ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

Oxime derivatives of betulonic and platanic acid as novel cytotoxic or antiviral agents

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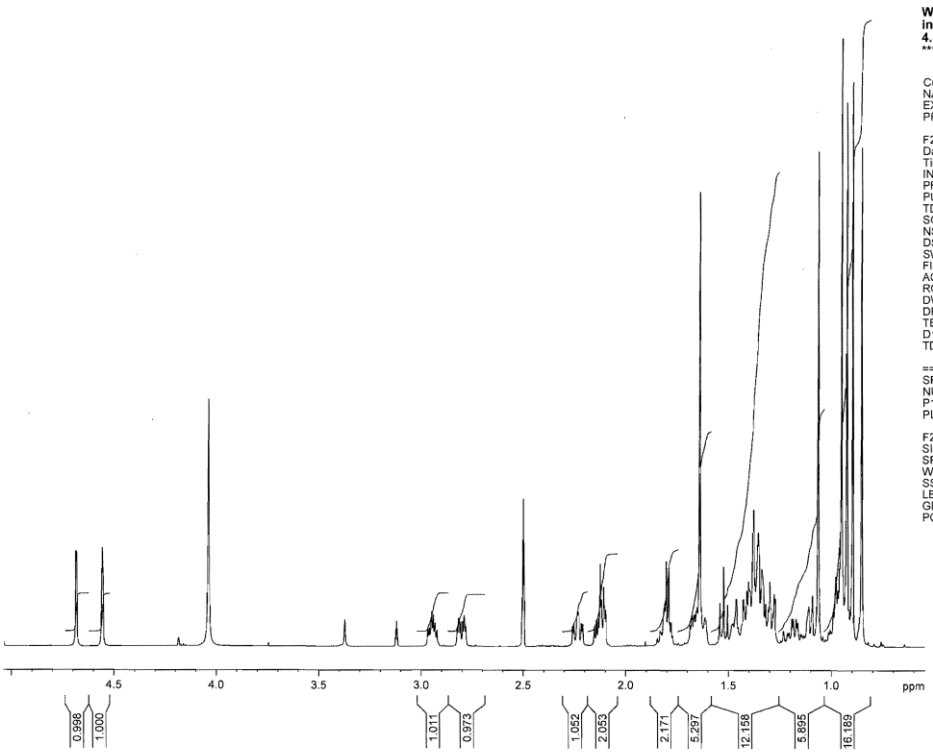
[#] These authors contributed equally in different topics of this paper.

Content

1. Analytical data

1.1. (3*E*)-3-(Hydroxyimino)lup-20(29)-en-28-oic acid (**3**)

^{1}H NMR (d_6-DMSO): δ 0.85 (3H, s, H25), 0.90 (3H, s, H26), 0.93 (3H, s, H27), 0.95 (3H, s, H24), 1.06 (3H, s, H23), 1.18 (2H, dq, J_1=4.4 Hz, J_2=4.4 Hz, J_3=4.4 Hz, J_4=12.7 Hz, H6), 1.52 (1H, t, J=11.3 Hz, H18), 1.64 (3H, dd, J_1=0.7 Hz, J_2=1.4 Hz, H29), 1.67 (2H, ddd, J_1=4.0 Hz, J_2=6.3 Hz, J_3=13.1 Hz, H1), 2.12 (1H, ddd, J_1=6.3 Hz, J_2=11.6 Hz, J_3=15.6 Hz, H2), 2.23 (1H, ddd, J_1=3.6 Hz, J_2=11.6 Hz, J_3=12.9 Hz, H13), 2.80 (1H, ddd, J_1=4.0 Hz, J_2=6.0 Hz, J_3=15.6 Hz, H2), 2.95 (1H, dt, J_1=4.7 Hz, J_2=11.0 Hz, J_3=11.0 Hz, H19), 4.56 (1H, dq, J_1=1.4 Hz, J_2=1.4 Hz, J_3=1.4 Hz, J_4=2.5 Hz, H30), 4.68 (1H, dq, J_1=0.7 Hz, J_2=0.7 Hz, J_3=0.7 Hz, J_4=2.5 Hz, H30). ^{13}C NMR (d_6-DMSO): δ 14.28 (q, C27), 15.47 (q, C25), 15.68 (q, C26), 16.62 (t, C2), 18.70 (t, C11), 18.95 (q, C29), 20.84 (t, C6), 23.04 (q, C24), 25.19 (t, C12), 27.59 (q, C23), 29.26 (t, C15), 30.16 (t, C21), 31.72 (t, C22), 33.52 (t, C16), 36.39 (t, C7), 36.81 (s, C4), 36.81 (s, C10), 37.76 (d, C13), 38.15 (t, C1), 40.35 (s, C8), 42.11 (s, C14), 46.70 (d, C19), 48.58 (d, C18), 49.56 (d, C9), 55.10 (d, C5), 55.49 (s, C17), 109.69 (t, C30), 150.38 (s, C20), 163.47 (s, C3), 177.24 (s, C28). MS (ES): *m/z* = 470.3 $[M+H]^+$, 468.3 $[M-H]^-$.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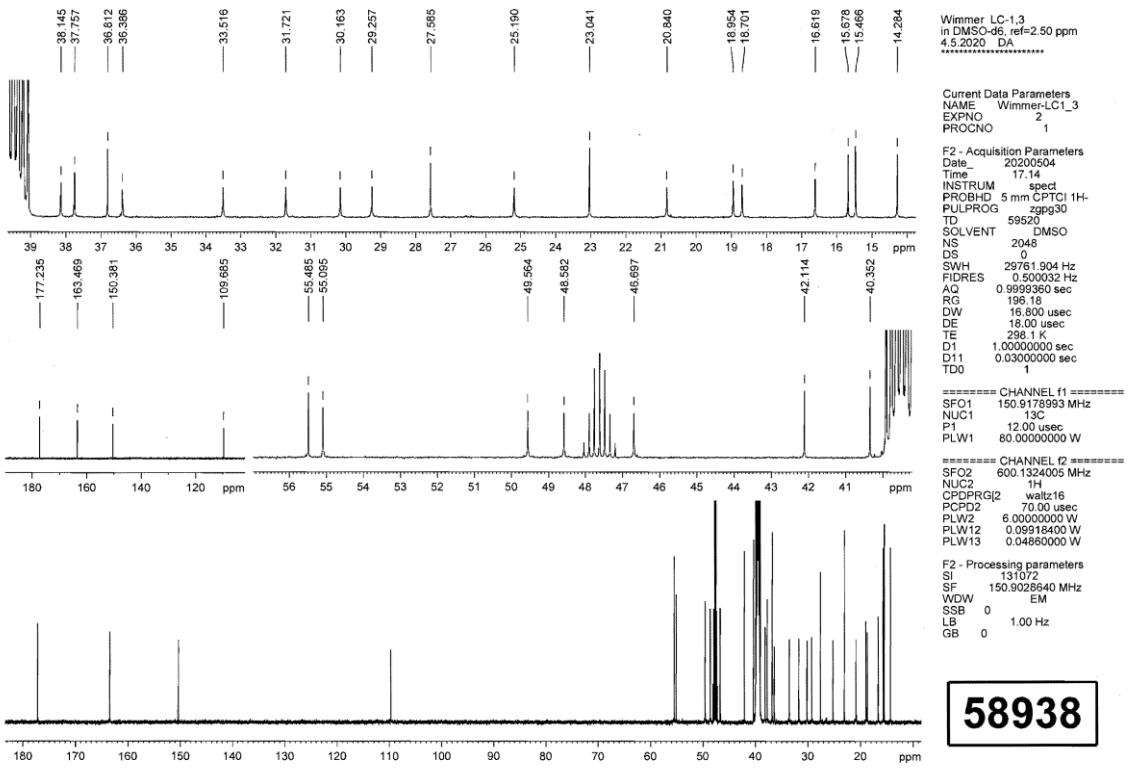
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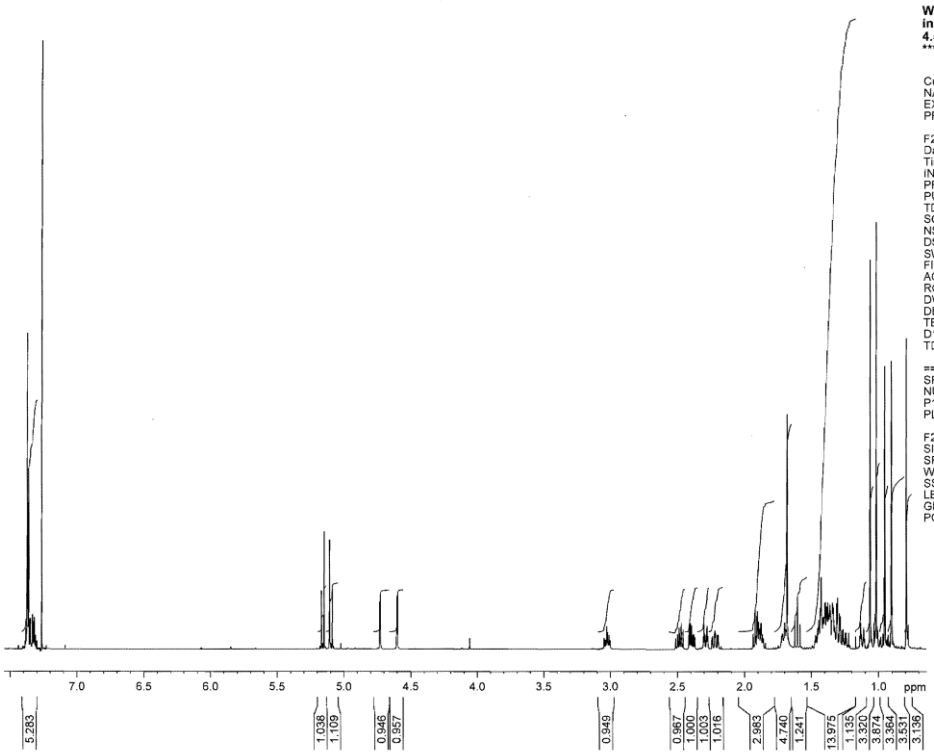
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
58938

1.2. Benzyl-3-oxolup-20(29)-en-28-oate (**4**)

^{1}H NMR ($CDCl_3$): δ 0.79 (3H, d, *J*=0.4 Hz, H25), 0.90 (3H, d, *J*=0.9 Hz, H26), 0.95 (3H, d, *J*=0.8 Hz, H27), 1.02 (3H, s, H24), 1.06 (3H, s, H23), 1.12 (2H, dt, J_1=3.3 Hz, J_2=3.3 Hz, J_3=13.5 Hz, H15), 1.30 (1H, t, *J*=11.4 Hz, H18), 1.30 (1H, dd, J_1=3.3 Hz, J_2=11.3 Hz, H5), 1.68 (3H, dd, J_1=0.7 Hz, J_2=1.4 Hz, H29), 1.68-1.73 (2H, m, H12), 1.84-1.94 (6H, m, H1+H7+H21), 2.22 (1H, ddd, J_1=3.7 Hz, J_2=11.5 Hz, J_3=12.9 Hz, H13), 2.29 (2H, ddd, J_1=3.1 Hz, J_2=3.5 Hz, J_3=13.0 Hz, H22), 2.39 (1H, ddd, J_1=4.4 Hz, J_2=7.6 Hz, J_3=15.6 Hz, H2), 2.48 (1H, ddd, J_1=7.6 Hz, J_2=9.8 Hz, J_3=15.6 Hz, H2), 3.03 (1H, dt, J_1=4.8 Hz, J_2=11.0 Hz, J_3=11.0 Hz, H19), 4.60 (1H, dq, J_1=1.4 Hz, J_2=1.4 Hz, J_3=1.4 Hz, J_4=2.3 Hz, H30), 4.73 (1H, dq, J_1=0.7 Hz, J_2=0.7 Hz, J_3=0.7 Hz, J_4=2.3 Hz, H30), 5.10 (1H, d, *J*=12.3 Hz, H1'), 5.15 (1H, d, *J*=12.3 Hz, H1'), 7.30-7.39 (5H, m, H3'-H5'). ^{13}C NMR ($CDCl_3$): δ 14.57 (q, C27), 15.61 (q, C25), 15.94 (q, C26), 19.35 (q, C29), 19.62 (t, C11), 21.01 (q, C24), 21.38 (t, C6), 25.52 (t, C12), 26.60 (q, C23), 29.52 (t, C15), 30.54 (t, C21), 32.03 (t, C22), 33.57 (t, C16), 34.13 (t, C2), 36.87 (s, C10), 36.89 (t, C7), 38.25 (d, C13), 39.61 (t, C1), 40.57 (s, C8), 42.42 (s, C14), 46.88 (d, C19), 47.31 (s, C4), 49.35 (d, C18), 49.89 (d, C9), 54.94 (d, C5), 56.50 (s, C17), 65.74 (t, C1'), 109.62 (t, C30), 128.06 (d, C5'), 128.24 (d, C4'), 128.48 (d, C3'), 136.45 (s, C2'), 150.48 (s, C20), 175.77 (s, C28), 218.20 (s, C3). MS (ES): *m/z* = 545.3 $[M+H]^+$.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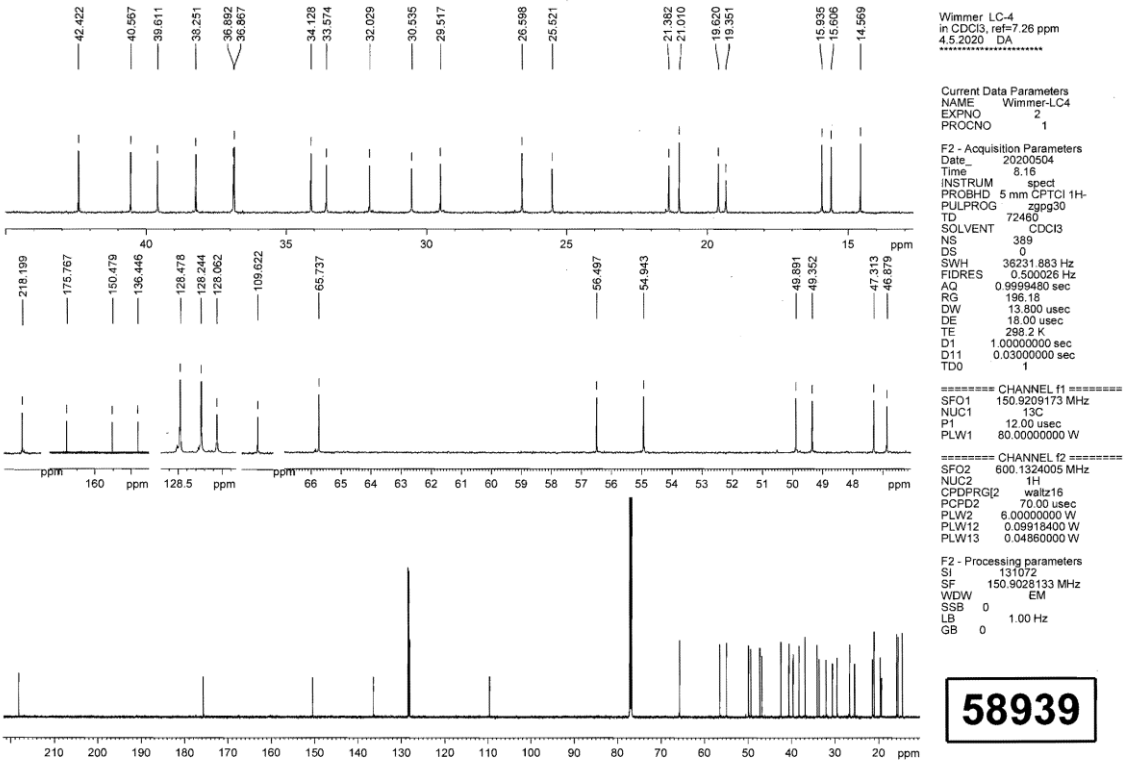
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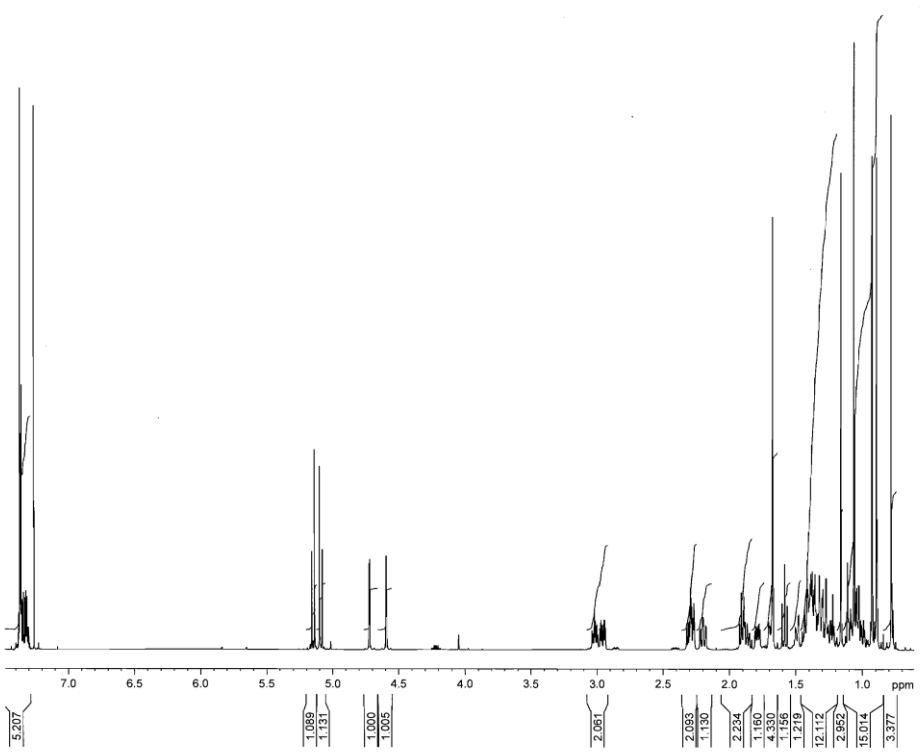
58939

