Electronic Supplementary Material (ESI) for CrystEngComm.

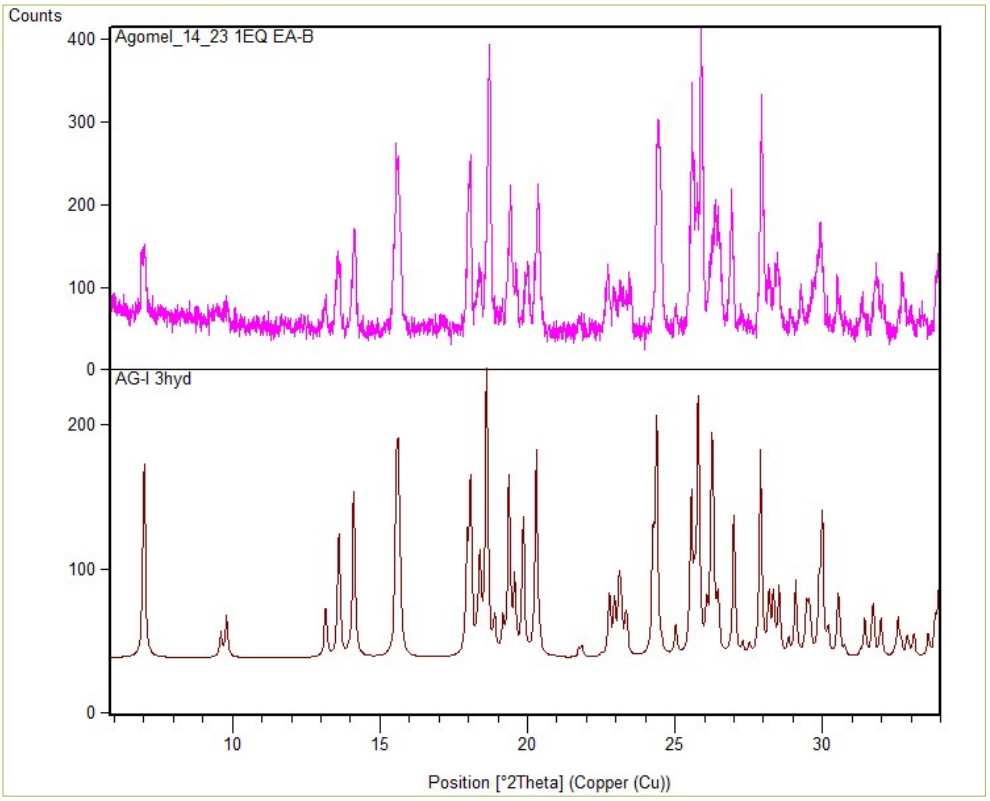

Fig. 1 AGI - experimental XRPD (top) compared with the corresponding one calculated from the single-crystal structure (bottom).

