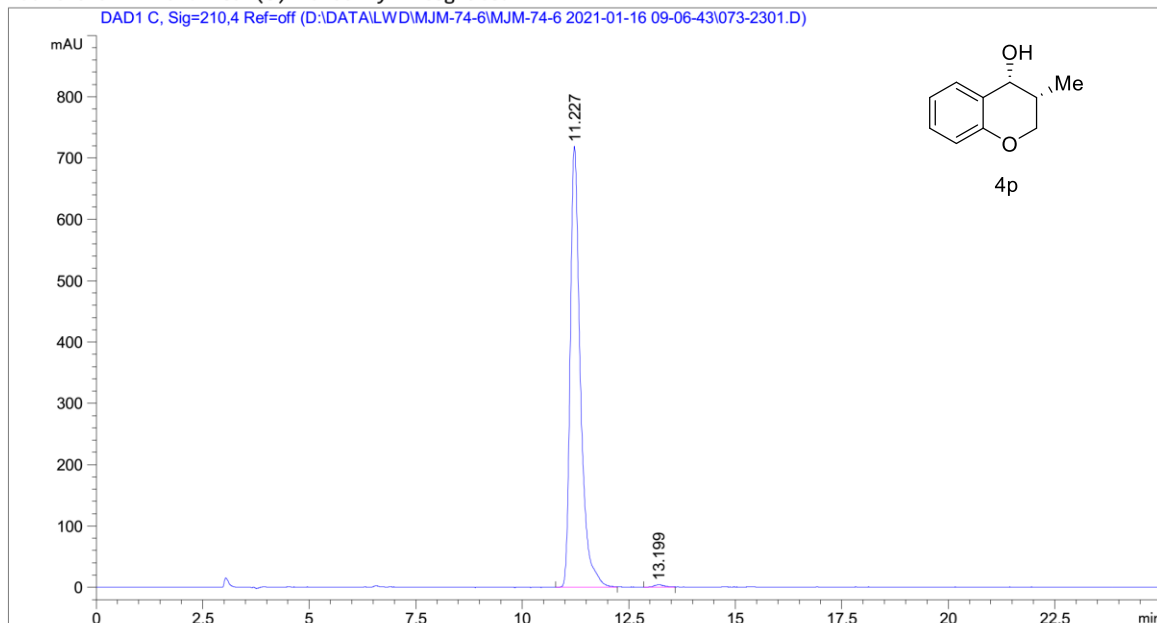
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.222	MF	0.2685	5813.52490	360.83945	49.9605
2	13.206	BB	0.2766	5822.70947	313.59488	50.0395

Totals : 1.16362e4 674.43433

Data File D:\DATA\LWD\MJM-74-6\MJM-74-6 2021-01-16 09-06-43\073-2301.D
Sample Name: LWD-6-167-12

=====

Acq. Operator	:		Seq. Line	:	23
Acq. Instrument	:	Instrument 2	Location	:	Vial 73
Injection Date	:	1/16/2021 10:31:43 PM	Inj	:	1
			Inj Volume	:	2.000 µl
Acq. Method	:	D:\DATA\LWD\MJM-74-6\MJM-74-6 2021-01-16 09-06-43\DAD-AD(1-2)-95-5-1ML-2UL-ALL-60MIN.M			
Last changed	:	1/4/2021 9:39:12 PM			
Analysis Method	:	D:\METHOD\LSL\DAD-0J(1-6)-100-0-0.5ML-5UL-ALL-120MIN.M			
Last changed	:	1/17/2021 10:00:47 AM			
		(modified after loading)			
Additional Info : Peak(s) manually integrated					



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.227	BV	0.2476	1.19373e4	719.36694	99.4027
2	13.199	BV	0.2072	71.73116	4.24284	0.5973

Totals : 1.20091e4 723.60978

Data File D:\DATA\LSL\LMZ-144-1-OD\LMZ-144-1-OD 2021-01-22 09-20-16\006-1901.D
Sample Name: LWD-6167-13-RAC

=====

Acq. Operator	:		Seq. Line	:	19
Acq. Instrument	:	Instrument 1	Location	:	Vial 6
Injection Date	:	1/22/2021 7:44:03 PM	Inj	:	1
			Inj Volume	:	3.000 µl

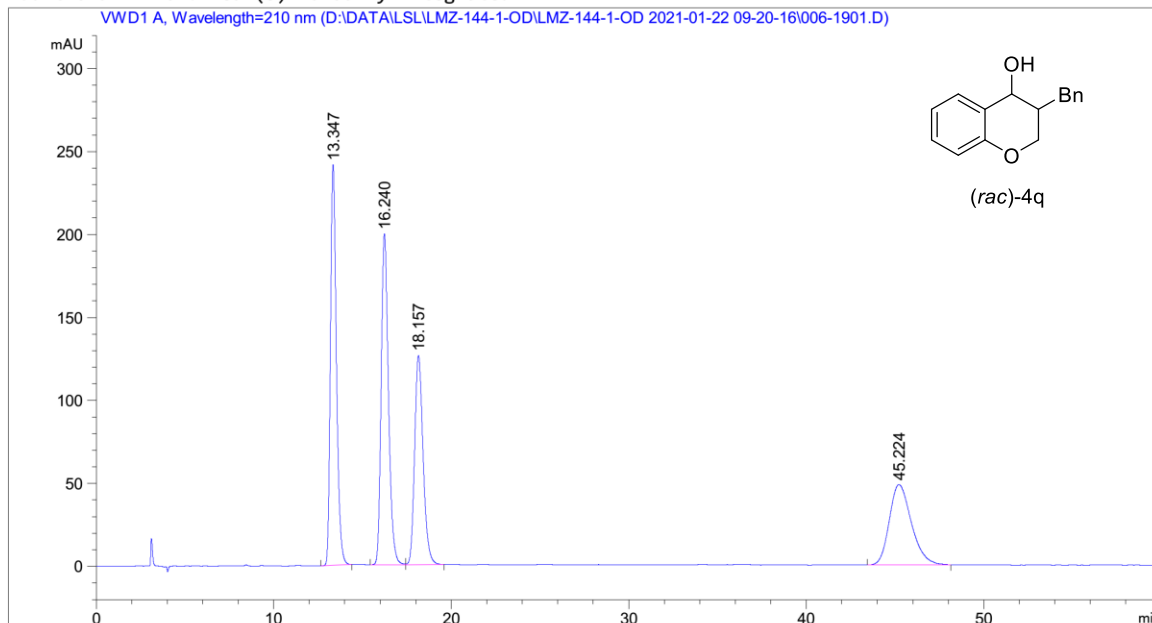
Acq. Method : D:\DATA\LSL\LMZ-144-1-OD\LMZ-144-1-OD 2021-01-22 09-20-16\VWD-OD(1-2)-95-5-1ML-3UL-210NM-60MIN.M