1.3. Benzyl-(3*E*)-3-(hydroxyimino)lup-20(29)-en-28-oate (**5**)

^{1}H NMR ($CDCl_3$): δ 0.78 (3H, s, H25), 0.89 (3H, d, *J*=0.7 Hz, H26), 0.92 (3H, d, *J*=0.7 Hz, H27), 1.06 (3H, s, H24), 1.16 (3H, s, H23), 1.58 (1H, t, *J*=11.4 Hz, H18), 1.67-1.71 (2H, m, H12), 1.67 (3H, dd, J_1=0.7 Hz, J_2=1.4 Hz, H29), 1.79 (2H, ddd, J_1=4.0 Hz, J_2=6.5 Hz, J_3=13.2 Hz, H1), 1.84-1.92 (2H, m, H7), 1.84-1.92 (2H, m, H21), 2.20 (1H, ddd, J_1=3.7 Hz, J_2=11.6 Hz, J_3=13.0 Hz, H13), 2.27-2.32 (1H, m, H2), 2.27-2.32 (2H, m, H16), 2.96 (1H, ddd, J_1=4.0 Hz, J_2=6.0 Hz, J_3=15.7 Hz, H2), 3.02 (1H, dt, J_1=4.7 Hz, J_2=11.0 Hz, J_3=11.0 Hz, H19), 4.60 (1H, dq, J_1=1.4 Hz, J_2=1.4 Hz, J_3=1.4 Hz, J_4=2.3 Hz, H30), 4.72 (1H, dq, J_1=0.7 Hz, J_2=0.7 Hz, J_3=0.7 Hz, J_4=2.3 Hz, H30), 5.09 (1H, d, *J*=12.3 Hz, H1'), 5.15 (1H, d, *J*=12.3 Hz, H1'), 7.29-7.38 (3H, m, H3'-H5'). ^{13}C NMR ($CDCl_3$): δ 14.50 (q, C27), 15.70 (q, C25), 15.70 (q, C26), 17.60 (t, C2), 19.00 (t, C11), 19.30 (q, C29), 21.20 (t, C6), 22.90 (q, C24), 25.50 (t, C12), 27.30 (q, C23), 29.50 (t, C15), 30.50 (t, C21), 32.10 (t, C22), 33.80 (t, C16), 36.90 (t, C7), 37.20 (s, C10), 38.20 (d, C13), 38.60 (t, C1), 40.30 (s, C4), 40.70 (s, C8), 42.40 (s, C14), 46.90 (d, C19), 49.40 (d, C18), 50.10 (d, C9), 55.50 (d, C5), 56.50 (s, C17), 65.70 (t, C1'), 109.60 (t, C30), 128.10 (d, C5'), 128.20 (d, C4'), 128.50 (d, C3'), 136.50 (s, C2'), 150.50 (s, C20), 168.50 (s, C3), 175.80 (s, C28). MS (ES): *m/z* = 560.4 $[M+H]^+$.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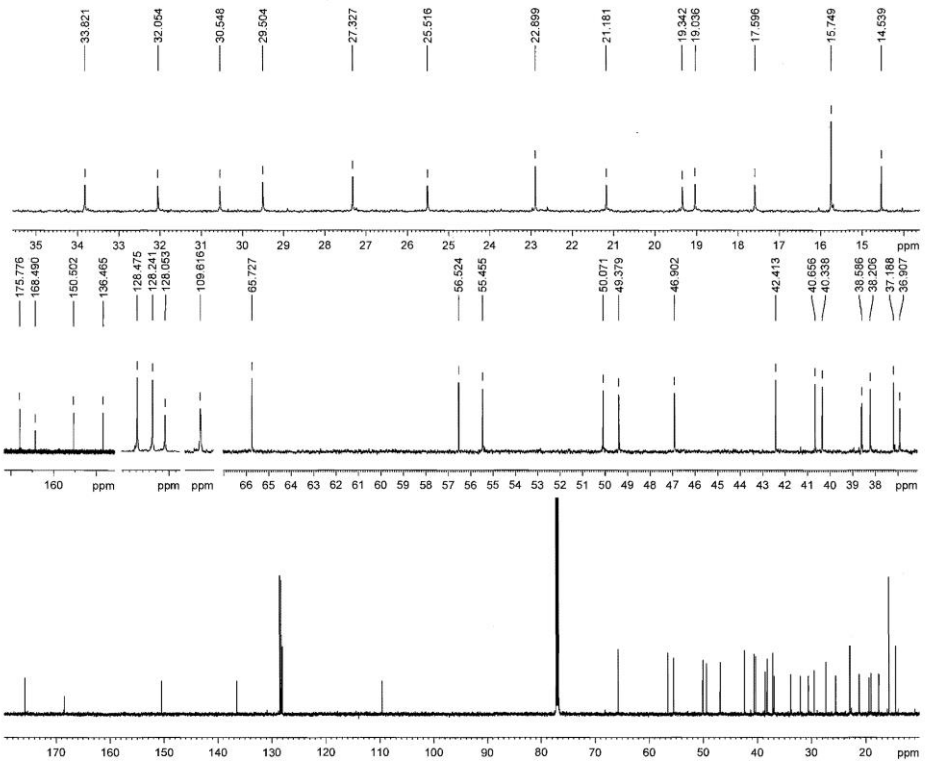
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37.188
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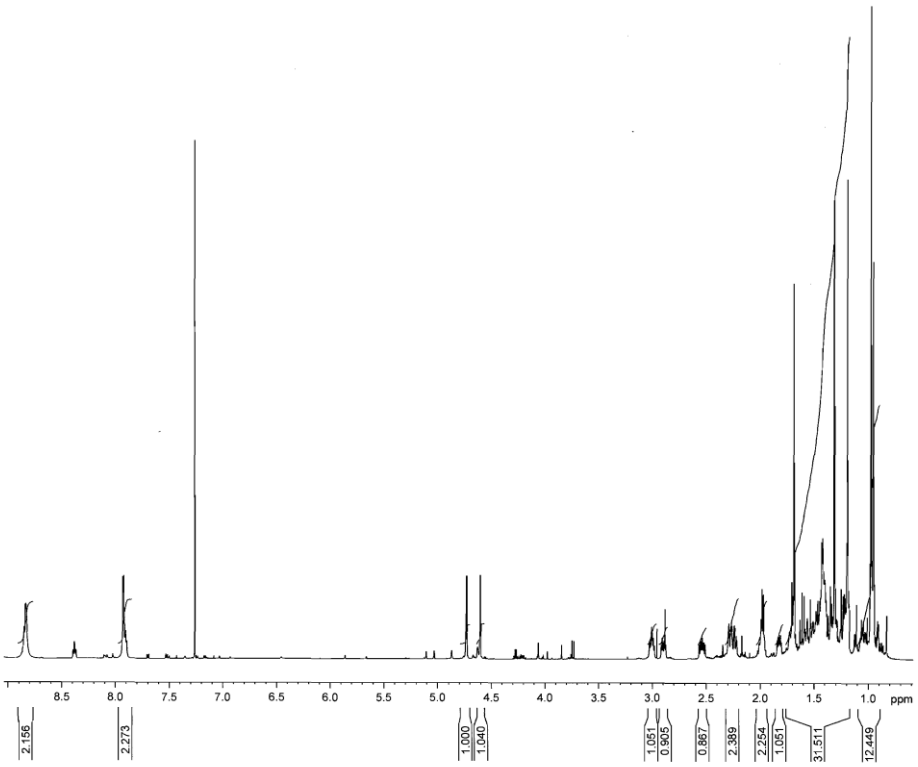
61270

1.4. (3*E*)-3-{[(Pyridin-3-ylcarbonyl)oxy]imino}lup-20(29)-en-28-oic acid (**6**)

^{1}H NMR ($CDCl_3$): δ 0.95 (3H, s, H26), 0.97 (3H, s, H25), 0.97 (3H, s, H27), 1.19 (3H, s, H24), 1.31 (3H, s, H23), 1.69 (3H, dd, J_1=0.7 Hz, J_2=1.4 Hz, H29), 1.82 (2H, ddd, J_1=4.7 Hz, J_2=6.3 Hz, J_3=13.2 Hz, H1), 1.95-2.02 (4H, m, H7+H21), 2.25 (1H, ddd, J_1=3.6 Hz, J_2=11.7 Hz, J_3=13.0 Hz, H13), 2.29 (2H, dt, J_1=3.4 Hz, J_2=3.4 Hz, J_3=12.8 Hz, H22), 2.54 (1H, ddd, J_1=6.3 Hz, J_2=10.9 Hz, J_3=15.4 Hz, H2), 2.90 (1H, ddd, J_1=4.7 Hz, J_2=6.5 Hz, J_3=15.4 Hz, H2), 3.01 (1H, dt, J_1=4.7 Hz, J_2=10.8 Hz, J_3=10.8 Hz, H19), 4.60 (1H, dq, J_1=1.4 Hz, J_2=1.4 Hz, J_3=1.4 Hz, J_4=2.4 Hz, H30), 4.73 (1H, dq, J_1=0.7 Hz, J_2=0.7 Hz, J_3=0.7 Hz, J_4=2.4 Hz, H30), 7.90 (1H, dd, J_1=5.7 Hz, J_2=7.7 Hz, H5'), 7.93 (1H, d, J=5.7 Hz, H6'), 8.84 (1H, bs, H3'), 8.84 (1H, bs, H4'). ^{13}C NMR ($CDCl_3$): δ 14.60 (q, C27), 15.90 (q, C26), 16.10 (q, C25), 19.00 (t, C11), 19.30 (q, C29), 20.10 (t, C2), 21.30 (t, C6), 22.70 (q, C24), 25.40 (t, C12), 27.40 (q, C23), 29.60 (t, C15), 30.50 (t, C21), 32.10 (t, C22), 33.70 (t, C16), 37.00 (t, C7), 37.20 (s, C10), 38.40 (d, C13), 39.10 (t, C1), 40.70 (s, C4), 41.70 (s, C8), 42.50 (s, C14), 46.90 (d, C19), 49.10 (d, C18), 50.10 (d, C9), 55.40 (d, C5), 56.30 (s, C17), 109.70 (t, C30), 123.20 (d, C6'), 126.60 (d, C5'), 137.90 (s, C2'), 142.10 (d, C3'), 149.70 (d, C4'), 150.40 (s, C20), 162.40 (s, C3), 177.60 (s, C1'), 180.90 (s, C28). MS (ES): *m/z* = 575.3 $[M+H]^+$.



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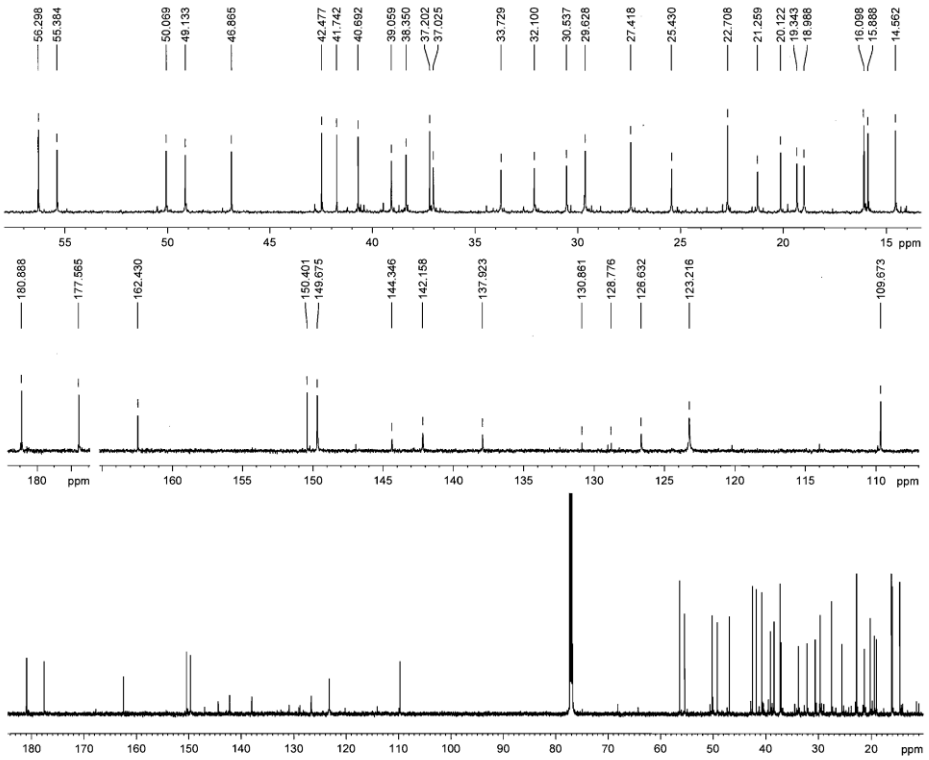
62285



Z.Wimmer LC-56
in CDCl3, ref=TMS
25.03.2022 DA
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Current Data Parameters
NAME Wimmer-LC56
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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Time 8.21 h
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PROBHD Z168380_0014 (
PULPROG zgpg30
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SOLVENT CDCl3
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SWH 29761.904 Hz
FIDRES 1.000064 Hz
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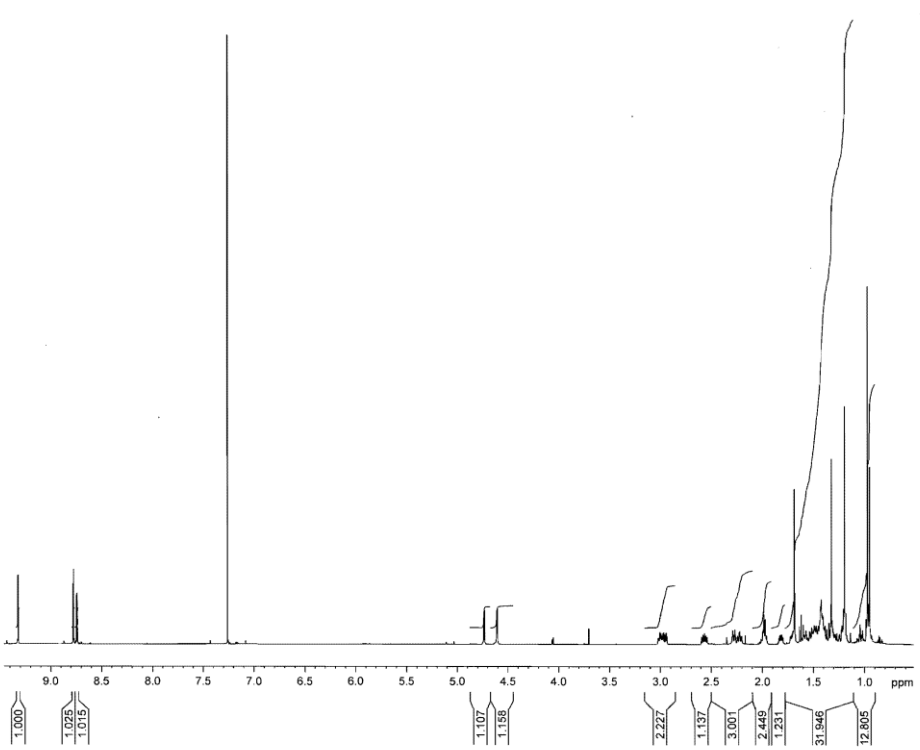
RG 196.18
DW 16.800 usec
DE 18.00 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178993 MHz
NUC1 13C
P0 4.00 usec
P1 12.00 usec
PLW1 104.66000366 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 6.34730005 W
PLW12 0.08290300 W
PLW13 0.04170000 W

F2 - Processing parameters
SI 131072
SF 150.9028137 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

62285

1.5. (3*E*)-3-{[(Pyrazin-2-ylcarbonyl)oxy]imino}lup-20(29)-en-28-oic acid (**7**)

