

New Cytotoxic Seco-Type Triterpene and Labdane-Type Diterpenes from *Nuxia oppositifolia*

Shaza M. Al-Massarani ¹, Ali A. El-Gamal ^{1,2,*}, Mohammad K. Parvez ¹, Mohammed S. Al-Dosari ¹, Mansour S. Al-Said ¹, Maged S. Abdel-Kader ^{3,4} and Omer A. Basudan ¹

Content

Spectral Data of known compounds2

Supplementary Table 1.....3

Spectral Data of known compounds

3-Oxolup-20(29)-en-30-al (3-oxolupenal) (**5**), white powder; ^{13}C -NMR data, see Table S1; HR-EI-MS m/z = 438.3685 calc. for $\text{C}_{30}\text{H}_{46}\text{O}_2$, 438.3498.

β -sitosterol (**6**), white powder; ^{13}C -NMR data: see Table S1; HR-EI-MS m/z = 414.39 calc. for $\text{C}_{29}\text{H}_{50}\text{O}$, 414.7067.

Stigmasterol (**7**), white powder; ^1H -and ^{13}C -NMR data: see Table S1; HR-EI-MS m/z = 412.36 calc. for $\text{C}_{29}\text{H}_{48}\text{O}$, 412.3705.

3-Oxoolean-12-en-29 α -oic acid (katononic acid) (**8**), white powder; ^{13}C -NMR data: see Table S1, HR-EI-MS m/z = 454.3447 calc. for $\text{C}_{30}\text{H}_{46}\text{O}_3$, 454.6844.

3-Oxours-12-en-30 α -oic acid (ifflaionic acid) (**9**), white powder; ^{13}C -NMR data: see Table S1; HR-EI-MS m/z = 454.3447 calc. for $\text{C}_{30}\text{H}_{46}\text{O}_3$, 454.6844.

Ursolic acid (**10**), white powder; ^1H -and ^{13}C -NMR data: see Table S1; HR-EI-MS m/z = 456.71 calc. for $\text{C}_{30}\text{H}_{48}\text{O}_3$, 456.3603.

30-Hydroxylup-20(29)-en-3-one (3-oxolupenol) (**11**), solid; ^1H -and ^{13}C -NMR data: see Table S1; HR-EI-MS m/z = 440.70 calc. for $\text{C}_{30}\text{H}_{48}\text{O}_2$, 440.3654.

2 α ,3 β -Dihydroxyolean-12-ene-28-oic acid (maslinic acid) (**12**), solid; ^{13}C -NMR data: see Table S1; HR-EI-MS m/z = 472.37 calc. for $\text{C}_{30}\text{H}_{48}\text{O}_4$, 472.3553.

2 α -Hydroxy-ursolic acid (asiatic acid) (**13**), solid; ^{13}C -NMR data: see Table S1; HR-EI-MS m/z = 488.70 calc. for $\text{C}_{30}\text{H}_{48}\text{O}_5$, 488.7022.

3-Hydroxyurs-12-en-30-oic acid (plectranthoic acid A) (**14**), solid; ^{13}C -NMR data: see Table S1; HR-EI-MS m/z = 456.70 calc. for $\text{C}_{30}\text{H}_{48}\text{O}_3$, 456.3603.

Oleanolic acid (**15**), white powder ^{13}C -NMR see Table S1, HR-EI-MS m/z = 456.70 calc. for $\text{C}_{30}\text{H}_{48}\text{O}_3$, 456.3603

3,11-Dioxoolean-12-en-28-oic acid (**16**), white powder; ^1H -and ^{13}C -NMR data: see Table S1, HR-EI-MS m/z = 468.32 calc. for $\text{C}_{30}\text{H}_{44}\text{O}_4$, 468.32.

