Supporting Information

An organocatalytic approach for assembling flavanones *via* a cascade 1,4-conjugate addition/*oxa*-Michael addition between propargylamines with water

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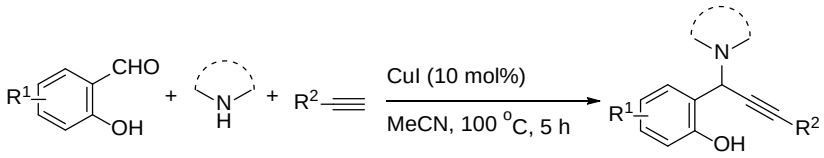
1. General consideration

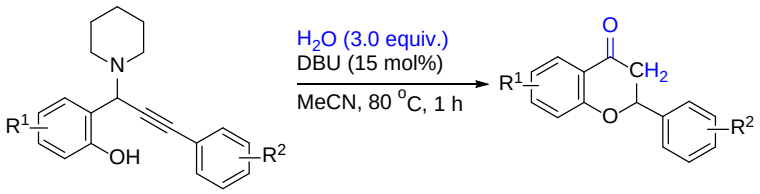
Unless otherwise specified, all reagents and starting materials were purchased from commercial sources and used as received, and the solvents were purified and dried using standard procedures. The chromatography solvents were technical grade and distilled prior to use. Flash chromatography was performed using 200-300 mesh silica gel with the indicated solvent system according to standard techniques. The ^{1}H and ^{13}C NMR data were recorded on 400 MHz or 500 MHz and 100 MHz or 125 MHz NMR spectrometers, unless otherwise specified. Chemical shifts (δ) in parts per million are reported relative to the residual signals of chloroform (7.26 ppm for ^{1}H and 77.16 ppm for ^{13}C), and all ^{13}C NMR were recorded with proton broadband decoupling and indicated as $^{13}C\{^{1}H\}$ NMR. Multiplicities are described as s (singlet), d (doublet), t (triplet), q (quartet), or m (multiplet), and the coupling constants (J) are reported in Hertz. HRMS analysis with a quadrupole time-of-flight mass spectrometer yielded ion mass/charge (m/z) ratios in atomic mass units. IR spectra were measured as dry films (KBr), and the peaks are reported in terms of wave number (cm^{-1}). The melting points were measured using SGWX-4 melting point apparatus.

2. General procedures for the synthesis of propargylamines



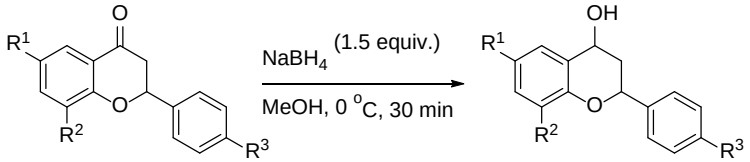
To a 25 mL round-bottom flask equipped with a magnetic stir bar were added amine (1.2 mmol), aldehyde (1.0 mmol), acetylene (1.2 mmol), copper (I) iodide (10 mol%) and toluene (3 mL). The mixture was degassed and backfilled with nitrogen, and then stirred in an oil bath preheated to 100 °C for 5 h (monitored by TLC). After the reaction completed (as determined using TLC), the reaction mixture was cooled to room temperature, diluted with CH_2Cl_2 (10 mL) and filtered through a thin pad of silica gel. The filter cake was washed with CH_2Cl_2, and the combined filtrate was concentrated in vacuum. The crude product was purified by flash column chromatography on silica gel to afford the corresponding propargylamines.

3. General procedures for the synthesis of flavanones 2



A mixture of propargylamines **1** (0.2 mmol), water (0.6 mmol), and DBU (15 mol%) in acetonitrile (2 mL) were heated to 80 °C in an oil bath for 1 h under air. After the reaction completed (as determined by TLC), the reaction mixture was cooled to room temperature, extracted with CH_2Cl_2 (3 × 10 mL), and washed with brine. The organic layers were combined, dried over Na_2SO_4, filtered, and then evaporated under vacuum. The residue was purified using flash column chromatography with silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:40, v/v) as the elution solvent to give desired products **2**.

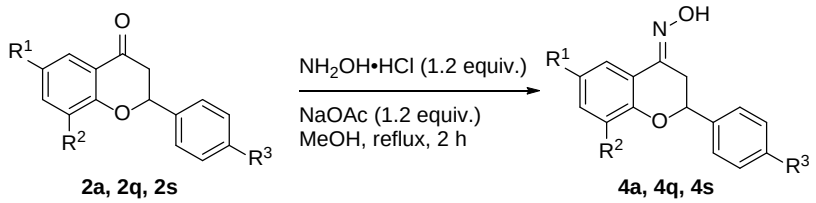
4. General procedures for the synthesis of chroman-4-ols 3



2a, 2q, 2v **3a, 3q, 3v**

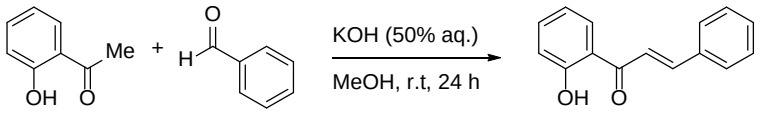
Following a reported procedure,[1] to a solution of flavanones **2** (0.2 mmol), in methanol (2 mL) was added solid sodium borohydride (1.5 equiv.) at 0 °C under air atmosphere. The mixture was stirred for 30 minutes at the same temperature, before it was quenched with 10 mL of saturated aqueous $NaHCO_3$. The aqueous layer was extracted with DCM (3×10 mL). The combined organic layers were dried over Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by recrystallization in ethyl acetate/petroleum ether (1:10, v/v) as the solvent to afford products **3**.

5. General procedures for the synthesis of chroman-4-one oximes 4



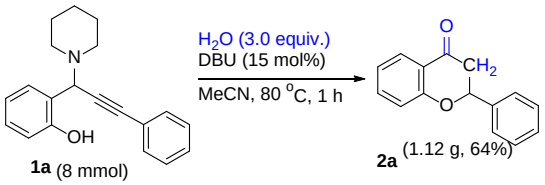
Following a reported procedure,[2] a mixture of flavanones **2** (0.2 mmol), sodium acetate (0.24 mmol, 1.2 equiv.) and hydroxylamine hydrochloride (0.24 mmol, 1.2 equiv) was heated to reflux in an oil bath. After 2 h, the reaction was allowed to cool to room temperature and evaporated to dryness *in vacuo*. EtOAc and an aqueous 2N NaOH solution were added to the residue. The organic layer was extracted with EtOAc (3×10 mL), washed with brine and then dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel (200-300 mesh) with EtOAc and petroleum ether (1:5, v/v) as the eluting solvents to produce the products **4**.

6. General procedures for the synthesis of 2’-hydroxychalcone (5aa)



Following a reported procedure,[3] 2′-hydroxyacetophenone (1 mmol) and benzaldehyde (1 mmol) were dissolved in methanol (3 mL) in a round bottom flask. The solution was cooled in an ice–water bath and 50% aq. KOH (0.6 mL) was added into the solution dropwise. After stirring at room temperature for 24 hours, the orange–red mixture was poured into an ice–water mixture (10 mL) and the solution was neutralized by 4N HCl solution. The yellow precipitate was filtered out, re–dissolved in DCM, dried by anhydrous Na_2SO_4, and concentrated. The resulting solid was purified by either recrystalization to give the corresponding 2’-hydroxychalcone **(5aa)** in 75% yield (168 mg) as a yellow amorphous solid.

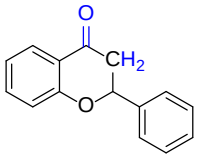
7. Gram-scale synthesis of compound 2a



A mixture of propargylamines **1** (2.32 g, 8 mmol), water (432 mg, 24 mmol), and DBU (182 mg, 1.2 mmol) in acetonitrile (10 mL) were heated to 80 °C in an oil bath for 1 h under air. After the reaction completed (as determined by TLC), the reaction mixture was cooled to room temperature, extracted with CH_2Cl_2 (3 × 20 mL), and washed with brine. The organic layers were combined, dried over Na_2SO_4, filtered, and then evaporated under a vacuum. The residue was purified using flash column chromatography with silica gel (200-300 mesh), using ethyl acetate and petroleum ether (1:40, v/v) as the elution solvent to give desired products **2a** in 64% yield.

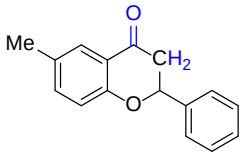
8. Characterization data for all compounds

2-Phenylchroman-4-one (Scheme 2, compound 2a)



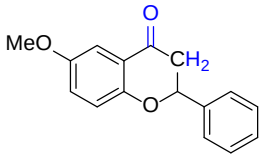
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a white solid in 84% yield (38 mg). m.p. 75−76 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00–7.88 (m, 1H), 7.54–7.51 (m, 1H), 7.50–7.48 (m, 2H), 7.46–7.42 (m, 2H), 7.41–7.37 (m, 1H), 7.08–7.04 (m, 2H), 5.49 (dd, J = 13.6, 2.8 Hz, 1H), 3.10 (dd, J = 16.8, 13.2 Hz, 1H), 2.90 (dd, J = 17.2, 3.2 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.1, 161.6, 138.8, 136.3, 128.9, 128.8, 127.1, 126.2, 121.7, 121.0, 118.2, 79.7, 44.7; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{13}O_2$ 225.0910; Found 225.0903.

6-Methyl-2-phenylchroman-4-one (Scheme 2, compound 2b)



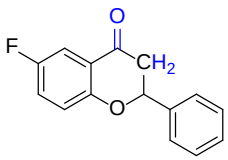
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 83% yield (40 mg). m.p. 103−104 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76–7.75 (m, 1H), 7.53–7.51 (m, 2H), 7.48–7.45 (m, 2H), 7.44–7.40 (m, 1H), 7.37–7.34 (dd, J = 10.0, 5.0 Hz, 1H), 7.00 (d, J = 8.5 Hz, 1H), 5.48 (dd, J = 13.0, 2.5 Hz, 1H), 3.10 (dd, J = 16.5, 13.0 Hz, 1H), 2.91 (dd, J = 17.0, 3.0 Hz, 1H), 2.36 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.3, 159.7, 138.9, 137.3, 131.1, 128.9, 128.8, 126.7, 126.2, 120.6, 118.0, 79.6, 44.8, 20.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{15}O_2$ 239.1067; Found 239.1064.

6-Methoxy-2-phenylchroman-4-one (Scheme 2, compound 2c)



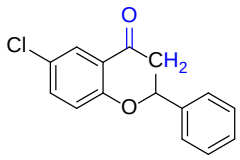
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 90% yield (46 mg). m.p. 138−139 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50–7.47 (m, 2H), 7.46–7.42 (m, 2H), 7.40-7.38 (m, 1H), 7.36 (d, J = 3.2 Hz, 1H), 7.13 (dd, J = 12.4, 3.2 Hz, 1H), 7.00 (d, J = 9.2 Hz, 1H), 5.45 (dd, J = 13.2, 2.8 Hz, 1H), 3.82 (s, 3H), 3.08 (dd, J = 18.0, 13.6 Hz, 1H), 2.88 (dd, J = 17.2, 3.2 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.2, 156.3, 154.3, 138.9, 128.9, 128.8, 126.2, 125.5, 120.8, 119.5, 107.3, 79.8, 55.9, 44.6; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{15}O_3$ 255.1016; Found 255.1017.

6-Fluoro-2-phenylchroman-4-one (Scheme 2, compound 2d)



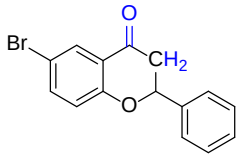
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 68% yield (33 mg). m.p. 72−73 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59–7.57 (dd, J = 8.0, 3.2 Hz,1H), 7.50–7.44 (m, 4H), 7.42–7.39 (m, 1H), 7.24–7.21 (m, 1H), 7.07–7.02 (dd, J = 8.8, 4.0 Hz, 1H), 5.47 (dd, J = 13.2, 2.8 Hz, 1H), 3.08 (dd, J = 16.8, 13.2 Hz, 1H), 2.91 (dd, J = 16.8, 2.8 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 191.3, 157.8, 157.4 (d, $J_{C\text{-}F}$ = 241.0 Hz), 138.5, 128.9, 126.2, 123.9, 123.6, 121.4 (d, $J_{C\text{-}F}$ = 6.8 Hz), 119. (d, $J_{C\text{-}F}$=7.3 Hz), 112.1 (d, $J_{C\text{-}F}$ = 23.2 Hz), 79.9, 44.4; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{12}FO_2$ 243.0816; Found 243.0811.

6-Chloro-2-phenylchroman-4-one (Scheme 2, compound 2e)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 70% yield (36 mg). m.p. 89−90 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.48–7.45 (m, 3H), 7.44–7.42 (m, 2H), 7.41–7.38 (m, 1H), 7.02 (d, J = 7.2 Hz, 1H), 5.47 (dd, J = 13.5, 3.0 Hz, 1H), 3.08 (dd, J = 17.0, 13.0 Hz, 1H), 2.91 (dd, J = 17.0, 3.0 Hz, 1H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 191.3, 160.4, 138.6, 136.5, 129.4, 129.3, 127.6, 126.8, 126.6, 122.1, 120.3, 80.2, 44.7; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{12}ClO_2$ 259.0520; Found 259.0516.

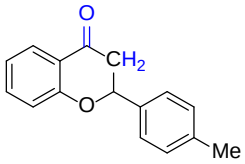
6-Bromo-2-phenylchroman-4-one (Scheme 2, compound 2f)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 63% yield (38 mg). m.p. 118−119 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 2.8 Hz, 1H), 7.59 (dd, J = 11.2, 2.4 Hz, 1H), 7.49–7.46 (m, 3H), 7.44–7.43 (m, 1H), 7.42–7.38 (m, 1H), 6.97 (d, J = 8.8 Hz, 1H), 5.48 (dd, J = 13.2, 3.2 Hz, 1H), 3.09 (dd, J = 16.8, 13.2 Hz, 1H), 2.91 (dd, J = 16.7, 2.8 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 190.8, 160.5, 138.9, 138.2, 129.6, 129.1, 129.0, 126.2, 122.2,

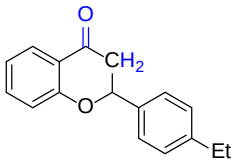
120.3, 114.4, 79.8, 44.3; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{12}BrO_2$ 303.0015; Found 303.0013.

2-(*p*-Tolyl)chroman-4-one (Scheme 2, compound 2g)



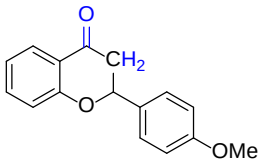
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 73% yield (35 mg). m.p. 60−62 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94–7.92 (dd, J = 8.4, 1.6 Hz, 1H), 7.53–7.48 (m, 1H), 7.39 (d, J = 8.0 Hz, 2H), 7.26 (d, J = 8.4 Hz, 2H), 7.08–7.02 (m, 2H), 5.46 (dd, J = 13.2, 2.8 Hz, 1H), 3.11 (dd, J = 16.8, 13.2 Hz, 1H), 2.88 (dd, J = 16.8, 2.8 Hz, 1H), 2.39 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.3, 161.7, 138.8, 136.2, 135.8, 129.6, 127.1, 126.3, 121.6, 120.9, 118.2, 79.6, 44.6, 21.3; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{15}O_2$ 239.1067; Found 239.1074.

2-(4-Ethylphenyl)chroman-4-one (Scheme 2, compound 2h)



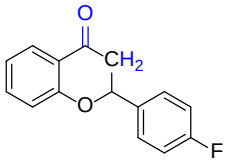
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 78% yield (39 mg). m.p. 62−63 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94–7.92 (dd, J = 8.0, 1.6 Hz, 1H), 7.52–7.48 (m, 1H), 7.41 (d, J = 8.0 Hz, 2H), 7.28 (d, J = 8.4 Hz, 2H), 7.07–7.03 (m, 2H), 5.46 (dd, J = 13.2, 2.8 Hz, 1H), 3.11 (dd, J = 16.8, 13.6 Hz, 1H), 2.88 (dd, J = 16.8, 2.8 Hz, 1H), 2.69 (q, J = 7.6 Hz, 2H), 1.26 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.3, 161.7, 145.1, 136.2, 136.0, 128.4, 127.1, 126.3, 121.6, 121.0, 118.2, 79.6, 44.6, 28.6, 15.6; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{17}H_{17}O_2$ 253.1223; Found 253.1228.

2-(4-Methoxyphenyl)chroman-4-one (Scheme 2, compound 2i)



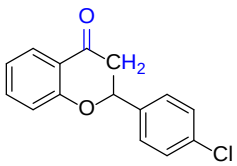
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 81% yield (41 mg). m.p. 82−83 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94–7.92 (dd, J = 8.0, 1.6 Hz, 1H), 7.52–7.48 (m, 1H), 7.42 (d, J = 8.8 Hz, 2H), 7.08–7.02 (m, 2H), 6.97 (d, J = 8.8 Hz, 2H), 5.44 (dd, J = 13.6, 2.8 Hz, 1H), 3.84 (s, 3H), 3.11 (dd, J = 16.9, 13.2 Hz, 1H), 2.87 (dd, J = 16.8, 2.8 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.3, 161.7, 160.0, 136.2, 130.8, 127.8, 127.1, 121.6, 121.0, 118.2, 114.2, 79.4, 55.4, 44.5; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{16}H_{15}O_3$ 255.1016; Found 255.1017.

2-(4-Fluorophenyl)chroman-4-one (Scheme 2, compound 2j)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 63% yield (30 mg). m.p. 74−75 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49–7.92 (d, J = 8.0, 1.6 Hz, 1H), 7.55–7.50 (m, 1H), 7.49–7.44 (m, 2H), 7.16–7.10 (m, 2H), 7.09–7.03 (m, 2H), 5.47 (dd, J = 13.6, 3.2 Hz, 1H), 3.07 (dd, J = 16.8, 13.2 Hz, 1H), 2.88 (dd, J = 17.2, 3.2 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 191.8, 162.8 (d, $J_{C\text{-}F}$ = 246.2 Hz), 161.4, 136.3, 134.6, 134.6, 128.1, 128.0, 127.1, 121.8, 120.9, 118.1, 115.9 (d, $J_{C\text{-}F}$ = 21.4 Hz), 78.9, 44.7; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{12}FO_2$ 243.0816; Found 243.0814.

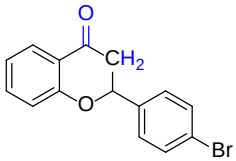
2-(4-Chlorophenyl)chroman-4-one (Scheme 2, compound 2k)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 66% yield (52 mg). m.p. 79−80 °C; ^{1}H NMR (400

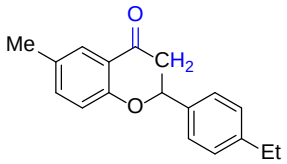
MHz, $CDCl_3$) δ 7.94–7.92 (dd, J = 7.6, 1.6 Hz, 1H), 7.54–7.50 (m, 1H), 7.44–7.40 (m, 4H), 7.09–7.04 (m, 2H), 5.47 (dd, J = 13.2, 3.2 Hz, 1H), 3.05 (dd, J = 16.8, 13.2 Hz, 1H), 2.88 (dd, J = 16.8, 3.2 Hz, 1H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 191.6, 161.3, 137.3, 136.4, 134.6, 129.1, 127.6, 127.1, 121.9, 120.9, 118.1, 78.9, 44.6; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{12}ClO_2$ 259.0520; Found 259.0520.

2-(4-Bromophenyl)chroman-4-one (Scheme 2, compound 2l)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 65% yield (39 mg). m.p. 111−113 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.94–7.91 (dd, J = 8.0, 1.6 Hz, 1H), 7.58 (d, J = 8.4 Hz, 2H), 7.52–7.50 (m, 1H), 7.37 (d, J = 8.4 Hz, 2H), 7.09–7.04 (m, 2H), 5.46 (dd, J = 13.2, 3.2 Hz, 1H), 3.04 (dd, J = 17.6, 12.8 Hz, 1H), 2.88 (dd, J = 17.6, 3.2 Hz, 1H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 191.6, 161.3, 137.8, 136.4, 132.1, 127.8, 127.1, 122.8, 121.9, 120.9, 118.1, 78.9, 44.6; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{12}BrO_2$ 303.0015; Found 303.0020.

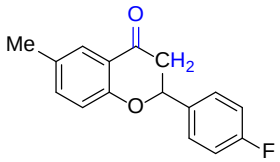
2-(4-Ethylphenyl)-6-methylchroman-4-one (Scheme 2, compound 2m)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 85% yield (45 mg). m.p. 160−162 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.41 (d, J = 8.4 Hz, 2H), 7.33–7.30 (dd, J = 8.4, 2.0 Hz, 1H), 7.28 (d, J = 8.0 Hz, 2H), 6.96 (d, J = 8.4 Hz, 1H), 5.42 (dd, J = 13.2, 2.8 Hz, 1H), 3.09 (dd, J = 16.8, 13.6 Hz, 1H), 2.86 (dd, J = 16.8, 2.8 Hz, 1H), 2.68 (q, J = 7.6 Hz, 2H), 2.33 (s, 3H), 1.26 (t, J = 7.6 Hz, 3H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 192.6, 159.8, 145.1, 137.3, 136.1, 131.0, 128.4, 126.6, 126.3, 120.5, 118.0, 79.6, 44.6, 28.7, 20.5, 15.6; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{18}H_{19}O_2$ 267.1380; Found

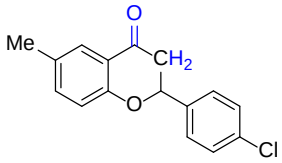
267.1381.

2-(4-Fluorophenyl)-6-methylchroman-4-one (Scheme 2, compound 2n)



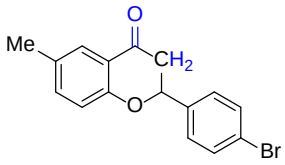
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 77% yield (39 mg). m.p. 105−107 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.48–7.44 (m, 2H), 7.34–7.31 (dd, J = 8.4, 2.4 Hz, 1H), 7.14–7.10 (m, 2H), 6.96 (d, J = 8.8 Hz, 1H), 5.43 (dd, J = 13.2, 2.8 Hz, 1H), 3.04 (dd, J = 16.8, 13.2 Hz, 1H), 2.85 (dd, J = 16.8, 2.8 Hz, 1H), 2.33 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.1, 162.8 (d, $J_{C\text{-}F}$ = 246.1 Hz), 159.5, 137.4, 134.8, 131.3, 128.1, 128.0, 126.7, 120.5, 117.9, 115.8 (d, $J_{C\text{-}F}$ = 21.6 Hz), 78.9, 44.7, 20.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{14}FO_2$ 257.0972; Found 257.0974.

2-(4-Chlorophenyl)-6-methylchroman-4-one (Scheme 2, compound 2o)



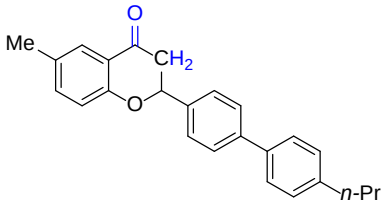
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 73% yield (40 mg). m.p. 128−129 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (s, 1H), 7.44–7.38 (m, 4H), 7.35–7.31 (dd, J = 8.4, 2.4 Hz, 1H), 6.95 (d, J = 8.4 Hz, 1H), 5.43 (dd, J = 12.8, 2.8 Hz, 1H), 3.02 (dd, J = 16.8, 13.2 Hz, 1H), 2.86 (dd, J = 17.2, 3.2 Hz, 1H), 2.33 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 191.9, 159.4, 137.5, 137.42, 134.6, 131.4, 129.1, 127.6, 126.7, 120.5, 117.9, 78.8, 44.7, 20.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{14}ClO_2$ 273.0677; Found 273.0673.

2-(4-Bromophenyl)-6-methylchroman-4-one (Scheme 2, compound 2p)



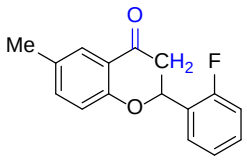
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 80% yield (51 mg). m.p. 144−145 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (s, 1H), 7.58–7.54 (m, 2H), 7.38–7.35 (m, 2H), 7.34–7.31 (m, 1H), 6.95 (d, *J* = 8.4 Hz, 1H), 5.41 (dd, *J* = 13.2, 3.2 Hz, 1H), 3.01 (dd, *J* = 16.8, 12.8 Hz, 1H), 2.85 (dd, *J* = 17.2, 3.2 Hz, 1H), 2.33 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 191.9, 159.4, 138.0, 137.4, 132.0, 131.4, 127.8, 126.7, 122.7, 120.5, 117.9, 78.8, 44.6, 20.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{14}BrO_2$ 317.0172; Found 317.0171.

6-Methyl-2-(4'-propyl-[1,1'-biphenyl]-4-yl)chroman-4-one (Scheme 2, compound 2q)



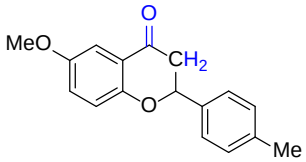
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a white solid in 66% yield (47mg). m.p. 160−161 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 2.0 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.55 (d, *J* = 7.6 Hz, 2H), 7.53 (d, *J* = 7.6 Hz, 2H), 7.35–7.32 (dd, *J* = 11.0, 2.0 Hz, 1H), 7.28 (d, *J* = 8.0 Hz, 2H), 6.98 (d, *J* = 8.4 Hz, 1H), 5.49 (dd, *J* = 13.2, 2.8 Hz, 1H), 3.12 (dd, *J* = 16.8, 13.2 Hz, 1H), 2.91 (dd, *J* = 16.8, 2.8 Hz, 1H), 2.67–2.61 (m, 2H), 2.34 (s, 3H), 1.73–1.65 (m, 2H), 0.98 (t, *J* = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.3, 159.7, 142.3, 141.8, 137.9, 137.5, 137.3, 131.1, 129.0, 127.4, 127.0, 126.7, 120.6, 118.0, 79.5, 44.6, 37.7, 24.6, 20.5, 13.9; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{25}H_{25}O_2$ 357.1849; Found 357.1846.

2-(2-Fluorophenyl)chroman-4-one (Scheme 2, compound 2r)



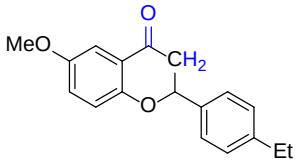
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 63% yield (32 mg). m.p. 80−82 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74–7.73 (m, 1H), 7.67–7.62 (m, 1H), 7.39–7.31 (m, 2H), 7.25– 7.22 (m, 1H), 7.14–7.08 (m, 1H), 6.97 (d, J = 8.4 Hz, 1H), 5.75 (dd, J = 13.2, 3.2 Hz, 1H), 3.04 (dd, J = 16.8, 13.3 Hz, 1H), 2.91 (dd, J = 16.8, 3.2 Hz, 1H), 2.34 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 191.9, 159.7 (d, $J_{C\text{-}F}$ = 250.0Hz), 159.6, 137.3, 131.3, 130.2(d, $J_{C\text{-}F}$ = 8.0 Hz), 127.5(d, $J_{C\text{-}F}$ = 3.0Hz) , 126.7, 126.4(d, $J_{C\text{-}F}$ = 13.0 Hz), 124.6 (d, $J_{C\text{-}F}$ = 3.0Hz), 120.6, 117.9, 115.8(d, $J_{C\text{-}F}$ = 21.0 Hz) , 73.8(d, $J_{C\text{-}F}$ = 3.0 Hz), 43.8, 20.5; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{16}H_{14}FO_2$ 257.0972; Found 257.0979.

6-Methoxy-2-(*p*-tolyl)chroman-4-one (Scheme 2, compound 2s)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 90% yield (48 mg). m.p. 118−119 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, J = 8.4 Hz, 2H), 7.34 (d, J = 3.2 Hz, 1H), 7.25 (d, J = 8.0 Hz, 2H), 7.14–7.09 (dd, J = 9.2, 3.2 Hz, 1H), 6.99 (d, J = 8.8 Hz, 1H), 5.41 (dd, J = 13.2, 2.8 Hz, 1H), 3.82 (s, 3H), 3.08 (dd, J = 17.2, 13.6 Hz, 1H), 2.86 (dd, J = 16.8, 2.8 Hz, 1H), 2.38 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.4, 156.4, 154.2, 138.7, 135.9, 129.5, 126.2, 125.5, 120.8, 119.5, 107.3, 79.7, 55.8, 44.5, 21.3; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{17}H_{17}O_3$ 269.1172; Found 269.1166.

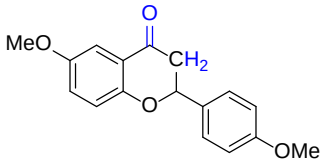
2-(4-Ethylphenyl)-6-methoxychroman-4-one (Scheme 2, compound 2t)



This compound was purified by column chromatography (ethyl acetate/petroleum ether

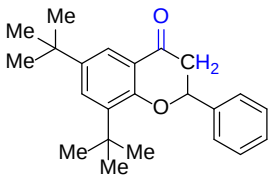
= 1:40) to afford a yellow solid in 88% yield (50 mg, 0.2 mmol). m.p. 99−101 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, J = 8.0 Hz, 2H), 7.35 (d, J = 3.2 Hz, 1H), 7.26 (d, J = 8.0 Hz, 2H), 7.14–7.09 (dd, J = 8.8, 3.2 Hz, 1H), 6.99 (d, J = 8.8 Hz, 1H), 5.41 (dd, J = 13.6, 2.8 Hz, 1H), 3.82 (s, 3H), 3.09 (dd, J = 17.2, 13.6 Hz, 1H), 2.86 (dd, J = 16.8, 2.8 Hz, 1H), 2.68 (q, J = 7.6 Hz, 2H), 1.25 (t, J = 7.6 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.4, 156.4, 154.2, 145.1, 136.1, 128.4, 126.32, 125.5, 120.8, 119.5, 107.3, 79.7, 55.9, 44.5, 28.7, 15.6; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{18}H_{19}O_3$ 283.1329; Found 283.1335.

