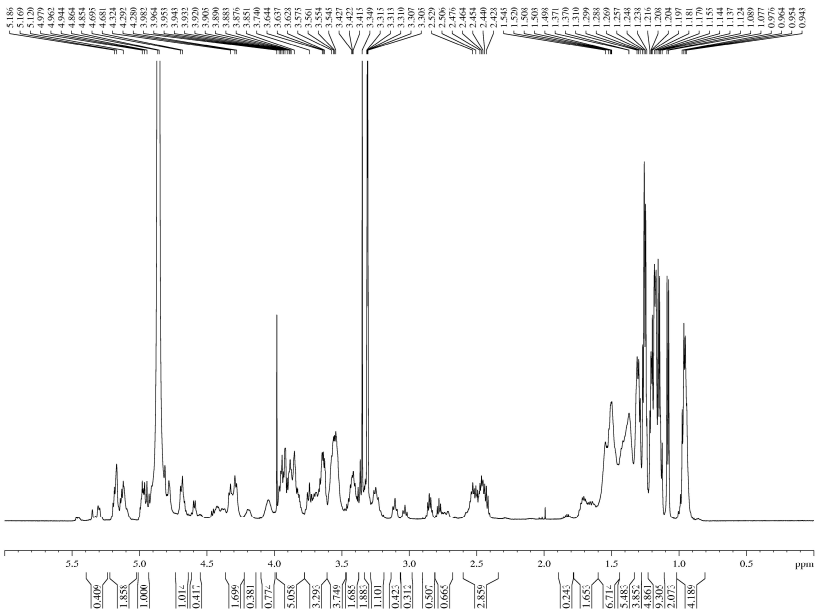
The Supplementary Materials for

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

1H



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RG                      101
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TE                 297.6 K
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NUC1                       1H
P1                     11.00 usec
PLW1            28.00000000 W

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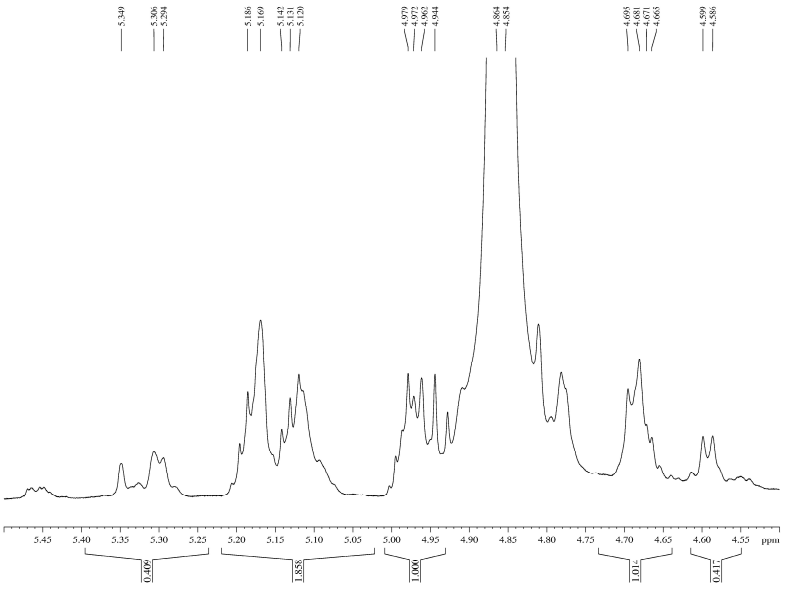
1H



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PULPROG                zg30
TD                    65536
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DS                        2
SWH               12336.634 Hz
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SF               600.1300141 MHz
WDW                       no
SSB                    0
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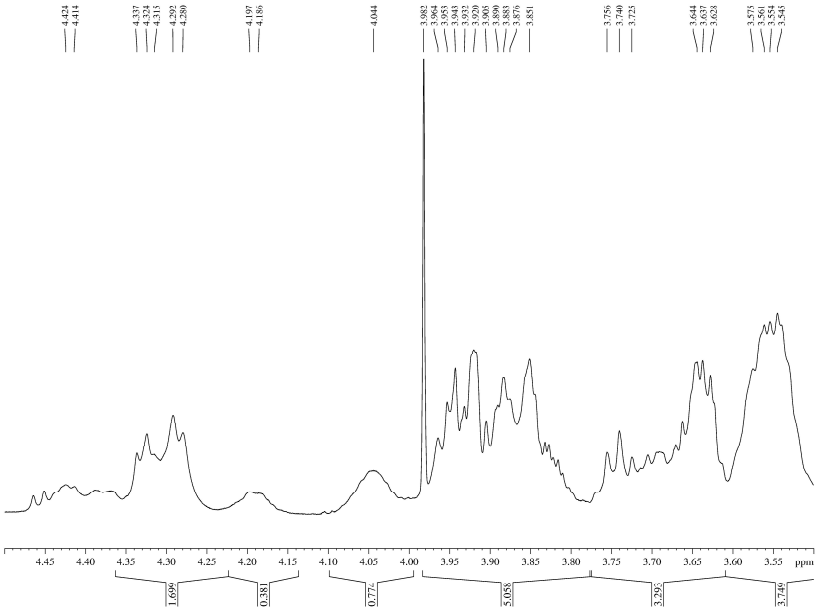
1H



