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Supporting information file

Green catalytic synthesis of symmetric and non-symmetric β-hydroxy-1,2,3-triazoles by using epichlorohydrin in the presence of Cu(II) coordination compounds containing oxazole ligands

Fatemeh Ajormal,[a] Rahman Bikas,[b,*] Nader Noshiranzadeh,[a,*] Anna Kozakiewicz-Piekarz,[c] Tadeusz Lis,[d]

[a] *Department of Chemistry, Faculty of Science, University of Zanjan, Zanjan, 45371-38791, Iran*

[b] *Department of Chemistry, Faculty of Science, Imam Khomeini International University, 34148-96818, Qazvin, Iran*

[c] *Department of Biomedical and Polymer Chemistry, Faculty of Chemistry, Nicolaus Copernicus University in Torun, 87-100, Torun, Poland*

[d] *Faculty of Chemistry, University of Wroclaw, Joliot-Curie 14, Wroclaw 50-383, Poland*

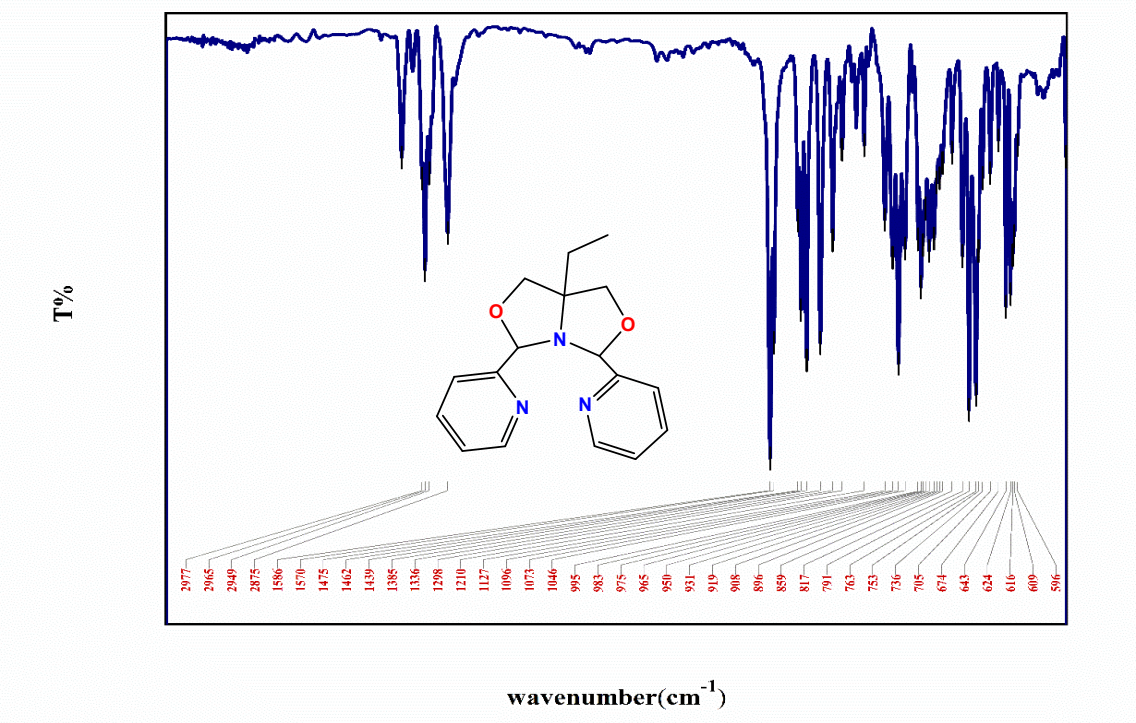


Fig. S1: The FT-IR spectrum of synthesized L^1 on KBr disk

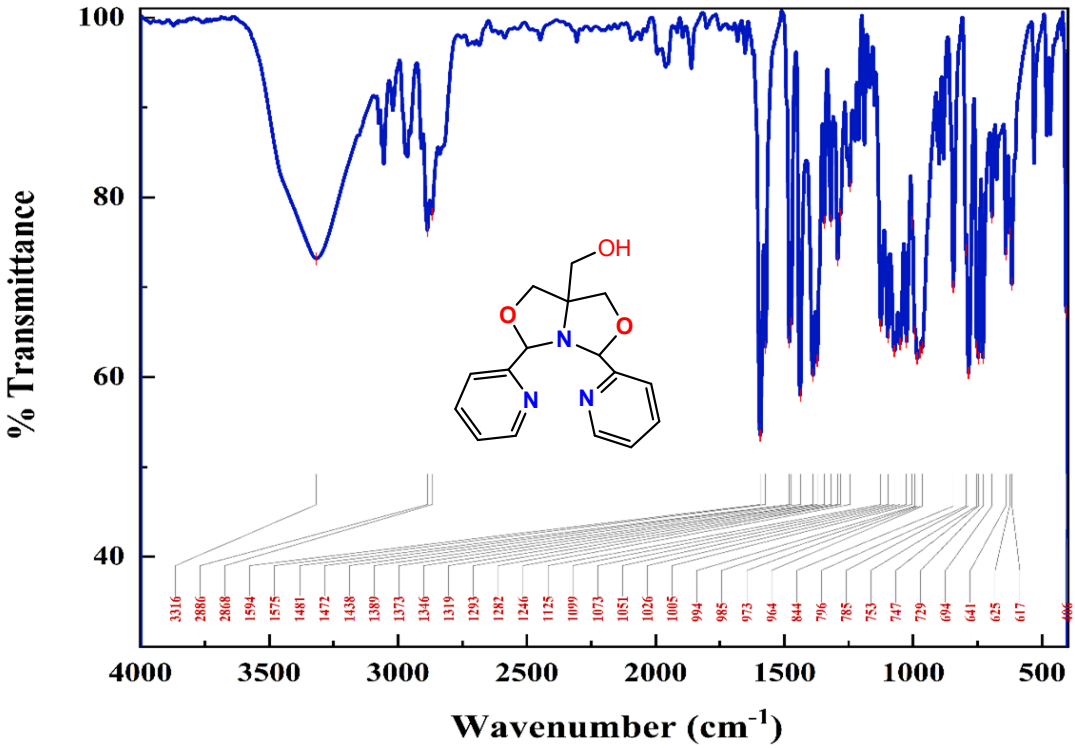


Fig. S2: The FT-IR spectrum of synthesized L^2 on KBr disk

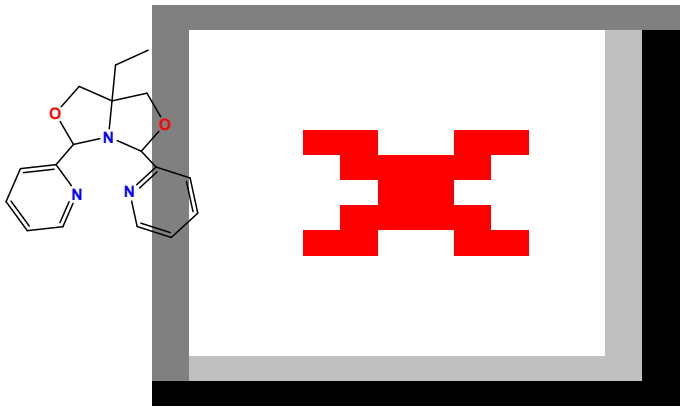


Fig. S3: ^{1}H-NMR spectrum of the ligand L^1 in $CDCl_3$ solution

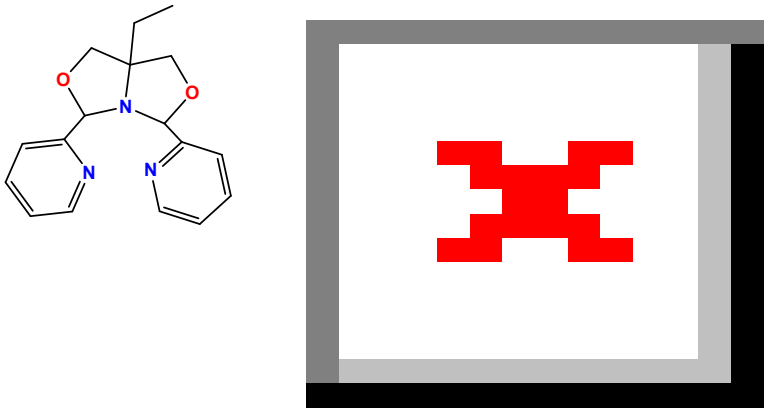


Fig. S4: ^{13}C-NMR spectrum of the ligand L^1 in $CDCl_3$ solution.

