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^{13}C NMR spectroscopy of eudesmane sesquiterpenes

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1. Introduction

In general, a phytochemical process involves five different phases of work:

1. choice of the plant to be studied;
2. botanical identification of the chosen plant;
3. preliminary analysis of the chemical composition;
4. isolation of the major components;
5. structure elucidation of the isolated compounds.

Each one of these phases has its relevance regarding the discovery of new substances of natural origin, but the structure elucidation is of particular importance being the main phase of the process. This phase demands vast experience in spectrum analysis in view of the high structure variety and diversity provided by structures in natural products chemistry as found for terpenoids [1] and alkaloids [2]. Among the terpenoids, sesquiterpenes are a class providing constant challenges for structure elucidation, due to the countless biogenetic pathways, that can produce several types of carbon skeletons [3]. Concerning this point, we decided to create, through the Expert System SISTEMAT [4–6], a specialist module for sesquiterpenoids, aimed at facilitating the process of structure elucidation.

As there are hundreds of substances of this class with reported ^{13}C NMR data, we began building this specialist module using one of the most representative skeletons of the sesquiterpenes, the eudesmane type (Fig. 1).

For building the database system all ^{13}C NMR data of sesquiterpenes with eudesmane skeleton were

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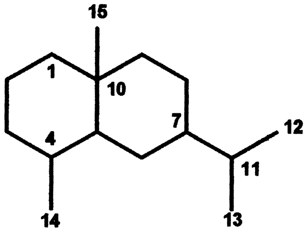


Fig. 1. Eudesmane skeleton.

collected from the literature. This procedure resulted in 350 substances that were then introduced in SISTEMAT.

The aim of this article is to indicate how SISTEMAT can be used to obtain useful rules for ^{13}C spectral analysis and can be used as an auxiliary tool in the process of structure elucidation for eudesmanes, and, also, to present a review on ^{13}C NMR data of eudesmanes.

2. The expert system SISTEMAT

SISTEMAT [4–6] was developed to help natural products researchers with the structure elucidation process. Several chemical classes of natural products have already been studied using SISTEMAT, for example, monoterpenes, diterpenes, triterpenes and flavonoids [7–10].

The specialist module in sesquiterpenes with an eudesmane skeleton was built by coding ^{13}C data obtained from the literature and introducing it in SISTEMAT [4]. These codes contained information on chemical formula, molecular mass and types of carbon atoms in a specific position that can be later accessed through the application of SISTEMAT [5–10]. A brief overview of SISTEMAT has been provided in Ref. [7]. SISTEMAT is available at the ftp site address ftp://143.107.53.186/PUB.

3. The search for heuristic rules

Heuristic rules are practical rules obtained from the experience from the experience of specialists, or originated from programs which perform “learning from machine” routines, and are aimed at solving a specific problem. In the SISTEMAT system, the search of these rules is done through the programs TIPCARB [7,8] and PICKUP [7,8,10]. The TIPCARB program can determine which carbon atoms are present in each position of a skeleton. This information helps in the search for heuristic rules because they define whether or not the skeleton is substituted and the kind of substituents. This could also be done manually by a careful analysis of the literature, but the huge data volume makes this task unfeasible for obtaining heuristic rules.

After the position of each carbon atom and the types of substituents have been defined these fragments, denominated substructures, are coded in the PICKUP program [7] that performs the search of the database for the chemical shift range for ^{13}C data of the carbons in the substructure. After the chemical shift estimation, this information is evaluated in relation to its degree of recognition using the complete database, allowing one to affirm that a certain group of chemical shifts characterises a certain probability of the occurrence of a substructure in the compound. In summary, the TIPCARB program indicates which substructure should be selected, and obtains the chemical shift ranges of its carbon atoms and the degree of recognition of these shifts within the database.

4. Structural data and tables of ^{13}C NMR shifts

For identification purposes and for structure elucidation of new compounds, it is useful to have access to an extensive list of eudesmanes and their structural data. Table 1 shows a collection of structural data of eudesmanes collected from the literature. The present compilation includes data from most of the relevant papers published up to 1996 [11–159]. The eudesmanes published from 1997 were used as test substances and are presented in Section 5. Table 1 presents data classified by the type and order of the substituents, and also contains information on the usual names and references. The structures can be determined from the data presented in Table 1, but in view of the structural complexity of some compounds a graphic representation in shown in Fig. 2.

The ^{13}C chemical shift data for all the 350 compounds are listed in Table 2, including information about the solvent used for the recorded sample.

Table 1
Structural information for eudesmanes

Subst.	Trivial names	Substituents	Stereochemistry	References
1	Balanitol	1,11-OH	11β,14β,15β	[11]
2		1β,4β,7α-OH	11β,14α,15β	[12]
3	Boarioside aglycone	1α,4β,11-OH	11α,14α,15α	[13]
4		1β,4α-OH, 6-OCin	11β,14β,15β	[14]
5		1β,4α-OH, 6β-OCin	11β,14β,15β	[15]
6		1β,4β-OH, 6-OCin	11β,14α,15β	[14]
7		1β,4α-OH, 6β-OAc	11β,14β,15β	[16]
8		1β,4β-OH, 6β-OAc	11β,14α,15β	[16]
9		1β,4β-OH, 6α,14-Oxy	11β,14α,15β	[17]
10		1β-OAc, 4β,7α-OH	11β,14α,15β	[12]
11	Boarioside	1α-OGly, 4β,11-OH	11α,14α,15α	[13]
12	Boarioside tetraacetyl	1α-OGly-$(OAc)_4$, 4β,11-OH	11α,14α,15α	[13]
13		1β,4β-Oxy, 6β-OCin	11β,14α,15α	[18]
14		1β,4β-Oxy, 6β-OCin	11β,14α,15β	[15]
15		1α,4α-Oxy, 6β-Cin	11β,14β,15β	[14]
16		1α,4α-Oxy, 6β-OAc	11β,14β,15β	[19]
17	Austradiol acetate	1-Br, 4α-OH, 6α-OAc	11α,14β,15β	[20]
18		1-Br, 4α-OAc, 6α-O-*trans*-(3′-OAc-2-butenoate)	11α,14β,15β	[20]
19		1-Br, 4α-OAc, 6α-O-*cis*-(3′-OAc-2-butenoate)	11α,14β,15β	[20]
20		1-Oxo, 11-OH	11β,14β,15β	[11]
21	Dihydro-α-agarofuran	5β,11-Oxy	11β,14α,15α	[21]
22	Dihydro-β-agarofuran	5β,11-Oxy	11β,14β,15α	[21]
23		1,6α,8α,9-OH, 5α,11-Oxy	11α,14β,15β	[22]
24	Angulatueoid-G	1,2-OH, 5α,11-Oxy, 6α-OAc, 8,9-OBzt	11α,14β,15β	[23]
25	Celahin-C	1α-OH, 2α,6β,15-OAc, 5β,11-Oxy, 9β-OBzt	11β,14α,15α	[24]
26	Emarginatine-D	See Fig. 2	11β,14α,15α	[25]
27	Emarginatine-E	See Fig. 2	11β,14α,15α	[25]
28	Triptogelin B-1	1β-OH, 5α,11-Oxy, 6α-OAc, 8β,9β-OBzt	11α,14β,15β	[26]
29	Triptogelin A-8	1β,2β,8β-OH, 5α,11-Oxy, 6α-OAc, 9β-OBzt	11α,14β,15β	[27]
30	Triptogelin A-3	1β,2β-OH, 5α,11-Oxy, 6α-OAc, 8β,9β-OBzt	11α,14β,15β	[26]
31	Triptogelin A-7	1β,2β-OH, 5α,11-Oxy, 6α-OAc, 8β-ONic, 9β-OBzt	11α,14β,15β	[27]
32	Triptogelin A-4	1β-OH, 2-Oxo, 5α,11-Oxy, 6α-OAc, 8β,9β-OBzt	11α,14β,15β	[26]
33		See Fig. 2	11α,14β,15β	[28]
34		See Fig. 2	11α,14β,15β	[28]
35		1-OAc, 5α,11-Oxy, 9α-OCin	11α,14β,15β	[22]
36		1-OAc, 5α,11-Oxy,9αOEpcin	11α,14β,15β	[29]
37	Angulatueoid-H	1,6α-OAc, 5α, 11-Oxy, 8,9-OBzt	11α,14β,15β	[23]
38		1,6α,8α-OAc, 5α,11-Oxy, 9β-OBzt	11α,14β,15β	[22]
39		1,6α,8-OAc, 5α,11-Oxy, 9-OBzt	11α,14β,15β	[3]
40	Angulatueoid-C	1,8α, 15-OAc, 5α,11-Oxy, 9-OBzt	11α,14β	[31,32]
41		1,8β, 15-OAc, 5α,11-Oxy, 9-OBzt	11α,14β	[32]
42		1,6α,8α, 15-OAc, 5α,11-Oxy, 9β-OBzt	11α,14β	[33]
43		1,8α, 15-OAc, 5α,11-Oxy, 9α-OFur	11α,14β	[33]
44		1,6α, 15-OAc, 4α-OH, 5α,11-Oxy, 8α,9α-OFur	11α,14β	[30]
45	Angulatueoid-D	1,8α-OAc, 5α,11-Oxy, 9-OBzt, 15-OPic	11α,14β	[31,34]
46	Angulatueoid-A	1,2,8α-OAc, 5α,11-Oxy, 9-OBzt, 15-OPic	11α,14β	[31,34]
47	Angulatueoid-B	1,2,8α,15-OAc, 5α,11-Oxy, 9-OBzt	11α,14β	[31]
48		1,2-OAc, 5α,11-Oxy, 9α-Oepcin	11α,14β,15β	[29]
49		1-OAc, 2-OBut, 5α,11-Oxy, 9α-OEpcin	11α,14β,15β	[29]
50		1-OAc, 2-OBzt, 5α,11-Oxy, 9α-OEpcin	11α,14β,15β	[29]

Table 1 (*continued*)

Subst.	Trivial names	Substituents	Stereochemistry	References
51		1-OAc, 2,8,9α-OBzt, 4α,6α-OH, 5α,11-Oxy	11α,14β,15β	[35]
52		1-OAc, 2,8β,9α-OBzt, 4α,6α-OH, 5α,11-Oxy	11α,14β,15β	[36]
53		1-OAc, 2β,6α,8β,9α-OBzt, 5α,11-Oxy	11α,14β,15β	[37]
54		1-OAc, 2-OFur, 4α,6α-OH, 5α,11-Oxy, 8,9α-OBzt	11α,14β,15β	[35]
55		1,8α-OAc, 2,15-OiBu, 4α,6α-OH, 5α,11-Oxy, 9-OBzt	11α,14β	[38]
56		1,6α,8-OAc, 2,15-OiBu, 4α-OH, 5α,11-Oxy, 9α-Ofur	11α,14β	[38]
57	Triptogelin G-2	1β-OAc, 5α,11-Oxy,9α-Obzt	11α,14β,15β	[39]
58	Triptogelin F-2	1β,6α-OAc, 5α,11-Oxy, 9α-Ocin	11α,14β,15β	[39]
59	Triptogelin F-1	1β-OAc, 5α,11-Oxy, 6α-Onic, 9α-OBzt	11α,14β,15β	[39]
60	Eumaitenin	1α,6β,8α-OAc, 5β,11-Oxy, 9β-OFur	11β,14α,15α	[40]
61	Triptofordin C-2	1β,6α-OAc, 2β, 4α-OH, 5α,11-Oxy, 8α,9α-Obzt	11α,14β,15β	[41]
62	Triptofordin C-1	1β,6α-OAc, 2-Oxo, 4α-OH, 5α,11-Oxy, 8α,9α-OBzt	11α,14β,15β	[41]
63	Triptogelin C-1	1β,2β,6α-OAc, 5α,11-Oxy, 9α-OBzt	11α,14β,15β	[42]
64	Triptogelin C-2	1β,2β-OAc, 5α,11-Oxy, 6α-ONic, 9α-OBzt	11α,14β,15β	[42]
65		1β,2β,6α,15-OAc, 4α-OH, 5α,11-Oxy, 9α-OBzt	11α,14β,15β	[43]
66		1β,2β,6α,15-OAc, 4α-OH, 5α,11-Oxy, 8-Oxo, 9β-OBzt	11α,14β,15β	[44,45]
67	Euonine	See Fig. 2	11α,14β,15β	[46]
68	Euonymine	See Fig. 2	11α,14β,15β	[46]
69	Triptogelin E-5	1β-OAc, 2β-OBut, 5α,11-Oxy, 9α-OBzt	11α,14β,15β	[39]
70	Triptogelin E-6	1β-OAc, 2β-OiBu, 5α,11-Oxy, 9α-OBzt	11α,14β,15β	[39]
71	Triptogelin E-8	1β-OAc, 2β-OiBu, 5α,11-Oxy, 9α-OCin	11α,14β,15β	[39]
72	Triptogelin E-7	1β-OAc, 2β-OBut, 5α,11-Oxy, 9α-OCin	11α,14β,15β	[39]
73	Triptogelin C-3	1β,6α-OAc, 2β-OBut-(2′-Me), 5α,11-Oxy, 9α-OBzt	11α,14β,15β	[42]
74		1β-OAc, 2β,8β,9α-OBzt, 4α,6α-OH, 5α,11-Oxy	11α,14β,15β	[47]
75	Wilfordine	See Fig. 2	11α,14β,15β	[28]
76		See Fig. 2	11α,14β,15β	[28]
77		1β-OAc, 2β-OFur, 4α,6α-OH, 5α,11-Oxy, 8β,9α-OBzt	11α,14β,15β	[47]
78		1α,6β, 15-OAc, 4β-OH, 5β,11-Oxy, 8α-OMeBu, 9α-OBzt	11β,14α,15α	[48]
79		1β-OAc, 2β-OMeBu, 4α,6α-OH, 5α,11-Oxy, 8β,9α-OBzt	11α,14β,15β	[48]
80	Celahin-B	1α,2α,6β,15-OAc, 5β,11-Oxy, 9β-OBzt	11β,14α,15α	[49]
81		1α,2α-OAc, 4β,6βOH, 5β,11-Oxy, 8β,15-OiBu, 9α-OBzt	11β,14α,15α	[50]
82	Emarginatine-C	See Fig. 2	11β,14α,15α	[25]
83	Emarginatine-A	See Fig. 2	11β,14α,15α	[25]
84	Emarginatinine	See Fig. 2	11β,14α,15α	[25]
85	Angulatueoid-F	1-OPro, 5α,11-Oxy, 8α-OAc, 9-OBzt, 15-ONic	11α,14β	[34]
86	Angulatueoid-E	1-OiBu, 5α,11-Oxy, 8α-OAc, 9-OBzt, 15-ONic	11α,14β	[34]
87		1β-OiBu, 2β,6α,15-OAc, 4α-OH, 5α,11-Oxy, 9α-OBzt	11α,14β,15β	[43]
88	Euonydin A-1	1β,2β-OBut, 4α,6α-OH, 5α,11-Oxy, 9α-OFur,15-OAc	11α,14β,15β	[51]
89	Euonydin A-2	1β,2β-OBut, 4α-OH, 5α,11-Oxy, 6α,15-OAc, 9α-OFur	11α,14β,15β	[51]
90	Euonydin A-3	1β,2β-OBut, 4α-OH, 5α,11-Oxy, 6α,15-OAc, 9α-OBzt	11α,14β,15β	[51]
91		1β-O2MeBu, 2β,6α,15-OAc, 4α-OH, 5α,11-Oxy, 9α-OBzt	11α,14β,15β	[43]
92		1,9-OBzt, 5α,11-Oxy, 6α-OH, 8-OAc	11α,14β,15β	[22]
93		1,8,9-OBzt, 5α,11-Oxy, 6α-OAc	11α,14β,15β	[32]
94		1,6α-OBzt, 5α,11-Oxy, 9α-OAc	11α,14β,15β	[22]
95		1,9-OBzt, 5α,11-Oxy, 8α,15-OAc	11α,14β	[32]
96		1,8-OBzt, 2-OHex, 5α,11-Oxy, 6α,9,15-OAc	11α,14β	[38]
97	Triptofordin-A	1β-OBzt, 4α-OH, 5α,11-Oxy, 9α-OCin	11α,14β,15β	[41]
98	Triptofordin-B	1β,9α-OBzt, 4α,6α-OH, 5α,11-Oxy	11α,14β,15β	[41]
99	Triptogelin A-2	1β,8β,9β-OBzt, 2β-OH, 5α,11-Oxy, 6α-OAc	11α,14β,15β	[26]
100	Ebenifoline E-I	See Fig. 2	11α,14β,15β	[46]
101	Euojaponine-C	See Fig. 2	11α,14β,15β	[46]

Table 1 (*continued*)