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EXPNO 2
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PULPROG zg30
TD 65536
SOLVENT MeOD
NS 320
DS 2
SWH 12336.636 Hz
FIDRES 0.188225 Hz
AQ 2.6563926 sec
RG 101
DW 40.533 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 20

======== CHANNEL f1 ========
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NUC1 1H
P1 11.00 usec
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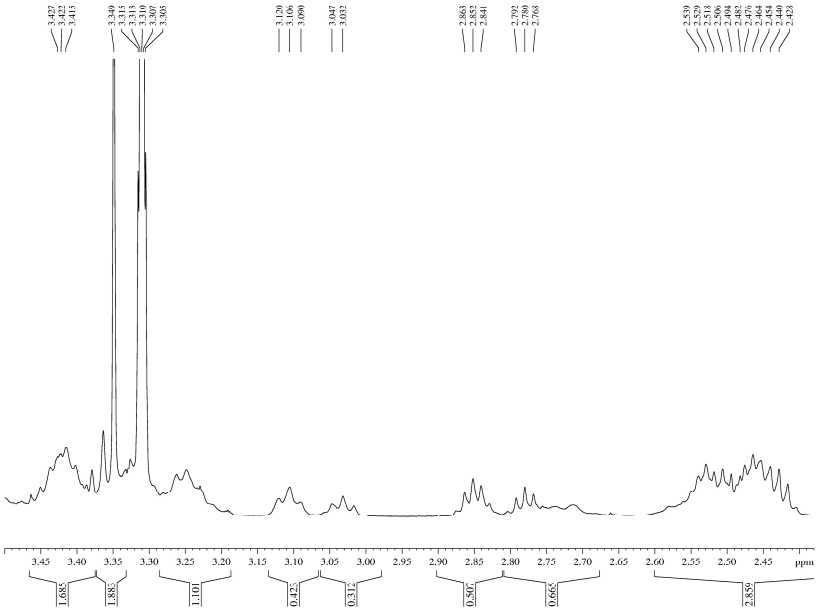

Current Data Parameters
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PULPROG zg30
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FIDRES 0.188225 Hz
AQ 2.6563926 sec
RG 101
DW 40.533 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 20

======== CHANNEL f1 ========
SFO1 600.1337061 MHz
NUC1 1H
P1 11.00 usec
PLW1 28.00000000 W

