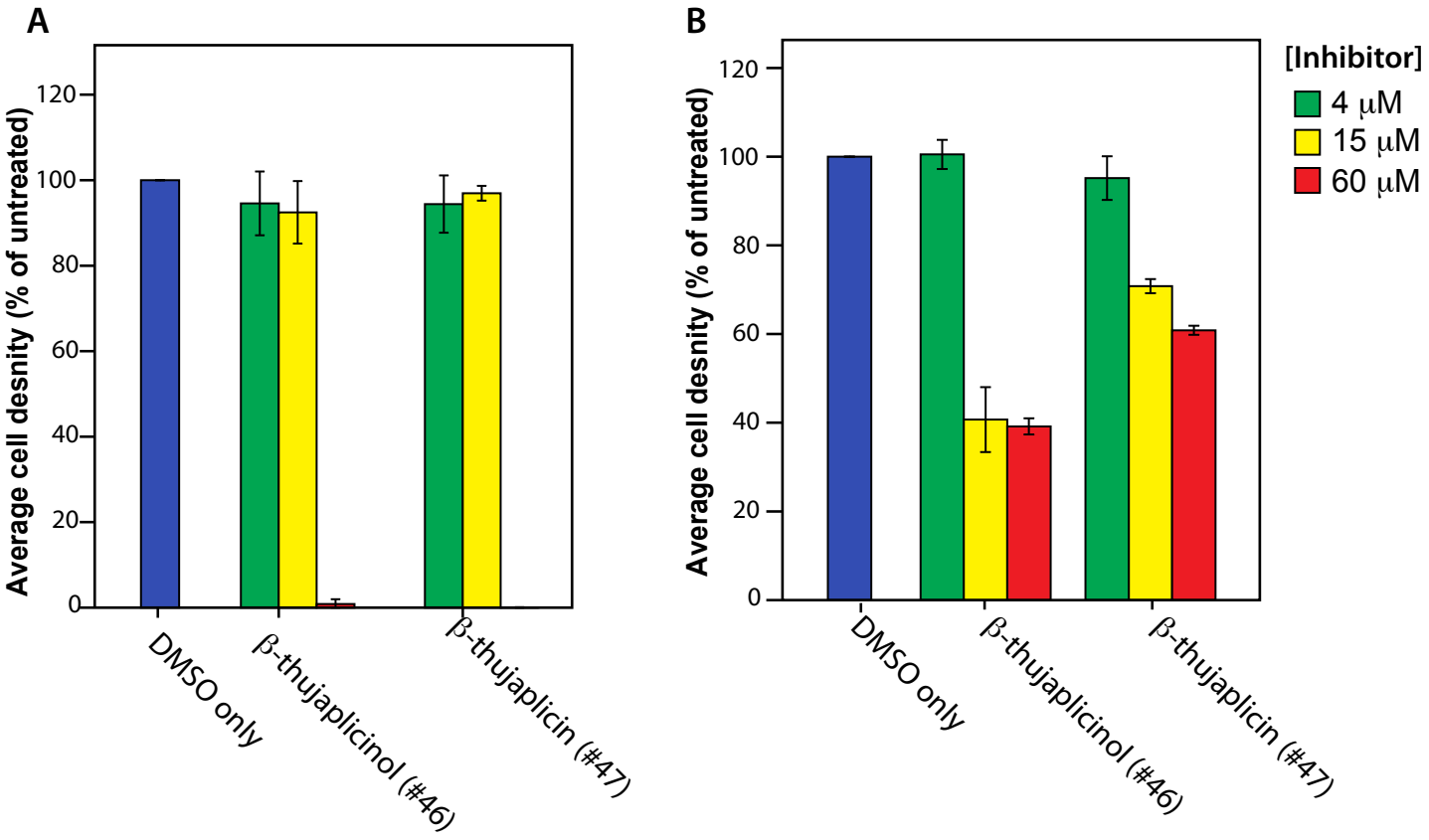
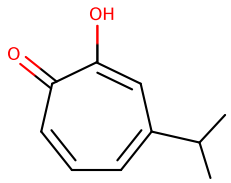
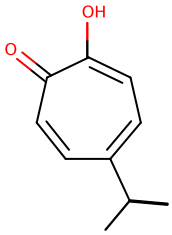


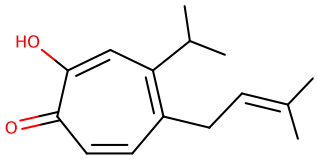
Supp. Fig. 1: Inhibition of KN99α cells by β-thujaplicinol and β-thujaplicin under conditions (A) YPD at 25˚C and (B) YNB-02 at 35˚C.



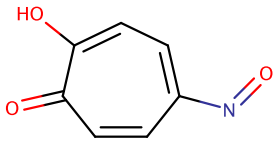
#47
MIC: 21 µM
CC_{50}: 66 µM
TI: 3



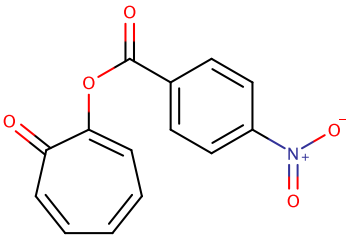
#48
MIC: 8 µM
CC_{50}: 45 µM
TI: 5



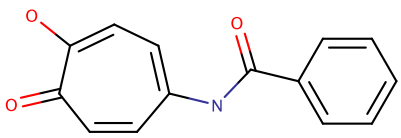
#49
MIC: 18 µM
CC_{50}: 18 µM
TI: 1



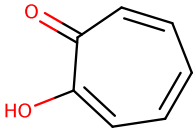
#50
MIC: 24 µM
CC_{50}: 17 µM
TI: <1



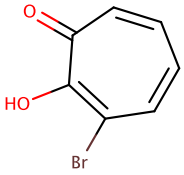
#51
MIC: 24 µM
CC_{50}: >100 µM
TI: 4



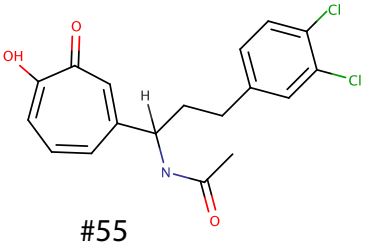
#52
MIC: 50 µM
CC_{50}: 100 µM
TI: 2



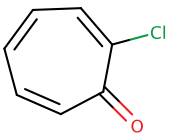
#53
MIC: 24 µM
CC_{50}: >100 µM
TI: 4



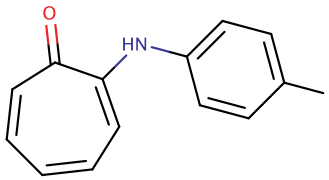
#54
MIC: 7 µM
CC_{50}: 95 µM
TI: 13



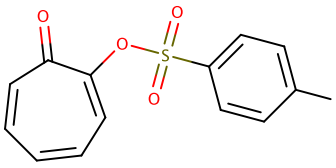
#55
MIC: 6 µM
CC_{50}: 4 µM
TI: <1



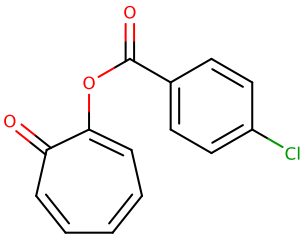
#57
MIC: 50 µM
CC_{50}: 57 µM
TI: 1



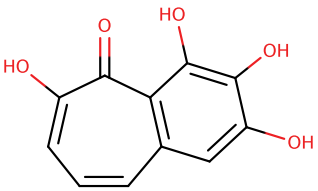
#60
MIC: 50 µM
CC_{50}: 100 µM
TI: 2



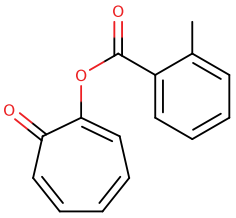
#61
MIC: 41 µM
CC_{50}: 30 µM
TI: <1



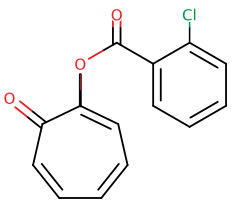
#63
MIC: 17 µM
CC_{50}: >100 µM
TI: 6



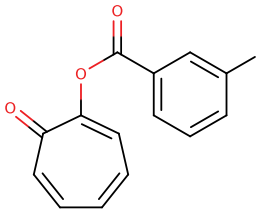
#195
MIC: 50 µM
CC_{50}: 92 µM
TI: 2



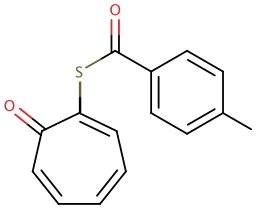
#281
MIC: >50 µM
CC_{50}: >100 µM
TI: 2



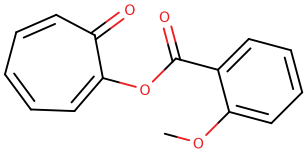
#282
MIC: 36 µM
CC_{50}: 96 µM
TI: 3



#283
MIC: 50 µM
CC_{50}: 74 µM
TI: 1



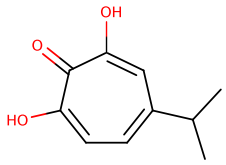
#284
MIC: 0.25 µM
CC_{50}: 91 µM
TI: >300



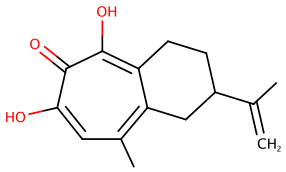
#285
MIC: 50 µM
CC_{50}: 100 µM
TI: 2

Supp. Fig 2: Structures of tropones and tropolones.

