(242–272 Å^3), the hydrogen bonding potential appears to be the only determining factor.

Although the correlations between $LogP_c$ and the quantum chemical parameters are very similar to those between $LogP_{app}$ and the quantum chemical parameters, they are somewhat different. Maybe $\Sigma\ Q'_{N,O,H}$ is the better parameter to predict the cell permeability in Caco-2 cell monolayers and $\Sigma\ Q_{N,O,H}$ is the better one in rat ileum and colon.

Because of their simplicity and excellent correlation with drug absorption, the quantum chemical parameters related to molecular charge distribution can be used to predict drug absorption.

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A new cyclolanostanol arabinoside from the rhizome of *Cimicifuga racemosa*

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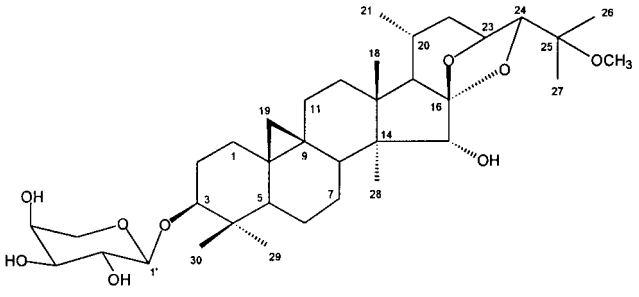
The most popular phytotherapeutic agent used in treatment of menopausal symptoms is the extract of *Cimicifuga racemosa* (L.) Nutt. which has been used in European phytotherapy for over 50 years. During a series of chemical investigations of *Cimicifuga* species, 9,19-cyclolanostane-type triterpenoids [1–3], fukiic and piscidic acid esters [4], and chromones have been isolated [5]. Our previous studies led to the isolation of a number of 9,19-cyclolanostane-type triterpenes from *C. racemosa* [6], and we have developed an analytical method for the separation of the main triterpene glycosides [7]. As a continuation of this work, a new triterpene glycoside has been isolated, 25-*O*-methylcimigenol-3-*O*-α-L-arabinopyranoside (**1**). This paper deals with the isolation and the structural elucidation of **1**.

The IR spectrum of **1** showed a strong hydroxyl absorption band at 3364 cm^{-1}. High resolution electrospray ionization mass spectrometry (HRESIMS) of **1** showed an ion peak for $[M + Na]^+$ at m/z 657.3933, in agreement with the molecular formula $C_{36}H_{58}O_9$. The ^{1}H NMR spectrum of **1** (Table) displayed signals characteristic of cyclopropane-methylene protons as an AX system (δ 0.28, 0.52, J = 3.0 Hz), a methoxy group [δ 3.18 ($OC\underline{H}_3$)], and six tertiary [1.26, 1.24 (×2), 1.17, 1.13 and 1.01] and a secondary methyl (δ 0.83, d, J = 6.4 Hz) group. Additionally, one anomeric proton signal was observed at δ 4.77 (d, J = 6.9 Hz). Thus, compound **1** was considered to be a 9,19-cyclolanostane-type triterpene monoglycoside. The ^{13}C NMR spectrum of **1** exhibited 36 signals. Thirty signals were accounted for the aglycon moiety. The remaining signals were in accordance with the presence of one pentose and one methoxy group. Full assignments of the proton and carbon signals of the aglycone part of **1** were secured by DQF-COSY and HMQC spectra. The carbon resonances attributed to the aglycon moiety supported the presence of 25-*O*-methyl-cimigenol as sapogenol moiety glycosylated at C-3 (δ 88.8 d) [1]. The glycosylation shifts observed for this carbon suggested that **1** was a monodesmosidic saponin. The structure of the sugar moiety was achieved using DQF-COSY and HMQC. The results of the DQF-COSY experiment allowed the sequential assignments of all proton resonances within the sugar resi-



Cimiracemoside B

Table: ^{1}H- and ^{13}C-assignments of 1* (in C_5D_5N)