F2 - Processing parameters
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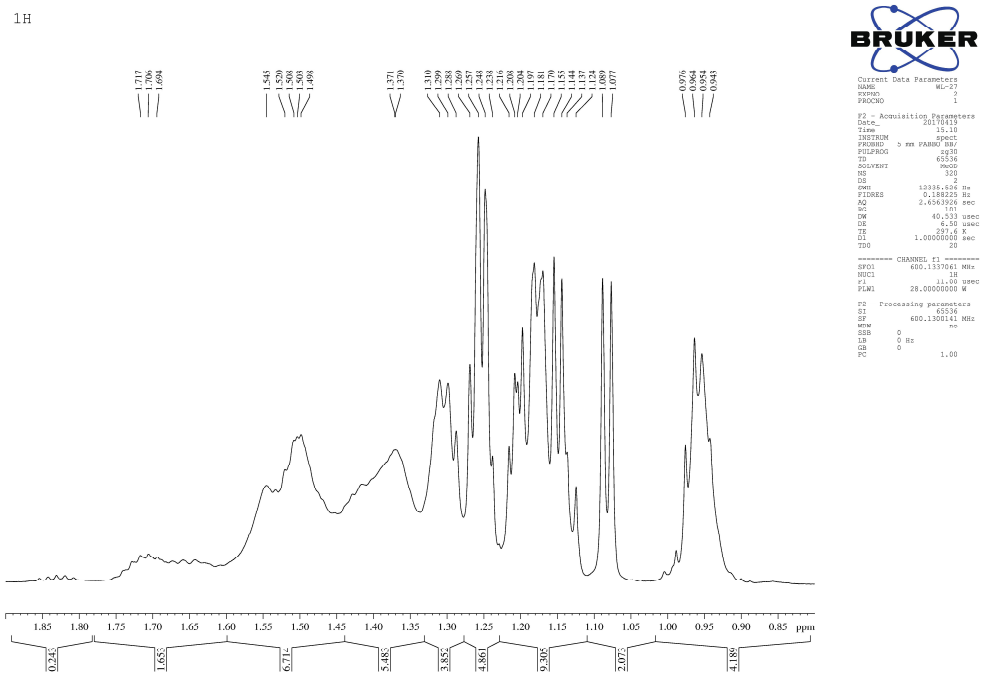
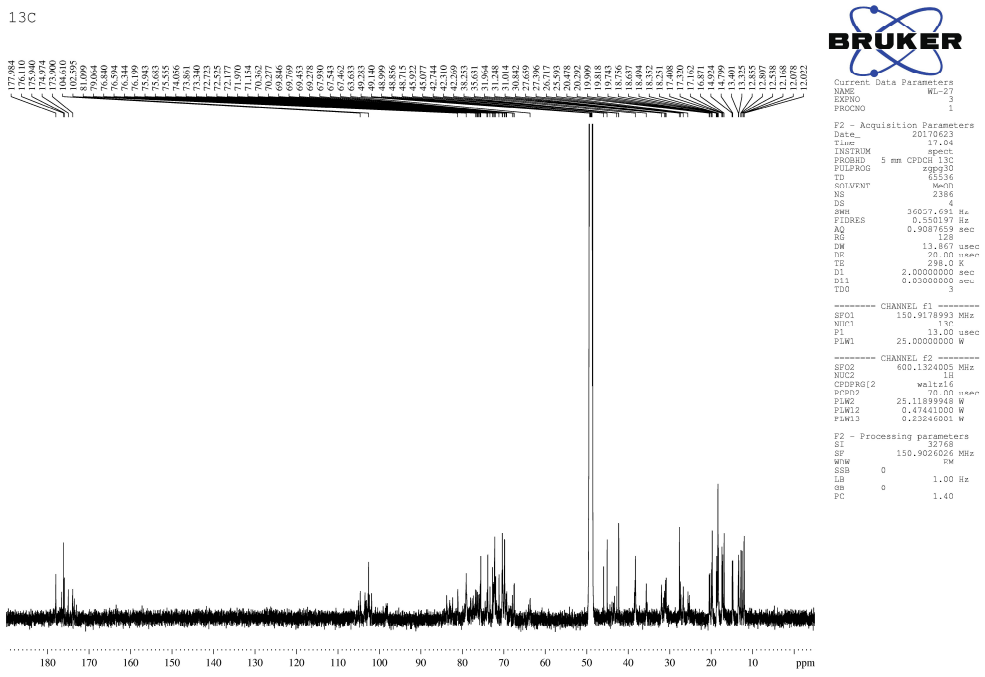
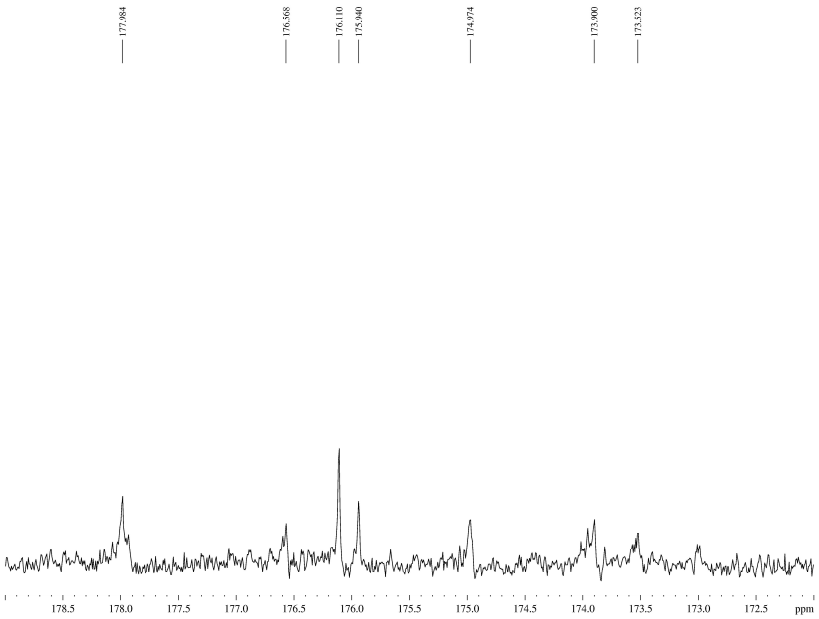


Figure. S1. [1]H-NMR spectrum of the active peak



13C



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TD                  65536
SOLVENT               MeOD
NS                     2386
DS                        4
SWH              36057.691 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
TD0                       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
CPDPRG[2            waltz16
PCPD2               70.00 usec
PLW2           25.11899948 W
PLW12           0.47441000 W
PLW13           0.23246001 W

