Electronic Supplementary Material (ESI) for CrystEngComm.

Supramolecular Synthons in the Gamma-Hydroxybutenolides

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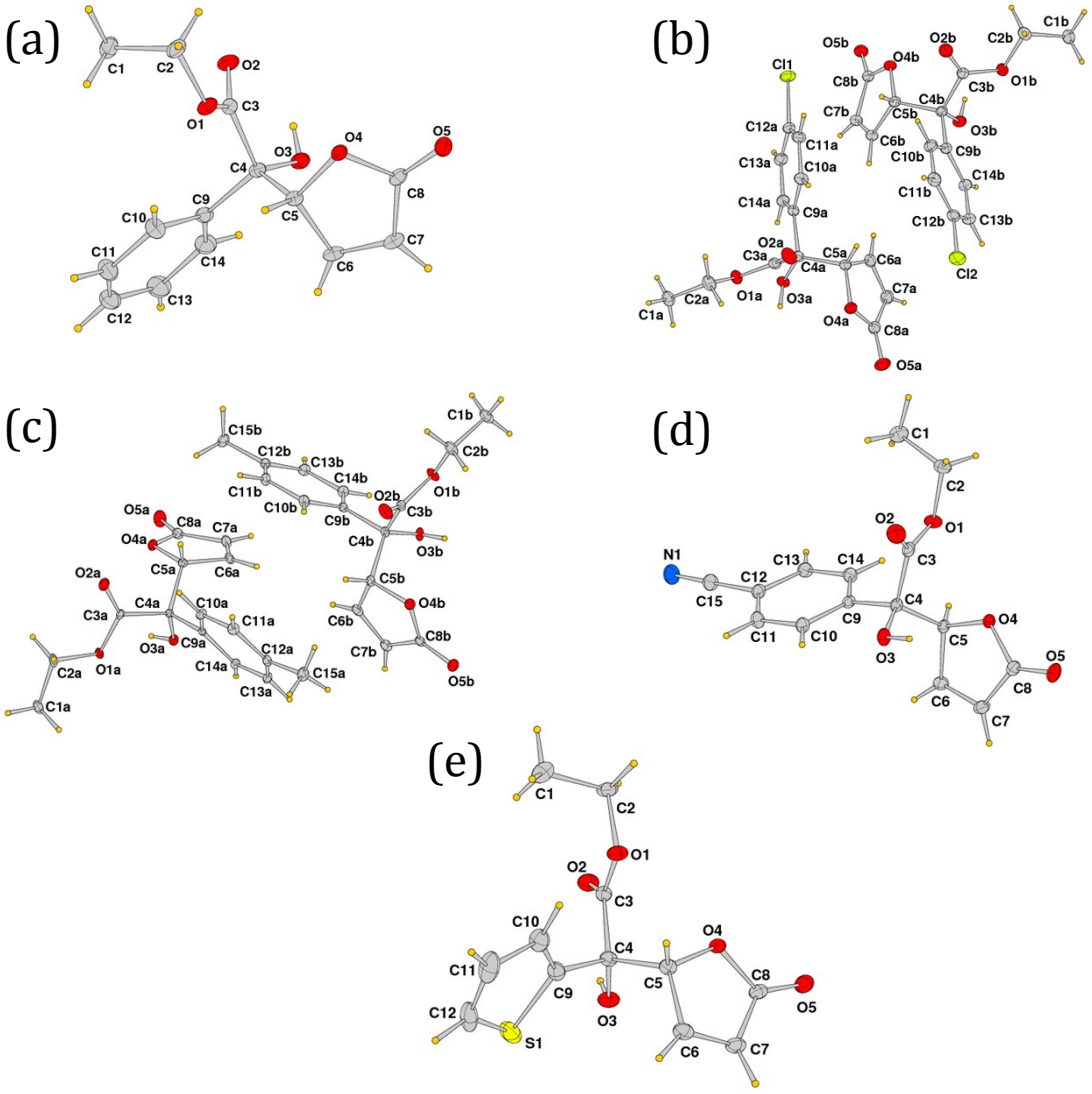

