Supporting information

Similar but Different: The Case of Metoprolol Tartrate and Succinate Salts

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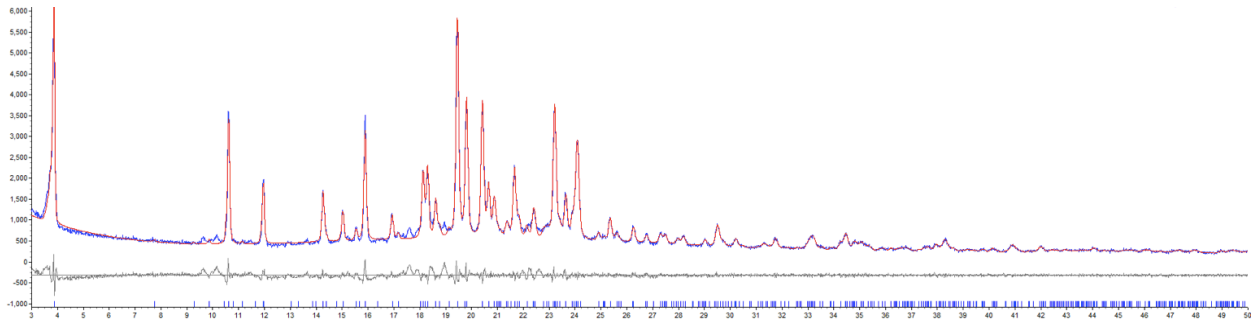

Figure S1. Experimental, calculated and difference diffraction patterns of **MT-o.**

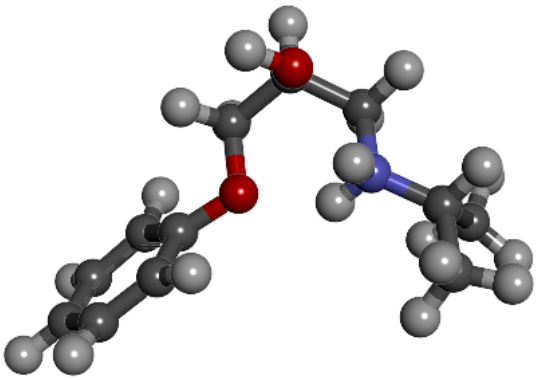

Figure S2. The “doubly-folded” conformation of the metoprolol cation model as found from MD simulations in vacuum at 300 K.

