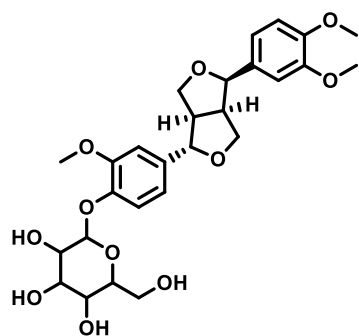


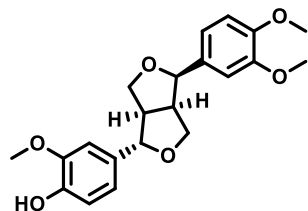
Supplemental File



Forsythin

^1H NMR (DMSO- d_6 , 600 MHz, ppm): δ 7.05 (m, 1H), 6.96 (m, 1H), 6.92 (m, 2H), 6.87 (m, 2H), 5.18 (m, 1H), 5.04 (m, 1H), 4.98 (m, 1H), 4.88 (m, 1H), 4.80 (m, 1H), 4.50 (m, 1H), 4.38 (m, 1H), 4.10 (m, 1H), 3.76–3.73 (m, 11H), 3.67–3.65 (m, 1H), 3.46–3.37 (m, 2H), 3.28–3.07 (m, 5H), 2.84–2.83 (m, 1H)

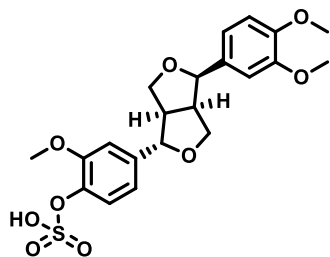
^{13}C NMR (DMSO- d_6 , 150 MHz, ppm): δ 148.90, 148.43, 147.57, 145.88, 135.26, 131.15, 118.11, 117.52, 115.17, 111.50, 110.39, 109.39, 100.11, 86.64, 81.22, 77.00, 76.84, 73.19, 70.29, 69.66, 68.93, 60.66, 55.65, 55.44, 53.99, 49.28



Aglycone (M1)

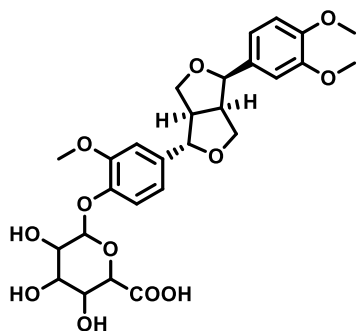
^1H NMR (DMSO- d_6 , exchanged by D_2O , 600 MHz, ppm): δ 6.91–6.86 (m, 4H), 6.75–6.73 (m, 2H), 4.77 (d, $J = 6$ Hz, 1H), 4.30 (d, $J = 7.2$ Hz, 1H), 4.02 (d, $J = 9.6$ Hz, 1H), 3.74 (s, 3H), 3.73 (s, 3H), 3.72 (s, 3H), 3.72–3.70 (m, 2H), 3.35 (m, 1H), 3.05 (m, 1H), 2.81 (m, 1H)

^{13}C NMR (DMSO- d_6 , 150 MHz, ppm): δ 148.44, 147.58, 147.51, 145.97, 132.30, 131.19, 118.62, 117.52, 115.14, 111.49, 110.25, 109.39, 86.98, 81.22, 70.29, 68.82, 55.56, 55.43, 53.89, 49.33



M1 sulfate (M2)

^1H NMR (DMSO- d_6 , 400 MHz, ppm): δ 7.41-7.39 (m, 1H), 6.94- 6.83 (m, 5H), 4.80 (m, 1H), 4.38 (m, 1H), 4.11 (m, 1H), 3.78 (m, 11H), 3.10 (m, 1H), 2.85 (m, 1H)

