Electronic Supplementary Material (ESI) for RSC Chemical Biology.

Supporting File 2

Containing chemical characterization data for:

Inhibition of SC4MOL and HSD17B7 shifts cellular sterol composition and promotes oligodendrocyte formation

Matthew J Pleshinger,[1] Ryan M. Friedrich,[2] Zita Hubler,[2] Adrianna M. Rivera-León,[2] Farrah Gao,[2] David Yan,[2] Joel Sax,[2] Ramya Srinivasan,[2] Ilya Bederman,[2] H. E. Shick,[2] Paul J. Tesar,[2] Drew J. Adams[2]

[1] Department of Pharmacology, Case Western Reserve University School of Medicine; Cleveland, Ohio 44106, USA.

[2] Department of Genetics and Genome Sciences, Case Western Reserve University School of Medicine; Cleveland, Ohio 44106, USA.

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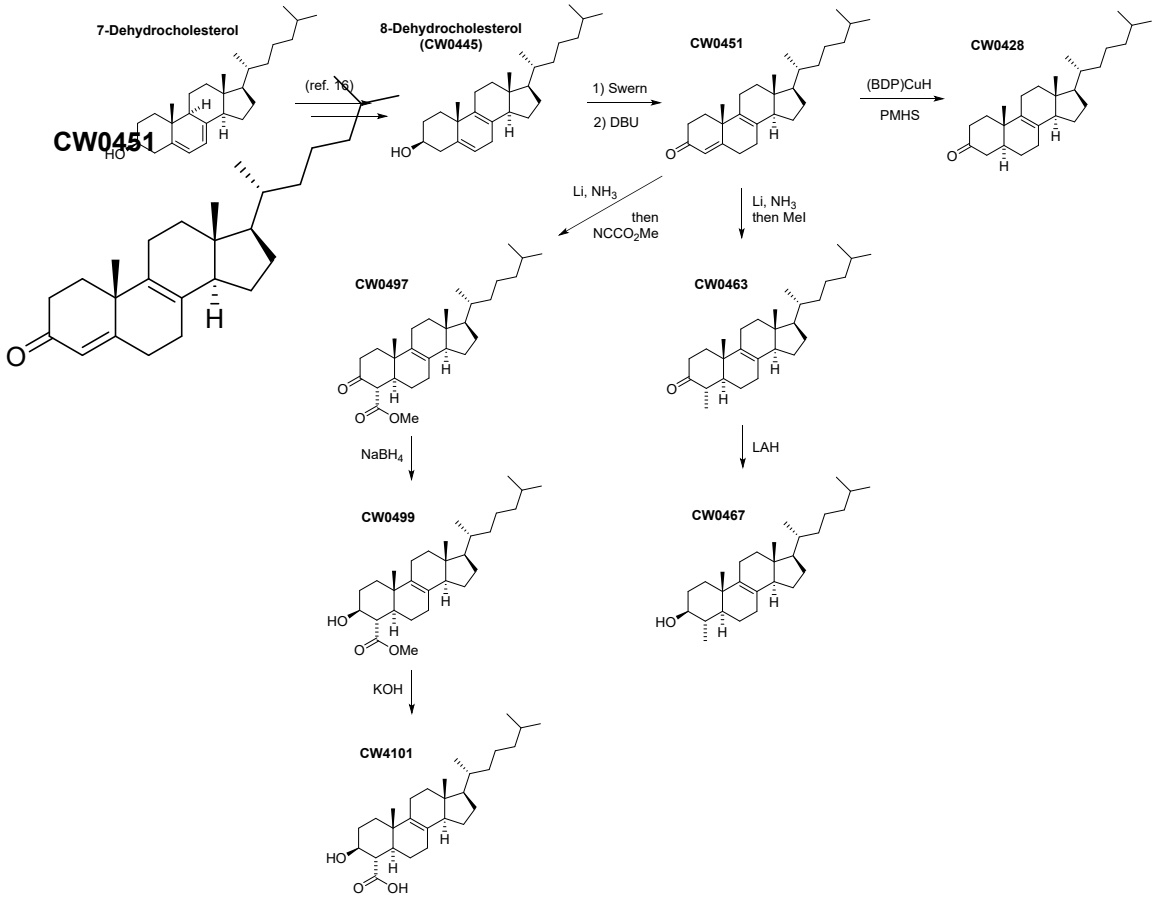
Synthetic Procedures

Materials and Methods

All commercially available reagents were used as received unless stated otherwise. Reactions were performed at ambient temperature unless otherwise noted. All air- or moisture-sensitive reactions utilized dry solvents, oven-dried glassware, and an argon atmosphere. TLC employed glass plates coated with a 250 μm layer of silica and a UV indicator. TLC plates were visualized with a UV lamp at 254 nm or by staining with $KMnO_4$ or PMA. Flash column chromatography was performed using 230-400 mesh silica gel and a gradient elution. Chemical shifts (δ) were calibrated to TMS (0 ppm) or the residual NMR solvent at ambient temperature. HRMS data was obtained from instrumentation facilities services. LC-MS (ESI) data was obtained using a C18 reversed-phase column (5 μm, 50 x 2.1 mm) and MeCN/H_2O (0.1% HCOOH) mobile phase.

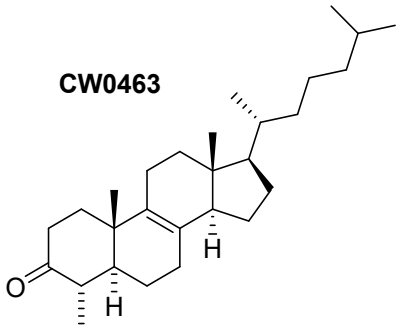
Sterol Standards

Figure 1: Synthetic scheme of C4DMC standards 4-methylzymostenone (**CW0463)**, 4-methylzymostenol (**CW0467)**, 4-carboxyzymostenol (**CW4101),** and zymostenone (**CW0428)**.



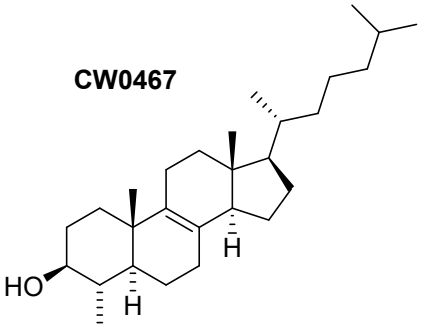
(10*S*,13*R*,14*R*,17*R*)-10,13-Dimethyl-17-((*R*)-6-methylheptan-2-yl)-1,2,6,7,10,11,12,13,14,15,16,17-dodecahydro-3*H*-cyclopenta[*a*]phenanthren-3-one (CW0451). To a solution of oxalyl chloride (0.96 mL, 11.2 mmol, 2 eq) in DCM (28 mL) at –78 °C was added DMSO (1.20 mL, 16.9 mmol, 3 eq). After 30 min, 8-dehydrocholesterol *(35)* (**CW0445**) (2.16 g, 5.6 mmol, 1 eq) in DCM (28 mL) was slowly added. After 3 h, Et_3N (3.92 mL, 28.1 mmol, 5 eq) was added and reaction allowed to warm to room temperature over 1 h. The reaction mixture was partitioned between H_2O (150 mL) and DCM (3 x 150 mL). The combined organic phase was washed with brine (50 mL), dried over Na_2SO_4, and concentrated to afford an orange solid (2.19 g). The crude saturated ketone was used in the next step without further purification.

To a solution of the crude saturated ketone in THF (22 mL) was added DBU (0.92 mL, 6.18 mmol, 1.1 eq) and the reaction heated at reflux. After 1 h, the reaction mixture was partitioned between saturated NH4Cl (aq) (50 mL) and DCM (3 x 50 mL). The combined organic phase was washed with brine (30 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0451** (1.07 g, 50% over 2 steps) as a yellow solid. TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.67; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 5.77 (s, 1H), 2.59-2.46 (m, 2H), 2.44-2.36 (m, 1H), 2.35-2.29 (m, 1H), 2.28-2.20 (m, 1H), 1.34 (s, 3H), 0.94 (d, *J* = 6.5 Hz, 3H), 0.871 (d, *J* = 6.6 Hz, 3H), 0.868 (d, *J* = 6.6 Hz, 3H), 0.68 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 199.2, 171.3, 132.0, 129.6, 123.2, 54.9, 51.7, 42.1, 39.5, 38.9, 36.7, 36.3, 36.1, 34.4, 34.3, 30.4, 28.62, 28.55, 28.0, 23.92, 23.86, 23.3, 22.8, 22.6, 22.0, 18.7, 11.6.

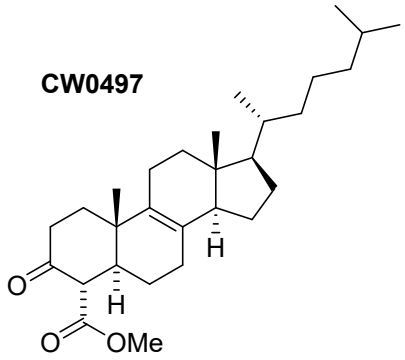


(4*S*,5*S*,10*S*,13*R*,14*R*,17*R*)-4,10,13-Trimethyl-17-((*R*)-6-methylheptan-2-yl)-1,2,4,5,6,7,10,11,12,13,14,15,16,17-tetradecahydro-3*H*-cyclopenta[*a*]phenanthren-3-one (CW0463). Lithium (12 mg, 1.57 mmol, 6 eq) was added to a solution of **CW0451** (100 mg, 0.26 mmol, 1 eq) in THF (2 mL) and NH_3 (~3 mL) at –78 °C. After slowly warming to –35 °C over 1 h (blue color maintained), the solution was cooled to –78 °C and iodomethane (0.24 mL, 3.92 mmol, 15 eq) was added. The reaction mixture was allowed to warm to room temperature overnight and ammonia evaporated. Water (5 mL) was slowly added, reaction mixture neutralized with HCl (aq) (2M, 1 mL), and extracted with Et_2O (3 x 15 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0463** (27 mg, 26%) as a white solid. TLC (Hex:EtOAc, 2:1 v/v): R_f = 0.69; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 2.46 (apparent dt, *J* = 13.8, 6.2 Hz, 1H), 2.40-2.34 (m, 1H), 2.34-2.26 (m, 1H), 1.20 (s,

3H), 1.02 (d, *J* = 6.5 Hz, 3H), 0.93 (d, *J* = 6.5 Hz, 3H), 0.869 (d, *J* = 6.6 Hz, 3H), 0.866 (d, *J* = 6.6 Hz, 3H), 0.64 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 213.5, 133.7, 129.0, 54.9, 51.7, 49.6, 45.0, 42.1, 39.5, 38.1, 37.2, 36.9, 36.5, 36.3, 36.1, 28.8, 28.0, 27.4, 23.9, 23.7, 22.9, 22.8, 22.6, 22.3, 18.7, 18.1, 11.4, 11.3. The observed 4α-Me,5α-H diastereoselectivity was consistent with that reported previously for similar compounds *(36)*. Additionally, an NOE correlation between the 4β-H and 10β-Me was observed, with the assignments confirmed by COSY coupling between the 4β-H and 4α-Me.

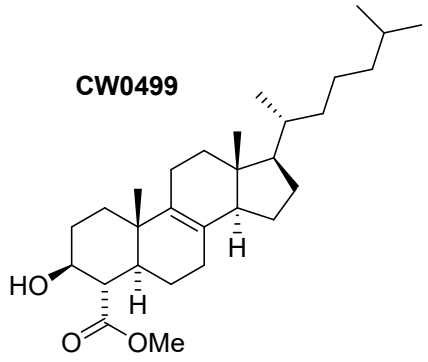


(3*S*,4*S*,5*S*,10*S*,13*R*,14*R*,17*R*)-4,10,13-Trimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,5,6,7,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-ol (CW0467). To a solution of **CW0463** (23 mg, 58 μmol, 1 eq) in THF (1.2 mL) at 0 °C was added $LiAlH_4$ (2.2 mg, 58 μmol, 1 eq). After 4 h, the reaction was quenched with H_2O (1 mL) and acidified with HCl (aq) (1M, 1 mL). The reaction mixture was extracted with Et_2O (3 x 10 mL) and the combined organic phase was washed with saturated $NaHCO_3$ (1 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0467** (10 mg, 43%, 3β/3α-OH > 95:5) as a white solid. TLC (Hex:EtOAc, 2:1 v/v): R_f = 0.50; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 3.15-3.05 (m, 1H), 0.99 (d, *J* = 6.3 Hz, 3H), 0.97 (s, 3H), 0.92 (d, *J* = 6.5 Hz, 3H), 0.865 (d, *J* = 6.6 Hz, 3H), 0.862 (d, *J* = 6.6 Hz, 3H), 0.60 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 135.0, 128.1, 76.5, 54.9, 51.9, 46.9, 42.1, 39.5, 39.2, 37.0, 36.29, 36.28, 36.2, 35.1, 31.2, 28.8, 28.0, 27.5, 23.9, 23.7, 22.83, 22.76, 22.6, 20.9, 18.9, 18.7, 15.1, 11.2. The observed 3α-H diastereoselectivity[2] and spectral data were consistent with that reported previously *(37)*.



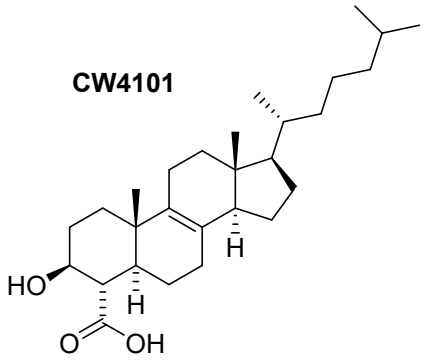
Methyl (4*S*,5*S*,10*S*,13*R*,14*R*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)-3-oxo-2,3,4,5,6,7,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-

cyclopenta[*a*]phenanthrene-4-carboxylate (CW0497). Lithium (29 mg, 4.18 mmol, 8 eq) was added to NH_3 (~5 mL) at –78 °C before adding a solution of **CW0451** (200 mg, 0.52 mmol, 1 eq) in Et_2O (2 mL) and *t*-BuOH (49 µL, 0.52 mmol, 1 eq). After 30 min, isoprene (0.3 mL) was added to discharge residual blue color and reaction slowly warmed to room temperature over 1.5 h under a stream of argon to evaporate solvents. After 5 min under high vacuum, the lithium enolate was suspended in Et_2O (5.2 mL) at –78 °C and methyl cyanoformate (62 µL, 0.78 mmol, 1.5 eq) was added dropwise. After 45 min, the reaction mixture was warmed to 0 °C. After 45 min, H_2O (5 mL) and Et_2O (5 mL) were added and reaction mixture warmed to room temperature. The reaction mixture was partitioned between H_2O (5 mL) and Et_2O (3 x 10 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0497** (36 mg, 16%) as a white solid. TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.68; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 3.76 (s, 3H), 3.29 (d, *J* = 13.1 Hz, 1H), 2.49-2.42 (m, 2H), 2.21 (apparent dt, *J* = 12.9, 2.5 Hz, 1H), 1.18 (s, 3H), 0.93 (d, *J* = 6.5 Hz, 3H), 0.869 (d, *J* = 6.6 Hz, 3H), 0.865 (d, *J* = 6.6 Hz, 3H), 0.63 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 206.1, 170.5, 133.1, 129.5, 60.1, 54.9, 51.9, 51.7, 45.0, 42.1, 39.5, 37.8, 36.8, 36.2, 36.10, 36.08, 35.6, 28.7, 28.0, 26.9, 23.9, 23.7, 22.84, 22.82, 22.6, 18.7, 17.8, 11.3. The observed 4α-CO_2Me,5α-H diastereoselectivity was consistent with that reported previously for similar compounds *(38)*. Additionally, an NOE correlation between the 4β-H and 10β-Me was observed, as well as a large coupling constant between the 4β-H and 5α-H ($J_{ax\text{-}ax}$ ~ 13 Hz) that was confirmed by COSY.

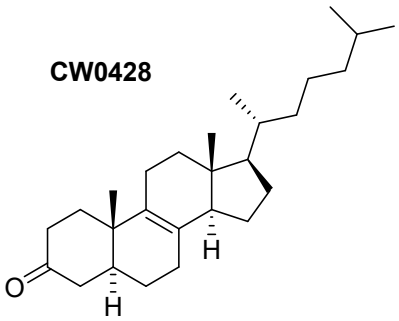


Methyl (3*S*,4*S*,5*S*,10*S*,13*R*,14*R*,17*R*)-3-hydroxy-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,5,6,7,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthrene-4-carboxylate (CW0499). To a solution of **CW0497** (33 mg, 75 µmol, 1 eq) in a mixture of MeOH (6 mL) and DCM (2 mL) was added $NaBH_4$ (6 mg, 150 µmol, 2 eq). After 1 day, the reaction was diluted with H_2O (10 mL) and acidified with HCl (aq) (1M, 1 mL). The reaction mixture was extracted with DCM (3 x 10 mL) and the combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0499** (15 mg, 45%, 3β/3α-OH > 95:5) as a white solid. TLC (Hex:EtOAc, 2:1 v/v): R_f = 0.27; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 3.86-3.78 (m, 1H), 3.73 (s, 3H), 2.37 (dd, *J* = 11.3, 10.5 Hz, 1H), 0.98 (s, 3H), 0.92 (d, *J* = 6.5 Hz, 3H), 0.865 (d, *J* = 6.6 Hz, 3H), 0.862 (d, *J* = 6.6

Hz, 3H), 0.60 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 175.7, 134.2, 128.5, 72.7, 54.8, 53.7, 51.8, 51.5, 43.5, 42.0, 39.5, 36.9, 36.3, 36.1, 35.8, 34.7, 30.5, 28.7 28.0, 26.9, 23.9, 23.7, 22.83, 22.78, 22.57, 22.56, 18.7, 18.4, 11.2. The observed 3α-H diastereoselectivity was consistent with that reported previously for similar compounds *(36)*. Additionally, an NOE correlation between the 3α-H and 5α-H was observed, as well as two large coupling constants for the 4β-H and 3α-H/5α-H ($J_{ax\text{-}ax}$ ~ 11 Hz) that were confirmed by COSY.



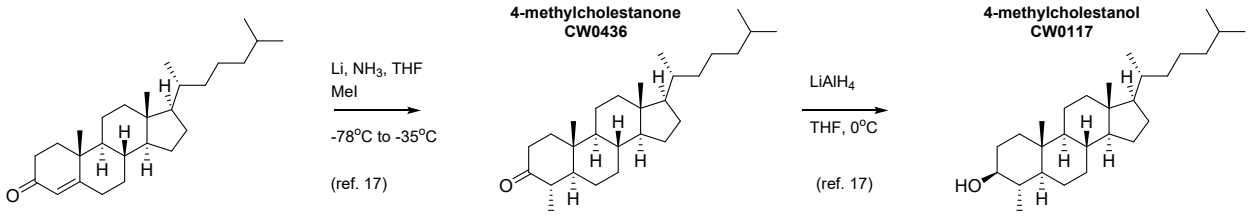
(3*S*,4*S*,5*S*,10*S*,13*R*,14*R*,17*R*)-3-Hydroxy-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,5,6,7,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthrene-4-carboxylic acid (CW4101). To **CW0499** (9 mg, 20 mol, 1 eq) was added methanolic KOH (20% by wt/v, 2.2 mL) and the reaction mixture heated at reflux. After 1 day, the reaction mixture was concentrated, dissolved in H_2O (10 mL), acidified with HCl (aq) (1M, 10 mL), and extracted with EtOAc (3 x 10 mL). The combined organic phase was washed with brine (3 mL), dried over Na_2SO_4, and concentrated to afford **CW4101** (9 mg, 100%) as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$/CD_3OD, representative signals): δ 3.74 (apparent dt, *J* = 11.0, 5.0 Hz, 1H), 2.30 (apparent t, *J* = 10.8 Hz, 1H), 0.99 (s, 3H), 0.93 (d, *J* = 6.5 Hz, 3H), 0.868 (d, *J* = 6.6 Hz, 3H), 0.864 (d, *J* = 6.6 Hz, 3H), 0.61 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$/CD_3OD): δ 177.8, 134.2, 128.4, 72.3, 54.8, 53.8, 51.7, 43.2, 42.0, 39.4, 36.8, 36.2, 36.0, 35.6, 34.7, 30.1, 28.7, 27.9, 26.9, 23.8, 23.6, 22.7, 22.4, 18.6, 18.2, 11.1.

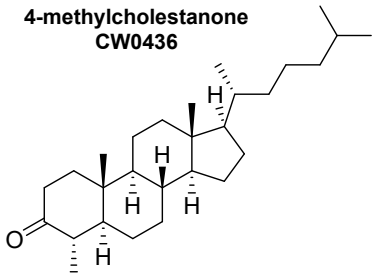


(5*S*,10*S*,13*R*,14*R*,17*R*)-10,13-Dimethyl-17-((*R*)-6-methylheptan-2-yl)-1,2,4,5,6,7,10,11,12,13,14,15,16,17-tetradecahydro-3*H*-cyclopenta[*a*]phenanthren-3-one (CW0428). A mixture of $Cu(OAc)_2 \cdot H_2O$ (5 mg, 23 μmol, 0.30 eq) and 1,2-bis(diphenylphosphino)benzene (BDP) (10 mg, 23 μmol, 0.30 eq) was dissolved in PhMe (0.16 mL). After 20 min, poly(methylhydrosiloxane) (PMHS) (26 μL, 390 μmol, 5

eq) and a solution of **CW0451** (30 mg, 78 µmol, 1 eq) in PhMe (0.16 mL) were added. After 1 day, the reaction mixture was diluted with EtOAc (10 mL) and washed with NaOH (aq) (1M, 5 mL), HCl (aq) (1M, 5 mL), and brine (5 mL). The organic phase was dried over Na_2SO_4 and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0428** (6 mg, 20%, 5α/5β-H ~ 80:20) as a white solid. TLC (Hex:EtOAc, 2:1 v/v): R_f = 0.56; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 1.14 (s, 3H), 0.93 (d, *J* = 6.5 Hz, 3H), 0.869 (d, *J* = 6.6 Hz, 3H), 0.866 (d, *J* = 6.6 Hz, 3H), 0.64 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): **major 5α epimer:** δ 212.0, 133.6, 129.2, 54.9, 51.8, 44.8, 42.8, 42.1, 39.5, 38.3, 36.9, 36.6, 36.3, 36.1, 35.8, 28.8, 28.0, 27.1, 25.6, 23.9, 23.8, 22.9, 22.8, 22.6, 18.7, 16.9, 11.3; **minor 5β epimer:** (representative signals) δ 213.4, 130.0, 54.8, 52.1. The observed 5α-H diastereoselectivity was consistent with that reported previously for similar compounds *(39)* and spectral data were consistent with that reported previously *(40)*.

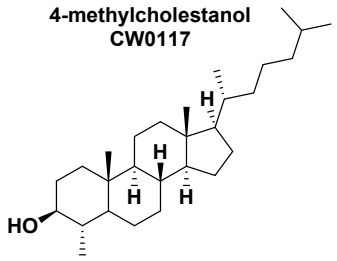
Figure 2: Synthetic scheme of C4DMC 8,9 saturated analogs 4-methylcholestanone (**CW0436)** and 4-methylcholestanol (**CW0117)**.





(4*S*,5*S*,8S,9S,10*S*,13*R*,14*R*,17*R*)-4,10,13-Trimethyl-17-((*R*)-6-methylheptan-2-yl)-hexadecahydro-1*H*-cyclopenta[*a*]phenanthran-3-one (CW0436). Lithium (12 mg, 1.73 mmol, 3.32 eq) was added to a solution of (+)- 4 -Cholesten-3-one (200 mg, 0.52 mmol, 1 eq) in THF (4 mL) and NH_3 (~3 mL) at –78 °C. After slowly warming to –35 °C over 1 h (blue color maintained), the solution was cooled to –78 °C and iodomethane (0.53 mL, 8.47 mmol, 16 eq) was added. The reaction mixture was allowed to warm to room temperature overnight and ammonia evaporated. Water (5 mL) was slowly added,

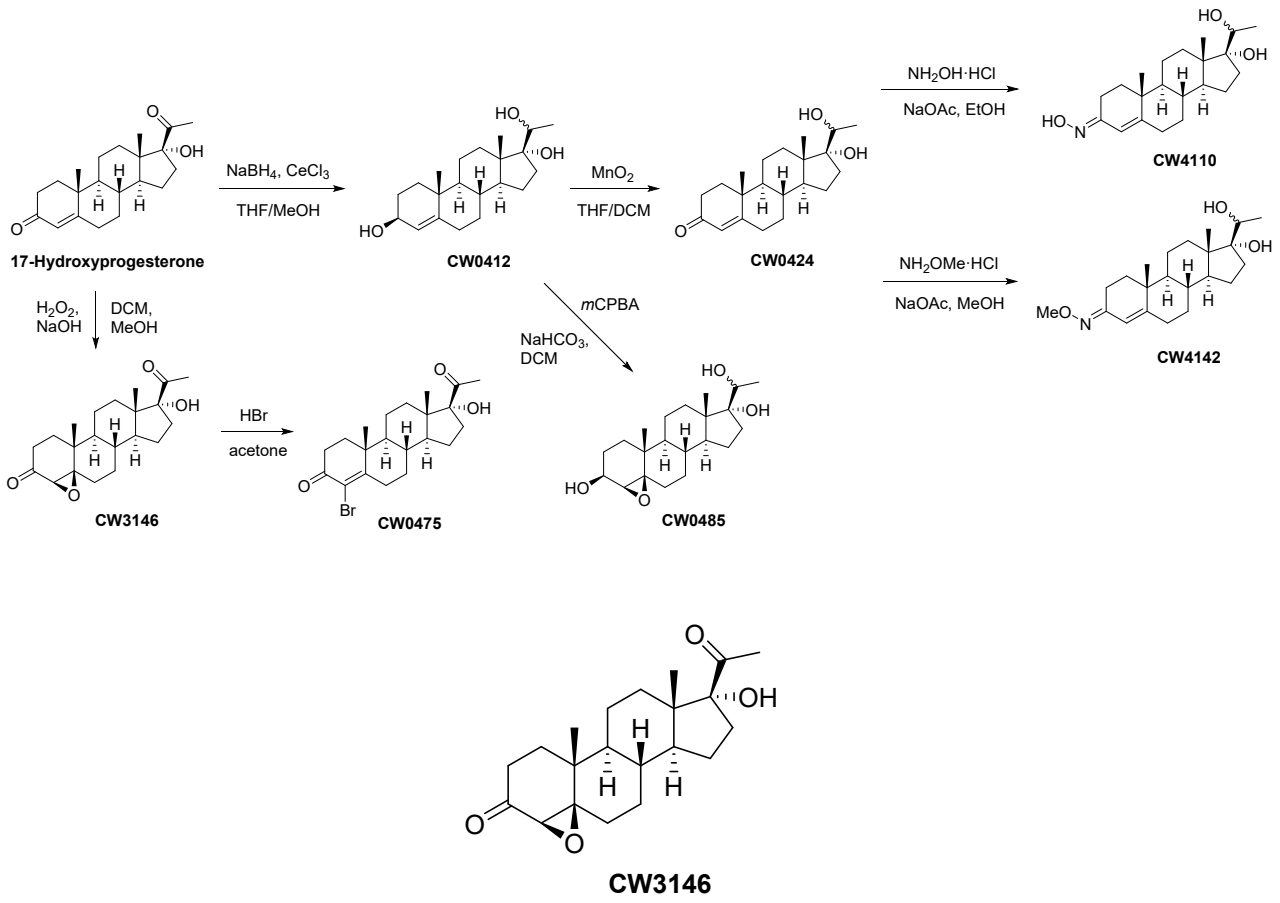
reaction mixture neutralized with HCl (aq) (2M, 10 mL), and extracted with Et_2O (3 x 20 mL). The combined organic phase was washed with brine (10 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0436** (40 mg, 19%) as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 0.67 (s, 3H), 0.65 – 0.71 (m, 1H), 0.85 (d, 3H), 0.87 (d, 3H), 0.90 (d, 3H), 0.93 – 1.01 (m, 2H), 0.97 (d, 3H), 1.04 – 1.19 (m, 8H), 1.07 (s, 3H), 1.20 – 1.27 (m, 1H), 1.31 – 1.39 (m, 6H), 1.49 – 1.59 (m, 4H), 1.65 – 1.68 (m, 1H), 1.72 – 1.76 (m, 1H), 1.77 – 1.85 (m, 1H), 1.97 – 2.05 (m, 2H), 2.27 – 2.34 (m, 2H), 2.41 – 2.46 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 11.50, 12.06, 12.71, 18.65, 21.38, 22.57, 22.82, 23.83, 24.20, 25.65, 28.02, 28.27, 31.95, 34.88, 35.79, 36.15, 36.34, 38.06, 39.28, 39.51, 39.93, 42.53, 45.06, 53.59, 54.08, 56.24, 56.32, 213.79. The observed 4α-Me,5α-H diastereoselectivity was consistent with that reported previously for similar compounds *(36)*.



(3*S*,4*S*,5*S*,8S,9S,10*S*,13*R*,14*R*,17*R*)-4,10,13-Trimethyl-17-((*R*)-6-methylheptan-2-yl)-hexadecahydro-1*H*-cyclopenta[*a*]phenanthran-3-ol (CW0117). To a solution of **CW0436** (11 mg, 27mmol) in anhydrous tetrahydrofuran (3 mL) at 0 °C, a 1M solution of lithium aluminum hydride in tetrahydrofuran (27 mL, 27mmol) was added. After stirring the solution for 4 h at 0 °C under an argon atmosphere, the reaction mixture was quenched with water (10 mL) and then acidified with 10% hydrochloric acid (10 mL). The aqueous layer was extracted with diethyl ether three times. The combined organic layers were washed with a saturated solution of sodium hydrogen carbonate and dried over anhydrous sodium sulfate. The ethereal solution was filtered, concentrated *in vacuo* and purified by flash chromatography (pentane/diethyl ether, 5:1) on silica gel to provide **CW0117** (4.3mg, 39%, 3β/3α-OH > 95:5) as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 0.58 - 0.60 (m, 1H), 0.63 (s, 3H), 0.64 - 0.67 (m, 1H), 0.71-0.77 (m, 1H), 0.81 (s, 3H), 0.84 – 0.86 (d,3H), 0.86 – 0.88 (d, 3H), 0.88 – 0.89 (d, 3H), 0.93 – 0.94 (d, 3H), 1.03 – 1.12 (m, 10H), 1.19 – 1.37 (m, 8H), 1.42 – 1.56 (m, 4H), 1.64 – 1.73 (m, 3H), 1.78 – 1.81 (m, 2H), 1.94 – 1.97 (d, 1H), 3.07 (m, 1H). The observed 3α-H diastereoselectivity and spectral data were consistent with that reported previously *(36)*.

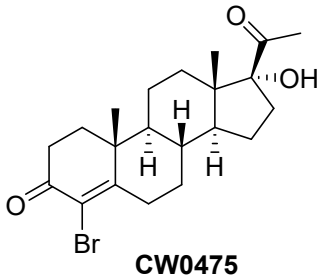
SC4MOL Inhibitors

Figure 3: Synthetic scheme of 17-hydroxyprogesterone analogs **CW0412**, **CW0424**, **CW0475**, **CW0485**, **CW4110**, and **CW4142**.



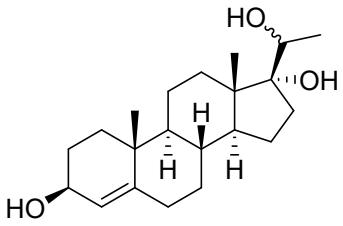
CW3146

(1a*R*,4a*R*,4b*S*,6a*S*,7*R*,9a*S*,9b*S*,11a*R*)-7-Acetyl-7-hydroxy-4a,6a-dimethyltetradecahydrocyclopenta[7,8]phenanthro[1,10a-*b*]oxiren-2(1a*H*)-one (CW3146). To a solution of 17α-hydroxyprogesterone (150 mg, 0.45 mmol, 1 eq) in a mixture of MeOH (1.8 mL) and DCM (1.5 mL) was added NaOH (aq) (2M, 0.25 mL, 0.50 mmol, 1.1 eq) and H_2O_2 (aq) (30% by wt, 0.25 mL, 2.21 mmol, 4.9 eq) dropwise. After 1 day, the reaction mixture was partially concentrated and partitioned between H_2O (5 mL) and DCM (3 x 5 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW3146** (100 mg, 64%, 4β,5β/4α,5α-epoxide ~ 3:1) as a white solid. TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.61; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ **major isomer**: 2.99 (s, 1H), 2.84 (s, 1H), 2.269 (s, 3H), 1.16 (s, 3H), 0.73 (s, 3H); **minor isomer**: 3.04 (s, 1H), 2.82 (s, 1H), 2.274 (s, 3H), 1.07 (s, 3H), 0.74 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, representative signals): δ **major isomer**: 211.59, 206.6, 89.7, 70.1, 62.6, 50.0, 48.3, 46.1; **minor isomer**: 211.60, 207.0, 89.9, 70.0, 62.8, 50.2, 49.8, 48.2. The observed major 4β,5β-epoxide diastereoselectivity was consistent with that reported previously for similar compounds *(41)*.



CW0475

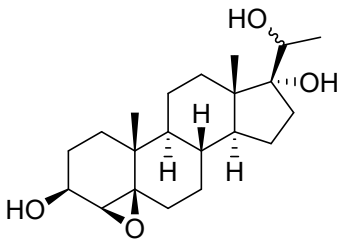
(8*R*,9*S*,10*R*,13*S*,14*S*,17*R*)-17-Acetyl-4-bromo-17-hydroxy-10,13-dimethyl-1,2,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-3*H*-cyclopenta[*a*]phenanthren-3-one (CW0475). To a solution of **CW3146** (50 mg, 0.144 mmol, 1 eq) in acetone (1.5 mL) was HBr (40% aq) (0.159 mmol, 1.1 eq) dropwise. After 1 day, the reaction mixture was poured into H_2O (10 mL), and extracted with DCM (3 x 10 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0475** (39 mg, 66%) as a white solid. TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.51; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 3.29 (ddd, *J* = 14.9, 3.5, 2.8 Hz, 1H), 2.79 (s, 1H), 2.28 (s, 3H), 1.24 (s, 3H), 0.76 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 211.6, 190.7, 167.8, 122.0, 89.7, 53.5, 49.9, 48.2, 42.5, 35.1, 34.6, 34.0, 33.6, 32.9, 31.3, 30.0, 27.9, 23.9, 20.7, 17.9, 15.4. Spectral data was consistent with that reported previously *(42)*.



CW0412

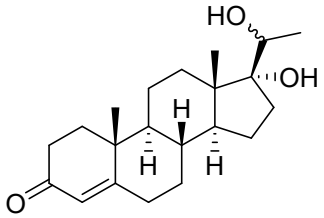
(3*S*,8*R*,9*S*,10*R*,13*S*,14*S*,17*R*)-17-(1-Hydroxyethyl)-10,13-dimethyl-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,17-diol (CW0412). To a solution of 17α-hydroxyprogesterone (50 mg, 0.151 mmol, 1 eq) in a mixture of THF (0.84 mL) and MeOH (0.42 mL) at 0 °C was added $CeCl_3 \cdot 7H_2O$ (56 mg, 0.151 mmol, 1 eq) and $NaBH_4$ (7 mg, 0.181 mmol, 1.2 eq). After 20 min, the reaction mixture was concentrated, dissolved in EtOAc (20 mL), and the organic phase successively washed with HCl (aq) (1M, 5 mL), saturated $NaHCO_3$ (aq) (5 mL), H_2O (5 mL), and brine (5 mL). The combined organic phase was dried over Na_2SO_4 and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0412** (21 mg, 42%, C3-OH β/α > 95:5, C20-OH *R*/*S* ~ 50:50) as a white solid. TLC (Hex:EtOAc, 1:2 v/v): R_f = 0.30; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ **C20 epimers**: 5.28 (s, 1H), 4.19-4.12 (m, 1H), 4.06-4.00 (m, 0.5H), 3.87-3.80 (m, 0.5H), 1.18 (d, *J* = 6.3 Hz, 1.5H), 1.17 (d, *J* = 6.3 Hz, 1.5H), 1.060 (s, 1.5H), 1.055 (s, 1.5H), 0.82 (s, 1.5H), 0.75 (s, 1.5H); ^{13}C NMR (125 MHz, $CDCl_3$, representative signals): δ **C20 epimers**: 147.5, 147.4, 123.5, 123.4, 85.6,

85.1, 72.3, 70.4, 67.95, 67.91, 54.0, 53.9, 50.8, 49.9, 47.3, 45.8. Spectral data and stereochemical assignments were consistent with that reported previously *(43)*.



CW0485

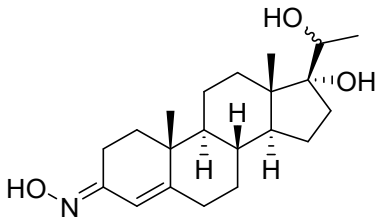
(1a*S*,2*S*,4a*R*,4b*S*,6a*S*,7*R*,9a*S*,9b*S*,11a*R*)-7-(1-Hydroxyethyl)-4a,6a-dimethylhexadecahydrocyclopenta[7,8]phenanthro[1,10a-*b*]oxirene-2,7-diol (CW0485). To a solution of **CW0412** (50 mg, 0.149 mmol, 1 eq) in DCM (3 mL) was added $NaHCO_3$ (19 mg, 0.224 mmol, 1.5 eq) and *m*CPBA (77% by wt, 37 mg, 0.164 mmol, 1.1 eq). After 1 day, the reaction mixture was diluted with DCM (20 mL) and washed with saturated $NaHCO_3$ (aq) (5 mL) then brine (5 mL). The combined organic phase was dried over Na_2SO_4 and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0485** (51 mg, 98%, C3-OH β/α > 95:5, C20-OH *R*/*S* ~ 50:50, 4β,5β/4α,5α-epoxide > 95:5) as a white solid. TLC (EtOAc): R_f = 0.30; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ **C20 epimers**: 4.09-3.99 (m, 1.5H), 3.85 (q, *J* = 6.3 Hz, 0.5H), 3.15 (d, *J* = 4.4 Hz, 1H), 1.19 (d, *J* = 6.3 Hz, 1.5H), 1.18 (d, *J* = 6.3 Hz, 1.5H), 1.04 (s, 1.5H), 1.03 (s, 1.5H), 0.81 (s, 1.5H), 0.74 (s, 1.5H); ^{13}C NMR (125 MHz, $CDCl_3$, representative signals): δ **C20 epimers**: 85.4, 85.1, 72.3, 70.3, 68.9, 68.8, 64.3, 64.2, 63.73, 63.70, 50.8, 49.9, 47.3, 46.8, 46.6, 45.8. The observed major 4β,5β-epoxide diastereoselectivity was consistent with that reported previously for similar compounds *(44)*. The stereochemistry of **CW0485** was also confirmed by DMP oxidation of the secondary alcohols to make the major diastereomer of **CW3146**, which was confirmed by ^{1}H NMR.



CW0424

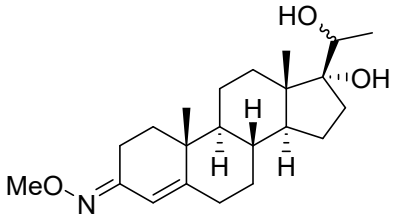
(8*R*,9*S*,10*R*,13*S*,14*S*,17*R*)-17-Hydroxy-17-(1-hydroxyethyl)-10,13-dimethyl-1,2,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-3*H*-cyclopenta[*a*]phenanthren-3-one (CW0424). To a solution of **CW0412** (8 mg, 24 μmol, 1 eq) in a mixture of THF (0.5 mL) and DCM (0.5 mL) was added MnO_2 (activated) (42 mg, 480 μmol, 20 eq). After 1 day, the reaction mixture was filtered through Celite with DCM and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0424** (7 mg, 88%, C20-OH epimers enriched to ~ 60:40) as a white solid. TLC (Hex:EtOAc, 1:2 v/v): R_f = 0.17; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals):

δ **major C20 epimer**: 5.73 (s, 1H), 4.07-4.01 (m, 1H), 0.85 (s, 3H); **minor C20 epimer**: 5.73 (s, 1H), 3.89-3.83 (m, 1H), 0.78 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, representative signals): δ **major C20 epimer**: 199.7, 171.5, 123.8, 85.0, 70.4, 53.4, 49.7, 47.2; **minor C20 epimer**: 199.6, 171.3, 123.9, 85.4, 72.3, 53.3, 50.6, 45.7. Spectral data was consistent with that reported previously *(43)*.



CW4110

(8*R*,9*S*,10*R*,13*S*,14*S*,17*R*,*E*)-17-Hydroxy-17-(1-hydroxyethyl)-10,13-dimethyl-1,2,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-3*H*-cyclopenta[*a*]phenanthren-3-one oxime (CW4110). To a solution of **CW0424** (149 mg, 0.45 mmol, 1 eq) in EtOH (95%, 23 mL) at 60 °C was added $NH_2OH{\cdot}HCl$ (47 mg, 0.67 mmol, 1.5 eq) and $NaOAc{\cdot}3H_2O$ (86 mg, 0.63 mmol, 1.4 eq). After 1 h, the reaction mixture was partitioned between H_2O (20 mL) and EtOAc (3 x 20 mL). The combined organic phase was washed with brine (10 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW4110** (124 mg, 79%, *E/Z* ~ 2:1, C20-OH epimers ~ 60:40) as a white solid. TLC (Hex:EtOAc, 1:4 v/v): R_f = 0.34; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ ***Z* isomer**: 6.47 (s, 1H); ***E* isomer**: 5.77 (s, 1H), 3.08-3.00 (m, 1H); **major C20 epimer**: 4.03 (q, *J* = 6.3 Hz, 1H), 0.84 (s, 3H); **minor C20 epimer**: 3.85 (q, *J* = 6.3 Hz, 1H), 0.76 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, representative signals): δ ***Z* isomer (C20 epimers)**: 159.7, 159.5, 154.1, 154.0, 110.3, 110.2, 85.59, 85.18, 72.4; ***E* isomer (C20 epimers)**: 157.1, 157.0, 155.6, 155.5, 117.3, 117.2, 85.65, 85.24, 70.5. The observed *E/Z* oxime selectivity was consistent with that reported previously for similar compounds *(45)*.

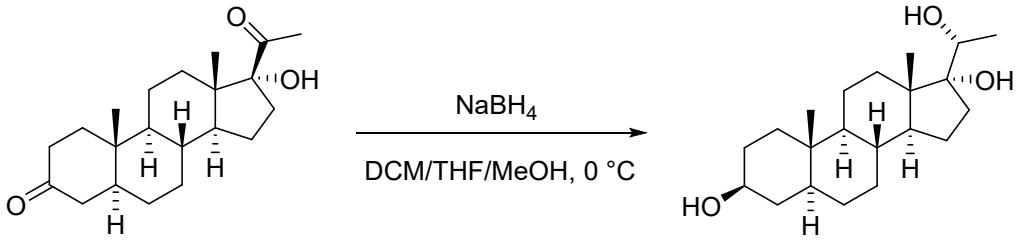


CW4142

(8*R*,9*S*,10*R*,13*S*,14*S*,17*R*,*E*)-17-Hydroxy-17-(1-hydroxyethyl)-10,13-dimethyl-1,2,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-3*H*-cyclopenta[*a*]phenanthren-3-one O-methyl oxime (CW4142). To a solution of **CW0424** (135 mg, 0.41 mmol, 1 eq) in MeOH (20 mL) was added $MeONH_2{\cdot}HCl$ (51 mg, 0.61 mmol, 1.5 eq) and $NaOAc{\cdot}3H_2O$ (77 mg, 0.57 mmol, 1.4 eq). After heating at 60 °C for 1 h, the reaction mixture was partially concentrated and partitioned between H_2O (10 mL) and EtOAc (3 x 10 mL). The combined organic phase was washed with brine (5 mL), dried over

Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW4142** (98 mg, 67%, *E/Z* ~ 60:40, C20-OH epimers ~ 60:40) as a white solid. TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.29; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ ***Z* isomer**: 6.36 (s, 1H), 3.848 (s, 3H); ***E* isomer**: 5.77 (s, 1H), 3.854 (s, 3H), 2.98-2.91 (m, 1H); **major C20 epimer**: 4.05-4.00 (m, 1H), 0.83 (s, 3H); **minor C20 epimer**: 3.88-3.81 (m, 1H), 0.76 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, representative signals): δ ***Z* isomer (C20 epimers)**: 159.8, 159.7, 153.42, 153.36, 110.73, 110.68, 85.54, 85.49, 72.29, 72.28, 61.29, 61.28; ***E* isomer (C20 epimers)**: 156.35, 156.29, 155.6, 155.4, 117.23, 117.17, 85.12, 85.06, 70.36, 70.35, 61.48, 61.47; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd. for $C_{22}H_{36}NO_3$, 362.2695; found, 362.2682. The observed *E/Z* oxime ether selectivity was consistent with that reported previously for similar compounds *(45)*.

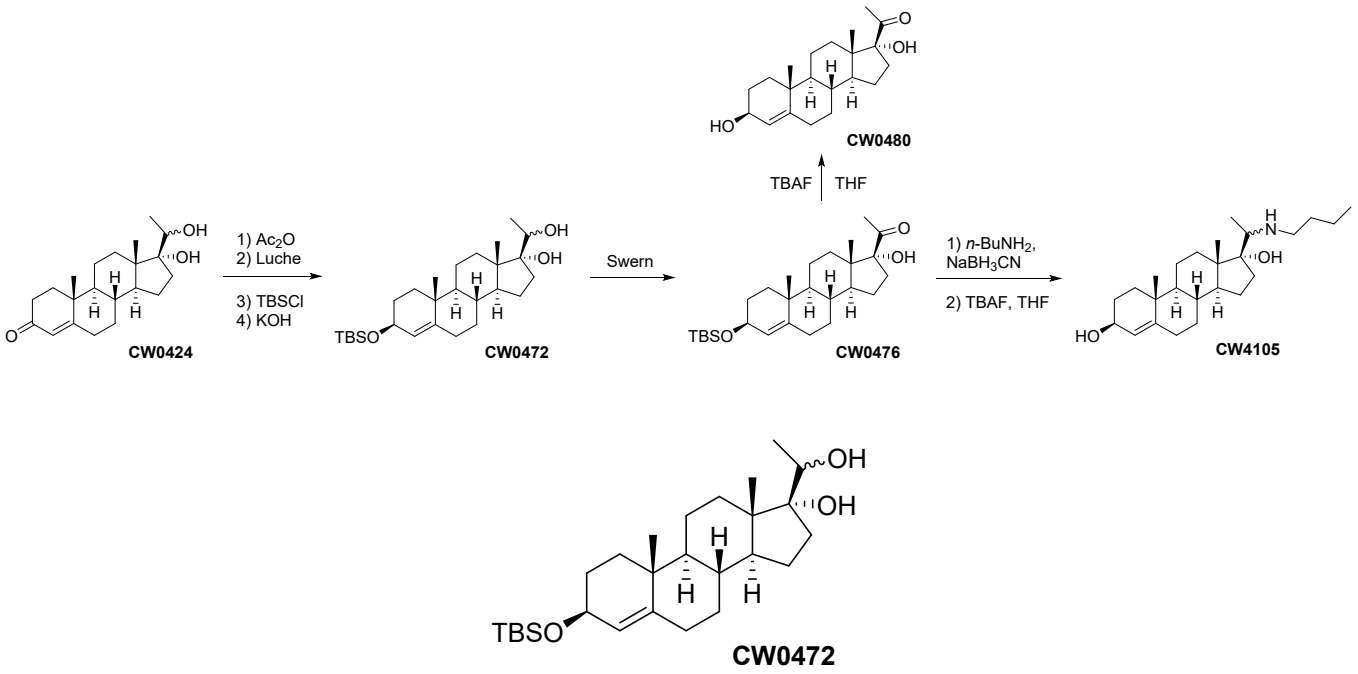
Figure 4: Synthetic scheme of 17-hydroxyprogesterone analogs **CW0464**



CW0464

(3*S*,5*S*,8*R*,9*S*,10*S*,13*S*,14*S*,17*R*)-17-((*R*)-1-Hydroxyethyl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,17-diol (CW0464). To a solution of 5α-pregnan-17α-ol-3,20-dione (10 mg, 30 μmol, 1 eq) in a mixture of DCM (0.2 mL), THF (0.2 mL), and MeOH (0.1 mL) at 0 °C was added $NaBH_4$ (~3 mg, 75 μmol, 2.5 eq). After 1 h, the reaction mixture was concentrated, dissolved in EtOAc (15 mL), and the organic phase successively washed with HCl (aq) (1M, 2 mL), saturated $NaHCO_3$ (aq) (2 mL), H_2O (2 mL), and brine (2 mL). The combined organic phase was dried over Na_2SO_4 and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0464** (6 mg, 59%, C3-OH β/α > 95:5, C20-OH *R*/*S* ~ 90:10) as a white solid with some minor impurities. TLC (EtOAc): R_f = 0.35; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ **major (*R*) C20 epimer**: 4.03 (q, *J* = 6.1 Hz, 1H), 3.64-3.56 (m, 1H), 1.17 (d, *J* = 6.3 Hz, 3H), 0.82 (s, 3H), 0.79 (s, 3H); **minor (*S*) C20 epimer**: 3.83 (q, *J* = 6.1 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ **major (*R*) C20 epimer**: 85.2, 71.3, 70.5, 54.0, 50.2, 47.4, 44.8, 38.2, 37.0, 35.7, 35.5, 33.9, 32.5, 32.1, 31.5, 28.7, 23.8, 20.9, 18.7, 15.3, 12.3. The observed diastereoselectivities were consistent with that reported previously for similar compounds *(43, 46)*.

Figure 5: Synthetic scheme of 17-hydroxyprogesterone analogs **CW0480**, **CW4105**, **CW4140**, **CW4148**, and **CW4154**.

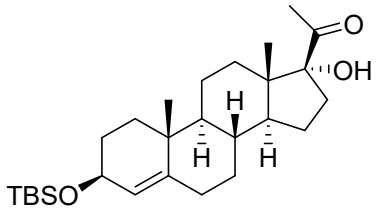


(3*S*,8*R*,9*S*,10*R*,13*S*,14*S*,17*R*)-3-((*tert*-Butyldimethylsilyl)oxy)-17-(1-hydroxyethyl)-10,13-dimethyl-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-17-ol (CW0472). To a solution of **CW0424** (323 mg, 0.972 mmol, 1 eq) in a mixture of DCM (4.5 mL) and pyridine (0.5 mL) was added DMAP (~6 mg, 0.05 mmol, 0.05 eq) and Ac_2O (0.92 mL, 9.72 mmol, 10 eq). After 2 days, the reaction mixture was diluted with DCM (50 mL) and successively washed with HCl (aq) (1M, 10 mL), saturated $NaHCO_3$ (aq) (10 mL), and brine (10 mL). The combined organic phase was dried over Na_2SO_4 and concentrated to afford a white solid (310 mg). The crude acetate was used in the next step without further purification.

To a solution of the crude acetate (310 mg) in a mixture of THF (5.5 mL) and MeOH (2.8 mL) at 0 °C was added $CeCl_3 \cdot 7H_2O$ (309 mg, 0.83 mmol, 1 eq) and $NaBH_4$ (38 mg, 1.00 mmol, 1.2 eq). After 1 h, the reaction mixture was concentrated, dissolved in EtOAc (50 mL), and the organic phase successively washed with HCl (aq) (1M, 10 mL), saturated $NaHCO_3$ (aq) (10 mL), H_2O (10 mL), and brine (10 mL). The combined organic phase was dried over Na_2SO_4 and concentrated to afford a white solid (310 mg). The crude alcohol was used in the next step without further purification.

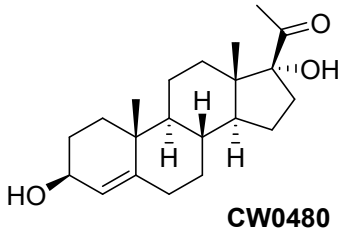
To a solution of the crude alcohol (310 mg) in DMF (4.2 mL) was added imidazole (280 mg, 4.2 mmol, 5 eq) and TBSCl (380 mg, 2.5 mmol, 3 eq). After heating at 50 °C for 1 day, the reaction mixture was diluted with EtOAc (50 mL) and washed with H_2O (3 x 10 mL). The combined organic phase was washed with brine (10 mL), dried over Na_2SO_4, and concentrated to afford a white solid (380 mg). The crude silyl ether was used in the next step without further purification.

To a solution of crude silyl ether (380 mg) in a mixture of THF (7 mL), MeOH (7 mL), and H_2O (0.7 mL) was added KOH (aq) (4M, 1.9 mL, 7.7 mmol, 10 eq). After 2 days, the reaction mixture was concentrated and partitioned between H_2O (20 mL) and EtOAc (3 x 20 mL). The combined organic phase was washed with brine (10 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0472** (230 mg, 53% over 4 steps, C3-OTBS β/α > 95:5, C20-OH epimers ~ 60:40) as a white solid. TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.56; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ **major C20 epimer**: 5.20 (s, 1H), 4.19-4.13 (m, 1H), 4.01 (q, *J* = 6.1 Hz, 1H), 1.16 (d, *J* = 6.4 Hz, 3H), 1.04 (s, 3H), 0.89 (s, 9H), 0.80 (s, 3H), 0.07 (s, 3H), 0.06 (s, 3H); **minor C20 epimer**: 5.20 (s, 1H), 4.19-4.13 (m, 1H), 3.82 (q, *J* = 6.1 Hz, 1H), 1.17 (d, *J* = 6.4 Hz, 3H), 1.04 (s, 3H), 0.89 (s, 9H), 0.73 (s, 3H), 0.07 (s, 3H), 0.06 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, representative signals): δ **major C20 epimer**: 146.1, 124.57, 85.1, 70.4, 68.92, 54.3, 49.9, 47.2; **minor C20 epimer**: 146.0, 124.62, 85.6, 72.3, 68.88, 54.1, 50.8, 45.8. The observed diastereoselectivities were consistent with that reported previously for similar compounds *(43)*.



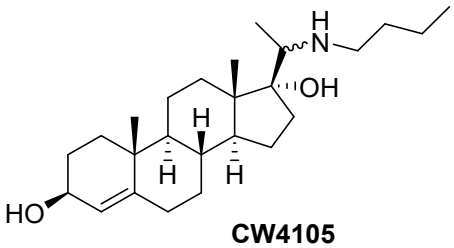
CW0476

1-((3*S*,8*R*,9*S*,10*R*,13*S*,14*S*,17*R*)-3-((*tert*-Butyldimethylsilyl)oxy)-17-hydroxy-10,13-dimethyl-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)ethan-1-one (CW0476). To a solution of oxalyl chloride (86 µL, 1.00 mmol, 2 eq) in DCM (2.5 mL) at –78 °C was added DMSO (107 µL, 1.50 mmol, 3 eq). After 30 min, **CW0472** (225 mg, 0.50 mmol, 1 eq) in DCM (2.5 mL) was slowly added. After 3 h, Et_3N (0.35 mL, 2.50 mmol, 5 eq) was added and reaction allowed to warm to room temperature over 1 h. The reaction mixture was partitioned between H_2O (10 mL) and DCM (3 x 10 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0476** (191 mg, 85%, C3-OTBS β/α > 95:5) as a white solid. TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.68; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 5.22 (s, 1H), 4.20-4.14 (m, 1H), 2.71 (s, 1H), 2.65 (ddd, *J* = 14.6, 11.6, 2.7 Hz, 1H), 2.26 (s, 3H), 1.04 (s, 3H), 0.90 (s, 9H), 0.73 (s, 3H), 0.08 (s, 3H), 0.07 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 211.8, 145.8, 124.8, 90.0, 68.9, 54.2, 50.2, 48.4, 37.3, 35.81, 35.78, 33.5, 33.2, 32.2, 30.2, 29.6, 28.0, 26.1, 24.0, 20.4, 18.7, 18.4, 15.5, –4.4, –4.6.



CW0480

1-((3*S*,8*R*,9*S*,10*R*,13*S*,14*S*,17*R*)-3,17-Dihydroxy-10,13-dimethyl-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)ethan-1-one (CW0480). To **CW0476** (15 mg, 34 µmol, 1eq) was added TBAF (1M in THF, 1.1 mL, 1.1 mmol, 30 eq). After 2 days, the reaction mixture was partitioned between H_2O (3 mL) and DCM (3 x 5 mL). The combined organic phase was washed with brine (3 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0480** (11 mg, 97%, C3-OH β/α > 95:5) as a white solid. TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.30; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 5.29 (s, 1H), 4.20-4.12 (m, 1H), 2.71 (s, 1H), 2.66 (ddd, *J* = 14.6, 11.5, 2.8 Hz, 1H), 2.27 (s, 3H), 1.06 (s, 3H), 0.74 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 211.8, 147.2, 123.6, 89.9, 67.9, 53.9, 50.2, 48.4, 37.3, 35.8, 35.4, 33.5, 33.1, 32.1, 30.1, 29.5, 27.9, 24.0, 20.5, 18.9, 15.5.



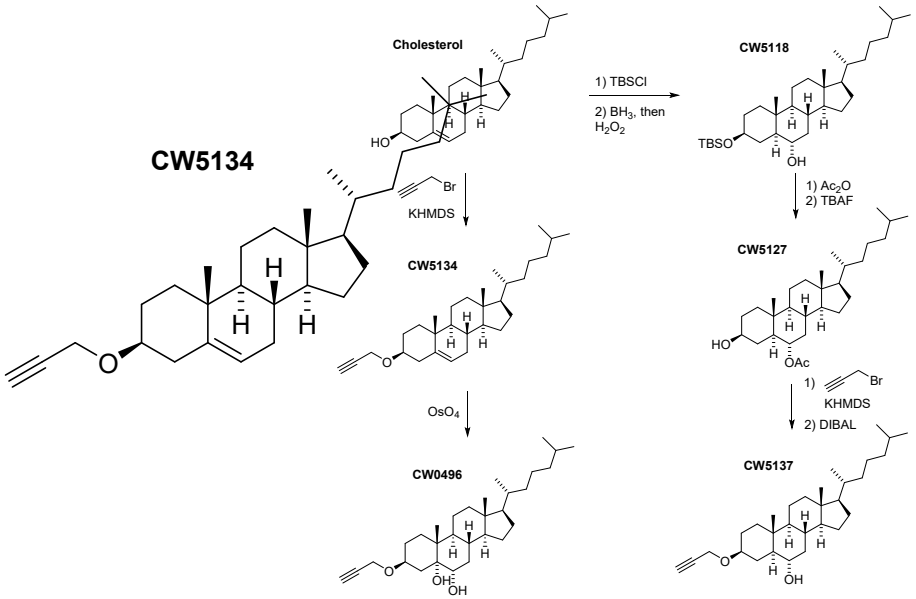
CW4105

(3*S*,8*R*,9*S*,10*R*,13*S*,14*S*,17*R*)-17-(1-(Butylamino)ethyl)-10,13-dimethyl-2,3,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,17-diol (CW4105). To a solution of **CW0476** (50 mg, 0.112 mmol, 1 eq) in a mixture of MeOH (0.50 mL) and THF (0.25 mL) was added *n*-$BuNH_2$ (55 µL, 0.560 mmol, 5 eq) and AcOH (glacial, 32 µL, 0.560 mmol, 5 eq). After 30 min, $NaBH_3CN$ (35 mg, 0.560 mmol, 5 eq) was added. After 2 days, the reaction mixture was partitioned between saturated $NaHCO_3$ (aq) (5 mL) and DCM (3 x 10 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated to afford a colorless oil. The crude amine was used in the next step without further purification.

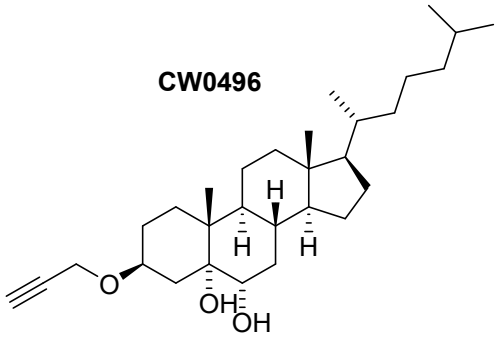
To a solution of crude amine was added TBAF (1M in THF, 3.4 mL, 3.4 mmol, 30 eq). After 3 days, the reaction mixture was partitioned between H_2O (5 mL) and DCM (3 x 10 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (DCM/MeOH/Me_2EtN) on silica and partitioned between H_2O/Et_2O to afford **CW4105** (25 mg, ~45% over 2 steps, C3-OH β/α > 95:5, C20 epimers ~2:1) as a white solid (~80% purity with ~20% **CW0480**). TLC (DCM:MeOH:Me_2EtN, 95:5:1 v/v/v): R_f = 0.07; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ **major C20 epimer**: 5.27 (s, 1H), 4.18-4.12 (m, 1H), 2.90 (q, *J* = 6.3 Hz, 1H), 0.76 (s, 3H); **minor C20 epimer**: 5.27

(s, 1H), 4.18-4.12 (m, 1H), 2.75 (q, *J* = 6.3 Hz, 1H), 0.75 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$, representative signals): δ **major C20 epimer**: 147.5, 123.43, 84.7, 67.9, 56.6; **minor C20 epimer**: 147.6, 123.37, 84.6, 67.8, 59.2.

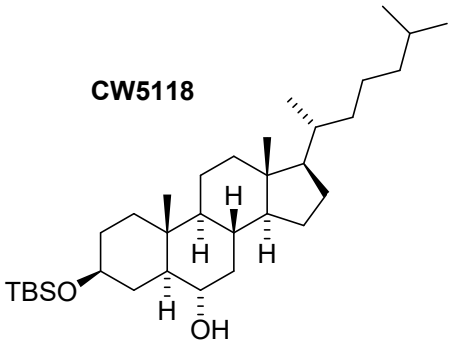
Figure 6: Synthetic scheme of cholesterol analogs **CW0496**, **CW4150**, **CW5131**, **CW5132**, **CW5134**, and **CW5137**.



(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-((*R*)-6-methylheptan-2-yl)-3-(prop-2-yn-1-yloxy)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthrene (CW5134). To a solution of cholesterol (150 mg, 0.388 mmol, 1 eq) in THF (3.9 mL) at 0 °C was added KHMDS (0.5 M in PhMe, 0.78 mL, 0.388 mmol, 1 eq) dropwise. After 15 min, propargyl bromide (80% by wt in PhMe, 43 µL, 0.388 mmol, 1 eq) was added and the reaction allowed to warm to room temperature. After 1 day, the reaction mixture was quenched with saturated NH_4Cl (aq) (5 mL) and H_2O (5 mL) and extracted with DCM (3 x 10 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW5134** (115 mg, 70%) as a white solid. TLC (Hex:EtOAc, 95:5 v/v): R_f = 0.58; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 5.38-5.34 (m, 1H), 4.19 (d, *J* = 2.3 Hz, 2H), 3.42-3.34 (m, 1H), 2.39 (t, *J* = 2.3 Hz, 1H), 2.26-2.18 (m, 1H), 1.00 (s, 3H), 0.91 (d, *J* = 6.5 Hz, 3H), 0.862 (d, *J* = 6.6 Hz, 3H), 0.860 (d, *J* = 6.6 Hz, 3H), 0.67 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 140.6, 121.9, 80.4, 78.2, 73.8, 56.8, 56.1, 55.1, 50.2, 42.3, 39.8, 39.5, 38.7, 37.1, 36.8, 36.2, 35.8, 31.94, 31.87, 28.2, 28.1, 28.0, 24.3, 23.8, 22.8, 22.6, 21.1, 19.3, 18.7, 11.9. Spectral data was consistent with that reported previously *(47)*.



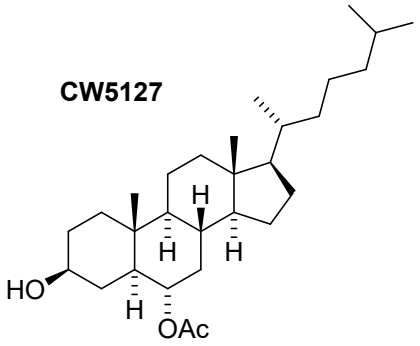
(3*S*,5*R*,6*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-((*R*)-6-methylheptan-2-yl)-3-(prop-2-yn-1-yloxy)hexadecahydro-5*H*-cyclopenta[*a*]phenanthrene-5,6-diol (CW0496). To a solution of **CW5134** (85 mg, 0.20 mmol, 1 eq) in a mixture of *t*-BuOH (5 mL) and H_2O (5 mL) was added $K_3Fe(CN)_6$ (0.66 g, 2.0 mmol, 10 eq), K_2CO_3 (0.28 g, 2.0 mmol, 10 eq), DABCO (22 mg, 0.20 mmol, 1 eq), and OsO_4 (aq) (4% by wt, 61 µL, 0.01 mmol, 0.05 eq). After 8 days, the reaction mixture was partitioned between H_2O (10 mL) and EtOAc (3 x 10 mL). The combined organic phase was washed with $Na_2S_2O_3$ (aq) (10% by wt, 5 mL) then brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0496** (2 mg, 2%, 5α,6α/5β,6β-diol > 95:5) as a white solid. TLC (Hex:EtOAc, 4:1 v/v): R_f = 0.12; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 4.19 (d, *J* = 2.3 Hz, 2H), 3.93-3.85 (m, 1H), 3.70-3.63 (m, 1H), 2.40 (t, *J* = 2.2 Hz, 1H), 2.25-2.20 (m, 1H), 0.95 (s, 3H), 0.90 (d, *J* = 6.5 Hz, 3H), 0.862 (d, *J* = 6.6 Hz, 3H), 0.860 (d, *J* = 6.6 Hz, 3H), 0.64 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 80.5, 76.7, 74.4, 73.8, 70.6, 56.2, 55.9, 55.4, 44.6, 42.7, 39.8, 39.5, 39.3, 36.1, 35.8, 35.2, 34.9, 33.5, 30.8, 28.2, 28.0, 27.1, 24.1, 23.8, 22.8, 22.6, 21.1, 18.6, 15.4, 12.1; HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd. for $C_{30}H_{50}O_3Na$, 481.3658; found, 481.3653. The observed major 5α,6α-diol diastereoselectivity was consistent with that reported previously for similar compounds *(48)*.



(3*S*,5*S*,6*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-3-((*tert*-Butyldimethylsilyl)oxy)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-1*H*-cyclopenta[*a*]phenanthren-6-ol (CW5118). To a solution of cholesterol (1.00 g, 2.59 mmol, 1 eq) in DMF (13 mL) was added imidazole (0.53 g, 7.76 mmol, 3 eq) and TBSCl (0.78 g, 5.17 mmol, 2 eq). After heating at 50 °C for 1 day, the reaction mixture was diluted with DCM (60 mL) and washed with H_2O (3 x 20 mL). The combined organic phase was washed with brine (20

mL), dried over Na_2SO_4, and concentrated to afford a white solid. The crude silyl ether was used in the next step without further purification.

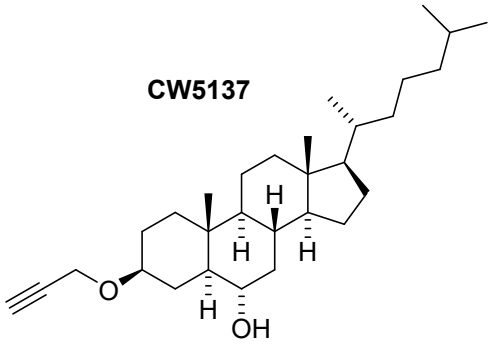
To a solution of crude silyl ether in THF (26 mL) was slowly added BH_3·DMS (5M in Et_2O, 1.6 mL, 7.77 mmol, 3 eq) and reaction heated at reflux. After 2 h, the reaction mixture was cooled to room temperature and H_2O (20 mL), NaOH (aq) (2M, 20 mL), and H_2O_2 (aq) (30% by wt, 4.4 mL) were slowly added before heating at reflux. After 1 h, the reaction mixture was extracted with DCM (3 x 30 mL) and the combined organic phase was washed with brine (20 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW5118** (1.06 g, 79% over 2 steps, α/β-hydration > 95:5) as a white solid. TLC (Hex:EtOAc, 2:1 v/v): R_f = 0.75; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 3.56-3.48 (m, 1H), 3.39 (apparent dt, *J* = 10.7, 4.5 Hz, 1H), 0.89 (d, *J* = 6.6 Hz, 3H), 0.88 (s, 9H), 0.86 (d, *J* = 6.6 Hz, 3H), 0.85 (d, *J* = 6.6 Hz, 3H), 0.80 (s, 3H), 0.64 (s, 3H), 0.05 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 72.1, 69.6, 56.2, 53.9, 51.8, 42.6, 41.6, 39.9, 39.5, 37.4, 36.3, 36.2, 35.8, 34.3, 32.6, 31.7, 28.2, 28.0, 26.0, 24.2, 23.8, 22.8, 22.6, 21.2, 18.7, 18.2, 13.5, 12.0, –4.5. The observed major *syn*-α diastereoselectivity and spectral data were consistent with that reported previously *(49)*.



(3*S*,5*S*,6*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-3-Hydroxy-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-1*H*-cyclopenta[*a*]phenanthren-6-yl acetate (CW5127). To a solution of **CW5118** (750 mg, 1.45 mmol, 1 eq) in pyridine (5.8 mL) was added DMAP (9 mg, 0.07 mmol, 0.05 eq) and Ac_2O (1.4 mL, 14.5 mmol, 10 eq). After 2 days, the reaction mixture was diluted with DCM (50 mL) and successively washed with HCl (aq) (1M, 25 mL), saturated $NaHCO_3$ (aq) (25 mL), and brine (25 mL). The combined organic phase was dried over Na_2SO_4 and concentrated to afford a white foam. The crude acetate was used in the next step without further purification.

To a solution of the crude acetate was added TBAF (1M in THF, 4.4 mL, 4.4 mmol, 3 eq). After 2 days, the reaction mixture was partitioned between H_2O (30 mL) and DCM (3 x 30 mL). The combined organic phase was washed with brine (15 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW5127** (505 mg, 78% over 2 steps) as a white solid. TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.39; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 4.67 (apparent dt, *J* = 10.9, 4.5 Hz, 1H), 3.57-3.49 (m, 1H), 2.02 (s, 3H), 1.75-1.69 (m, 1H), 0.90 (d, *J* = 6.6 Hz, 3H), 0.88-0.84 (m, 9H), 0.65 (s,

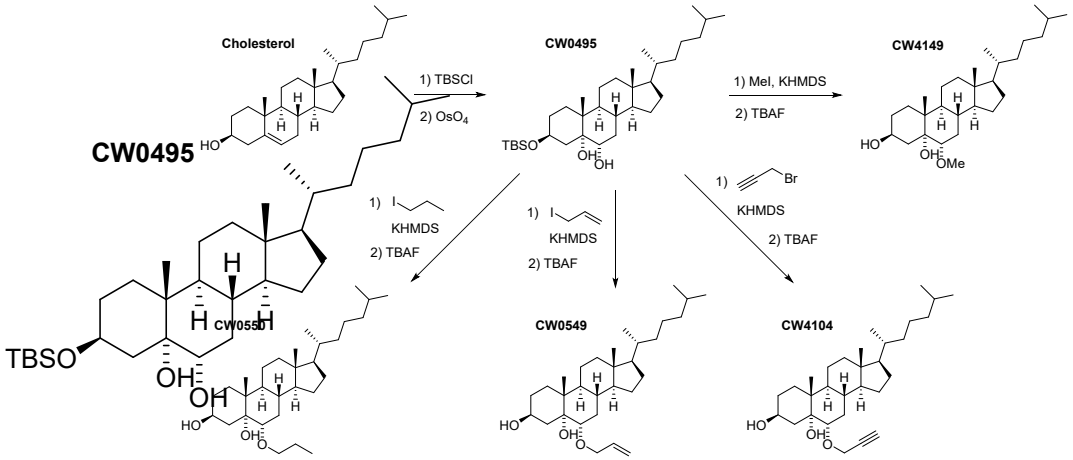
3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 170.8, 72.6, 70.9, 56.21, 56.19, 53.7, 48.7, 42.6, 39.8, 39.5, 37.7, 37.2, 36.6, 36.1, 35.7, 34.1, 32.2, 31.1, 28.2, 28.0, 24.1, 23.8, 22.8, 22.6, 21.3, 21.1, 18.7, 13.4, 12.0. Spectral data was consistent with that reported previously *(49)*.



(3*S*,5*S*,6*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-((*R*)-6-methylheptan-2-yl)-3-(prop-2-yn-1-yloxy)hexadecahydro-1*H*-cyclopenta[*a*]phenanthren-6-ol (CW5137). To a solution of **CW5127** (450 mg, 1.0 mmol, 1 eq) in THF (10 mL) at 0 °C was added KHMDS (0.5 M in PhMe, 2.0 mL, 1.0 mmol, 1 eq) dropwise. After 10 min, propargyl bromide (80% by wt in PhMe, 115 µL, 1.0 mmol, 1 eq) was added and the reaction allowed to warm to room temperature. After 1 day, the reaction mixture was quenched with saturated NH_4Cl (aq) (15 mL) and H_2O (15 mL) and extracted with DCM (3 x 30 mL). The combined organic phase was washed with brine (20 mL), dried over Na_2SO_4, and concentrated. The crude mixture was partially purified by flash column chromatography (Hex/EtOAc) on silica to afford a colorless oil. The impure propargyl ether was used as is in the next step.

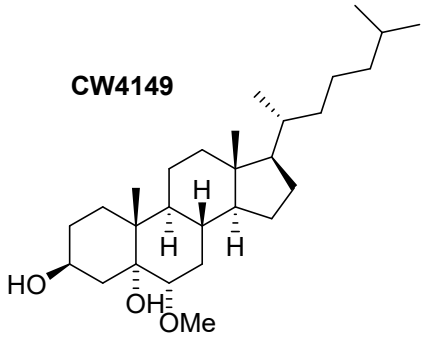
To a solution of the impure propargyl ether in PhMe (3.8 mL) at –78 °C was added DIBAL-H (1M in hexanes, 0.42 mL, 0.42 mmol, 1.1 eq). After 2 h, the reaction mixture was quenched with HCl (aq) (1M, 10 mL) and extracted with DCM (3 x 10 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW5137** (19 mg, 4% over 2 steps) as a white solid. TLC (Hex:EtOAc, 2:1 v/v): R_f = 0.54; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 4.23 (dd, *J* = 15.8, 2.3 Hz, 1H), 4.19 (dd, *J* = 15.8, 2.3 Hz, 1H), 3.48-3.37 (m, 2H), 2.39 (apparent t, *J* = 2.3 Hz, 1H), 2.33-2.27 (m, 1H), 0.90 (d, *J* = 6.5 Hz, 3H), 0.865 (d, *J* = 6.7 Hz, 3H), 0.862 (d, *J* = 6.6 Hz, 3H), 0.80 (s, 3H), 0.65 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 80.5, 77.5, 73.7, 69.6, 56.21, 56.18, 55.1, 53.8, 51.6, 42.6, 41.7, 39.8, 39.5, 37.2, 36.5, 36.1, 35.8, 34.3, 28.3, 28.2, 28.0, 27.8, 24.2, 23.8, 22.8, 22.6, 21.1, 18.7, 13.4, 12.0; HRMS (EI-TOF) *m/z*: $[M]^+$ calcd. for $C_{30}H_{50}O_2$, 442.3811; found, 442.3824.