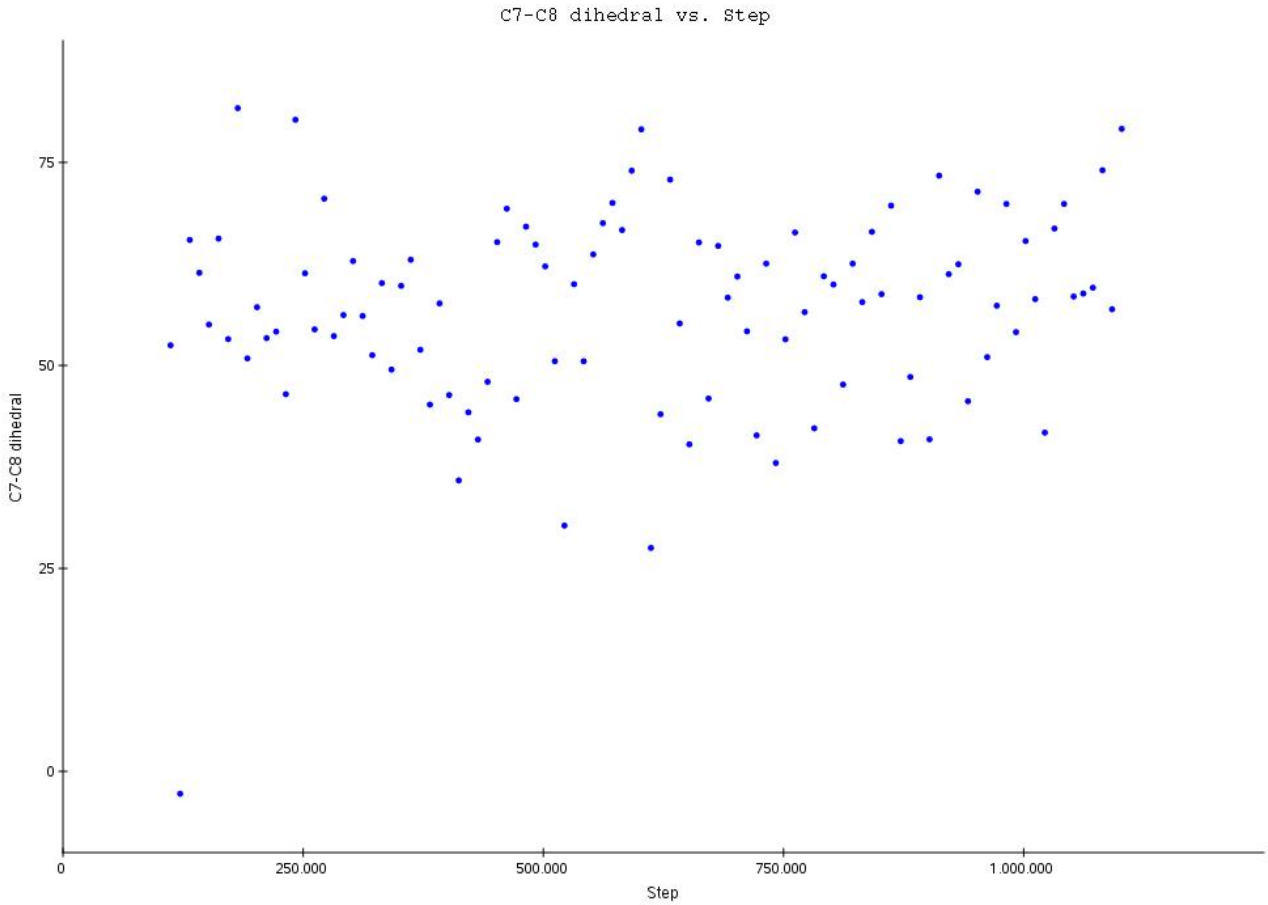

Figure S3. Plot of the C7-C8 dihedral angle (°) from MD trajectory (in vacuum, T=300K).

