

Supplementary Materials

Determination of Propionylbrassinolide and Its Impurities by High-Performance Liquid Chromatography with Evaporative Light Scattering Detection

Lidong Cao¹, Hong Zhang¹, Hongjun Zhang², Li Yang¹, Miaomiao Wu¹, Puguo Zhou^{2,*}, and Qiliang Huang^{1,*}

¹ Institute of Plant Protection, Chinese Academy of Agricultural Sciences, No. 2 Yuanmingyuan West Road, Beijing 100193, China; caolidong@caas.cn (L.C.); hongapplezh@163.com (H.Z.); huaweimian666666@163.com (L.Y.); wumiaomiao2016@163.com (M. W.)

² Institute for the Control of Agrochemicals, Ministry of Agriculture, No. 22 Maizidian Street, Beijing 110000, China; hongjun-zh1975@163.com (H.Z.)

*Correspondence: zhoupuguo@sohu.com, Tel./Fax: +86 10 59195230; qlhuang@ippcaas.cn; Tel./Fax: (+86) 10 62816909

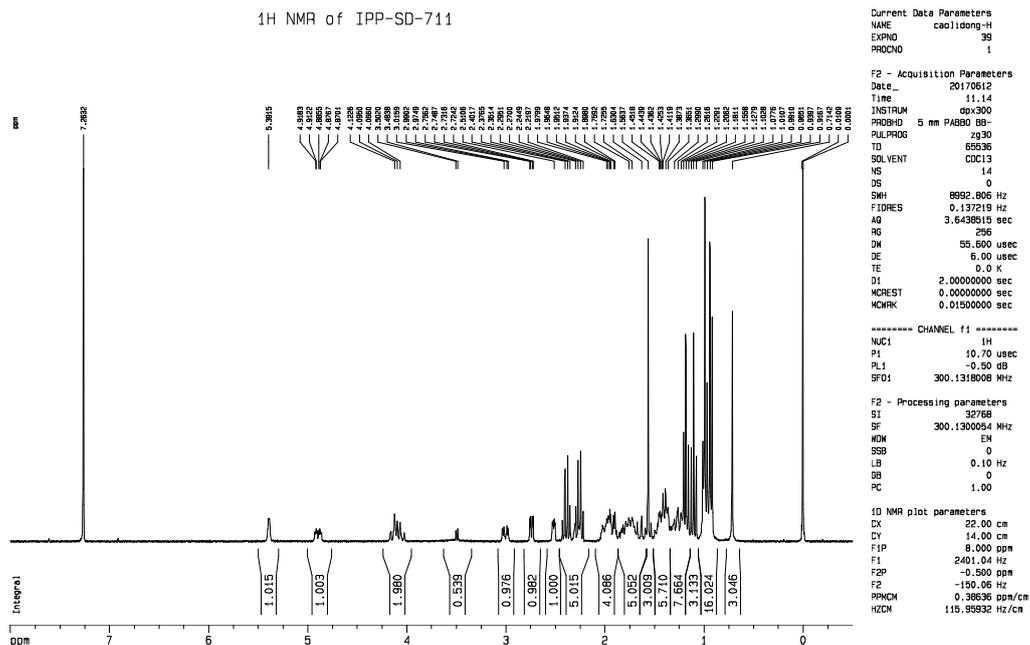


Figure S1. ¹H NMR of propionylbrassinolide

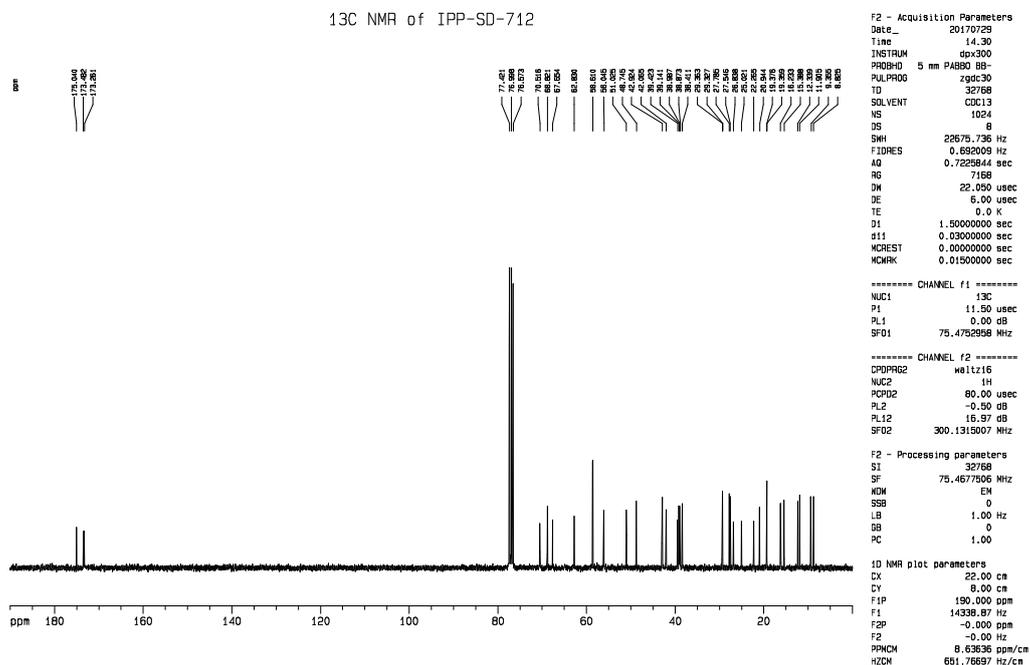


Figure S2. ¹³C NMR of propionylbrassinolide

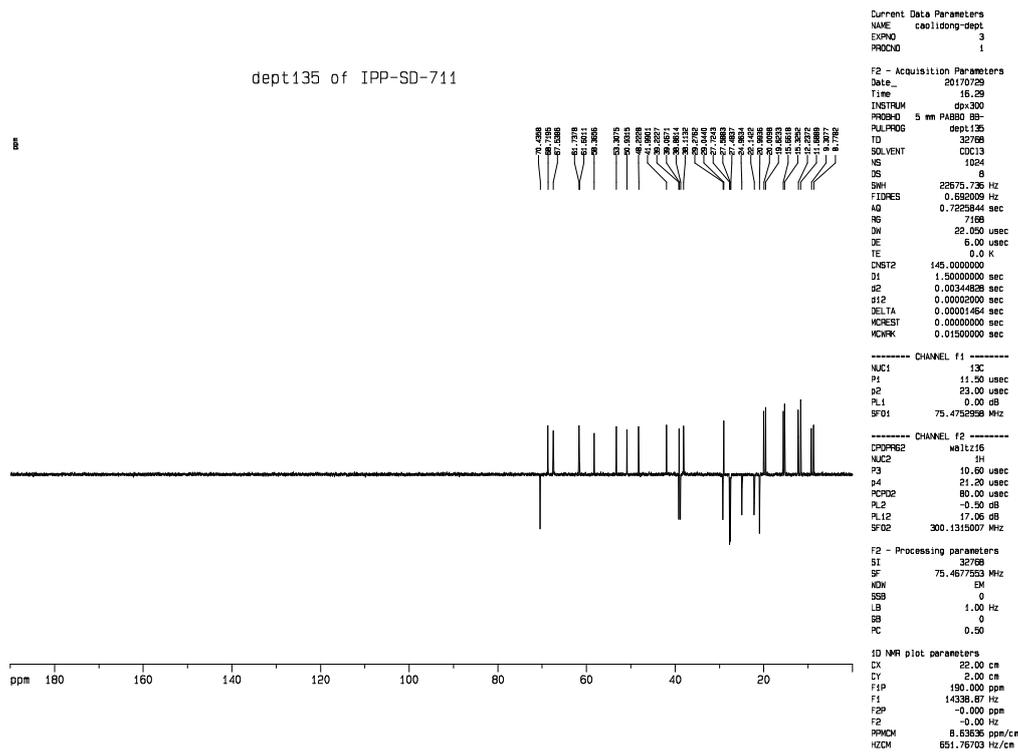


Figure S3. ¹³C NMR (DEPT 135) of propionylbrassinolide

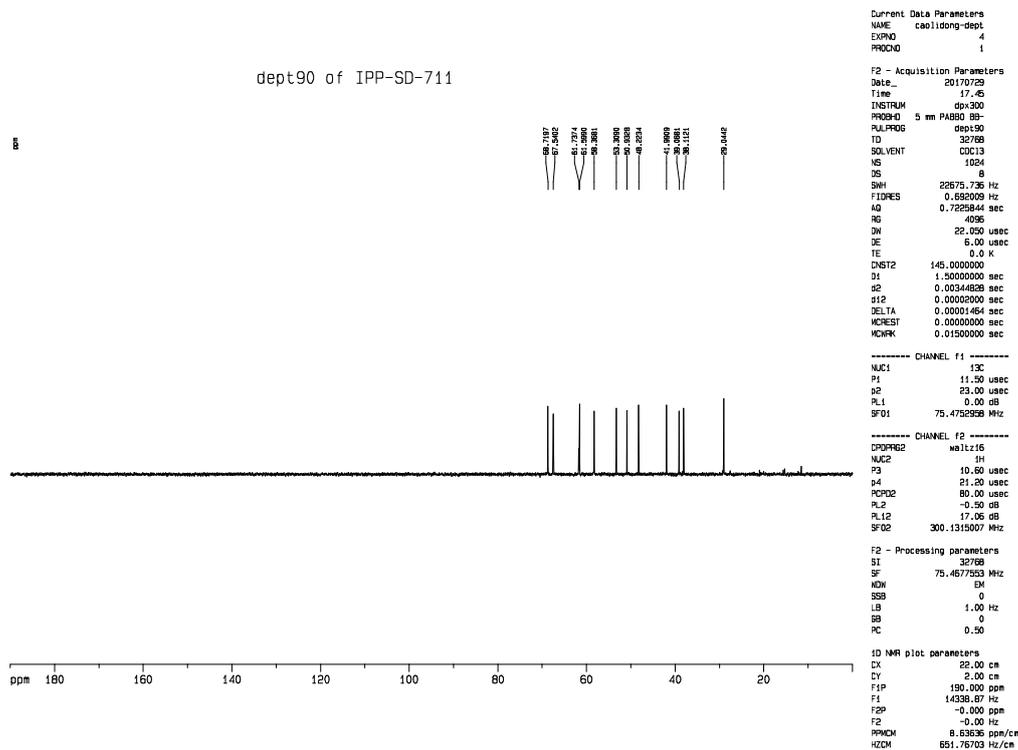
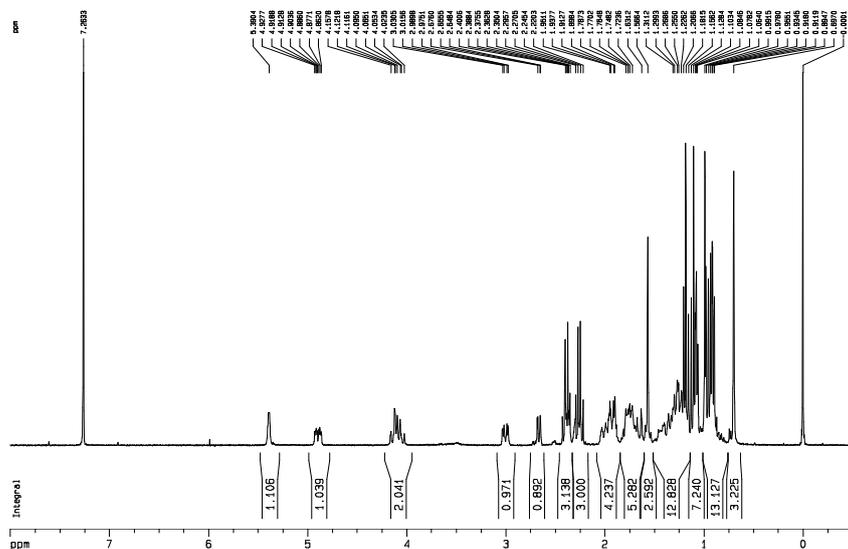