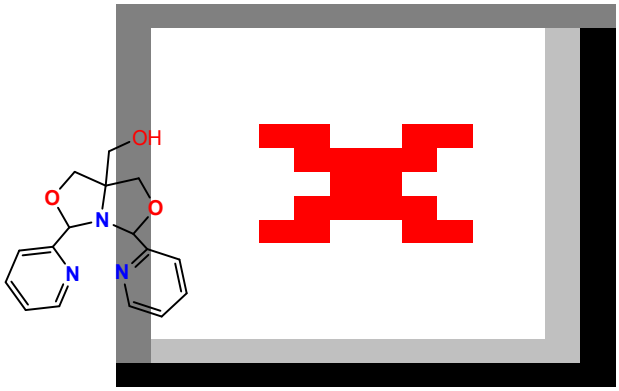


Fig. S5: ^{1}H-NMR spectrum of the ligand L^2 in DMSO-d6 solution.

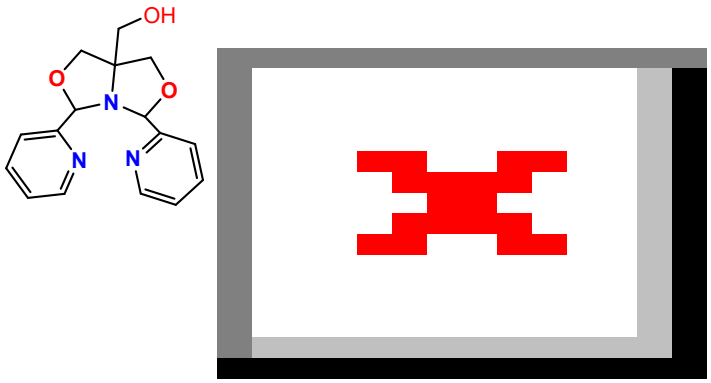


Fig. S6: ^{13}C-NMR spectrum of the ligand L^2 in DMSO-d6 solution.