Figure 7: Synthetic scheme of cholesterol analogs **CW4104**, **CW4149**, **CW0549**, **CW0550**, and **CW0556**.



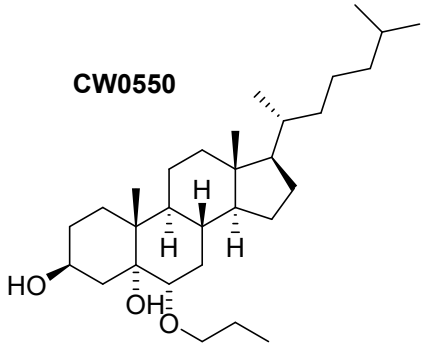
(3*S*,5*R*,6*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-3-((*tert*-Butyldimethylsilyl)oxy)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-5*H*-cyclopenta[*a*]phenanthrene-5,6-diol (CW0495). To a solution of cholesterol (300 mg, 0.776 mmol, 1 eq) in DMF (4 mL) was added imidazole (264 mg, 3.88 mmol, 5 eq) and TBSCl (351 mg, 2.33 mmol, 3 eq). After heating at 50 °C for 1 day, the reaction mixture was diluted with DCM (50 mL) and washed with H_2O (3 x 10 mL). The combined organic phase was washed with brine (10 mL), dried over Na_2SO_4, and concentrated to afford a white foam. The crude silyl ether was used in the next step without further purification.

To a solution of the crude silyl ether in a mixture of *t*-BuOH (20 mL), DCM (10 mL), and H_2O (20 mL) was added $K_3Fe(CN)_6$ (2.55 g, 7.76 mmol, 10 eq), K_2CO_3 (1.07 g, 7.76 mmol, 10 eq), DABCO (87 mg, 0.776 mmol, 1 eq), and OsO_4 (aq) (4% by wt, 0.48 mL, 0.078 mmol, 0.10 eq). After 9 days, the reaction mixture was partitioned between H_2O (50 mL) and EtOAc (3 x 50 mL). The combined organic phase was washed with $Na_2S_2O_3$ (aq) (10% by wt, 20 mL) then brine (20 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0495** (269 mg, 65% over 2 steps, 5α,6α/5β,6β-diol > 95:5) as a white solid. TLC (Hex:EtOAc, 4:1 v/v): R_f = 0.65; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 4.06-3.98 (m, 1H), 3.69-3.62 (m, 1H), 2.02-1.94 (m, 2H), 1.87-1.78 (m, 1H), 0.96 (s, 3H), 0.89 (d, *J* = 6.6 Hz, 3H), 0.88 (s, 9H), 0.862 (d, *J* = 6.6 Hz, 3H), 0.859 (d, *J* = 6.6 Hz, 3H), 0.64 (s, 3H), 0.06 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 76.9, 70.7, 68.2, 56.2, 55.9, 44.6, 42.7, 39.9, 39.5, 39.1, 38.8, 36.1, 35.8, 35.2, 33.5, 31.13, 31.05, 28.2, 28.0, 26.0, 24.1, 23.8, 22.8, 22.6, 21.2, 18.6, 18.2, 15.6, 12.1, –4.5, –4.6. The observed major 5α,6α-diol diastereoselectivity was consistent with that reported previously for similar compounds *(48)*.



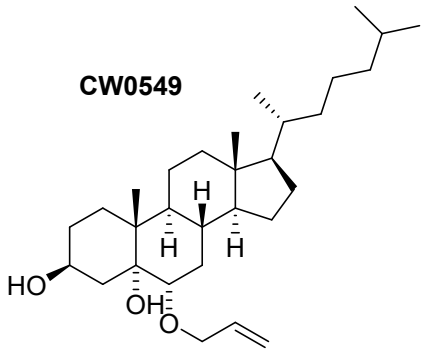
(3*S*,5*R*,6*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-6-Methoxy-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-5*H*-cyclopenta[*a*]phenanthrene-3,5-diol (CW4149). To a solution of **CW0495** (125 mg, 0.234 mmol, 1 eq) in THF (2.3 mL) was added KHMDS (0.5 M in PhMe, 0.70 mL, 0.351 mmol, 1.5 eq) dropwise. After 1 h, iodomethane (22 µL, 0.351 mmol, 1.5 eq) was added. After 1 day, the reaction mixture was quenched with saturated NH_4Cl (aq) (5 mL) and H_2O (5 mL) and extracted with DCM (3 x 10 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was partially purified by flash column chromatography (Hex/EtOAc) on silica to afford a white solid (110 mg). The impure methyl ether was used as is in the next step.

To the impure methyl ether was added TBAF (1M in THF, 6.0 mL, 6.0 mmol, 30 eq). After 2 days, the reaction mixture was partitioned between H_2O (20 mL) and DCM (3 x 20 mL). The combined organic phase was washed with brine (10 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW4149** (65 mg, 64% over 2 steps) as a white solid. TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.22; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 4.11-4.02 (m, 1H), 3.35 (s, 3H), 3.13 (dd, *J* = 11.3, 5.1 Hz, 1H), 2.22-2.16 (m, 1H), 1.99-1.93 (m, 1H), 0.94 (s, 3H), 0.90 (d, *J* = 6.5 Hz, 3H), 0.863 (d, *J* = 6.6 Hz, 3H), 0.859 (d, *J* = 6.6 Hz, 3H), 0.64 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 79.9, 77.0, 67.6, 57.5, 56.1, 56.0, 44.3, 42.7, 39.8, 39.5, 39.0, 38.7, 36.1, 35.8, 33.4, 31.0, 30.8, 30.6, 28.2, 28.0, 24.2, 23.9, 22.8, 22.6, 21.2, 18.6, 15.6, 12.0; HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd. for $C_{28}H_{50}O_3Na$, 457.3658; found, 457.3646. The regioselectivity of the methylation was confirmed by HSQC and HMBC NMR experiments.



(3*S*,5*R*,6*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-((*R*)-6-methylheptan-2-yl)-6-propoxyhexadecahydro-5*H*-cyclopenta[*a*]phenanthrene-3,5-diol (CW0550). To a solution of **CW0495** (100 mg, 0.187 mmol, 1 eq) in THF (1.9 mL) was added KHMDS (0.5 M in PhMe, 1.12 mL, 0.561 mmol, 3 eq) dropwise. After 5 min, iodopropane (55 µL, 0.561 mmol, 3 eq) was added and reaction heated to 50 °C. After 1 day, the reaction mixture was quenched with saturated NH_4Cl (aq) (5 mL) and H_2O (5 mL) and extracted with DCM (3 x 10 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was partially purified by flash column chromatography (Hex/EtOAc) on silica to afford a yellow oil (57 mg). The impure propyl ether was used as is in the next step.

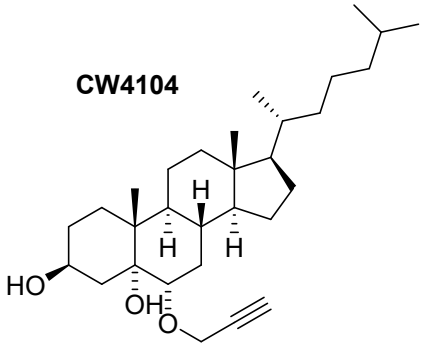
To the impure propyl ether was added TBAF (1M in THF, 0.17 mL, 0.17 mmol, 10 eq). After 2 days, the reaction mixture was partitioned between H_2O (2 mL) and DCM (3 x 5 mL). The combined organic phase was washed with brine (2 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0550** (6 mg, 7% over 2 steps) as a white solid. TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.57; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 4.12-4.03 (m, 1H), 3.52 (apparent dt, *J* = 9.0, 6.6 Hz, 1H), 3.28 (apparent dt, *J* = 8.9, 6.7 Hz, 1H), 3.20 (dd, *J* = 11.2, 5.1 Hz, 1H), 2.24-2.17 (m, 1H), 1.99-1.93 (m, 1H), 0.94 (s, 3H), 0.91 (t, *J* = 7.5 Hz, 3H), 0.90 (d, *J* = 6.5 Hz, 3H), 0.863 (d, *J* = 6.6 Hz, 3H), 0.859 (d, *J* = 6.6 Hz, 3H), 0.64 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 78.1, 77.1, 71.4, 67.7, 56.2, 56.0, 44.2, 42.7, 39.8, 39.5, 39.0, 38.7, 36.2, 35.8, 33.4, 31.7, 30.8, 30.7, 28.2, 28.0, 24.2, 23.9, 23.4, 22.8, 22.6, 21.2, 18.6, 15.5, 12.0, 10.7; HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd. for $C_{30}H_{54}O_3Na$, 485.3971; found, 485.3966.



(3*S*,5*R*,6*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-6-(Allyloxy)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-5*H*-cyclopenta[*a*]phenanthrene-3,5-diol (CW0549). To a solution of **CW0495** (100 mg, 0.187 mmol, 1 eq) in THF (1.9 mL) was added KHMDS (0.5 M in PhMe, 1.12 mL, 0.561 mmol, 3 eq) dropwise. After 5 min, allyl iodide (52 µL, 0.561 mmol, 3 eq) was added and reaction heated to 50 °C. After 1 day, the reaction mixture was quenched with saturated NH_4Cl (aq) (5 mL) and H_2O (5 mL) and extracted with DCM (3 x 10 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was partially purified by flash column chromatography (Hex/EtOAc) on silica to afford a colorless oil (100 mg). The impure allyl ether was used as is in the next step.

To the impure allyl ether was added TBAF (1M in THF, 1.7 mL, 1.7 mmol, 10 eq). After 2 days, the reaction mixture was partitioned between H_2O (10 mL) and DCM (3 x 10 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0549** (54 mg, 63% over 2 steps) as a white solid. TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.46; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 5.94-5.84 (m, 1H), 5.25 (dd, *J* = 17.2, 1.4 Hz, 1H), 5.15 (dd, *J* = 10.4, 0.8 Hz, 1H), 4.12-4.02 (m, 2H), 3.92 (dd, *J* = 12.6, 5.7 Hz, 1H), 3.29 (dd, *J* = 11.2, 5.0 Hz, 1H), 2.24-2.17 (m, 1H), 1.99-1.93 (m, 1H), 0.94 (s, 3H), 0.90 (d, *J* = 6.5 Hz, 3H), 0.863 (d, *J* = 6.6 Hz, 3H), 0.860 (d, *J* = 6.6 Hz, 3H), 0.64 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 135.2, 116.7, 77.8, 77.0, 70.6, 67.6, 56.2, 56.0, 44.2, 42.7, 39.8, 39.5, 39.1, 38.8, 36.2, 35.8, 33.5, 31.6, 30.8, 30.7, 28.2, 28.0, 24.2, 23.9, 22.8, 22.6, 21.2, 18.6, 15.6, 12.1; HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd. for $C_{30}H_{52}O_3Na$, 483.3814; found, 483.3806.

CW4104



(3*S*,5*R*,6*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-((*R*)-6-methylheptan-2-yl)-6-(prop-2-yn-1-yloxy)hexadecahydro-5*H*-cyclopenta[*a*]phenanthrene-3,5-diol (CW4104). To a solution of **CW0495** (130 mg, 0.243 mmol, 1 eq) in THF (2.4 mL) was added KHMDS (0.5 M in PhMe, 1.5 mL, 0.73 mmol, 3 eq) dropwise. After 45 min, propargyl bromide (80% by wt in PhMe, 81 µL, 0.73 mmol, 3 eq) was added and reaction heated to 50 °C. After 1 day, the reaction mixture was quenched with saturated NH_4Cl (aq) (5 mL) and H_2O (5 mL) and extracted with DCM (3 x 10 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was partially purified by flash column chromatography (Hex/EtOAc) on silica to afford a yellow oil (73 mg). The impure propargyl ether was used as is in the next step.

To the impure propargyl ether was added TBAF (1M in THF, 3.7 mL, 3.7 mmol, 30 eq). After 3 days, the reaction mixture was partitioned between H_2O (10 mL) and DCM (3 x 10 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW4104** (30 mg, 27% over 2 steps) as a white solid. TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.33; ^{1}H NMR (500 MHz, $CDCl_3$, representative signals): δ 4.22 (dd, *J* = 15.8, 2.3 Hz, 1H), 4.14 (dd, *J* = 15.9, 2.3 Hz, 1H), 4.11-4.02 (m, 1H), 3.48 (dd, *J* = 11.3, 5.1 Hz, 1H), 2.41 (apparent t, *J* = 2.3 Hz, 1H), 2.24-2.17 (m, 1H), 1.99-1.94 (m, 1H), 0.96 (s, 3H), 0.90 (d, *J* = 6.6 Hz, 3H), 0.864 (d, *J* = 6.6 Hz, 3H), 0.860 (d, *J* = 6.6 Hz, 3H), 0.64 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$):

δ 80.1, 77.6, 76.9, 74.1, 67.5, 56.5, 56.1, 55.9, 44.2, 42.7, 39.8, 39.5, 39.2, 38.7, 36.1, 35.8, 33.5, 31.1, 30.8, 30.6, 28.2, 28.0, 24.2, 23.9, 22.8, 22.6, 21.1, 18.6, 15.6, 12.1; HRMS (ESI-TOF) *m/z*: $[M+Na]^+$ calcd. for $C_{30}H_{50}O_3Na$, 481.3658; found, 481.3651. The regioselectivity of the propargylation was confirmed by HSQC and HMBC NMR experiments.

HSD17B7 Inhibitors:

General Procedure A: To a solution of commercially available carboxylic acid (1 eq) in DCM (0.25 M) was added oxalyl chloride (2 eq) followed by slow addition of DMF (0.05 eq). After 2 h, the reaction mixture was concentrated and resuspended in THF or DMF (0.25 M). The commercially available amine (1.1 eq) and $NaHCO_3$ or K_2CO_3 (2 eq) were then added. After stirring overnight, the reaction mixture was poured into H_2O and the aqueous layer extracted with EtOAc. The combined organic phase was washed with brine, dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford the desired amide.

General Procedure B: To a solution of the crude material obtained from General Procedure A in THF/H_2O (10:1, 0.1 M) was added LiOH (5 eq). After 1 day, the reaction mixture was poured into H_2O and the aqueous layer extracted with EtOAc. The combined organic phase was washed with brine, dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford the desired amide.

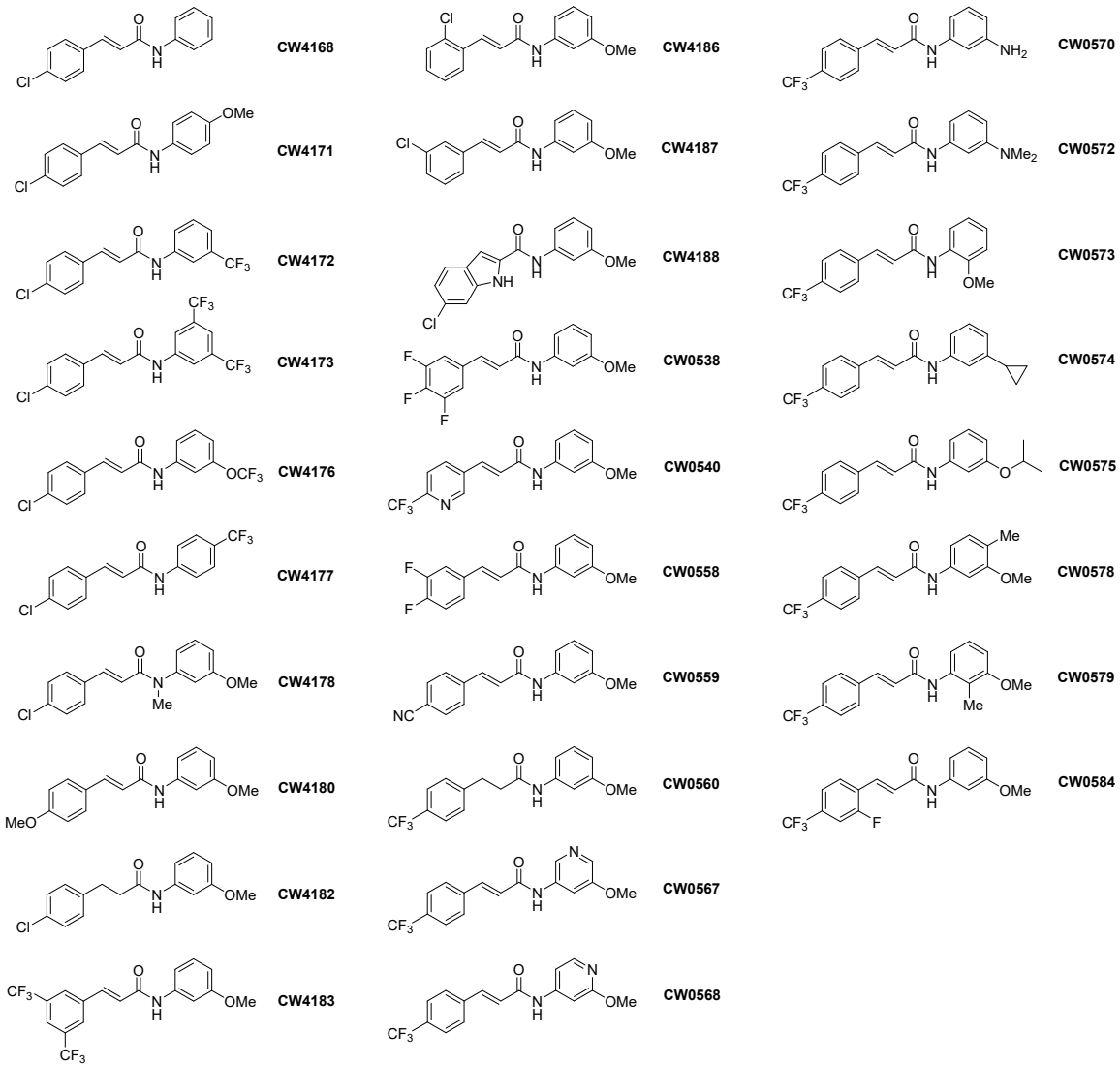
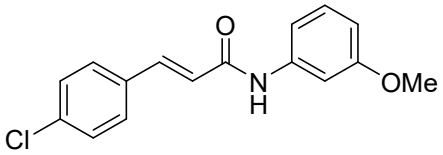


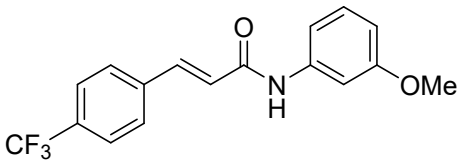
Figure 8: Compounds synthesized via General Procedure A.



CW4170

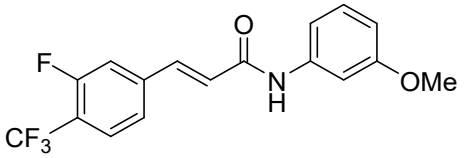
(*E*)-3-(4-Chlorophenyl)-*N*-(3-methoxyphenyl)acrylamide (CW4170). Synthesized via General Procedure A to afford a white solid (13% yield). TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.53; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.21 (s, 1H), 7.65 (d, *J* = 8.3 Hz, 2H), 7.57 (d, *J* = 15.8 Hz, 1H), 7.51 (d, *J* = 8.2 Hz, 2H), 7.41 (s, 1H), 7.26-7.19 (m, 2H), 6.82 (d, *J* = 15.7 Hz, 1H), 6.66 (d, *J* = 7.2 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ

163.3, 159.5, 140.3, 138.8, 134.2, 133.7, 129.6, 129.4, 129.1, 123.1, 111.6, 108.8, 105.1, 55.0. Spectral data was consistent with that reported previously *(50)*.



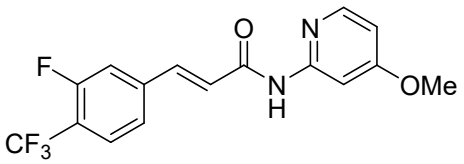
CW4181

(*E*)-*N*-(3-Methoxyphenyl)-3-(4-(trifluoromethyl)phenyl)acrylamide (CW4181). Synthesized via General Procedure A to afford a white solid (54% yield). TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.54; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.29 (s, 1H), 7.84 (d, *J* = 8.3 Hz, 2H), 7.81 (d, *J* = 8.4 Hz, 2H), 7.66 (d, *J* = 15.8 Hz, 1H), 7.42 (s, 1H), 7.27-7.20 (m, 2H), 6.95 (d, *J* = 15.6 Hz, 1H), 6.67 (d, *J* = 7.3 Hz, 1H), 3.75 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 163.1, 159.6, 140.2, 138.8, 138.5, 129.7, 129.5 (q, $^2J_{C-F}$ = 31.8 Hz), 128.3, 125.9 (q, $^3J_{C-F}$ = 3.7 Hz), 125.1, 124.1 (q, $^1J_{C-F}$ = 271.9 Hz), 111.6, 109.0, 105.1, 55.0; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd. for $C_{17}H_{15}F_3NO_2$, 322.1055; found, 322.1044.



CW0539

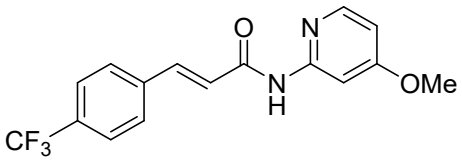
(*E*)-3-(3-Fluoro-4-(trifluoromethyl)phenyl)-*N*-(3-methoxyphenyl)acrylamide (CW0539). Synthesized via General Procedure A to afford a white solid (46% yield). TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.56; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.32 (s, 1H), 7.86 (app t, *J* = 7.9 Hz, 1H), 7.77 (d, *J* = 11.9 Hz, 1H), 7.68-7.60 (m, 2H), 7.41 (s, 1H), 7.27-7.20 (m, 2H), 6.97 (d, *J* = 15.6 Hz, 1H), 6.70-6.66 (m, 1H), 3.75 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 162.8, 159.6, 159.1 (app dd, J_{C-F} = 253.5, 1.8 Hz), 142.0 (d, J_{C-F} = 8.4 Hz), 140.1, 137.3, 129.7, 128.0 (q, J_{C-F} = 4.3 Hz), 126.6, 123.9 (d, J_{C-F} = 3.2 Hz), 122.6 (q, J_{C-F} = 271.6 Hz), 116.8 (dq, J_{C-F} = 32.3, 12.2 Hz), 115.9 (d, J_{C-F} = 21.0 Hz), 111.7, 109.0, 105.2, 55.0; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd. for $C_{17}H_{14}F_4NO_2$, 340.0961; found, 340.0954.



CW5107

(*E*)-3-(3-Fluoro-4-(trifluoromethyl)phenyl)-*N*-(4-methoxypyridin-2-yl)acrylamide (CW5107). Synthesized via General Procedure B to afford a white solid (9% yield). TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.37; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.89 (s, 1H), 8.11 (d, *J* =

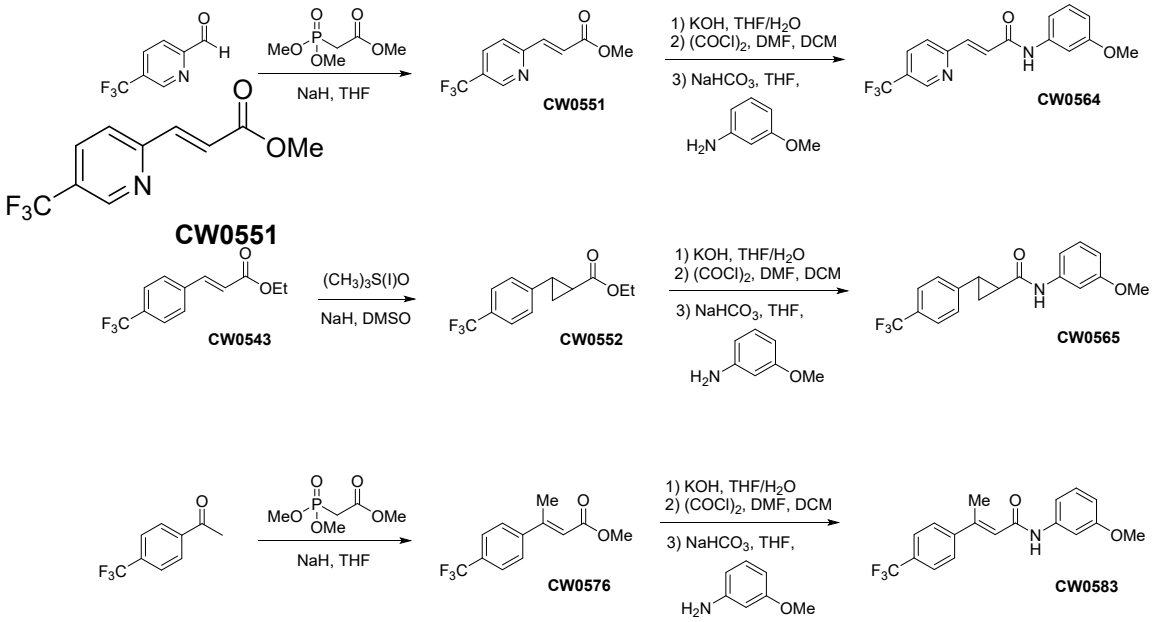
5.8 Hz, 1H), 8.00 (s, 1H), 7.73 (d, *J* = 15.5 Hz, 1H), 7.64 (app t, *J* = 7.7 Hz, 1H), 7.38 (d, *J* = 8.1 Hz, 1H), 7.33 (d, *J* = 10.9 Hz, 1H), 6.66 (dd, *J* = 5.8, 2.3 Hz, 1H), 6.62 (d, *J* = 15.5 Hz, 1H), 3.92 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 167.7, 163.1, 160.0 (d, J_{C-F} = 258.4 Hz), 153.0, 148.5, 140.5 (d, J_{C-F} = 8.3 Hz), 140.0, 127.8 (dq, J_{C-F} = 4.6, 1.9 Hz), 124.3, 123.7 (d, J_{C-F} = 3.5 Hz), 122.3 (q, J_{C-F} = 271.9 Hz), 119.4 (dq, J_{C-F} = 32.9, 12.5 Hz), 115.6 (d, J_{C-F} = 21.5 Hz), 108.1, 99.3, 55.5; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd. for $C_{16}H_{13}F_4N_2O_2$, 341.0913; found, 341.0904.



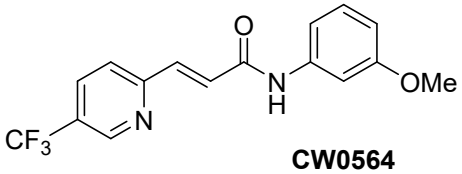
CW5124

(*E*)-*N*-(4-Methoxypyridin-2-yl)-3-(4-(trifluoromethyl)phenyl)acrylamide (CW5124). Synthesized via General Procedure B to afford a white solid (21% yield). TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.47; ^{1}H NMR (500 MHz, $CDCl_3$/CD_3OD): δ 8.08 (d, *J* = 5.7 Hz, 1H), 8.00 (s, 1H), 7.77 (d, *J* = 15.7 Hz, 1H), 7.70 (d, *J* = 8.1 Hz, 2H), 7.67 (d, *J* = 8.2 Hz, 2H), 6.87 (d, *J* = 15.6 Hz, 1H), 6.66 (dd, *J* = 5.6, 1.6 Hz, 1H), 3.92 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$/CD_3OD): δ 168.0, 164.8, 153.3, 148.4, 141.3, 138.3, 131.7 (q, $^2J_{C-F}$ = 32.6 Hz), 128.4, 126.0 (app d, $^3J_{C-F}$ = 3.4 Hz), 124.2 (q, $^1J_{C-F}$ = 272.0 Hz), 123.4, 108.0, 99.9, 55.6; HRMS (ESI-TOF) *m/z*: $[M+H]^+$ calcd. for $C_{16}H_{14}F_3N_2O_2$, 323.1007; found, 323.0995.

Figure 9: Synthetic schemes of **CW0564**, **CW0565**, and **CW0583**.



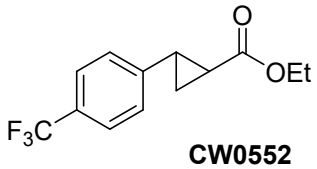
Methyl (*E*)-3-(5-(trifluoromethyl)pyridin-2-yl)acrylate (CW0551). To a solution of NaH (60% by wt, 110 mg, 2.74 mmol, 1.2 eq) in THF (15.0 mL) was added trimethyl phosphonoacetate (0.44 mL, 2.74 mmol, 1.2 eq) dropwise. After 1 h, 5-(trifluoromethyl)picolinaldehyde (400 mg, 2.28 mmol, 1 eq) in THF (2.3 mL) was slowly added. After 1 day, the reaction was carefully quenched with saturated NH_4Cl (aq) (10 mL) and partitioned between H_2O (10 mL) and EtOAc (3 x 20 mL). The combined organic phase was washed with brine (10 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0551** (260 mg, 49%, *E/Z* > 95:5) as a white solid. TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.73; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.90 (s, 1H), 7.96 (dd, *J* = 8.1, 0.9 Hz, 1H), 7.71 (d, *J* = 15.7 Hz, 1H), 7.53 (d, *J* = 8.1 Hz, 1H), 7.04 (d, *J* = 15.6 Hz, 1H), 3.84 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 166.7, 156.1, 147.0 (q, $^3J_{C-F}$ = 3.9 Hz), 141.8, 134.1 (q, $^3J_{C-F}$ = 3.4 Hz), 126.6 (q, $^2J_{C-F}$ = 33.2 Hz), 124.6, 123.6, 123.3 (q, $^1J_{C-F}$ = 272.5 Hz), 52.1.



CW0564

(*E*)-*N*-(3-Methoxyphenyl)-3-(5-(trifluoromethyl)pyridin-2-yl)acrylamide (CW0564). To a solution of **CW0551** (260 mg, 1.12 mmol, 1 eq) in a mixture of THF (5.0 mL) and H_2O (2.5 mL) was added KOH (315 mg, 5.62 mmol, 5 eq). After 1 day, the reaction was acidified with HCl (aq) (1M, ~7 mL) and extracted with EtOAc (3 x 10 mL). The combined organic phase was washed with brine (10 mL), dried over Na_2SO_4, and concentrated to afford a white solid. The crude carboxylic acid was used directly in the next reaction without further purification.

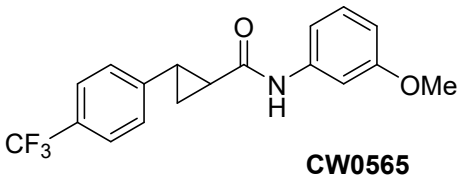
The crude carboxylic acid was used in General Procedure A to afford **CW0564** as a pink solid (43% yield over 2 steps). TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.60; ^{1}H NMR (500 MHz, CD_3CN): δ 8.90 (s, 1H), 8.72 (s, 1H), 8.06 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.69 (d, *J* = 15.2 Hz, 1H), 7.64 (d, *J* = 8.2 Hz, 1H), 7.42 (s, 1H), 7.29 (d, *J* = 15.2 Hz, 1H), 7.23 (app t, *J* = 8.1 Hz, 1H), 7.17 (d, *J* = 8.0 Hz, 1H), 6.68 (dd *J* = 8.1, 1.6 Hz, 1H), 3.77 (s, 3H); ^{13}C NMR (125 MHz, CD_3CN): δ 164.1, 161.1, 157.7, 147.7 (q, $^3J_{C-F}$ = 3.9 Hz), 141.0, 139.4, 135.4 (q, $^3J_{C-F}$ = 3.5 Hz), 130.7, 129.0, 126.6 (q, $^2J_{C-F}$ = 32.9 Hz), 125.2, 124.8 (q, $^1J_{C-F}$ = 271.7 Hz), 112.8, 110.5, 106.3, 55.8.



CW0552

Ethyl 2-(4-(trifluoromethyl)phenyl)cyclopropane-1-carboxylate (CW0552). To a solution of trimethylsulfoxonium iodide (673 mg, 3.06 mmol, 3 eq) in DMSO (6.1 mL)

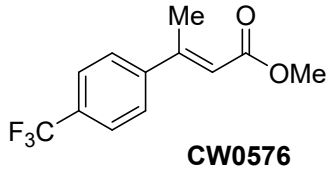
was added NaH (60% by wt, 126 mg, 3.16 mmol, 3.1 eq) portionwise over 5 min. After 10 min, **CW0543** (250 mg, 1.02 mmol, 1 eq) in DMSO (2.0 mL) was added dropwise *(51)*. After 4 h, the reaction was carefully quenched with saturated NH_4Cl (aq) (5 mL) and partitioned between H_2O (5 mL) and EtOAc (3 x 10 mL). The combined organic phase was washed with H_2O (10 mL) then brine (10 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0552** (47 mg, 18%) as a colorless oil. TLC (Hex:EtOAc, 4:1 v/v): R_f = 0.58; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.53 (d, *J* = 8.2 Hz, 2H), 7.19 (d, *J* = 8.2 Hz, 2H), 4.18 (q, *J* = 7.1 Hz, 2H), 2.59-2.53 (m, 1H), 1.97-1.92 (m, 1H), 1.68-1.63 (m, 1H), 1.36-1.31 (m, 1H), 1.29 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 172.9, 144.4, 128.8 (q, $^2J_{C-F}$ = 32.3 Hz), 126.4, 125.4 (q, $^3J_{C-F}$ = 3.6 Hz), 124.3 (q, $^1J_{C-F}$ = 272.1 Hz), 60.9, 25.7, 24.5, 17.3, 14.2.



CW0565

***N*-(3-Methoxyphenyl)-2-(4-(trifluoromethyl)phenyl)cyclopropane-1-carboxamide (CW0565).** To a solution of **CW0552** (45 mg, 0.17 mmol, 1 eq) in a mixture of THF (1.0 mL) and H_2O (0.5 mL) was added KOH (49 mg, 0.87 mmol, 5 eq). After 1 day, the reaction was acidified with HCl (aq) (1M, ~2 mL) and extracted with EtOAc (3 x 10 mL). The combined organic phase was washed with brine (5 mL), dried over Na_2SO_4, and concentrated to afford a white solid. The crude carboxylic acid was used directly in the next reaction without further purification.

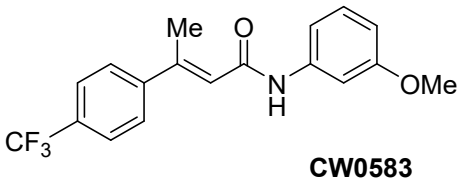
The crude carboxylic acid was used in General Procedure A to afford **CW0565** as a white solid (57% yield over 2 steps). TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.56; ^{1}H NMR (500 MHz, CD_3CN): δ 8.60 (s, 1H), 7.60 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 7.30 (s, 1H), 7.20 (app t, *J* = 8.2 Hz, 1H), 7.07 (d, *J* = 7.9 Hz, 1H), 6.64 (dd *J* = 8.3, 1.9 Hz, 1H), 3.75 (s, 3H), 2.54-2.48 (m, 1H), 2.04-1.99 (m, 1H), 1.66-1.59 (m, 1H), 1.39-1.33 (m, 1H); ^{13}C NMR (125 MHz, CD_3CN): δ 170.8, 161.1, 147.0, 141.2, 130.6, 128.6 (q, $^2J_{C-F}$ = 32.2 Hz), 127.6, 126.2 (q, $^3J_{C-F}$ = 3.9 Hz), 125.5 (q, $^1J_{C-F}$ = 270.6 Hz), 112.4, 110.0, 106.0, 55.8, 28.1, 25.8, 17.0.



CW0576

Methyl (*E*)-3-(4-(trifluoromethyl)phenyl)but-2-enoate (CW0576). To a solution of NaH (60% by wt, 510 mg, 12.76 mmol, 1.2 eq) in THF (85 mL) was added trimethyl phosphonoacetate (2.07 mL, 12.76 mmol, 1.2 eq) dropwise. After 1 h, 1-(4-(trifluoromethyl)phenyl)ethan-1-one (2.00g, 10.63 mmol, 1 eq) in THF (11 mL) was

slowly added. After 1 day, the reaction was carefully quenched with saturated NH_4Cl (aq) (50 mL) and partitioned between H_2O (50 mL) and EtOAc (3 x 100 mL). The combined organic phase was washed with brine (50 mL), dried over Na_2SO_4, and concentrated. The crude mixture was purified by flash column chromatography (Hex/EtOAc) on silica to afford **CW0576** (2.50 g, 96%, *E/Z* 60:40) as a colorless oil. TLC (Hex:EtOAc, 2:1 v/v): R_f = 0.61; ^{1}H NMR (500 MHz, $CDCl_3$): ***(E)*-isomer:** δ 7.63 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 8.2 Hz, 2H), 6.15 (d, *J* = 1.0 Hz, 1H), 3.77 (s, 3H), 2.58 (d, *J* = 1.0 Hz, 3H); ***(Z)*-isomer:** δ 7.61 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 5.98 (d, *J* = 1.1 Hz, 1H), 3.57 (s, 3H), 2.19 (d, *J* = 1.2 Hz, 3H).



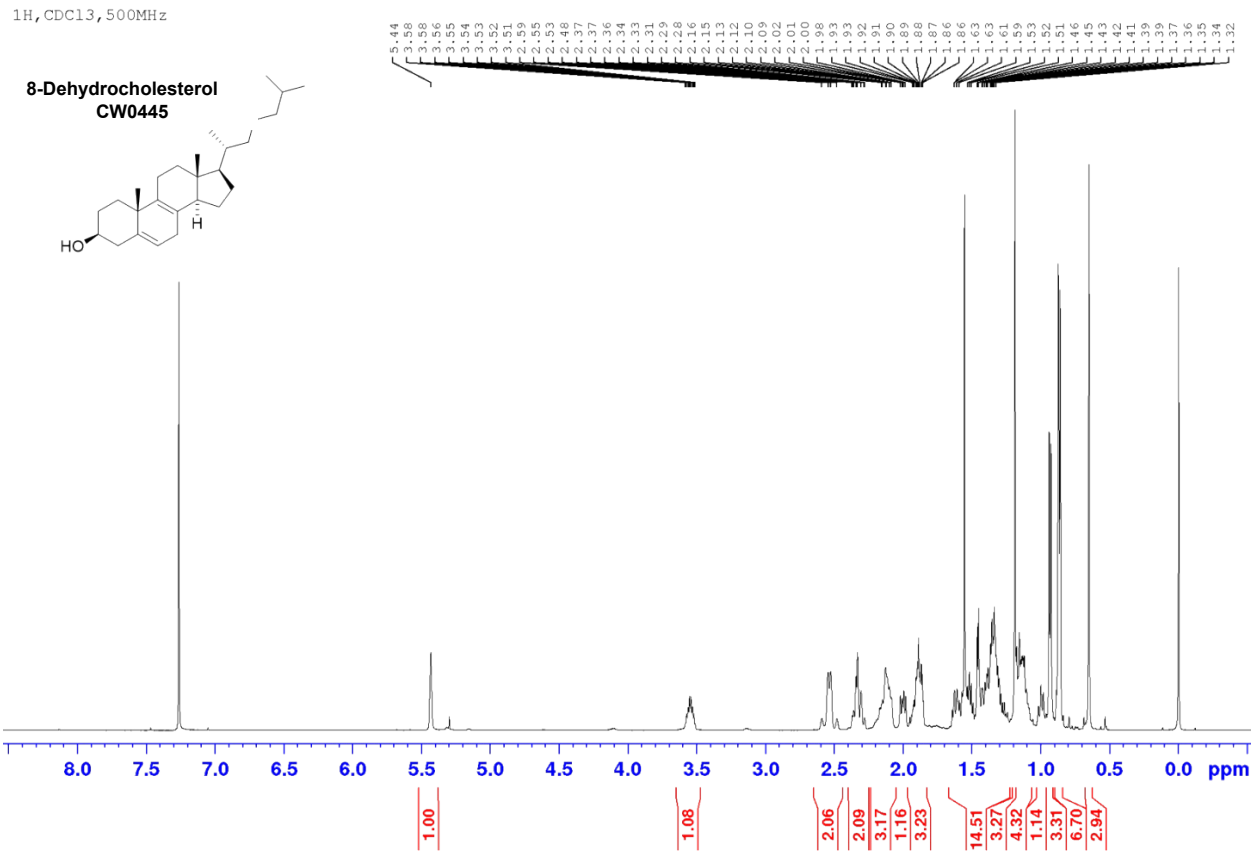
CW0583

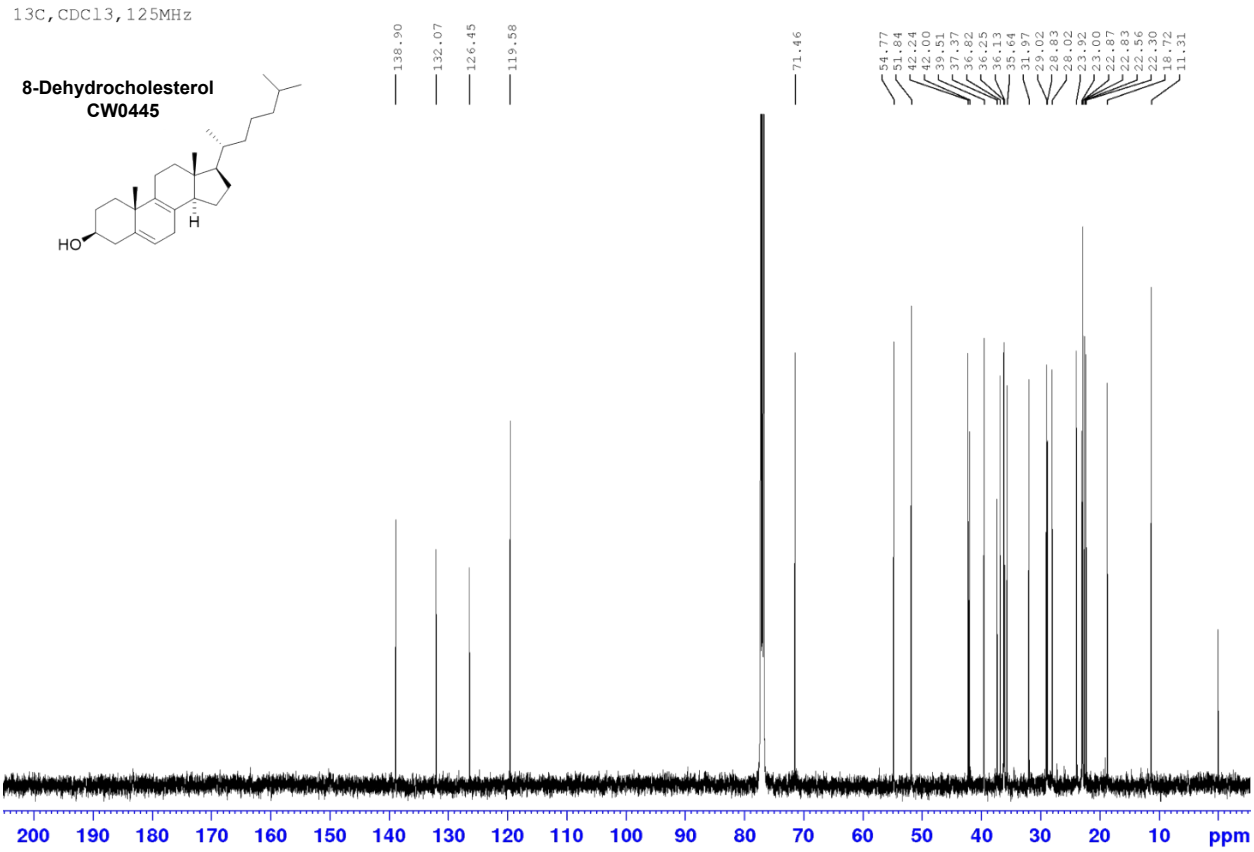
(*E*)-*N*-(3-Methoxyphenyl)-3-(4-(trifluoromethyl)phenyl)but-2-enamide (CW0583). To a solution of **CW0576** (*E/Z* 60:40, 2.50 g, 10.2 mmol, 1 eq) in a mixture of THF (45 mL) and H_2O (23 mL) was added KOH (2.87 g, 51.2 mmol, 5 eq). After 1 day, additional KOH (5.74 g, 102.4 mmol, 10 eq) was added. After 1 day, the THF was removed and reaction mixture extracted with Et_2O (3 x 20 mL). The combined organic phase was then triturated with hexanes and resulting yellow oil separated, diluted with EtOAc, dried over Na_2SO_4, and concentrated to afford a white solid. The crude carboxylic acid was used directly in the next reaction without further purification.

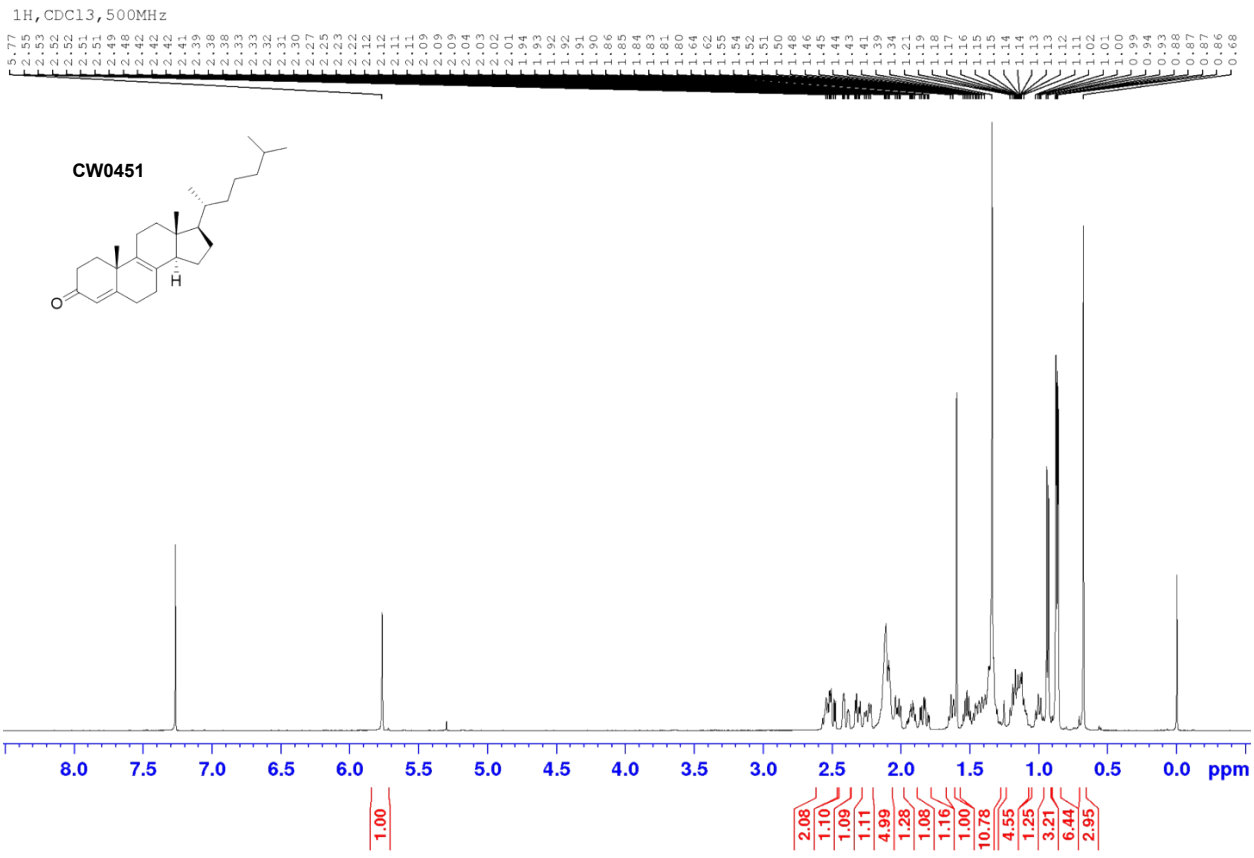
The crude carboxylic acid was used in General Procedure A to afford **CW0583** as a white solid (*E/Z* 95:5, 24% yield over 2 steps). TLC (Hex:EtOAc, 1:1 v/v): R_f = 0.68; ^{1}H NMR (500 MHz, DMSO-d_6): δ 10.15 (s, 1H), 7.80 (d, *J* = 8.4 Hz, 2H), 7.76 (d, *J* = 8.3 Hz, 2H), 7.39 (s, 1H), 7.22 (app t, *J* = 8.1 Hz, 1H), 7.17 (d, *J* = 7.8 Hz, 1H), 6.65 (dd *J* = 7.9, 1.2 Hz, 1H), 6.50 (s, 1H), 3.74 (s, 3H), 2.56 (s, 3H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 164.2, 159.5, 148.6, 146.2, 140.4, 129.6, 128.8 (q, $^2J_{C\text{-}F}$ = 31.8 Hz), 126.9, 125.5 (q, $^3J_{C\text{-}F}$ = 3.8 Hz), 124.2 (q, $^1J_{C\text{-}F}$ = 272.2 Hz), 122.7, 111.4, 108.8, 104.8, 55.0, 16.7. The major (*E*)-isomer was confirmed by the absence of an NOE correlation between the vinyl methyl and vinyl hydrogen.

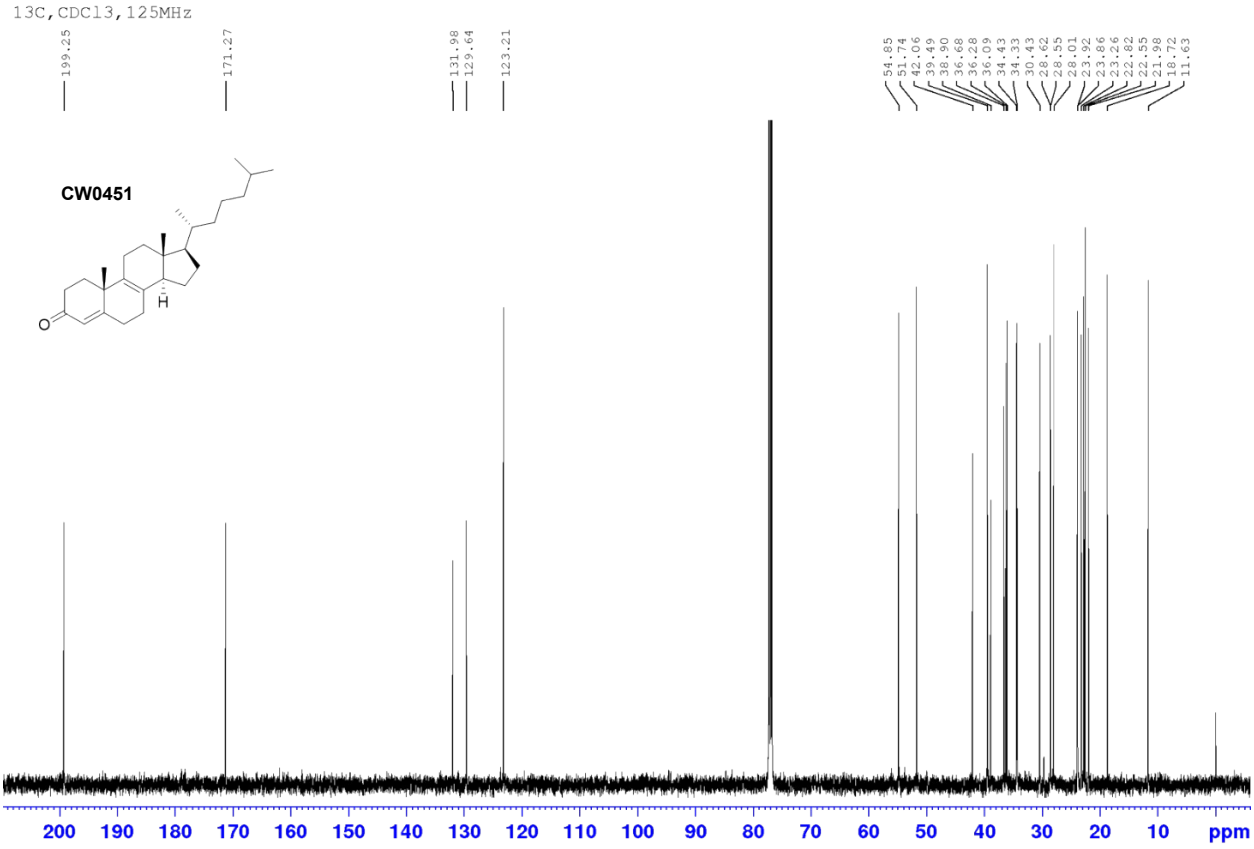
NMR Spectra

Sterol Standards




13C,CDCl3,125MHz
8-Dehydrocholesterol
CW0445
HO
H
138.90
132.07
126.45
119.58
71.46
54.77
51.84
42.24
42.00
39.51
37.37
36.82
36.25
36.13
35.64
31.97
29.02
28.83
28.02
23.92
23.00
22.87
22.83
22.56
22.30
18.72
11.31
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


1H,CDCl3,500MHz
CW0451
O
H
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
2.08
1.10
1.09
1.11
4.99
1.28
1.08
1.16
1.00
10.78
4.55
1.25
3.21
6.44
2.95


13C,CDCl3,125MHz
199.25
171.27
131.98
129.64
123.21
54.85
51.74
42.06
39.49
38.90
36.68
36.28
36.09
34.43
34.33
30.43
28.62
28.55
28.01
23.92
23.86
23.26
22.82
22.55
21.98
18.72
11.63
CW0451
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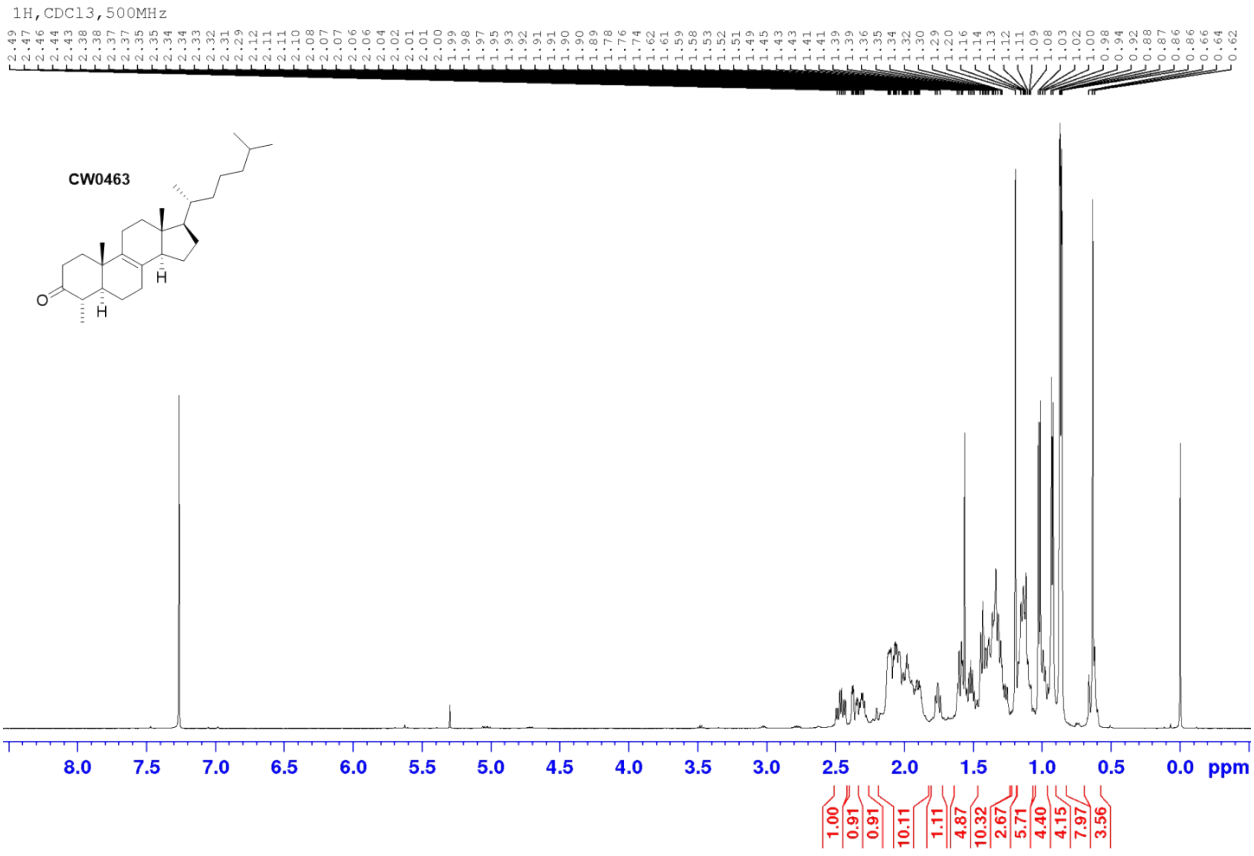
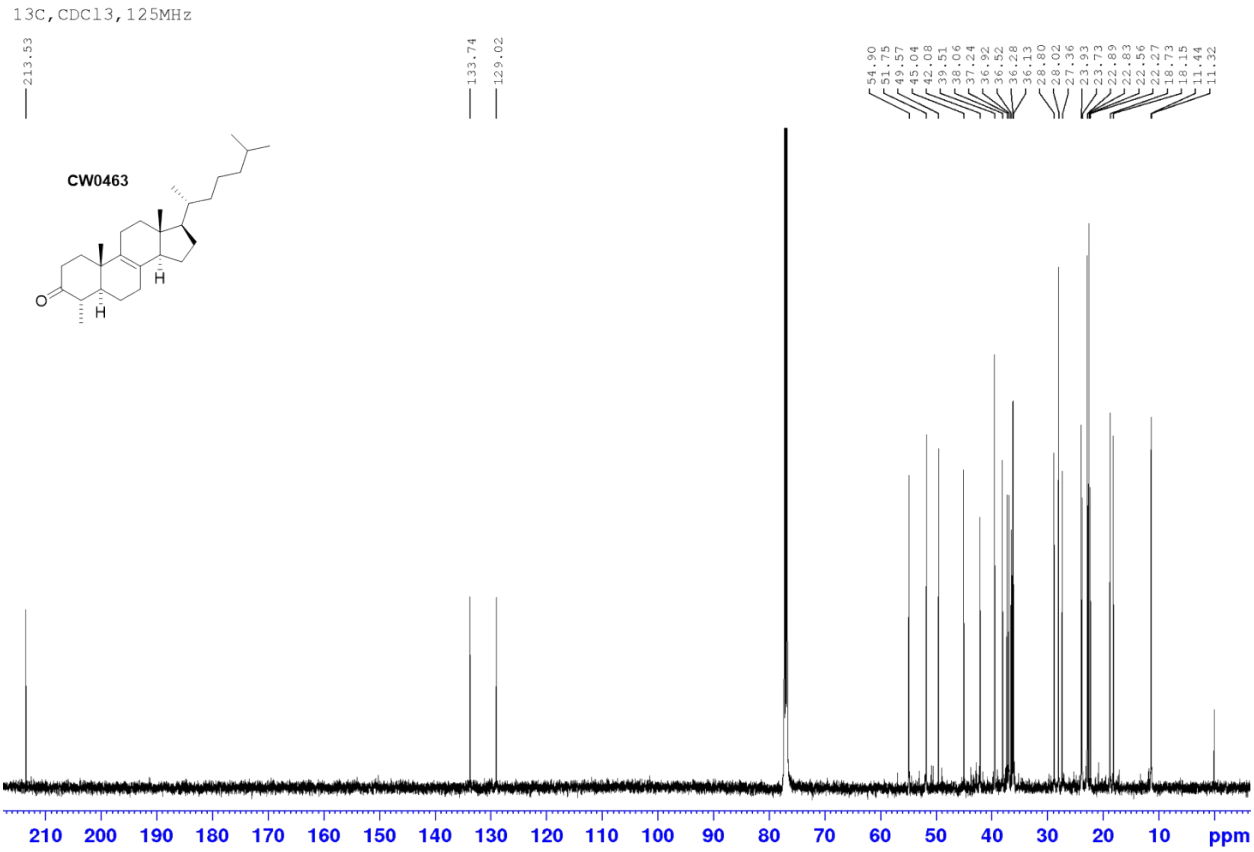

1H,CDCl3,500MHz
CW0463
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
0.91
0.91
10.11
1.11
4.87
10.32
2.67
5.71
4.40
4.15
7.97
3.56


13C,CDCl3,125MHz
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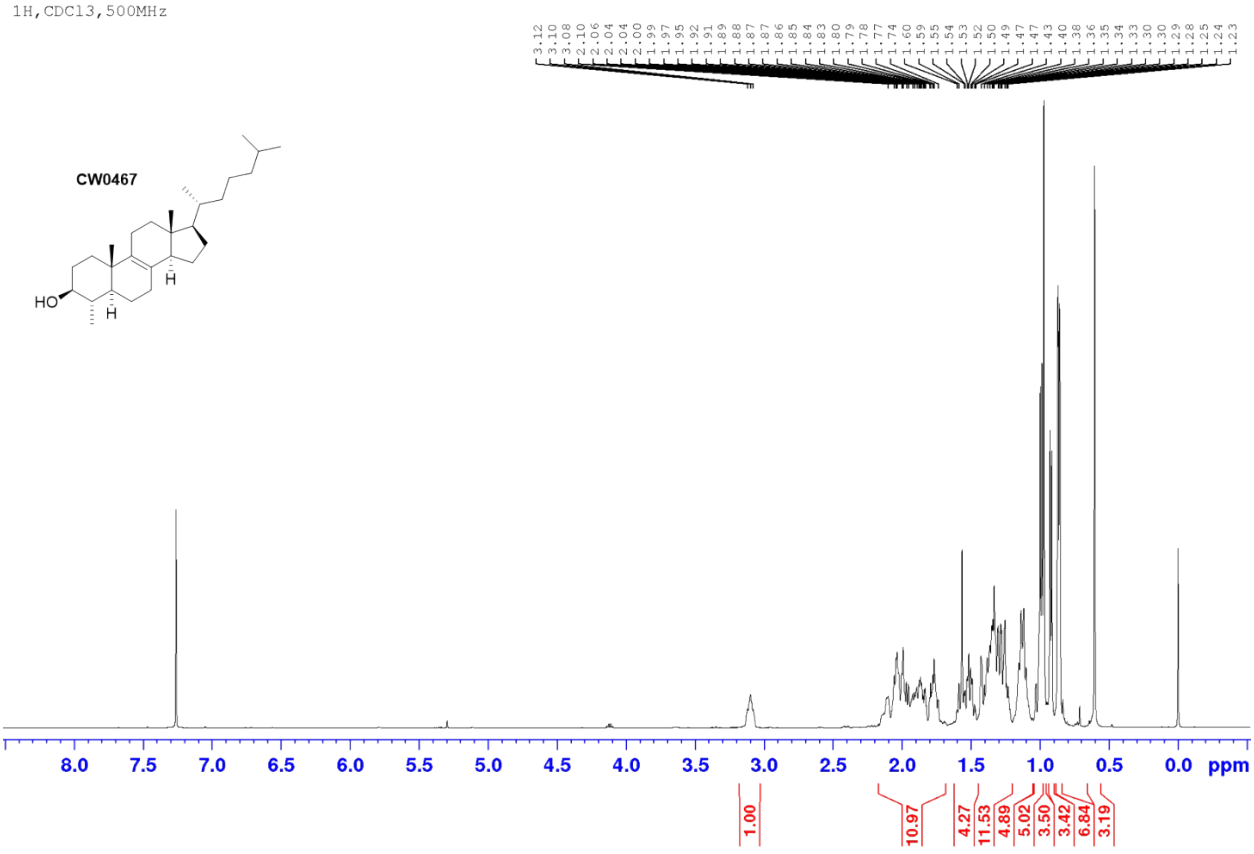
133.74
129.02
54.90
51.75
49.57
45.04
42.08
39.51
38.06
37.24
36.92
36.52
36.28
36.13
28.80
28.02
27.36
23.93
23.73
22.83
22.83
22.56
22.27
18.73
18.15
11.44
11.32
CW0463
O
H
H
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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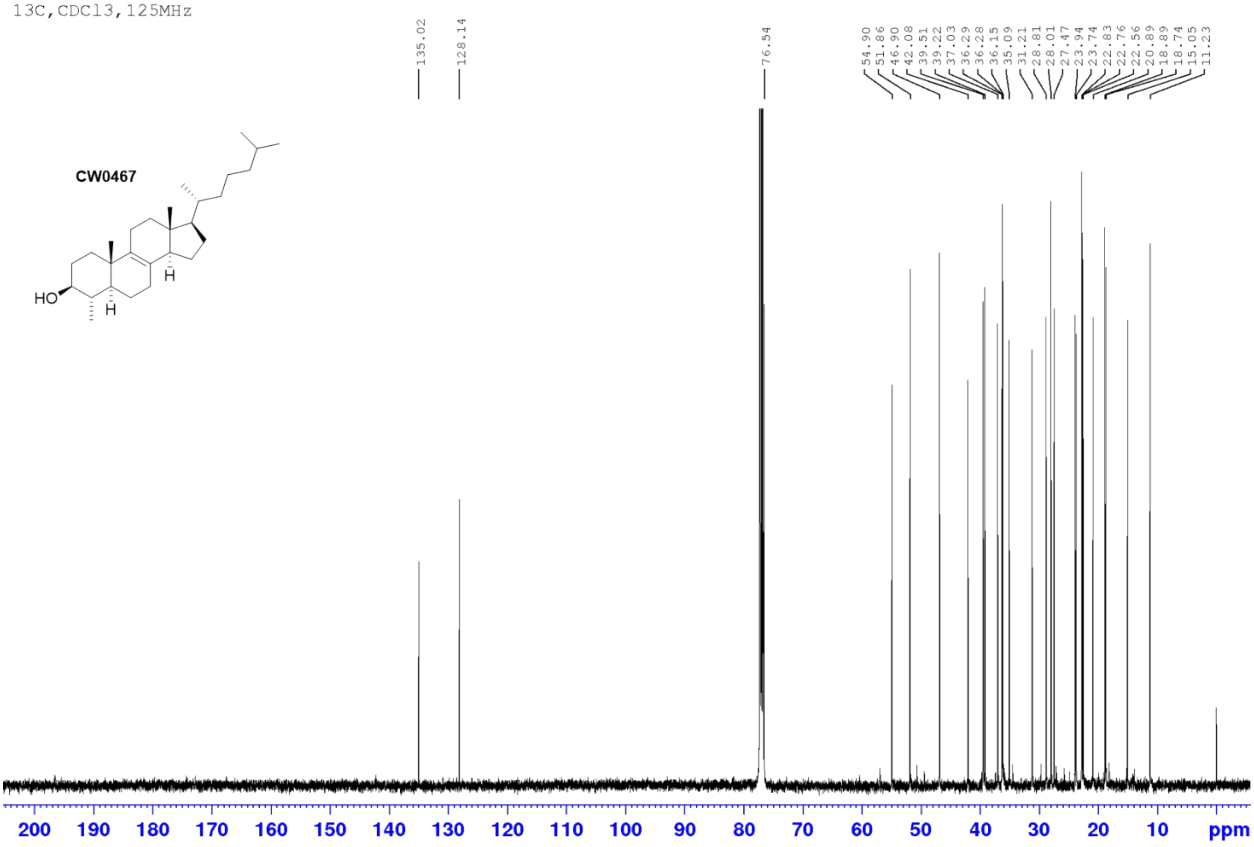
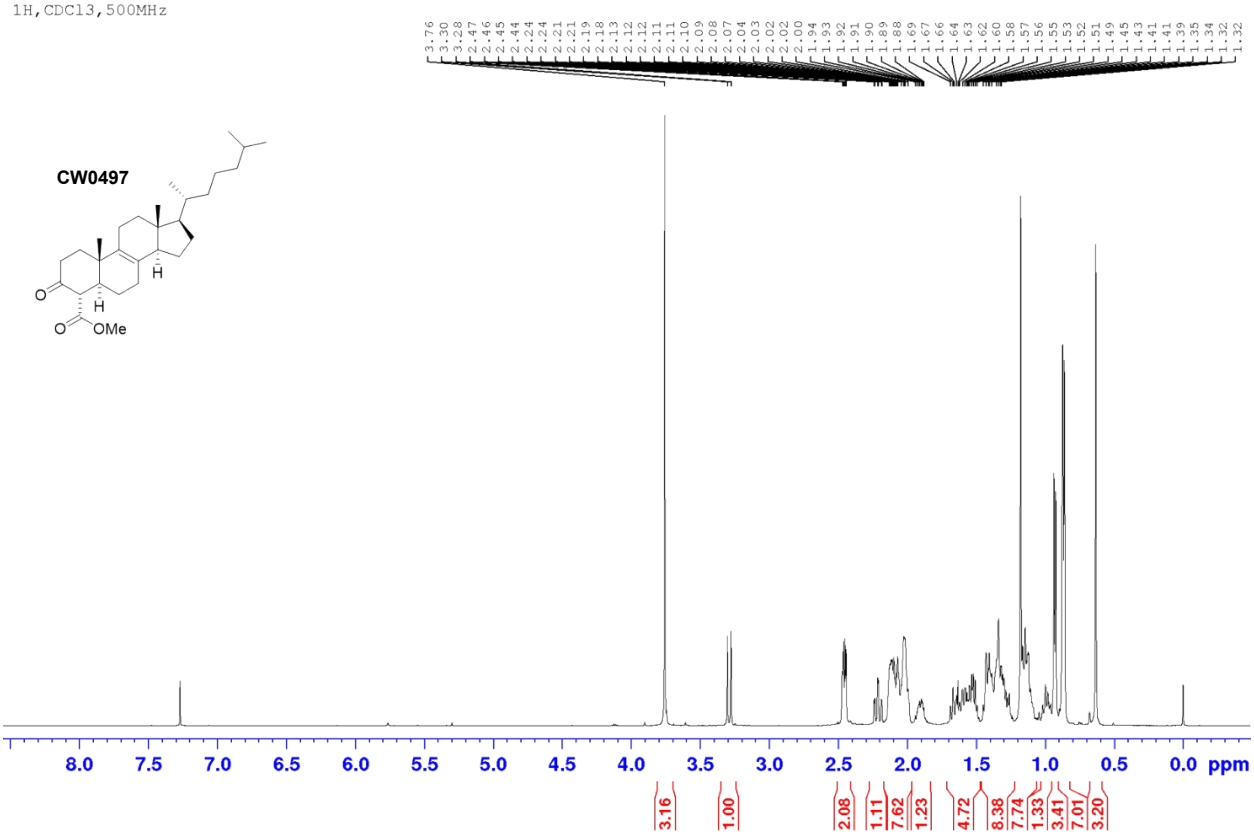
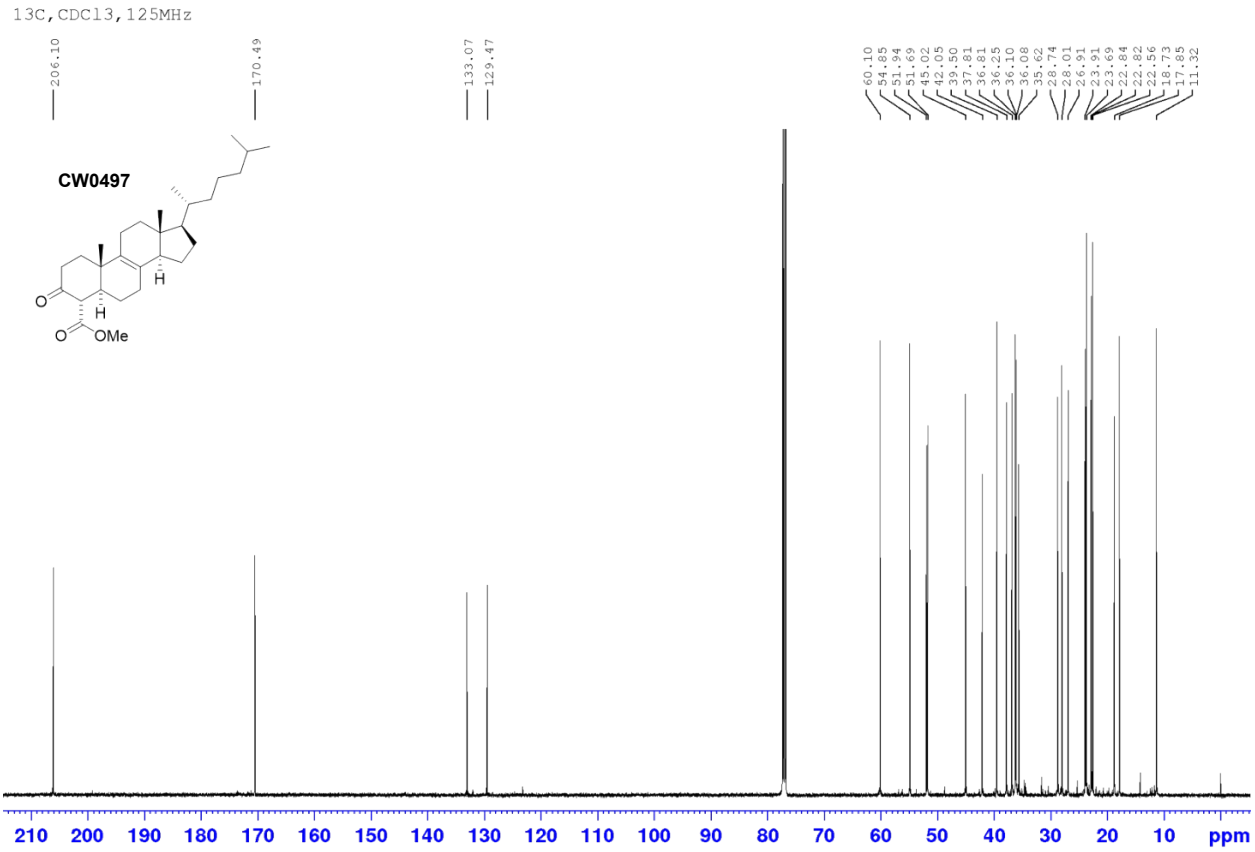
3.12
3.10
3.08
2.10
2.06
2.04
2.04
2.00
1.99
1.97
1.95
1.92
1.91
1.89
1.88
1.87
1.87
1.86
1.85
1.84
1.83
1.80
1.79
1.78
1.77
1.74
1.60
1.59
1.55
1.54
1.53
1.52
1.50
1.49
1.47
1.47
1.43
1.40
1.38
1.36
1.35
1.34
1.33
1.30
1.29
1.28
1.25
1.24
1.23
CW0467
HO
H
H
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
10.97
4.27
11.53
4.89
5.02
3.50
3.42
6.84
3.19