Figure S4. ¹³C NMR (DEPT 90) of propionylbrassinolide

1H NMR of IPP-SD-710



Current Data Parameters
NAME cao1dong-H
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170512
Time 11:17
INSTRUM dpx300
PROBHD 5 mm PABBO B9-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 40
DS 0
SWH 8992.906 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 295
DM 55.500 usec
DE 6.00 usec
TE 0.0 K
D1 2.0000000 sec
MCREST 0.0000000 sec
MCHRK 0.0150000 sec

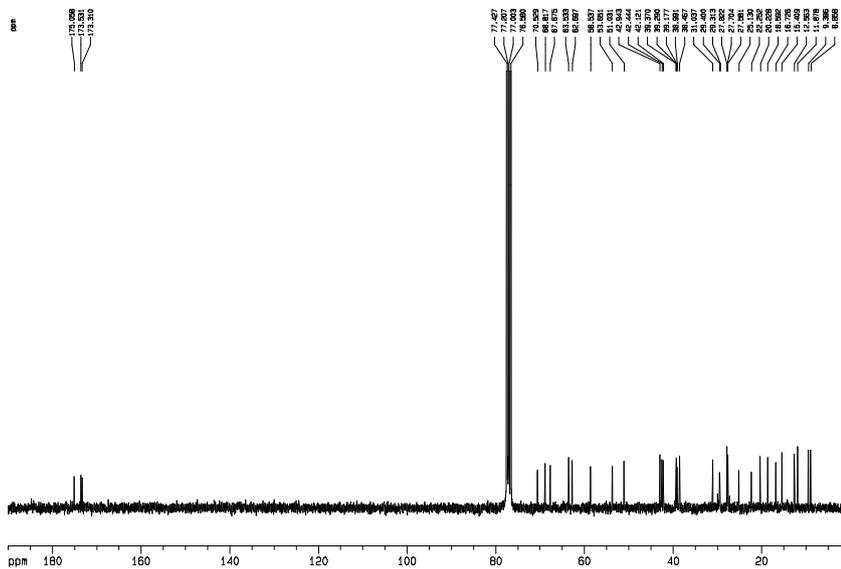
----- CHANNEL f1 -----
NUC1 1H
P1 10.70 usec
PL1 -0.50 dB
SFO1 300.1318008 MHz

F2 - Processing parameters
SI 32768
SF 300.1300054 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 16.00 cm
F1P 8.000 ppm
F1 2401.04 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPCM 0.36536 ppm/cm
HZCM 115.95932 Hz/cm

Figure S5. ¹H NMR of impurity 1

¹³C NMR of IPP-SD-710



Current Data Parameters
NAME cao1dong-13C
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170730
Time 23:22
INSTRUM dpx300
PROBHD 5 mm PABBO B9-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 4096
DS 8
SWH 22675.736 Hz
FIDRES 0.692009 Hz
F1P 8152
AQ 0.7229844 sec
RG 8152
DM 22.050 usec
DE 6.00 usec
TE 0.0 K
D1 1.5000000 sec
d11 0.0300000 sec
MCREST 0.0000000 sec
MCHRK 0.0150000 sec

----- CHANNEL f1 -----
NUC1 13C
P1 11.50 usec
PL1 0.00 dB
SFO1 75.4752958 MHz

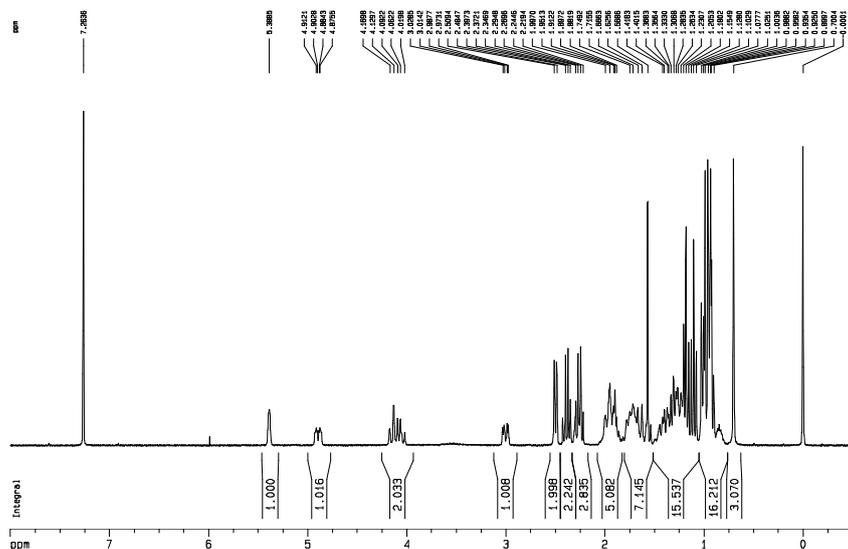
----- CHANNEL f2 -----
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NUC2 1H
PCPD2 80.00 usec
PL2 -0.50 dB
PL12 16.97 dB
SFO2 300.1315007 MHz