Last changed : 1/14/2021 10:11:39 AM

Analysis Method : D:\METHOD\LWD\VWD-OD(1-2)-97-3--1ML-3UL-210-10MIN.M

Last changed : 1/22/2021 9:19:43 PM
(modified after loading)

Additional Info : Peak(s) manually integrated



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=210 nm

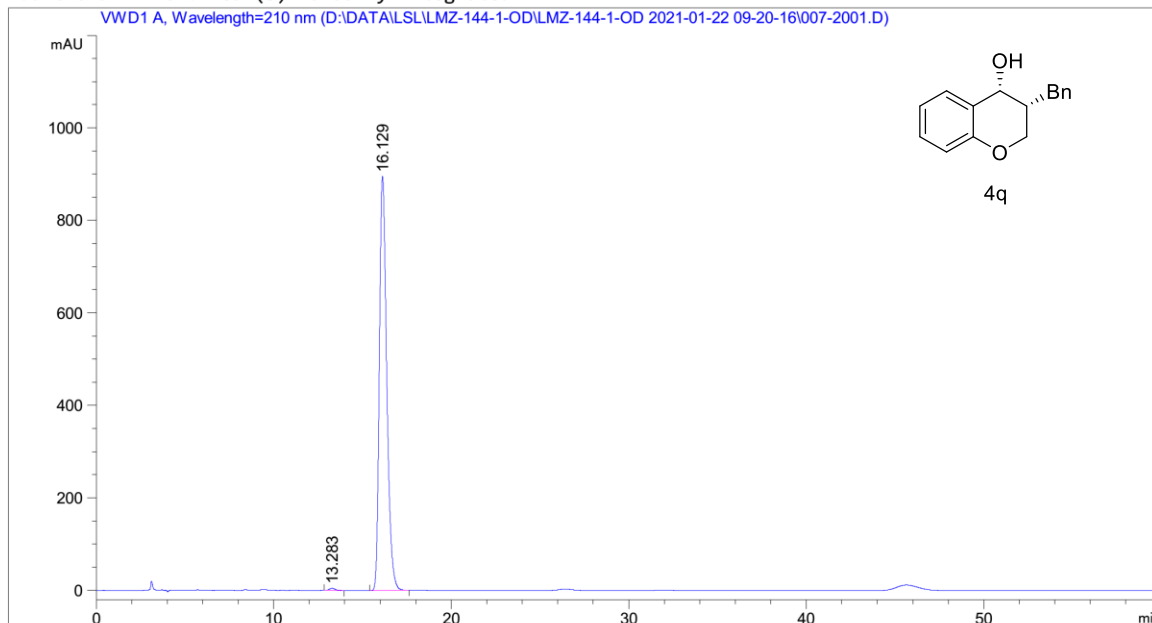
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.347	BB	0.3590	5651.01904	241.46303	28.7214
2	16.240	BV	0.4358	5668.40869	199.33913	28.8098
3	18.157	VB	0.5116	4184.05420	125.94888	21.2655
4	45.224	BB	1.3251	4171.80762	48.37503	21.2033

Totals : 1.96753e4 615.12606

Data File D:\DATA\LSL\LMZ-144-1-OD\LMZ-144-1-OD 2021-01-22 09-20-16\007-2001.D
Sample Name: LWD-6167-13-EE

```
=====
Acq. Operator   :                               Seq. Line :   20
Acq. Instrument : Instrument 1                   Location  : Vial 7
Injection Date  : 1/22/2021 8:44:53 PM           Inj       :    1
                                                Inj Volume: 3.000 µl

Acq. Method     : D:\DATA\LSL\LMZ-144-1-OD\LMZ-144-1-OD 2021-01-22 09-20-16\VWD-OD(1-2)-95-5-
                  1ML-3UL-210NM-60MIN.M
Last changed    : 1/14/2021 10:11:39 AM
Analysis Method : D:\METHOD\LWD\VWD-OD(1-2)-97-3--1ML-3UL-210-10MIN.M
Last changed    : 1/22/2021 9:52:10 PM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
=====
```



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=210 nm

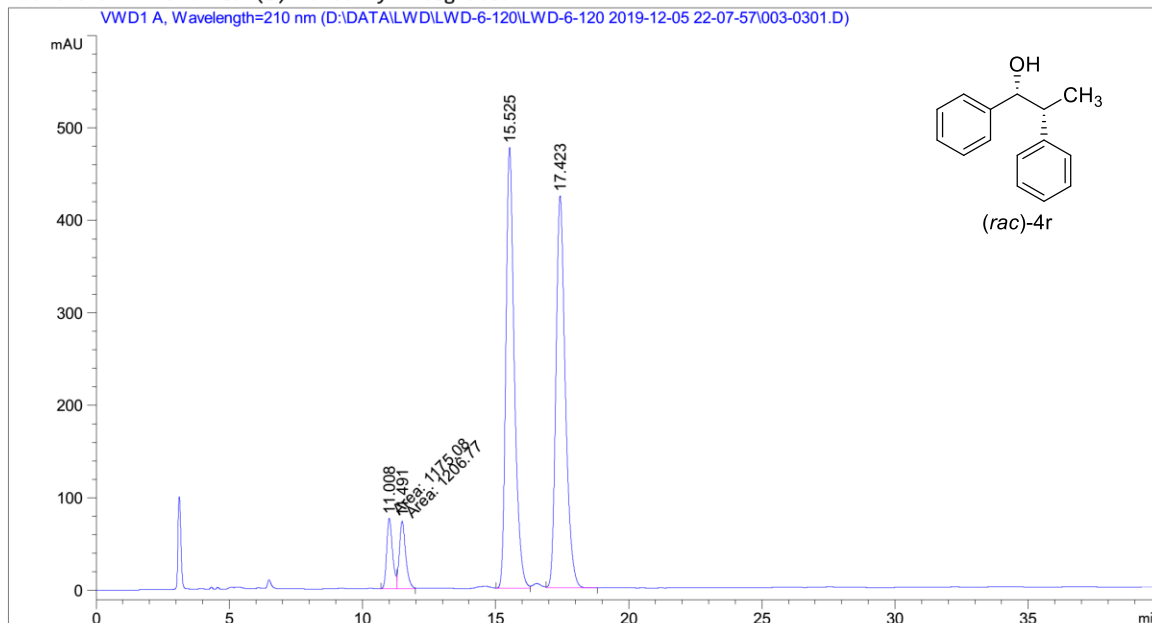
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.283	BB	0.3508	104.81422	4.56545	0.4042
2	16.129	BB	0.4437	2.58238e4	894.81628	99.5958