Subst.	Trivial names	Substituents	Stereochemistry	References
102	Triptofordin-E	1β,9β-OBzt, 2β,6α,15-OAc, 4α-OH, 5α,11-Oxy, 8-Oxo	11α,14β,15β	[45]
103	Euosachalidin-A	1β-OBzt, 2β,6α,9β,15-OAc, 5α,11-Oxy, 8-Oxo	11α,14β,15β	[52]
104	Euojaponine-F	See Fig. 2	11α,14β,15β	[46]
105	Ebenifoline E-II	See Fig. 2	11α,14β,15β	[46]
106	Ebenifoline E-III	See Fig. 2	11α,14β,15β	[46]
107	Ebenifoline E-IV	See Fig. 2	11α,14β,15β	[46]
108	Ebenifoline E-V	See Fig. 2	11α,14β,15β	[46]
109	Mayteine	See Fig. 2	11α,14β,15β	[46]
110	Triptogelin A-9	1β,9β-OBzt, 2β-OMeBu, 6α-OAc, 5α,11-Oxy, 8β-ONic	11α,14β,15β	[27]
111		1β,2β,8β,9β-OBzt, 5α,11-Oxy, 6α-OH	11α,14β,15β	[26]
112	Triptogelin A-1	1β,2β,8β,9β-OBzt, 5α,11-Oxy, 6α-OAc	11α,14β,15β	[26]
113	Triptogelin A-11	1β,2β,9β-OBzt, 5α,11-Oxy, 6α,8β-OAc	11α,14β,15β	[42]
114	Triptogelin A-6	1β,2β,9β-OBzt, 5α,11-Oxy, 6α-OAc, 8β-ONic	11α,14β,15β	[27]
115	Ebenifoline W-II	See Fig. 2	11α,14β,15β	[46]
116	Ebenifoline W-I	See Fig. 2	11α,14β,15β	[46]
117	Mortonol A	1α,9β-OBzt, 4β-OH, 6-Oxo, 5β,11-Oxy	14α,15α	[53]
118		1α-OBzt, 4β,6β-OH, 9β-OAc, 5β,11-Oxy	11β,14α,15α	[54]
119		1α-OBzt, 4β-OH, 5β,11-Oxy, 6β,9β-OAc	11β,14α,15α	[54]
120		1α-OBzt, 4β,8β-OH, 5β,11-Oxy, 6β,9α-OAc	11β,14α,15α	[54]
121		1α-OBzt, 4β-OH, 5β,11-Oxy, 6β,8β,9α-OAc	11β,14α,15α	[54]
122		1α-OBzt, 4β-OH, 5β,11-Oxy, 6β,9β,15-OAc	11β,14α,15α	[54]
123		1α,9α-OBzt, 4β-OH, 5β,11-Oxy, 6β,8α,15-OAc	11β,14α,15α	[55]
124	Mortonol B	1α,9β-OBzt, 2β-OAc, 4β-OH, 5β,11-Oxy, 6-Oxo	11β,14α,15α	[56–58]
125		1α,9β-OBzt, 4β-OH, 6-Oxo, 2β-OGly-(2′,6′-OAc), 5β,11-Oxy	14α,15α	[58]
126		1α,9β-OBzt, 4β-OH, 6-Oxo, 2β-OGly-$(OAc)_4$, 5β,11-Oxy	14α,15α	[58]
127		1α,9β-OBzt, 2β,3β-OAc, 4β-OH, 5β,11-Oxy	14α,15α	[59]
128		1α-OBzt, 2β,6β-OAc, 3β, 4β-OH, 5β,11-Oxy, 9β-OCin	11β,14α,15α	[60]
129		1α-OBzt, 2β,3β,6β-OAc, 4β-OH, 5β,11-Oxy, 9β-OCin	11β,14α,15α	[60]
130		1α-OCin, 4β-OH, 5β,11-Oxy, 6β,8α,15-OAc, 9α-OBzt	11β,14α,15α	[48]
131	Triptofordin D-2	1β-OCin, 4α-OH, 5α,11-Oxy, 6α,8β,15-OAc, 9β-OBzt	11α,14β,15β	[45]
132	Triptofordin D-1	1β-OCin, 4α-OH, 5α,11-Oxy, 6α,15-OAc, 8-Oxo, 9β-OBzt	11α,14β,15β	[45]
133		1β-OCin, 2β,6α,15-OAc, 4α-OH, 5α,11-Oxy, 8-Oxo, 9β-OBzt	11α,14β,15β	[45]
134		1α-OCin, 2β,4β-OH, 5β,11-Oxy, 6β,9β-OAc	11β,14α,15α	[54,56]
135	Rzedowskin C	1α-OEpcin, 2β,4β-OH, 5β,11-Oxy, 6β,9β-OAc	11β,14α,15α	[56]
136	Euonydin A-5	1β,9α-OFur, 2β-OBut, 4α,6α-OH, 5α,11-Oxy, 15-OAc	11α,14β,15β	[51]
137	Euonydin A-4	1β,2β,9α-OFur, 4α,6α-OH, 5α,11-Oxy, 15-OAc	11α,14β,15β	[51]
138	Triptogelin B-2	1β-ONic, 5α,11-Oxy, 6α-OAc, 8β,9β-OBzt	11α,14β,15β	[42]
139	Triptogelin A-5	1β-ONic, 2β,9β-OBzt, 5α,11-Oxy, 6α-OAc, 8β-OMeBu	11α,14β,15β	[27]
140	Triptogelin A-10	1β-ONic, 2β,8β,9β-OBzt, 5α,11-Oxy, 6α-OAc	11α,14β,15β	[42]
141		1α-ONic, 2α,6-OAc, 4β-OH, 5,11-Oxy, 9-OFur, 15-OiBu	14α,15α	[61]
142		1α-ONic, 2α,6-OAc, 4β-OH, 5,11-Oxy, 9-OFur, 15-OMeBu	14α,15α	[61]
143		1α-ONic, 2α,6,15-OAc, 4β-OH, 5,11-Oxy, 9-OFur	14α,15α	[61]
144		1α-ONic, 2α,6,15-OAc, 4β-OH, 5,11-Oxy, 9-OBzt	14α,15α	[61]
145	11,12,13-Trinor-3,4-diepicuauhtemone	3β,4β-OH, 8-Oxo, 11,12,13-Trinor	14α,15β	[62]
146		3β,4α-OH, 6β-OCin	11β,14β,15β	[15]
147		3α-OEpang, 4α-OAc, 8-Oxo	14β	[63]
148		3α-OEpang, 4α-OAc, 8-Oxo, 7β,11β-Epoxy	14β,15β	[64]
149	*trans*-Dihydrocarisone	3-Oxo, 11-OH	11β,14α,15β	[65,66]
150		4-$O(CH_2)_2O$-4; 8α,11-OH, 14-Nor	11β,15β	[67]
151		4-$O(CH_2)_2O$-4; 8-Oxo, 11-OH, 14-Nor	11β,15β	[67]

Table 1 (*continued*)

Subst.	Trivial names	Substituents	Stereochemistry	References
152		4-Oxo, 8α,11-OH, 14-Nor	11β,15β	[67]
153		4,12,13-Oxo, 12,13-OMe, 14-Nor	11β,15β	[67]
154	Verbesindiol	4α,6β-OH	11β,14β,15β	[68]
155		4α-OH, 6β-O-*trans*-Cou	11β,14β,15β	[68]
156		4α-OH, 6α-OAc	11α,14β	[20]
157	5β-Acetoxyvitranoxide	4α,7α-Oxy, 6β-OAc	11β,14β,15β	[69]
158		4α-OH, 6-Oxo	11β,14β,15β	[68]
159	8α-Acetoxycryptomeridiol	4α,11-OH, 8α-OAc	14β,15β	[70]
160		4α-OH, 11-OAc	11β,14β,15β	[71]
161	1-Oxoisocryptomeridiol	1-Oxo, 4α,11-OH	11β,14β,15β	[72]
162		4β-OH, 6-OCin	11β,14α,15β	[14]
163		4β,9β-OH, 6β-OCin	11β,14α,15β	[73]
164		4β,5β-OH	11β,14α,15α	[74]
165		4β,11-OH	11β,14α,15α	[74]
166	Geosmin	5α-OH, 11,12,13-Trinor	14α,15β	[75]
167	Eudesmane-5α,11-diol	5α,11-OH	11β,14β,15β	[71]
168		5β,11-OH	11β,14β,15α	[76]
169		5β,11-OH	11β,14α,15α	[76]
170	α-Dihydroeudesmol	11-OH	11β,14α,15β	[75]
171	β-Dihydroeudesmol	11-OH	11β,14β,15β	[11,75]
172	4-Epi-Aubergenone	3-Oxo, 11-OH, Δ^1	11β,14α,15β	[65,77,78]
173		3-Oxo, 11-OH, Δ^1	11β,14β,15α	[77]
174		6α-OAc, 7α-OH, Δ^3	11β,15β	[79]
175	Eudesm-3-ene-7α-ol	7α-OH, Δ^3	11β,15β	[79]
176	7-epi-α-Eudesmol	11-OH, Δ^3	11α,15β	[80]
177	5,7-Diepi-α-eudesmol	5β-H, 11-OH, Δ^3	11α,15β	[81]
178		11-OGly[$(OAc)_3$,6′-OTig], Δ^3	11β,15β	[82]
179	3-Eudesmene-1β,11-diol	1β,11-OH, Δ^3	11β,15β	[71]
180		1β-OAc, 11-OH, Δ^3	11β,15β	[71]
181		1β-OH, 6β-OCin, Δ^3	11β,15β	[73]
182	5α-OH-Isopterocarpolone	2-Oxo, 5α, 11-OH, Δ^3	11β,15β	[72]
183		1α-OCin, 2-Oxo, 5β,11-Oxy, 6β, 9β-OAc, Δ^3	11β,15α	[54]
184		11-OH, Δ^4	11β,15β	[83]
185	7-epi-γ-Eudesmol	11-OH, Δ^4	11α,15β	[71]
186		11-OXyl-$(OAc)_3$, 14-OAc, Δ^4	11β,15β	[84]
187	4-Eudesmene-1β,11-diol	1β,11-OH, Δ^4	11β,15β	[71]
188		1β,11-OH, Δ^4	11α,15β	[71]
189		1β-OAc, 11-OH, Δ^4	11β,15β	[71]
190	Acorusnol	1β-OH, 6-Oxo, Δ^4	11β,15β	[85]
191	Acorusdiol	1β,3α-OH, 6-Oxo, Δ^4	11β,15β	[85]
192		1β-OH, 3α-OOH, 6β-OCin, Δ^4	11β,15β	[73]
193		1β-OH, 3-Oxo, 6β-OCin, Δ^4	11β,15β	[15]
194	α-Carissanol	2α,11-OH, 3-Oxo, Δ^4	11β,15β	[86]
195	Carissone	3-Oxo, 11-OH, Δ^4	11β,15β	[86]
196	6β-Carissanol	3-Oxo, 6β, 11-OH, Δ^4	11β,15β	[86]
197		3,12-Oxo, 8α-OH, 12-OMe, Δ^4	11β,13α,15β	[87]
198		3,12-Oxo, 8β-OH, 12-OMe, Δ^4	11β,13α,15β	[87]
199		3,8,12-Oxo, 12-OMe, Δ^4	11β,13α,15β	[87]
200	10-Epijunenol	5α-H, 6α-OH, $\Delta^{4(14)}$	11β,15α	[88]
201	Junenol	6α-OH, $\Delta^{4(14)}$	11β,15β	[88]
202	β-Eudesmol	11-OH, $\Delta^{4(14)}$	11β,15β	[89,90]

Table 1 (*continued*)

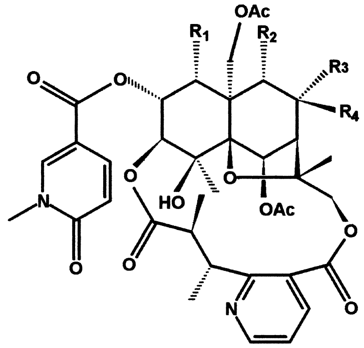
Subst.	Trivial names	Substituents	Stereochemistry	References
203		11-OAra, $\Delta^{4(14)}$	11β,15β	[90]
204	Arctiol	8α,11-OH, $\Delta^{4(14)}$	11β,15β	[67]
205		8-Oxo, 11-OH, $\Delta^{4(14)}$	11β,15β	[67]
206		12,13-Oxo, 12,13-OMe, $\Delta^{4(14)}$	11β,15β	[67]
207		1β,6α-OH, $\Delta^{4(14)}$	15β	[91]
208		1β,6α-OH, $\Delta^{4(14)}$	11β,15β	[72,92]
209		1β-OH, 6β-OCin, $\Delta^{4(14)}$	11β,15β	[73]
210	Selin-4(14)en-1,11diol	1β,11-OH, $\Delta^{4(14)}$	11β,15β	[93]
211		1-Oxo, 11-OH, $\Delta^{4(14)}$	11β,15β	[93]
212		1β-OAc, 11-OH, $\Delta^{4(14)}$	11β,15β	[71]
213		1α-OBzt, 5β,11-Oxy, 6β,9β-OAc, $\Delta^{4(14)}$	11β,15α	[54]
214		1α-OBzt, 5β,11-Oxy, 6β,8β,9α-OAc, $\Delta^{4(14)}$	11β,15α	[54]
215		1α-OBzt, 5β,11-Oxy, 6β,9α-OAc, 8-Oxo, $\Delta^{4(14)}$	11β,15α	[54]
216	Pterocarpol	2α,11-OH, $\Delta^{4(14)}$	11β,15β	[94]
217	Pterocarpol-acetate	2α-OAc, 11-OH, $\Delta^{4(14)}$	11β,15β	[94]
218		3α,11-OH, $\Delta^{4(14)}$	11β,15β	[66]
219		11-OH, Δ^{5}	11β,14α,15α	[95]
220		11-NC, Δ^{5}	11α,14β,15β	[96]
221	Stylotelline	5α-NC, Δ^{6}	14α,15β	[97]
222		1β-OH, 4β-OCin, Δ^{6}	14α,15β	[73]
223		1β,2α-OH, 4β-OCin, Δ^{6}	14α,15β	[73]
224		1β-OAc, 4β-OH, Δ^{6}	14α,15β	[98]
225	Erigeside A	3-OGly, 5α,9α-OH, Δ^{6}	14α,15β	[99]
226	4-Epiplucheinol	3α,4β,11-OH, 8-Oxo, Δ^{6}	14α,15β	[100]
227	Plucheinol	3α,4α,11-OH, 8-Oxo, Δ^{6}	14β,15β	[100]
228		3α,4β,5α,11-OH, 8-Oxo, Δ^{6}	14α,15β	[101]
229		3α-OAng,4α, 11-OH, 8-Oxo, Δ^{6}	14β,15β	[102]
230	Arguticinin	3α-OEpang, 4β-OAc, 8-Oxo, 11-OH, Δ^{6}	14α,15β	[103]
231	Odontinin	3α-O2MeBu-(2’OAc, 3’OH), 4α-OAc, 8-Oxo, 11-OH, Δ^{6}	14β,15β	[101]
232		3β-OAng, 4α, 11-OH, 8-Oxo, Δ^{6}	14β,15β	[104]
233		3β-OAng, 4α-OH, 8-Oxo, 11-OOH, Δ^{6}	14β,15β	[104]
234		3β-OAng, 4β-OAc, 8-Oxo, 11-OH, Δ^{6}	14α,15β	[104]
235	6-Eudesmene-4α-ol	4α-OH, Δ^{6}	11β,14β,15β	[17]
236	Oplodiol	1β,4β-OH, Δ^{7}	14α,15β	[98]
237		1β-OH, 4β-OCin, Δ^{7}	14α,15β	[73]
238	Oplodiol-monoacetate	1β-OAc, 4β-OH, Δ^{7}	14α,15β	[98]
239		1β,2α-OH, 4β-OCin, Δ^{7}	14α,15β	[73,105]
240		1β,3α-OH, 4β-OCin, Δ^{7}	14α,15β	[105]
241		1β,4-OH, 8-Oxo, $\Delta^{7(11)}$	15β	[106]
242		1α,4α-OH, 8-Oxo, $\Delta^{7(11)}$	14β,15α	[106]
243		1α,4β-OH, 8-Oxo, $\Delta^{7(11)}$	14α,15α	[107]
244	Cuathemone	3α,4α-OH, 8-Oxo, $\Delta^{7(11)}$	14β,15β	[108]
245		3α-OEpang, 4α-OAc, 8-Oxo, $\Delta^{7(11)}$	14β,15β	[108]
246	Argutin	3α-O2MeBu-(2’OAc,3’-OH), 4α-OAc, 8-Oxo, $\Delta^{7(11)}$	14β,15β	[109]
247		3α-OAng, 4α-OAc, 8-Oxo, $\Delta^{7(11)}$	14β	[110]
248		3β-OAng, 4α-OAc, 8-Oxo, $\Delta^{7(11)}$	14β,15β	[110]
249		3β-OAng, 4α-OH, 8-Oxo, $\Delta^{7(11)}$	14β,15β	[104]
250		3β-OAng, 4β-OAc, 8-Oxo, $\Delta^{7(11)}$	14α,15β	[104]
251		3β-OAng, 4β-OAc, 8β-OH, 8α,12-Oxy, $\Delta^{7(11)}$	14α,15β	[104]
252		1β-OH, 4β-OCin, 7α-OOH, Δ^{8}	11β,14α,15β	[73]
253	α-Corymbolol	1α,5α-OH, Δ^{11}	11β,14β,15β	[111]

Table 1 (*continued*)

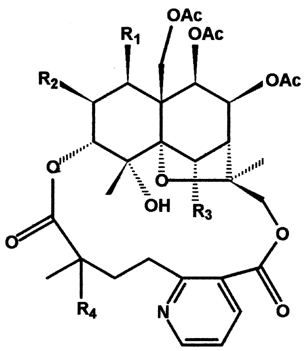
Subst.	Trivial names	Substituents	Stereochemistry	References
254	β-Corymbolol	1β,5α-OH, Δ^{11}	11β,14β,15β	[111]
255		1β-O(αOH-dihydroCou), 6α-OH, 13-Oxo, 13-OMe, 14-OGly, Δ^{11}	11β,14α,15β	[112]
256		see Fig. 2	11β,14α,15β	[112]
257		1β,4β,6α,8α, 14-OH, 13-Oxo, 13-OMe, Δ^{11}	11β,14α,15β	[113]
258		1β,4β,6α,14-OH, 13-Oxo, 8α-OMeAcr-(4’OH), 13-OMe, Δ^{11}	11β,14α,15β	[113]
259		1β,4β,6α-OH, 13-Oxo, 13-OMe, 14-OGly, Δ^{11}	11β,14α,15β	[112]
260	Ixerisoide-J	1β-O(α-OH-iVa), 4β,6α-OH, 13-Oxo, 13-OMe, 14-OGly, Δ^{11}	11β,14α,15β	[112]
261	Ixerisoside-K	1β-O(α-OH-dihydroCou), 4β,6α-OH, 13-Oxo, 13-OMe, 14-OGly, Δ^{11}	11β,14α,15β	[112]
262	Ixerisoside-L	see Fig. 2	11β,14α,15β	[112]
263		1β,6α-OH, 4α,14-Epoxy, 8α-OMeAcr-(4’-OH), 13-Oxo, 13-OMe, Δ^{11}	14β,15β	[114]
264	Corymbolone	1-Oxo, 5α-OH, Δ^{11}	11β,14β,15β	[111]
265	Isocorymbolone acetate	1-Oxo, 9α-OAc, Δ^{11}	11β,14α,15β	[115]
266	Pluchecinin	3β-OEpang, 4α-OH, 8,13-Oxo, 13-OMe, Δ^{11}	14β,15β	[62]
267		3α-OAc, 4α-OH, 13-Oxo, 13-OMe, Δ^{11}	11β,14β,15β	[116]
268		3,13-Oxo, 4α,5α-Epoxy, 13-OMe, Δ^{11}	11β,14β,15β	[117]
269		4α-OH, Δ^{11}	11β,14β,15β	[118]
270	Ilicic acid	4α-OH, 13-Oxo, 13-OMe, Δ^{11}	11β,14β,15β	[119]
271	Arbusculin-E-methylester	4α,6α-OH, 13-Oxo, 13-OMe, Δ^{11}	14β,15β	[120]
272	Isointermedeol	4α-OH, Δ^{11}	11α,14β,15β	[121]
273		4α-OAc, Δ^{11}	11β,14β,15α	[122]
274		4β-OFuc, Δ^{11}	11β,14α,15α	[122]
275		4β-OFuc-(2’-OMeBu), Δ^{11}	11β,14α,15α	[122]
276		4β-OFuc-$(OAc)_3$, Δ^{11}	11β,14α,15α	[122]
277		4β-OFuc-(2’OMeBu, 3’,4’OAc), Δ^{11}	11β,14α,15α	[122]
278		4β-OFuc(3’,4’Oisopropylidene), Δ^{11}	11β,14α,15α	[122]
279		4β-OFuc-(2’-OMeBu, 3’,4’Oisopropylidence), Δ^{11}	11β,14α,15α	[122]
280	4αH-Eudesm-5α-ol	5α-OH, Δ^{11}	11β,14β,15β	[123,124]
281	Occidentalol	11-OH, 5α-H, $\Delta^{1,3}$	11β,15α	[125]
282	Dehydrocarissone	3-Oxo, 11-OH, $\Delta^{1,4}$	11β,15β	[65]
283		3-Oxo, 8α-OH, 12-Oxo, 12-OMe, $\Delta^{1,4}$	11β,13α,15β	[87]
284		3,12-Oxo, 8β-OH, 12-OMe, $\Delta^{1,4}$	11β,13α,15β	[87]
285		3,8,12-Oxo, 12-OMe, $\Delta^{1,4}$	11β,13α,15β	[87]
286	Benghalesin-A	3-Oxo, 6β-OH, 6α,14-Peroxy, $\Delta^{1,4}$	11β,15β	[126]
287	Benghalesin-B	3-Oxo, 6β,7α-OH, 6α,14-Oxy, $\Delta^{1,4}$	11β,15β	[126]
288		6α-OAc, $\Delta^{1,4(14)}$	11α,15β	[20]
289		4β-OH, 13-Oxo, 13-OMe, $\Delta^{2,11}$	11β,14α,15β	[127]
290		$\Delta^{3,5}$	11β,15α	[74]
291		11-OXyl-$(OAc)_3$, $\Delta^{3,5}$	11β,15β	[84]
292		11-OCin, $\Delta^{3,5}$	11β,15β	[15]
293	α-Selinene	$\Delta^{3,11}$	11β,15β	[128]
294	Hypochoeroside-L	1β-OGly, 14-Oxo, 14-OH, $\Delta^{3,11}$	15β	[129]
295		1β-OH, 13-OGly, $\Delta^{3,11}$	—	[130]
296		1β-O(α-OH-dihydroCou), 6α-OH, 13-Oxo, 13-OMe, 14-OGly, $\Delta^{3,11}$	11β,15β	[112]
297	1α-Tigloyloxypolyachyrol	1α-OTig, 2α, 9/3-OAc, 15-OH, $\Delta^{3,11}$	11β,15α	[131]
298		1-Oxo, 2α,5α-Peroxy, $\Delta^{3,11}$	11β,15β	[132]
299		2α-OMe, 13-Oxo, 13-OH, $\Delta^{3,11}$	11β,15β	[127]
300	7-epi-Teucrenone	2-Oxo, 7α-OH, $\Delta^{3,11}$	11β,15α	[133]

