Structure of Floranol, a flavonoid isolated from *Dioclea grandiflora*.

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Palavras Chave: floranol; prenylated flavanonol, X-ray structure

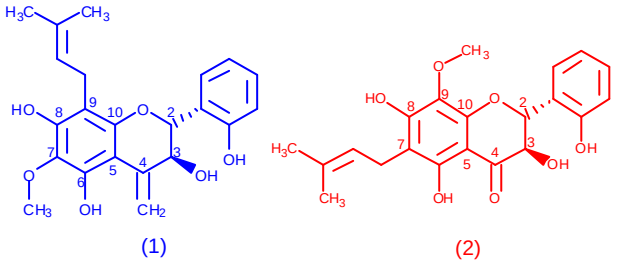
Introduction

Dioclea grandiflora is a Brazilian vine commonly known as "olho de boi". Its root is used for the treatment of kidney stones and prostate gland disorders.[1] Previous works have reported the presence of flavonoids in this plant (e.g. Jenking et al., 1999).[2] The promising biological activities of flavonoids prompted us to investigate potential pharmacological properties of the flavonoids from *Dioclea grandiflora*. In the course of our continuing interest in *D. grandiflora*, we have isolated a biological active prenylated flavanonol named by us as floranol. The aim of the present work is to determine its crystal structure by X-ray diffraction (XRD).

Results and Discussion

The roots of Dioclea grandiflora Mart. ex Benth. (Fabaceae) were collected from the municipality of Santa Rita, Paraíba state, Brazil. After the isolation procedures described in Lemos et al. (2002),[3] floranol was recrystallized in ethyl acetate. A well-shaped prismatic single crystal of 0.26 x 0.12 x 0.10 mm^3 was used for data collection. The X-ray data were measured at 100 K on an Enraf-Nonius Kappa-CCD diffractometer with graphite monochromated radiation. The structure was solved using direct methods and the model was refined by full-matrix least-squares procedures on F^2.

The initial aim in performing a XRD study for the floranol was to solve the ambiguity arising from the difficulties to identify, from spectroscopic data analysis, which isomer, (1) or (2), (see scheme) have been isolated from *D. grandiflora*.



(1) (2)

The XRD technique has allowed us to establish unambiguously the presence of the isopropyl group at C9 (see scheme) position confirming isomer (1). Another interesting crystallographic feature in this study is the highly symmetric space group found for this organic compound (Trigonal, R3). It is important to emphasize that in the Cambridge Structural Database (CSD) only 186 of the organic structures deposited crystallize in the R3 space group. This number represents ~0.05% of the total one deposited (355067 structures – update august 2005). The inter-molecular interactions are, of course, the main responsible by the high symmetrical space group observed for this compound. One water of crystallization was observed, which forms an H bond with the O3 atom.

The crystal structure of (1) is shown in Figure 1. It is shown that floranol exhibits two intra-molecular hydrogen bonds. The packing revels that there are three cavities along the c axis, which take place exactly on the position of the 3-fold symmetry axis 3 and 3_2. Considering one of these cavities, which has a mean diameter of ~8 Å, this polymorph of floranol can be regarded as a zeolite type of compound.

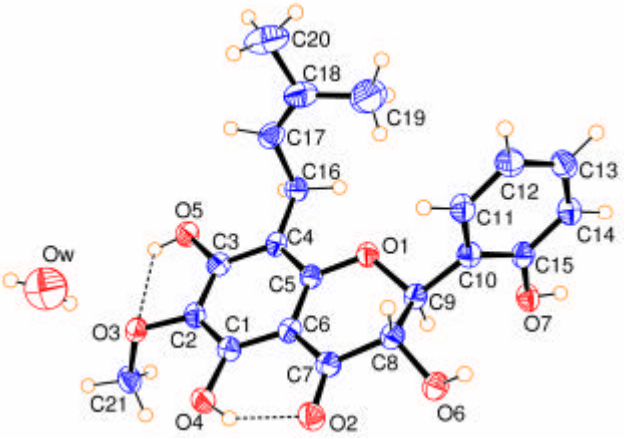


Figure 1. ORTEP view of floranol.

Conclusion

The structure of the prenylated flavanonol, floranol, isolated from the roots of *Dioclea grandiflora* (Fabaceae), was unambiguously determined by crystallographic X-ray analysis.

Acknowledgments

The authors are grateful to CNPq and FAPESP.

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