Supporting Information

Using Systematic Comparisons of 2D and 3D Structures to Reveal Principles of Molecular Organization. Linear Bis-Isophthalic Acids and their Tetraesters

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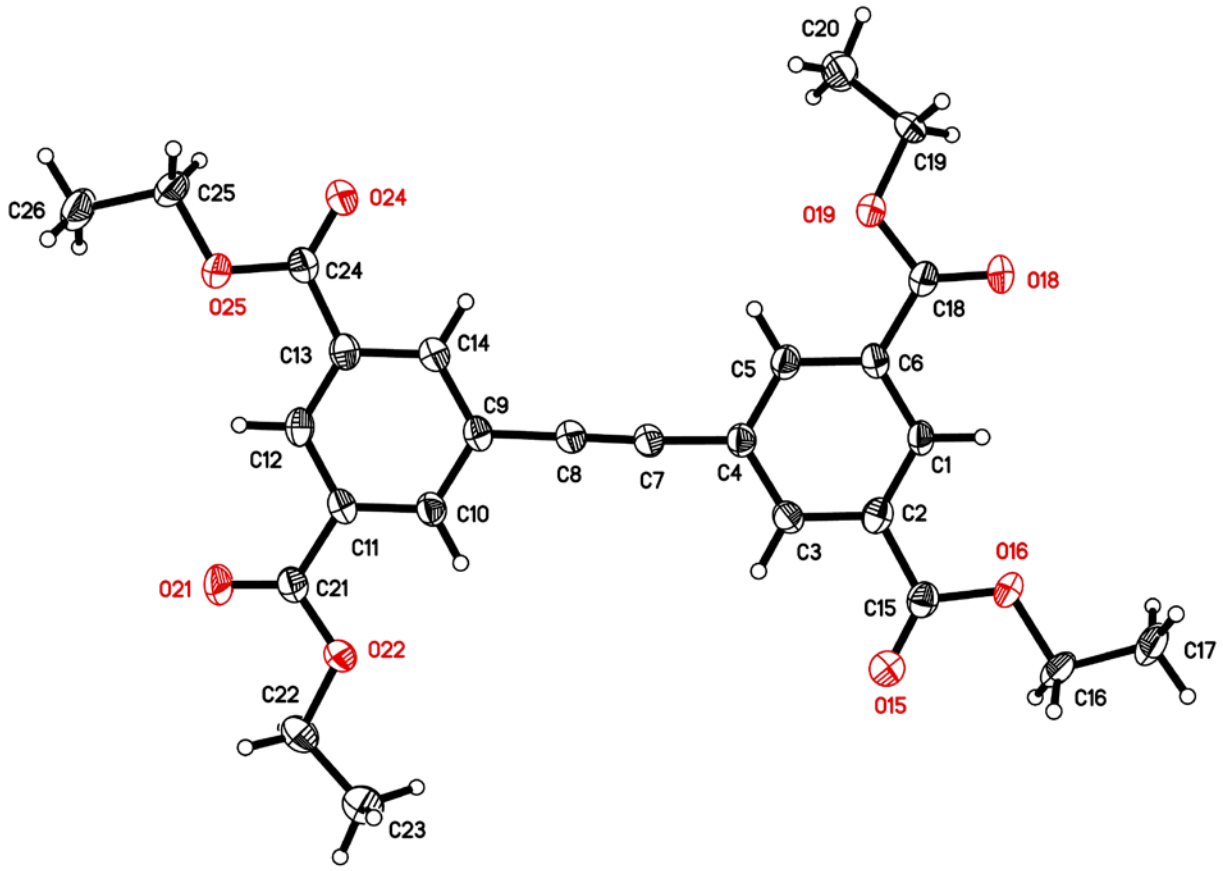

Figure S1. Thermal atomic displacement ellipsoid plot of the structure of crystals of tetraester **3** grown from hexane/$CHCl_3$. The ellipsoids of non-hydrogen atoms are drawn at the 50% probability level, and hydrogen atoms are represented by a sphere of arbitrary size.

