

Kauralexin A3 <sup>1</sup>H (600 MHz), <sup>13</sup>C (151 MHz), HMBC and NOESY NMR spectroscopic data for diterpene acid aldehydes in CDCl<sub>3</sub>. Chemical shifts referenced to δ(CHCl<sub>3</sub>) = 7.26 ppm for <sup>1</sup>H and δ(CHCl<sub>3</sub>) = 77.36 ppm for <sup>13</sup>C. Coupling constants are given in Hertz [Hz].

Position	δ <sup>13</sup> C [ppm]	δ <sup>1</sup> H [ppm]	J coupling constants [Hz]	HMBC correlations (C. No)	NOESY
1	40.1	2H 1.83α* and 0.80β*	0.80, 1H, dt, J = 13.3, 4.0; 1.83, 1H, "dt", J = 13.1, 3	Hα - C3 (weak), C5 (weak)	Hβ - 0.99, 1.05, 1.15
2	18.6	2H 1.62α* and 1.45β*	1.45, 1H, J = 14.5		
3	34.4	2H 2.14α* and 0.99β*#	2.14 1H, "br d" J = 13.5; 0.99 1H, m	Hα - C1,C5; Hβ - C19	
4	48.7	-	-	-	-
5	56.8	1H 1.15*	dd J=12.7, 1.9	C1, C4, C18,C19, C6, C7, C20, C9	0.99, 1.05, 1.53
6	20.5	2H 1.90β and 1.68α*	1.90 1H, ddt J = 13.1, 2.4, 3.4		H β - 0.99, 9.73 (weak); Hα-9.73
7	41.1	2H 1.53β and 1.63α			
8	45.3	-	-	-	-
9	54.7	1H 1.05*	br d J = 6.6	C20, C11, C10, C8, C12, C14, C16 (weak)	0.80, 1.15, 1.68, 1.53
10	39.4	-	-	-	-
11	18.8	2H 1.53α* and 1.65β			Hβ - 0.85
12	31.24	2H 1.53*			2.67
13	41.5	1H 2.54*	m		1.88, 1.53, 1.24
14	38.4	2H 1.24* and 1.88*	1.24, 1H, m; 1.88, 1H, d, J = 12	H(1.24) - C8, C13; H(1.88) - C12	H (1.88) - 0.85, 2.54
15	44.6	2H 1.68β* and 1.74α*	1.74, 1H, dd, J = 5.9, 13.5	Hβ - C9, C14, C17; Hα - C9, C17	Hβ -1.05
16	45.2	1H 2.67*	dd J = 5.9, 9.1	C12, C13, C14, C17	1.53
17	181.9				
H of COOH		10.1	br s		
18	24.5	3H 0.99*#	s	C3, C4#, C19#, C5#	1.15, 1.90
19	206.2	1H 9.73*	d J = 1.3 Hz	C3, C4	0.85, 0.99, 1.68, 1.90 (weak), 2.14 (weak)
20	16.4	3H 0.85*	s	C5, C10, C9, C1 and/or C10	9.73, 1.68, 1.53, 1.65, 1.88, 1.62

\*Distinct proton chemical shifts from <sup>1</sup>H NMR 1D or 2D (COSY). The rest of the <sup>1</sup>H chemical shifts were deduced from HSQC. #Hβ at C3 and/or H at C18 have HMBC to C4, C5 and C19.