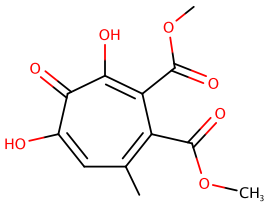
A



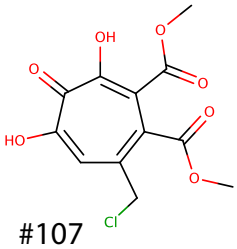
#46
MIC: 8 μM
CC_{50}: 23 μM
TI: 3



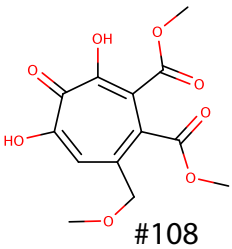
#56
MIC: 50 μM
CC_{50}: 27 μM
TI: <1



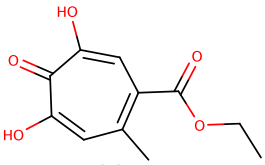
#106
MIC: 41 μM
CC_{50}: 24 μM
TI: <1



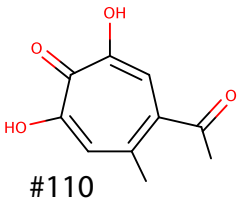
#107
MIC: 50 μM
CC_{50}: 85 μM
TI: 2



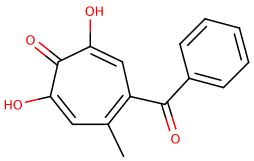
#108
MIC: 50 μM
CC_{50}: 90 μM
TI: 2



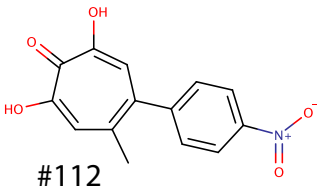
#109
MIC: 50 μM
CC_{50}: 87 μM
TI: 2



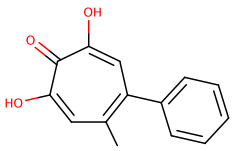
#110
MIC: 50 μM
CC_{50}: 19 μM
TI: <1



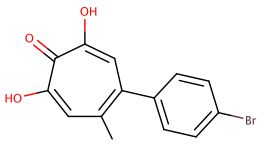
#111
MIC: 36 μM
CC_{50}: 26 μM
TI: <1



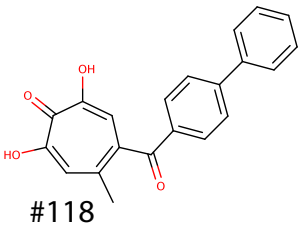
#112
MIC: 49 μM
CC_{50}: 79 μM
TI: 1



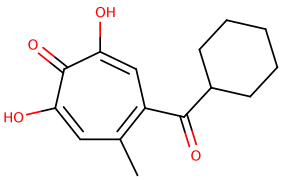
#113
MIC: 24 μM
CC_{50}: 37 μM
TI: 1



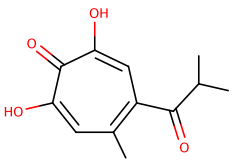
#114
MIC: 11 μM
CC_{50}: 19 μM
TI: 1



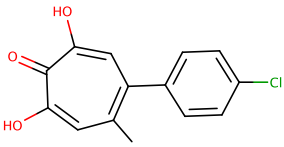
#118
MIC: 18 μM
CC_{50}: 18 μM
TI: 1



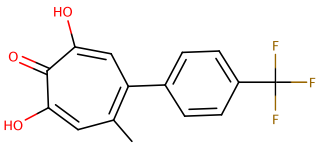
#120
MIC: 12 μM
CC_{50}: 22 μM
TI: 2



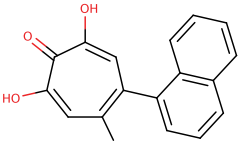
#143
MIC: 50 μM
CC_{50}: >100 μM
TI: 2



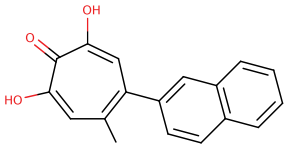
#144
MIC: 50 μM
CC_{50}: nd
TI: nd



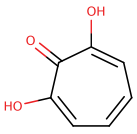
#145
MIC: 15 μM
CC_{50}: 10 μM
TI: 1



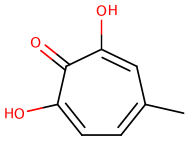
#146
MIC: 20 μM
CC_{50}: 20 μM
TI: 1



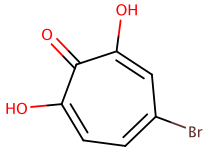
#147
MIC: 15 μM
CC_{50}: nd
TI: nd



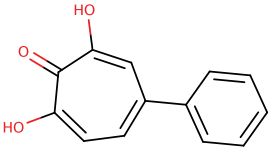
#172
MIC: 24 μM
CC_{50}: 95 μM
TI: 4



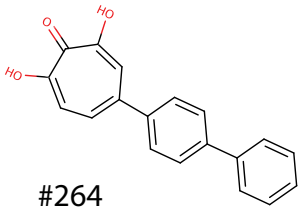
#210
MIC: 15 μM
CC_{50}: 71 μM
TI: 5



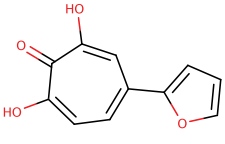
#261
MIC: 49 μM
CC_{50}: 100 μM
TI: 2



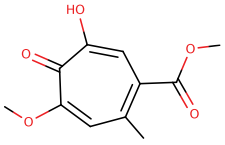
#262
MIC: 18 μM
CC_{50}: 96 μM
TI: 5



#264
MIC: 35 μM
CC_{50}: 28 μM
TI: <1



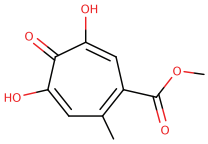
#265
MIC: 11 μM
CC_{50}: 29 μM
TI: 2



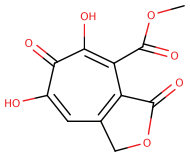
#273
MIC: 50 μM
CC_{50}: >100 μM
TI: 2

Supp. Fig. 3: Structures of α-hydroxytropolones and α-methoxytropolones

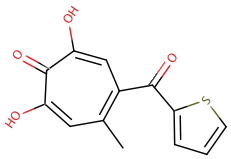
B



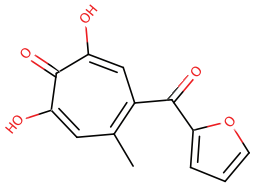
#274
MIC: >50 μM
CC_{50}: 95 μM
TI: 2



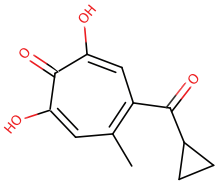
#280
MIC: >50 μM
CC_{50}: 66 μM
TI: 1



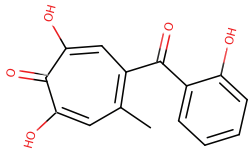
#308
MIC: 11 μM
CC_{50}: 24 μM
TI: 2



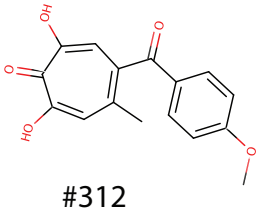
#309
MIC: 24 μM
CC_{50}: 32 μM
TI: 1



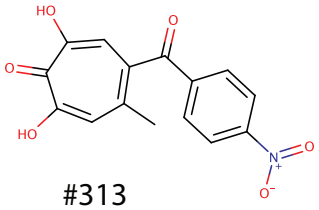
#310
MIC: 11 μM
CC_{50}: 35 μM
TI: 3



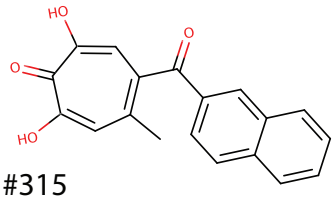
#311
MIC: 15 μM
CC_{50}: 20 μM
TI: 1



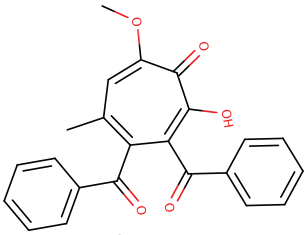
#312
MIC: 24 μM
CC_{50}: 18 μM
TI: <1



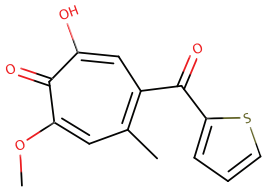
#313
MIC: 24 μM
CC_{50}: 46 μM
TI: 2



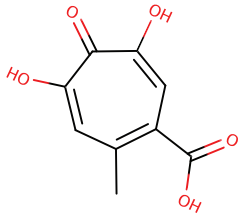
#315
MIC: 24 μM
CC_{50}: 17 μM
TI: 1



#317
MIC: >50 μM
CC_{50}: nd
TI: nd

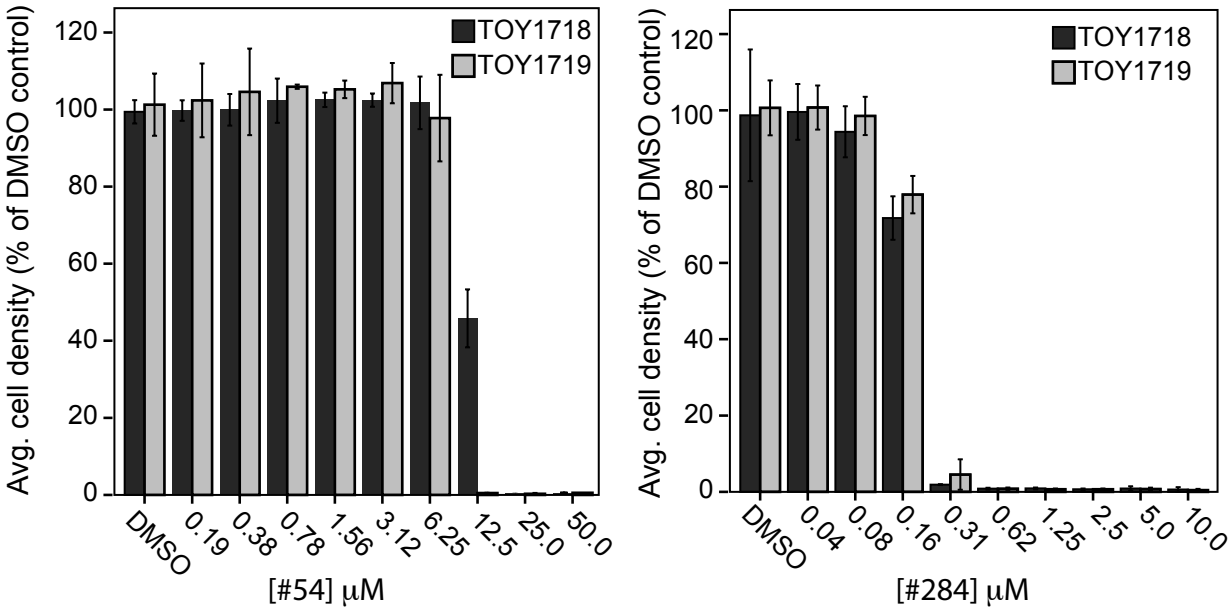


#318
MIC: >50 μM
CC_{50}: nd
TI: nd



#319
MIC: 50 μM
CC_{50}: 100
TI: 2

Supp. Fig. 3: Structures of α-hydroxytropolones and α-methoxytropolones


Avg. cell density (% of DMSO control)
120
100
80
60
40
20
0
TOY1718
TOY1719
DMSO
0.19
0.38
0.78
1.56
3.12
6.25
12.5
25.0
50.0
[#54] μM
Avg. cell density (% of DMSO control)
120
100
80
60
40
20
0
TOY1718
TOY1719
DMSO
0.04
0.08
0.16
0.31
0.62
1.25
2.5
5.0
10.0
[#284] μM

Supp. Fig 4

Troponoids can inhibit growth of the human fungal pathogen *Cryptococcus neoformans*

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[2]Department of Molecular Microbiology and Immunology, Saint Louis University School of Medicine, St. Louis, Missouri USA
[3]Department of Chemistry, Brooklyn College, The City University of New York, Brooklyn, New York USA
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Electronic Supplementary Information

Table of Contents

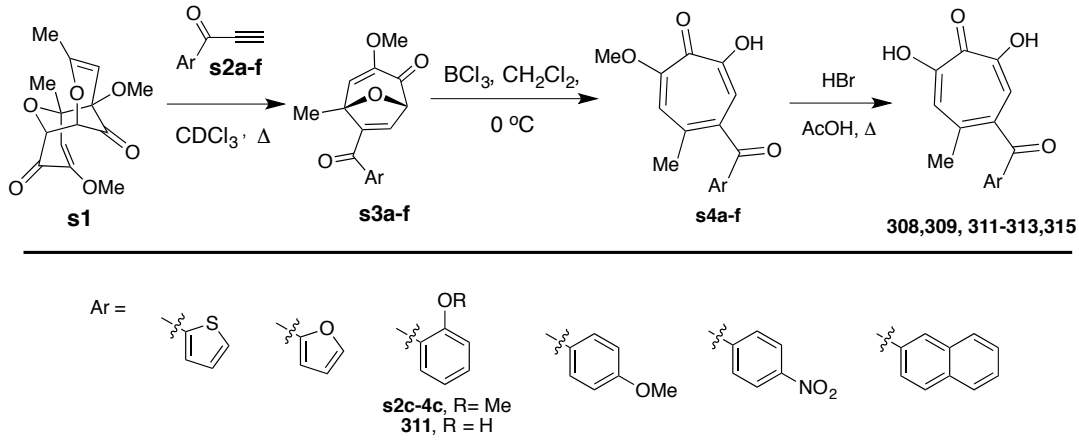
I. General Information

Synthesis: All starting materials and reagents were purchased from commercially available sources and used without further purification, with exception of CH_2Cl_2 and benzene, which was purified on a solvent purification system prior to the reaction. ^1H NMR shifts are measured using the solvent residual peak as the internal standard ($CHCl_3$ d 7.26, D_2O d 4.79), and reported as follows: chemical shift, multiplicity (s = singlet, bs = broad singlet, d = doublet, t = triplet, dd = doublet of doublet, q = quartet, m = multiplet), coupling constant (Hz), integration. ^{13}C NMR shifts are measured using the solvent residual peak as the internal standard ($CDCl_3$ d 77.20 or D_2O), and reported as chemical shifts. Infrared (IR) spectral bands are characterized as broad (br), strong (s), medium (m), and weak (w). Microwave reactions were preformed via the Biotage Intiator 2.5. Purification via normal phase column chromatography was performed on the Biotage Isolera Prime, with Biotage SNAP 10-25g cartridges, in a solvent system of Ethylacetate in Hexane. Purification for final compounds via reverse phase column chromatography was preformed on the Biotage Isolera Prime, with Biotage SNAP 12g cartridges, in a solvent system of CH_3CN in water each solvent containing 0.05% trifluoroacetic acid (TFA).

II. Synthesis of Aryl Ketone αHTs (308, 309, 311-313, 315)

IIa. General Synthetic Overview

Scheme S1. Schematic Overview of Aryl Ketone αHT Synthesis



Synthesis of Alkynones (s2a-e).

Closely following literature precedent,[1] in a round bottom flask, to a solution of acid chloride (1-2 g, 4.5 mM-9 mM, 1.0 eq) in CH_2Cl_2 (0.056 M), TMS acetylene (480-1000 mg, 4.95-9.9 mmol, 1.1 eq) is added. The flask was cooled to 0 ^{0}C, then $AlCl_3$ (14-28 mmol, 3.1 eq) is added with vigorous stirring and left at 0 ^{o}C for 30 minutes. Then, the temperature was raised to room temperature, for 30 minutes. The reaction was quenched with 2M HCl and extracted with CH_2Cl_2. The organic layers were washed twice with saturated $NaHCO_3$ solution, followed by brine wash. After drying with Na_2SO_4, organic layers were filtered and concentrated under reduced pressure, to be used as such in next step. (Crude yields 80->100%)

Oxidopyrylium Cycloaddition: Synthesis of s3a-e.

