Supplementary data: Rietveld refinement results

**Figure 1** Rietveld refinement results: Observed (black), calculated (red) and difference (observed-calculated, blue) diffraction patterns of the refined $\beta_1$-structure of MOM.

**Figure 2** Rietveld refinement results: Observed (black), calculated (red) and difference (observed-calculated, blue) diffraction patterns of the refined $\beta_1$-structure of POP.
Figure 3  Rietveld refinement results: Observed (black), calculated (red) and difference (observed-calculated, blue) diffraction patterns of the refined $\beta_1$-structure of SOS-POP.

Figure 4  Rietveld refinement results: Observed (black), calculated (red) and difference (observed-calculated, blue) diffraction patterns of the refined $\beta_1$-structure of SOS.

Figure 5  Rietveld refinement results: Observed (black), calculated (red) and difference (observed-calculated, blue) diffraction patterns of the refined $\beta_1$-structure of POS.

Figure 6  (Rietveld refinement results: Observed (black), calculated (red) and difference (observed-calculated, blue) diffraction patterns of the refined $\beta_1$-structure of SOA)
Figure 7  Rietveld refinement results: Observed (black), calculated (red) and difference (observed-calculated, blue) diffraction patterns of the refined β-VI-structure of Bahia cocoa butter.

Figure 8  Rietveld refinement results: Observed (black), calculated (red) and difference (observed-calculated, blue) diffraction patterns of the refined β-VI-structure of Ivory Coast cocoa butter.

Figure 9  Different orientation of glycerol in flat conformation (left) and rotated conformation (right). View parallel to the S1 and S3m direction.