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(+)-Tephrocin - A New Flavone from *Tephrosia purpurea*

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Tephrosia species are widely used in East African traditional medicinal practice to treat various infectious diseases. In our continued search for antiparasitic agents from *Tephrosia* species found in Kenya a new flavone [(+)-Tephrocin] from the stem of *T. purpurea* was isolated.¹

Its ¹H NMR spectrum is identical with the spectrum reported for tephrocin which was isolated from *T. polystachyoides*.²

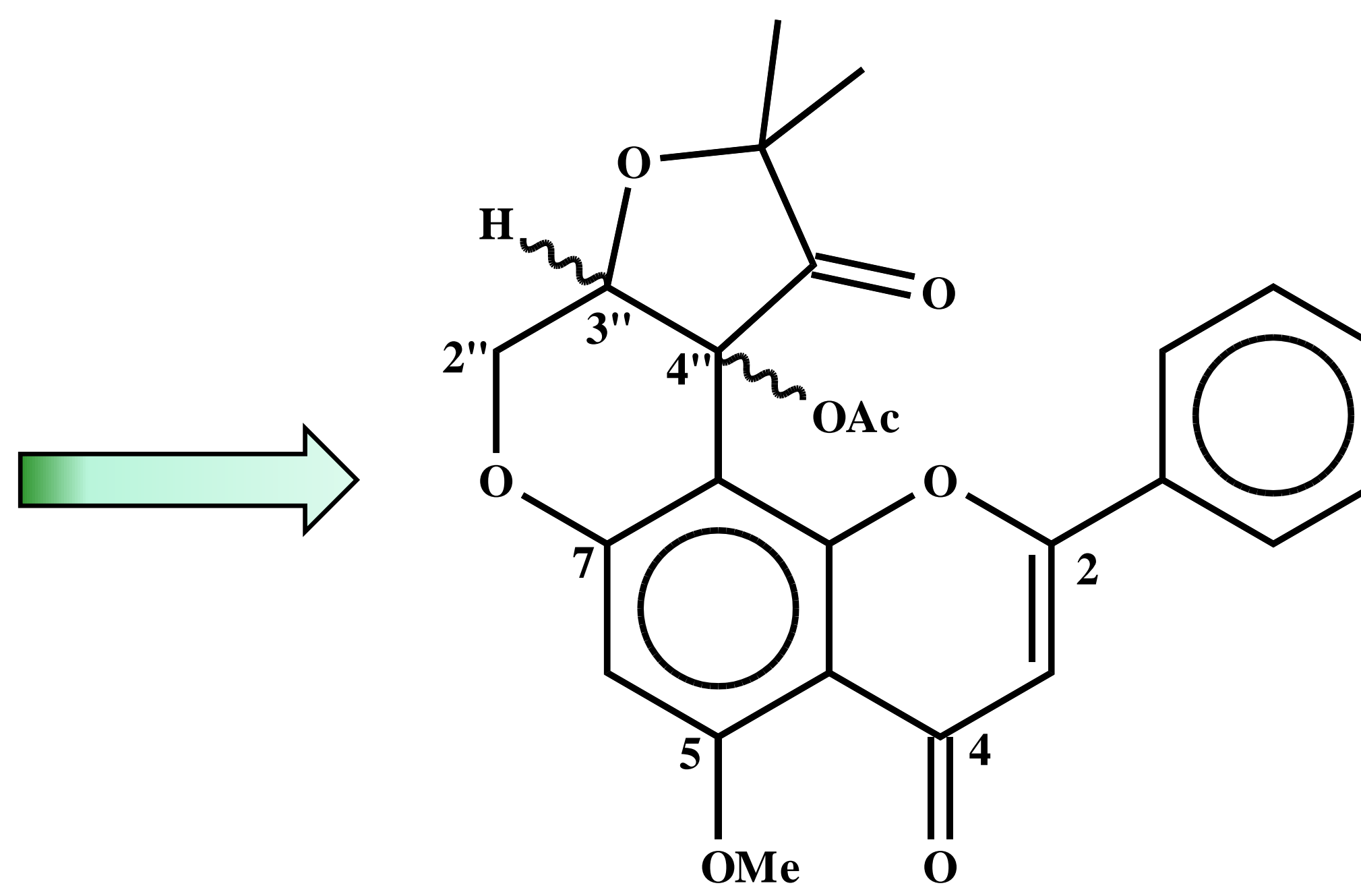
However, in contrast to the levorotatory tephrocin found by Vleggar et al. our compound showed dextrorotatory behaviour ($[\alpha]_D^{20} = +4.7^\circ$). This suggests that both compounds must be stereoisomers.

