

Poster Presentations

[MS38-P05] Salts of (+)-deoxycholic acid with amines: Structure and chiral resolution

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(+)-deoxycholic acid (DCA) is a bile acid involved in the solubilization of fats in the gastrointestinal tract. The bile acids contain hydroxyl groups directed below the plane and methyl groups pointing above the plane, thus providing both a hydrophilic side and a hydrophobic side. The inclusion compounds of the bile acids have attracted much interest and Giglio [1] has reviewed the inclusion compounds of DCA. Miyata *et al.* [2,3] related the inclusion ability of different bile acids and their derivatives with various organic guests. The bile acids are also chiral, enabling their application in chiral studies. Thus the use of DCA as a chiral resolving agent has been explored. [4,5,6] In this study we focus on the salts formed between DCA and the chiral amines *sec*-butylamine and 3-methyl-2-butylamine. The salts were characterized using thermal analysis and single crystal X-ray diffraction. In the structures we observed proton transfer from the carboxylic acid moiety of DCA to the nitrogen of the amine guest. The chiral discrimination of DCA for racemic mixtures of *sec*-butylamine and 3-methyl-2-butylamine yielded interesting results. A mixture of DCA and racemic *sec*-butylamine yielded exclusively crystals of the (*R*)-2-butylammonium deoxycholate. A similar experiment with DCA and racemic 3-methyl-2-butylamine resulted in only crystals of the (*S*)-3-methyl-2-butylammonium deoxycholate.

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