Table 1 (*continued*)

Subst.	Trivial names	Substituents	Stereochemistry	References
301		5-OH, $\Delta^{3,11}$	11β,15β	[124]
302	Selina-3,11-dien-9-ol	9β-OH, $\Delta^{3,11}$	11β,15β	[134]
303	Selina-3,11-dien-9-one	9-Oxo, $\Delta^{3,11}$	11β,15β	[134]
304	β-Costol	13-OH, $\Delta^{3,11}$	11β,15β	[66]
305		13-OH, 13-Oxo, $\Delta^{3,11}$	11β,15β	[135]
306	Selina-3,11-dien-14-al	14-Oxo, $\Delta^{3,11}$	11β,15β	[136]
307		14-Oxo, 14-OMe, $\Delta^{3,11}$	11β,15β	[136]
308	Selina-4,11-dien-14-al	14-Oxo, $\Delta^{4,11}$	11β,15β	[136]
309		14-Oxo, 14-OMe, $\Delta^{4,11}$	11β,15β	[136]
310	1β-OH-α-Ciperone	1β-OH, 3-Oxo, $\Delta^{4,11}$	11β,15β	[132]
311		8α,13-OH, 13-Oxo, $\Delta^{4,11}$	15β	[137]
312		9β-OH, 14-Oxo, 14-OMe, $\Delta^{4,11}$	11β,15β	[136]
313		9β,13-OH, 13-Oxo, $\Delta^{4,11}$	–-	[63]
314		9β-OAc, 13-OH, 13-Oxo, $\Delta^{4,11}$	15β	[138]
315		9β-OAc, 13-OH, 13-Oxo, $\Delta^{4,11}$	–-	[63]
316		9,13-Oxo, 13-OH, $\Delta^{4,11}$	–-	[63]
317	γ-Costol	13-OH, $\Delta^{4,11}$	11β,15β	[66]
318		1β-OAc, $\Delta^{4(14),7}$	15β	[91]
319	Ventricosin-A	8-Oxo, $\Delta^{4(14),7(11)}$	15α	[139]
320		9α-OH, $\Delta^{4(14),7(11)}$	15β	[75]
321		12-Oxo, 12-OMe, 13-OH, $\Delta^{4(14),7(11)}$	15β	[140]
322	β-Selinene	$\Delta^{4(14),11}$	11β,15β	[128]
323		1β,3β-OH, $\Delta^{4(14),11}$	15β	[129]
324	Hypochoeroside-K	1β-OH, 3β-OGly, $\Delta^{4(14),11}$	15β	[129]
325		1β-OH, 3-Oxo, $\Delta^{4(14),11}$	11β,15β	[141]
326		1β-O(Val-2’OH), 6α-OH, 13-Oxo, 13-OMe, 14-OGly, $\Delta^{4(14),11}$	11β,15β	[112]
327		6α-OH, 13-Oxo, 13-OMe, $\Delta^{4(14),11}$	15β	[120]
328		7α-OH, 13-Oxo, 13-OMe, $\Delta^{4(14),11}$	15β	[140]
329		9,13-OH, 13-Oxo, $\Delta^{4(14),11}$	15β	[142]
330	α-Costol	13-OH, $\Delta^{4(14),11}$	11β,15β	[66,67]
331		13-Oxo, $\Delta^{4(14),11}$	11β,15β	[67]
332	Coralloidin-D	12,13-OAc, $\Delta^{4,7(11)}$	15β	[143]
333	Coralloidin-E	11-OH, $\Delta^{5,7}$	14α,15β	[143]
334	Deacetylcoralloidin-A	8β-OH, $\Delta^{5,7(11)}$	14α,15β	[144]
335	Coralloidin-A	8β-OAc, $\Delta^{5,7(11)}$	14α,15β	[144]
336	Deacetylcoralloidin-C	15α-OH, $\Delta^{5,7(11)}$	14α,15β	[143]
337	Coralloidin-C	15α-OAc, $\Delta^{5,7(11)}$	14α,15β	[143]
338	Rishitin	2α-OH, 3β-OGly, $\Delta^{5(10),11}$; 15-Nor	11β,14α	[145–148]
339	Rishitin-aglycone	2α,3β-OH, $\Delta^{5(10),11}$; 15-Nor	11β,14α	[147]
340		2α-OAc, 3β-OGly(2’-OGly), $\Delta^{5(10),11}$; 15-Nor	11β,14α	[147]
341		2α-OH, 3β-[OGly(OAc)$_3$-(2′OGly(OAc)$_4$))], $\Delta^{5(10),11}$; 15-Nor	11β,14α	[147]
342	Argentone	2-OMe, 3-Oxo, $\Delta^{1,4,6}$	15β	[149]
343	8-Oxo-argentone	2-OMe, 3,8-Oxo, $\Delta^{1,4,6}$	15β	[149]
344	14-hydroxy-argentone	2-OMe, 3-Oxo, 14-OH, $\Delta^{1,4,6}$	15β	[149]
345	14-Nor-argentone	2-OMe, 3-Oxo, $\Delta^{1,4,6}$; 14-Nor	15β	[149]
346	8Oxo-14Norargentone	2-OMe, 3,8-Oxo, $\Delta^{1,4,6}$; 14Nor	15β	[149]
347		3,13-Oxo, 13-OH, $\Delta^{1,4,11}$	11β,15β	[150]
348		1α,13-OH, 13-Oxo, $\Delta^{2,4(14),11}$	11β,15β	[150]
349		8,12-Oxy, $\Delta^{1,3,7,11}$		[151]
350		6-Oxo, 8,12-Oxy, $\Delta^{1,4,7,11}$		[151]



	R_1	R_2	R_3	R_4	Name
26	OH	OAc	OAc	H	Emarginatine D
27	OH	OH	H	OAc	Emarginatine E
82	OAc	OH	OAc	H	Emarginatine C
83	OAc	OAc	OAc	H	Emarginatine A

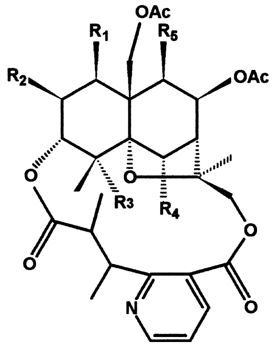


	R_1	R_2	R_3	R_4	Name
33	OH	OBz	OAc	OH	1-Desacetylwilfordine
34	OH	OFur	OAc	OH	1-Desacetylwilfortrine
67	OAc	OAc	OAc	H	Euonine
75	OAc	OBz	OAc	OH	Wilfordine
76	OAc	ONic	OAc	H	---
104	OBz	OAc	OAc	H	Euojaponine F
115	OBz	OBz	OH	H	Ebenifoline W-II
116	OBz	OBz	OAc	H	Ebenifoline W-I

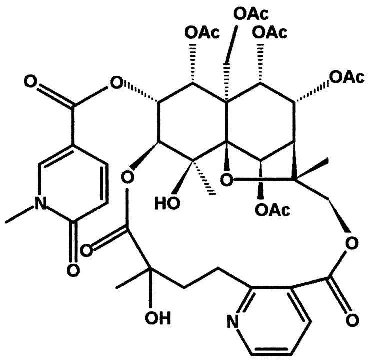
Fig. 2. Compounds not described in Table 1.

5. Results

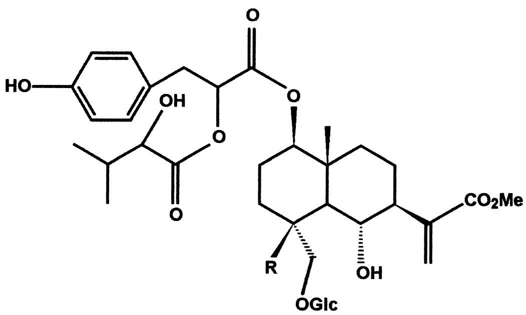
The PICKUP program afforded countless chemical shift ranges that characterise several substructures present in eudesmanes. These results and the percentage success of recognition are presented in Table 3. The use of these groups of chemical shifts can be applied in the processes of structure elucidation for new eudesmanes, for example, if the ^{13}C NMR data of an unpublished eudesmanes showed chemical shifts in the range of the first group presented in Table 3, it is possible to affirm with 100% recognition, that the structure of the new substance presents a carbonyl group at carbon 8, and that carbons 5, 9 and 10 do not bear substituents, for example, the eudesmanes XXVI, XXVII and XXVIII shown in Table 4. In



	R_1	R_2	R_3	R_4	R_5	Name
68	OAc	OAc	OAc	OH	OH	1-Desacetylwilfordine
100	OBz	OH	OAc	OH	OH	1-Desacetylwilfortrine
101	OBz	OH	OAc	H	H	Euonine
105	OBz	OBz	OAc	OH	OH	Wilfordine
106	OBz	ONic	OAc	H	H	---
107	OBz	OAc	OAc	H	H	Euojaponine F
108	OBz	OBz	OH	H	H	Ebenifoline W-II
109	OBz	OBz	OAc	H	H	Ebenifoline W-I



84 - Emarginatinine



	R
256	H
262	OH

Fig. 2. (*continued*)

Table 2
Chemical shifts and multiplicity data of the eudesmanes presented in Table 1 (solvents: $CDCl_3$; A = $(CD_3)_2CO$; B = C_6D_6; D = $(CD_3)_2SO$; P = C_5D_5N)

Site	1	2	3	4	5	6	7	8	9	10	11	12	13	14[B]	15
1	80.3	80.5	80.0	78.9	80.5	80.4	80.3	80.3	80.5	81.0	91.3	90.9	84.5	84.5	84.5
2	27.3[a]	40.1	28.6	26.7	26.8	28.7	28.5	28.8	28.0	34.4	28.6	27.3	23.7	23.4	23.4
3	31.5[b]	40.6	37.7	45.2	39.6	41.6[a]	41.3	40.8	39.7	39.4	38.8	37.5	41.9	43.0	42.7
4	33.1[b]	72.1	72.0	75.4	71.8	71.2	71.1	71.7	80.4	71.4	72.5	72.8	82.5	82.5	82.4
5	45.9[c]	46.1	47.3	55.3	53.1	55.3	55.1	53.0	57.6	44.9	48.6	47.3	53.2	57.4	57.2
6	26.4[a]	29.3	20.9	69.7	70.9	69.8	69.7	70.4	75.6	29.0	21.6	20.8	72.0	69.4	69.5
7	49.7[c]	74.8	41.3	49.9	49.9	49.9	49.6	49.6	51.2	73.6	43.0	41.0	43.3	49.8	49.9
8	22.6	30.1	20.6	21.2	20.9	20.8	20.6	21.2	22.2	29.0	21.6	20.7	21.2	23.8	23.2
9	40.3	27.7	41.2	41.0	40.5	41.4[a]	41.5	38.6	39.1	23.4	41.9	41.0	28.9	33.1	33.0
10	39.2	35.8	38.7	34.8	39.4	39.1	39.1	39.4	33.2	37.9	40.2	38.8	48.4	48.5	48.3
11	72.5	40.5	74.8	28.9	28.7	28.8	28.8	29.7	29.6	39.1	75.2	74.6	27.4	29.6	29.3
12	27.3	17.4	29.7	21.2	21.4	21.3	21.2	21.6	18.5	17.0	29.6	29.6	23.6	21.8	21.6
13	26.9	17.5	29.7	20.8	20.5	20.7	20.6	20.9	20.7	16.9	29.0	29.5	19.9	21.0	20.6
14	14.9	29.9	22.2	21.6	29.8	24.7	24.6	20.5	76.5	29.8	22.1	22.1	23.6	17.8	22.5
15	14.0	12.2	13.2	15.3	13.9	14.9	14.7	13.5	12.8	12.6	14.5	13.6	17.1	22.8	17.3

Site	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
1	84.9	65.9	65.1	65.2	216.0	37.6	36.1	74.8	72.1	69.6[a]	72.5	74.5	76.4	76.4	76.1
2	23.5	31.1	31.3	31.2	34.0	17.0	21.4	28.1	71.4	73.3[a]	72.1	70.5	26.9	71.4	71.3
3	42.8	41.9	37.9[a]	38.0[a]	32.6[a]	29.5	32.2	26.3	32.5	29.7	75.6	75.2	25.6	32.5	32.4
4	82.6	71.0	84.3	83.9	32.3[a]	40.5	32.2	34.8	33.7	33.1	69.9	70.2	34.0	33.5	33.5
5	57.1	51.0	45.8[b]	46.4[b]	47.0[b]	87.8	87.3	93.3	91.6	89.3	93.8	93.8	91.3	91.6	91.4
6	69.6	77.3	73.9	73.8	26.8	38.4	38.1	75.9	75.2	78.3	73.7	74.5	72.0	74.9	75.1
7	49.9	43.8	44.5[b]	44.3[b]	49.2[b]	44.6	43.8	57.7	53.1	48.8	50.5	49.3	53.1	54.3	53.0
8	23.2	22.9	22.6	22.4	22.3	25.1	25.1	78.1	76.3	34.3	69.3	74.5	75.3[a]	70.5	72.0
9	33.1	37.1	37.6[a]	37.7[a]	35.1	38.1	38.1	80.9	75.9	69.3[a]	71.2	76.3	75.5[a]	78.0	75.7
10	48.4	41.9	42.5	42.3	48.2	38.4	38.6	46.8	49.2	54.6	52.2	51.2	49.7	49.0	49.0
11	29.4	23.9	23.5	23.6	72.4	81.2	81.0	82.7	81.4	82.6	84.0	85.5	81.4	81.1	81.3
12	21.5	22.1	22.1	22.1	27.5	23.6	23.5	26.7	24.2	31.9	18.5	19.3	24.2	24.1	24.1
13	20.8	25.1	25.3	25.4	26.8	30.6	30.2	32.4	18.2	26.0	70.2	70.2	30.7	30.8	30.7
14	22.3	23.1	21.9	21.5	14.8	17.7	15.7	18.0	13.3	17.9	23.3	24.3	16.8	18.7	18.7
15	17.5	15.5	16.6	16.7	19.2	22.9	23.0	11.5	30.8	65.2	60.7	60.5	11.0	13.4	13.3

Table 2 (*continued*)

Site	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45
1	76.9	80.6	72.9	72.7	73.6	73.1	71.8	73.4	78.8	75.7	79.0[a]	78.0	72.9	71.7	75.5
2	71.0	210.0	73.5	72.7	27.0	22.1	26.7	26.5	22.1	26.5	23.4	22.8	22.2	23.8	26.5
3	32.5	42.8	76.5	76.5	22.0	26.7	22.2	22.0	26.5	22.8	26.7	26.0	26.6	38.2	22.8
4	33.0	38.8	69.7	69.7	40.0	39.9	33.9	33.9	33.8	39.8	39.9	33.2	39.7	70.2	39.8
5	91.0	89.8	93.6	93.8	87.7	87.3	91.2	91.2	90.0	88.2	88.5	90.8	86.4	91.2	88.1
6	75.0	73.6	73.8	73.7	36.6	36.4	74.6	76.2	75.1	36.3	32.0	75.2	36.6	75.8	36.5
7	52.5	53.0	50.8	50.9	43.9	43.6	53.0	52.1	52.4	47.2	48.0	52.0	48.2	53.7	47.2
8	72.5	72.0	69.4	69.3	31.6	31.5	78.9	76.8	71.3	76.7	70.0[a]	74.0	71.7	70.1	76.8
9	76.0	75.3	72.4	72.0	74.0	74.6	75.0	79.0	74.3	76.1	74.3[a]	75.4	68.4	68.0	76.1
10	49.0	55.3	51.4	51.7	47.9	47.9	48.9	46.7	48.8	50.1	49.0	49.4	51.2	52.9	50.2
11	81.5	82.7	84.8	84.7	82.0	81.9	81.7	82.5	81.6	81.7	80.5	82.3	82.0	84.4	81.6
12	24.0	24.2	17.9	17.9	24.3	24.1	24.2	25.7	24.1	24.4	22.9	30.6	24.9	26.2	24.4
13	31.0	30.7	69.7	69.7	30.3	30.2	16.8	30.8	30.6	30.8	29.9	25.9	31.0	30.0	30.7
14	18.0	17.9	23.6	23.2	17.8	17.5	12.3	16.9	16.8	16.9	16.1	15.9	17.3	23.7	17.1
15	13.0	12.7	62.6	61.9	18.3	18.0	30.6	12.5	12.0	61.6	61.2	60.9	63.8	64.1	60.0