Figure S1. Ellipsoid plots at 50% probability for γ-hydroxybutenolides **3a** (a),**3b** (b), **3c** (c), **3d**(d) and **3e** (e)**.**

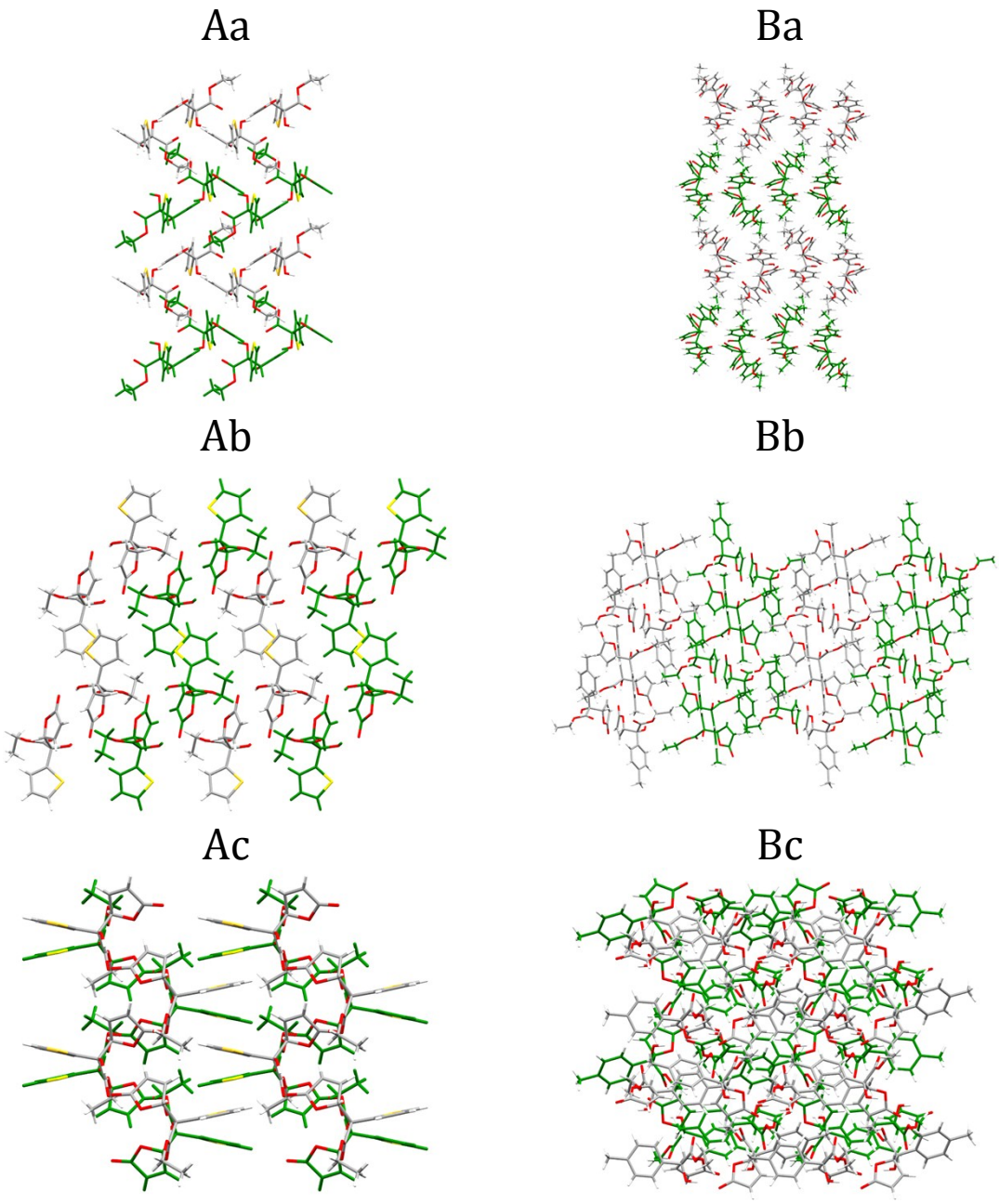

Figure S2. The packing arrangements of syn-γ-hydroxybutenolide **3e** (A) and syn-γ-hydroxybutenolide **3c** (B), as viewed along the a-axis (a), b-axis (b) and c-axis (c). Carbon atoms are represented in different colours (grey and green) to distinguish between the enantiomers.

