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A New Isopimarane Diterpene from *Nepeta prattii*

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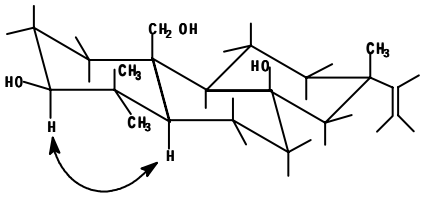
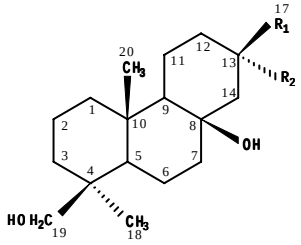
Abstract: A new isopimarane diterpene, isopimar-15-en-3β,8β,20-triol, was isolated from *Nepeta prattii*. Its structure was elucidated by spectral methods (EIMS, 1D and 2D NMR).

Keywords: *Nepeta prattii*; isopimarane diterpene; prattol.

Some plants of the *Nepeta* genus were used as Chinese folk medicine to 'dissipate wind and cold'. In order to find the active principles from the genus, studies on the chemical constituents of *Nepeta prattii* were carried out. From the methanol extracts we have isolated a new isopimarane diterpene, prattol **I.**





I

II R_1=CH_3, R_2= -CH=CH_2

III R_1= -CH=CH_2, R_2=CH_3

I was obtained as colorless cubic crystals from methanol, m.p. 222-224°C. The EIMS revealed the peak m/z 322, and the ^{13}C-NMR and DEPT showed the presence of three CH_3, nine CH_2, four CH and four C. Then the molecular composition was deduced to be $C_{20}H_{34}O_3$. The ^{1}H-NMR spectra indicated the presence of a –CH=CH_2 group, a –CH_2OH unit and three methyl singlets. The ^{1}H-^{1}HCOSY and HMQC spectra revealed the following partial structure –CH_2-CH_2-CHOH- and two >CH-CH_2-CH_2-. The C-C interconnectivity of all the fragments was established through HMBC experiment. The above information suggested compound **I** to be a pimarane or isopimarane diterpene, and three hydroxyl groups were located at C-3, C-8 and C-20. By further comparison of ^{13}C-NMR of **I** with those of the compound isopimar-15-en-8β, 19-diol **II**[1] and pimar-15-en-8β, 19-diol **III**[2], it was found that ^{13}C-NMR spectral data at C-15, C-16 and C-17

of **I** were parallel to compound **II** but not compound **III**. Moreover, in the ^{1}H-NMR spectra, the coupling constant values of 14-H (1.74, dd, J=13.8, 1.7; 1.43, d, J=13.8) indicated the presence of W-coupling of 17-CH_3 and 14 α -H. The fact suggested 17-CH_3 and 14 α -H could be axial. The 3 β -configuration of the hydroxyl group was determined on the basis of the coupling constant values (3.53, dd, J=9.7, 6.7) and the correlation between 3 α -H and 5 α -H in NOESY spectra of I. Thus prattol I was elucidated to be isopimar-15-en-3 β , 8 β , 20-triol.

Table 1 NMR Spectral Data of Compound **I**, **II**, and III
(**I**, 100MHz, C_5D_5N; **II**, III, 25MHz, $CDCl_3$)

	^{1}HNMR	^{13}CNMR		
No.	**I**	**I**	**II**	**III**
1	1.64, 0.90	35.67	39.59	39.5
2	1.91	29.27	18.07	18.1
3	3.53 (dd, 9.7, 6.7)	78.35	35.74	35.6
4		39.71	38.68	38.7
5	1.05 (d, 12.3)	55.91	57.21	56.5
6	2.62 (m)	18.66	18.35	18.1
7	2.01, 1.43	43.99	43.99	42.3
8		70.27	72.49	72.5
9	0.93 (d, 11.7)	58.41	58.21	57.2
10		40.90	36.43	36.4
11	1.99	18.01	17.18	17.4
12	1.61, 1.38	39.09	38.13	36.1
13		37.20	37.20	37.1
14	1.74 (dd, 13.8, 1.7), 1.43 (d, 13.8)	50.79	51.57	53.4
15	5.88 (dd, 17.4, 10.7)	152.42	151.59	147.5
16	5.00 (d, 17.4), 4.91 (d,10.7)	108.65	108.57	111.9
17	1.49 (s)	24.73	24.28	32.3
18	1.30 (s)	29.08	27.08	27.0
19	1.39 (s)	16.37	65.25	65.1
20	4.25 (d, 12.1), 3.79 (d, 12.1)	63.70	16.21	16.1

References

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