Totals : 2.59286e4 899.38173

Data File D:\DATA\LWD\LWD-6-120\LWD-6-120 2019-12-05 22-07-57\003-0301.D
Sample Name: LWD-6-120-RAC

```
=====
Acq. Operator   :                               Seq. Line :    3
Acq. Instrument : Instrument 1                   Location  : Vial 3
Injection Date  : 12/5/2019 10:31:58 PM          Inj       :    1
                                                Inj Volume : 3.000 µl

Acq. Method     : D:\DATA\LWD\LWD-6-120\LWD-6-120 2019-12-05 22-07-57\VWD-AD(1-2)-95-5-1ML-
                  3UL-210NM-60MIN.M
Last changed    : 9/3/2018 10:35:53 AM
Analysis Method : D:\METHOD\LSL\DAD-OD(1-2)-95-5-1ML-5UL-ALL-20MIN.M
Last changed    : 12/6/2019 9:01:24 AM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
=====
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: VWD1 A, Wavelength=210 nm

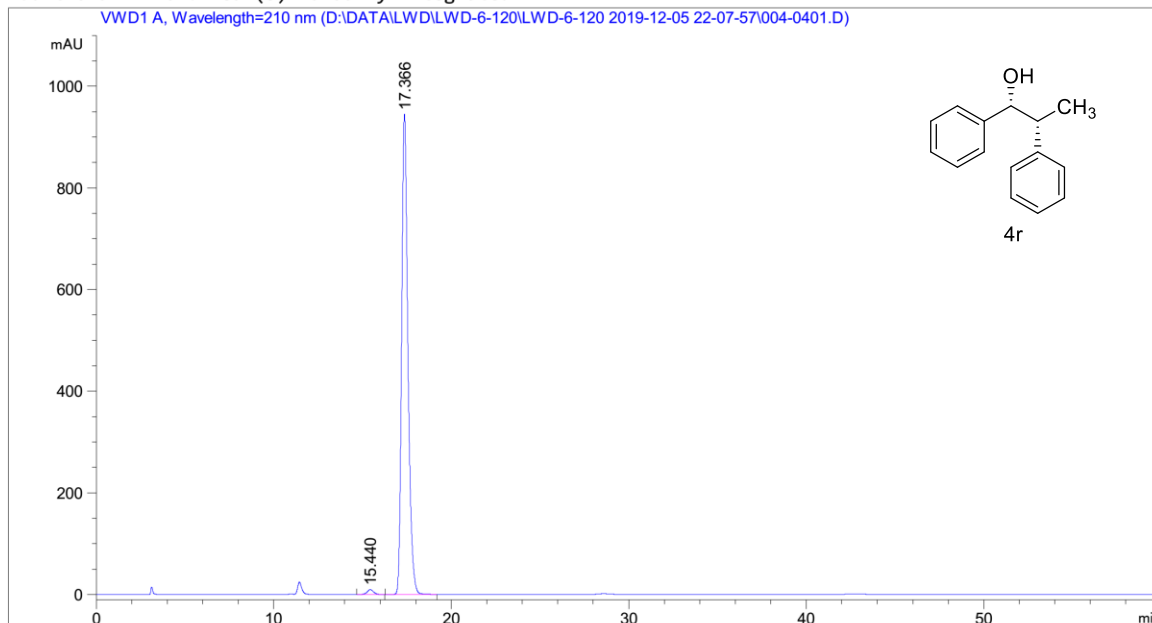
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.008	MF	0.2575	1175.08167	76.06036	5.0613
2	11.491	FM	0.2757	1206.76550	72.95611	5.1977
3	15.525	BV	0.3313	1.04668e4	476.36560	45.0825
4	17.423	VB	0.3705	1.03684e4	423.66904	44.6585

Totals : 2.32171e4 1049.05111

Data File D:\DATA\LWD\LWD-6-120\LWD-6-120 2019-12-05 22-07-57\004-0401.D
Sample Name: LWD-6-120

=====

Acq. Operator	:		Seq. Line	:	4
Acq. Instrument	:	Instrument 1	Location	:	Vial 4
Injection Date	:	12/5/2019 11:32:47 PM	Inj	:	1
			Inj Volume	:	3.000 µl
Acq. Method	:	D:\DATA\LWD\LWD-6-120\LWD-6-120 2019-12-05 22-07-57\VWD-AD(1-2)-95-5-1ML-3UL-210NM-60MIN.M			