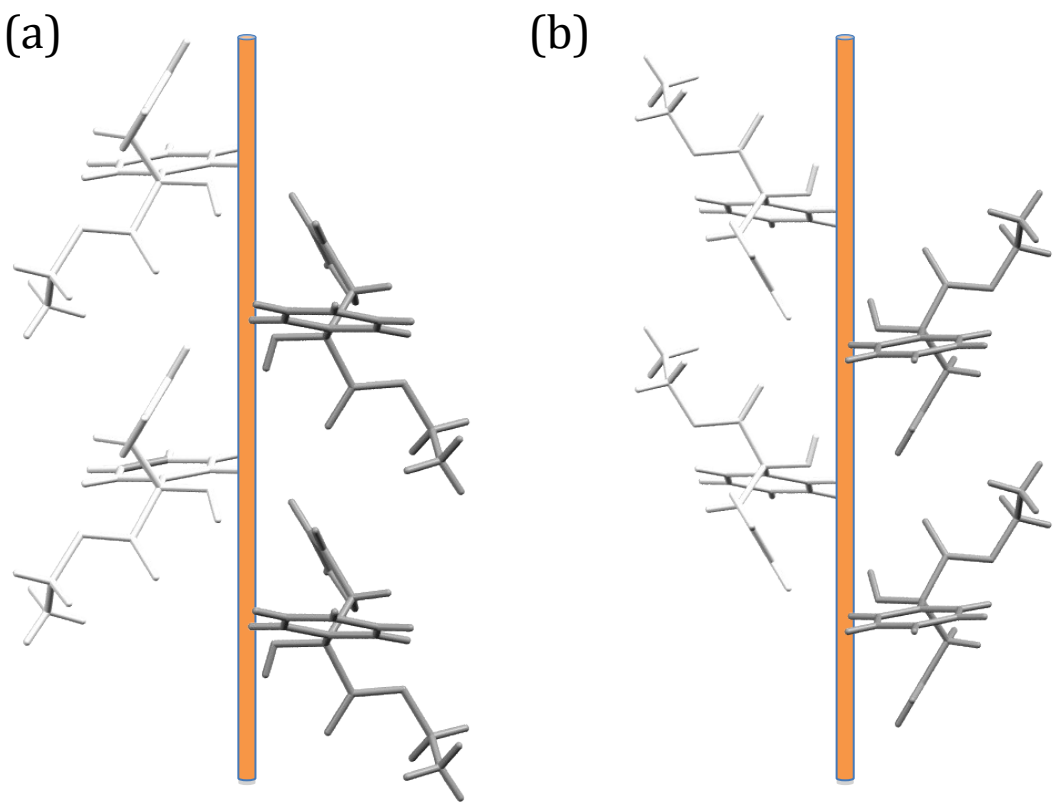

Figure S3. Handedness of 2_1 helices, on the basis of supramolecular-tilt-chirality (STC) proposed by Miyata and co-workers.[1] For clarity, molecules in front of the 2_1 screw axis (orange cylinder) are depicted entirely in a darker shade of grey with respect to those behind the axis. The handedness of the helix is determined by the direction the tilt of the molecule in front of the 2_1axis. Thus, (a) represents a left-handed helix and (b) a right-handed helix.

