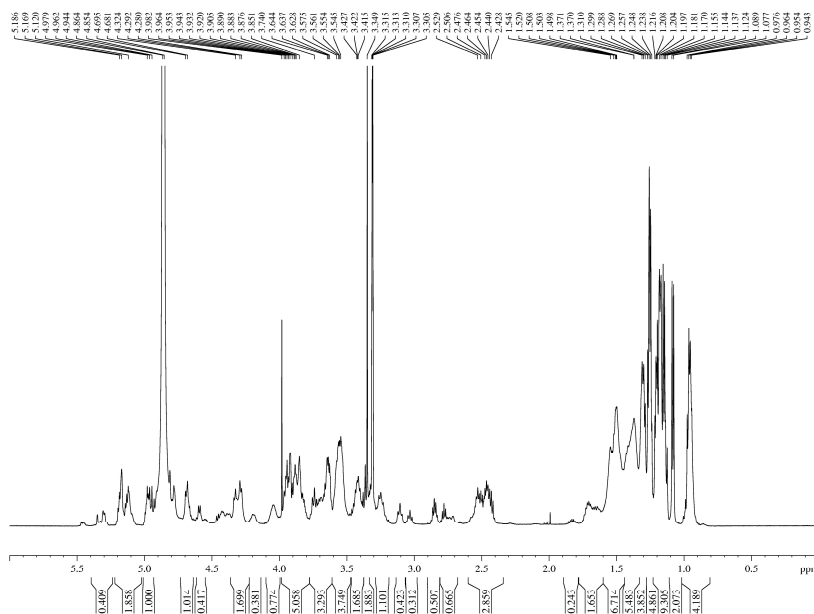


The Supplementary Materials for

**Bioassay-guided isolation of anthelmintic components from *Semen Pharbitidis*, and the mechanism of action of pharbitin**

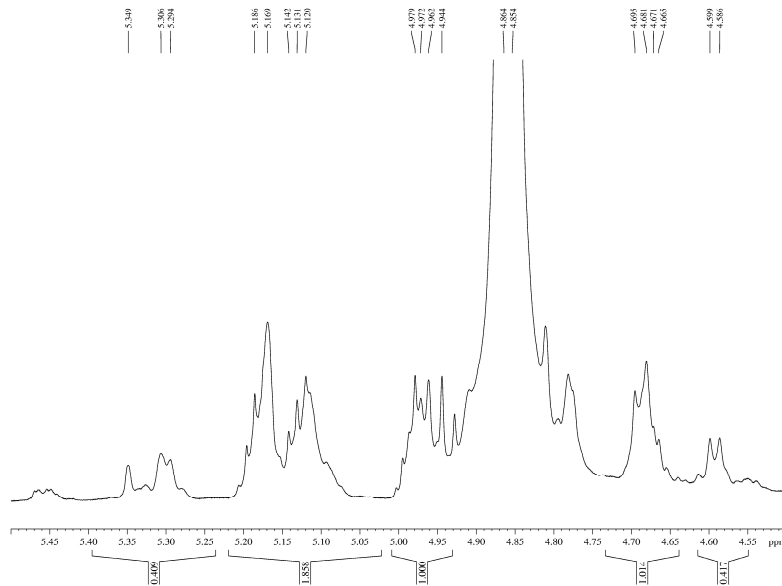
Maoxuan Liu, Jing-Guang Lu, Ming-Rong Yang, Zhi-Hong Jiang, Xiaochun Wan and  
Walter Luyten

<sup>1</sup>H



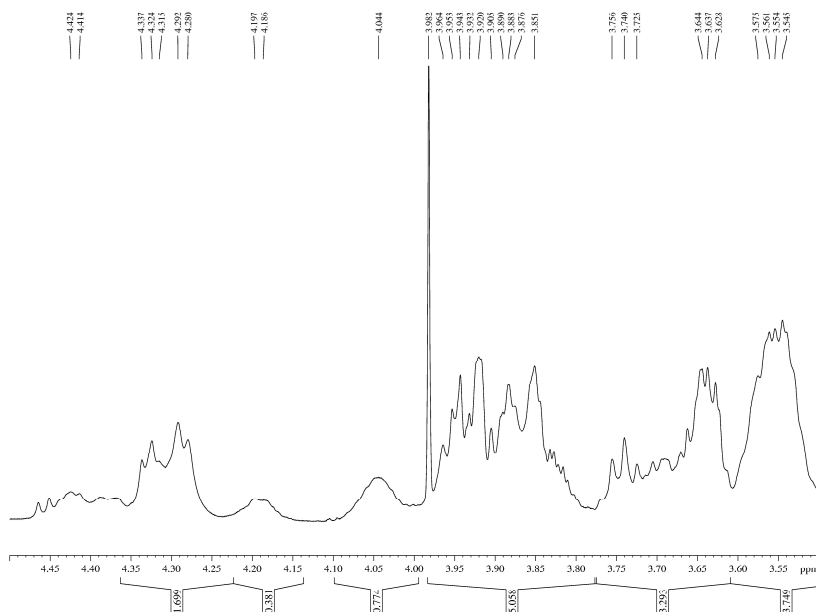
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PROBHD: 5 mm PABBO 500  
PULPROG: zgpg30  
TD: 65536  
SOLVENT: H2O  
NUC1: 13C  
QNP1: 101318.624 Hz  
FIDRES: 0.188325 Hz  
AQ: 2.6363926 sec  
RG: 101  
DM: 40.533 usec  
DE: 6.30 usec  
TE: 297.2 K  
D1: 1.00000000 sec  
D20: 20  
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NUC2: 13C  
P2: 101.324 usec  
PLW1: 28.00000000 W  
P2 Processing parameters  
SI: 65536  
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SSB: 0  
LB: 0 Hz  
GB: 0  
PC: 1.00

