Supplementary Materials to article Crystals_ 317884

Cryochemically obtained nanoforms of antimicrobial drug substance dioxidine and their physico-chemical and sructural properties

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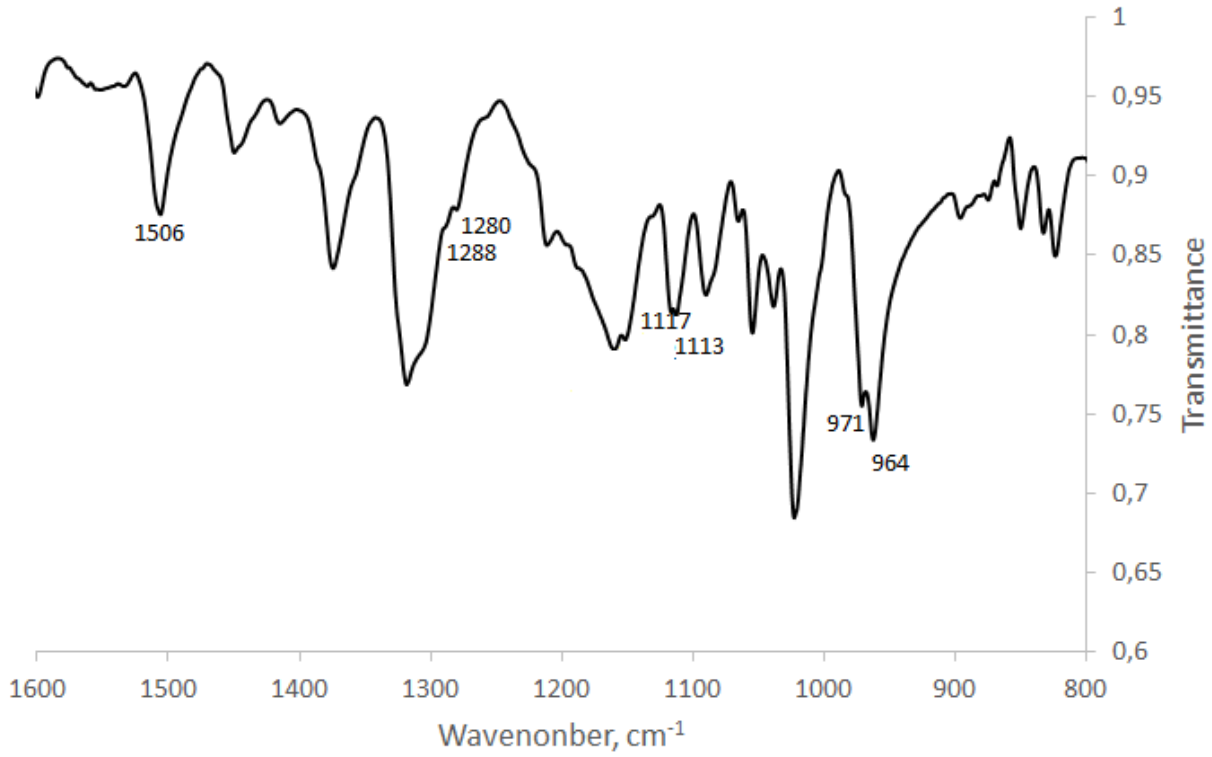
1. FTIR spectra of the samples were recorded in KBr discs between 4000 and 400 cm−1 using spectrometer Bruker Tensor II (Germany). The FTIR spectra of the cryomodified (C) and commercial source (S) samples of dioxidine are presented in Figure S1.

Dioxidine commercial source (S)



Dioxidine cryomodified (C)

