

Kauralexin B3 ^1H (600 MHz), ^{13}C (151 MHz), HMBC and NOESY NMR spectroscopic data for diterpene acid aldehydes in CDCl_3 . ^{13}C was also detected directly (126 MHz) using a 5 mm broadband (BBO) probe. Chemical shifts referenced to $\delta(\text{CHCl}_3) = 7.26$ ppm for ^1H and $\delta(\text{CDCl}_3) = 77.16$ ppm for ^{13}C . Coupling constants are given in Hertz [Hz].

Position	$\delta^{13}\text{C}$ [ppm]	$\delta^1\text{H}$ [ppm]	J coupling constants [Hz]	HMBC correlations (C. No)	NOESY
1	39.79	2H 0.81 β^* and 1.86 α^*	0.81, 1H, dt, J = 13.3, 4.0; 1.86, 1H, "br dt", J = 13.5, 3	H α - C3, C5, C9 (weak)	H α - 1.59, 0.92 (weak); H β - 1.09, 1.18 (weak), 1.46 (weak)
2	18.43 18.53 18.63	2H 1.645 α^* and 1.46 β			H β - 2.145
3	34.38	2H 2.145 α^* and 1.02 β^*	2.145, 1H, "br d", J = 14; 1.02, 1H, ~ddt, J = 1, 4.5, 13.8	H α - C1 (weak), C5	H α - 9.74 (very weak)
4	48.57	-	-	-	-
5	56.33	1H 1.18 *		C1, C6 (18.43-18.63), C7, C19, C4 (weak)	1.01, 1.09
6	18.43 18.53 18.63	2H 1.90 β^* and 1.67 α^* ^s	1.67, 1H, "d" J = 9		H β - 1.01, 9.74; H α - 9.74 (strong)
7	38.33	2H 1.67 β^* ^s and 1.75 α^*		H α - C5, C6, C9, C8; H β - C14, C15	H β - 6.64; H α - 6.64 (weak)
8	50.62	-	-	-	-
9	45.39	1H 1.09 *	"br d", J = 7		0.81, 6.64, 1.18
10	39.85	-	-	-	-
11	18.43 18.53 18.63	2H (1.59, 151) [#]			1.86, 0.92 (weak)
12	25.23	2H 1.51 * and 1.640 *		H (1.51) - C16	
13	40.36	1H 2.95 *	m		2.140, 1.53
14	43.47	2H 2.140 * and 1.53 *	2.140, 1H, d, J = 10.6	H (2.140) - C12, C15, C16; H (1.53) - C8, C9	H (2.140) - 2.95, 0.92; H (1.53) - 2.95
15	155.69	1H 6.64 *	s	C8, C13, C14, C17, C7 (weak)	1.67, 1.09, 1.75 (weak)
16	137.74	-	-	-	-
17	170.25	-	-	-	-
H of COOH		11.3 *	br s		
18	24.38	3H 1.01 *	s	C4, C19, C3, C5	9.74, 1.18, 1.90
19	205.85	1H 9.74 *	d, J = 1.2	C3, C4	0.92 (strong), 1.67 (strong), 1.01, 1.90, 2.145 (very weak)
20	16.46	3H 0.92 *	s	C5, C9, C1 and/or C10	9.74 (strong), 2.140, 1.59, 1.67, 151, 1.86 (weak)

*Distinct proton chemical shifts from ^1H NMR 1D or 2D (COSY). The rest of the ^1H chemical shifts were deduced from HSQC. H of COOH at C17 was obtained from 1H NMR (500MHz). ^ssignal composed of two overlapping ^1H signal. [#]ambiguous assignment of 1.51, 1.59 at C11.