13C,CDCl3,125MHz



1H,CDCl3,500MHz

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206.10
170.49
133.07
129.47
60.10
54.85
51.94
51.69
45.02
42.05
39.50
37.81
36.81
36.25
36.10
36.08
35.62
28.74
28.01
26.91
23.91
23.69
22.84
22.82
22.56
18.73
17.85
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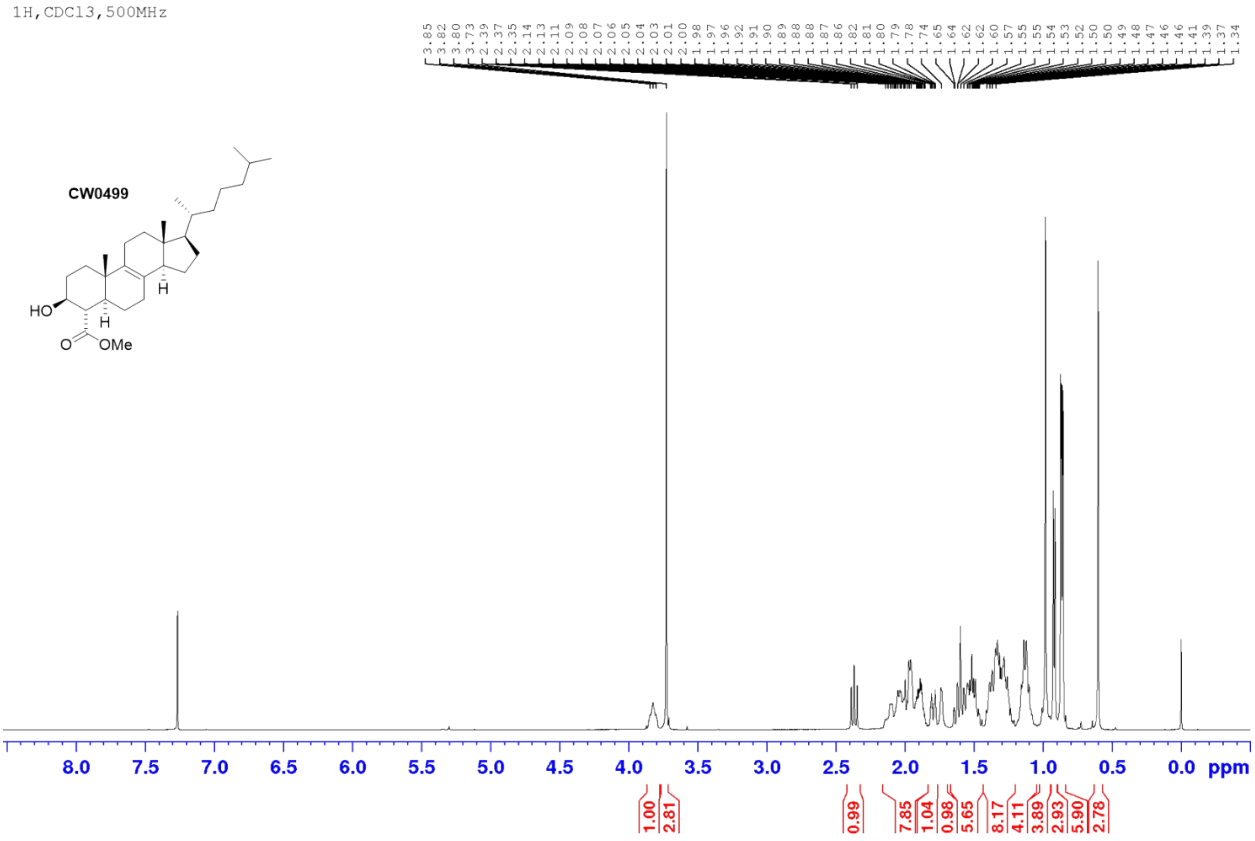
OMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


1H,CDCl3,500MHz
3.85
3.82
3.80
3.73
2.39
2.37
2.35
2.14
2.13
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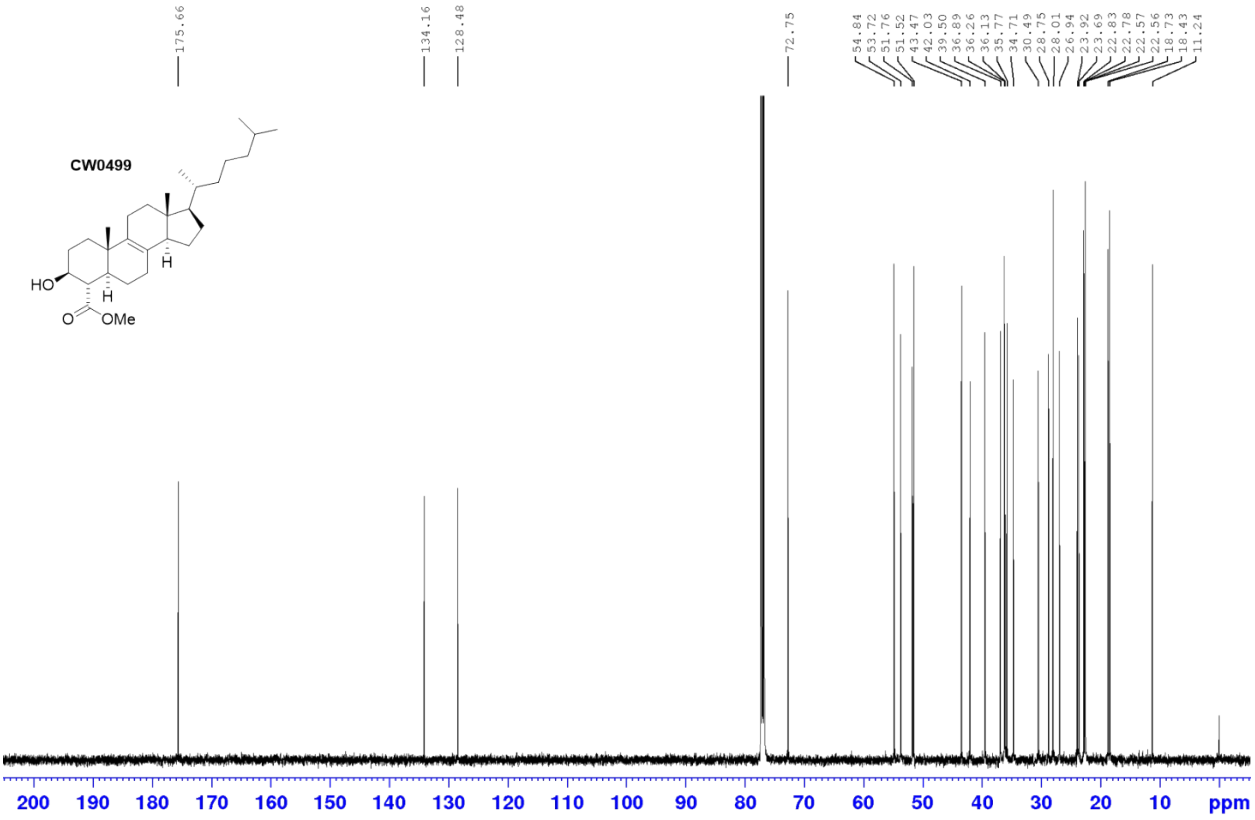
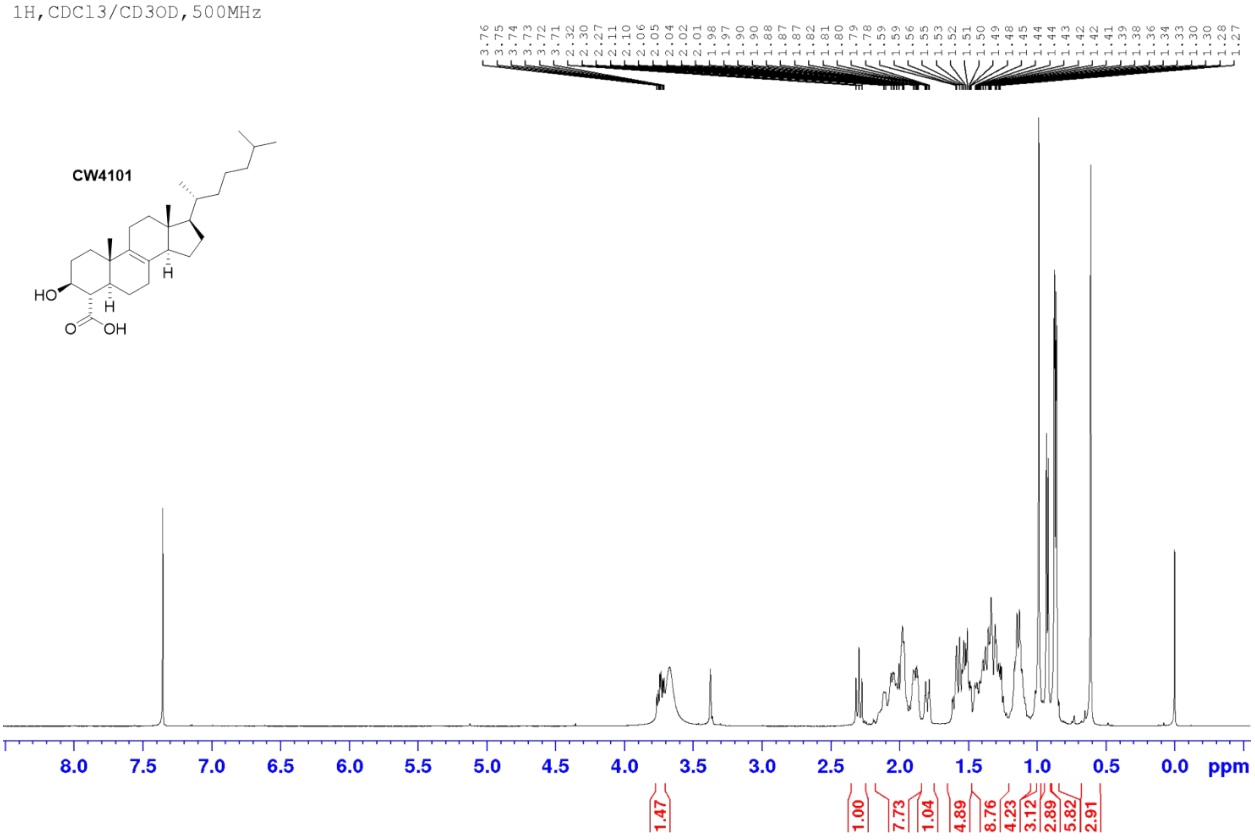
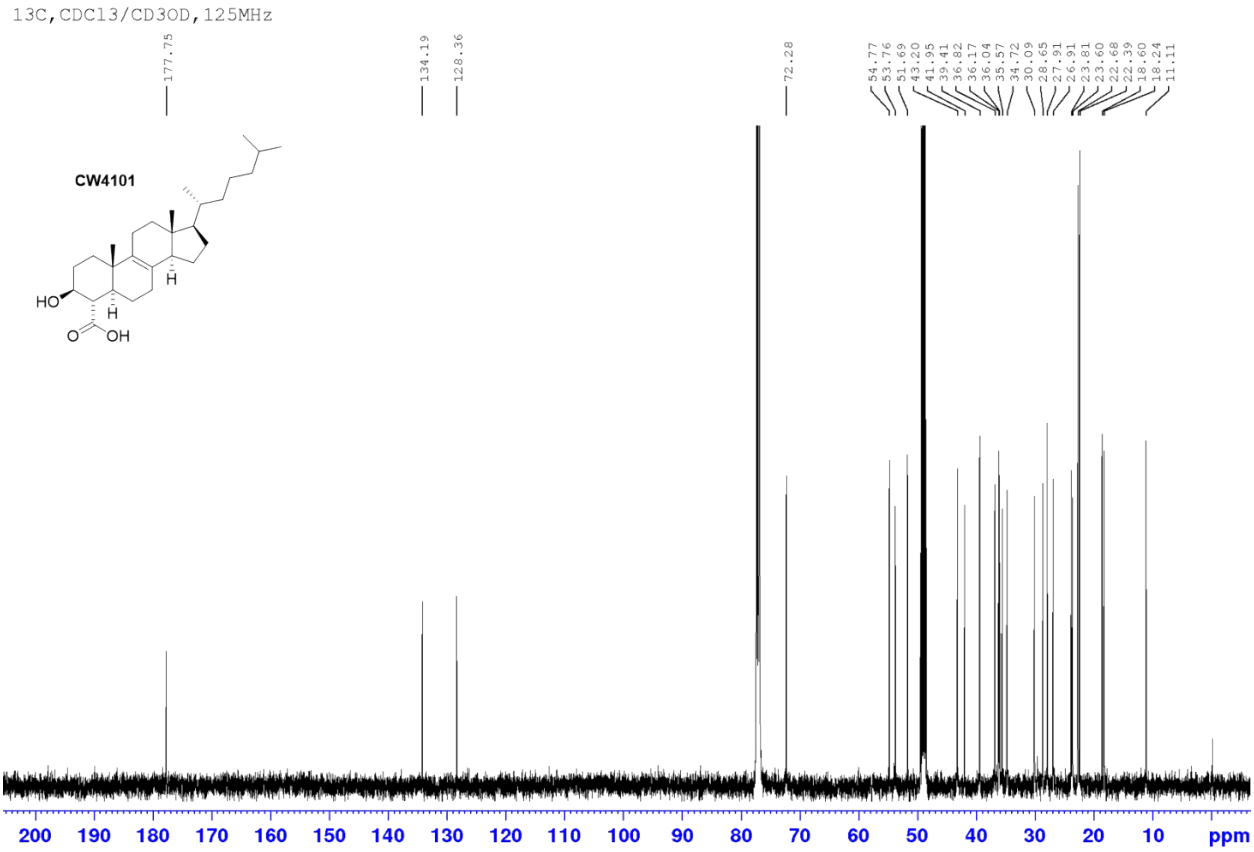
2.09
2.08
2.07
2.06
2.05
2.04
2.03
2.01
2.00
1.98
1.97
1.96
1.92
1.91
1.90
1.89
1.88
1.88
1.87
1.86
1.82
1.81
1.80
1.79
1.78
1.74
1.65
1.64
1.62
1.62
1.60
1.57
1.55
1.55
1.54
1.53
1.52
1.50
1.50
1.49
1.48
1.47
1.46
1.46
1.41
1.39
1.37
1.34
CW0499
HO
H
O
OMe
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
2.81
0.99
7.85
1.04
0.98
5.65
8.17
4.11
3.89
2.93
5.90
2.78

13C,CDCl3,125MHz



1H,CDCl3/CD3OD,500MHz




13C,CDCl3/CD3OD,125MHz
177.75
134.19
128.36
72.28
54.77
53.76
51.69
43.20
41.95
39.41
36.82
36.17
36.04
35.57
34.72
30.09
28.65
27.91
26.91
23.81
23.60
22.68
22.39
18.60
18.24
11.11
CW4101
HO
H
H
O
OH
200
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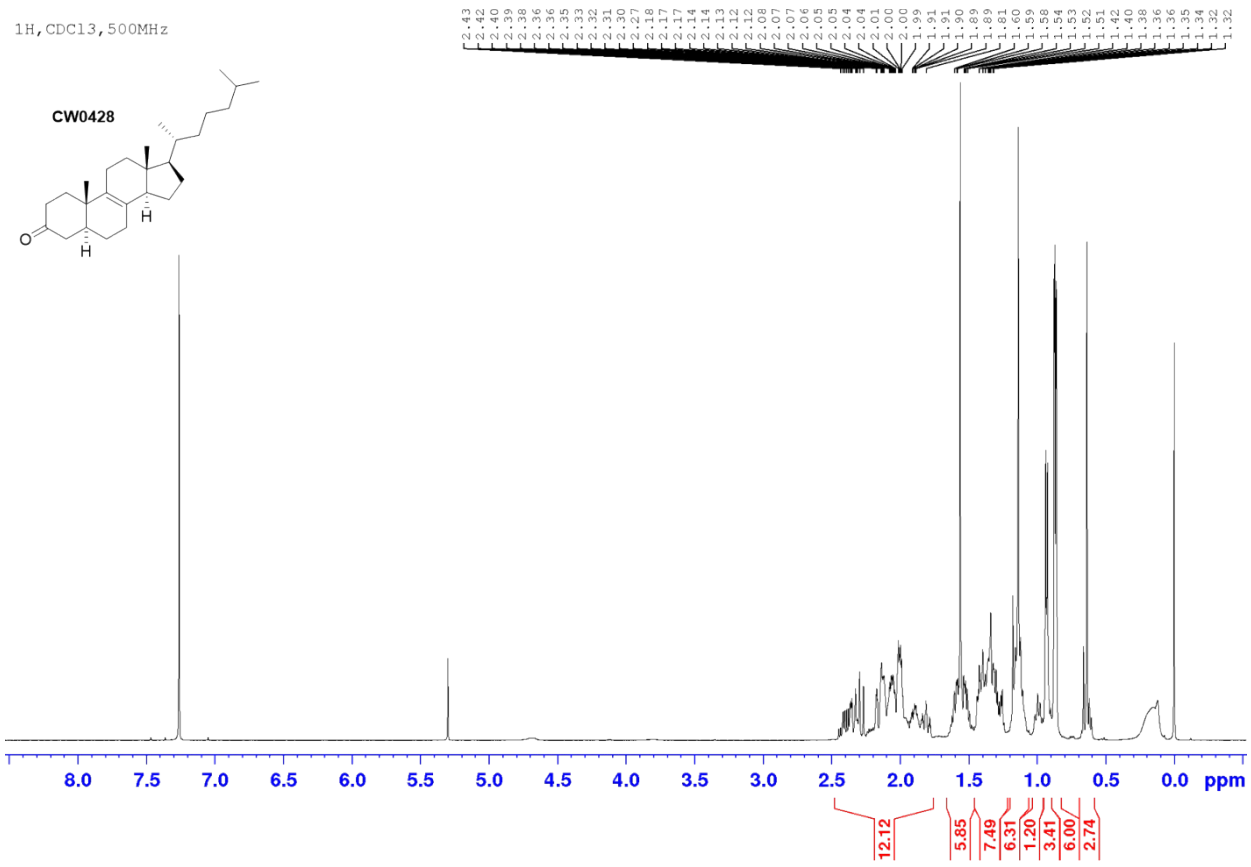
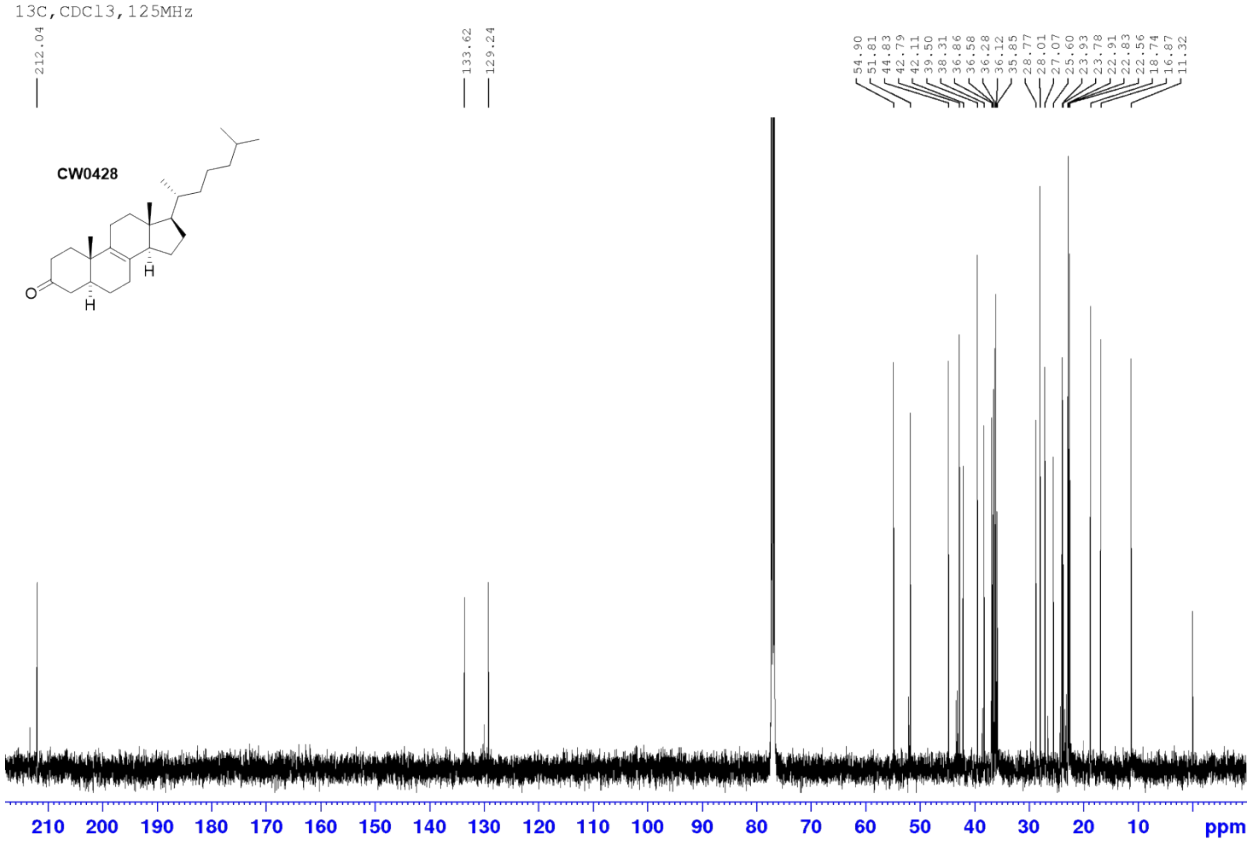
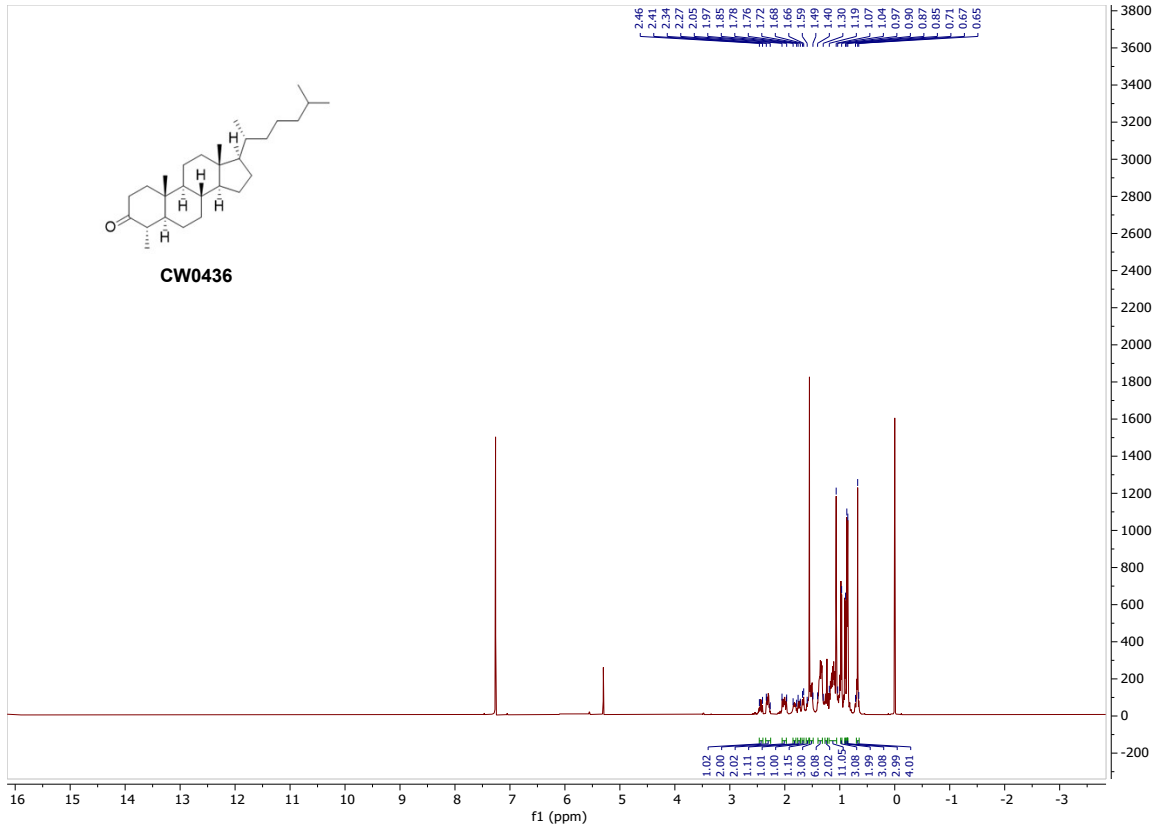
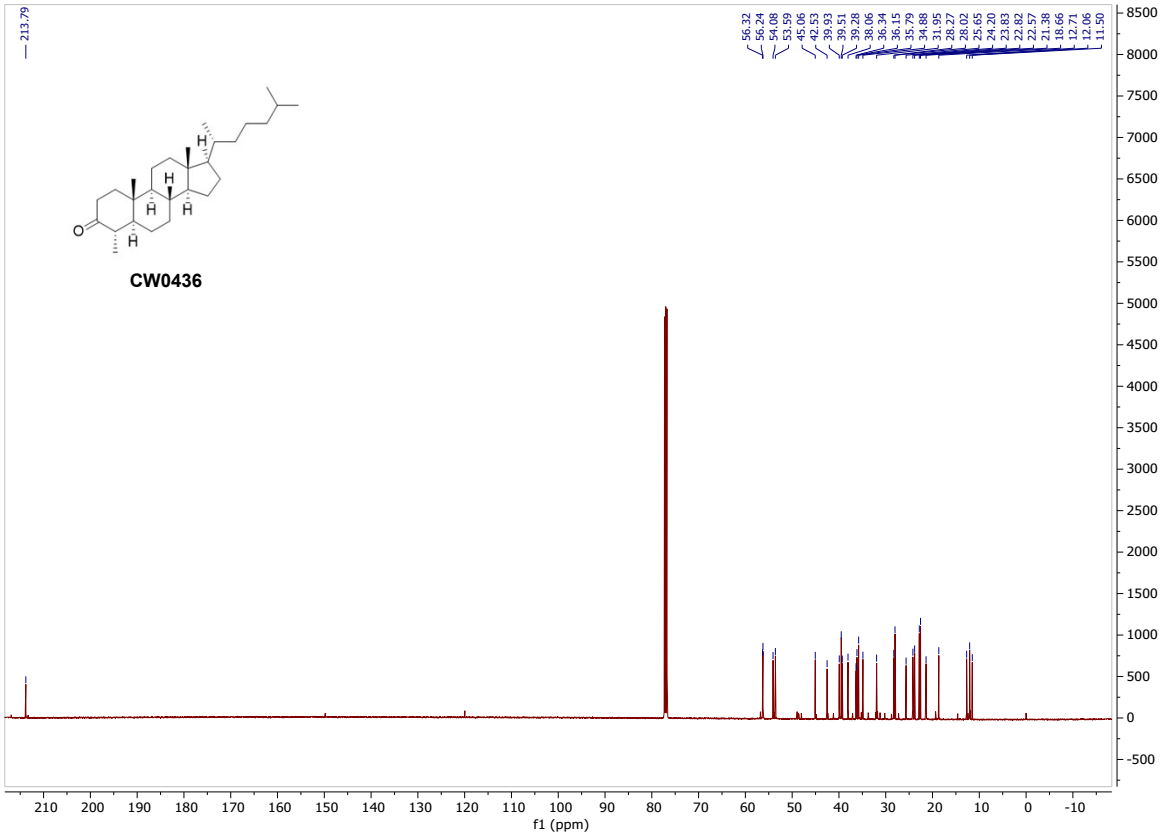
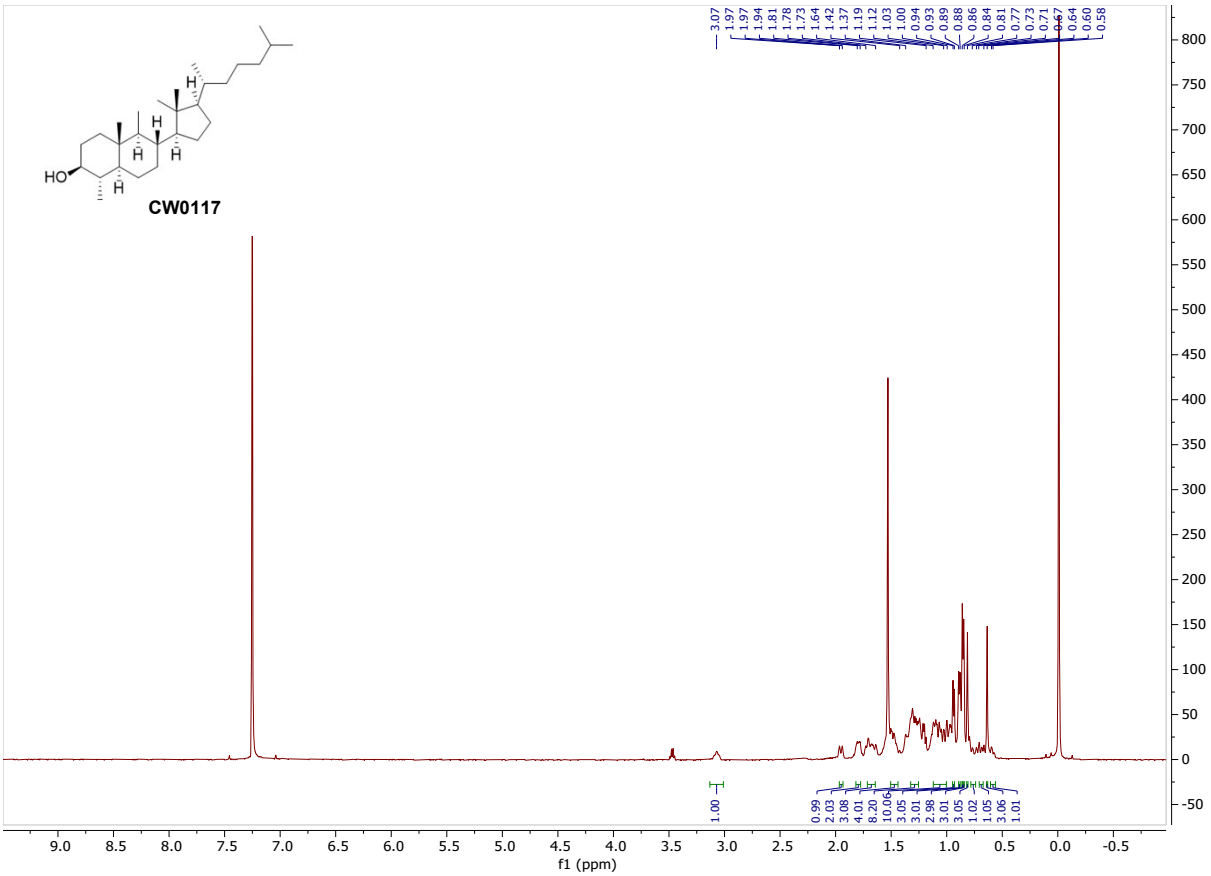
90
80
70
60
50
40
30
20
10
ppm


1H,CDCl3,500MHz
CW0428
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
12.12
5.85
7.49
6.31
1.20
3.41
6.00
2.74

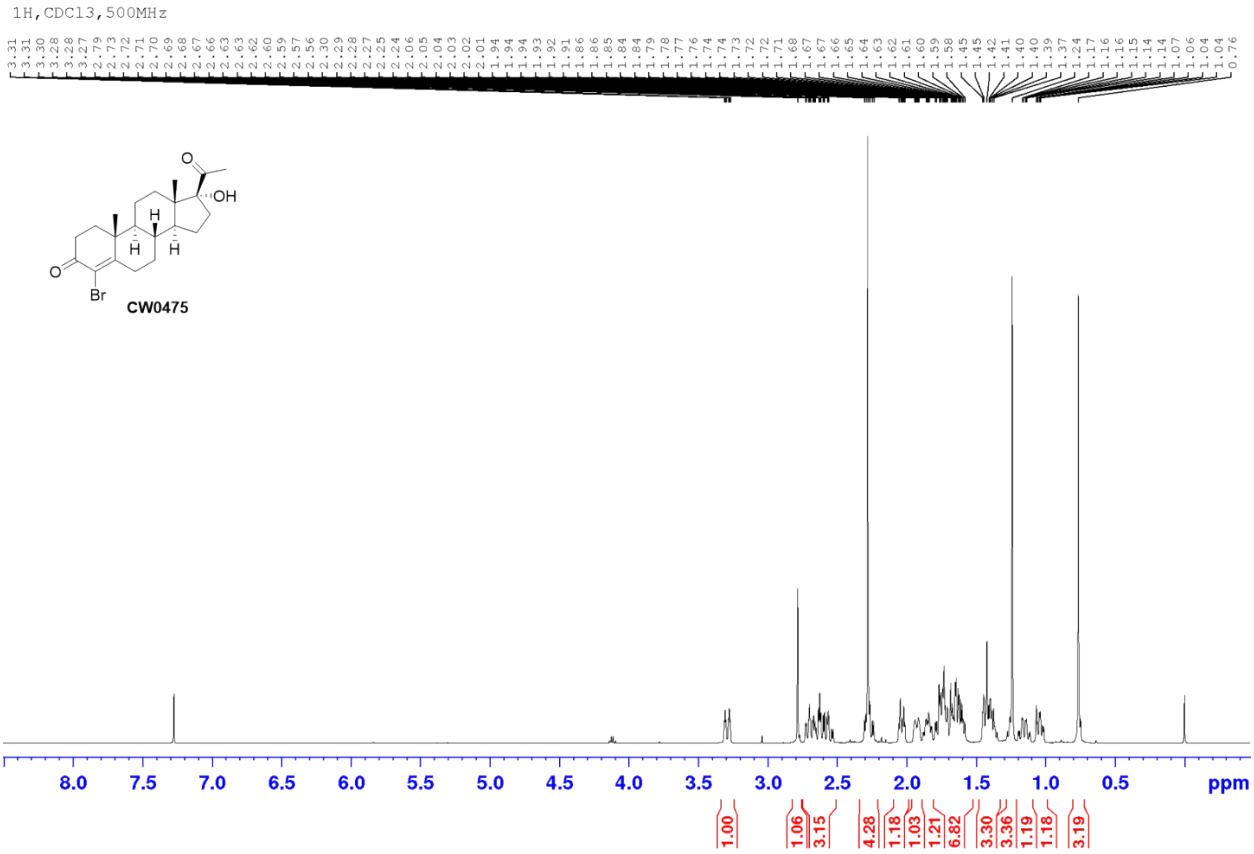

13C,CDCl3,125MHz
CW0428
212.04
133.62
129.24
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

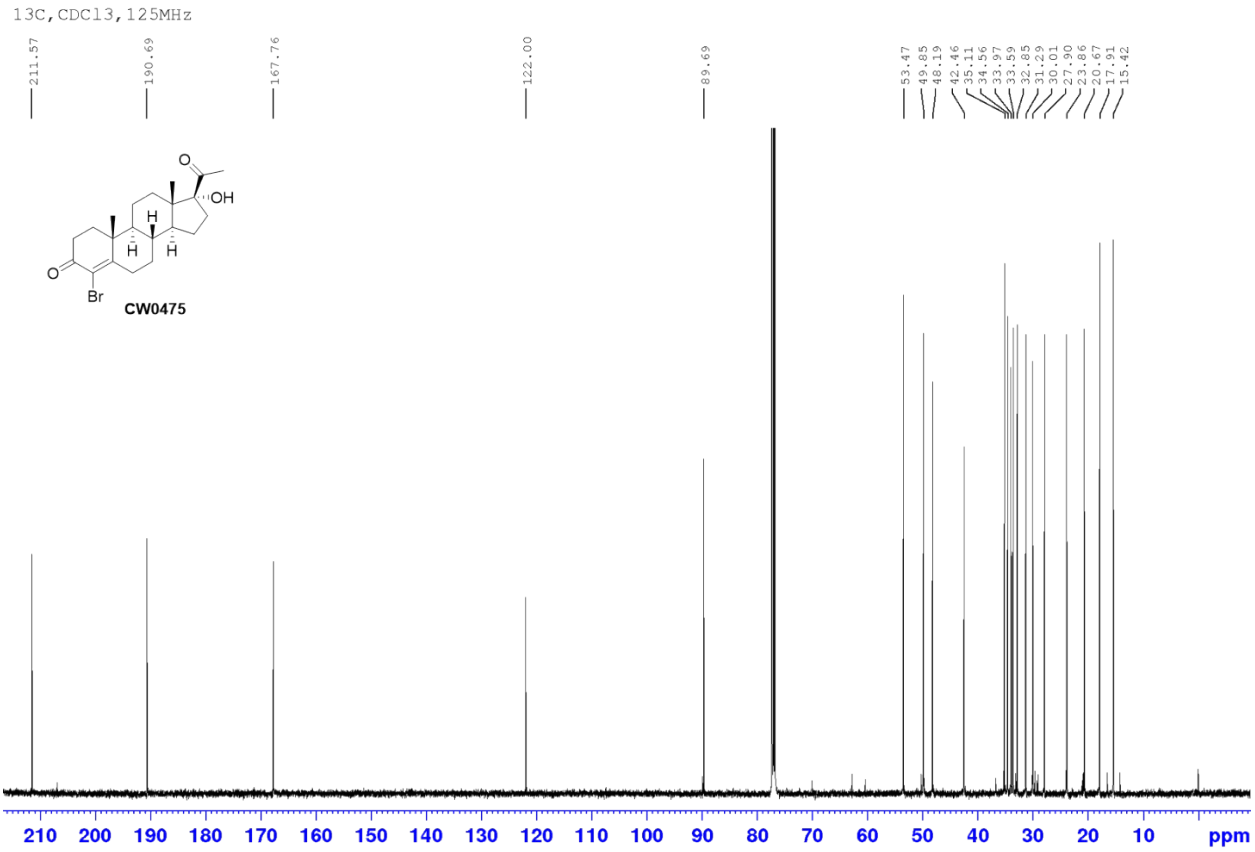

CW0436
f1 (ppm)

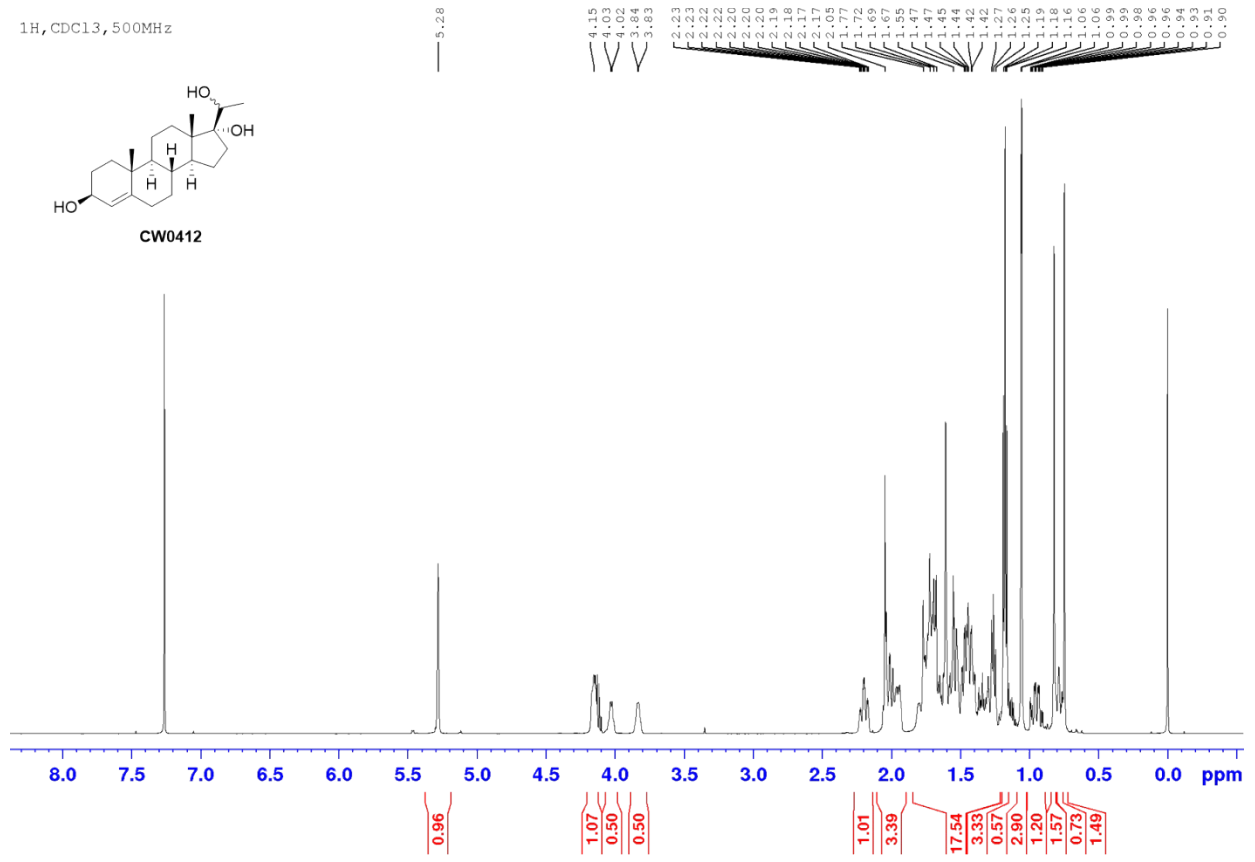

CW0436
f1 (ppm)

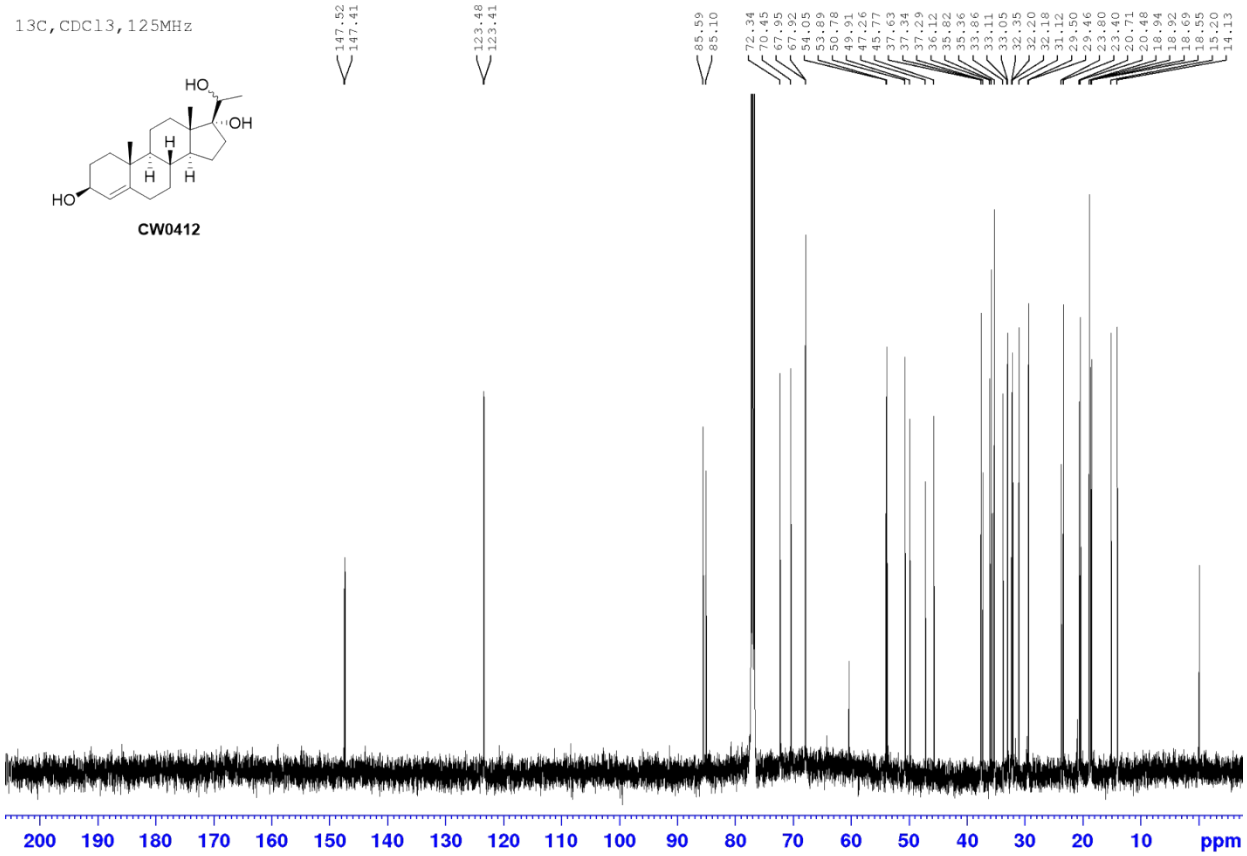

CW0117
HO
3.07
1.97
1.97
1.94
1.81
1.78
1.73
1.64
1.42
1.37
1.19
1.12
1.03
1.00
0.94
0.93
0.89
0.88
0.86
0.84
0.81
0.77
0.73
0.71
0.67
0.64
0.60
0.58
1.00
0.99
2.03
3.08
4.01
8.20
10.06
3.05
3.01
2.98
3.01
3.05
1.02
1.05
3.06
1.01
f1 (ppm)

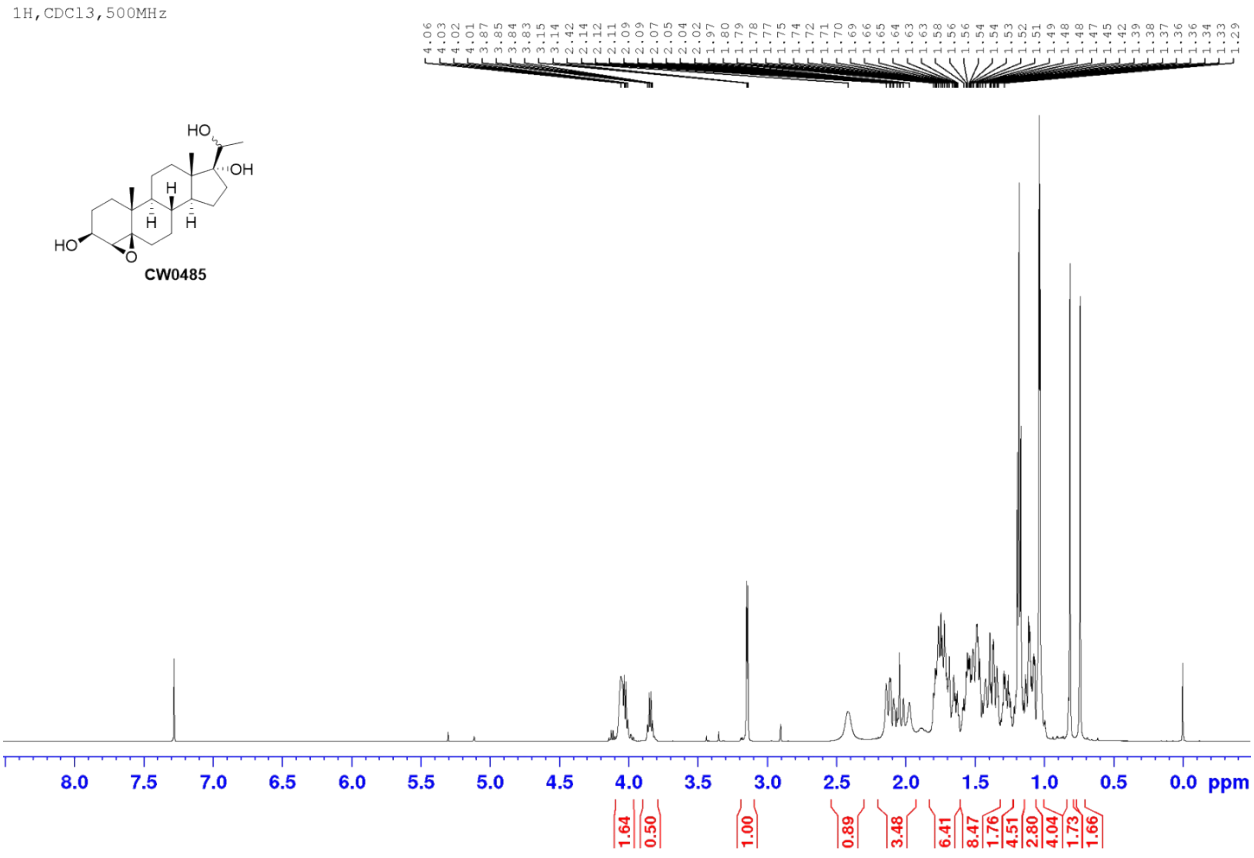
SC4MOL Inhibitors

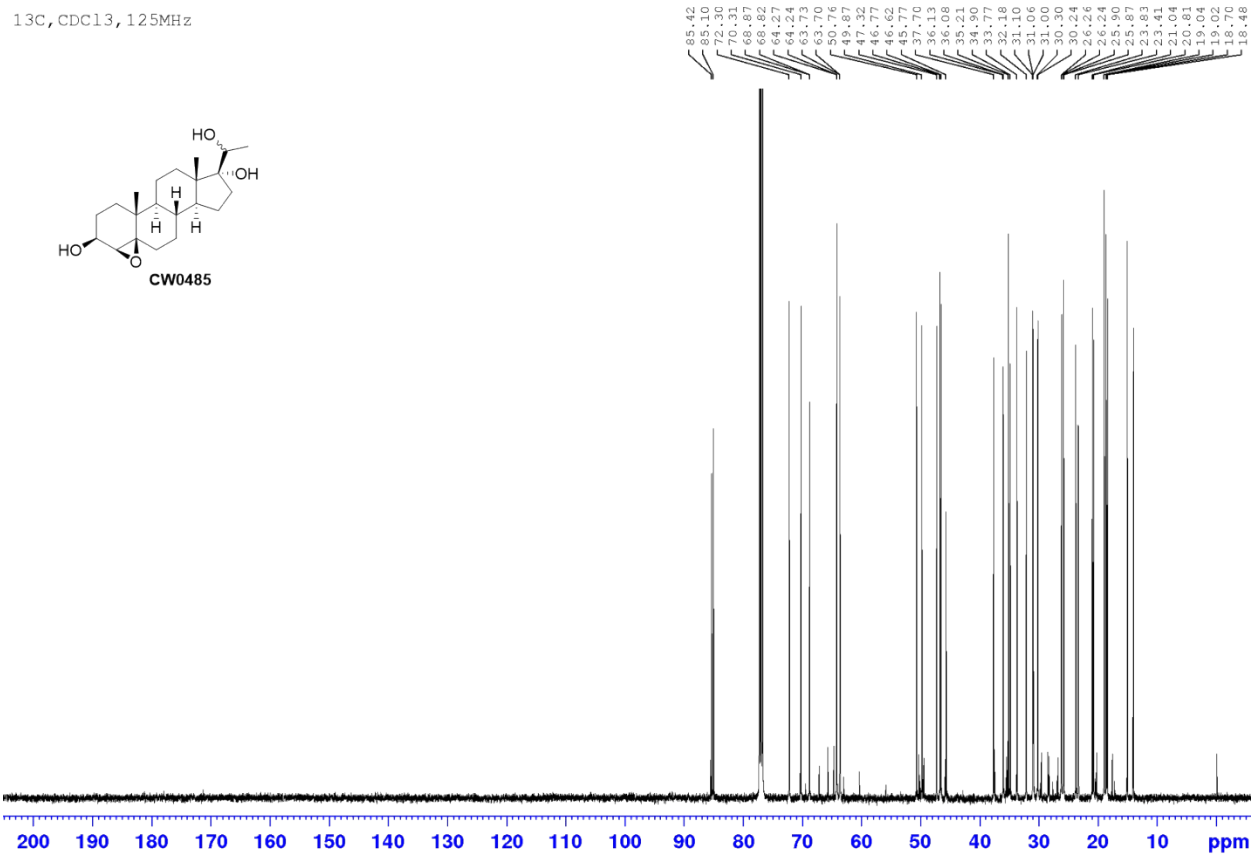


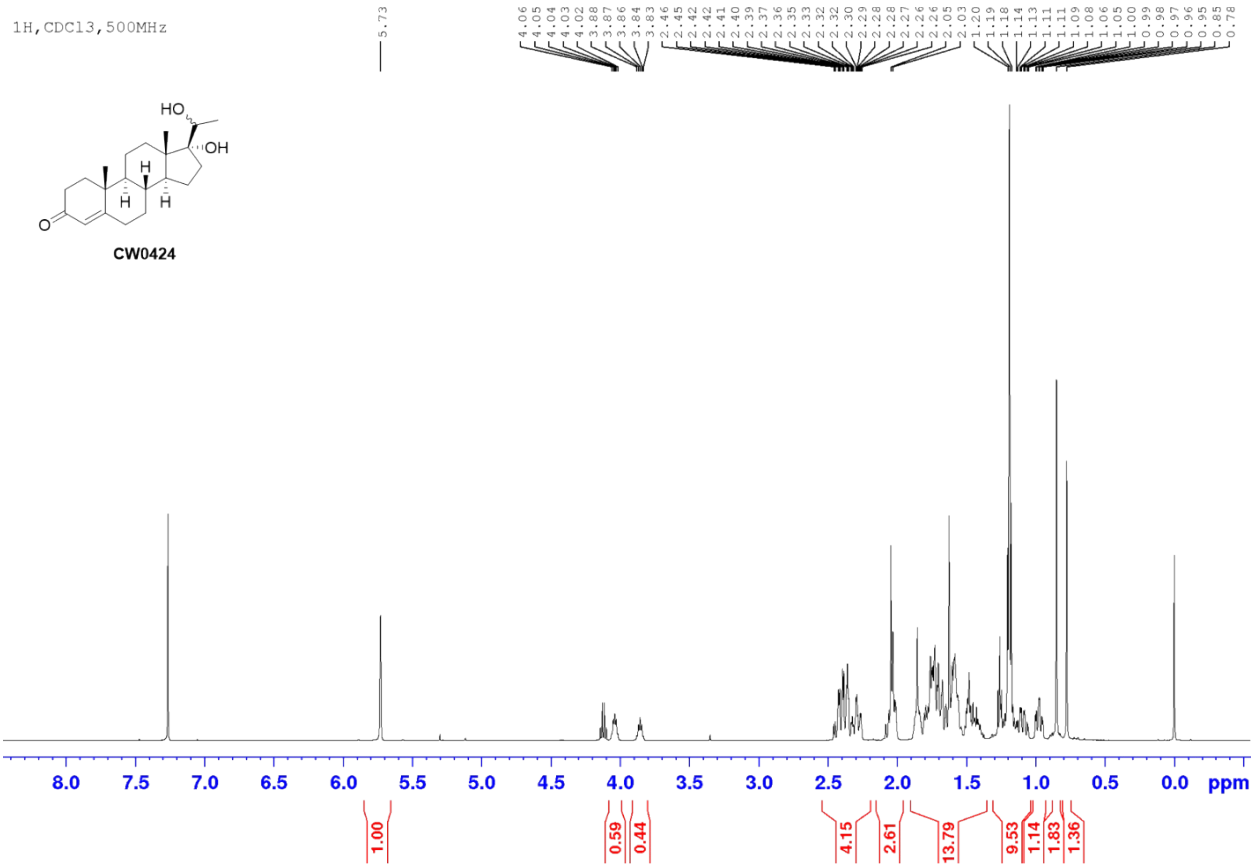

13C,CDCl3,125MHz
211.57
190.69
167.76
122.00
89.69
53.47
49.85
48.19
42.46
35.11
34.56
33.97
33.59
32.85
31.29
30.01
27.90
23.86
20.67
17.91
15.42
CW0475
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

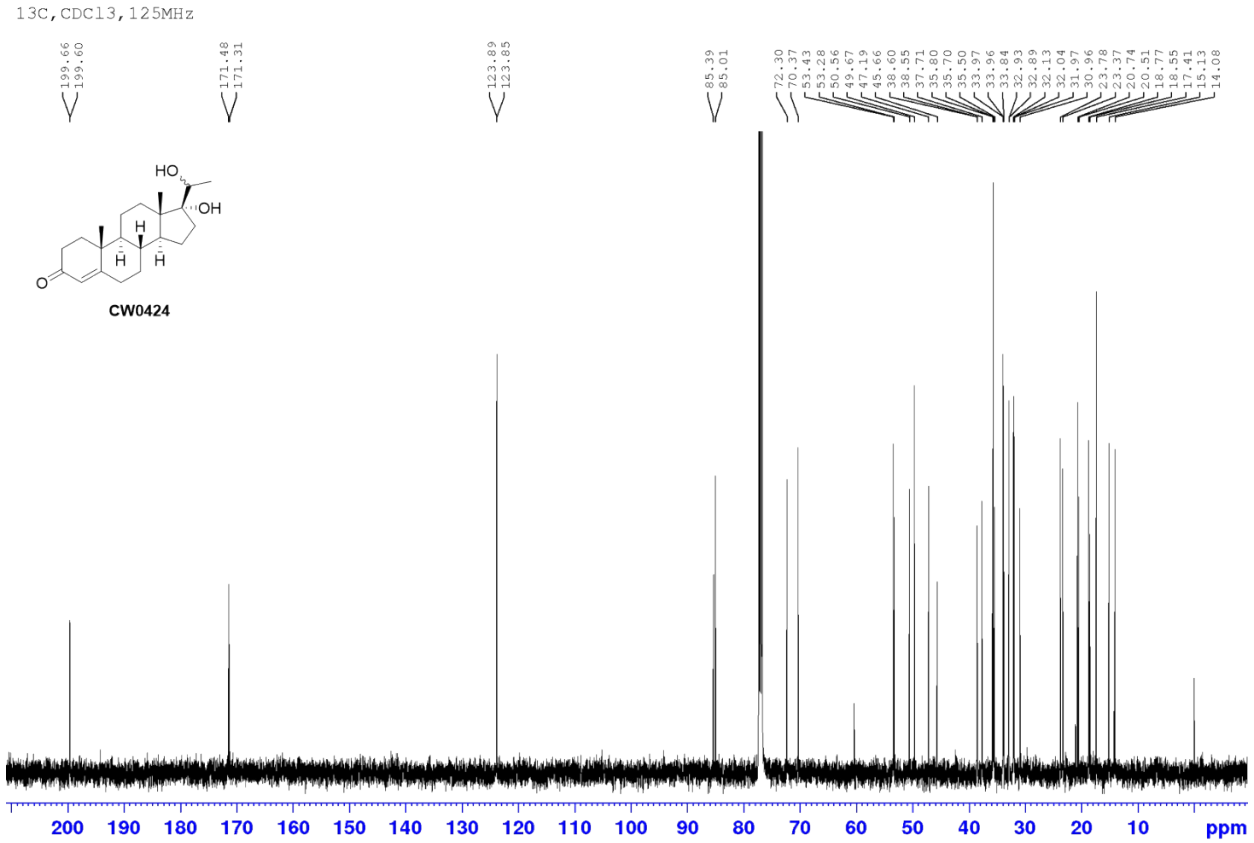

1H,CDCl3,500MHz
5.28
4.15
4.03
4.02
3.84
3.83
CW0412
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.96
1.07
0.50
0.50
1.01
3.39
17.54
3.33
0.57
2.90
1.20
1.57
0.73
1.49

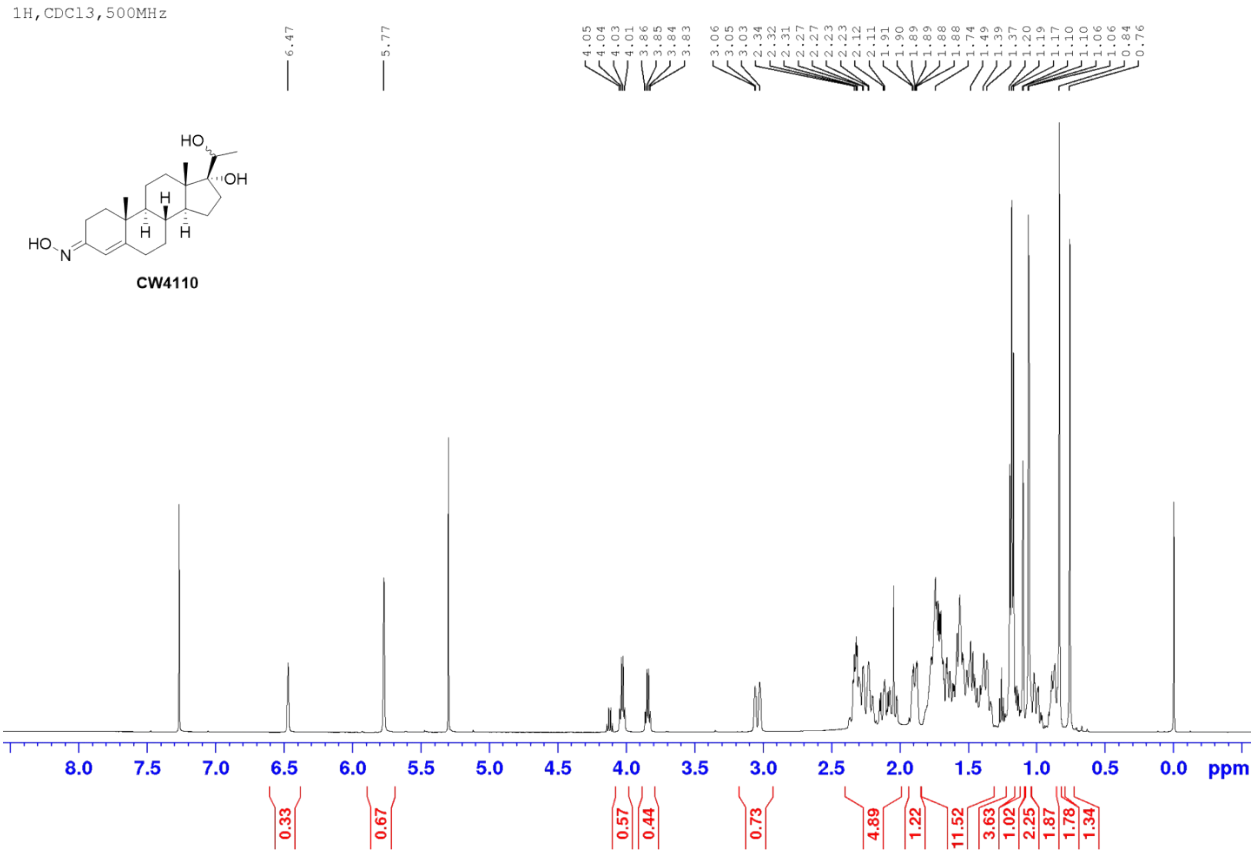

13C,CDCl3,125MHz
147.52
147.41
123.48
123.41
85.59
85.10
72.34
70.45
67.95
67.92
54.05
53.89
50.78
49.91
47.26
45.77
37.63
37.34
37.29
36.12
35.82
35.36
33.86
33.11
33.05
32.35
32.20
32.18
31.12
29.50
29.46
23.80
23.40
20.71
20.48
18.94
18.92
18.69
18.55
15.20
14.13
HO
OH
H
H
H
HO
CW0412
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

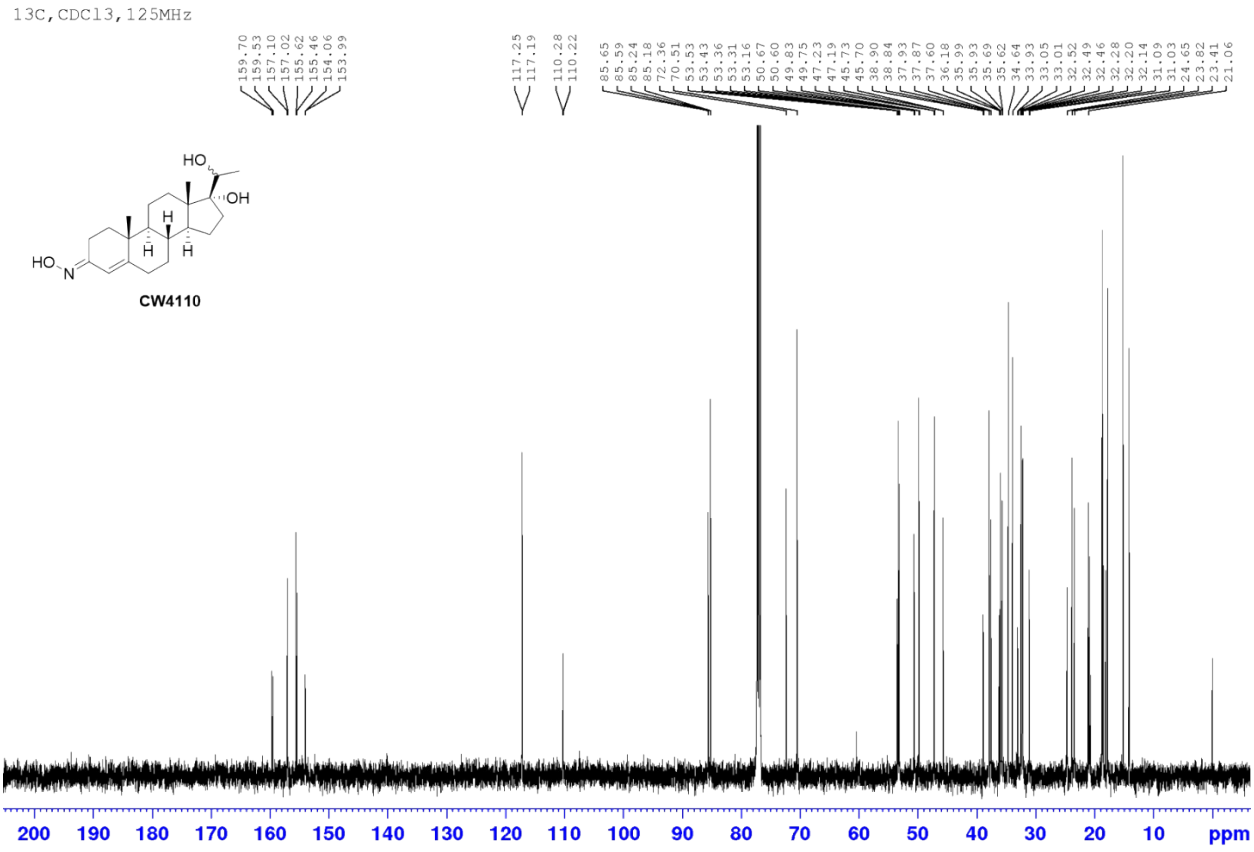

1H,CDCl3,500MHz
4.06
4.03
4.02
4.01
3.87
3.85
3.84
3.83
3.15
3.14
2.42
2.14
2.12
2.11
2.09
2.09
2.07
2.05
2.04
2.02
1.97
1.80
1.79
1.78
1.77
1.75
1.74
1.72
1.71
1.70
1.69
1.66
1.65
1.64
1.63
1.63
1.58
1.56
1.56
1.54
1.54
1.53
1.52
1.51
1.49
1.48
1.48
1.47
1.45
1.42
1.39
1.38
1.37
1.36
1.36
1.34
1.33
1.29
HO
OH
H
H
H
HO
O
CW0485
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.64
0.50
1.00
0.89
3.48
6.41
8.47
1.76
4.51
2.80
4.04
1.73
1.66


13C,CDCl3,125MHz
85.42
85.10
72.30
70.31
68.87
68.82
64.27
64.24
63.73
63.70
50.76
49.87
47.32
46.77
46.62
45.77
37.70
36.13
36.08
35.21
34.90
33.77
32.18
31.10
31.06
31.00
30.30
30.24
26.26
26.24
25.90
25.87
23.83
23.41
21.04
20.81
19.04
19.02
18.70
18.48
HO
OH
H
H
H
HO
O
CW0485
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