To a solution of **(1R, 2S, 6S, 7R)-6,9-dimethoxy-4,7-dimethyl-3,11-dioxatricyclo[5.3.1.12,6]dodeca-4,8-diene-10,12-dione (s1)**[1] (150-250 mg) in $CDCl_3$ (0.4-0.5 M, 1.1 mL) in a sealed tube, was added alkynones **s2a-f** (700-1200 mg, 4.2-6.36

[1] Schubert, T.; Werner, H.; Maria-Regina, K.; Müller, M. *Eur. J. Org. Chem.* **2001**, *22*, 4181-4187.

mmol, 4-12 eq). After stirring at 120 ^{0}C, for 3 hr in an oil bath, the solvent was evaporated and crude material loaded onto column cartridge using 1-1.5 mL toluene, was purified by chromatography (Biotage Isolera Prime, SNAP 25g silica gel, 18cm x 1.8cm, solvent gradient: 5% EtOAc in hexanes (100 mL); 10% EtOAc in hexanes (200 mL); 20% EtOAc in hexanes (200 mL)). Product fractions were concentrated to yield **s3a-f** (60-95 % yield)

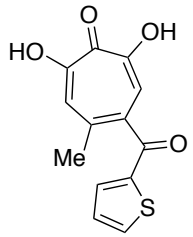
BCl_3-mediated Ring-Opening: Synthesis of s4a-e.

A solution of BCl_3 (1.0 M in CH_2Cl_2, 7eq, 2.955-5.91 mmol) was diluted with CH_2Cl_2 (0.014 M, 30-60 mL) and cooled to 0°C. In a separate round bottom flask, **s3a-f** (120-250 mg, 0.42-0.84 mmol) was dissolved in CH_2Cl_2 (0.014M, 30-60 mL), was cooled to 0°C and was added to the BCl_3 solution. After 10 min of stirring at 0°C, the reaction mixture was quenched with H_2O (60.3 mL), stirred for 2 min at 0°C, and then warmed to room temperature where it continued to stir for 1 hr. The organic layer was isolated and the aqueous layer was extracted with CH_2Cl_2, (5 x 10 mL). Combined organics were dried over Na_2SO_4, filtered, and concentrated under reduced pressure to yield **s4a-e** as solids. Reactions were immediately carried to next step.

HBr/AcOH Demethylation: Synthesis of œ-Hydroxytropolones.

A round bottom flask containing methoxytropolones **s4a-f** (100-200 mg) fitted with reflux condenser and base trap, a 33% HBr in acetic acid (0.09 M) was added to flask, and the reaction was heated to 120 °C for 1 hr. After 1 hour, reaction mixture was let to cool to room temperature, quenched with phosphate buffer (pH=7), and diluted with CH_2Cl_2. The organic layer was washed several times with the phosphate buffer. The organic layer was dried over Na_2SO_4, and evaporated under reduced pressure to yield pale yellow to brown solids **308, 309, 311-313, 315** (50-70% crude yield over two steps from **s3a-e**). They were further purified using reverse phase column chromatography conditions (Biotage Isolera Prime, SNAP 12g C18 silica gel column, solvent gradient: 2-85% acetonitrile in water (35 CV); acetonitrile and water each contained 0.05% TFA)). Crude material loaded onto column cartridge using 1-1.5 mL DMSO. Product fractions were concentrated to yield **308, 309, 311-313, 315** (10-60 mg, 20-60 % yields).

IIb. 4-(thiopene-2-carbonyl)-2,7-dihydroxy-5-methylcyclohepta-2,4,6-trien-1-one. (**308)**

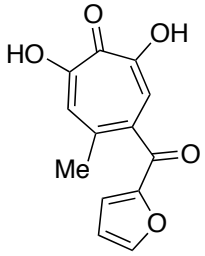


308

1-(thiophen-2-yl) prop-2-yn-1-one **(s2a)** (340 mg, 2.5 mmol, 4 eq), was synthesized as described in the general synthetic method using thiophene-2-carbonyl chloride and carried through oxidopyrylium cycloaddition procedure with **s1** (175 mg, 0.625 mmol, 1eq) in $CDCl_3$ (0.4 M, 1.5 mL) to yield **s3a** as a pale brown oil**.** (250 mg, 0.71 mmol, 56 % yield) **^{1}H NMR (200 MHz, $CDCl_3$)** δ 7.75 (dd, *J* = 3.8 Hz, 0.8 Hz 2H), 7.18 (t, *J* = 5 Hz, 4.4 Hz, 1H), 6.96 (d, *J* = 2.4 Hz, 1H), 6.24 (s, 1H), 5.17 (d, *J* = 2 Hz, 1H), 3.58 (s, 3H), 1.74 (s, 3H). Ring opening of **s3a** (250 mg, 0.905mmol, 1eq) was carried out with BCl_3 solution (6.34mL, 6.34mmol, 7eq) to yield **318** as a pale brown solid (213 mg, 0.768 mmol, 85% yield). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.80 (dd, *J* = 4.9, 1.2 Hz, 1H), 7.42 (dt, *J* = 6.7, 3.4 Hz, 1H), 7.31 (s, 1H), 7.16 – 7.12 (m, 1H), 7.07 (s, 1H), 4.05 (s, 3H), 2.40 (s, 3H). Demethylation of **s4a** (190 mg, 0.76 mmol, 1 eq) with HBr/AcOH (8.5mL, 0.09M) followed by reverse phase column chromatography (Biotage Isolera Prime, SNAP 12g C18 silica gel column, solvent gradient: 2-85% acetonitrile in water (35 CV); acetonitrile and water each contained 0.05% TFA)) yielded **308** (69 mg, 38% yield). **4-(thiopene-2-carbonyl)-2,7-dihydroxy-5-methylcyclohepta-2,4,6-trien-1-one**. Pale brown liquid. **IR (ATR, ZnSe)** 3265 (b), 2862 (w), 1652 (s), 1533(s), 1518(s), 1400 (s), 1356 (m), 1287 (m), 1232 (m), 1090 (w), 913 (w), 803 (w), 728 (w) cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 (dd, *J* = 4 Hz, 0.8 Hz 1H), 7.51 (s, 1H), 7.42 (s, 1H), 7.40 (t, *J* = 3.2 Hz, 1H), 7.14 (dd, *J* = 4 Hz, 0.8 Hz, 1H), 2.39 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 189.29, 168.29, 159.08, 156.85, 157.05, 142.97, 139.28, 138.25, 136.49, 135.98, 128.66, 124.56, 119.10, 24.45. **HRMS (ESI+):** *m/z* calc'd for $C_{13}H_{10}O_4SH^+$: 262.0372 Found: 263.0384.

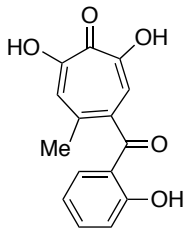
IIc. **4-(furan-2-carbonyl)-2,7-dihydroxy-5-methylcyclohepta-2, 4,6-trien-1-one. (309)**

1-(furan-2-yl) prop-2-yn-1-one **(s2b)** (900 mg, 8 mmol, 7eq) was synthesized as described in the general synthetic method using furan-2-carbonyl chloride and carried through oxidopyrylium cycloaddition procedure with **s1** (280 mg, 1 mmol, 1eq) in $CDCl_3$ (0.5 M, 2 mL) to yield **s3b** as a pale brown oil (220mg, 0.85 mmol, 42 % yield) **^{1}H NMR (200 MHz, $CDCl_3$)** δ 7.66 (dd, *J* = 3.8 Hz, 0.8 Hz 2H), 7.26 (m, 2H), 6.60 (t, *J* = 1.6 Hz, 2 Hz, 1H), 6.23 (s, 1H), 5.17 (dd, *J* = 1.2 Hz, 1H), 3.57 (s, 3H), 1.77 (s, 3H). Ring opening of **s3b** (250 mg, 0.905 mmol, 1 eq) was carried out with BCl_3 solution (5.91mL, 5.91mmol, 7eq) to yield a mixture of **s4b** and **309** (220 mg, ~85% crude yield), which was homogenized with HBr/AcOH (9 mL, 0.09 M) and chromatographed (Biotage Isolera Prime, SNAP 12g C18 silica gel column, solvent gradient: 2-85% acetonitrile in water (35 CV); acetonitrile and water each contained 0.05% TFA)) to yield **309** as a pale yellow solid **309** (12mg, 5% yield over 2 steps). **IR (ATR, ZnSe)** 3259 (b), 2924 (w), 1662 (s), 1389 (m), 1300 (m), 1226 (m), 1161 (w), 1090 (w) cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.71 (dd, *J* = 1.6 Hz 1H), 7.51 (s, 1H), 7.41 (s, 1H), 7.09 (d, *J* = 3.2 Hz, 1H), 6.60 (dd, *J* = 3.6 Hz, 1.6 Hz, 1H), 2.39 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 184.24, 168.35, 158.97, 156.85, 151.45, 148.61, 138.90, 138.24, 124.36, 121.88, 119.12, 112.92, 24.35. **HRMS (ESI+):** *m/z* calc'd for $C_{13}H_{10}O_5H^+$: 247.0600 Found: 247.0606.



309

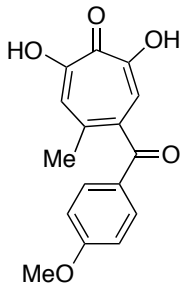
IId. 4-(2-hydroxybenzoyl)-2,7-dihydroxy-5-methylcyclohepta-2,4,6-trien-1-one (311)



311

1-(2-methoxyphenyl)prop-2-yn-1-one **(s2c)** (430 mg, 2.68 mmol, 5 eq) was synthesized as described in the general synthetic method using 2-methoxybenzoyl chloride and carried through oxidopyrylium cycloaddition procedure with (150 mg, 0.53 mmol, 1 eq) in $CDCl_3$ (0.4 M, 1.32 mL) to yield **s3c** as a pale brown oil (230 mg, 0.76 mmol, 71% yield). **^{1}H NMR (200 MHz, $CDCl_3$)** δ 7.42-7.32 (m, 2H), 6.95 (t, *J* = 8.2 Hz, 2H), 6.58 (d, *J* = 2.8 Hz, 1H), 6.21 (s, 1H), 5.01 (dd, *J* = 2.6 Hz, 1H), 3.77 (s, 3H), 3.55 (s, 3H), 1.78 (s, 3H). Ring opening of **s3c** (230 mg, 0.76 mmol, 1 eq) was carried out with BCl_3 solution (5.36 mL, 5.36 mmol, 7eq) to yield a mixture of **s4c** and **311** (200 mg, ~85% crude yield), which was homogenized with HBr/AcOH to yield **311** as a pale brown solid (60 mg, 0.22 mmol, 28% yield over 2 steps). **IR (ATR, ZnSe)** 3055 (b), 2925 (w), 2847 (w), 1625 (s), 1531(s), 1486 (s), 1400 (s), 1356 (m), 1287 (m), 1232 (m), 1144 (m), 1063 (w), 906 (w) cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.55 (dt, *J* = 7.2 Hz, 5.6 Hz, 1.6 Hz, 1H), 7.51 (s, 1H), 7.30 (s, 1H), 7.09 (dd, *J* = 8 Hz, 0.4 Hz, 1H), 6.86 (d, *J* = 0.8 Hz, 1H), 6.83 (t, *J* = 7.2 Hz, 1H), 2.34 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 202.62, 168.39, 163.65, 159.01, 157.16, 137.89, 137.81, 137.58, 132.81, 124.34, 119.56, 118.80, 118.74, 118.57, 24.45. **HRMS (ESI+):** *m/z* calc'd for $C_{15}H_{12}O_5H^+$: 273.0757 Found: 273.0994.