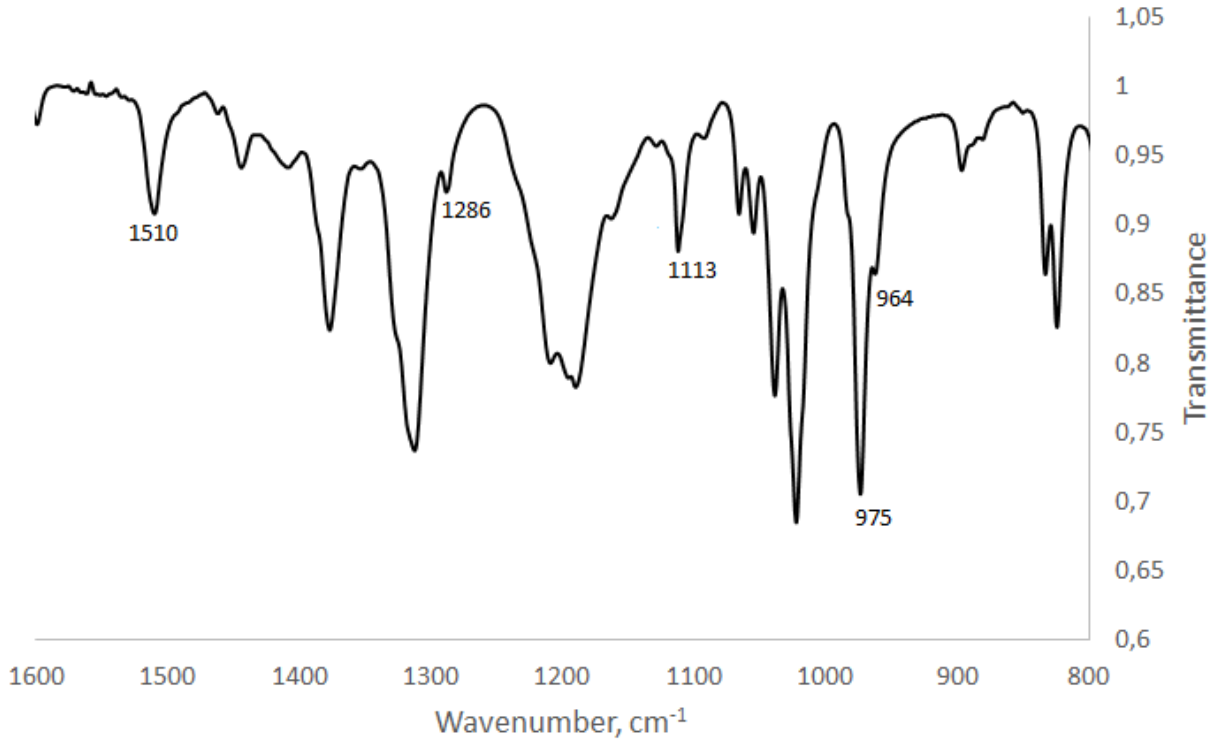


Figure S1. The FTIR spectra of the cryomodified (C) and commercial source (S) samples of dioxidine.

In the case cryomodified dioxidine quinoxaline ring is at 1510 cm-1, the vibrations of C-H of benzene ring appear at 975, 113cm^{-1}, and the band of vibrations of C-O-H is shown at 1288 cm^{-1}. While in the case of original dioxidine, the oscillation of the quinoxaline ring is at 1506 cm^{-1}, and the vibrational bands of the C-Hof aromatic ring are manifested by the peak at 971 cm^{-1} and doublet at 1117 and 1113cm^{-1}, the vibration band of the C-O-H is also doublet at 1280 and 1288 cm^{-1}.

2. **X-ray powder** patterns of the commercial source (**S**) and just after cryomodification (**C**) samples were measured on a Guinier-Huber camera in a transmission mode, CuK $_1$-radiation. Their powder patterns are shown in Figures S2 and S3, respectively.