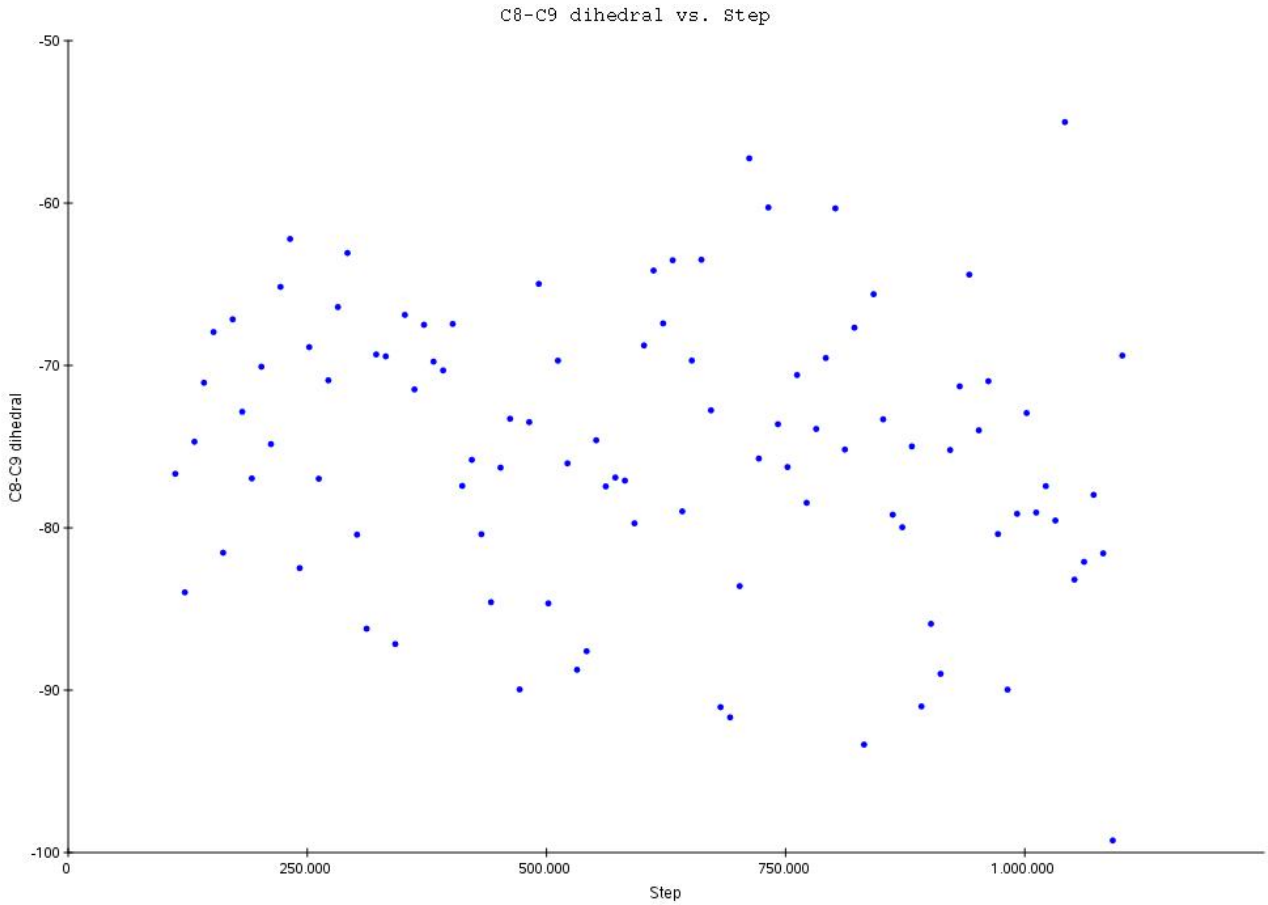

Figure S4. Plot of the C8-C9 dihedral angle (°) from MD trajectory (in vacuum, T=300K).