Site	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60
1	75.4[a]	75.5	70.4	70.1	70.7	70.1	70.1	71.6	70.0	76.5	68.1	73.9	73.1	73.6	73.3
2	69.2[a]	69.1	70.7	70.8	71.3	69.0	69.0	70.9	68.5	73.9	70.8	21.8	21.3	21.5	21.3
3	31.0	31.0	30.9	30.9	30.9	40.9	40.9	31.4	40.8	41.3	42.2	27.0	26.8	26.8	26.6
4	39.1	39.2	39.4	39.4	39.2	72.2	72.2	33.4	72.2	72.2	70.0	40.0	34.0	34.4	33.7
5	87.7	87.8	87.1	87.1	87.0	91.8	91.8	90.7	91.9	91.6	91.5	87.7	89.8	90.0	90.3
6	36.4	36.1	35.9	35.9	35.9	75.0	75.0	73.5	75.0	75.2	71.6	36.6	79.6	80.9	76.4
7	47.2	47.2	43.6	43.6	43.7	54.5	54.5	55.4	54.2	53.7	53.1	43.8	48.9	49.0	52.9
8	76.8[a]	76.3	31.0	31.1	31.1	76.0	76.0	77.0	76.1	75.5	75.6	31.6	32.0	32.2	76.0
9	76.3[a]	76.2	74.3	74.4	74.3	76.4	76.4	77.3	76.4	77.0	76.2	74.2	73.4	73.4	75.7
10	50.6	50.6	47.2	47.2	47.0	49.5	49.5	49.0	49.5	50.7	54.1	48.0	50.4	50.7	49.7
11	82.0	81.9	82.2	82.3	82.3	84.2	84.2	82.5	84.2	84.6	83.5	82.1	82.5	82.6	81.7
12	24.4	24.4	24.0	24.0	24.0	26.2	26.2	26.1	26.2	26.4	25.5	17.9	17.4	17.6	25.4
13	30.6	30.7	30.2	30.2	30.2	30.5	30.5	31.4	30.5	30.1	30.0	18.4	18.7	18.9	30.8
14	18.6	18.4	19.1	19.1	19.4	25.2	25.2	19.5	25.2	24.3	24.6	24.3	26.0	26.0	17.3
15	63.3	61.8	19.6	20.0	20.0	21.7	21.7	20.7	21.5	61.8	65.5	30.2	30.7	32.1	18.6

Table 2 (*continued*)

Site	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75
1	72.6	76.6	71.2	71.1	70.5	74.1[a]	73.6	73.4	71.3	71.2	71.6	71.1	71.2	70.1	73.2
2	67.7	200.5	70.0	69.7	68.9	68.3	69.5	68.9	70.3	70.2	70.4	70.5	69.4	69.0	69.3
3	44.1	54.7	31.0	31.0	41.9	42.0	76.0	75.9	31.1	31.2	31.5	31.1	31.2	40.9	76.9
4	70.2	74.1	33.8	34.2	69.7	69.8	69.9	70.7	39.4	39.4	39.8	39.5	33.7	72.2	69.8
5	91.7	91.3	89.6	89.7	91.1	93.3	93.9	94.2	87.3	87.3	87.6	87.3	89.6	91.8	94.0
6	69.2	69.4	79.2	80.4	68.1	74.4[a]	73.9	73.9	36.1	36.1	36.1	36.0	79.2	75.0	73.6
7	54.1	53.9	48.9	49.0	49.1	64.9	51.3	50.7	43.8	43.7	44.0	43.7	48.8	54.5	51.0
8	77.3	77.1	31.6	31.6	34.7	197.0	–	69.1	31.1	31.2	31.3	31.2	31.6	76.0	68.9
9	72.3	72.1	73.1	72.8	78.1	79.7	71.1	70.8	73.8	73.8	73.8	73.5	73.0	76.4	70.8
10	50.1	51.9	50.0	50.1	55.0	52.6	52.3	52.3	47.2	47.1	47.4	47.0	49.8	49.5	51.9
11	84.8	85.8	82.9	82.8	84.6	85.1	84.5	84.3	82.3	82.3	82.6	82.2	82.9	84.2	84.8
12	26.7	26.5	26.9	26.1	29.4	25.2	18.0	18.6	19.3	19.3	19.3	19.3	26.0	26.2	17.9
13	30.3	30.3	30.7	30.9	25.7	29.2	70.4	70.0	20.1	20.2	20.1	20.1	30.6	30.5	69.8
14	25.5	25.0	18.6	18.5	25.1	24.5	22.8	23.0	24.3	24.3	24.5	24.2	18.9	25.2	23.0
15	20.7	19.9	20.4	20.4	65.5	61.0	60.3	60.1	30.2	30.2	30.4	30.2	20.6	21.7	60.6

Site	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90
1	73.3	70.0	75.3	79.0	71.5	75.0	70.8	73.1	73.5	75.4[a]	73.4[a]	70.1	69.7	69.8	70.0
2	70.7	68.5	25.2	67.7	69.5	67.3	69.6	69.4	68.7	26.7	26.7	69.5	67.6	67.9	67.9
3	75.8	40.8	37.9	41.1	29.7	41.1	75.4	75.7	76.6	23.0	22.9	41.9	41.2	42.2	42.2
4	69.7	72.2	70.7	72.3	33.1	72.1	70.5	70.5	69.2	40.0	40.0	69.7	72.2	69.6	69.6
5	93.8	91.9	92.2	91.9	89.2	91.5	93.7	94.1	94.2	88.2	88.2	91.1	91.1	91.2	91.2
6	73.6	75.0	73.3	75.0	78.1	76.9	73.6	73.8	70.4	36.7	36.7	67.9	78.7	78.1	78.1
7	51.2	54.2	53.4	54.6	48.8	53.6	50.2	50.7	51.2	47.3	47.8	49.1	50.2	49.2	49.2
8	68.9	76.1	78.3	76.1	34.8	73.8	71.3	69.0	70.4	78.4[a]	78.4	34.6	34.4	34.5	34.5
9	70.3	76.4	69.7	76.5	69.5	75.3	71.8	70.6	69.9	76.4[a]	76.3	78.1	68.8	69.3	69.8
10	52.1	49.5	52.2	49.6	53.3	50.6	54.0	52.2	52.1	50.3	50.5	55.1	53.6	54.9	55.1
11	84.5	84.2	82.9	84.2	82.7	84.4	84.8	84.4	84.8	81.9	81.9	84.6	84.8	84.5	84.6
12	18.0	26.2	24.4	25.0	30.3	30.0	18.3	18.7	17.9	24.6	24.6	29.4	26.4	26.5	25.7
13	70.6	30.5	29.5	21.8	25.9	26.7	70.1	70.0	70.7	30.8	30.8	25.7	30.0	29.4	29.4
14	23.0	25.2	22.6	26.2	17.7	24.2	23.7	23.4	22.8	17.1	17.1	25.0	24.6	25.0	25.1
15	60.3	21.5	60.9	30.5	65.4	61.7	60.4	60.5	60.2	63.1	63.1	65.5	65.8	65.9	65.9

Table 2 (*continued*)

Site	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105
1	70.1	71.5	71.6	73.5	75.6	69.3	73.1[a]	73.5	79.2	75.5	75.5	74.3	76.2	73.6	73.5
2	69.5	26.8	22.2	26.9	22.7	70.8	24.0	23.4	69.3	70.1	70.2	68.8	70.7	69.9	69.2
3	41.8	22.6	26.5	21.6	26.4	31.4	37.1	37.3	32.7	78.4	78.4	42.1	31.7	76.0	78.4
4	69.7	33.7	33.8	34.5	39.8	32.8	70.3	73.1	33.7	70.6	70.8	69.8	34.2	70.0	70.7
5	91.1	92.6	91.1	90.2	88.2	90.4	90.7	91.5	91.0	94.6	94.3	93.4	92.4	93.9	93.8
6	68.1	72.8	74.3	73.8	36.2	72.6	31.2	79.7	74.9[a]	74.1	75.1	74.6	75.5	73.9	74.9
7	49.1	54.5	52.8	49.1	47.3	53.6	43.7	50.2	53.0	50.5	50.4	65.0	65.8	51.2	50.4
8	34.4	74.7	74.9	32.2	76.0	74.9	31.6	32.0	74.8[a]	69.1	69.2	197.1	198.7	69.1	69.1
9	78.1	79.6	79.0	80.3	78.2	77.6	73.8[a]	73.2	74.9[a]	71.8	72.0	79.7	80.4	71.7	71.6
10	55.1	48.7	49.0	50.7	50.1	51.1	48.2	50.6	49.0	53.0	53.1	53.1	52.7	52.6	52.7
11	84.6	81.8	81.7	82.6	81.6	81.2	83.5	84.5	81.7	84.2	84.3	85.2	84.1	84.7	84.4
12	29.4	24.5	24.1	26.1	24.3	24.6	24.0	26.6	24.2	18.5	18.4	25.2	25.6	17.9	18.4
13	25.7	31.1	30.5	30.8	30.7	30.4	30.1	30.1	30.7	70.2	70.2	29.3	31.2	70.4	70.0
14	25.0	17.4	16.7	17.6	16.6	16.4	24.4	23.8	18.6	23.1	23.2	24.6	18.6	22.8	22.9
15	65.4	12.3	12.4	18.9	61.5	60.9	19.3	20.3	15.5	60.5	60.5	61.1	61.0	60.4	60.2

Site	106	107	108	109	110	111[P]	112	113	114	115	116	117	118	119	120
1	73.6	74.4	73.5	73.6	76.4	79.0	76.5	76.5	76.4	73.5	73.5	72.6	72.6	72.6	73.7
2	69.3	70.0	69.1	69.3	69.8	71.4	70.8	71.0	70.8	70.7	70.5	23.9	23.4	23.3	24.2
3	75.9	75.8	75.2	75.8	31.2	34.6	31.3	31.4	31.3	75.2	75.9	38.5	37.2	38.5	38.3
4	70.7	36.0	72.7	70.7	33.5	34.8	33.5	33.5	33.5	72.0	69.9	70.6	73.0	70.3	70.5
5	94.2	90.8	93.2	94.2	90.7	93.7	90.9	90.9	90.8	93.0	93.9	86.1	91.5	91.5	92.5
6	74.0	74.4	74.5	74.0	74.8	72.1	74.7[a]	74.5	74.7	74.3	73.9	212.0	79.7	79.7	78.2
7	50.5	50.4	51.9	50.6	52.8	57.6	53.1	52.7	53.0	52.6	51.2	55.2	50.2	49.0	54.2
8	69.3	69.2	69.4	69.1	72.4	72.1	71.7	71.4	72.4	69.3	69.0	33.5	32.0	31.8	72.8[a]
9	71.6	71.8	71.8	71.5	74.5	77.1	74.8[a]	75.0	74.7	72.0	71.7	72.3	73.3	72.9	80.2[a]
10	53.2	51.3	52.1	52.7	49.0	48.5	48.9	49.1	49.0	51.2	52.5	56.0	50.3	51.4	48.1
11	84.5	82.6	85.0	84.5	81.9	81.2	82.1	82.0	82.1	85.4	84.7	78.1	84.6	84.3	84.3
12	18.6	18.2	18.8	18.5	24.2	24.5	24.2	24.1	24.2	18.2	18.0	21.2[a]	30.2	29.6	30.0
13	70.0	69.9	70.9	70.1	30.6	31.9	30.7	30.7	30.7	71.4	70.4	23.5[a]	26.7	25.7	25.7
14	23.1	14.2	23.5	23.0	18.3	20.1	18.5	18.5	18.5	23.9	23.2	29.6	23.9	24.0	23.9
15	60.2	60.1	61.0	60.2	14.2	13.8	14.1	14.2	14.6	61.6	60.8	17.1	19.9	19.6	13.6

Table 2 (*continued*)

Site	121	122	123	124	125[D]	126	127	128	129	130	131	132	133	134	135
1	73.4	9.37[d]	72.7	72.1	72.2	72.0	73.4	68.2	67.8	75.4	75.3	76.0	74.3	72.7	72.7
2	24.0	23.7	25.2	69.0	73.3	73.0	69.0	70.8	68.3	25.2	25.1	25.3	68.8	67.6	67.6
3	38.1	38.2	37.9	44.4	42.8	45.0	70.0	78.1	77.2	38.0	37.9	38.3	42.1	49.1	49.1
4	70.4	70.2	70.6	71.0	69.9	70.7	68.1	71.6	70.1	70.7	70.5	70.5	69.8	84.6	84.6
5	92.6	91.4	92.2	85.8	84.9	85.5	89.9	93.0	91.1	92.2	92.1	93.6	93.4	91.2	91.2
6	78.1	78.2	78.6	211.0	212.7	211.3	30.3	80.4	78.8	72.8	72.6	74.5	74.6	76.2	76.2
7	52.1	49.1	53.2	55.3	55.5	55.4	43.0	48.4	48.3	53.3	53.2	65.1	65.0	57.9	57.9
8	77.2[a]	34.5	75.5	33.1	32.6	33.1	32.8	32.0	31.2	78.3	78.1	197.6	197.1	48.6	48.6
9	76.5[d]	72.4	70.2	72.2	72.2	72.0	76.0	73.1	72.4	70.4	70.3	79.5	79.7	79.6	79.6
10	47.9	54.1	52.6	55.8	55.5	55.8	48.0	52.1	51.1	52.5	52.4	52.2	53.1	51.6	51.6
11	84.1	84.3	82.7	78.6	77.5	78.7	84.1	82.6	85.0	82.8	82.7	84.8	85.2	71.0	71.0
12	29.7	29.4	24.3	22.2	23.1	22.4	19.9	29.9	29.8	24.4	24.3	24.6	25.3	21.5	21.5
13	25.5	25.7	29.5	23.6	23.3	23.6	20.5	26.1	26.0	29.6	29.5	29.3	29.3	24.9	24.9
14	23.7	23.8	22.8	17.9	28.6	29.6	30.0	24.4	24.0	22.8	22.7	23.8	24.6	20.2	20.2
15	13.3	65.1	60.6	29.6	17.1	17.9	20.9	22.0	21.5	60.7	60.5	60.6	61.1	29.7	29.7

Site	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150
1	70.6	70.5	79.6	76.9	77.1	68.2	68.3	68.4	69.2	34.5	40.7	32.9	33.4	41.2	40.4
2	67.8	68.7	26.5	70.6	70.6	68.1	68.2	68.2	68.4	26.9	26.5	23.1	26.8	40.7	19.2
3	41.3	41.0	22.4	31.2	31.3	41.9	42.1	41.9	42.0	75.2	78.8	73.5	71.6	213.1	35.5
4	72.2	72.1	33.8	33.3	33.4	69.7	69.9	69.6	69.8	73.9	75.1	82.8	82.7	45.6	109.9
5	91.0	91.0	91.2	90.8	90.8	91.1	91.1	91.1	91.1	47.5	55.1	46.5	46.8	51.0	50.8
6	78.8	78.8	71.6	74.7	74.8	71.6	71.7	71.7	72.0	23.0	69.5	23.0	23.1	26.3	21.3
7	50.1	50.1	52.9	52.7	53.0	48.9	49.0	49.0	49.2	42.6	49.7	55.5	70.2	48.7	54.1
8	34.6	34.6	74.6	70.7	71.6	34.2	34.5	34.6	34.7	214.3	21.1	209.8	204.8	22.0	68.9
9	68.0	68.0	74.9	75.0	74.7	78.5	78.6	78.1	78.2	59.6	45.0	59.1	60.1	38.0	51.1
10	53.9	53.7	49.1	48.7	48.8	55.1	55.2	55.2	55.5	39.5	34.6	38.4	38.3	33.4	36.1
11	84.8	84.9	81.9	82.2	82.2	84.6	84.6	84.5	84.7	–	28.7	25.8	63.1	72.7	75.2
12	26.4	26.4	24.2	24.1	24.2	25.6[a]	25.6[a]	25.5[a]	25.8[a]	–	21.1	19.2	19.7	26.8	23.9
13	30.0	30.0	30.6	30.7	30.7	25.2[a]	25.2[a]	25.1[a]	25.2[a]	–	20.8	20.6	19.0	27.5	30.2
14	24.6	24.8	12.5	18.5	18.5	29.3	29.4	29.2	29.3	21.6	21.6	18.2	17.7	11.2	-
15	65.7	66.0	16.7	14.1	14.4	65.3	65.2	65.2	65.4	19.0	18.0	17.2	19.1	16.3	18.9

Table 2 (*continued*)

Site	151	152	153	154	155	156	157	158	159[D]	160	161[A]	162	163	164	165
1	40.4	41.1	–	45.3[a]	45.2[a]	41.6	38.6	43.1[a]	40.0	41.0	215.6	44.2[a]	40.5	33.7	41.4
2	19.5	22.2	22.5	20.3	19.9	19.2	18.0	19.7	22.2	20.2	41.1	20.0	20.8	19.2	20.1
3	–	40.0	40.2	43.9[a]	43.7[a]	41.6	43.6	40.6[a]	29.6	43.6	35.9[a]	45.4[a]	39.5	37.0	44.5
4	109.8	221.5	211.7	73.0	72.8	71.9	72.6	71.0	70.3[a]	72.2	73.7	71.7	71.8	74.6	77.0
5	50.4	56.9	56.8	57.7	56.8	51.0	47.9	66.7	52.9	54.8	47.8	57.2	53.0	78.8	48.5
6	35.6	22.2	–	66.3	69.3	77.9	72.0	213.3	35.1	21.2	22.1	69.4	70.9	26.0	20.5
7	59.1	53.2	37.5	50.9	50.0	44.4	74.5	56.0	51.6	47.2	42.5	50.2	49.8	40.5	41.7
8	214.7	68.5	–	21.1	21.4	23.2	28.0	22.3	70.6	22.1	21.6	21.3	26.7	22.4	21.3
9	58.8	49.5	41.1	45.3[a]	43.1[a]	39.1	44.3	41.0[a]	43.0	44.4	33.6[a]	43.5[a]	80.5	34.7	41.5
10	23.7	40.5	39.2	34.9	34.9	37.3	33.8	39.8	50.1	34.6	46.6	34.5	39.4	37.6	34.2
11	71.8	75.5	57.7	28.8	28.7	24.0	32.7	25.6	70.1[a]	85.1	70.7	28.8	28.7	29.3	74.6
12	25.5	23.8	168.7	20.8	21.2	22.3	15.9	20.7	21.5	23.5	23.4	21.3	21.3	21.9	29.9
13	28.6	30.4	168.7	20.8	21.2	25.3	16.2	20.7	27.9	23.7	29.9	20.7	20.4	22.9	29.5
14	–	–	–	25.7	20.7	23.4	30.0	24.1	21.0	18.6	29.7	24.6	29.7	24.0	21.8
15	18.6	17.9	16.8	21.7	24.5	19.5	20.7	20.4	18.6	22.5	29.0	21.3	13.7	22.7	18.4