F2 - Processing parameters
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SF              150.9026026 MHz
WDW                      EM
SSB       0
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GB        0
PC                  1.40
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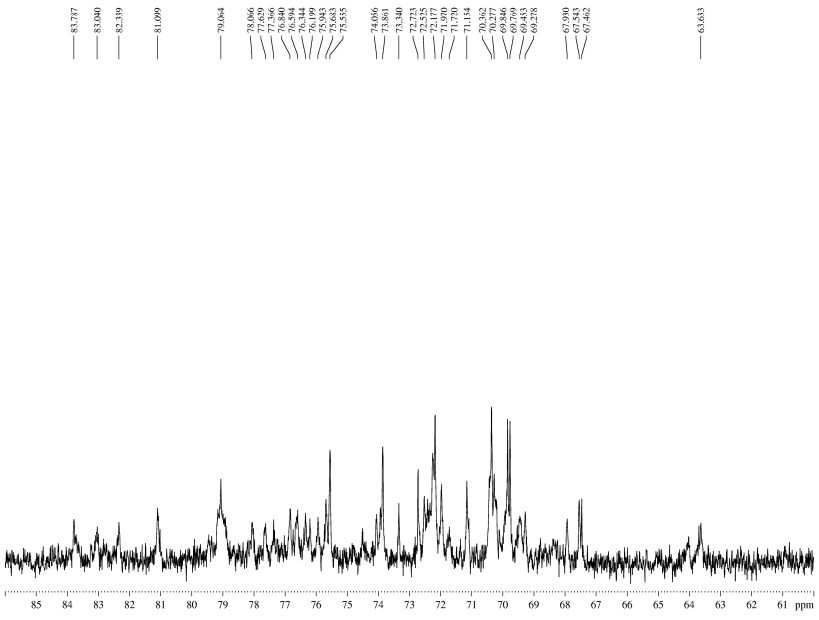
13C

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Current Data Parameters
NAME                  WL-27
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PROCNO                    1

F2 - Acquisition Parameters
Date_              20170623
Time                  17.04
INSTRUM                spect
PROBHD   5 mm CPDCH 13C
PULPROG             zgpg30
TD                  65536
SOLVENT               MeOD
NS                     2386
DS                        4
SWH              36057.691 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
TD0                       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
CPDPRG[2            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                      EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
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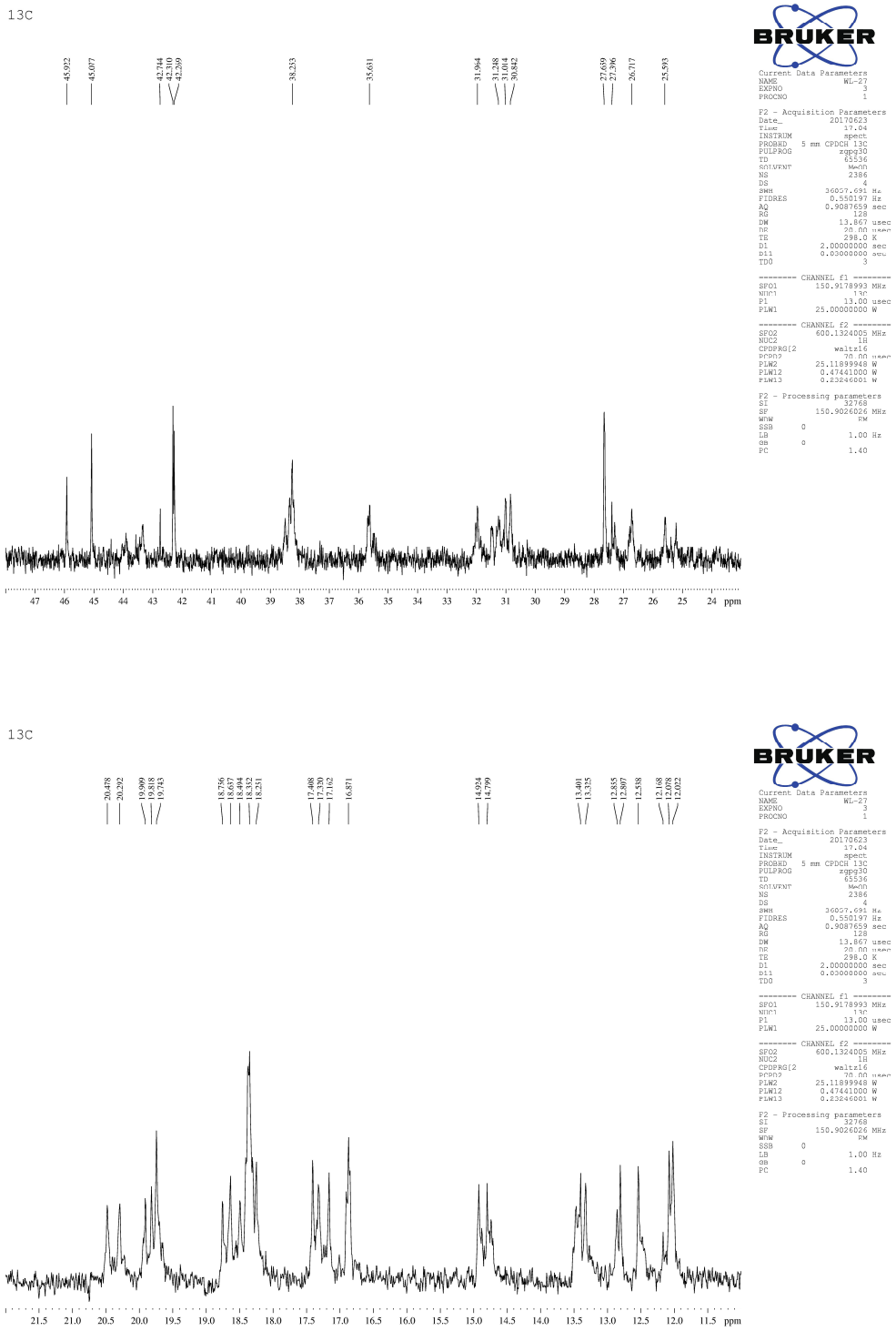