[1]I. Hisaki, T. Sasaki, N. Tohnai, M. Miyata, Chemistry - A European Journal, 2012, **18**, 10066

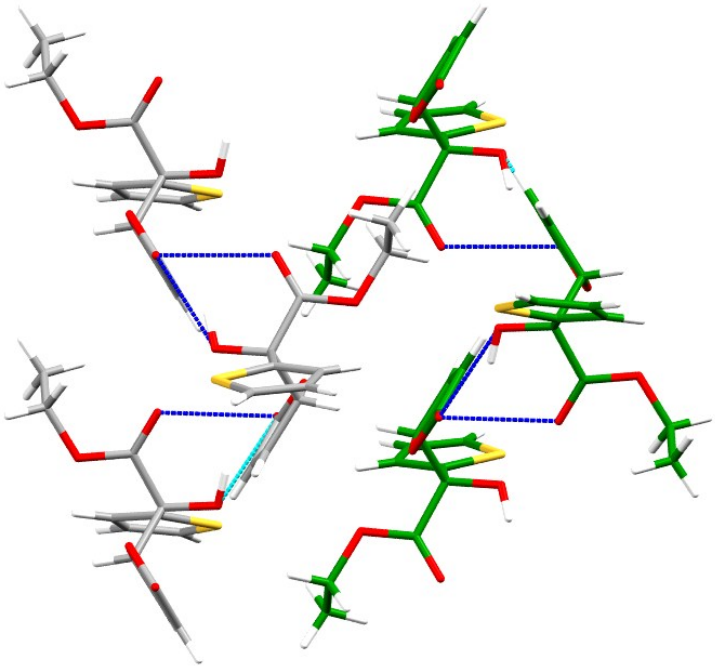

Figure S4. Helical arrangement, viewed down the a-axis, of the enantiomers around the 2_1 screw axis for *syn*-γ-hydroxybutenolide **3e**. 3 molecules, representing a full turn, are shown for each enantiomer. The carbon atoms are depicted in grey and green to distinguish between the two enantiomorphic helices.