F2 - Processing parameters
SI 32768
SF 75.4677465 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 30.00 cm
F1P 190.000 ppm
F1 14338.87 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPCM 8.63636 ppm/cm
HZCM 651.76697 Hz/cm

Figure S6. ¹³C NMR of impurity 1

1H NMR of IPP-SD-712



Current Data Parameters
 NAME caolidong-H
 EXPNO 36
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170512
 Time 11:05
 INSTRUM dpx300
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 36
 DS 0
 SWH 8992.806 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 295
 DM 55.500 usec
 DE 6.00 usec
 TE 0.0 K
 D1 2.0000000 sec
 MCREST 0.0000000 sec
 MCNRK 0.0150000 sec

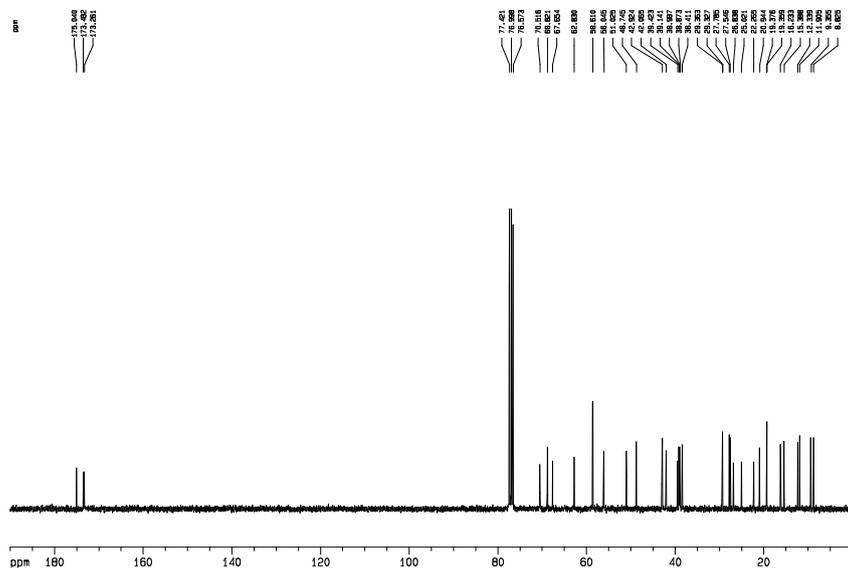
----- CHANNEL f1 -----
 NUC1 1H
 P1 10.70 usec
 PL1 -0.50 dB
 SFO1 300.1318008 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300054 MHz
 MDW EN
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 9.00 cm
 FIP 8.000 ppm
 F1 2401.04 Hz
 F2P -0.500 ppm
 F2 -150.06 Hz
 PPMCM 0.36536 ppm/cm
 HZCM 115.95932 Hz/cm

Figure S9. ¹H NMR of impurity 2

¹³C NMR of IPP-SD-712



Current Data Parameters
 NAME caolidong-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170729
 Time 14:30
 INSTRUM dpx300
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1024
 DS 8
 SWH 22675.736 Hz
 FIDRES 0.692009 Hz
 AQ 0.7225844 sec
 RG 7168
 DM 22.050 usec
 DE 6.00 usec
 TE 0.0 K
 D1 1.5000000 sec
 S11 0.0300000 sec
 MCREST 0.0000000 sec
 MCNRK 0.0150000 sec

