

Electronic Supplementary Information

Supramolecular homochiral helicity and zigzag hydrogen bonded networks in 1,2,4-triazole derived aminoester and aminoacid

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General procedures

Infrared spectra in KBr were recorded with a BioRad FTS 135 spectrometer in the range 400–3600 cm⁻¹. ¹H NMR spectra were recorded on Bruker Avance 300 MHz spectrometer at 25 °C. Mass spectra were recorded on a Thermo Finnigan LCQ Ion Trap spectrometer using APCI mode and detecting positive ions. Elemental analyses were carried out at the University College of London (UK).

Table S1 Crystallographic data and structure refinements for ethyl-4H-1,2,4-triazol-4-yl-acetate (**1**) and 4-(4H-1,2,4-Triazol-4-yl)l-propionic acid (**2**).

Crystal data	1	2
Empirical formula	C ₆ H ₉ N ₃ O ₂	C ₅ H ₇ N ₃ O ₂
T (K)	293(2)	150(2)
M (g/mol)	155.16	141.14
Crystal system	Tetragonal	Orthorhombic
Space group	P4 ₁ (n° 76)	P2 ₁ 2 ₁ 2 ₁ (n° 19)
a/Å	9.025(4)	9.7498(5)
b/Å	9.025(4)	10.7110(4)
c/Å	10.200(4)	12.7361(6)
V/Å ³	830.8(6)	1330.04(11)
Z	4	8
D/g.cm ⁻³	1.241	1.410
Crystal size (mm)	0.4 x 0.4 x 0.05	0.44 x 0.27 x 0.22
F(000)	328	592
Reflections collected	9692	9867
Independent reflections	1164 [R(int) = 0.063]	2490 [R(int) = 0.0505]
No. parameters	147	231
Goodness of fit on F ²	1.096	1.089
R ₁ , wR ₂ [I>2σ(I)]	0.0317 , 0.0820	0.0438 , 0.0981
R ₁ , wR ₂ [all data]	0.0357 , 0.0854	0.0529 , 0.1038
Largest difference peak and hole	0.079 and -0.079 e.Å ⁻³	0.159 and -0.148 e.Å ⁻³

No flack parameter has been given for the reported structures; both datasets lack enough anomalous scattering power to accurately determine the chirality. In **1** the molecule is achiral and the chirality is expressed as the handedness of the helix as explained in the main text. Both P4₁ and P4₃ crystals will be present in the bulk material. In **2** the starting material was L-alanine, but partial racemization was observed (see main text), the asymmetric unit consist of a 3/1 ratio between both enantiomers, given that L-alanine was used as source material, the L configuration chosen as reference in the initial structure refinement, the minor contribution of the other enantiomer was thus assigned as being the D-configuration.

Table S2 (a) Selected bond distances (\AA) and (b) inter-atomic distances and angles ($^\circ$) for hydrogen bonds interactions in ethyl-4H-1,2,4-triazol-4-yl-acetate (**1**).

(a)

N1-C5	1.296(5)	C6-H6B	1.02(6)
N1-N2	1.383(5)	C7-O8	1.202(4)
N2-C3	1.306(5)	C7-O9	1.312(4)
C3-N4	1.348(5)	O9-C10	1.467(7)
C3-H3	1.06(7)	C10-C11	1.263(10)
N4-C5	1.351(5)	C10-H10A	0.970(0)
N4-C6	1.452(4)	C10-H10B	0.970(0)
C5-H5	1.06(6)	C11-H11A	0.960(0)
C6-C7	1.485(5)	C11-H11B	0.960(0)
C6-H6A	0.88(7)	C11-H11C	0.960(0)

C5-N1-N2	106.5(3)	N4-C6-C7	111.7(3)
C3-N2-N1	106.9(3)	N4-C6-H6A	105(4)
N2-C3-N4	110.7(3)	C7-C6-H6A	116(4)
N2-C3-H3	130(3)	N4-C6-H6B	115(3)
N4-C3-H3	120(3)	C7-C6-H6B	101(4)
C3-N4-C5	104.4(3)	H6A-C6-H6B	108(5)
C3-N4-C6	127.6(3)	O8-C7-O9	124.6(3)
C5-N4-C6	127.9(3)	O8-C7-C6	125.9(3)
N1-C5-N4	111.4(3)	O9-C7-C6	109.5(3)
N4-C5-H5	116(3)	C7-O9-C10	117.6(4)
		C11-C10-O9	115.2(6)