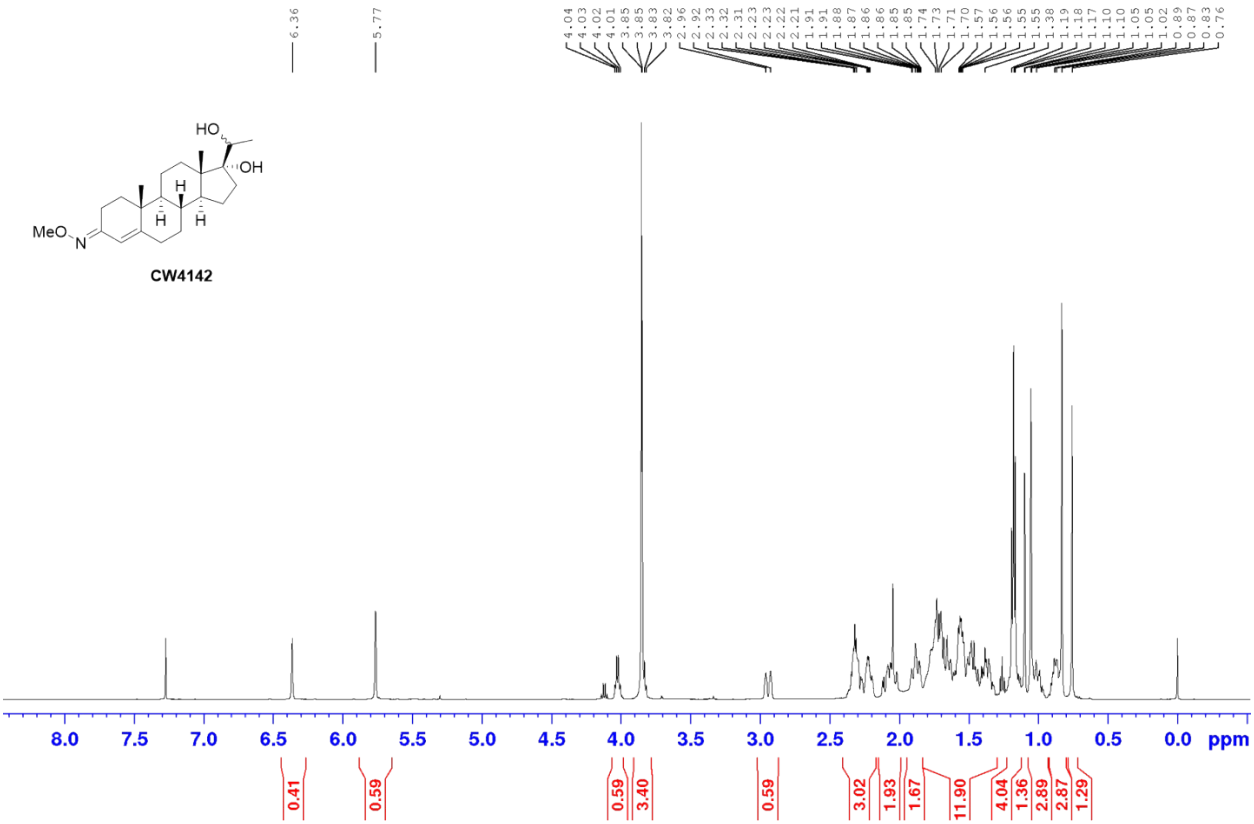

1H,CDCl3,500MHz
CW0424
ppm


13C,CDCl3,125MHz
CW0424
ppm

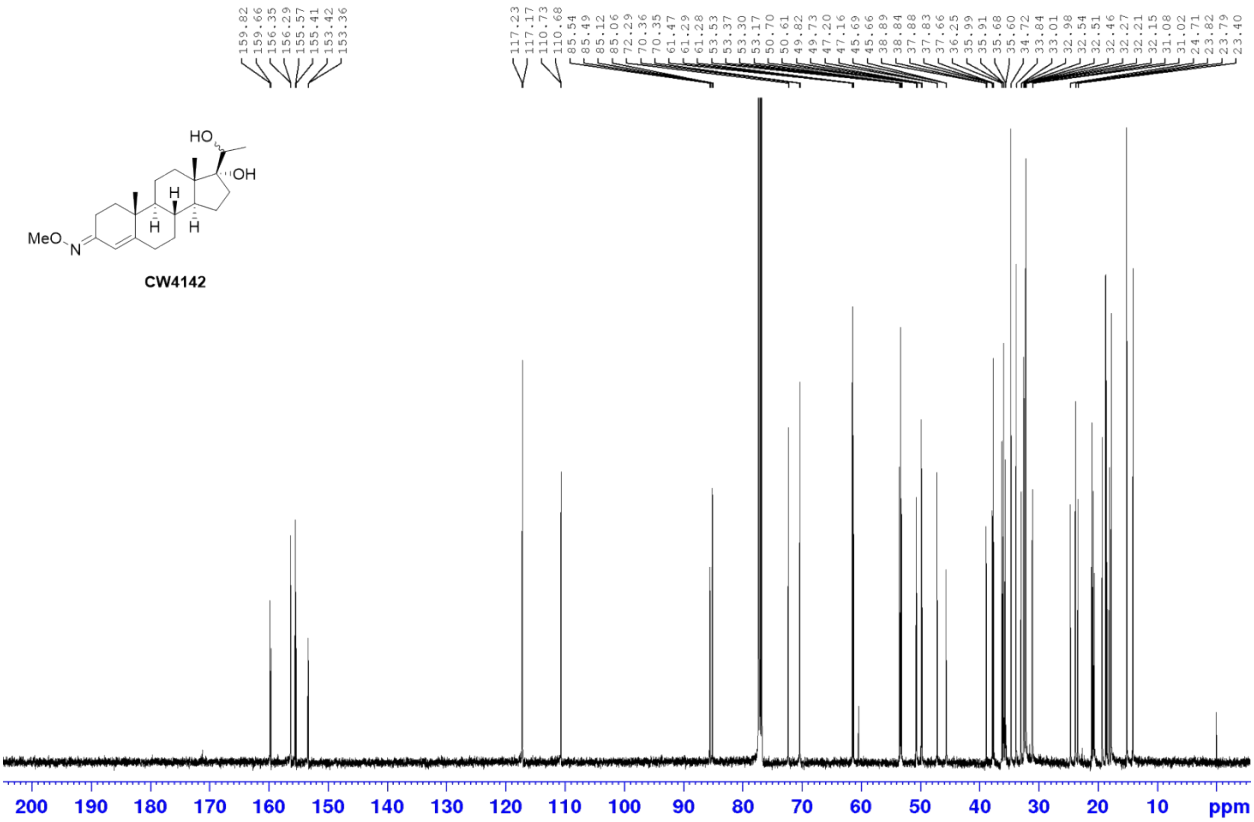

1H,CDCl3,500MHz
CW4110
ppm


13C,CDCl3,125MHz
CW4110
ppm

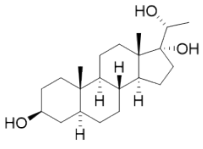
1H,CDCl3,500MHz



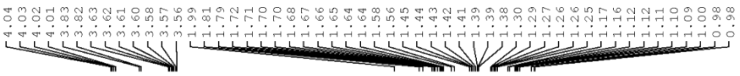
13C,CDCl3,125MHz



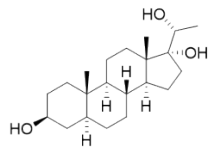
1H,CDCl3,500MHz



CW0464

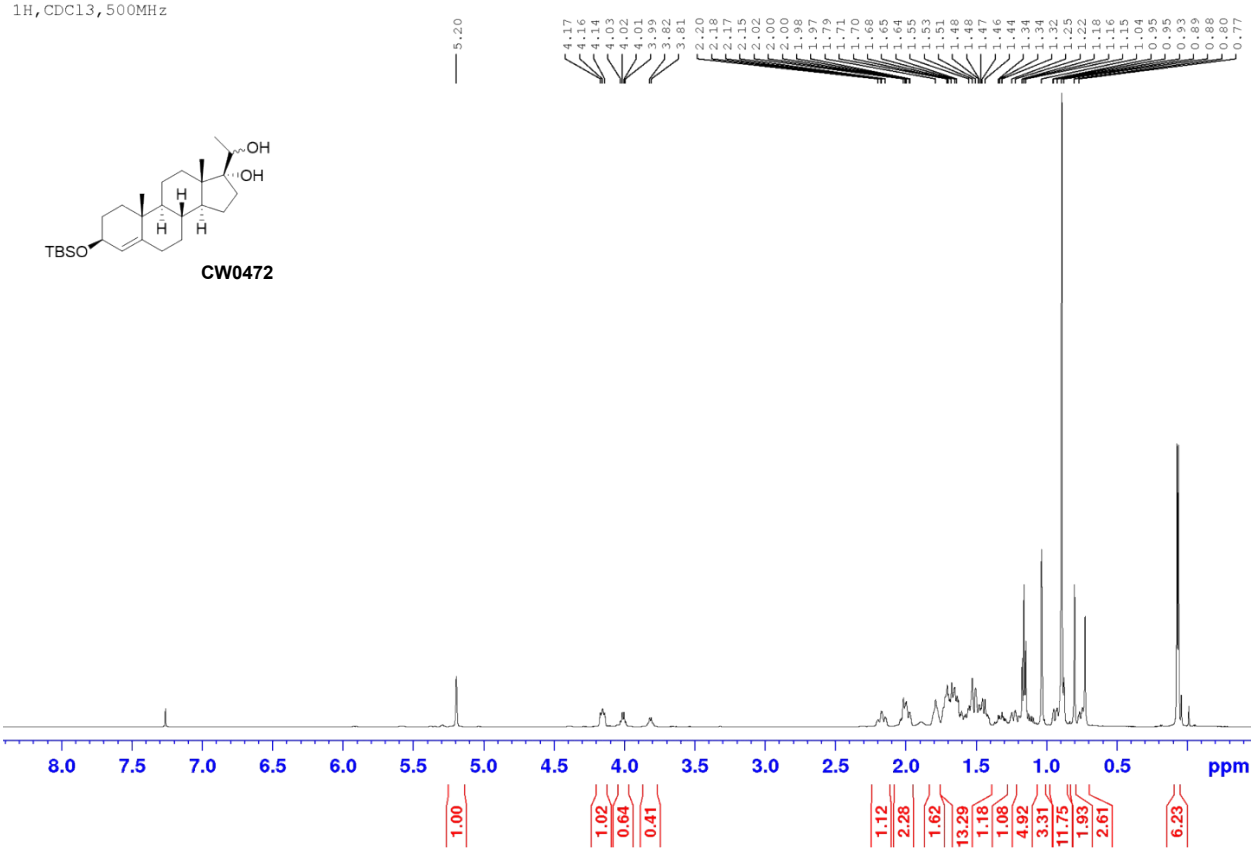


13C,CDCl3,125MHz

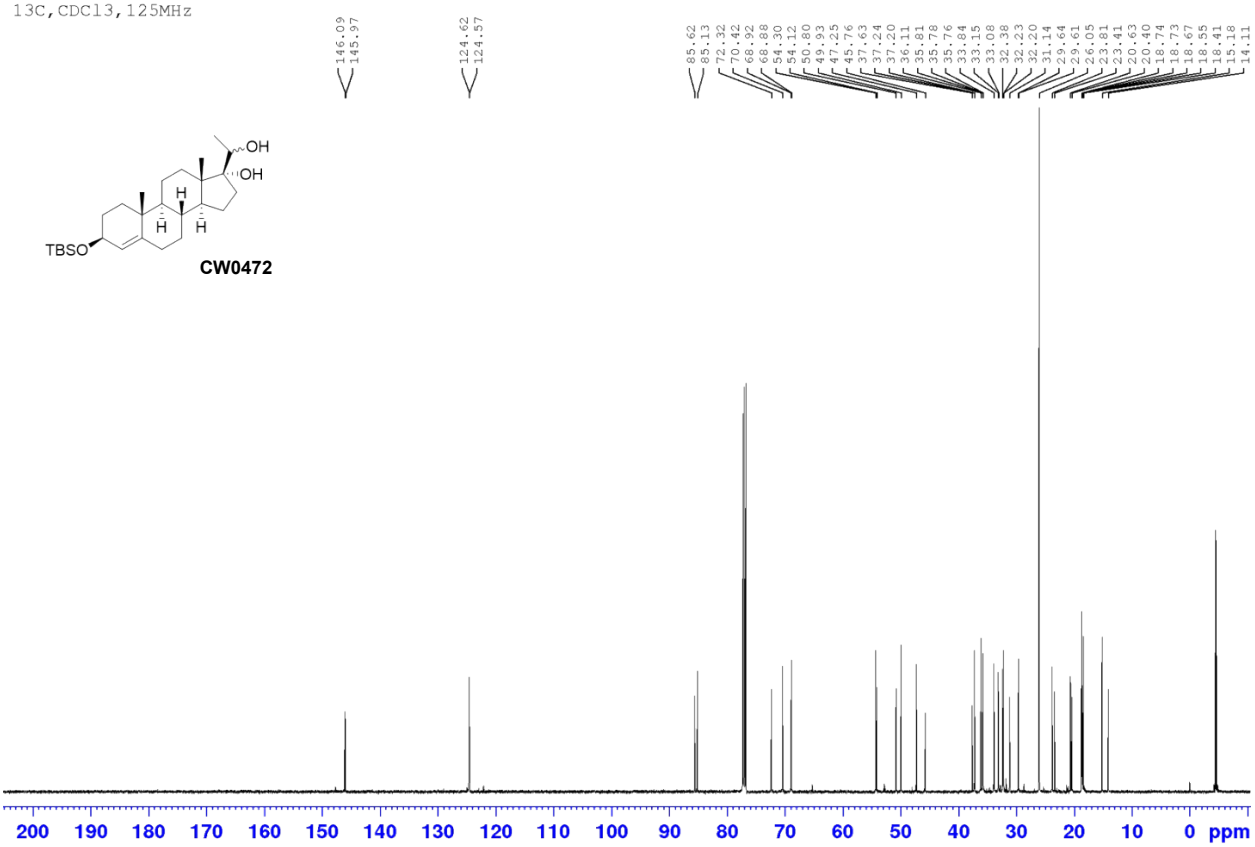


CW0464

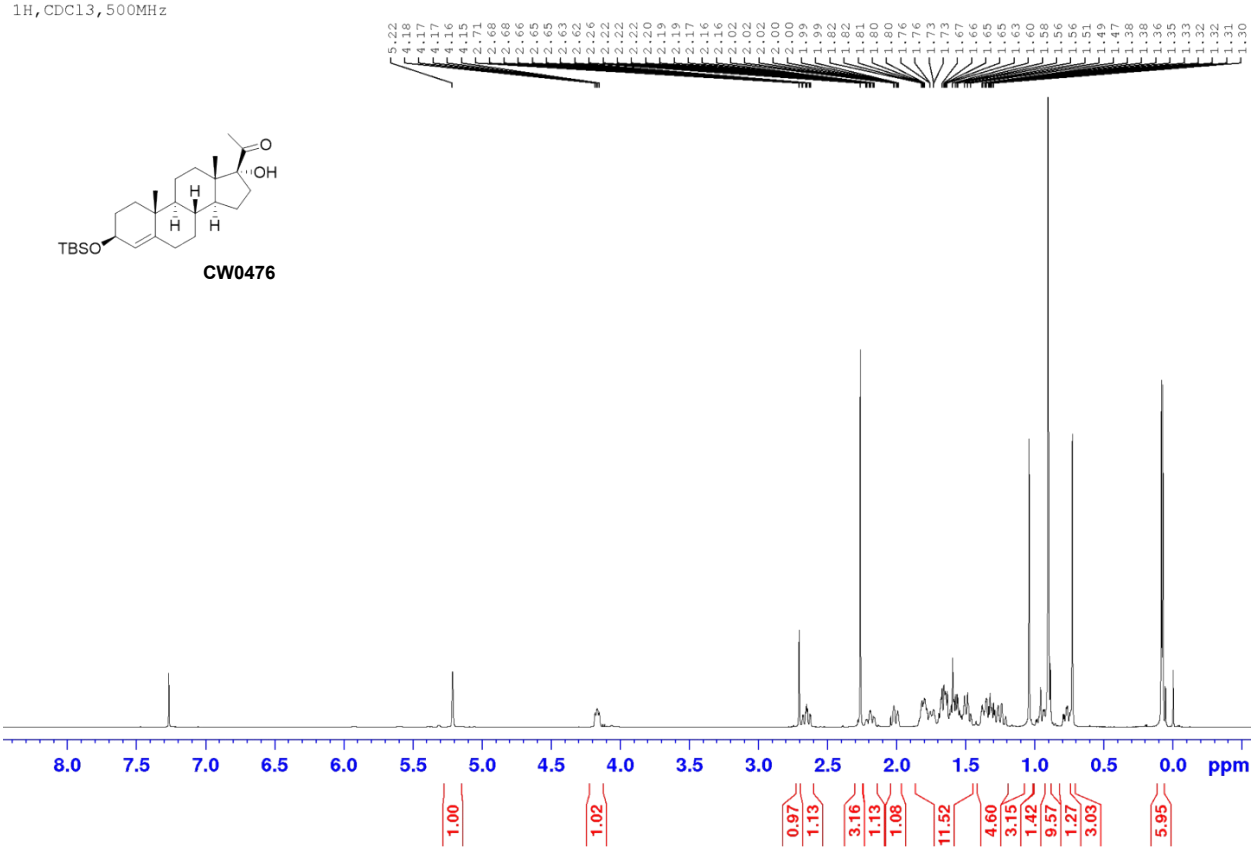
1H,CDCl3,500MHz



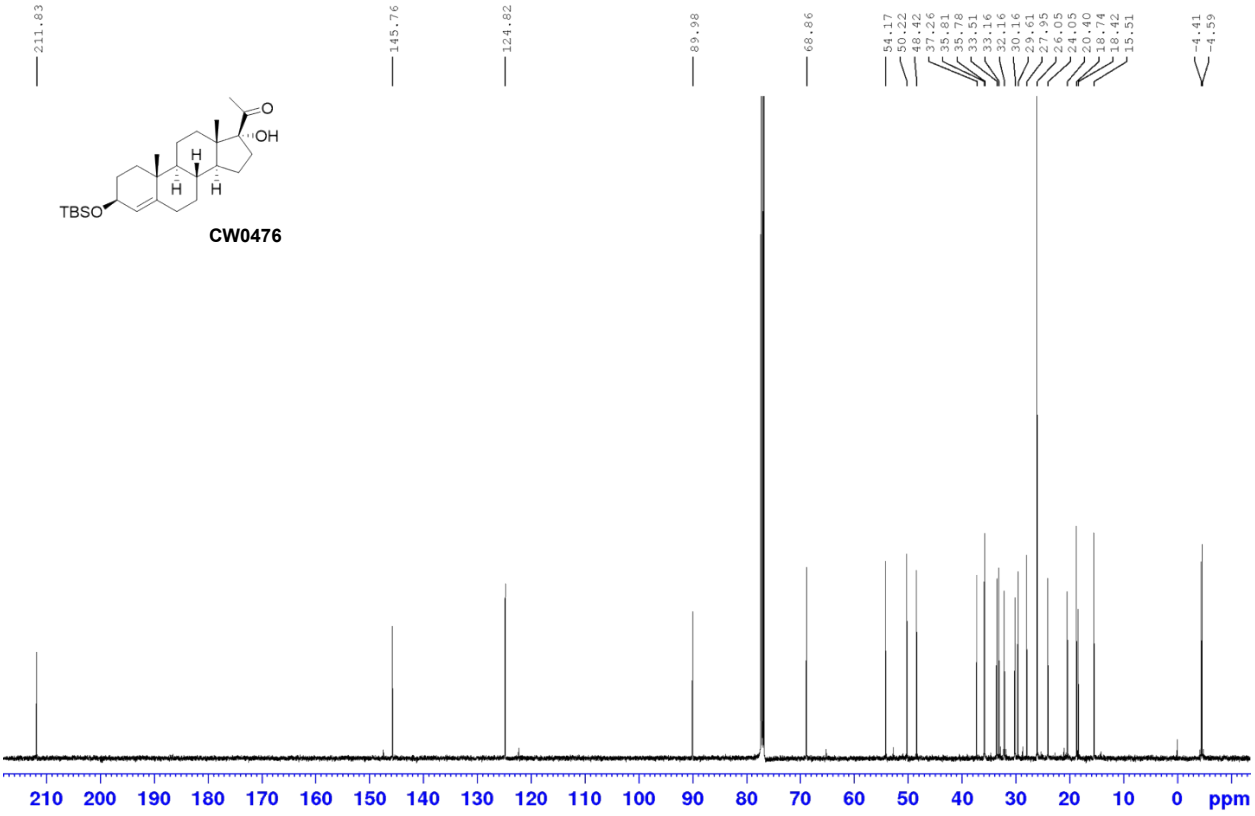
13C,CDCl3,125MHz

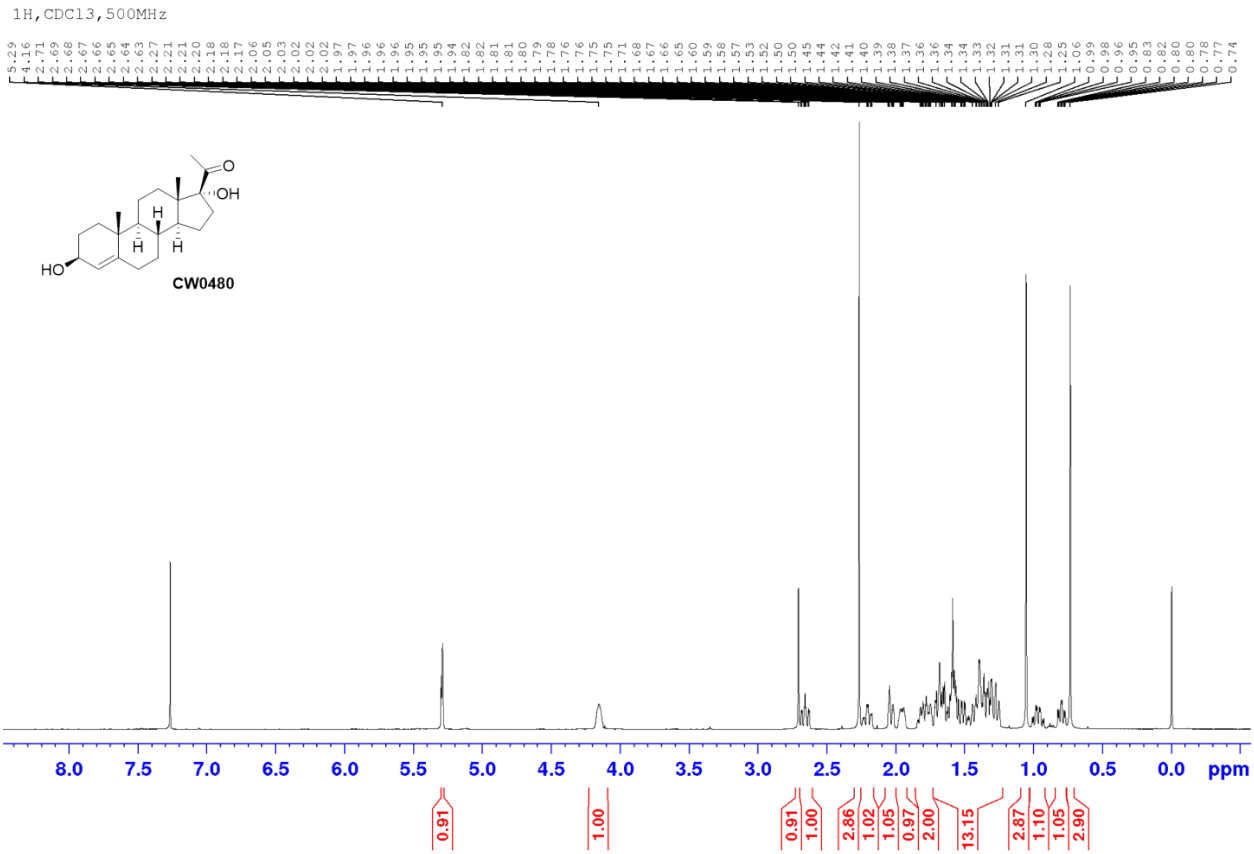


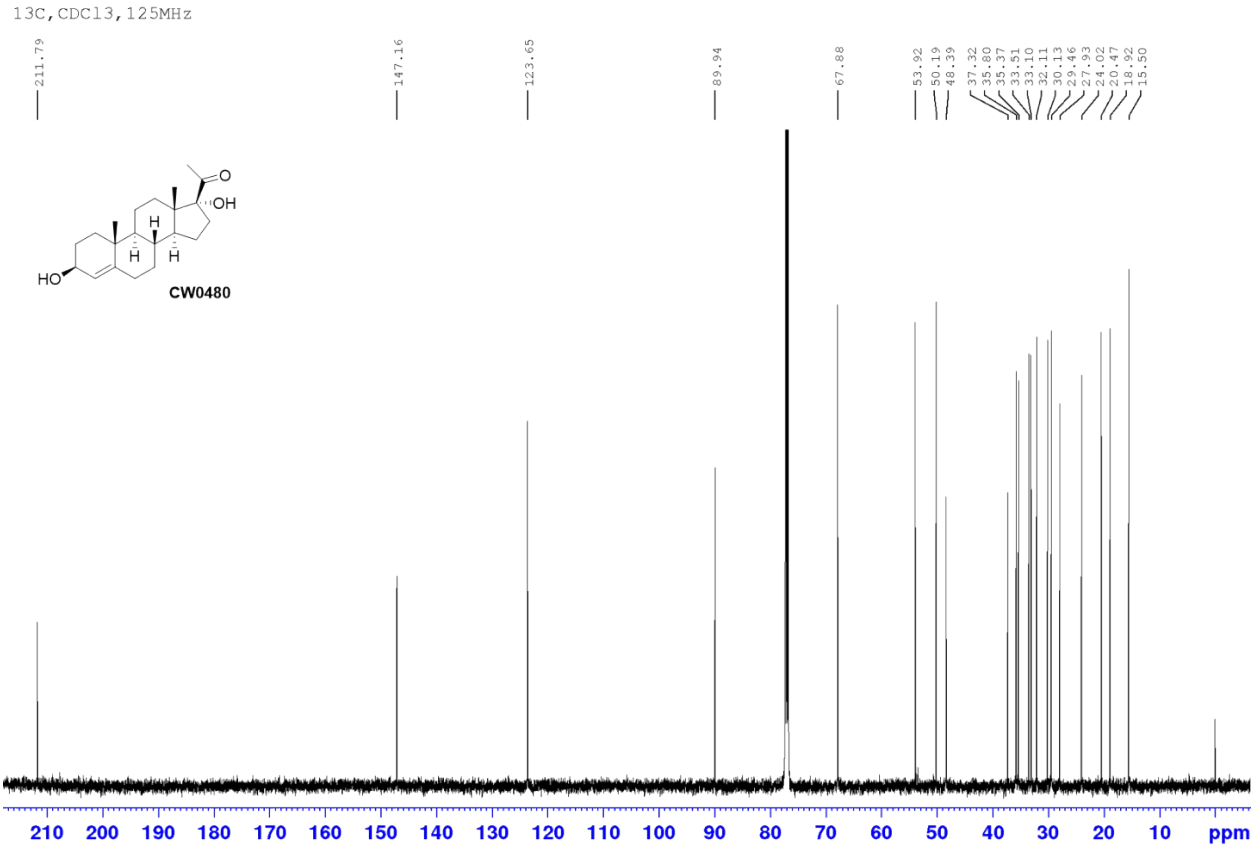
1H,CDCl3,500MHz



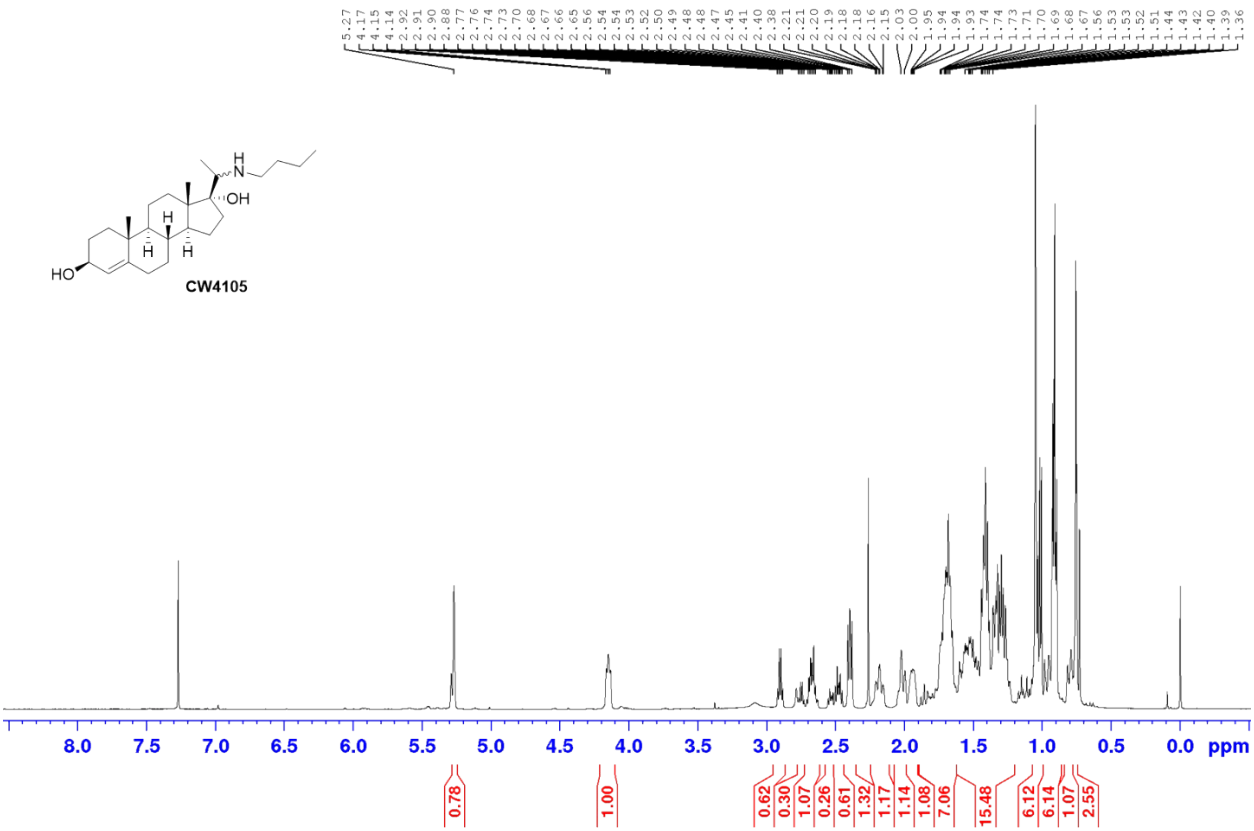
13C,CDCl3,125MHz



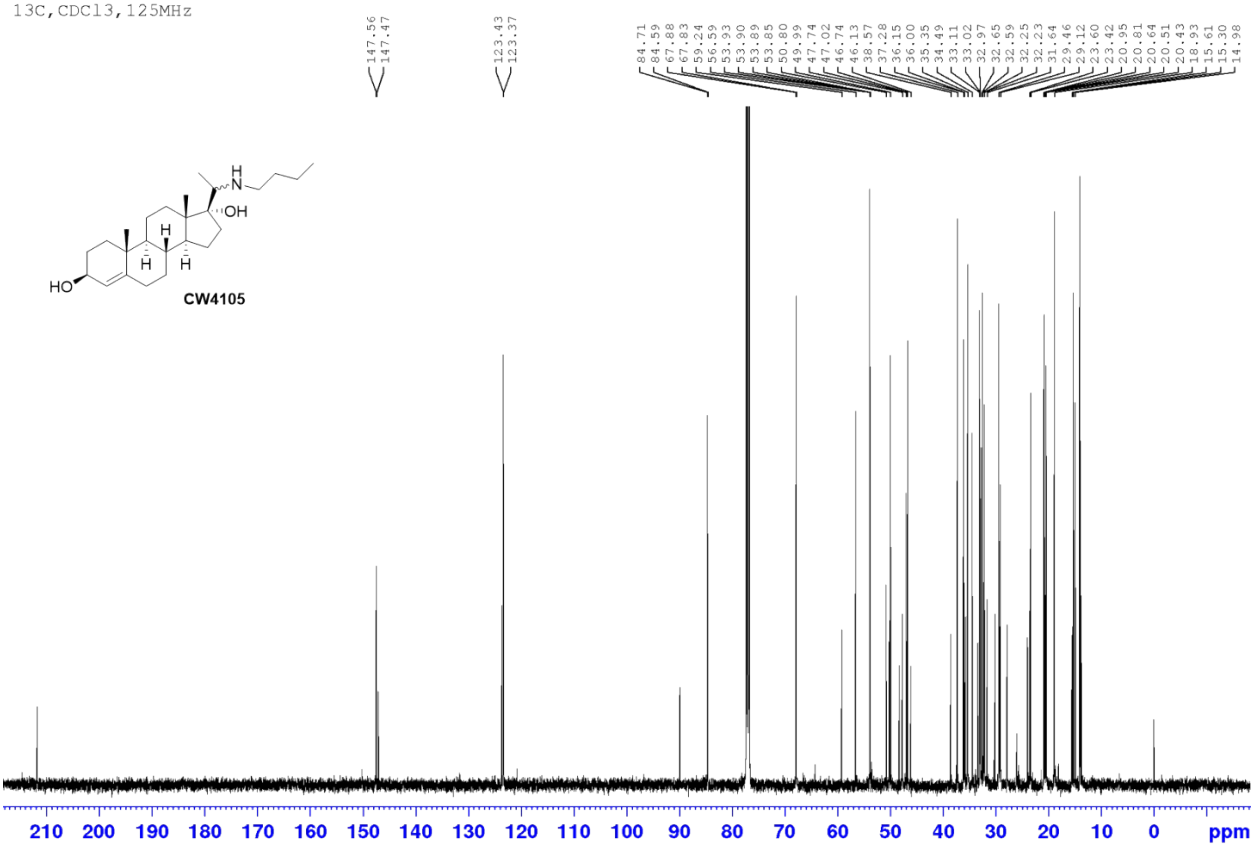

1H,CDCl3,500MHz
CW0480
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.91 1.00 0.91 1.00 2.86 1.02 1.05 0.97 2.00 13.15 2.87 1.10 1.05 2.90

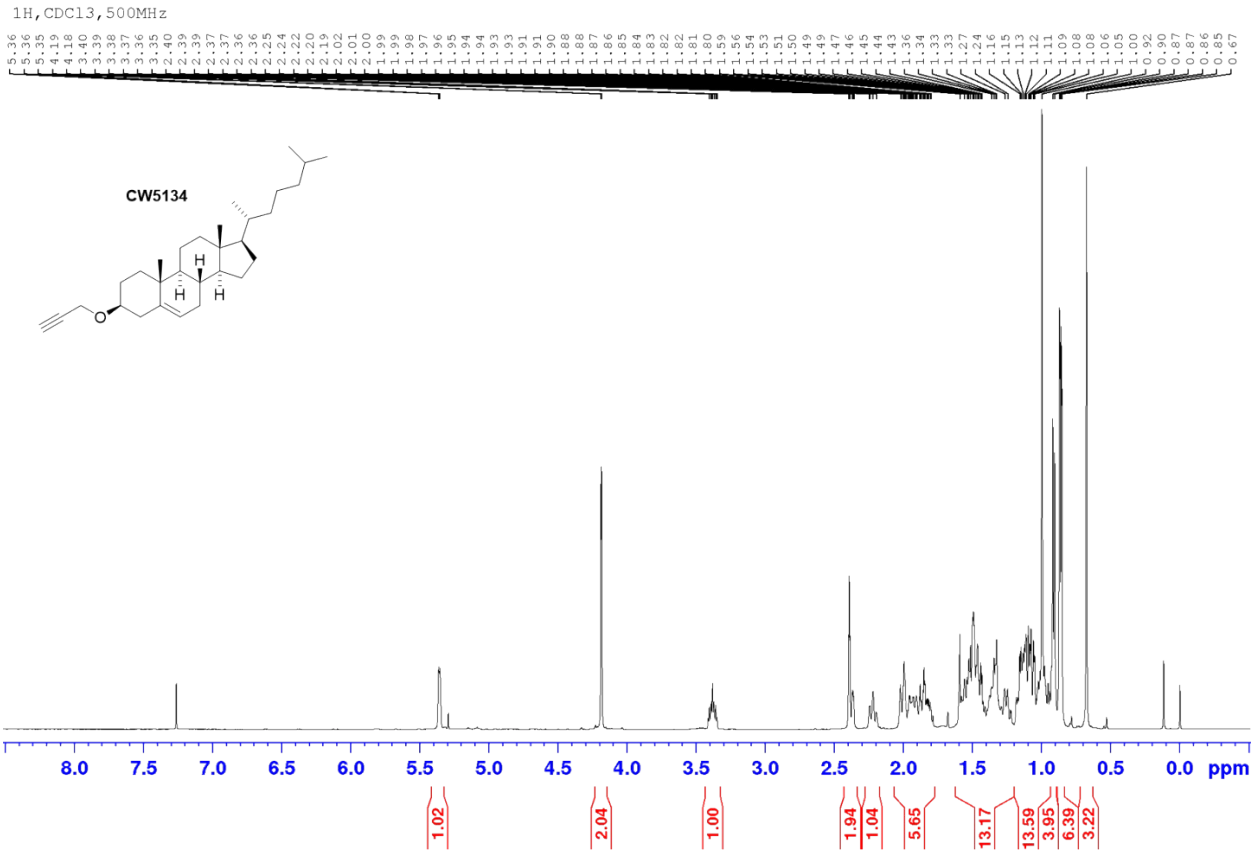

13C,CDCl3,125MHz
211.79
147.16
123.65
89.94
67.88
53.92
50.19
48.39
37.32
35.80
35.37
33.51
33.10
32.11
30.13
29.46
27.93
24.02
20.47
18.92
15.50
CW0480
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

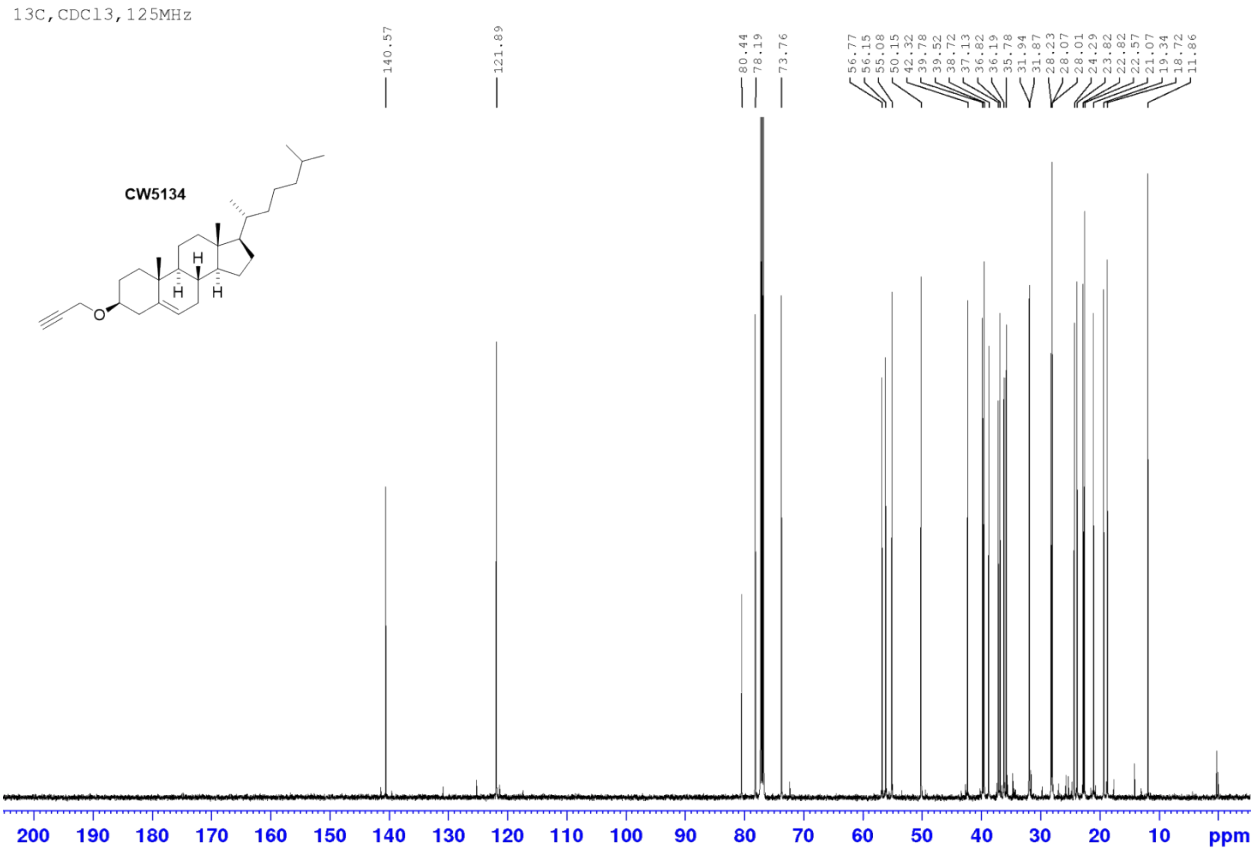
1H,CDCl3,500MHz

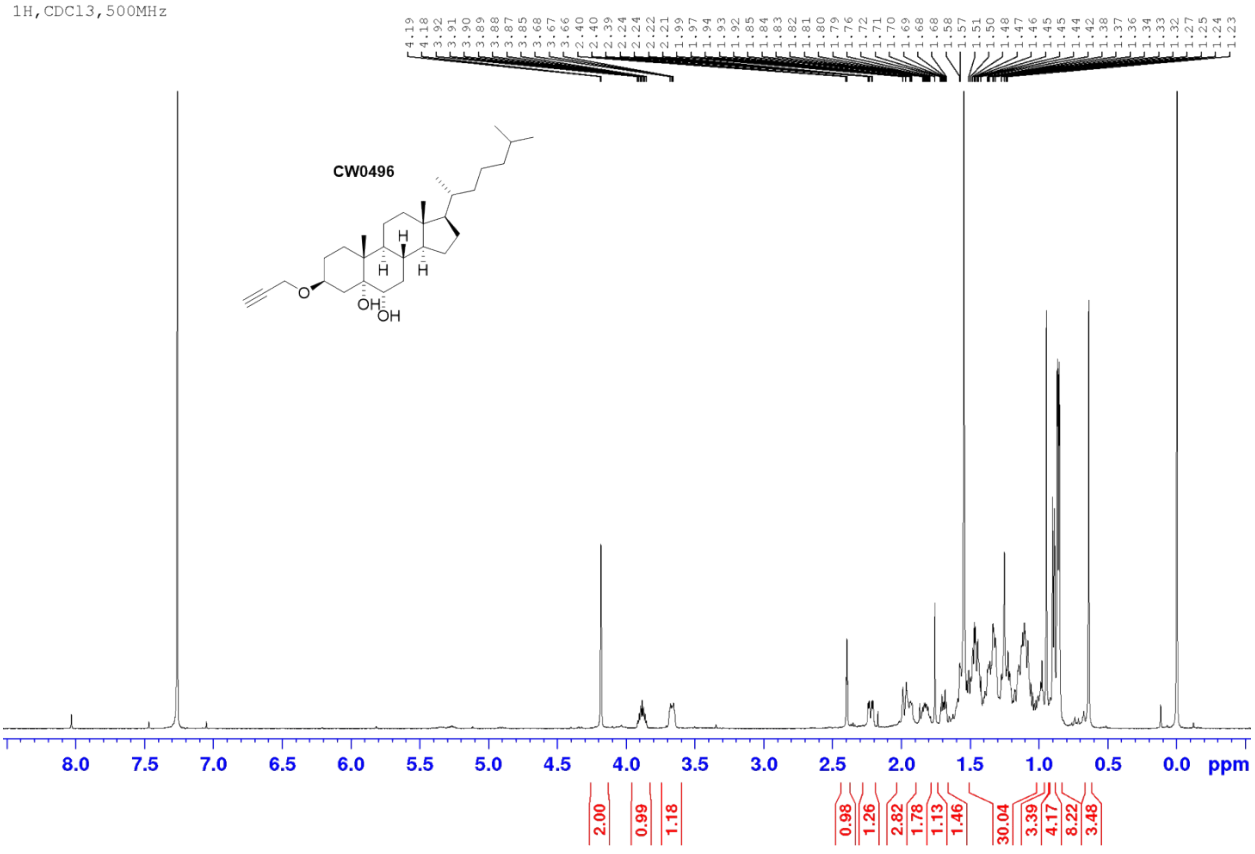


13C,CDCl3,125MHz

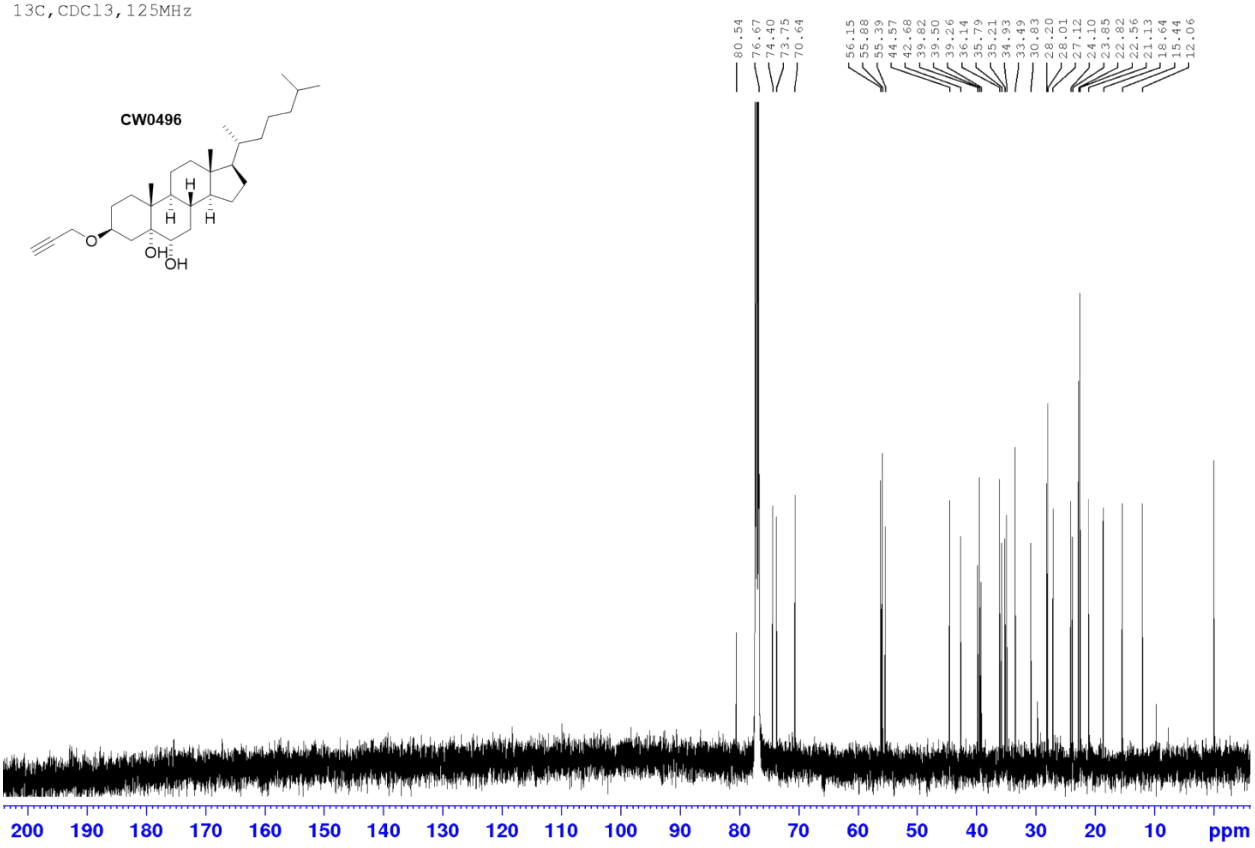



1H,CDCl3,500MHz
CW5134
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.02
2.04
1.00
1.94
1.04
5.65
13.17
13.59
3.95
6.39
3.22

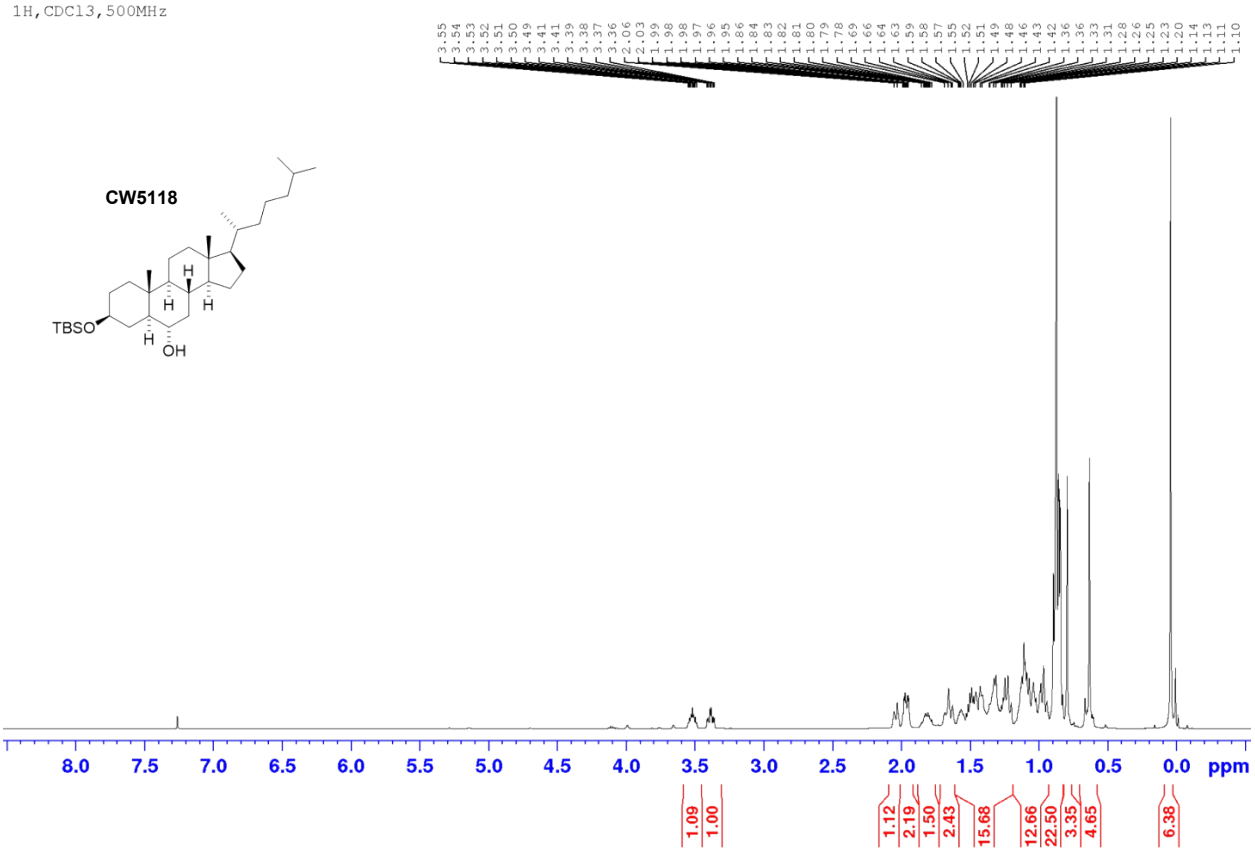

13C,CDCl3,125MHz
CW5134
140.57
121.89
80.44
78.19
73.76
56.77
56.15
55.08
50.15
42.32
39.78
39.52
38.72
37.13
36.82
36.19
35.78
31.94
31.87
28.23
28.07
28.01
24.29
23.82
22.82
22.57
21.07
19.34
18.72
11.86
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


1H,CDCl3,500MHz
CW0496
4.19
4.18
3.92
3.91
3.90
3.89
3.88
3.87
3.85
3.68
3.67
3.66
2.40
2.40
2.39
2.24
2.24
2.22
2.21
1.99
1.97
1.94
1.93
1.92
1.85
1.84
1.83
1.82
1.81
1.80
1.79
1.76
1.72
1.71
1.70
1.69
1.68
1.68
1.58
1.57
1.51
1.50
1.48
1.47
1.46
1.45
1.45
1.44
1.42
1.38
1.37
1.36
1.34
1.33
1.32
1.27
1.25
1.24
1.23
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.00
0.99
1.18
0.98
1.26
2.82
1.78
1.13
1.46
30.04
3.39
4.17
8.22
3.48

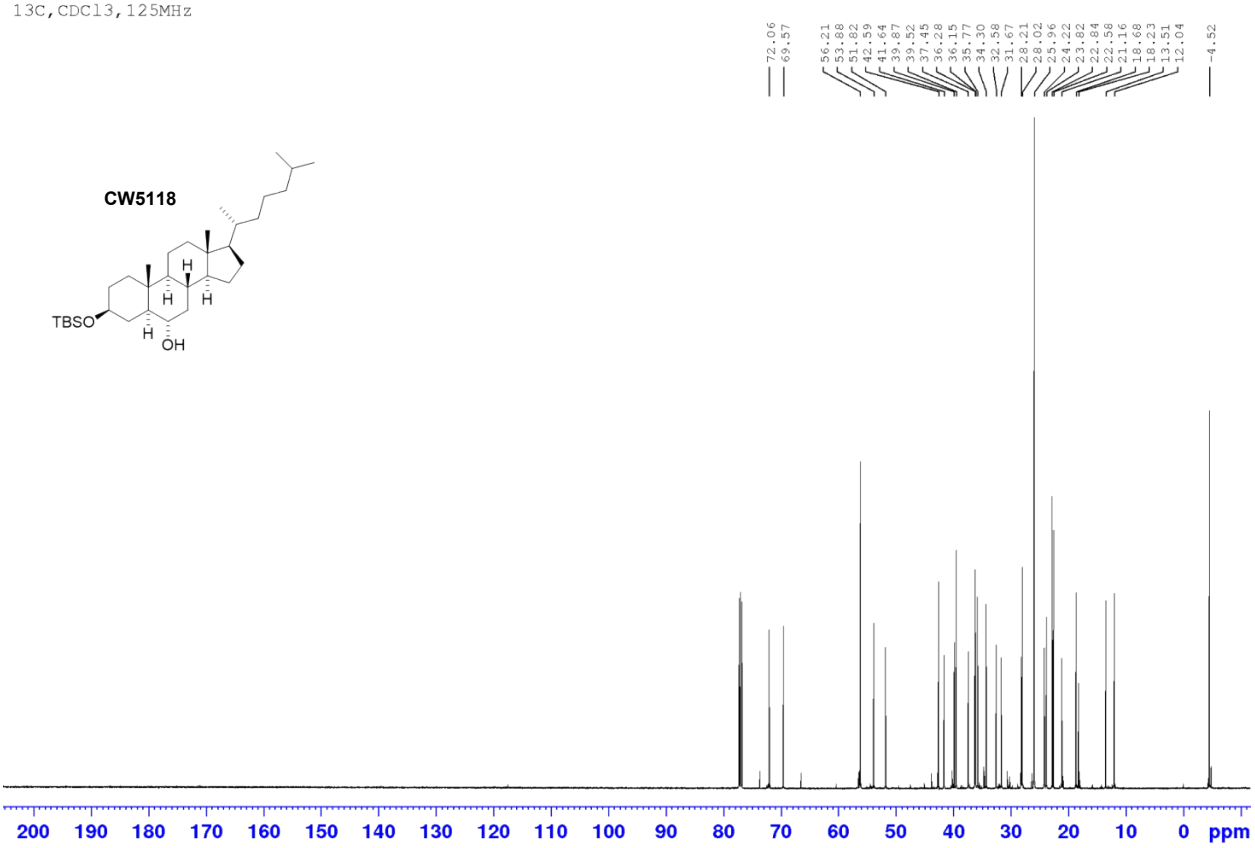
13C,CDCl3,125MHz



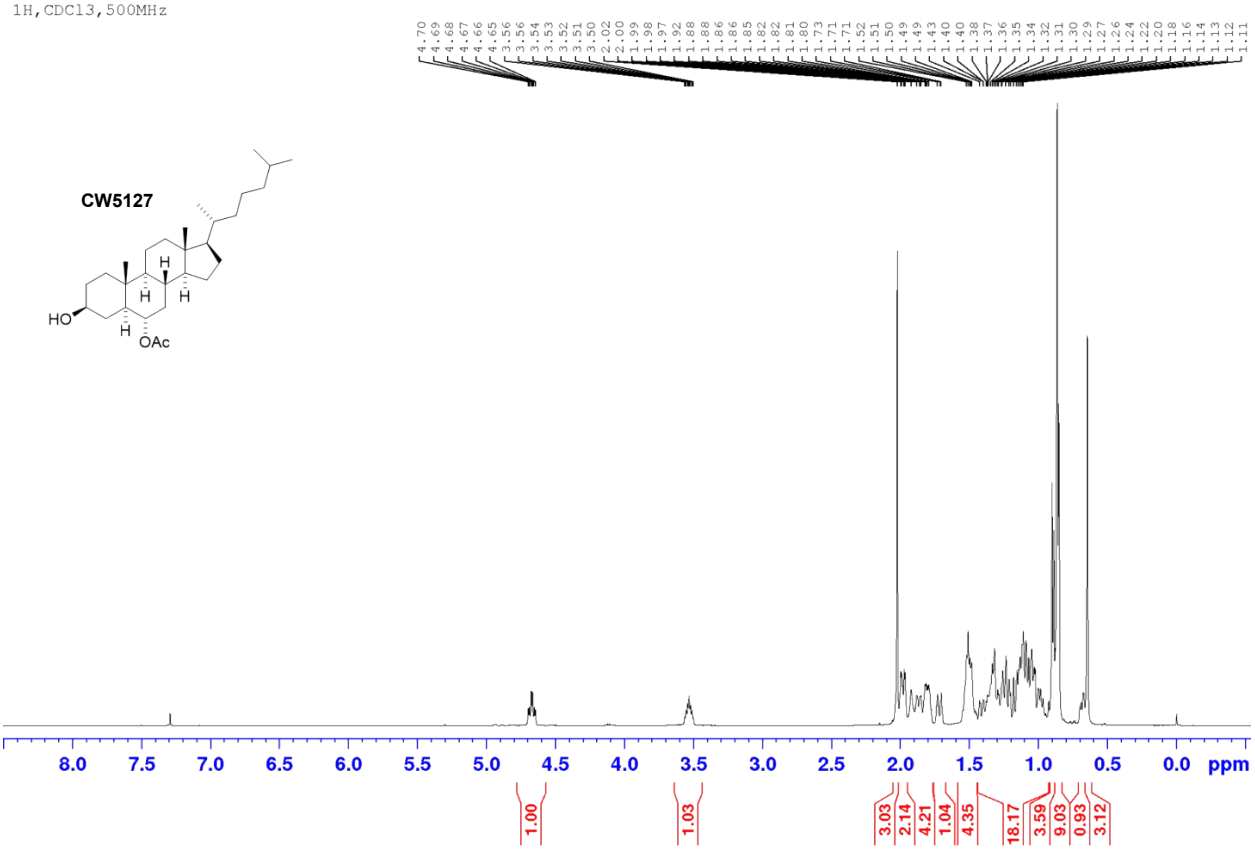
1H,CDCl3,500MHz

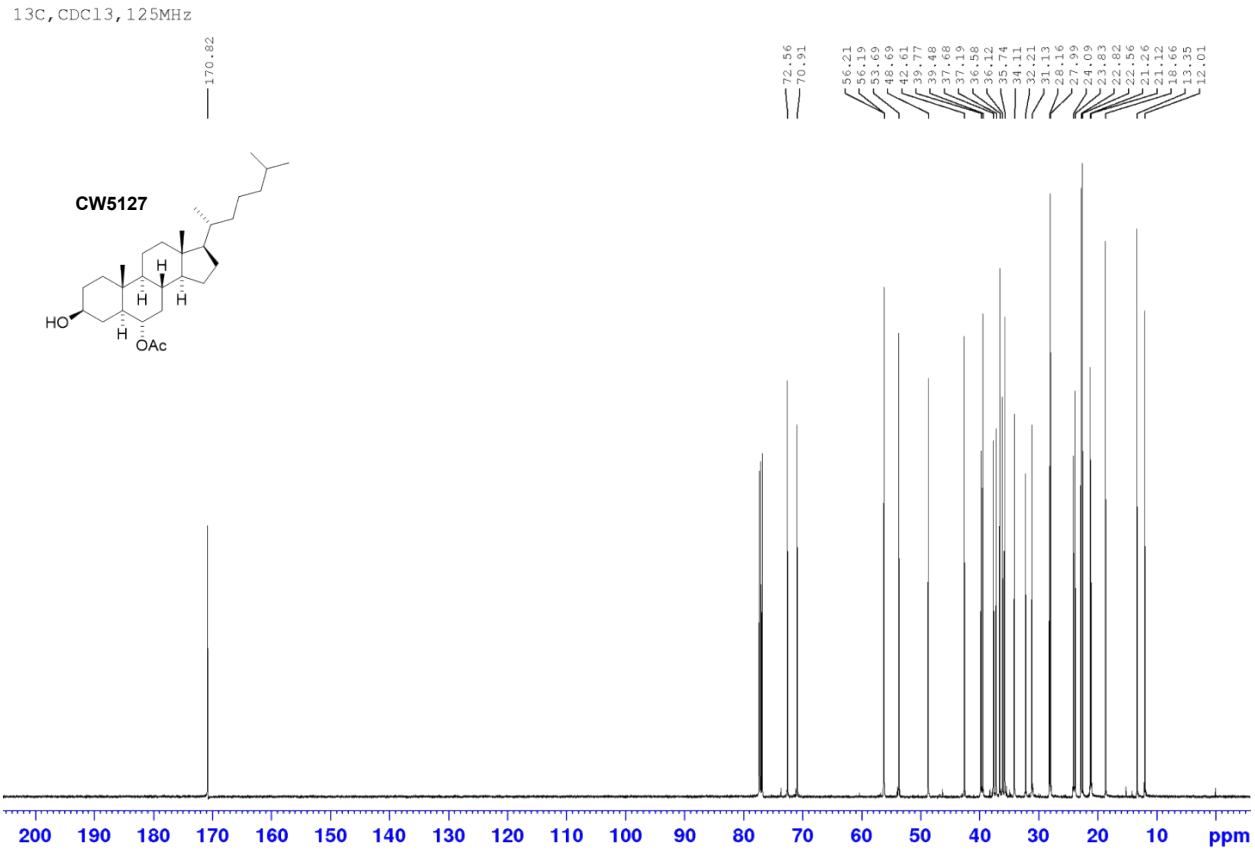


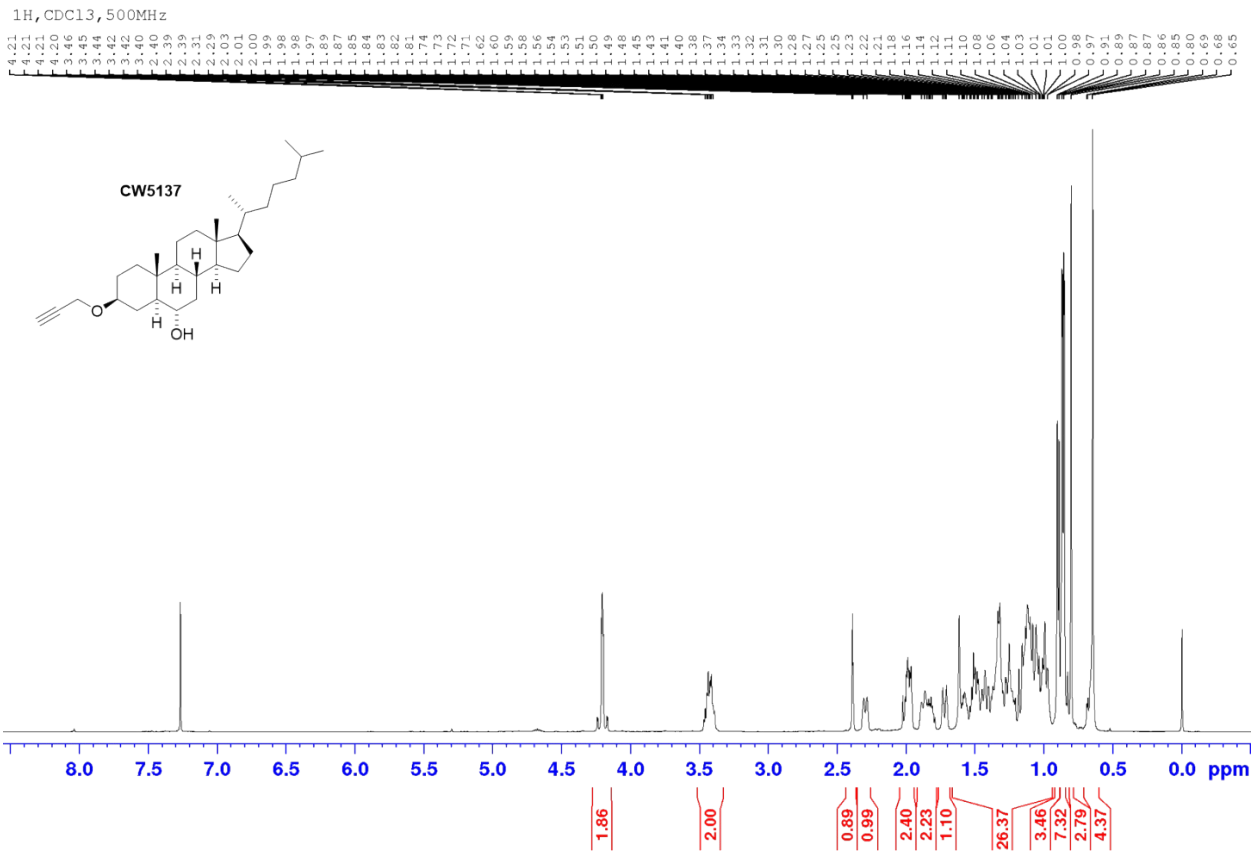
13C,CDCl3,125MHz



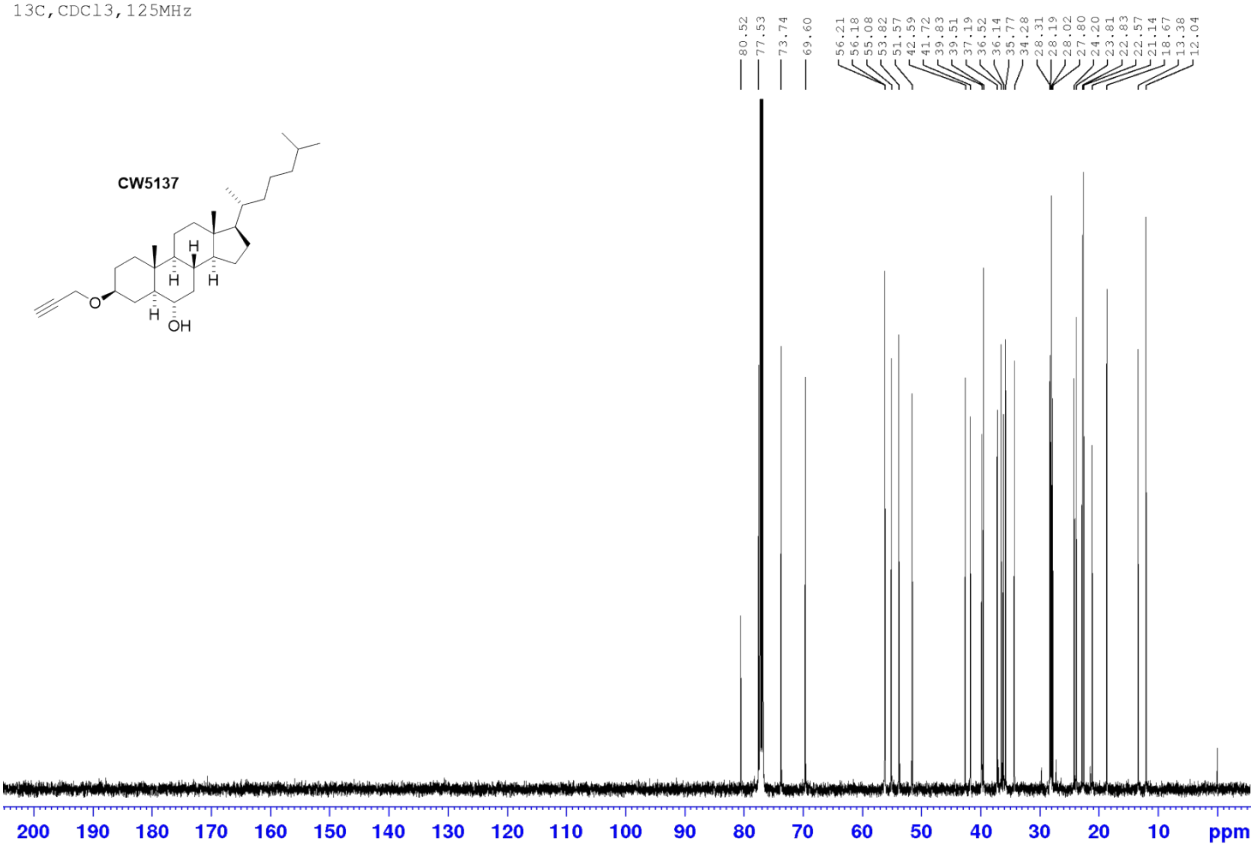
1H,CDCl3,500MHz



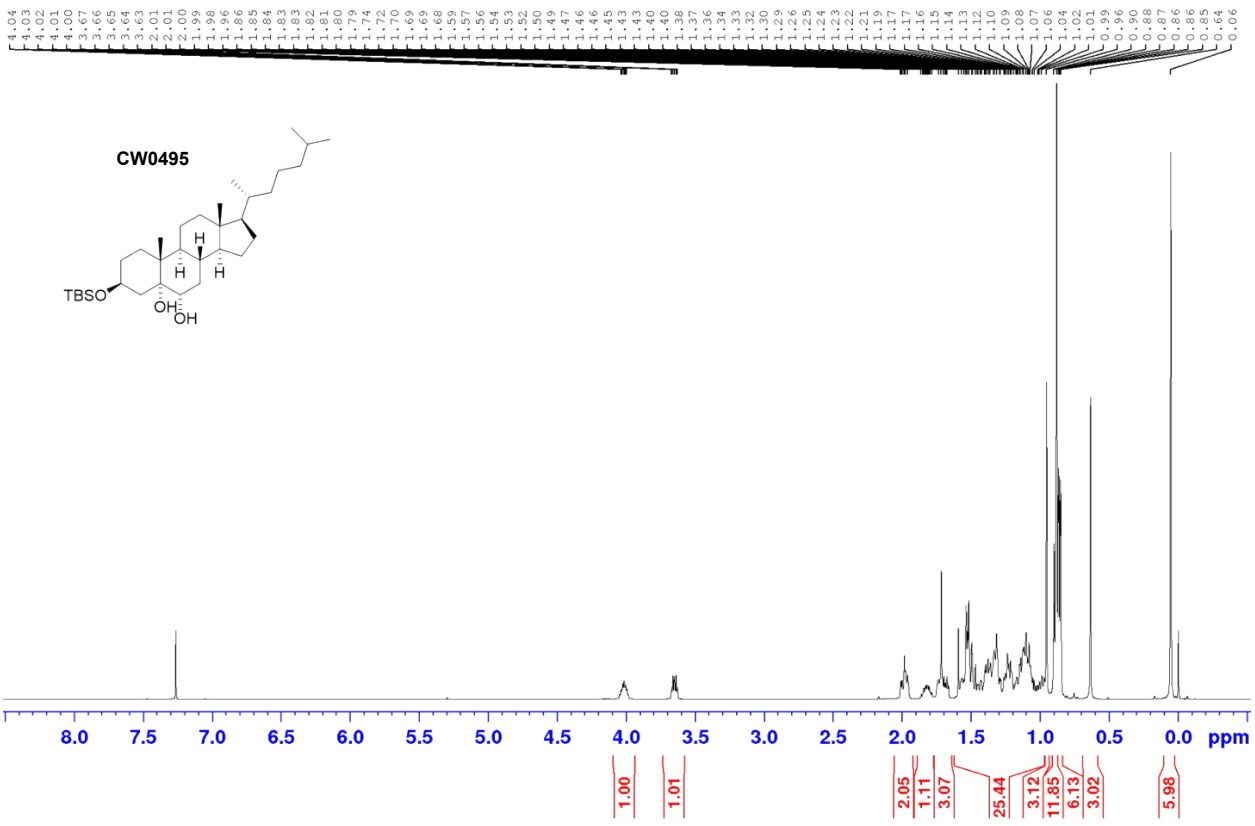

13C,CDCl3,125MHz
CW5127
HO
OAc
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


1H,CDCl3,500MHz
CW5137
OH
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.86
2.00
0.89
0.99
2.40
2.23
1.10
26.37
3.46
7.32
2.79
4.37

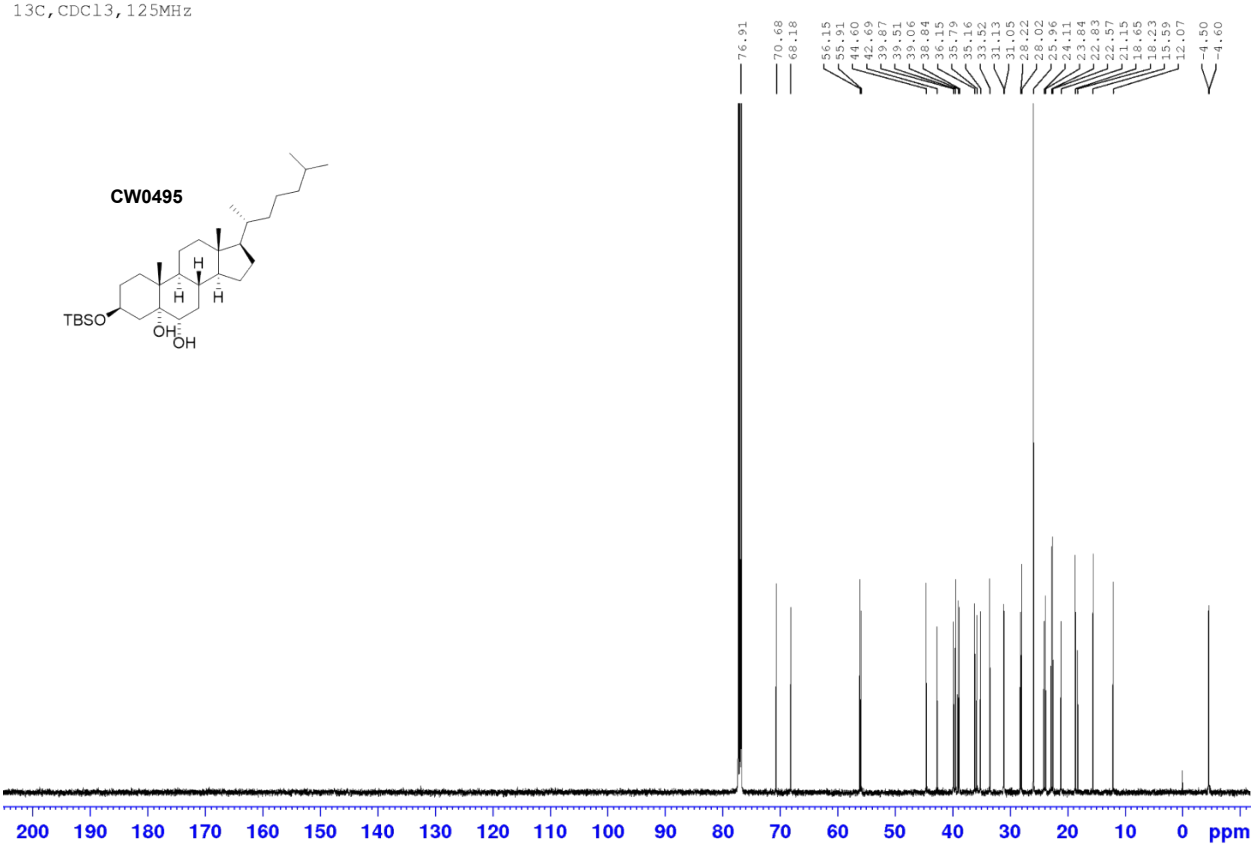
13C,CDCl3,125MHz



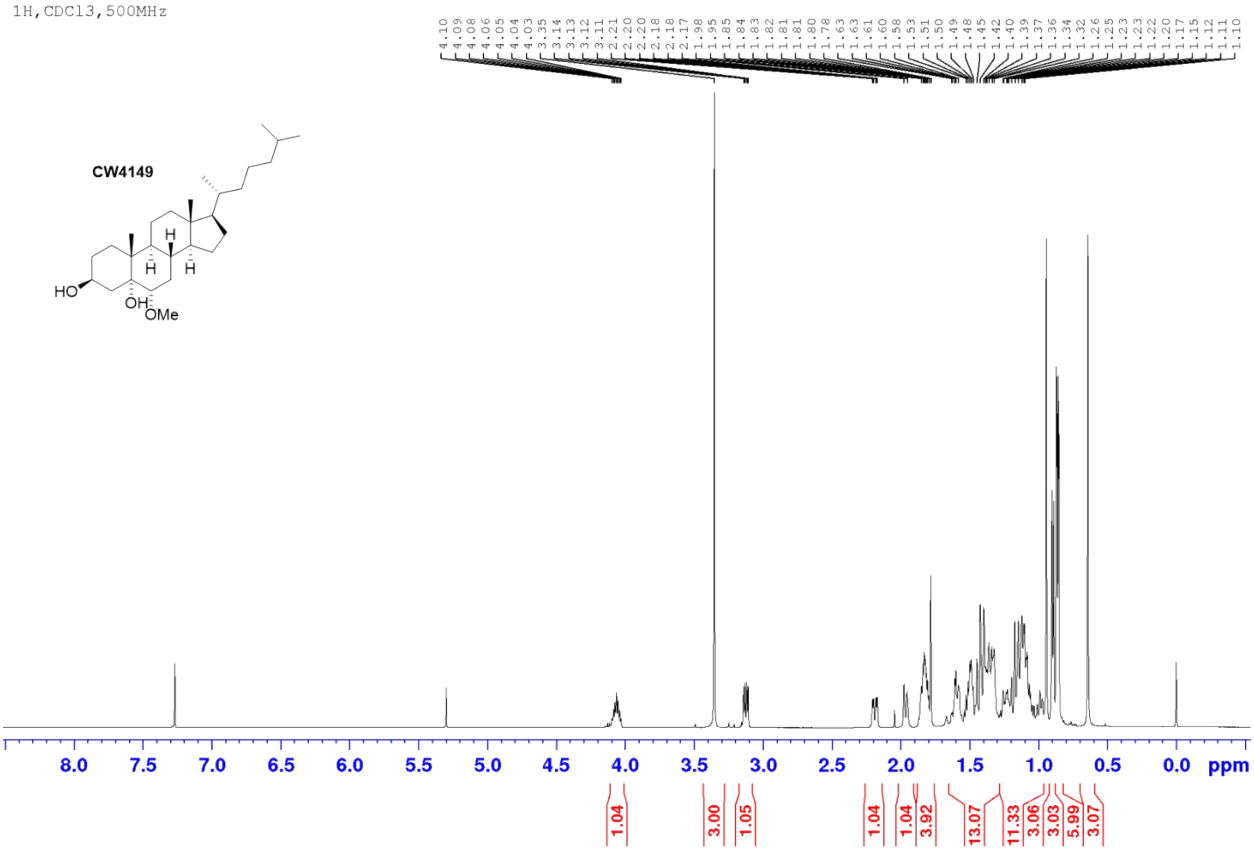
1H,CDCl3,500MHz

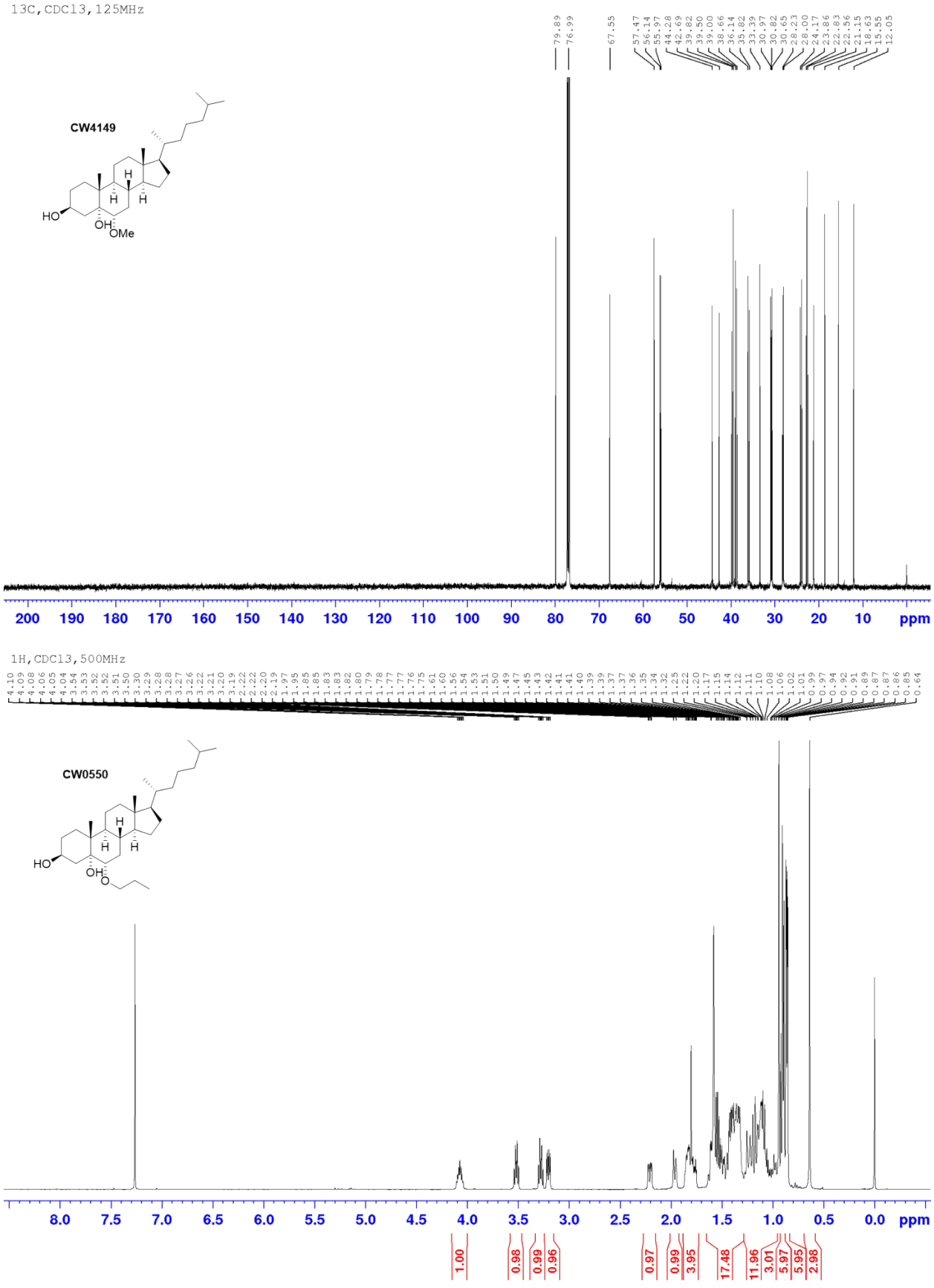


13C,CDCl3,125MHz

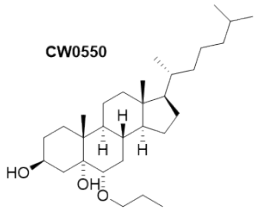


1H,CDCl3,500MHz

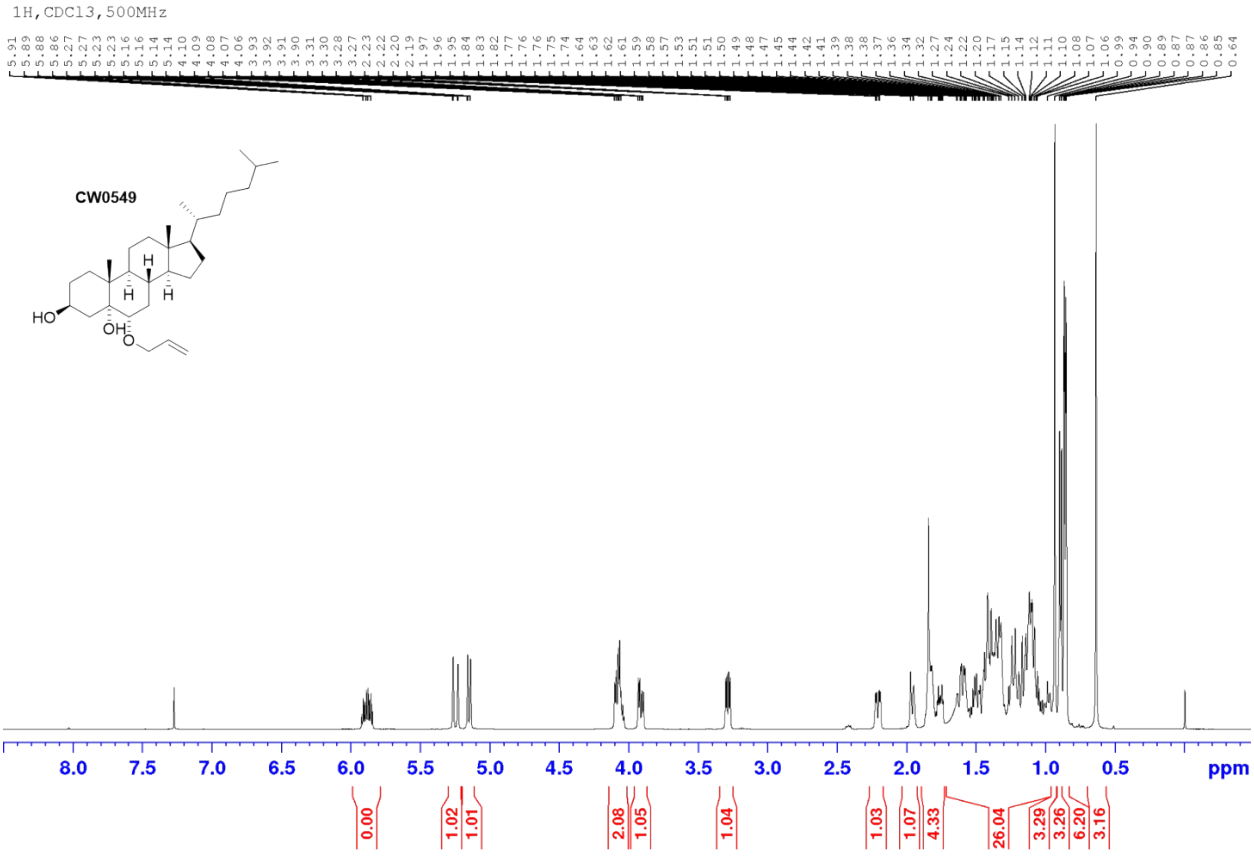


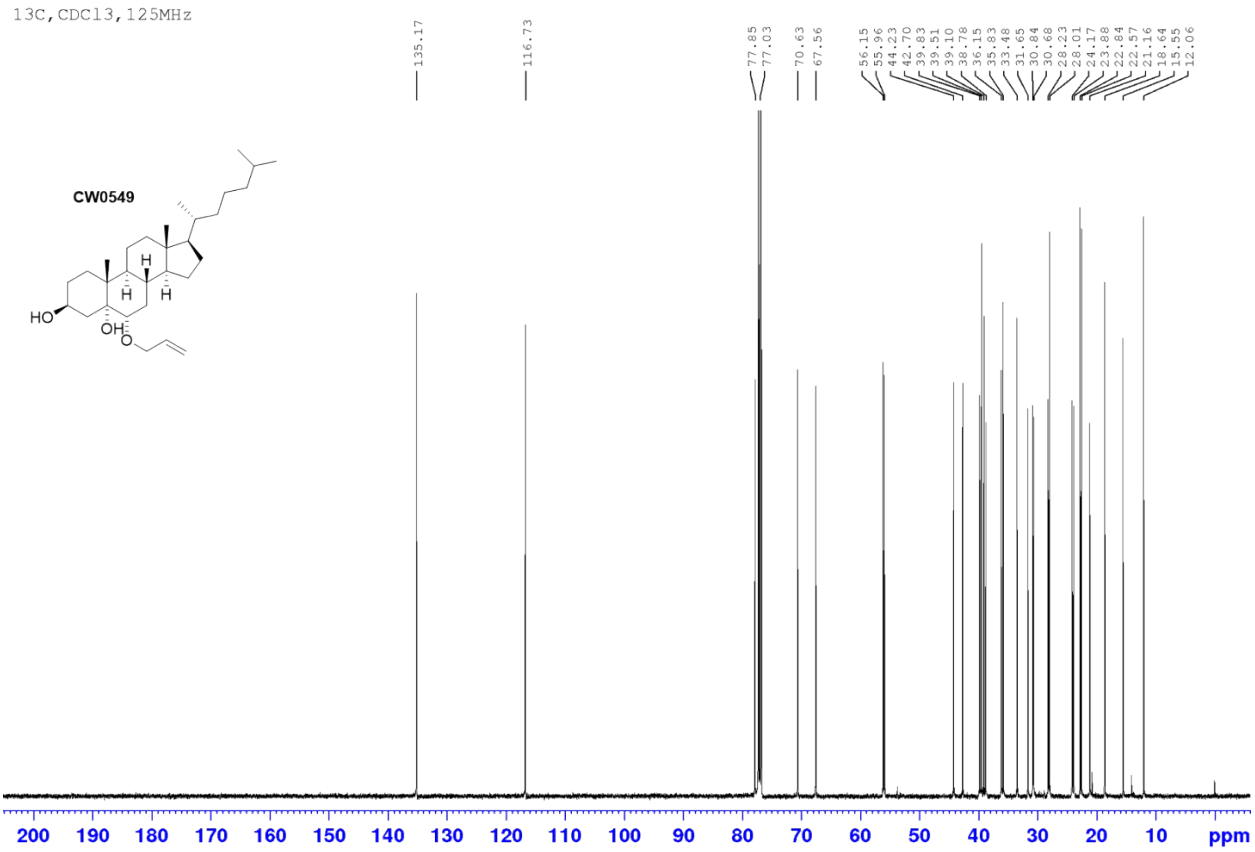

13C,CDCl3,125MHz
CW4149
HO
OH
OMe
79.89
76.99
67.55
57.47
56.14
55.97
44.28
42.69
39.82
39.50
39.00
38.66
36.14
35.82
33.39
30.97
30.82
30.65
28.23
28.00
24.17
23.86
22.83
22.56
21.15
18.63
15.55
12.05
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
1H,CDCl3,500MHz
CW0550
HO
OH
O
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
0.98
0.99
0.96
0.97
0.99
3.95
17.48
11.96
3.01
5.97
5.95
2.98