6-Methoxy-2-(4-methoxyphenyl)chroman-4-one (Scheme 2, compound 2u)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 86% yield (49 mg). m.p. 156−158 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, J = 8.8 Hz, 2H),7.35 (d, J = 3.2 Hz, 1H), 7.37–7.33 (m, 1H), 7.14–7.08 (dd, J = 9.0, 1.6 Hz, 1H), 6.98 (d, J = 6.4 Hz, 2H), 6.96 (d, J = 6.4 Hz, 1H), 5.39 (dd, J = 13.2, 2.8 Hz, 1H), 3.83 (s, 3H), 3.82 (s, 3H), 3.08 (dd, J = 16.8, 13.2 Hz, 1H), 2.85 (dd, J = 17.6, 2.8 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.4, 160.0, 156.4, 154.2, 130.9, 127.7, 125.4, 120.8, 119.5, 114.2, 107.4, 79.5, 55.8, 55.4, 44.4; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{17}H_{17}O_4$ 285.1121; Found 285.1118.

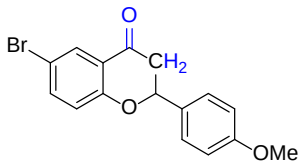
6,8-Di-*tert*-butyl-2-phenylchroman-4-one (Scheme 2, compound 2v)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 83% yield (56 mg). m.p. 134−136 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, J = 2.4 Hz, 1H), 7.60 (d, J = 2.4 Hz, 1H), 7.53–7.50 (m, 2H), 7.47–7.43 (m, 2H), 7.41–7.37 (m, 1H), 5.44 (dd, J = 14.0, 2.8 Hz, 1H), 3.03 (dd, J =

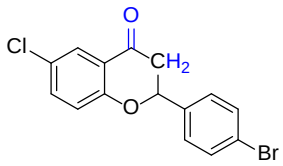
16.8, 13.6 Hz, 1H), 2.88 (dd, *J* = 17.2, 3.2 Hz, 1H), 1.41 (s, 9H), 1.33 (s, 9H); $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 193.2, 158.7, 143.7, 139.5, 138.6, 131.0, 128.9, 128.5, 125.9, 121.2, 121.1, 79.6, 45.3, 35.1, 34.6, 31.4, 29.8; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{23}H_{29}O_2$ 337.2162; Found 337.2153.

6-Bromo-2-(4-methoxyphenyl)chroman-4-one (Scheme 2, compound 2w)



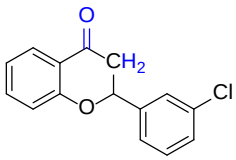
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 68% yield (45 mg). m.p. 109−111 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.58–7.56 (dd, *J* = 11.0, 2.8 Hz, 1H), 7.40 (d, *J* = 8.8 Hz, 2H), 6.97–6.903(m, 3H), 5.42 (dd, *J* = 13.2, 2.8 Hz, 1H), 3.84 (s, 3H), 3.10 (dd, *J* = 16.8, 13.2 Hz, 1H), 2.88 (dd, *J* = 16.8, 2.8 Hz, 1H) ; $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ 191.0, 160.5, 160.1, 138.8, 130.2, 129.5, 127.8, 122.2, 120.3, 114.3, 79.6, 55.4, 44.0; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{16}H_{14}BrO_3$ 333.0121; Found 333.0128.

2-(4-Bromophenyl)-6-chlorochroman-4-one (Scheme 2, compound 2x)



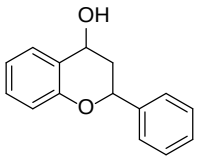
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 60% yield (40 mg). m.p. 145−146 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (d, *J* = 2.4 Hz, 1H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.46–7.44 (dd, *J* = 8.5, 3.0 Hz, 1H), 7.35 (d, *J* = 8.5 Hz, 2H), 7.02 (d, *J* = 8.5 Hz,1H), 5.44 (dd, *J* = 12.5, 3.0 Hz, 1H), 3.02 (dd, *J* = 17.0, 13.0 Hz, 1H), 2.89 (dd, *J* = 17.0, 3.5 Hz, 1H); $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$) δ 190.7, 160.1, 137.7, 136.5, 132.5, 128.2, 127.8, 126.8, 123.3, 122.1, 120.2, 79.5, 44.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ Calcd for $C_{15}H_{11}BrClO_2$ 336.9625; Found 336.9627.

2-(3-Chlorophenyl)chroman-4-one (Scheme 2, compound 2y)



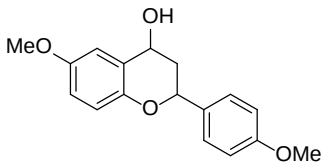
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:40) to afford a yellow solid in 70% yield (36 mg). m.p. 81−82 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95–7.92 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.56–7.50 (m, 2H), 7.39–7.36 (m, 2H), 7.35–7.33 (m, 1H), 7.10– 7.05 (m, 2H), 5.47 (dd, *J* = 13.2, 2.8 Hz, 1H), 3.04 (dd, *J* = 16.8, 13.2 Hz, 1H), 2.90 (dd, *J* = 16.8, 2.8 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) *δ* 191.4, 161.3, 140.8, 136.4, 134.9, 130.2, 128.9, 127.1, 126.4, 124.2, 121.9, 120.9, 118.1, 78.8, 44.7; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{12}ClO_2$ 259.0520; Found 259.0510.

2-Phenylchroman-4-ol (Scheme 3, compound 3a)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:6) to afford a white solid in 70% yield (32 mg). m.p. 145−147 °C; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.53 (d, *J* = 7.6 Hz, 1H), 7.47–7.45 (m, 2H), 7.43–7.39 (m, 2H), 7.37–7.35 (m, 1H), 7.23–7.19 (m, 1H), 7.01–6.97 (m, 1H), 6.91–6.89 (m, 1H), 5.19 (dd, *J* = 11.6, 2.0 Hz, 1H), 5.15–5.08 (m, 1H), 2.64–2.46 (m, 1H), 2.24–2.09 (m, 1H), 1.80 (s, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) *δ* 154.5, 140.5, 129.2, 128.7, 128.3, 127.0, 126.1, 125.8, 121.0, 116.8, 76.9, 65.9, 40.1; HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{15}H_{14}O_2Na$ 249.0880; Found 249.0887.

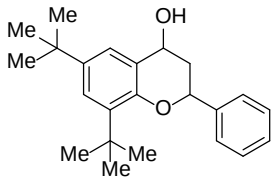
6-Methoxy-2-(4-methoxyphenyl)chroman-4-ol (Scheme 3, compound 3u).



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:6) to afford a white solid in 64% yield (37 mg). m.p. 148−149 °C; ^{1}H NMR (400

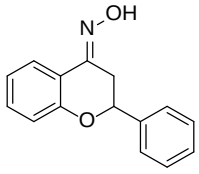
MHz, $CDCl_3$) δ 7.38–7.36 (m, 1H), 7.06 (d, J = 2.8 Hz, 1H), 6.94–6.92 (m, 2H), 6.82–6.76 (m, 2H), 5.13–5.01 (m, 1H), 3.82 (s, 3H), 3.79 (s, 3H), 2.71–2.30 (m, 1H), 2.21–2.07 (m, 1H), 1.74 (d, J = 8.8 Hz, 1H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 159.6, 154.0, 148.6, 132.7, 127.6, 126.1, 117.6, 115.8, 114.1, 111.1, 76.5, 66.2, 55.8, 55.4, 40.0; HRMS (ESI-TOF) m/z: [M+ Na]+ Calcd for $C_{17}H_{18}O_4Na$ 309.1097; Found 309.1098.

6,8-Di-*tert*-butyl-2-(*p*-tolyl)chroman-4-ol (Scheme 3, compound 3v)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:6) to afford a white solid in 64% yield (43 mg). m.p. 134−135 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.51–7.46 (m, 3H), 7.44–7.41 (m, 2H), 7.37–7.34 (m, 1H), 7.31–7.30 (m, 1H), 5.15 (d, J = 10.8 Hz, 2H), 2.63–2.49 (m, 1H), 2.21–2.07 (m, 1H), 1.82 (s, 1H), 1.40 (s, 9H), 1.35 (s, 9H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 151.2, 142.8, 141.2, 137.1, 128.6, 127.9, 126.0, 125.2, 123.8, 121.7, 76.9, 66.8, 40.7, 35.2, 34.5, 31.6, 30.0; HRMS (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{23}H_{30}O_2Na$ 361.2138; Found 361.2142.

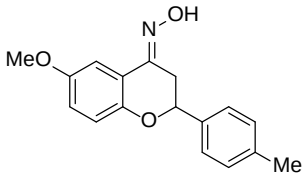
2-Phenylchroman-4-one oxime (Scheme 3, compound 4a)



This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:5) to afford a white solid in 90% yield (43 mg, 0.2 mmol). m.p. 164−166 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.87–7.85 (m, 1H), 7.76 (s, 1H), 7.51–7.48 (m, 2H), 7.44–7.41 (m, 2H), 7.39–7.35 (m, 1H), 7.32–7.87 (m, 1H), 7.00–6.96 (m, 2H), 5.11 (dd, J = 12.4, 2.8 Hz, 1H), 3.58 (dd, J = 17.2, 2.8 Hz, 1H), 2.76 (dd, J = 17.2, 12.4 Hz, 1H); $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 156.7, 150.4, 139.8, 131.3, 128.7, 128.5, 126.2,

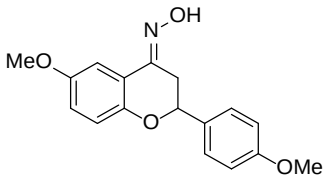
124.0, 121.7, 118.1, 77.1, 30.4; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{14}NO_2$ 240.1019; Found 240.1014.

6-Methoxy-2-(*p*-tolyl)chroman-4-one oxime (Scheme 3, compound 4s)



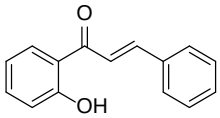
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:5) to afford a white solid in 84% yield (48 mg). m.p. 176−178 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (s, 1H), 7.38–7.34 (m, 3H), 7.23 (d, J = 8.0 Hz, 2H), 6.93– 6.88 (m, 2H), 5.03 (dd, J = 12.4, 3.2 Hz, 1H), 3.80 (s, 3H), 3.52 (dd, J = 17.2, 2.8 Hz, 1H), 2.76 (dd, J = 17.2, 12.4 Hz, 1H), 2.38 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 154.1, 151.3, 150.7, 138.3, 136.9, 129.4, 126.3, 119.4, 119.1, 118.1, 106.2, 77.2, 55.8, 30.4, 21.2; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{17}H_{18}NO_3$ 284.1281; Found 284.1285.

6-Methoxy-2-(4-methoxyphenyl)chroman-4-one oxime (Scheme 3, compound 4u)



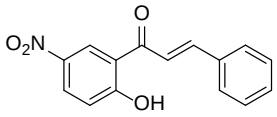
This compound was purified by column chromatography (ethyl acetate/petroleum ether = 1:5) to afford a white solid in 87% yield (52 mg). m.p. 191−192 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (s, 1H), 7.41–7.39 (m, 2H), 7.34–7.33 (m, 1H), 6.96–6.93 (m, 2H), 6.92–6.88 (m, 2H), 5.01 (dd, J = 12.8, 3.2 Hz, 1H), 3.83 (s, 3H), 3.80 (s, 3H), 3.49 (dd, J = 17.2, 3.2 Hz, 1H), 2.75 (dd, J = 17.3, 12.5 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 159.7, 154.1, 151.3, 150.8, 132.0, 127.7, 119.5, 119.1, 118.1, 114.1, 106.1, 76.9, 55.7, 55.4, 30.2; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{17}H_{18}NO_4$ 300.1230; Found 300.1235.

(*E*)-1-(2-Hydroxyphenyl)-3-phenylprop-2-en-1-one (Scheme 4, compound 5aa)



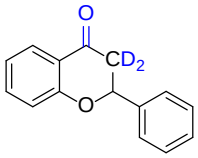
This compound was synthesized by the reported procedure in 75% (168 mg). Yellow amorphous solid; m.p. 84−86 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.82 (s, 1H), 7.95–7.91 (m, 2H), 7.68–7.65 (m, 3H), 7.53–7.48 (m, 1H), 7.45–7.42 (m, 3H), 7.05–7.02 (m, 1H), 6.97–6.93 (m, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.8, 163.7, 145.5, 136.5, 134.6, 131.0, 129.7, 129.1, 128.7, 120.2, 120.1, 118.9, 118.7; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{13}O_2$ 225.0910; Found 225.0906.

(*E*)-1-(2-Hydroxy-5-nitrophenyl)-3-phenylprop-2-en-1-one (Scheme 4, compound 5ab)



This compound was synthesized using the standard procedure for compounds **2**, and purified by column chromatography (ethyl acetate/petroleum ether = 1:20) to afford a white solid in 75% yield (40 mg). m.p. 67−69 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.58 (s, 1H), 8.90 (d, J = 2.8 Hz, 1H), 8.39 (dd, J = 9.2, 2.8 Hz, 1H), 8. 07 (d, J = 7.6 Hz, 1H), 7.75–7.72 (m, 2H), 7.70 (d, J = 15.2 Hz, 1H), 7.56–7.50–7.49 (m, 2H), 7.48–7.47 (m, 1H), 7.14 (d, J = 9.2 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.9, 168.5, 148.2, 139.6, 134.0, 131.8, 131.0, 129.3, 129.2, 126.1, 119.7, 118.9, 118.5, 76.71; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{12}NO_4$ 270.0766; Found 270.0769.

2-Phenylchroman-4-one (Scheme 4, compound 2a-*d*$_2$)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95–7.92 (dd, J = 8.0, 1.6 Hz, 1H), 7.54–7.48 (m, 3H), 7.46–7.42 (m, 2H), 7.41–7.38 (m, 1H), 7.08–7.04 (m, 2H), 5.56–5.39 (m, 1H), 3.13–2.87 (m, 1H); HRMS (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{15}H_{11}D_2O_2$ 227.1036; Found 227.1035.

References

1 (a) Yue, G.; Lei, K.; Hirao, H.; Zhou, J. *Angew. Chem. Int. Ed.* **2015**, *54*, 6531–6535. (b) Yahiaoui, S.; Pouget, C.; Buxeraud, J.; Chulia, A. J.; Fagnère, C. *Eur. J. Med. Chem.* **2011**, *46*, 2541-2545.

2 (a) Zhao, H.; Vandenbossche, C. P.; Koenig, S. G.; Singh, S. P.; Bakale, R. P. *Org. Lett.* **2008**, *10*, 505-507. (b) Pal, S.; Gaumont, A.-C.; Lakhdar, S.; Gillaizeau, I. *Org. Lett.* **2019**, *21*, 5621-5625.

3 Thornton, M. T.; Henderson, L. C.; Byrne, N.; Pfeffer, F. M. *Curr. Org. Chem.* **2012**, *16*, 121-126.

9. X-ray crystallographic data of compound 2p

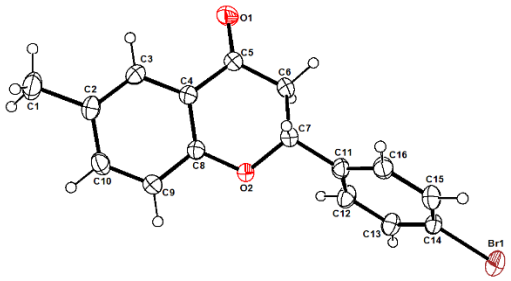


Figure S1. ORTEP drawing of compound **2p** (30% probability for the thermal ellipsoid).

The purified compound **2p** is dissolved in a mixed solvent of ethyl acetate and petroleum ether, and placed in a dark cabinet to slowly evaporate. After several days, a colourless bulk crystal is obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart CCDC APEX-2 diffractometer (graphite- monochromated Mo *Kα* radiation, λ=0.71073 nm) at 293(2) K.

A similar structure to compound **2p** was reported in 2010. (enone structure).

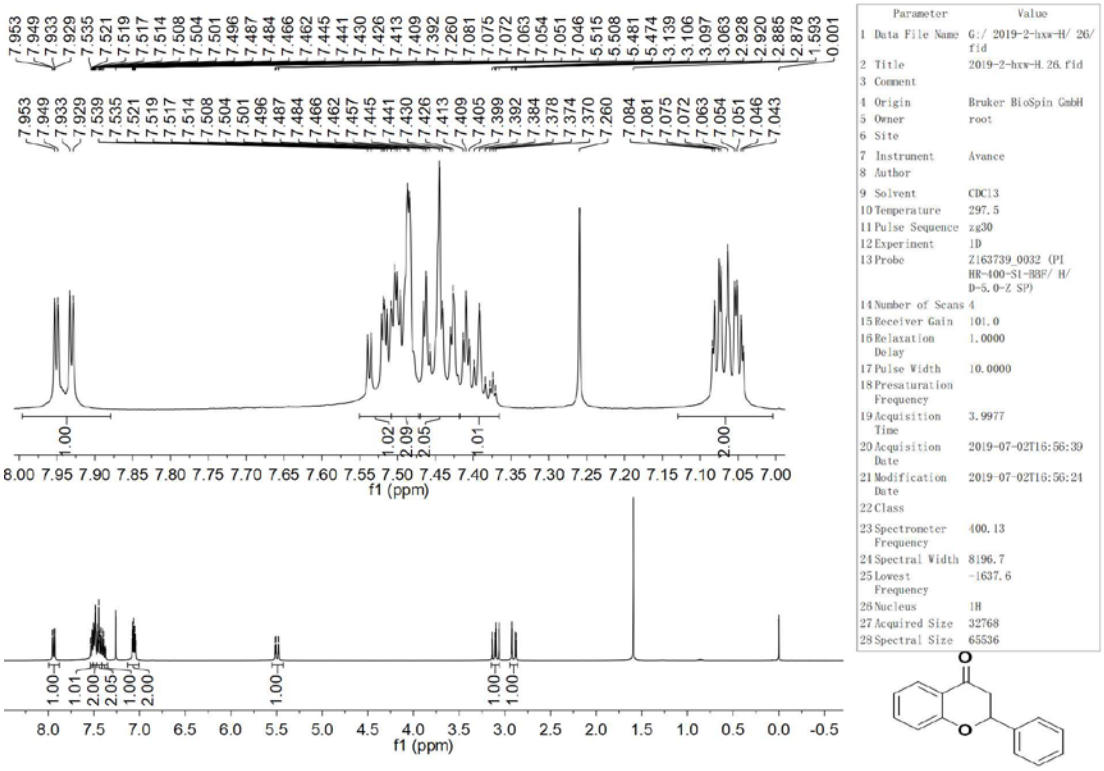
Ref: Janeczko, T.; Bialonska, A.; Kostrzewa-Suslow, E. *Acta Crystallogr., Sect.E: Struct. Rep. Online*, **2010**, *66*, o966

Table S1. Crystal data and structure refinement for 190513a_0m_a.

CCDC number	1966545
Identification code	190513a_0m_a
Empirical formula	C16 H13 Br O2
Formula weight	317.17
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 6.7796(6) Å α= 90°. b = 16.3362(14) Å β= 105.720(4)°. c = 12.5109(10) Å γ= 90°.
Volume	1333.8(2) $Å^3$
Z	4
Density (calculated)	1.579 Mg/m^3
Absorption coefficient	3.076 mm^{-1}
F(000)	640
Crystal size	0.210 x 0.230 x 0.240 mm^3
Theta range for data collection	2.101 to 27.534°.
Index ranges	-8<=h<=8, -21<=k<=21, -16<=l<=16
Reflections collected	7401
Independent reflections	2139 [R(int) = 0.0299]
Completeness to theta = 25.242°	63.2 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2139 / 0 / 173
Goodness-of-fit on F^2	1.021
Final R indices [I>2sigma(I)]	R1 = 0.0394, wR2 = 0.1034
R indices (all data)	R1 = 0.0603, wR2 = 0.1101
Extinction coefficient	n/a
Largest diff. peak and hole	0.494 and -0.319 $e.Å^{-3}$

10. ^{1}H and ^{13}C NMR spectra for all listed compounds

2-Phenylchroman-4-one (Table 2, compound 2a)



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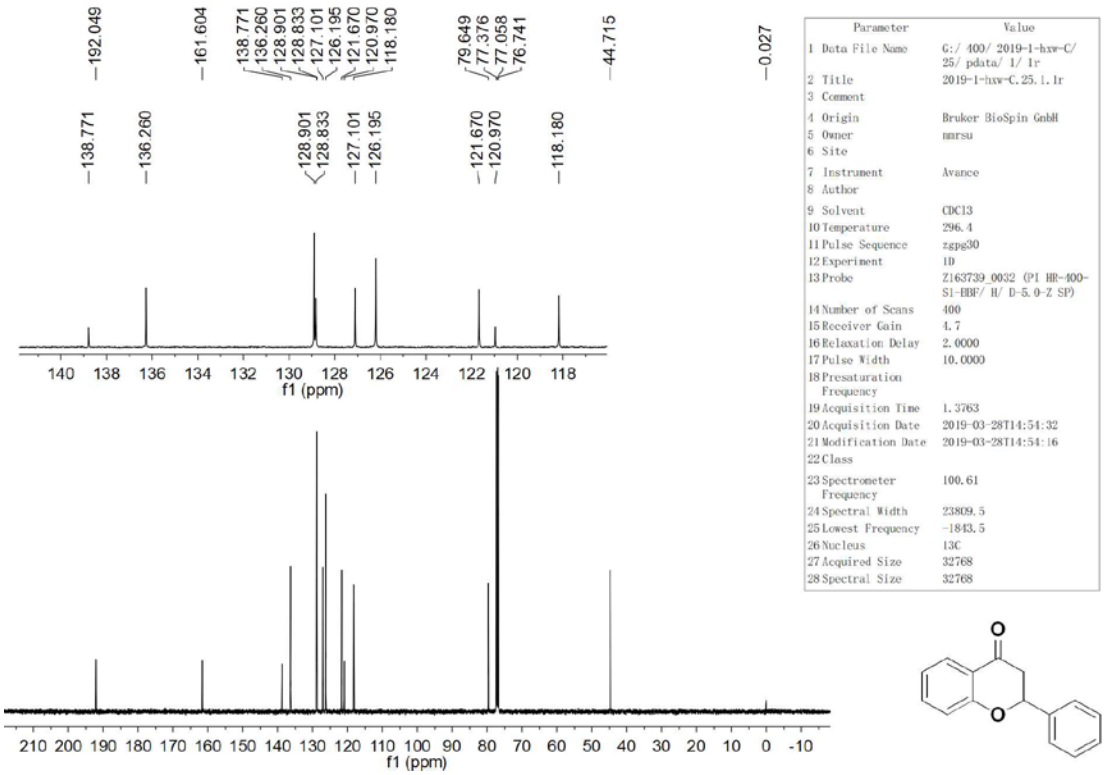
5 Owner	root
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297. 5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-SI-BBF/ H/ D-5. 0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101. 0
16 Relaxation Delay	1. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	3. 9977
20 Acquisition Date	2019-07-02T16:56:39
21 Modification Date	2019-07-02T16:56:21
22 Class	
23 Spectroneter Frequency	400. 13
24 Spectral Width	8196. 7
25 Lowest Frequency	-1637. 6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



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5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	296. 4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-SI-BBF/ H/ D-5. 0-Z SP)
14 Number of Scans	400
15 Receiver Gain	4. 7
16 Relaxation Delay	2. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
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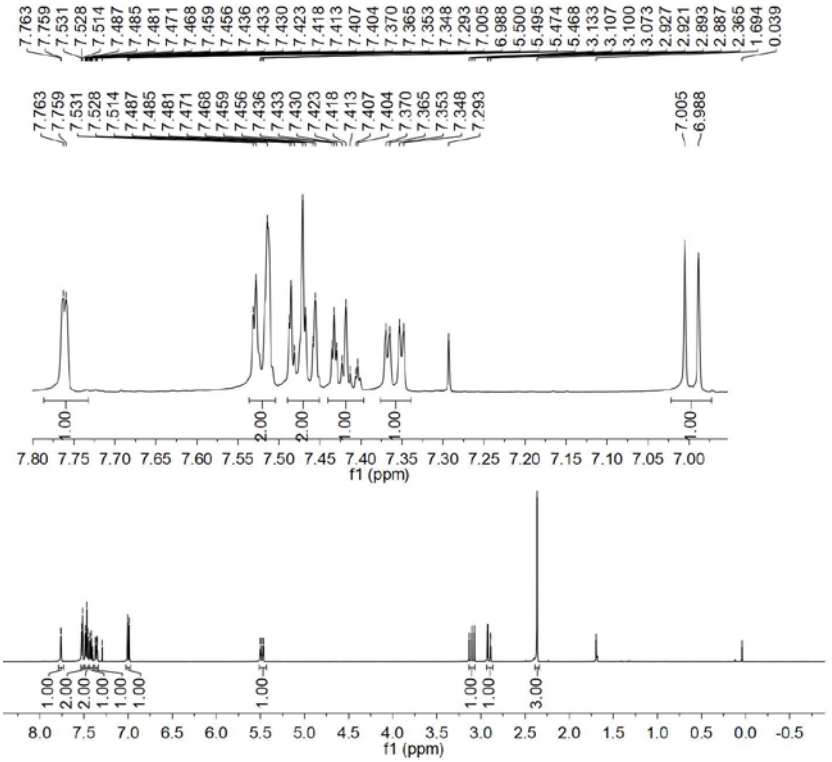
20 Acquisition Date	2019-03-28T14:54:32
21 Modification Date	2019-03-28T14:54:16
22 Class	
23 Spectrometer Frequency	100. 61
24 Spectral Width	23809. 5
25 Lowest Frequency	-1843. 5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

6-Methyl-2-phenylchroman-4-one (Table 2, compound 2b)



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5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.8
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12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117
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15 Receiver Gain	76.5
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17 Pulse Width	12.0000
18 Presaturation Frequency	
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26 Nucleus	1H
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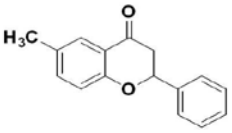

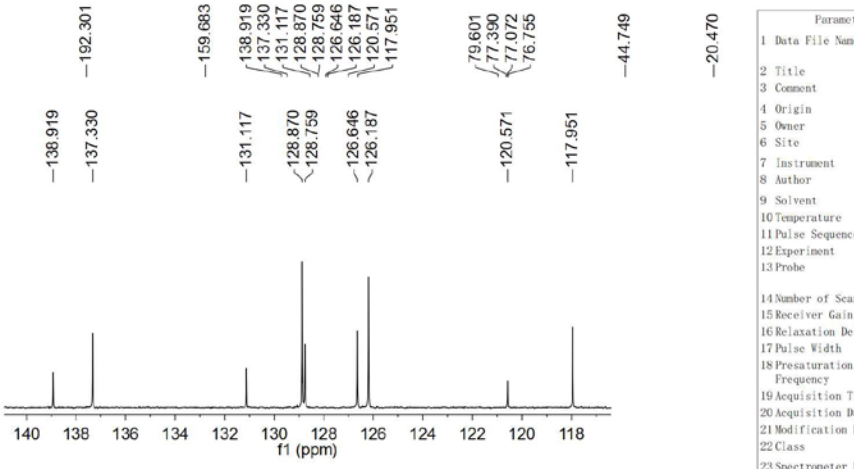

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6 Site	
7 Instrument	Avance
8 Author	
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11 Pulse Sequence	zgpg30
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13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
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19 Acquisition Time	1.3763
20 Acquisition Date	2019-03-28T14:25:36
21 Modification Date	2019-03-28T14:25:20
22 Class	
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24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
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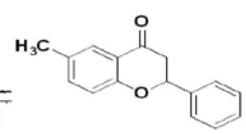
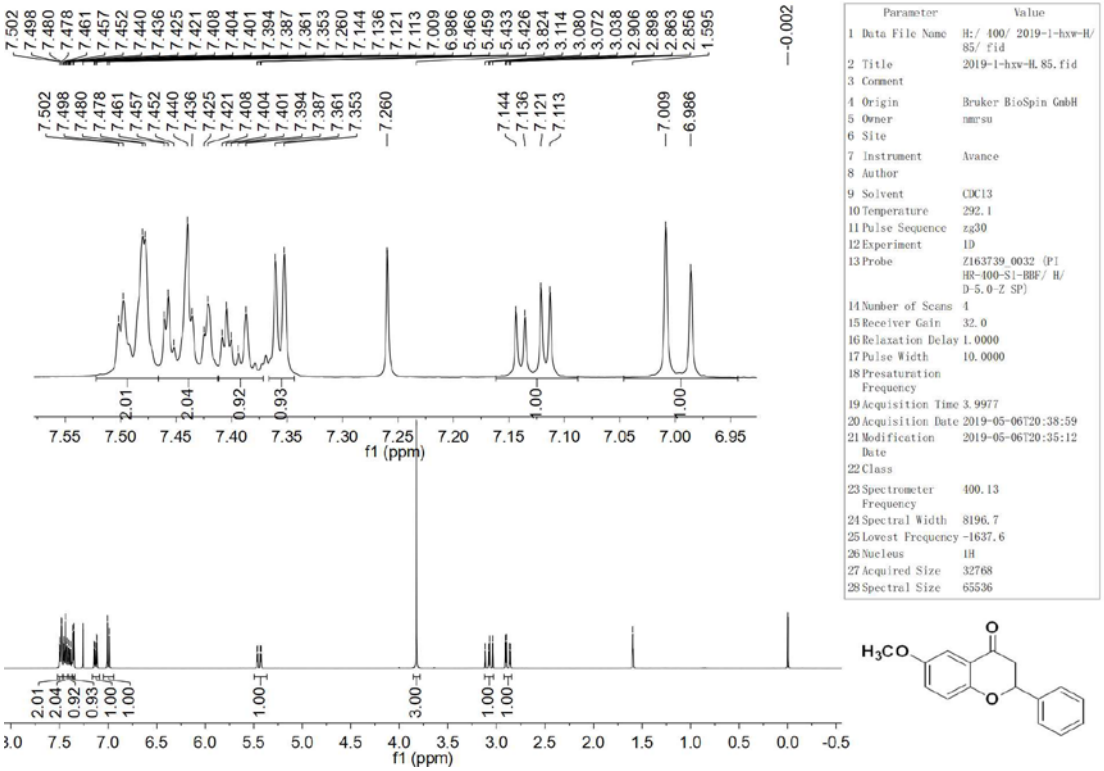


6-Methoxy-2-phenylchroman-4-one (Table 2, compound 2c)