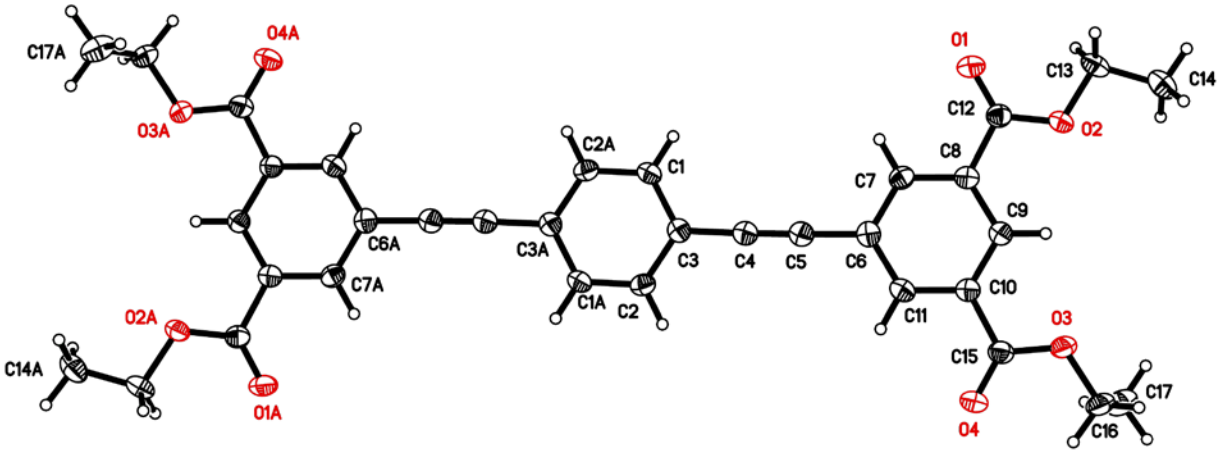

Figure S2. Thermal atomic displacement ellipsoid plot of the structure of crystals of tetraester **4a** grown from hexane/$CHCl_3$. The ellipsoids of non-hydrogen atoms are drawn at the 50% probability level, and hydrogen atoms are represented by a sphere of arbitrary size.

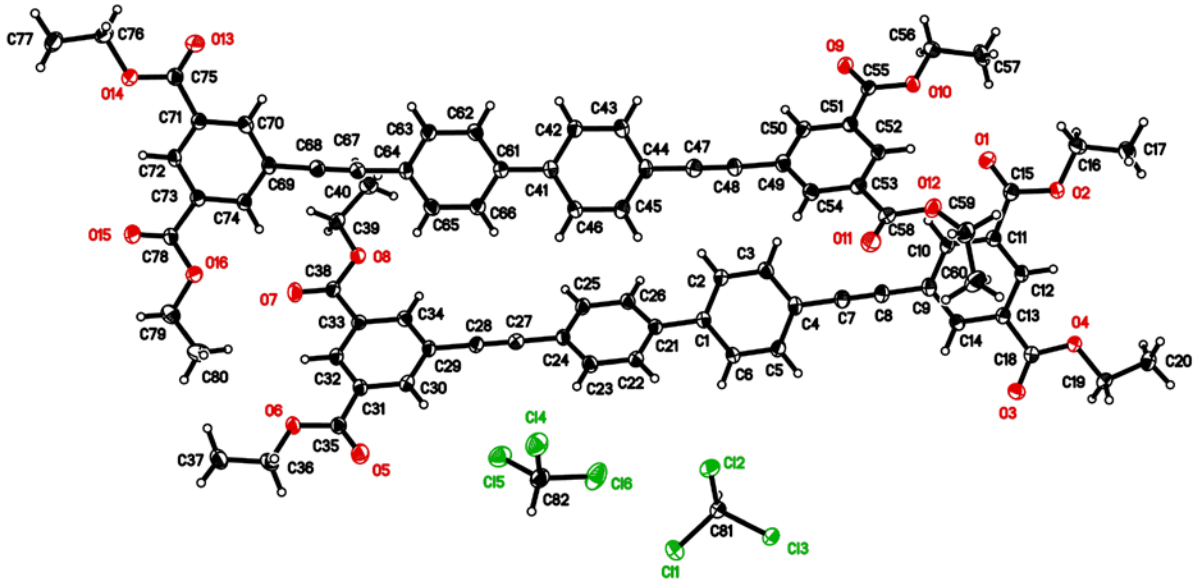

Figure S3. Thermal atomic displacement ellipsoid plot of the structure of crystals of tetraester **5** • $CHCl_3$ grown from hexane/$CHCl_3$. The ellipsoids of non-hydrogen atoms are drawn at the 50% probability level, and hydrogen atoms are represented by a sphere of arbitrary size.