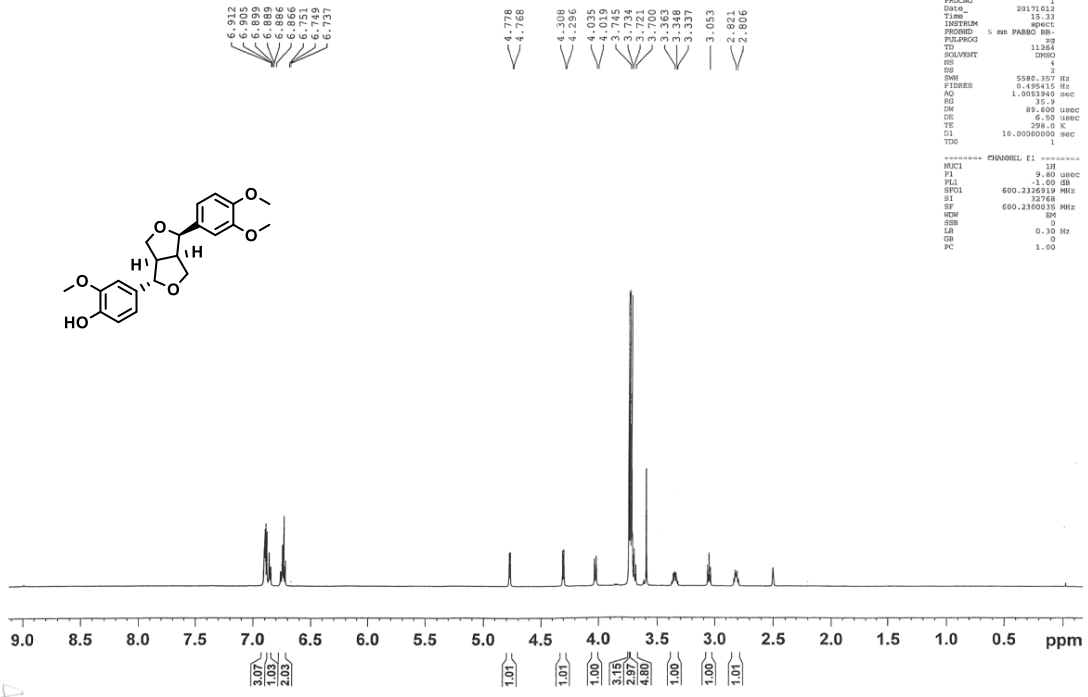


M1 glucuronide (M7)

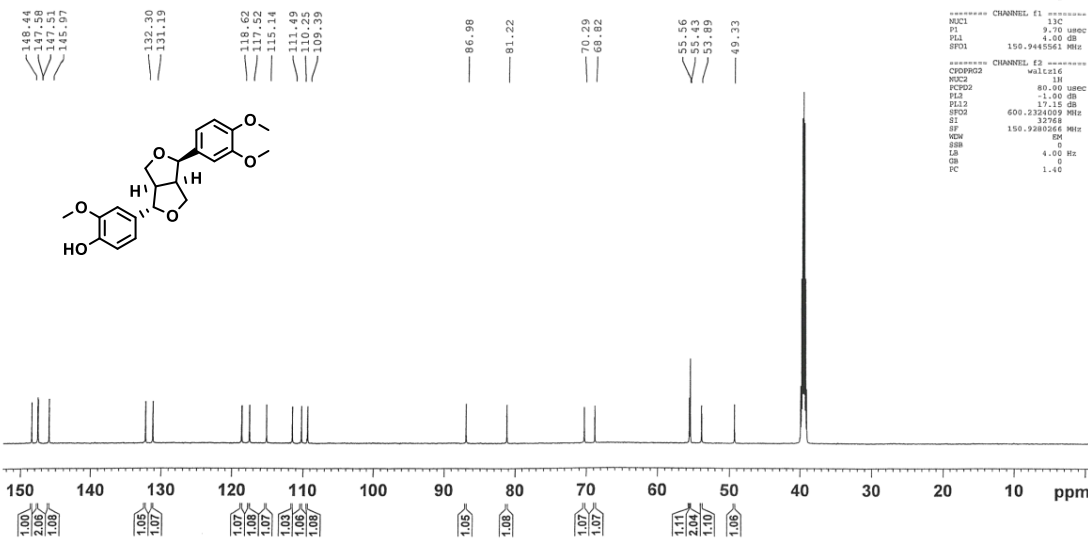
^1H NMR (DMSO- d_6 , 600 MHz, ppm): δ 7.26 (bra, 1H), 7.04 (m, 1H), 6.96 (m, 1H), 6.92 (m, 2H), 6.87 (m, 2H), 5.09 (m, 1H), 4.94 (m, 1H), 4.83- 4.79 (m, 2H), 4.39 (m, 1H), 4.10 (m, 1H), 3.77– 3.74 (m, 11H), 3.38 (m, 1H), 3.31 (m, 2H), 3.21 (m, 2H), 3.09 (m, 2H), 2.86– 2.84 (m, 1H)

^{13}C NMR (DMSO- d_6 , 150 MHz, ppm): δ 171.54, 148.94, 148.41, 147.53, 146.05, 135.17, 131.18, 118.04, 117.50, 115.56, 111.49, 110.44, 109.38, 100.22, 86.63, 81.22, 76.99, 73.48, 73.11, 72.07, 70.33, 68.89, 55.71, 55.42, 54.01, 49.22