^{1}H NMR ($CDCl_3$): δ 0.95 (3H, s, H26), 0.97 (3H, s, H25), 0.97 (3H, s, H27), 1.20 (3H, s, H24), 1.32 (3H, s, H23), 1.62 (1H, t, *J*=11.4 Hz, H18), 1.69 (3H, dd, J_1=0.7 Hz, J_2=1.4 Hz, H29), 1.82 (2H, ddd, J_1=4.7 Hz, J_2=6.5 Hz, J_3=13.3 Hz, H1), 1.95-2.02 (4H, m, H7+H21), 2.22 (1H, ddd, J_1=3.6 Hz, J_2=11.6 Hz, J_3=12.8 Hz, H13), 2.28 (2H, dt, J_1=3.4 Hz, J_2=3.4 Hz, J_3=12.5 Hz, H22), 2.57 (1H, ddd, J_1=6.5 Hz, J_2=10.8 Hz, J_3=15.3 Hz, H2), 2.96 (1H, ddd, J_1=4.7 Hz, J_2=6.3 Hz, J_3=15.3 Hz, H2), 3.00 (1H, dt, J_1=4.7 Hz, J_2=10.6 Hz, J_3=10.6 Hz, H19), 4.61 (1H, dq, J_1=1.4 Hz, J_2=1.4 Hz, J_3=1.4 Hz, J_4=2.4 Hz, H30), 4.74 (1H, dq, J_1=0.7 Hz, J_2=0.7 Hz, J_3=0.7 Hz, J_4=2.4 Hz, H30), 8.74 (1H, dd, J_1=1.5 Hz, J_2=2.4 Hz, H4'), 8.78 (1H, d, *J*=2.4 Hz, H5'), 9.32 (1H, d, *J*=1.5 Hz, H3'). ^{13}C NMR ($CDCl_3$): δ 14.60 (q, C27), 15.90 (q, C26), 16.10 (q, C25), 19.00 (t, C11), 19.30 (q, C29), 20.20 (t, C2), 21.20 (t, C6), 22.70 (q, C24), 25.40 (t, C12), 27.40 (q, C23), 29.60 (t, C15), 30.50 (t, C21), 32.10 (t, C22), 33.70 (t, C16), 37.00 (t, C7), 37.20 (s, C10), 38.40 (d, C13), 39.10 (t, C1), 40.70 (s, C4), 41.80 (s, C8), 42.50 (s, C14), 46.90 (d, C19), 49.10 (d, C18), 50.10 (d, C9), 55.40 (d, C5), 56.30 (s, C17), 109.70 (t, C30), 143.60 (s, C2'), 144.50 (d, C4'), 146.10 (d, C3'), 147.50 (d, C5'), 150.30 (s, C20), 161.70 (s, C3), 181.30 (s, C28). MS (ES): *m/z* = 576.2 $[M+H]^+$, 574.2 $[M-H]^-$.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in CDCl3, ref=TMS
25.03.2022 DA
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EXPNO 100
PROCNO 1
F2 - Acquisition Parameters
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Time 9.59 h
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PULPROG zg30
TD 48076
SOLVENT CDCl3
NS 16
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FIDRES 0.250005 Hz
AQ 3.9999232 sec
RG 14.7
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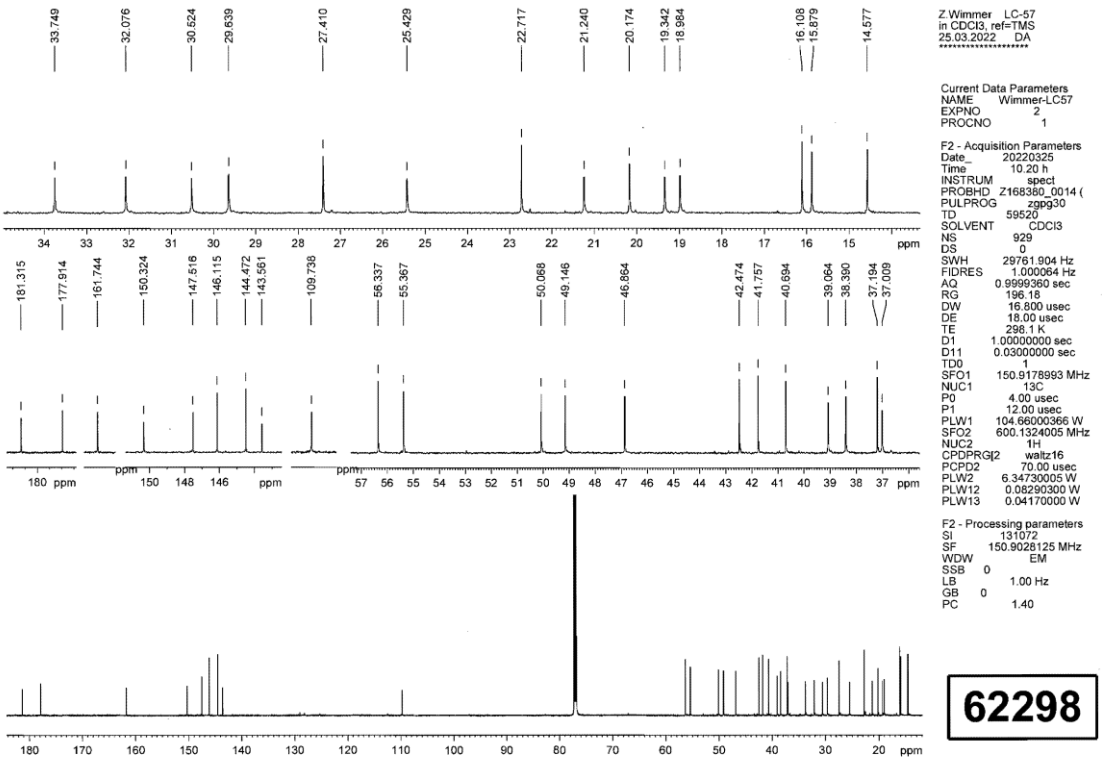
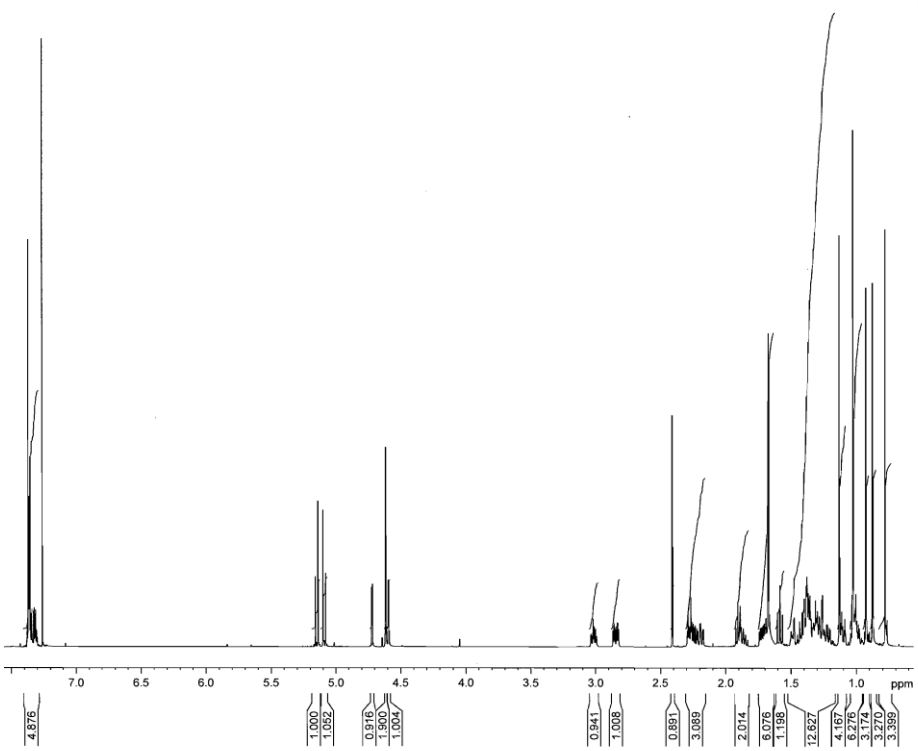
DE 10.00 usec
TE 298.2 K
D1 0 sec
TD0 1
SFO1 600.1330006 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 6.34730005 W
F2 - Processing parameters
SI 131072
SF 600.1300138 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.000 1.025 1.015 1.107 1.158 2.227 1.137 3.001 2.449 1.231 31.946 12.805
62298


33.749 32.076 30.624 29.639 27.410 25.429 22.717 21.240 20.174 19.342 18.984 16.108 15.879 14.577
181.315 177.914 161.744 150.324 147.516 146.115 144.472 143.561 109.738 56.337 55.367 50.068 49.146 46.864 42.474 41.757 40.694 39.064 38.390 37.194 37.009
180 ppm 150 148 146 ppm 57 56 55 54 53 52 51 50 49 48 47 46 45 44 43 42 41 40 39 38 37 ppm
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
Z.Wimmer LC-57
in CDCl3, ref=TMS
25.03.2022 DA
****
Current Data Parameters
NAME Wimmer-LC57
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220325
Time 10.20 h
INSTRUM spect
PROBHD Z168380_0014 (
PULPROG zgpg30
TD 59520
SOLVENT CDCl3
NS 929
DS 0
SWH 29761.904 Hz
FIDRES 1.000064 Hz
AQ 0.9999360 sec
RG 196.18
DW 16.800 usec
DE 18.00 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178993 MHz
NUC1 13C
P0 4.00 usec
P1 12.00 usec
PLW1 104.66000366 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 6.34730005 W
PLW12 0.08290300 W
PLW13 0.04170000 W
F2 - Processing parameters
SI 131072
SF 150.9028125 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
62298

1.6. Benzyl-(3*E*)-3-[(prop-2-yn-1-yloxy)imino]lup-20(29)-en-28-oate (**8**)

^{1}H NMR ($CDCl_3$): δ 0.78 (3H, s, H25), 0.88 (3H, d, *J*=0.8 Hz, H26), 0.93 (3H, d, *J*=0.8 Hz, H27), 1.03 (3H, s, H24), 1.10 (2H, dt, J_1=3.3 Hz, J_2=3.3 Hz, J_3=13.6 Hz, H15), 1.13 (3H, s, H23), 1.21 (2H, dq, J_1=4.6 Hz, J_2=12.7 Hz, J_3=12.7 Hz, J_4=12.7 Hz, H6), 1.58 (1H, t, J_1=11.4 Hz, J_2=11.4 Hz, H18), 1.68 (3H, dd, J_1=0.8 Hz, J_2=1.4 Hz, H29), 1.72 (2H, ddd, J_1=4.1 Hz, J_2=6.4 Hz, J_3=13.1 Hz, H1), 2.20 (1H, ddd, J_1=3.8 Hz, J_2=11.7 Hz, J_3=13.0 Hz, H13), 2.25 (1H, ddd, J_1=6.4 Hz, J_2=11.4 Hz, J_3=15.5 Hz, H2), 2.28 (2H, dt, J_1=3.6 Hz, J_2=3.6 Hz, J_3=13.0 Hz, H22), 2.41 (1H, t, *J*=2.4 Hz, H8'), 2.85 (1H, ddd, J_1=4.1 Hz, J_2=6.0 Hz, J_3=15.5 Hz, H2), 3.02 (1H, dt, J_1=4.8 Hz, J_2=10.9 Hz, J_3=10.9 Hz, H19), 4.60 (1H, dq, J_1=1.4 Hz, J_2=1.4 Hz, J_3=1.4 Hz, J_4=2.4 Hz, H30), 4.60 (1H, dd, J_1=2.4 Hz, J_2=15.6 Hz, H6'), 4.63 (1H, dd, J_1=2.4 Hz, J_2=15.6 Hz, H6'), 4.72 (1H, dq, J_1=0.7 Hz, J_2=0.7 Hz, J_3=0.7 Hz, J_4=2.4 Hz, H30), 5.09 (1H, d, *J*=12.3 Hz, H1'), 5.15 (1H, d, *J*=12.3 Hz, H1'), 7.29-7.39 (3H, m, H3'-H5'). ^{13}C NMR ($CDCl_3$): δ 14.60 (q, C27), 15.70 (q, C26), 15.80 (q, C25), 18.00 (t, C2), 19.00 (t, C11), 19.40 (q, C29), 21.20 (t, C6), 23.00 (q, C24), 25.60 (t, C12), 27.50 (q, C23), 29.50 (t, C15), 30.60 (t, C21), 32.10 (t, C22), 33.80 (t, C16), 36.90 (t, C7), 37.10 (s, C10), 38.20 (d, C13), 38.70 (t, C1), 40.20 (s, C4), 40.70 (s, C8), 42.40 (s, C14), 46.90 (d, C19), 49.40 (d, C18), 50.10 (d, C9), 55.40 (d, C5), 56.50 (s, C17), 60.70 (t, C6'), 65.70 (t, C1'), 73.60 (d, C8'), 80.90 (s, C7'), 109.60 (t, C30), 128.10 (d, C5'), 128.20 (d, C4'), 128.50 (d, C3'), 136.50 (s, C2'), 150.50 (s, C20), 167.80 (s, C3), 175.80 (s, C28). MS (ES): *m/z* = 598.4 $[M+H]^+$.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22.9.2021 DA
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PROCNO 1
F2 - Acquisition Parameters
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Time 8.19 h
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PROBHD Z168380_0014 (
PULPROG zg30
TD 38362
SOLVENT CDCl3
NS 16
DS 0
SWH 4795.396 Hz
FIDRES 0.250008 Hz
AQ 3.9998779 sec
RG 12.83
DW 104.267 usec
DE 10.00 usec
TE 298.1 K
D1 0 sec
TD0 1
SFO1 600.1324005 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 6.34730005 W
F2 - Processing parameters
SI 131072
SF 600.1300148 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
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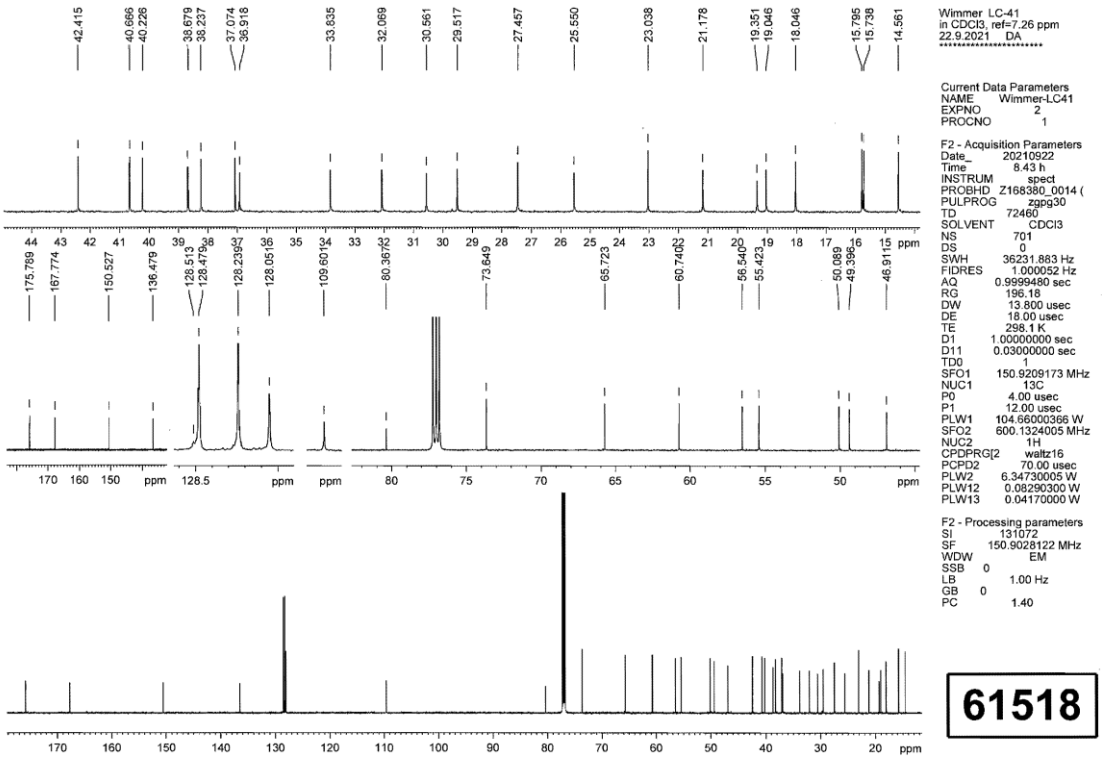
1.000 1.052
0.916 1.900 1.000 1.004
0.941 1.008
0.891 3.089
2.014 6.076 1.198
12.627
4.167 6.276 3.174 3.270 3.399
61518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175.769 167.774 150.527 136.479 128.513 128.479 128.239 128.051 109.601 80.367 73.649 65.723 60.748 56.540 55.423 50.089 49.396 46.911
Wimmer LC-41
in CDCl3, ref=7.26 ppm
22.9.2021 DA
Current Data Parameters
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EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
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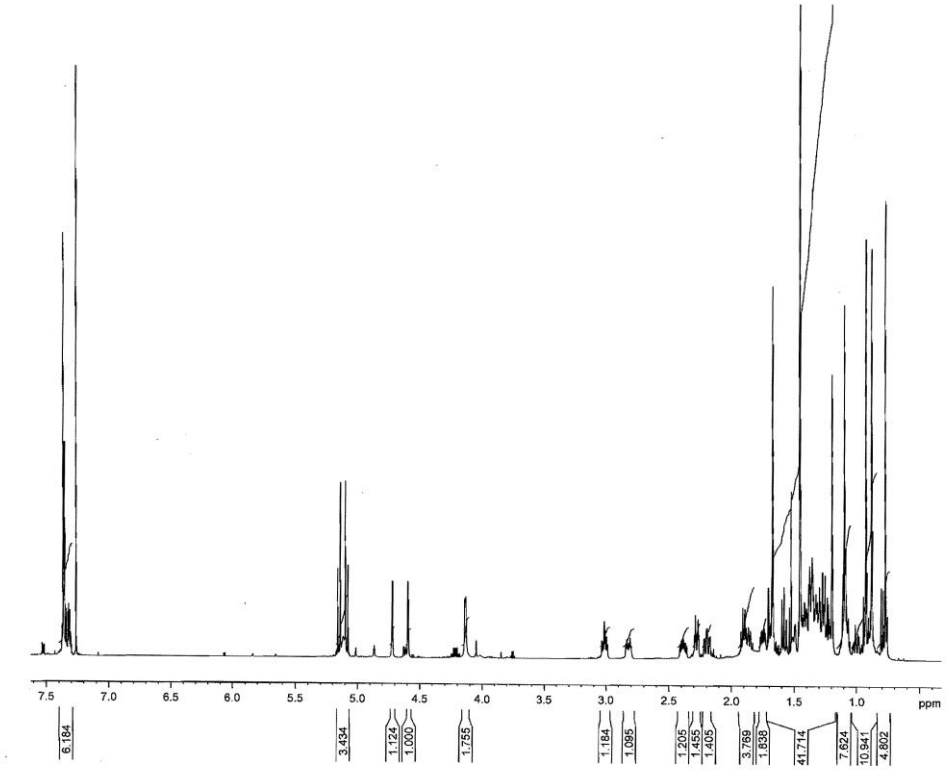
INSTRUM spect
PROBHD Z168380_0014 (
PULPROG zgpg30
TD 72460
SOLVENT CDCl3
NS 701
DS 0
SWH 36231.883 Hz
FIDRES 1.000052 Hz
AQ 0.9999480 sec
RG 196.18
DW 13.800 usec
DE 18.00 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9209173 MHz
NUC1 13C
P0 4.00 usec
P1 12.00 usec
PLW1 104.66000366 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 6.34730005 W
PLW12 0.08290300 W
PLW13 0.04170000 W
F2 - Processing parameters
SI 131072
SF 150.9028122 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
61518