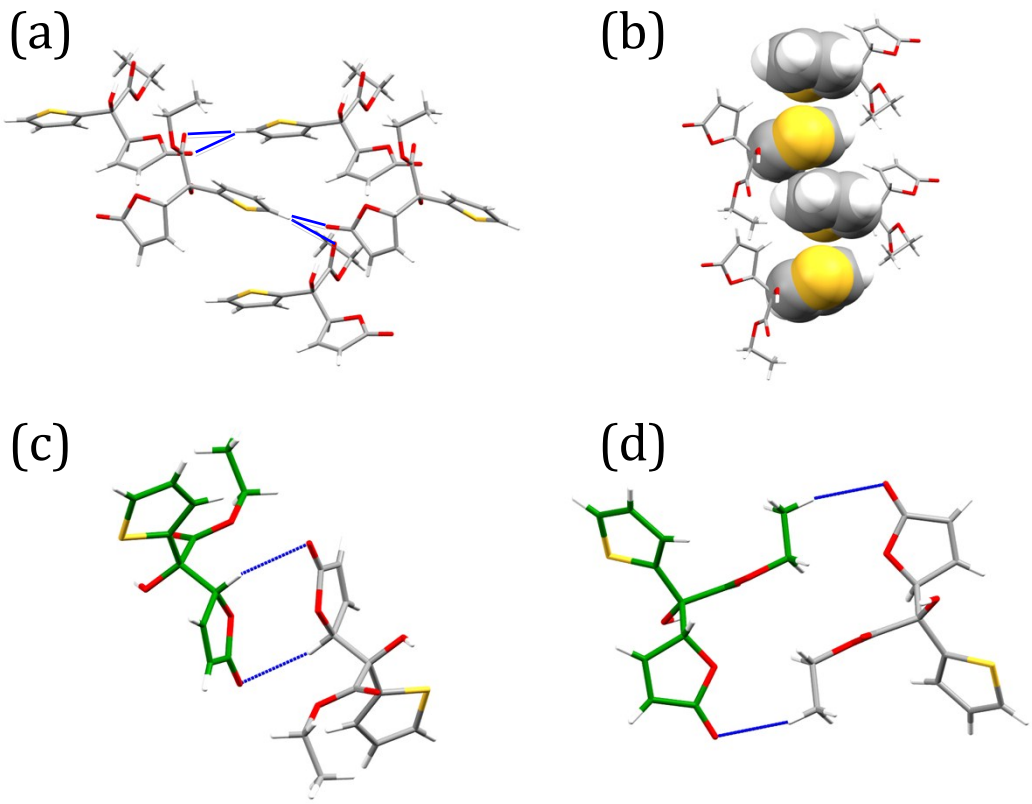

Figure S5. Overview of the weak non-covalent packing contacts in syn-γ-hydroxybutenolide **3e**. (a) bridged C12H12···O2 / C12H12···O5 interactions between adjacent helical strands of molecules with the same chirality; (b) interlocking, zipper-like stacking of the phenyl rings which arises between adjacent helical strands of molecules with the same chirality; (c) reciprocal C7H7···O5 interactions between helical strands of different enantiomers; (d) reciprocal C1H1C···O5 interactions between helical strands of different enantiomers. The carbon atoms are depicted in grey and green to distinguish between the enantiomers.