Figure. S2. ^{13}C-NMR spectrum of the active peak

11-(D-glucopyranosyloxy)-3-hydroxy-tetradecanoic acid ($C_{20}H_{38}O_9$, exact mass: 422.2516)

HRMS-ESI: $[M+H]^+$ calcd. 423.2589, found 423.2588. $[M+Na]^+$ calcd. 445.2408, found 445.2403. $[M-H]^-$ calcd. 421.2443, found 421.2448.

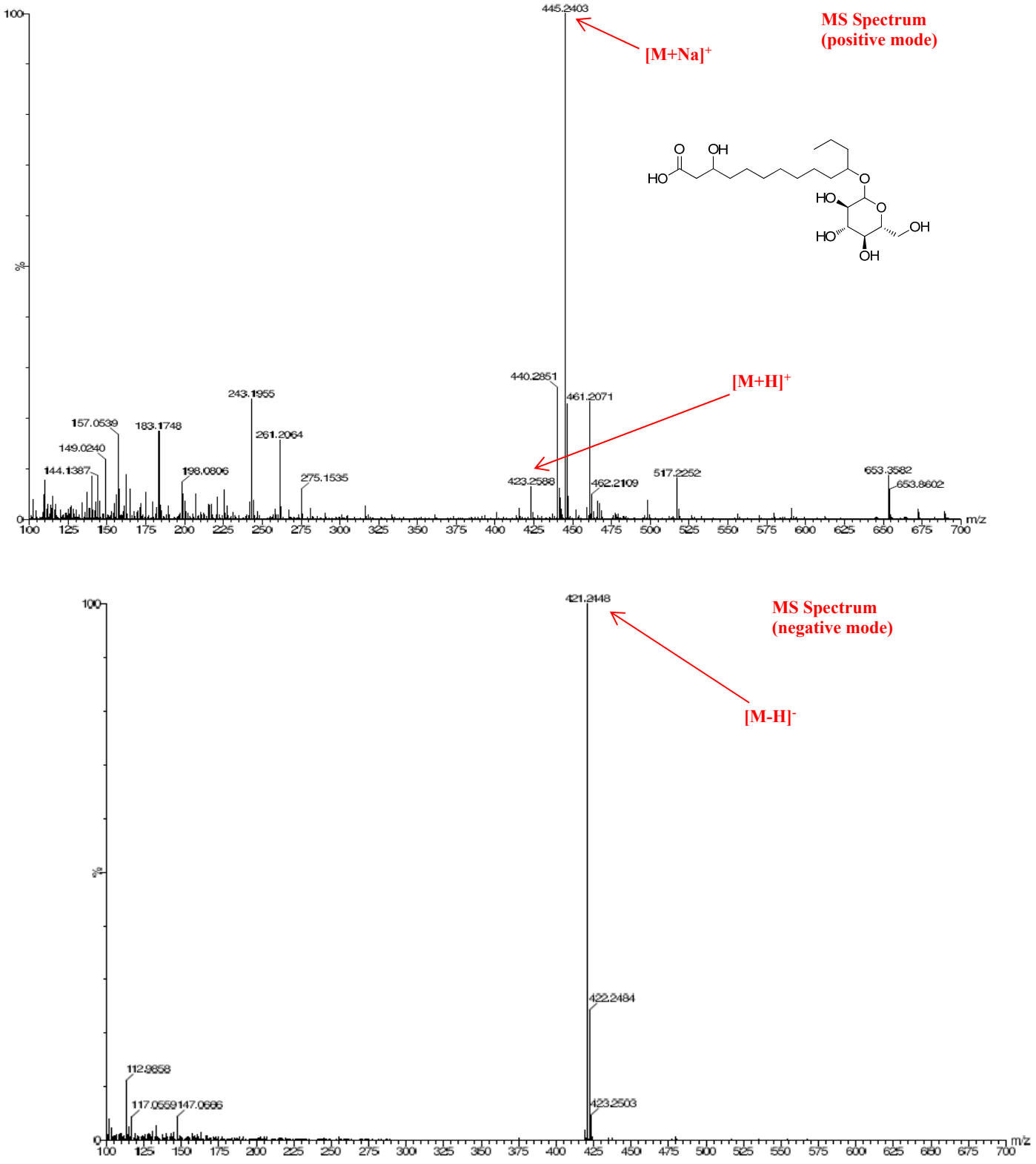


Figure. S3. HRMS spectra of 11-(D-glucopyranosyloxy)-3-hydroxy-tetradecanoic acid

Ipurolic acid ($C_{14}H_{28}O_4$, exact mass: 260.1988)

HRMS-ESI: $[M+Na]^+$ calcd. 283.1880, found 283.1877. $[M-H]^-$ calcd. 259.1915, found 259.1923.

