Maleate Salts of Bedaquiline

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Supporting Information

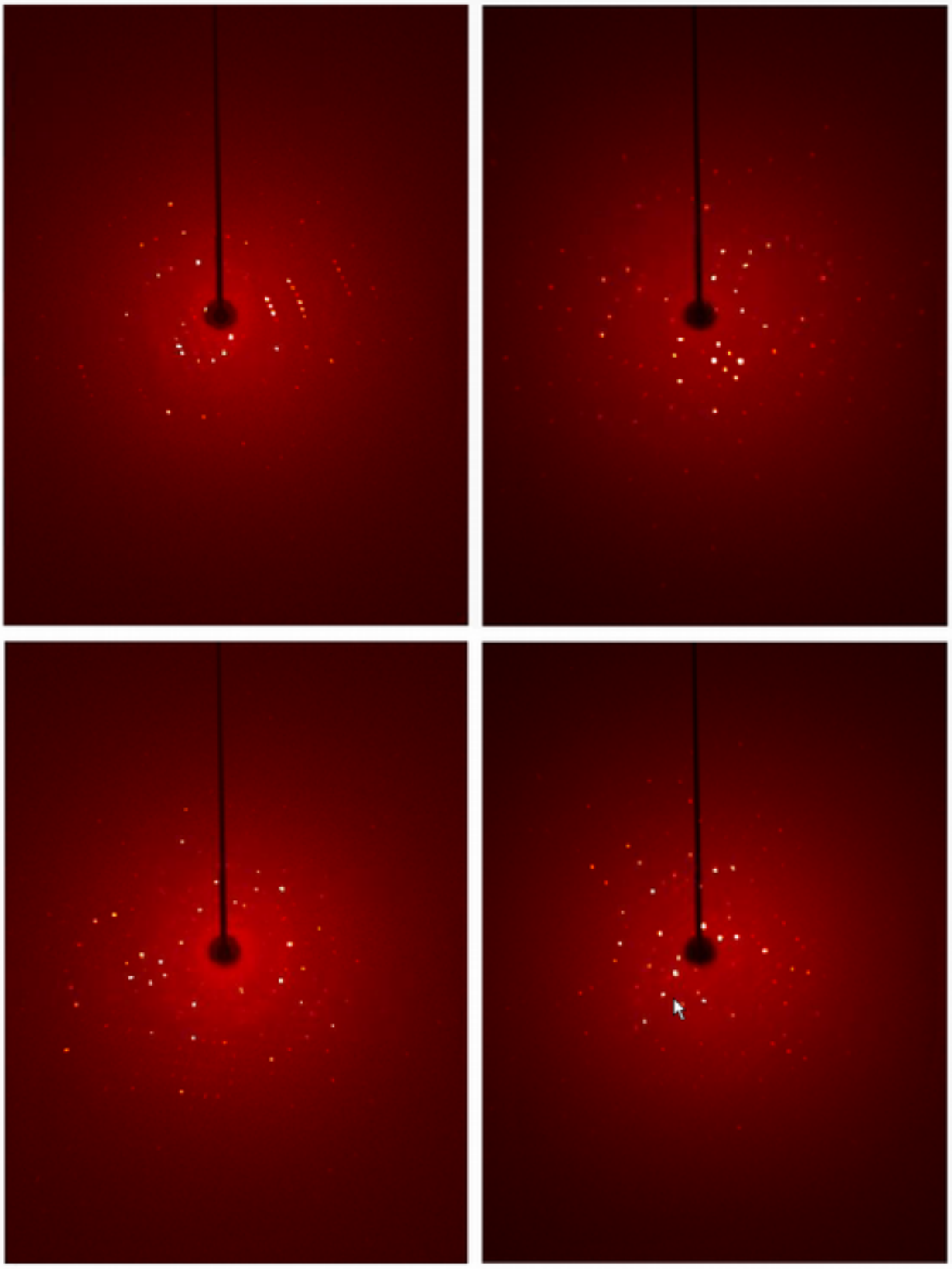

Figure S1. Comparison of diffraction patterns from crystals fresh out of mother liquor and after storing in atmosphere for 14 hrs. Patterns are from different but similar sized crystals. Top left: acetone/hexane solvate, native. Top right: acetone/hexane solvate, after 14hrs. Bottom left: ethyl acetate solvate, native. Bottom right: ethyl acetate, after 14hrs.