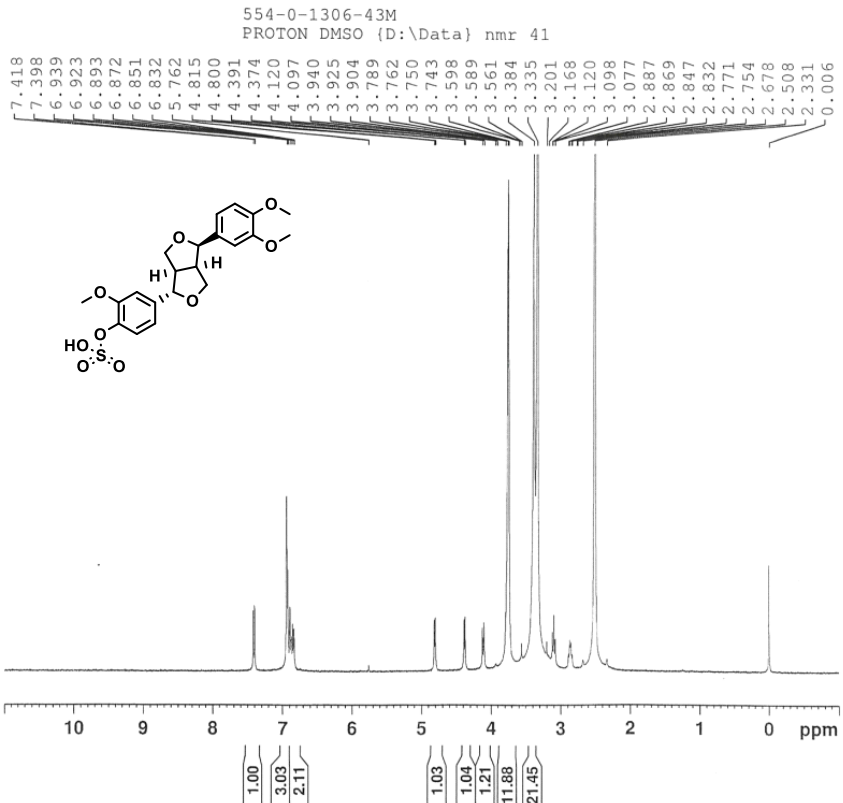
H1 in D2O



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F2RES 0.195418 Hz
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RG 35
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DE 6.50 usec
TE 298.0 K
D1 10.0000000 sec
TD0 1
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SI 32768
SF 600.2300035 MHz
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
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TD 20480
SOLVENT DMSO
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F2RES 1.637604 Hz
AQ 0.1078050 sec
RG 7298.2
DM 15.000 usec
DE 6.50 usec
TE 298.0 K
D1 7.0000000 sec
D11 0.0300000 sec
TD0 1
----- CHANNEL f1 -----
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P1 9.70 usec
PL1 0
SFO1 150.9445561 MHz
----- CHANNEL f2 -----
CHPROG waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
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GB 0
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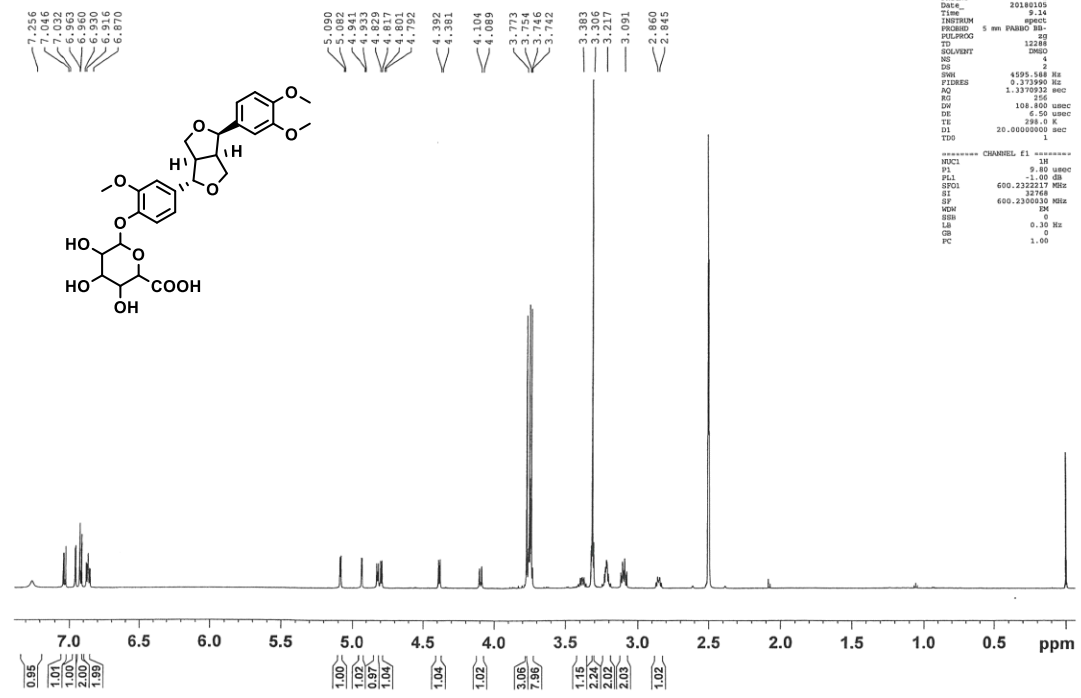
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EXPNO 1
PROCNO 1

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SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203.15
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

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NUC1 1H
P1 8.70 usec
PLW1 20.00000000 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 0.30 Hz
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PC 1.00

kd-2-glu H1



NAME k1andoy
EXPNO 21
PROCNO 1
Date_ 20180105
Time 9.14
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TD 12288
SOLVENT DMSO
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FIDRES 0.373990 Hz
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RG 256
DW 108.800 usec
DE 6.50 usec
TE 298.0 K
D1 20.00000000 sec
TDO 1

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NUC1 1H
P1 8.00 usec
PLW1 1.00000000 W
SF 600.322217 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kd-2-glu nne