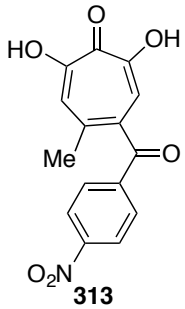
IIe. **4-(4-methoxybenzoyl)-2,7-dihydroxy-5-methylcyclohepta-2,4,6-trien-1-one (312)**



312

1-(4-methoxyphenyl) prop-2-yn-1-one **(s2d)** (430 mg, 2.68 mmol, 5 eq) was synthesized as described in the general synthetic method using 4-methoxybenzoyl chloride and carried through oxidopyrylium cycloaddition procedure with **s1** (150 mg, 0.53 mmol, 1 eq) in $CDCl_3$ (0.4 M, 1.32 mL) to yield **s3d** as a pale brown solid (230mg, 0.76 mmol, 71 % yield) **^{1}H NMR (200 MHz, $CDCl_3$)** δ 7.42-7.32 (m, 2H), 6.95 (t, *J* = 8.2 Hz, 2H), 6.58 (d, *J* = 2.8 Hz, 1H), 6.21 (s, 1H), 5.01 (dd, *J* = 2.6 Hz, 1H), 3.77 (s, 3H), 3.55 (s, 3H), 1.78 (s, 3H). Ring opening of **s3d** (530 mg, 1.76 mmol, 1eq) was carried out with BCl_3 solution (12.36 mL, 12.36 mmol, 7eq) to yield a mixture of **s4d** and **312** (375 mg, ~70% crude yield), which was homogenized with HBr/AcOH (14 mL, 0.09M) and chromatographed (Biotage Isolera Prime, SNAP 12g C18 silica gel column, solvent gradient: 2-85% acetonitrile in water (35 CV); acetonitrile and water each contained 0.05% TFA)) to yield **312** as a pale yellow solid (66 mg, 0.23 mmol, 13% yield over 2 steps). **IR (ATR, ZnSe)** 3243 (b), 1661(s), 1598 (s), 1568 (s), 1531 (s), 1504 (s), 1389 (b), 1290 (m), 1163 (s), 1093 (s), 1021 (s), 903 (s) cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.77 (d, *J = 8 Hz,* 2H), 7.50 (s, 1H), 7.31 (s, 1H), 6.95 (d, *J* = 8.4 Hz 2H), 3.88(s, 3H), 2.25 (s, 3H). **^{13}C NMR (400 MHz, $CDCl_3$)** δ 195.68, 168.11, 164.56, 158.80, 157.23, 140.26, 137.91, 132.56, 128.48, 124.56, 119.16, 114.28, 55.65, 24.37. **HRMS (ESI+):** *m/z* calc'd for $C_{16}H_{14}O_5\,H^+$: 287.0913. Found: 287.0926.

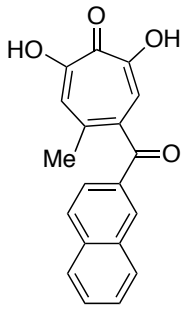
IIe. **2,7-dihydroxy-4-methyl-5-(4-nitrobenzoyl)cyclohepta-2,4,6-trien-1-one (313)**



313

1-(4-nitrophenyl) prop-2-yn-1-one **(s2e**) (1.20 g, 6.85 mmol, 12 eq) was synthesized as described in the general synthetic method using 4-methoxybenzoyl chloride and carried through oxidopyrylium cycloaddition procedure with **s1** (150 mg, 0.53 mmol, 1 eq) in $CDCl_3$ (0.4 M, 4.6 mL) to yield **s3e** as a pale brown solid (120 mg, 0.38 mmol, 35 % yield). **^{1}H NMR (200 MHz, $CDCl_3$)** δ 7.42-7.32 (m, 2H), 6.95 (t, *J* = 8.2 Hz, 2H), 6.58 (d, *J* = 2.8 Hz, 1H), 6.21 (s, 1H), 5.01 (dd, *J* = 2.6 Hz, 1H), 3.77 (s, 3H), 3.55 (s, 3H), 1.78 (s, 3H). Ring opening of **s3e** (120 mg, 0.38 mmol, 1eq) was carried out with BCl_3 solution (2.66 mL, 2.66 mmol, 7eq) to yield a mixture of **s4e** and **313** (>120 mg crude yield), which was homogenized with HBr/AcOH (4.55 mL, 0.09M) and chromatographed (Biotage Isolera Prime, SNAP 12g C18 silica gel column, solvent gradient: 2-85% acetonitrile in water (35 CV); acetonitrile and water each contained 0.05% TFA)) to yield **313** as a pale yellow solid (40 mg, 0.13 mmol, 32% yield over 2 steps). **IR (ATR, ZnSe)** 2957 (b), 2940 (s), 2858 (s), 1673 (s), 1598 (s), 1454 (s), 1394 (b), 1349 (s), 1286 (m), 1078 (s), 1021 (s), 907 (s) cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.34 (d, *J = 8.4 Hz,* 2H), 7.98 (d, *J = 8.4 Hz,* 2H), 7.53 (s, 1H), 7.26 (s, 1H), 2.32 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 195.44, 168.70, 159.05, 156.89, 150.94, 140.21, 138.33, 137.78, 130.98, 124.24, 118.33, 24.62. **HRMS (ESI+):** *m/z* calc'd for $C_{15}H_{11}NO_6$ H^+: 302.0658. Found: 302.0660

IIg. **4-(2-naphthoyl)-2,7-dihydroxy-5-methylcyclohepta-2, 4,6-trien-1-one (315)**

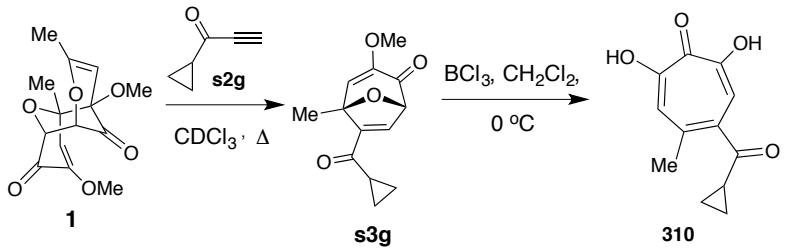


315

1-(naphthalen-2-yl) prop-2-yn-1-one **(s2f)** (763 mg, 4.24 mmol, 8 eq) was synthesized as described in the general synthetic method using 2-naphthoyl chloride and carried through oxidopyrylium cycloaddition procedure with **s1** (150 mg, 0.53 mmol, 1eq) in $CDCl_3$ (0.4 M, 1.32 mL) as described previously to yield **s3g** as a pale brown solid**.** (101 mg, 0.31 mmol, 30 % yield). **^{1}H NMR (200 MHz, $CDCl_3$)** δ 8.37 (d, *J* = 0.8 Hz, 1H), 7.99 (d, *J* = 8.2 Hz, 1H), 7.87 (d, *J* = 5.8 Hz, 1H), 7.71 (d, *J* = 7.4 Hz, 1H), 7.42-7.32 (m, 2H), 6.65 (s,1H), 6.33 (d, *J* = 1.2 Hz, 1H), 5.09 (dd, *J* = 1.6 Hz, 1.4 Hz, 1H), 3.60 (s, 3H), 1.86 (s, 3H). Ring opening of **s3f** (101 mg, 0.31 mmol, 1eq) was carried out with BCl_3 solution (2.2 mL, 2.2 mmol, 7 eq) to yield a mixture of **s4f** and **315** (68 mg, ~68% crude yield), which was homogenized with HBr/AcOH (2.4 mL, 0.09 M) and chromatographed (Biotage Isolera Prime, SNAP 12g C18 silica gel column, solvent gradient: 2-85% acetonitrile in water (35 CV); acetonitrile and water each contained 0.05% TFA)) to yield **315** as a pale yellow solid (11 mg, 0.03 mmol, 11% yield over 2 steps). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.10 (s, 1H), 8.02-7.87 (m, 4H), 7.65 (dt, *J* = 1.6 Hz, 1.2Hz, 1H), 7.56 (dt, *J* = 1.6 Hz, 1.2Hz, 1H), 7.55 (s, 1H), 7.34 (s, 1H), 2.35 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 197.13, 168.37, 158.75, 157.02, 139.91, 138.20, 136.13, 133.07, 132.96, 132.41, 129.80, 129.39, 129.19, 127.95, 127.21, 124.42, 124.39, 118.98, 24.55. **HRMS (ESI+):** *m/z* calc'd for $C_{19}H_{14}O_4H^+$: 307.0964 Found: 307.0967.

III. Synthesis and Characterization of Hydroxytropolone 310

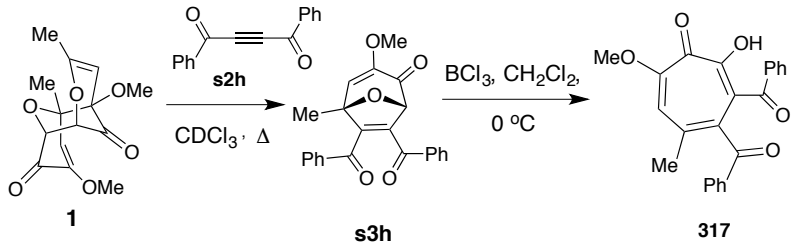
Scheme S2. Synthesis of αHT **310**



1-cyclopropylprop-2-yn-1-one **(s2g)** (1.12 g, 4.24 mmol, 22 eq) was synthesized as described in the general synthetic method using cyclopropanecarbonyl chloride and carried through oxidopyrylium cycloaddition procedure with **s1** (150 mg, 0.53 mmol, 1 eq) as described previously to yield **s3g** as a pale brown solid**.** (122 mg, 0.55 mmol, 52% yield) **^{1}H NMR (200 MHz, $CDCl_3$)** δ 7.14 (s, 1H), 6.09 (s, 1H), 5.80 (s, 1H), 7.71 (d, *J* = 7.4 Hz, 1H), 3.53 (s, 3H), 2.28 (m, 1H), 1.71 (s, 3H), 1.13-0.98 (m, 4H). Ring opening of **s3g** (122 mg, 0.55 mmol, 1 eq) with BCl_3 solution (3.91 mL, 3.91 mmol, 7 eq) yielded direct conversion to **310** as a pale yellow oil. (22 mg, 0.1 mmol, 20% yield) **IR (ATR, ZnSe)** 3253 (b), 3004 (w), 1683 (s), 1611 (s), 1539 (m), 1434 (m), 1376 (m), 1281 (m), 1197 (m), 1156 (w), 1124 (w), 1095 (w), 974 (m) cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.49 (s, 2H), 2.47 (s, 3H), 2.22 (t, *J= 4.8 Hz, 4.4 Hz*, 1H), 1.339 (t, *J= 4.4 Hz, 3.6 Hz,* 2H), 1.34-1.15 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 206.66, 168.16, 158.67, 157.18, 142.11, 137.62, 124.61, 118.61, 24.64, 21.99, 13.40, 13.29. **HRMS (ESI+):** *m/z* calc'd for $C_{12}H_{12}O_4H^+$: 221.0808. Found: 221.0815.

IV. Synthesis and Characterization of Methoxytropolone 317

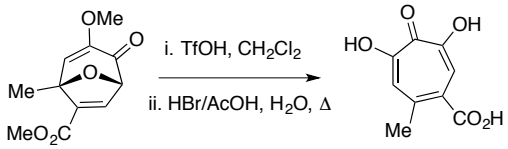
Scheme S3. Synthesis of α-Methoxytropolone **317**



To a solution of **s1** (44 mg, 0.32 mmol, 1.5 eq) in $CDCl_3$ (0.14 M, 1.5 mL) was added 1,4-diphenylbut-2-yne-1,4-dione **s2h** (50 mg, 0.213 mmol, 1 eq). After microwave irradiation at 100 °C for 15 minutes, the reaction mixture was purified by chromatography (Biotage Isolera Prime, SNAP 10 g silica gel column, solvent gradient: 5% EtOAc in hexanes (3 CV); 5-30% EtOAc in hexanes (20 CV)). Product fractions were concentrated to yield **s3h** as a pale yellow liquid (52 mg, 0.13 mmol, 65% yield). R_f = 0.50 in 40% EtOAc in hexanes. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.46 – 7.36 (m, 1H), 7.31 – 7.27 (m, 1H), 7.24 – 7.16 (m, 1H), 6.33 (s, 1H), 5.61 (s, 1H), 3.69 (d, *J* = 20.0 Hz, 1H), 1.70 (d, *J* = 30.3 Hz, 1H).**^{13}C NMR (100 MHz, $CDCl_3$)** δ 192.27, 189.66, 187.54, 155.05, 145.45, 143.28, 137.36, 136.99, 133.92, 133.51, 128.59, 128.54, 128.51, 128.38, 119.87, 89.54, 88.69, 77.36, 77.05, 76.73, 55.08, 20.95. Ring opening of **s3h** (100 mg, 0.26 mmol, 1eq) was carried out with BCl_3 solution (1.86 mL, 1.86 mmol, 7 eq) according to previous procedure to yield **317** (100 mg, 0.26 mmol, 100% yield) **(7-hydroxy-5-methoxy-3-methyl-6-oxocyclohepta-2, 4,7-triene-1, 2-diyl) bis (phenyl methanone)** pale brown solid. **IR (ATR, ZnSe)** 2898 (w), 1671(s), 1592 (s), 1571 (m), 1556 (m), 1444 (m), 1389 (s), 1175 (m), 1090 (w), 1021 (s), 845 (w), 770 (s) cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.81 – 7.66 (m, 1H), 7.54 (dt, *J* = 11.0, 7.5 Hz, 1H), 7.39 (dt, *J* = 11.1, 7.8 Hz, 1H), 7.11 (s, 1H), 4.07 (s, 1H), 2.24 (s, 1H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ 196.95, 194.60, 170.52, 158.88, 156.14, 138.09, 136.61, 136.37, 134.22, 133.97, 133.88, 133.81, 129.77, 129.46, 128.83, 128.63, 128.51, 122.09, 77.41, 77.29, 77.09, 76.77, 56.73, 25.57. **HRMS (ESI+):** *m/z* calc'd for $C_{16}H_{14}O_5$ H^+: 375.1226. Found: 375.1233.

