Supplementary material

Triterpenoids, megastigmanes and hydroxycinnamic acid derivatives

from Anisomeles indica

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Abstract: Six triterpenoids (1 - 6), four megastigmanes (7 - 10) and five hydroxycinnamic acid derivatives (11 - 15) were isolated from the aerial part of *Anisomeles indica* (Lamiaceae). Of these components, compound 1 was identified to be a new triterpenoid with the structure of $2 \square, 3 \square, 19 \square$ -trihydroxyurs-12,20(30)-dien-28-oic acid based on extensive analysis of MS, 1D and 2D NMR spectroscopic data, while compounds 2 - 13 were obtained for the first time from Anisomeles species.

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 $2\Box$, $3\Box$, $19\Box$ -trihydroxyurs-12, 20(30)-dien-28-oic acid (1)

No.	$\square_{\rm H}$, mult. (<i>J</i> in Hz)	\Box_{C}	mult.	No.	$\Box_{\rm H}$, mult. (<i>J</i> in Hz)	□ _C ,	mult.
1	1.58, dd (12.1, 4.0)	42.5	CH_2	16	2.71, td (13.2, 4.0)	27.0	CH_2
	1.29, t (12.0)				1.66, dd (12.9, 4.8)		
2	3.93, ddd (12.0, 4.0, 2.8)	67.2	CH	17		49.1	С
3	3.32, d (2.8)	80.1	CH	18	2.65, s	55.8	CH
4		39.5	С	19		73.6	С
5	1.26, br. d (10.2)	49.3	CH	20		156.5	С
6	1.46, br. d (13.1)	19.3	CH_2	21	2.78, td-like (13.0, 4.4)	29.2	CH_2
	1.38, qd-like (12.8, 3.1)				2.09 dt (13.2, 4.3)		
7	1.60, br. d (13.1)	34.3	CH_2	22	1.90, dt (12.9, 4.3)	39.7	CH_2
	1.34, td-like (13.1, 3.1)				1.65, td-like (12.9, 4.8)		
8		41.1	С	23	0.99, s	29.3	CH_3
9	1.86, dd (10.8, 7.1)	48.2	CH	24	0.87, s	22.5	CH_3
10		39.4	С	25	0.99, s	17.0	CH_3
11	2.04, ddd (18.4, 7.1, 3.3)	24.7	CH_2	26	0.80, s	17.7	CH_3
	1.98, ddd (18.4, 10.8, 3.3)			27	1.36, s	24.2	CH_3
12	5.33, t (3.3)	129.4	CH	28		182.0	С
13		139.9	С	29	1.37, s	27.7	CH_3
14		42.9	С	30	4.88, s	106.1	CH_2
15	1.79, td-like (13.7, 4.3)	29.5	CH_2		4.70, s		
	1.04, dt (13.2, 4.4)						

Table 1S. ¹H and ¹³C NMR spectroscopic data of $\mathbf{1}$ (400 and 100 MHz, in CD₃OD).

Elemental Composition Report

Monoisotopic Mass, Odd and Even Electron Ions

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Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0 Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

6 formula(e) evaluated	d with 1 re	esults wit	hin limits (up to 20 clo	sest results	for each mas	ss)	1		
SIMM-Mass S	pec				Q-Tof Ultima					02-Mar-2016	
20160302_ES	IH_TCH_CC	H_160392 :	246 (4.653)	AM (Cen,4, 485.3	80.00, Ht,9000 278	0.0,318.10,0.70	0); Sm (SG, 2x1	.00); Cm (236:250)	TOF	MS ES- 1.40e3	
100											
1											
%-					486.3300						
479.139	⁹⁸ 480.0916	482.9306	483.3817	485.1889	487	.3330 488.	3383_489.3448	491.2075 493.249	494.1717	m/z	
480	0.0	482.0	484	1.0	486.0	488.0	490.0	492.0	494.0	1 . 102	
Minimum: Maximum:	50.00 100.00			200.0	20.0	-1.5 50.0					
Mass	RA	Calc.	Mass	mDa	PPM	DBE	Score	Formula			
485.3278	100.00	485.32	267	1.1	2.3	8.5	1	СЗО Н45 С)5		

Figure 1S. (-)-HR-ESI-MS spectrum of 1



Figure 2S. IR spectrum of 1





Figure 4S. ¹³C NMR spectrum of **1** in CD₃OD (100 MHz)









Figure 7S. Selected HMBC (H to C, upper) and NOESY (under) correlations of 1.



Figure 8S. NOESY spectrum of 1 in CD₃OD