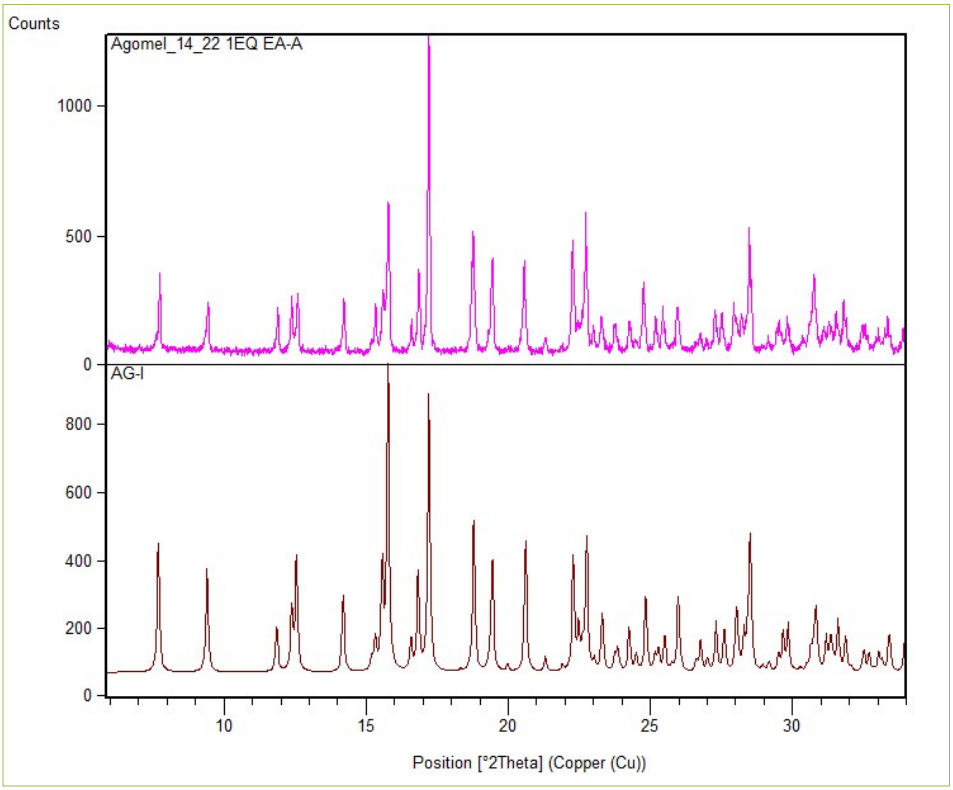

Fig. 2 AG_2I_3 - experimental XRPD (top) compared with the corresponding one calculated from the single-crystal structure (bottom).

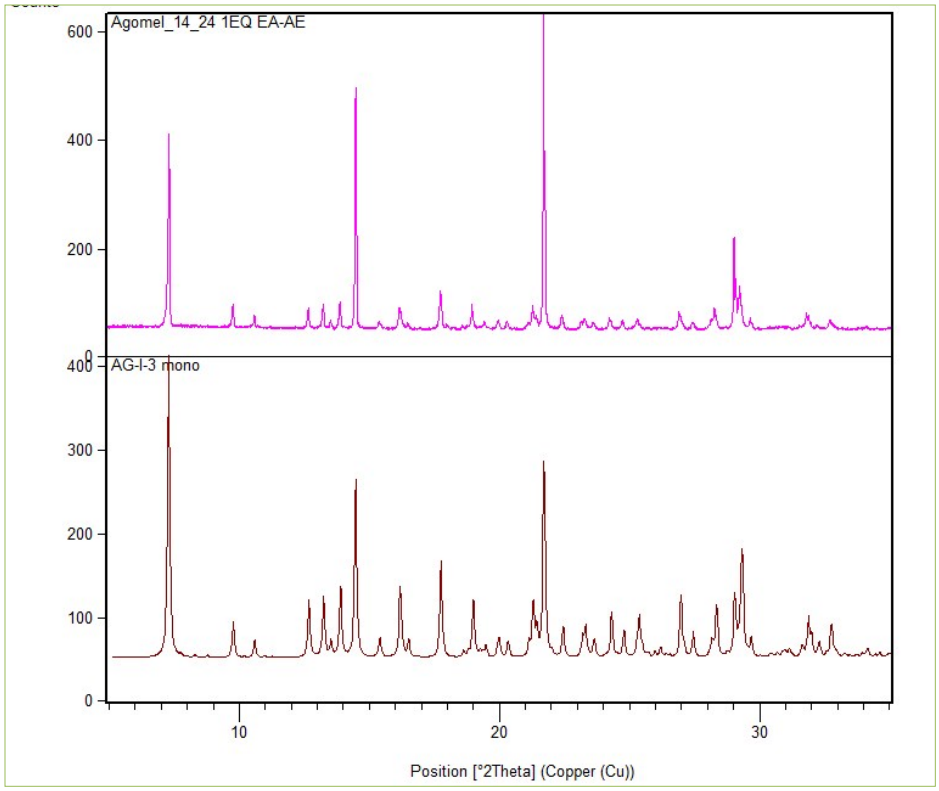

Fig. 3 AGI_2 - experimental XRPD (top) compared with the corresponding one calculated from the single-crystal structure (bottom).