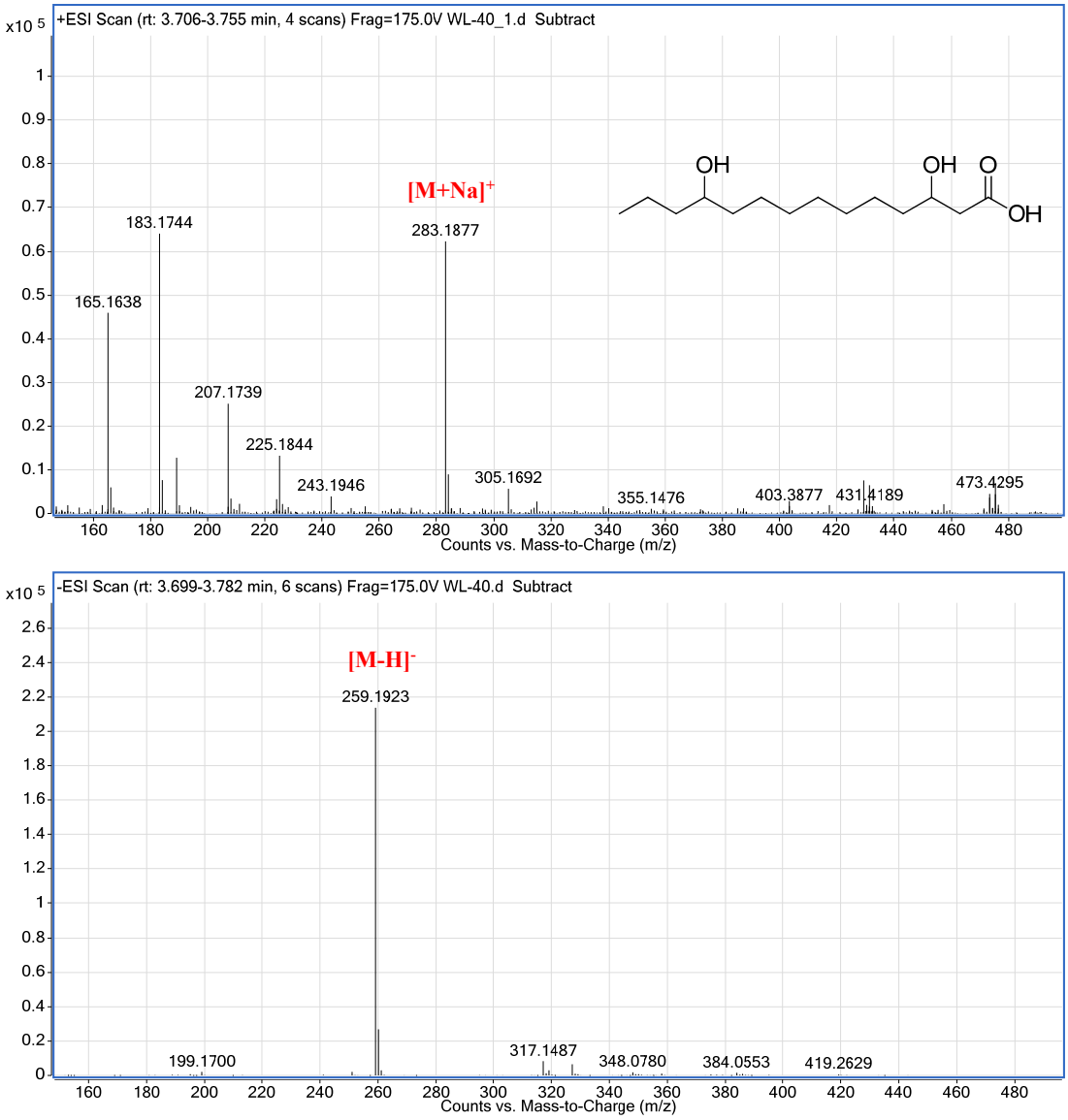
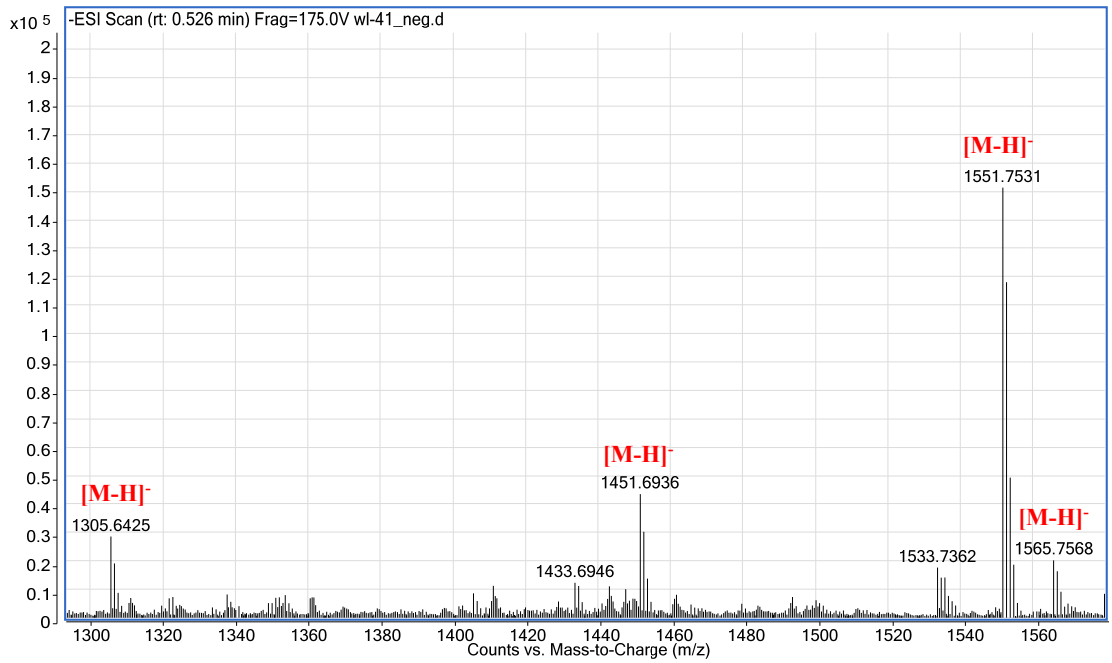
