Structure of Diastereomeric 10-Bromo-10,11-dihydroquinines

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Cinchona Alkaloids, 10-Bromo-10,11-dihydroquinines, New Chiral Center Configuration

The absolute configurations of new chiral centers in the side chains of diastereomeric 10,11-dihydroquinines, C_{20}H_{25}BrN_{2}O_{2}, have been determined. Both diastereomers with either 10R or 10S configuration adopt the conformations in which quinuclidine nitrogen atom points away from the quinoline ring (open conformations). The bulky C3-side chain in the 10R diastereomer hinders intermolecular hydrogen bond formation to the quinuclidinic, more basic nitrogen atom. Instead, the hydrogen bond to the quinolinic N atom is formed which is an unusual case for Cinchona alkaloid crystal packing. The same bulky C3-substituent in the 10S diastereomer does not hinder the common packing mode via intermolecular hydrogen bonding to the quinuclidinic N-atom.