Last changed	:	9/3/2018 10:35:53 AM			
Analysis Method	:	D:\METHOD\LSL\DAD-OD(1-2)-95-5-1ML-5UL-ALL-20MIN.M			
Last changed	:	12/6/2019 9:02:47 AM			
		(modified after loading)			
Additional Info : Peak(s) manually integrated					



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: VWD1 A, Wavelength=210 nm

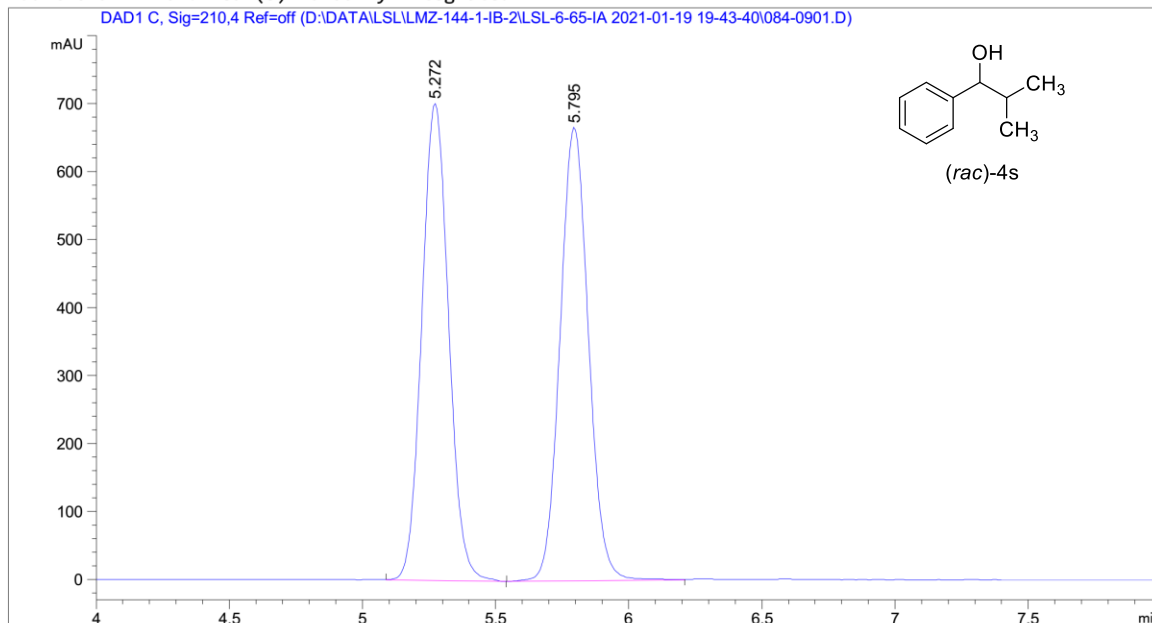
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.440	BB	0.3668	242.16133	9.85193	1.0305
2	17.366	BB	0.3731	2.32566e4	944.95715	98.9695

Totals : 2.34988e4 954.80908

Data File D:\DATA\LSL\LMZ-144-1-IB-2\LSL-6-65-IA 2021-01-19 19-43-40\084-0901.D
Sample Name: LWD-6-171-13-RAC

=====

Acq. Operator	:		Seq. Line	:	9
Acq. Instrument	:	Instrument 2	Location	:	Vial 84
Injection Date	:	1/19/2021 10:54:13 PM	Inj	:	1
			Inj Volume	:	3.000 µl
Acq. Method	:	D:\DATA\LSL\LMZ-144-1-IB-2\LSL-6-65-IA 2021-01-19 19-43-40\DAD-IC(1-2)-95-5-1ML-3UL-ALL-20MIN.M			
Last changed	:	1/18/2021 8:54:41 AM			
Analysis Method	:	D:\METHOD\LWD\DAD-IA(1-6)-95-5-1ML-2UL-ALL-10MIN.M			
Last changed	:	1/20/2021 8:53:28 AM			
		(modified after loading)			
Additional Info : Peak(s) manually integrated					



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

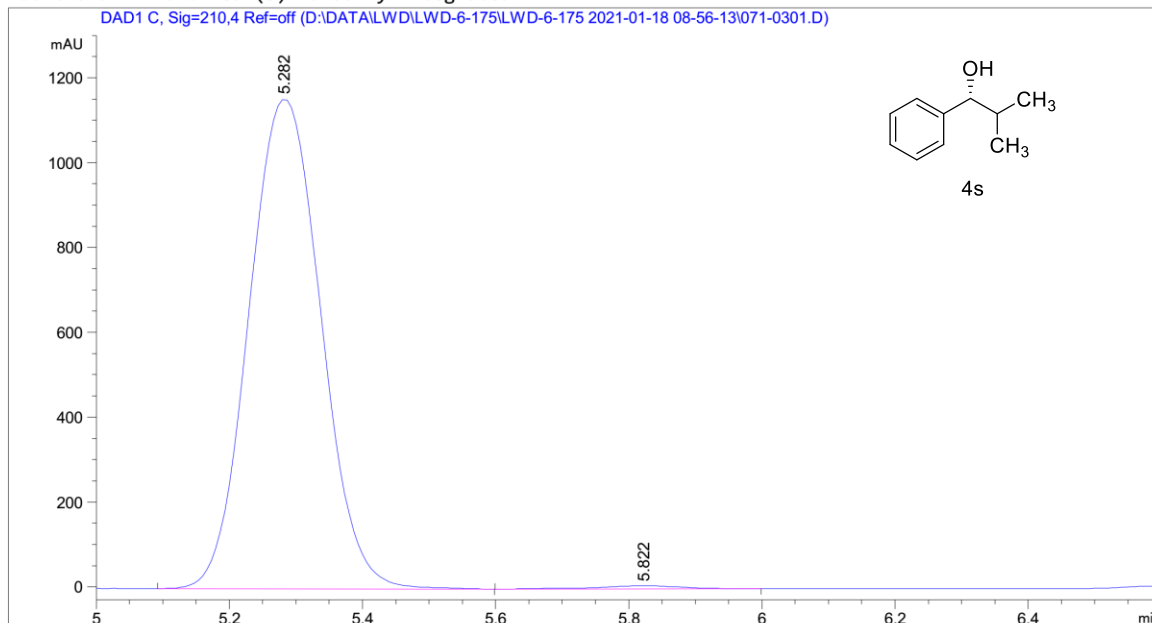
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.272	VB	0.1094	4901.08301	702.11841	49.7264
2	5.795	BV	0.1166	4955.01270	667.40308	50.2736

Totals : 9856.09570 1369.52148

Data File D:\DATA\LWD\LWD-6-175\LWD-6-175 2021-01-18 08-56-13\071-0301.D
Sample Name: LWD-6-175-1