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6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	292.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	32.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
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19 Acquisition Time	3.9977
20 Acquisition Date	2019-05-06T20:38:59
21 Modification Date	2019-05-06T20:35:12
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	1H
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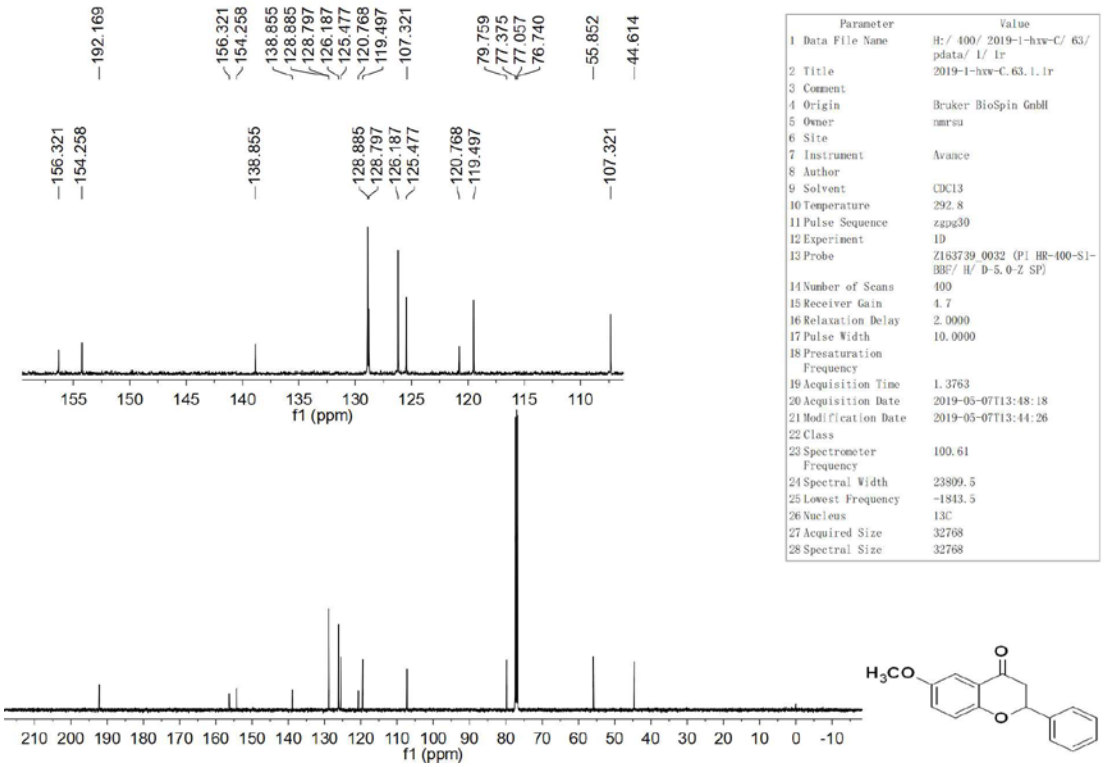
28 Spectral Size	65536



Parameter	Value
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5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	292.8
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17 Pulse Width	10.0000
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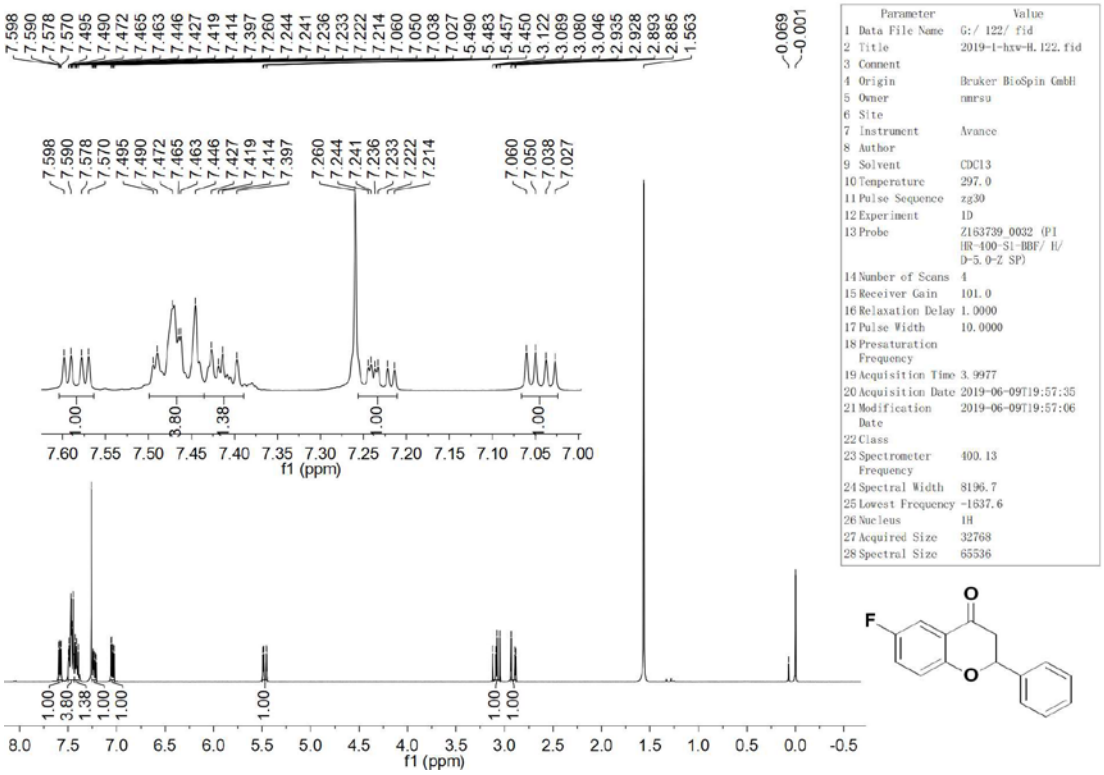
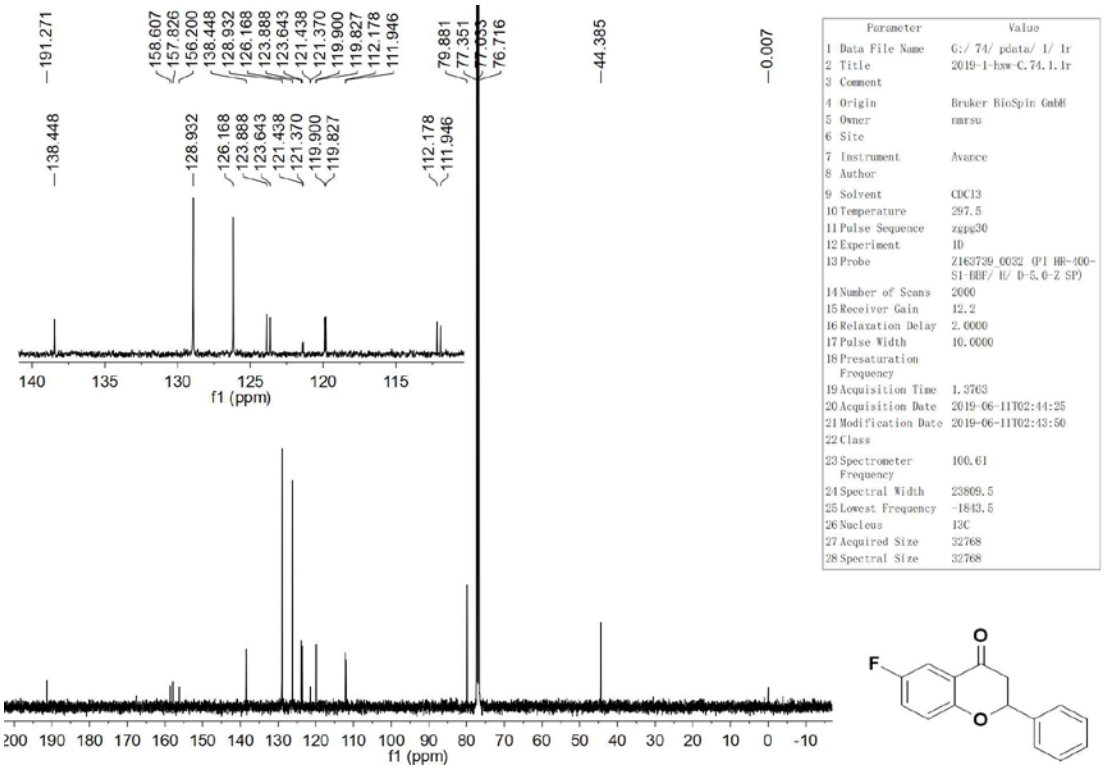
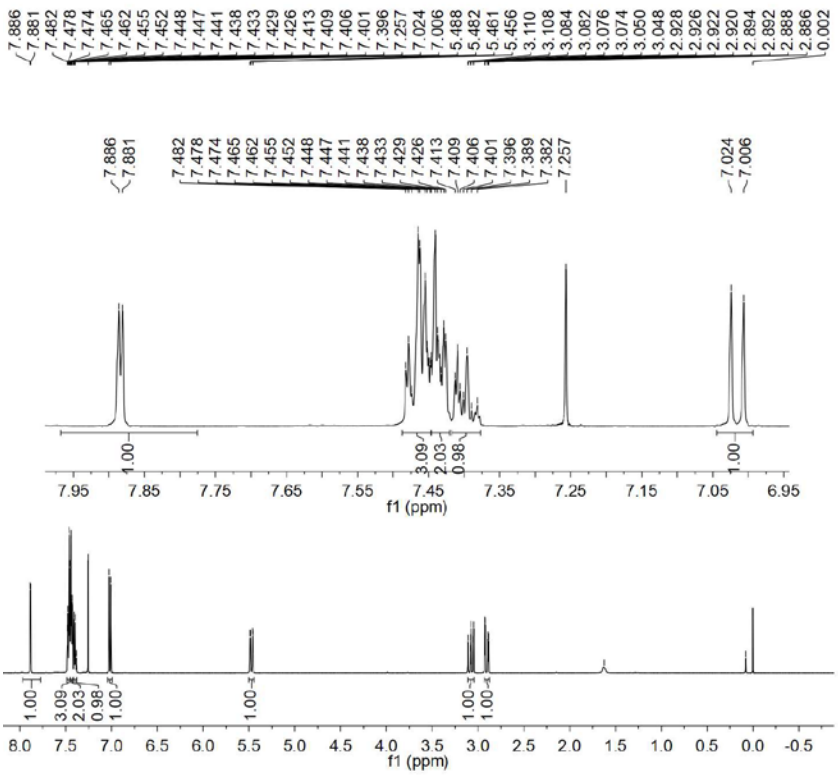
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

6-Fluoro-2-phenylchroman-4-one (Table 2, compound 2d)

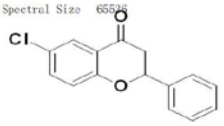


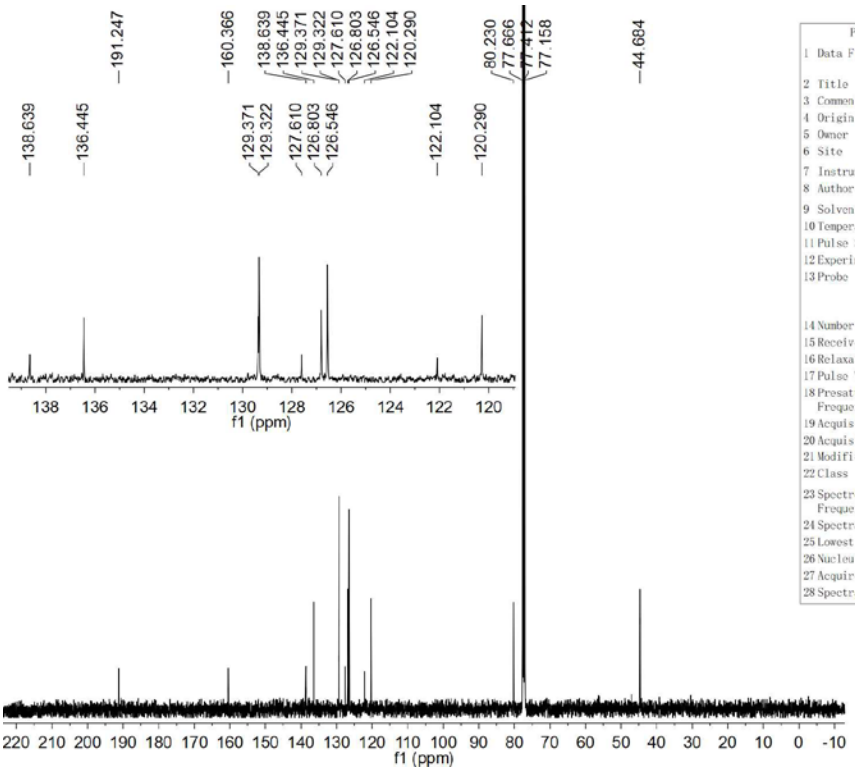


6-Chloro-2-phenylchroman-4-one (Table 2, compound 2e)

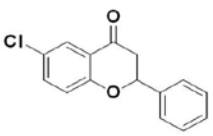


Parameter	Value
1 Data File Name	F:/ 处理的数据/ 2018-1-hxw-H/ 26/ fid
2 Title	2018-1-hxw-H. 26. fid
3 Comment	1H
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298. 4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117
14 Number of Scans	2
15 Receiver Gain	66. 5
16 Relaxation Delay	2. 0000
17 Pulse Width	12. 0000
18 Presaturation Frequency	
19 Acquisition Time	1. 8175
20 Acquisition Date	2018-06-12T10:03:00
21 Modification Date	2018-06-12T10:03:48
22 Class	
23 Spectrometer Frequency	500. 16
24 Spectral Width	9014. 4
25 Lowest Frequency	-1519. 4
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536

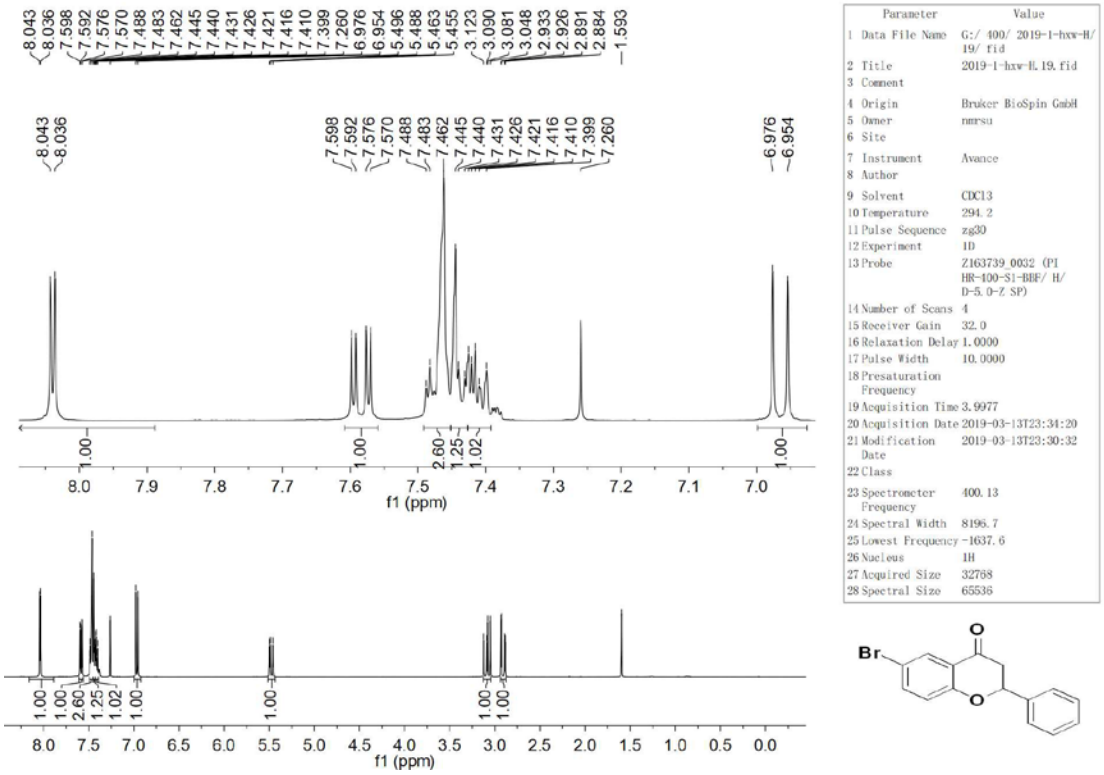




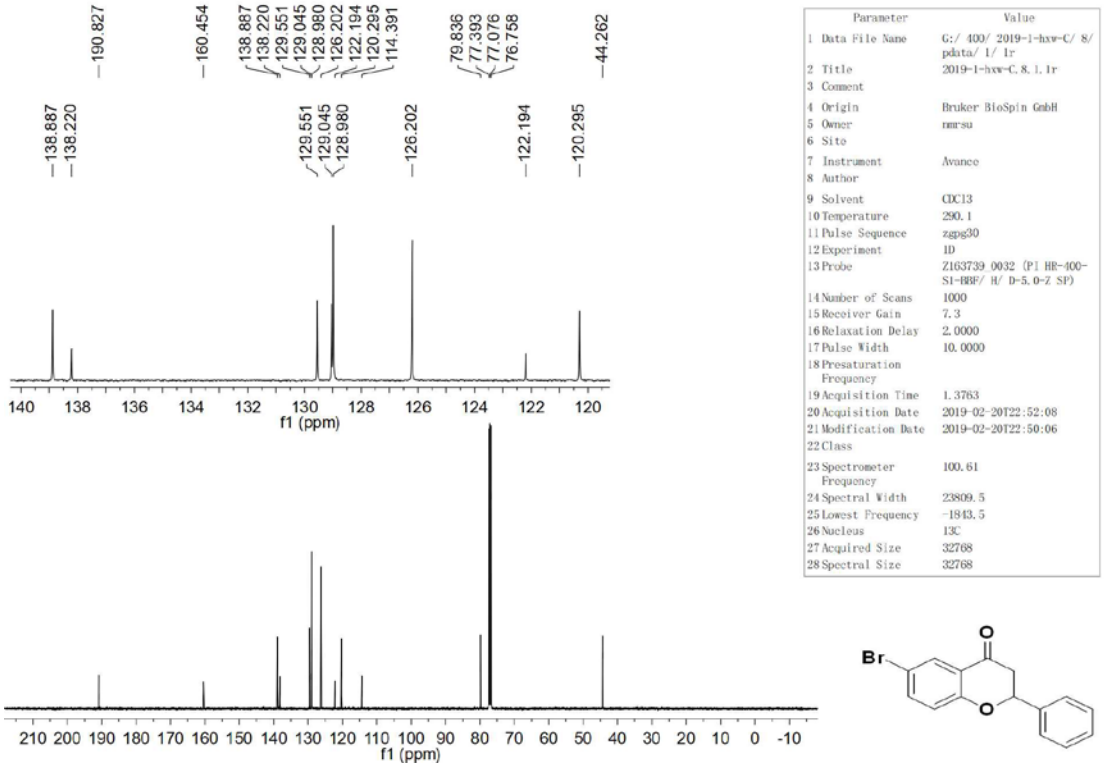
Parameter	Value
1 Data File Name	F:/ 处理的数据/ 2018-2-hxw-C/ 42/ fid
2 Title	2018-2-hxw-C. 42. fid
3 Comment	13C
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296. 5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117
14 Number of Scans	238
15 Receiver Gain	188. 8
16 Relaxation Delay	2. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	0. 5505
20 Acquisition Date	2018-09-06T09:46:00
21 Modification Date	2018-09-06T09:52:00
22 Class	
23 Spectrometer Frequency	125. 78
24 Spectral Width	29761. 9
25 Lowest Frequency	-1627. 5
26 Nucleus	13C
27 Acquired Size	16384
28 Spectral Size	65536



6-Bromo-2-phenylchroman-4-one (Table 2, compound 2f)

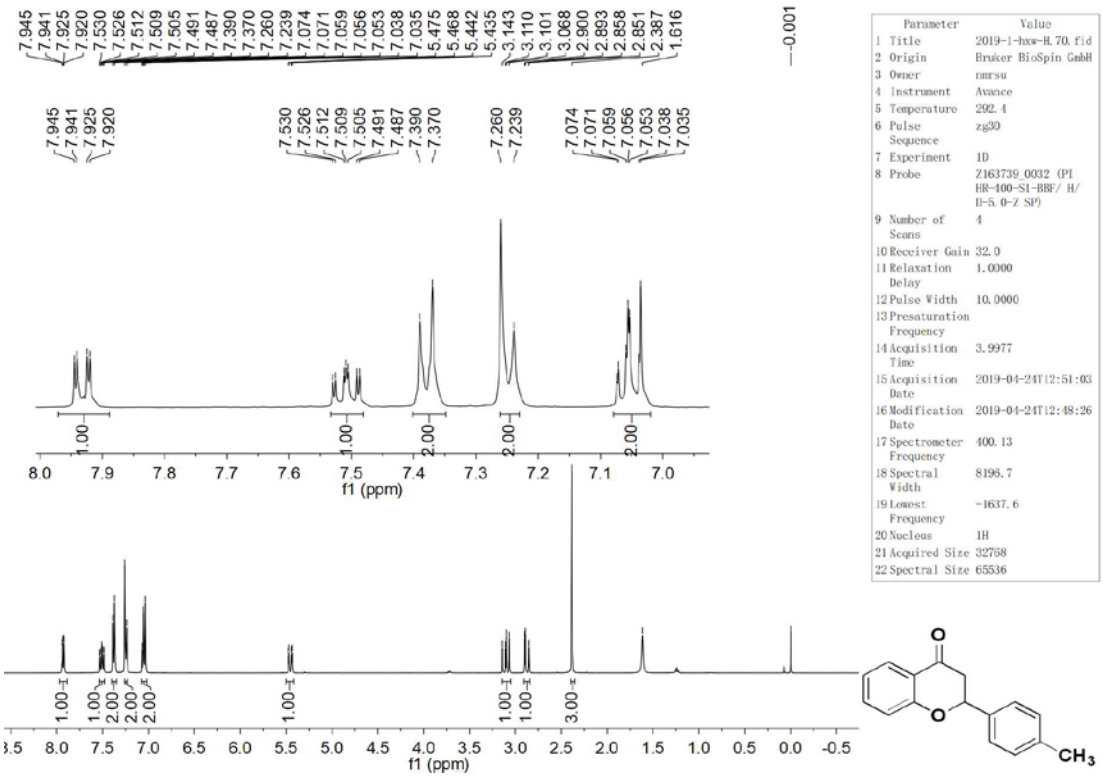


Parameter	Value
1 Data File Name	G:/ 400/ 2019-1-hxw-H/ 19/ fid
2 Title	2019-1-hxw-H. 19. fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	294. 2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5. 0-Z SP)
14 Number of Scans	4
15 Receiver Gain	32. 0
16 Relaxation Delay	1. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	3. 9977
20 Acquisition Date	2019-03-13T23:34:20
21 Modification Date	2019-03-13T23:30:32
22 Class	
23 Spectrometer Frequency	400. 13
24 Spectral Width	8196. 7
25 Lowest Frequency	-1637. 6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

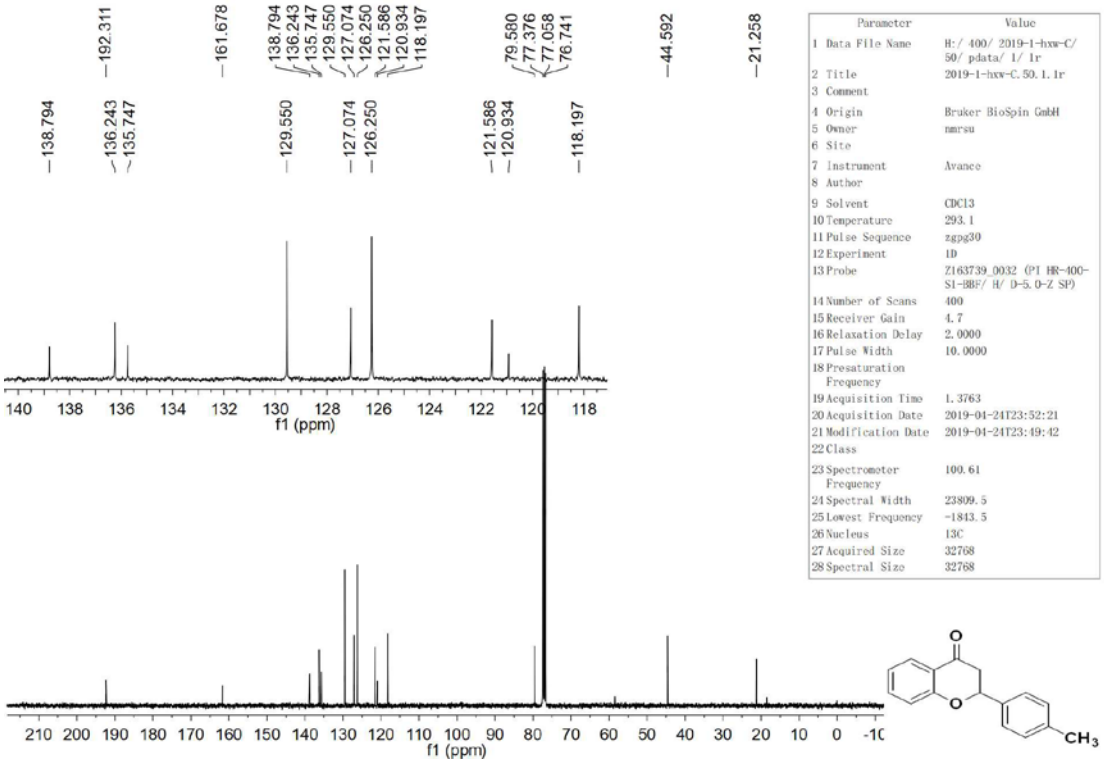


Parameter	Value
1 Data File Name	G:/ 400/ 2019-1-hxw-C/ 8/ pdata/ 1/ 1r
2 Title	2019-1-hxw-C. 8. 1. 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	290. 1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5. 0-Z SP)
14 Number of Scans	1000
15 Receiver Gain	7. 3
16 Relaxation Delay	2. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	1. 3763
20 Acquisition Date	2019-02-20T22:52:08
21 Modification Date	2019-02-20T22:50:06
22 Class	
23 Spectrometer Frequency	100. 61
24 Spectral Width	23809. 5
25 Lowest Frequency	-1843. 5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-(*p*-Tolyl)chroman-4-one (Table 2, compound 2g)

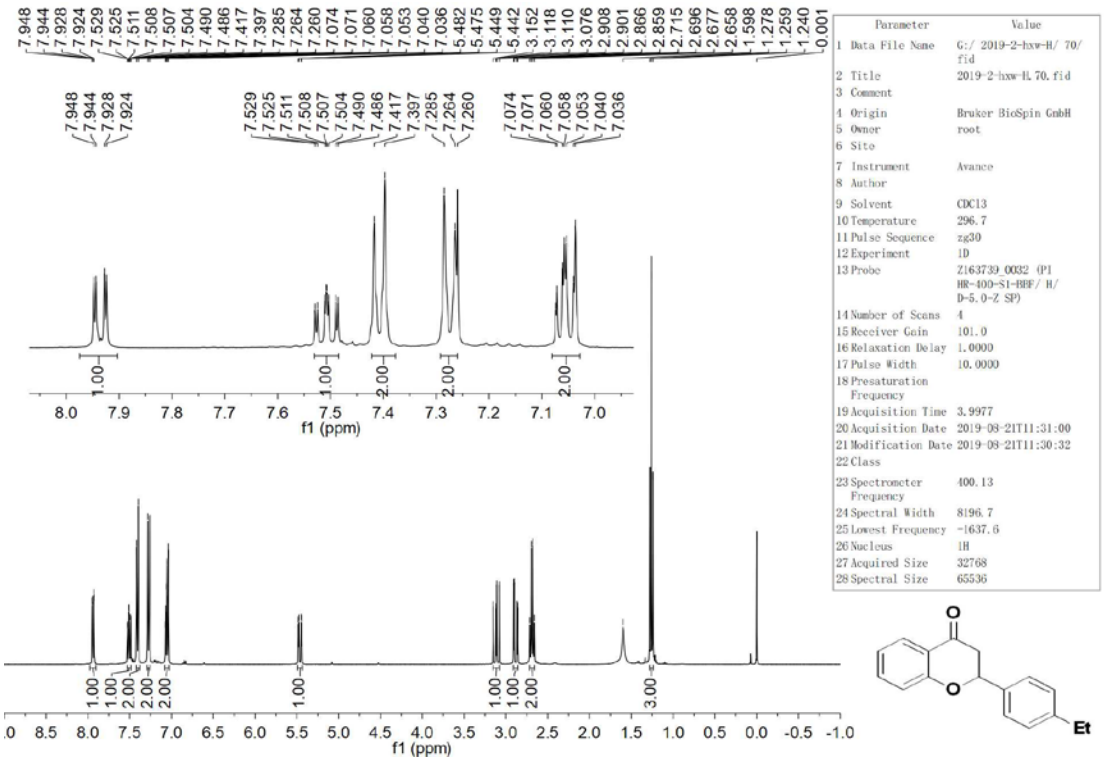


Parameter	Value
1 Title	2019-1-hxw-H. 70. fid
2 Origin	Bruker BioSpin GmbH
3 Owner	nmrsu
4 Instrument	Avance
5 Temperature	292. 4
6 Pulse Sequence	zg30
7 Experiment	1D
8 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5. 0-Z SP)
9 Number of Scans	4
10 Receiver Gain	32. 0
11 Relaxation Delay	1. 0000
12 Pulse Width	10. 0000
13 Presaturation Frequency	
14 Acquisition Time	3. 9977
15 Acquisition Date	2019-04-24T12:51:03
16 Modification Date	2019-04-24T12:48:26
17 Spectrometer Frequency	400. 13
18 Spectral Width	8196. 7
19 Lowest Frequency	-1637. 6
20 Nucleus	1H
21 Acquired Size	32768
22 Spectral Size	65536