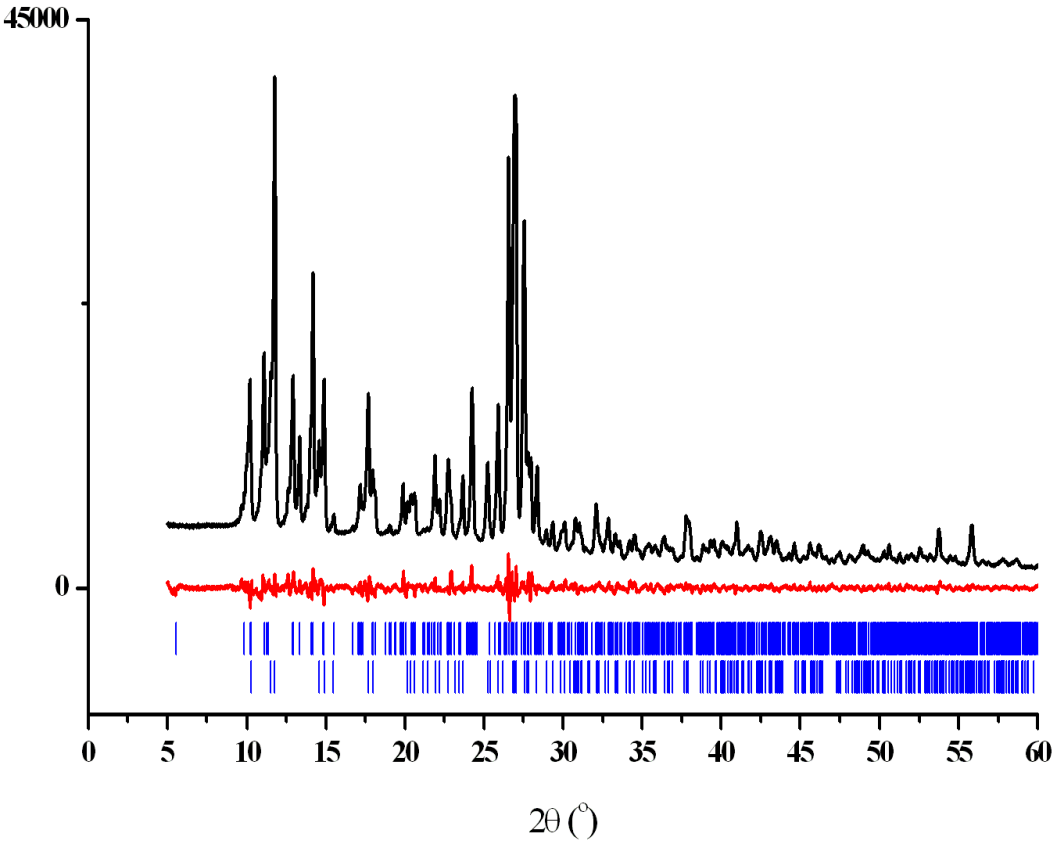


Figure S2. Rietveld plot for the two-phase pattern of **S** showing the experimental (black) and difference (red) curves. The vertical blue bars denote the calculated positions of diffraction peaks for crystalline phases **H** (top raw) and **M** (bottom raw).

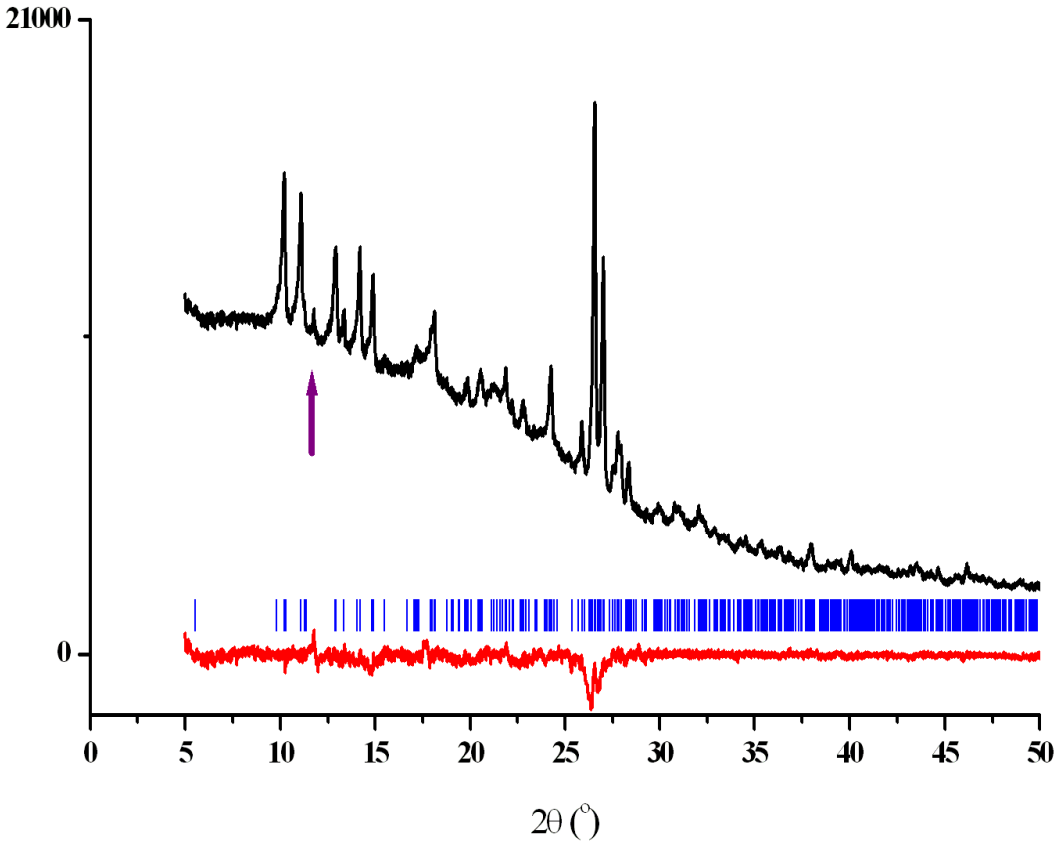


Figure S3. Rietveld plot for the pattern of **C** showing the experimental (black) and difference (red) curves. The vertical blue bars denote the calculated positions of diffraction peaks for crystalline phase **H**. Position of the strongest peak of crystalline phase **M** at 2 = 11.78° is shown by magenta arrow.