Site	166	167	168	169	170	171	172	173	174[e]	175[e]	176	177	178	179	180
1	34.9[a]	33.0	36.6	34.2	41.9[a]	44.6[a]	160.4	156.7	37.9	37.5	38.7	29.7	40.1	76.3	78.2
2	20.6	22.2	17.0	20.8	21.6[b]	17.4	126.3	128.5	22.9	22.9	20.8	23.0	23.7	32.3	29.1
3	30.3[b]	30.5	28.1	29.7	36.7	33.6[b]	202.3	201.9	124.6	121.2	121.0	119.0	120.7	119.5	119.0
4	34.1	32.4	41.2	34.7	31.5	33.7[b]	42.7	48.6[a]	133.2	134.9	135.4	137.0	135.3	135.4	135.3
5	74.3	75.2	75.1	74.3	51.3	47.0	48.3[a]	48.5[a]	45.0	40.9	42.6	47.4	46.5	46.5	46.4
6	29.7[b]	32.1	31.8	29.7	24.9	28.0	25.2	24.5	76.9	32.3	24.0	26.0	22.3	23.9	23.7
7	21.2[c]	45.2	40.2	40.8	49.6	50.1	48.5[a]	42.1[a]	73.8	74.2	41.0	49.4	48.7	49.2	49.1
8	20.6[c]	21.3	20.3	20.5	22.3[b]	22.7	21.9	23.9	22.8	29.2	23.1	22.7	22.9	21.9	21.8
9	35.5[a]	36.3	34.8	34.2	41.7[a]	41.6[a]	37.9	41.0	34.2	35.6	37.6	40.8	37.8	35.0	34.9
10	37.1	37.6	36.6	36.8	33.4	33.6	36.2	38.2	34.3	32.1	31.3	30.3	32.2	37.4	36.3
11	–	72.5	72.8	73.1	73.0	72.8	72.6	72.7	34.0	39.1	74.2	72.8	80.9	72.9	72.8
12	–	26.9	29.6	29.5	21.8[c]	26.9[c]	26.9[b]	27.1	15.8	14.4	28.1	26.8[a]	25.0	26.7	26.7
13	–	27.0	30.0	30.6	27.2[c]	27.1[c]	27.6[b]	27.1	16.2	16.8	28.8	27.2[a]	22.4	27.6	27.1
14	14.7	22.7	17.2	14.8	20.1	19.5	11.8	12.0	21.8	21.0	20.9	29.3	21.1	20.9	21.2
15	20.1	14.9	21.8	20.1	16.7	14.8	17.2	27.1	17.8	16.9	18.4	22.8	14.4	9.5	10.2

Table 2 (*continued*)

Site	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195
1	76.7	42.3	70.5[a]	42.3	39.4	41.7	78.3	75.4	80.3	76.8	72.9	73.8	75.1	45.7	37.4
2	32.1	199.0	192.9	19.2	18.9	26.0	27.1	26.9	23.9	26.7	35.9	30.7	42.4	68.9	33.8
3	121.2	125.4	129.2	33.2	32.7	29.3	31.9	31.3	31.5	32.1	69.9	85.1	198.2	200.4	199.0
4	133.5	167.0	153.6	124.5	126.0	124.2	123.8	125.1	124.0	139.2	142.5	138.3	133.8	125.9	128.9
5	50.8	76.0	87.9	134.9	135.0	142.5	133.4	133.6	133.4	136.4	133.7	140.3	154.7	164.2	162.6
6	71.4	34.3[a]	81.7	26.4	25.4	22.6	26.3	25.2	26.3	206.8	207.8	70.7	70.5	28.9	28.8
7	49.3	47.0	49.3	50.6	44.1	49.3	49.7	44.1	49.7	57.5	58.2	48.6	48.5	49.8	49.7
8	20.3	22.7	32.0	23.3	22.6	18.7	22.8	21.8	22.7	21.7	22.6	20.3	20.0	22.5	22.6
9	35.4	35.0[a]	74.9[a]	40.3	38.1	39.7	38.8	33.5	38.6	37.0	37.0	38.2	37.8	42.7	42.0
10	37.7	40.1	51.5	34.5	34.4	34.9	39.4	39.5	38.4	43.0	44.0	39.6	41.0	37.0	35.9
11	28.6	72.6	85.0	72.9	74.6	79.9	72.7	74.1	72.6	25.8	25.8	29.0	28.9	72.4	72.4
12	22.2	25.5	29.9	27.2	27.8	23.3	26.7	27.4	26.7	18.2	17.8	20.8	20.9	26.7[a]	26.8[a]
13	20.1	28.6	25.7	26.9	29.8	24.7	27.1	29.4	27.2	21.0	21.1	20.8	20.7	27.7[a]	27.5[a]
14	20.7	22.7	22.0	19.3	25.9	64.6	17.3	19.2	18.4	20.7	16.3	17.6	11.1	11.0	10.9
15	12.2	18.8	20.2	24.7	19.6	24.3	18.9	19.3	18.9	18.3	18.4	16.9	16.7	22.9	22.6

Site	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210
1	39.1	37.2	37.8	36.6	30.8[a]	39.8	41.1	41.0	41.4	41.3	40.5	79.2	77.2	80.1	79.1
2	34.1	33.4	33.3	33.7	22.7	22.7	23.5	22.2	22.9	23.0	23.4	32.5	31.9	34.5	31.5
3	200.3	198.7	198.9	198.0	30.2[a]	30.8	36.9	36.8	36.6	36.6	36.7	35.2	35.1	30.8	34.2
4	131.3	129.4	128.9	130.4	146.8	146.8	151.1	151.1	150.0	148.4	150.2	146.4	146.2	147.8	148.6
5	158.9	159.4	161.6	156.7	60.3	60.3	49.4	49.8	49.4	48.4	49.3	56.2	55.9	51.8	48.9
6	68.6	29.2	26.5	30.5	67.4	67.4	25.0	24.7	26.0	28.2	28.3	67.2	67.0	71.2	24.8
7	49.7	47.9	45.2	51.4	48.9	48.9	49.8	48.1	54.3	59.0	38.4	49.6	49.3	50.4	47.5
8	16.1	67.0	66.7	207.8	18.5	18.5	22.4	23.4	69.2	214.4	25.7	18.5	16.2	20.4	22.2
9	41.6	50.2	49.0	54.6	39.8	30.2	41.8	41.8	50.2	57.1	41.7	36.5	36.3	37.4	37.0
10	35.0	37.0	35.7	40.0	35.5	35.5	35.9	35.9	37.7	40.9	35.8	41.8	41.7	40.4	40.1
11	73.4	39.9	42.1	38.6	26.3	26.3	72.9	80.7	75.2	71.5	58.0	26.3	26.0	28.1	72.5
12	28.8[a]	176.4	176.8	175.1	16.1	16.1	27.2	23.7	24.0	25.6	169.0	21.1	16.2	22.0	27.0[a]
13	28.9[a]	12.9	15.3	14.6	20.8	20.8	27.2	24.0	30.3	28.6	169.0	16.4	21.1	20.3	27.2[a]
14	10.4	11.1	10.7	11.3	112.3	112.3	105.3	105.4	105.5	107.3	105.6	107.9	107.8	108.9	108.0
15	24.6	23.3	25.0	24.4	28.2	28.2	16.3	16.3	17.3	17.1	16.2	11.7	11.6	13.2	10.2

Table 2 (*continued*)

Site	211	212	213	214	215	216	217	218	219	220[B]	221	222	223	224	225
1	214.5	80.7	71.3	74.0	75.1	51.0	46.8	35.8	39.6	41.3	30.8	78.2	83.0	80.3	49.4
2	38.1	28.0	27.7	28.0	28.7	67.9	70.7	29.8	17.7	18.1	22.0	27.0	68.2	39.4	36.6
3	34.5	33.8	32.7	31.5	31.8	46.6	42.3	73.6	33.6	33.8	28.7	33.6	41.5	38.7	74.6
4	146.8	148.2	143.1	142.1	141.8	148.2	147.1	152.1	38.8	39.3	39.7	81.9	82.5	71.0	38.7
5	48.7	48.7	88.8	90.3	91.2	49.4	49.4	43.6	133.2	151.6	68.7	52.0	52.1	50.3	75.5
6	24.6	24.2	79.4	78.1	77.4[a]	40.9	40.8	24.6	121.0	129.2	122.4	116.2	115.7	115.3	128.8
7	48.0[a]	47.6	48.5	52.2	65.6	49.2	49.3	49.4	45.4	44.1	143.9	143.7	142.3	146.2	145.1
8	22.1	21.9	31.8	72.2[a]	199.3	24.7	24.6	22.5	20.3	20.6	23.0	22.7	22.6	23.7	42.2
9	32.3	36.6	73.0	75.9[a]	81.2[a]	22.0	21.8	40.8	41.3	39.5	36.1	35.5	35.7	22.9	65.3
10	48.4[a]	39.1	51.6	48.8	50.3	35.3	35.5	35.8	34.4	34.8	35.8	38.3	38.5	37.4	38.4
11	72.5	72.7	82.7	82.4	82.7	72.8	72.9	73.0	73.5	60.5	34.7	35.1	35.1	35.3	30.6
12	27.1[b]	27.0	31.2	31.3	31.0	27.4	27.4	27.3	27.2	26.9[a]	21.5	21.7	21.7	21.8	21.7
13	27.6[b]	27.2	26.2	26.3	25.7	27.1	27.2	27.0	27.4	27.0[a]	21.2	21.6	21.6	21.3	23.5
14	108.9	107.2	112.3	112.8	113.6	108.0	109.1	109.0	27.8	27.3[a]	16.4	24.4	24.6	29.5	25.4
15	16.6	11.2	19.3	13.3	13.1	17.3	16.7	15.6	22.4	22.4	24.1	12.2	13.4	12.8	15.7

Site	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240
1	32.0	31.9	32.1	33.2	32.0	31.7	37.0	37.0	36.5	40.7	80.0	79.5	81.5	83.8	73.6
2	25.9	25.1	26.8	24.1	25.9	23.1	25.4	25.5	25.6	20.4	40.7	26.7	40.6	67.4	41.1
3	73.4	73.4[a]	70.7	75.7	73.7	73.9	81.0	81.0	72.9	43.2	39.7	33.4	39.4	41.2	69.9
4	72.1	75.4[a]	68.7	71.9	80.1	81.8	73.3	73.6	85.7	72.3	71.0	82.4	70.9	83.5	84.6
5	49.0	48.9	70.2	50.6	49.9	48.6	54.1	54.2	48.6	54.4	46.5	52.0	46.8	48.9	42.9
6	143.6	143.2	143.4	142.6	140.2	140.9	141.7	143.4	140.1	117.2	26.9	23.2	23.5	23.1	33.9
7	144.9	145.4	147.9	145.1	142.3	145.4	144.6	142.3	145.1	143.8	142.1	141.8	142.1	141.7	142.0
8	201.5	201.3	201.7	200.8	201.0	200.0	200.8	197.8	200.3	23.4	116.2	115.8	116.1	115.8	116.2
9	57.8	57.7	53.6	58.6	57.5	57.7	57.5	57.8	57.6	39.5	23.2	41.0	23.1	41.2	33.9
10	39.3	39.2	36.9	39.2	39.0	39.1	39.0	39.0	40.0	33.8	37.9	37.9	36.9	38.0	27.7
11	72.0	72.0	72.1	71.2	72.4	75.9	71.9	83.4	71.7	35.0	35.1	34.8	35.1	34.8	35.0
12	29.4	29.3	29.5	29.4	29.4	29.2	29.2	25.0	28.9	21.6	21.9	21.7	21.9	21.7	21.8
13	28.9	28.8	28.7	28.8	28.9	28.8	28.9	24.4	29.1	21.8	21.3	21.2	21.3	21.3	21.3
14	22.4	22.4	22.8	22.7	18.6	18.9	19.5	19.4	18.7	22.3	29.9	24.7	29.9	24.8	23.0
15	17.8	17.7	16.8	17.9	17.8	18.2	18.1	18.1	18.5	17.6	11.8	12.3	12.9	13.4	12.3

Table 2 (*continued*)

Site	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255
1	78.5	78.7	78.0	32.9	32.9	32.6	38.0	33.4	38.3	37.7	38.5	75.3	76.2	74.2	82.3
2	28.9	30.0	28.3	25.7	23.0	25.1	26.0	23.1	25.5	25.8	25.4	27.2	24.8	26.5[a]	26.7[a]
3	41.2	39.7	40.3	74.3	73.7	73.3	74.2	72.3	81.3	74.0	73.8	33.7	22.4	26.9[a]	27.4[a]
4	71.9	71.0	71.5	73.1	82.9	82.6	87.7	83.4	74.4	87.4	87.6	82.4	41.4	41.3	33.7
5	50.7	47.6	50.4	45.6	45.1	44.8	45.1	45.6	51.1	44.9	47.5	46.6	77.7	77.3	53.1
6	26.0	26.8	26.0	25.7	25.8	25.4	25.8	26.1	25.5	25.6	20.9	23.0	38.2	38.2	70.1
7	130.0	129.9	130.5	131.2	130.1	129.7	130.2	130.5	130.3	129.9	129.5	85.8	39.8	39.8	50.1
8	202.1	202.0	204.0	202.0	201.4	200.9	202.1	210.7	202.1	201.8	97.1	141.9	26.0	26.1	23.6
9	56.8	55.4	56.7	60.2	60.1	59.7	60.2	60.4	59.8	59.9	49.7	124.0	32.7	33.4	39.5
10	41.2	40.3	41.2	36.3	35.9	35.4	37.1	36.0	36.4	36.9	35.6	41.1	39.7	41.9	40.9
11	145.0	146.4	146.0	144.1	145.5	146.0	144.7	146.1	144.8	144.5	125.1	32.4	150.0	150.2	144.5
12	22.8	23.1	22.3	23.4	23.6	23.1	23.5	23.7	23.4	23.3	72.9	17.7	108.4	108.6	124.7
13	22.8	23.8	22.8	22.7	22.8	22.6	22.9	23.1	22.7	22.5	13.3	16.8	21.1	21.0	168.1
14	23.5	25.9	23.6	21.4	19.1	18.9	19.6	19.3	17.5	16.7	17.0	24.9	17.0	15.5[b]	69.1
15	12.7	12.7	12.7	18.6	18.0	17.6	16.9	18.3	18.9	19.4	19.7	13.5	21.8	16.8[b]	15.8

Site	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270
1	83.1	76.1	75.9	75.3[a]	76.0	75.5	75.5	77.2	215.5	215.3	32.1	34.1	31.7[a]	41.1	44.5[a]
2	26.6[a]	29.6	29.6	29.3	27.7	27.8	27.8	29.1	34.1	33.0	23.3	27.3	37.9	20.2	20.1
3	27.4[a]	39.1	39.1	36.5	35.5	35.6	35.5	33.0	30.1	30.5	79.3	77.6	207.7	43.4	43.4[a]
4	33.6	65.9	66.8	78.8	81.3	81.3	82.1	60.8	40.5	31.7	71.5	71.7	71.7	72.3	72.0
5	53.1	60.6	60.5	57.0	56.6	56.7	56.5	49.4	78.5	53.7	46.9	49.6	65.4	54.9	54.9
6	70.1	66.3	66.8	72.3	71.6	71.7	71.6	68.2	28.0	25.6	29.4	23.7	26.9	26.1	27.3[b]
7	50.2	56.3	52.6	50.6	50.6	50.7	50.6	54.9	39.3	39.5	36.2	40.4	38.0	46.4	40.4
8	23.5	67.5	70.8	28.3	25.3	25.2	25.1	70.4	25.4	26.7	205.8	26.0	31.5[a]	26.9	26.4[b]
9	39.4	44.5	41.2	40.8[b]	39.9[a]	39.9[a]	39.7	42.2	37.2	79.0	58.9	44.2	33.3[a]	44.7	40.9[a]
10	40.4	42.4	42.6	41.7[b]	40.2[a]	40.8[a]	40.4	41.2	51.2	51.2	32.8	34.3	33.8	34.7	34.6
11	144.4	137.7	137.5	144.2	143.6	143.7	143.6	137.5	149.4	150.6	144.3	145.5	144.3	150.7	145.7
12	168.1	128.8	128.4	124.7	125.2	125.2	125.1	128.2	108.8	108.5	124.1	122.5	123.7	108.2	122.5
13	124.7	167.4	167.0	168.1	167.8	167.9	167.8	166.8	21.0	21.0	174.0	167.8	167.1	21.1	167.8
14	69.0	63.7	63.6	76.0[a]	74.7	74.8	74.6	51.4	20.3	19.6	22.4	21.0	20.7	22.8	22.5
15	15.7	12.9	12.7	15.0	15.3	15.3	15.3	12.8	17.7	17.4	18.2	18.4	11.4	18.7	18.7

Table 2 (*continued*)

Site	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285
1	42.9[a]	41.4	41.8	41.0	41.0	40.9	40.7	41.0	41.0	26.1	133.2	156.6	155.2	156.2	153.1
2	19.5	20.2	23.0	22.5	23.4	22.7	23.5	23.2	23.0	17.0	123.5	126.1	126.1	125.4	126.9
3	43.6	43.6	35.6	40.0	40.1	39.7	40.9	40.1	39.8	28.1	116.8	186.5	186.2	186.4	185.7
4	73.5	72.1	83.4	77.2	79.4	79.7	79.8	79.4	79.2	41.2	139.8	129.2	129.8	129.2	131.2
5	57.9	49.2	48.6	47.6	47.5	47.3	47.4	47.3	47.4	75.7	47.7	160.5	157.3	159.8	153.8
6	73.3	22.8	18.2	19.2	19.8	19.6	19.7	19.6	19.7	37.6	27.3	28.7	28.5	26.9	29.4
7	50.3	39.4	39.4	39.0	39.5	39.4	39.5	39.2	39.5	40.0	47.3	50.5	48.4	46.6	50.8
8	26.8	23.6	23.4	23.1	23.0	23.3	23.0	23.2	22.9	34.9	24.8	22.0	66.7	66.2	206.0
9	42.6[a]	40.4	40.1	40.4	40.7	40.6	39.9	40.4	40.6	38.0	39.1	38.0	45.3	44.6	51.2
10	36.3	35.3	34.6	34.6	35.1	35.0	35.2	35.0	35.1	36.7	35.7	40.3	40.8	40.3	42.4
11	142.3	147.0	147.1	146.5	146.7	146.6	146.7	146.6	146.7	150.5	72.8	72.3	39.6	41.9	38.0
12	125.8	110.9	110.7	110.7	110.9	110.8	110.9	110.8	110.8	108.2	26.9[a]	26.9[a]	176.1	176.8	175.1
13	168.3	22.8	22.8	22.7	22.9	22.7	22.9	22.6	22.6	21.0	27.1[a]	27.7[a]	13.3	15.4	14.4
14	23.8	22.3	25.0	17.9	18.2	18.1	18.4	18.1	18.4	16.7	26.0	10.4	10.6	10.2	10.9
15	19.7	18.5	18.8	18.6	19.0	18.8	19.0	18.8	19.0	21.6	22.2	23.4	24.6	26.3	25.1