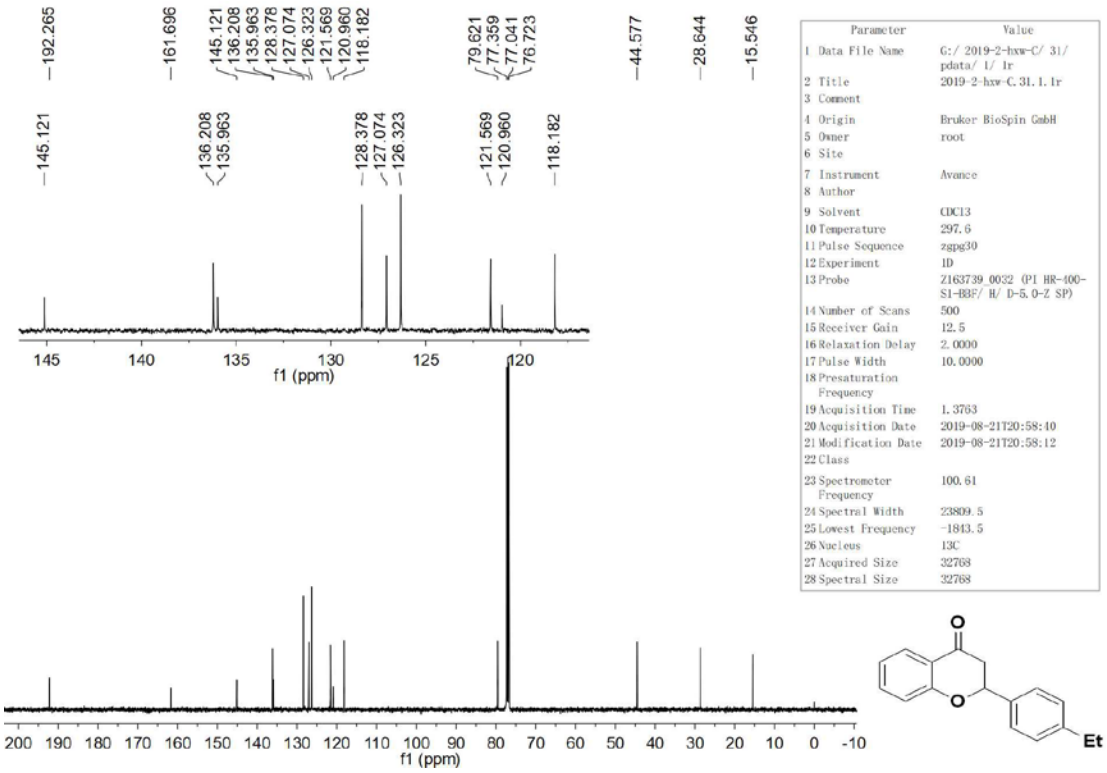


Parameter	Value
1 Data File Name	H:/ 400/ 2019-1-hxw-C/ 50/ pdata/ 1/ 1r
2 Title	2019-1-hxw-C. 50. 1. 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	293. 1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5. 0-Z SP)
14 Number of Scans	400
15 Receiver Gain	4. 7
16 Relaxation Delay	2. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	1. 3763
20 Acquisition Date	2019-04-24T23:52:21
21 Modification Date	2019-04-24T23:49:42
22 Class	
23 Spectrometer Frequency	100. 61
24 Spectral Width	23809. 5
25 Lowest Frequency	-1843. 5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-(4-Ethylphenyl)chroman-4-one (Table 2, compound 2h)

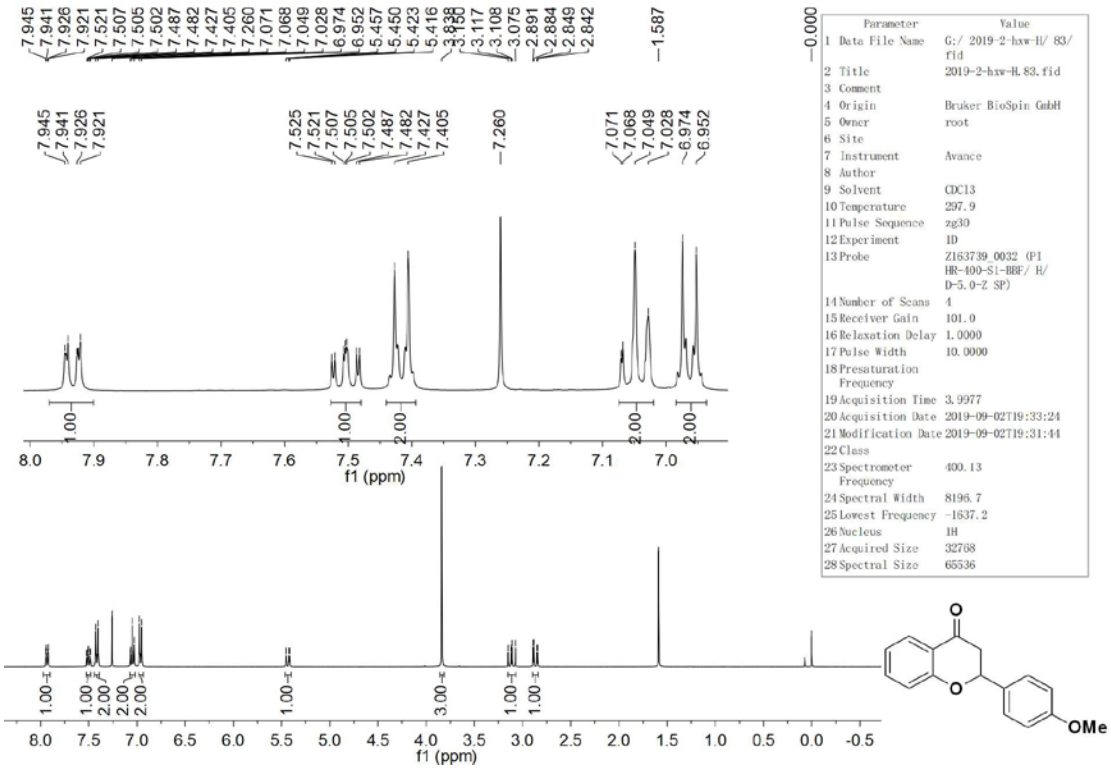


Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-H/ 70/ fid
2 Title	2019-2-hxw-H. 70. fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	296.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-08-21T11:31:00
21 Modification Date	2019-08-21T11:30:32
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

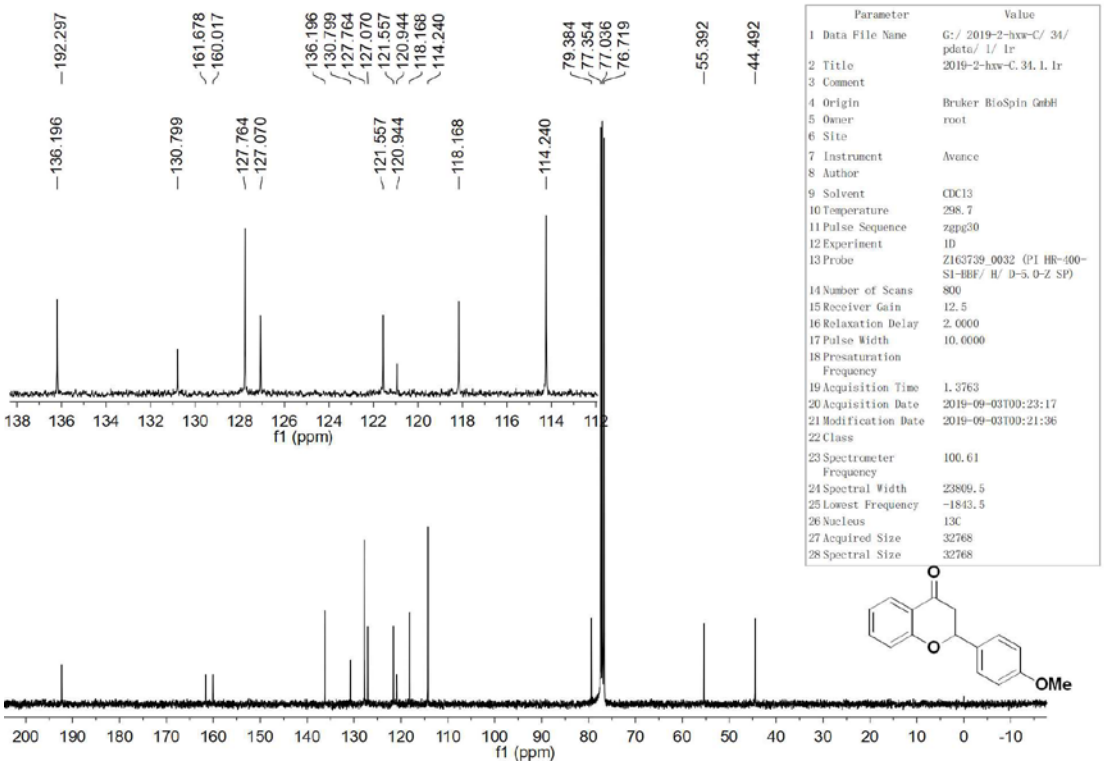


Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-C/ 31/ pdata/ 1/ 1r
2 Title	2019-2-hxw-C. 31. 1. 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	500
15 Receiver Gain	12.5
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-08-21T20:58:40
21 Modification Date	2019-08-21T20:58:12
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-(4-Methoxyphenyl)chroman-4-one (Table 2, compound 2i)

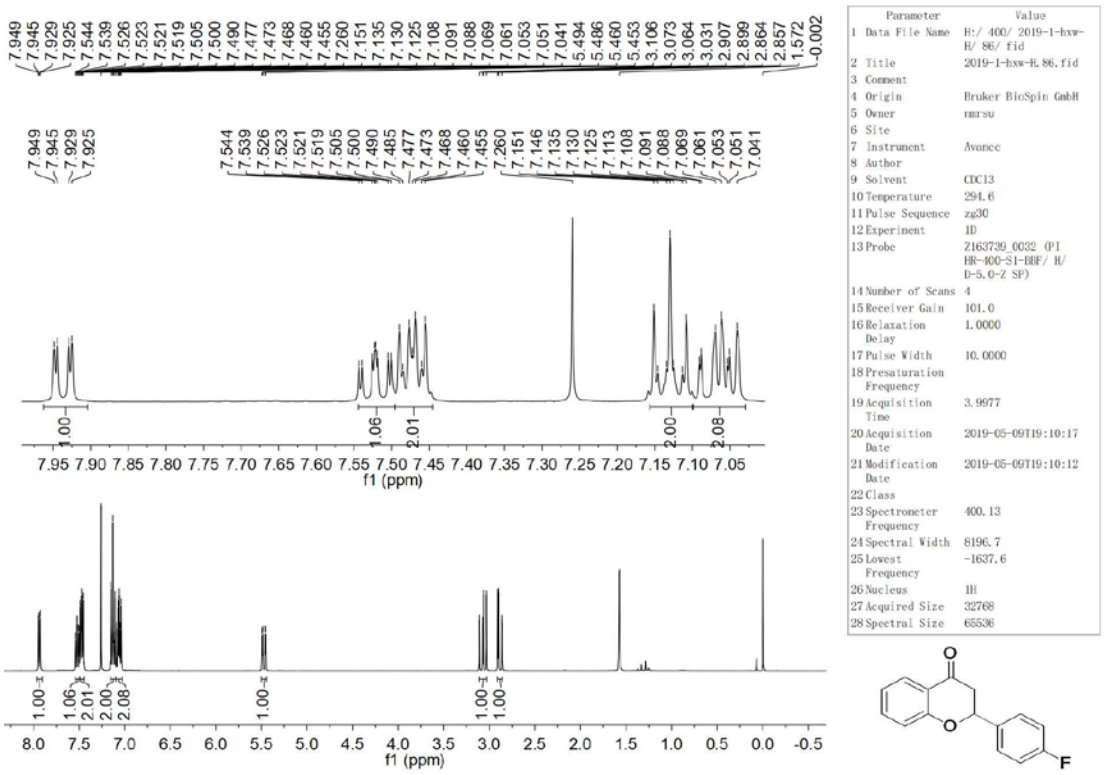


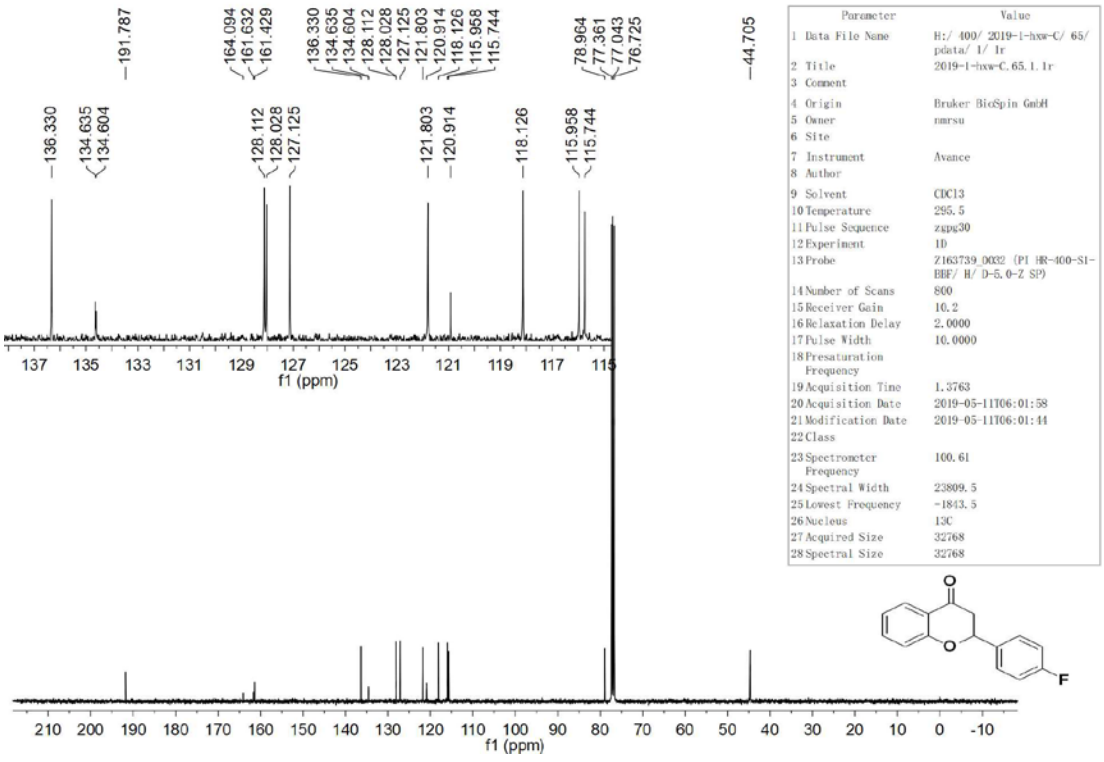
Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-H/ 83/ fid
2 Title	2019-2-hxw-H.83.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (P1 HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-09-02T19:33:24
21 Modification Date	2019-09-02T19:31:44
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



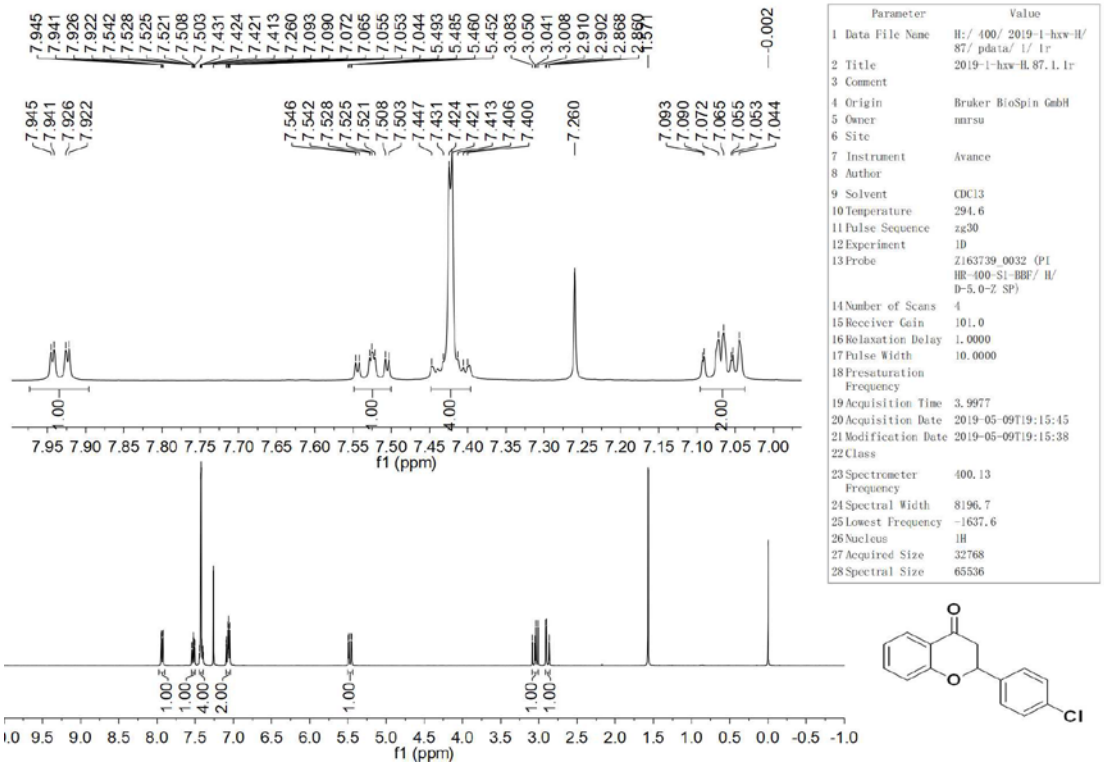
Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-C/ 34/ pdata/ 1/ 1r
2 Title	2019-2-hxw-C.34.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (P1 HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	800
15 Receiver Gain	12.5
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-09-03T00:23:17
21 Modification Date	2019-09-03T00:21:36
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-(4-Fluorophenyl)chroman-4-one (Table 2, compound 2j)

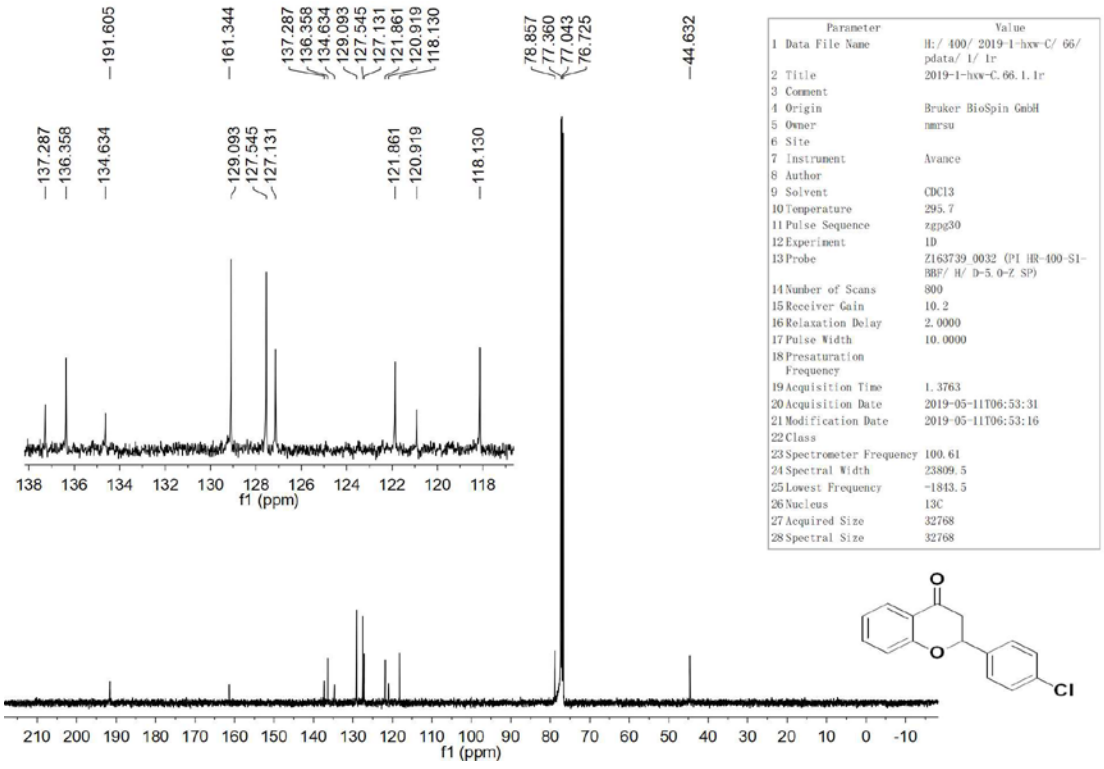




2-(4-Chlorophenyl)chroman-4-one (Table 2, compound 2k)

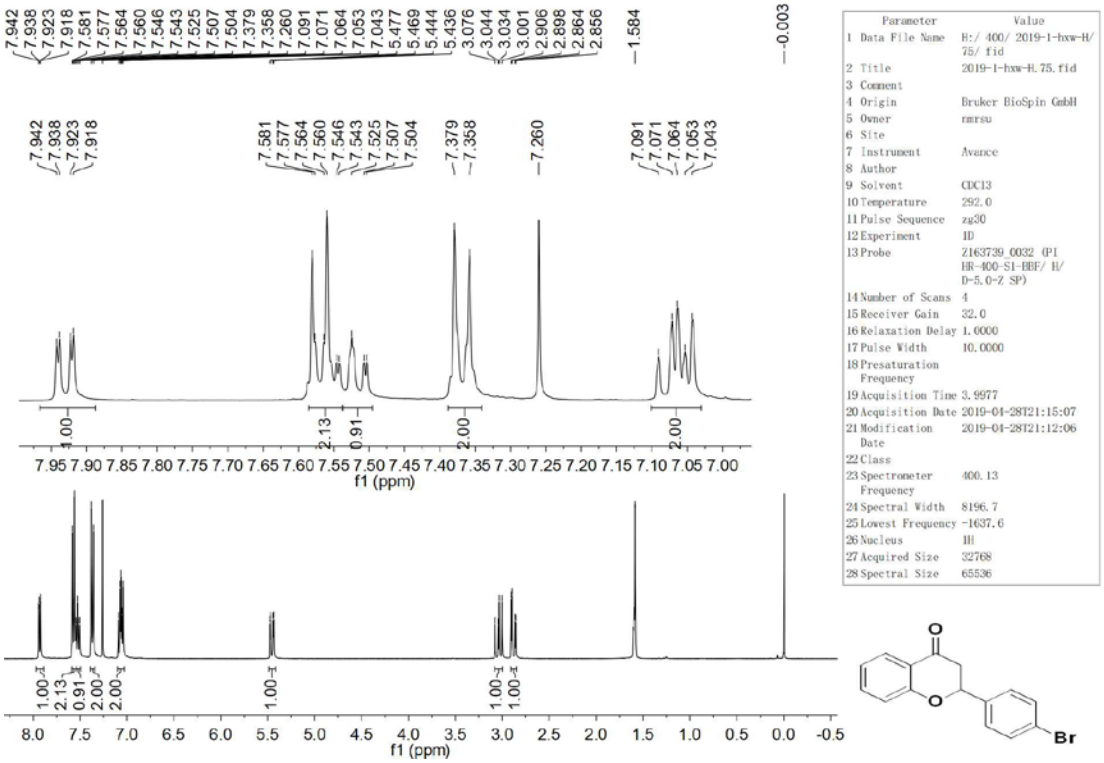


Parameter	Value
1 Data File Name	H:/ 400/ 2019-1-hxw-H/ 87/ pdata/ 1/ 1r
2 Title	2019-1-hxw-H. 87. 1. 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	294.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-05-09T19:15:45
21 Modification Date	2019-05-09T19:15:38
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

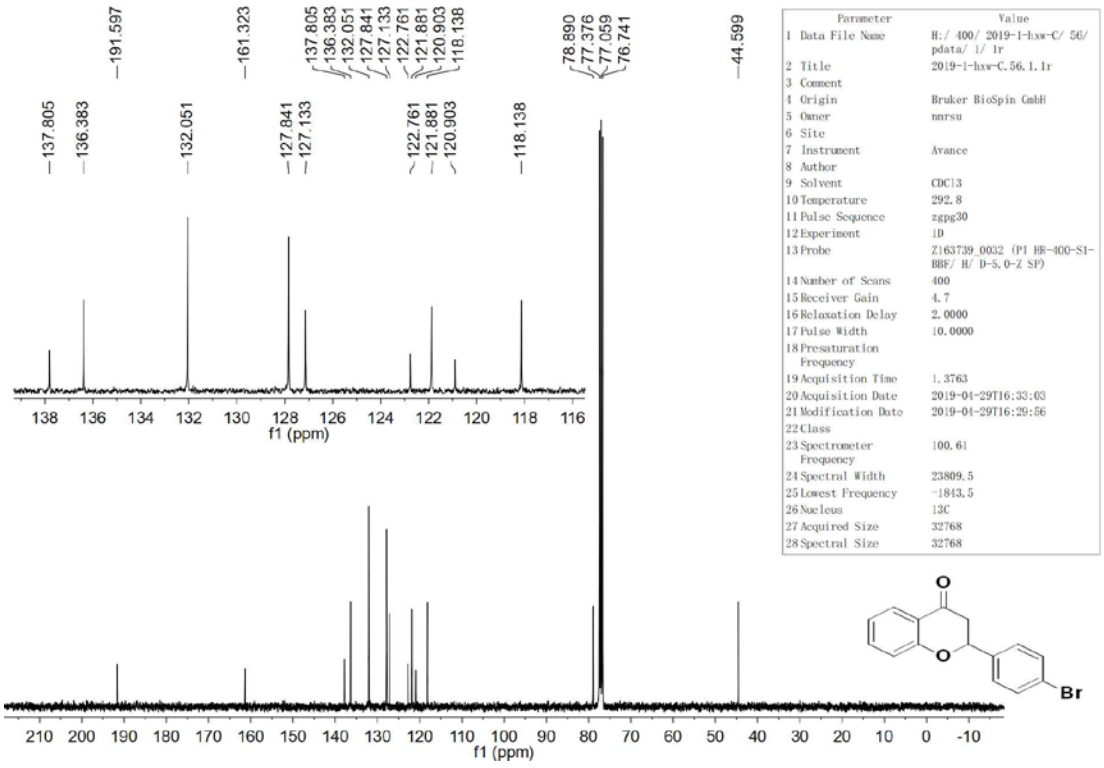


Parameter	Value
1 Data File Name	H:/ 400/ 2019-1-hxw-C/ 66/ pdata/ 1/ 1r
2 Title	2019-1-hxw-C. 66. 1. 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	295.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	800
15 Receiver Gain	10.2
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-05-11T06:53:31
21 Modification Date	2019-05-11T06:53:16
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-(4-Bromophenyl)chroman-4-one (Table 2, compound 2l)

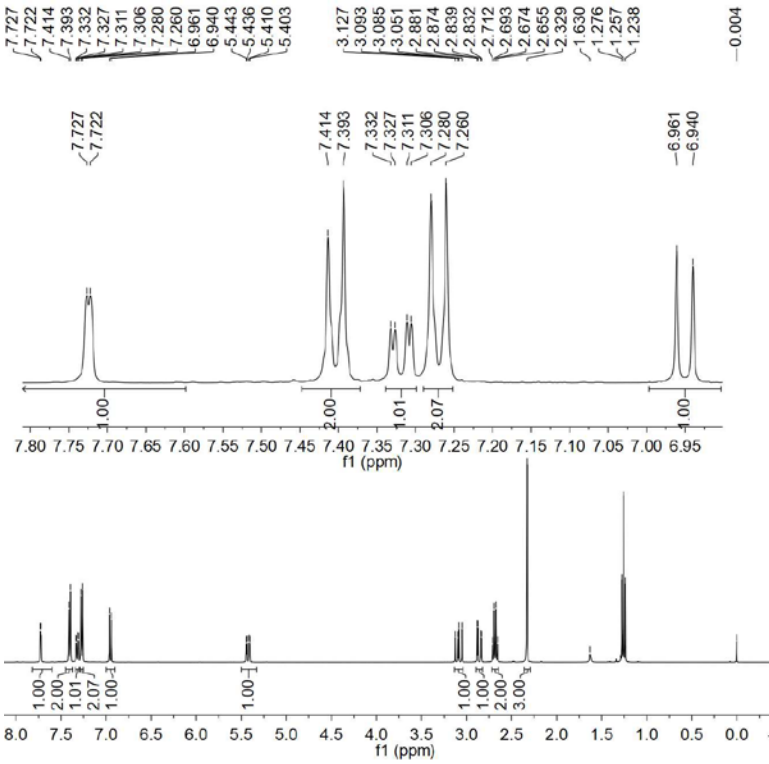


Parameter	Value
1 Data File Name	H:/ 400/ 2019-1-hxw-H/ 75/ fid
2 Title	2019-1-hxw-H.75.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	292.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	32.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-04-28T21:15:07
21 Modification Date	2019-04-28T21:12:06
22 Class	
23 Spectroneter Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

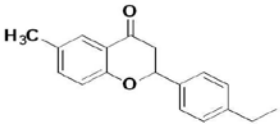


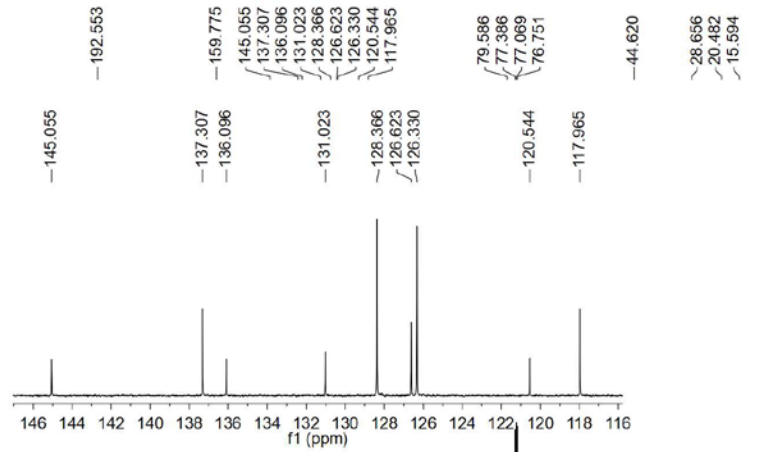
Parameter	Value
1 Data File Name	H:/ 400/ 2019-1-hxw-C/ 56/ pdata/ 1/ 1r
2 Title	2019-1-hxw-C.56.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	292.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	400
15 Receiver Gain	4.7
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-04-29T16:33:03
21 Modification Date	2019-04-29T16:29:56
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-(4-Ethylphenyl)-6-methylchroman-4-one (Table 2, compound 2m)