V. Synthesis of αHT Carboxylic acid 319

Scheme S4. Synthesis of αHT **319**

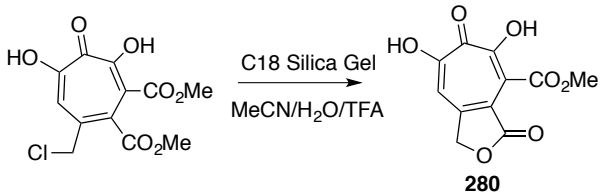


319

4,6-dihydroxy-2-methyl-5-oxocyclohepta-1, 3,6-triene-1-carboxylic acid 319. To a solution of methyl 3-methoxy-5-methyl-2-oxo-8-oxabicyclo [3.2.1] octa-3, 6-diene-6-carboxylate[2] (300 mg, 1.34 mmol) in CH_2Cl_2 (13.4 mL) was added triflic acid (473 μL, 5.36 mmol). The reaction was allowed to stir for 30 min at rt, at which point NaOAc (1.1 g, 13.4 mmol) was added and stirred for an additional 10 min at rt. The reaction mixture was concentrated under reduced pressure, and H_2O (724 μL, 40.2 mmol) in 13 mL of 33% HBr/AcOH solution was added. The reaction was heated to 120 °C for 4 h before being quenched with pH 7 phosphate buffer to a pH of 4. The reaction mixture was extracted with CH_2Cl_2 (5 x 20 mL) followed by EtOAc (3 x 20 mL). The combined organics were dried over Na_2SO_4, filtered, and concentrated under reduced pressure to yield **1** as a brown solid (135 mg, 51% yield) that decomposes at 235 °C. **IR (ATR, ZnSe)** 3302 (m), 3157 (b), 2925 (m), 2853 (m), 1708 (s), 1611 (w), 1533 (s), 1495 (w), 1431 (w), 1176 (s), 1137 (m), 906 (m), 782 (w), 713 (w) cm^{-1}. **^{1}H NMR (400 MHz, MeOD)** δ 7.62 (s, 1H), 7.45 (s, 1H), 2.53 (s, 3H). **^{13}C NMR (100 MHz, DMSO-d_6)** δ 170.15, 168.48, 159.87, 157.16, 137.56, 131.99, 123.67, 119.29, 24.56. **HRMS (ESI+):** *m/z* calc'd for $C_9H_9O_5^+$: 197.0444. Found: 197.0443

VI. Synthesis of αHT Lactone 280

Scheme S5. Synthesis of αHT Lactone 280



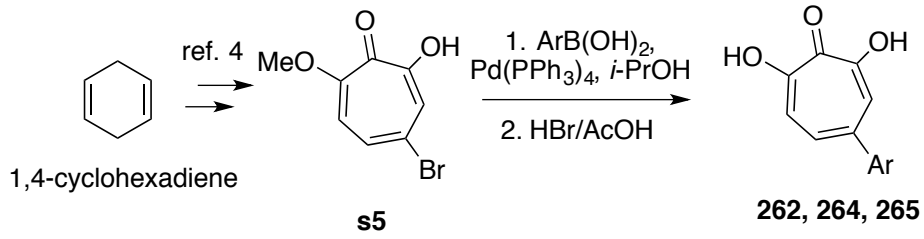
Methyl 5,7-dihydroxy-3,6-dioxo-3,6-dihydro-1*H*-cyclohepta[*c*]furan-4-carboxylate (280). Dimethyl 3- (chloromethyl)-5,7-dihydroxy-6-oxocyclohepta-2,4,7-triene-1,2-dicarboxylate [2] (26 mg, 0.086 mmol) was subjected to reverse phase column chromatography conditions (Biotage Isolera Prime, SNAP 12g C18 silica gel column, solvent gradient: 2-85% acetonitrile in water (35 CV); acetonitrile and water each contained 0.05% TFA)). Product fractions were concentrated to yield **280** as a yellow solid (12 mg, 55% yield). MP= 252-255 °C. **IR (ATR, ZnSe)** 3325 (b), 2930 (w), 1737 (s), 1723 (s), 1714 (s), 1623 (w), 1569 (m), 1471 (m), 1438 (m), 1354 (s), 1303 (s), 1259 (m), 1146 (s), 1034 (m), 980 (m), 793 (m) cm^{-1}. **^{1}H NMR (400 MHz, Acetone-d_6)** δ 7.62 (s, 1H), 5.39 (s, 2H), 3.92 (s, 3H). **^{13}C NMR (150 MHz, Acetone-d_6)** δ 173.61, 170.64, 165.61, 162.70, 155.70, 149.87, 122.38, 118.98, 113.06, 71.49, 52.95. **HRMS (ESI+):** *m/z* calc'd for $C_{11}H_8O_7Na^+$: 275.0162. Found: 275.0163.

[2] Meck, C.; Mohd, N.; Murelli, R. P. *Org. Lett.* **2012**, 14, 5988-5991.

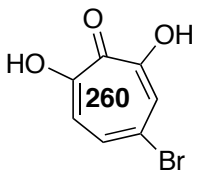
VI. Synthesis of Monosubstituted αHTs

The following procedures are derived from the work of Banwell *et al*, whereby 1,4-cyclohexadiene was converted into 4-bromo-2,7-dihydroxycyclohepta-2,4,6-trien-1-one (**s5**),[3] which subsequently serves as an intermediate for various αHTs through cross-coupling and demethylation sequence.[4]

Scheme S5. General Overview of Banwell αHT synthesis strategy

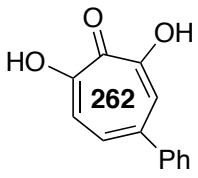


VIa. 4-bromo-2,7-dihydroxycyclohepta-2,4,6-trien-1-one (260)



4-bromo-2,7-dihydroxycyclohepta-2,4,6-trien-1-one (**s5**) (100.8 mg, 0.436 mmol) was dissolved in 33% HBr in acetic acid to a concentration of 0.1M, and heated to 120°C in a sealed vessel for 1hr. The reaction was diluted 20 fold with CH_2Cl_2 and 0.2M phosphate buffer was added until the pH of the aqueous layer was ~6. The reaction was then extracted 3 x with CH_2Cl_2 and the combined organic extracts dried over Na_2SO_4, and the solvent evaporated under reduced pressure to afford the product, 4-bromo-2,7-dihydroxycyclohepta-2,4,6-trien-1-one**,** as a brown solid. (94 mg, >95% yield) **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.34 (br s, 1H), 7.80 (d, J = 2.0 Hz, 1H), 7.51(dd, J = 11.0, 2.0 Hz, 1H), 7.25 (d, J = 11.0 Hz, 1H). **HRMS** (TOF MS ES+) *m/z* Calcd for $C_8H_5BrO_3$: 216.9500. Mass Found: 216.9513

VIb. 2,7-dihydroxy-4-phenylcyclohepta-2,4,6-trien-1-one (262)

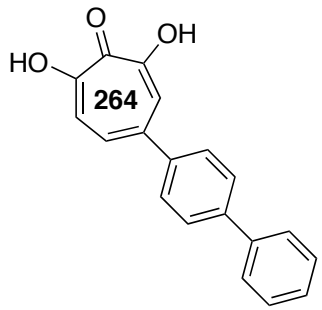


4-bromo-2,7-dihydroxycyclohepta-2,4,6-trien-1-one (**s5**) (19.6 mg, 0.085mmol) and benzene boronic acid (14.5 mg, 0.119 mmol) were dissolved in 4.25 mL of 2-propanol. 1.19 mL of 1 M aq. Na_2CO_3 was

[3] Amon, C. M.; Banwell, M. G.; Gravatt, G. L. *J. Org. Chem.* **1987**, *52*, 4851.
[4] Banwell, M. G.; Cameron, J. M.; Collis, M. P.; Crisp, G. T.; Gable, R. W.; Hamel, E.; Lambert, J. N.; Mackay, M. F.; Reum, M. E.; Scoble, J. A. *Aust. J. Chem.* **1991**, *44*, 705.

then added and the solution was purged with Ar for 15min, and $Pd(PPh_3)_4$ (9.8 mg, 0.008 mmol) was added, and the reaction was stirred in a sealed vessel at 85°C for 48hrs. The reaction was poured into water, and extracted 3 x DCM. The combined organic extracts were dried over Na_2SO_4, and the solvent evaporated under reduced pressure. The product, 7-hydroxy-2-methoxy-4-phenylcyclohepta-2,4,6-trien-1-one (15mg, 77% isolated yield) , was purified by RP-Flash chromatography using a C18 column and eluting with a linear gradient of 20%-60% acetonitrile in water containing 0.05% trifluoroacetic acid over 20 column volumes. Isolated 7-hydroxy-2-methoxy-4-phenylcyclohepta-2,4,6-trien-1-one (19.7 mg, 0.086 mmol) was then dissolved in 33% HBr in acetic acid to a concentration of 0.1M, and heated to 120°C in a sealed vessel for 1hr. The reaction was diluted 20 fold with DCM and 0.2M phosphate buffer was added until the pH of the aqueous layer was ~6. The reaction was then extracted 3 x DCM and the combined organic extracts dried over Na_2SO_4, and the solvent evaporated under reduced pressure to yield a yellow oil. The residue was subjected RP-Flash chromatography using a C18 column and eluting with a linear gradient of 20%-60% acetonitrile in water containing 0.05% trifluoroacetic acid over 20 column volumes. Fractions containing product were redissolved in CH_2Cl_2 and treated with saturated aq. K_2CO_3. The DCM layer was discarded, then the pH of the aqueous layer was adjusted to ~6, and extracted 3 x DCM. The combined organic extracts were dried over Na_2SO_4, and the solvent evaporated under reduced pressure to afford pure 2,7-dihydroxy-4-phenylcyclohepta-2,4,6-trien-1-one (5.8 mg, 31% yield). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.56 – 7.36 (m, 7H) .**HRMS** (TOF MS ES+) *m/z* Calcd for $C_{13}H_{11}O_3$: 215.0708. Mass Found: 215.0726.

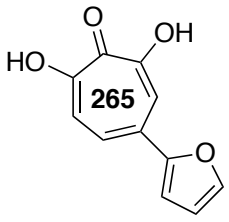
VIc. 4-([1,1'-biphenyl]-4-yl)-2,7-dihydroxycyclohepta-2,4,6-trien-1-one (264)



4-bromo-2,7-dihydroxycyclohepta-2,4,6-trien-1-one (**s5**) (20.7 mg, 0.090 mmol) and 4-biphenyl boronic acid (25 mg, 0.125 mmol) were dissolved in 4.5mL of 2-propanol. 1.25mL of 1M aq. K_2CO_3 was then added and the solution was purged with Ar for 15min, and $Pd(PPh_3)_4$ (10.4 mg, 0.009 mmol) was added, and the reaction was stirred in a sealed vessel at 85°C for 48hrs. The reaction was poured into water, and extracted 3 x DCM. The combined

organic extracts were dried over Na_2SO_4, and the solvent evaporated under reduced pressure. The product, 4-([1,1'-biphenyl]-4-yl)-7-hydroxy-2-methoxycyclohepta-2,4,6-trien-1-one (9.6mg, 35% isolated yield) , was purified by RP-Flash chromatography using a C18 column and eluting with a linear gradient of 20%-60% acetonitrile in water containing 0.05% trifluoroacetic acid over 20 column volumes. Isolated 4-([1,1'-biphenyl]-4-yl)-7-hydroxy-2-methoxycyclohepta-2,4,6-trien-1-one (9.6mg, 0.032mmol) was then dissolved in 33% HBr in acetic acid to a concentration of 0.1M, and heated to 120°C in a sealed vessel for 1hr. The reaction was diluted 20 fold with DCM and 0.2M phosphate buffer was added until the pH of the aqueous layer was ~6. The reaction was then extracted 3 x DCM and the combined organic extracts dried over Na_2SO_4, and the solvent evaporated under reduced pressure to yield a pale yellow oil. The product, 4-([1,1'-biphenyl]-4-yl)-2,7-dihydroxycyclohepta-2,4,6-trien-1-one (1.8mg, 19% isolated yield), was isolated as an off-white yellow solid by RP-Flash chromatography using a C18 column and eluting with a linear gradient of 20%-60% acetonitrile in water containing 0.05% trifluoroacetic acid over 20 column volumes. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 1.7 Hz, 1H), 7.74 – 7.68 (m, 2H), 7.63 (ddd, *J* = 18.6, 10.0, 6.0 Hz, 5H), 7.51 – 7.43 (m, 3H), 7.39 (ddd, *J* = 7.3, 3.8, 1.2 Hz, 1H). **HRMS** (TOF MS ES+) *m/z* Calcd for $C_{19}H_{15}O_3$: 291.1021. Mass Found: 291.1015.

