Tephrosia species are widely used in East African traditional medicinal practice to treat various infectious diseases. In our continued search for antiplasmodial agents from Tephrosia species found in Kenya a new flavone [(+)-Tephrodin] from the stem of *T. purpurea* was isolated. Its 1H NMR spectrum is identical with the spectrum reported for tephrodin which was isolated from *T. polystachyoides*. However, in contrast to the levorotary tephrodin found by Vleeggar et al. our compound showed dextrorotatory behaviour (δC20 = +4.7°). This suggests that both compounds must be stereoisomers.

To clarify the relative configuration of our compound experimental data are compared with theoretical quantum chemical calculations (DFT B3LYP 6-311G**).

For configurational and conformational analysis the coupling constants between H-3° and both protons H-2° (2.3 and 1.0 Hz, resp.) can be used:

Theoretical calculations gave a global energy minimum of the gauche-gauche conformation between H-3° and both H-2° for the cis linked R*R* diastereomer (A). The next local energy minimum (ΔAG°=1.83 kcal/mole) for the R*R* diastereomer was found also to have a gauche-gauche conformation between H-3° and both H-2°, it differs only in rotational angle of the acetyl group (B). The conformation with a local energy minimum for an antiperiplanar-gauche conformation between H-3° and both H-2° has an energy difference to the global minimum of 5.13 kcal/mole (C). Considering the Boltzmann distribution, this energy is too high to be found by NMR in solution. The trans-linked R*S* diastereomer did not give any local minimum with a gauche-gauche conformation, all calculations went to the global minimum with an antiperiplanar-gauche conformation between H-3° and both protons at C-2° (D). The coupling constants observed between H-3° and both protons at C-2° (J = 2.3 and 1.0 Hz), together with NOESY results, allow only gauche-gauche conformation. Thus, it can be assumed that our compound is one of the two R*R* stereoisomers, and since the optical rotation observed (dextrorotatory) is opposite to the one reported for (+)-tephrodin it must be the other R*R* stereoisomer.

The intensities of the NOESY cross peaks between H-3° and both of the H-2° protons are about the same size. Thus, also their distances must be very similar.

(+)-Tephrodin was tested *in vitro* against D6 and W2 strains of *Plasmodium falciparum* and showed good to moderate activities (IC50 = 14.0±1.5 μM and 18.0±2.4 μM, resp.). No significant cytotoxicity was observed (IC50 >100 μM).

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