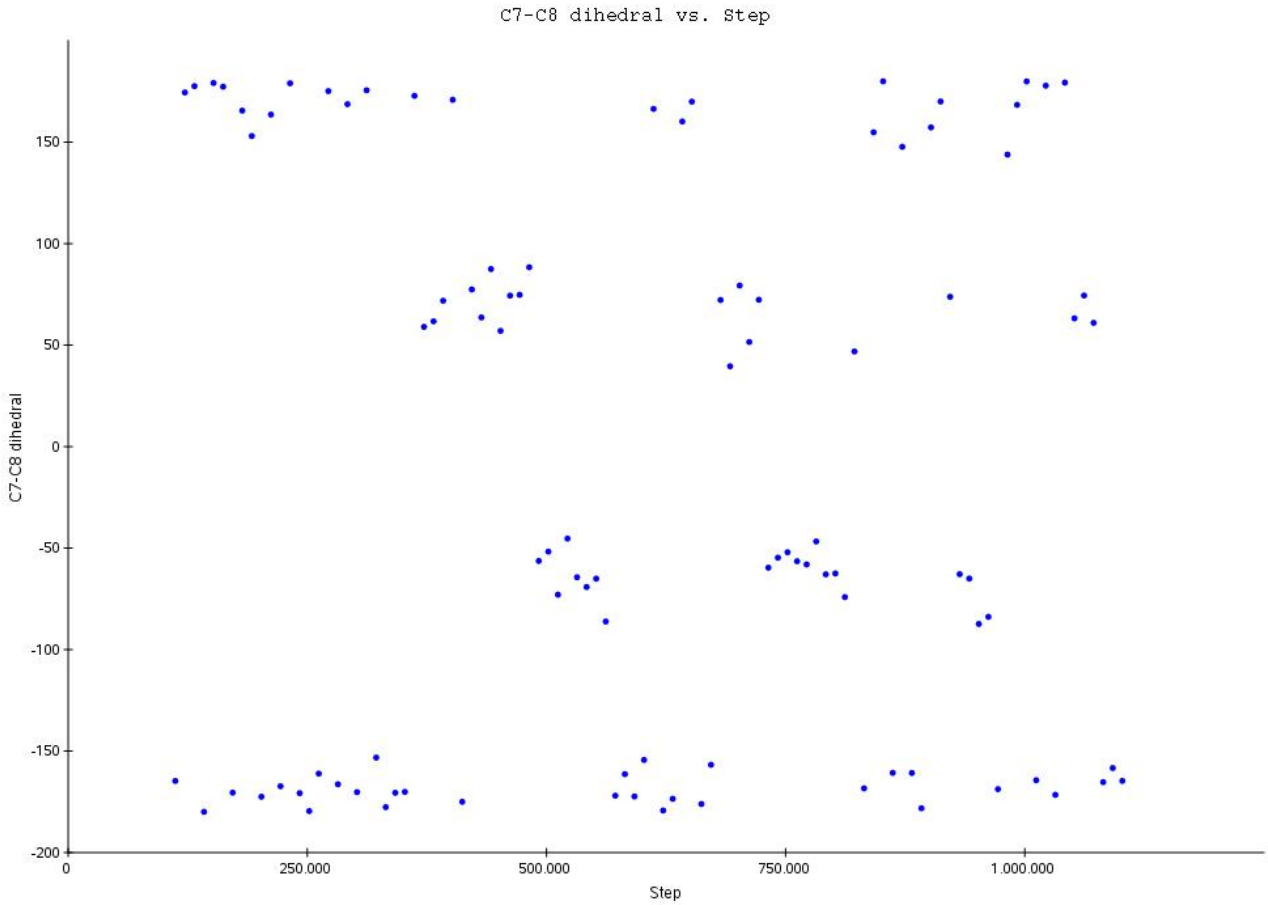

Figure S5. Plot of the C7-C8 dihedral angle (°) from MD trajectory (in an implicit water model, T=300K).