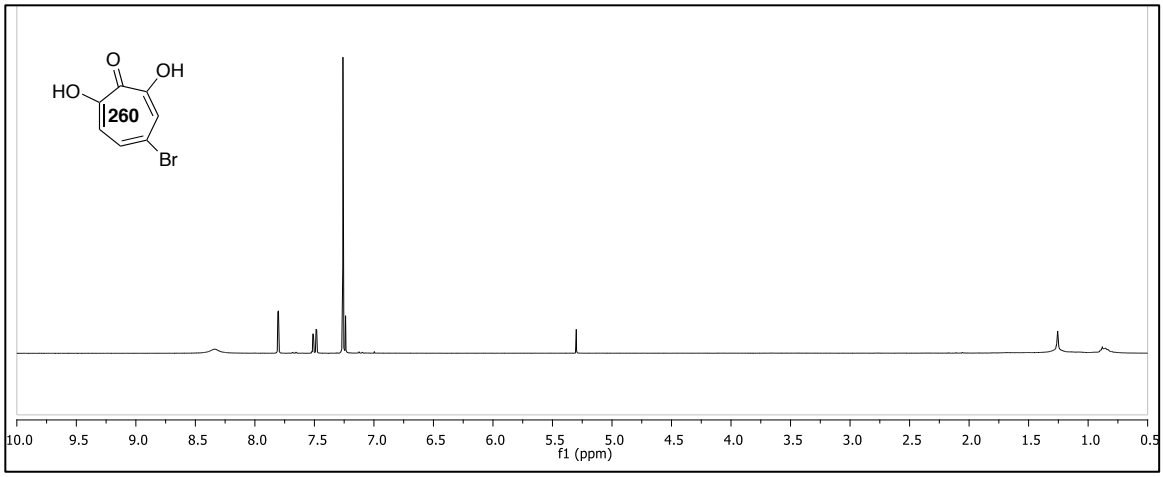
VId. 4-(furan-2-yl)-2,7-dihydroxycyclohepta-2,4,6-trien-1-one (265)

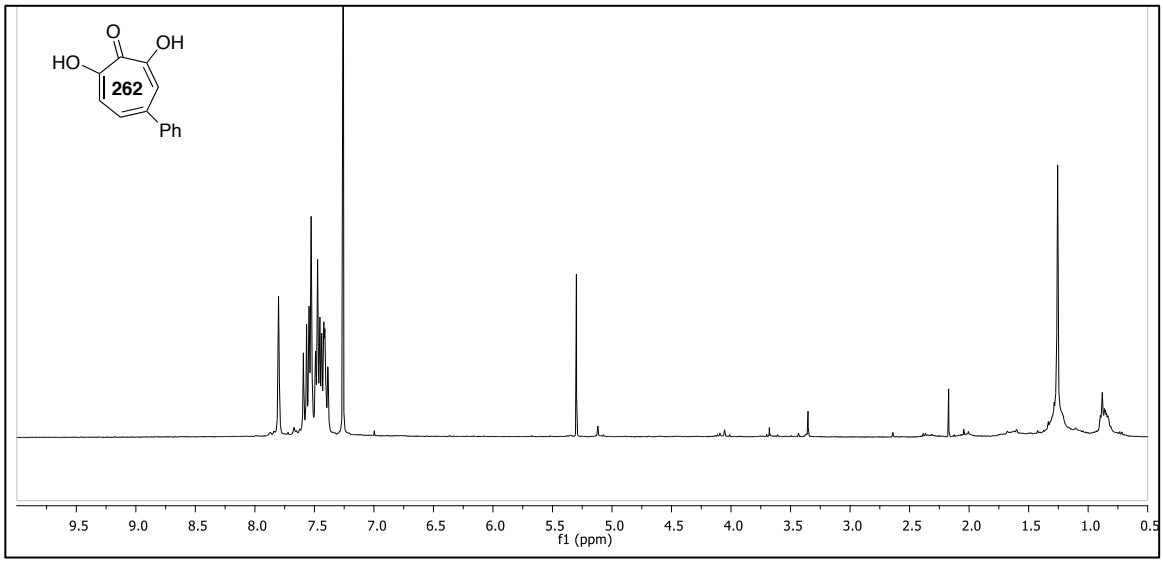


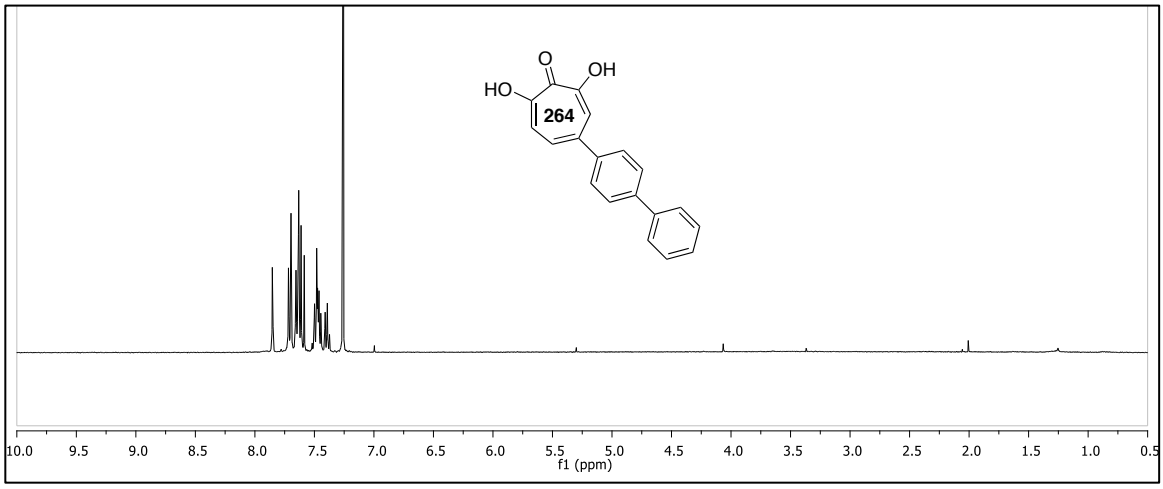
4-bromo-2,7-dihydroxycyclohepta-2,4,6-trien-1-one (**s5**) (19.3 mg, 0.063 mmol) and 2-furan boronic acid (9.8 mg, 0.124 mmol) were dissolved in 3.15mL of 2-propanol. 0.88mL of 1M aq. K_2CO_3 was then added and the solution was purged with Ar for 15min, and $Pd(PPh_3)_4$ (7.3 mg, 0.006 mmol) was added, and the reaction was stirred in a sealed vessel at 85°C for 48 hrs. The reaction was poured into water, and extracted 3 x DCM. The combined organic extracts were dried over Na_2SO_4, and the solvent evaporated under reduced pressure. The product, 44-(furan-2-yl)-7-hydroxy-2-methoxycyclohepta-2,4,6-trien-1-one (8.8 mg, 48% isolated yield), was purified by RP-Flash chromatography using a C18 column and eluting with a linear gradient of 20%-60% acetonitrile in water containing 0.05% trifluoroacetic acid over 20 column volumes.

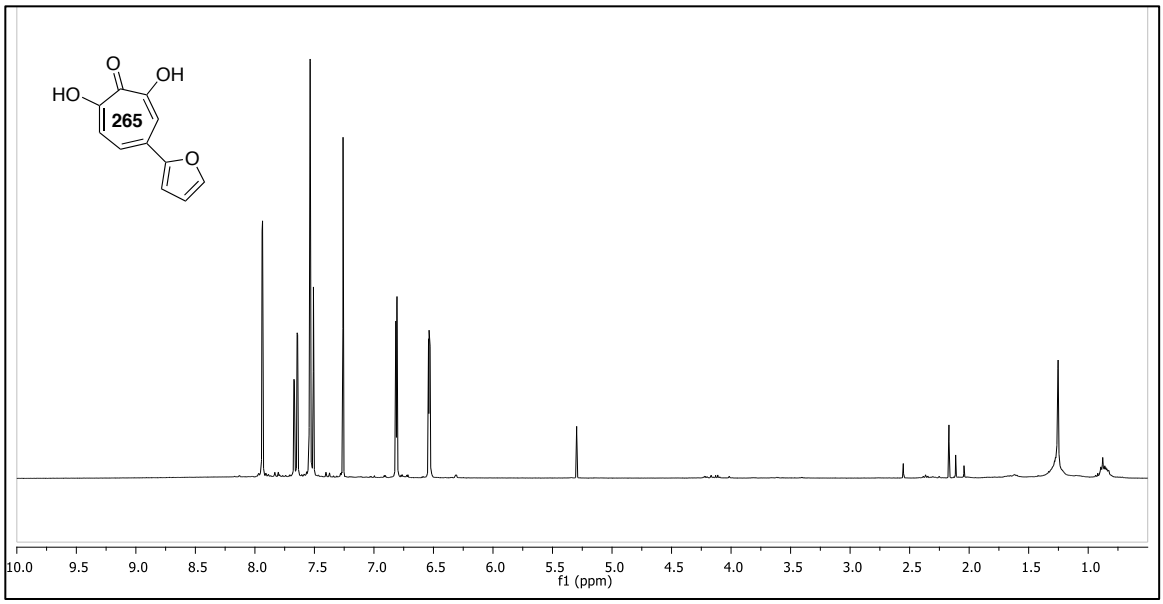
Isolated 4-([1,1'-biphenyl]-3-yl)-7-hydroxy-2-methoxycyclohepta-2,4,6-trien-1-one (13.1mg, 0.06mmol) was then dissolved in 33% HBr in acetic acid to a concentration of 0.1M, and heated to 120°C in a sealed vessel for 1hr. The reaction was diluted 20 fold with DCM and 0.2 M phosphate buffer was added until the pH of the aqueous layer was ~6. The reaction was then extracted 3 x DCM and the combined organic extracts dried over Na_2SO_4, and the solvent evaporated under reduced pressure to yield the product, 4-(furan-2-yl)-2,7-dihydroxycyclohepta-2,4,6-trien-1-one (12.4 mg, >95%) was isolated as a light yellow solid. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 1.6 Hz, 1H), 7.66 (dd, *J* = 10.9, 1.6 Hz, 1H), 7.54 (s, 1H), 7.52 (d, *J* = 10.9 Hz, 1H,), 6.81 (d, *J* = 3.5 Hz, 1H), 6.53 (dt, *J* = 8.8, 4.4 Hz, 1H). **HRMS** (TOF MS ES+) *m/z* Calcd for $C_{11}H_9O_4$: 205.0501. Mass Found: 205.0558

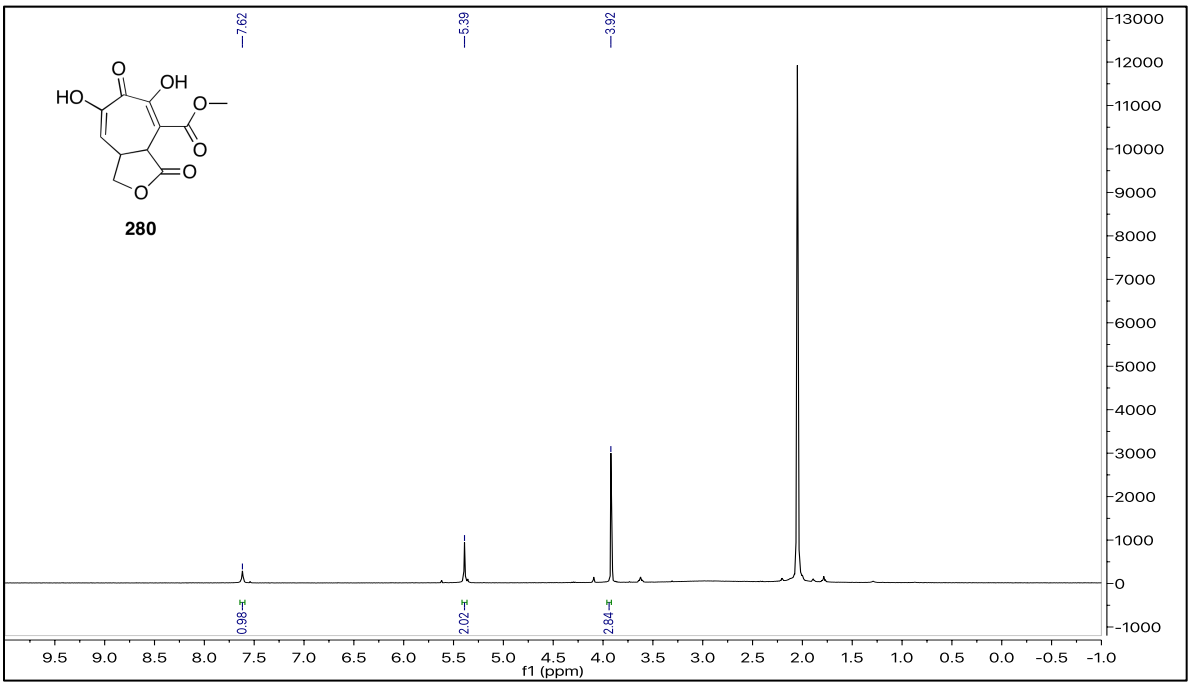
VII. ^{1}H Spectra of New Compounds Tested (In Numerical Order)