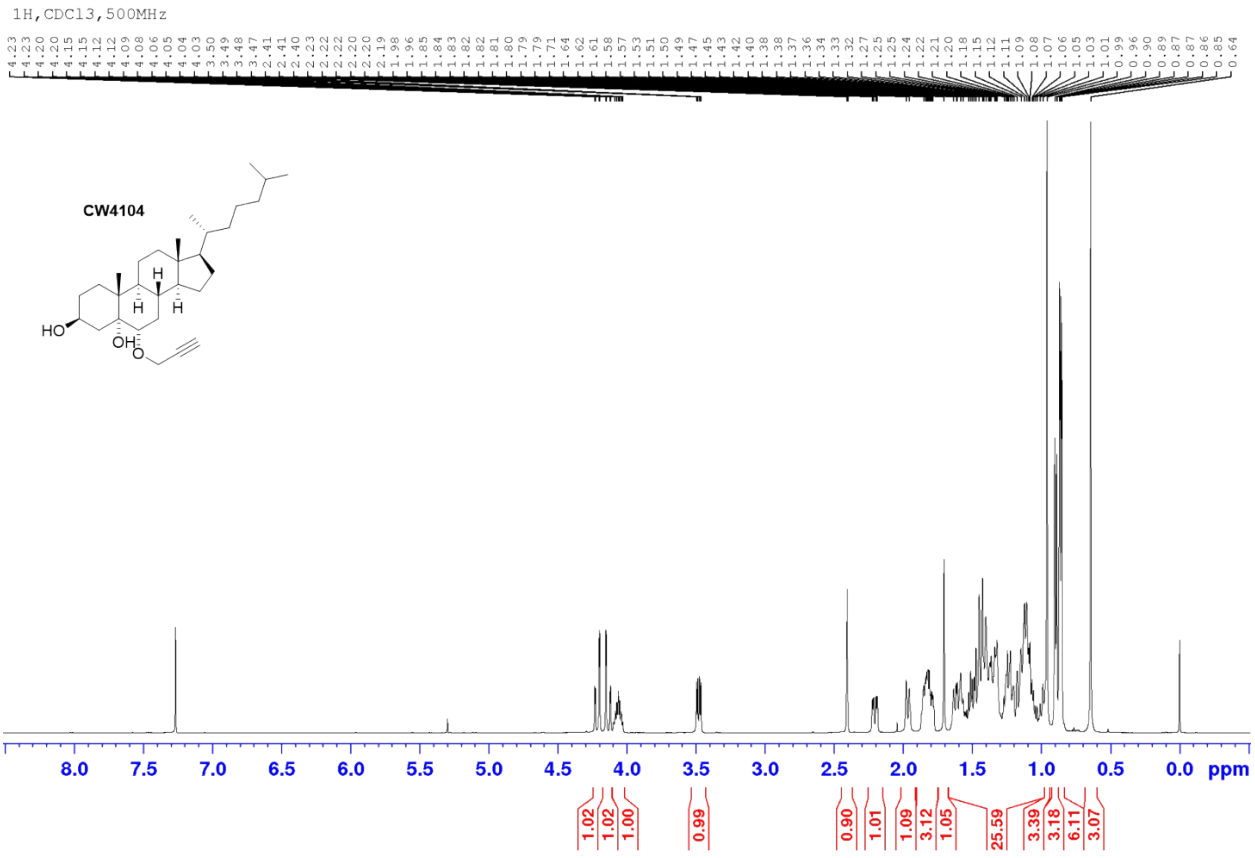
13C,CDCl3,125MHz

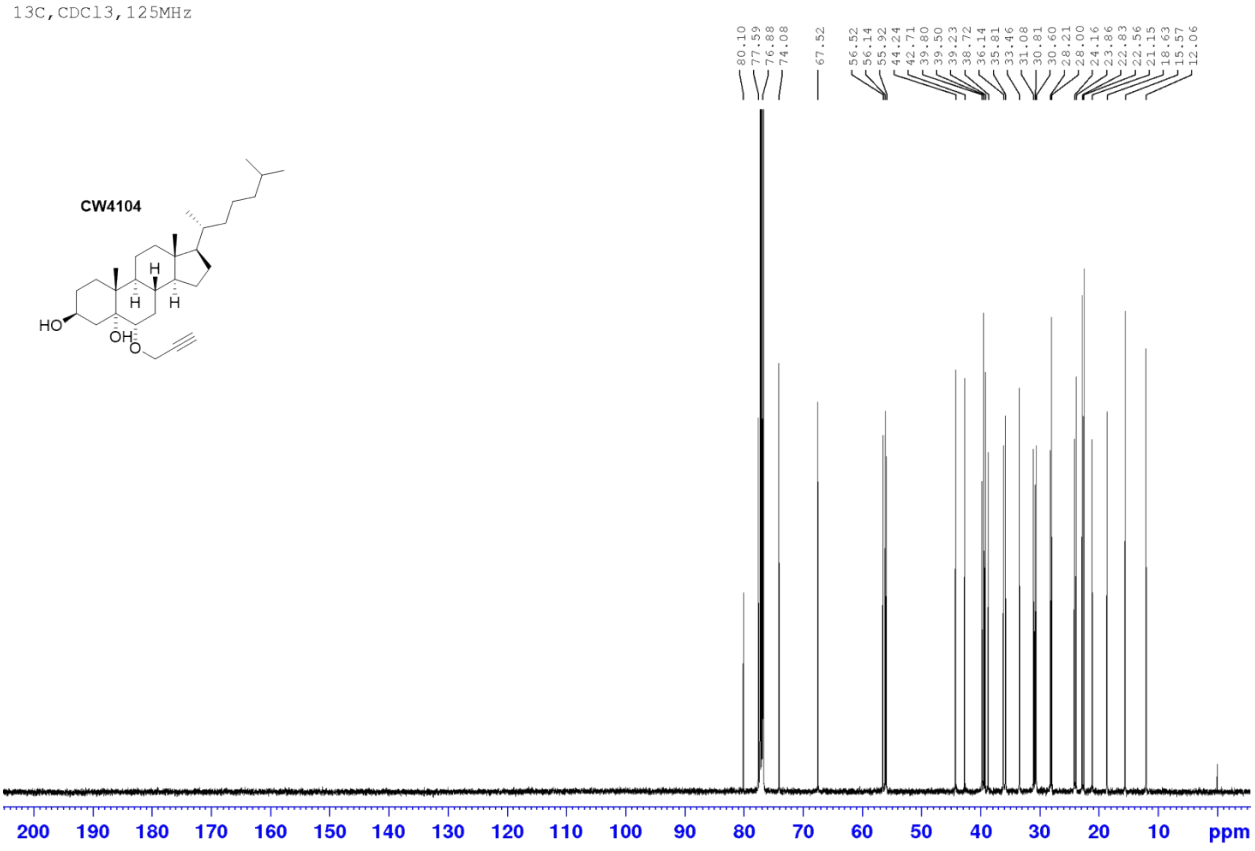


1H,CDCl3,500MHz

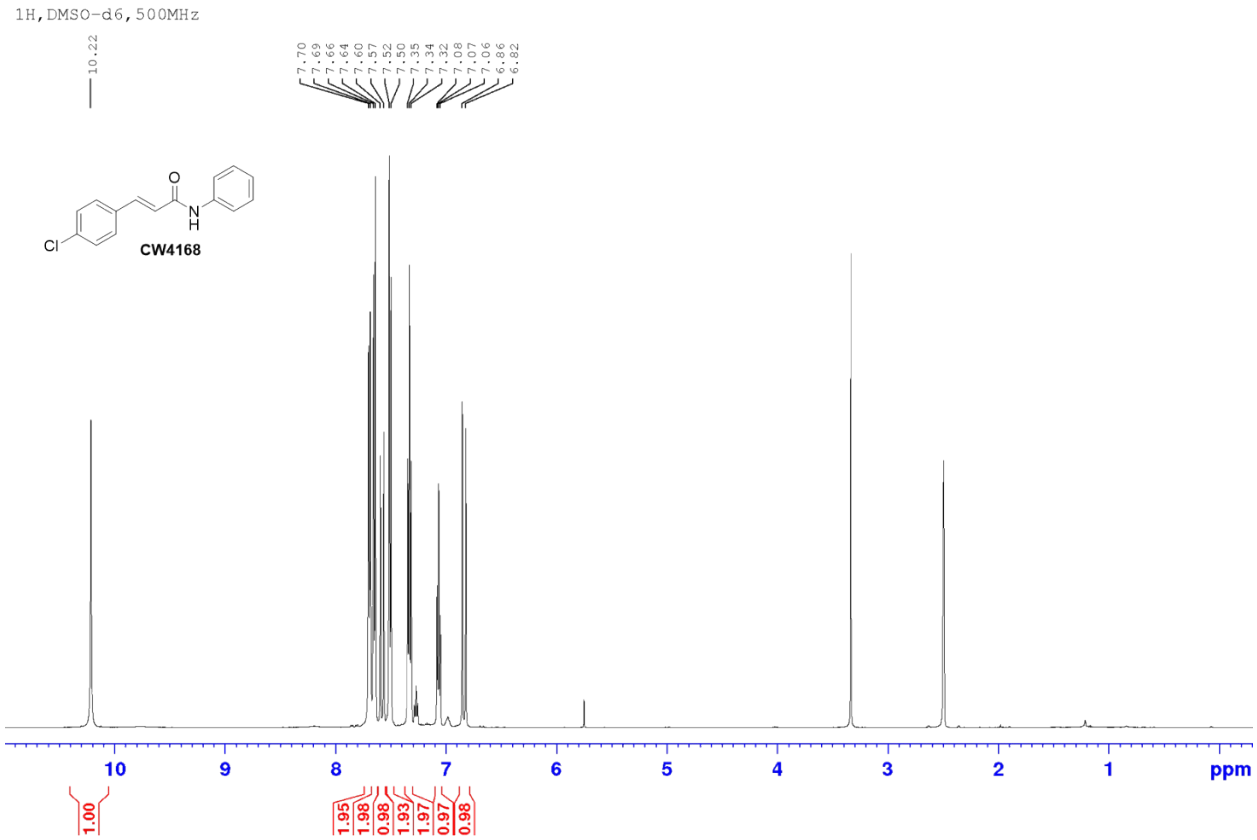



13C,CDCl3,125MHz
CW0549
135.17
116.73
77.85
77.03
70.63
67.56
56.15
55.96
44.23
42.70
39.83
39.51
39.10
38.78
36.15
35.83
33.48
31.65
30.84
30.68
28.23
28.01
24.17
23.88
22.84
22.57
21.16
18.64
15.55
12.06
HO
OH
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

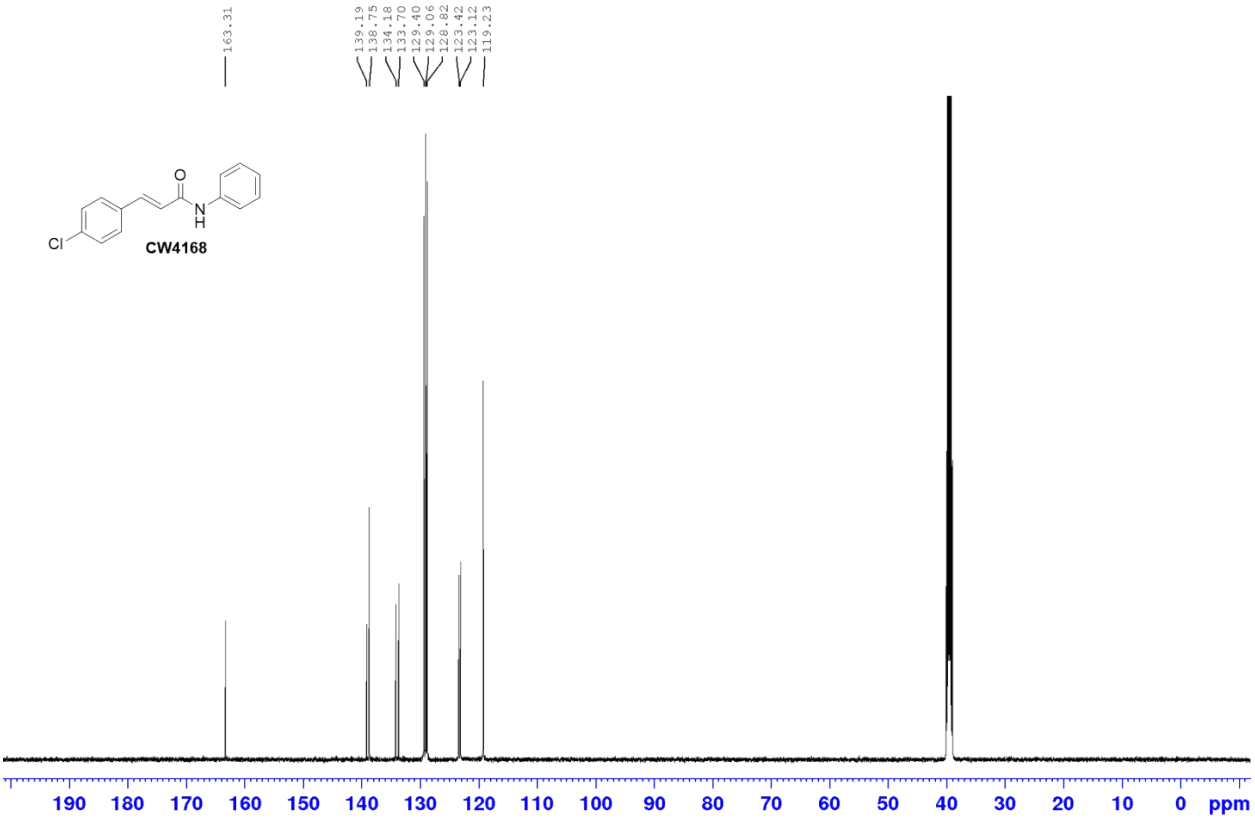

1H,CDCl3,500MHz
CW4104
HO
OH
O
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.02
1.02
1.00
0.99
0.90
1.01
1.09
3.12
1.05
25.59
3.39
3.18
6.11
3.07


13C,CDCl3,125MHz
80.10
77.59
76.88
74.08
67.52
56.52
56.14
55.92
44.24
42.71
39.80
39.50
39.23
38.72
36.14
35.81
33.46
31.08
30.81
30.60
28.21
28.00
24.16
23.86
22.83
22.56
21.15
18.63
15.57
12.06
CW4104
HO
OH
O
H
H
H
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

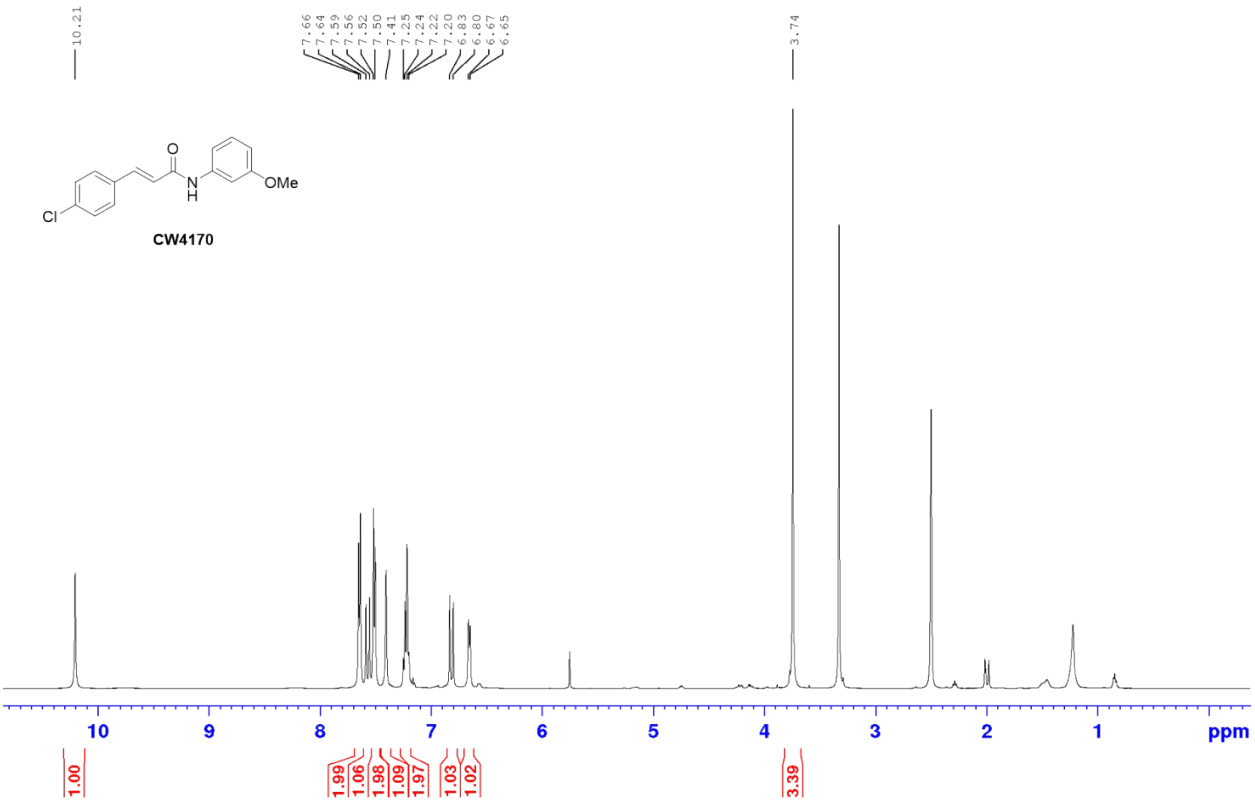
HSD17B7 Inhibitors



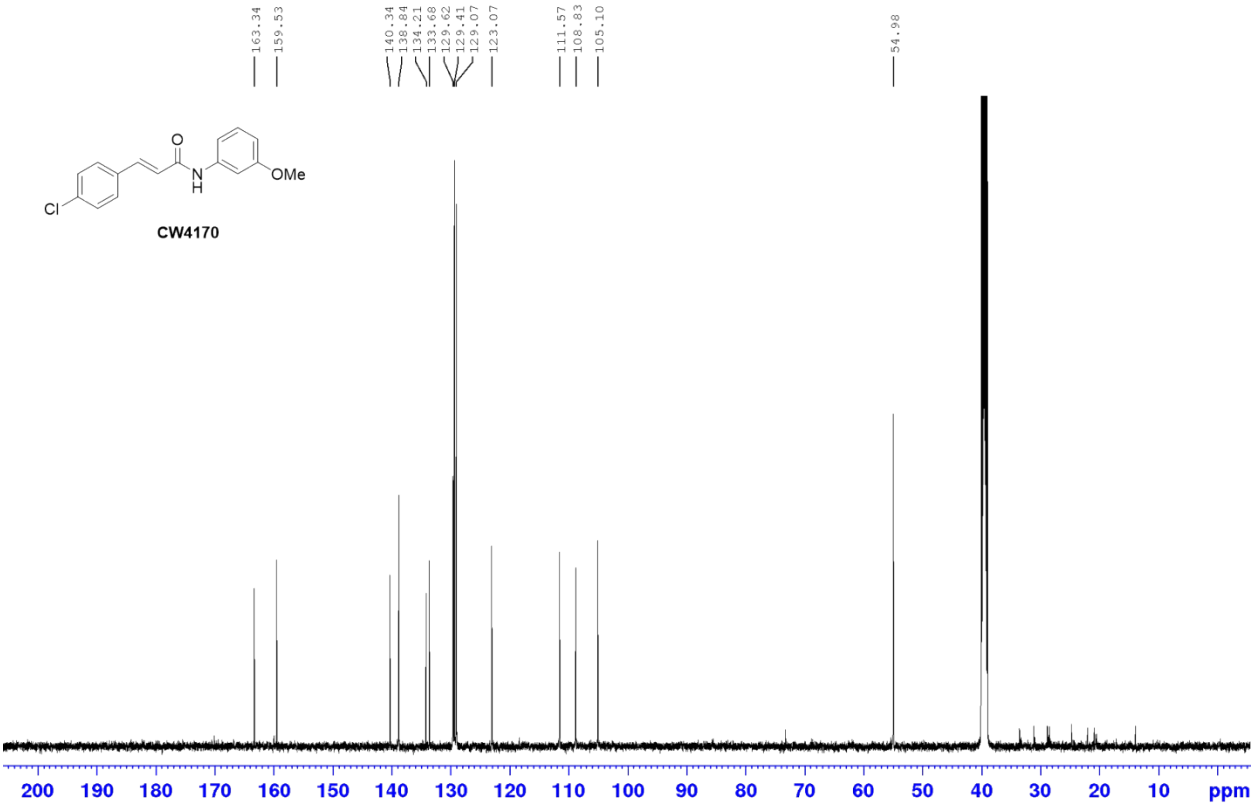
13C,DMSO-d6,125MHz



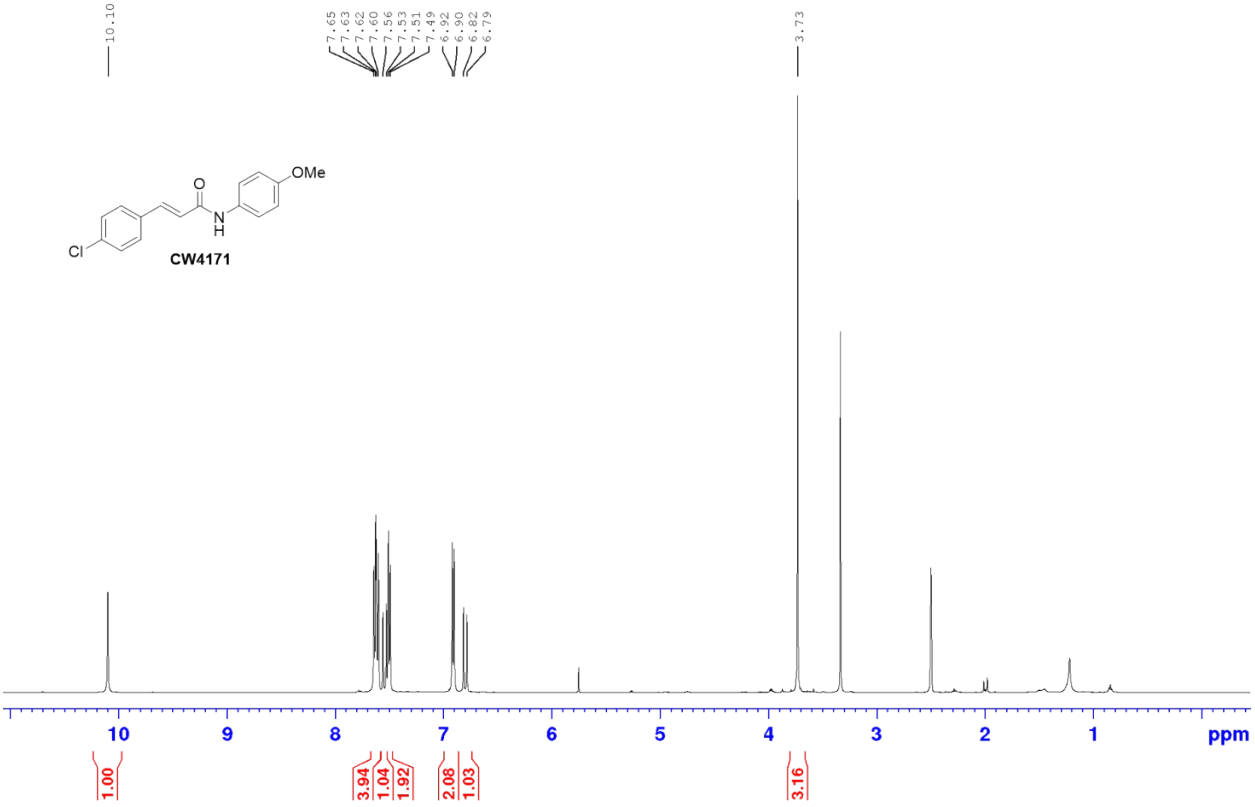
1H,DMSO-d6,500MHz



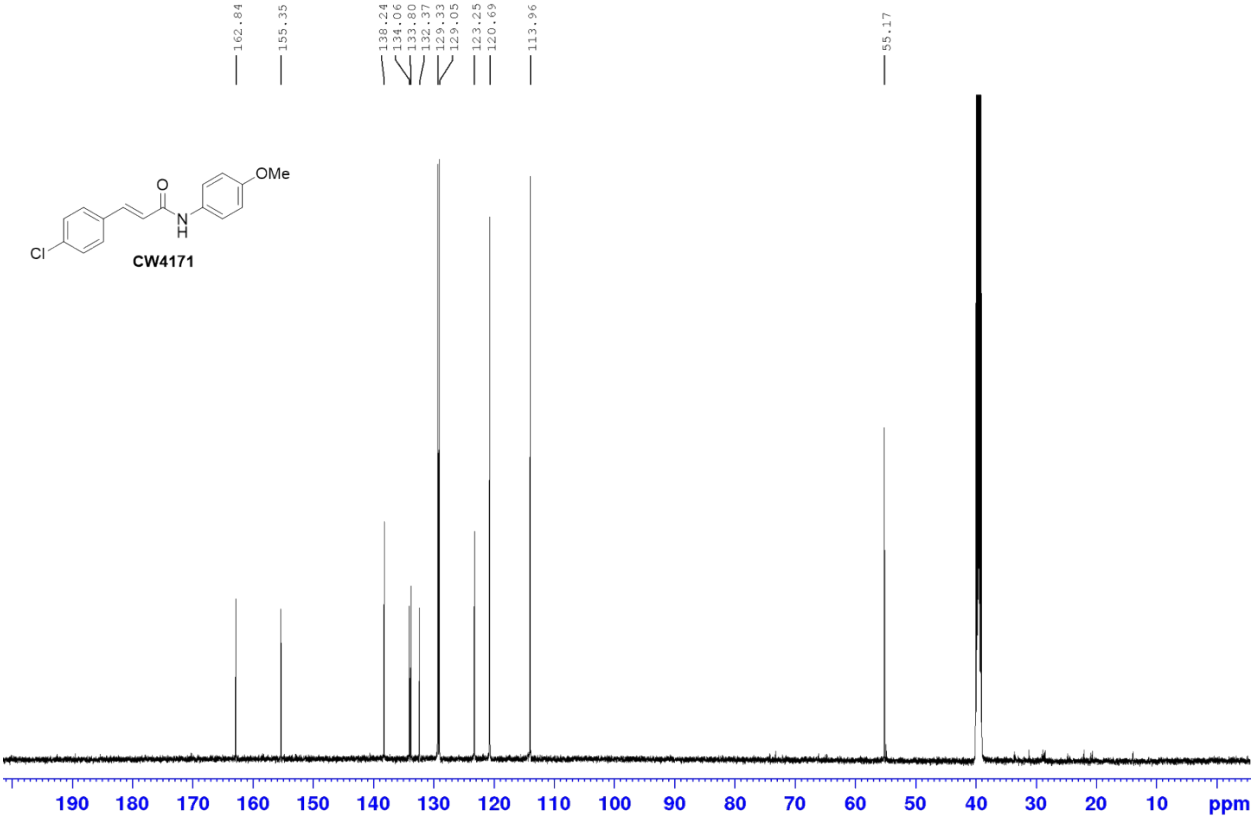
13C,DMSO-d6,125MHz



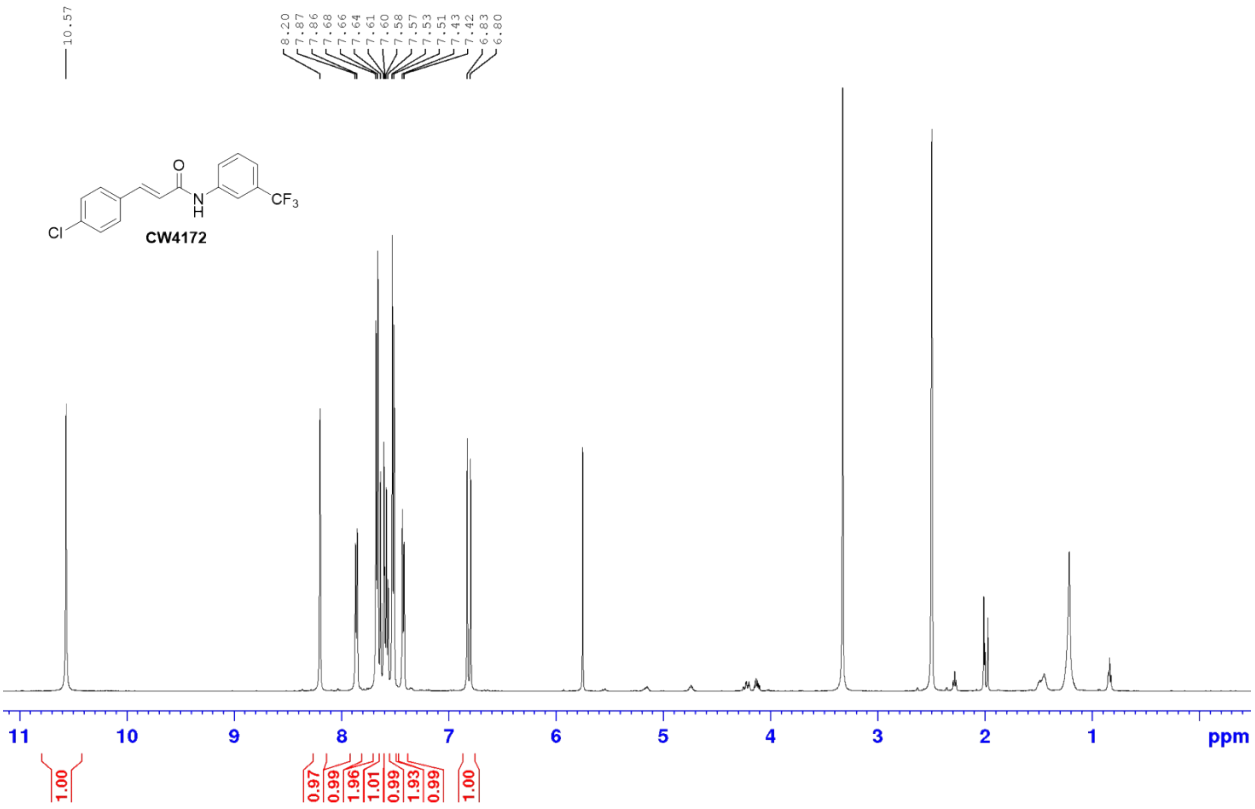
1H,DMSO-d6,500MHz



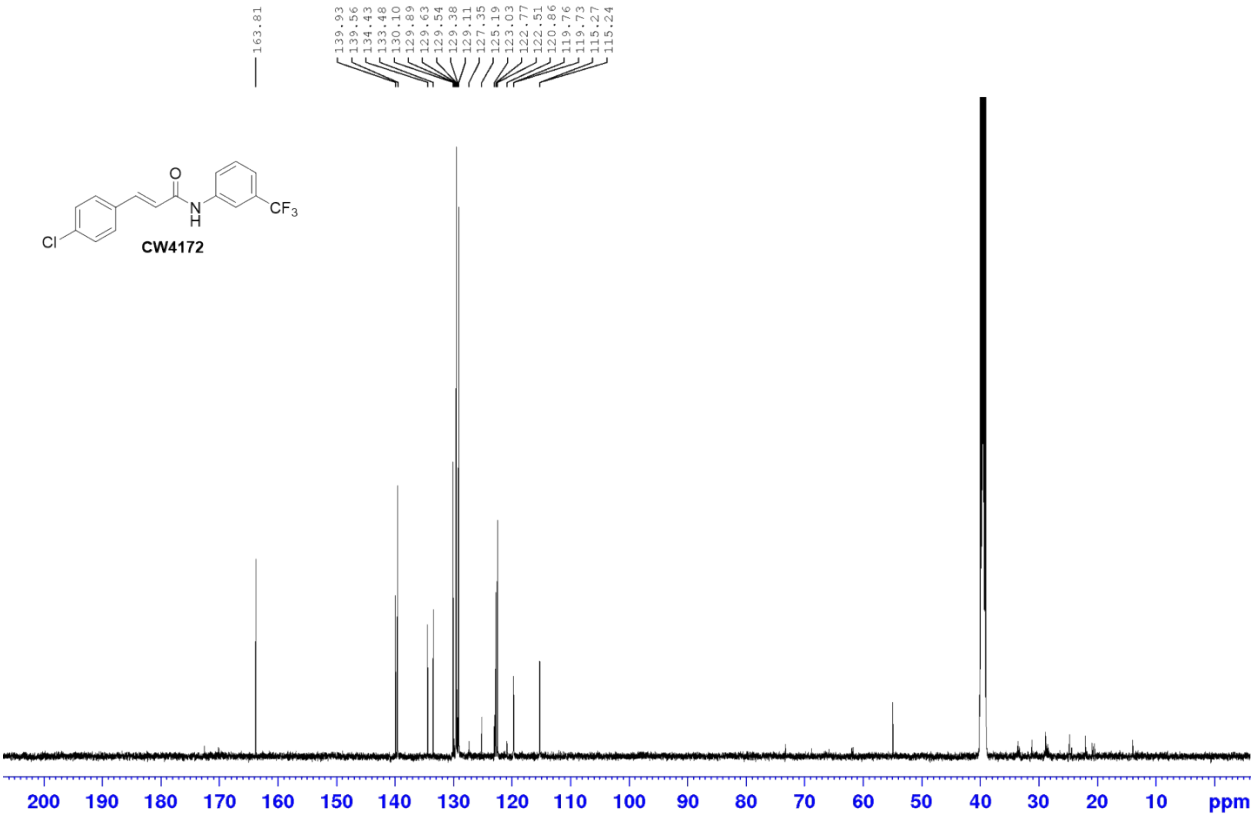
13C,DMSO-d6,125MHz



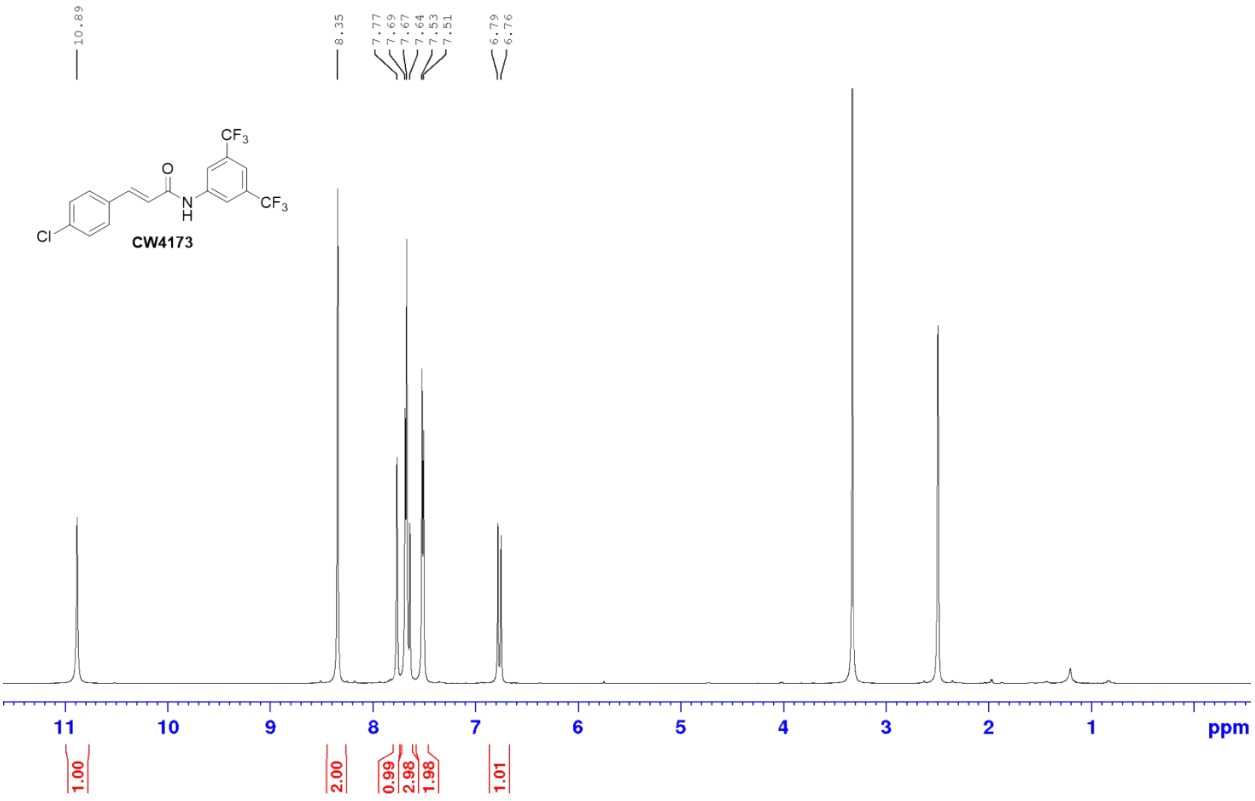
1H,DMSO-d6,500MHz



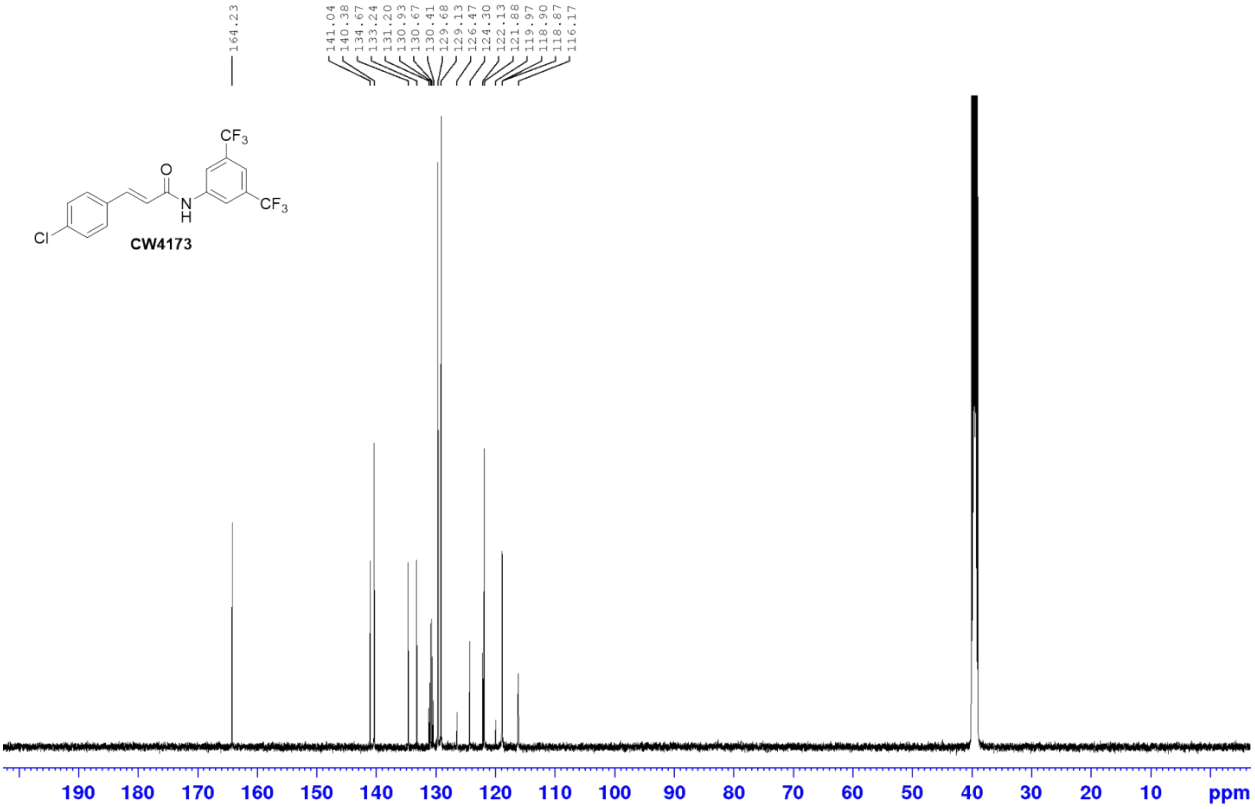
13C,DMSO-d6,125MHz



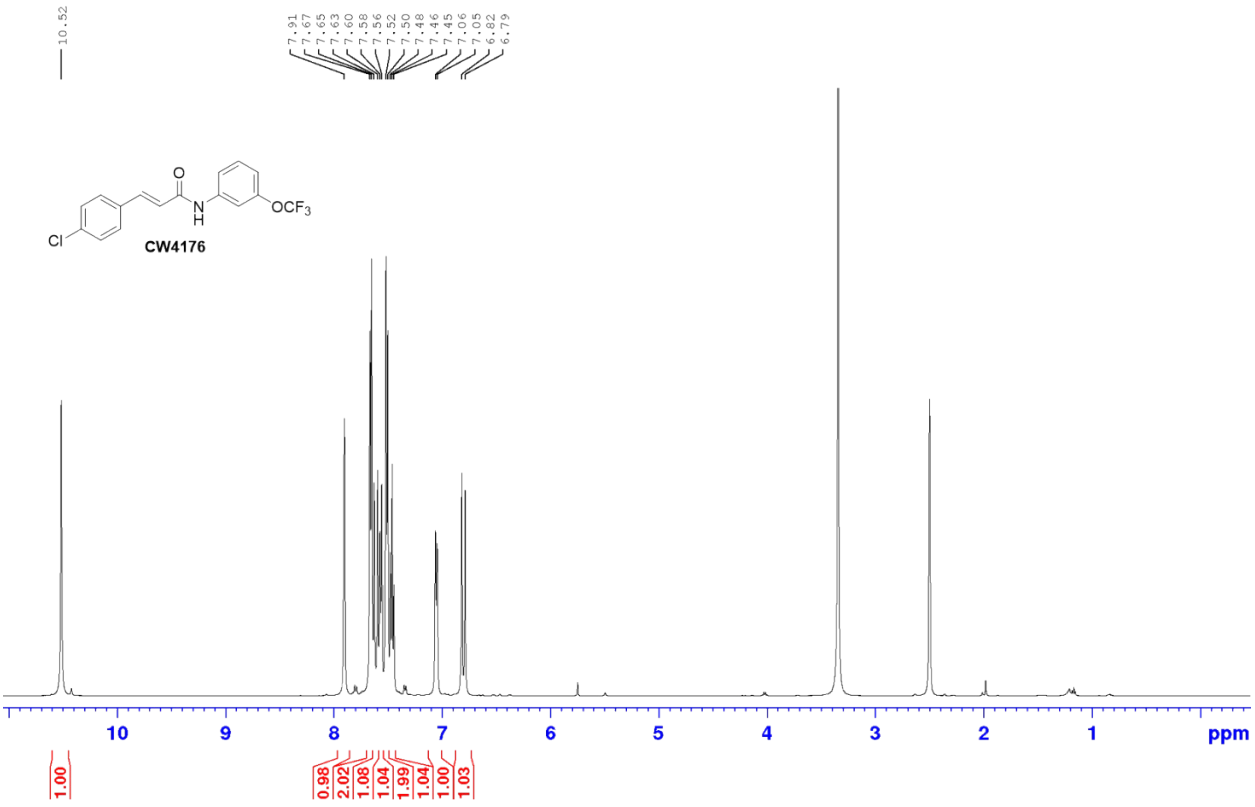
1H,DMSO-d6,500MHz



13C,DMSO-d6,125MHz



1H,DMSO-d6,500MHz



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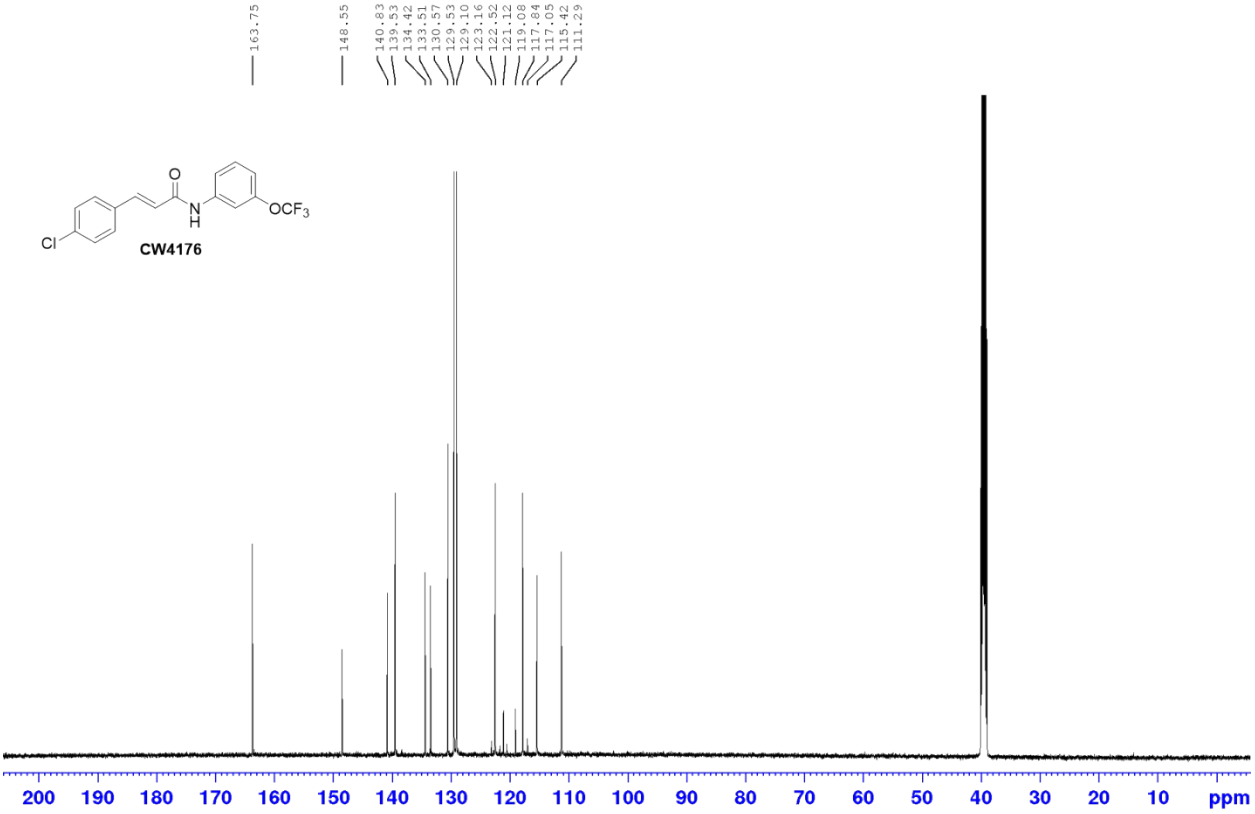

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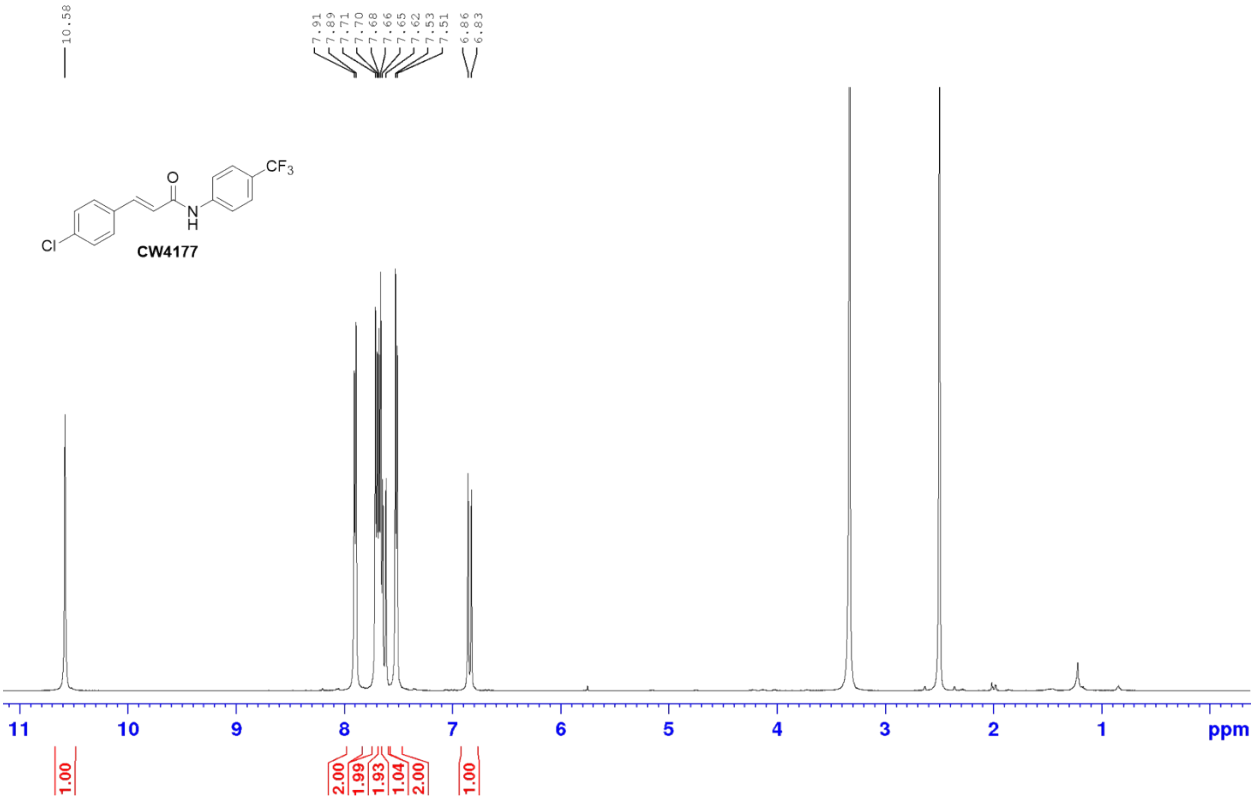

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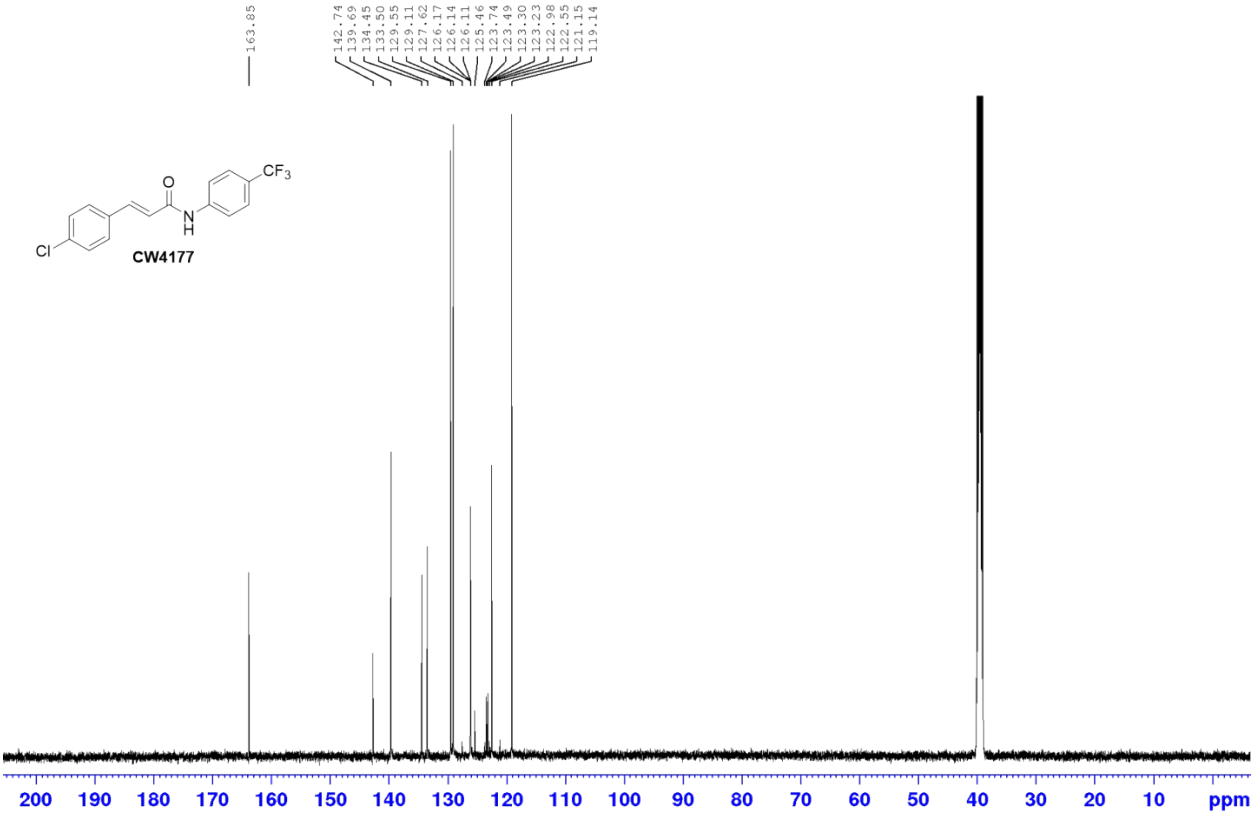

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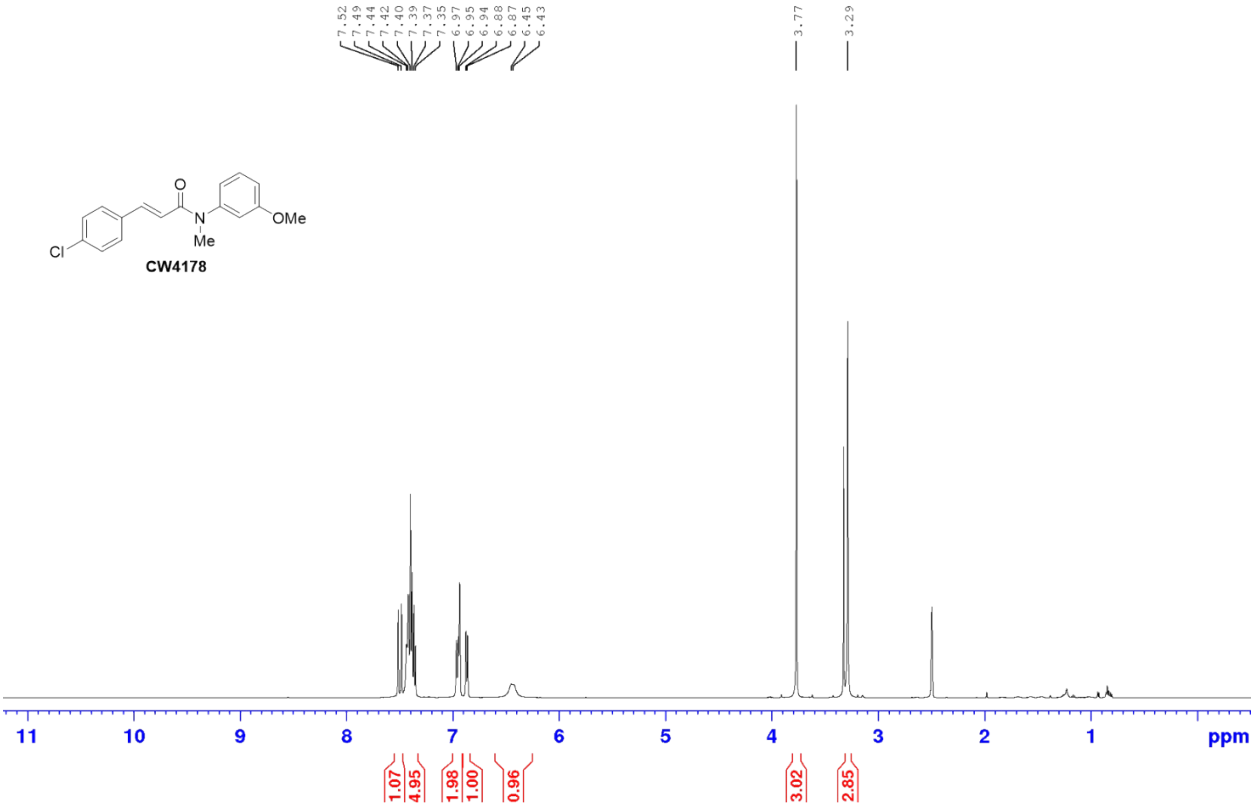
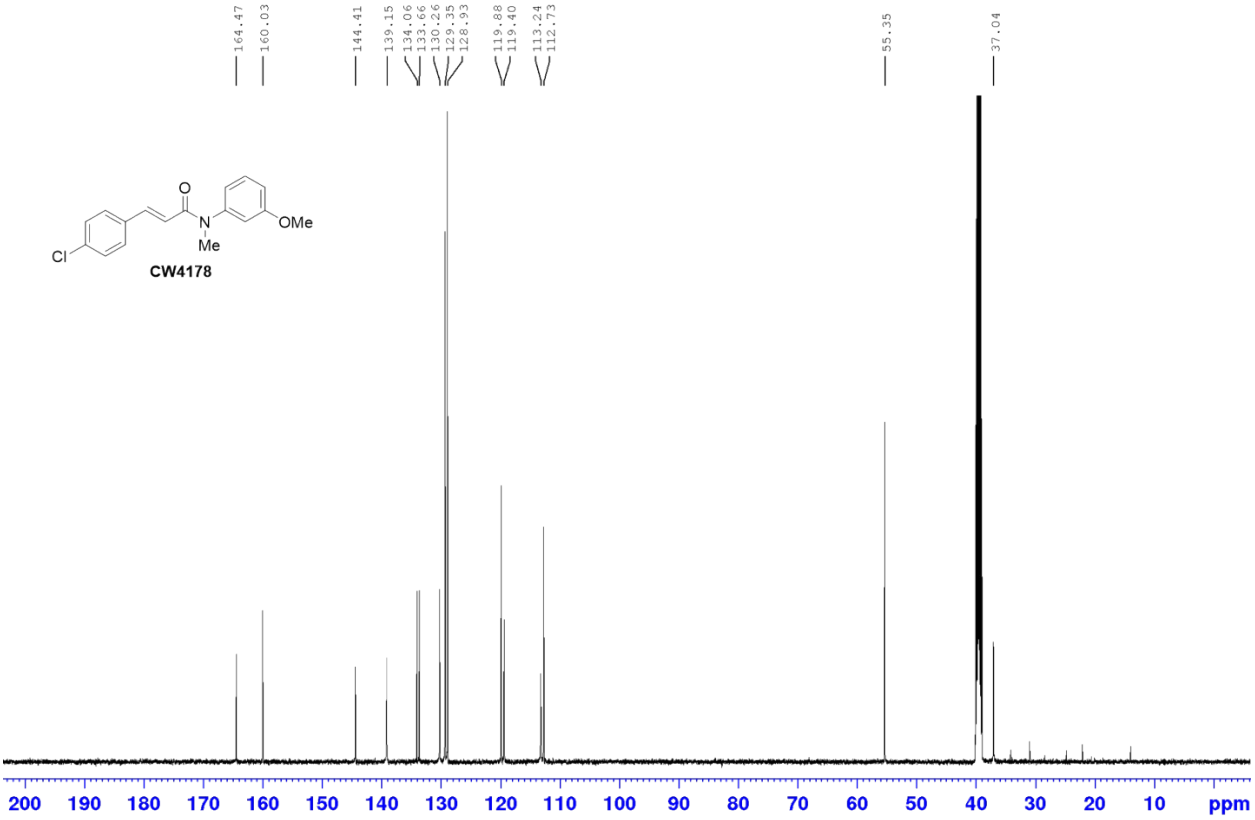


13C,DMSO-d6,125MHz



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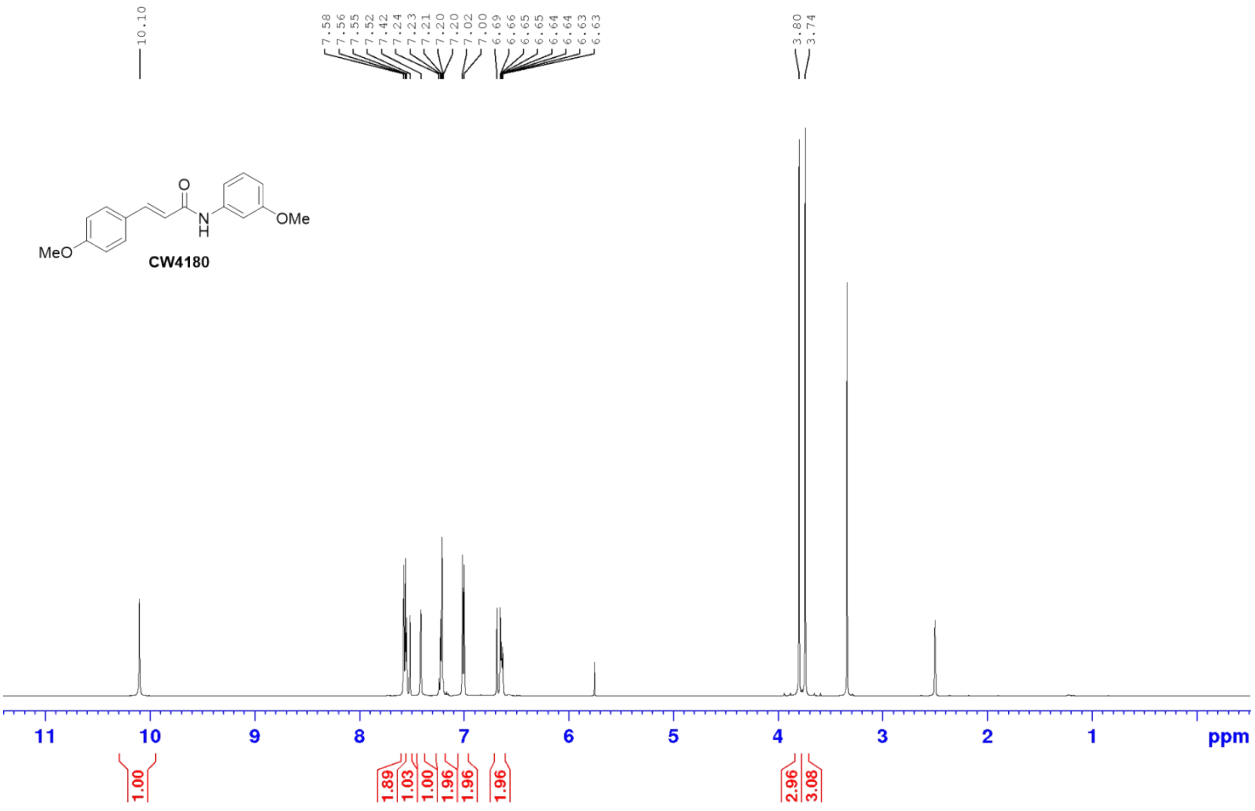

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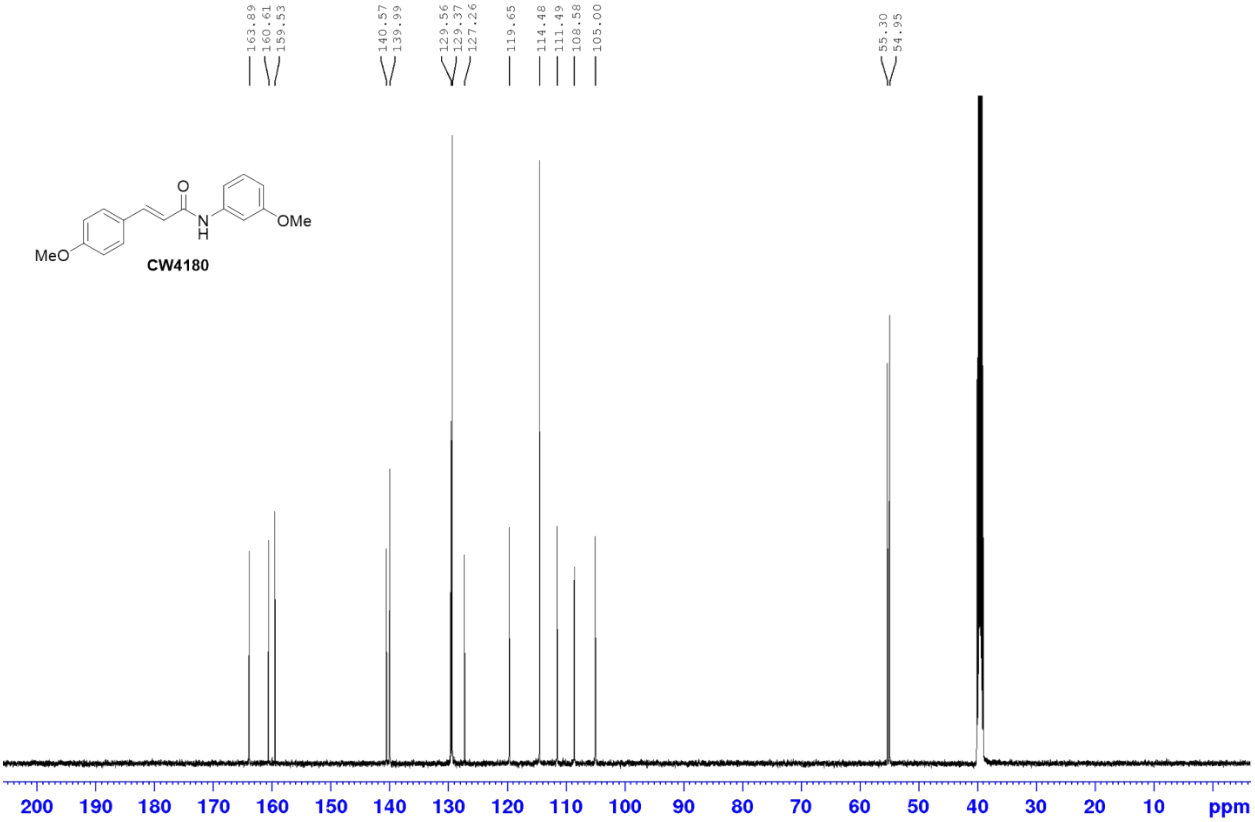