<sup>1</sup>H



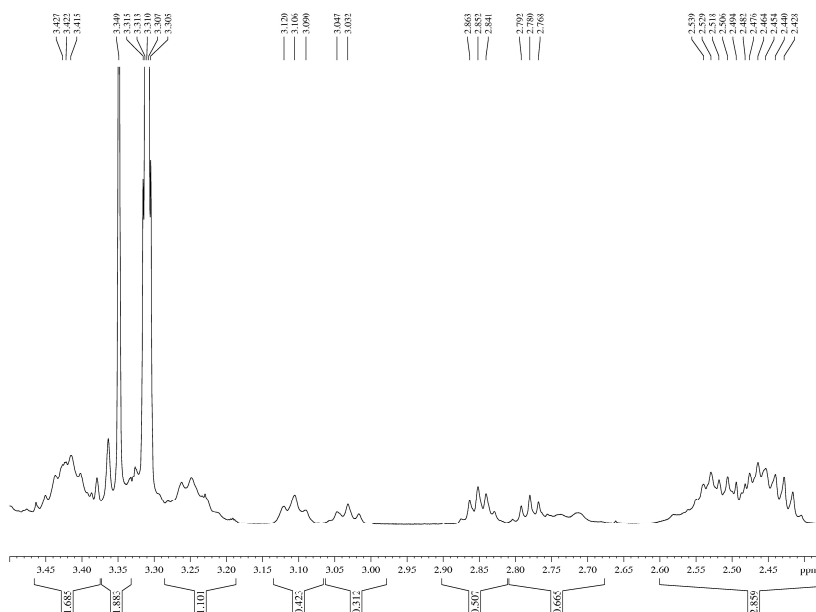
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PULPROG: zgpg30  
TD: 65536  
SOLVENT: H2O  
NUC1: 13C  
QNP1: 101318.624 Hz  
FIDRES: 0.188325 Hz  
AQ: 2.6363926 sec  
RG: 101  
DM: 40.533 usec  
DE: 6.30 usec  
TE: 297.2 K  
D1: 1.00000000 sec  
D20: 20  
===== CHANNEL f1 =====  
NUC2: 13C  
P2: 101.324 usec  
PLW1: 28.00000000 W  
P2 Processing parameters  
SI: 65536  
SF: 600.130141 MHz  
WDW: Hanning  
SSB: 0  
LB: 0 Hz  
GB: 0  
PC: 1.00

<sup>1</sup>H



Current Data Parameters  
NAME: WC-27  
PROCNO: 1  
P2 - Acquisition Parameters  
DATE\_: 20110113  
Time: 15.19  
INSTRUM: spect  
PROBHD: 5 mm PABBO BB7  
PULPROG: zgpg30  
TD: 65536  
SOLVENT: H<sub>2</sub>O  
DS: 320  
SWH: 10338.424 Hz  
FIDRES: 0.1888220 Hz  
AQ: 2.6569720 sec  
RG: 170  
WDW: EM  
SSB: 40.573 usec  
GB: 4.50 usec  
TE: 297.2 K  
DE: 1.00000000 sec  
DT: 20  
===== CHANNEL f1 =====  
NUC1: 600.137041 MHz  
P1: 11.00 usec  
PL1: 28.00000000 W  
P2 Processing parameters  
SI: 65536  
SF: 600.130141 MHz  
WDW: EM  
SSB: 0  
GB: 0 Hz  
TE: 297.2 K  
DE: 1.00

<sup>1</sup>H



Current Data Parameters  
NAME: WC-27  
PROCNO: 1  
P2 - Acquisition Parameters  
DATE\_: 20110113  
Time: 15.19  
INSTRUM: spect  
PROBHD: 5 mm PABBO BB7  
PULPROG: zgpg30  
TD: 65536  
SOLVENT: H<sub>2</sub>O  
DS: 320  
SWH: 10338.424 Hz  
FIDRES: 0.1888220 Hz  
AQ: 2.6569720 sec  
RG: 170  
WDW: EM  
SSB: 40.573 usec  
GB: 4.50 usec  
TE: 297.2 K  
DE: 1.00000000 sec  
DT: 20  
===== CHANNEL f1 =====  
NUC1: 600.137041 MHz  
P1: 11.00 usec  
PL1: 28.00000000 W  
P2 Processing parameters  
SI: 65536  
SF: 600.130141 MHz  
WDW: EM  
SSB: 0  
GB: 0 Hz  
TE: 297.2 K  
DE: 1.00



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PROGRAM       1

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PULPROG       zpgzpg
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TD            65536
CONVENTION    1
NS            320
DS            1
SS            1
AQ            19356.624 Hz
FIDRES        0.188225 Hz
AQ           2.6563926 sec
SI            160
DE            40.533 usec
DK            6.30 usec
TL            297.6 Hz
D1            1.00000000 sec
TD0           20