1.7. Benzyl-(3*E*)-3-[({[(*tert*-butoxycarbonyl)amino]acetyl}oxy)imino]lup-20(29)-en-28-oate (**9**)

^{1}H NMR ($CDCl_3$): δ 0.78 (3H, s, H26), 0.88 (3H, s, H25), 0.92 (3H, s, H27), 1.00 (2H, dq, J_1=4.9 Hz, J_2=13.0 Hz, J_3=13.0 Hz, J_4=13.0 Hz, H12), 1.10 (3H, s, H24), 1.20 (3H, s, H23), 1.45 (3H, s, H10'), 1.67 (3H, dd, J_1=0.7 Hz, J_2=1.4 Hz, H29), 1.75 (2H, ddd, J_1=4.6 Hz, J_2=6.5 Hz, J_3=13.2 Hz, H1), 1.83-1.93 (4H, m, H7+H21), 2.20 (1H, ddd, J_1=3.7 Hz, J_2=11.6 Hz, J_3=12.9 Hz, H13), 2.28 (2H, dt, J_1=3.5 Hz, J_2=3.5 Hz, J_3=12.7 Hz, H22), 2.39 (1H, ddd, J_1=6.5 Hz, J_2=11.0 Hz, J_3=15.3 Hz, H2), 2.82 (1H, ddd, J_1=4.6 Hz, J_2=6.2 Hz, J_3=15.3 Hz, H2), 3.01 (1H, dt, J_1=4.6 Hz, J_2=10.9 Hz, J_3=10.9 Hz, H19), 4.14 (2H, d, J=4.6 Hz, H7'), 4.59 (1H, dq, J_1=1.4 Hz, J_2=1.4 Hz, J_3=1.4 Hz, J_4=2.3 Hz, H30), 4.72 (1H, dq, J_1=0.7 Hz, J_2=0.7 Hz, J_3=0.7 Hz, J_4=2.3 Hz, H30), 5.09 (1H, d, J=12.3 Hz, H1'), 5.15 (1H, d, J=12.3 Hz, H1'), 7.30-7.38 (3H, m, H3'-H5'). ^{13}C NMR ($CDCl_3$): δ 14.50 (q, C27), 15.70 (q, C26), 16.00 (q, C25), 19.00 (t, C11), 19.30 (q, C29), 19.50 (t, C2), 21.20 (t, C6), 22.60 (q, C24), 25.50 (t, C12), 27.30 (q, C23), 28.30 (q, C10'), 29.50 (t, C15), 30.00 (t, C22), 30.50 (t, C21), 33.70 (t, C16), 36.90 (t, C7), 37.10 (s, C10), 38.20 (d, C13), 39.00 (t, C1), 40.60 (s, C4), 41.40 (s, C8), 42.20 (t, C7'), 42.40 (s, C14), 46.90 (d, C19), 49.30 (d, C18), 50.10 (d, C9), 55.40 (d, C5), 56.50 (s, C17), 65.70 v(t, C1'), 80.00 (s, C9'), 109.60 (t, C30), 128.10 (d, C5'), 128.20 (d, C4'), 128.50 (d, C3'), 136.50 (s, C2'), 150.50 (s, C20), 155.70 (s, C8'), 170.50 (s, C3), 175.70 (s, C28), 175.80 (s, C6'). MS (ES): *m/z* = 717.4 $[M+H]^+$.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in CDCl3, ref=7.26 ppm
19.04.2022 DA
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EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220419
Time 7.30 h
INSTRUM spect
PROBHD Z168380_0014 (
PULPROG zg30
TD 38362
SOLVENT CDCl3
NS 16
DS 0
SWH 4795.396 Hz
FIDRES 0.250008 Hz
AQ 3.9998779 sec
RG 16.14
DW 104.267 usec
DE 10.00 usec
TE 298.1 K
D1 0 sec
TD0 1
SFO1 600.1324005 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 6.34730005 W
F2 - Processing parameters
SI 131072
SF 600.1300148 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
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3.434
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1.000
1.755
1.184
1.085
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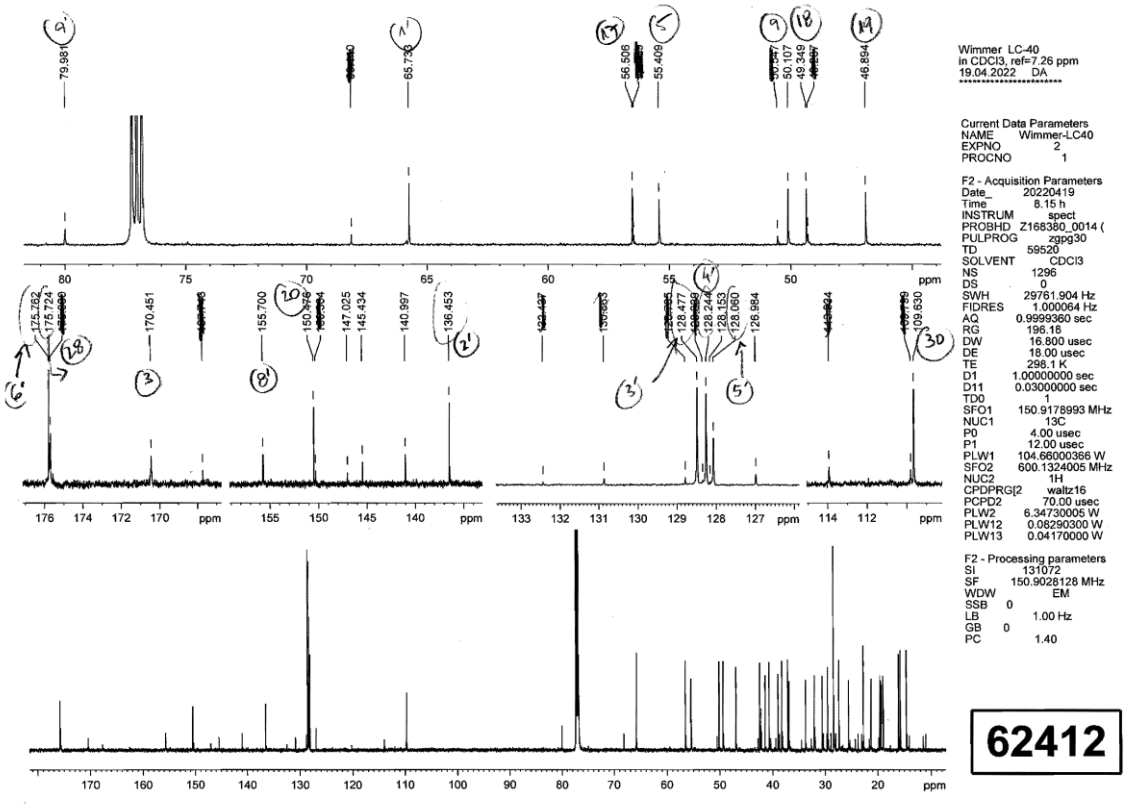
41.714
7.624
10.941
4.802
62412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55.409
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49.349
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Wimmer LC-40
in CDCl3, ref=7.26 ppm
19.04.2022 DA
Current Data Parameters
NAME Wimmer-LC40
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220419
Time 8.15 h
INSTRUM spect
PROBHD Z168380_0014 (
PULPROG zgpg30
TD 59520
SOLVENT CDCl3
NS 1296
DS 0
SWH 29761.904 Hz
FIDRES 1.000064 Hz
AQ 0.9999360 sec
RG 196.16
DW 16.800 usec
DE 18.00 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178993 MHz
NUC1 13C
P0 4.00 usec
P1 12.00 usec
PLW1 104.66000366 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 6.34730005 W
PLW12 0.08290300 W
PLW13 0.04170000 W
F2 - Processing parameters
SI 131072
SF 150.9028128 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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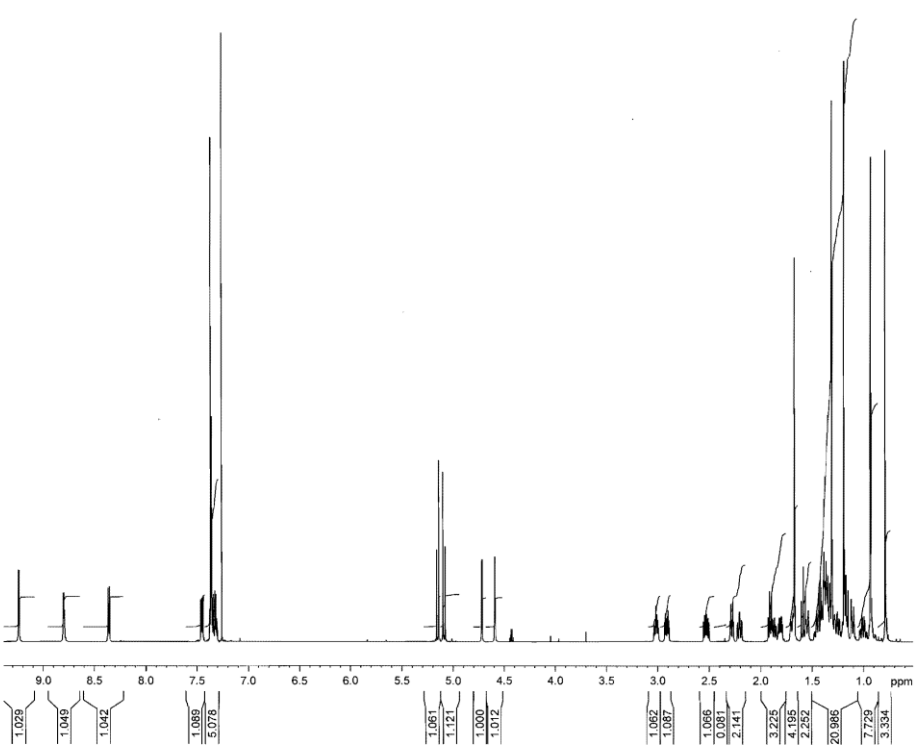
175.724
170.451
155.700
150.469
147.025
145.434
140.997
136.453
128.477
128.244
128.153
128.060
126.984
109.830
176 174 172 170 ppm
155 150 145 140 ppm
133 132 131 130 129 128 127 ppm
114 112 ppm
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
62412

1.8. Benzyl-(3*E*)-3-{[(pyridin-3-ylcarbonyl)oxy]imino}lup-20(29)-en-28-oate (**10**)

^{1}H NMR ($CDCl_3$): δ 0.79 (3H, s, H26), 0.93 (3H, d, *J*=0.6 Hz, H25), 0.93 (3H, d, *J*=0.6 Hz, H27), 1.01 (2H, dq, J_1=4.5 Hz, J_2=12.9 Hz, J_3=12.9 Hz, J_4=12.9 Hz, H12), 1.11 (2H, dt, J_1=3.4 Hz, J_2=3.4 Hz, J_3=13.5 Hz, H15), 1.19 (3H, s, H24), 1.31 (3H, s, H23), 1.58 (1H, t, *J*=11.4 Hz, H18), 1.67 (3H, dd, J_1=0.7 Hz, J2=1.4 Hz, H29), 1.81 (2H, ddd, J_1=4.6 Hz, J_2=6.4 Hz, J_3=13.2 Hz, H1), 1.85-1.93 (4H, m, H7+H21), 2.21 (1H, ddd, J_1=3.6 Hz, J_2=11.6 Hz, J_3=12.8 Hz, H13), 2.29 (2H, dt, J_1=3.5 Hz, J_2=3.5 Hz, J_3=12.7 Hz, H22), 2.53 (1H, ddd, J_1=6.4 Hz, J_2=10.9 Hz, J_3=15.3 Hz, H2), 2.91 (1H, ddd, J_1=4.6 Hz, J_2=6.2 Hz, J_3=15.3 Hz, H2), 3.02 (1H, dt, J_1=4.8 Hz, J_2=11.0 Hz, J_3=11.0 Hz, H19), 4.59 (1H, dq, J_1=1.4 Hz, J_2=1.4 Hz, J_3=1.4 Hz, J_4=2.3 Hz, H30), 4.72 (1H, dq, J_1=0.7 Hz, J_2=0.7 Hz, J_3=0.7 Hz, J_4=2.3 Hz, H30), 5.09 (1H, d, *J*=12.3 Hz, H7'), 5.15 (1H, d, *J*=12.3 Hz, H7'), 7.30-7.38 (5H, m, H9'-H11'), 7.45 (1H, dd, J_1=4.8 Hz, J_2=8.0 Hz, H5'), 8.36 (1H, dt, J_1=2.0 Hz, J_2=2.0 Hz, J_3=8.0 Hz, H6'), 8.80 (1H, bdd, J_1=1.7 Hz, J_2=4.8 Hz, H4'), 9.24 (1H, dd, J_1=0.6 Hz, J_2=2.1 Hz, H3'). ^{13}C NMR ($CDCl_3$): δ 14.50 (q, C27), 15.70 (q, C26), 16.10 (q, C25), 19.00 (t, C11), 19.30 (q, C29), 20.10 (t, C2), 21.30 (t, C6), 22.70 (q, C24), 25.50 (t, C12), 27.40 (q, C23), 29.50 (t, C15), 30.50 (t, C21), 32.00 (t, C22), 33.70 (t, C16), 36.90 (t, C7), 37.20 (s, C10), 38.20 (d, C13), 39.10 (t, C1), 40.60 (s, C4), 41.70 (s, C8), 42.40 (s, C14), 46.90 (d, C19), 49.30 (d, C18), 50.10 (d, C9), 55.40 (d, C5), 56.50 (s, C17), 65.70 (t, C7'), 109.60 (t, C30), 123.70 (d, C5'), 126.20 (s, C2'), 128.10 (d, C11'), 128.20 (d, C10'), 128.50 (d, C9'), 136.50 (s, C8'), 137.80 (d, C6'), 149.80 (d, C3'), 150.50 (s, C20), 152.60 (d, C4'), 162.60 (s, C3), 175.80 (s, C1'), 177.20 (s, C28). MS (ES): *m/z* = 665.3 $[M+H]^+$.



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in CDCl3, ref=TMS
31.03.2022 DA
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PROCNO 1

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PULPROG zg30
TD 48076
SOLVENT CDCl3
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FIDRES 0.250005 Hz
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DE 10.00 usec
TE 298.1 K
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NUC1 1H
P0 2.67 usec
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F2 - Processing parameters
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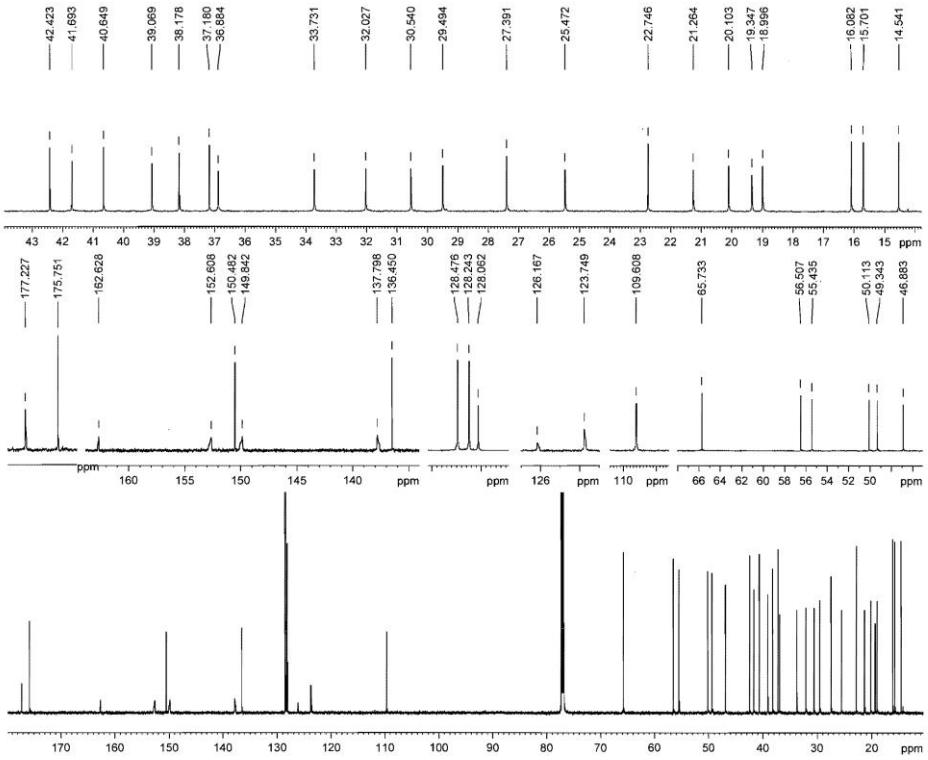
SF 600.1300138 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

62334



Z.Wimmer LC-68
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31.03.2022 DA
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Current Data Parameters
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EXPNO 2
PROCNO 1

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SOLVENT CDCl3
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SWH 29761.904 Hz
FIDRES 1.000064 Hz
AQ 0.9999360 sec
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DW 16.800 usec
DE 18.00 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178993 MHz
NUC1 13C
P0 4.00 usec
P1 12.00 usec
PLW1 104.66000366 W
SFO2 600.1324005 MHz
NUC2 1H
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PCPD2 70.00 usec
PLW2 6.34730005 W
PLW12 0.08290300 W
PLW13 0.04170000 W

F2 - Processing parameters
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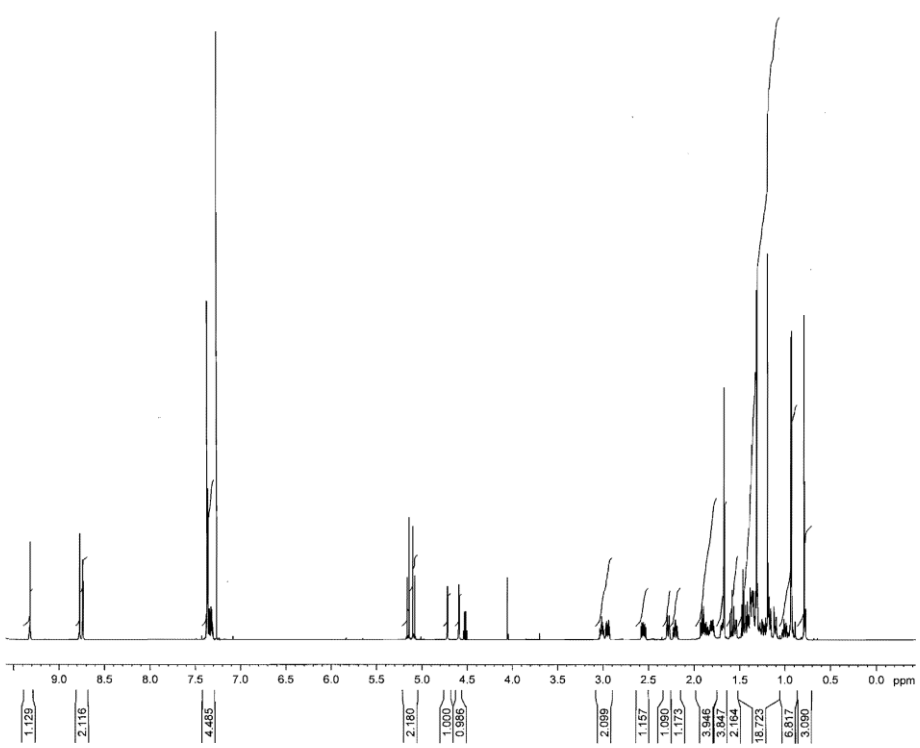
SF 150.9028133 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

62334

1.9. Benzyl-(3*E*)-3-{[(pyrazin-2-ylcarbonyl)oxy]imino}lup-20(29)-en-28-oate (**11**)

^{1}H NMR ($CDCl_3$): δ 0.79 (3H, s, H26), 0.93 (3H, s, H25), 0.93 (3H, s, H27), 1.19 (3H, s, H24), 1.31 (3H, s, H23), 1.58 (1H, t, *J*=11.4 Hz, H18), 1.67 (3H, dd, J_1=0.7 Hz, J_2=1.4 Hz, H29), 1.80 (2H, ddd, J_1=4.5 Hz, J_2=6.5 Hz, J_3=13.2 Hz, H1), 1.85-1.94 (4H, m, H7+H21), 2.21 (1H, ddd, J_1=3.6 Hz, J_2=11.5 Hz, J_3=12.9 Hz, H13), 2.28 (2H, dt, J_1=3.4 Hz, J_2=3.4 Hz, J_3=12.5 Hz, H22), 2.56 (1H, ddd, J_1=6.5 Hz, J_2=10.8 Hz, J_3=15.3 Hz, H2), 2.95 (1H, ddd, J_1=4.5 Hz, J_2=6.3 Hz, J_3=15.3 Hz, H2), 3.02 (1H, dt, J_1=4.8 Hz, J_2=11.0 Hz, J_3=11.0 Hz, H19), 4.59 (1H, dq, J_1=1.4 Hz, J_2=1.4 Hz, J_3=1.4 Hz, J_4=2.3 Hz, H30), 4.72 (1H, dq, J_1=0.7 Hz, J_2=0.7 Hz, J_3=0.7 Hz, J_4=2.3 Hz, H30), 5.09 (1H, d, *J*=12.3 Hz, H6'), 5.15 (1H, d, *J*=12.3 Hz, H6'), 7.31-7.37 (5H, m, H8'+H9'+H10'), 8.74 (1H, dd, J_1=1.5 Hz, J_2=2.5 Hz, H4'), 8.77 (1H, d, *J*=2.5 Hz, H5'), 9.32 (1H, d, *J*=1.5 Hz, H3'). ^{13}C NMR ($CDCl_3$): δ 14.50 (q, C27), 15.70 (q, C26), 16.10 (q, C25), 19.00 (t, C11), 19.30 (q, C29), 20.20 (t, C2), 21.30 (t, C6), 22.70 (q, C24), 25.50 (t, C12), 27.40 (q, C23), 29.50 (t, C15), 30.50 (t, C21), 32.00 (t, C22), 33.70 (t, C16), 36.90 (t, C7), 37.20 (s, C10), 38.20 (d, C13), 39.10 (t, C1), 40.60 (s, C4), 41.70 (s, C8), 42.40 (s, C14), 46.90 (d, C19), 49.30 (d, C18), 50.10 (d, C9), 55.40 (d, C5), 56.50 (s, C17), 65.70 (t, C6'), 109.60 (t, C30), 128.10 (d, C10'), 128.20 (d, C9'), 128.50 (d, C8'), 136.40 (s, C7'), 143.60 (s, C2'), 144.50 (d, C4'), 146.10 (d, C3'), 147.50 (d, C5'), 150.50 (s, C20), 161.80 (s, C3), 175.80 (s, C1'), 177.90 (s, C28). MS (ES): *m/z* = 666.8 $[M+H]^+$.