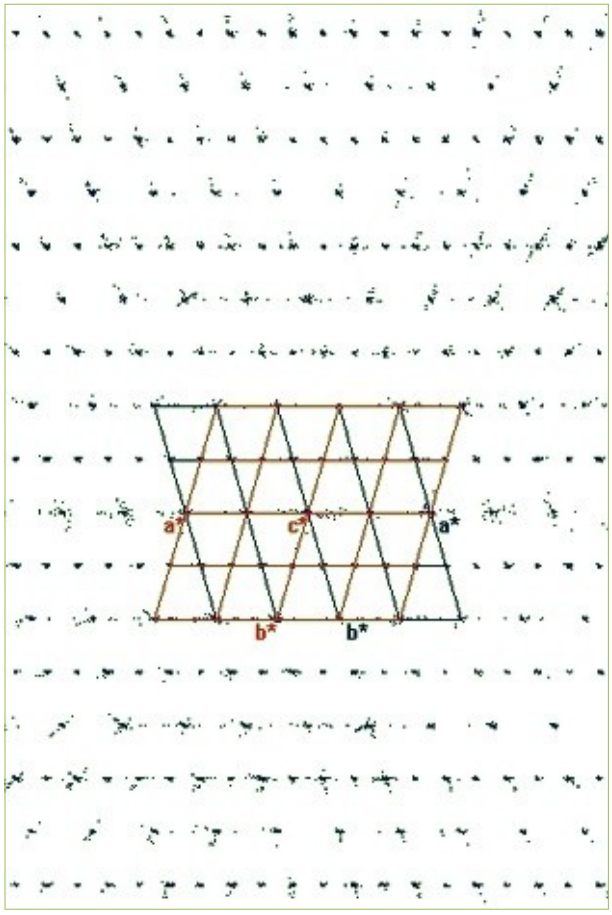

Fig. 4 c* projection of peak positions found for AGI_2.

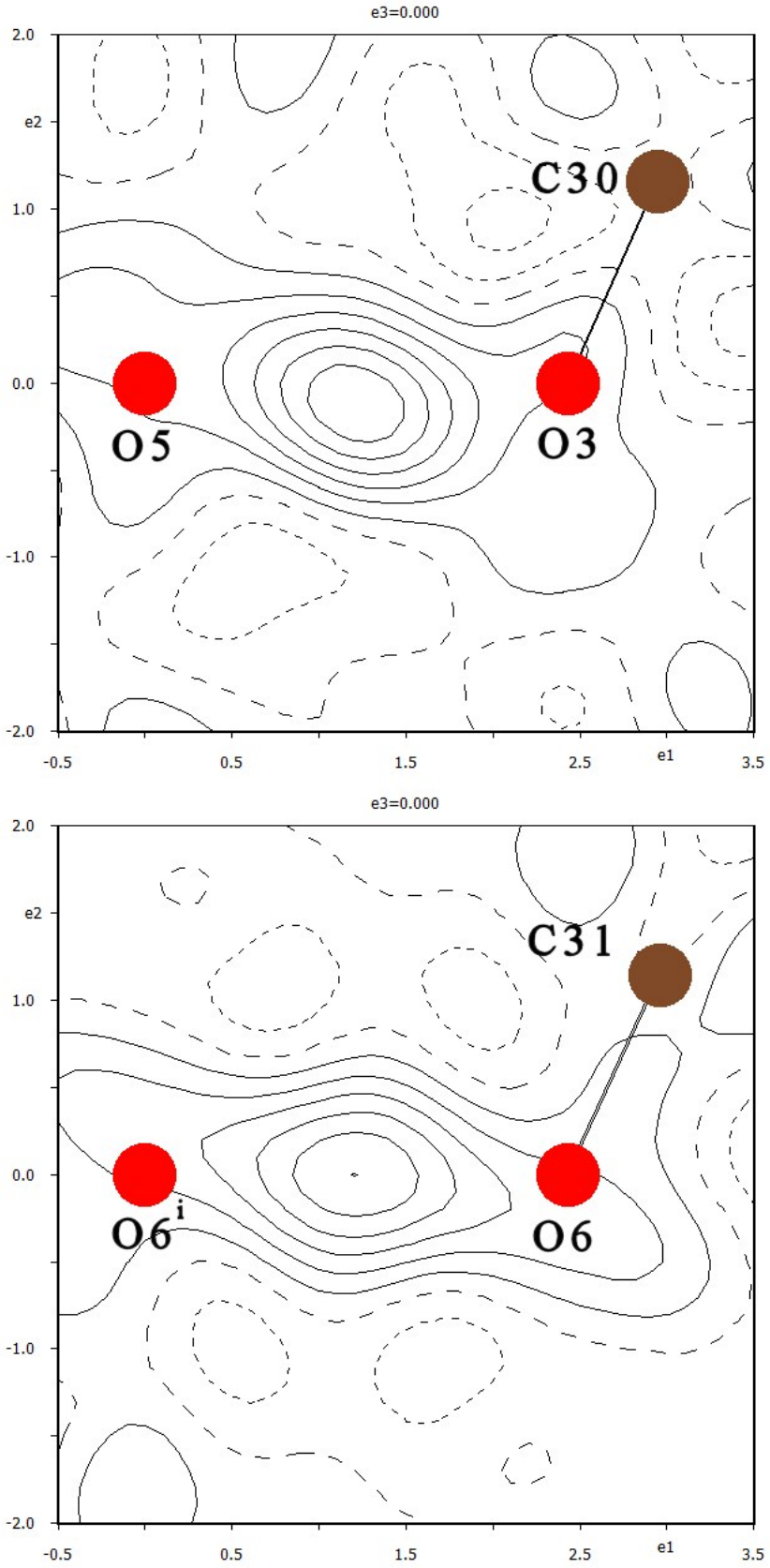

Fig. 5 Difference Fourier maxima corresponding to hydrogen atoms of the symmetric hydrogen bonds in AGI_2. Section planes were calculated from the indicated atoms, contour step was 0.05 eA^{-3}.
Symmetry code: (i) -x+1, -y+2, -z;

