Present work intends to quantify the degree of isostucturation of these pairs by means of packing coefficients, hydrogen bond parameters and analysis of the corresponding atomic coordinates of eleven steroids possessing a common flexible 14-iso-cholesterol skeleton. E.g. solitarein (reported by us earlier as 4,4-thiodibenzylothiol, Ribar et al [1993] J. Chem. Res. 321) is quasi-isostuctural with bufalin (Roemer et al [1982] Acta Cryst. B 38, 1865) although there is a quite relevant difference between the puckering of their A rings.

Fig. 1. Eleven steroids having a common sp. gr. P2_{1}2_{1}2

DIGITOGENICIN  DIGITOXIGENIN

METHYLDIGITOXIGENIN: = R = Methyl

DIGIREZIGENIN: = R = 0-Acetyl

GAMAEUFOTALIN: R = OH

ARENOBUFAGIN: R = OH

SCILLARENIN (reported in atomic coordinates of eleven steroids possessing a common flexible 14-iso-cholesterol skeleton. E.g. solitarein (reported by us earlier as 4,4-thiodibenzylothiol, Ribar et al [1993] J. Chem. Res. 321) is quasi-isostuctural with bufalin (Roemer et al [1982] Acta Cryst. B 38, 1865) although there is a quite relevant difference between the puckering of their A rings.)

In the plot presented below the dotted area show the possible values of \( \Phi_1 \) and \( \Phi_2 \). The plot also shows the conformations of four diphenylsulphide derivatives determined experimentally:

1. diphenylsulphide, \( \Phi_1 = 35.5 \) (Rozsnyai et al., Acta Chim. Budapest 1977, 26, 321);
2. 4,4-thiodibenzylothiol, \( \Phi_1 = 33.4 \) (Ratajczak-Sitarz et al., Acta Cryst. C – in press);
3. 1,4-bis(phenylthio)benzene, \( \Phi_1 = 9.2 \) (Andreatti et al., Cryst. Struct. Comm. 1981, 10, 789);

In three of these structures the phenyl rings are related by the twofold axis passing through the central S atom and, consequently, \( \Phi_1 \) and \( \Phi_2 \) have the same values. The plot shows that angles \( \Phi_1 \) and \( \Phi_2 \) in all above structures fall in the region least limited by steric hindrances, where \( \Phi_1 \) and \( \Phi_2 \) have the same sign. The close van der Waals contacts were found only in the molecule of 4,4-thiodibenzylothiol: \( \Phi_2 = 35.5 \) (Rozsnyai et al., Acta Chim. Budapest 1977, 26, 321).

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