===== CHANNEL 1 Parameters =====
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P1            1.00 usec
PL1           28.00000000 dB
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F2 Processing Parameters
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12.586  
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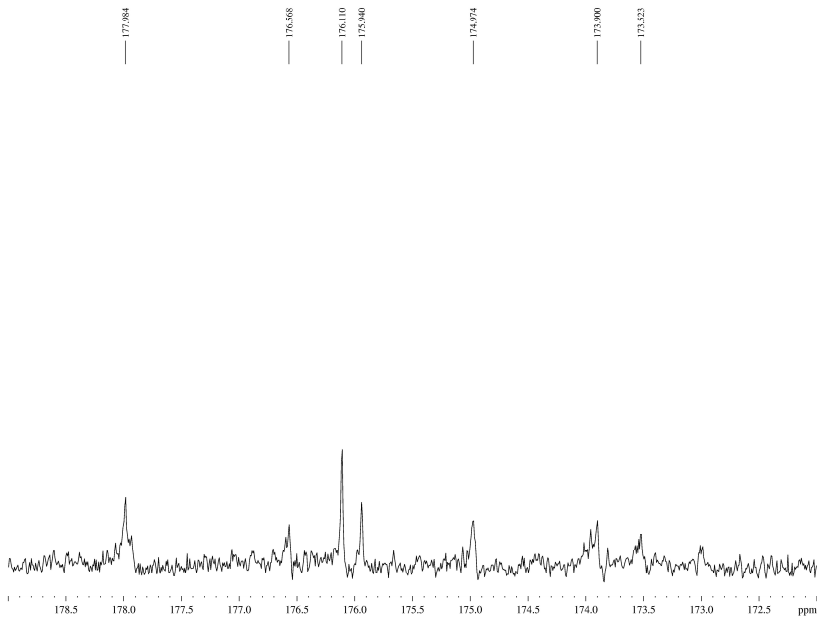
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SOLVENT                             DMS
NS                                  2386
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FIDRES                             0.550197 Hz
AQ                                  0.900189 s
RG                                  128
DM                                  1
QM                                  0
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d11                                  0.000000000 s
DELTA                               3
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NUC1                               15N
P1                                  1.00
PL1                                 0.000000000 W
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NUC2                               13C
P2                                  1.00
PL2                                 0.000000000 W
===== CHANNEL f3 =====
P3                                  1.00
PL3                                 0.000000000 W

F2 - Processing parameters
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13C



Current Data Parameters  
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PROCNO 1

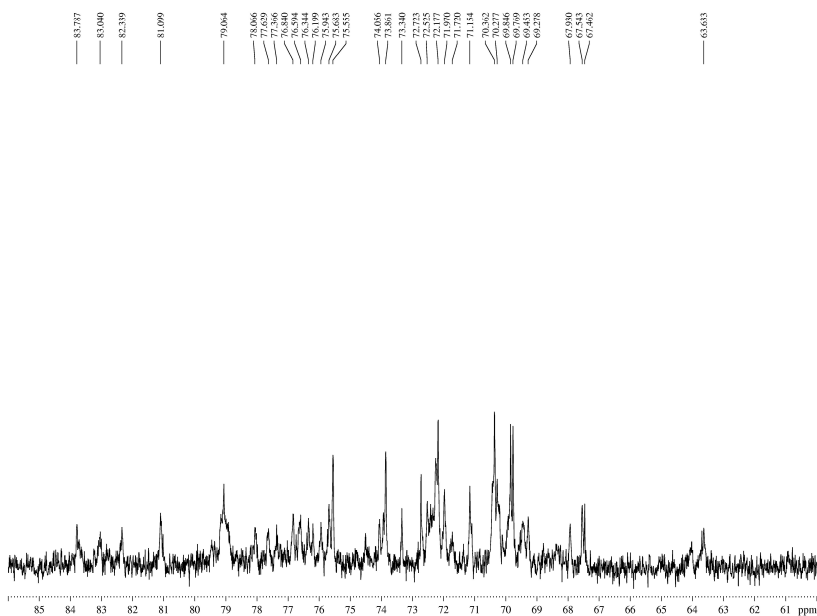
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SOLVENT MeOH  
NS 2386  
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SWH 36027.691 Hz  
FIDRES 0.550197 Hz  
AQ 0.9087659 sec  
RG 128  
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DE 20.00 usec  
TE 298.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
TDO 3

----- CHANNEL f1 -----  
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NUC1 13C  
P1 13.00 usec  
PLW1 25.00000000 W

----- CHANNEL f2 -----  
SFO2 600.1324005 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 70.00 usec  
PLW2 25.11899948 W  
PLW12 0.47441000 W  
PLW13 0.23246001 W

F2 - Processing parameters  
SI 32768  
SF 150.9026026 MHz  
WDW RM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

