2-Hexanoyl-1-tribromomethyl-1,2,3,4-tetrahydro-β-carboline: Crystal Structure Analysis of a Potent Inhibitor of Complex I of Mitochondrial Respiration*

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The molecular structure of the title compound 2-hexanoyl-1-tribromomethyl-1,2,3,4-tetrahydro-β-carboline (3), a potent inhibitor of complex I of the mammalian mitochondrial respiratory chain, has been studied by single-crystal X-ray diffraction analysis. In the crystal, two heterochiral molecules of 3 (i.e., one $R$- and one $S$-configured molecule each) were found to be connected with one other in pairs via two intermolecular hydrogen bonds [O(215)···H(212)' and O(215)''···H(212)] to form an overall achiral ‘dimeric’ subunit.