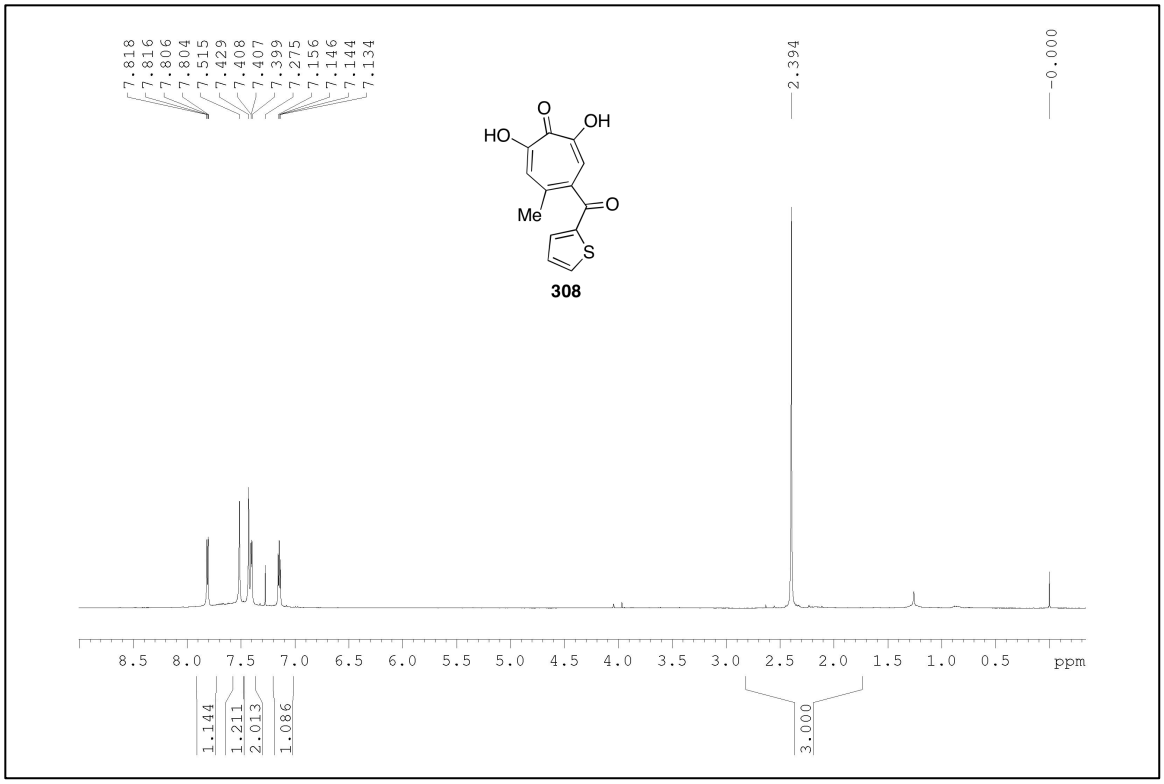


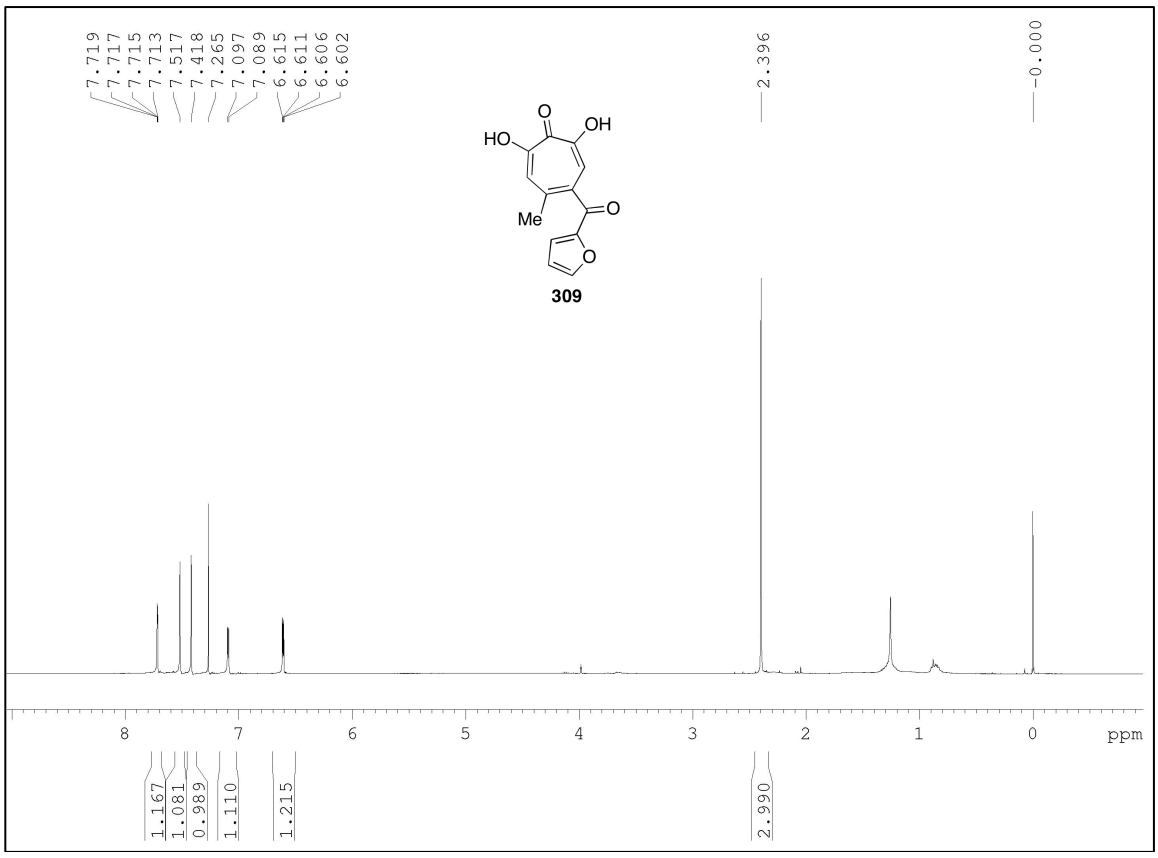


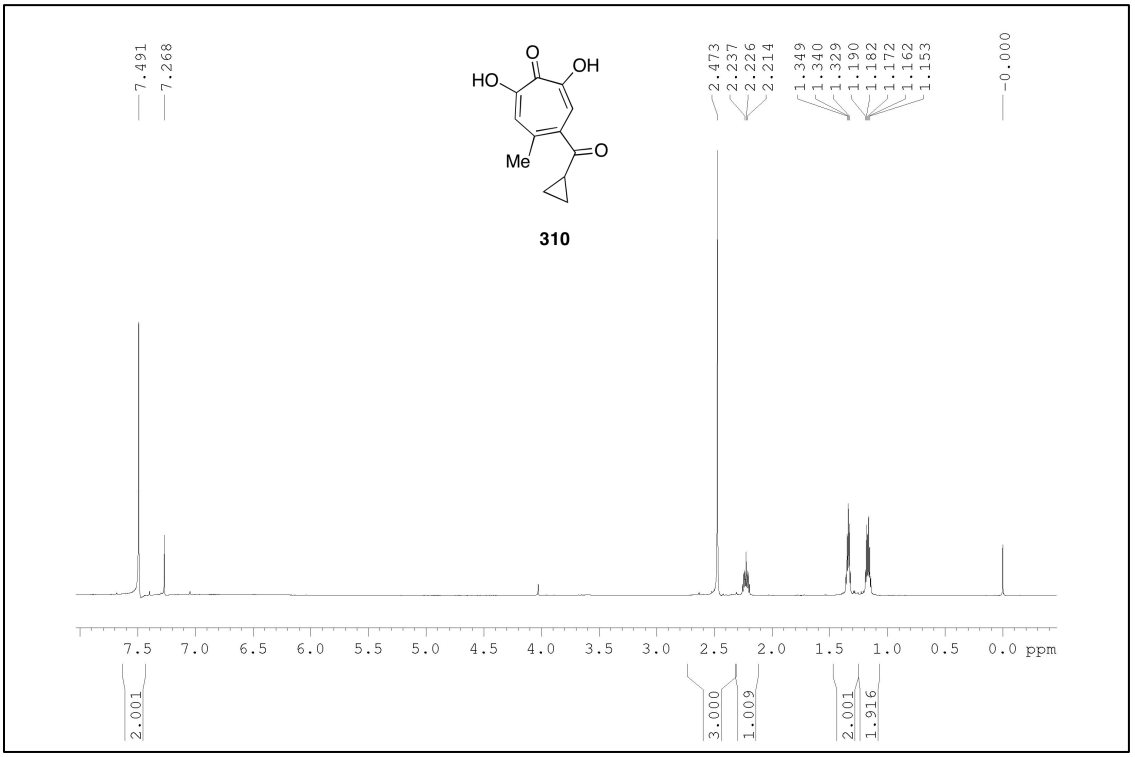


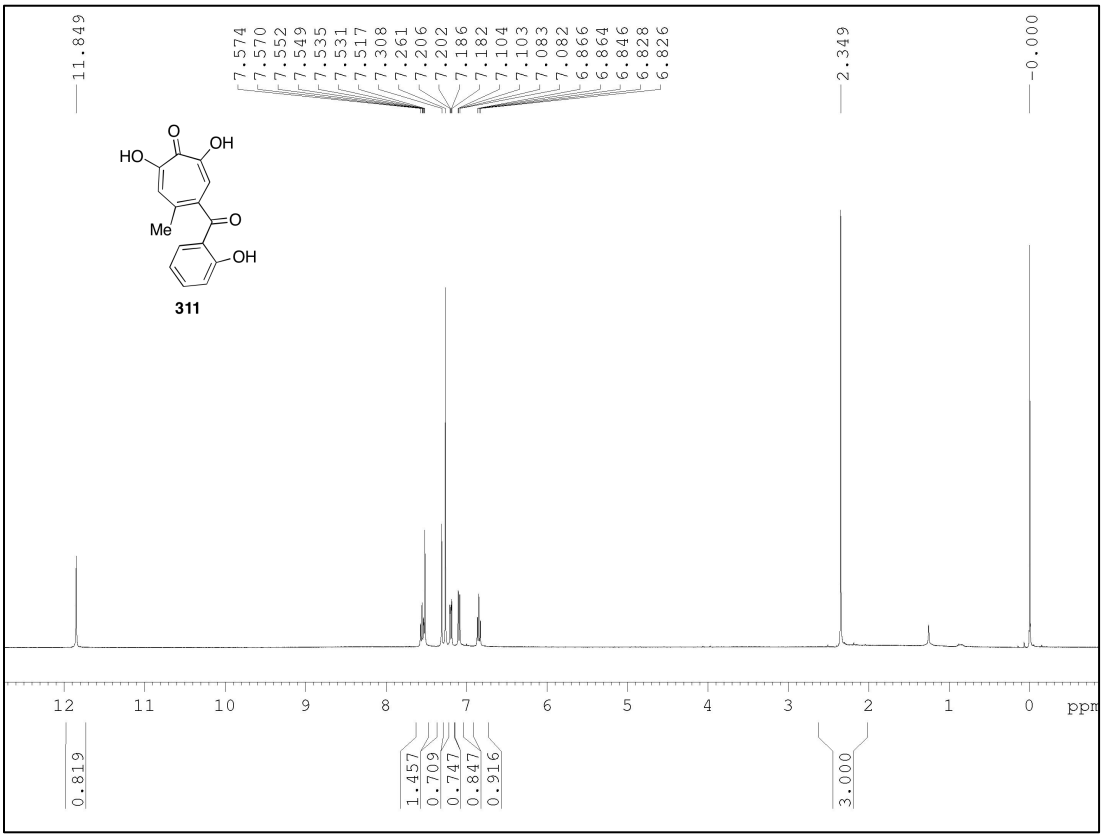

O
OH
HO
265
O
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0
f1 (ppm)