Site	286[P]	287[P]	288[B]	289	290	291	292	293	294[P]	295	296	297	298	299	300
1	157.5	157.5	139.4	42.5	37.1	38.0	37.9	37.9	80.2	81.8	74.4	66.8	206.3	44.3	54.0
2	125.2	127.3	123.7	126.2	22.9	20.2	22.9	22.9	27.9	29.0	29.7	72.5	78.4	75.3	199.1
3	184.9	183.7	33.3	134.0	124.1	124.3	124.7	120.9	NO[f]	118.9	125.0	118.4	119.7	121.6	126.8
4	129.9	133.2	143.4	69.4	131.2	131.5	131.2	135.1	NO[f]	153.8	136.2	141.8	151.6[a]	139.0	162.5
5	154.7	159.8	47.9	49.9	132.0	142.9	143.4	46.8[a]	46.1	47.2	52.3[a]	36.1	85.3	47.2	44.9
6	98.7	112.6	72.3	27.8	123.7	120.4	120.2	28.9	29.8	28.6	78.1	24.1	29.7[b]	28.9	33.0
7	49.5	75.7	43.7	39.8	40.7	47.2	45.6	46.7[a]	45.1	41.5	50.4[a]	36.2	38.5	40.1	74.7
8	18.6	28.1	22.9	27.0	20.8	20.6	20.1	26.8	26.9	26.9	27.5	25.9	24.8	26.7	31.5
9	36.5	32.0	37.5	41.6	35.7	37.1	37.1	40.2	37.4	35.5	34.7	68.2	29.5[b]	39.8	37.6
10	39.5	39.6	39.5	31.9	32.3	32.2	32.3	32.3	35.4	36.6	40.9	43.9	44.7	35.2	37.4
11	26.3	32.1	24.3	145.7	33.2	81.0	85.4	151.0	150.7	135.2	144.4	147.3	148.7[a]	145.1	145.9
12	23.4[a]	21.7[a]	22.3	122.7	20.8	22.8	23.2	108.2	108.7	108.0	125.2	108.7	109.5	125.1	114.1
13	24.5[a]	18.0[a]	25.6	167.9	20.7	23.2	23.2	20.9	21.0	64.8	168.1	20.6	20.0[c]	172.3	18.6
14	68.9	71.8	107.5	29.0	23.0	22.0	20.2	21.2	NO	10.4	69.8	22.4	20.9[c]	21.0	16.9
15	19.3	17.5[a]	20.8	18.9	20.1	24.4	23.7	15.6	10.9	20.6	12.1	60.8	17.7[c]	16.4	22.0

Table 2 (*continued*)

Site	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315
1	31.1	33.0	28.8	37.9	37.8	36.5	36.6	39.4	39.4	74.4	39.7	35.4	27.5	30.7	31.2
2	22.7	22.4	22.3	23.0	23.0	24.5	23.3	17.8	18.4	42.4	18.7	18.1	27.0	18.5	23.7
3	121.9	121.1	121.8	121.1	121.1	152.7	137.1	23.8	28.0	197.5	32.8[a]	27.9	31.8	32.2	31.3
4	138.8	133.8	132.6	134.9	134.8	142.5	134.0	132.7	124.3	129.5	126.1	126.8	144.7	143.4	144.6
5	75.5	45.1	46.1	46.9	46.9	43.5	43.7	164.2	149.4	161.9	142.0	146.7	124.5	129.0	124.7
6	39.4	28.1	28.2	29.4	29.4	26.8	28.0	29.3	32.9	32.8	30.5[a]	32.1	31.4	32.9	31.2
7	40.2	43.6	45.7	42.4	40.1	46.0	46.1	47.4	46.9	45.1	48.3	42.8	39.5	37.1	38.4
8	26.6	35.0	41.9	27.5	27.4	26.5	26.7	27.0	27.2	26.5	70.6	35.4	38.6	35.7	38.3
9	36.6	78.1	215.3	40.3	40.1	39.7	39.8	41.4	41.7	37.7	50.3	78.1	78.2	79.9	80.1
10	35.7	37.6	46.7	32.3	32.3	32.2	32.4	36.7	35.3	41.3	35.8	40.9	39.3	39.1	39.4
11	150.2	149.3	147.7	154.5	145.3	150.3	150.4	148.9	149.7	148.9	132.4	148.2	132.9	131.6	132.6
12	108.5	109.0	109.9	107.3	172.4	108.5	108.4	109.3	108.6	109.4	126.5	109.2	124.6	125.5	124.8
13	20.9	20.8	20.3	65.1	125.0	21.0	20.9	20.7	20.8	20.6	171.9	20.7	171.9	170.8	170.8
14	17.4	21.7	21.6	21.2	21.1	194.8	168.7	190.7	170.9	16.3	19.4	170.7	18.9	19.8	18.9
15	21.8	10.0	16.2	15.7	15.7	15.7	15.7	25.1	24.9	11.0	25.4	18.1	17.2	19.0	18.3

Site	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330
1	34.7	42.3	81.0	37.0	36.8[a]	41.0	41.9	76.8	76.4	76.2	81.5	41.9[a]	41.3	38.9	41.7
2	27.1	19.1	28.2	23.4	23.3	29.4	23.5	42.7	41.0	46.4	27.1[a]	26.7	23.4	24.5	23.5
3	32.0	33.2	34.1	41.4	37.3[a]	41.8	36.9	70.5	76.7	198.8	27.7[a]	37.8	36.8	37.8	36.8
4	144.3	125.0	147.9	149.1	149.5	149.8	150.9	154.0	149.4	148.6	114.1	143.0	150.3	151.0	150.7
5	125.2	134.6	43.4	47.1	48.3	50.6	49.9	45.9[a]	45.9	44.6	53.9	57.9	43.7	49.8	50.0
6	31.5	31.2	25.5	29.3	27.9	27.4	29.5	29.4[b]	29.4	29.2	68.3	69.3	34.3	30.8	30.0
7	39.5	42.7	141.6	131.5	126.9	154.0	45.8	45.5[a]	45.3	46.5	50.0	48.1	72.9	38.5	41.2
8	36.0	28.3	115.8	201.8	34.6	23.1	26.8	27.0[b]	27.1	26.7	24.7	23.9	31.3	36.5	27.3
9	216.1	40.3	38.1	57.6	79.6	36.4	41.2	37.9	37.9	36.8	36.1	40.4[a]	35.9	80.0	41.9
10	47.0	34.6	38.1	38.0	41.2	36.1	35.9	40.9	40.7	38.9	41.4	37.4	35.4	42.3	36.0
11	133.5	154.2	35.0	144.1	123.1	125.1	151.0	150.7	150.7	150.1	144.4	147.3	146.7	146.9	154.1
12	125.2	107.6	21.2	22.2	20.2	169.7	108.1	21.0	109.0	109.5	124.9	124.6	167.8	123.4	107.8
13	172.4	65.3	21.2	23.2	20.2	59.0	21.0	108.7	21.1	21.3	168.1	168.1	123.3	170.4	65.3
14	22.1	19.4	108.0	107.0	106.9	105.8	105.3	103.6	105.5	118.5	141.6	106.9	105.1	106.9	105.4
15	18.9	24.7	11.5	17.3	10.1	15.9	16.3	10.9	10.9	10.0	13.0	17.6	15.4	11.2	16.4

Table 2 (*continued*)

Site	331	332[B]	333[B]	334[B]	335[B]	336	337[B]	338	339	340	341	342	343	344	345
1	41.0	42.0	42.8	43.6	43.0	35.7	36.3	38.4	26.6	27.7	26.6	121.7	121.7	122.8	121.8
2	23.5	19.3	22.7	22.1	22.1	22.1	22.3	71.5	71.5	71.5	69.0	149.7	150.1	149.7	150.8
3	36.5	33.1	35.7	37.7	37.5	36.9	37.1	79.2	79.3	81.9	93.4	181.4	180.8	182.4	181.8
4	150.8	133.5	33.2	33.6	33.6	33.8	34.0	41.7	40.5	39.2	40.5	126.5	133.1	128.8	122.0
5	49.8	147.9	149.6	147.7	147.3	143.3	142.5	129.1	129.1	129.3	128.6	154.6	150.1	157.5	162.1
6	29.5	30.6	115.5	114.6	115.4	120.2	120.6	31.2	31.1	32.7	31.1	117.7	133.5	116.6	120.1
7	36.9	125.7	142.8	131.8	131.4	127.7	128.2	40.5	41.7	41.9	40.5	153.7	147.9	156.4	155.4
8	27.0	26.8	114.1	65.5	67.9	23.0	23.0	26.6	38.4	33.1	37.7	23.6	196.2	23.7	24.1
9	41.9	39.5	41.0	46.7	44.2	34.5	34.4	29.7	29.7	30.3	29.6	33.6	49.8	33.3	33.6
10	35.9	34.9	34.9	34.5	34.3	40.3	39.0	124.9	124.8	123.2	124.7	36.5	40.6	37.1	37.7
11	155.5	120.6	71.4	128.8	127.4	126.2	125.5	148.9	148.9	-	148.8	35.4	29.0	35.5	35.2
12	133.0	62.3	29.3[a]	25.8	25.2	20.7	20.7	109.0	109.0	109.4	108.9	20.9	21.4	20.9	20.9
13	194.9	62.1	29.5[a]	19.0	18.9	19.8	19.7	21.1	21.1	20.9	20.5	21.2	21.7	21.1	21.2
14	105.6	19.3	18.7	19.8	19.9	18.9	19.1	16.5	16.4	17.9	16.4	9.9	11.0	55.9	–
15	16.4	24.5	22.4	20.2	20.6	65.2	64.8	–	–	–	–	25.4	26.8	26.5	26.5

Site	346	347	348	349	350
1	126.0	156.6	72.8	135.6	133.8
2	153.2	126.3	133.0	122.1	120.5
3	185.4	186.6	127.0	120.1	38.6
4	112.8	129.8	145.0	136.9	133.8
5	156.2	158.8	38.7	42.9	163.1
6	145.7	26.6	27.2	36.7	188.2
7	144.3	40.6	38.1	116.7	150.7
8	191.1	33.2	29.6	149.9	140.1
9	48.3	37.8	33.4	19.8	35.1
10	40.4	40.2	37.4	35.3	39.5
11	28.8	143.4	145.0	119.4	119.6
12	21.6	125.8	125.0	137.5	139.4
13	21.6	170.7	171.8	8.2	9.1
14	–	10.6	113.1	20.4	28.0
15	26.0	23.6	17.0	15.4	20.9

[a,b,c] Identically marked assignments within a column are interchangeable.
[d] Incorrect data from literature.
[e] Data not attributed by the authors from the original papers.
[f] NO = Not observed.

Table 3
^{13}C NMR shift ranges for several substructures

Substructure	No. of C	^{13}C NMR shifts range	% Recognition
[8OXO]	5	50.5–44.7 d	100.0
	8	214.3–200.0 s	
	9	60.4–56.7 t	
	10	41.2–32.7 s	
[1,9OR; 5,11OXY]	1	80.5–66.8 d	100.0
	5	94.5–57.4 s	
	7	65.8–43.0 d	
	9	80.9–66.0 d	
	10	56.0–43.9 s	
	11	85.8–69.8 s	
[1,6,9OR; 5,11OXY]	1	80.5–67.8 d	100.0
	5	94.5–88.0 s	
	6	80.9–67.9 d	
	7	57.5–48.2 d	
	9	80.9–68.0 d	
	10	55.5–45.7 s	
	11	85.8–69.8 s	
[5,11OXY; 6OXO]	5	86.0–84.9 s	100.0
	6	212.6–211.0 s	
	7	55.5–55.2 d	
	11	78.6–77.5 s	
[1,4,9OR; 5,11OXY; 6OXO]	1	72.5–72.0 d	100.0
	4	71.0–69.9 s	
	5	86.0–84.9 s	
	6	212.6–211.0 s	
	7	55.5–55.2 d	
	9	72.3–72.0 d	
	10	56.0–55.0 s	
	11	78.6–77.5 s	
[1,4,6,9OR; 5,11OXY]	1	76.5–67.8 d	100.0
	4	85.1–69.5 s	
	5	94.5–91.0 s	
	6	80.4–67.9 d	
	7	65.0–48.2 d	
	9	79.6–68.0 d	
	11	85.8–69.8 s	
[1OR]	1	83.0–80.3 d	100.0
	2	27.2–26.6 t	
	3	31.5–27.3 t	
	4	33.7–33.0 d	
	5	53.0–45.9 d	
	10	40.9–39.2 s	
[1,2,3,4,8,9,15OR; 5,11OXY]	1	75.5–70.8 d	100.0
	2	73.5–69.0 d	
	3	78.4–75.1 d	
	4	72.6–69.6 s	
	5	94.5–93.0 s	
	7	52.5–49.2 d	
	8	74.5–68.9 d	
	9	76.3–70.5 d	
	11	85.5–84.0 s	
	15	62.5–60.2 t	

Table 3 (*continued*)

Substructure	No. of C	^{13}C NMR shifts range	% Recognition
[4OR]	1	45.2–40.5 t	55.8
	2	23.3–19.2 t	
	3	45.4–35.5 t	
	4	83.4–71.6 s	
	5	57.2–46.2 d	
	10	39.4–33.7 s	
[6OR]	5	60.2–45.7 d	72.3
	6	78.0–66.3 d	
	7	51.2–43.2 d	
	8	28.2–16.2 t	
	9	45.2–28.8 t	
	10	48.5–33.2 s	
[11OH]	5	54.9–42.5 d	90.6
	6	40.9–20.5 t	
	7	50.7–41.0 d	
	8	24.7–20.6 t	
	9	44.7–21.7 t	
	10	48.2–30.2 s	
	11	85.0–72.4 s	
	12	29.8–23.5 q	
[1,4OR]	1	91.3–75.3 d	52.8
	2	40.7–23.3 t	
	3	45.2–33.0 t	
	4	82.5–65.9 s	
	5	60.5–44.9 d	
	10	48.5–33.2 s	
[3,4OR]	1	40.7–31.7 t	71.4
	2	27.2–23.0 t	
	3	79.3–71.5 d	
	4	87.6–71.5 s	
	5	55.0–44.7 d	
	10	39.2–32.7 s	
[3,4OR]	1	40.7–31.7 t	73.9
	2	27.2–23.0 t	
	3	79.3–70.6 d	
	4	87.6–68.6 s	
	10	39.2–32.7 s	
[4,6OR]	4	84.3–71.0 s	78.9
	5	57.7–45.7 d	
	6	77.9–66.3 d	
	7	51.2–43.2 d	
	11	29.7–23.5 d	
[4,11OR]	4	77.0–72.0 s	100.0
	5	54.9–47.2 d	
	6	21.6–20.5 t	
	7	50.7–41.0 d	
	11	85.0–73.0 s	
[1,11OH]	1	91.3–76.3 d	100.0
	5	48.9–45.4 d	
	10	40.2–36.2 s	
	11	75.1–72.5 s	

Table 3 (*continued*)

Substructure	No. of C	^{13}C NMR shifts range	% Recognition
[1OR; 4,11OH]	1	91.3–80.0 d	100.0
	4	72.8–72.0 s	
	5	48.5–47.2 d	
	10	40.2–38.7 s	
	11	75.1–74.5 s	
[1EN; 3OXO]	1	160.8–153.1 d	100.0
	2	127.3–125.1 d	
	3	204.0–183.6 s	
	10	42.4–36.0 s	
[3EN]	1	40.0–28.7 t	81.8
	2	23.7–20.2 t	
	3	124.6–119.0 d	
	4	138.8–131.1 s	
	5	47.4–42.5 d	
	10	46.7–30.2 s	
[1OR; 3EN]	1	81.0–74.4 d	100.0
	2	32.2–29.0 t	
	3	125.0–118.9 d	
	4	153.8–133.5 s	
	5	52.2–46.4 d	
	10	40.9–36.2 s	
[1OR; 4EN]	1	80.3–75.4 d	50.0
	2	27.7–23.8 t	
	3	32.7–31.2 t	
	4	133.3–123.8 s	
	5	133.6–125.4 s	
[3OXO; 4EN]	3	200.3–180.8 s	100.0
	4	133.8–125.9 s	
	5	164.1–150.1 s	
	10	42.4–35.0 s	
[3OXO; 4EN; 11OR]	3	200.3–186.5 s	100.0
	4	131.3–125.9 s	
	5	164.1–158.8 s	
	7	50.5–49.5 d	
	11	73.4–72.0 s	
[4EN; 11OR]	4	215.0–123.8 s	56.2
	5	208.1–133.3 s	
	6	39.2–25.2 t	
	7	50.5–44.0 d	
	11	78.6–72.0 s	
	14	29.5–10.3 q	
[4(14)EN]	1	41.9–30.7 t	61.5
	2	29.3–22.2 t	
	3	41.7–30.2 t	
	4	154.1–146.8 s	
	5	60.2–43.7 d	
	10	42.2–35.4 s	
	14	112.3–104.9 t	
	15	28.2–10.1 q	

Table 3 (*continued*)

Substructure	No. of C	^{13}C NMR shifts range	% Recognition
[4(14)EN]	3	46.5–30.2 t	69.2
	4	154.1–143.3 s	
	5	60.2–43.4 d	
	10	42.2–35.2 s	
	14	112.3–104.9 t	
[4(14)EN; 11OH]	4	151.1–147.1 s	81.8
	5	49.7–43.5 d	
	6	40.9–24.2 t	
	7	59.0–47.5 d	
	11	80.6–71.5 s	
	14	109.0–105.3 t	
[5EN]	1	43.5–39.5 t	100.0
	2	22.7–17.7 t	
	3	37.7–33.2 t	
	4	39.2–33.2 d	
	5	152.6–133.1 s	
	6	129.1–114.5 d	
	10	34.9–34.2 s	
	14	27.7–18.7 q	
	15	22.3–20.2 q	
[5EN; 11OR]	5	152.6–133.1 s	62.5
	6	129.1–119.6 d	
	7	47.2–44.0 d	
	11	85.4–60.5 s	
[4OR; 6EN]	4	82.5–71.0 s	100.0
	5	54.4–48.5 d	
	6	140.8–115.3 d	
	7	146.1–142.3 s	
	10	39.0–33.7 s	
[6EN; 8OXO]	6	145.6–133.5 d	100.0
	7	147.8–142.3 s	
	8	201.6–191.1 s	
	9	58.5–48.2 t	
	10	40.5–36.9 s	
[4OR; 7EN]	4	84.5–70.9 s	100.0
	5	52.0–42.9 d	
	6	33.9–23.1 t	
	7	142.1–141.6 s	
	8	116.1–115.8 d	
[7(11)EN]	7	131.8–126.9 s	76.9
	10	41.2–34.2 s	
	11	146.1–123.0 s	
	12	25.7–20.2 q	
	13	23.2–18.8 q	
[7(11)EN; 8OXO]	7	131.5–129.6 s	100.0
	8	210.6–200.8 s	
	9	60.0–56.7 t	
	10	41.2–35.4 s	
	11	146.1–144.1 s	