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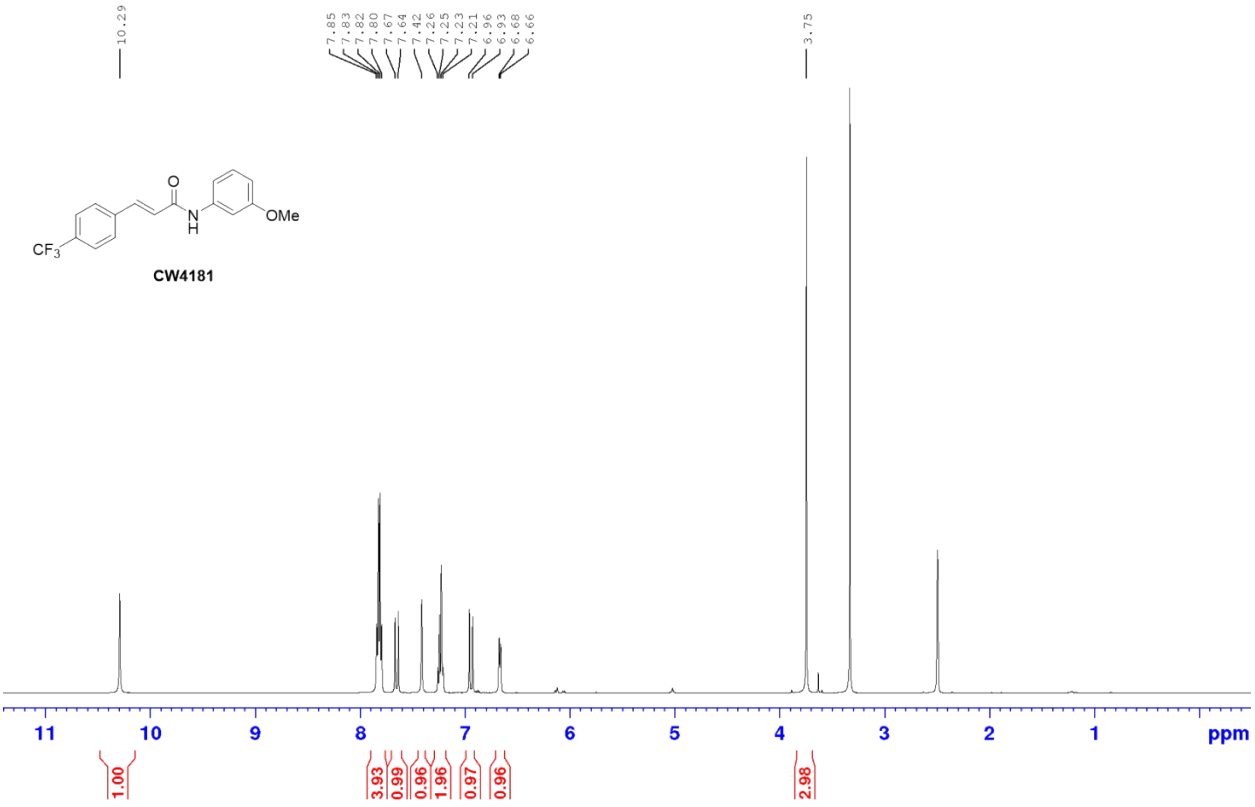

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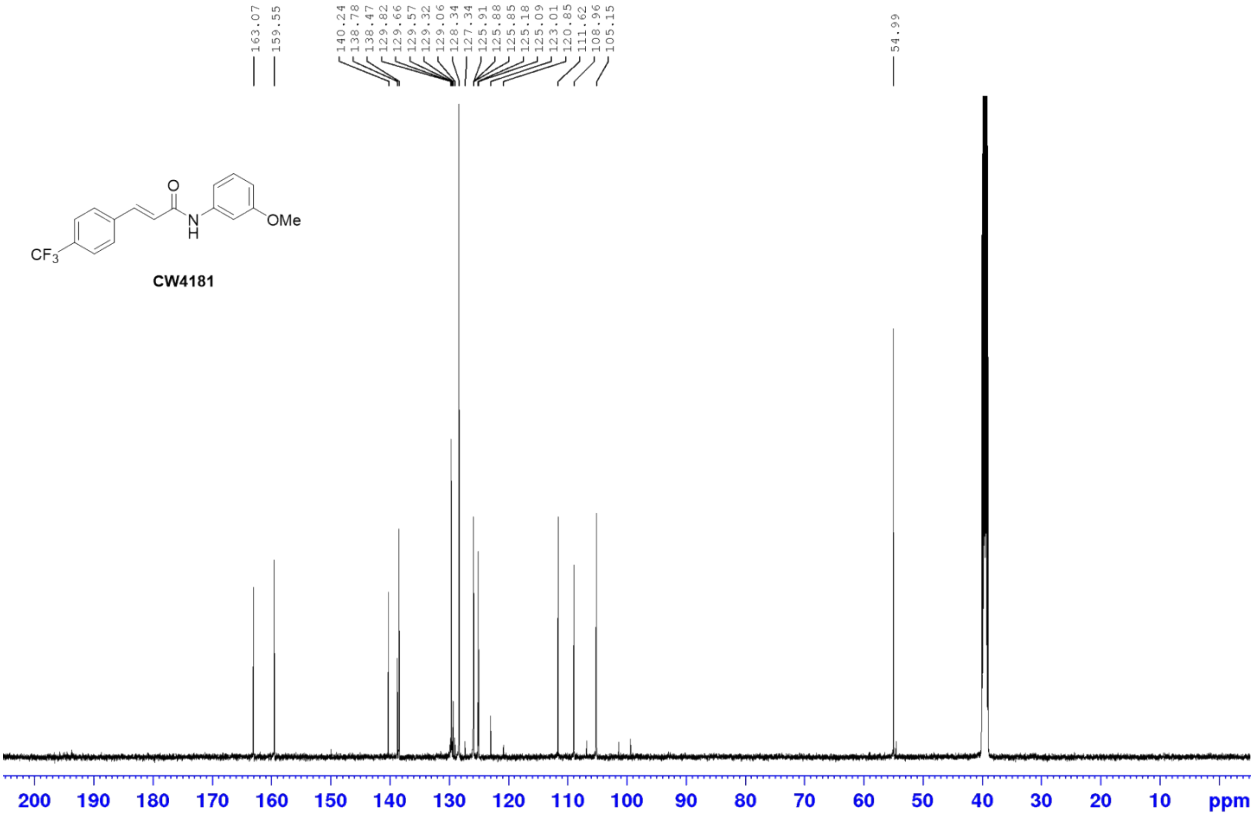

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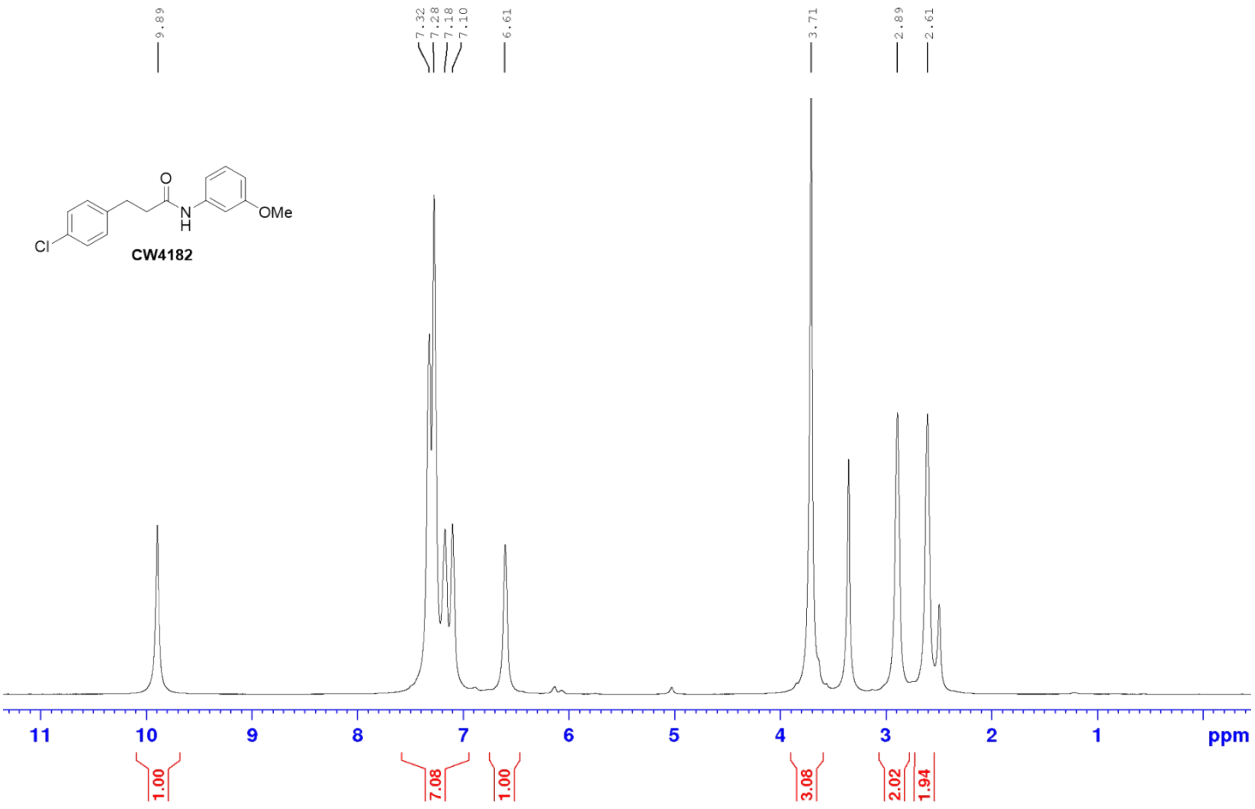

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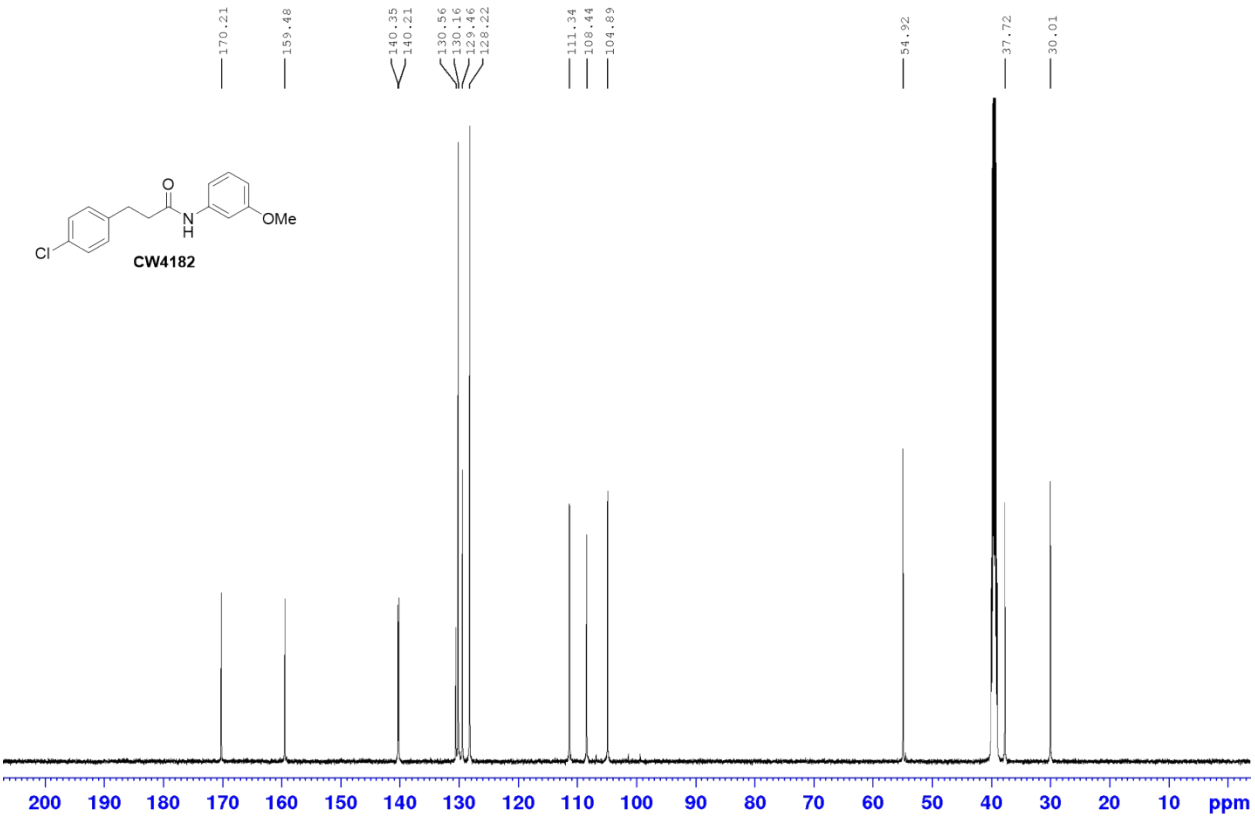

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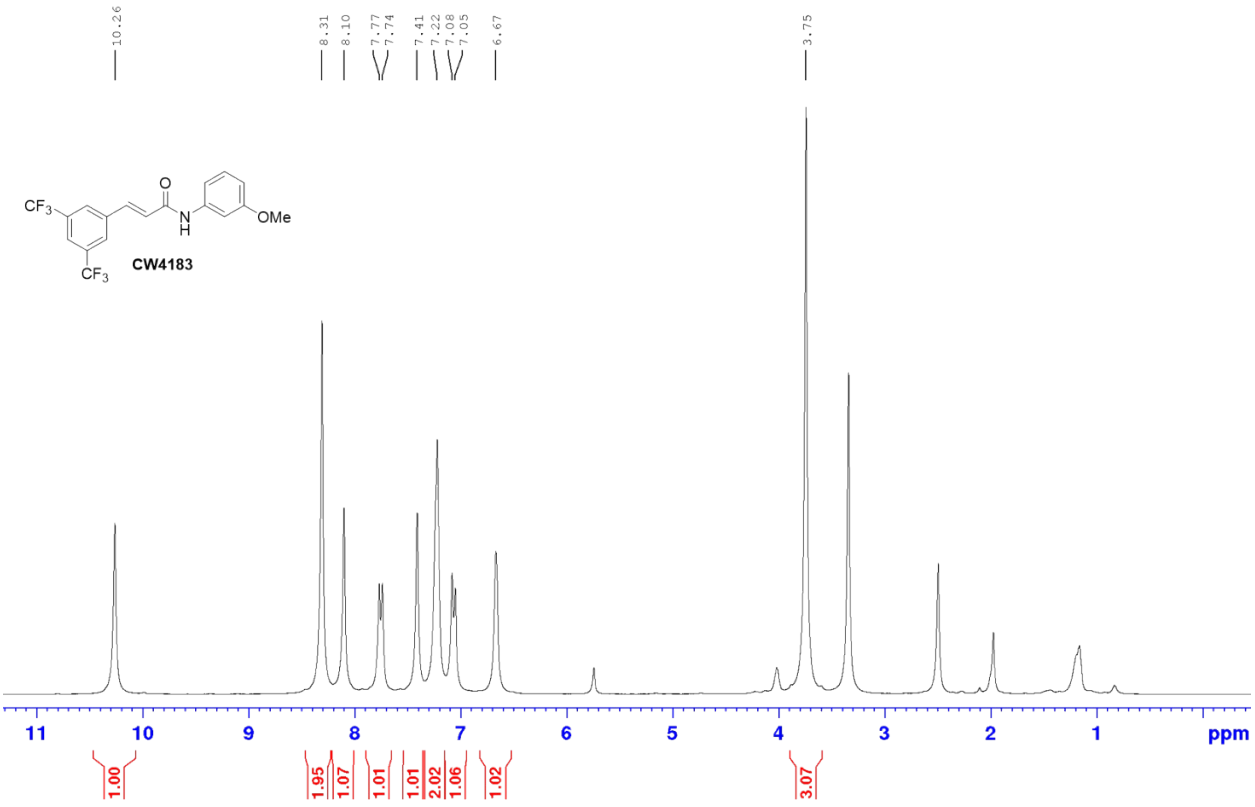

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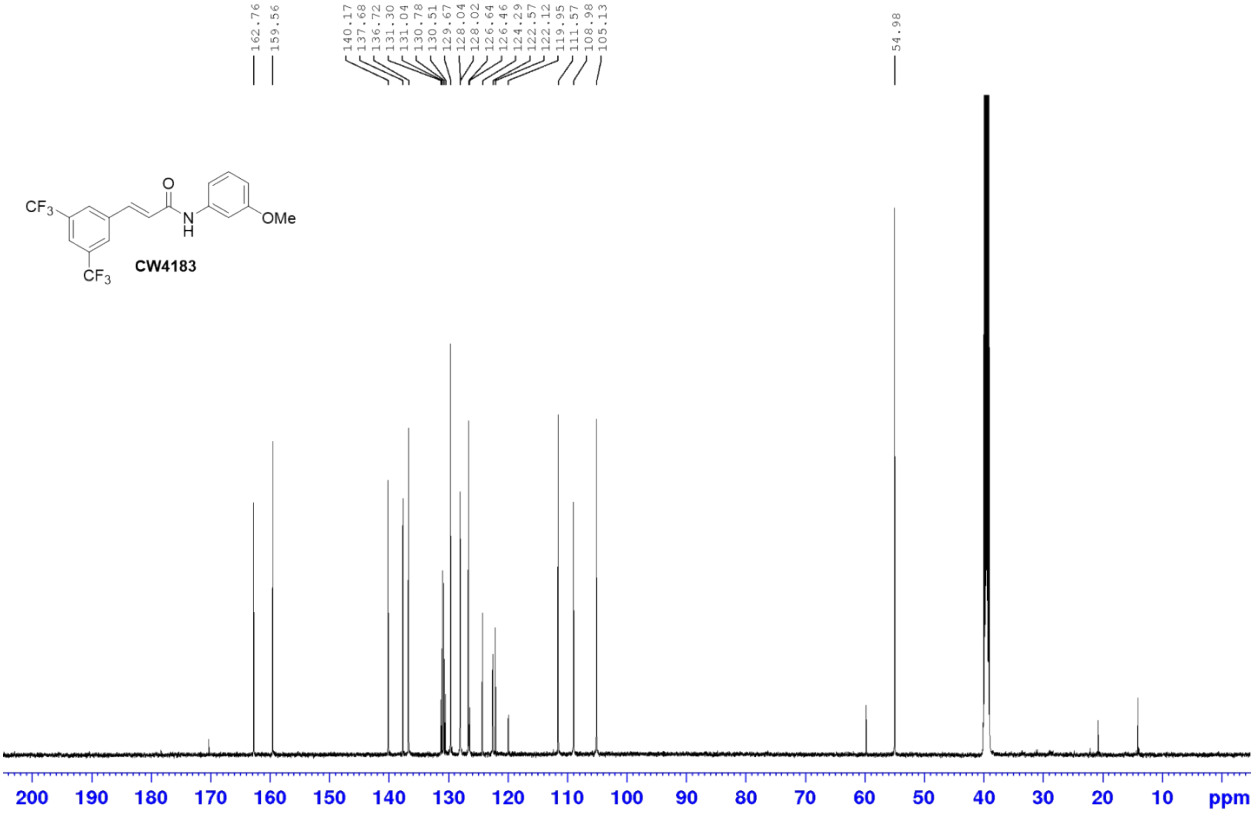

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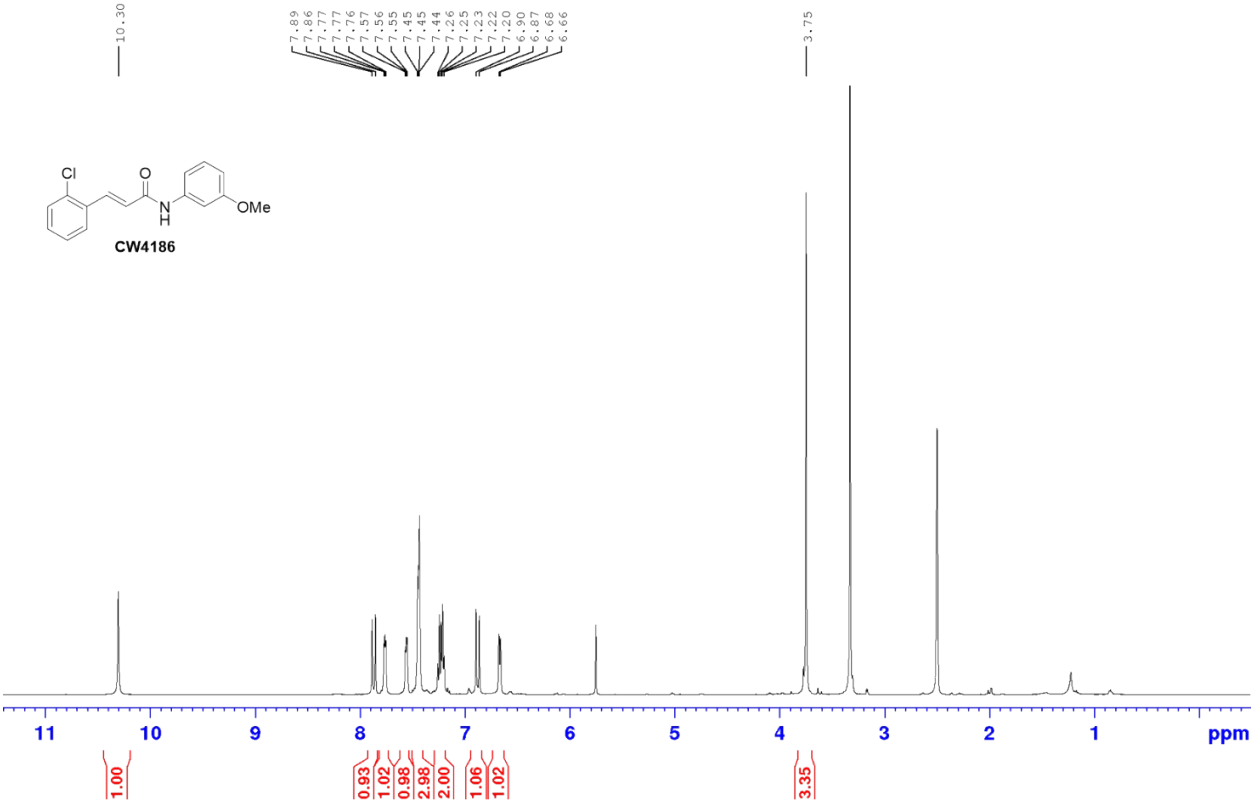

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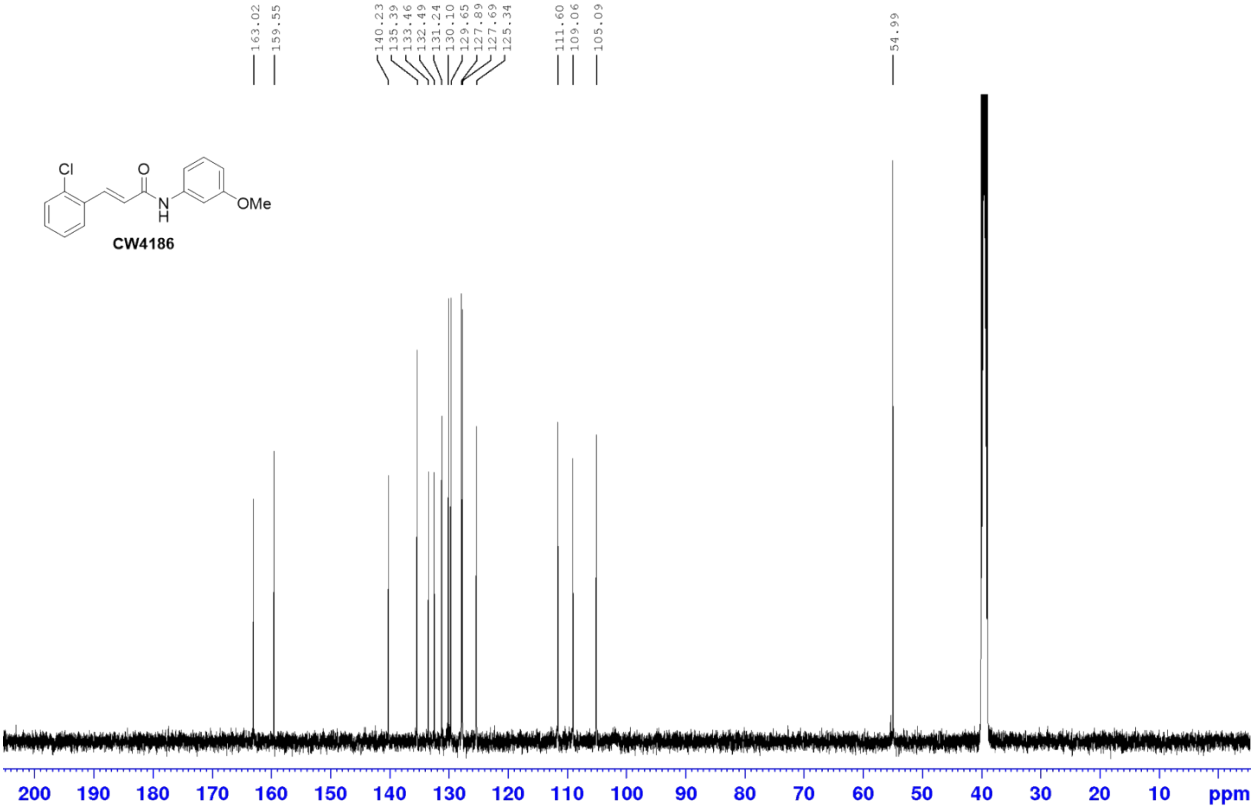

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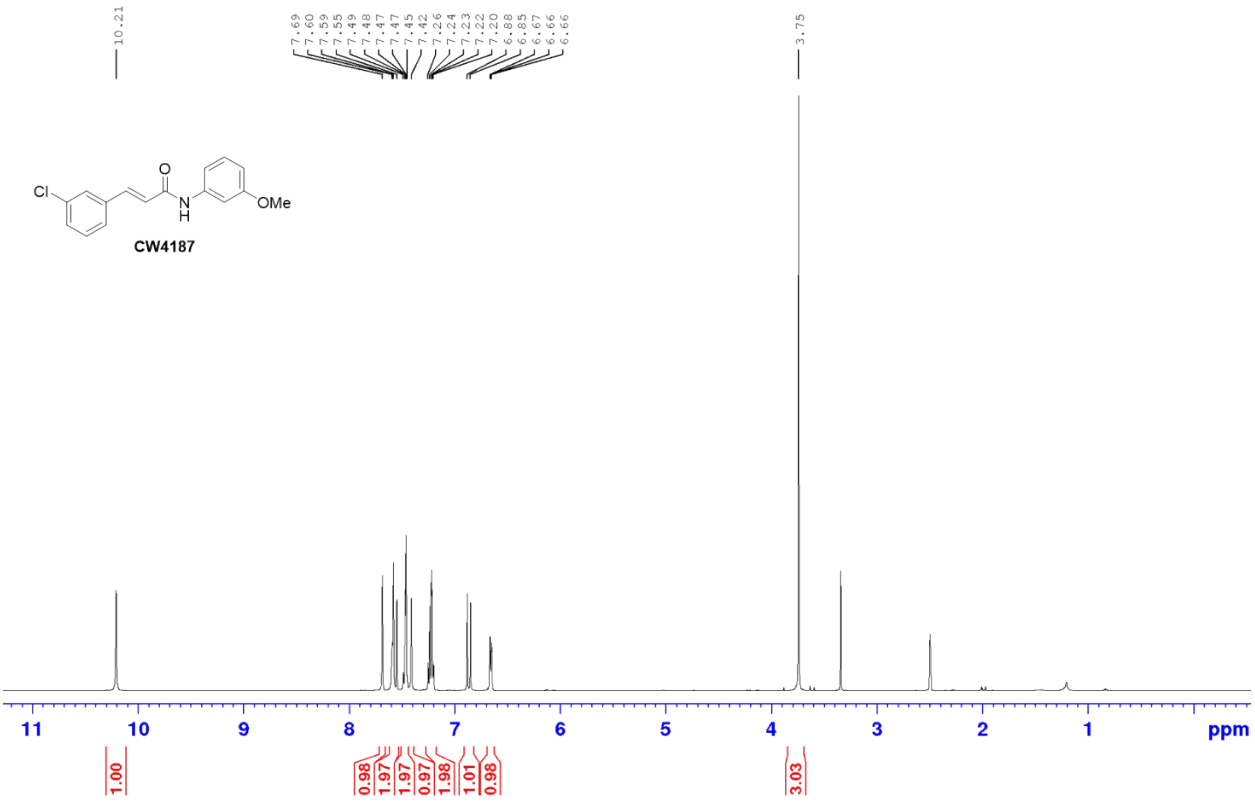

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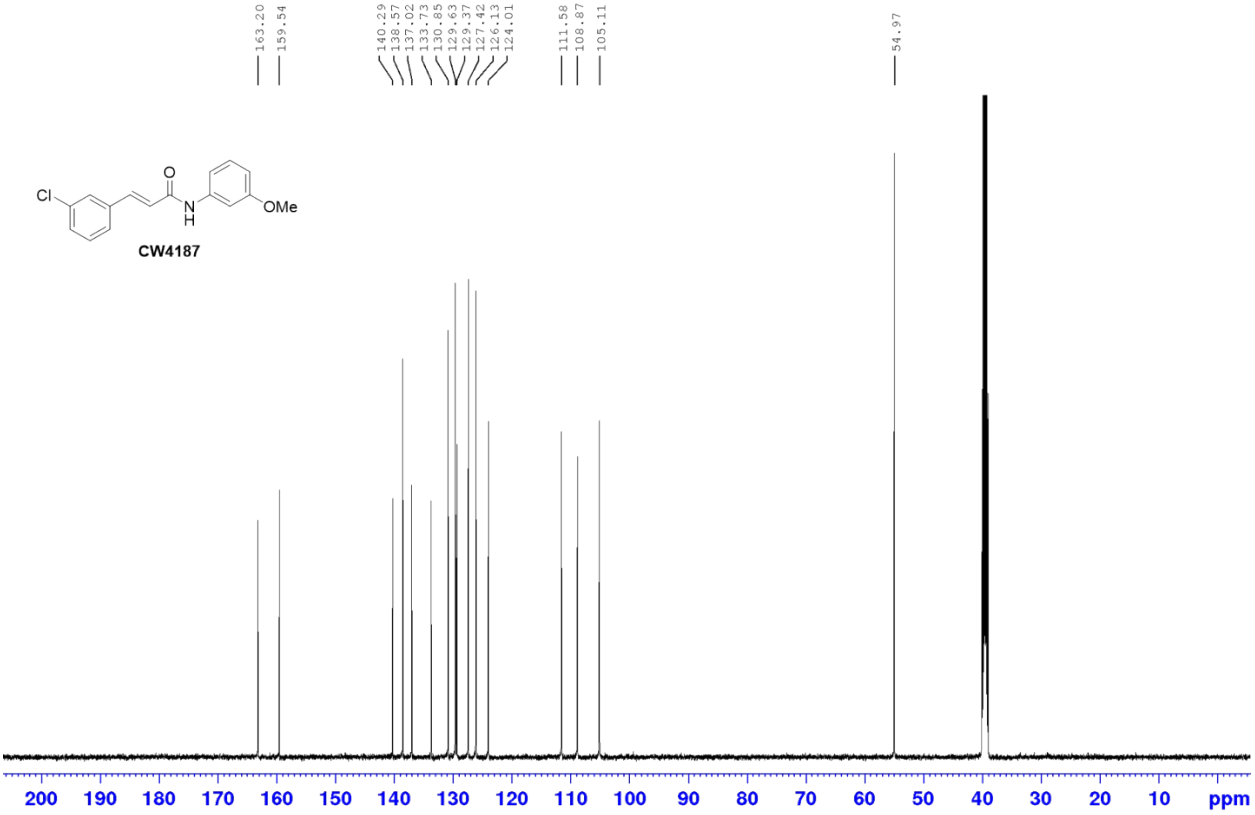

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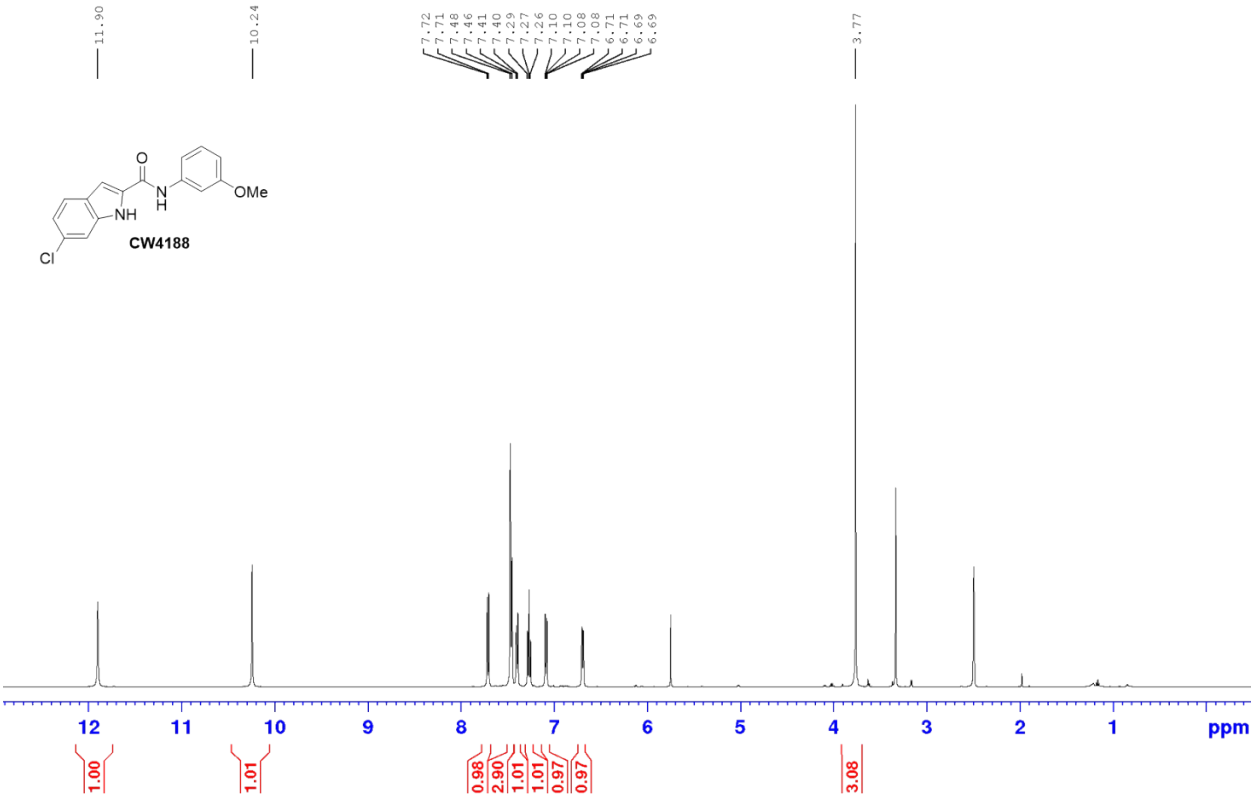

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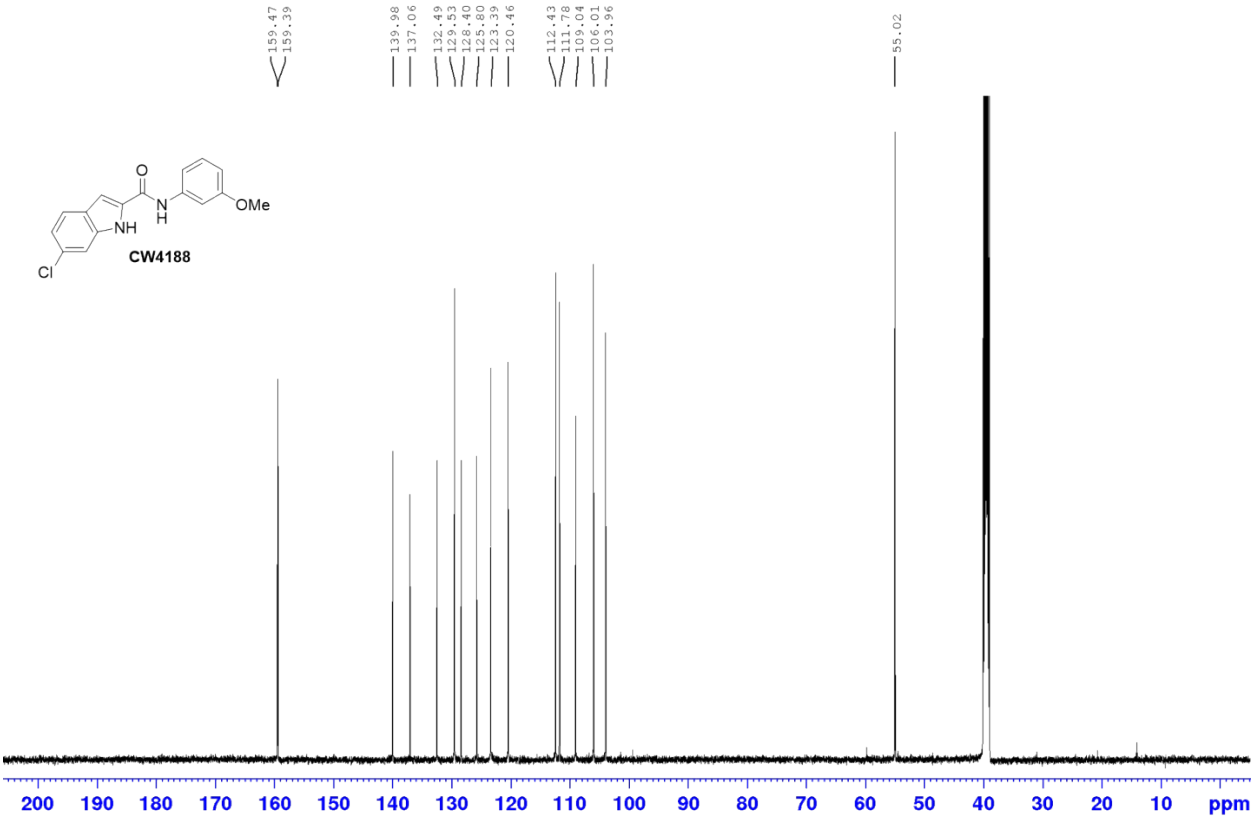

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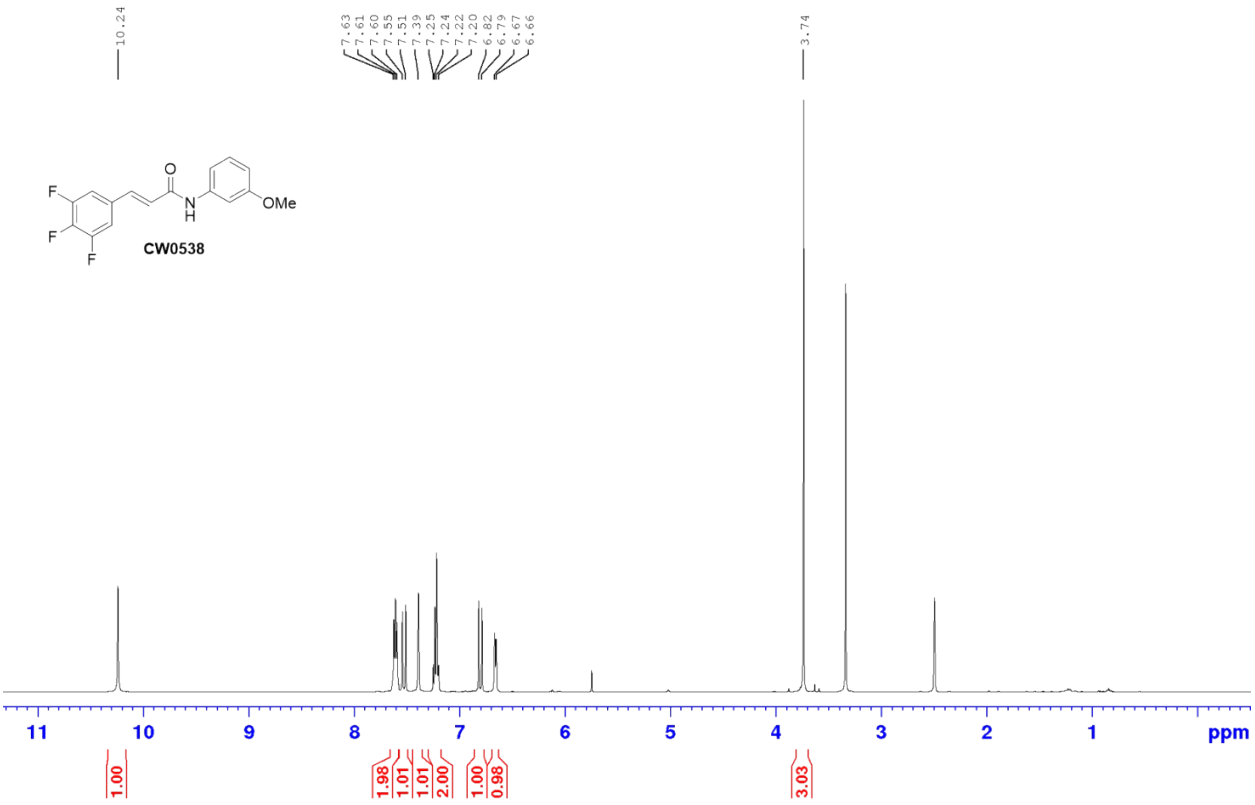
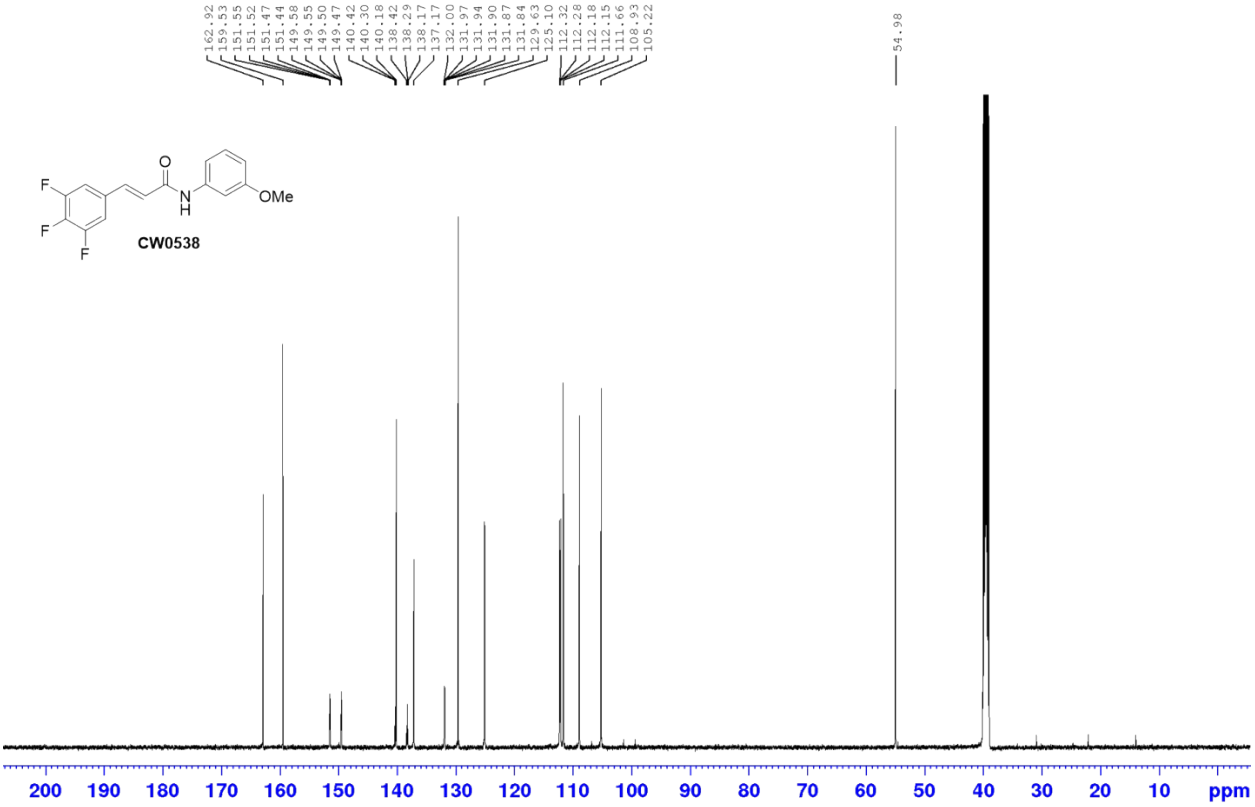


13C,DMSO-d6,125MHz



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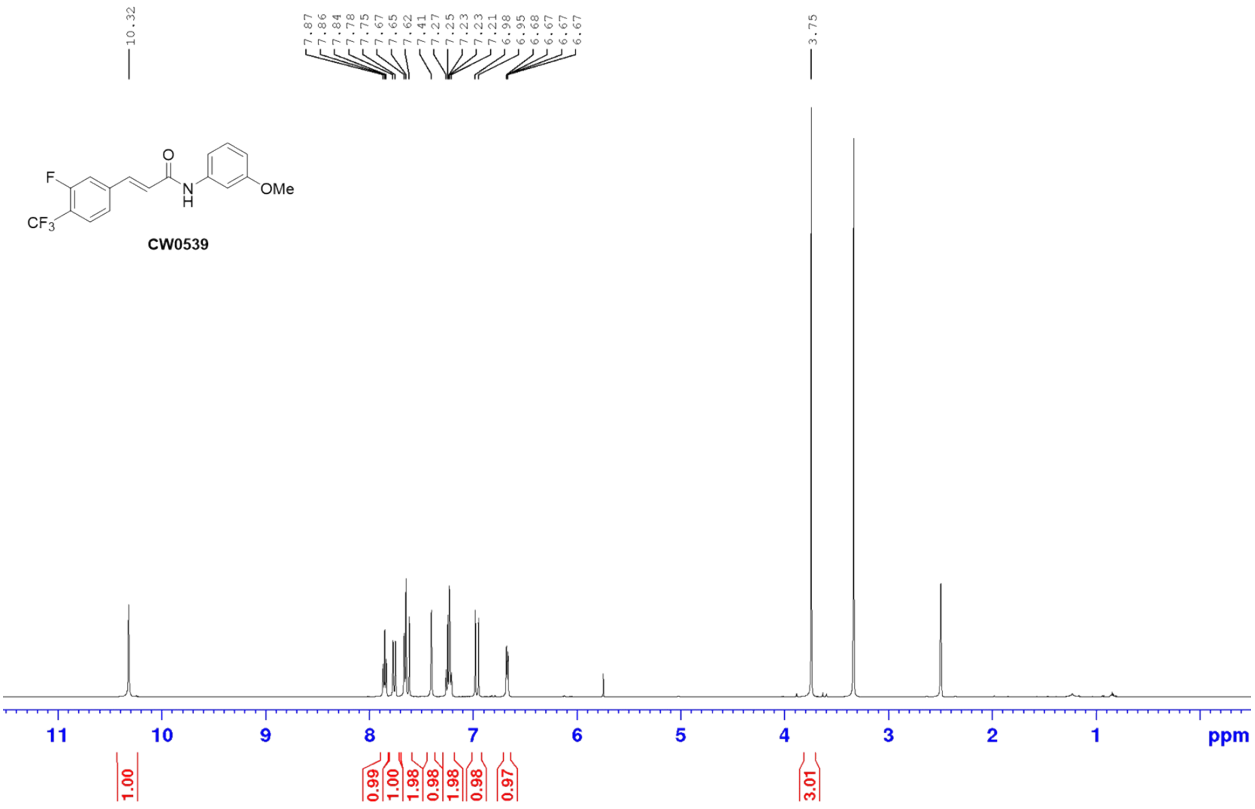

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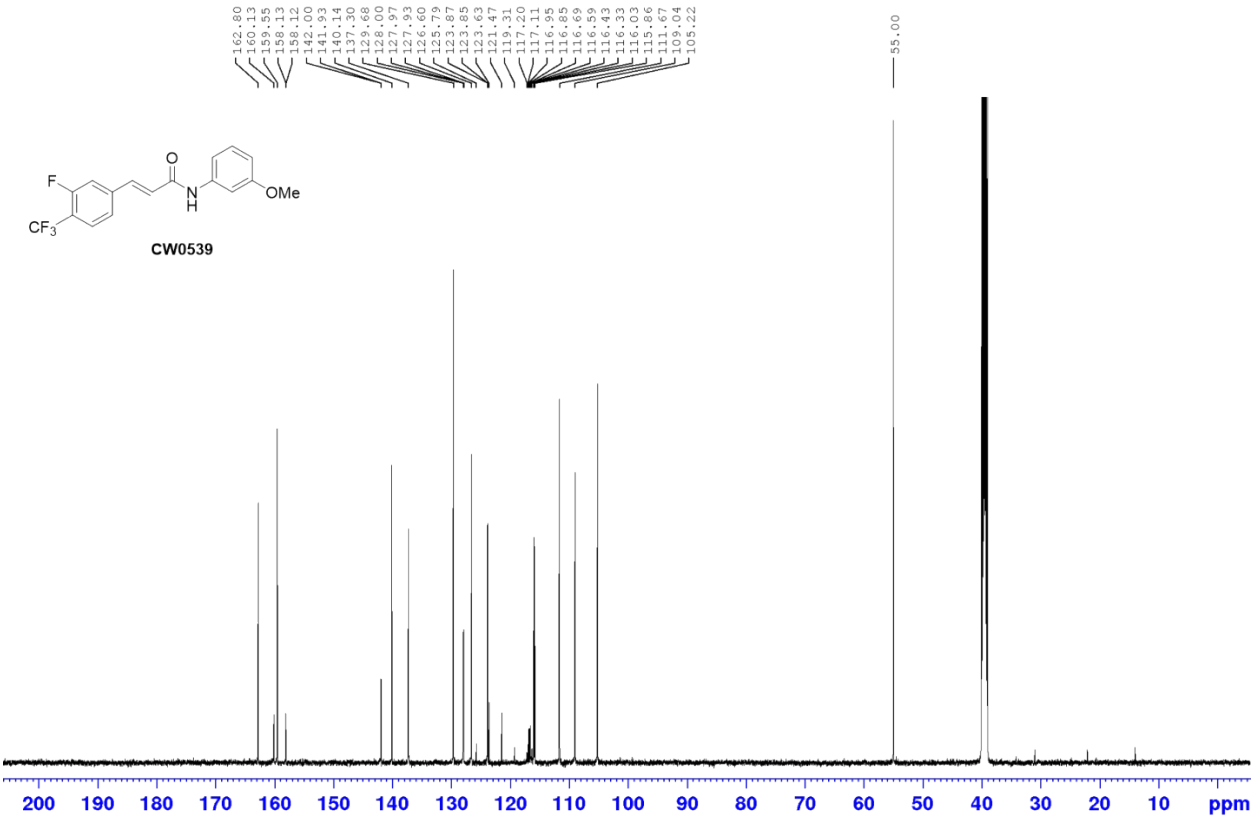

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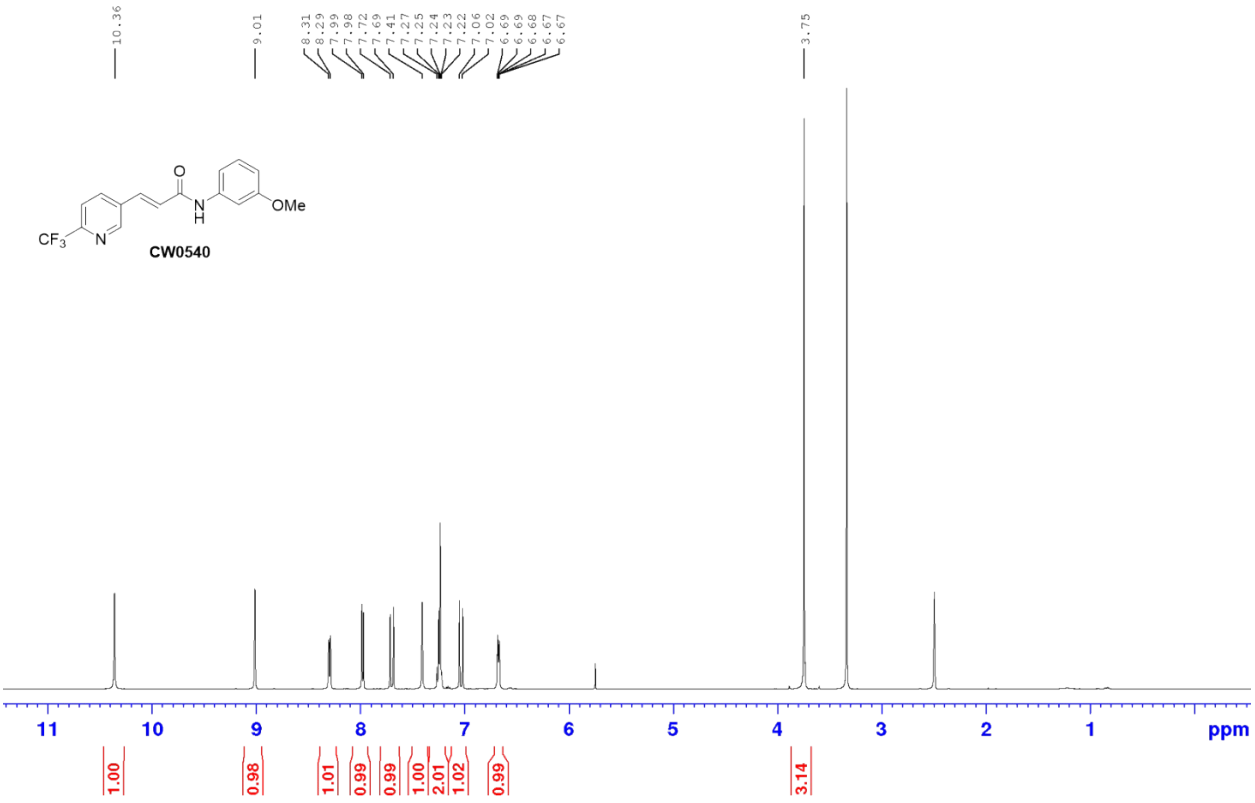
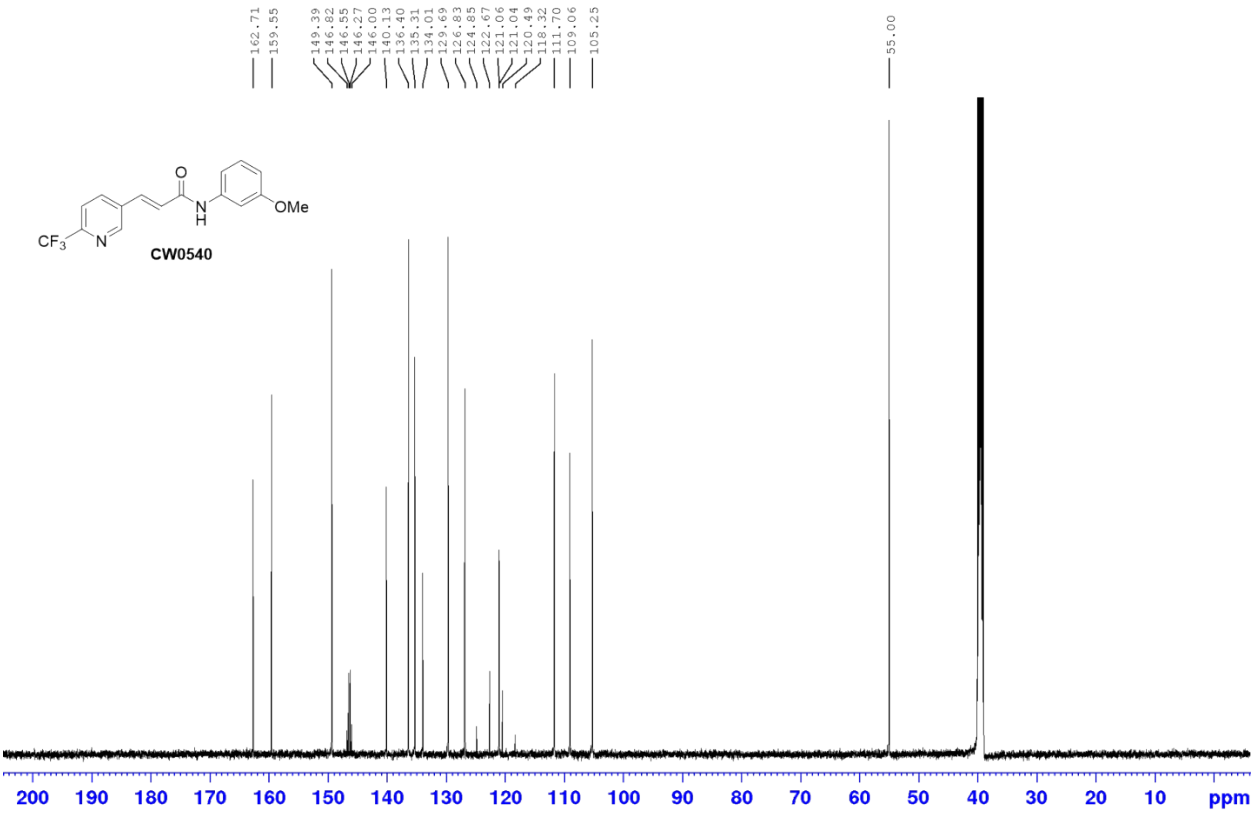
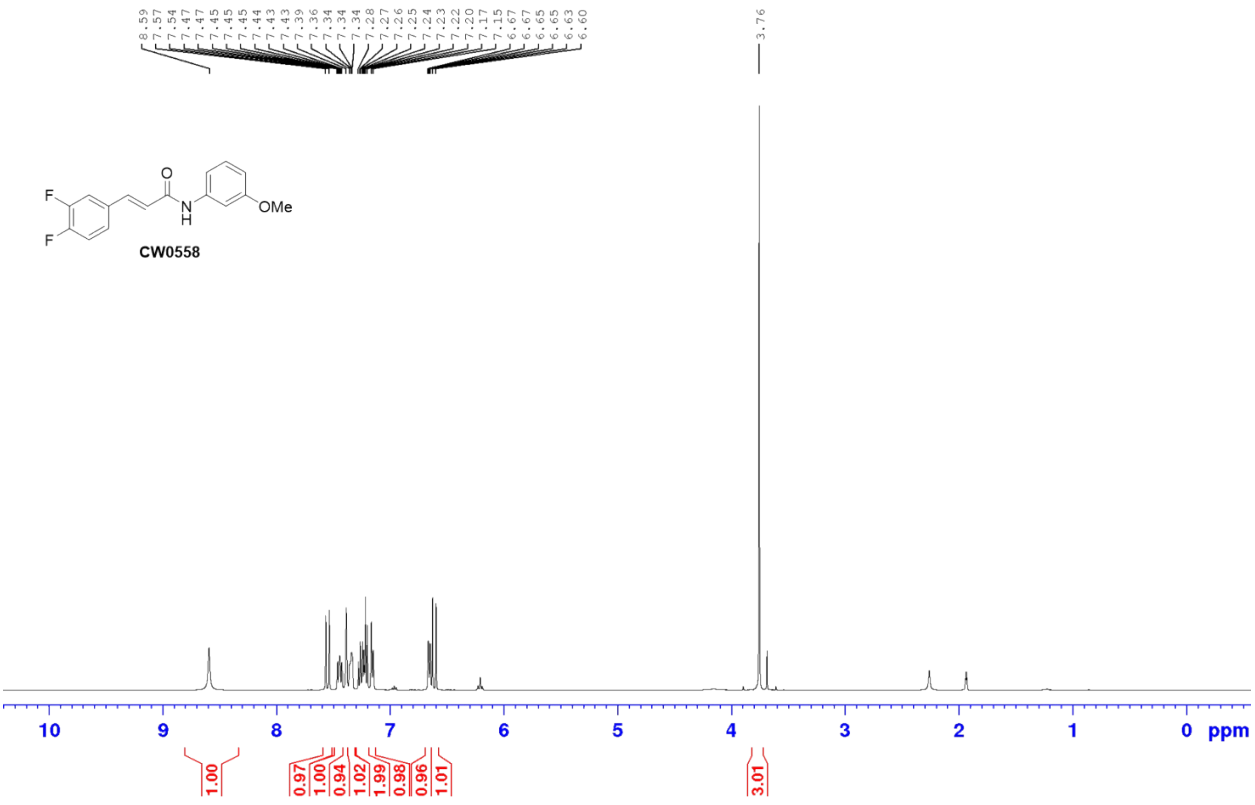


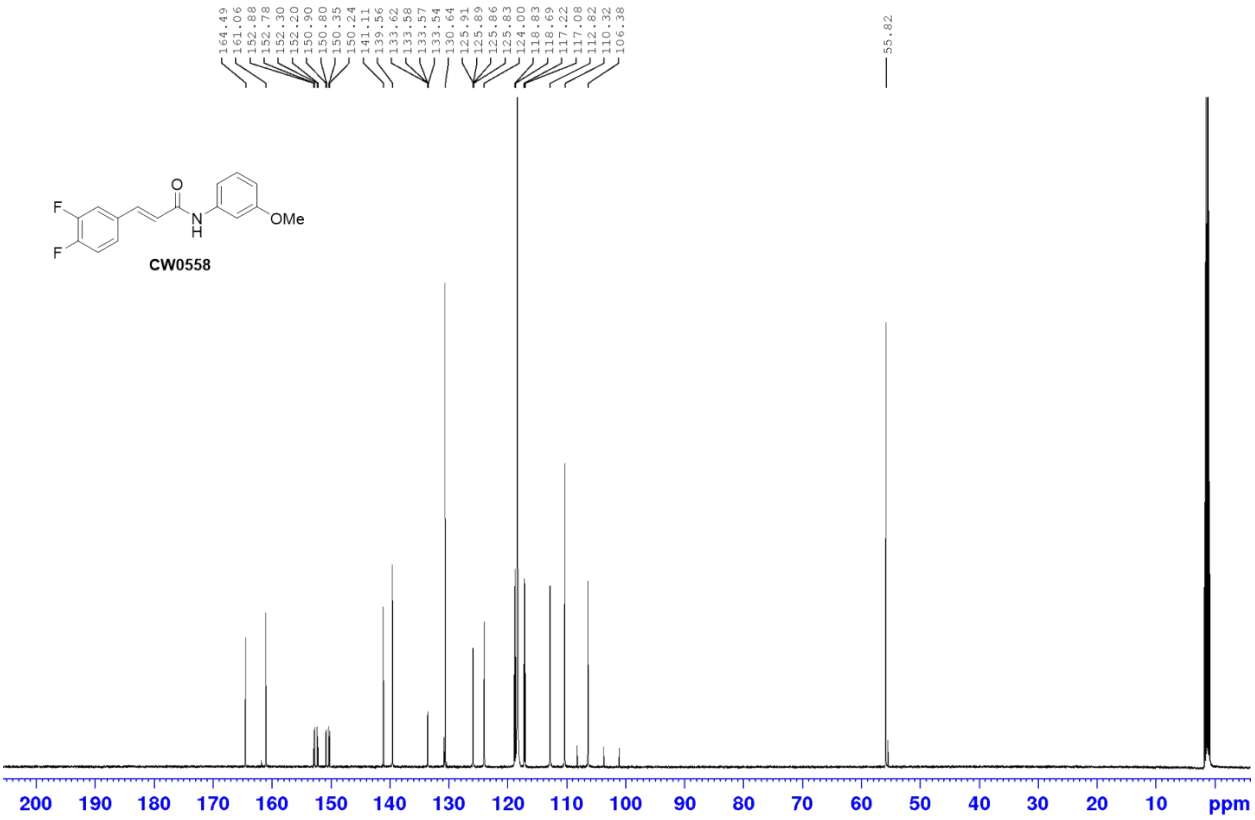
13C,DMSO-d6,125MHz



1H,CD3CN,500MHz



13C,CD3CN,125MHz



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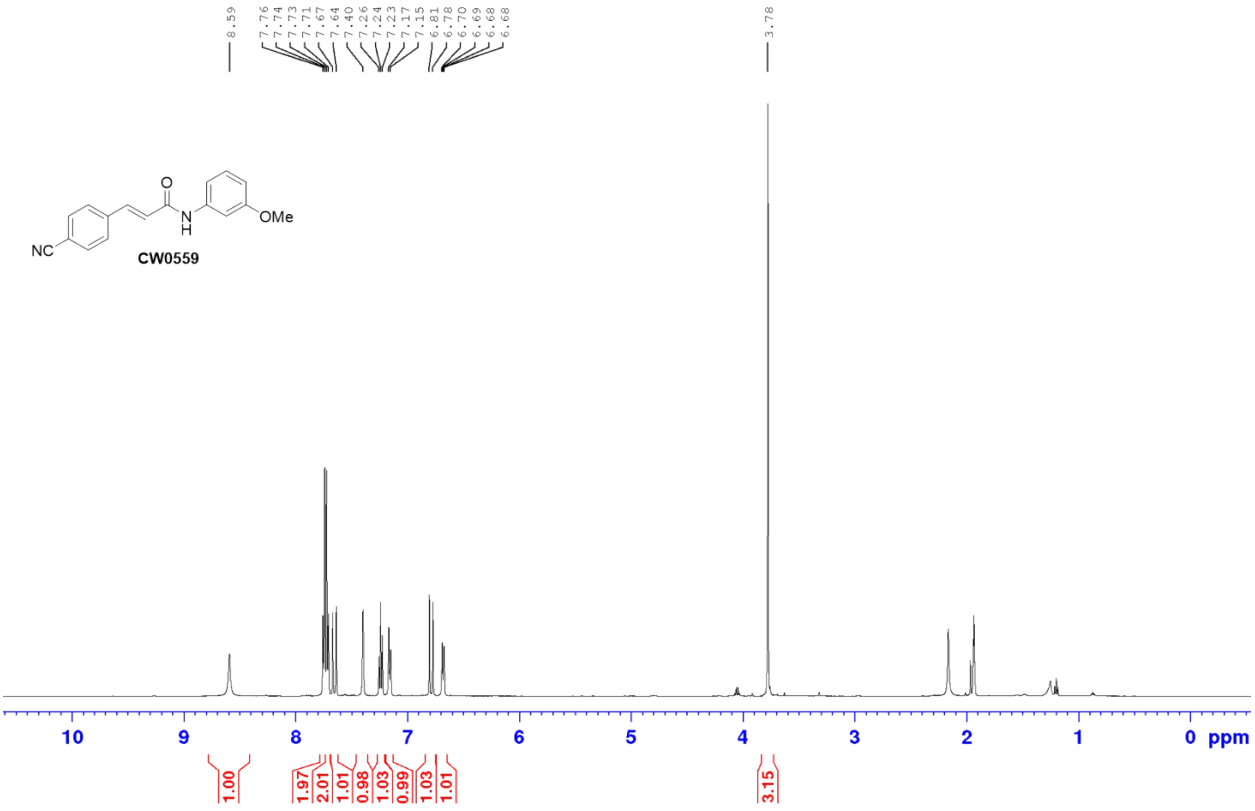
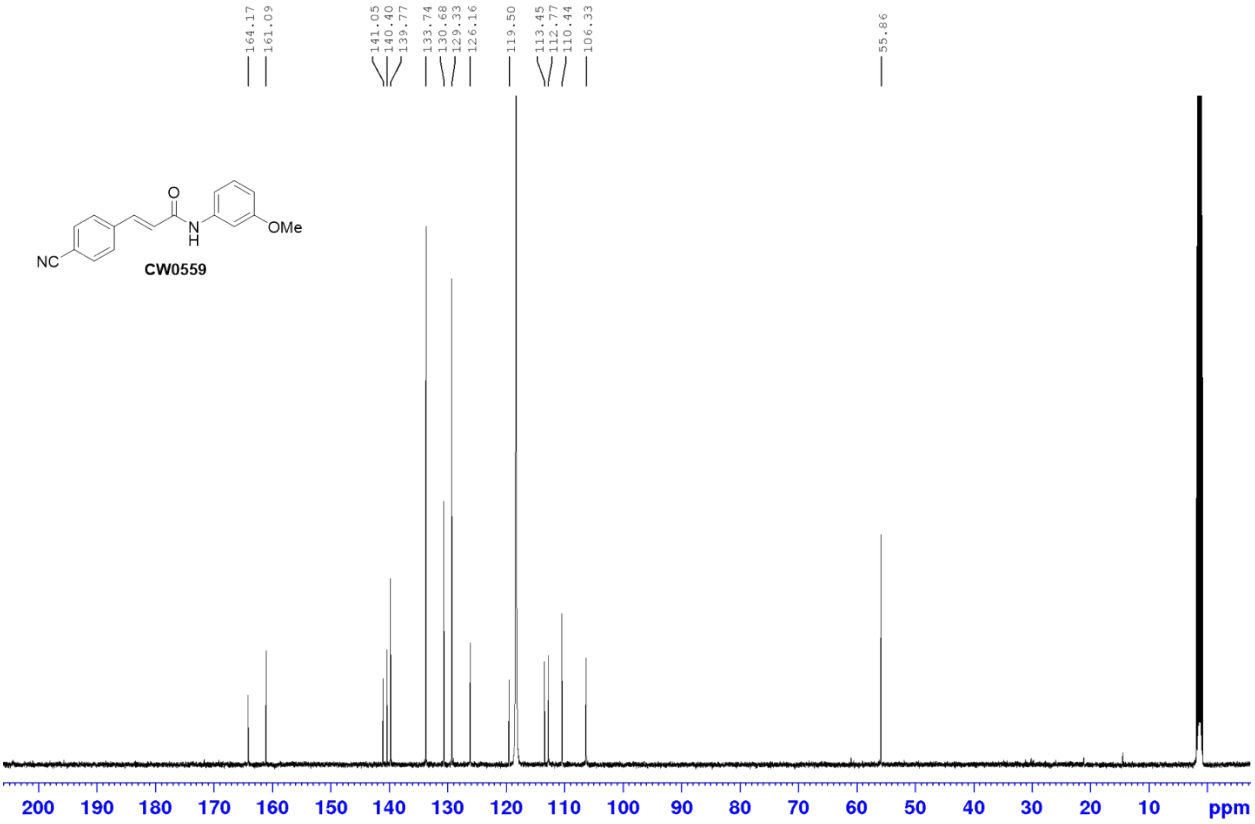


13C,CD3CN,125MHz



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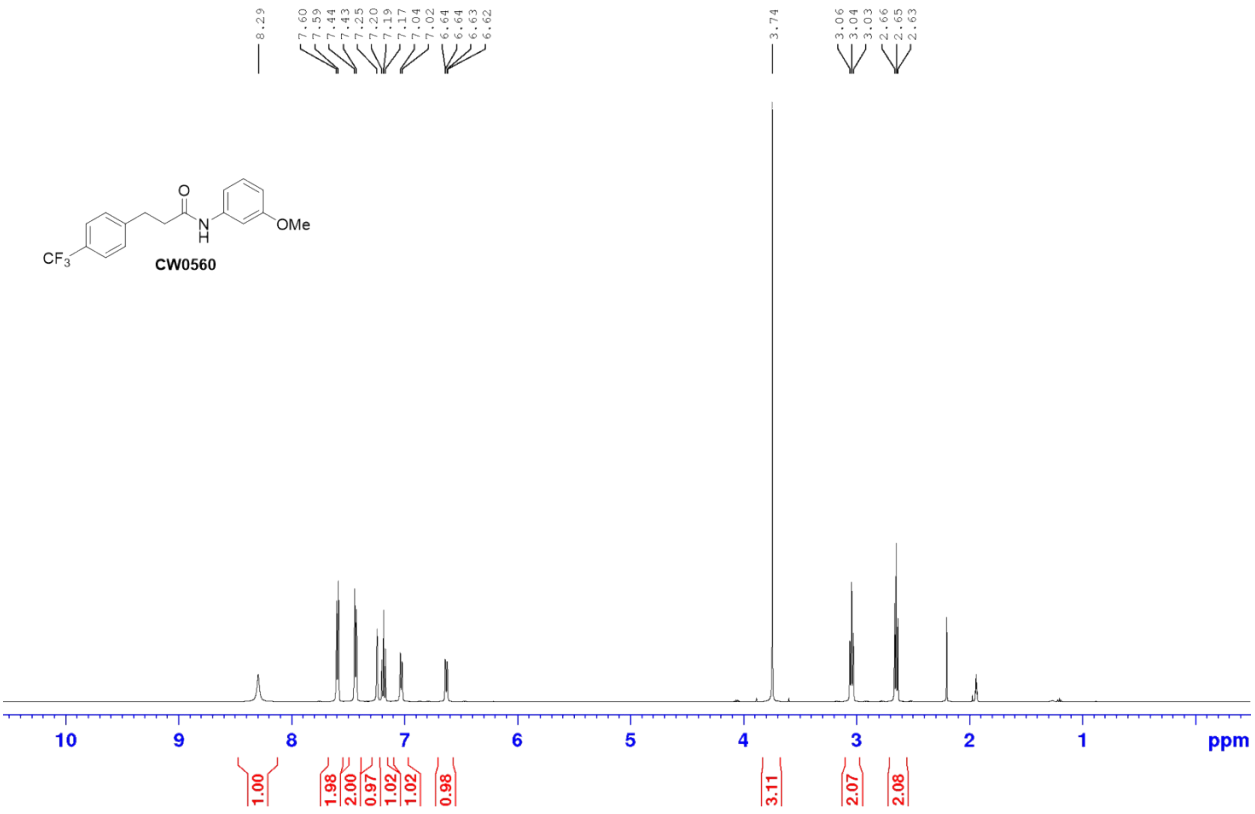
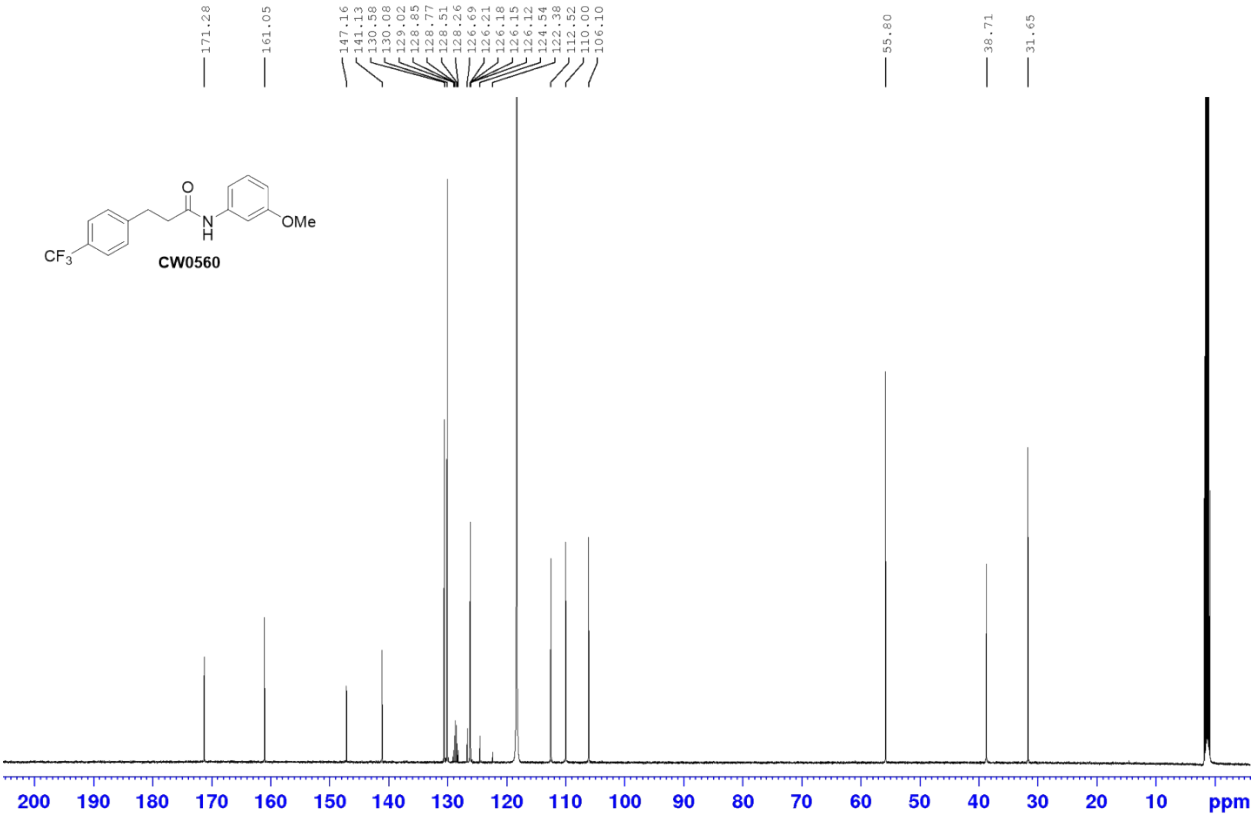
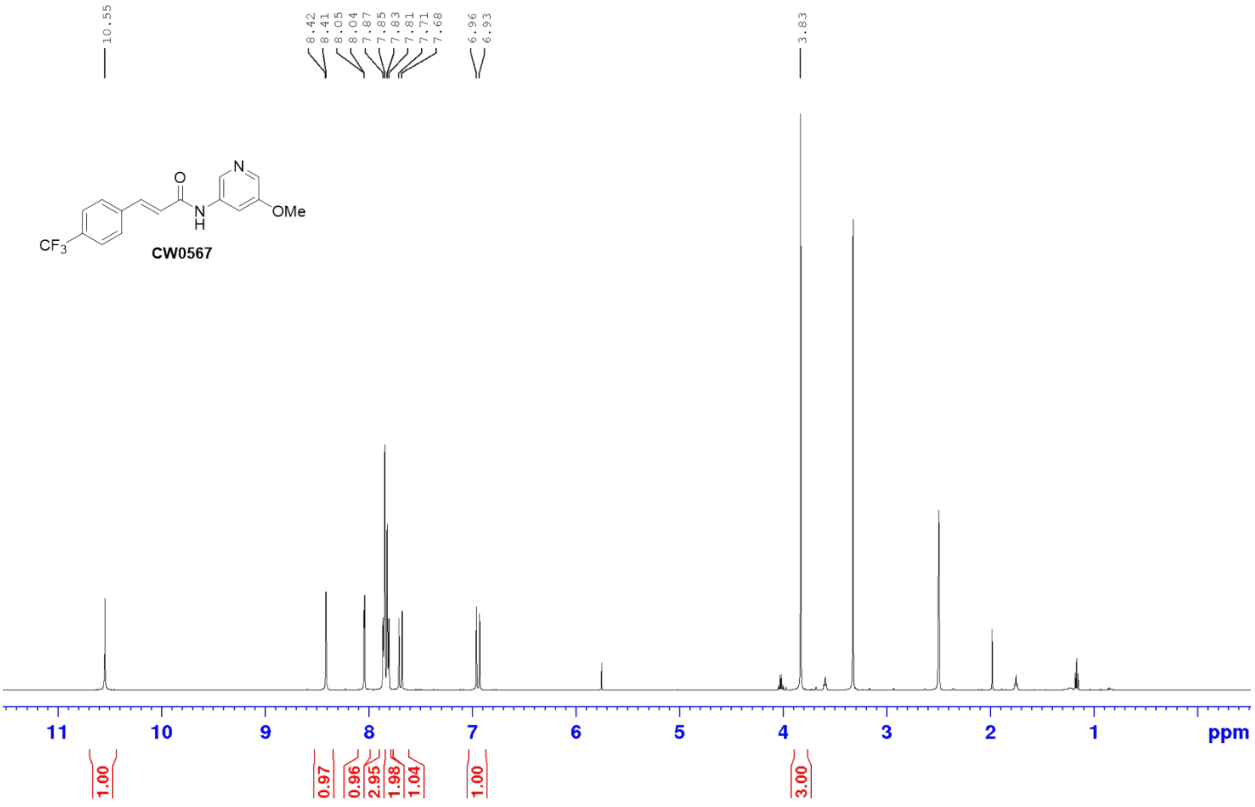