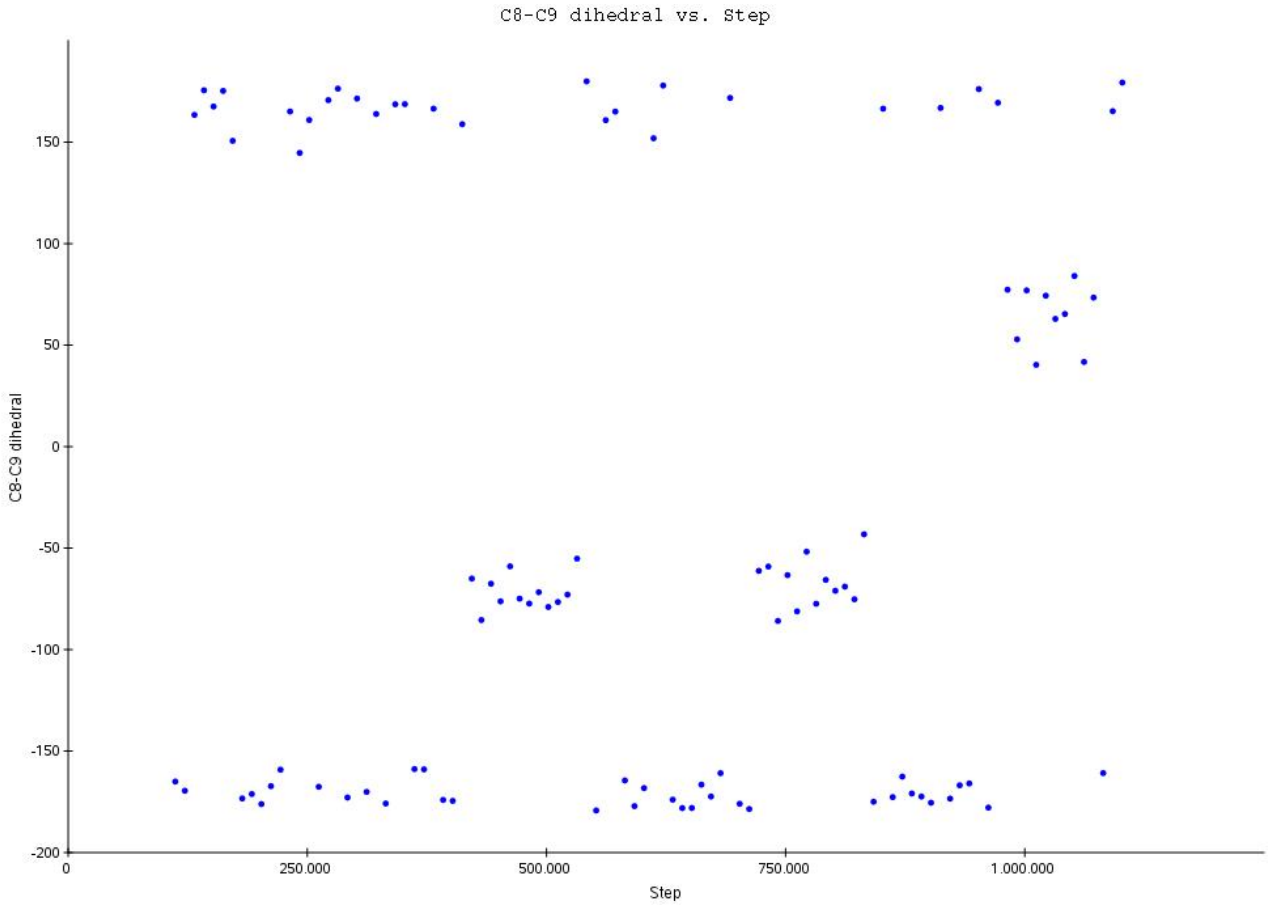

Figure S6. Plot of the C8-C9dihedral angle (°) from MD trajectory (in an implicit water model, T=300K).

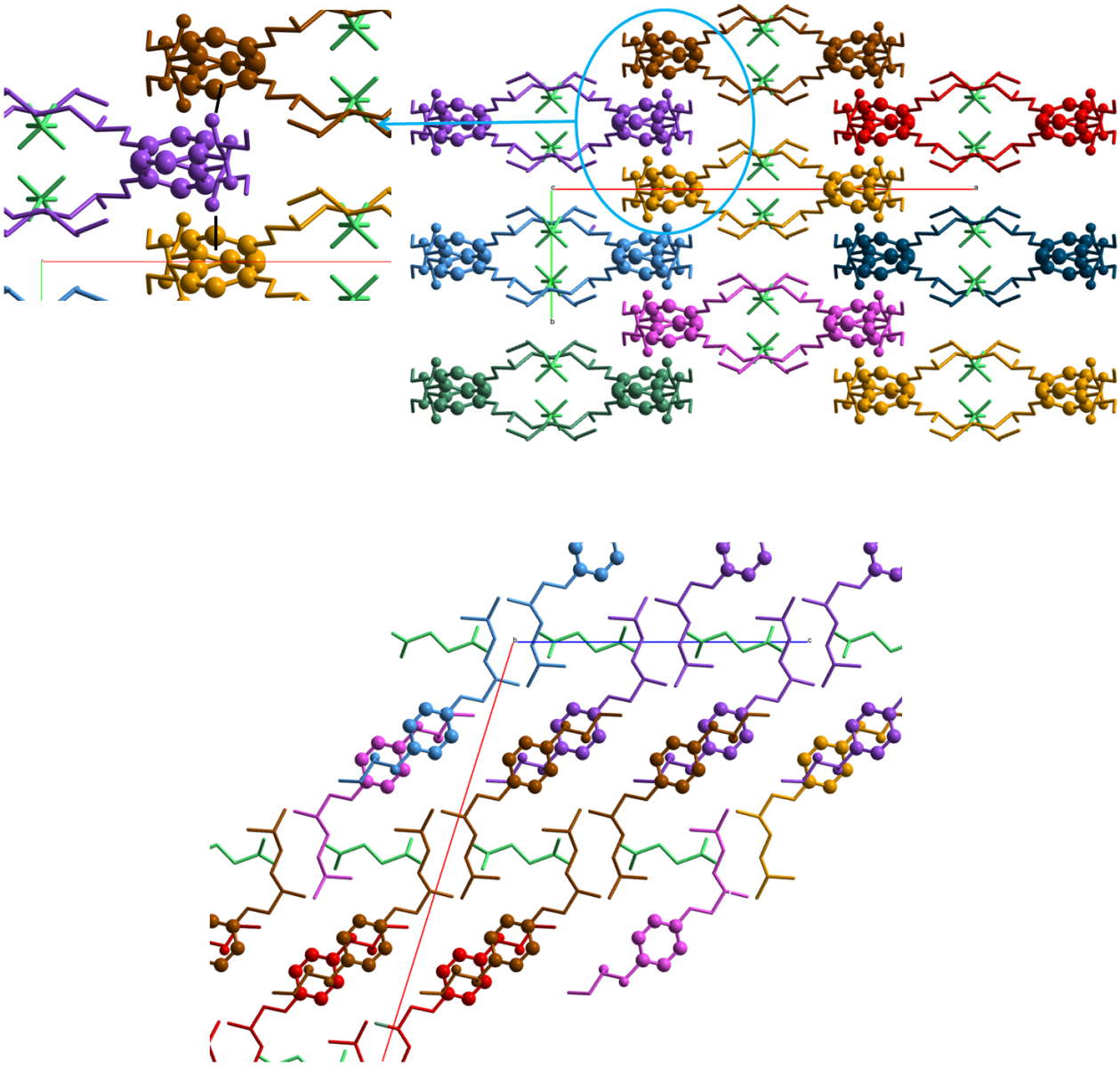

Figure S7. Crystal packing of **MS-m** along the *c* axis (top) and along the *b* axis (bottom). The atoms displayed as ball and stick are those involved in CH···π interactions.