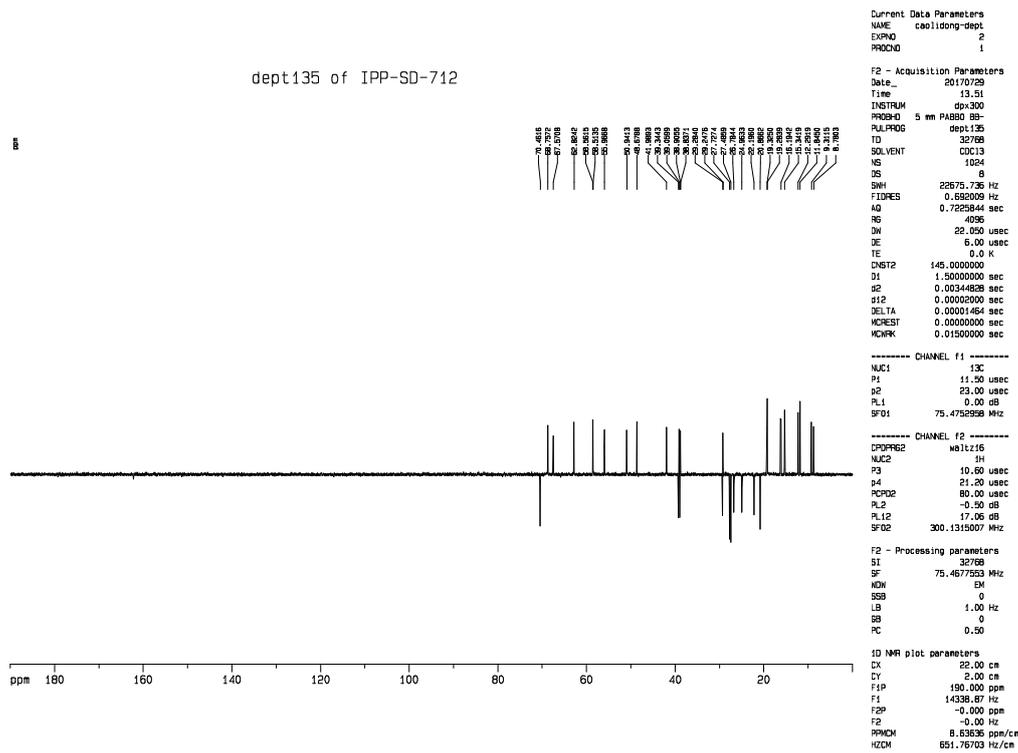
----- CHANNEL f1 -----
 NUC1 13C
 P1 11.50 usec
 PL1 0.00 dB
 SFO1 75.4752958 MHz

----- CHANNEL f2 -----
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 -0.90 dB
 PL12 16.97 dB
 SFO2 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677506 MHz
 MDW EN
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 8.00 cm
 FIP 130.000 ppm
 F1 14338.87 Hz
 F2P -0.000 ppm
 F2 -0.00 Hz
 PPMCM 8.63536 ppm/cm
 HZCM 651.76697 Hz/cm