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:

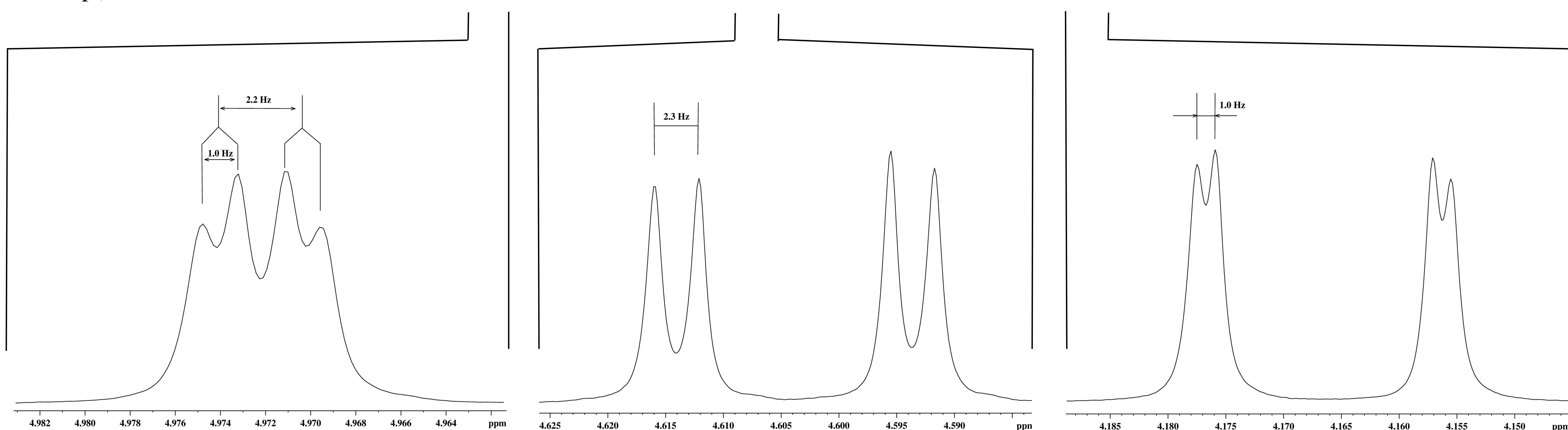
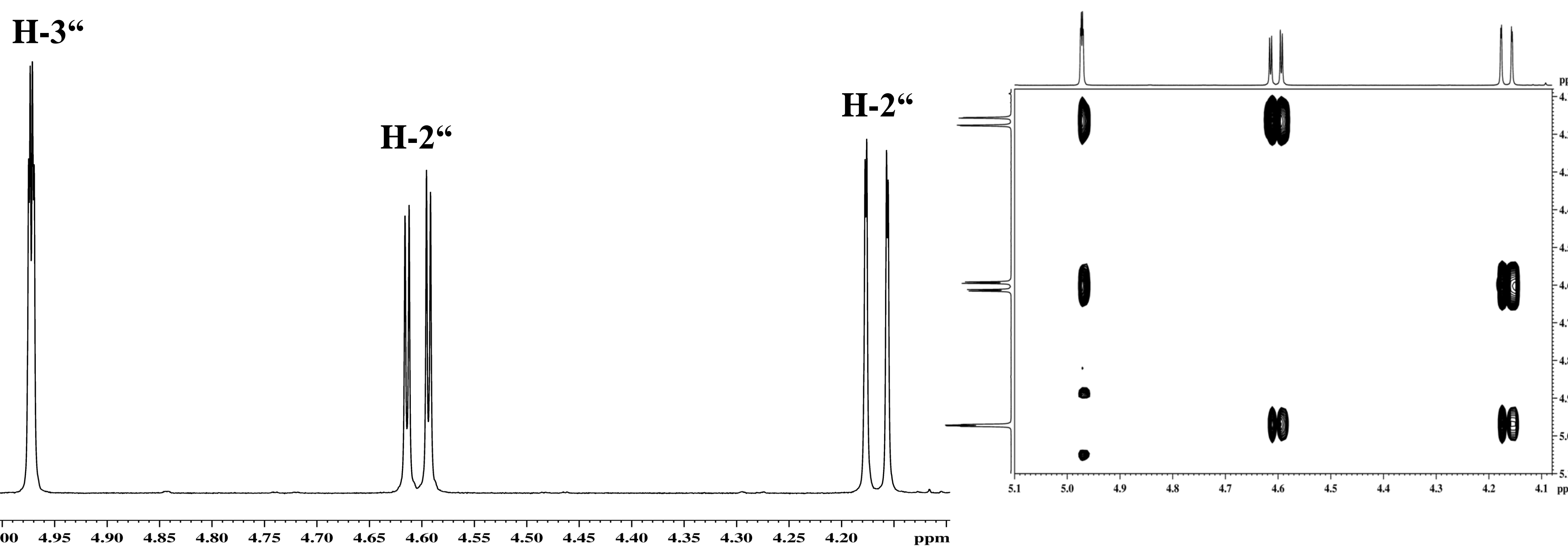