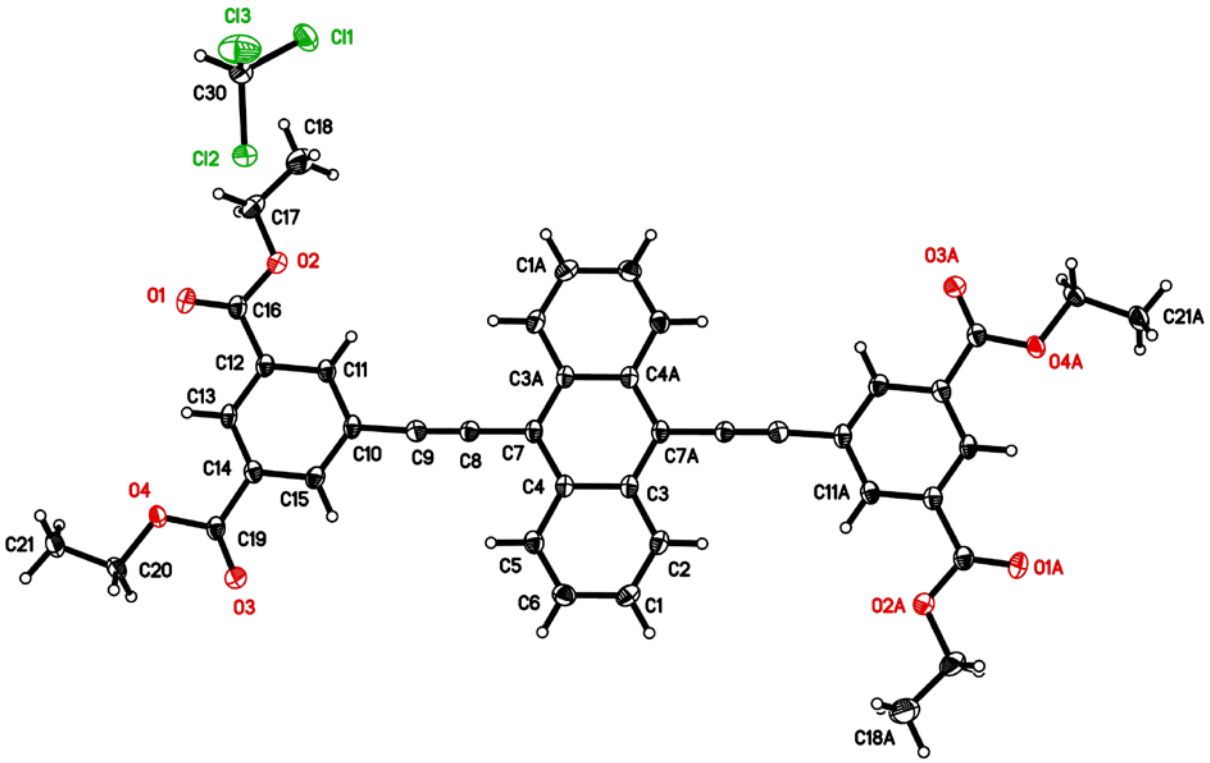

Figure S4. Thermal atomic displacement ellipsoid plot of the structure of crystals of tetraester **7** • 2 $CHCl_3$ grown from hexane/$CHCl_3$. The ellipsoids of non-hydrogen atoms are drawn at the 30% probability level, and hydrogen atoms are represented by a sphere of arbitrary size.