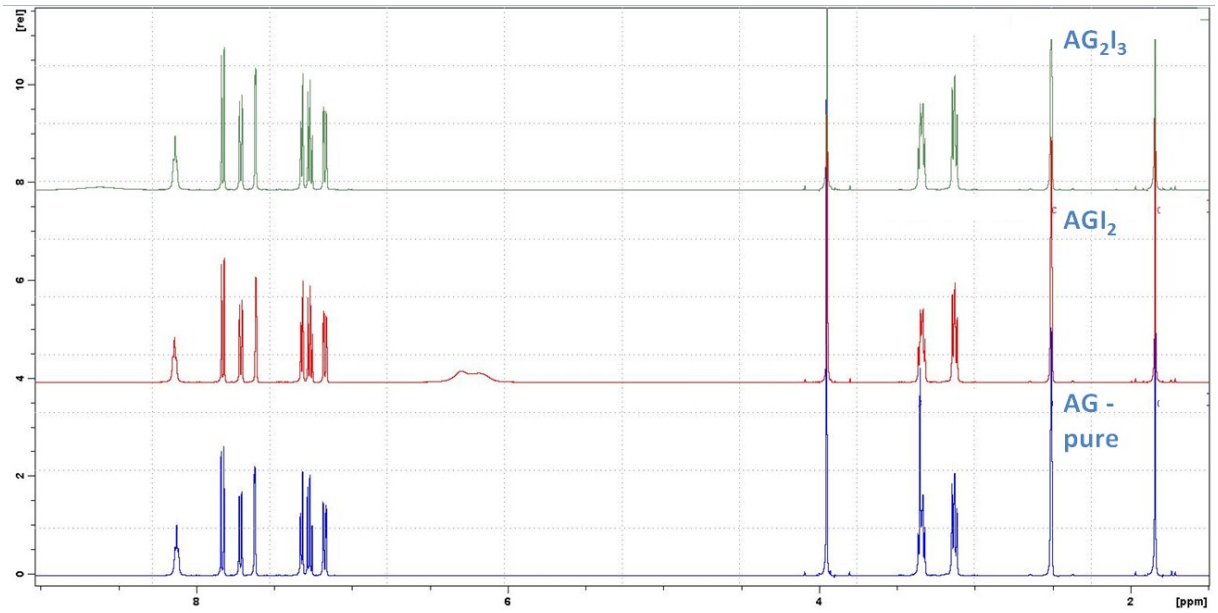

Fig. 6 Solution ^{1}H NMR of agomelatine solid forms measured in DMSO at the same molar concentration. The changes of chemical shift of NH signal as compared to the pure API were not significant (less than 5 Hz).