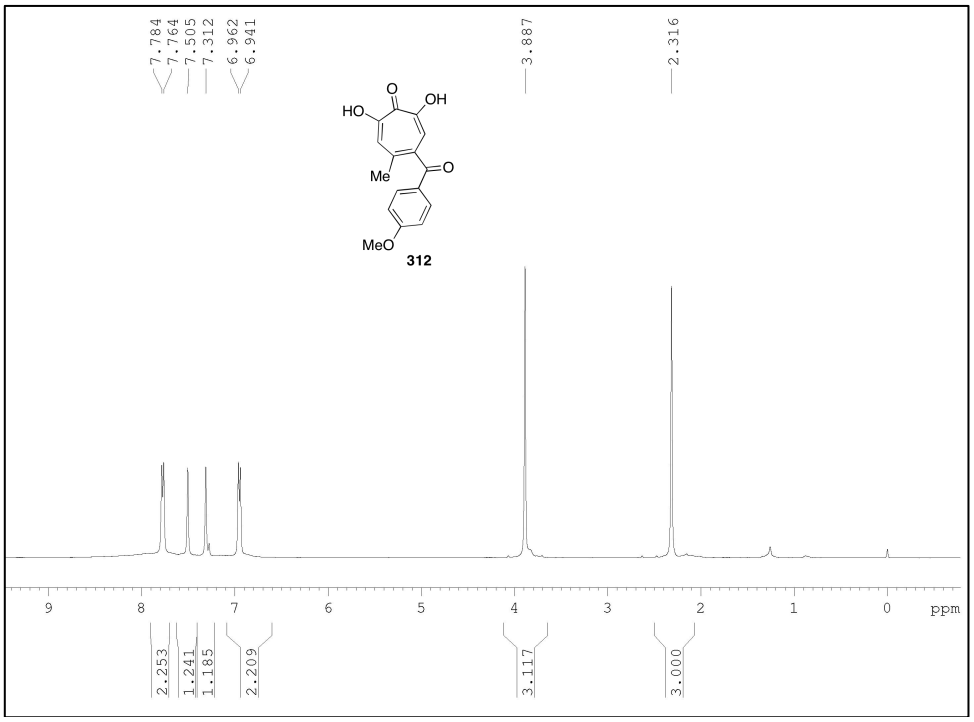

7.62
5.39
3.92
O
OH
HO
O
O
O
O
280
0.98
2.02
2.84
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

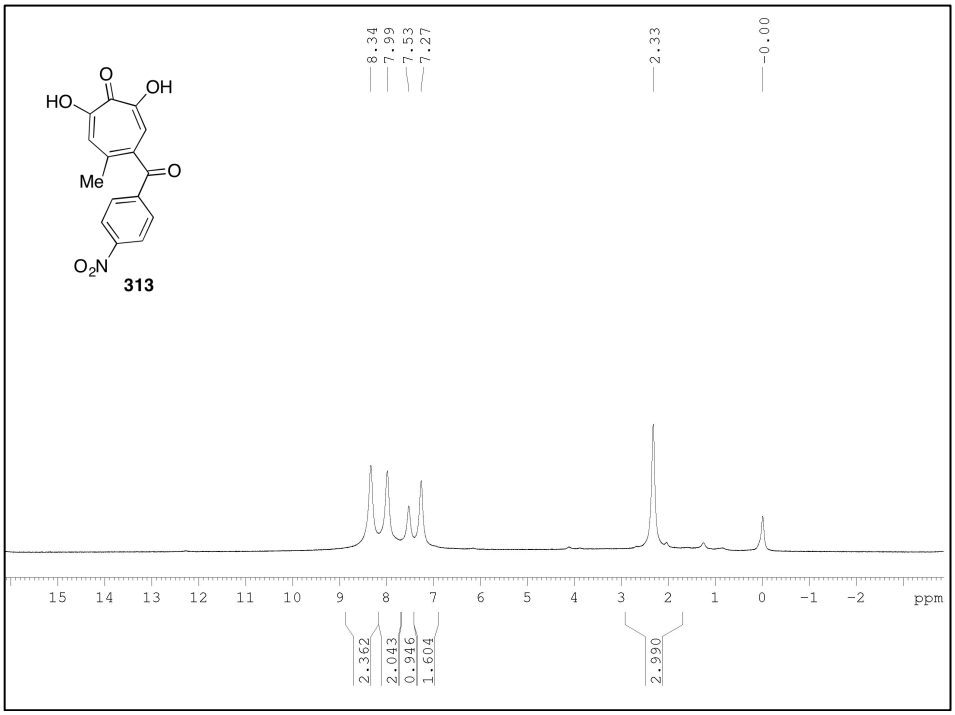

7.818
7.816
7.806
7.804
7.515
7.429
7.408
7.407
7.399
7.275
7.156
7.146
7.144
7.134
2.394
0.000
HO
OH
O
Me
O
S
308
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.144
1.211
2.013
1.086
3.000

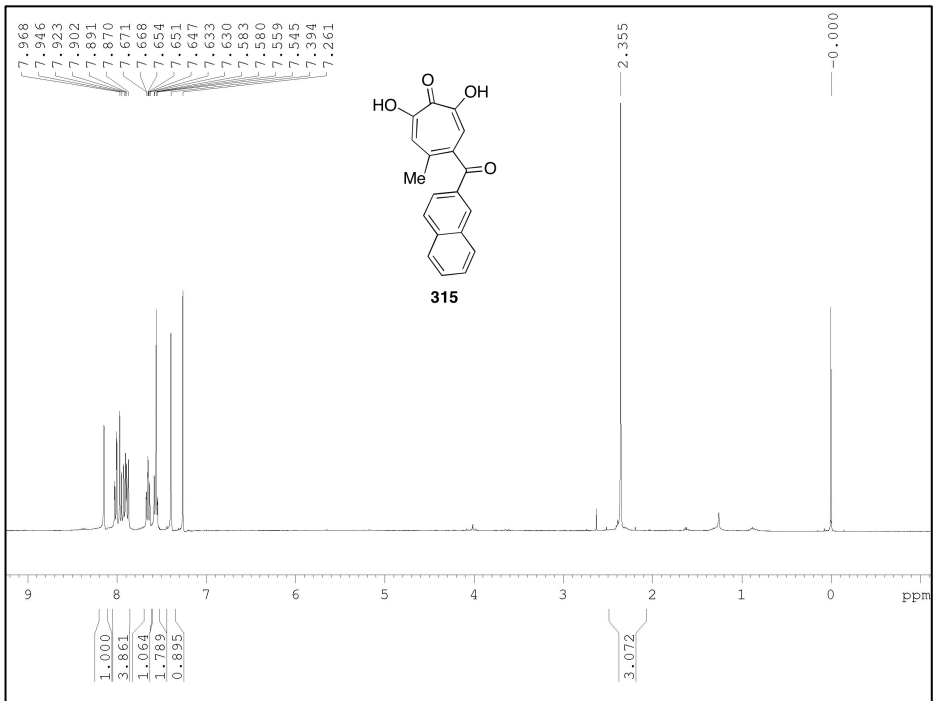

7.719
7.717
7.715
7.713
7.517
7.418
7.265
7.097
7.089
6.615
6.611
6.606
6.602
2.396
0.000
HO
OH
O
Me
O
O
309
8 7 6 5 4 3 2 1 0 ppm
1.167
1.081
0.989
1.110
1.215
2.990

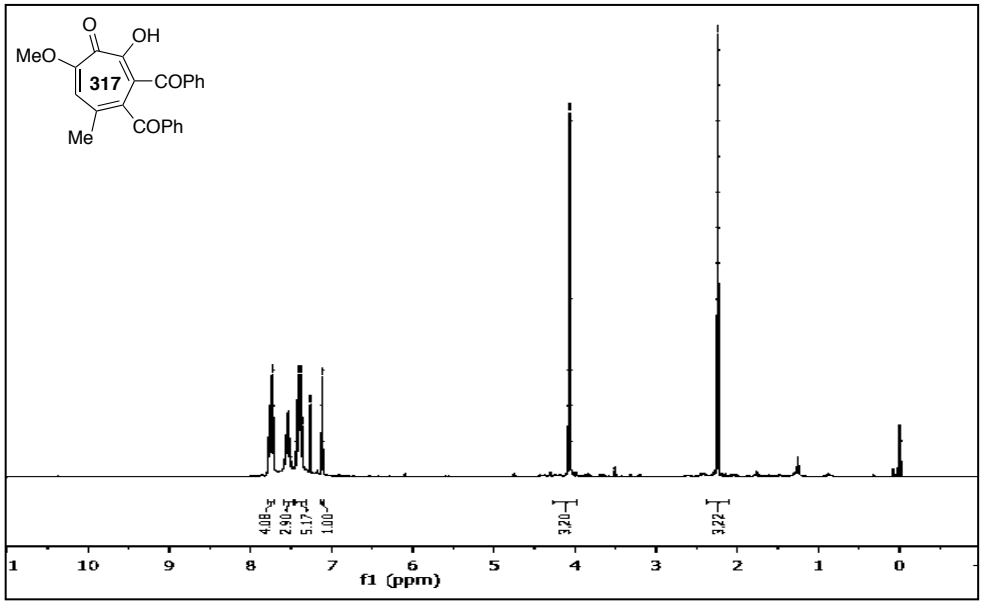

7.491
7.268
2.473
2.237
2.226
2.214
1.349
1.340
1.329
1.190
1.182
1.172
1.162
1.153
-0.000
HO
OH
Me
O
O
310
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.001
3.000
1.009
2.001
1.916

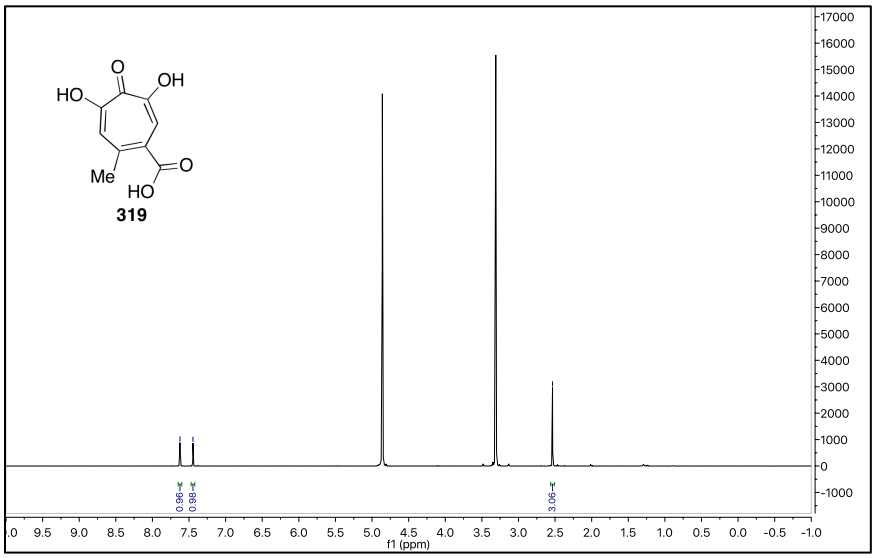

11.849
7.574
7.570
7.552
7.549
7.535
7.531
7.517
7.308
7.261
7.206
7.202
7.186
7.182
7.104
7.103
7.083
7.082
6.866
6.864
6.846
6.828
6.826
2.349
-0.000
HO
OH
Me
O
OH
311
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.819
1.457
0.709
0.747
0.847
0.916
3.000


7.784
7.764
7.505
7.312
6.962
6.941
3.887
2.316
HO
OH
Me
MeO
312
9
8
7
6
5
4
3
2
1
0
ppm
2.253
1.241
1.185
2.209
3.117
3.000


8.34
7.99
7.53
7.27
2.33
-0.00
HO
OH
Me
O2N
313
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
ppm
2.362
2.043
0.946
1.604
2.990


7.968
7.946
7.923
7.902
7.891
7.870
7.671
7.668
7.654
7.651
7.647
7.633
7.630
7.583
7.580
7.559
7.545
7.394
7.261
2.355
-0.000
HO
O
OH
Me
O
315
9
8
7
6
5
4
3
2
1
0
ppm
1.000
3.861
1.064
1.789
0.895
3.072


MeO
O
OH
317
COPh
Me
COPh
4.08
2.90
5.17
1.00
3.20
3.22
1
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


O
OH
HO
Me
HO
O
319
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
0.96
0.98
3.06
9.5 9.0 8.5 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 -0.5 -1.0
f1 (ppm)