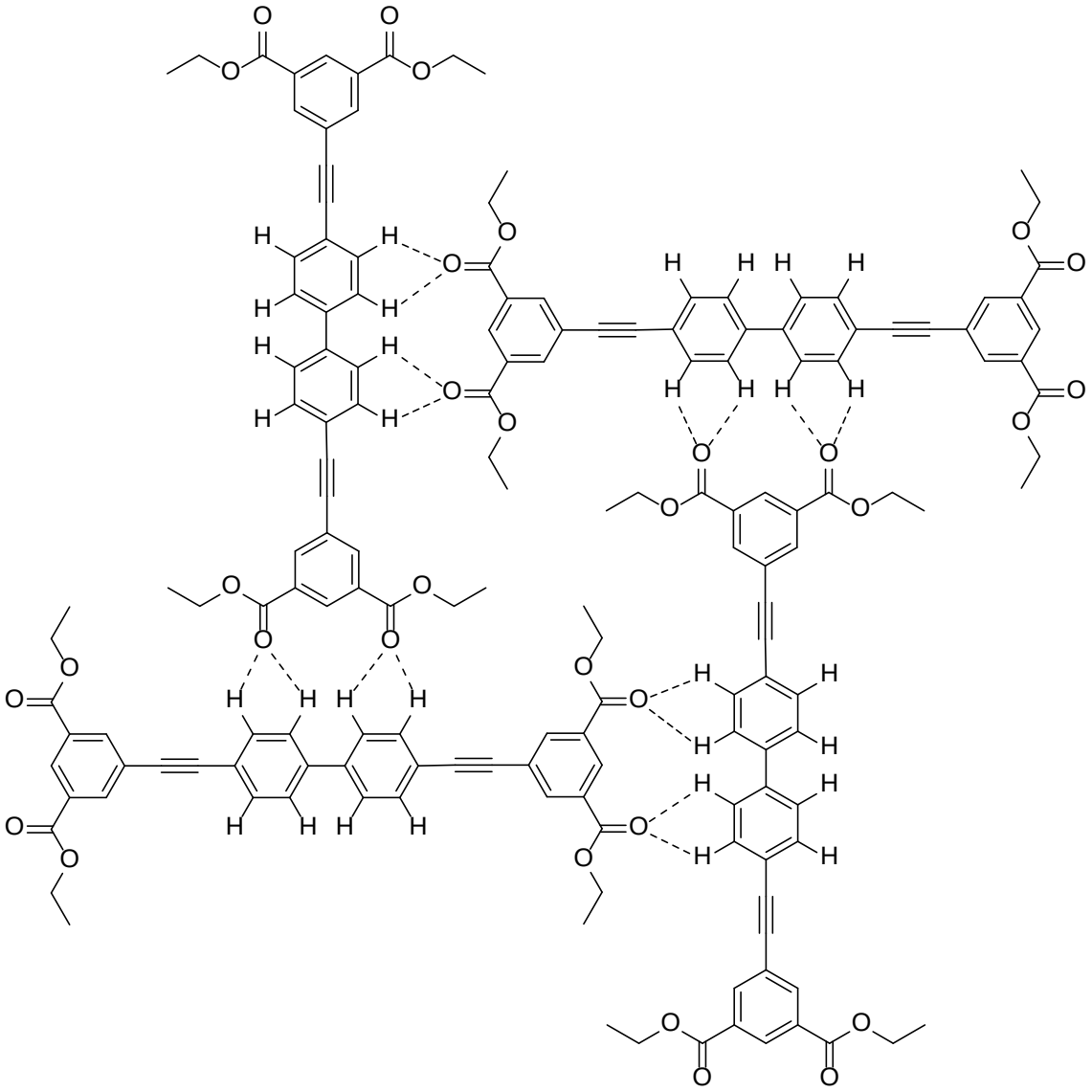

Figure S5. Representation of the square grid formed by adsorption of tetraester **5** on HOPG, showing perpendicular molecules in a planar D_{2h} conformation linked to neighbors by multiple C-H···O interactions.