13C



Current Data Parameters  
NAME WL-27  
EXNO 3  
PROCNO 1

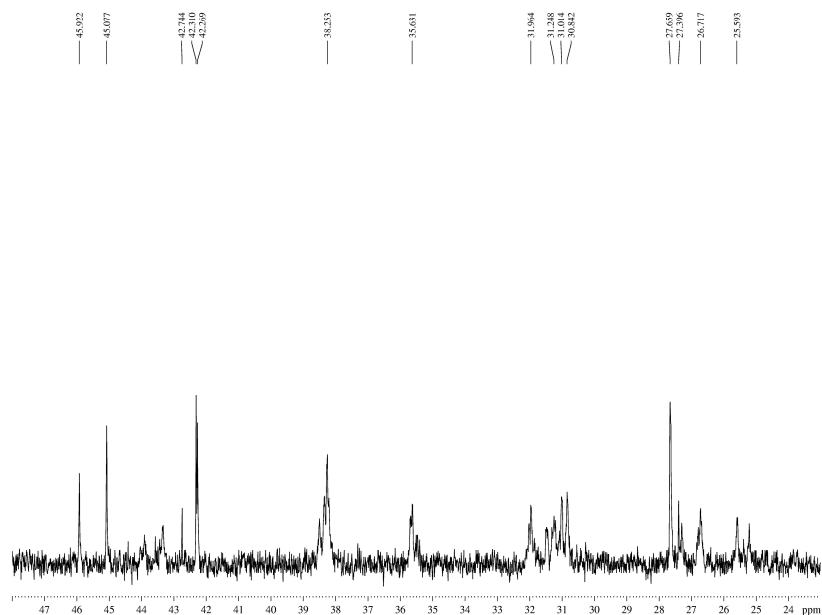
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INSTRUM spect  
PROBHD 5 mm CPDCH 13C  
PULPROG zgpg30  
TD 65536  
SOLVENT MeOH  
NS 2386  
DS 4  
SWH 36027.691 Hz  
FIDRES 0.550197 Hz  
AQ 0.9087659 sec  
RG 128  
DW 13.867 usec  
DE 20.00 usec  
TE 298.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
TDO 3

----- CHANNEL f1 -----  
SFO1 150.9178993 MHz  
NUC1 13C  
P1 13.00 usec  
PLW1 25.00000000 W

----- CHANNEL f2 -----  
SFO2 600.1324005 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 70.00 usec  
PLW2 25.11899948 W  
PLW12 0.47441000 W  
PLW13 0.23246001 W

F2 - Processing parameters  
SI 32768  
SF 150.9026026 MHz  
WDW RM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>13</sup>C



Current Data Parameters  
NAME WL-27  
EXNO 3  
PROCNO 1

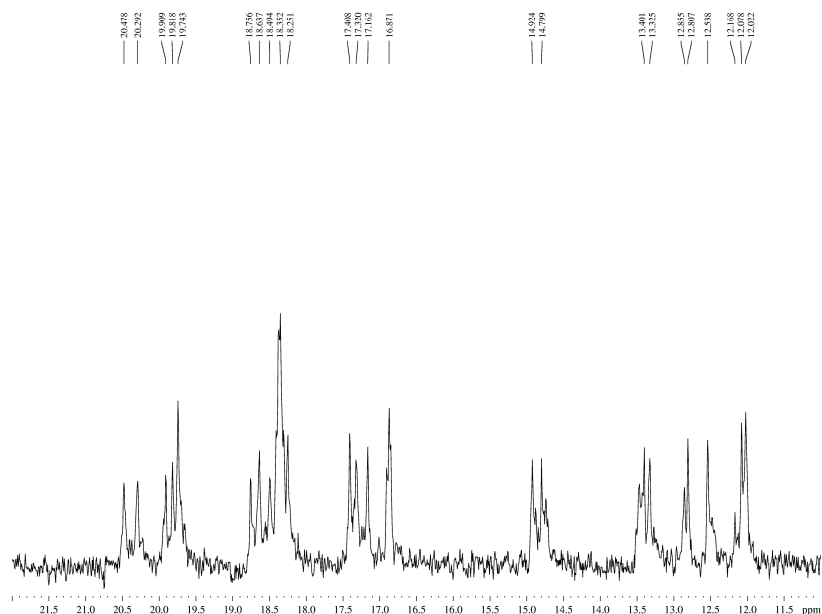
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PULPROG zgpg30  
TD 65536  
SOLVENT MeOH  
NS 2386  
DS 4  
SWH 36027.691 Hz  
FIDRES 0.550197 Hz  
AQ 0.9087659 sec  
RG 128  
DW 13.867 usec  
DE 20.00 usec  
TE 298.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
TDO 3

===== CHANNEL f1 =====  
SFO1 150.9178993 MHz  
NUC1 13C  
P1 13.00 usec  
PLW1 25.00000000 W

===== CHANNEL f2 =====  
SFO2 600.1324005 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD 70.00 usec  
PLW2 25.11899948 W  
PLW12 0.47441000 W  
PLW13 0.23246001 W

F2 - Processing parameters  
SI 32768  
SF 150.9026026 MHz  
WDW RM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

<sup>13</sup>C



Current Data Parameters  
NAME WL-27  
EXNO 3  
PROCNO 1

F2 - Acquisition Parameters  
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Time 17.04  
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PULPROG zgpg30  
TD 65536  
SOLVENT MeOH  
NS 2386  
DS 4  
SWH 36027.691 Hz  
FIDRES 0.550197 Hz  
AQ 0.9087659 sec  
RG 128  
DW 13.867 usec  
DE 20.00 usec  
TE 298.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
TDO 3

===== CHANNEL f1 =====  
SFO1 150.9178993 MHz  
NUC1 13C  
P1 13.00 usec  
PLW1 25.00000000 W