Table. S1 (^{13}C -NMR, 125 MHz for compounds **5-16**, **5-8** and **15** were measured in CDCl_3 , while **9-14** and **16** were measured in $\text{DMSO-}d_6$)

#	5	6	7	8	9	10	11
1	39.5 CH ₂	37.2 CH ₂	37.3 CH ₂	39.3 CH ₂	38.7 CH ₂	38.2 CH ₂	38.8 CH ₂
2	34.0 CH ₂	31.6 CH ₂	31.8 CH ₂	34.2 CH ₂	33.6 CH ₂	26.9 CH ₂	33.6 CH ₂
3	217.6 C	71.7 CH	71.8 CH	217.6 C	216.0 C	76.8 CH	216.5 C
4	47.2 C	42.2 CH ₂	42.3 CH ₂	47.5 C	46.6 C	46.8 C	46.5 C
5	54.8 CH	140.8 C	140.8 C	55.3 CH	54.2 CH	54.7 CH	53.8 CH
6	19.6 CH ₂	121.6 CH ₂	121.7 CH	19.6 CH ₂	19.1 CH ₂	18.0 CH ₂	19.1 CH ₂
7	33.5 CH ₂	31.6 CH ₂	31.7 CH ₂	32.2 CH ₂	31.8 CH ₂	32.7 CH ₂	33.0 CH ₂
8	40.6 C	31.8 CH	31.9 CH	39.7 C	39.8 C	39.1 C	40.2 C
9	49.5 CH	50.0 CH	50.1 CH	48.0 CH	36.0 CH	47.0 CH	48.9 CH
10	36.7 C	36.2 C	36.2 C	36.7 C	38.8 C	36.5 C	36.3 C
11	21.4 CH ₂	21.1 CH ₂	21.1 CH ₂	23.6 CH ₂	23.1 CH ₂	23.7 CH ₂	21.0 CH ₂
12	27.5 CH ₂	39.6 CH ₂	39.7 CH ₂	122.5 CH	124.4 CH	124.5 CH	25.9 CH ₂
13	37.7 CH	42.1 C	42.3 C	144.3 C	138.2 C	138.1 CH	37.6 CH
14	42.7 C	56.8 CH	56.8 CH	41.6 C	41.6 C	41.6 C	42.4 C
15	27.5 CH ₂	24.3 CH ₂	24.3 CH ₂	26.1 CH ₂	25.1 CH ₂	27.5 CH ₂	27.0 CH ₂
16	35.2 CH ₂	28.8 CH ₂	28.3 CH ₂	26.9 CH ₂	26.0 CH ₂	22.8 CH ₂	34.9 CH ₂
17	43.2 C	55.8 CH	56.1 CH	32.0 C	33.1 C	47.0 C	42.5 C
18	51.0 CH	12.2 CH ₃	11.9 CH ₃	47.0 CH	57.1 CH	52.3 CH	47.9 CH
19	51.0 CH	19.9 CH ₃	19.4 CH ₃	42.5 CH ₂	33.9 CH	38.4 CH	43.8 CH
20	157.2 C	40.7 CH	36.5 CH	44.1 C	51.6 CH	38.5 CH	155.0 C
21	32.7 CH ₂	21.0 CH ₃	19.1 CH ₃	31.1 CH ₂	31.8 CH ₂	30.1 CH ₂	31.1 CH ₂
22	39.8 CH ₂	138.2 CH	34.0 CH ₂	38.3 CH ₂	40.0 CH ₂	36.3 CH ₂	39.3 CH ₂
23	26.6 CH ₃	129.5 CH	26.2 CH ₂	26.4 CH ₃	26.2 CH ₃	28.2 CH ₃	26.3 CH ₃
24	21.0 CH ₃	51.2 CH	45.9 CH	21.5 CH ₃	21.1 CH ₃	16.9 CH ₃	20.7 CH ₃
25	15.6 CH ₃	32.0 CH	29.2 CH	15.2 CH ₃	15.0 CH ₃	16.0 CH ₃	15.6 CH ₃
26	16.0 CH ₃	21.2 CH ₃	19.8 CH ₃	16.7 CH ₃	16.4 CH ₃	15.2 CH ₃	15.4 CH ₃
27	14.3 CH ₃	19.0 CH ₃	18.8 CH ₃	25.9 CH ₃	23.0 CH ₃	23.2 CH ₃	14.2 CH ₃
28	17.8 CH ₃	25.5 CH ₂	23.1 CH ₃	28.2 CH ₃	28.0 CH ₃	178.3 C	17.4 CH ₃
29	133.2 CH ₂	12.3 CH ₃	12.0 CH ₃	28.7 CH ₃	18.4 CH ₃	17.0 CH ₃	105.6 CH ₂
30	194.8 C	---	---	183.9	177.1 C	21.0 CH ₃	62.5 CH ₂