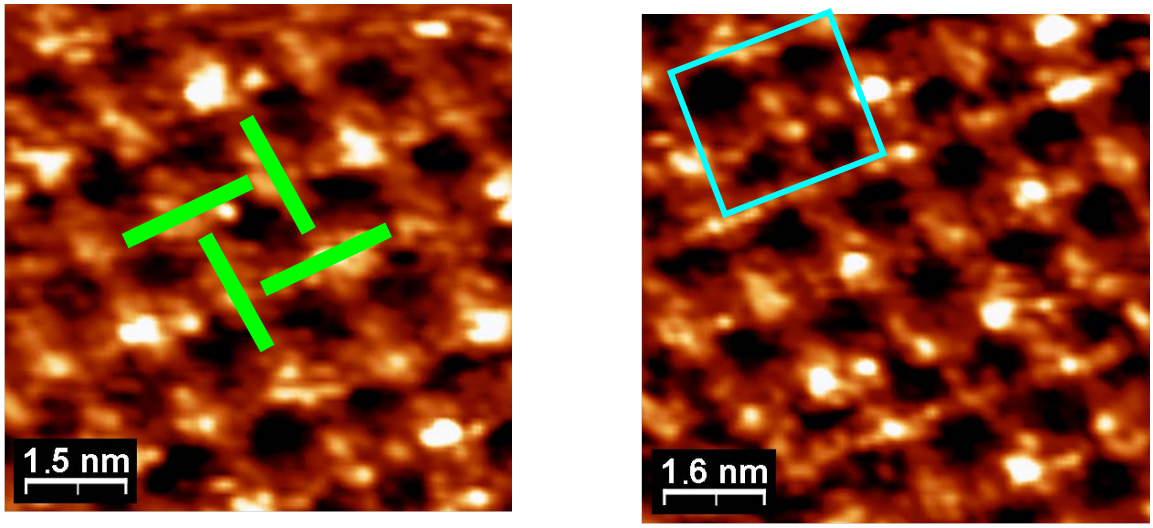

Figure S6. Supplementary STM images of the adsorption of tetraester **6** on HOPG (deposition from heptanoic acid, with V_{bias} = -1.5 V and I_{set} = 50 pA). (a) View of the square-grid network, with individual molecules represented by green bars to facilitate interpretation of the pattern of contrasts. (b) Additional view of the network, with local geometric irregularities highlighted in blue.