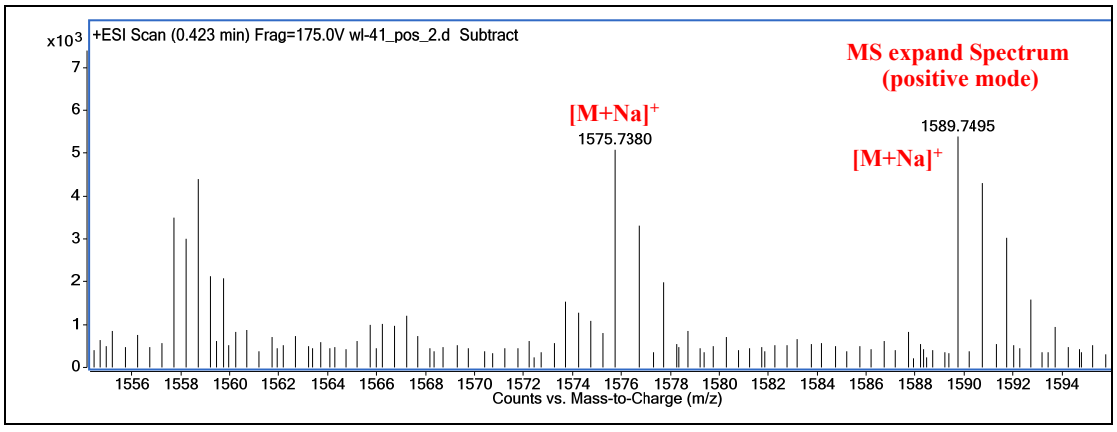