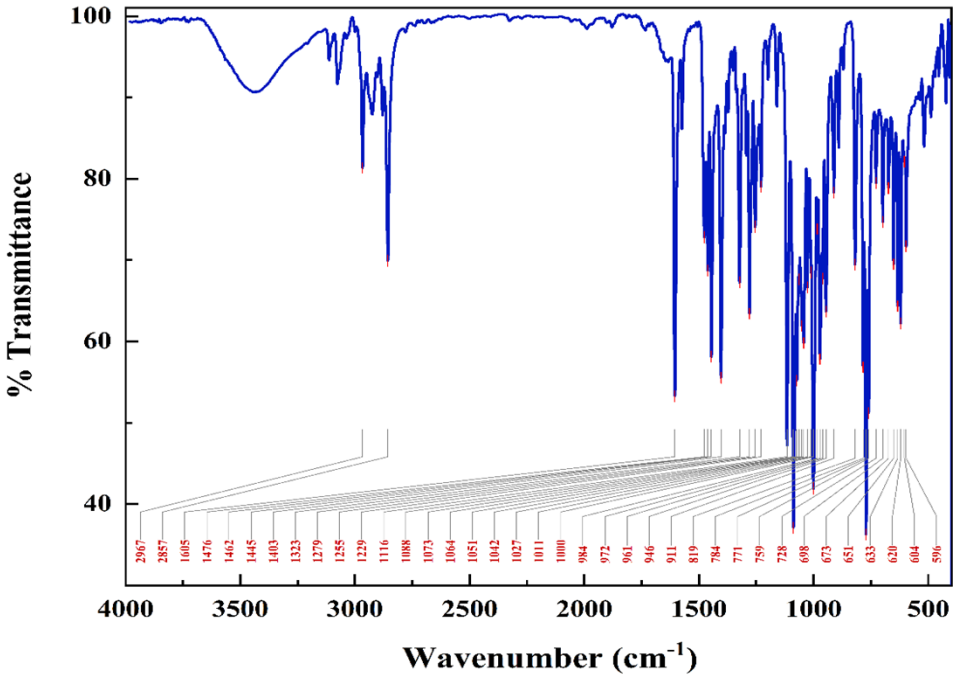


Fig. S7: The FT-IR spectrum of compound **1** on KBr disk

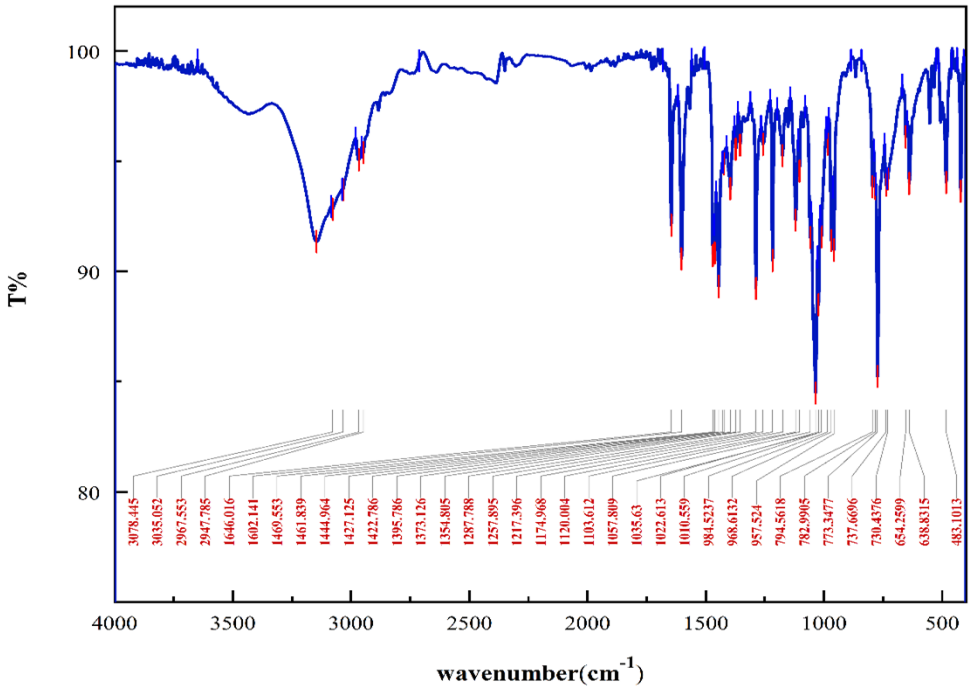


Fig. S8: The FT-IR spectrum of compound **2** on KBr disk

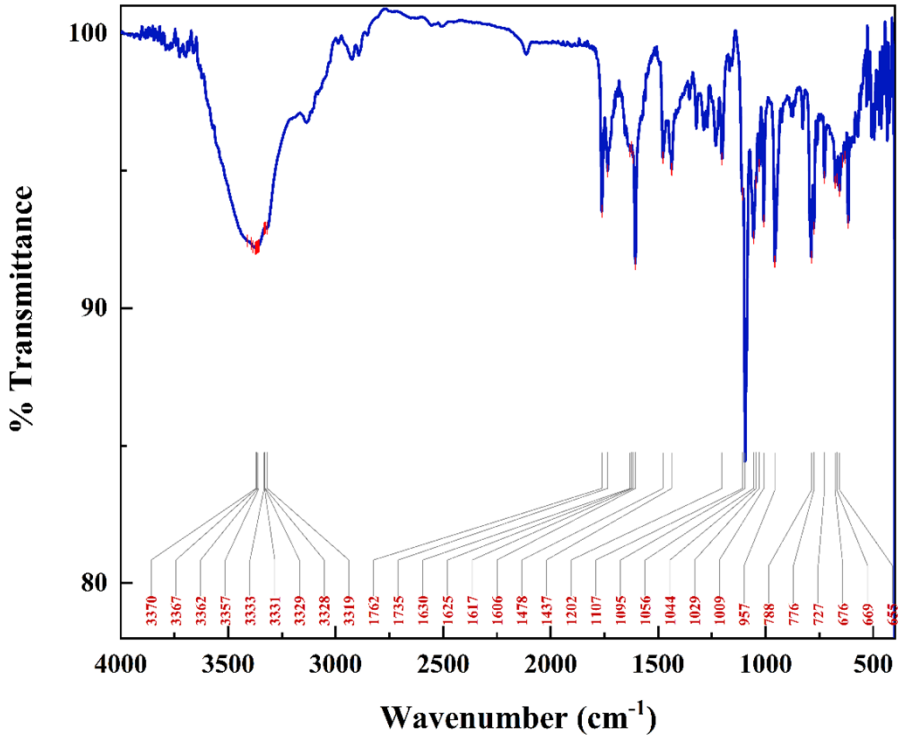


Fig. S9: The FT-IR spectrum of compound **3** on KBr disk

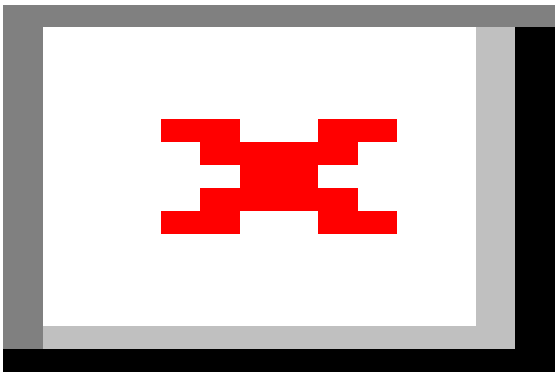


Fig. S10: Intermolecular C−H···O (green dashed lines) and C−H···Cl (pink dashed lines) hydrogen bond interactions in the structure of compound **1**

