Supporting Information

Solvent mediated phase transformation between two tegafur polymorphs in several solvents.

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Table S1. EpiCalc calculation for potential lattice matching between {100}, {110} and {010} face of β tegafur and {001}, {011} and {010} face of α tegafur. V/V_0 is the dimensionless potential energy parameter used to measure the goodness-of-fit.

α face (hkl)	β face (hkl)	V/V_0
010	100	0.9941
010	110	0.9675
010	010	0.9836
001	100	0.9908
001	110	0.9925
001	010	0.9902
011	100	0.9985
011	110	0.9923
011	010	0.9908

The value of V/V_0 indicates the goodness-of-fit between the substrate lattice and the overlayer lattice, where $V/V_0=1$ indicates that there is no match between lattice points, $V/V_0=0.5$ – a partial match (for non-hexagonal substrate), and $V/V_0=0$ – complete matching of the lattice points or crystal faces.

The default setting for overlayer dimensions (25 x 25) and the orientation angle (60º with a step size of 0.25º) was used to test α and β tegafur lattice match.