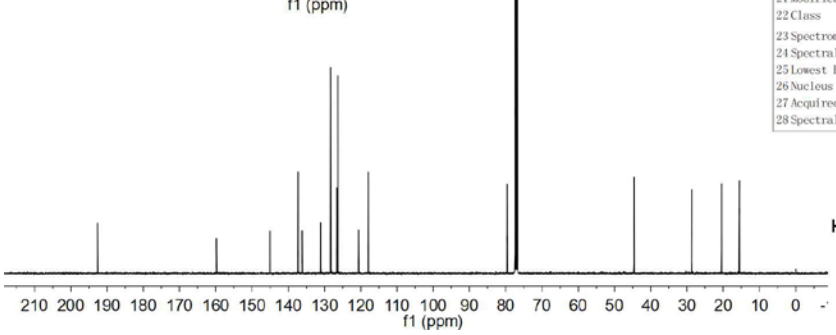


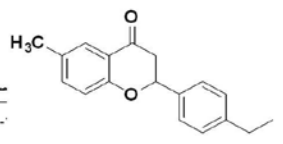
Parameter	Value
1 Data File Name	H:/ 480/ fid
2 Title	2019-1-syj-H 480. fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	292.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739 0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	32.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-05-05T14:34:03
21 Modification Date	2019-05-05T14:30:22
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



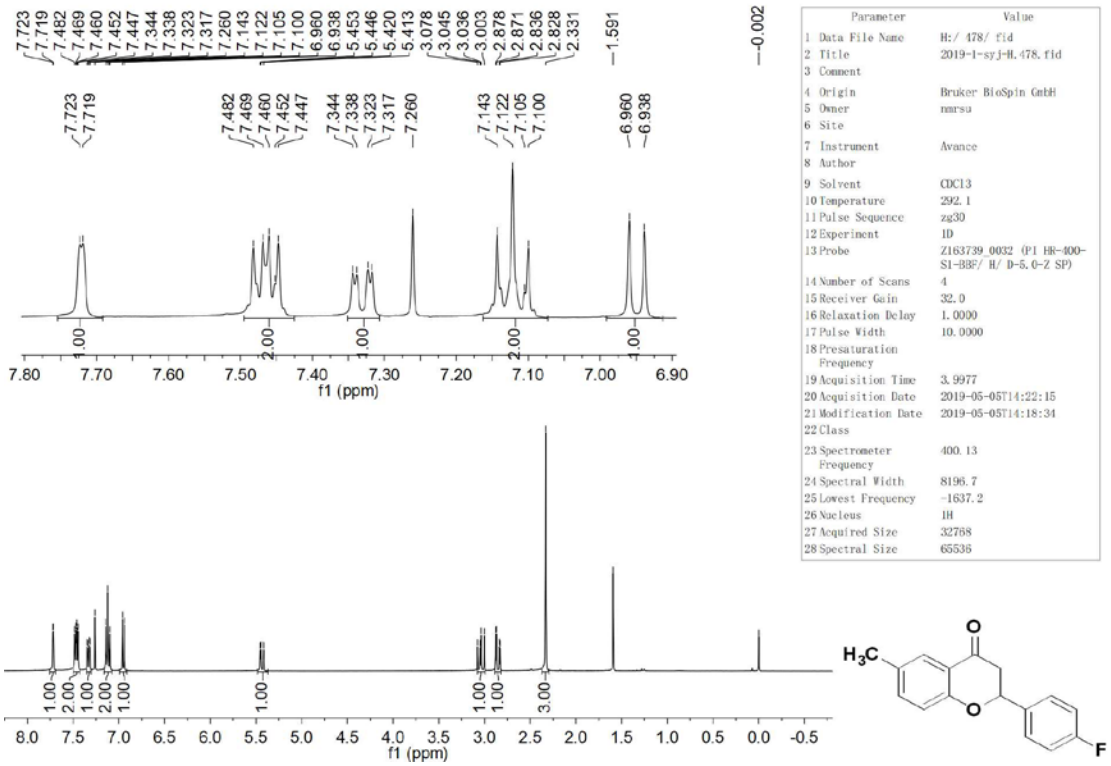


Parameter	Value
1 Data File Name	H:/ 400/ 2019-1-hxw-C/ 61/ pdata/ 1/ 1r
2 Title	2019-1-hxw-C. 61. 1. 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	292.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	800
15 Receiver Gain	7.3
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-05-06T00:23:08
21 Modification Date	2019-05-06T00:19:26
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

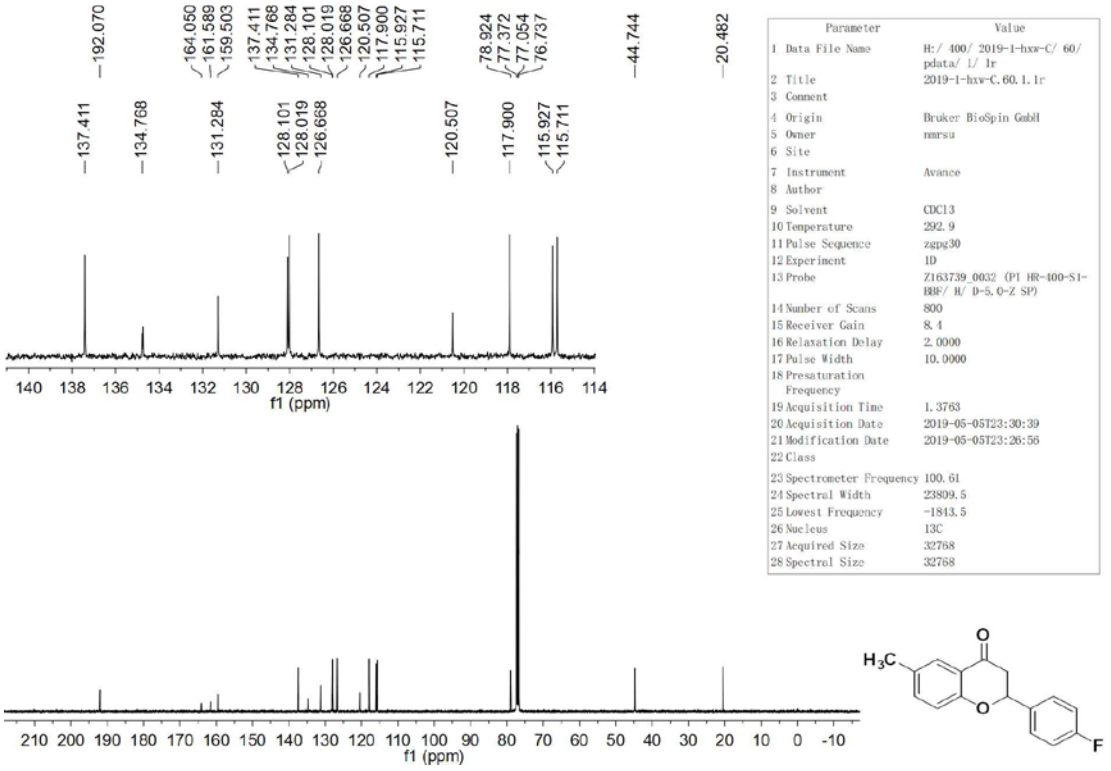




2-(4-Fluorophenyl)-6-methylchroman-4-one (Table 2, compound 2n)

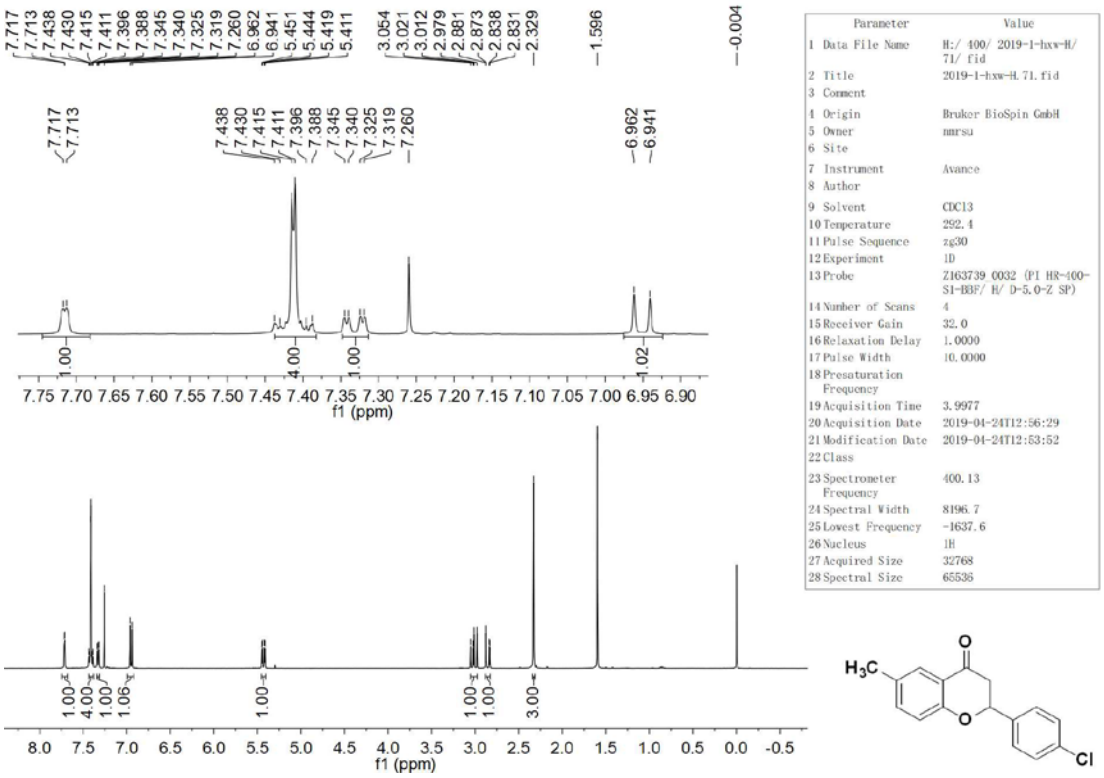


Parameter	Value
1 Data File Name	H:/ 478/ fid
2 Title	2019-1-syj-H. 478. fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	292. 1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5. 0-Z SP)
14 Number of Scans	4
15 Receiver Gain	32. 0
16 Relaxation Delay	1. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	3. 9977
20 Acquisition Date	2019-05-05T14:22:15
21 Modification Date	2019-05-05T14:18:34
22 Class	
23 Spectrometer Frequency	400. 13
24 Spectral Width	8196. 7
25 Lowest Frequency	-1637. 2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

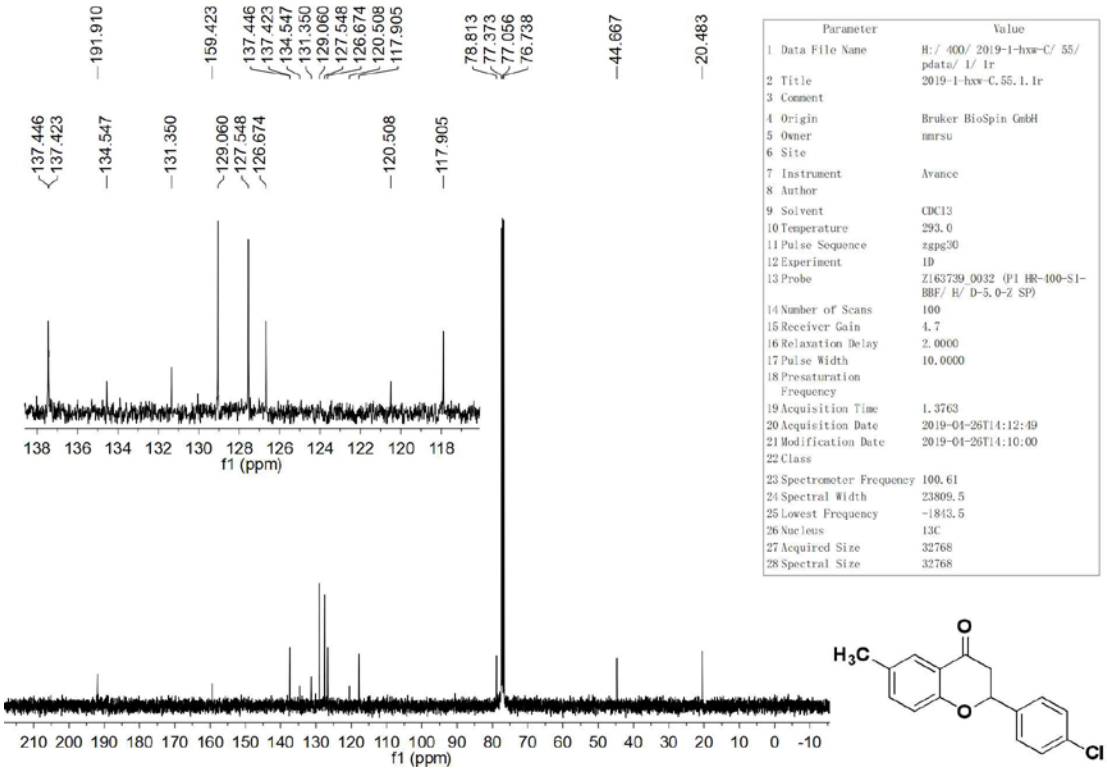


Parameter	Value
1 Data File Name	H:/ 400/ 2019-1-hxw-C/ 60/ pdata/ 1/ 1r
2 Title	2019-1-hxw-C. 60. 1. 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	292. 9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5. 0-Z SP)
14 Number of Scans	800
15 Receiver Gain	8. 4
16 Relaxation Delay	2. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	1. 3763
20 Acquisition Date	2019-05-05T23:30:39
21 Modification Date	2019-05-05T23:26:56
22 Class	
23 Spectrometer Frequency	100. 61
24 Spectral Width	23809. 5
25 Lowest Frequency	-1843. 5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-(4-Chlorophenyl)-6-methylchroman-4-one (Table 2, compound 2o)

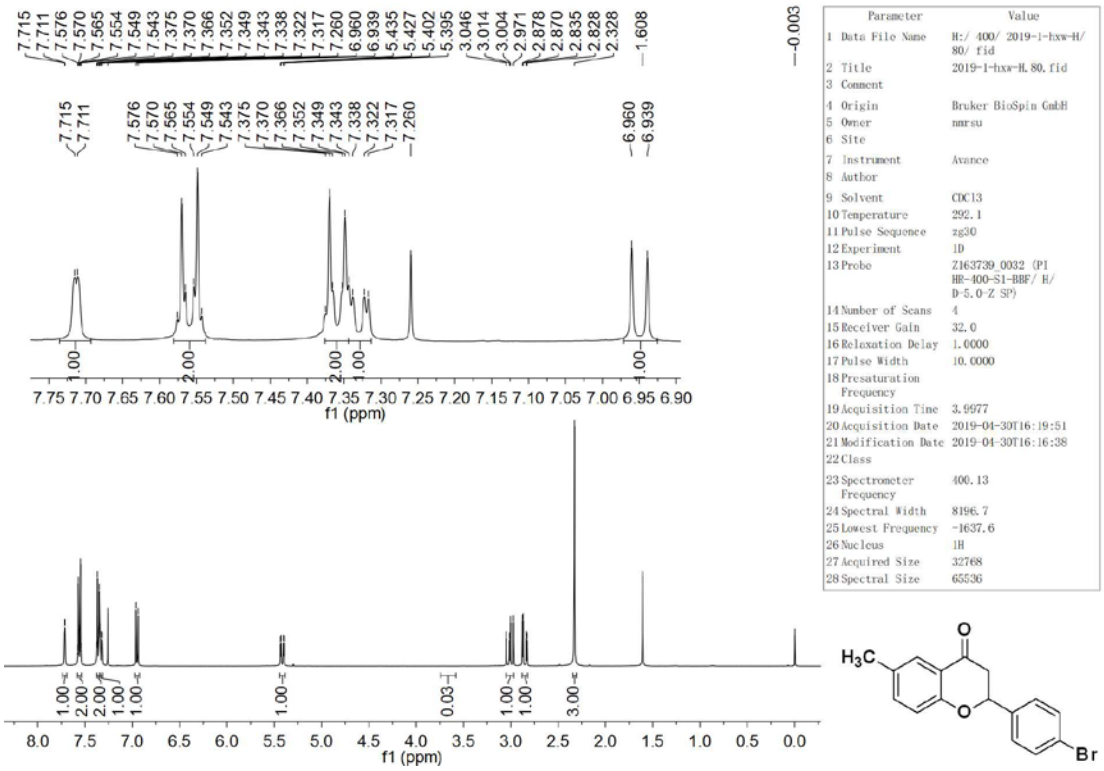


Parameter	Value
1 Data File Name	H:/ 400/ 2019-1-hxw-H/ 71/ fid
2 Title	2019-1-hxw-H. 71. fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	292. 4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5. 0-Z SP)
14 Number of Scans	4
15 Receiver Gain	32. 0
16 Relaxation Delay	1. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	3. 9977
20 Acquisition Date	2019-04-24T12:56:29
21 Modification Date	2019-04-24T12:53:52
22 Class	
23 Spectrometer Frequency	400. 13
24 Spectral Width	8196. 7
25 Lowest Frequency	-1637. 6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

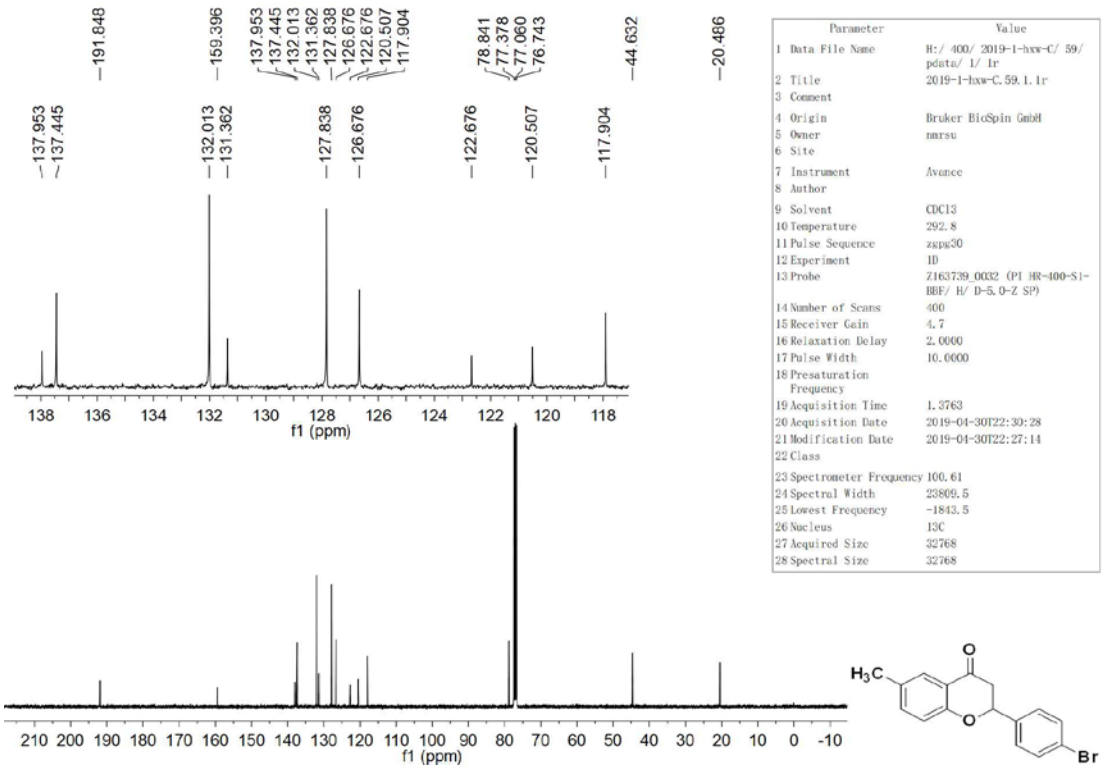


Parameter	Value
1 Data File Name	H:/ 400/ 2019-1-hxw-C/ 55/ pdata/ 1/ 1r
2 Title	2019-1-hxw-C. 55. 1. 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	293. 0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5. 0-Z SP)
14 Number of Scans	100
15 Receiver Gain	4. 7
16 Relaxation Delay	2. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	1. 3763
20 Acquisition Date	2019-04-26T14:12:49
21 Modification Date	2019-04-26T14:10:00
22 Class	
23 Spectrometer Frequency	100. 61
24 Spectral Width	23809. 5
25 Lowest Frequency	-1843. 5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-(4-Bromophenyl)-6-methylchroman-4-one (Table 2, compound 2p)

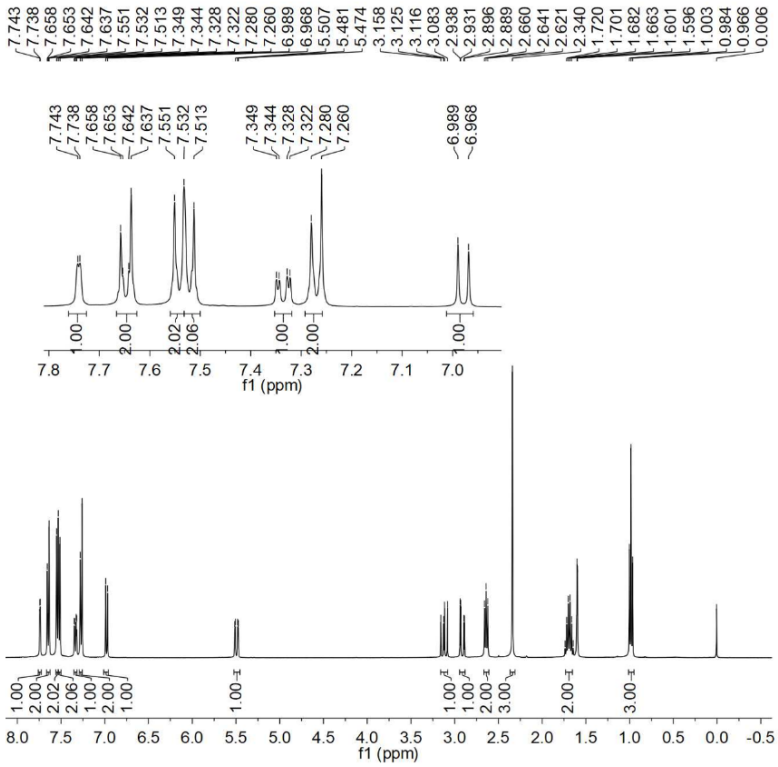


Parameter	Value
1 Data File Name	H:/ 400/ 2019-1-hxw-H/ 80/ fid
2 Title	2019-1-hxw-H, 80, fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	292.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	32.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-04-30T16:19:51
21 Modification Date	2019-04-30T16:16:38
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

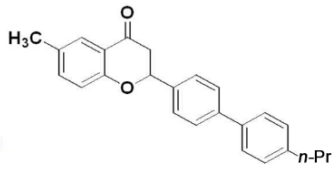


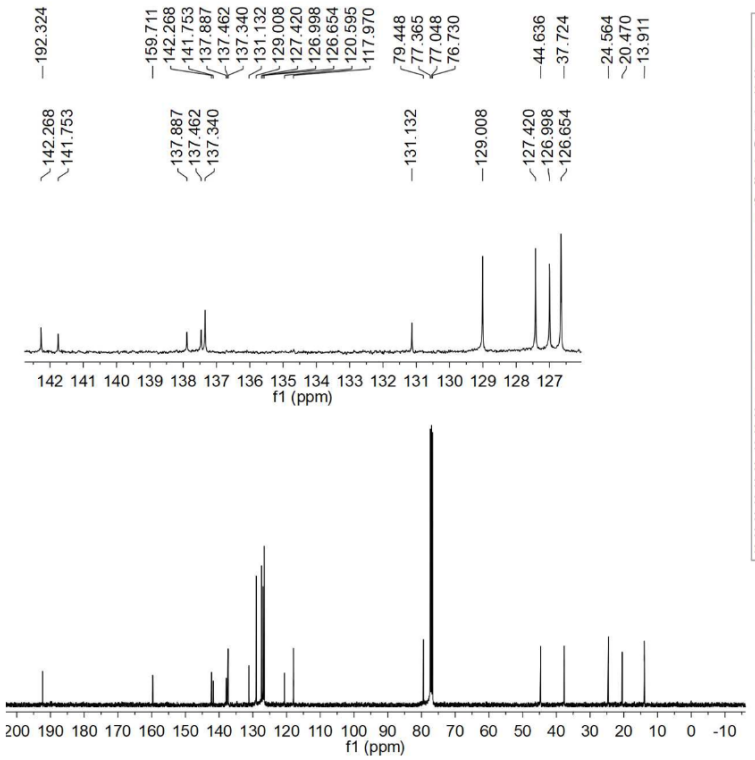
Parameter	Value
1 Data File Name	H:/ 400/ 2019-1-hxw-C/ 59/ pdata/ 1/ 1r
2 Title	2019-1-hxw-C, 59, 1, 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	292.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	400
15 Receiver Gain	4.7
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-04-30T22:30:28
21 Modification Date	2019-04-30T22:27:14
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

6-Methyl-2-(4'-propyl-[1,1'-biphenyl]-4-yl)chroman-4-one (Table 2, compound 2q)

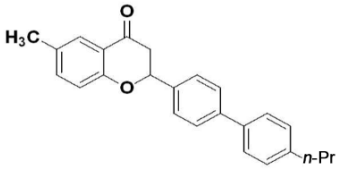


Parameter	Value
1 Data File Name	F:/ 处理的数据/ 2019-2-hxw-H/ 31/ fid
2 Title	2019-2-hxw-H.31.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	296.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (P1 HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-07-08T07:40:06
21 Modification Date	2019-07-08T07:39:20
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

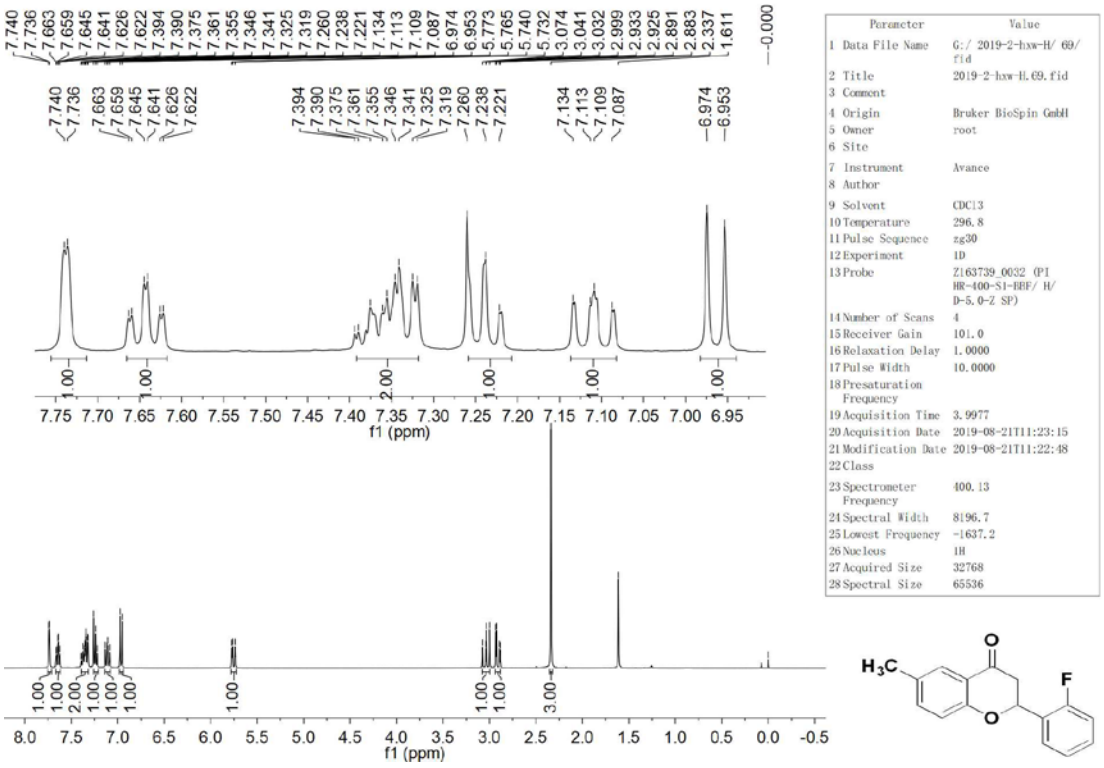




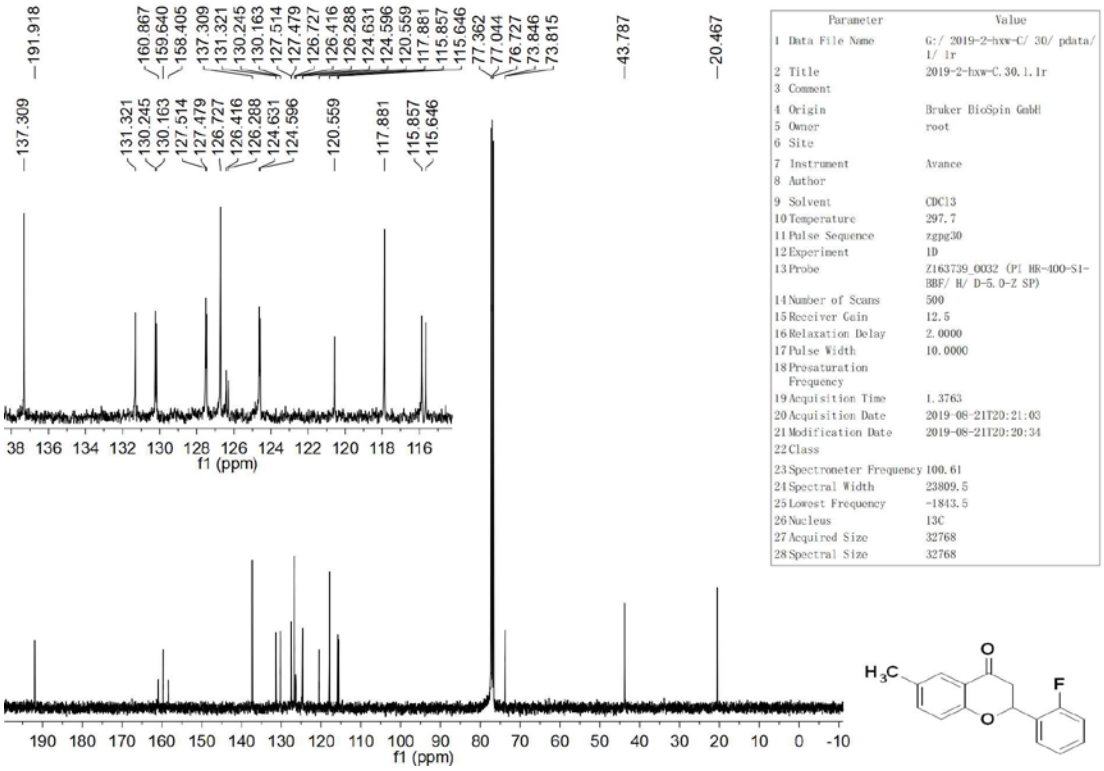
Parameter	Value
1 Data File Name	F:/ 处理的数据/ 2019-2-hxw-H/ 37/ pdata/ 1/ 1r
2 Title	2019-2-hxw-H.37.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (P1 HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	600
15 Receiver Gain	14.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-07-08T21:12:18
21 Modification Date	2019-07-08T21:11:28
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768