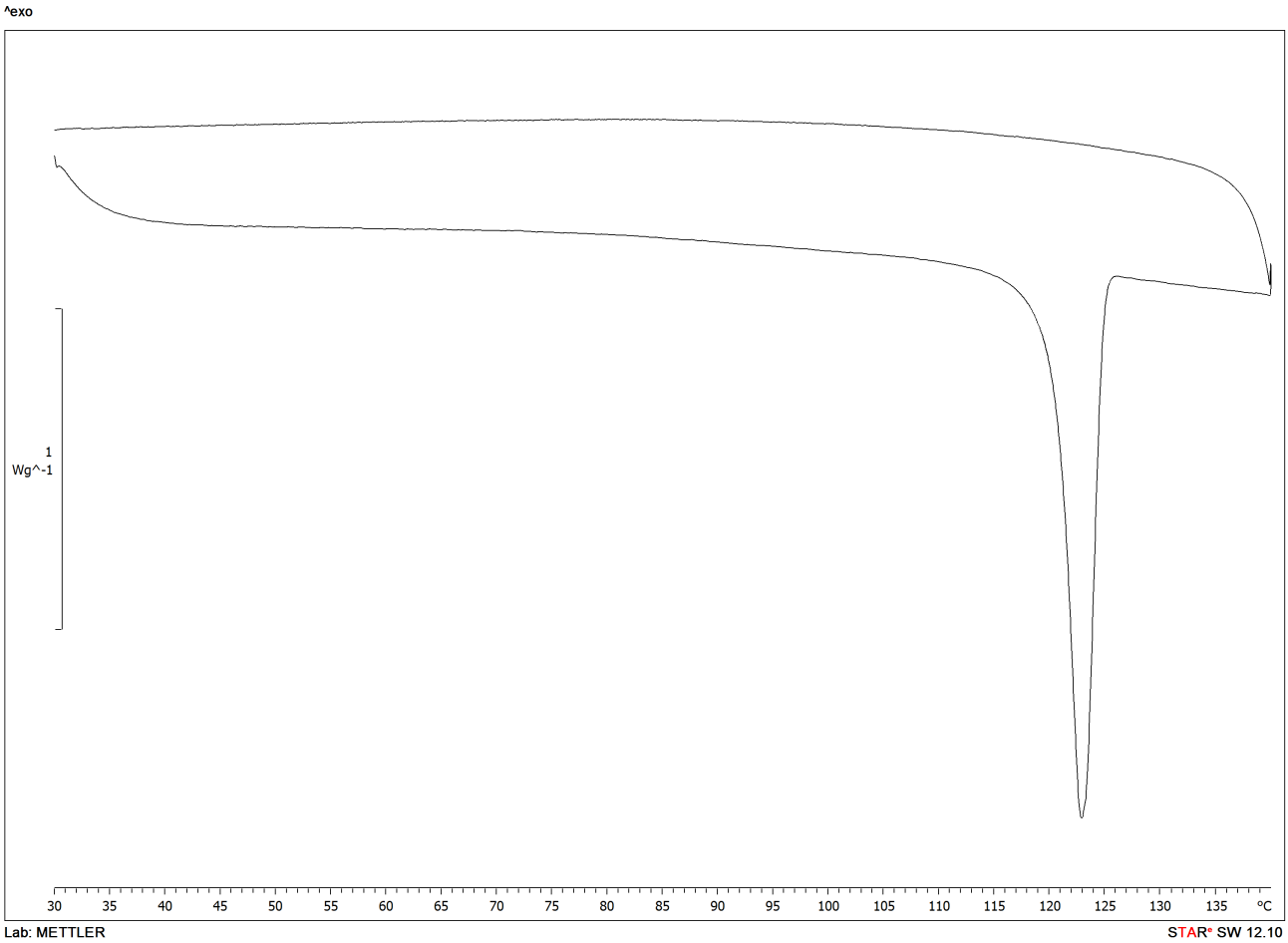

Figure S8. Experimental DSC curves of **MT-o** relative to the heating (bottom) and cooling (top) steps. The experiments were performed at a rate of 5 K/min.

