

**MS33-1-1 Self-assembly and conformation of three novel benzothiazolyl azo dyes
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The majority of synthetic aromatic dyes are azo dyes (65-70 %), in which one or more N=N groups are linked to aromatic or heteroaromatic ring substituted with some functional groups. Azo dyes are mostly used in textile industry (80%), because of their low cost, high stability and colour variety, but also for colouring different substrates in many other industrial fields. Besides, they are used in a number of high-tech applications such as for optical data storage and non-linear optics [1,2]. Compounds which contain heterocyclic ring, compared to those that have aromatic ring, are used in the design of new azo dyes due to the fact that they exhibit better colour strength and brightness. From variety of such dyes interest for those with benzothiazole ring is growing. We have previously reported synthesis and structural studies of several azo dyes that comprise benzothiazole ring [3,4]. Herein we present the synthesis and X-ray structures of three novel benzothiazolyl azo derivatives that have potential to be used as textile disperse dyes. These derivatives differ in the substituent at 2-position of the benzothiazole ring (Fig. 1). The focus in this study is on conformation of the molecules and especially on their supramolecular assembling as it is known that small difference on surface of the molecule may significantly influence its supramolecular architecture. The results reveal that hydrogen-bonding in all structures is governed by two strong intermolecular hydrogen bonds, one O-H...N and one O-H...O. While both interactions in **1** form dimers, in **2** and **3** they link neighbouring molecules into infinite chains. Further difference in the supramolecular aggregation arise from a number of weaker C-H...O hydrogen bonds. Thus, two bifurcated C-H...O hydrogen bonds are present in **2** and **3**, while only one is observed in **1**. Interestingly, hydrogen-bonded dimers generated by O-H...N and O-H...O hydrogen bonds in **1** give rise to a parallel arrangement of aromatic rings and formation of $\pi\cdots\pi$ interactions (Fig. 2), which are completely absent in **2** and **3**. All above mentioned interactions in these three structures are reinforced by C-H... π interactions, so forming three-dimensional networks.

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References

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Fig. 1.

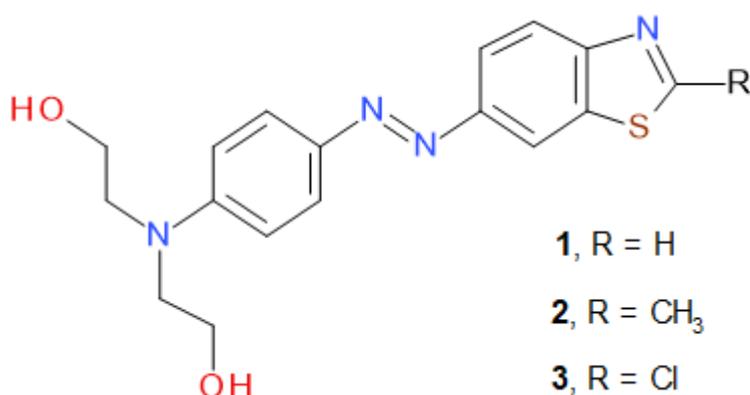


Fig. 2.