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31.03.2022 DA

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PROCNO 1

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SOLVENT CDCl3
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RG 16.14
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DE 10.00 usec
TE 298.2 K
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TD0 1
SFO1 600.1327606 MHz
NUC1 1H
P0 2.67 usec
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PLW1 6.34730005 W

F2 - Processing parameters
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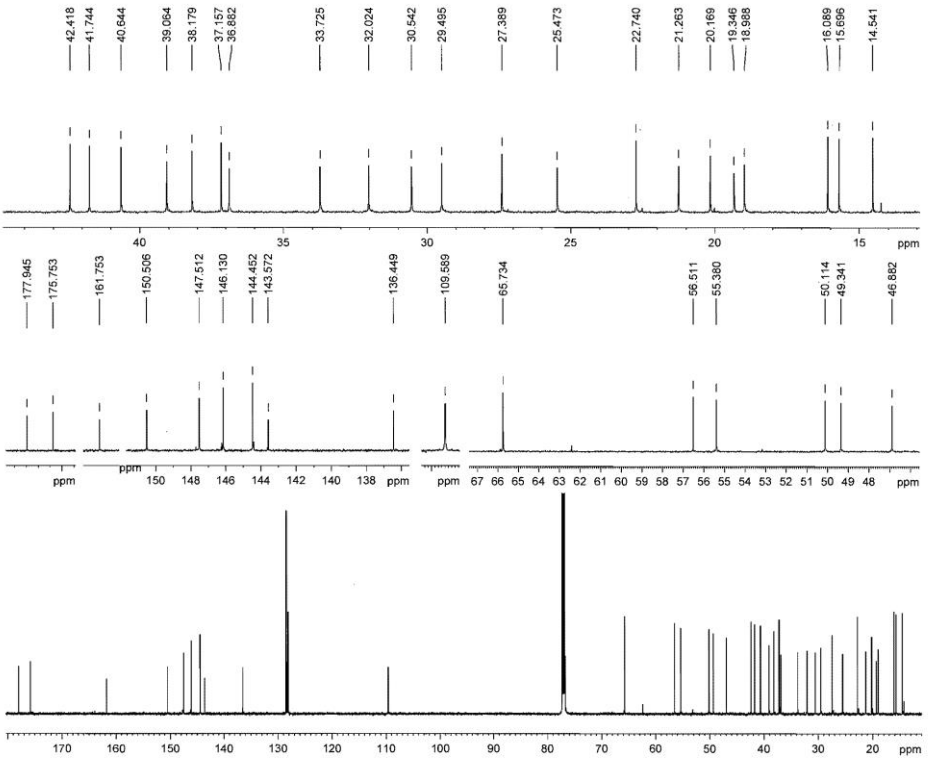
PC 1.00

62335



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31.03.2022 DA

Current Data Parameters
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EXPNO 2
PROCNO 1

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TD 59520
SOLVENT CDCl3
NS 1024
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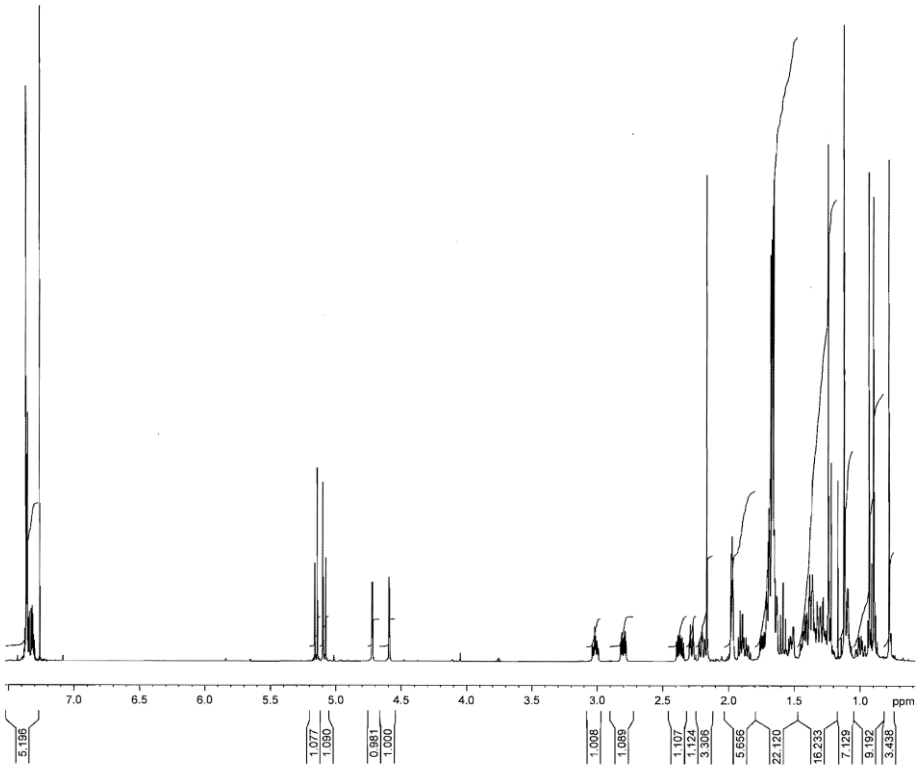
SWH 29761.904 Hz
FIDRES 1.000064 Hz
AQ 0.9999360 sec
RG 196.18
DW 16.800 usec
DE 18.00 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178993 MHz
NUC1 13C
P0 4.00 usec
P1 12.00 usec
PLW1 104.66000366 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 6.34730005 W
PLW12 0.08290300 W
PLW13 0.04170000 W

F2 - Processing parameters
SI 131072
SF 150.9028133 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

62335

1.10. Benzyl-(3*E*)-3-{[(tricyclo[3.3.1.1^{3,7}]dec-1-ylacetyl)oxy]imino}lup-20(29)-en-28-oate (**12**)

^{1}H NMR ($CDCl_3$): δ 0.78 (3H, s, H26), 0.89 (3H, d, *J*=0.6 Hz, H25), 0.93 (3H, d, *J*=0.6 Hz, H27), 1.00 (2H, dq, J_1=4.8 Hz, J_2=12.9 Hz, J_3=12.9 Hz, J_4=12.9 Hz, H12), 1.12 (3H, s, H24), 1.24 (3H, s, H23), 1.62-1.72 (10H, m, H9'+H11'), 1.67 (3H, dd, J_1=0.7 Hz, J_2=1.4 Hz, H29), 1.74 (2H, ddd, J_1=4.7 Hz, J_2=6.3 Hz, J_3=13.2 Hz, H1), 1.83-1.93 (2H, m, H7), 1.96-1.99 (2H, m, H10'), 2.16 (2H, s, H7'), 2.20 (1H, ddd, J_1=3.7 Hz, J_2=11.6 Hz, J_3=13.0 Hz, H13), 2.28 (2H, dt, J_1=3.6 Hz, J_2=3.6 Hz, J_3=13.0 Hz, H22), 2.37 (1H, ddd, J_1=6.3 Hz, J_2=11.0 Hz, J_3=15.2 Hz, H2), 2.80 (1H, ddd, J_1=4.7 Hz, J_2=6.1 Hz, J_3=15.2 Hz, H2), 3.02 (1H, dt, J_1=4.7 Hz, J_2=11.0 Hz, J_3=11.0 Hz, H19), 4.59 (1H, dq, J_1=1.4 Hz, J_2=1.4 Hz, J_3=1.4 Hz, J_4=2.3 Hz, H30), 4.72 (1H, dq, J_1=0.7 Hz, J_2=0.7 Hz, J_3=0.7 Hz, J_4=2.3 Hz, H30), 5.09 (1H, d, *J*=12.3 Hz, H1'), 5.15 (1H, d, *J*=12.3 Hz, H1'), 7.30-7.38 (5H, m, H3'-H5'). ^{13}C NMR ($CDCl_3$): δ 14.60 (q, C27), 15.70 (q, C26), 16.10 (q, C25), 19.00 (t, C11), 19.40 (q, C29), 19.80 (t, C2), 21.20 (t, C6), 22.70 (q, C24), 25.50 (t, C12), 27.20 (q, C23), 28.60 (d, C10'), 29.50 (t, C15), 30.50 (t, C21), 32.00 (t, C22), 32.90 (s, C8'), 33.80 (t, C16), 36.70 (t, C11'), 36.90 (t, C7), 37.10 (s, C10), 38.20 (d, C13), 39.10 (t, C1), 40.70 (s, C4), 41.40 (s, C8), 42.40 (s, C14), 42.40 (t, C9'), 46.90 (d, C19), 47.60 (t, C7'), 49.40 (d, C18), 50.10 (d, C9), 55.50 (d, C5), 56.50 (s, C17), 65.70 (t, C1'), 109.60 (t, C30), 128.10 (d, C5'), 128.20 (d, C4'), 128.50 (d, C3'), 136.50 (s, C2'), 150.60 (s, C20), 169.30 (s, C3), 175.10 (s, C28), 175.80 (s, C6'). MS (ES): *m/z* = 736.2 $[M+H]^+$.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07.03.2022 DA
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PROCNO 1
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FIDRES 0.250008 Hz
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RG 16.14
DW 104.267 usec
DE 10.00 usec
TE 298.2 K
D1 0 sec
TD0 1
SFO1 600.1324003 MHz
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P0 2.67 usec
P1 8.00 usec
PLW1 6.34730005 W
F2 - Processing parameters
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LB 0 Hz
GB 0
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16.233
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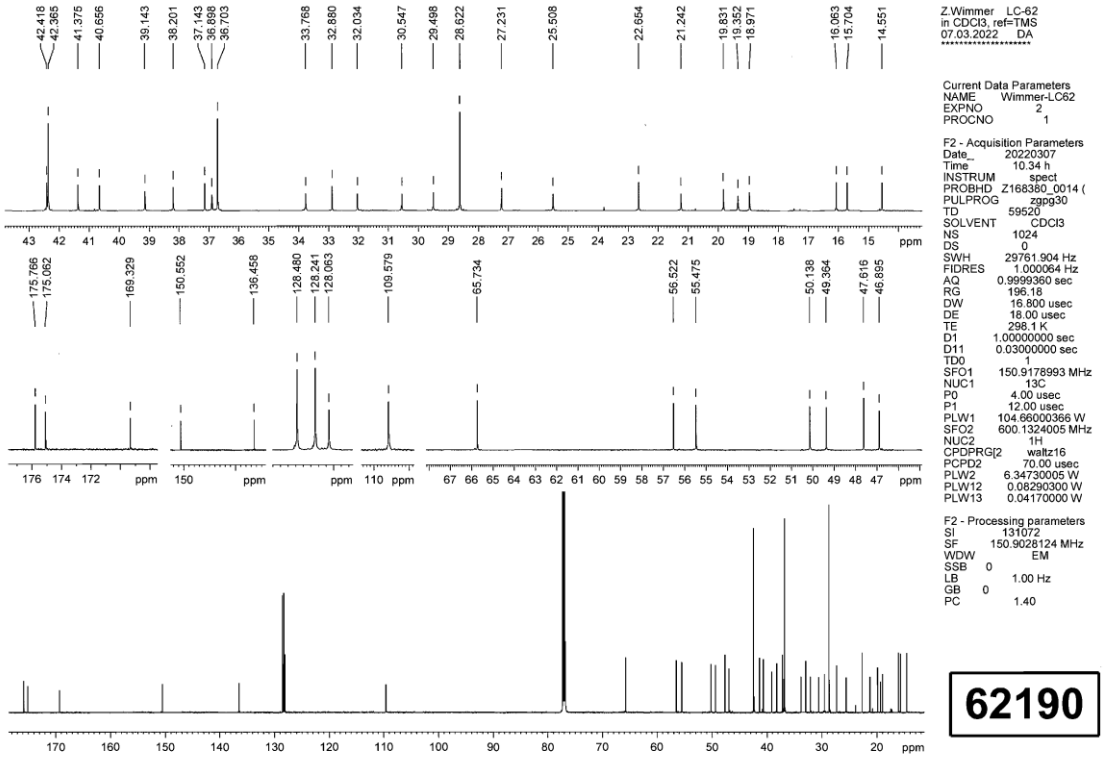
3.438
62190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46.895
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in CDCl3, ref=TMS
07.03.2022 DA
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PROCNO 1
F2 - Acquisition Parameters
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SOLVENT CDCl3
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FIDRES 1.000064 Hz
AQ 0.9999360 sec
RG 196.18
DW 16.800 usec
DE 18.00 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178993 MHz
NUC1 13C
P0 4.00 usec
P1 12.00 usec
PLW1 104.66000366 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 6.34730005 W
PLW12 0.08290300 W
PLW13 0.04170000 W
F2 - Processing parameters
SI 131072
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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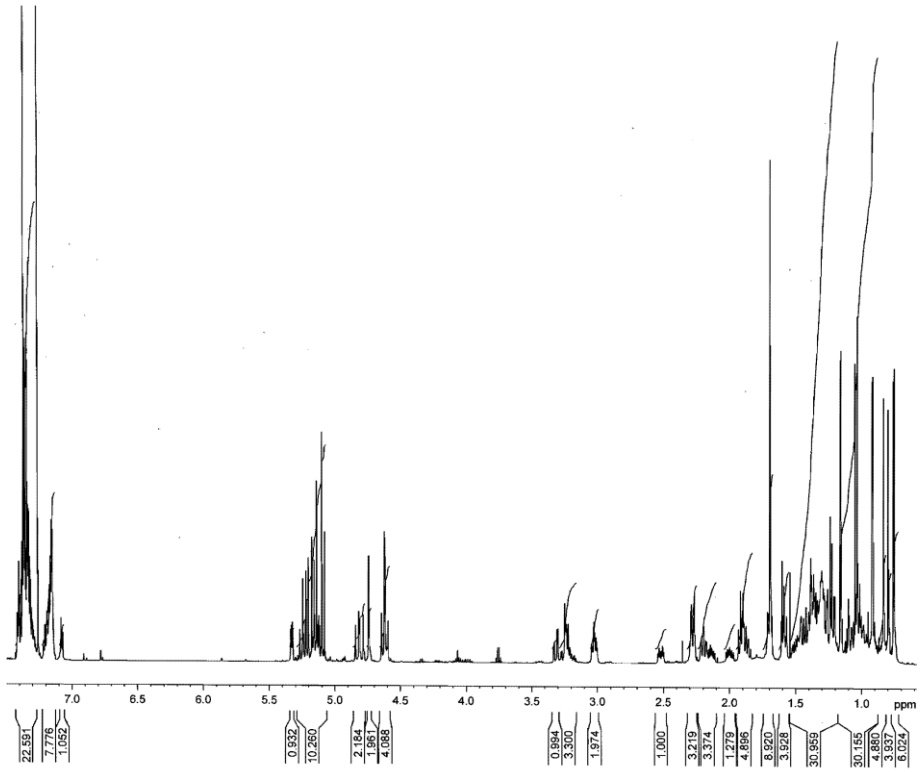
176 174 172 ppm
150 ppm
110 ppm
67 66 65 64 63 62 61 60 59 58 57 56 55 54 53 52 51 50 49 48 47 ppm
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
62190

1.11. Benzyl-(3*E*)-3-{[({(3*S*)-2-[(benzyloxy)carbonyl]-1,2,3,4-tetrahydroisoquinolin-3-yl}carbonyl)oxy]imino}lup-20(29)-en-28-oate (**13**)