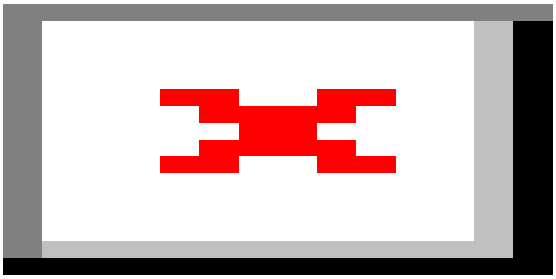


Fig. S11: Intermolecular C−H···O (green dashed lines) and C−H···Br (pink dashed lines) hydrogen bond interactions for compound **2**

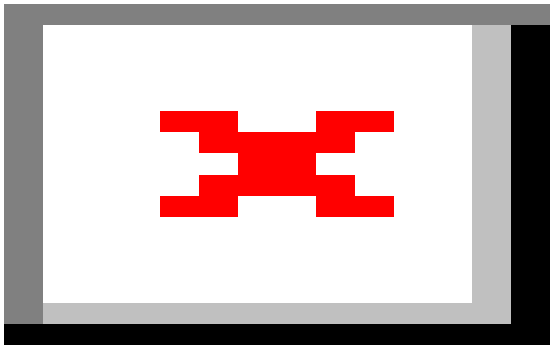


Fig. S12: Intermolecular hydrogen bond interactions in the crystal structure of **T1**

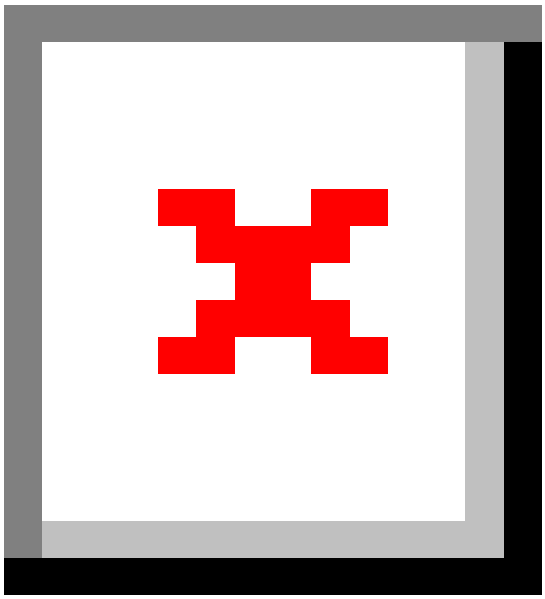


Fig. S13: Intermolecular hydrogen bond interactions in the crystal structure of **T2**

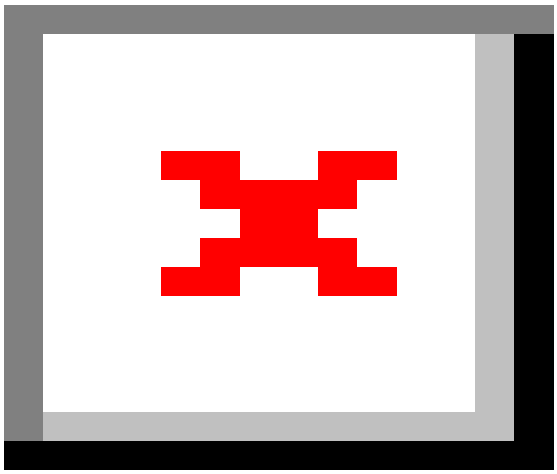


Fig. S14: Intermolecular hydrogen bond interactions in the crystal structure of **T4**