Table. S1 Cont.

#	12	13	14	15	16
1	46.7 CH ₂	47.0 CH ₂	39.9 CH ₂	38.5 CH ₂	39.7 CH ₂
2	67.1 CH	67.1 CH	27.0 CH ₂	27.3 CH ₂	34.2 CH ₂
3	82.2 CH	82.2 CH	76.8 CH	79.2 CH	217.4 C
4	39.9 C	39.2 C	39.3 C	38.5 C	47.8 C
5	54.7 CH	54.7 CH	54.7 CH	55.3 CH	55.4 CH ₂
6	18.0 CH ₂	18.0 CH ₂	17.9 CH ₂	18.4 CH ₂	18.8 CH ₂
7	32.3 CH ₂	32.6 CH ₂	32.4 CH ₂	32.7 CH ₂	32.1 CH ₂
8	38.9 C	38.9 C	39.1 C	39.4 C	43.8 C
9	47.0 CH	46.9 CH	47.0 CH	47.8 CH	61.1 CH
10	37.6 C	37.5 C	36.4 C	37.2 C	36.7 C
11	22.9 CH ₂	22.9 CH ₂	22.9 CH ₂	23.0 CH ₂	199.8 C
12	121.4 CH	124.4 CH	124.5 CH	122.8 CH	128.4 CH
13	143.8 C	138.2 C	138.2 C	143.7 C	170.0 C
14	41.3 C	41.6 C	41.5 C	41.7 C	43.3 C
15	27.1 CH ₂	27.5 CH ₂	27.3 CH ₂	27.8 CH ₂	26.4 CH ₂
16	23.0 CH ₂	22.9 CH ₂	25.1 CH ₂	23.5 CH ₂	26.5 CH ₂
17	45.4 C	46.9 C	33.1 C	46.7 C	45.3 C
18	40.7 CH	52.3 CH	57.0 CH	41.1 CH	48.2 CH
19	45.7 CH ₂	40.7 CH	33.9 CH	46.0 CH ₂	40.9 CH ₂
20	30.3 C	38.4 CH ₂	51.6 CH	30.8 C	31.9 C
21	33.3 CH ₂	30.2 CH ₂	32.4 CH ₂	33.9 CH ₂	37.7 CH ₂
22	32.3 CH ₂	36.3 CH ₂	38.3 CH ₂	32.6 CH ₂	34.2 CH ₂
23	28.7 CH ₃	28.8 CH ₃	28.2 CH ₃	28.2 CH ₃	26.4 CH ₃
24	16.8 CH ₃	16.9 CH ₃	16.5 CH ₃	15.7 CH ₃	21.5 CH ₃
25	16.3 CH ₃	16.4 CH ₃	16.0 CH ₃	15.5 CH ₃	15.7 CH ₃
26	17.0 CH ₃	17.1 CH ₃	15.4 CH ₃	17.2 CH ₃	18.5 CH ₃
27	25.6 CH ₃	25.4 CH ₃	23.1 CH ₃	26.1 CH ₃	23.4 CH ₃
28	178.6 C	178.6 C	28.0 CH ₃	183.9 C	182.0 C
29	32.6 CH ₃	23.3 CH ₃	18.4 CH ₃	33.2 CH ₃	28.6 CH ₃
30	22.6 CH ₃	21.1 CH ₃	177.1 C	23.7 CH ₃	28.5 CH ₃