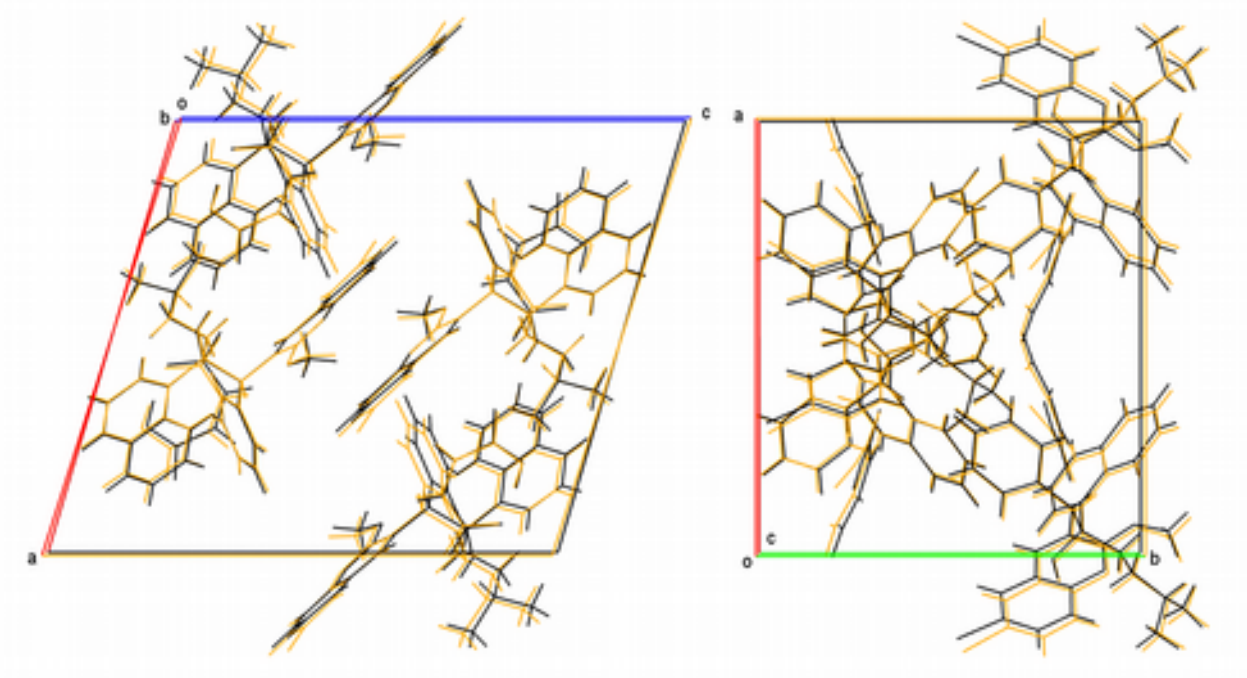

Figure S2. Unit cell overlay of the acetone/hexane solvate (orange, solvate molecules omitted for clarity) and the structure of the desolvated structure (black, derived from the acetone/hexane solvate).