```
=====
Acq. Operator   :                               Seq. Line :    3
Acq. Instrument : Instrument 2                   Location  : Vial 71
Injection Date  : 1/18/2021 9:20:04 AM           Inj       :    1
                                                Inj Volume : 3.000 µl
Acq. Method     : D:\DATA\LWD\LWD-6-175\LWD-6-175 2021-01-18 08-56-13\DAD-IC(1-2)-95-5-1ML-
                  3UL-ALL-20MIN.M
Last changed    : 1/18/2021 8:54:41 AM
Analysis Method : D:\METHOD\LWD\DAD-IA(1-6)-95-5-1ML-2UL-ALL-10MIN.M
Last changed    : 1/19/2021 8:23:04 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
DAD1 C, Sig=210,4 Ref=off (D:\DATA\LWD\LWD-6-175\LWD-6-175 2021-01-18 08-56-13\071-0301.D)
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

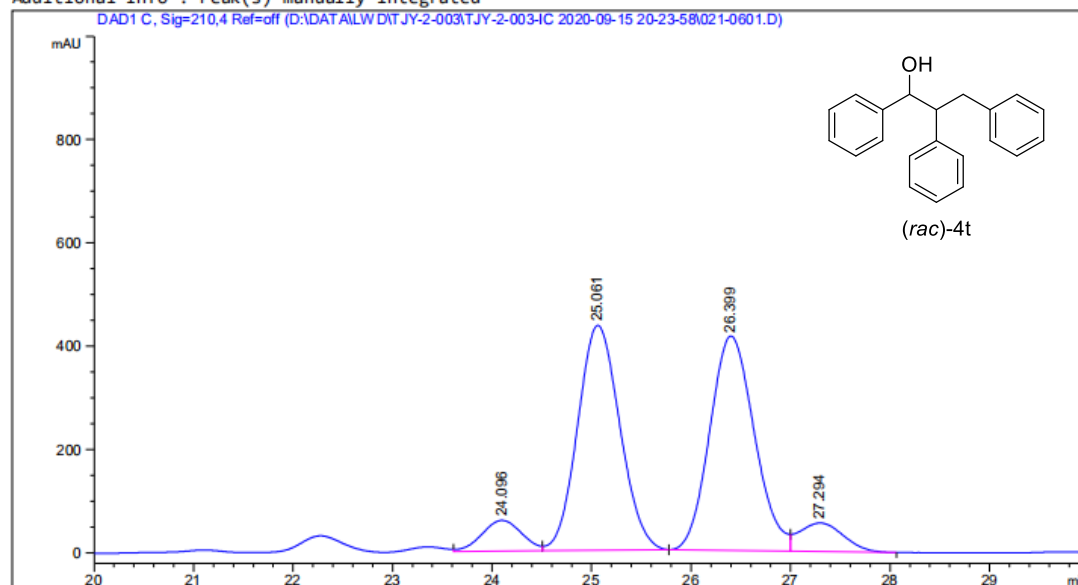
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.282	BB	0.1192	8634.29688	1154.75830	99.2365
2	5.822	BB	0.1325	66.42905	7.41661	0.7635

Totals : 8700.72592 1162.17491

Acq. Operator : Seq. Line : 6
 Acq. Instrument : Instrument 2 Location : Vial 21
 Injection Date : 9/15/2020 10:50:09 PM Inj : 1
 Inj Volume : 2.000 µl
 Acq. Method : D:\DATA\LWD\TJY-2-003\TJY-2-003-IC 2020-09-15 20-23-58\DAD-IC(1-6)-98-2-0.
 SML-2UL-ALL-80MIN.M
 Last changed : 9/10/2020 8:49:16 AM
 Analysis Method : D:\METHOD\LYH\DAD-OD(1-2)-90-10-0.5ML-1UL-ALL-60MIN.M
 Last changed : 9/16/2020 10:16:57 AM
 (modified after loading)

Additional Info : Peak(s) manually integrated



Area Percent Report

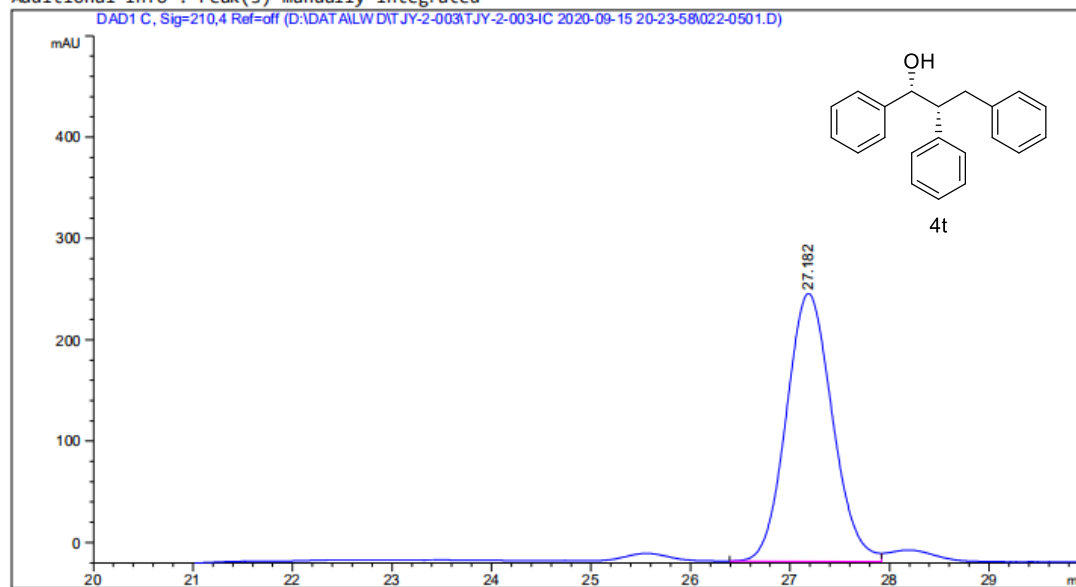
Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.096	VV	0.4422	1667.80310	59.65076	5.7262
2	25.061	VB	0.4595	1.28238e4	435.51529	44.0286
3	26.399	BV	0.4835	1.29255e4	414.85364	44.3777
4	27.294	VB	0.4720	1708.95447	55.37924	5.8675

