Limonene-based thiosemicarbazones as inhibitors of *Leishmania amazonensis:* crystal structures with a pseudo-center of symmetry

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The current treatment to the human protozoan leishmaniasis disease shows limited effectiveness, pathogen resistance and toxicity, thereby causing adverse side effects, which justify the search for new drug candidates. Compounds with the essential structural unit thiosemicarbazone are known to possess antineoplastic, antitubercular, antiviral properties, and are also antiparasitic. The large monoterpene family provides many examples of renewable natural products that meet the non-toxicity required for new candidates. Aiming to discover compounds with antileishmania activity, (R)-limonene was selected as the chiral building block to thiosemicarbazones due to the reactivity of the terminal double bond toward the acid addition, with retention of the chiral integrity of the natural product. We present the structure of two novel chiral limonene-based thiosemicarbazone derivatives, *m*-nitrobenzaldehyde – 4-limonene-3-thiosemicarbazone (Figure 1a) and *o*-clorobenzaldehyde -4 limonene-3-thiosemicarbazone (Figure 1b), elucidated by x-ray crystallography. The crystal structure, both of $P2_1$ space group, is formed by packing dimers joined by N—H…S intermolecular H-bonds related by a pseudo-center of symmetry.

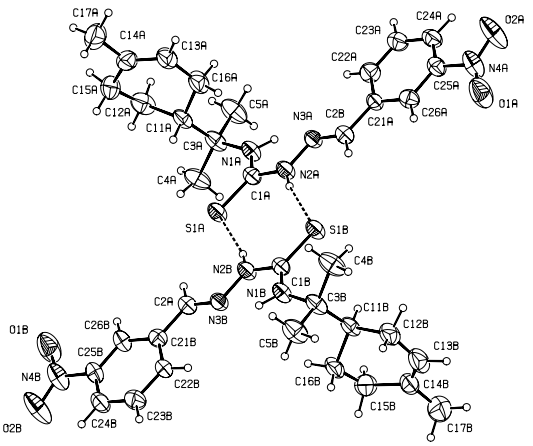

Figure 1a

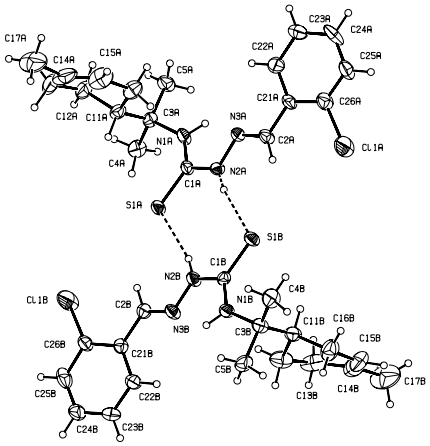

Figure 1b

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