===== CHANNEL f2 =====  
SFO2 600.1324005 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD 70.00 usec  
PLW2 25.11899948 W  
PLW12 0.47441000 W  
PLW13 0.23246001 W

F2 - Processing parameters  
SI 32768  
SF 150.9026026 MHz  
WDW RM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Figure. S2. <sup>13</sup>C-NMR spectrum of the active peak

**11-(D-glucopyranosyloxy)-3-hydroxy-tetradecanoic acid** (C<sub>20</sub>H<sub>38</sub>O<sub>9</sub>, exact mass: 422.2516)

HRMS-ESI: [M+H]<sup>+</sup> calcd. 423.2589, found 423.2588. [M+Na]<sup>+</sup> calcd. 445.2408, found 445.2403. [M-H]<sup>-</sup> calcd. 421.2443, found 421.2448.

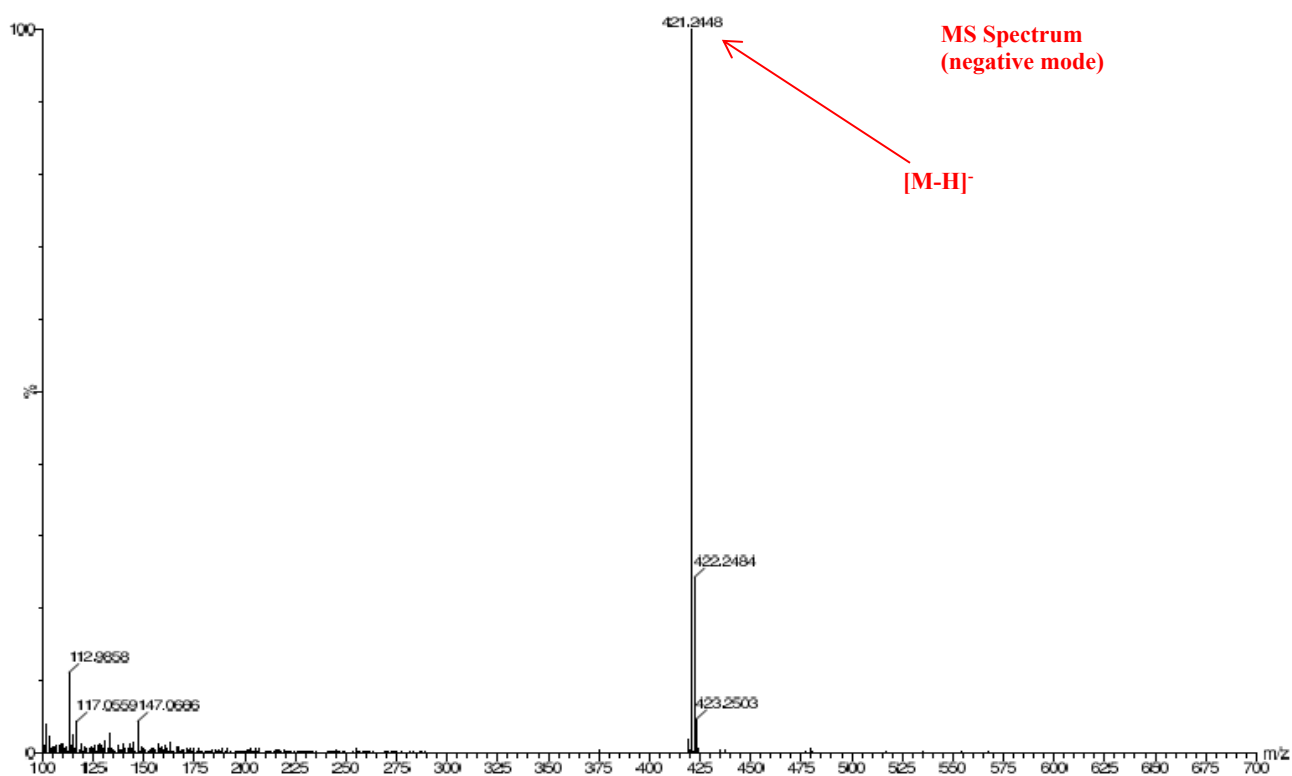
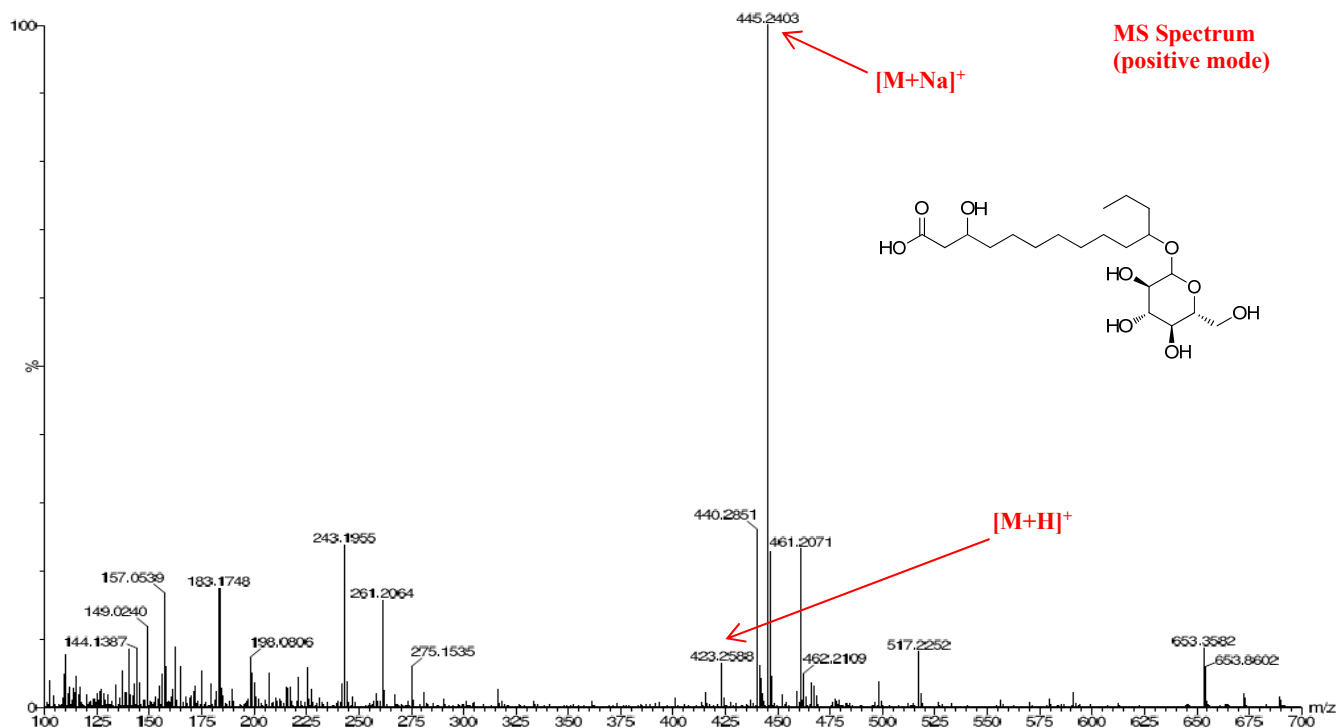