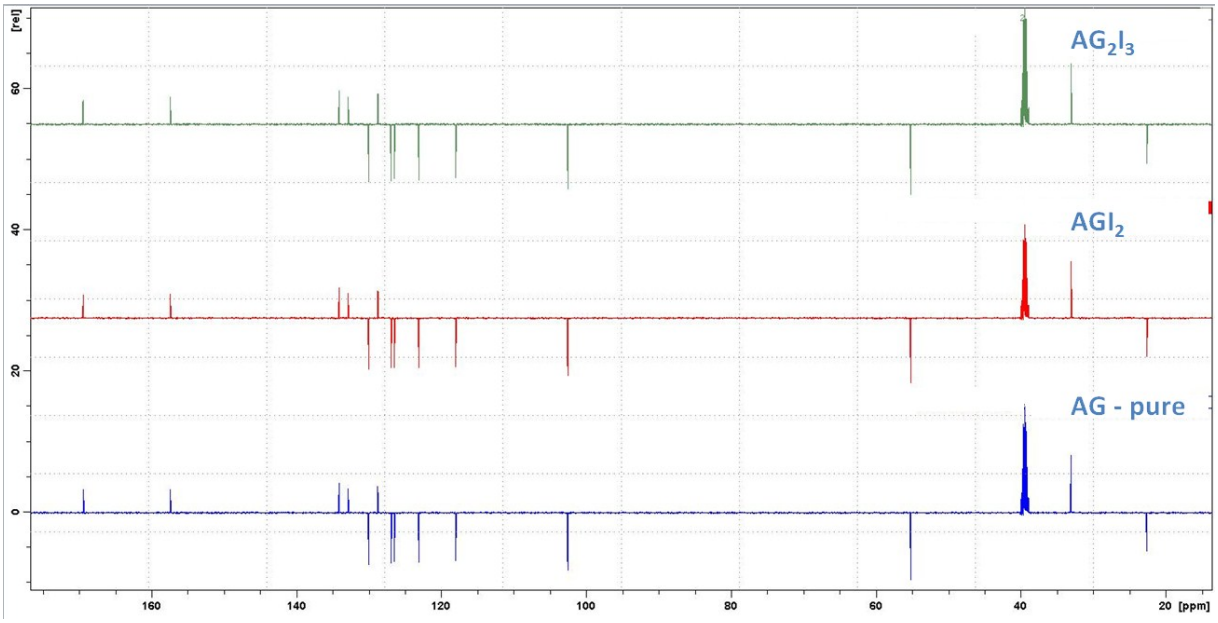

Fig. 7 Solution ^{13}C NMR of agomelatine solid forms measured in DMSO at the same molar concentration. The changes of chemical shift of C=O signal as compared to the pure API were not significant (less than 5 Hz).

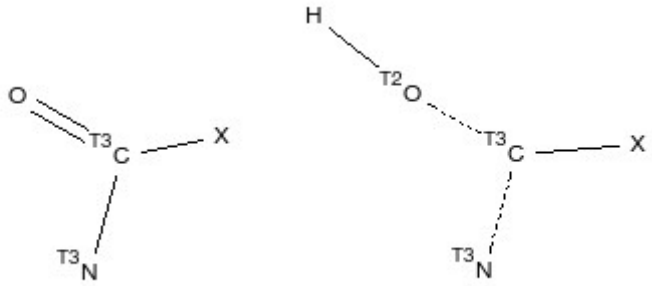

Fig. 8 Search motifs in CSD to determine the number of amides (left, 100,070 hits) and of protonated amides (right, 324 hits). T stands for the number of bonded atoms; dotted line for any type of chemical bond; X for any type of atom.

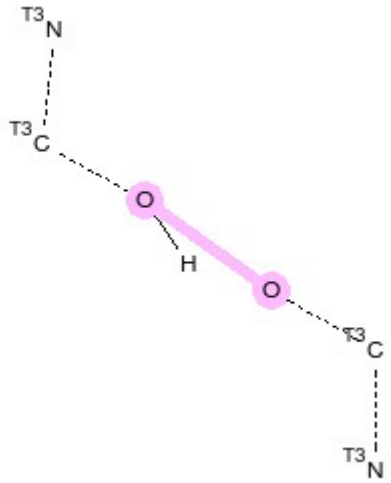

Fig. 9 Search motifs in CSD to determine the number of protonated amides forming O-H-O strong hydrogen bond. The distance between oxygens was set to 2.2 – 2.6 Å. 60 such structures were found, however, when the hydrogen atom was removed, the number increased to 153.

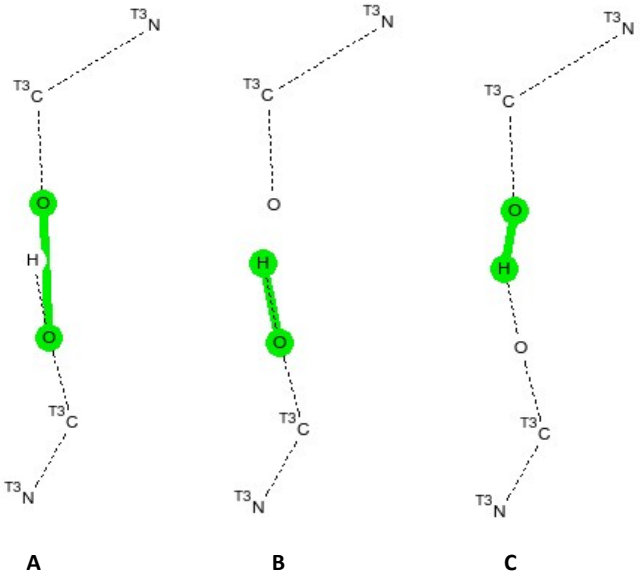

Fig. 10 Search motifs in CSD to determine the ratio between symmetric and non-symmetric H-bonds in the structures 60 structures of protonated amides forming O-H-O strong hydrogen bond. Symmetric: A = 2.2 - 2.6 Å, B = 1.15 – 1.30 Å, C = 1.15 – 1.30 Å, 7 hits. Non-symmetric: A = 2.2 - 2.6 Å, B = 0.60 – 1.15 Å, C = not specified, 53 hits.