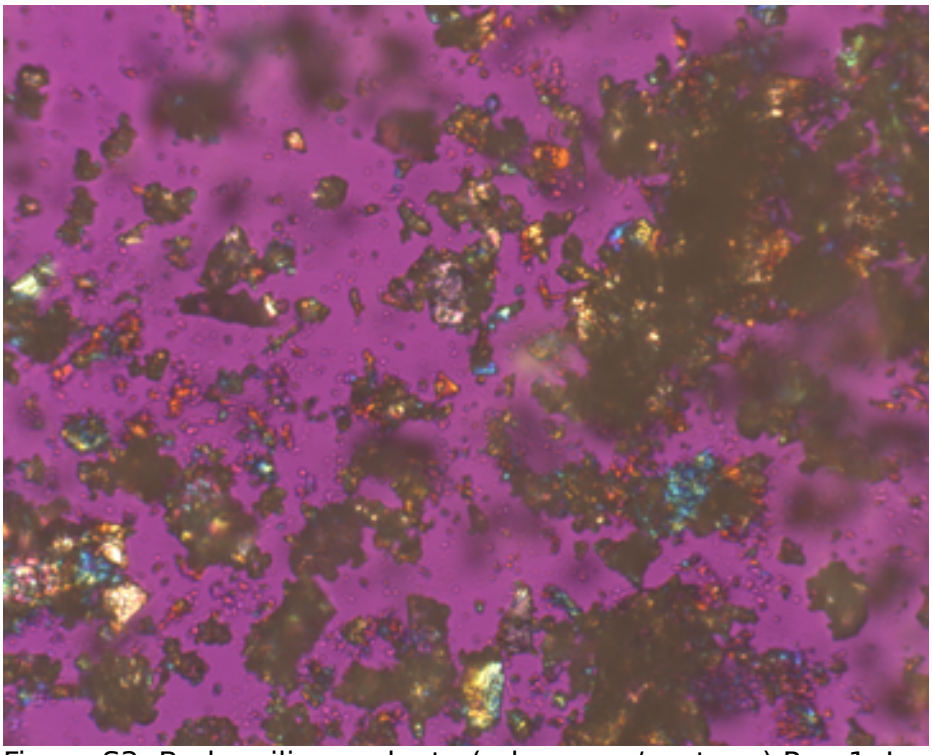

Figure S3: Bedaquiline maleate (n-hexanes/acetone) Run 1, Image file: 1-91-2-001, Temperature: 32.3 °C, start of heating.

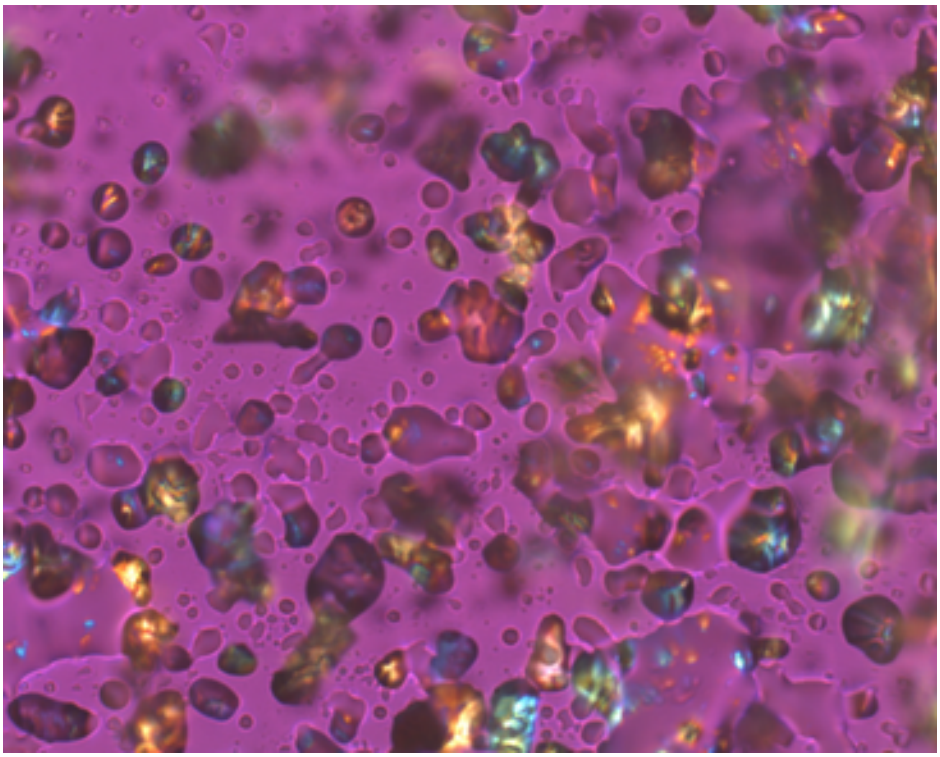

Figure S4: Bedaquiline maleate (n-hexanes/acetone) Run 1, Image file: 1-91-2-003, Temperature: 130.6 °C, melting.