C/H	δ_C	δ_H (J Hz)	C/H	δ_C	
1	32.6 t	1.20 m, 1.60 m	**20**	24.2 d	1.65 m
2	30.2 t	1.90 m, 2.33 m	**21**	19.8 q	0.83 d (6.4)
3	88.8 d	3.48 dd (4.2, 11.6)	**22**	38.3 t	0.97 m, 2.08 m
4	41.5 s		**23**	71.8 d	4.59 d (9.0)
5	47.4 d	1.32 dd (3.9, 12.3)	**24**	88.4 d	3.63 s
6	21.3 t	0.71 m, 1.53 m	**25**	76.4 s	
7	26.6 t	1.08 m, 2.08 m	**26**	19.5 q	1.24 s
8	48.8 d	1.69 **	**27**	22.3 q	1.24 s
9	20.1 s		**28**	11.9 q	1.17 s
10	26.8 s		**29**	25.9 q	1.26 s
11	26.6 t	1.15 m, 2.08 m	**30**	15.6 q	1.01 s
12	34.2 t	1.55 m, 1.68 m			
13	42.0 s		**1′**	107.5 d	4.77 d (6.9)
14	47.8 s		**2′**	73.1 d	4.41 dd (7.0, 8.5)
15	88.8 d	4.21 s	**3′**	74.8 d	4.14 dd (3.2, 8.8)
16	112.1 s		**4′**	69.6 d	4.32 dd (2.7, 3.2)
17	59.6	1.44 d (11.0)	**5′**	66.8 t	3.77 dd (2.7, 14.2),
18	19.7 q	1.13 s			4.30 dd (2.7, 14.2)
19	31.0 t	0.28 (3.0), 0.52 (3.0)	**OMe**	49.4 q	3.18 s

* Assignments confirmed by COSY, HMQC and HMBC experiments
** Signal pattern was unclear due to overlapping

due, starting from the well isolated anomeric proton signals (Table). Thus on the basis of the chemical shifts, the multiplicity of the signals, the absolute values of the coupling constants, the sugar residue was identified as α-L-arabinopyranosyl [8]. The position of the sugar residue was unambigously determined by the HMBC experiment which showed long-range correlations between C-3 (δ 88.8) of the aglycon and H-1_{ara} (δ 4.77). On the basis of these evidences, compound **1** was established as 25-*O*-methylcimigenol-3-*O*-α-L-arabinopyranoside, named cimiracemoside B.

Experimental

1. General procedures

Details have been published previously [6].

2. Plant material

For information regarding plant material, see Bedir et al. [6].

3. Extraction and isolation

Plant material (4.2 kg) was extracted with dichloromethane (8 l) under reflux and the extract was filtered. The filtrate was concentrated to dryness in vacuo (210 g). An aliquot of the extract (125 g) was applied to vacuum liquid chromatography using normal phase silica gel (500 g) as eluents, employing n-hexane (1 l), Et_2O (4 l), EtOAc (4 l), $CHCl_2$ (4 l), Me_2CO (4 l), and MeOH (8 l). Fractions EtOAc, $CHCl_2$, Me_2CO, and MeOH (80 g), rich in saponins, were combined and then subjected to open column chromatography (silica gel, 1.5 kg), eluted with $CHCl_3$–MeOH mixtures (99 : 1, 1.5 l; 98 : 2, 0.5 l; 97 : 3, 0.5 l; 96 : 4, 0.5 l; 95 : 5, 10 l; 94 : 6, 1 l) to give seven main fractions (Frs. A–G). Fr D (9.3 g) further subjected to flash column chromatography using reversed phase material (C-18, 350 g). Elution with increasing amount of MeOH in H_2O (50 : 50 → 70 : 30) yielded eight fractions (Frs. D1-D8). Fr. D-8 (1.1 g) was applied to chromatotron system (Model 8924, 4 mm plate, flow rate: 8–10 ml/min.) n-Hexane-EtOAc-MeOH (10 : 10 : 0.2) was used as the eluents to yield compound **1** (135.0 mg).
Cimiracemoside B (**1**): IR (KBr) ν_{max}: 3364, 2348, 2291 cm^{-1}. ^{1}H- and ^{13}C-NMR: see Table 1. HRESIFTMS m/z: 657.3933 $[M + Na]^+$.

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