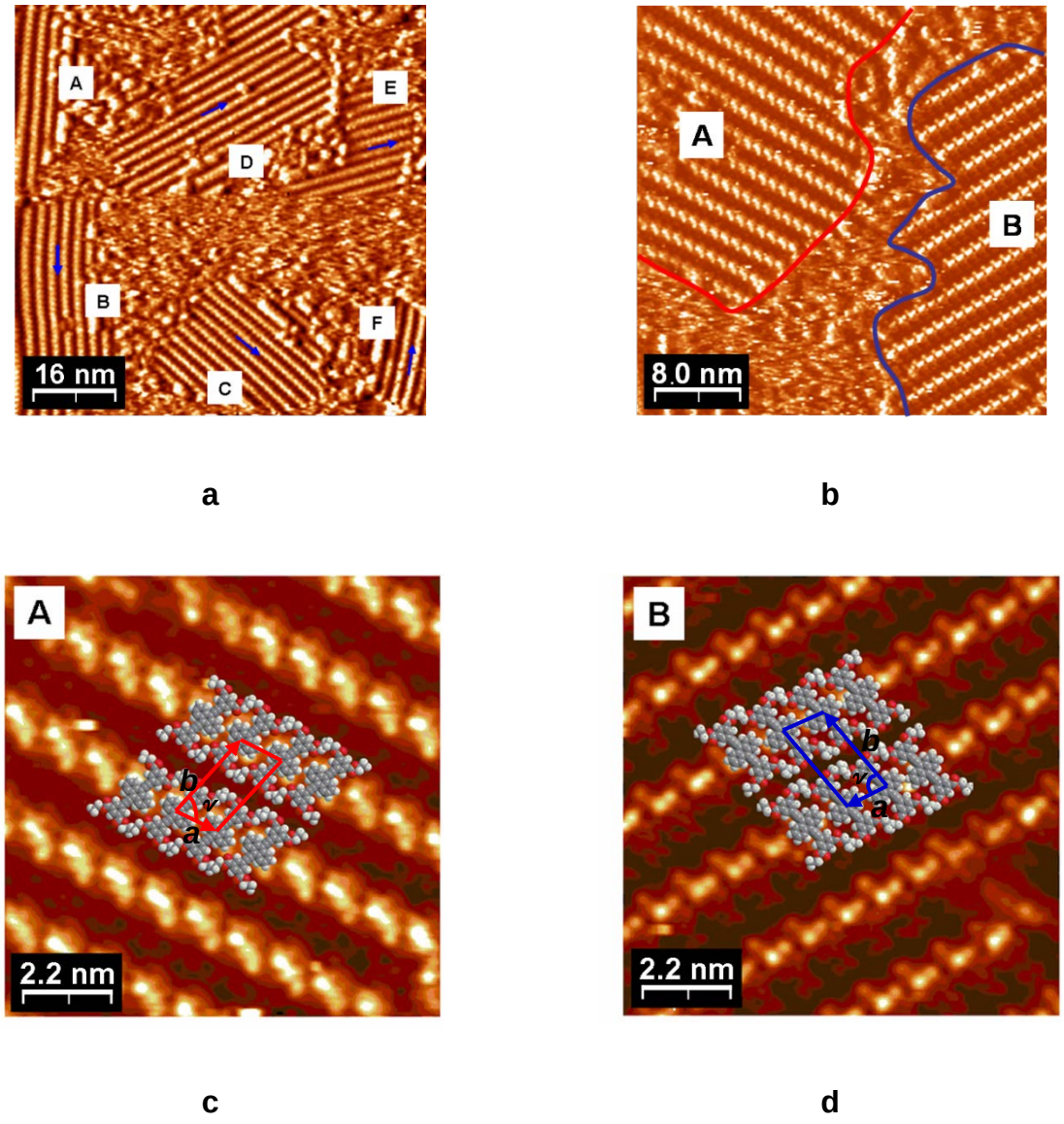

Figure S7. Supplementary STM images of the adsorption of tetraester **7** on HOPG (deposition from heptanoic acid, with V_{bias} = -1.5 V, I_{set} = 50 pA in Figure S7a, and I_{set} = 100 pA in Figures S7b-d). (a) View of an area of 80 nm × 80 nm, showing six domains labeled A-F with diverse orientations relative to the underlying HOPG. (b) Additional image showing enantiomorphous domains A and B. (c) Enlarged view of domain A, with superimposed molecular models to show 2D chirality. (d) Similar enlarged view of domain B.

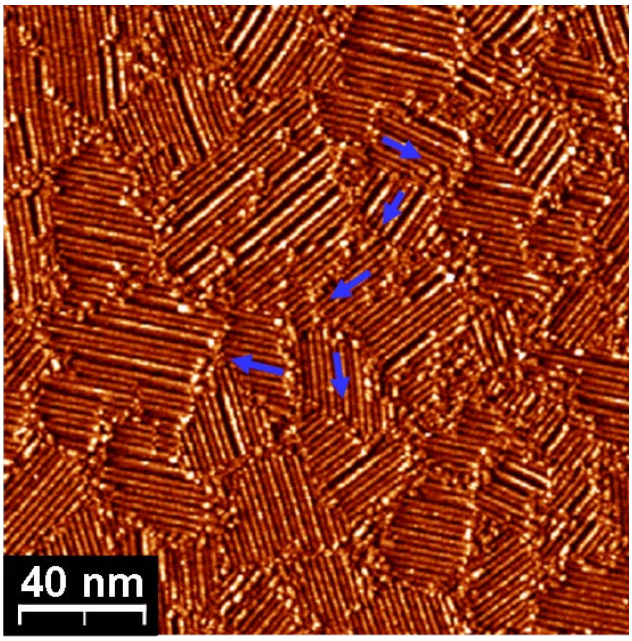

Figure S8. Supplementary STM image of the competitive adsorption of tetraesters **3** and **7** on HOPG (deposition of an equimolar mixture in heptanoic acid, with V_{bias} = -1.5 V and I_{set} = 100), showing multiple domains of pure tetraester **7**. Rows in adjacent domains tend to interact at angles that are multiples of 60°.