Acq. Operator : Seq. Line : 5
 Acq. Instrument : Instrument 2 Location : Vial 22
 Injection Date : 9/15/2020 9:29:11 PM Inj : 1
 Inj Volume : 2.000 µl
 Acq. Method : D:\DATA\LWD\TJY-2-003\TJY-2-003-IC 2020-09-15 20-23-58\DAD-IC(1-6)-98-2-0.
 5ML-2UL-ALL-80MIN.M
 Last changed : 9/10/2020 8:49:16 AM
 Analysis Method : D:\METHOD\LYH\DAD-OD(1-2)-90-10-0.5ML-1UL-ALL-60MIN.M
 Last changed : 9/16/2020 10:24:35 AM
 (modified after loading)

Additional Info : Peak(s) manually integrated



Area Percent Report

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

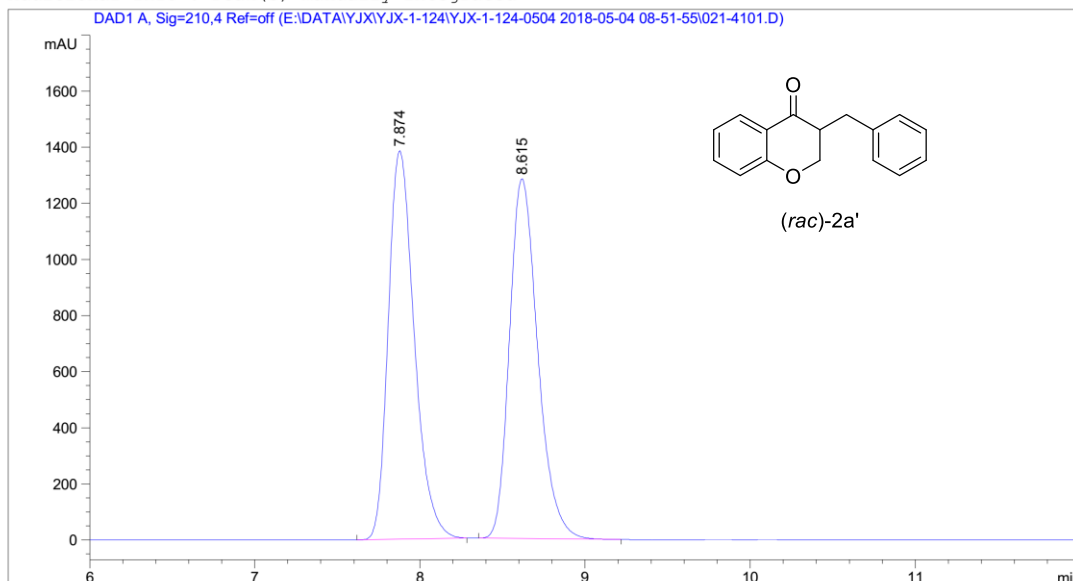
Signal 1: DAD1 C, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	27.182	BV	0.4978	8464.92480	264.18637	100.0000

Totals : 8464.92480 264.18637

Data File E:\DATA\YJX\YJX-1-124\YJX-1-124-0504 2018-05-04 08-51-55\021-4101.D
Sample Name: LWD-4-37-1

```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   41
Acq. Instrument : 1260HPLC-DAD                Location  : Vial 21
Injection Date  : 5/5/2018 10:45:21 AM        Inj       :    1
                                           Inj Volume: 3.000 µl
Acq. Method     : E:\DATA\YJX\YJX-1-124\YJX-1-124-0504 2018-05-04 08-51-55\
DAD-OD(1-2)-95-5-1ML-3UL-ALL-15MIN.M
Last changed    : 5/5/2018 10:15:59 AM by SYSTEM
Analysis Method : E:\DATA\YJX\YJX-1-124\YJX-1-124-0504 2018-05-04 08-51-55\
DAD-OD(1-2)-95-5-1ML-3UL-ALL-15MIN.M (Sequence Method)
Last changed    : 7/27/2018 11:46:37 AM by SYSTEM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
DAD1 A, Sig=210,4 Ref=off (E:\DATA\YJX\YJX-1-124\YJX-1-124-0504 2018-05-04 08-51-55\021-4101.D)
```



Area Percent Report

```
=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs
```

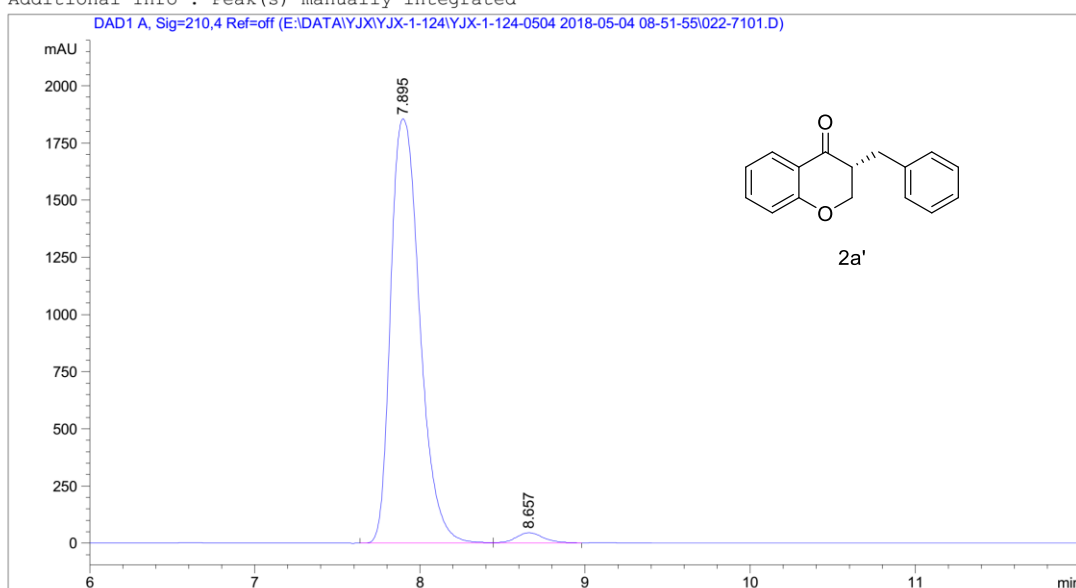
Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.874	BB	0.1696	1.51469e4	1384.87122	49.8046
2	8.615	BB	0.1848	1.52657e4	1282.89966	50.1954