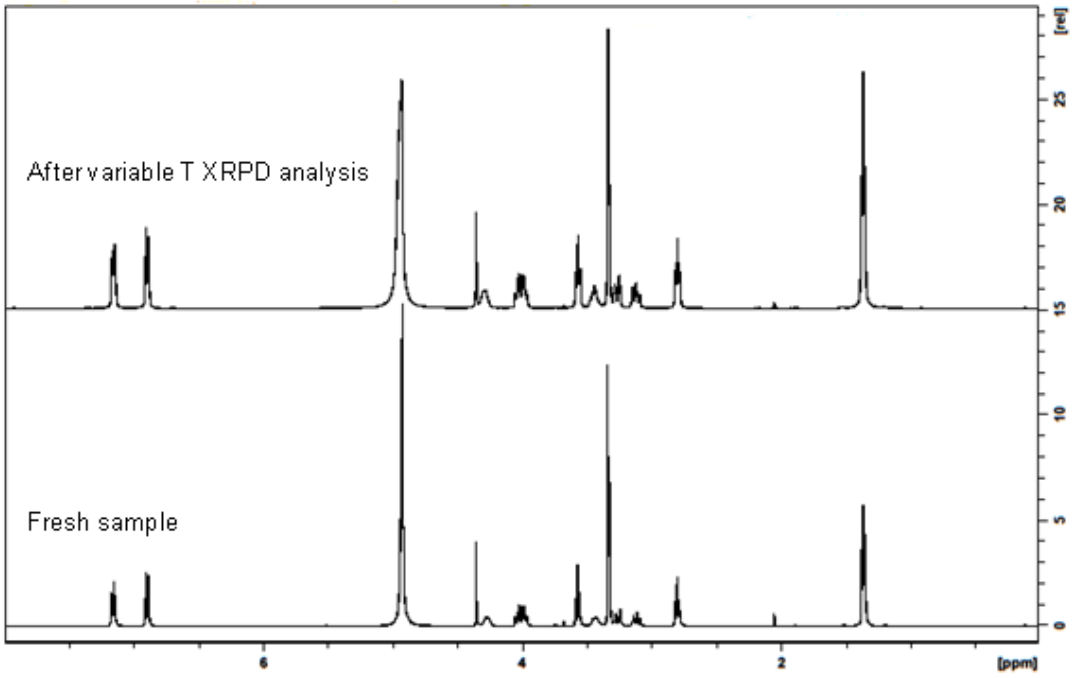

Figure S9. ^{1}H NMR recorded in CD_3OD on **MT-o** samples as received from Sigma Aldrich and after recrystallization from the melt.