2-(2-Fluorophenyl)chroman-4-one (Table 2, compound 2r)

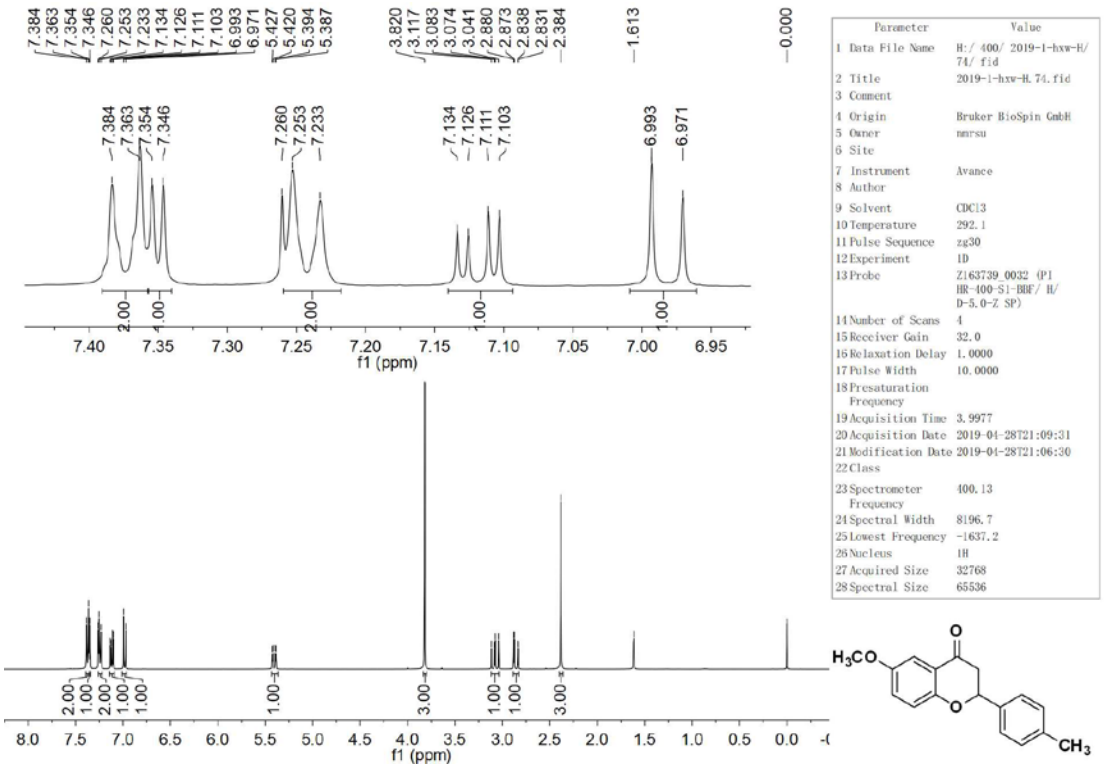


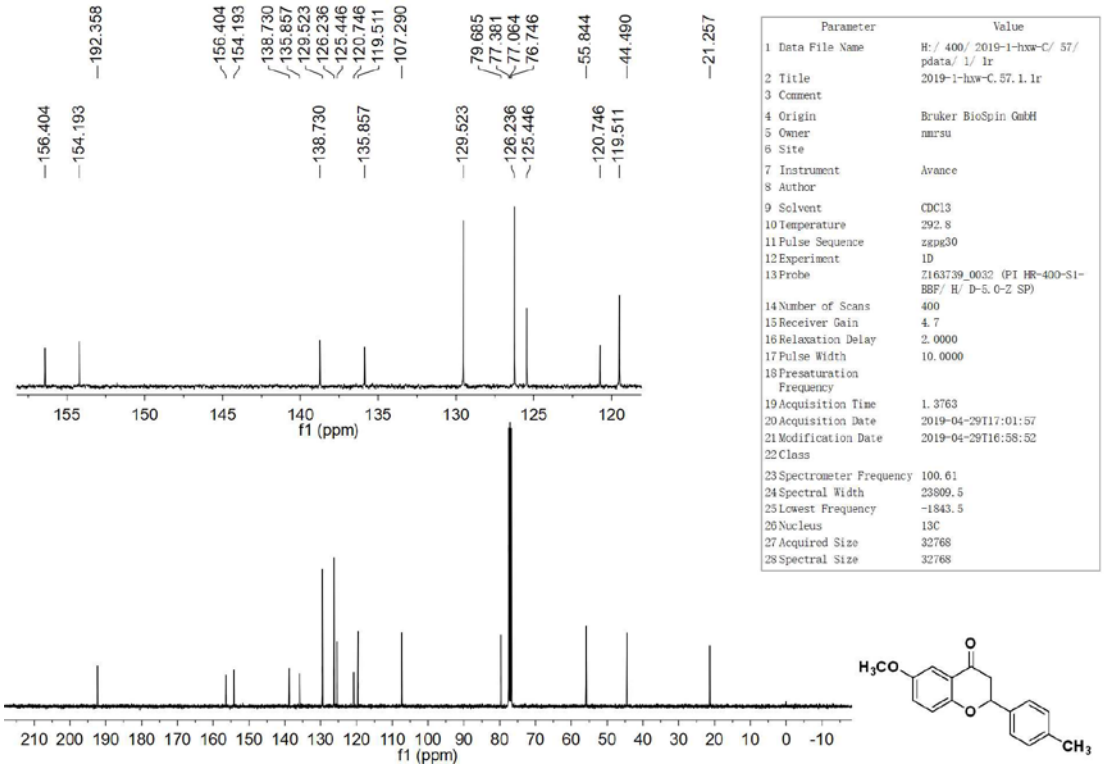
Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-H/ 69/ fid
2 Title	2019-2-hxw-H.69.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	296.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-08-21T11:23:15
21 Modification Date	2019-08-21T11:22:48
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



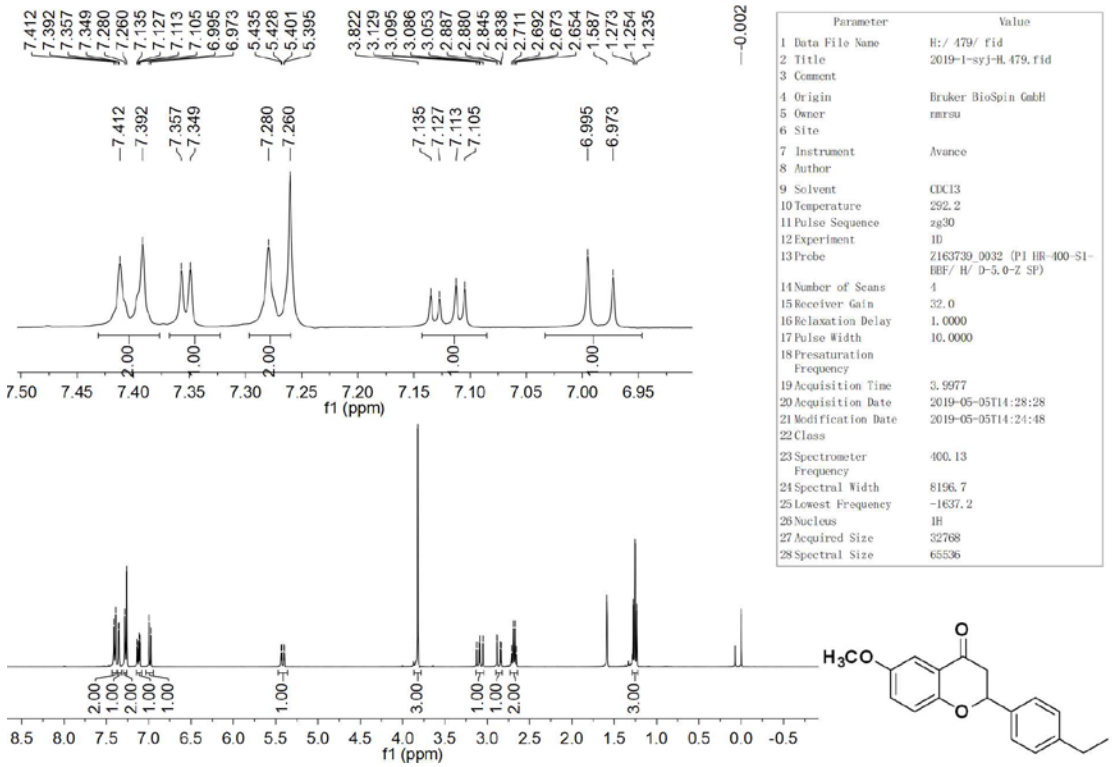
Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-C/ 30/ pdata/ 1/ 1r
2 Title	2019-2-hxw-C.30.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	500
15 Receiver Gain	12.5
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-08-21T20:21:03
21 Modification Date	2019-08-21T20:20:34
22 Class	
23 Spectroneter Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

6-Methoxy-2-(p-tolyl)chroman-4-one (Table 2, compound 2s)

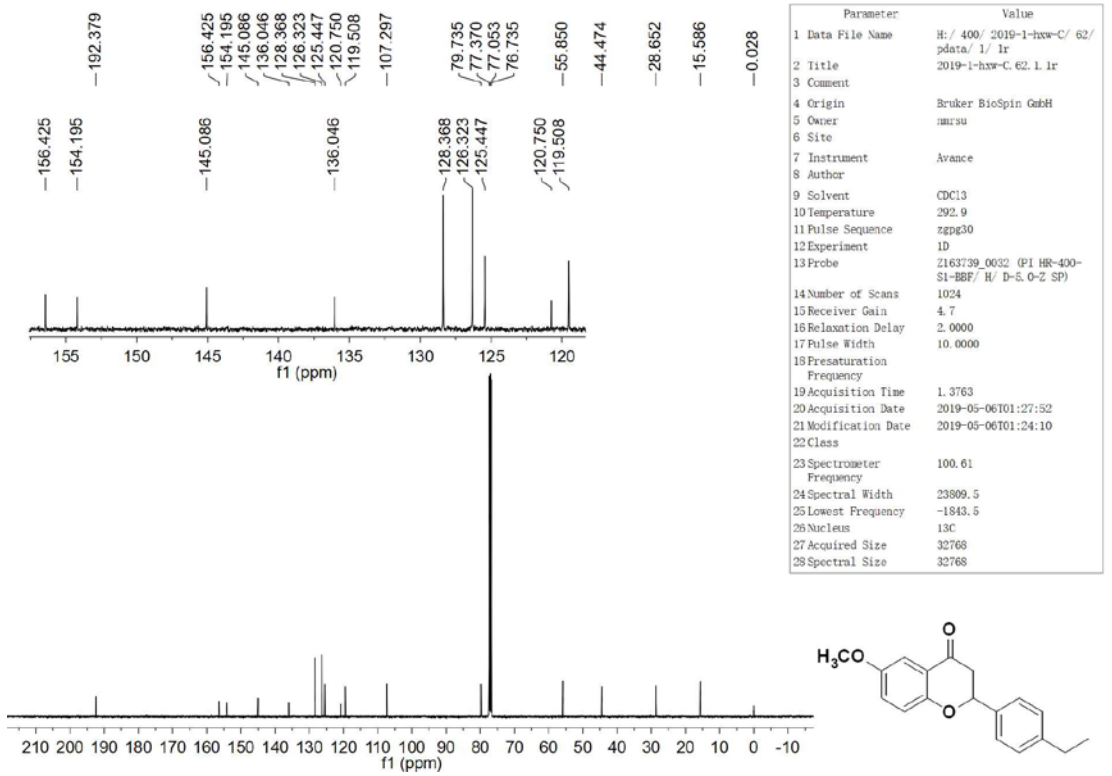




2-(4-Ethylphenyl)-6-methoxychroman-4-one (Table 2, compound 2t)

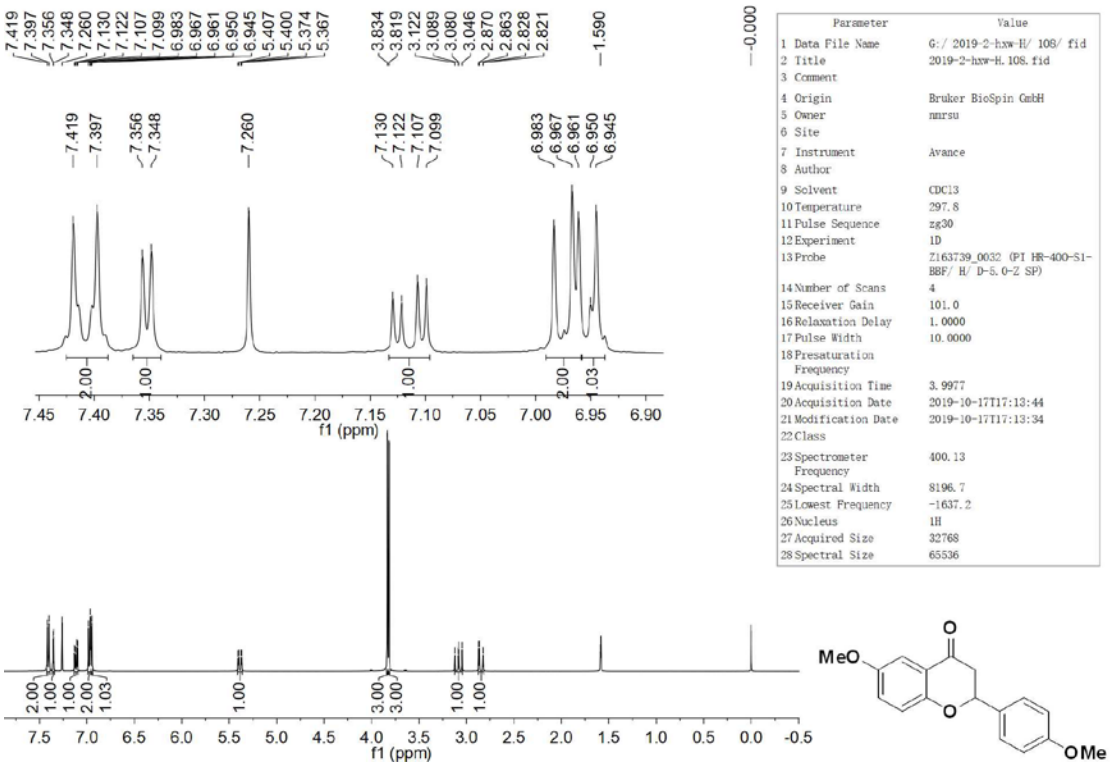


Parameter	Value
1 Data File Name	H:/ 479/ fid
2 Title	2019-1-syj-H 479.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	292.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	32.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-05-05T14:28:28
21 Modification Date	2019-05-05T14:24:48
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

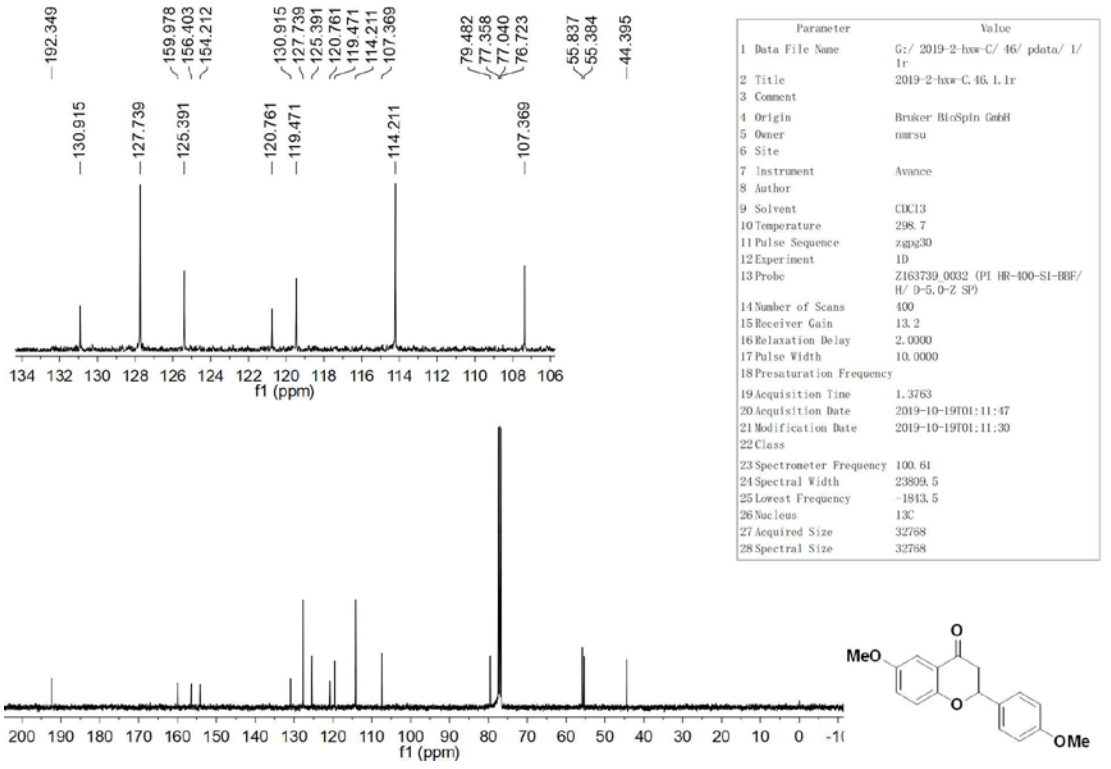


Parameter	Value
1 Data File Name	H:/ 400/ 2019-1-hxw-C/ 62/ pdata/ 1/ 1r
2 Title	2019-1-hxw-C.62.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	292.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	1024
15 Receiver Gain	4.7
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-05-06T01:27:52
21 Modification Date	2019-05-06T01:24:10
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

6-Methoxy-2-(4-methoxyphenyl)chroman-4-one (Table 2, compound 2u)

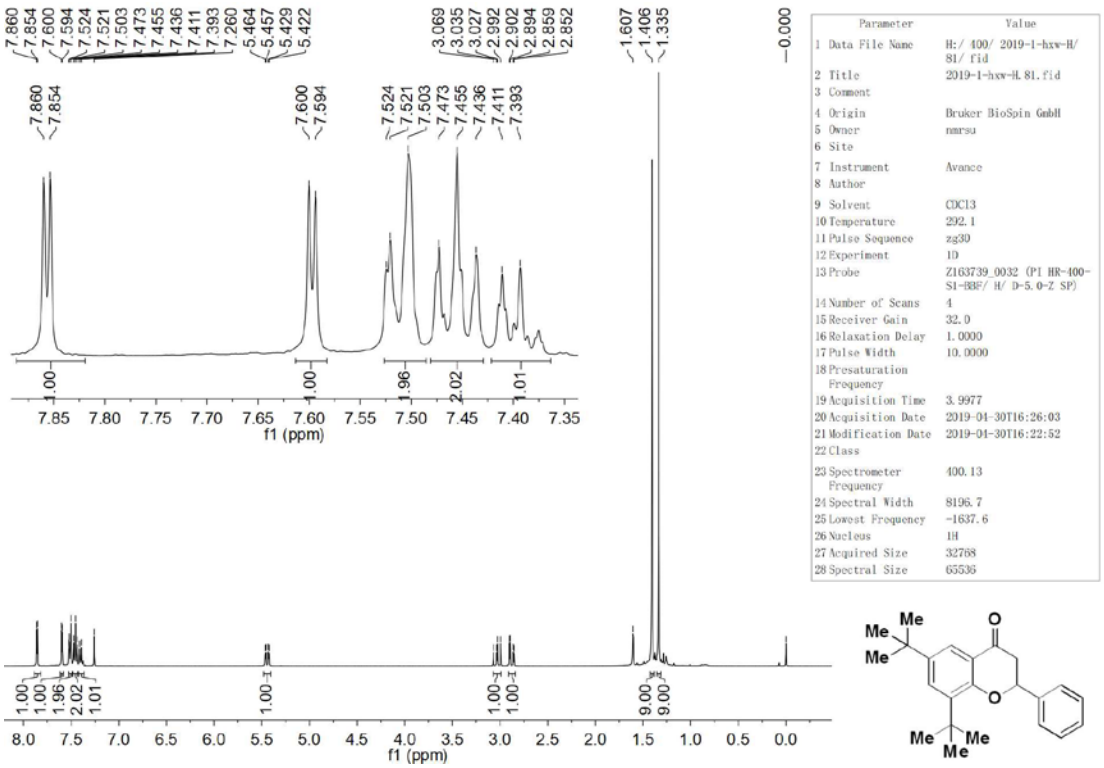


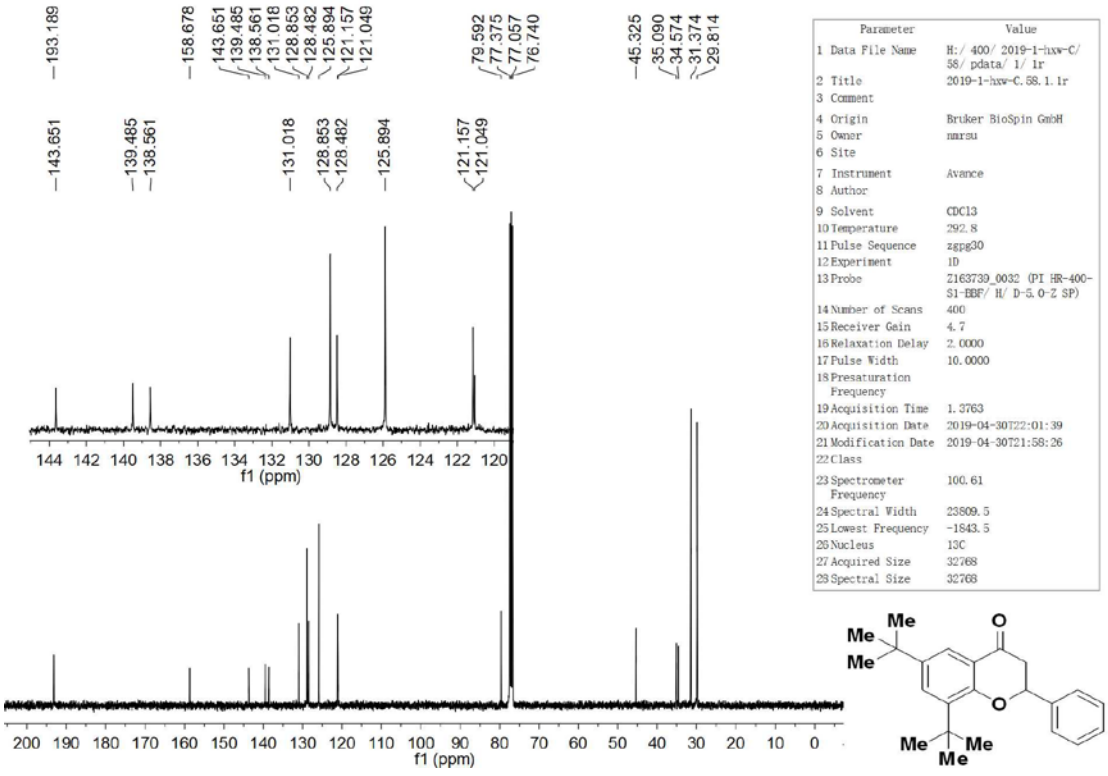
Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-H/ 108/ fid
2 Title	2019-2-hxw-H. 108. fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-10-17T17:13:44
21 Modification Date	2019-10-17T17:13:34
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



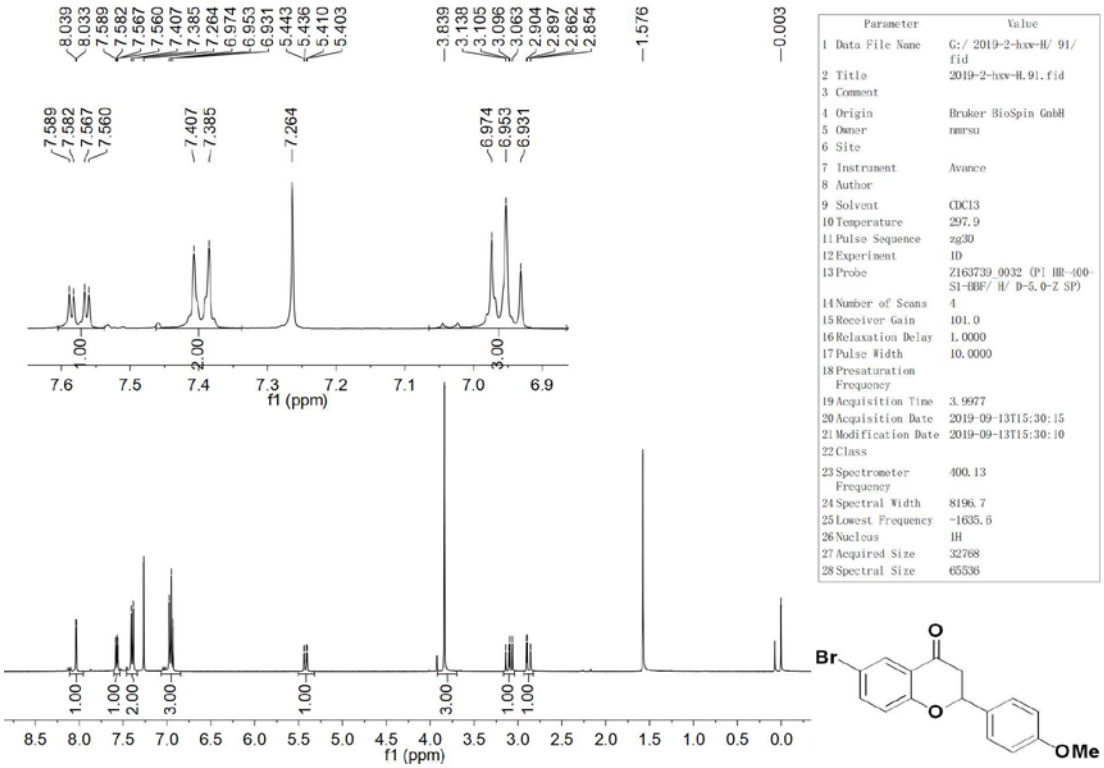
Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-C/ 46/ pdata/ 1/ 1r
2 Title	2019-2-hxw-C. 46. 1. 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	400
15 Receiver Gain	13.2
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-10-19T01:11:47
21 Modification Date	2019-10-19T01:11:30
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

6,8-Di-tert-butyl-2-phenylchroman-4-one (Table 2, compound 2v)

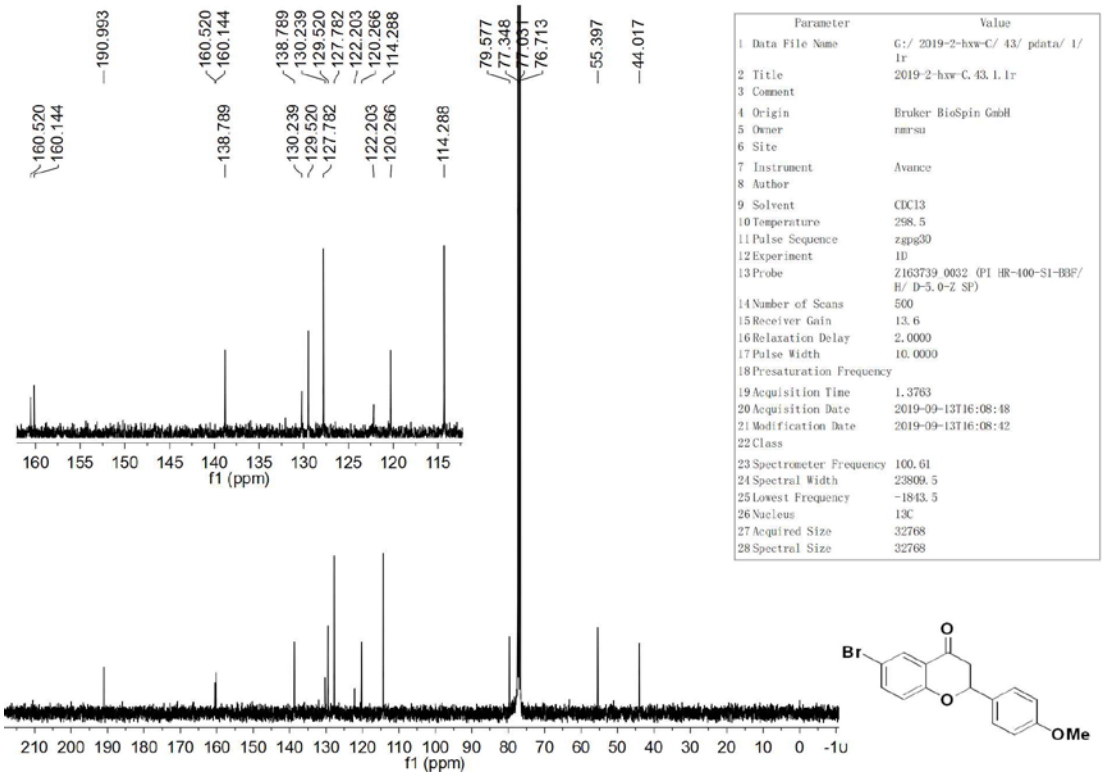




6-Bromo-2-(4-methoxyphenyl)chroman-4-one (Table 2, compound 2w)