Totals : 3.04126e4 2667.77087

Data File E:\DATA\YJX\YJX-1-124\YJX-1-124-0504 2018-05-04 08-51-55\022-7101.D
Sample Name: LWD-4-35-2

```
=====
Acq. Operator   : SYSTEM                      Seq. Line :   71
Acq. Instrument : 1260HPLC-DAD                Location  : Vial 22
Injection Date  : 5/6/2018 3:17:56 AM          Inj       :    1
                                           Inj Volume: 3.000 µl
Acq. Method     : E:\DATA\YJX\YJX-1-124\YJX-1-124-0504 2018-05-04 08-51-55\DAD-OD(1-2)-95-5-
                  1ML-3UL-ALL-15MIN.M
Last changed    : 5/5/2018 10:15:59 AM by SYSTEM
Analysis Method : E:\DATA\YJX\YJX-1-124\YJX-1-124-0504 2018-05-04 08-51-55\DAD-OD(1-2)-95-5-
                  1ML-3UL-ALL-15MIN.M (Sequence Method)
Last changed    : 7/27/2018 11:47:23 AM by SYSTEM
                  (modified after loading)
Additional Info  : Peak(s) manually integrated
DAD1 A, Sig=210,4 Ref=off (E:\DATA\YJX\YJX-1-124\YJX-1-124-0504 2018-05-04 08-51-55\022-7101.D)
```



Area Percent Report

```
=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs
```

Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.895	BV	0.1907	2.26907e4	1855.42444	97.6244
2	8.657	VV	0.1849	552.16425	45.72316	2.3756

Totals : 2.32429e4 1901.14760

WVD1 A, Wavelength=210 nm (D:\DATA\LWD\LWD-4-101-6-RAC\LWD-4-101-6-RAC 2018-07-24 20-43-01\031-0301.D)

Chromatogram showing four peaks at retention times 28.248, 29.997, 35.508, and 40.655 minutes. The y-axis is labeled mAU (milliabsorbance units) and ranges from 0 to 100. The x-axis represents time in minutes, ranging from 26 to 42. A chemical structure of (rac)-2x is shown in the top right corner.

Chemical structure of (rac)-2x:

COc1ccc(cc1COC2=CC=C(C=C2)OC3=CC=CC=C3OC4=CC=CC=C4)C(=O)OC

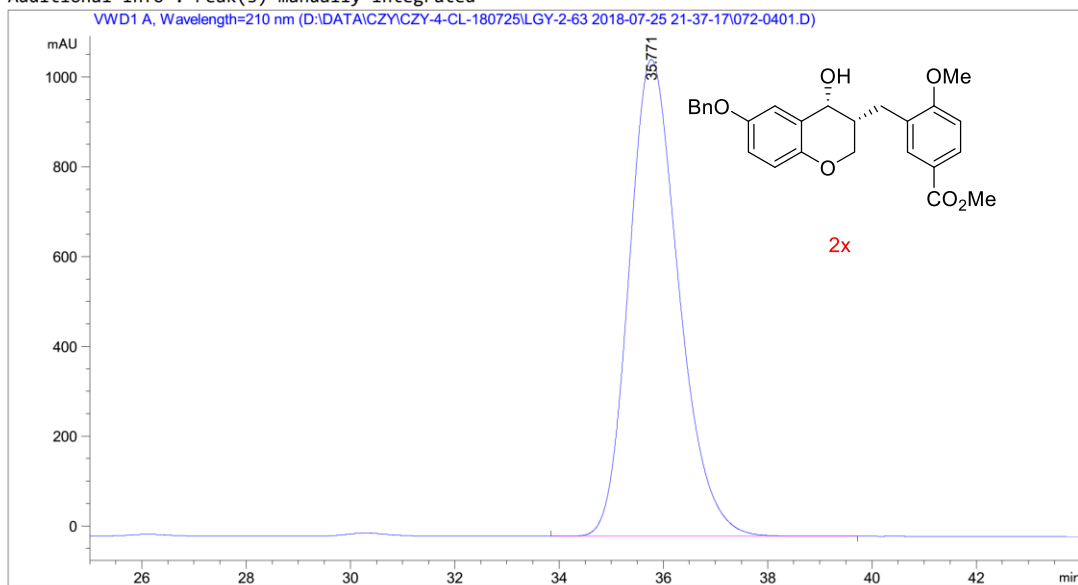
(rac)-2x

```
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	28.248	BV	0.7821	5942.21094	117.09351	24.2602
2	29.997	VB	0.8449	5945.02393	107.04466	24.2717
3	35.508	BB	0.9988	6506.79639	99.78468	26.5652
4	40.655	BB	1.1595	6099.63574	81.98985	24.9029

Data File D:\DATA\CZY\CZY-4-CL-180725\LGY-2-63 2018-07-25 21-37-17\072-0401.D
Sample Name: LWD-4-100-5-100-6