Figure S10. ¹³C NMR of impurity 2



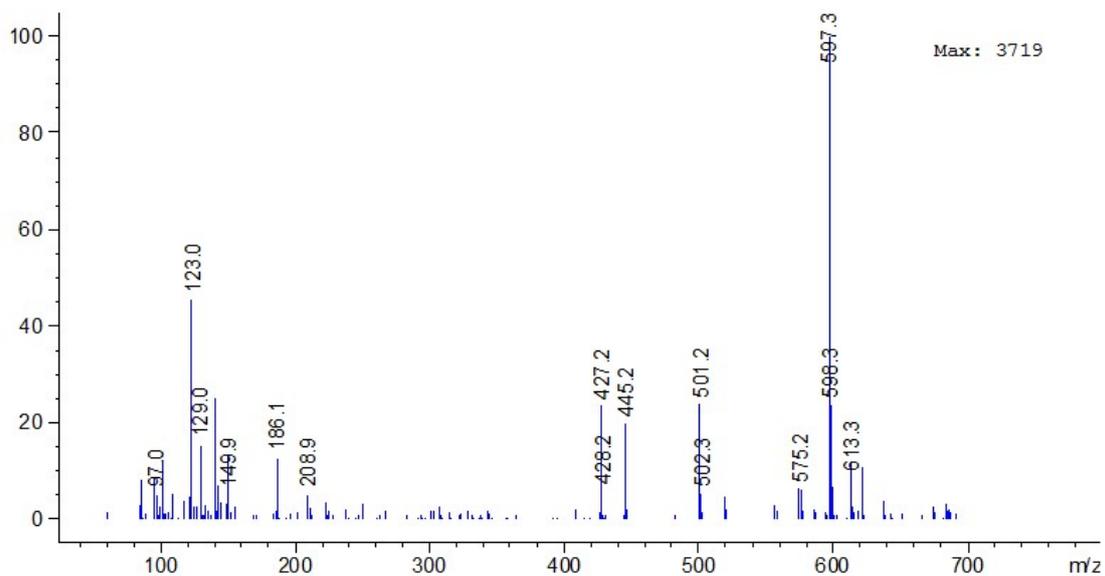


Figure S13. Mass spectrum of propionylbrassinolide impurity 1 recorded in the positive mode.

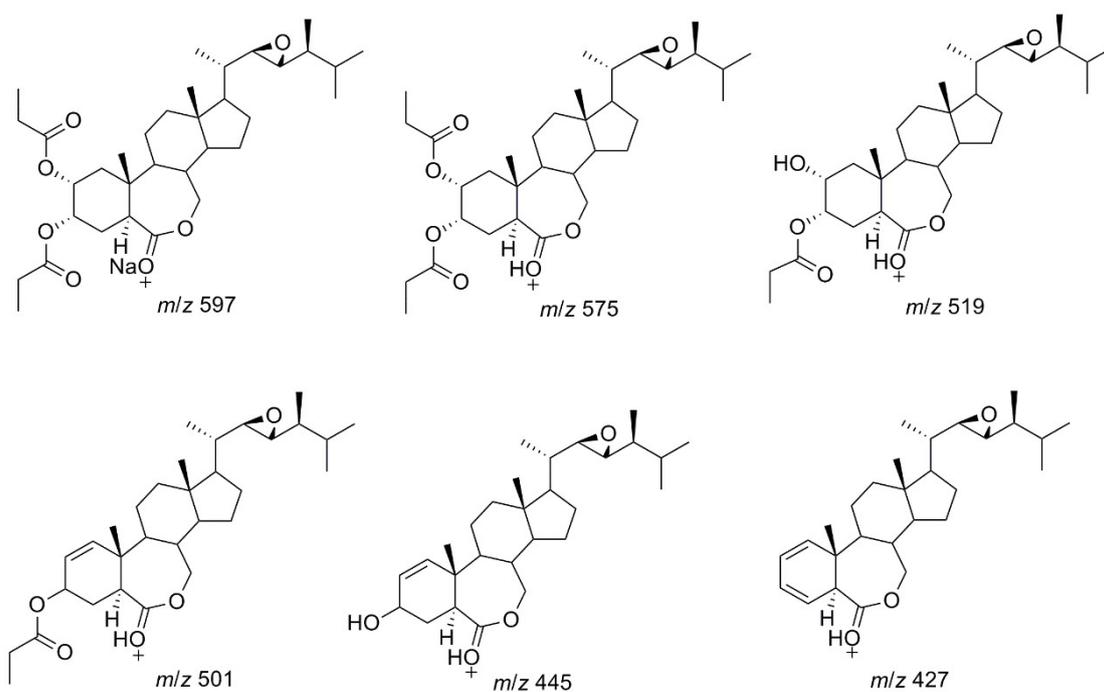


Figure S14. Proposed structure of the major mass ions for propionylbrassinolide impurity 1.