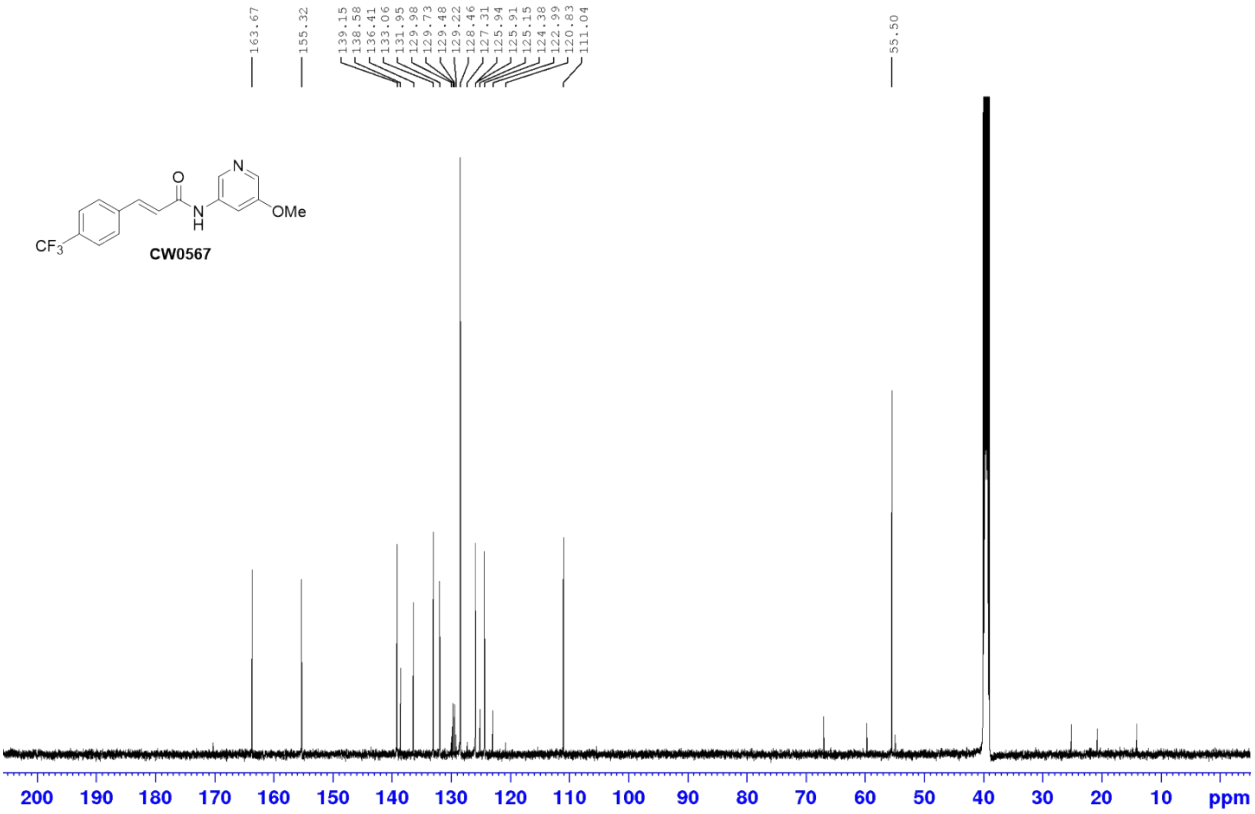
13C,CD3CN,125MHz



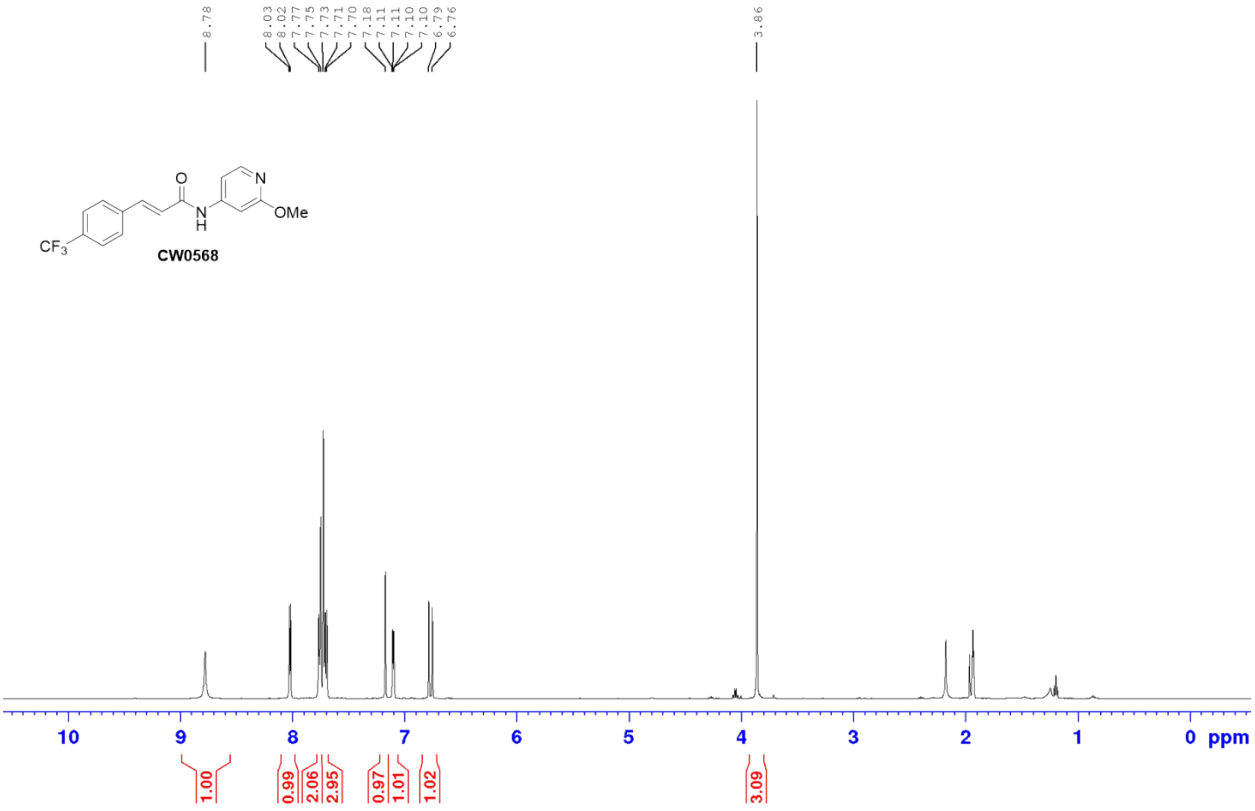
1H,DMSO-d6,500MHz



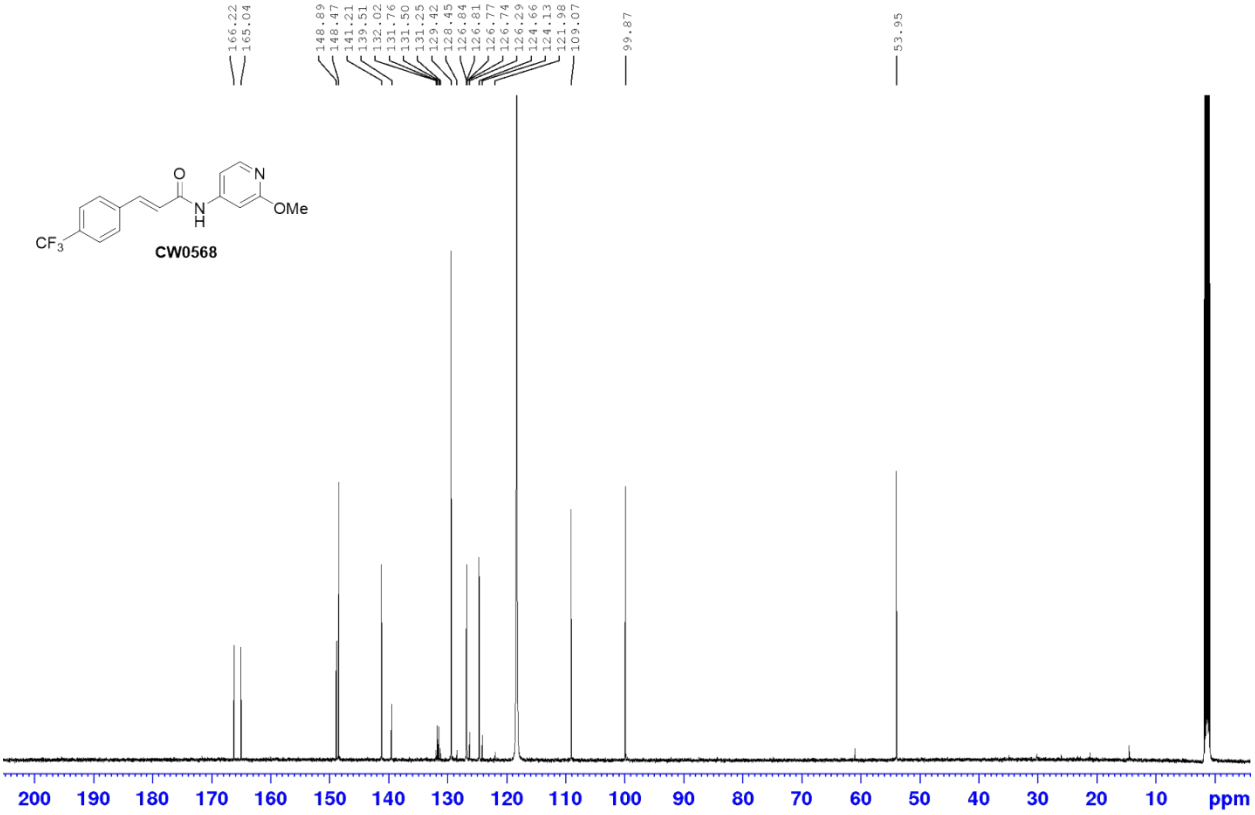
13C,DMSO-d6,125MHz



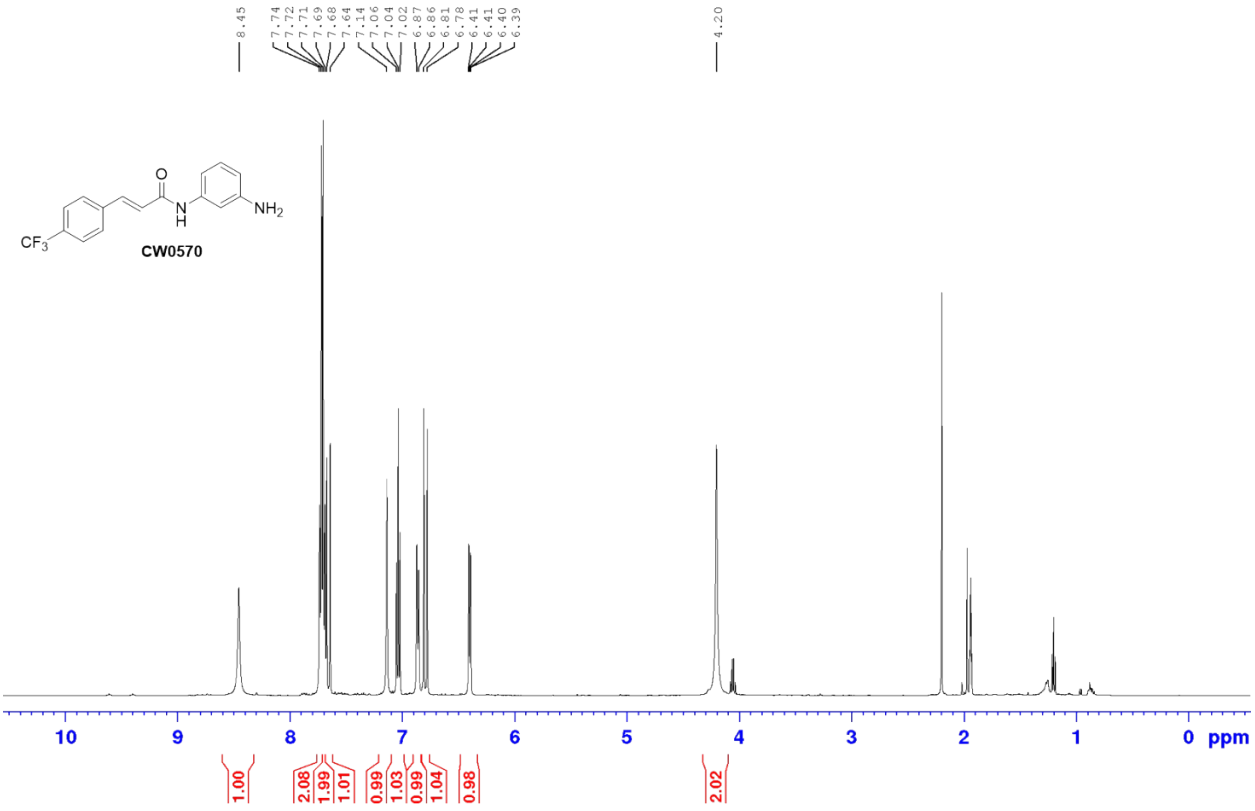
1H,CD3CN,500MHz



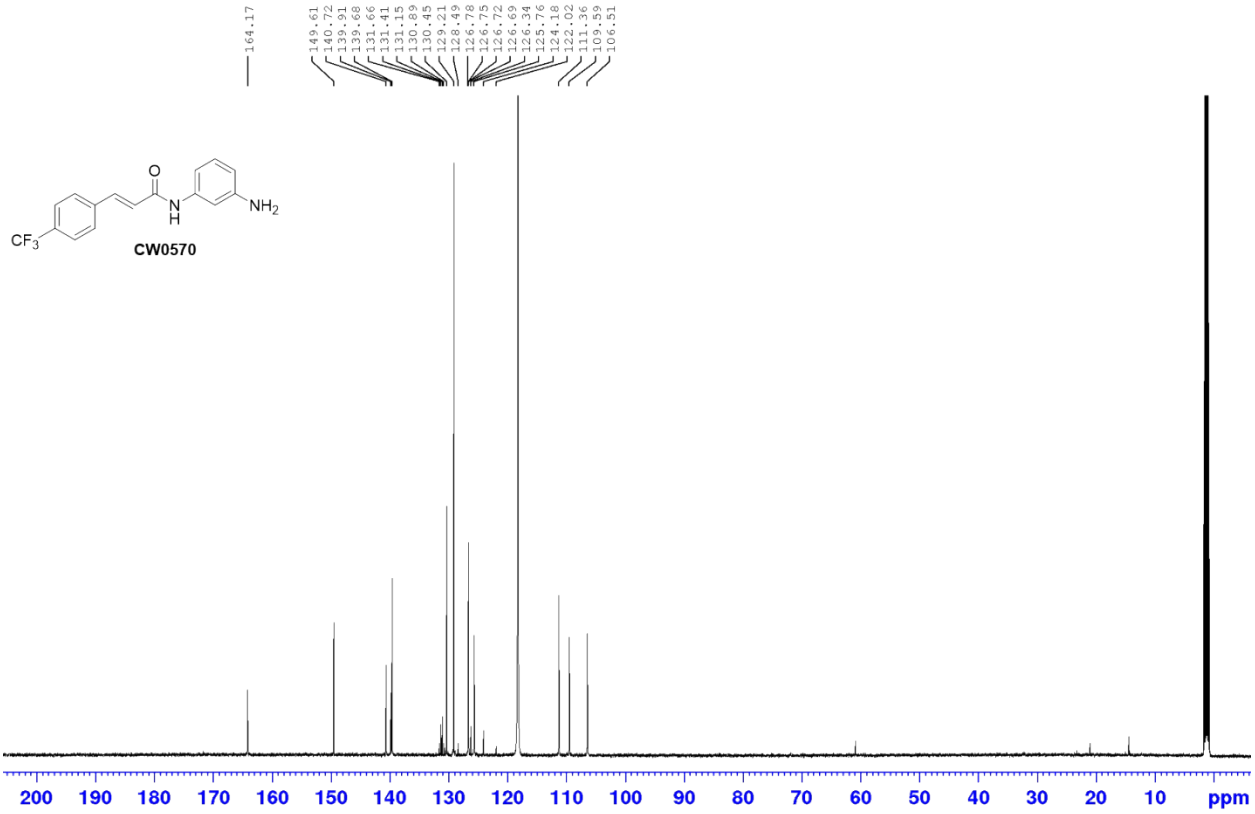
13C,CD3CN,125MHz



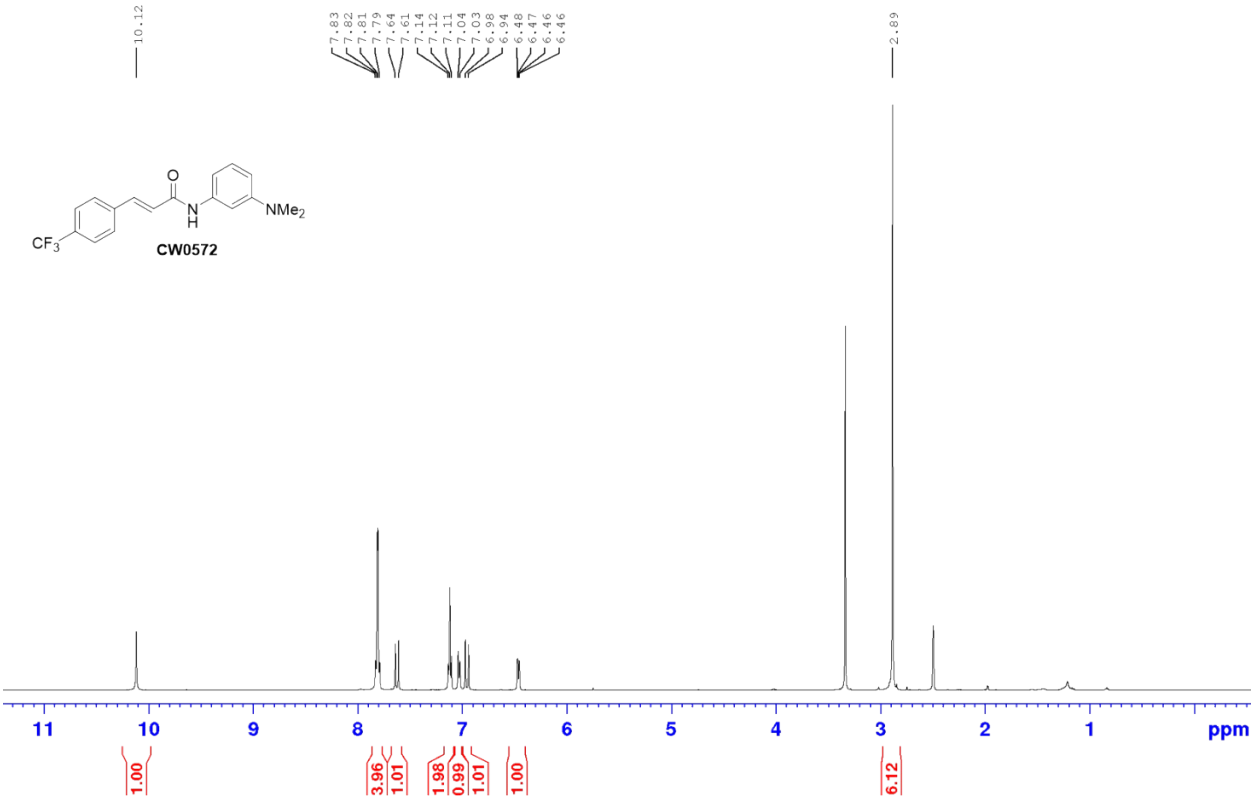
1H,CD3CN,500MHz



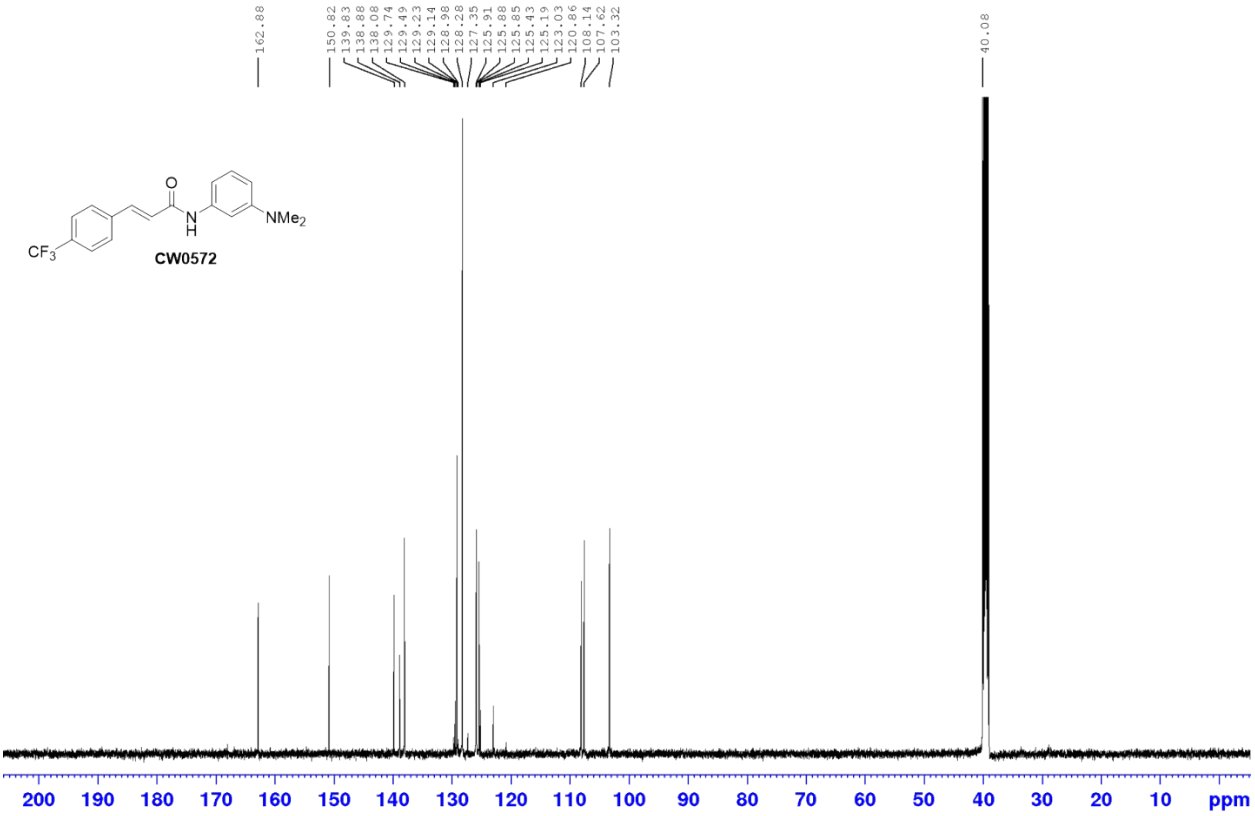
13C,CD3CN,125MHz



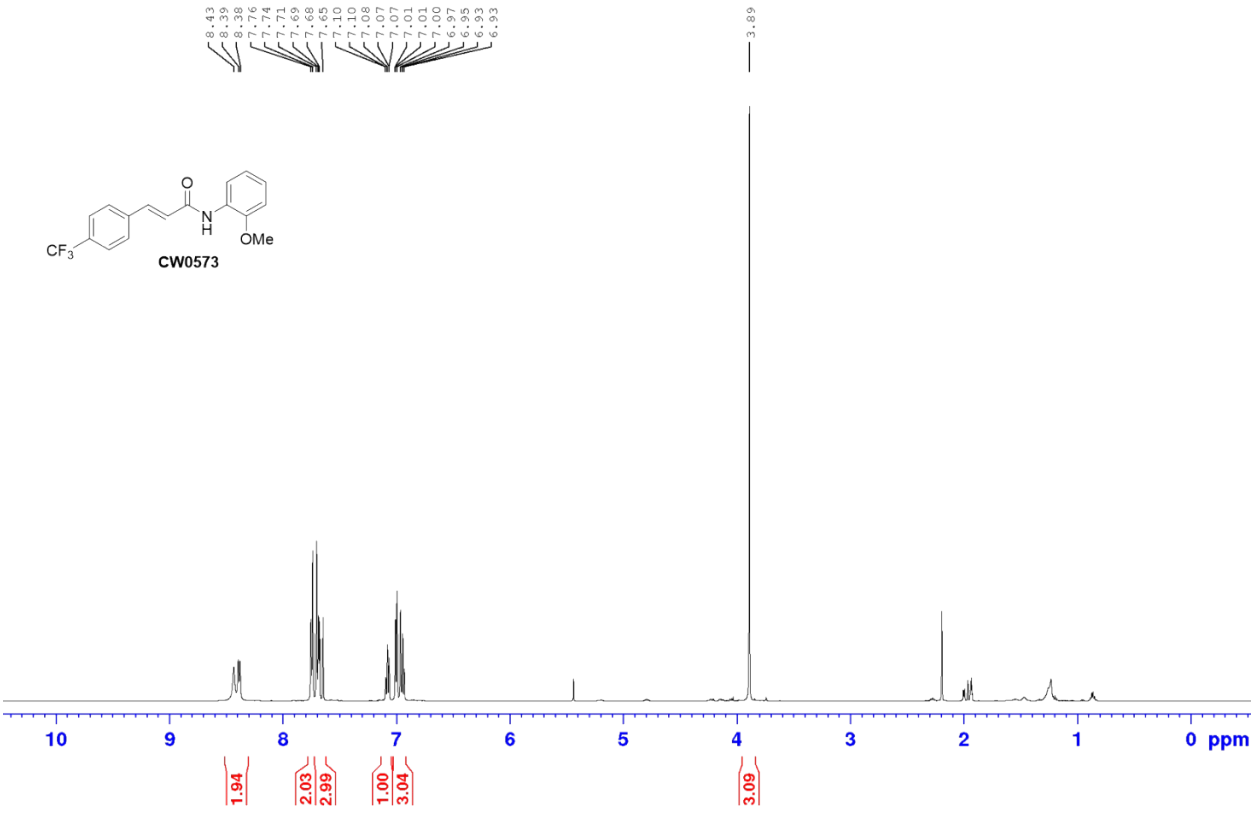
1H,DMSO-d6,500MHz



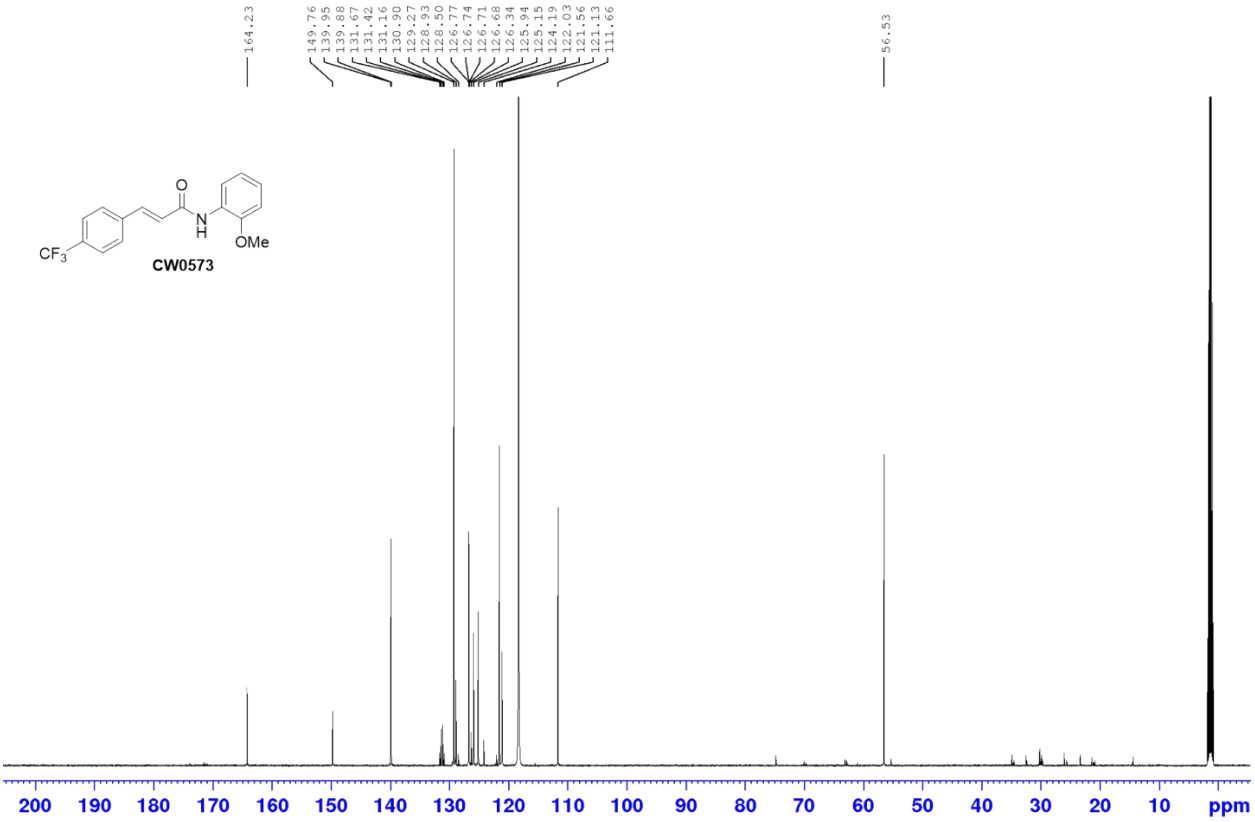
13C,DMSO-d6,125MHz



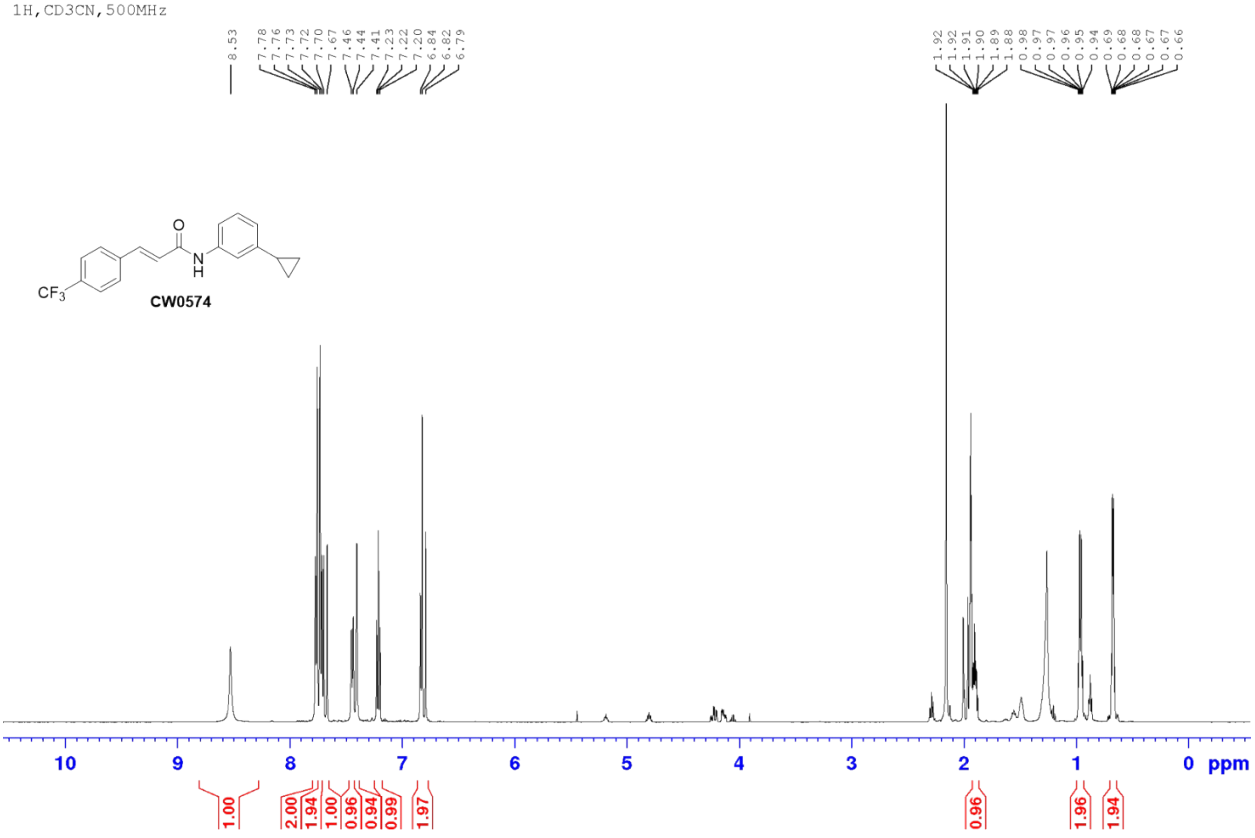
1H,CD3CN,500MHz



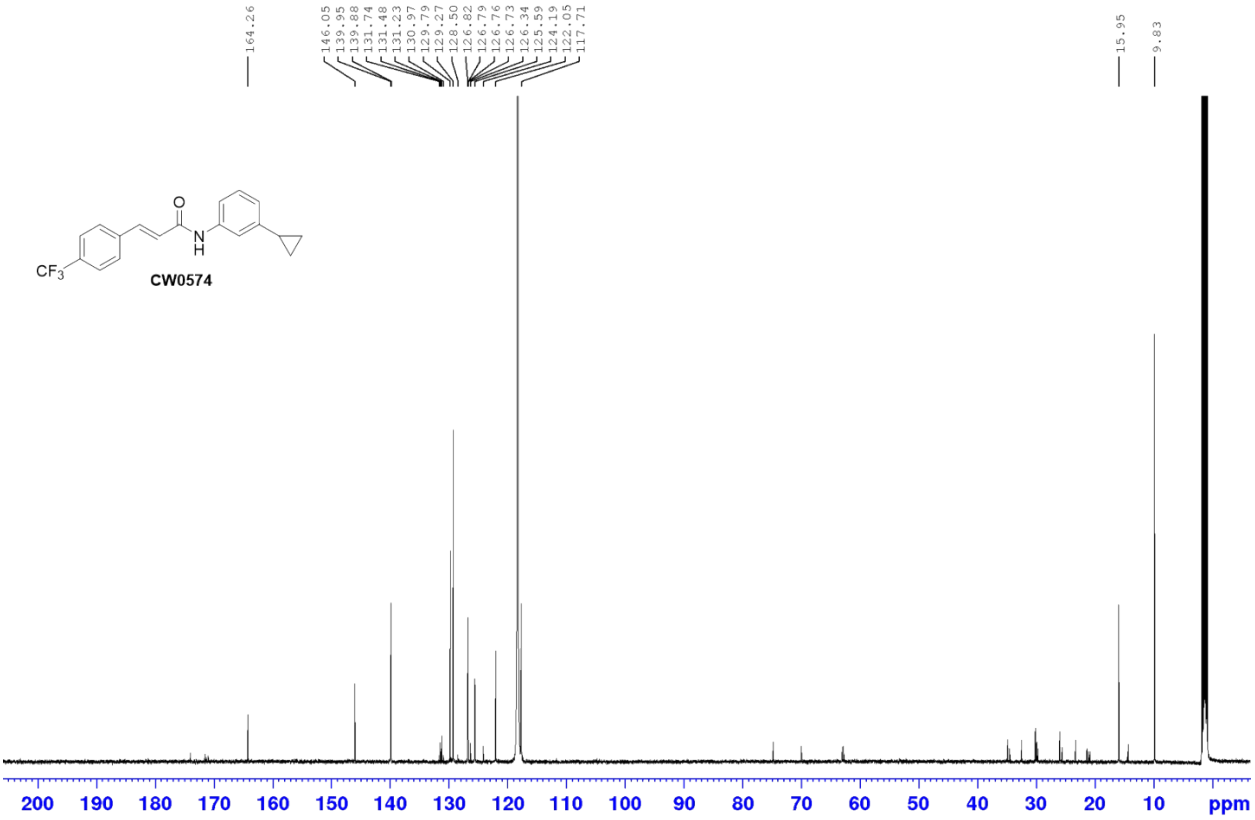
13C,CD3CN,125MHz



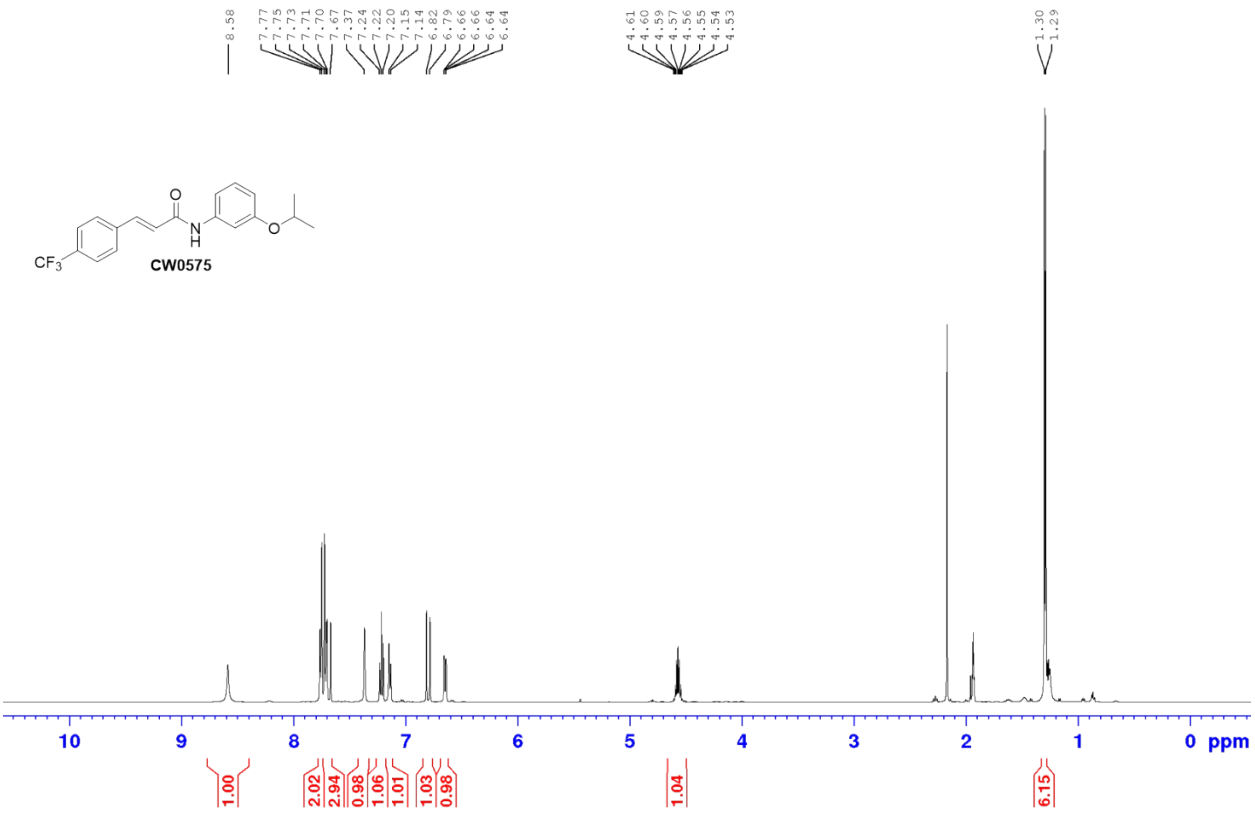
1H,CD3CN,500MHz



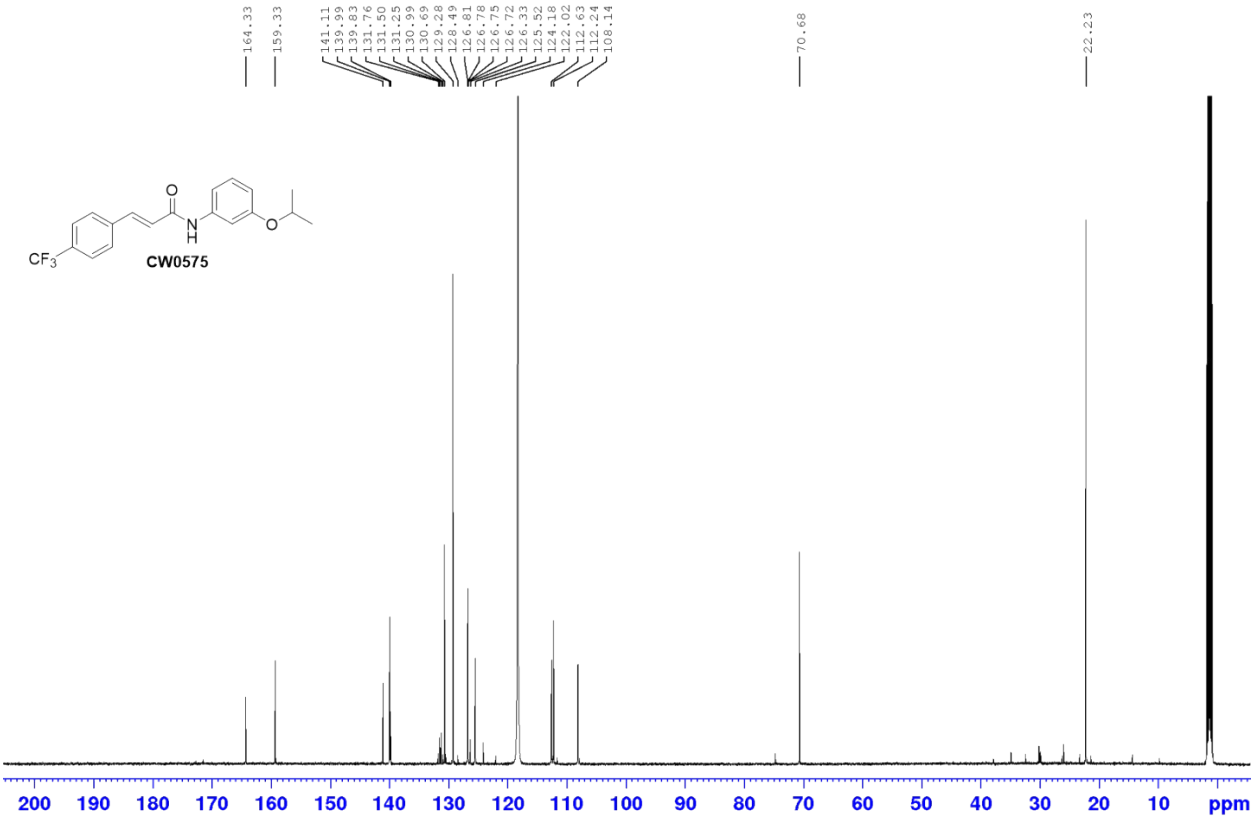
13C,CD3CN,125MHz



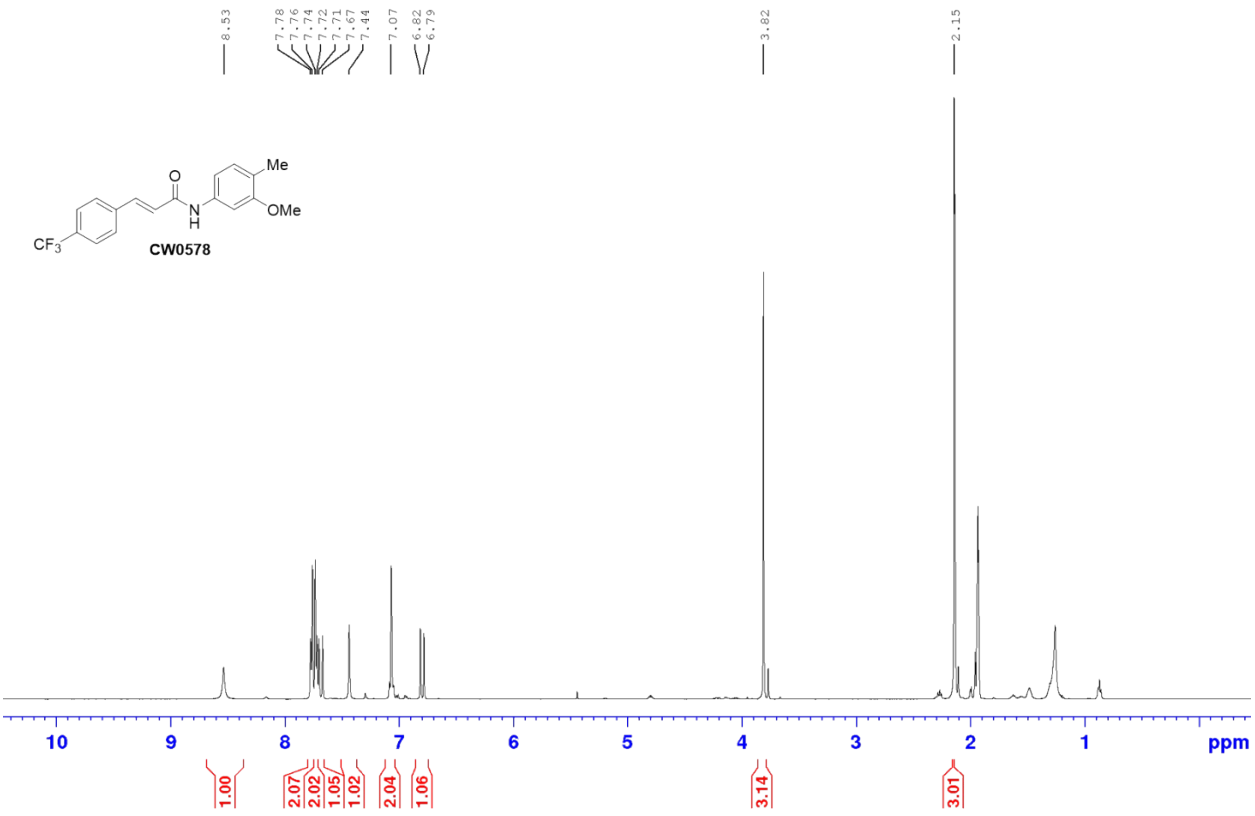
1H,CD3CN,500MHz

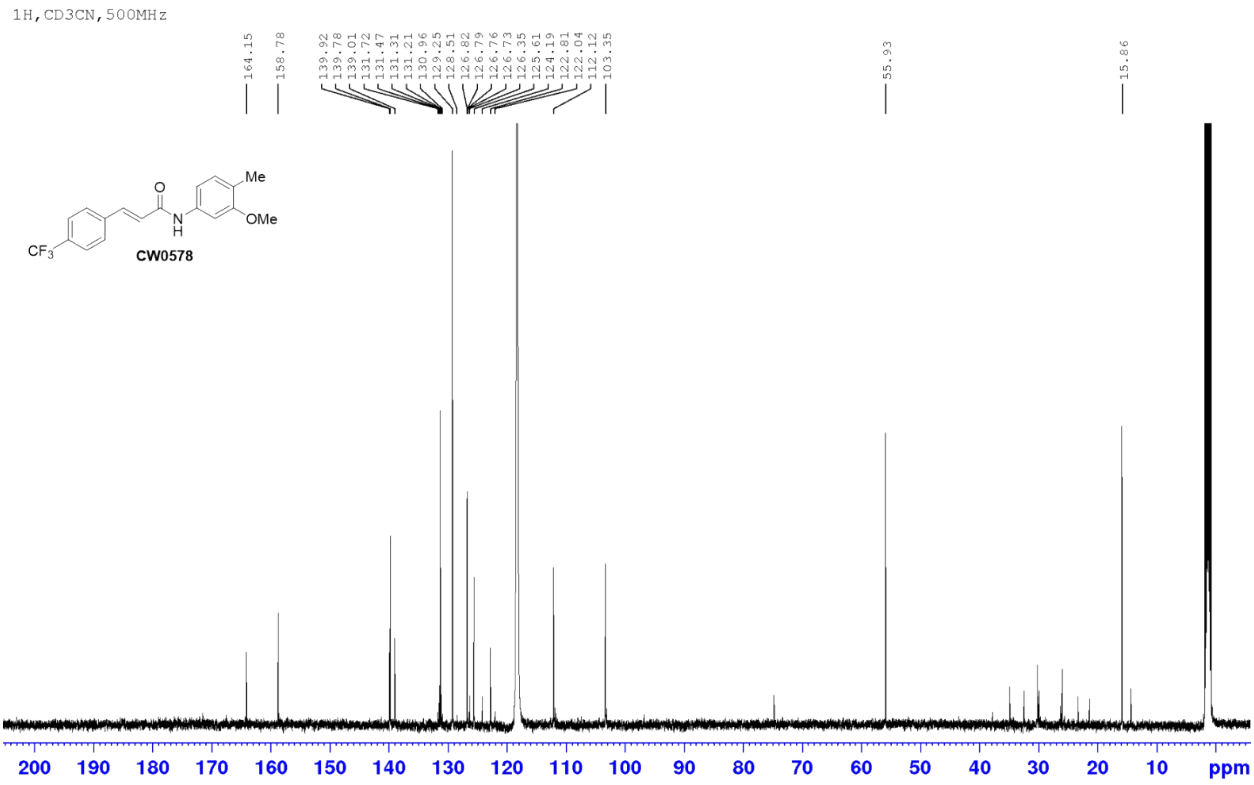


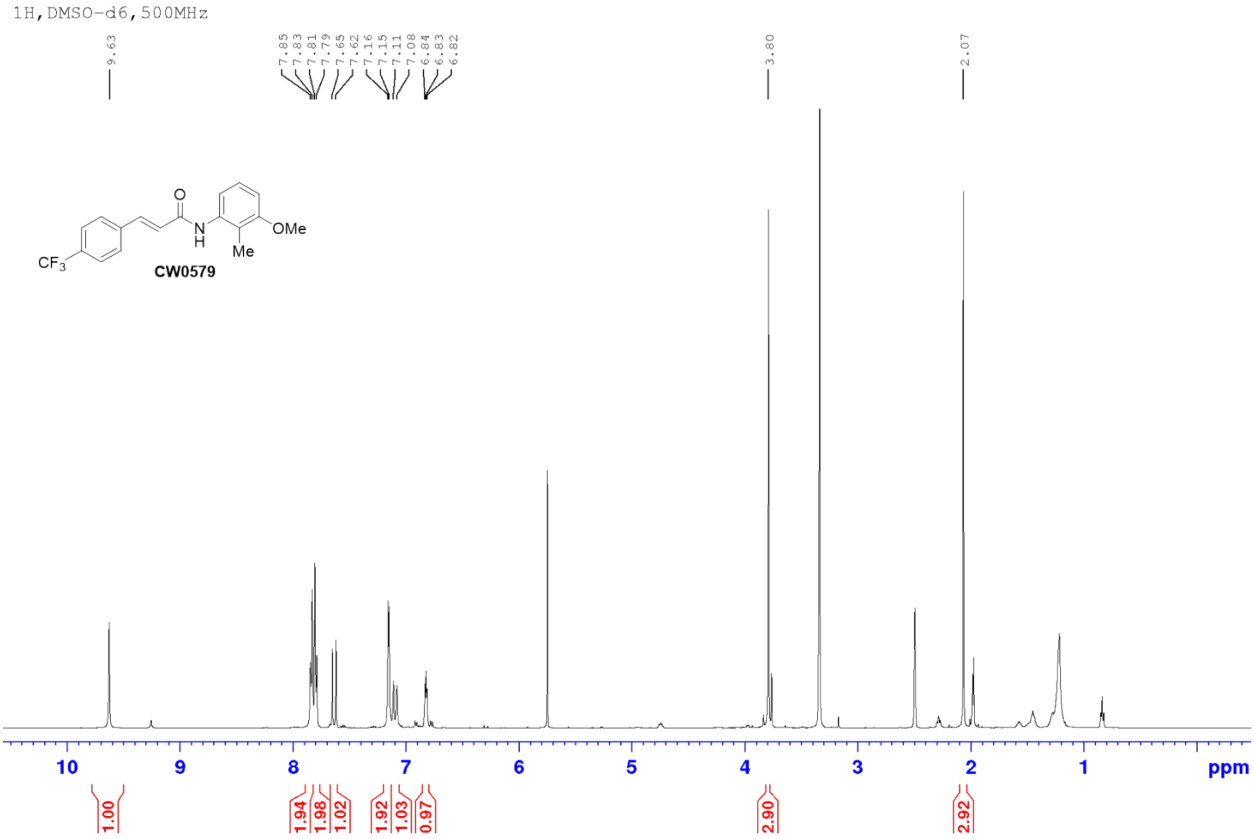
13C,CD3CN,125MHz



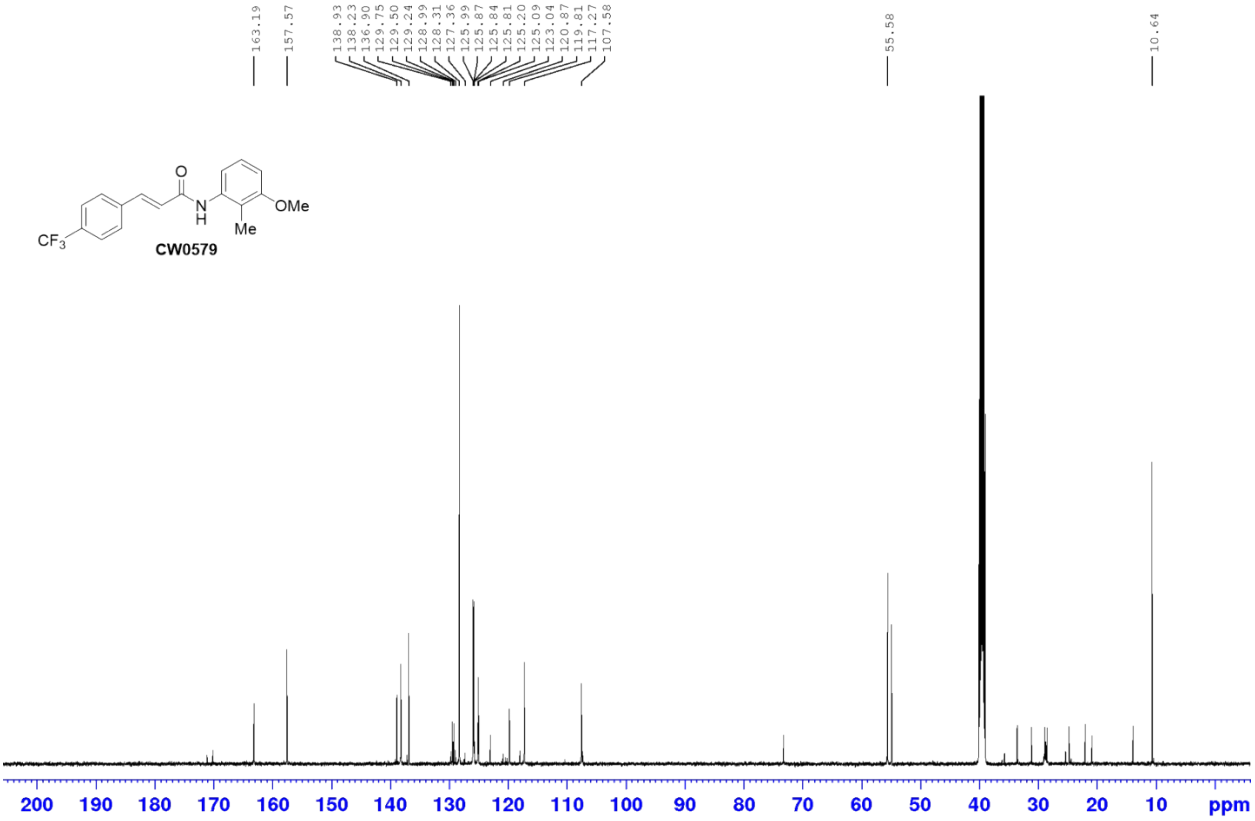
1H,CD3CN,500MHz



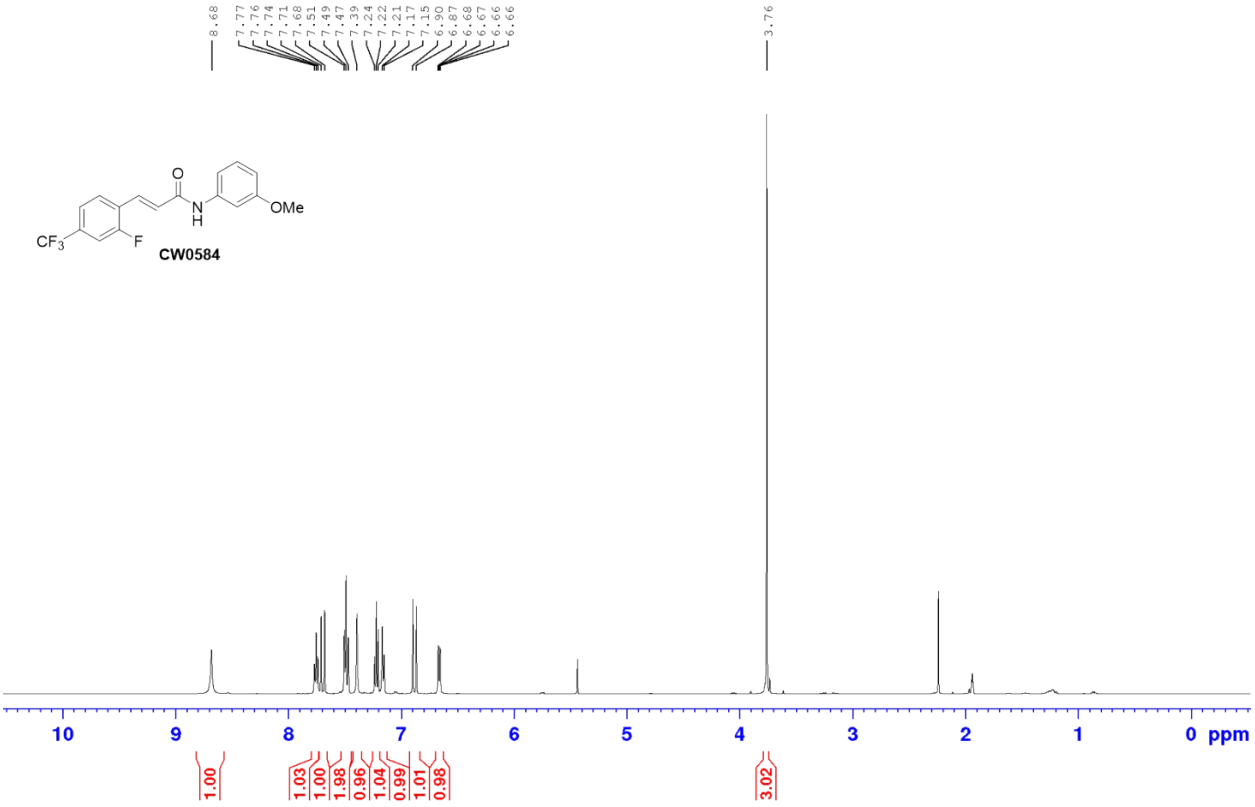

1H,CD3CN,500MHz
164.15
158.78
139.92
139.78
139.01
131.72
131.47
131.31
131.21
130.96
129.25
128.51
126.82
126.79
126.76
126.73
126.35
125.61
124.19
122.81
122.04
112.12
103.35
55.93
15.86
Me
OMe
CF3
CW0578
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


1H,DMSO-d6,500MHz
9.63
7.85
7.83
7.81
7.79
7.65
7.62
7.16
7.15
7.11
7.08
6.84
6.83
6.82
3.80
2.07
OMe
Me
CF3
CW0579
10 9 8 7 6 5 4 3 2 1 ppm
1.00
1.94
1.98
1.02
1.92
1.03
0.97
2.90
2.92