^{1}H NMR ($CDCl_3$): δ 0.75 (3H, s, H26), 0.80 (3H, s, H25), 0.91 (3H, s, H27), 1.03 (3H, s, H24), 1.16 (3H, s, H23), 1.59 (2H, dt, J_1=1.3 Hz, J_2=11.4 Hz, H1), 1.69 (3H, dd, J_1=0.7 Hz, J_2=1.4 Hz, H29), 1.87 (2H, m, H7), 1.89 (2H, m, H21), 2.00 (1H, ddd, J_1=6.2 Hz, J_2=11.1 Hz, J_3=15.1 Hz, H2), 2.21 (1H, ddd, J_1=3.7 Hz, J_2=11.8 Hz, J_3=12.9 Hz, H13), 2.26-2.30 (2H, m, H22), 2.52 (1H, ddd, J_1=4.5 Hz, J_2=6.5 Hz, J_3=15.1 Hz, H2), 3.03 (1H, dt, J_1=4.7 Hz, J_2=11.0 Hz, J_3=11.0 Hz, H19), 3.23 (1H, dd, J_1=6.2 Hz, J_2=16.0 Hz, H11'), 3.32 (1H, dd, J_1=3.1 Hz, J_2=16.0 Hz, H11'), 4.62 (1H, dq, J_1=1.4 Hz, J_2=1.4 Hz, J_3=1.4 Hz, J_4=2.4 Hz, H30), 4.63 (1H, d, *J*=16.3 Hz, H4'), 4.74 (1H, dq, J_1=0.7 Hz, J_2=0.7 Hz, J_3=0.7 Hz, J_4=2.4 Hz, H30), 4.83 (1H, d, *J*=16.3 Hz, H4'), 5.09 (1H, d, *J*=12.2 Hz, H18'), 5.16 (1H, d, *J*=12.2 Hz, H18'), 5.21 (1H, d, *J*=12.2 Hz, H13'), 5.26 (1H, d, *J*=12.2 Hz, H13'), 5.33 (1H, dd, J_1=3.1 Hz, J_2=6.2 Hz, H2'), 7.31-7.44 (3H, m, H15'-H17'), 7.31-7.44 (3H, m, H20'-H22'). ^{13}C NMR ($CDCl_3$): δ 14.50 (q, C27), 15.70 (q, C26), 15.90 (q, C25), 18.90 (t, C11), 19.40 (q, C29), 19.50 (t, C2), 21.20 (t, C6), 22.50 (q, C24), 25.50 (t, C12), 27.00 (q, C23), 29.50 (t, C15), 30.60 (t, C21), 31.00 (t, C11'), 32.00 (t, C22), 33.70 (t, C16), 36.90 (t, C7), 37.00 (s, C10), 38.20 (d, C13), 39.00 (t, C1), 40.60 (s, C4), 41.50 (s, C8), 42.40 (s, C14), 44.40 (t, C4'), 46.90 (d, C19), 49.40 (d, C18), 50.00 (d, C9), 52.70 (d, C2'), 55.40 (d, C5), 56.50 (s, C17), 65.70 (t, C18'), 67.60 (t, C13'), 73.60 (d, C9'), 109.60 (t, C30), 126.20 (d, C6'), 126.80 (d, C7'), 127.90 (d, C22'), 128.00 (d, C17'), 128.20 (d, C16'), 128.20 (d, C21'), 128.50 (d, C15'), 128.50 (d, C20'), 128.60 (d, C8'), 131.50 (s, C5'), 133.10 (s, C10'), 136.30 (s, C14'), 136.40 (s, C19'), 150.60 (s, C20), 155.40 (s, C12'), 168.80 (s, C3), 175.80 (s, C28), 176.90 (s, C1'). MS (ES): *m/z* = 853.8 $[M+H]^+$.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28.03.2022 DA
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SOLVENT CDCl3
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FIDRES 0.250008 Hz
AQ 3.9998779 sec
RG 16.14
DW 104.267 usec
DE 10.00 usec
TE 298.2 K
D1 0 sec
TD0 1
SFO1 600.1324005 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
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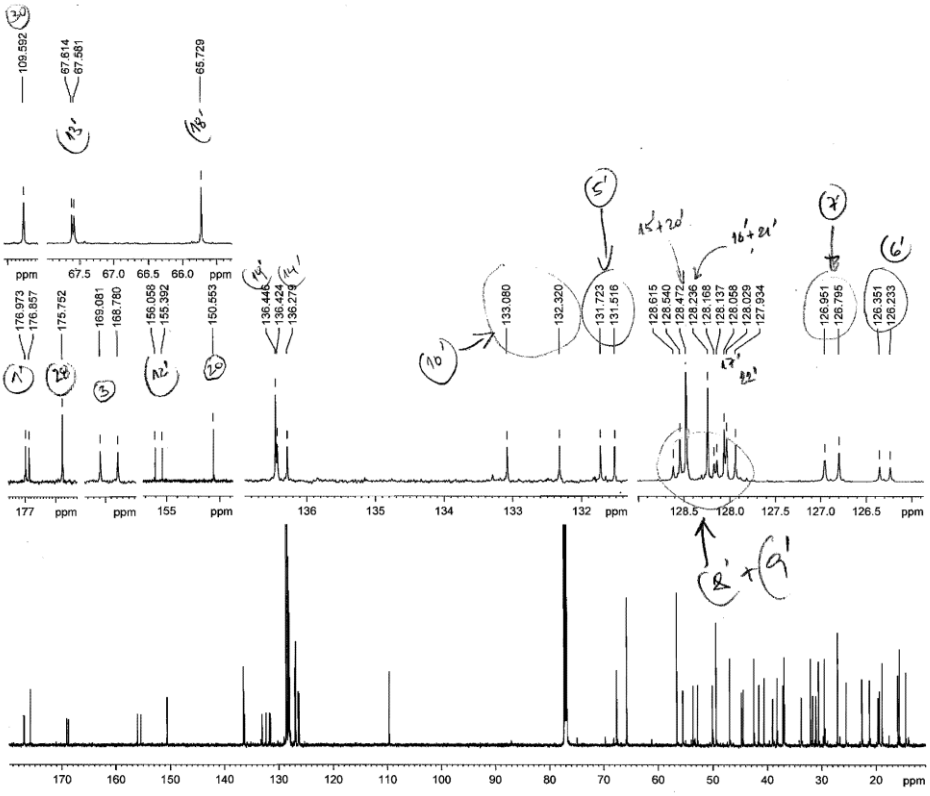
SSB 0
LB 0 Hz
GB 0
PC 1.00
62299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28.03.2022 DA
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SOLVENT CDCl3
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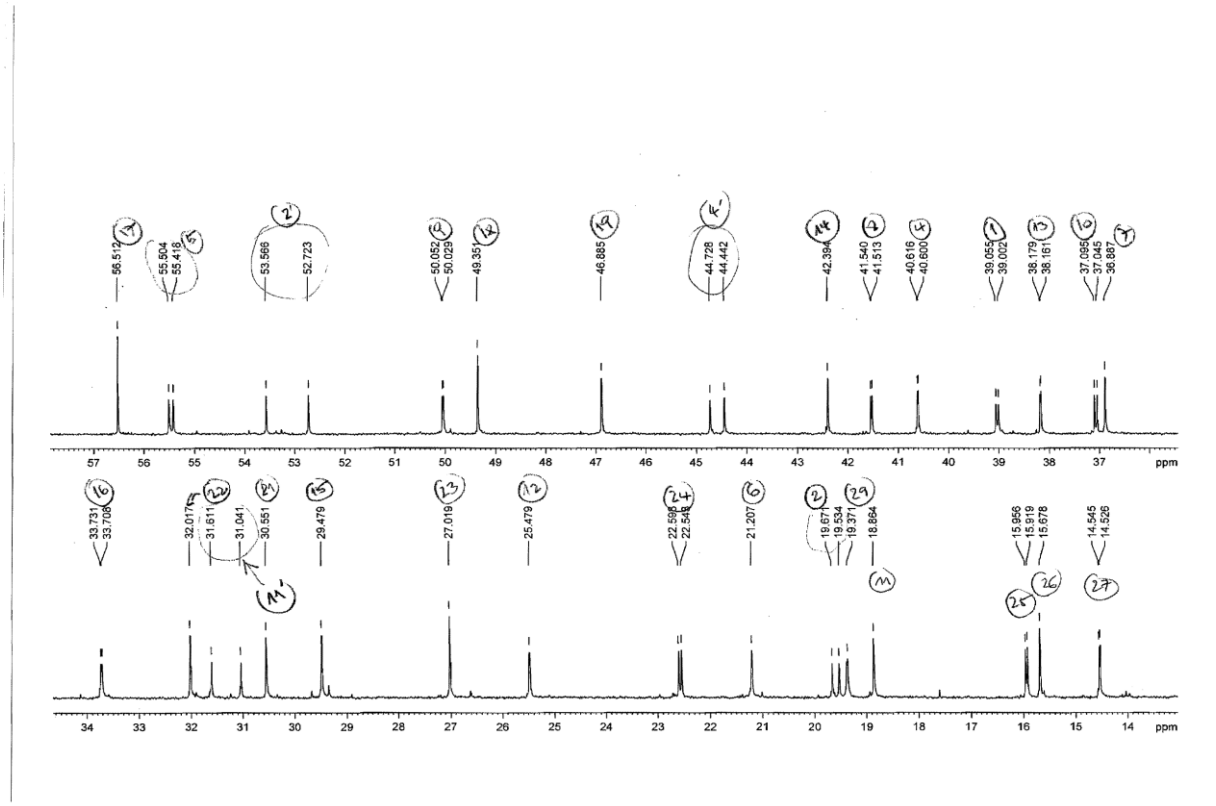
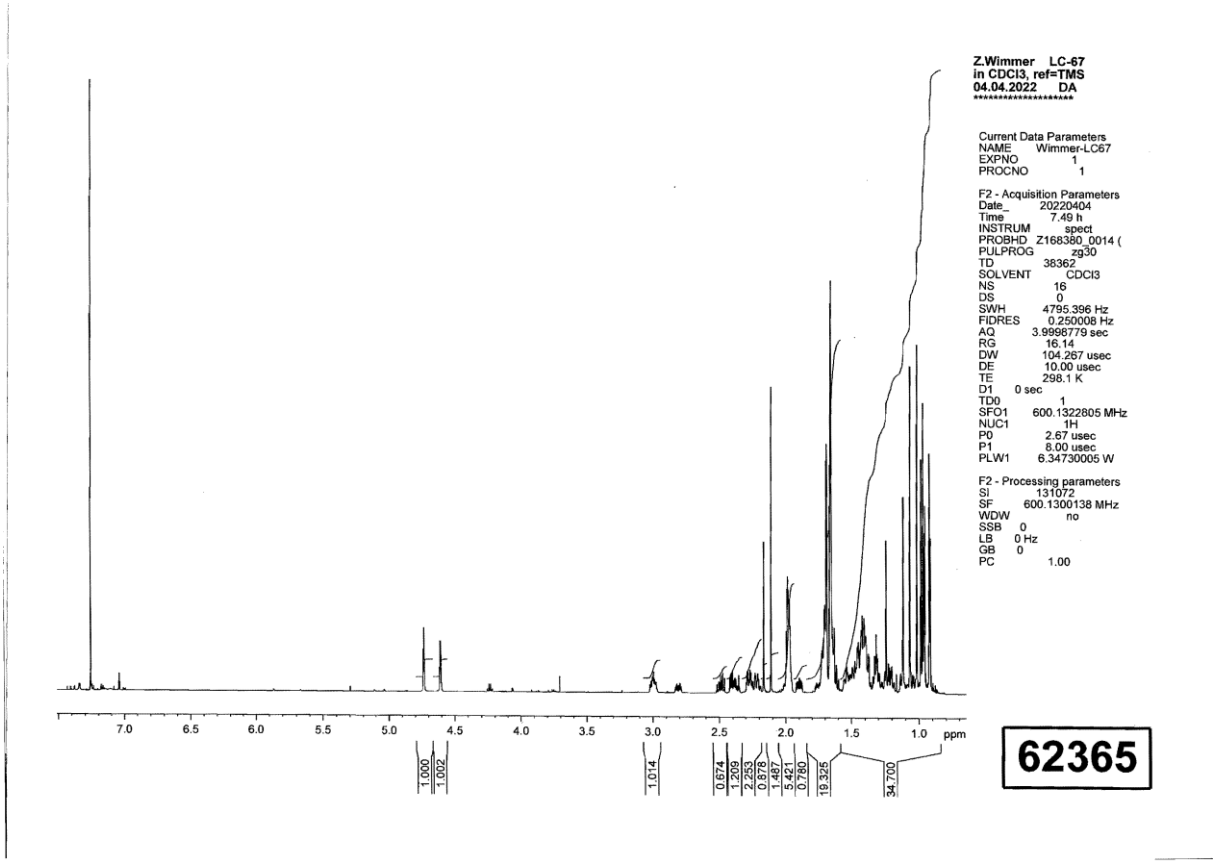
62299

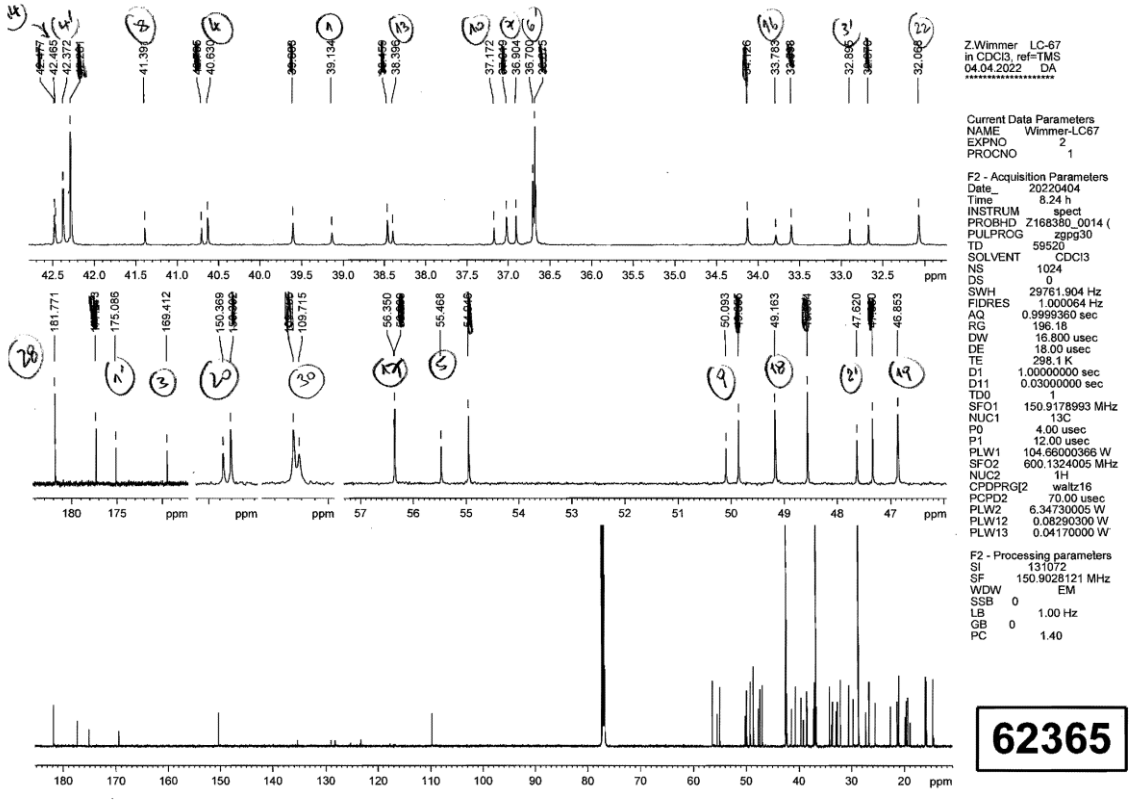


1.12. (3*E*)-3-{[(Tricyclo[3.3.1.1^{3,7}]dec-1-ylacetyl)oxy]imino}lup-20(29)-en-28-oic acid (**14**)

^{1}H NMR ($CDCl_3$): δ 0.92 (3H, d, *J*=0.7 Hz, H26), 0.95 (3H, s, H25), 0.98 (3H, d, *J*=0.7 Hz, H27), 1.12 (3H, s, H24), 1.24 (3H, s, H23), 1.65-1.68 (2H, m, H4'), 1.65-1.68 (1H, m, H5'), 1.69 (3H, dd, J_1=0.7 Hz, J_2=1.4 Hz, H29), 1.90 (2H, ddd, J_1=4.6 Hz, J_2=6.4 Hz, J_3=13.4 Hz, H1), 1.95-2.00 (4H, m, H7+H21), 1.95-2.00 (2H, m, H6'), 2.12 (2H, s, H2'), 2.22 (1H, ddd, J_1=3.6 Hz, J_2=11.6 Hz, J_3=13.0 Hz, H13), 2.27 (2H, dt, J_1=3.8 Hz, J_2=3.8 Hz, J_3=13.0 Hz, H22), 2.38 (1H, ddd, J_1=6.4 Hz, J_2=10.8 Hz, J_3=15.2 Hz, H2), 2.81 (1H, ddd, J_1=4.6 Hz, J_2=6.0 Hz, J_3=15.2 Hz, H2), 3.00 (1H, dt, J_1=4.6 Hz, J_2=11.0 Hz, J_3=11.0 Hz, H19), 4.61 (1H, dq, J_1=1.4 Hz, J_2=1.4 Hz, J_3=1.4 Hz, J_4=2.4 Hz, H30), 4.74 (1H, dq, J_1=0.7 Hz, J_2=0.7 Hz, J_3=0.7 Hz, J_4=2.4 Hz, H30). ^{13}C NMR ($CDCl_3$): δ 14.60 (q, C27), 15.90 (q, C26), 16.10 (q, C25), 19.00 (t, C11), 19.30 (q, C29), 19.60 (t, C2), 21.20 (t, C6), 22.60 (q, C24), 25.50 (t, C12), 27.20 (q, C23), 28.60 (d, C5'), 29.60 (t, C15), 30.50 (t, C21), 32.10 (t, C22), 32.90 (s, C3'), 33.80 (t,

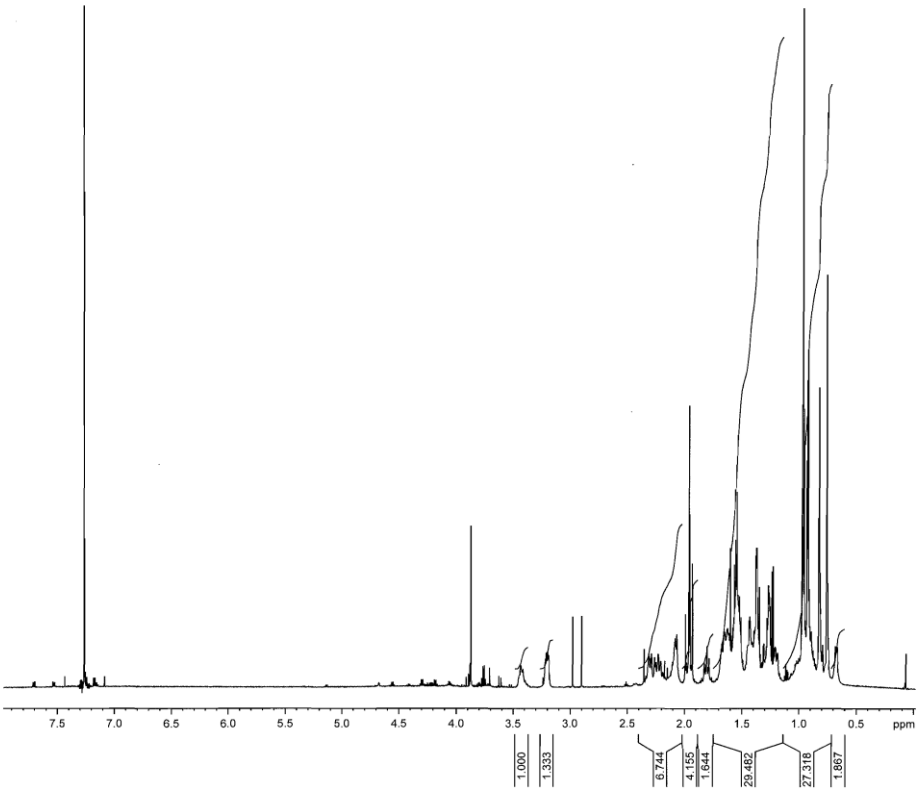
C16), 36.70 (t, C6'), 36.90 (t, C7), 37.20 (s, C10), 38.40 (d, C13), 39.10 (t, C1), 40.60 (s, C4), 41.40 (s, C8), 42.40 (t, C4'), 42.50 (s, C14), 46.90 (d, C19), 47.60 (t, C2'), 49.20 (d, C18), 50.10 (d, C9), 55.50 (d, C5), 56.40 (s, C17), 109.70 (t, C30), 150.40 (s, C20), 169.40 (s, C3), 175.10 (s, C1'), 181.80 (s, C28). MS (ES): *m/z* = 646.4 $[M+H]^+$, 644.4 $[M-H]^-$.