Figure. S4. HRMS spectra of ipurolic acid

Table S1. HRMS results of pharbitin

compound	formula	exact mass	calcd. $[M-H]^-$	$[M-H]^-$	calcd. $[M+Na]^+$	$[M+Na]^+$
1	$C_{65}H_{112}O_{35}$	1452.6984	1451.6911	1451.6936	1475.6876	1475.6933
2	$C_{65}H_{112}O_{35}$	1452.6984	1451.6911	1451.6936	1475.6876	1475.6933
3	$C_{59}H_{102}O_{31}$	1306.6405	1305.6332	1305.6425	1329.6297	1329.6827
4	$C_{59}H_{102}O_{31}$	1306.6405	1305.6332	1305.6425	1329.6297	1329.6827
5	$C_{70}H_{120}O_{37}$	1552.7508	1551.7435	1551.7531	1575.7400	1575.7380
6	$C_{70}H_{120}O_{37}$	1552.7508	1551.7435	1551.7531	1575.7400	1575.7380
7	$C_{71}H_{122}O_{37}$	1566.7665	1565.7592	1565.7568	1589.7557	1589.7495
8	$C_{71}H_{122}O_{37}$	1566.7665	1565.7592	1565.7568	1589.7557	1589.7495





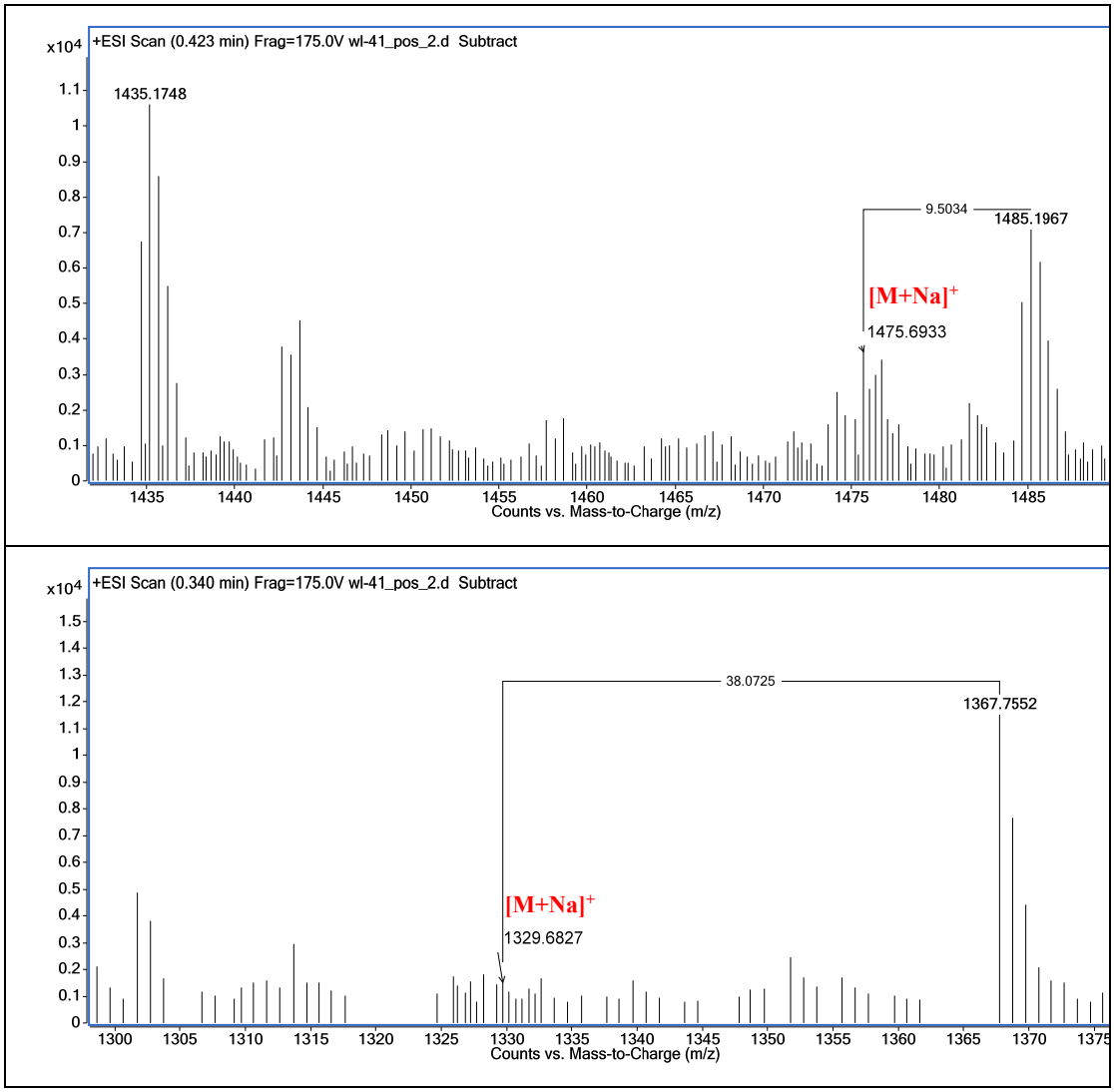


Figure. S5. HRMS spectra of the active peak (pharbitin)