Table 3 (*continued*)

Substructure	No. of C	^{13}C NMR shifts range	% Recognition
[11EN]	5	55.0–44.5 d	73.7
	6	29.5–18.2 t	
	7	46.7–39.0 d	
	8	27.3–23.0 t	
	9	44.7–36.7 t	
	10	40.9–32.2 s	
	11	151.0–146.5 s	
	12	110.9–108.0 t	
	13	22.8–20.8 q	
[5OR; 11EN]	4	41.4–40.5 d	100.0
	5	85.3–75.5 s	
	11	150.5–145.6 s	
	12	109.5–108.1 t	
	13	21.1–20.0 q	
	14	20.2–15.5 q	
[11EN; 13OH]	7	42.7–41.5 d	100.0
	11	154.5–135.1 s	
	12	108.0–107.1 t	
	13	65.3–64.8 t	
[11EN; 13OXO; 13 OR]	6	31.5–23.7 t	94.0
	7	40.4–35.9 d	
	8	38.5–25.1 t	
	11	149.5–132.8 s	
	12	125.1–121.9 t	
	13	172.3–167.1 s	
[1,4EN; 3OXO]	1	158.1–153.1 d	100.0
	2	127.3–125.1 d	
	3	187.6–183.6 s	
	4	133.1–129.1 s	
	5	160.5–153.8 s	
[1,4(14)EN]	1	139.3–124.8 d	100.0
	2	133.1–123.6 d	
	3	35.0–33.2 t	
	4	143.6–143.3 s	
	14	114.5–107.5 t	
[3,5EN]	3	124.6–124.0 d	100.0
	4	131.5–131.1 s	
	5	143.3–132.0 s	
	6	123.6–120.1 d	
	14	23.0–20.2 q	
[5,7(11)EN]	5	147.6–142.5 s	100.0
	6	120.5–114.5 d	
	7	131.8–127.6 s	
	10	40.2–34.2 s	
	11	128.8–125.5 s	
[7,11EN; 8,12OXY]	7	117.3–115.6 s	100.0
	8	150.1–149.2 s	
	11	119.9–118.8 s	
	12	138.2–136.9 d	
	13	8.7–8.1 q	

Table 4
Substructures proposed by the system for eudesmanes in Fig. 3

Eudesmane	^{13}C NMR data (C_1–C_{15})	Proposed substructures	References
I	73.4d, 38.6t, 23.5t, 70.5s 91.6s, 73.4d, 49.1d, 31.9t 79.8d, 51.8s, 84.4s, 25.8q 29.6q, 24.1q, 20.0q	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0%	[153]
II	73.4d, 39.0t, 23.5t, 70.8s 91.6s, 73.4d, 49.1d, 31.9t 80.6d, 51.8s, 84.5s, 25.9q 29.7q, 24.0q, 20.1q	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0%	[153]
III	72.5d, 23.6t, 37.1t, 73.0s 91.2s, 79.2d, 49.9d, 34.2t 68.4d, 53.4s, 84.7s, 30.0q 26.6q, 23.3q, 65.0t	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0%	[154]
IV	73.2d, 23.5t, 38.9t, 70.8s 91.6s, 80.9d, 49.1d, 31.9t 73.3d, 51.8s, 84.5s, 29.7q 26.0q, 24.0q, 20.1q	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0%	[154]
V	73.2d, 68.7d, 75.7d, 70.6s 93.7s, 73.9d, 50.3d, 68.9d 70.6d, 52.1s, 84.1s, 18.5q 69.8t, 22.9q, 60.0t	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0% [1,2,3,4,8,9,15OR; 5,11Oxy]—100.0%	[155]
VI	73.1d, 68.7d, 75.6d, 70.6s 94.0s, 74.2d, 50.5d, 68.8d 70.2d, 52.7s, 84.3s, 18.6q 69.8t, 23.8q, 60.0t	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0% [1,2,3,4,8,9,15OR; 5,11Oxy]—100.0%	[155]
VII	73.2d, 69.0d, 75.6d, 70.7s, 94.0s, 74.2d, 50.4d, 69.0d 70.6d, 52.6s, 84.4s, 18.6q 69.9t, 24.1q, 61.0t	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0% [1,2,3,4,8,9,15OR; 5,11Oxy]—100.0%	[155]
VIII	73.2d, 68.7d, 75.8d, 70.6s 93.7s, 74.8d, 50.4d, 69.1d 70.8d, 52.2s, 84.2s, 18.4q 69.9t, 22.9q, 60.0t	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0% [1,2,3,4,8,9,15OR; 5,11Oxy]—100.0%	[155]
IX	72.4d, 68.5d, 75.2d, 70.6s 94.5s, 74.6d, 49.3d, 74.5d 73.7d, 51.3s, 85.7s, 19.6q 69.8t, 23.8q, 60.7t	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0% [1,2,3,4,8,9,15OR; 5,11Oxy]—100.0%	[156]
X	74.5d, 69.3d, 77.1d, 70.7s 94.4s, 74.6d, 51.8d, 74.5d 77.2d, 52.0s, 85.5s, 19.5q 70.1t, 23.8q, 61.3t	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0% [1,2,3,4,8,9,15OR; 5,11Oxy]—100.0%	[156]
XI	72.2d, 68.3d, 75.1d, 70.6s 94.2s, 74.8d, 51.1d, 74.1d 76.9d, 51.3s, 85.5s, 19.6q 70.2t, 23.5q, 60.7t	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0% [1,2,3,4,8,9,15OR; 5,11Oxy]—100.0%	[157]

Table 4 (*continued*)

Eudesmane	^{13}C NMR data (C_1–C_{15})	Proposed substructures	References
XII	72.4d, 68.5d, 75.2d, 70.6s 94.5s, 74.9d, 49.4d, 74.6d 73.7d, 52.6s, 85.6s, 19.7q 69.8t, 23.8q, 60.7t	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0% [1,2,3,4,8,9,15OR; 5,11Oxy]—100.0%	[157]
XIII	73.1d, 68.8d, 78.0d, 70.9s 93.6s, 75.4d, 51.0d, 69.2d 71.1d, 53.4s, 83.8s, 18.7q 70.0t, 23.4q, 60.4t	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0% [1,2,3,4,8,9,15OR; 5,11Oxy]—100.0%	[158]
XIV	73.0d, 68.3d, 77.9d, 71.7s 93.6s, 74.7d, 51.1d, 69.3d 71.2d, 52.8s, 83.6s, 18.7q 69.9t, 22.8q, 60.6t	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0% [1,2,3,4,8,9,15OR; 5,11Oxy]—100.0%	[158]
XV	72.8d, 68.4d, 77.5d, 70.3s 93.2s, 74.1d, 50.6d, 68.8d 70.6d, 52.2s, 83.3s, 18.6q 69.7t, 22.6q, 60.3t	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0% [1,2,3,4,8,9,15OR; 5,11Oxy]—100.0%	[158]
XVI	73.3d, 69.1d, 76.0d, 71.0s 94.4s, 74.4d, 50.8d, 69.0d 70.4d, 53.0s, 84.6s, 18.7q 70.3t, 23.8q, 60.1t	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0% [1,2,3,4,8,9,15OR; 5,11Oxy]—100.0%	[158]
XVII	73.3d, 69.0d, 76.6d, 70.4s 93.1s, 74.6d, 50.7d, 68.3d 70.6d, 52.7s, 83.5s, 17.9q 70.1t, 23.4q, 60.0t	[1,9OR; 5,11Oxy]—100.0% [1,6,9OR; 5,11Oxy]—100.0% [1,4,6,9OR; 5,11Oxy]—100.0% [1,2,3,4,8,9,15OR; 5,11Oxy]—100.0%	[159]
XVIII	52.7t, 65.3d, 54.3t, 72.7s 48.1d, 21.8t, 42.5d, 21.6t 42.7t, 34.3s, 81.5s, 25.9q 27.1q, 20.5q, 23.9q	[4,11OR]—100.0%	[160]
XIX	79.4d, 29.4t, 39.1t, 79.3s 47.0d, 21.6t, 42.5d, 21.6t 42.6t, 39.5s, 73.7s, 29.5q 30.3q, 14.6q, 19.6q	[1,11OH]—100.0% [1,4OR]—52.8%	[160]
XX	52.7t, 65.7d, 54.4t, 72.4s 49.4d, 21.7t, 43.1d, 21.8t 42.8t, 34.4s, 73.8s, 29.7q 30.6q, 20.5q, 24.0q	[4,11OR]—100.0%	[160]
XXI	215.8s, 33.6t, 36.0t, 70.3s 48.0d, 21.6t, 42.4d, 22.1t 41.2t, 46.5s, 73.4s, 29.5q 30.1q, 23.7q, 19.2q	[11OH]—90.6%	[161]
XXII	43.5t, 21.0t, 44.3t, 71.6s 52.0d, 21.5t, 48.4d, 68.6d 52.0t, 35.2s, 73.9s, 25.8q 30.1q, 23.8q, 23.3q	[4,11OR]—100.0% [4OR]—55.8%	[161]

Table 4 (*continued*)

Eudesmane	^{13}C NMR data (C_1–C_{15})	Proposed substructures	References
XXIII	79.3d, 29.4t, 36.7t, 72.7s 47.9d, 73.1d, 51.2d, 23.4t 41.4t, 41.5s, 25.9d, 24.5q 25.1q, 22.6q, 14.7q	[1,4OR]—52.8% [4,6OR]—78.9% [6OR]—72.3%	[161]
XXIV	36.0t, 24.6t, 75.7d, 72.8s 49.0d, 70.4d, 50.2d, 21.2t 44.9t, 34.2s, 28.9d, 20.3q 20.8q, 21.1q, 23.8q	[4,6OR]—78.9% [3,4OR]—73.9% [6OR]—72.3% [1,4OR]—52.8%	[162]
XXV	36.1t, 24.7t, 75.7d, 72.9s 49.0d, 70.0d, 50.0d, 21.3t 45.0t, 34.3s, 28.8d, 20.7q 21.1q, 21.1q, 23.8q	[4,6OR]—78.9% [3,4OR]—73.9% [6OR]—72.3% [1,4OR]—52.8%	[162]
XXVI	38.2t, 25.5t, 81.0d, 73.8s 52.0d, 26.2t, 70.1s, 205.5s 59.4t, 38.4s, 63.7s, 19.7q 19.4q, 18.9q, 18.0q	[8OXO]—100.0% [4OR]—55.8% [3,4OR]—73.9% [3,4OR]—71.4%	[163]
XXVII	38.1t, 25.6t, 74.0d, 85.5s 44.4d, 26.4t, 67.2s, 206.0s 57.8t, 37.9s, 65.7s, 20.8q 21.0q, 20.0q, 16.9q	[8OXO]—100.0% [4OR]—55.8% [3,4OR]—73.9% [3,4OR]—71.4%	[163]
XXVIII	38.6t, 25.6t, 81.3d, 74.0s 57.6d, 23.9t, 47.4d, 213.6s 56.0t, 39.2s, 28.1d, 20.7q 20.9q, 18.9q, 17.9q	[8OXO]—100.0% [3,4OR]—73.9% [3,4OR]—71.4%	[164]
XXIX (not attributed)	83.3s, 74.9d, 72.0s, 71.7d 70.1t, 56.2d, 49.9s, 43.9d 40.9t, 30.5q, 30.3t, 29.4q 22.8t, 22.6q, 17.6t	[1,4OR]—52.8% [6OR]—72.3%	[165]
XXX	80.4d, 30.4t, 42.3t, 72.0s 59.9d, 80.5d, 46.1d, 18.1d 28.5t, 44.1s, 71.4s, 30.4q 30.1q, 24.1q, 62.9t	[1,4OR]—52.8% [1,11OH]—100.0% [6OR]—72.3%	[165]
XXXI	77.4d, 32.2t, 120.9d, 135.1s 50.3d, 69.5d, 45.1d, 19.6t 33.5t, 36.3s, 27.3d, 22.2q 22.0q, 21.4q, 15.4q	[1OR; 3EN]—100.0%	[166]
XXXII	76.6d, 32.3t, 121.9d, 133.7s 50.8d, 68.4d, 49.0t, 20.5t 35.3t, 37.0s, 29.1d, 20.7q 21.0q, 20.3q, 11.8q	[1OR; 3EN]—100.0%	[166]

Table 4 (*continued*)

Eudesmane	^{13}C NMR data (C_1–C_{15})	Proposed substructures	References
XXXIII	47.7t, 198.4s, 125.5d, 168.2s 76.2s, 35.4t, 42.9d, 23.0t 76.2t, 41.5s, 71.8s, 23.2q 27.1q, 28.1q, 18.9q	–	[161]
XXXIV	78.7d, 35.2t, 121.5d, 134.9s 51.4d, 79.1d, 44.9d, 18.2t 26.5t, 42.2s, 72.4s, 30.1q 30.6q, 22.9q, 61.9t	[1,11OH]—100.0% [1OR; 3EN]—100% [6OR]—72.3%	[165]
XXXV	38.2t, 19.0t, 32.8t, 126.0s 135.1s, 27.0t, 44.2d, 22.7t 39.5t, 34.5s, 74.6s, 29.9q 28.0q, 19.7q, 26.0q	[4EN; 11OH]—56.2%	[167]
XXXVI	42.6t, 21.1t, 37.3t, 151.5s 44.5d, 24.1t, 42.4d, 23.8t 38.3t, 35.4s, 74.7s, 29.7q 29.3q, 105.4t, 17.2q	[11OH]—90.6% [4(14)EN]—61.5% [4(14)EN]—69.2%	[167]
XXXVII	81.4d, 33.7t, 36.2t, 147.2s 51.3d, 77.4d, 46.1d, 20.1t 28.4t, 42.9s, 72.6s, 31.1q 28.8q, 106.6t, 63.8t	[1,11OH]—100.0% [4(14)EN; 11OH]—81.8% [4(14)EN]—69.2% [6OR]—72.3%	[165]
XXXVIII	88.6d, 74.8d, 40.5t, 141.5s 47.6d, 72.5d, 43.0d, 22.2t 31.5t, 39.1s, 27.2d, 22.2q 24.1q, 113.2t, 12.6q	[4(14)EN]—69.2% [6OR]—72.3%	[168]
XXXIX	80.0d, 32.4t, 35.5t, 150.8s 48.9d, 24.7t, 45.2d, 23.4t 38.4t, 41.4s, 75.5s, 20.8q 69.1t, 107.0t, 10.7q	[4(14)EN; 11OH]—81.8% [11OH]—90.6% [4(14)EN]—69.2%	[169]
XL	80.1d, –, 34.8t, 144.5s, 55.4d 68.7d, 53.0d, 22.1t, 36.1t 40.6s, 74.3s, 24.2q, 29.8q 108.9t, 12.7q	[4(14)EN]—69.2% [6OR]—72.3%	[170]
XLI	35.2t, 29.7t, 73.5d, 151.8s 38.3d, 28.9t, 75.4s, 26.5t 35.9t, 35.4s, 76.4s, 24.6q 24.7q, 108.8t, 14.5q	–	[171]
XLII	41.0t, 22.2t, 36.8t, 151.0s 49.7d, 24.9t, 48.3d, 23.4t 41.7t, 35.5s, 80.8s, 23.6q 24.2q, 105.3t, 16.3q	[11OH]—90.6% [4(14)EN]—61.5% [4(14)EN]—69.2% [4(14)EN; 11OH]—81.8%	[172]

Table 4 (*continued*)

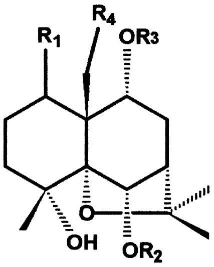
Eudesmane	^{13}C NMR data (C_1–C_{15})	Proposed substructures	References
XLIII	41.0t, 22.2t, 36.8t, 151.1s 49.8d, 25.0t, 48.2d, 23.4t 41.8t, 35.9s, 80.6s, 23.7q 24.1q, 105.4t, 16.3q	[11OH]—90.6% [4(14)EN]—61.5% [4(14)EN]—69.2% [4(14)EN;11OH]—81.8%	[172]
XLIV	37.9t, 25.3t, 79.1d, 75.2s 156.2s, 121.3d, 66.9s, 203.2s 57.8t, 41.3s, 66.6s, 19.3q 20.6q, 26.7q, 24.7q	[3,4OR]—73.9%	[163]
XLV	42.0t, 20.8t, 44.1t, 71.5s 56.2d, 26.2t, 132.9s,25.3t 56.2t, 35.3s, 120.5s, 20.1q 20.1q, 22.6q, 18.5q	[4OR]—55.8% [7(11)EN]—76.9%	[161]
XLVI	41.4t, 20.2t, 43.5t, 72.1s 49.1d, 22.7t, 39.4d, 23.5t 40.4t, 35.2s, 146.9s, 110.8t 22.6q, 22.3q, 18.5q	[4OR]—55.8% [11EN]—73.7%	[173]
XLVII	37.6t, 25.6t, 73.7d, 86.7s 44.5d, 33.3t, 80.3s, 211.3s 55.0t, 40.5s, 143.9s, 115.1t 18.2q, 19.3q, 16.8q	[8OXO]—100.0% [3,4OR]—73.9% [3,4OR]—71.4%	[164]
XLVIII	41.1t, 20.2t, 43.5t, 72.0s 55.0d, 26.6t, 40.6d, 27.4t 44.6t, 34.6s, 145.9s, 122.3t 167.9s, 22.5q, 18.7q	[11EN; 13OXO; 13OR]—100.0% [4OR]—55.8%	[174]
XLIX	33.5t, 14.7t, 31.9t, 68.1s 72.3s, 26.8t, 37.6d, 19.9t 37.4t, 33.6s, 143.5s, 126.0t 171.3s, 201.9d, 20.7q	[11EN; 13OXO; 13OR]—100.0%	[166]
L	32.0t, 15.5t, 34.4t, 68.5s 71.3s, 26.9t, 38.3d, 22.1t 34.6t, 34.1s, 143.3s, 125.4t 170.5s, 201.4d, 23.1q	[11EN; 13OXO; 13OR]—100.0%	[166]
LI (not attributed)	150.8s, 108.2t, 80.0s, 52.1d 46.3d, 45.0t, 40.8t, 39.2t 26.9t, 26.1t, 19.8t, 27.5q 21.0q, 20.4q, 34.8s	[4OR]—55.8% [11EN]—73.7%	[175]
LII (not attributed)	150.8s, 108.2t, 80.0s, 52.1d 46.3d, 45.0t, 40.8t, 39.2t 26.9t, 26.1t, 19.8t, 20.7q 20.7q, 19.8q, 34.8s	[4OR]—55.8% [11EN]—73.7%	[175]
LIII	39.5t, 27.4t, 79.7d, 75.8s 47.1d, 22.5t, 38.8d, 23.4t	[3,4OR]—73.9% [3,4OR]—71.4%	[176]