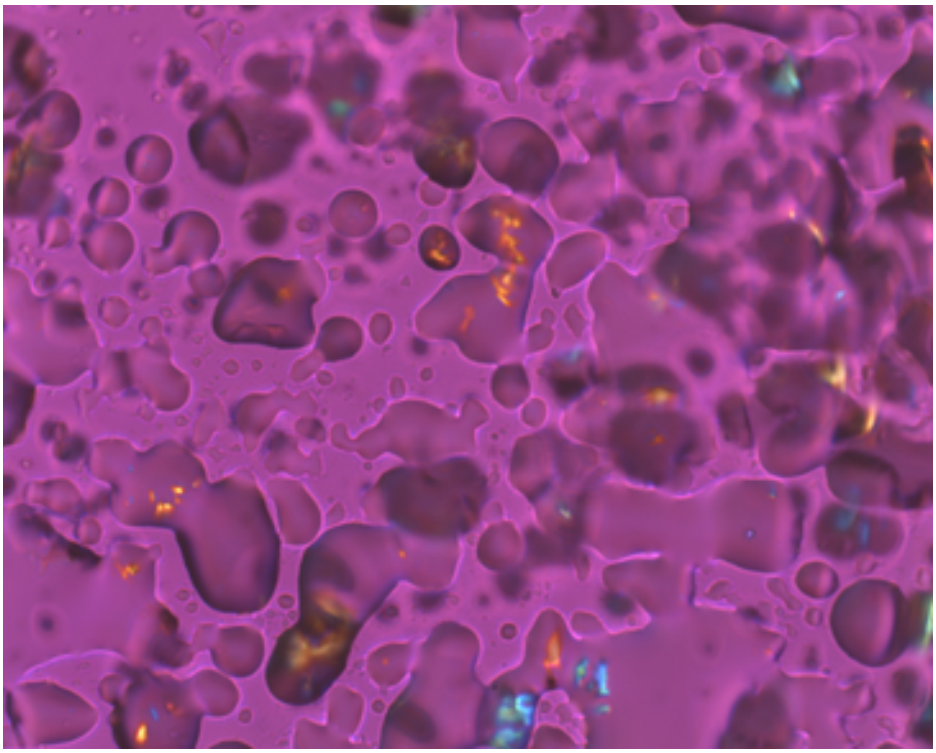

Figure S5: Bedaquiline maleate (n-hexanes/acetone) Run 1, Image file: 1-91-2-004, Temperature: 131.5 °C, melting.

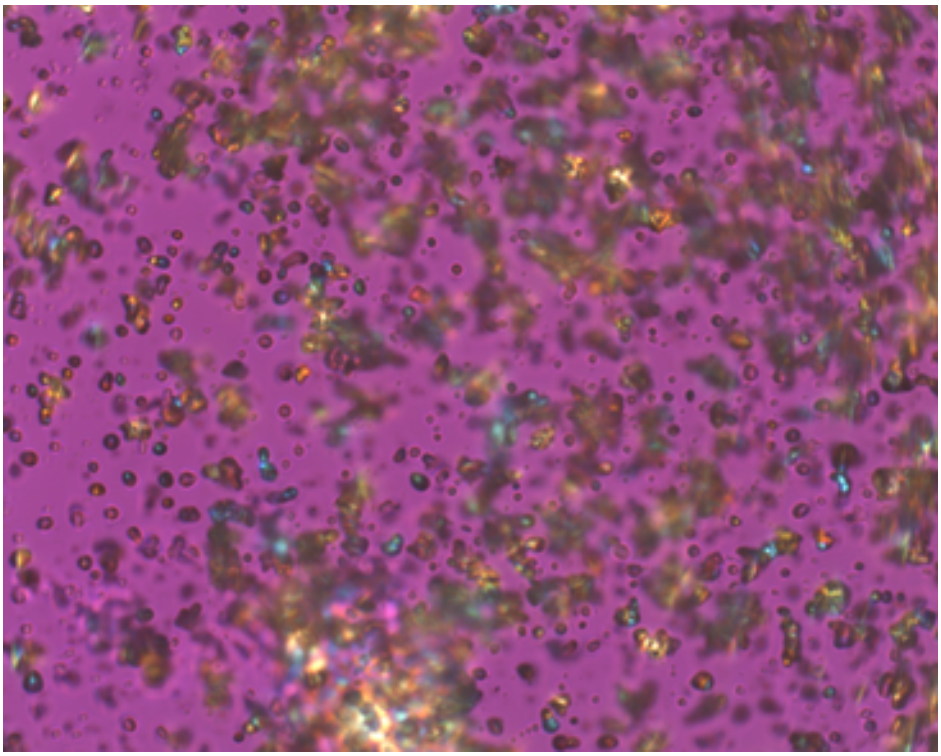

Figure S6: Bedaquiline maleate (n-hexanes/acetone) Run 2, Image file: 1-91-2-008, Temperature: 124.7 °C, melting.