1.13. (3β)-3-Hydroxy-20-hydroximino-29-norlupan-28-oic acid (**15**)

^{1}H NMR ($CDCl_3$): δ 0.67 (1H, bd, *J*=10.8 Hz, H5), 0.75 (3H, s, H24), 0.82 (3H, s, H26), 0.93 (3H, s, H25), 0.96 (3H, s, H23), 0.96 (3H, s, H27), 1.80 (1H, t, *J*=11.5 Hz, H18), 2.30 (2H, dt, J_1=3.3 Hz, J_2=3.3 Hz, J_3=12.9 Hz, H16), 2.33 (1H, ddd, J_1=3.5 Hz, J_2=11.5 Hz, J_3=13.0 Hz, H13), 3.20 (1H, dd, J_1=5.6 Hz, J_2=11.2 Hz, H3), 3.43 (1H, dt, J_1=4.4 Hz, J_2=10.5 Hz, J_3=10.5 Hz, H19). ^{13}C NMR ($CDCl_3$): δ 13.10 (q, C29), 14.60 (q, C27), 15.40 (q, C24), 16.00 (q, C25), 16.10 (q, C26), 18.30 (t, C6), 20.70 (t, C11), 25.70 (t, C12), 27.30 (t, C2), 28.00 (q, C23), 28.40 (t, C15), 29.40 (t, C21), 31.90 (t, C16), 34.20 (t, C22), 37.00 (t, C7), 37.20 (s, C10), 37.80 (d, C13), 38.70 (s, C4), 38.80 (t, C1), 40.70 (s, C8), 42.30 (s, C14), 44.50 (d, C19), 49.60 (d, C18), 50.40 (d, C9), 55.30 (d, C5), 55.90 (s, C17), 79.10 (d, C3), 170.40 (s, C20), 180.90 (s, C28). MS (ES): *m/z* = 474.3 $[M+H]^+$, 472.2 $[M-H]^-$.



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10.03.2022 DA
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F2 - Processing parameters
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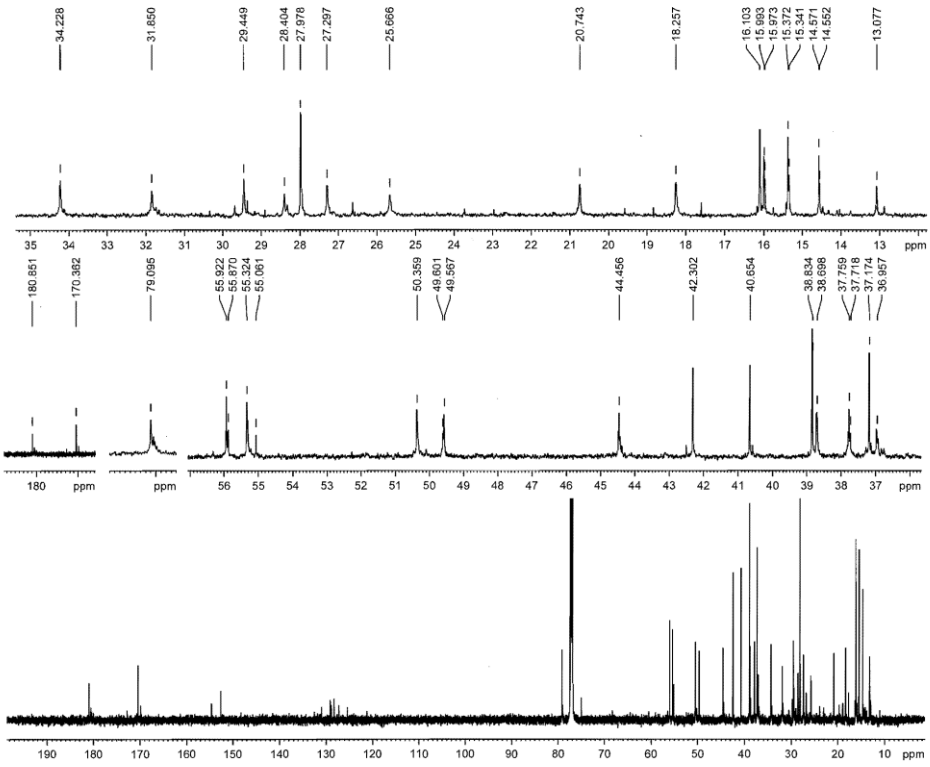
62209



Z.Wimmer LC-28
in CDCl3, ref=TMS
10.03.2022 DA
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Current Data Parameters
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PROCNO 1

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SOLVENT CDCl3
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SWH 29761.904 Hz
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AQ 0.9999360 sec
RG 196.18
DW 16.800 usec
DE 18.00 usec
TE 298.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178993 MHz
NUC1 13C
P0 4.00 usec
P1 12.00 usec
PLW1 104.66000366 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 6.34730005 W
PLW12 0.08290300 W
PLW13 0.04170000 W

F2 - Processing parameters
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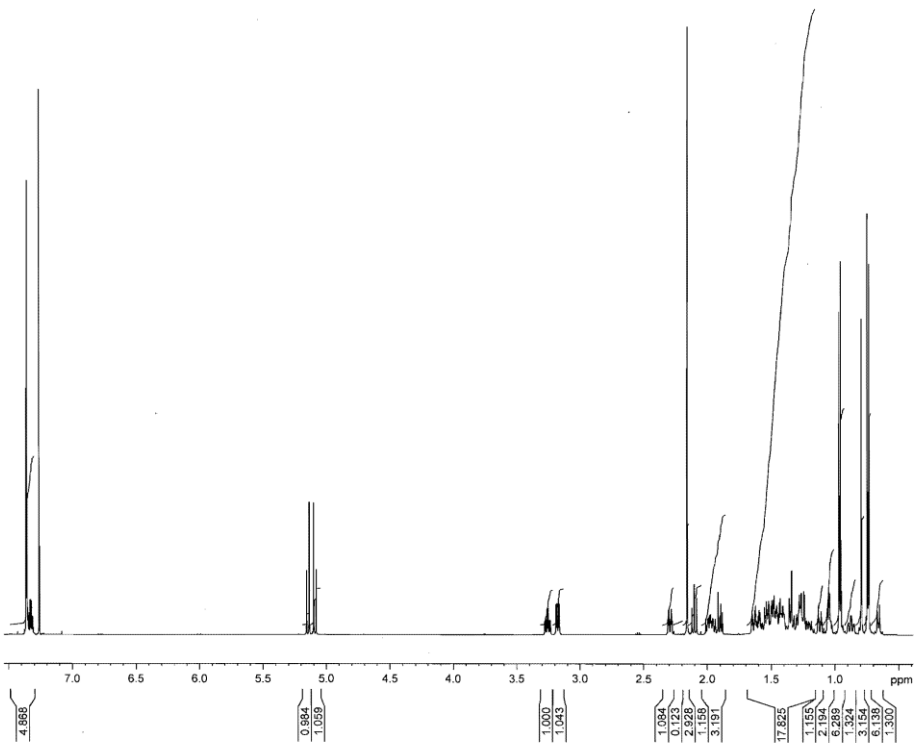
SF 150.9028125 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

62209

1.14. Benzyl-(3β)-3-hydroxy-20-oxo-29-norlupan-28-oate (**16**)

^{1}H NMR ($CDCl_3$): δ 0.66 (1H, dd, J_1=2.0 Hz, J_2=11.4 Hz, H5), 0.73 (3H, s, H27), 0.75 (3H, s, H23), 0.79 (3H, d, J=0.7 Hz, H25), 0.87 (1H, dt, J_1=4.0 Hz, J_2=13.0 Hz, J_3=13.0 Hz, H1), 0.95 (3H, s, H24), 0.97 (3H, d, J=0.7 Hz, H26), 1.12 (2H, dt, J_1=3.4 Hz, J_2=3.4 Hz, J_3=13.7 Hz, H15), 1.64 (1H, dt, J_1=3.5 Hz, J_2=3.5 Hz, J_3=13.1 Hz, H1), 2.10 (1H, dd, J_1=11.0 Hz, J_2=11.7 Hz, H18), 2.16 (3H, s, H29), 2.29 (2H, ddd, J_1=3.1 Hz, J_2=3.7 Hz, J_3=13.1 Hz, H16), 3.18 (1H, dd, J_1=4.6 Hz, J_2=11.6 Hz, H3), 3.26 (1H, dt, J_1=4.9 Hz, J_2=11.2 Hz, J_3=11.2 Hz, H19), 5.09 (1H, d, J=12.2 Hz, H1'), 5.15 (1H, d, J=12.2 Hz, H1'), 7.30-7.38 (3H, m, H3'-H5'). ^{13}C NMR ($CDCl_3$): δ 14.70 (q, C27), 15.30 (q, C24), 15.70 (q, C26), 16.10 (q, C25), 18.30 (t, C6), 20.90 (t, C11), 27.30 (t, C12), 27.40 (t, C2), 28.00 (q, C23), 28.20 (t, C21), 29.60 (t, C15), 30.20 (q, C29), 31.40 (t, C16), 34.20 (t, C7), 36.60 (t, C22), 37.20 (s, C10), 37.20 (d, C13), 38.70 (s, C4), 38.80 (t, C1), 40.50 (s, C8), 42.20 (s, C14), 49.40 (d, C18), 50.40 (d, C9), 51.10 (d, C19), 55.30 (d, C5), 56.40 (s, C17), 65.90 (t, C1'), 78.90 (d, C3), 128.20 (d, C5'), 128.30 (d, C4'), 128.50 (d, C3'), 136.30 (s, C2'), 175.70 (s, C28), 212.30 (s, C20). MS (ES): *m/z* = 549.4 $[M+H]^+$.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GB 0
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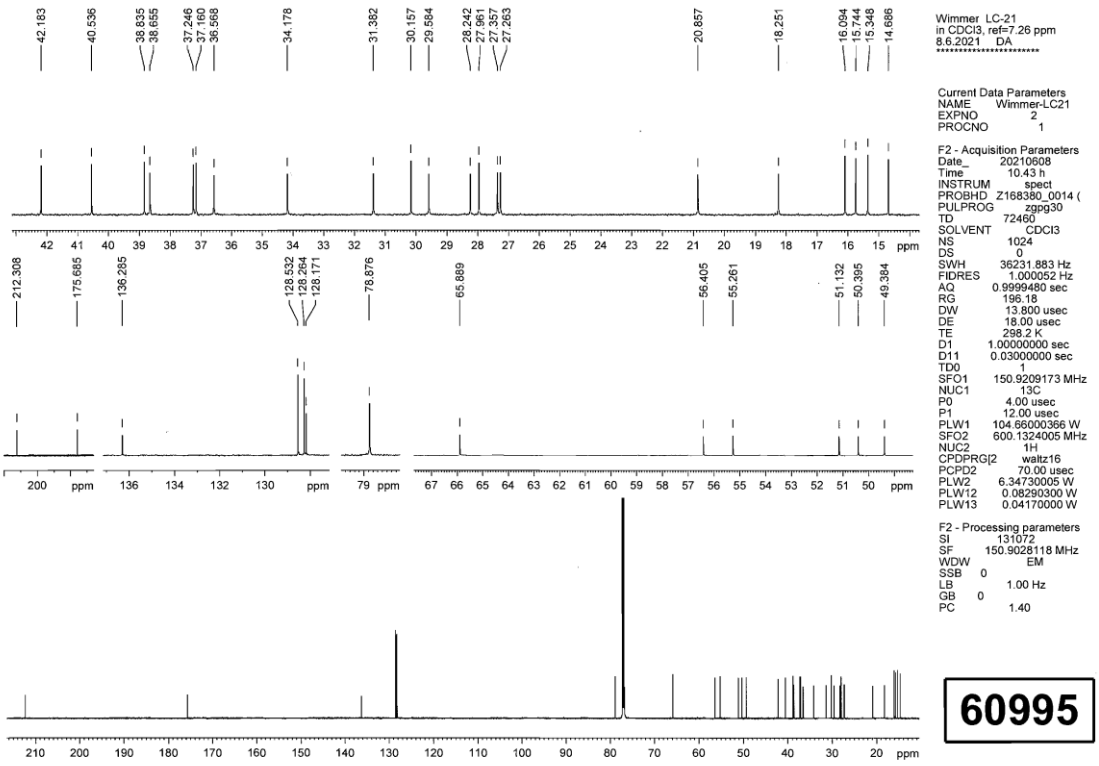
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8.6.2021 DA
Current Data Parameters
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PROCNO 1
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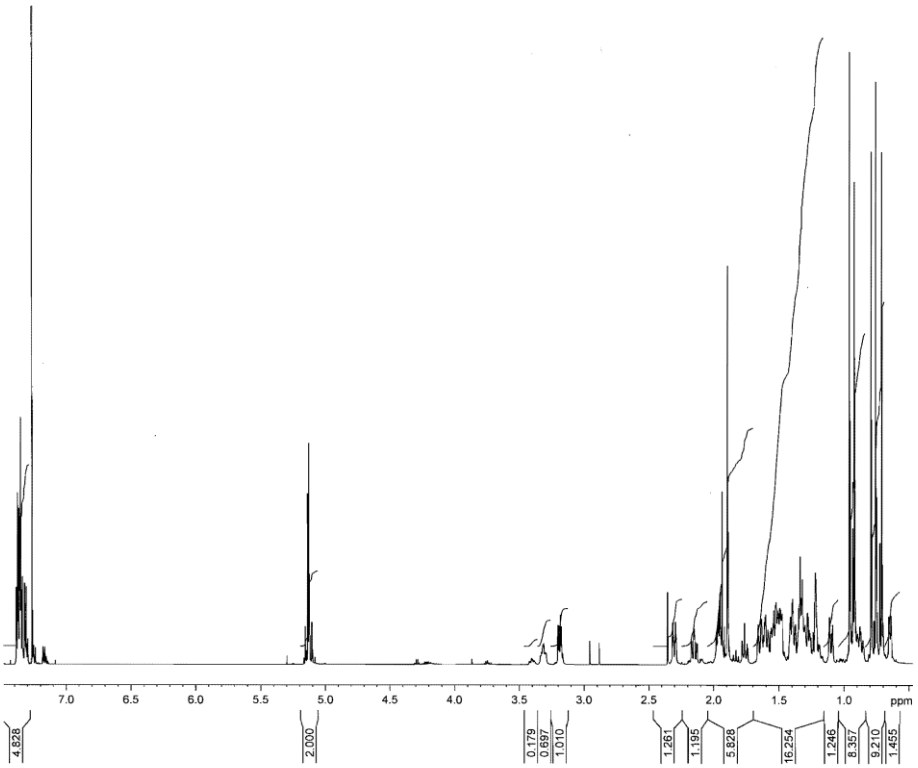
D11 0.03000000 sec
TD0 1
SFO1 150.9209173 MHz
NUC1 13C
P0 4.00 usec
P1 12.00 usec
PLW1 104.66000366 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 6.34730005 W
PLW12 0.08290300 W
PLW13 0.04170000 W
F2 - Processing parameters
SI 131072
SF 150.9028118 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
60995