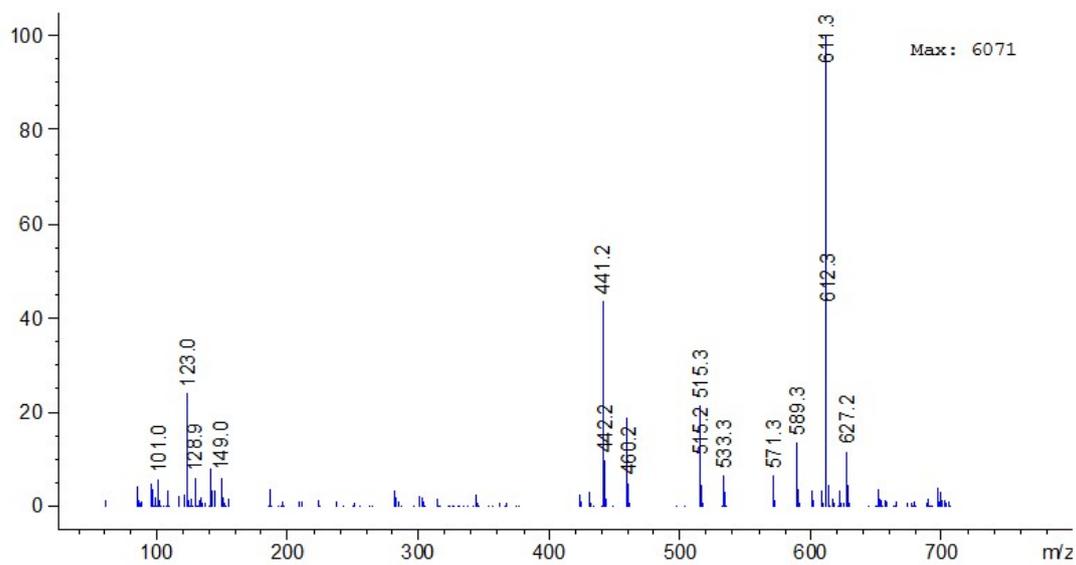


Figure S15. Mass spectrum of propionylbrassinolide impurity 2 recorded in the positive mode.

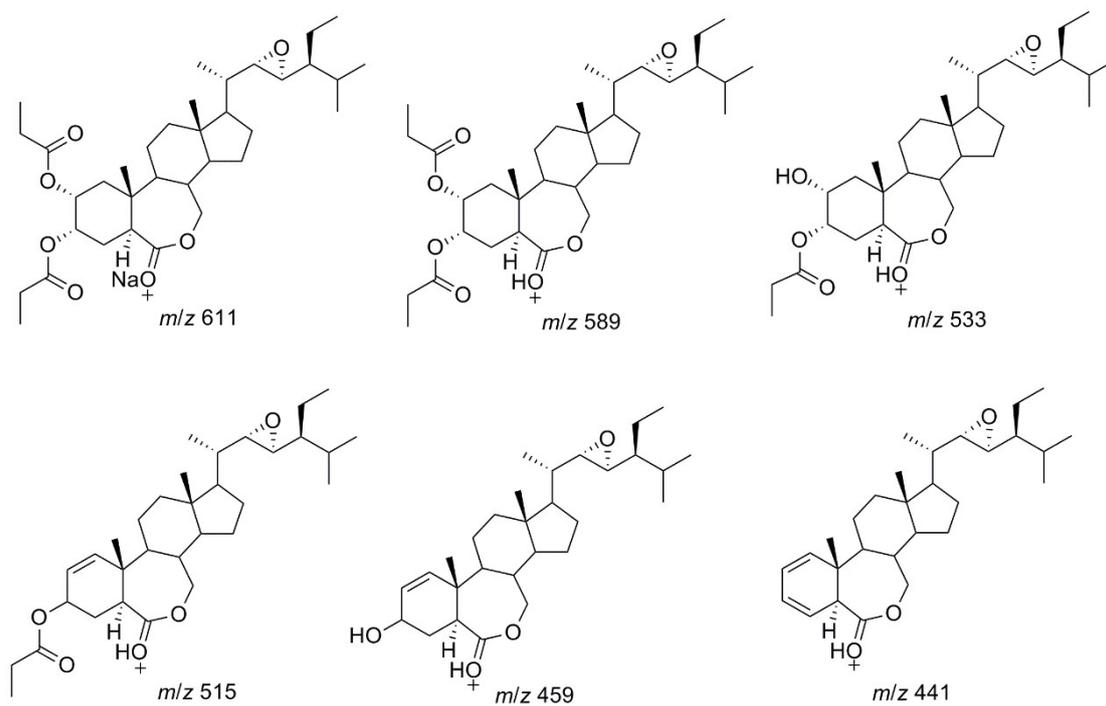


Figure S16. Proposed structure of the major mass ions for propionylbrassinolide impurity 2.