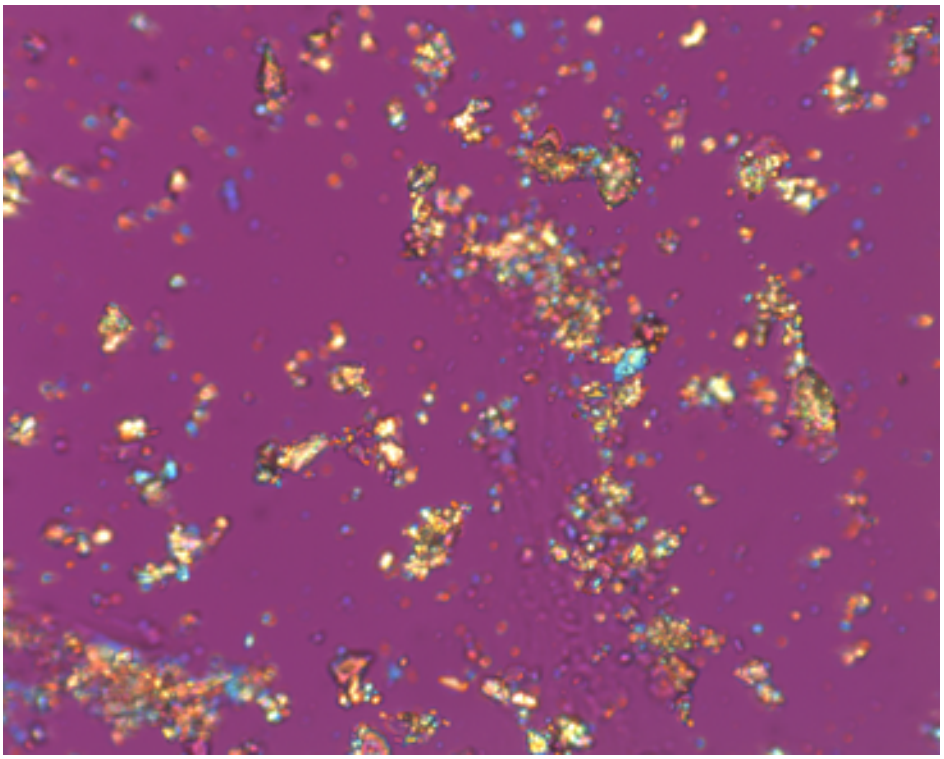

Figure S7: Bedaquiline maleate (n-hexanes/acetone) Run 3, Image file: 1-91-2-012, Temperature: 36.2 °C, start of heating.

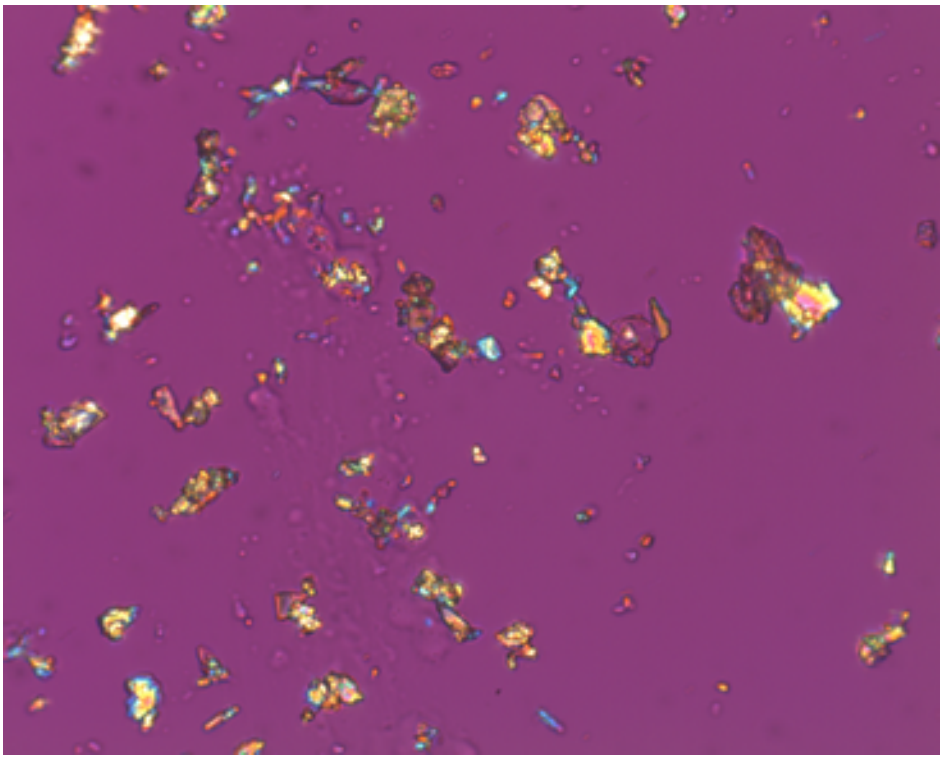

Figure S8: Bedaquiline maleate (n-hexanes/acetone) Run 3, Image file: 1-91-2-013, Temperature: 119.9 °C, onset melting.