Figure. S3. HRMS spectra of 11-(D-glucopyranosyloxy)-3-hydroxy-tetradecanoic acid

**Ipurolic acid** (C<sub>14</sub>H<sub>28</sub>O<sub>4</sub>, exact mass: 260.1988)

HRMS-ESI: [M+Na]<sup>+</sup> calcd. 283.1880, found 283.1877. [M-H]<sup>-</sup> calcd. 259.1915, found 259.1923.

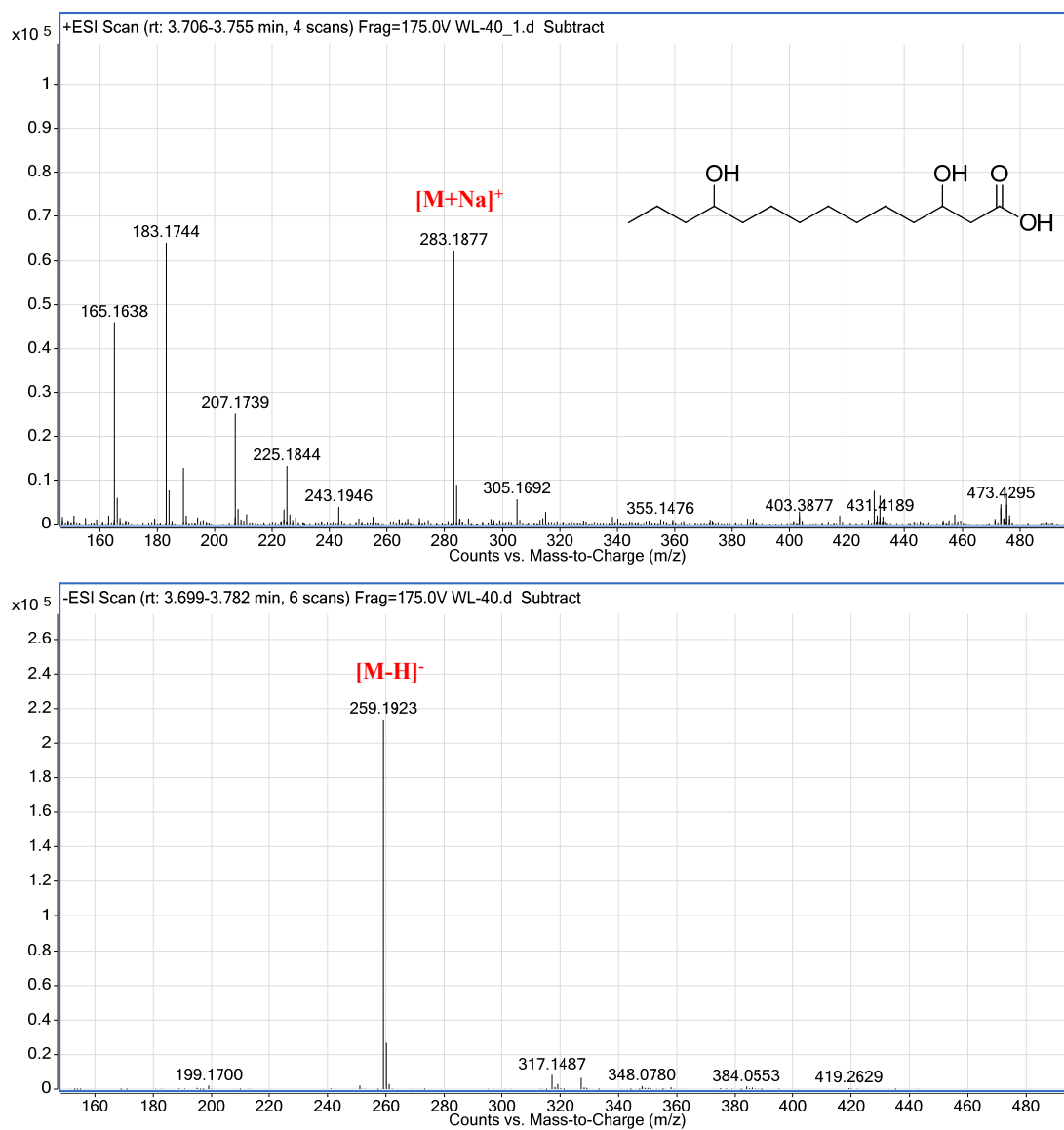
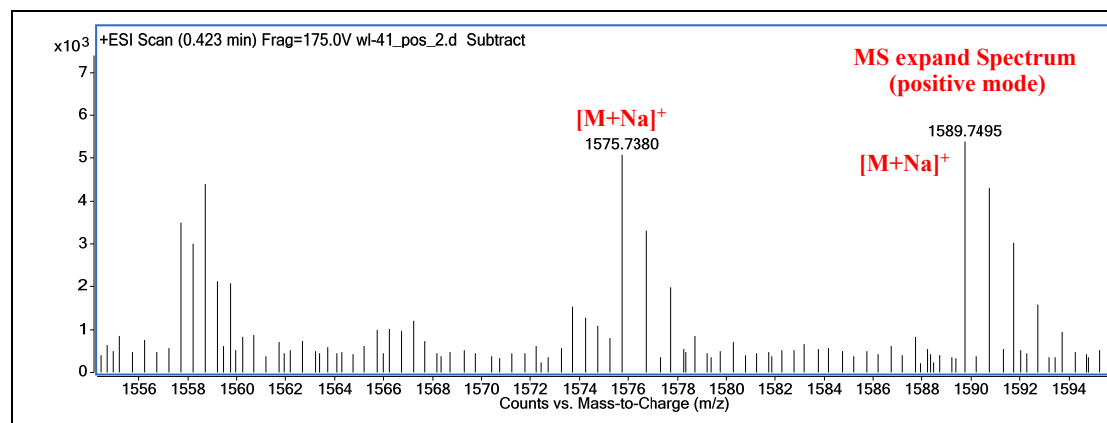
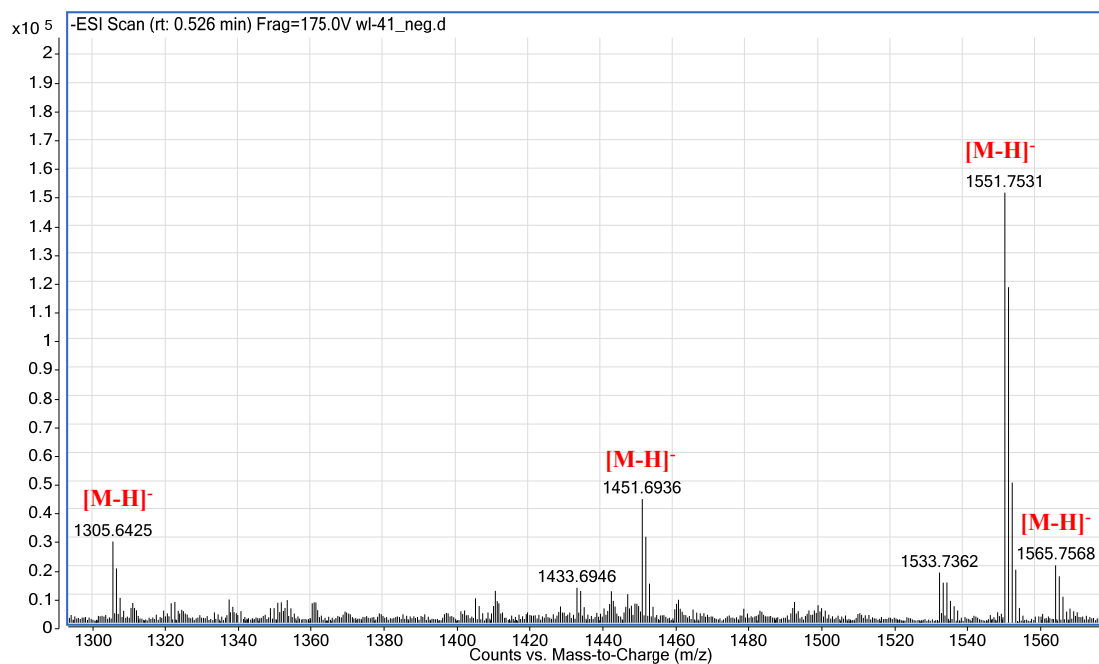