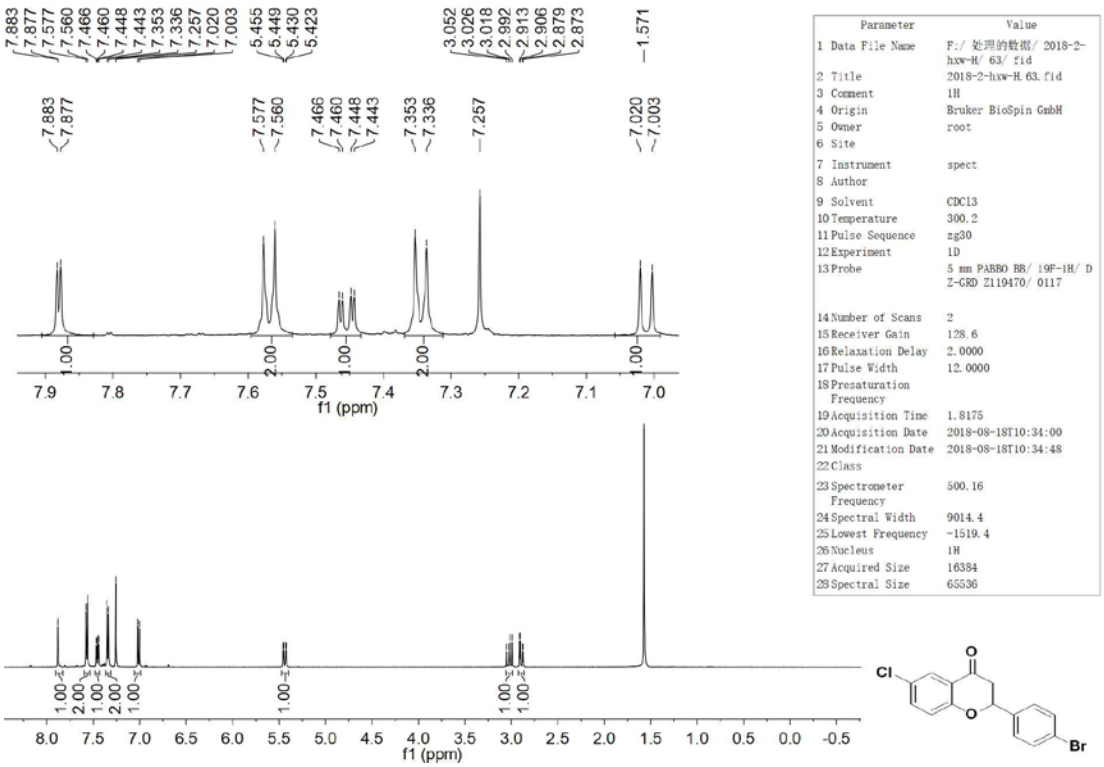


Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-H/ 91/ fid
2 Title	2019-2-hxw-H. 91. fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-09-13T15:30:15
21 Modification Date	2019-09-13T15:30:10
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1635.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

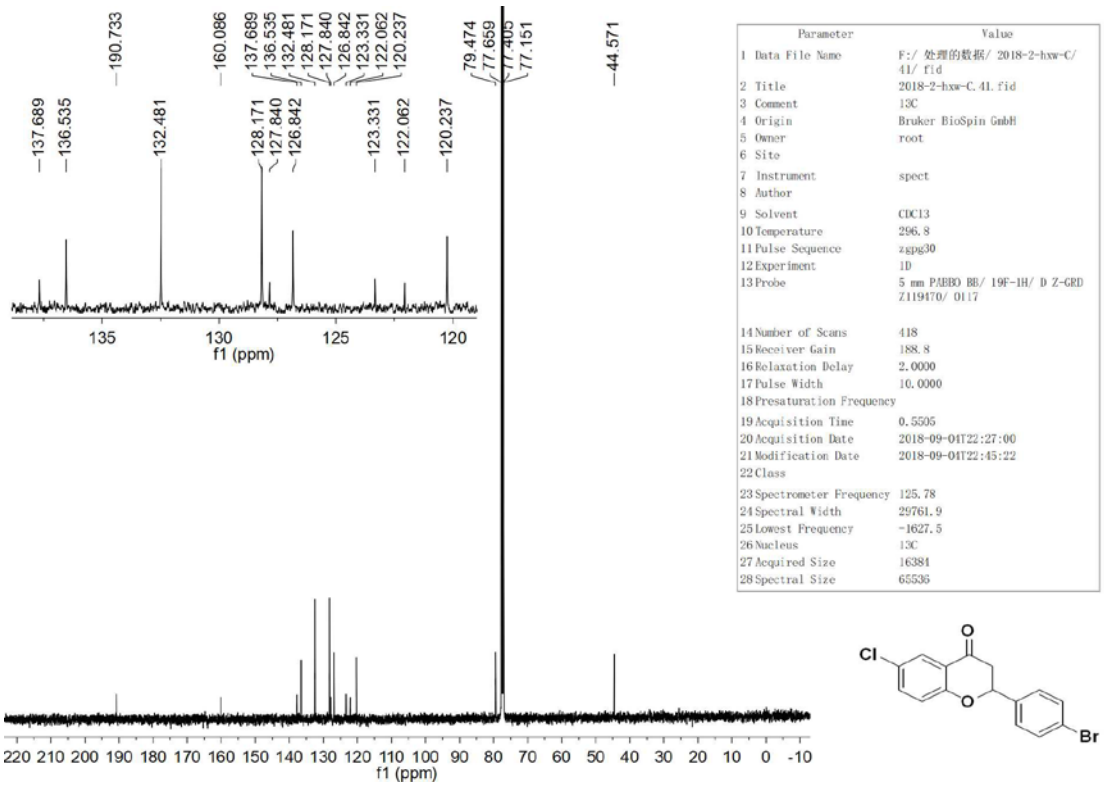


Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-C/ 43/ pdata/ 1/ 1r
2 Title	2019-2-hxw-C. 43. 1. 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	500
15 Receiver Gain	13.6
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-09-13T16:08:48
21 Modification Date	2019-09-13T16:08:42
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-(4-Bromophenyl)-6-chlorochroman-4-one (Table 2, compound 2x)

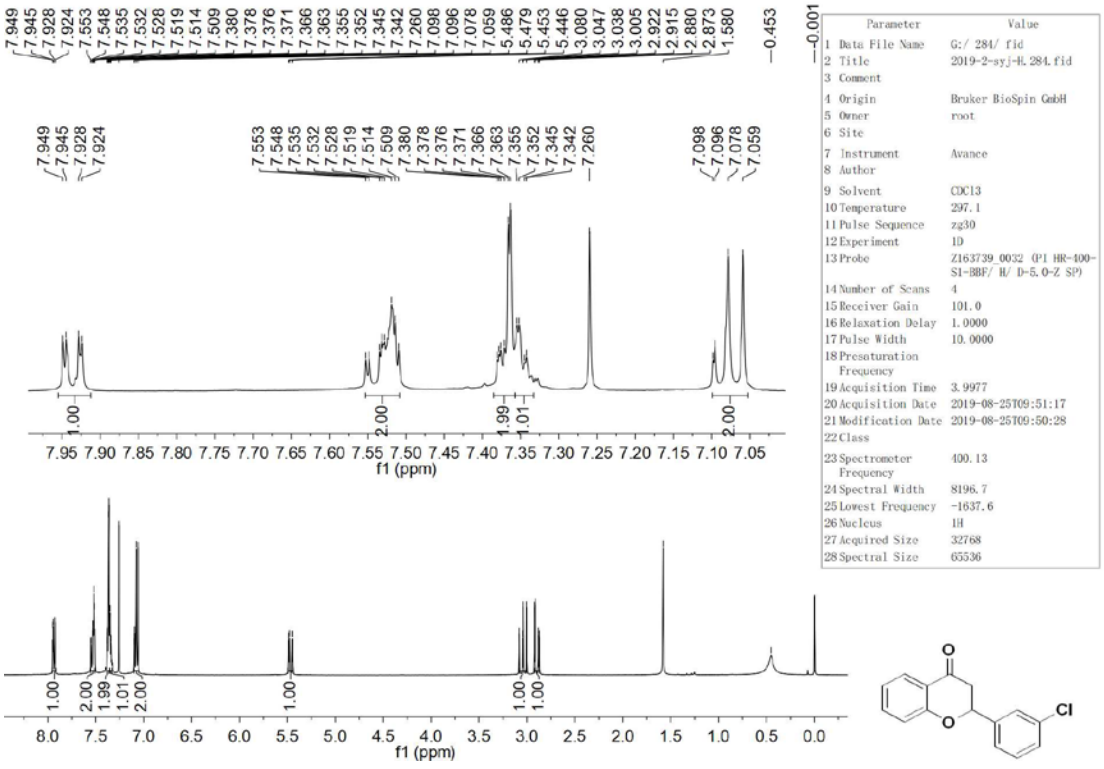


Parameter	Value
1 Data File Name	F:/ 处理的数据/ 2018-2-hxw-H/ 63/ fid
2 Title	2018-2-hxw-H 63.fid
3 Comment	1H
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117
14 Number of Scans	2
15 Receiver Gain	128.6
16 Relaxation Delay	2.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	1.8175
20 Acquisition Date	2018-08-18T10:34:00
21 Modification Date	2018-08-18T10:34:48
22 Class	
23 Spectrometer Frequency	500.16
24 Spectral Width	9014.4
25 Lowest Frequency	-1519.4
26 Nucleus	1H
27 Acquired Size	16384
28 Spectral Size	65536

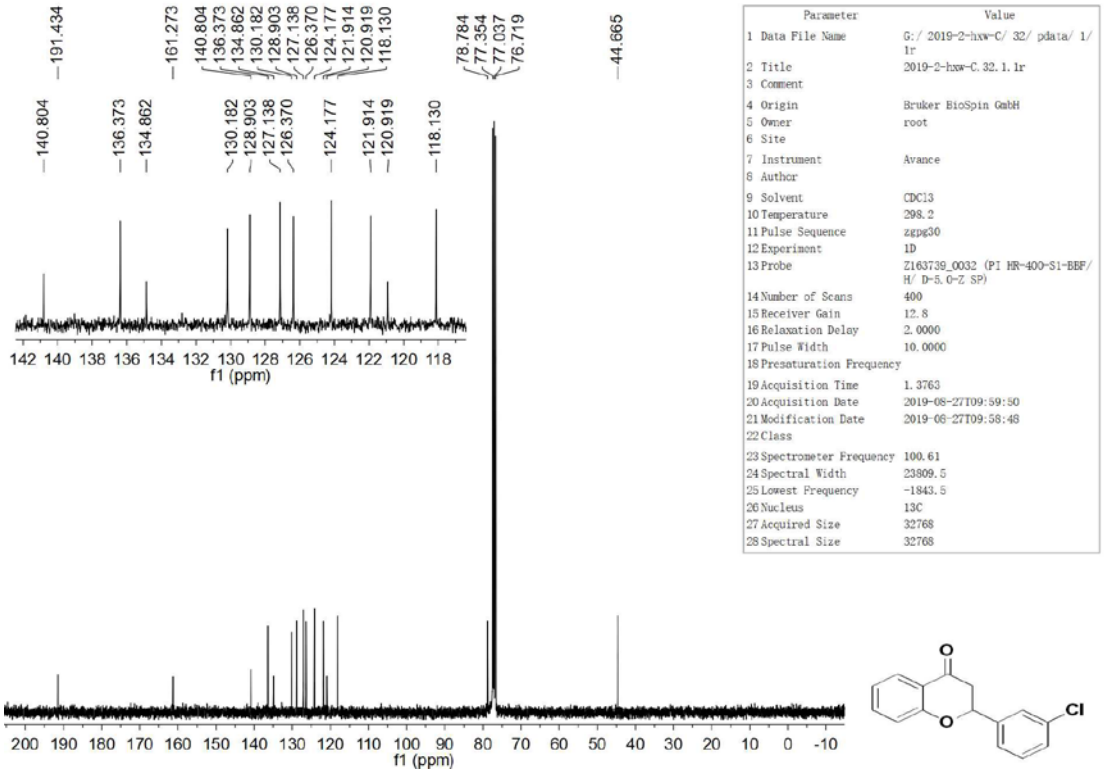


Parameter	Value
1 Data File Name	F:/ 处理的数据/ 2018-2-hxw-C/ 41/ fid
2 Title	2018-2-hxw-C 41.fid
3 Comment	13C
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z119470/ 0117
14 Number of Scans	418
15 Receiver Gain	188.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.5505
20 Acquisition Date	2018-09-04T22:27:00
21 Modification Date	2018-09-04T22:45:22
22 Class	
23 Spectrometer Frequency	125.78
24 Spectral Width	29761.9
25 Lowest Frequency	-1627.5
26 Nucleus	13C
27 Acquired Size	16384
28 Spectral Size	65536

2-(3-Chlorophenyl)chroman-4-one (Table 2, compound 2y)

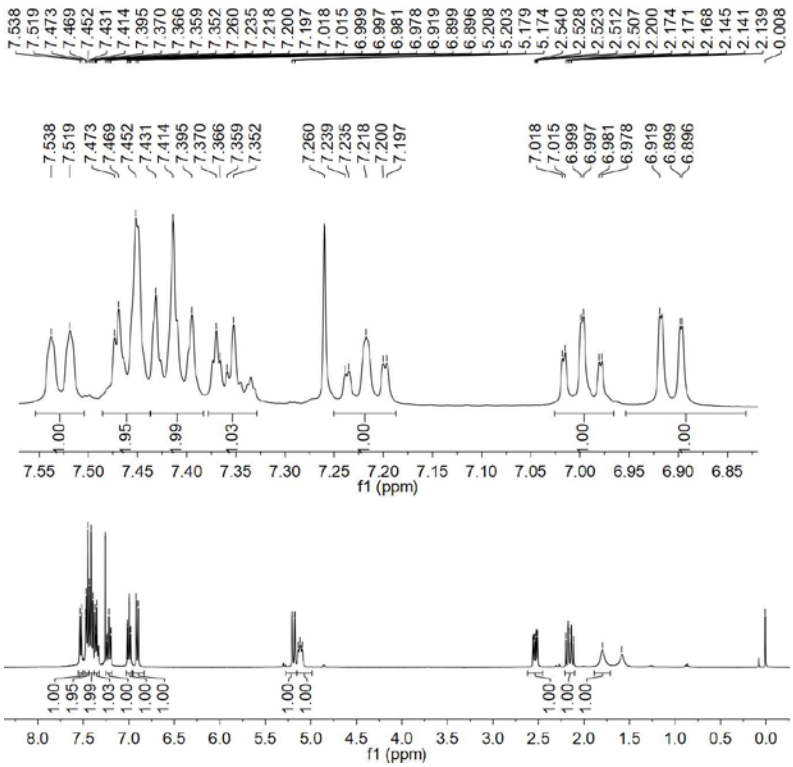


Parameter	Value
1 Data File Name	G:/ 284/ fid
2 Title	2019-2-syj-H. 284. fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-08-25T09:51:17
21 Modification Date	2019-08-25T09:50:28
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

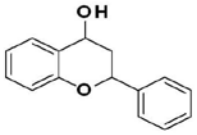


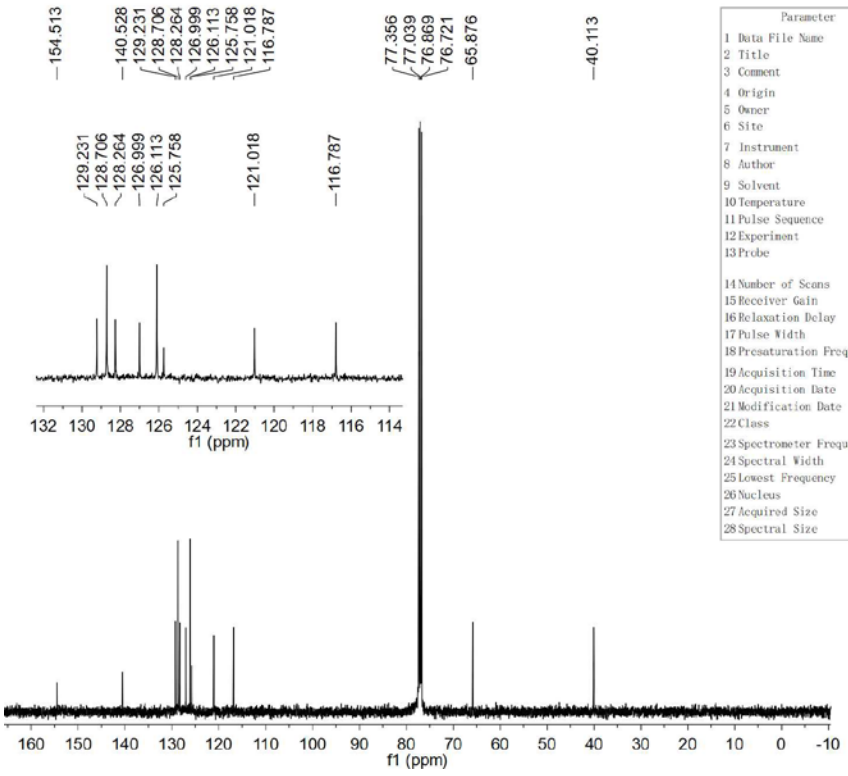
Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-C/ 32/ pdata/ 1/ 1r
2 Title	2019-2-hxw-C. 32. 1. 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	400
15 Receiver Gain	12.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-08-27T09:59:50
21 Modification Date	2019-08-27T09:58:48
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-Phenylchroman-4-ol (Scheme 2, compound 3a)

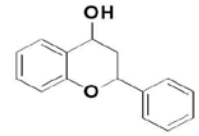


Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-H/ 111/ fid
2 Title	2019-2-hxw-H 111.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-10-21T19:57:31
21 Modification Date	2019-10-21T19:56:58
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

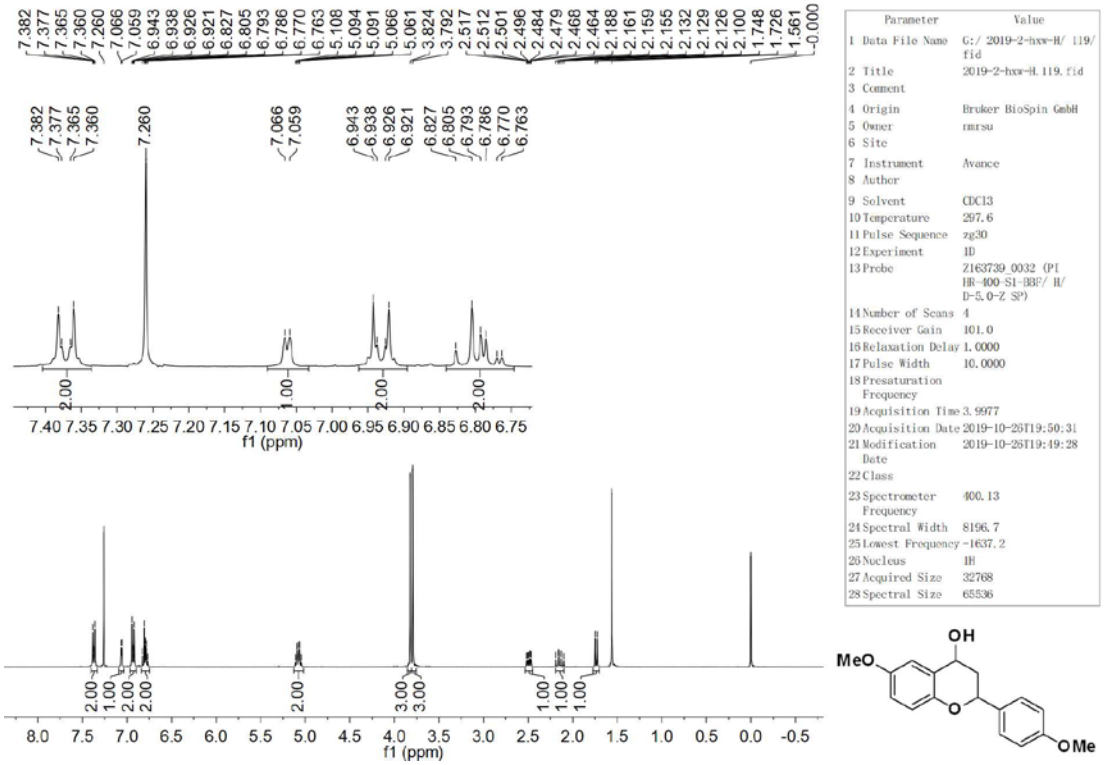




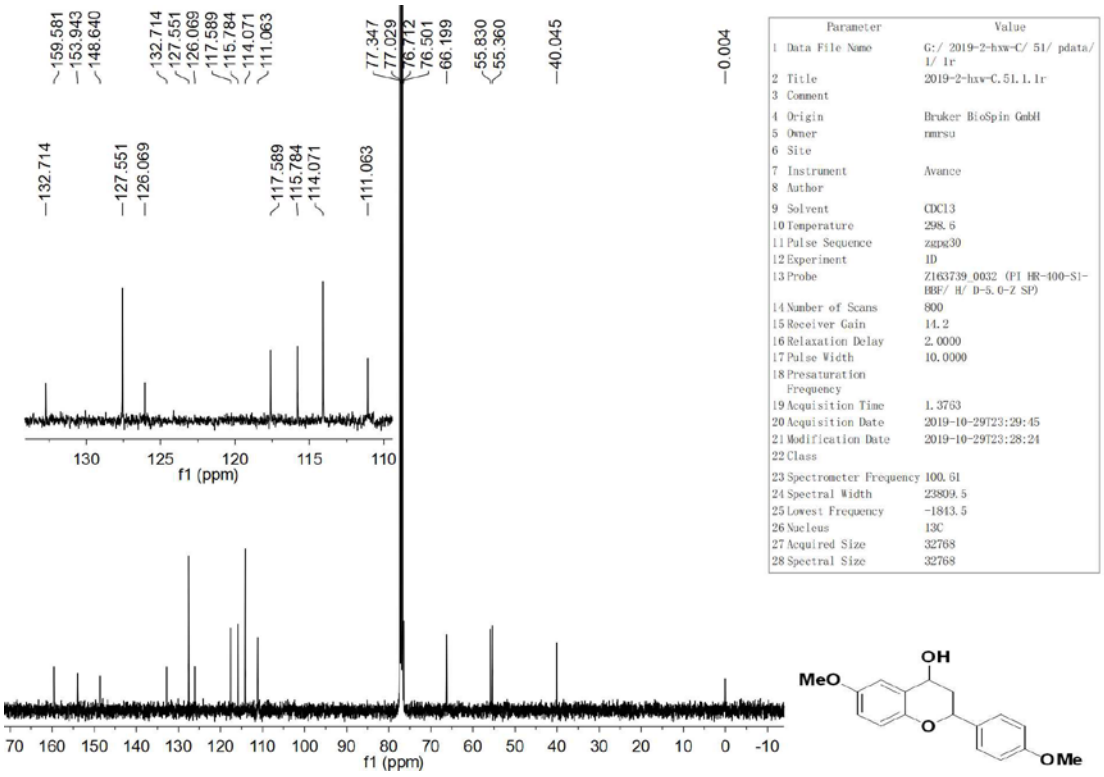
Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-C/ 47/ pdata/ 1/ 1r
2 Title	2019-2-hxw-C 47.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	400
15 Receiver Gain	13.2
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-10-23T10:37:16
21 Modification Date	2019-10-23T10:36:34
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768



6-Methoxy-2-(4-methoxyphenyl)chroman-4-ol (Scheme 2, compound 3u)

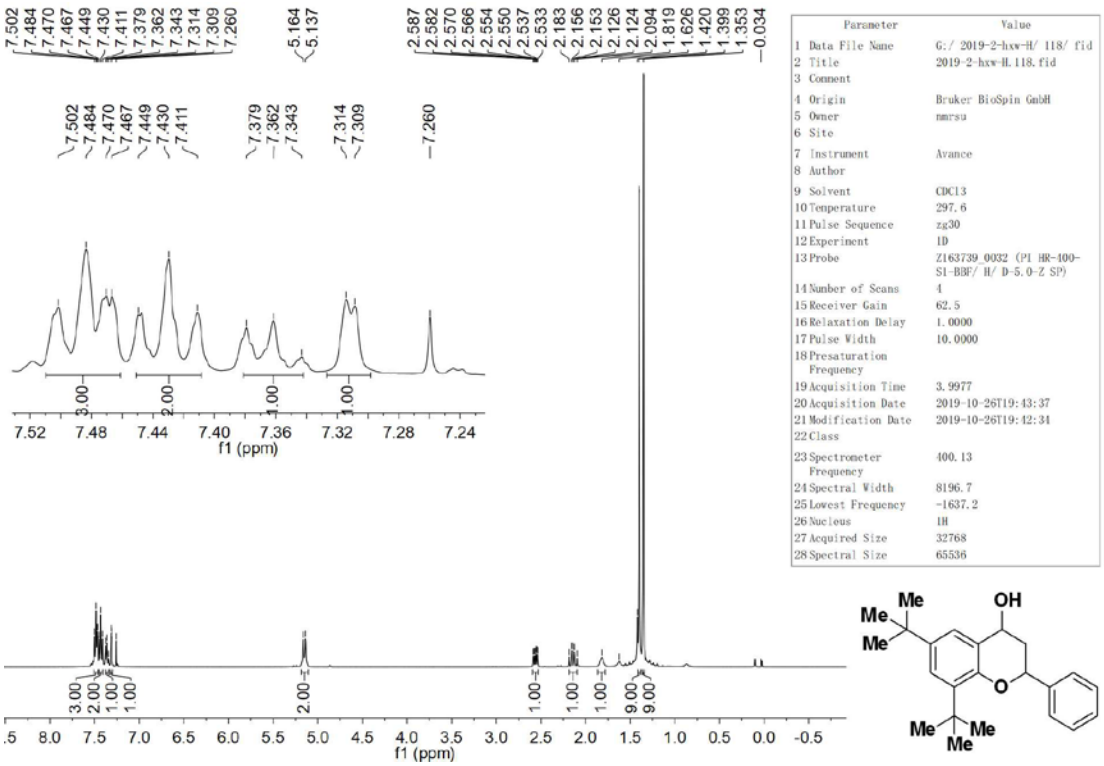


Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-H/ 119/ fid
2 Title	2019-2-hxw-H. 119. fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-10-26T19:50:31
21 Modification Date	2019-10-26T19:49:28
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

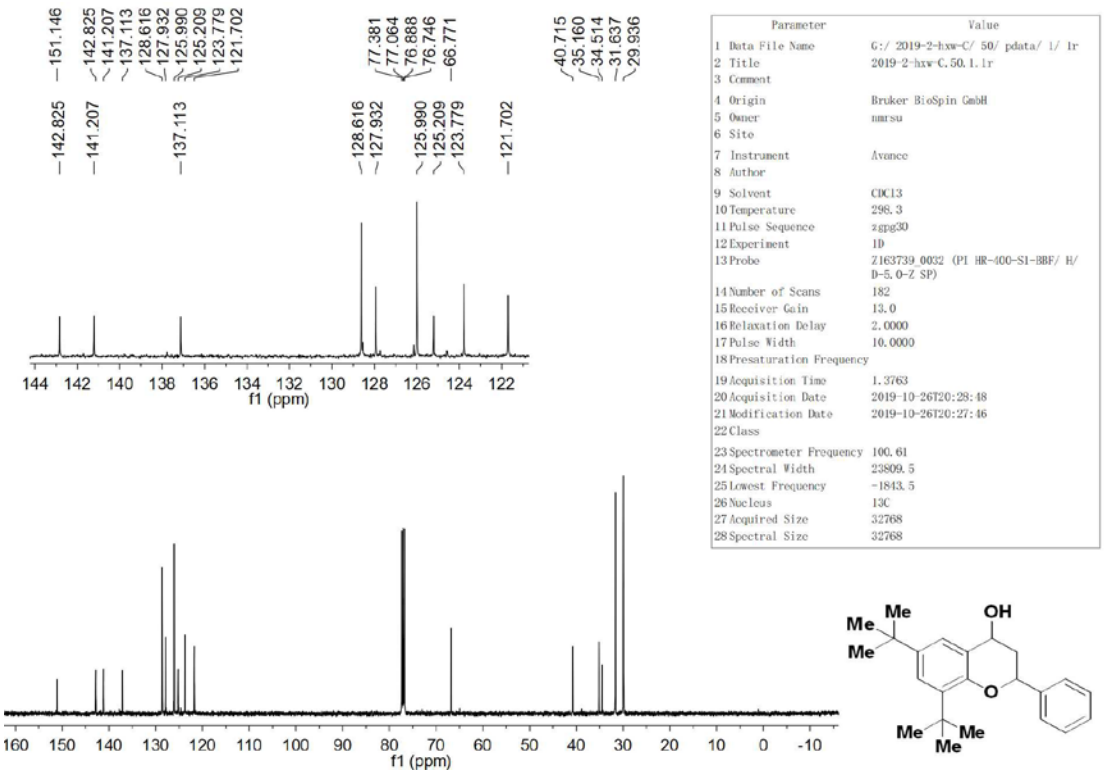


Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-C/ 51/ pdata/ 1/ 1r
2 Title	2019-2-hxw-C. 51. 1. 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	800
15 Receiver Gain	14.2
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-10-29T23:29:45
21 Modification Date	2019-10-29T23:28:24
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

6,8-Di-*tert*-butyl-2-phenylchroman-4-ol (Scheme 2, compound 3v)

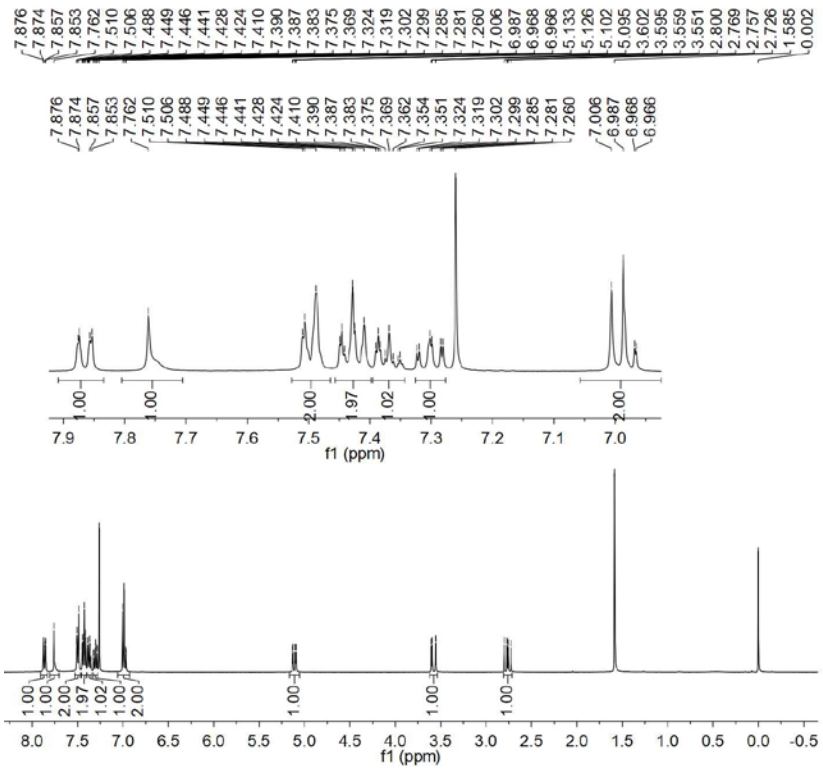


Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-H/ 118/ fid
2 Title	2019-2-hxw-H. 118. fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	62.5
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-10-26T19:43:37
21 Modification Date	2019-10-26T19:42:34
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