Tephrosia purpurea



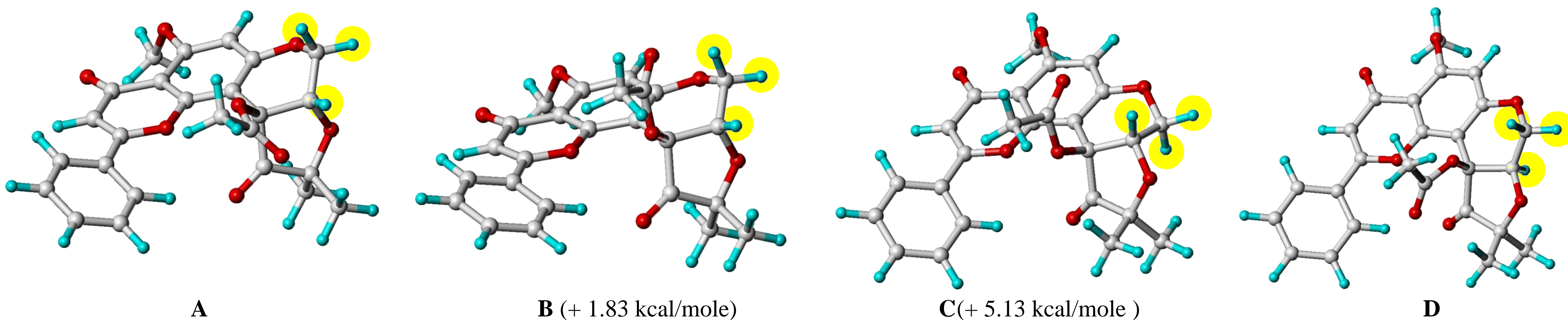
R*R*- or R*S*-Tephrocin?

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:



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 ($\Delta\Delta G^\circ = 1.83$ 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 (-)-tephrocin it must be the other

R*R* stereoisomer.



(+)-Tephrocin was tested *in vitro* against D6 and W2 strains of *Plasmodium falciparum* and showed good to moderate activities ($IC_{50} = 14.0 \pm 1.5$ μ M and 18.0 ± 2.4 μ M, resp.). No significant cytotoxicity was observed ($IC_{50} > 100$ μ M).

¹ Muiva-Mutisya L., Macharia B., Heydenreich M., Koch A., Akala H.M., Derese S., Omosa L.K., Yusuf A.O., Kamau E., Yenesew, A. *Phytochem. Lett.*, in press.

² Vleggar R., Smalberger T.M., de Waal H.L. *Tetrahedron Lett.* **13** (1972) 703