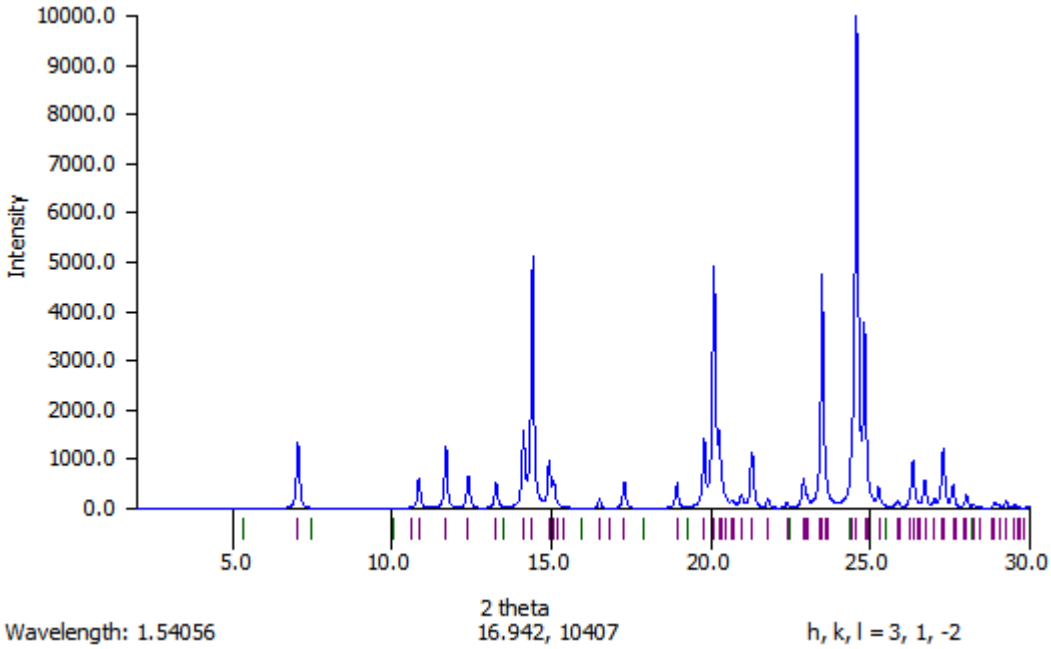

Figure S10. XRPD theoretical pattern (determined by using Mercury v.3.5, the data used are those deposited for **MS-m** in the CSD, refcode YOTXOV).

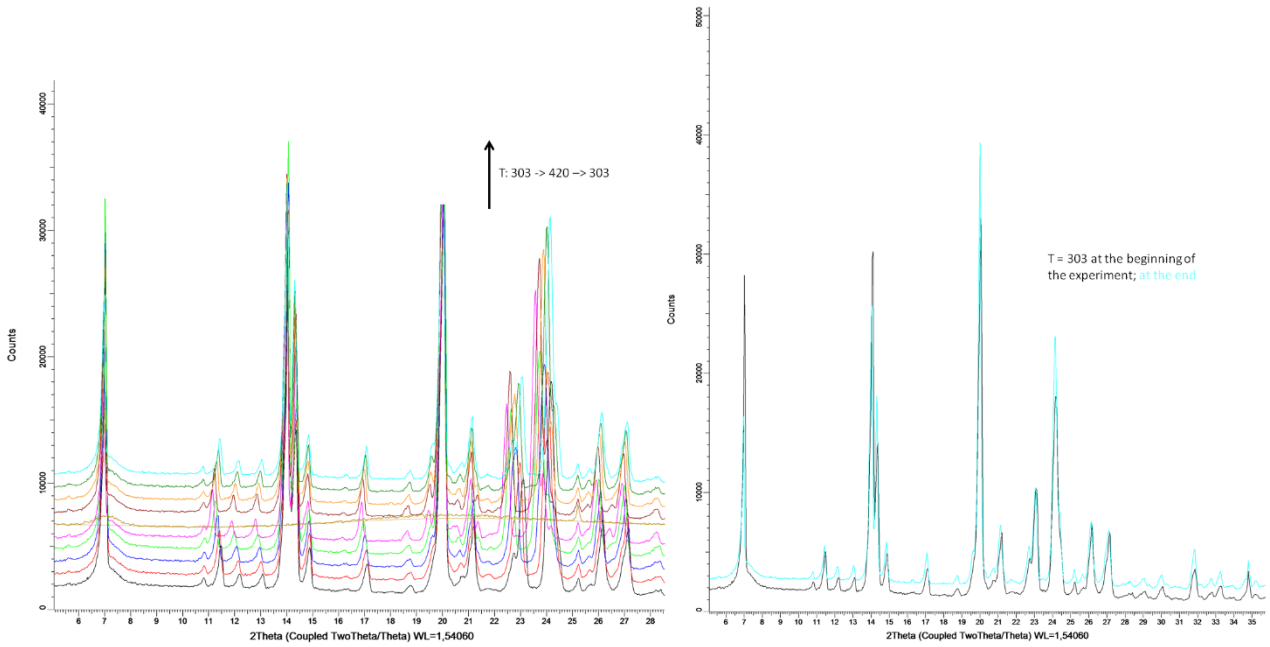

Figure S11. XRPD patterns of compound **MS-m** collected in the 303 – 420 – 303 K range (data were collected at 303, 323, 348, 373, 393, 420 K and 373, 348, 323, 303 K under nitrogen atmosphere). The anisotropic variation of the lattice is reversible as provided by the fact that the XRPD patterns collected at 303K at the beginning of the experiment and at the end are well superimposable.

Table S1. Intramolecular H-bonds in tartrate anions in **MT-o**.

	X···Y (Å)	H···Y (Å)	X-H···Y (°)
O6a-H6aa···O4a[1]	2.62(2)	2.10	121
O6b-H6bb···O5b[2]	3.24(2)	2.65	130.3

[1] = -x+1,+y,-z+1; [2] = -x+1, y, -z+2