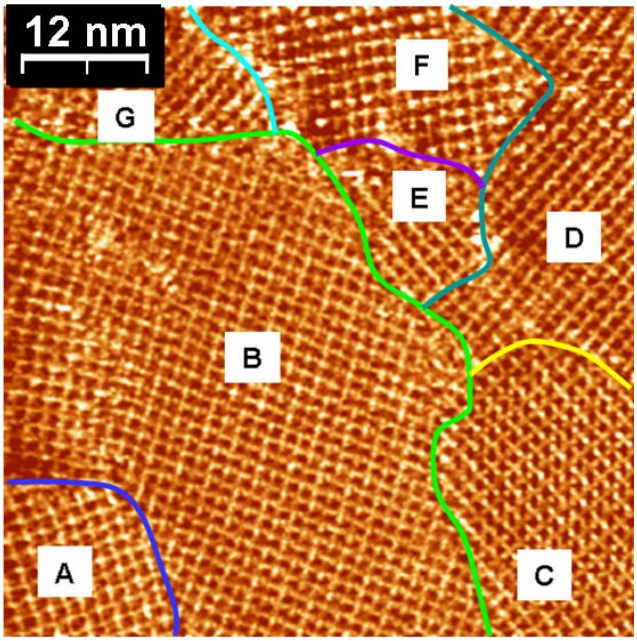

Figure S9. Supplementary STM image of the competitive adsorption of tetraesters **3** and **4a** on HOPG (deposition of an equimolar mixture in heptanoic acid, with V_{bias} = -1.5 V and I_{set} = 100), showing multiple domains of pure tetraester **4a**.

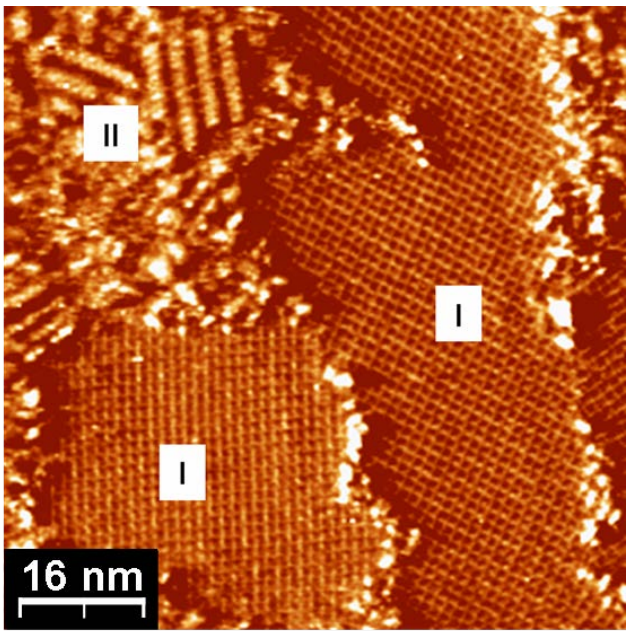

Figure S10. Supplementary STM image of the competitive adsorption of tetraesters **4a** and **7** on HOPG (deposition of an equimolar mixture in heptanoic acid, with V_{bias} = -1.5 V and I_{set} = 100), showing the predominant adsorption of tetraester **4a**.

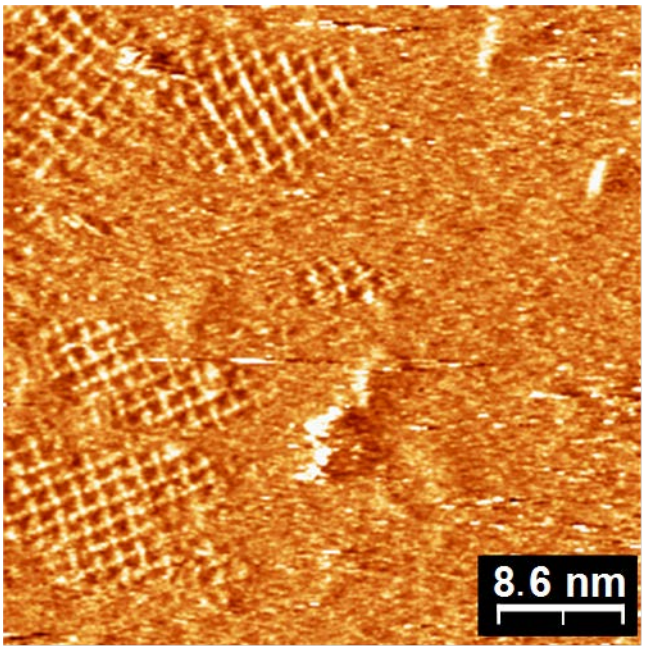

Figure S11. Supplementary STM image of the adsorption of tetramethyl ester **4b** on HOPG to form small areas of square grids (deposition from heptanoic acid, with V_{bias} = -1.5 V and I_{set} = 50 pA).