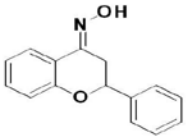


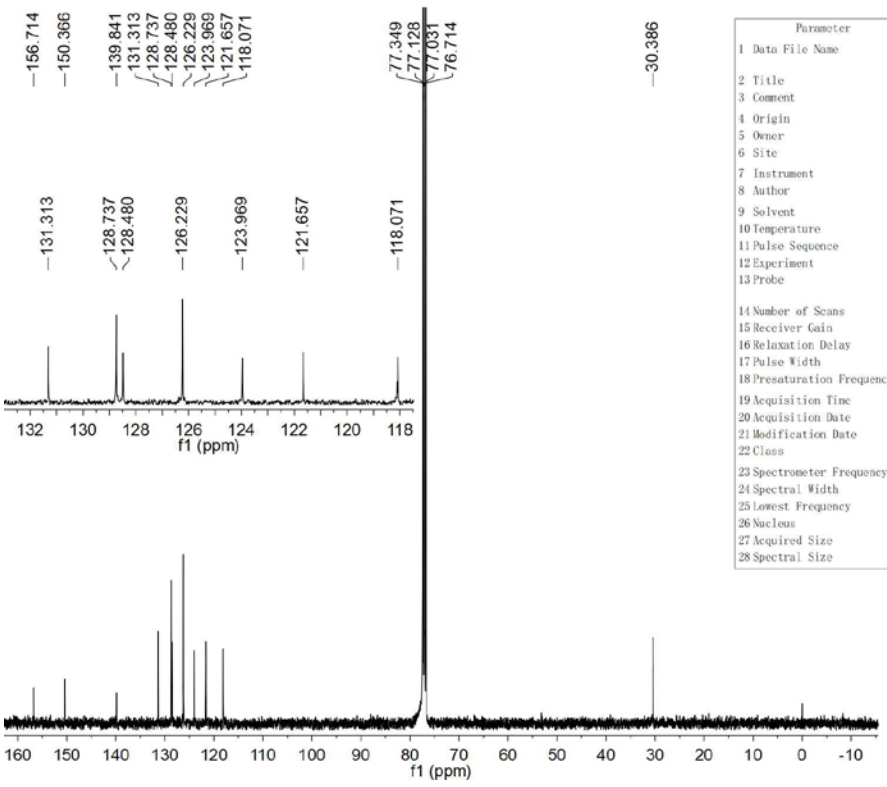
Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-C/ 50/ pdata/ 1/ 1r
2 Title	2019-2-hxw-C. 50. 1. 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.3
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	182
15 Receiver Gain	13.0
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-10-26T20:28:48
21 Modification Date	2019-10-26T20:27:46
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-Phenylchroman-4-one oxime (Scheme 2, compound 4a)

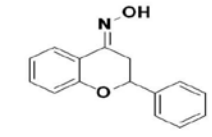


Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-H/ 96/ fid
2 Title	2019-2-hxw-H.96.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-09-26T20:13:18
21 Modification Date	2019-09-26T20:12:20
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

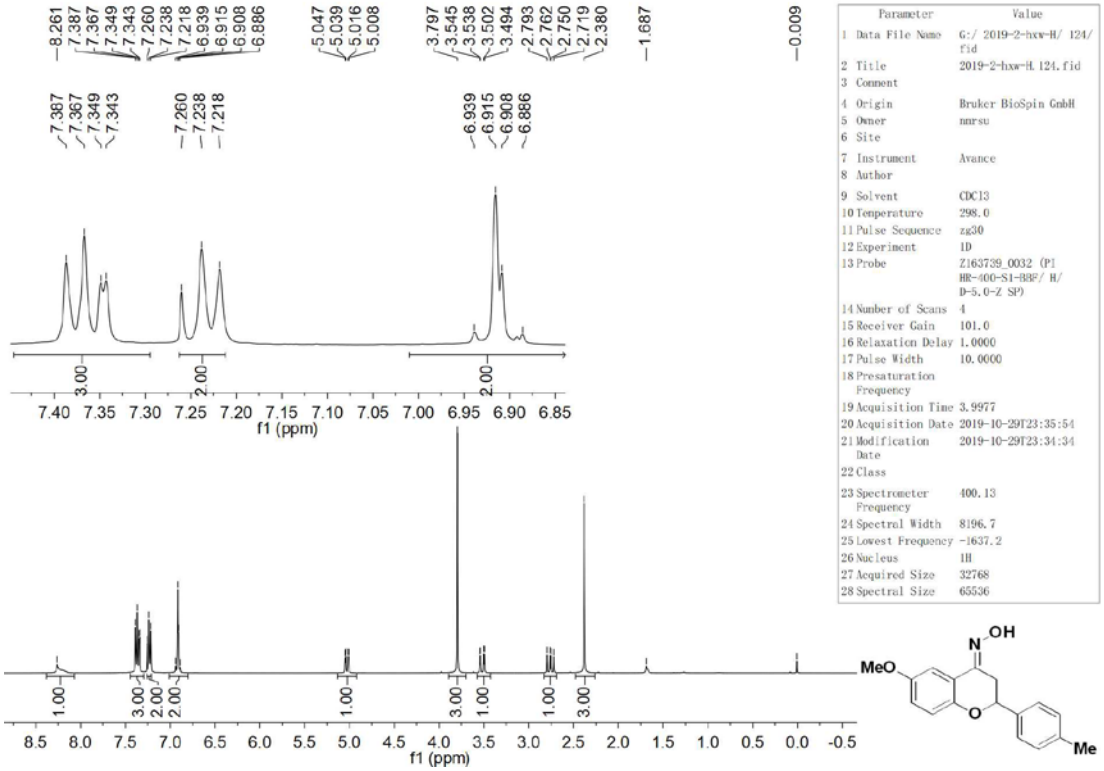




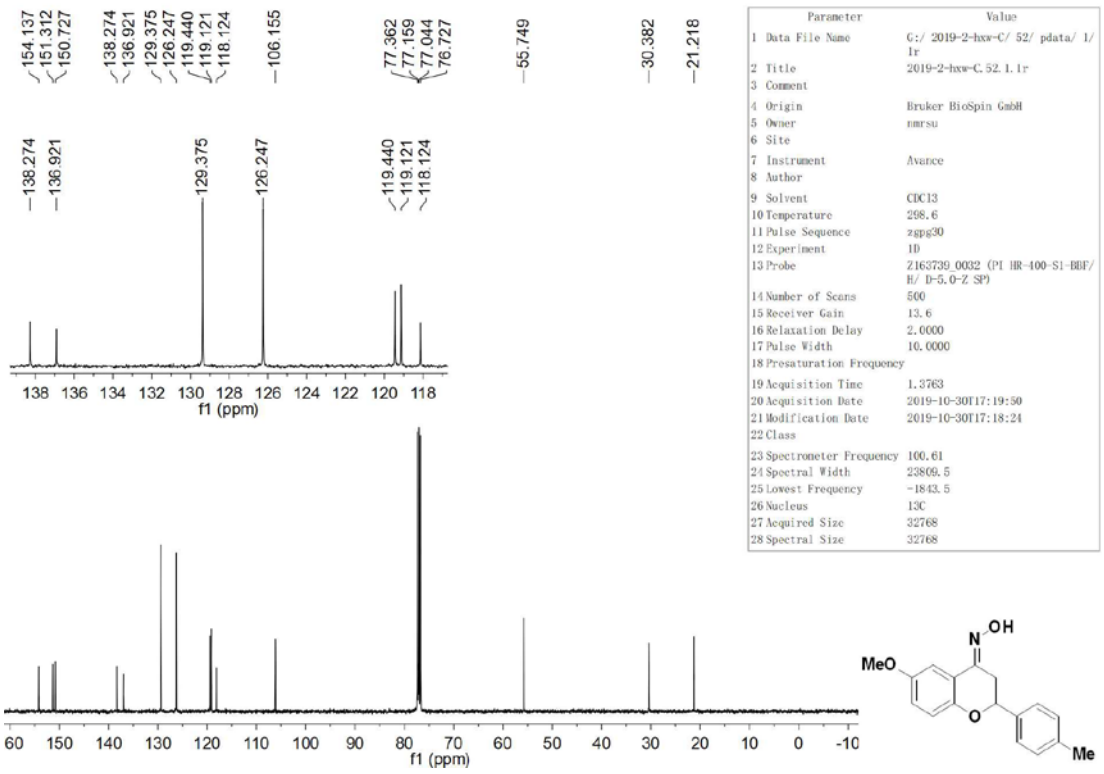
Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-C/ 45/ pdata/ 1/ 1r
2 Title	2019-2-hxw-C.45.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	1000
15 Receiver Gain	13.2
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-09-26T23:27:54
21 Modification Date	2019-09-26T23:26:56
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768



6-Methoxy-2-(*p*-tolyl)chroman-4-one oxime (Scheme 2, compound 4s)

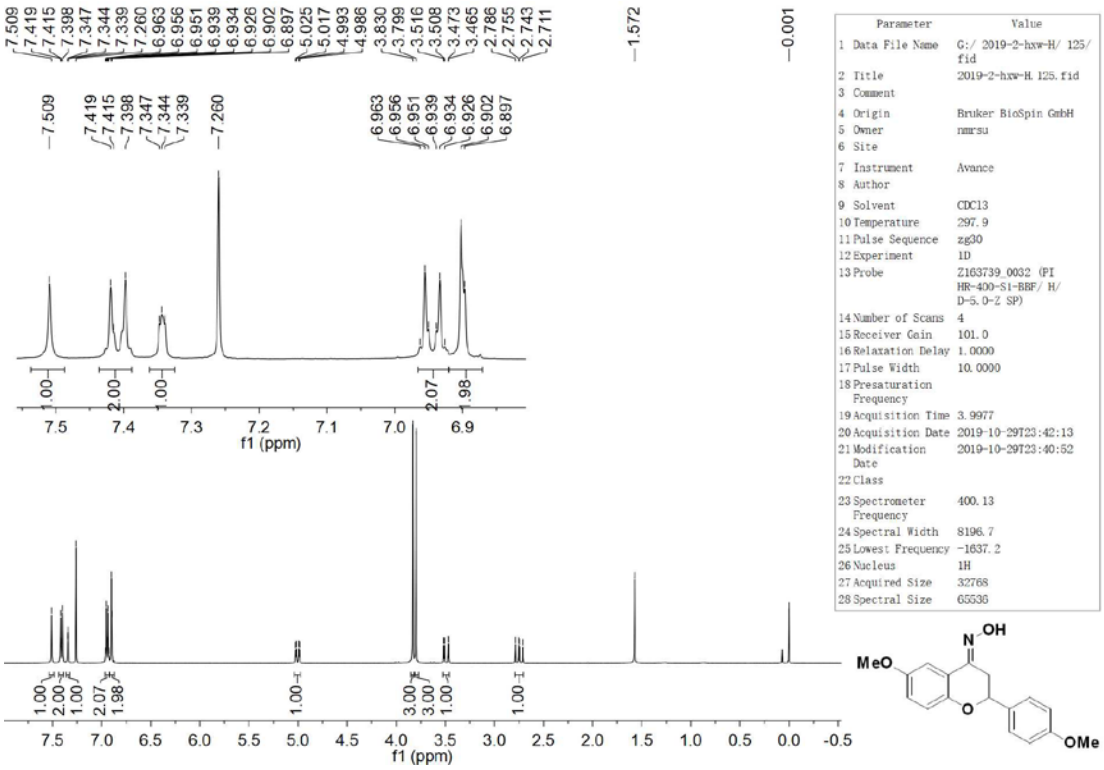


Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-H/ 124/ fid
2 Title	2019-2-hxw-H 124.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-10-29T23:35:54
21 Modification Date	2019-10-29T23:34:34
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

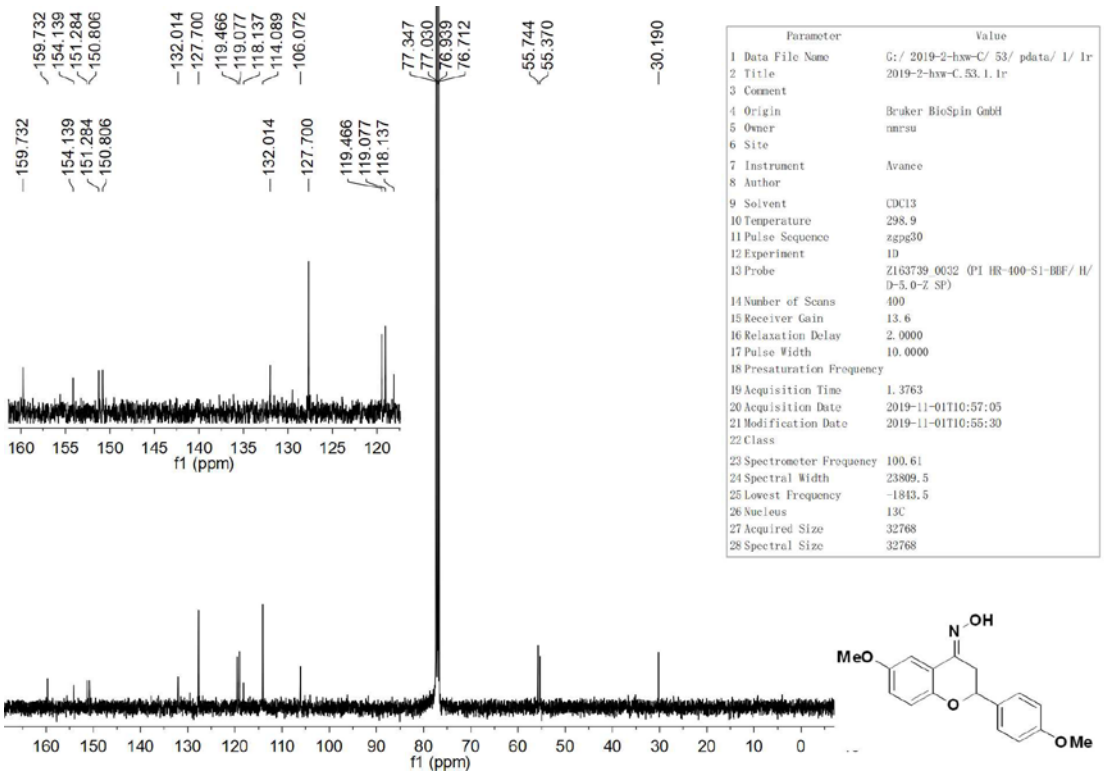


Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-C/ 52/ pdata/ 1/ 1r
2 Title	2019-2-hxw-C.52.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	500
15 Receiver Gain	13.6
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-10-30T17:19:50
21 Modification Date	2019-10-30T17:18:24
22 Class	
23 Spectroneter Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

6-Methoxy-2-(4-methoxyphenyl)chroman-4-one oxime (Scheme 2, compound 4u)

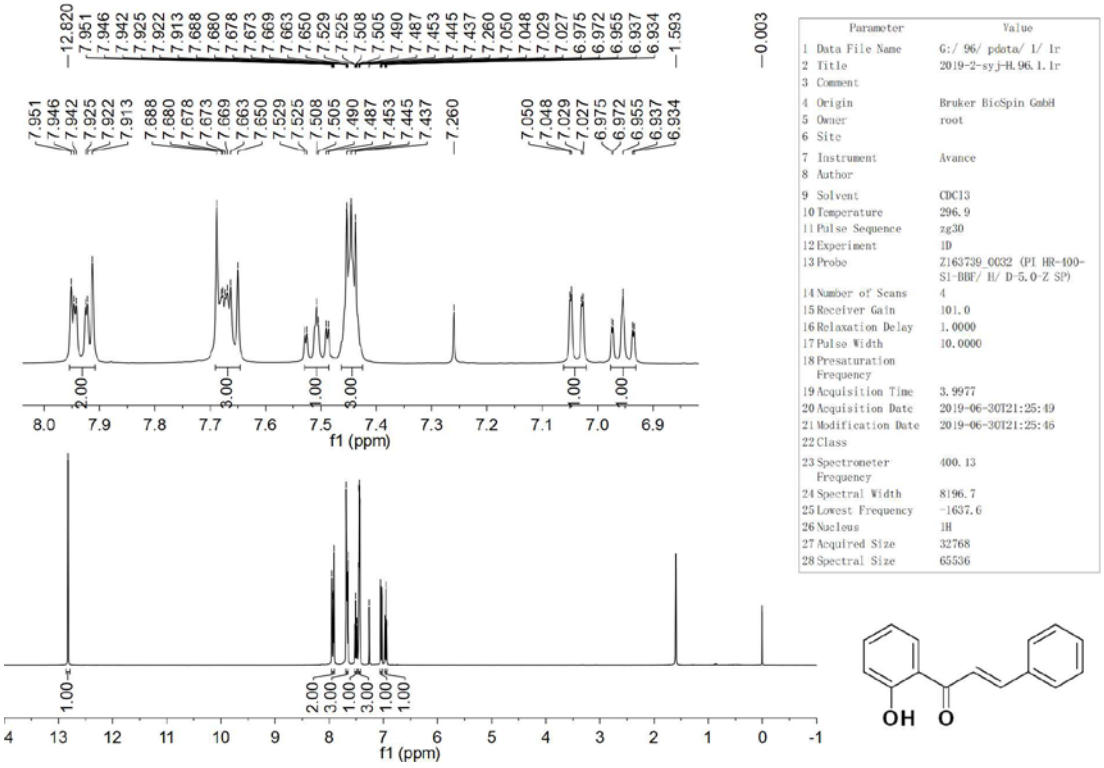


Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-H/ 125/ fid
2 Title	2019-2-hxw-H. 125. fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-10-29T23:42:13
21 Modification Date	2019-10-29T23:40:52
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

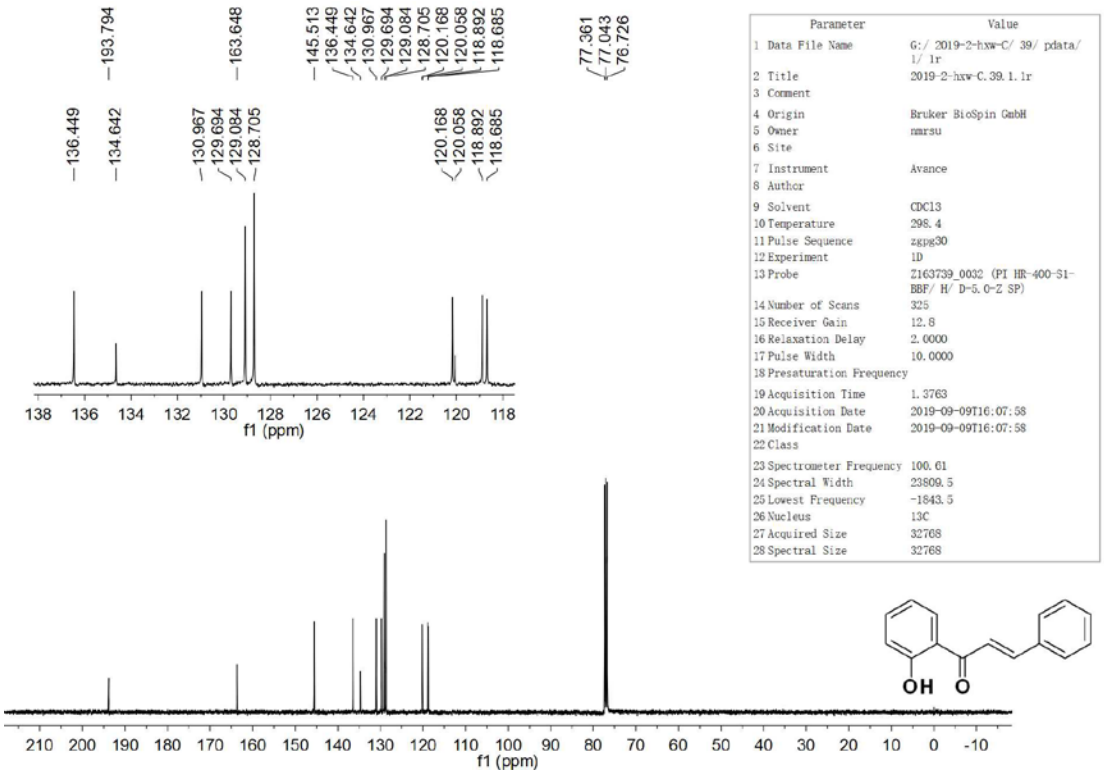


Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-C/ 53/ pdata/ 1/ 1r
2 Title	2019-2-hxw-C. 53. 1. 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	400
15 Receiver Gain	13.6
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-11-01T10:57:05
21 Modification Date	2019-11-01T10:55:30
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

(*E*)-1-(2-Hydroxyphenyl)-3-phenylprop-2-en-1-one (Scheme 3, compound 5aa)

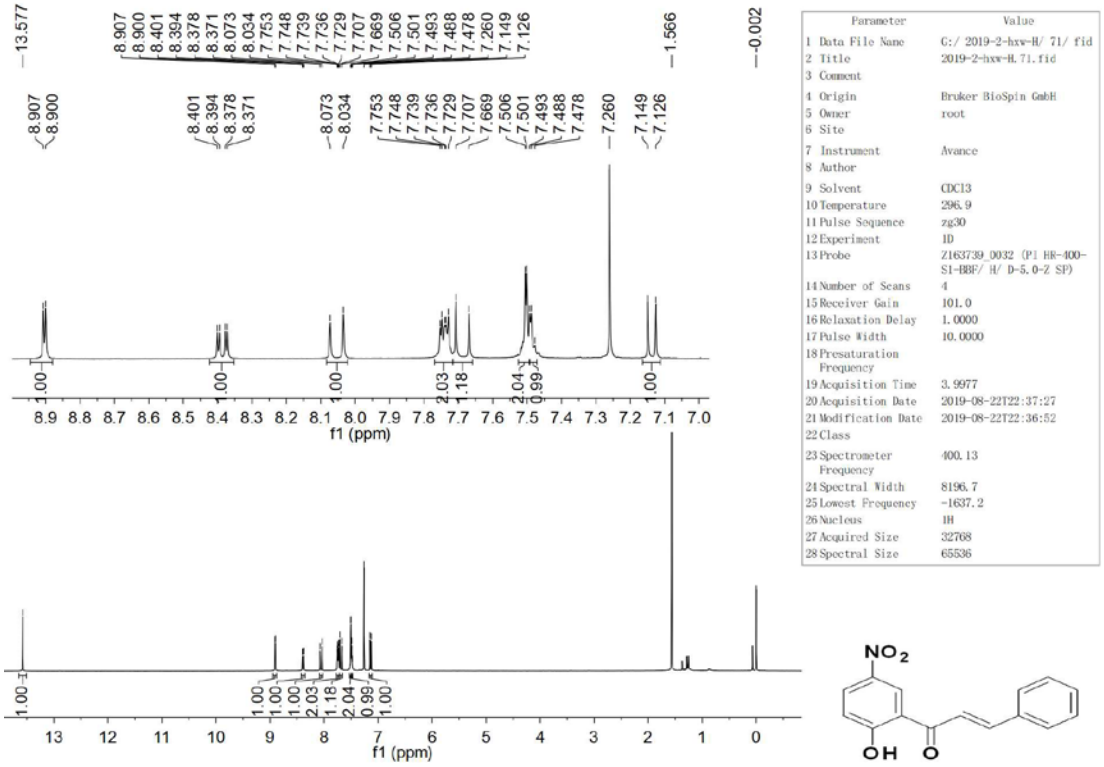


Parameter	Value
1 Data File Name	G:/ 96/ pdata/ 1/ 1r
2 Title	2019-2-syj-H.96.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	296.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-06-30T21:25:49
21 Modification Date	2019-06-30T21:25:46
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

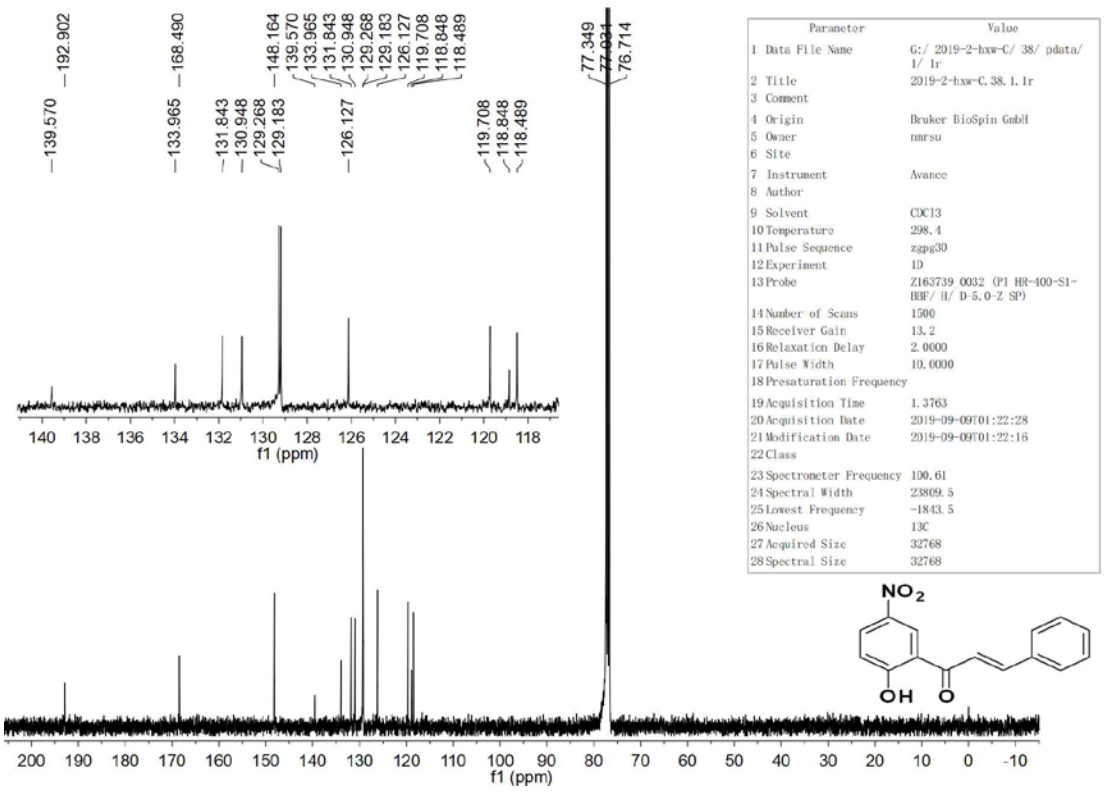


Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-C/ 39/ pdata/ 1/ 1r
2 Title	2019-2-hxw-C.39.1.1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	325
15 Receiver Gain	12.8
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-09-09T16:07:58
21 Modification Date	2019-09-09T16:07:58
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

(*E*)-1-(2-Hydroxy-5-nitrophenyl)-3-phenylprop-2-en-1-one (Scheme 3, compound 5ab)

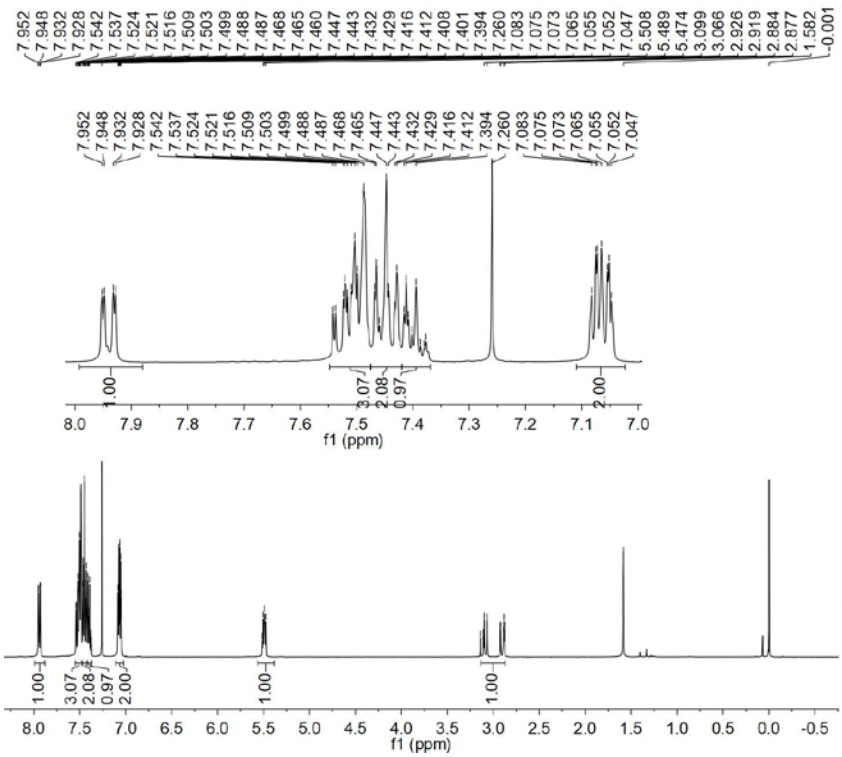


Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-H/ 71/ fid
2 Title	2019-2-hxw-H. 71. fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	296.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (P1 HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2019-08-22T22:37:27
21 Modification Date	2019-08-22T22:36:52
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



Parameter	Value
1 Data File Name	G:/ 2019-2-hxw-C/ 38/ pdata/ 1/ 1r
2 Title	2019-2-hxw-C. 38. 1. 1r
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (P1 HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	1500
15 Receiver Gain	13.2
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2019-09-09T01:22:28
21 Modification Date	2019-09-09T01:22:16
22 Class	
23 Spectrometer Frequency	100.61
24 Spectral Width	23809.5
25 Lowest Frequency	-1843.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	32768

2-Phenylchroman-4-one (Scheme 3, compound 2a-d_2)



Parameter	Value
1 Data File Name	H:/ 400/ 2019-1-hxw-H/ 84/ fid
2 Title	2019-1-hxw-H. 84. fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	292. 2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (P1 HR-400-S1-BBF/ H/ D-5. 0-Z SP)
14 Number of Scans	4
15 Receiver Gain	32. 0
16 Relaxation Delay	1. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	3. 9977
20 Acquisition Date	2019-05-06T20:32:46
21 Modification Date	2019-05-06T20:28:58
22 Class	
23 Spectrometer Frequency	400. 13
24 Spectral Width	8196. 7
25 Lowest Frequency	-1637. 6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536