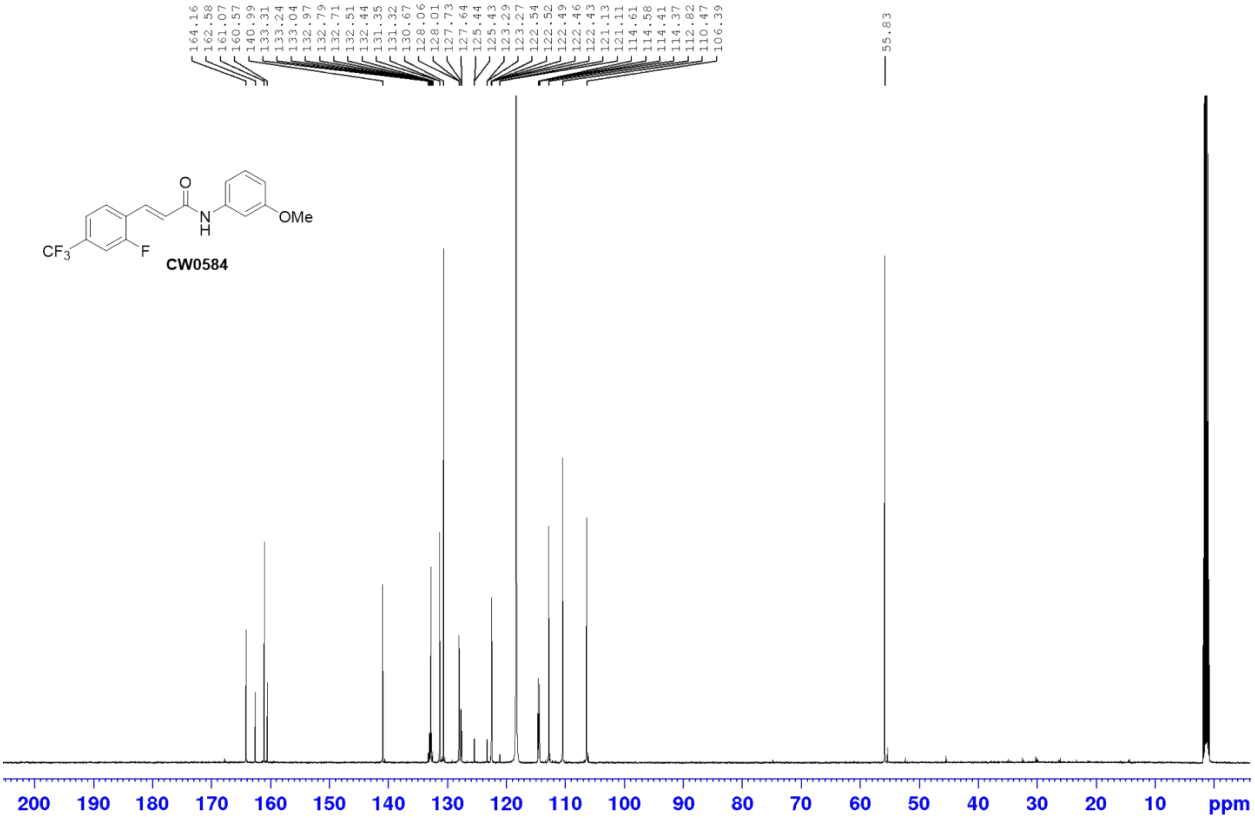
13C,DMSO-d6,125MHz



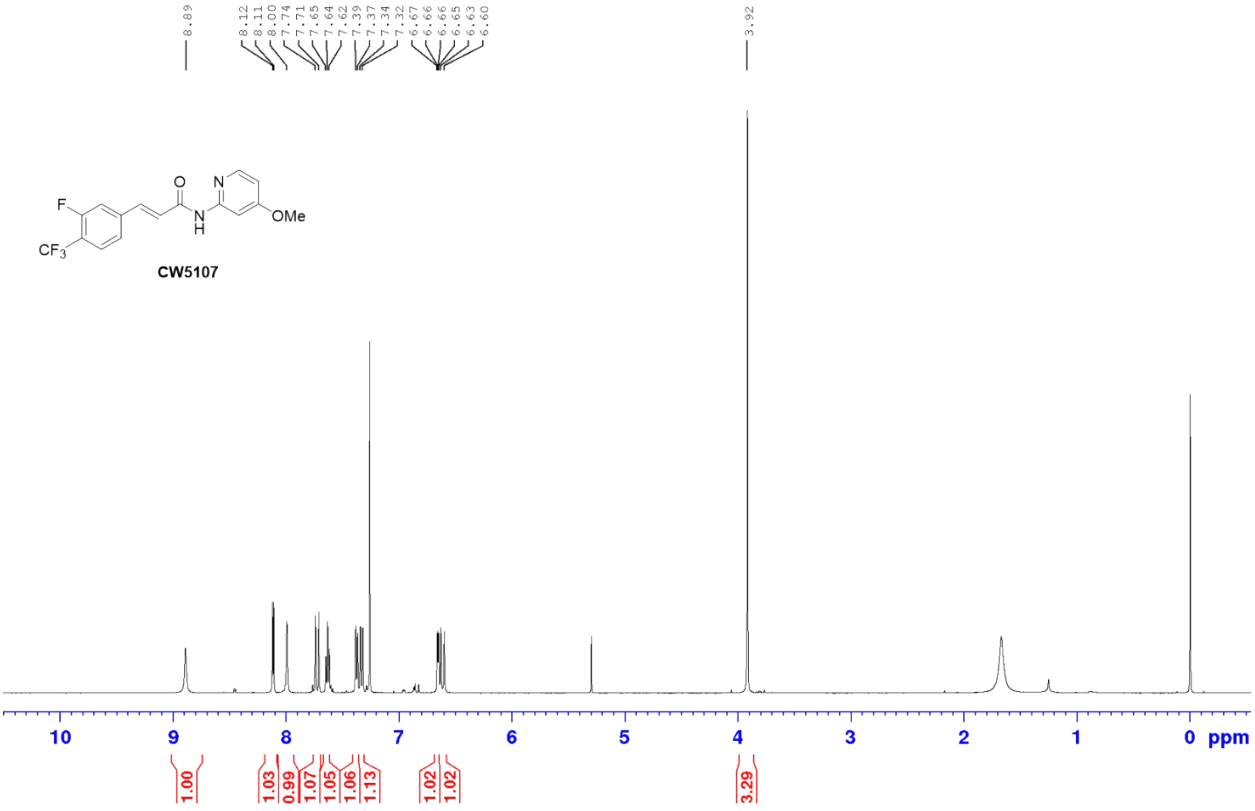
1H,CD3CN,500MHz



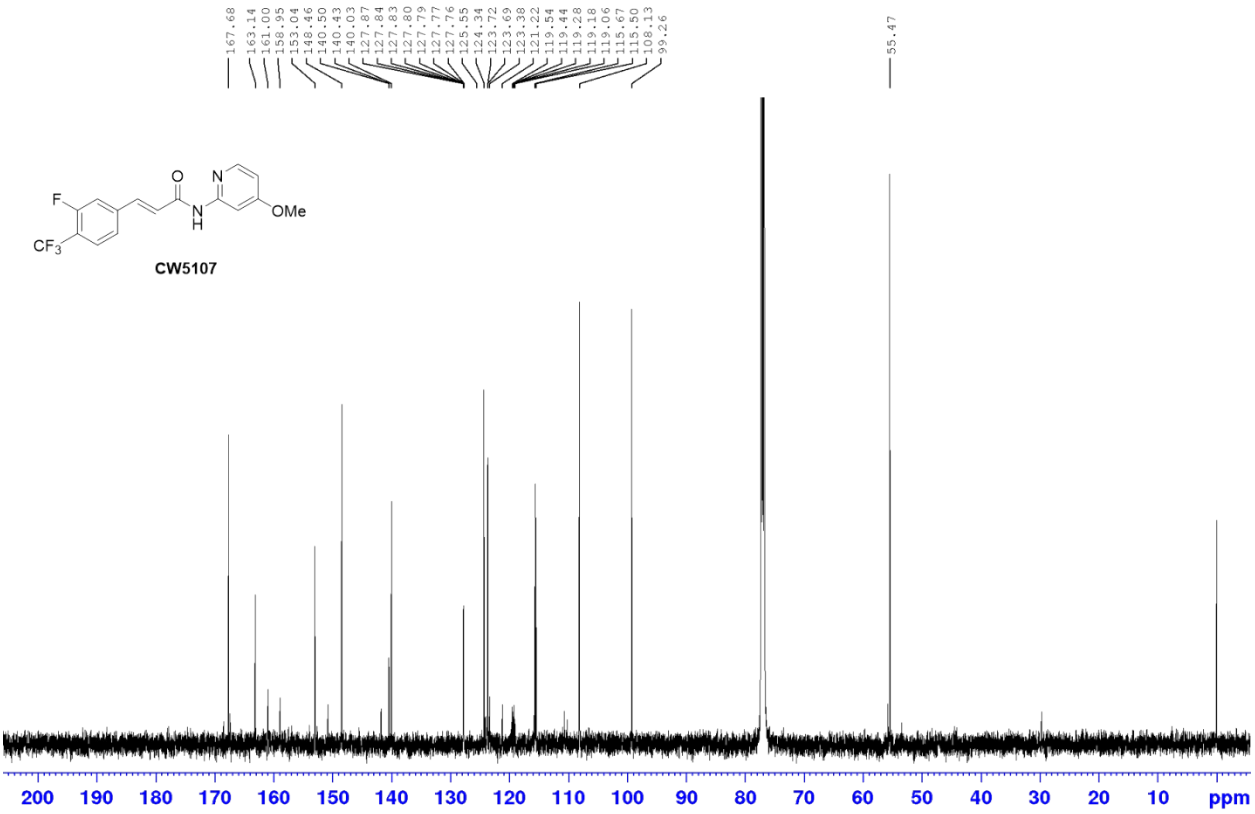
13C,CD3CN,125MHz



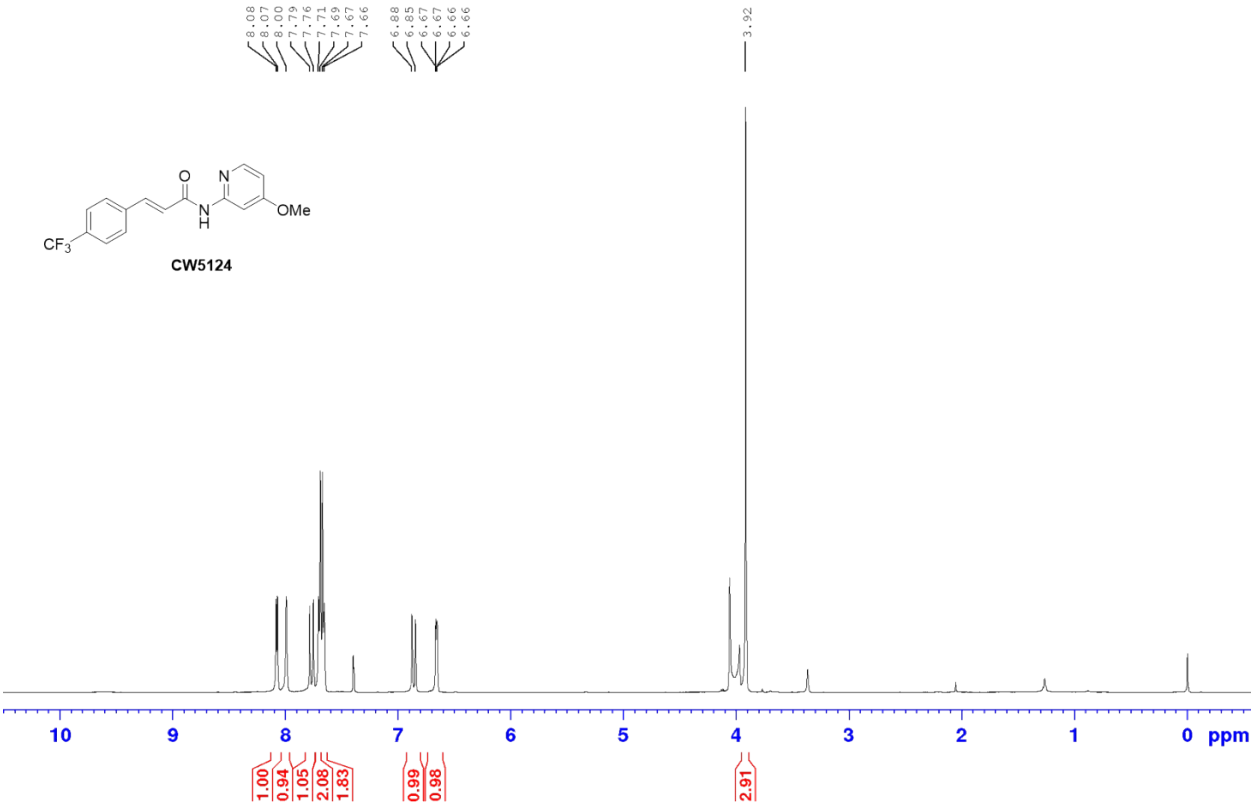
1H,CDCl3,500MHz



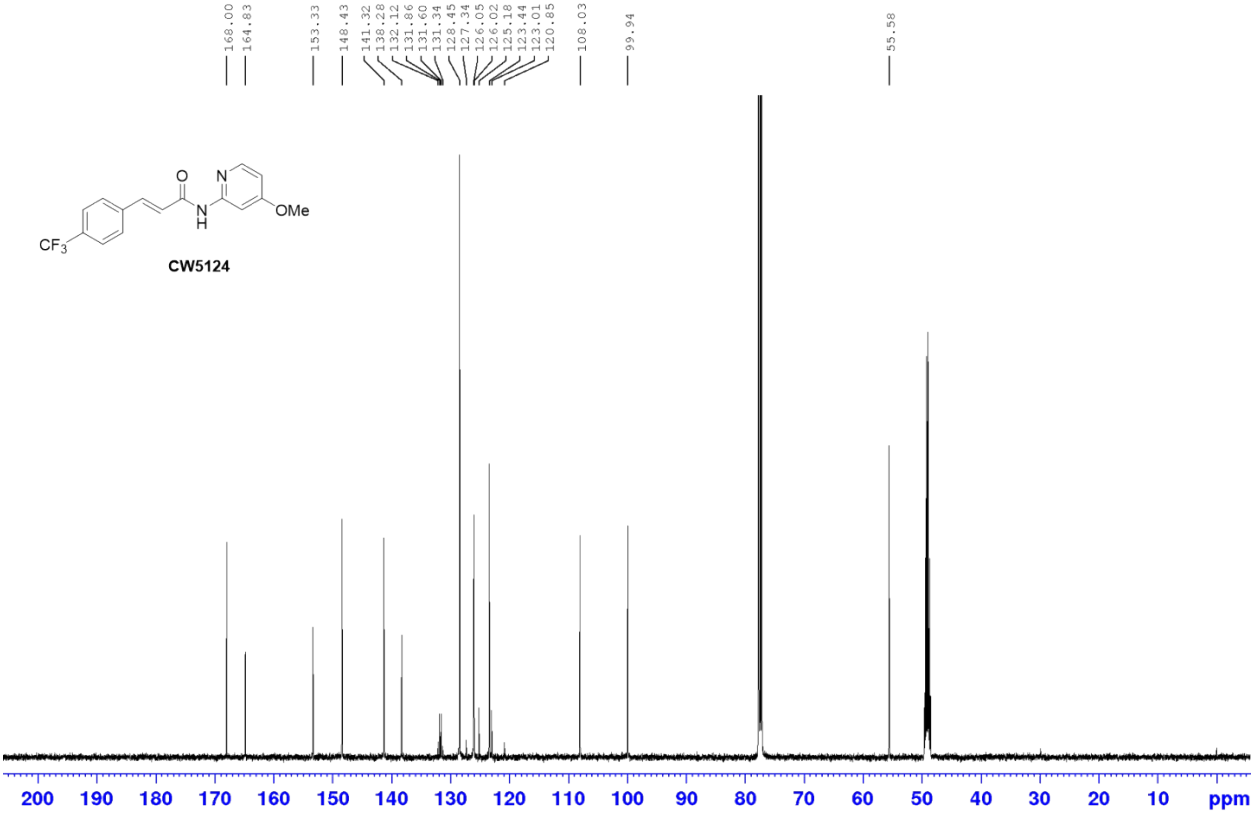
13C,CDCl3,125MHz



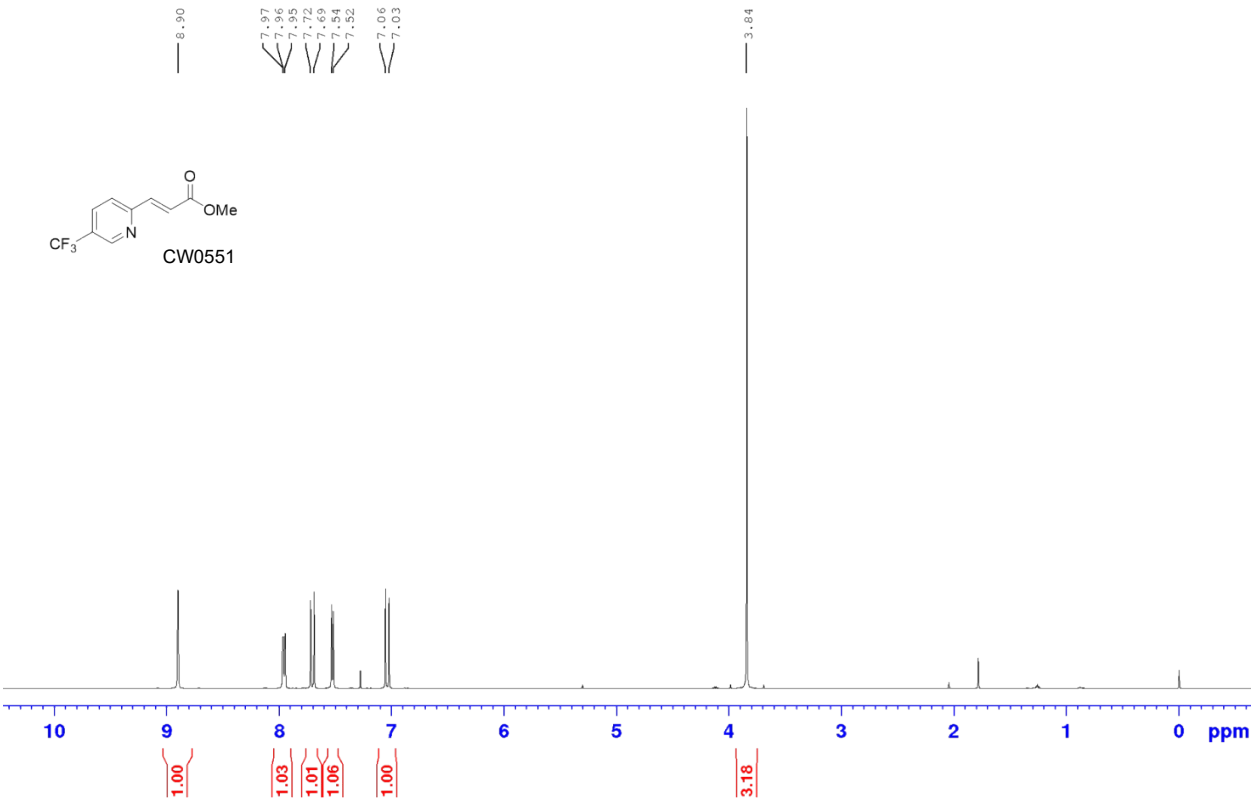
1H,CDCl3/CD3OD,500MHz



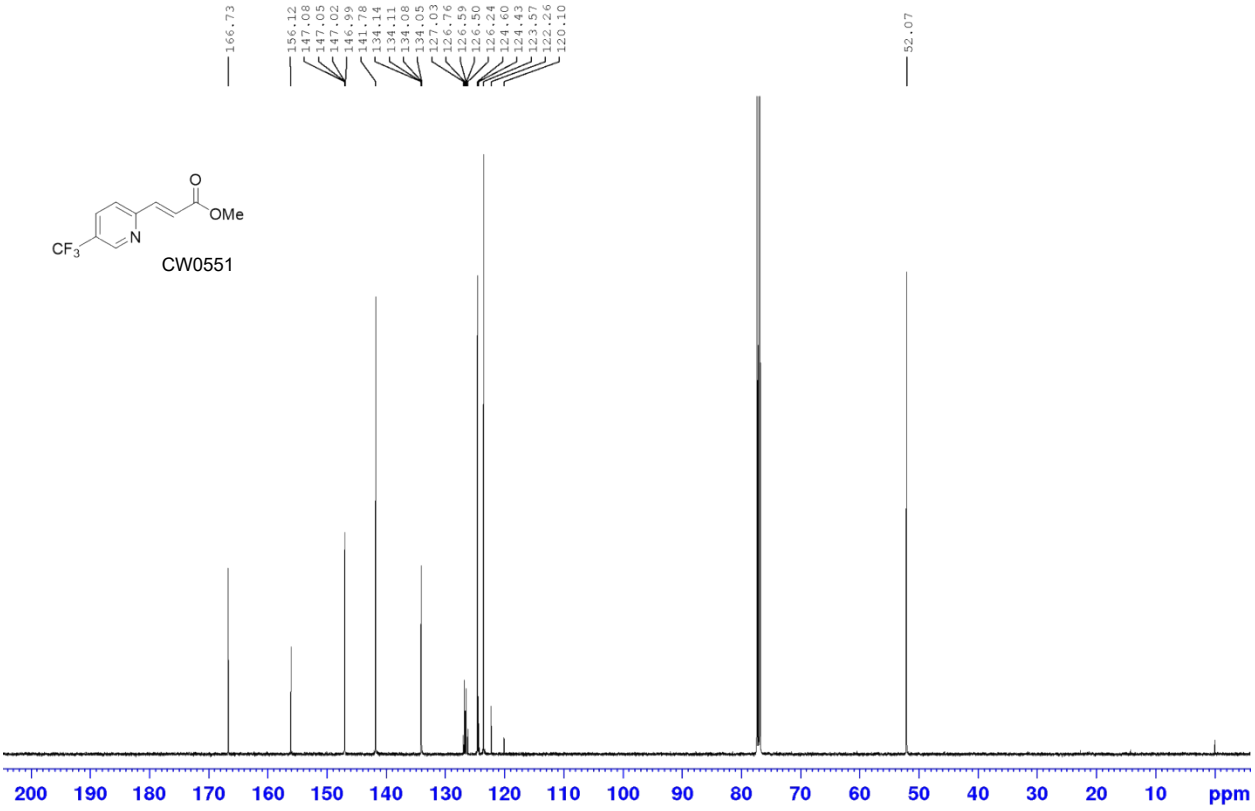
13C,CDCl3/CD3OD,125MHz



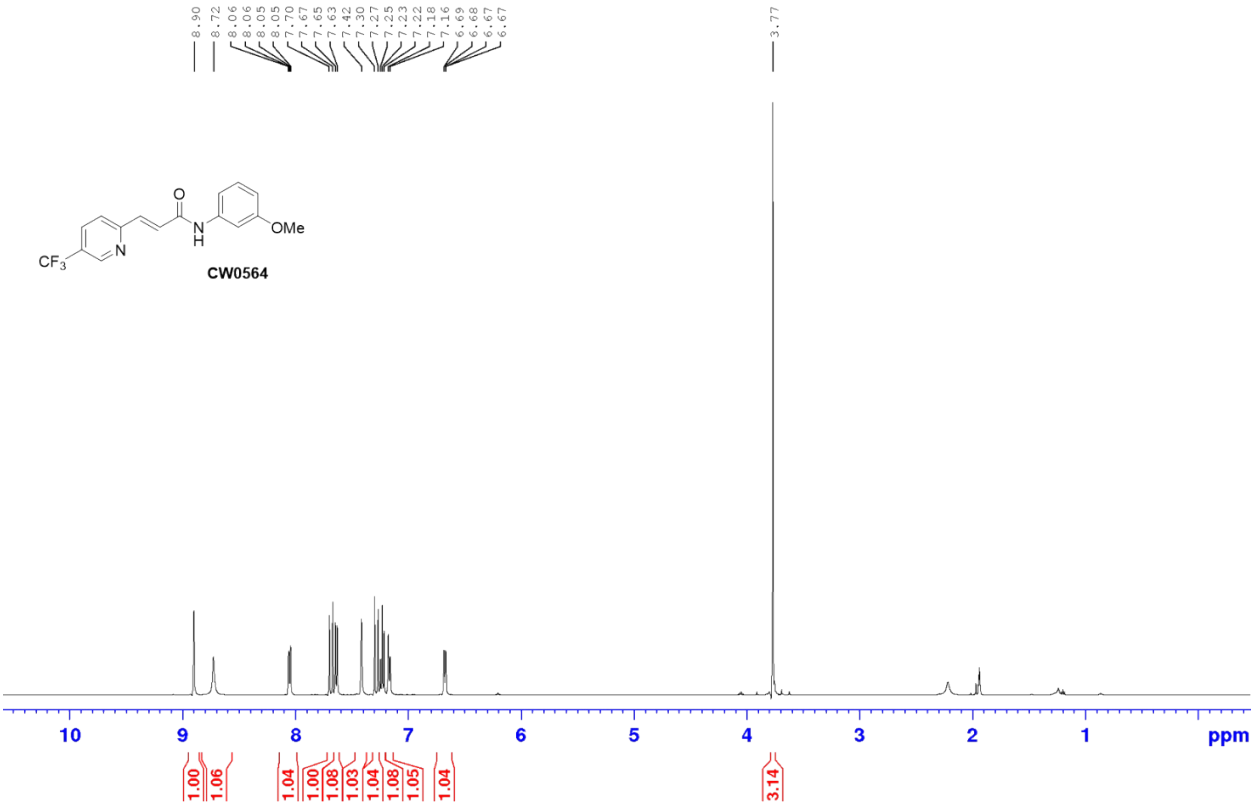
1H,CDCl3,500MHz



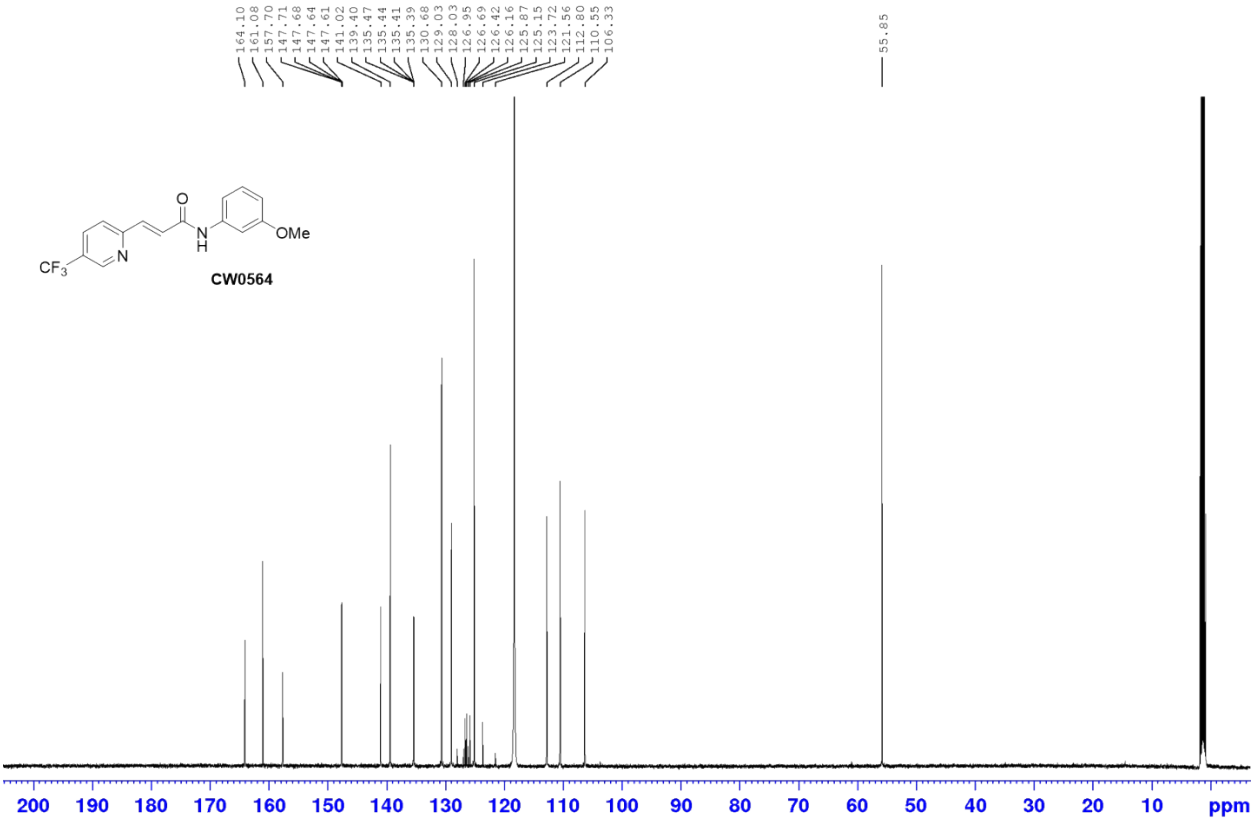
13C,CDCl3,125MHz



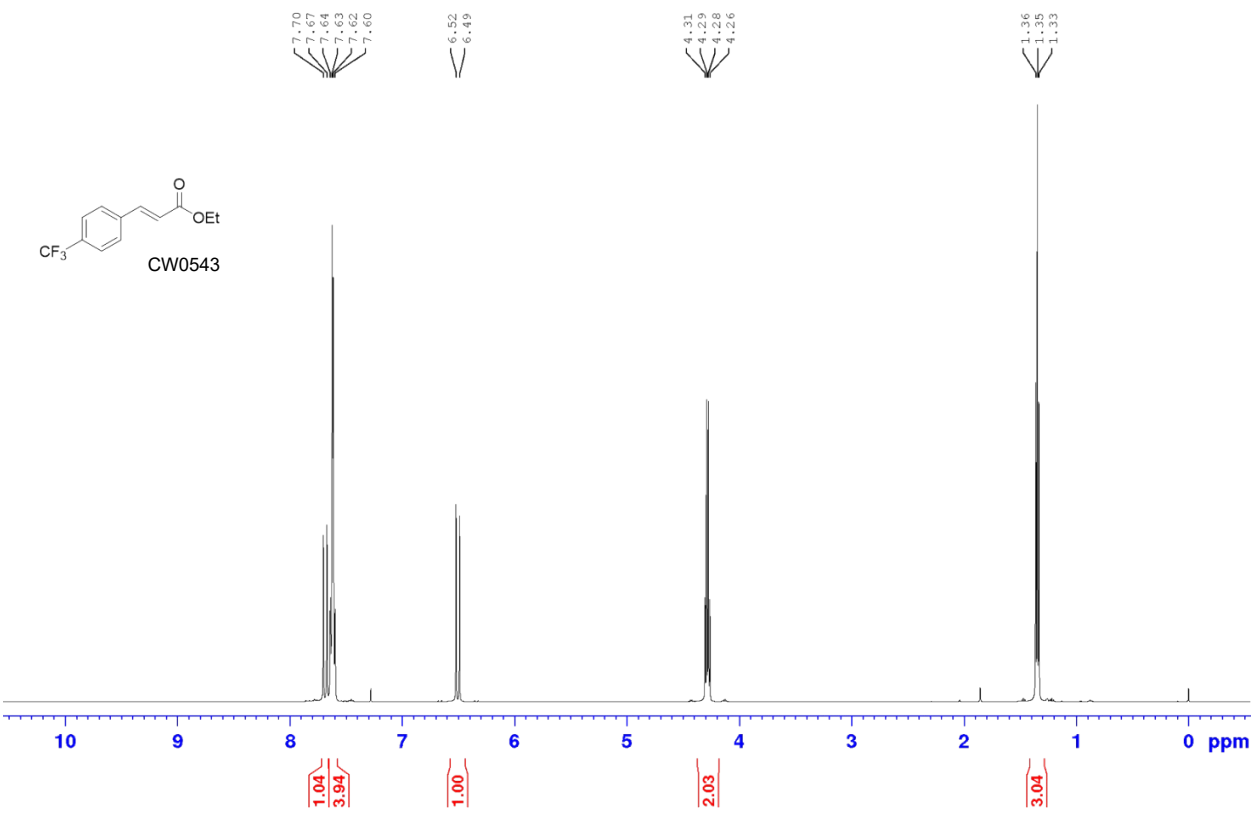
1H,CD3CN,500MHz



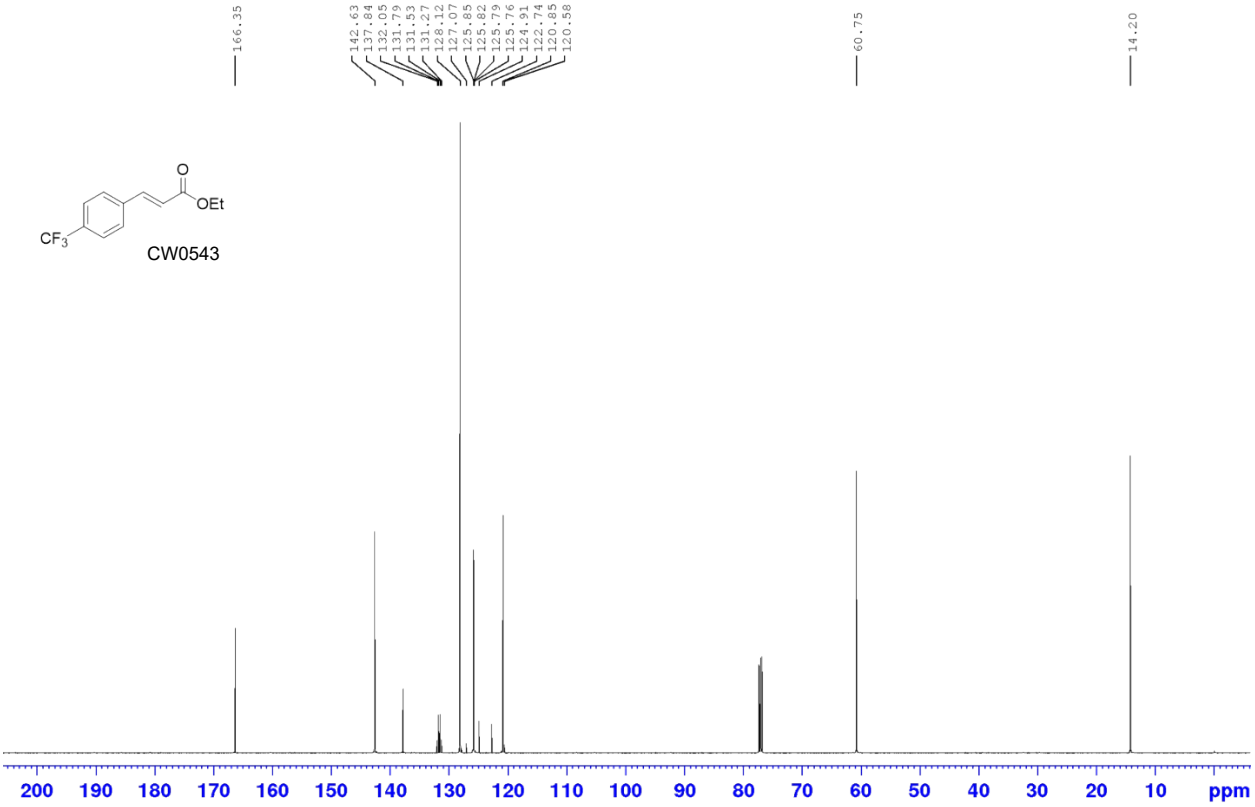
13C,CD3CN,125MHz



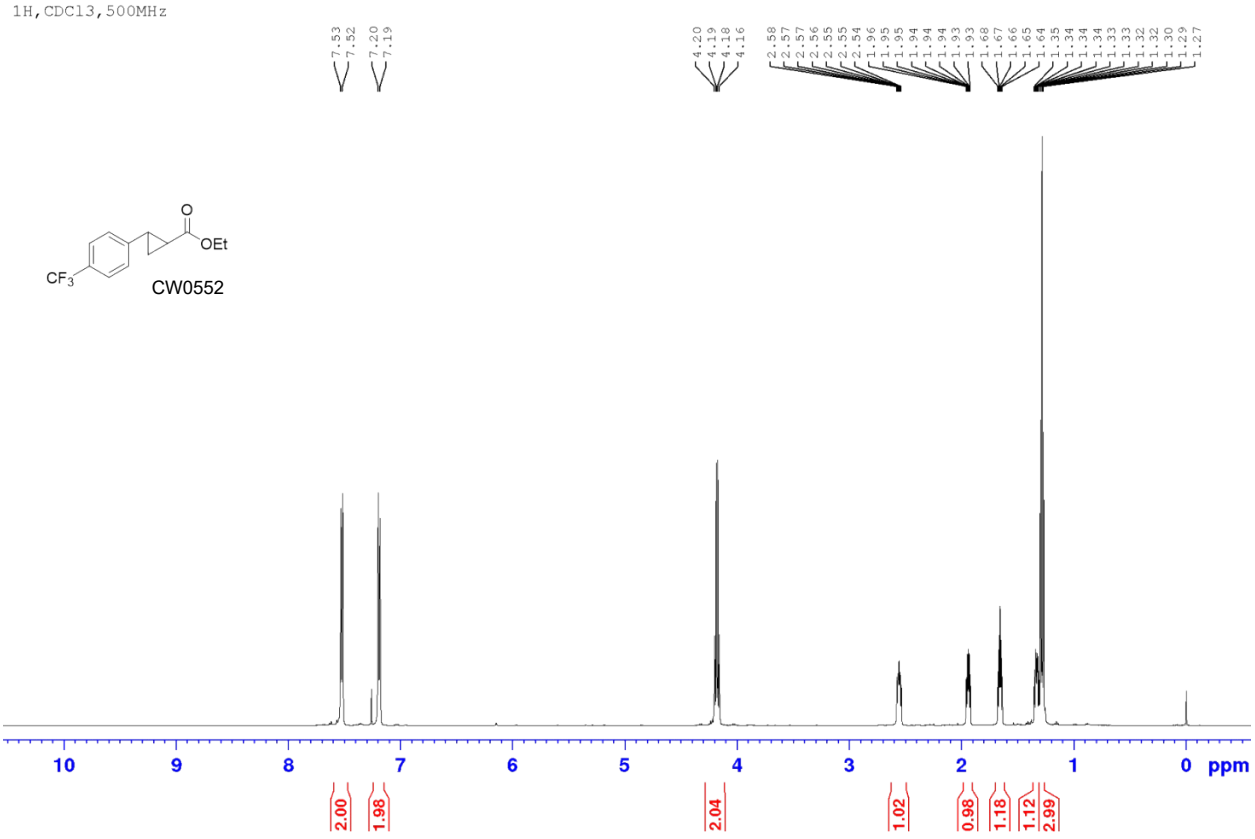
1H,CDCl3,500MHz



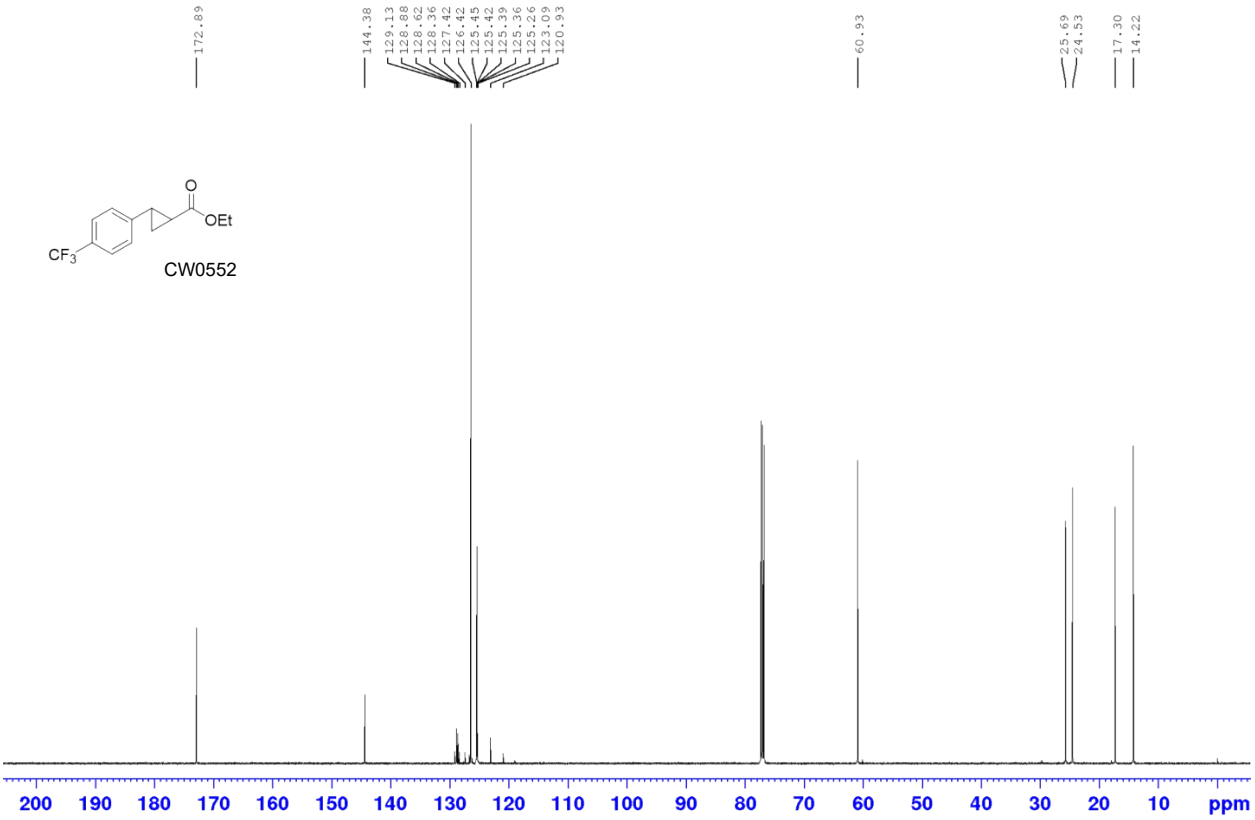
13C,CDCl3,125MHz



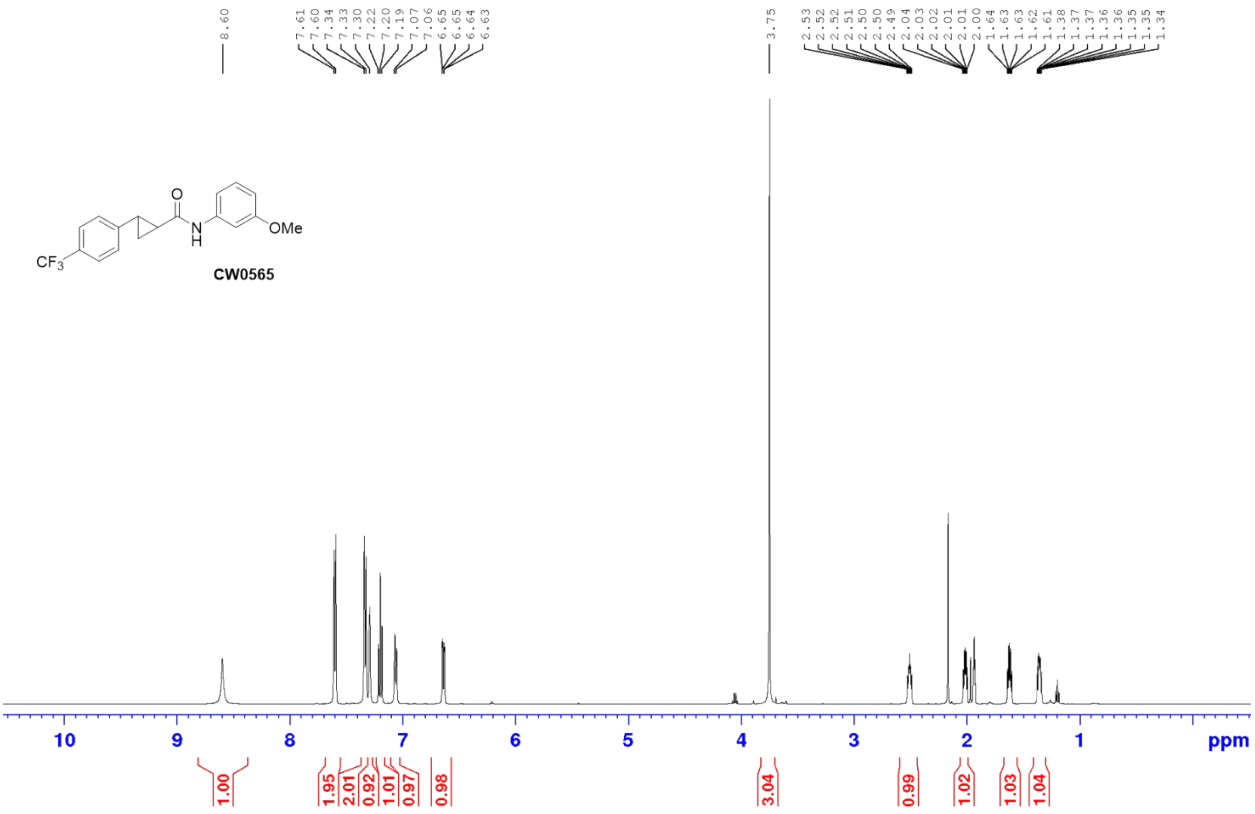
1H,CDCl3,500MHz

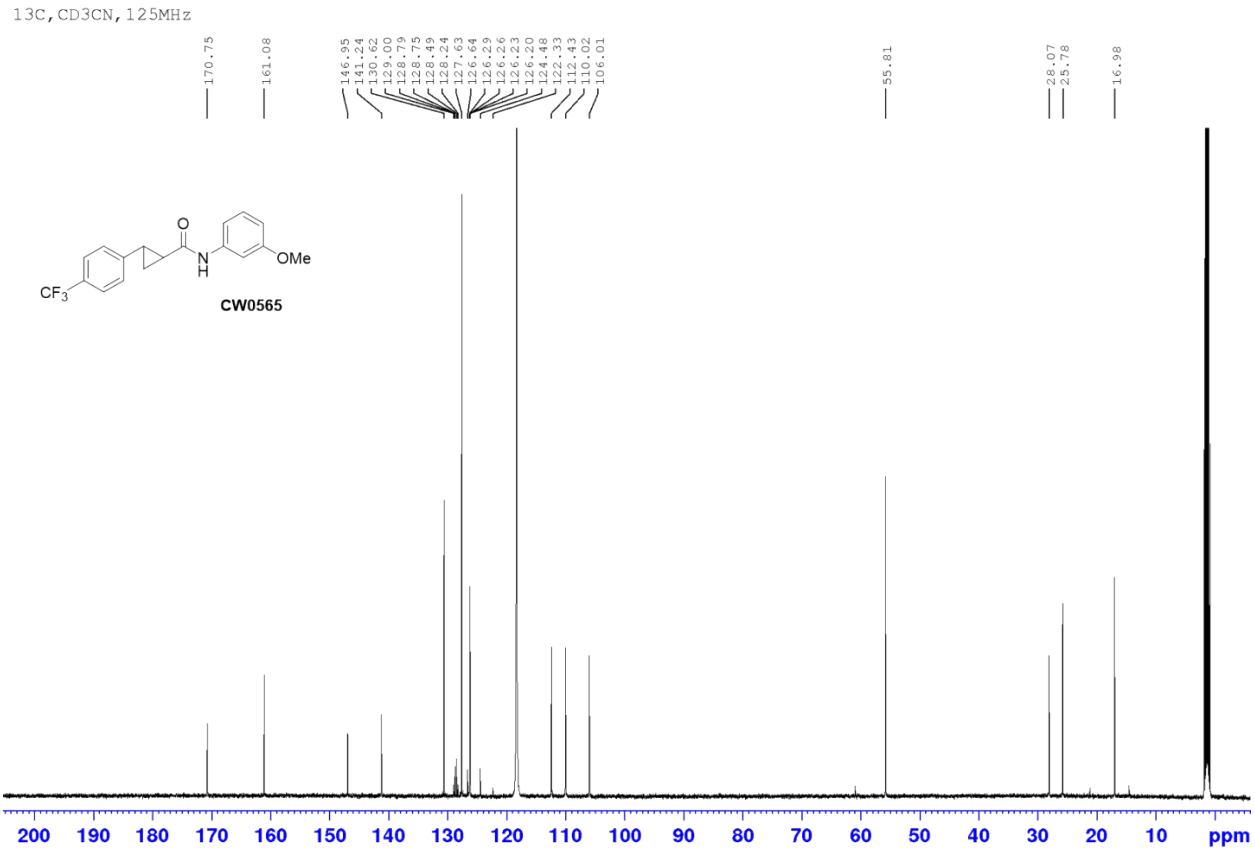


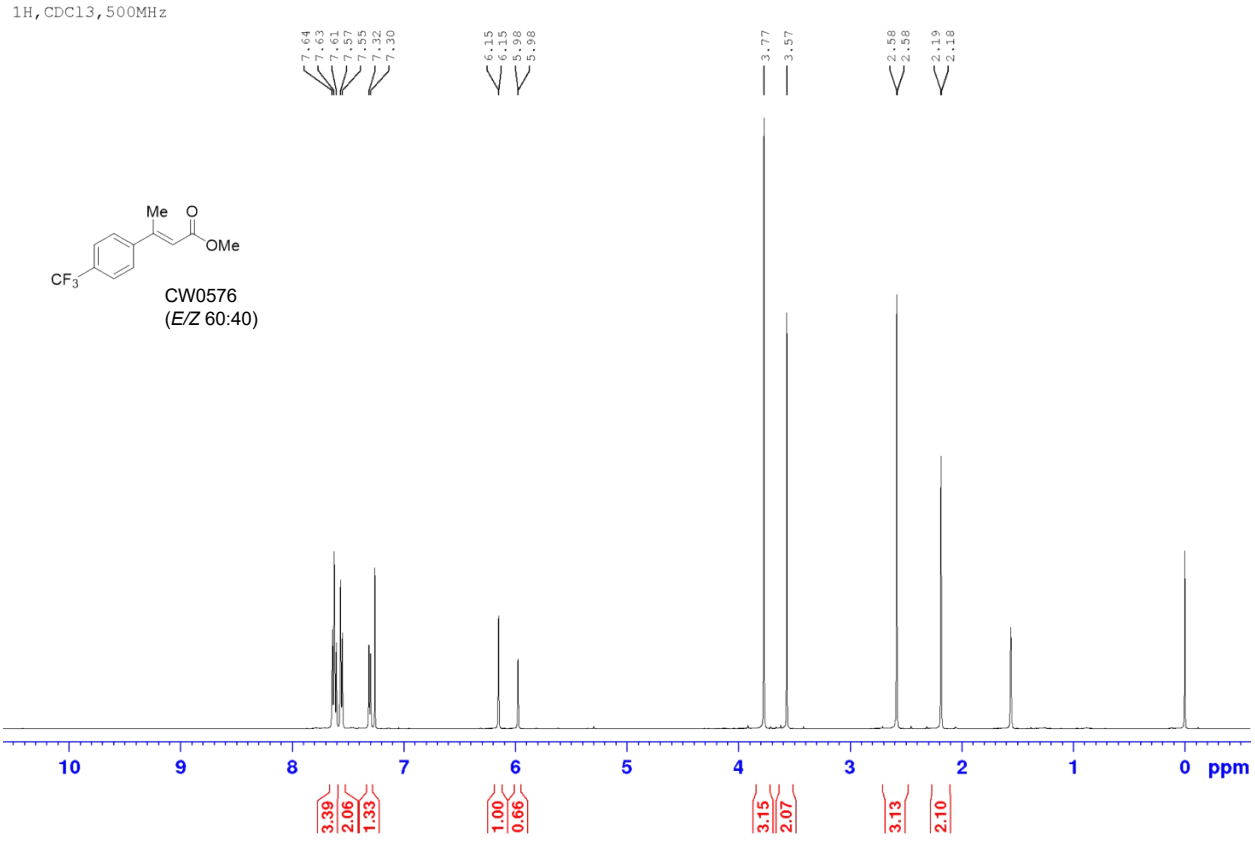
13C,CDCl3,125MHz

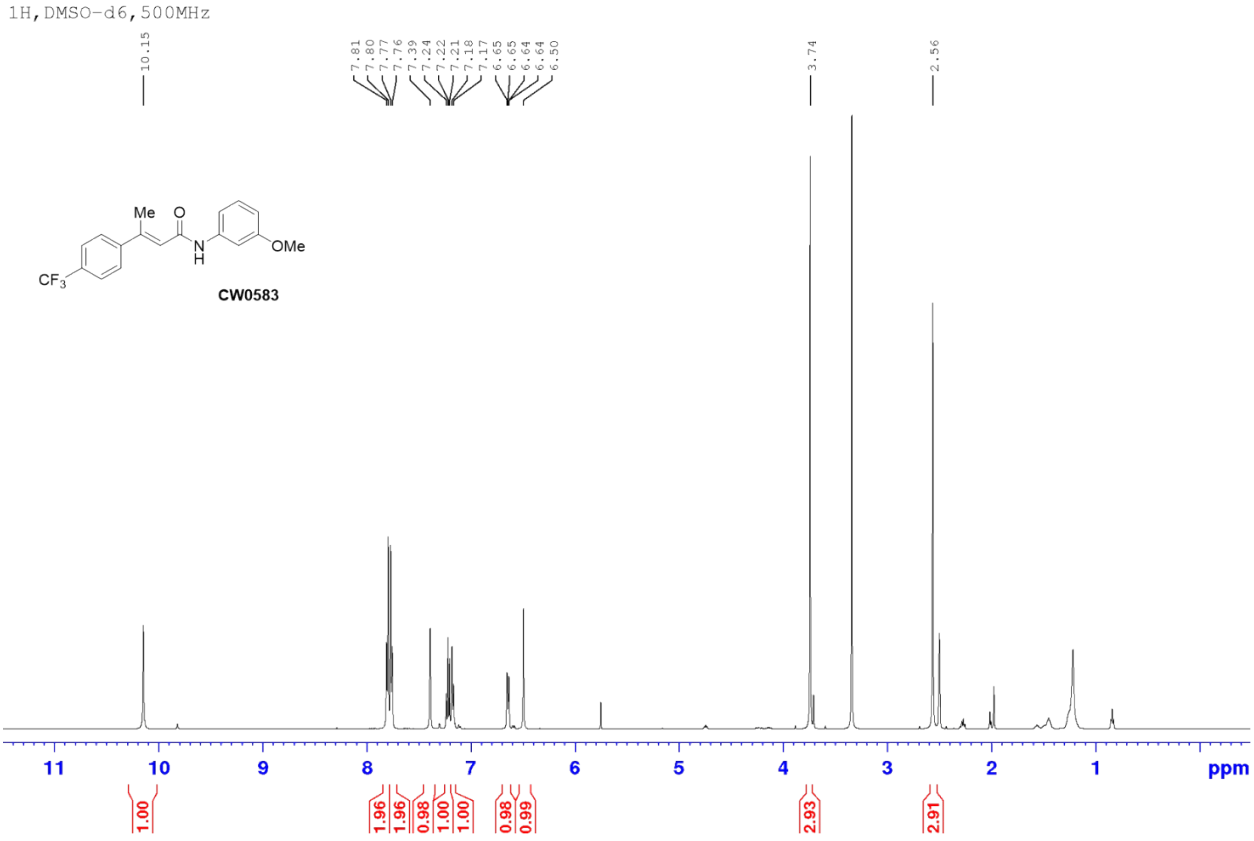


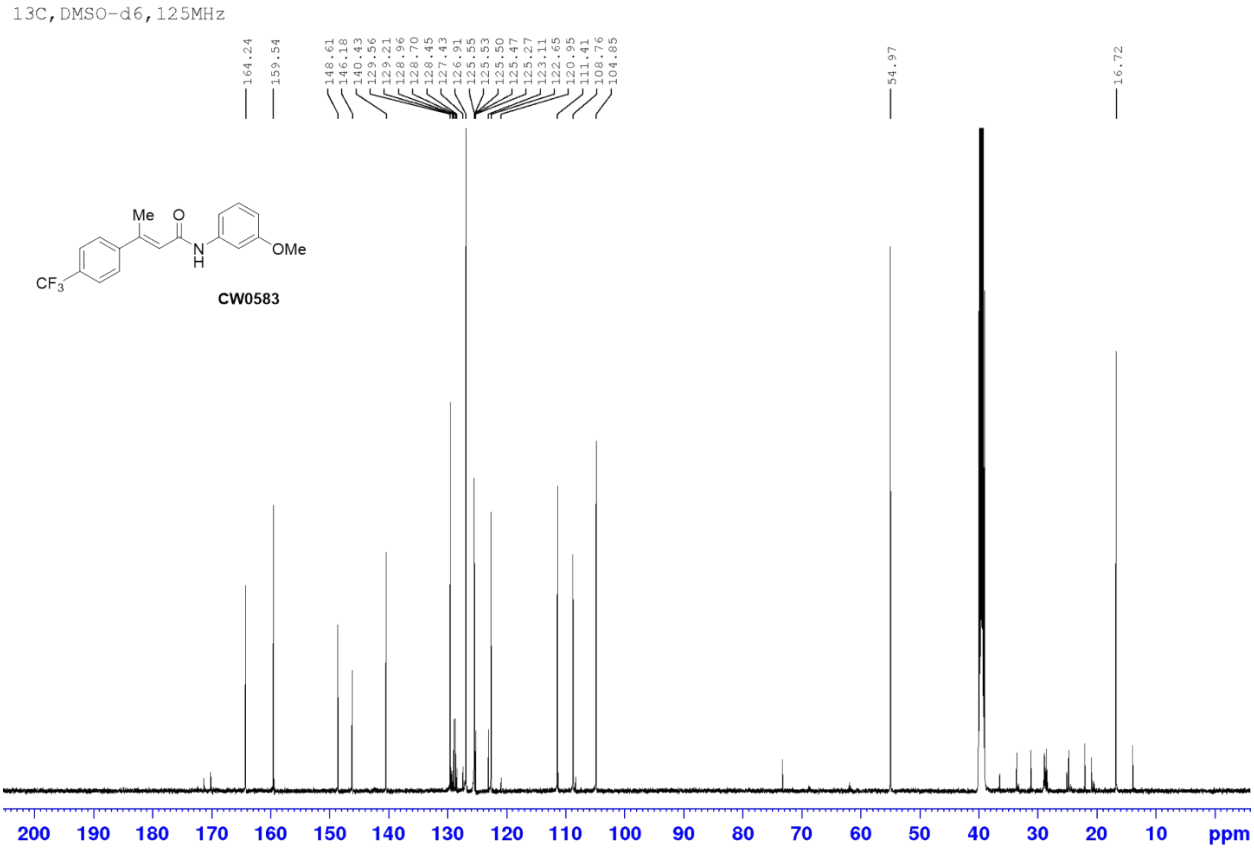
1H,CD3CN,500MHz



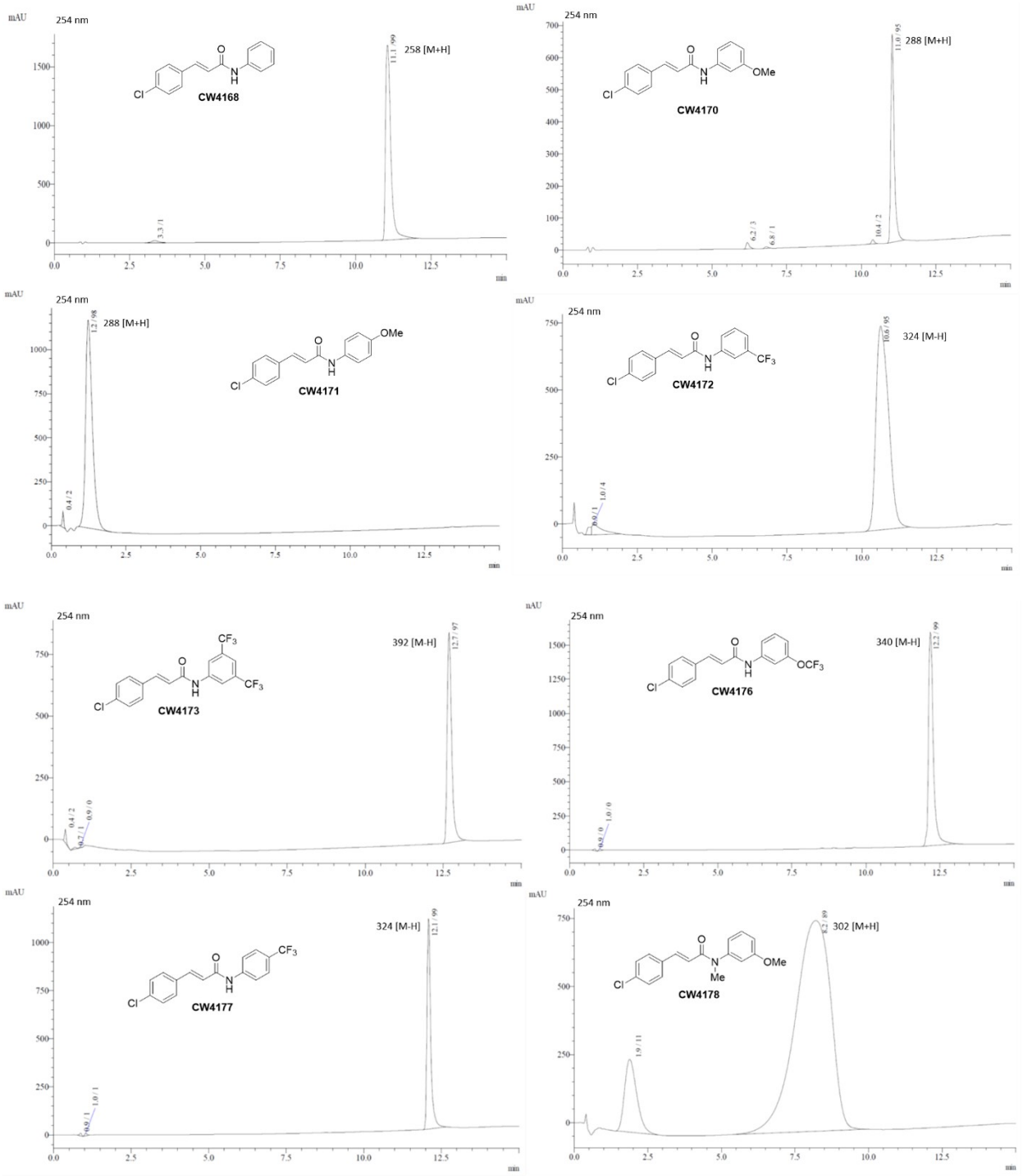

13C,CD3CN,125MHz
170.75
161.08
146.95
141.24
130.62
129.00
128.79
128.75
128.49
128.24
127.63
126.64
126.29
126.26
126.23
126.20
124.48
122.33
112.43
110.02
106.01
55.81
28.07
25.78
16.98
O
N
H
OMe
CF3
CW0565
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

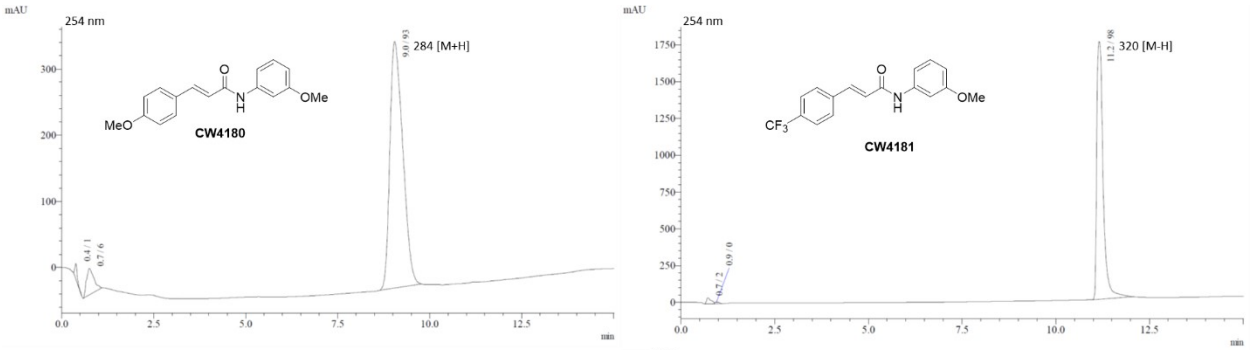

1H,CDCl3,500MHz
7.64
7.63
7.61
7.57
7.55
7.32
7.30
6.15
6.15
5.98
5.98
3.77
3.57
2.58
2.58
2.19
2.18
Me
O
OMe
CF3
CW0576
(E/Z 60:40)
10 9 8 7 6 5 4 3 2 1 0 ppm
3.39
2.06
1.33
1.00
0.66
3.15
2.07
3.13
2.10

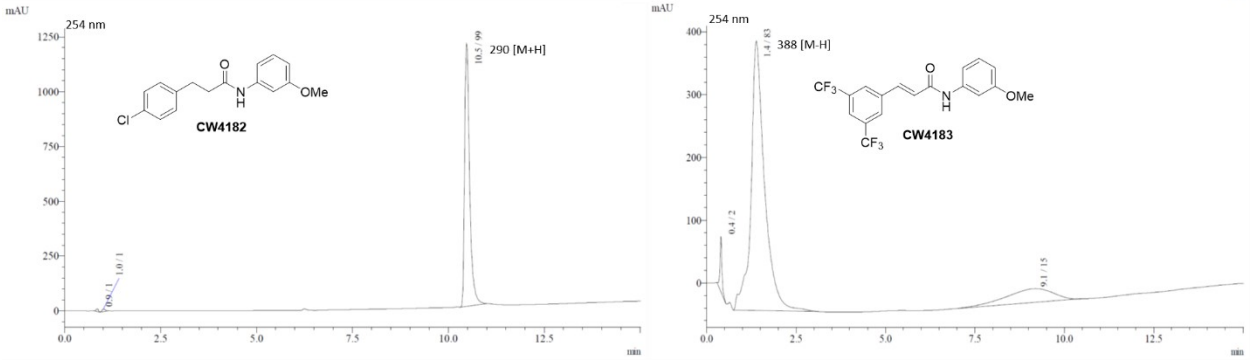

1H,DMSO-d6,500MHz
10.15
7.81
7.80
7.77
7.76
7.39
7.24
7.22
7.21
7.18
7.17
6.65
6.65
6.64
6.64
6.50
3.74
2.56
Me
O
N
H
OMe
CF3
CW0583
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.96
1.96
0.98
1.00
1.00
0.98
0.99
2.93
2.91

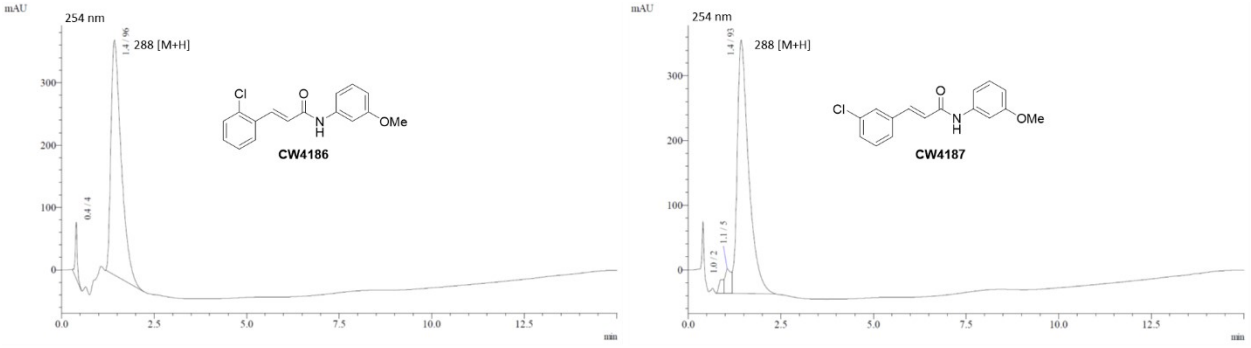

13C,DMSO-d6,125MHz
164.24
159.54
148.61
146.18
140.43
129.56
129.21
128.96
128.70
128.45
127.43
126.91
125.55
125.53
125.50
125.47
125.27
123.11
122.65
120.95
111.41
108.76
104.85
54.97
16.72
Me
O
N
H
OMe
CF3
CW0583
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

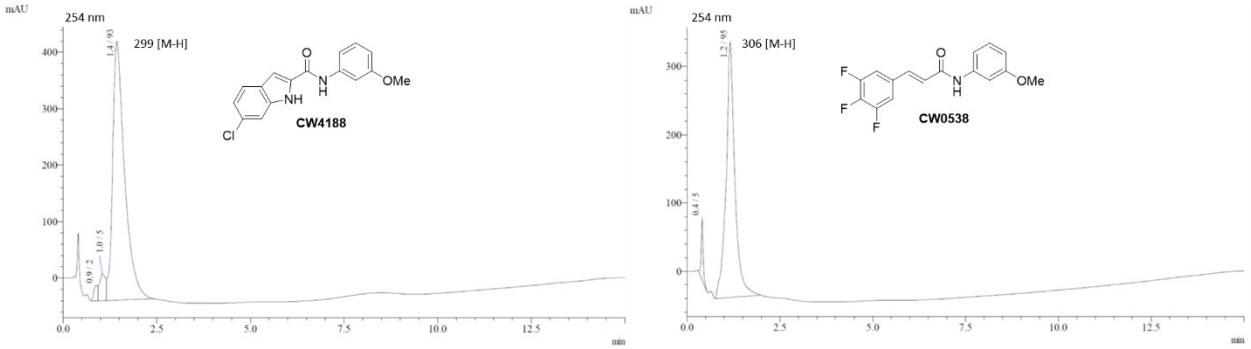
LC/MS Chromatogram HSD17B7 Inhibitors

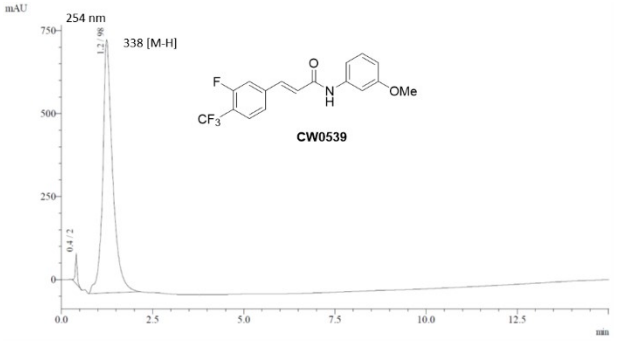


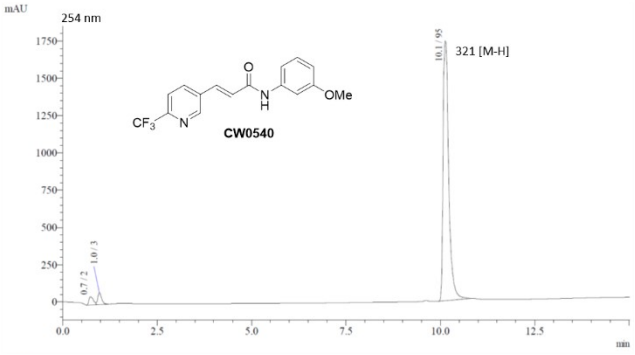

mAU
254 nm
284 [M+H]
MeO
OMe
CW4180
mAU
254 nm
320 [M-H]
CF3
OMe
CW4181

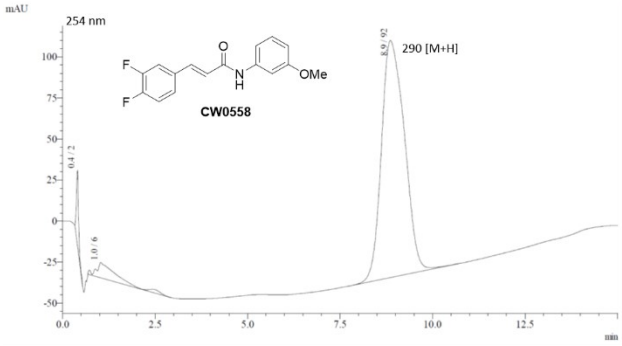

mAU
254 nm
290 [M+H]
Cl
OMe
CW4182
mAU
254 nm
388 [M-H]
CF3
CF3
OMe
CW4183

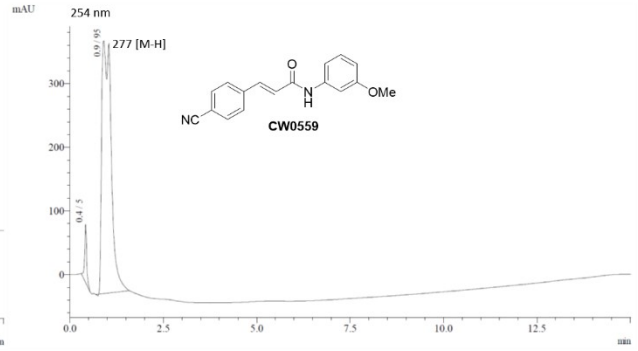

mAU
254 nm
288 [M+H]
Cl
OMe
CW4186
mAU
254 nm
288 [M+H]
Cl
OMe
CW4187

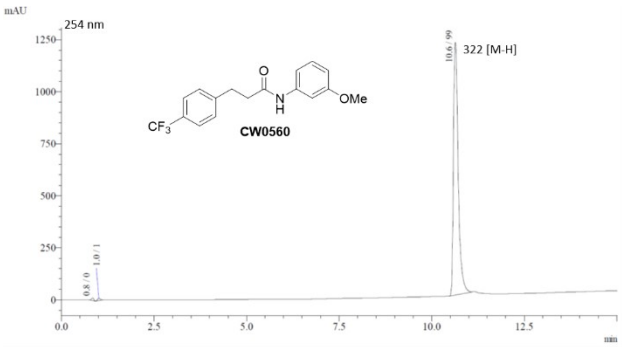

mAU
254 nm
299 [M-H]
NH
Cl
OMe
CW4188
mAU
254 nm
306 [M-H]
F
F
F
OMe
CW0538

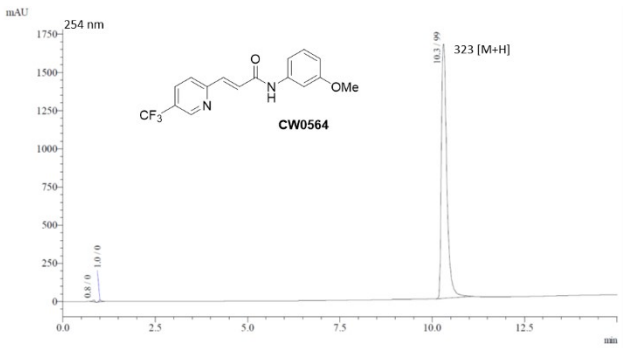

mAU
254 nm
338 [M-H]
CW0539

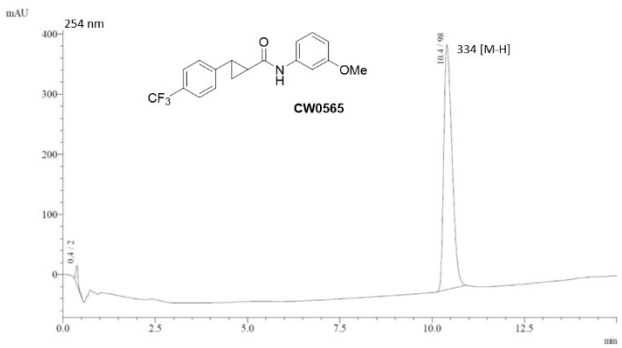

mAU
254 nm
321 [M-H]
CW0540

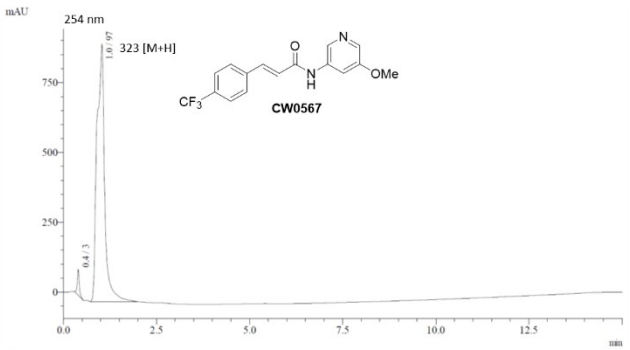

mAU
254 nm
290 [M+H]
CW0558

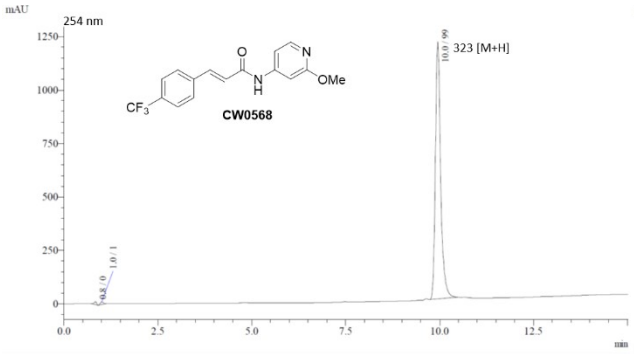

mAU
254 nm
277 [M-H]
CW0559

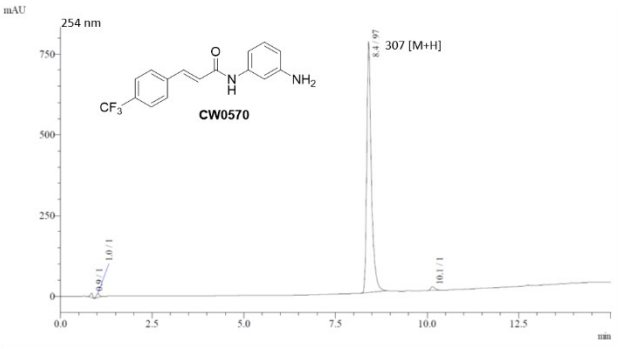

mAU
254 nm
322 [M-H]
CW0560

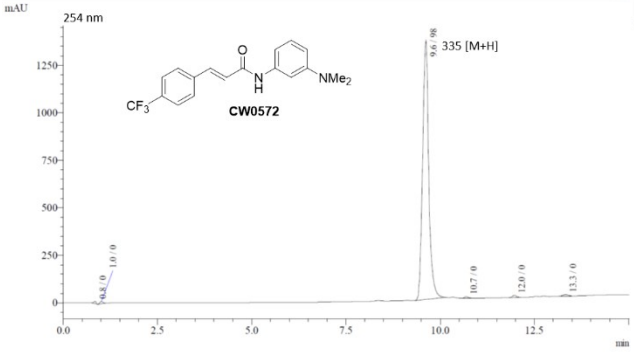

mAU
254 nm
323 [M+H]
CW0564

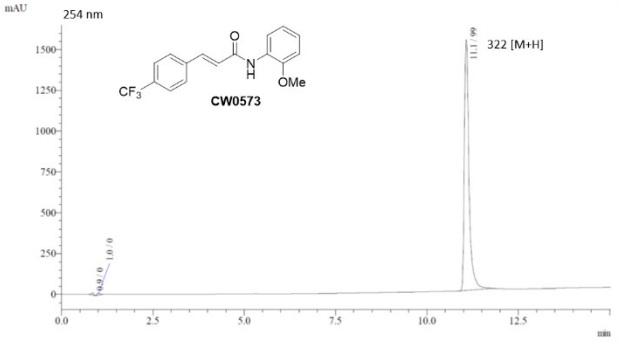

mAU
254 nm
334 [M-H]
CW0565

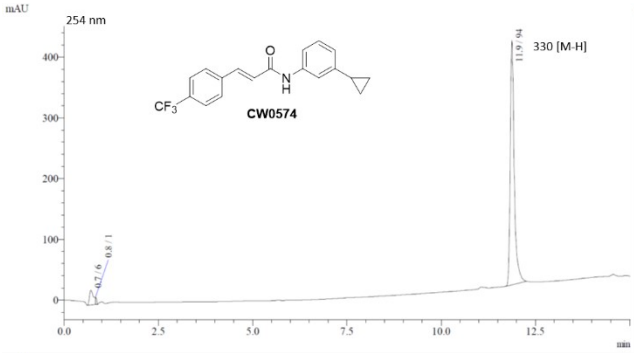

mAU
254 nm
323 [M+H]
CW0567

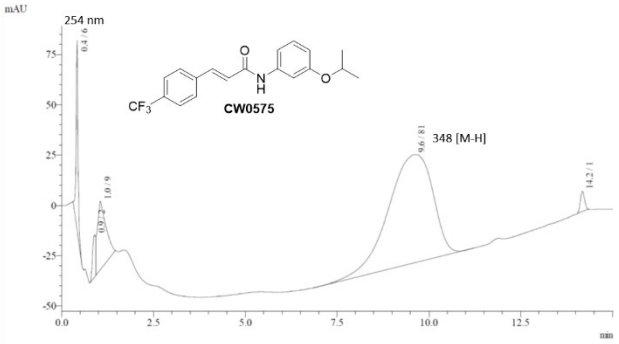

mAU
254 nm
323 [M+H]
CW0568

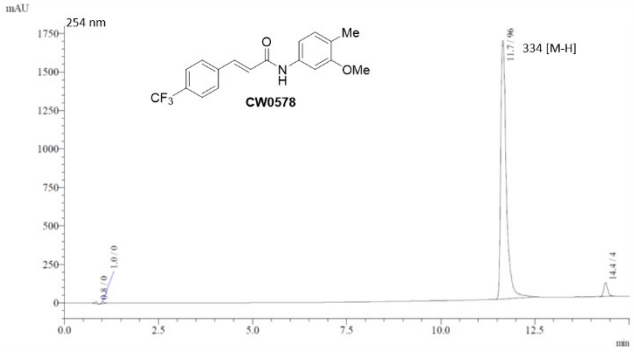

mAU
254 nm
307 [M+H]
CW0570

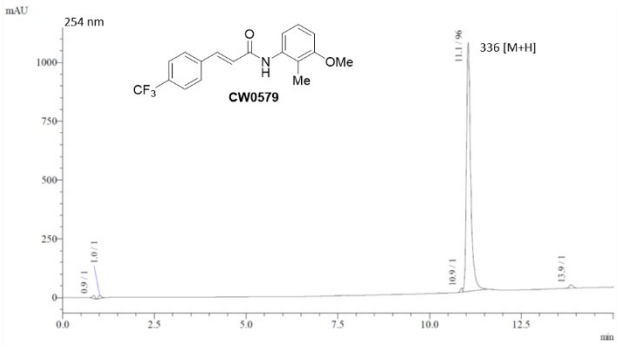

mAU
254 nm
335 [M+H]
CW0572

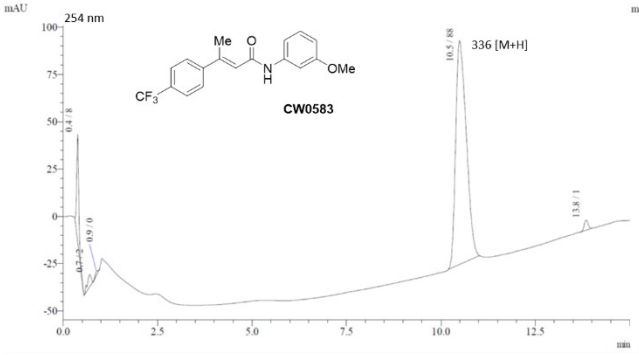

mAU
254 nm
322 [M+H]
CW0573

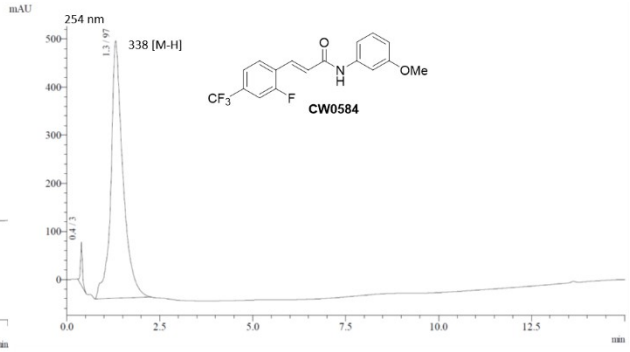

mAU
254 nm
330 [M-H]
CW0574

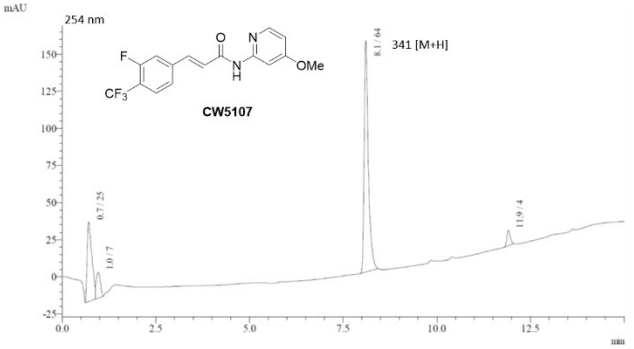

mAU
254 nm
348 [M-H]
CW0575

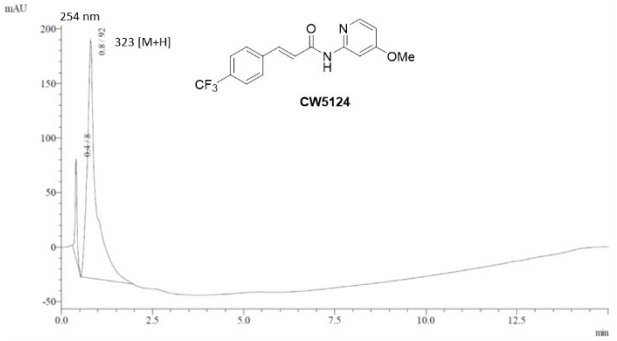

mAU
254 nm
334 [M-H]
CW0578


mAU
254 nm
336 [M+H]
CW0579


mAU
254 nm
336 [M+H]
CW0583
mm


mAU
254 nm
338 [M-H]
CW0584
mm


mAU
254 nm
341 [M+H]
CW5107
mm


mAU
254 nm
323 [M+H]
CW5124
mm