1.5 Benzyl-(3β)-3-hydroxy-20-hydroximino-29-norlupan-28-oate (**17**)

^{1}H NMR ($CDCl_3$): δ 0.65 (1H, dd, J_1=2.2 Hz, J_2=11.5 Hz, H5), 0.71 (3H, s, H25), 0.75 (3H, s, H24), 0.79 (3H, s, H26), 0.92 (3H, s, H27), 0.95 (3H, s, H23), 1.10 (2H, dt, J_1=3.3 Hz, J_2=3.3 Hz, J_3=13.4 Hz, H21), 1.77 (1H, t, J=11.3 Hz, H18), 1.89 (3H, s, H29), 2.15 (1H, ddd, J_1=3.6 Hz, J_2=11.7 Hz, J_3=13.0 Hz, H13), 2.30 (2H, dt, J_1=3.2 Hz, J_2=3.2 Hz, J_3=12.5 Hz, H16), 3.19 (1H, dd, J_1=4.8 Hz, J_2=11.3 Hz, H3), 3.32 (1H, dt, J_1=3.7 Hz, J_2=10.5 Hz, J_3=10.5 Hz, H19), 5.12 (1H, d, J=12.2 Hz, H1'), 5.14 (1H, d, J=12.2 Hz, H1'), 7.29-7.40 (5H, m, H3'+H4'+H5'). ^{13}C NMR ($CDCl_3$): δ 11.90 (q, C29), 14.50 (q, C27), 15.40 (q, C24), 15.70 (q, C25), 16.00 (q, C26), 18.20 (t, C6), 20.80 (t, C11), 25.90 (t, C12), 27.30 (t, C2), 28.00 (q, C23), 28.60 (t, C15), 29.30 (t, C21), 31.90 (t, C16), 34.20 (t, C22), 36.80 (t, C7), 37.10 (s, C10), 37.70 (d, C13), 38.80 (t, C1), 38.80 (s, C4), 40.60 (s, C8), 42.30 (s, C14), 44.50 (d, C19), 50.10 (d, C18), 50.30 (d, C9), 55.30 (d, C5), 56.10 (s, C17), 65.90 (t, C1'), 79.00 (d, C3), 128.20 (d, C5'), 128.50 (d, C3'), 128.50 (d, C4'), 136.20 (s, C2'), 164.40 (s, C20), 175.20 (s, C28). MS (ES): *m/z* = 564.2 $[M+H]^+$, 562.2 $[M-H]^-$.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10.03.2022 DA
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PROCNO 1
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TD 38362
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RG 16.14
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TE 298.2 K
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TD0 1
SFO1 600.1324003 MHz
NUC1 1H
P0 2.67 usec
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PLW1 6.34730005 W
F2 - Processing parameters
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SF 600.1300136 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
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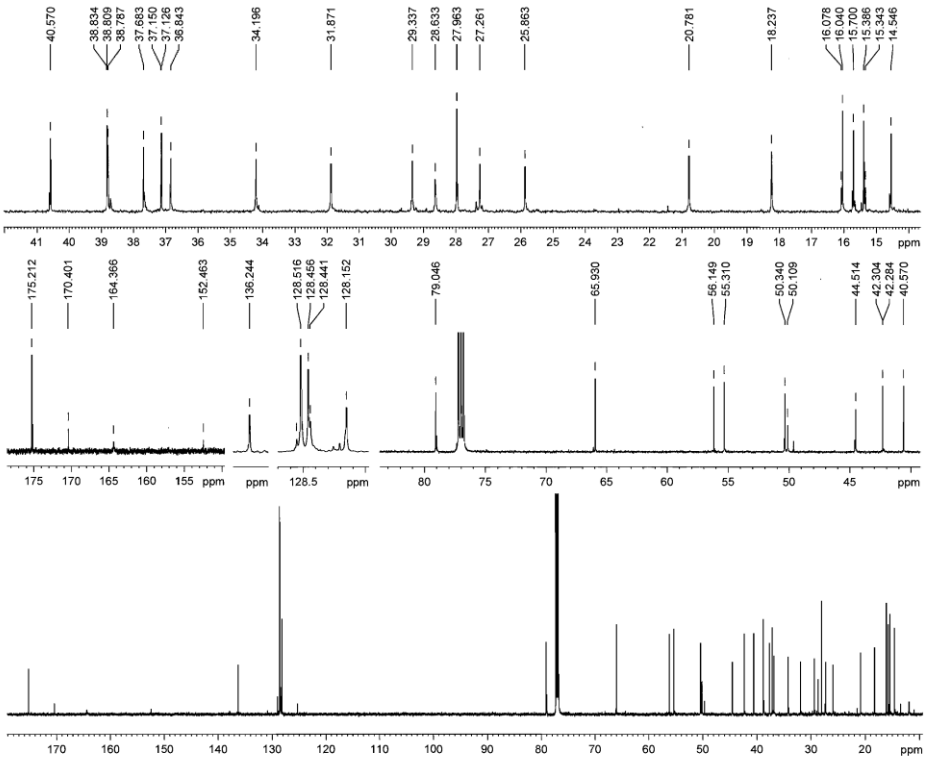
62210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10.03.2022 DA
Current Data Parameters
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PROCNO 1
F2 - Acquisition Parameters
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Time 8.30 h
INSTRUM spect
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FIDRES 1.000064 Hz
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RG 196.18
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D11 0.03000000 sec
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SFO1 150.9178993 MHz
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PLW1 104.66000366 W
SFO2 600.1324005 MHz
NUC2 1H
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F2 - Processing parameters
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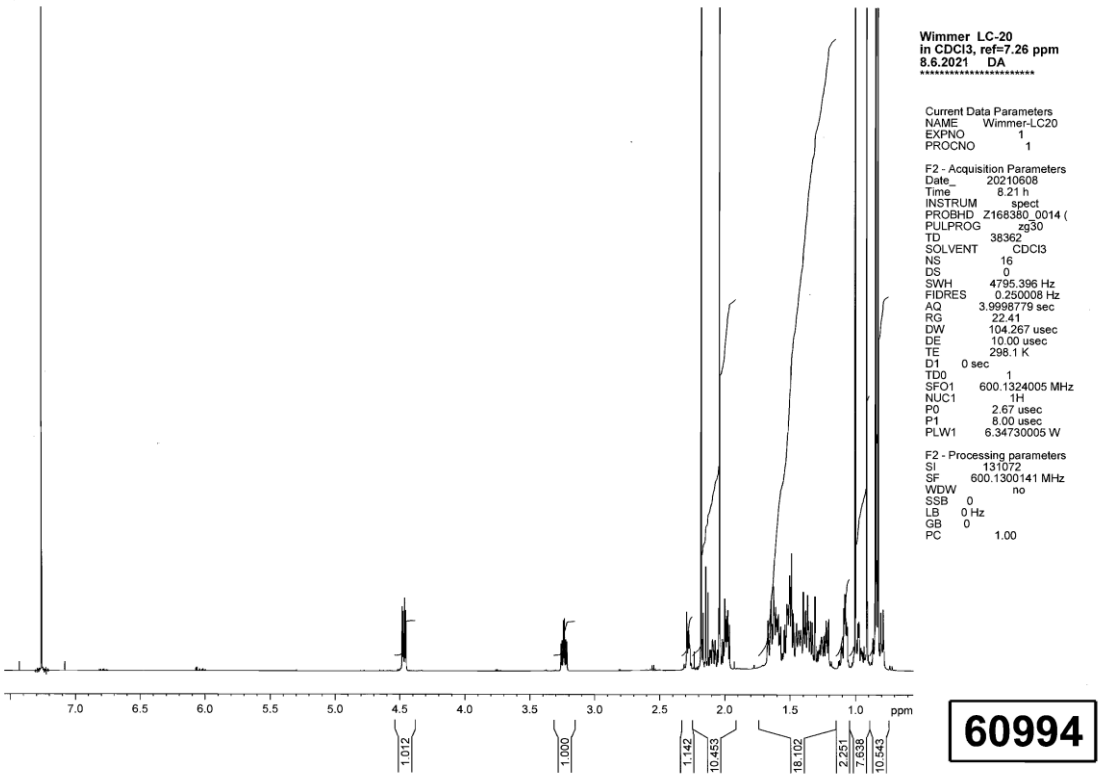
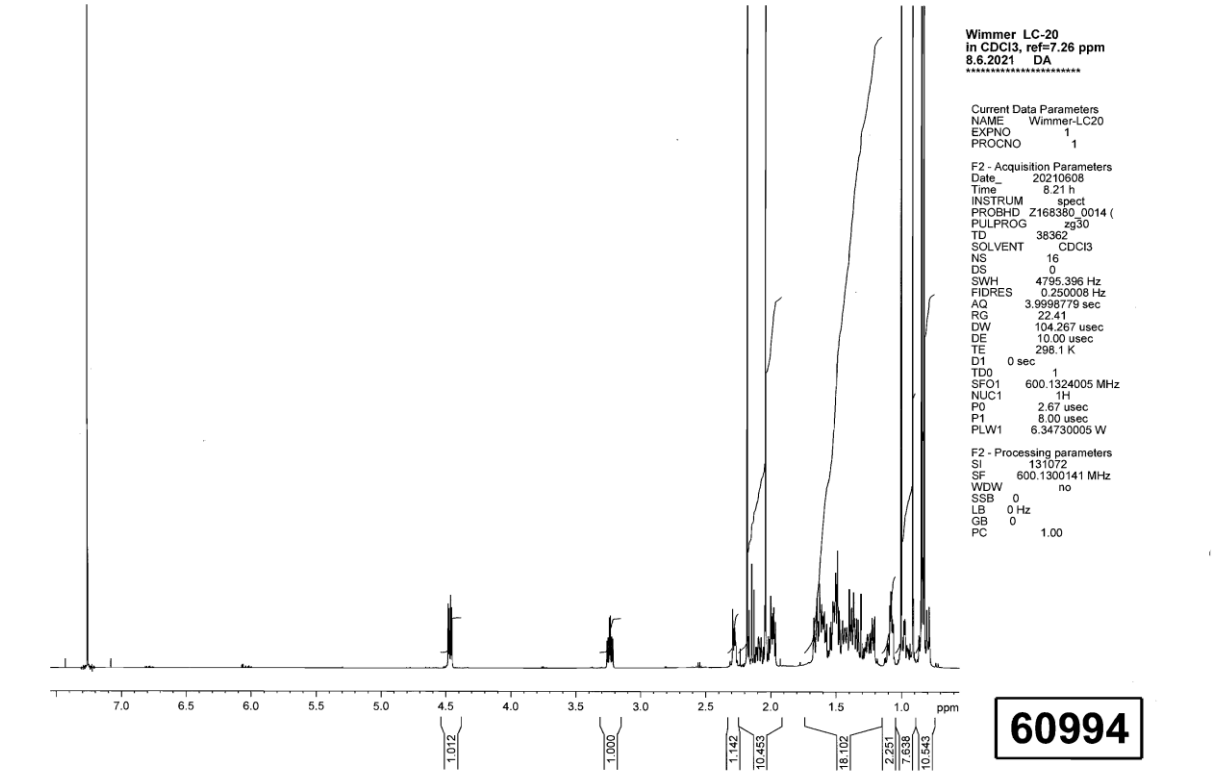
SF 150.9028128 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
62210

3.16. (3β)-3-(Acetyloxy)-20-oxo-29-norlupan-28-oic acid (**18**)

^{1}H NMR ($CDCl_3$): δ 0.80 (1H, dd, J_1=2.0 Hz, J_2=11.3 Hz, H5), 0.83 (3H, s, H23), 0.84 (3H, s, H25), 0.85 (3H, s, H26), 0.91 (3H, s, H24), 1.60 (3H, s, H27), 2.04 (3H, s, OAc), 2.15 (1H, t, *J*=11.3 Hz, H18), 2.18 (3H, s, H29), 2.26-2.30 (2H, m, H16), 3.24 (1H, dt, J_1=5.0 Hz, J_2=11.4 Hz, J_3=11.4 Hz, H19), 4.47 (1H, dd, J_1=4.8 Hz, J_2=11.4 Hz, H3). ^{13}C NMR ($CDCl_3$): δ 14.70 (q, C27), 15.90 (q, C24), 16.20 (q, C26), 16.50 (q, C25), 18.10 (t, C6), 20.80 (t, C11), 21.30 (q, C2'), 23.60 (t, C2), 27.20 (t, C12), 27.90 (q, C23), 28.20 (t, C21), 29.70 (t, C15), 30.10 (q, C29), 31.40 (t, C16), 34.10 (t, C7), 36.70 (t, C22), 37.10 (s, C10), 37.50 (d, C13), 37.80 (s, C4), 38.30 (t, C1), 40.60 (s, C8), 42.20 (s, C14), 49.20 (d, C18), 50.20 (d, C9), 51.20 (d, C19), 55.30 (d, C5), 56.20 (s, C17), 80.80 (d, C3), 171.00 (s, C1'), 180.70 (s, C28), 212.10 (s, C20). MS (ES): *m/z* = 501.4 $[M+H]^+$, 499.3 $[M-H]^-$.

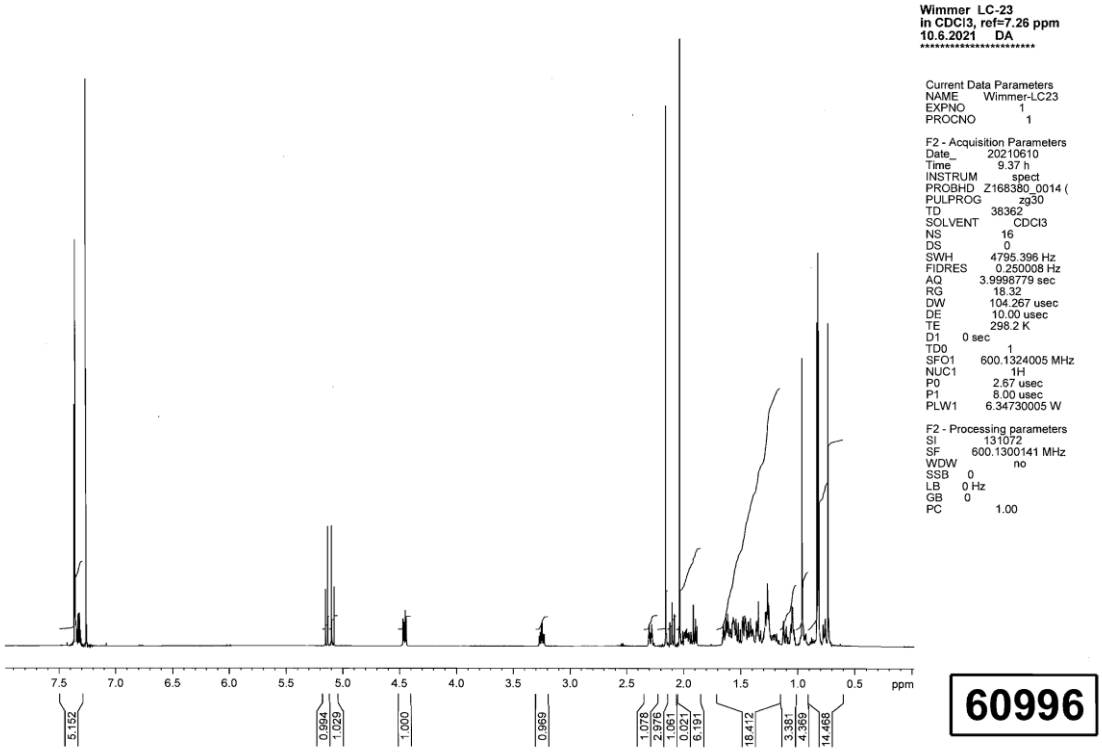


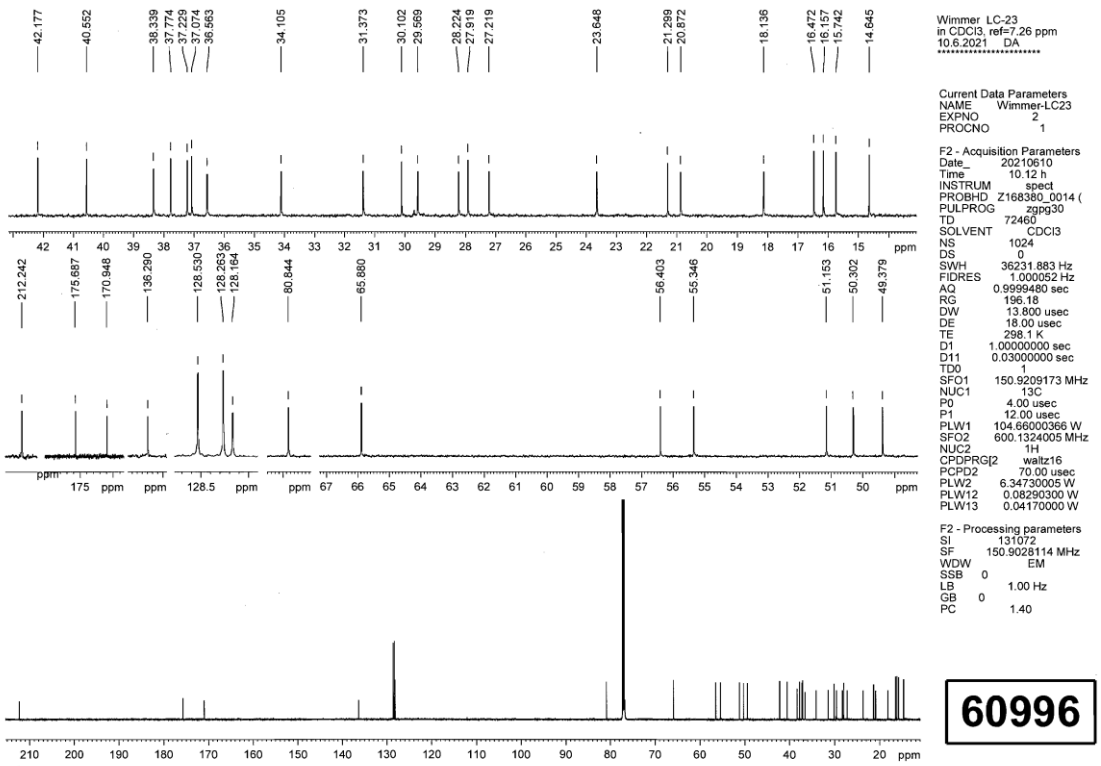


3.17. Benzyl-(3β)-3-(acetyloxy)-20-oxo-29-norlupan-28-oate (**19**)

^{1}H NMR ($CDCl_3$): δ 0.73 (3H, s, H24), 0.76 (1H, dd, J_1=2.1 Hz, J_2=11.5 Hz, H5), 0.82 (3H, d, J=0.5 Hz, H25), 0.82 (3H, s, H26), 0.83 (3H, s, H23), 0.95 (1H, dt, J_1=4.2 Hz, J_2=13.0 Hz, J_3=13.0 Hz, H1), 0.96 (3H, d, J=0.7 Hz, H27), 1.11 (2H, dt, J_1=3.4 Hz, J_2=3.4 Hz, J_3=13.7 Hz, H15), 1.64 (1H, dt, J_1=3.5 Hz, J_2=3.5 Hz, J_3=13.0 Hz, H1), 2.03 (3H, s, H2'), 2.10 (1H, dd, J_1=10.9 Hz, J_2=11.6 Hz, H18), 2.16 (3H, s, H29), 2.29 (2H, ddd, J_1=3.2 Hz, J_2=3.7 Hz, J_3=13.1 Hz, H16), 3.25 (1H, dt, J_1=4.9 Hz, J_2=11.3 Hz, J_3=11.3 Hz, H19), 4.45 (1H, dd, J_1=5.0 Hz, J_2=11.2 Hz, H3), 5.09 (1H, d, J=12.2 Hz, H3'), 5.14 (1H, d, J=12.2 Hz, H3'), 7.30-7.38 (3H, m, H5'-H7'). ^{13}C NMR ($CDCl_3$): δ 14.60 (q, C27), 15.70 (q, C24), 16.20 (q, C26), 16.50 (q, C25), 18.10 (t, C6), 20.90 (t, C11), 21.30 (q, C2'), 23.60 (t, C2), 27.20 (t, C12), 27.90 (q, C23), 28.20 (t, C21), 29.60 (t, C15), 30.10 (q, C29), 31.40 (t, C16), 34.10 (t, C7), 36.60 (t, C22), 37.10 (s, C10), 37.20 (d, C13), 37.80 (s, C4), 38.30 (t, C1), 40.60 (s, C8), 42.20 (s, C14), 49.40 (d, C18),

50.30 (d, C9), 51.20 (d, C19), 55.30 (d, C5), 56.40 (s, C17), 65.90 (t, C3'), 80.80 (d, C3), 128.20 (d, C7'), 128.30 (d, C6'), 128.50 (d, C5'), 136.30 (s, C4'), 170.90 (s, C1'), 175.70 (s, C28), 212.20 (s, C20). MS (ES): *m/z* = 591.5 $[M+H]^+$.





2. Elucidation of the oxime configuration

To elucidate the configuration of the oximes and their derivatives, we have studied the so far published results from the literature. The search has been based on the analysis of the ^{1}H and ^{13}C NMR spectra of the studied compounds. Here, we summarize the findings in ESI, Table S1 and Table S2.

Table S1. Platanic acid oxime derivatives

^{13}C NMR (δ [ppm])	**15**	**17**	Compound **14** (20*E*) taken from ref.[39]	Compound **15** (20*Z*) taken from ref.[39]
C(18)	49.6	50.1	49.7	50.4
C(19)	44.5	44.5	45.1	44.9
C(20)	170.4	164.4	162.6	162.6
C(21)	29.4	29.3	28.7	27.7
C(29)	**13.1**	**11.9**	**11.5**	16.1

^{1}H NMR (δ [ppm])	**15**	**17**	Compound **14** (20*E*) taken from ref.[40]	Compound **15** (20*Z*) taken from ref.[40]
H-C(19)	**3.43**	**3.32**	**3.44**	4.63

Table S2. Betulonic acid oxime derivatives

^{13}C NMR (δ [ppm])	**3**	**5**	Compound **3** (3*E*) taken from ref.[41]
C-2	16.6	17.6	23.4
C-3	163.5	168.5	168.0
C-4	36.8	40.3	41.5
C-23	**27.6**	**27.3**	**27.9**
C-24	**14.3**	**14.5**	**14.3**
^{1}H NMR (δ [ppm])			
H-C(23)	1.06	1.16	1.06
H-C(24)	0.86	0.78	0.83

3. Antiviral activity

To determine the anti-HIV-1 and anti-HSV-1 activity of prepared derivatives of betulonic and platanic acids, the ability of derivatives to inhibit virus-induced cytopathic effect (CPE) in MT-4 and Vero cells, respectively, was measured. While the results of testing the compounds **17** and **18** were presented in the main text of this paper (Table 2; Figure 1; Figure 2), the results obtained with less active compounds (**4**, **5**, **8** and **15**), as well as those obtained with the parent triterpenoids (**1** and **2**), and with saquinavir or acyclovir, are presented in ESI, Figure S1.

Figure S1. Antiviral and cytotoxicity evaluation of **1**, **2**, **4**, **5**, **8**, **15** and saquinavir or acyclovir. Anti-HIV-1 activity (**A**) and cytotoxicity (**B**) in MT-4 cells and anti-HSV-1 activity (**C**) and cytotoxicity (**D**) in Vero cells.

HIV-1 in MT-4 cells		HSV-1 in Vero cells