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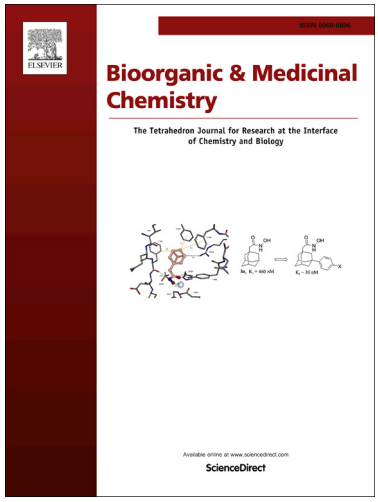

Dibenzosuberyl substituted polyamines and analogs of clomipramine as effective inhibitors of trypanothione reductase; molecular docking, and assessment of trypanocidal activities

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Title:
Dibenzosuberyl substituted polyamines and analogs of clomipramine as effective inhibitors of trypanothione reductase; molecular docking, and assessment of trypanocidal activities.

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Abstract:

Trypanothione reductase (TR) is an enzyme critical to the maintenance of the thiol redox balance in trypanosomatids, including the genera *Trypanosoma* and *Leishmania* that are parasites responsible for several serious diseases. Analogs of clomipramine were prepared since clomipramine is reported to inhibit TR and cure mice infected with trypanosomes, however its psychotropic activity precludes its use as an anti-trypanosomal therapeutic. The clomipramine analogs contained a tricyclic dibenzosuberyl moiety. Additionally a series of polyamines with *N*-dibenzosuberyl substituents were prepared. All compounds studied were competitive inhibitors of TR and showed trypanocidal activities against *T. brucei in vitro*. The analogs of clomipramine were poor inhibitors of TR, whereas the polyamine derivatives were effective TR