(b)

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$\angle DHA$	<i>symmetry</i>
$C(3)-H(3) \cdots N(2)$	0.93	2.55	3.392(6)	150	$-1+y, 2-x, -1/4+z$
$C(6)-H(6A) \cdots N(1)$	0.97	2.50	3.423(5)	158	$-1+y, 2-x, -1/4+z$

Table S3 (a) Selected bond distances (\AA) and (b) inter-atomic distances and angles ($^\circ$) for hydrogen bonds interactions in 4-(4H-1,2,4-triazol-4-yl)l-propionic acid (**2**).

C1–N2	1.302(4)	C21–N22	1.302(7)
C1–N5	1.360(4)	C21–N25	1.376(8)
N2–N3	1.385(4)	N22–N23	1.374(7)
N3–C4	1.301(4)	N23–C24	1.307(7)
C4–N5	1.338(4)	C24–N25	1.327(8)
N5–C6	1.469(3)	N25–C26	1.461(6)
C6–C7	1.514(4)	C26–C27	1.515(7)
C6–C8	1.525(4)	C26–C28	1.527(7)
C8–O9	1.209(3)	C28–O29	1.207(7)
C8–O10	1.302(3)	C28–O30	1.326(7)

C21B N22B	1.305(8)	N25B C26B	1.476(6)
C21B N25B	1.365(8)	C26B C27B	1.513(7)
N22B N23B	1.376(8)	C26B C28B	1.527(7)
N23B C24B	1.309(8)	C28B O29B	1.210(7)
C24B N25B	1.334(8)	C28B O30B	1.323(8)

(b)

D-H\cdotsA	D - H	H\cdotsA	D\cdotsA	<D HA	symmetry
O(10)-H(10)...N(3)	0.84	1.74	2.569(4)	171	1/2-x,-y,1/2+z
O(30)-H(30)...N(22)	0.84	2.41	3.24(3)	170	1/2-x,1-y,-1/2+z
O(30)-H(30)...N(23)	0.84	1.78	2.57(3)	156	1/2-x,1-y,-1/2+z

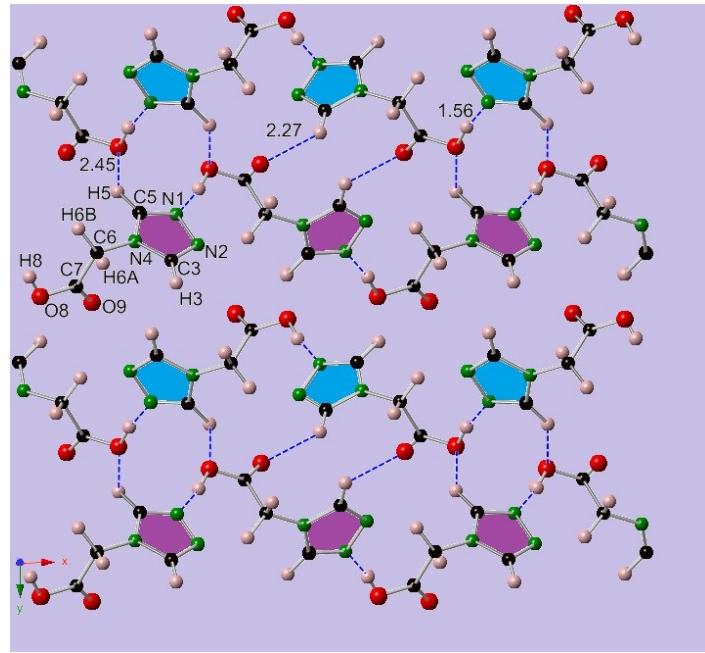


Figure S1 View of the zig-zag parallel chains of $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonding network in the crystal packing of **2** along *ab* plane. Opposite 1D chains are marked with blue and mauve colours.