```
=====
Acq. Operator   :                               Seq. Line :    4
Acq. Instrument : Instrument 1                   Location  : Vial 72
Injection Date  : 7/25/2018 11:00:52 PM          Inj       :    1
                                                Inj Volume: 3.000 µl
Acq. Method     : D:\DATA\CZY\CZY-4-CL-180725\LGY-2-63 2018-07-25 21-37-17\VWD-AD(1-2)-80-20-
                  1ML-3UL-210NM-60MIN.M
Last changed    : 7/24/2018 8:42:32 PM
Analysis Method : D:\METHOD\CZY\DAD-OD(1-2)-98-2-1ML-3UL-ALL-30MIN.M
Last changed    : 7/27/2018 12:02:34 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Area Percent Report

```
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```

Signal 1: VWD1 A, Wavelength=210 nm

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	35.771	BB	1.0189	7.04453e4	1062.01050	100.0000

Totals : 7.04453e4 1062.01050

IV. Reference

- 1 X. Zong, J. Cai, J. Chen, C. Sun, L. Li and M. Ji, *RSC Adv.*, 2015, **5**, 24814-24823.
- 2 A. Riahi, C. Thorey, F. Hénin and J. Muzart, *Synth. Commun.*, 1998, **28**, 4339-4344.
- 3 (a) R. B. Gammill, *Synthesis*, 1979, **11**, 901-903; (b) G. Priyadarshani, S. Amrutkar, A. Nayak, U. C. Banerjee, C. N. Kundu and S. K. Guchhait, *Eur. J. Med. Chem.*, 2016, **122**, 43-54.
- 4 P. Bichovski, T. M. Haas, D. Kratzert and J. Streuff, *Chemistry* 2015, **21**, 2339-2342.
- 5 T. Patonay, Z. Dinya, A. Levai and D. Molnar, *Tetrahedron* 2001, **57**, 2895-2907.
- 6 Z. Zhao, P. R. Bagdi, S. Yang, J. Liu, W. Xu and X. Fang, *Org. Lett.*, 2019, **21**, 5491-5494.
- 7 J. A. R. Rodrigues, E. P. Siqueira-Filho, M. d. Mancilha and P. J. S. Moran, *Synth. Commun.*, 2003, **33**, 331-340.
- 8 J.-P. Wan, Z. Tu and Y. Wang, *Chem. Eur. J.*, 2019, **25**, 6907-6910.
- 9 D. A. Vasselin, A. D. Westwell, C. S. Matthews, T. D. Bradshaw and M. F. G. Stevens, *J. Med. Chem.*, 2006, **49**, 3973-3981.
- 10 Y. Hoshino, N. Miyaura and A. Suzuki, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 3008-3010.
- 11 A. E. Nibbs, A. L. Baize, R. M. Herter and K. A. Scheidt, *Org. Lett.*, 2009, **11**, 4010-4013.
- 12 X. Zhao, J. Zhou, S. Lin, X. Jin and R. Liu, *Org. Lett.*, 2017, **19**, 976-979.
- 13 O. V. Zatolochnaya, S. Rodríguez, Y. Zhang, K. S. Lao, S. Tcyrulnikov, G. Li, X.-J. Wang, B. Qu, S. Biswas, H. P. R. Mangunuru, D. Rivalti, J. D. Sieber, J.-N. Desrosiers, J. C. Leung, N. Grinberg, H. Lee, N. Haddad, N. K. Yee, J. J. Song, M. C. Kozlowski and C. H. Senanayake, *Chem. Sci.*, 2018, **9**, 4505-4510.
- 14 J. Tsoung, K. Krämer, A. Zajdlík, C. Liébert and M. Lautens, *J. Org. Chem.*, 2011, **76**, 9031-9045.
- 15 K. Fujita, C. Asai, T. Yamaguchi, F. Hanasaka and R. Yamaguchi, *Org. Lett.*, 2005, **7**, 4017-4019.
- 16 L. Fang, S. Liu, L. Han, H. Li and F. Zhao, *Organometallics* 2017, **36**, 1217-1219.
- 17 T. Qin and P. Metz, *Org. Lett.*, 2017, **19**, 2981-2984.
- 18 R. Fernandez, A. Ros, A. Magriz, H. Dietrich and J. M. Lassaletta, *Tetrahedron* 2007, **63**, 6755-6763.
- 19 J. S. Bandar, E. Ascic and S. L. Buchwald, *J. Am. Chem. Soc.*, 2016, **138**, 5821-5824.
- 20 W. Wu, S. Liu, M. Duan, X. Tan, C. Chen, Y. Xie, Y. Lan, X. Q. Dong and X. Zhang, *Org. Lett.*, 2016, **18**, 2938-2941.
- 21 T. Miura, O. Kose, F. Li, S. Kai and S. Saito, *Chem. Eur. J.*, 2011, **17**, 11146-11151.
- 22 C. Conti and N. Desideri, *Biorg. Med. Chem.*, 2009, **17**, 3720-3727.

- 23 M. Kawasaki, N. Toyooka, Y. Matsui, A. Tanaka, M. Goto, H. Kakuda, S. Kawabata and T. Kometani, *Heterocycles* 2005, **65**, 761-765.
- 24 J. P. Wan, Z. Tu and Y. Wang, *Chem. Eur. J.*, 2019, **25**, 6907-6910.
- 25 R. J. Chambers, A. Marfat, G. W. Antognoli, J. B. Cheng, D. B. Damon, A. V. Kuperman, T. C. Liston, C. Mebus, J. S. Pillar, J. T. Shirley and J. W. Watson, *Bioorg. Med. Chem. Lett.*, 1999, **9**, 2773-2778
- 26 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams; F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Gaussian 16* Wallingford, CT, 2016.
- 27 (a) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456-1465; (b) B. Miehlich, A. Savin, H. Stoll and H. Preuss, *Chem. Phys. Lett.*, 1989, **157**, 200-206; (c) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B* 1988, **37**, 785-789; (d) A. D. Becke, *J. Chem. Physics.*, 1993, **98**, 5648-5652.
- 28 (a) M. Dolg, U. Wedig, H. Stoll and H. Preuss, *J. Chem. Physics.*, **1987**, **86**, 866-872; (b) D. Andrae, U. Häußermann, M. Dolg, H. Stoll and H. Preuß, *Theor. Chem. Acc.*, 1990, **77**, 123-141.
- 29 (a) G. A. Petersson, A. Bennett, T. G. Tensfeldt, M. A. Al-Laham, W. A. Shirley and J. Mantzaris, *J. Chem. Physics.*, 1988, **89**, 2193-2218; (b) G. A. Petersson and M. A. Al-Laham, *J. Chem. Physics.*, 1991, **94**, 6081-6090; (c) T. Clark, J. Chandrasekhar, G. W. Spitznagel and P. V. R. Schleyer, Efficient diffuse function-augmented basis sets for anion calculations. III. The 3-21+G basis set for first-row elements, Li-F. 1983, **4**, 294-301.
- 30 A. Ehlers, M. Böhme, S. Dapprich, A. Gobbi, A. Höllwarth, V. Jonas, K. Köhler, R. Stegmann, A. Veldkamp and G. Frenking, *Chem. Phys. Lett.*, 1993, **208**, 111-114.
- 31 K. Fukui, *Acc. Chem. Res.*, 1981, **14**, 363-368.
- 32 A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B* 2009, **113**, 6378-6396.