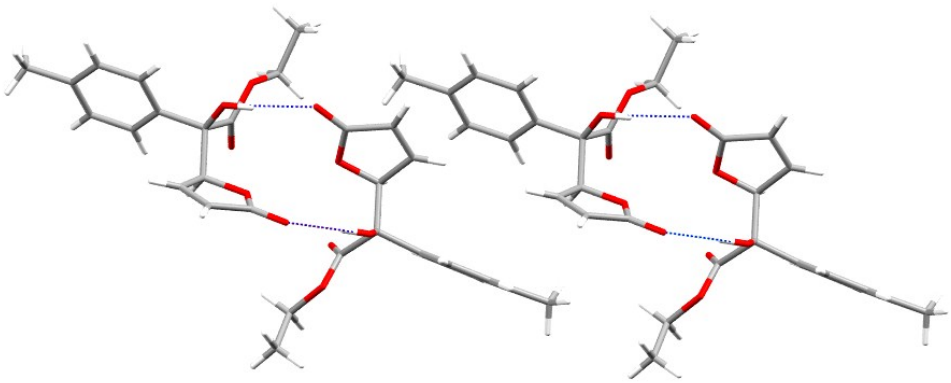

Figure S6. Homochiral dimers of syn—hydroxybutenolide **3c.**

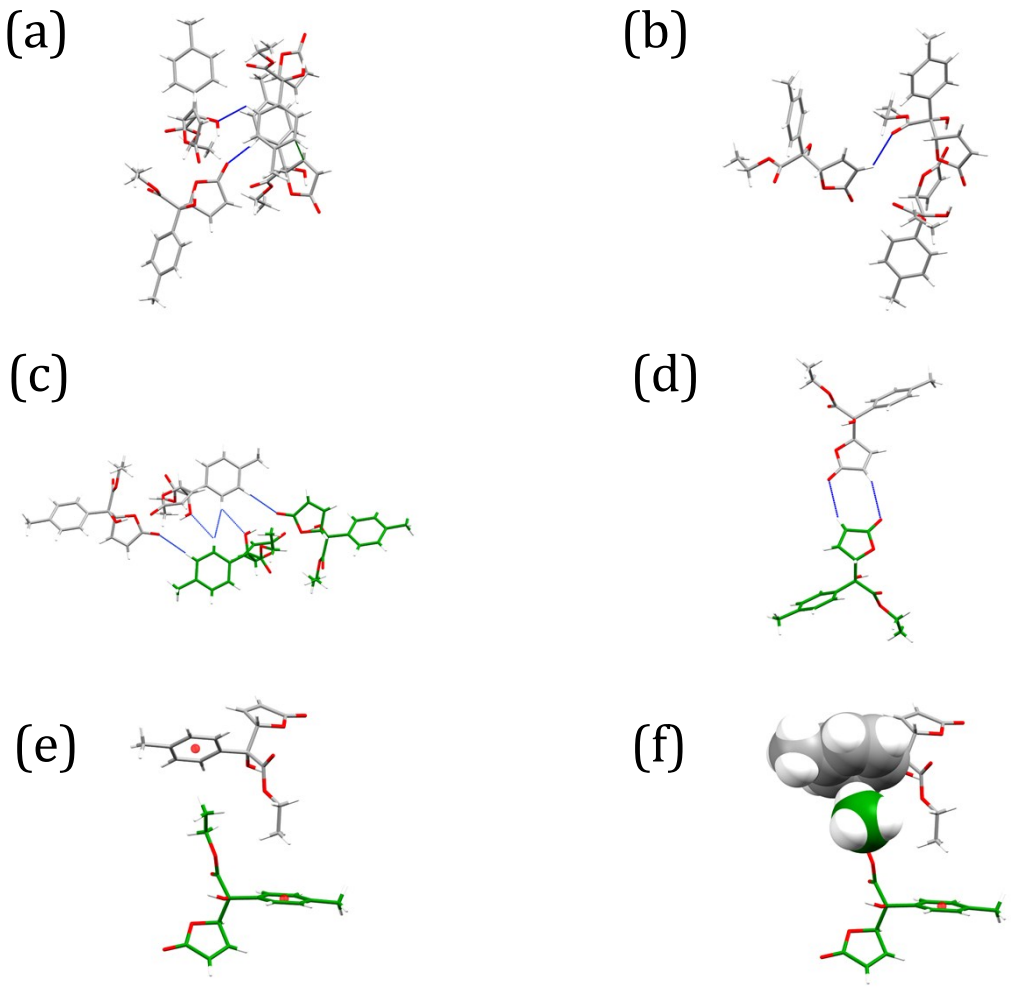

Figure S7. Overview of the weak, non-covalent packing contacts in syn-γ-hydroxybutenolide **3c**. (a) network of interactions between the hydrogen bond oxygen atoms (O3A, O5B) of one dimer with aromatic hydrogens on two adjacent dimers; (b) interaction between the H7 butenolide hydrogen and the O2 carbonyl oxygen atom of an adjacent molecule; (c) reciprocal interactions between the hydrogen bond oxygen atoms (O3B, O5A) of one dimer with phenyl hydrogens on an adjacent molecule; (d) reciprocal interactions between a vinylic hydrogen and the carbonyl oxygen of two facing butenolide rings; (e) CH-π interaction between a methyl hydrogen and a phenyl ring, with reciprocal CH···O interactions between a methyl hydrogen of the phenyl acceptor molecule and the O1 oxygen atom of the methyl donor molecule; (f) as in (e), with the CH-π interaction shown as a space fill model. The carbon atoms are depicted in grey and green to distinguish between the enantiomers.

Table S1. Crystallographic data for compound 3d

CCDC code	CCDC 1523707
Formula	C_{15} H_{13} N O_5
Formula weight	287.26
Temperature (K)	100
Wavelength (Å)	0.7
Crystal system	Orthorhombico
Space group	$Pn2_1a$
a (Å)	10.2780 (3)
b (Å)	10.4130 (16)
c (Å)	12.405 0 (11)
α (°)	90
β (°)	90
γ (°)	90
V (Å^3)	1327.6 (2)
Z, ρ_{calc} (g.mm^{-3})	4, 1.437
μ (mm^{-1})	0.104
F (000)	600
Data collection θ range	2.515 – 29.983
Refl. Collected / unique	24594 / 3912
R_{int}	0.0269
Completeness (%)	96.3
Refinement method[a]	FMLS on F^2
Data/Restraints/Parameters	3912 /0 / 193
GooF	1.056
R_1, wR_2 [I>2σ(I)]	0.0277, 0.0764
R_1, wR_2 all data	0.0278, 0.0764
ls shift su max/mean	0.001 / 0
Largest. Diff. peak/hole (e. Å^3)	0.043 / -0.19
Absoulte structure parameter (Flack)	0.03 (9)

[a]Full-matrix least-squares (FMLS) on F^2