Supporting Information

First- and Second-Generation Practical Syntheses of Chroman-4-one Derivative: A Key Intermediate for the Preparation of SERT/5-HT$_{1A}$ Dual Inhibitors

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Contents

NMR spectra of 3, 11, 12, 4, 5, 8, 9, 19 and 22
Chemical Formula: C_{12}H_{16}O_{4}

Exact Mass: 224.10

Molecular Weight: 224.25
Chemical Formula: $C_{16}H_{22}O_7$

Exact Mass: 326.14

Molecular Weight: 326.34
Chemical Formula: $\text{C}_{16}\text{H}_{22}\text{O}_7$

Exact Mass: 326.14
Molecular Weight: 326.34
Chemical Formula: C_{14}H_{20}O_{5}
Exact Mass: 268.13
Molecular Weight: 268.31
Chemical Formula: C_{14}H_{20}O_{5}
Exact Mass: 268.13
Molecular Weight: 268.31
Chemical Formula: C_{12}H_{14}O_{5}
Exact Mass: 238.08
Molecular Weight: 238.24
Chemical Formula: $\text{C}_{12}\text{H}_{14}\text{O}_5$

Exact Mass: 238.08

Molecular Weight: 238.24
Chemical Formula: \( C_{12}H_{12}O_4 \)
Exact Mass: 220.07
Molecular Weight: 220.22
Chemical Formula: $C_{12}H_{12}O_4$

Exact Mass: 220.07

Molecular Weight: 220.22
Chemical Formula: $C_{11}H_{12}O_3$

Exact Mass: 192.08

Molecular Weight: 192.21
Chemical Formula: C_{11}H_{12}O_{3}

Exact Mass: 192.08
Molecular Weight: 192.21
Chemical Formula: $C_{18}H_{18}O_5S$

Exact Mass: 346.09

Molecular Weight: 346.40
Chemical Formula: C₁₁H₁₄O₄
Exact Mass: 210.09
Molecular Weight: 210.23
## NMR Spectral Data

**Chemical Formula:** C$_{11}$H$_{14}$O$_{4}$

**Exact Mass:** 210.09

**Molecular Weight:** 210.23

| PPM  | 172.32 | 156.62 | 131.56 | 129.82 | 114.14 | 100.14 | 93.29 | 86.54 | 84.17 | 75.82 | 72.01 | 63.51 | 62.45 | 61.45 | 40.34 | 40.06 | 39.78 | 39.50 | 39.23 | 39.06 | 38.78 | 38.50 | 38.23 | 38.06 | 37.78 | 37.50 |
|------|--------|--------|--------|--------|--------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|

**Diagram:**

![NMR Spectrum](image)

**Notes:**

- **DFILE:** K0612-150-OH2bcm_E83_FT.als
- **COMNT:** K0612-150-OH
- **DATIM:** Sun Oct 16 17:31:51 2011
- **OBNUC:** 13C
- **EXMOD:** bcm
- **OBFRQ:** 75.45 MHz
- **OBSET:** 0.00 KHz
- **OBFIN:** 125840.00 Hz
- **POINT:** 32768
- **FREQU:** 20366.60 Hz
- **SCANS:** 1024
- **ACQTM:** 1.6089 sec
- **PD:** 1.3911 sec
- **PW1:** 5.00 usec
- **IRNUC:** 1H
- **CTEMP:** 22.8 c
- **SLVNT:** DMSO
- **EXREF:** 39.50 ppm
- **BF:** 1.20 Hz
- **RGAIN:** 27
Chemical Formula: C_{18}H_{20}O_{6}S
Exact Mass: 364.10
Molecular Weight: 364.41
Chemical Formula: C_{18}H_{20}O_{6}S

Exact Mass: 364.10

Molecular Weight: 364.41