Figure. S4. HRMS spectra of ipurolic acid

Table S1. HRMS results of pharbitin

compound	formula	exact mass	calcd. [M-H] <sup>-</sup>	[M-H] <sup>-</sup>	calcd. [M+Na] <sup>+</sup>	[M+Na] <sup>+</sup>
1	C <sub>65</sub> H <sub>112</sub> O <sub>35</sub>	1452.6984	1451.6911	1451.6936	1475.6876	1475.6933
2	C <sub>65</sub> H <sub>112</sub> O <sub>35</sub>	1452.6984	1451.6911	1451.6936	1475.6876	1475.6933
3	C <sub>59</sub> H <sub>102</sub> O <sub>31</sub>	1306.6405	1305.6332	1305.6425	1329.6297	1329.6827
4	C <sub>59</sub> H <sub>102</sub> O <sub>31</sub>	1306.6405	1305.6332	1305.6425	1329.6297	1329.6827
5	C <sub>70</sub> H <sub>120</sub> O <sub>37</sub>	1552.7508	1551.7435	1551.7531	1575.7400	1575.7380
6	C <sub>70</sub> H <sub>120</sub> O <sub>37</sub>	1552.7508	1551.7435	1551.7531	1575.7400	1575.7380
7	C <sub>71</sub> H <sub>122</sub> O <sub>37</sub>	1566.7665	1565.7592	1565.7568	1589.7557	1589.7495
8	C <sub>71</sub> H <sub>122</sub> O <sub>37</sub>	1566.7665	1565.7592	1565.7568	1589.7557	1589.7495



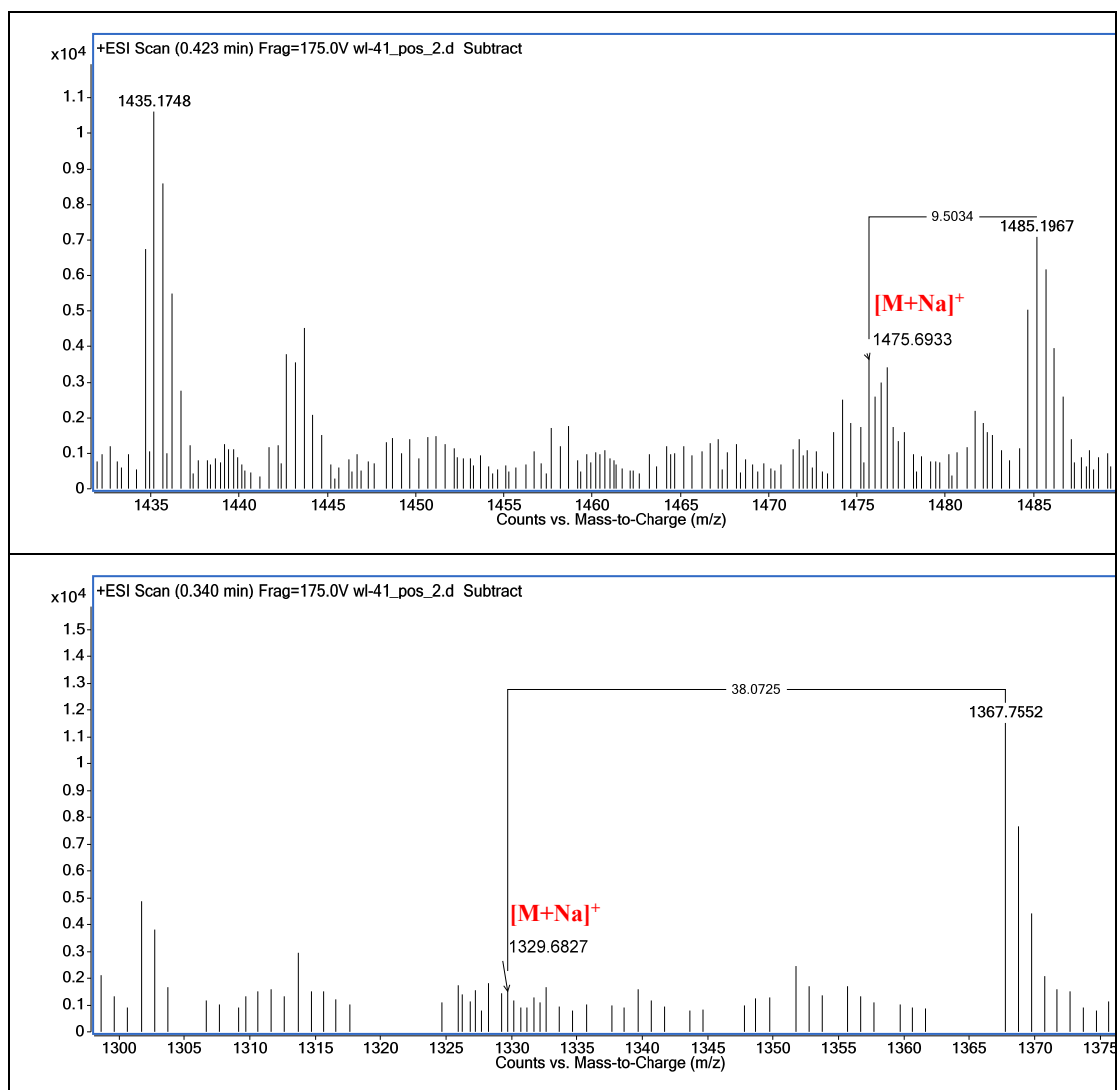


Figure. S5. HRMS spectra of the active peak (pharbitin)