Table 4 (*continued*)

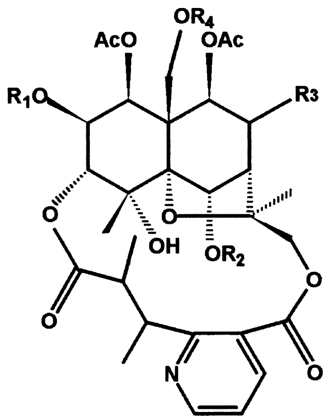
Eudesmane	^{13}C NMR data (C_1–C_{15})	Proposed substructures	References
	40.1t, 35.2s, 146.7s, 111.0t 22.8q, 16.2q, 18.7q	[11EN]—73.7%	
LIV	39.2t, 25.8t, 82.1d, 74.5s 48.3d, 22.1t, 38.8d, 23.1t 40.2t, 35.2s, 146.8s, 111.5t 22.7q, 17.5q, 18.9q	[3,4OR]—73.9% [3,4OR]—71.4% [11EN]—73.7%	[176]
LV	37.3t, 20.6t, 120.1d, 144.1s 131.5s, 124.9d, 48.5d, 23.0t 38.2t, 32.3s, 73.3s, 25.9q 28.1q, 20.3q, 23.4q	[3.5EN]—100.0%	[170]
LVI	40.3t, 71.5d, 124.3d, 143.3s 81.6s, 30.2t, 34.6d, 26.4t 36.2t, 33.2s, 144.2s, 125.9t 171.1s, 25.1q, 17.4q	[11EN; 13OXO; 13OR]—100.0%	[174]
LVII (not attributed)	199.1s, 171.5s, 161.0s, 143.8s 129.1s, 35.7s, 39.6d, 125.6t 41.7t, 37.3t, 33.7t, 33.2t 27.1t, 22.4q, 10.8q	[3OXO; 4EN]—100.0% [11EN; 13OXO; 13OR]—100.0%	[177]
LVIII	40.0t, 19.0t, 27.2t, 129.0s 140.5s, 32.0t, 41.2d, 29.9t 41.7t, 35.0s, 144.8s, 124.2t 171.3s, 62.9t, 24.8q	[11EN; 13OXO; 13OR]—100.0%	[166]
LIX	39.3t, 17.7t, 23.7t, 133.0s 163.6s, 29.9t, 40.9d, 26.9t 41.2t, 36.6s, 143.6s, 125.6t 171.6s, 191.7d, 25.1q	[11EN; 13OXO; 13OR]—100.0%	[166]
LX	35.0t, 22.2t, 31.7t, 151.9s 75.8s, 35.4t, 40.0d, 26.0t 34.3t, 37.7s, 150.5s, 108.5t 21.1q, 107.6t, 19.9q	[5OR; 11EN]—100.0%	[178]
LXI	47.3t, 70.8d, 42.8t, 146.5s 49.8d, 26.6t, 40.4d, 30.0t 41.2t, 35.9s, 146.6s, 123.7t 168.3s, 109.1t, 24.0q	[11EN; 13OXO; 13OR]—100.0% [4(14)EN]—69.2%	[161]
LXII	30.2t, 28.2t, 74.9d, 146.9s 76.9s, 36.6t, 36.0d, 25.6t 33.0t, 38.6s, 144.4s, 124.2t 171.3s, 116.4t, 22.3q	[11EN; 13OXO; 13OR]—100.0%	[179]
LXIII	79.3d, 31.5t, 34.2t, 148.7s 47.6d, 26.5t, 45.3d, 28.9t	[4(14)EN]—69.2% [11EN]—73.7%	[180]

Table 4 (*continued*)

Eudesmane	^{13}C NMR data (C_1–C_{15})	Proposed substructures	References
	37.0t, 40.2s, 150.3s, 108.3t 20.9q, 106.8t, 10.2q		
LXIV	A-41.9t, 23.5t, 36.9t, 150.6s 50.0d, 29.9t, 39.9d, 27.4t 41.2t, 36.0s, 145.3s, 123.7t 168.8s, 105.6t, 16.4q B-126.7s, 195.6s, 82.9d 75.3s, 54.6d, 82.2d, 50.0d 24.9t, 38.5t, 158.2s, 137.8s 166.3s, 120.2t, 24.7q, 17.6q	[11EN; 13OXO;13OR]—100.0% [4(14)EN]—61.5% [4(14)EN]—69.2%	[181]
LXV	47.2t, 67.8d, 39.0t, 39.4d 147.8s, 126.0d, 42.0d, 27.5t 42.0t, 39.4s, 146.7s, 123.1t 168.5s, 19.3q, 28.2q	–	[161]
LXVI (not attributed)	19.4q, 21.4q, 26.8t, 29.0t 35.7t, 37.3s, 38.8t, 46.2d 48.4d, 106.4t, 108.7t, 123.3d 139.7d, 148.0s, 151.0s	[1,4(14)EN]—100.0% [11EN]—73.7%	[182]
LXVII	40.9t, 126.9d, 130.1d, 145.3s 45.1d, 27.5t, 39.1d, 29.7t 42.8t, 33.6s, 146.0s, 125.1t 172.5s, 109.6t, 17.0q	[11EN; 13OXO; 130R]—100.0%	[174]
LXVIII	77.1d, 29.0t, 119.7d, 134.6s 44.2d, 21.2t, 116.6s, 150.1s 35.0t, 37.5s, 119.4s, 137.8d 8.1q, 20.8q, 11.4q	[1OR; 3EN]—100.0% [7,11EN; 8,12OXY]—100.0%	[183]
LXIX	80.1d, 28.3t, 34.0t, 147.4s 44.1d, 20.7t, 115.7s, 149.1s 36.0t, 40.2s, 119.3s, 137.8d 8.1q, 109.0t, 12.0q	[4(14)EN]—69.2% [7,11EN; 8,12OXY]—100.0%	[183]
LXX	210.8s, 38.7t, 34.7t, 146.1s 44.9d, 20.7t, 114.9s, 149.7s 32.0t, 49.2s, 119.1s, 138.1d 8.1q, 109.9t, 17.3q	[7,11EN; 8,12OXY]—100.0%	[184]



	R_1	R_2	R_3	R_4	Name
I	OBz	Ac	Bz	H	---
II	OBz	Bz	Bz	H	---
III	β-OAc	H	Bz	OCin	TWHR-1
IV	β-OBz	Nic	Bz	H	Regelidine

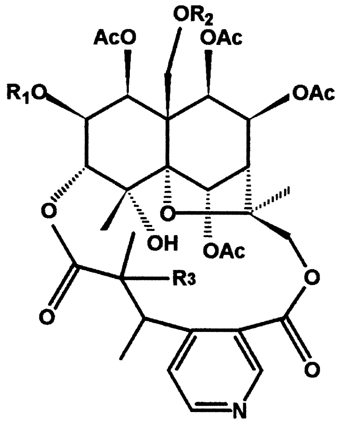


	R_1	R_2	R_3	R_4	Name
V	Ac	Fur	β-OAc	Ac	Hyponine-A
VI	Ac	Ac	β-OAc	Fur	Hyponine-B
VII	Ac	Ac	β-OAc	Bz	Hyponine-C
VIII	Ac	Bz	β-OAc	Ac	Cangorinine E-I
IX	Ac	Ac	α-OBz	Ac	Aquifoliunine E-I
X	H	Ac	α-OH	Ac	Aquifoliunine E-II
XI	Ac	Ac	α-OH	Ac	Aquifoliunine E-III
XII	Ac	Ac	α-ONic	Ac	Aquifoliunine E-IV

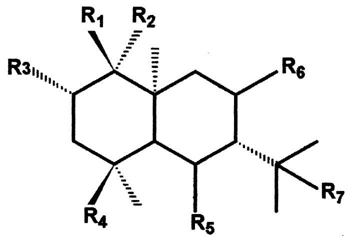
Fig. 3. Eudesmanes used to test the program.

this way, through the overlap of two or more presented substructures, we can achieve a complete structure for the new eudesmane.

In order to check if the chemical shift ranges obtained were useful for structure determination of new substances, eudesmanes published in the literature from 1997 (included in Fig. 3) were deliberately not fed into the database for calculating the ranges



	R_1	R_2	R_3	Name
XIII	Ac	Fur	OH	Hypoglaunine A
XIV	Fur	Ac	OH	Hypoglaunine B
XV	Bz	Ac	OH	Hypoglaunine C
XVI	Ac	Fur	H	Hypoglaunine D
XVII	Ac	Fur	OH	Hypoglaunine



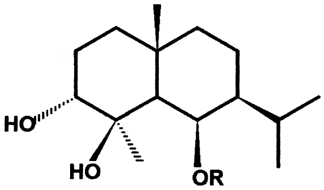
	R_1	R_2	R_3	R_4	R_5	R_6	R_7	Name
XVIII	H	H	OH	OH	H	H	OGlu	Pterodontoside A
XIX	H	OH	H	OGlu	H	H	OH	Pterodontoside B
XX	H	H	OH	OH	H	H	OH	Pterodontriol A
XXI	OXO		H	OH	H	H	OH	---
XXII	H	H	H	OH	H	OH	OH	Pterodontriol C
XXIII	OH	H	H	OH	OH	H	H	Pterodontriol D

Fig. 3. (*continued*)

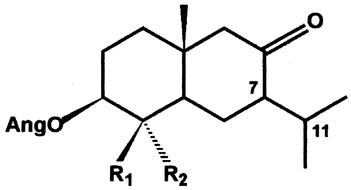
shown in Table 3, and these values were then used to test the efficiency of obtaining substructures from the chemical shifts of a new substances. The results of these tests are presented in Table 4, where only the first 15 chemical shifts of the compound are given, after the chemical shifts of the substituents had been previously removed by the MACRONO program [152].

6. Discussion of results and conclusions

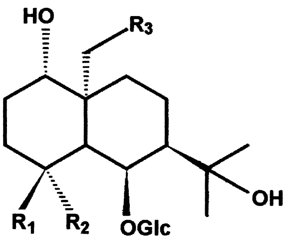
The system used here was able to propose substructures in 95.7% of the cases considered. The negative results for a few cases (eudesmanes XXXIII, XLI and LXV) were probably due to the non-existence of precise rules for these compounds. A more detailed



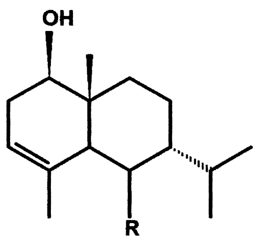
	R
XXIV	Bz
XXV	Cin



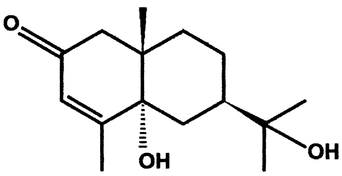
	R_1	R_2	
XXVI	CH_3	OH	7,11β-epoxy
XXVII	OAc	CH_3	7,11α-epoxy
XXVIII	OH	CH_3	---



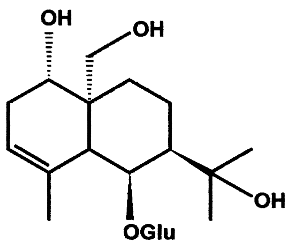
	R_1	R_2	R_3
XXIX	CH_3	OXY	
XXX	OH	CH_3	OH



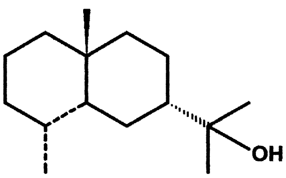
	R
XXXI	α-OH
XXXII	β-OH



XXXIII

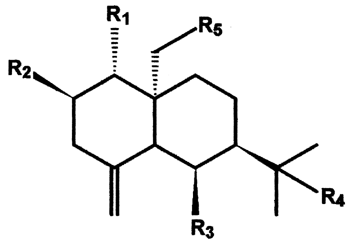


XXXIV - Dictamnoside C

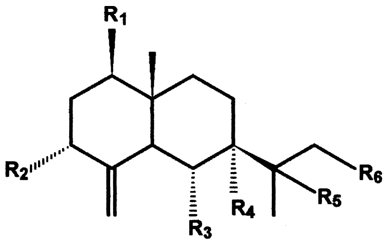


XXXV - Δ^4 - 7-epi-γ-eudesmol
XXXVI - $\Delta^{4(14)}$ - 7-epi-β-eudesmol

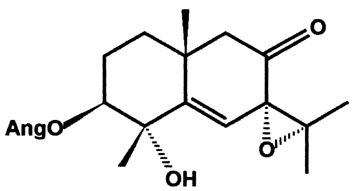
Fig. 3. (*continued*)



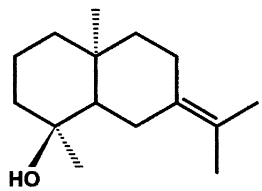
	R_1	R_2	R_3	R_4	R_5	Name
XXXVII	OH	H	OGlu	OH	OH	Dictamnoside B
XXXVIII	-OC(Me)$_2$O-		OAc	H	H	---



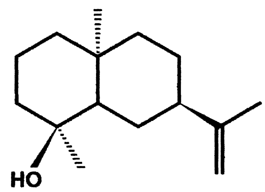
	R_1	R_2	R_3	R_4	R_5	R_6	Name
XXXIX	OH	H	H	H	OH	OH	---
XL	OAc	H	OH	H	OH	H	---
XLI	H	OH	H	OH	OH	H	Clypeotriol
XLII	H	H	H	H	O[α]Ara	H	---
XLIII	H	H	H	H	O[β]Ara	H	---



XLIV



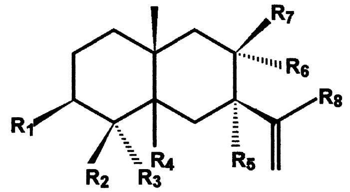
XLV



XLVI - Intermedeol

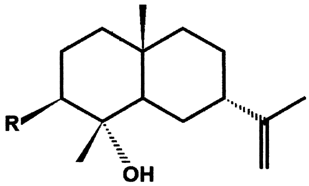
Fig. 3. (*continued*)

analysis of the cases where the program was able to propose overlapping substructures gave a 98.8% success rate, where it was possible to build up a complex molecular structure. A few imprecise assignments occurred in some cases (tests XXIV and XXV). In both tests, four substructures were proposed with incorrect positioning of one of the groups "–OR" (position 1 or 6 of the skeleton), but the correct structure was always displayed as one the three first options. It is worth noting that in many

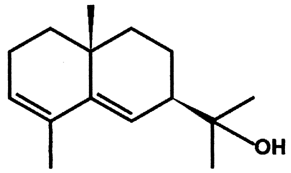


	R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8
XLVII	OAng	OAc	CH_3	α-H	OH	OXO		CH_3
XLVIII	H	CH_3	OH	α-H	H	H	H	CO_2Me
XLIX	H	OH	CHO	α-OH	H	H	H	CO_2H
L	H	OH	CHO	β-OH	H	H	H	CO_2H
LI	H	CH_3	A	α-H	H	H	H	CH_3
LII	H	CH_3	B	α-H	H	H	H	CH_3

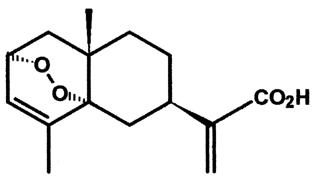
A - 3’-senecioyloxy-6’-deoxyglucopyranoside
B - 3’-tigloyloxy-6’-deoxyglucopyranoside



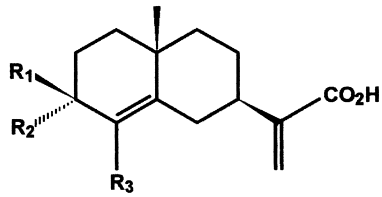
	R
LIII	OH
LIV	OAc



LV



LVI

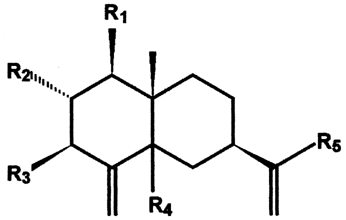


	R_1	R_2	R_3	Name
LVII	OXO		CH_3	---
LVIII	H	H	CH_2OH	---
LIX	H	H	CHO	Isocostic Acid

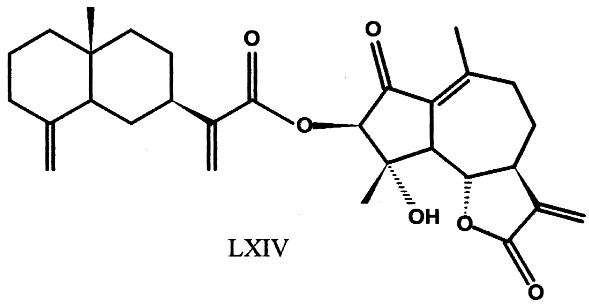
Fig. 3. (*continued*)

cases the overlapping of two or more proposed substructures resulted in the correct assignment of the compound structure. For example, in tests I–XVII, the user selection could choose the correct position of the groups indicated by the MACRONO program [152].

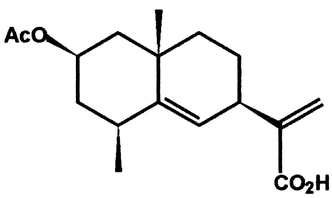
The results obtained with this new class of compounds, not previously presented in the SISTEMAT



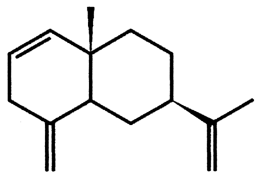
	R_1	R_2	R_3	R_4	R_5	Name
LX	H	H	H	α-OH	CH_3	---
LXI	H	OAc	H	α-H	CO_2H	2α-Acetoxycostoate
LXII	H	H	OH	β-OH	CO_2H	---
LXIII	OH	H	H	α-H	CH_3	β-Dictyopterol



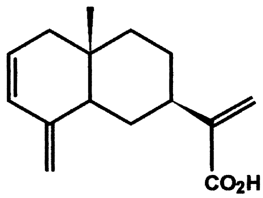
LXIV



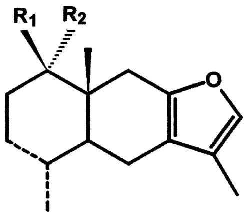
LXV - 2β-Acetoxy pterodontic acid



LXVI



LXVII



	R_1	R_2	
LXVIII	OAc	H	Δ^3
LXIX	OAc	H	$\Delta^{4(14)}$
LXX	OXO		$\Delta^{4(14)}$

Fig. 3. (*continued*)

system, confirm the power of these expert systems in the field of structural elucidation and as a new tool for use in the search for heuristic rules.

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