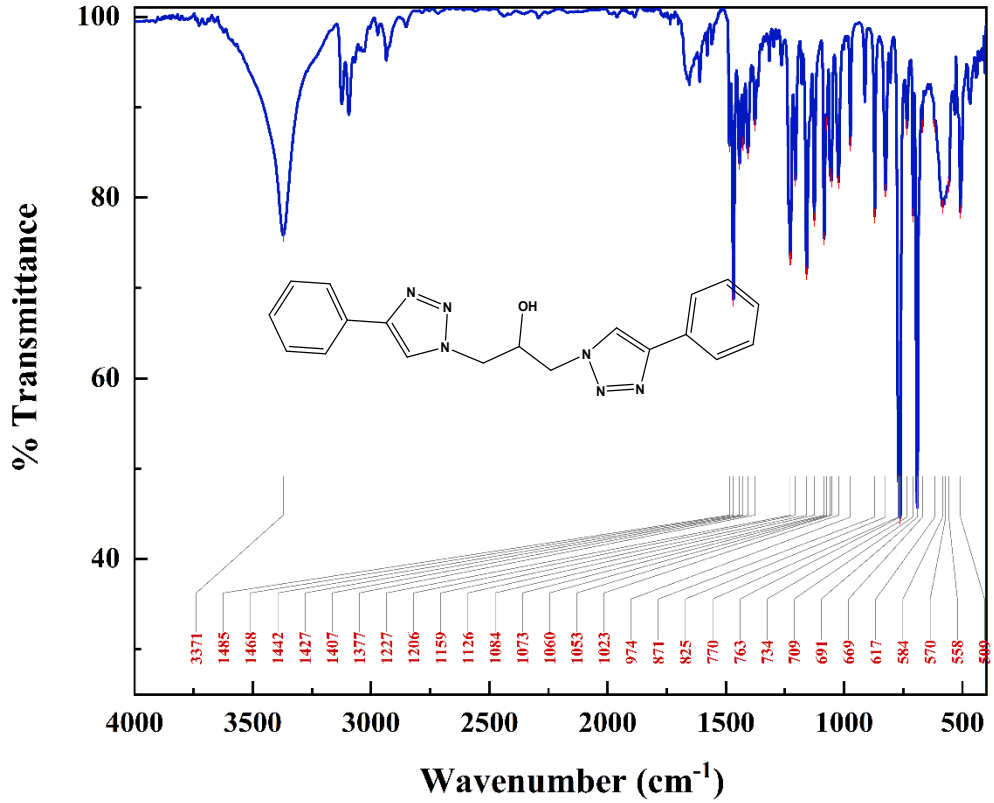


Fig. S15: The FT-IR spectrum of synthesized **T1** on KBr disk

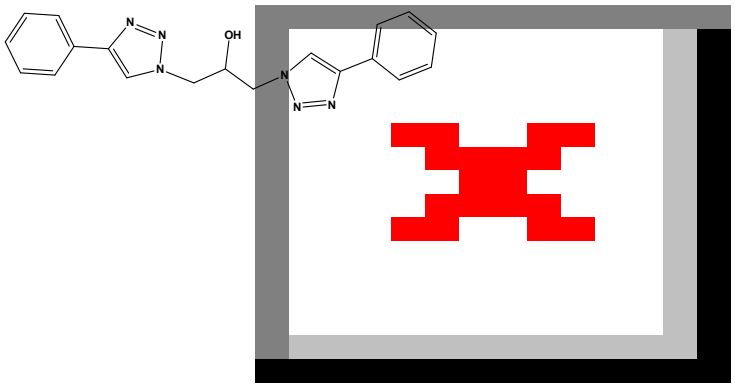


Fig. S16: ^{1}H-NMR spectrum of the **T1** in DMSO-d_6 solution

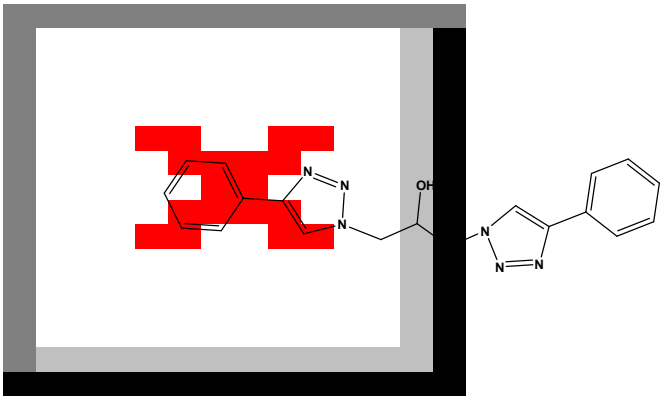


Fig. S17: ^{13}C-NMR spectrum of the **T1** in DMSO-d_6 solution.

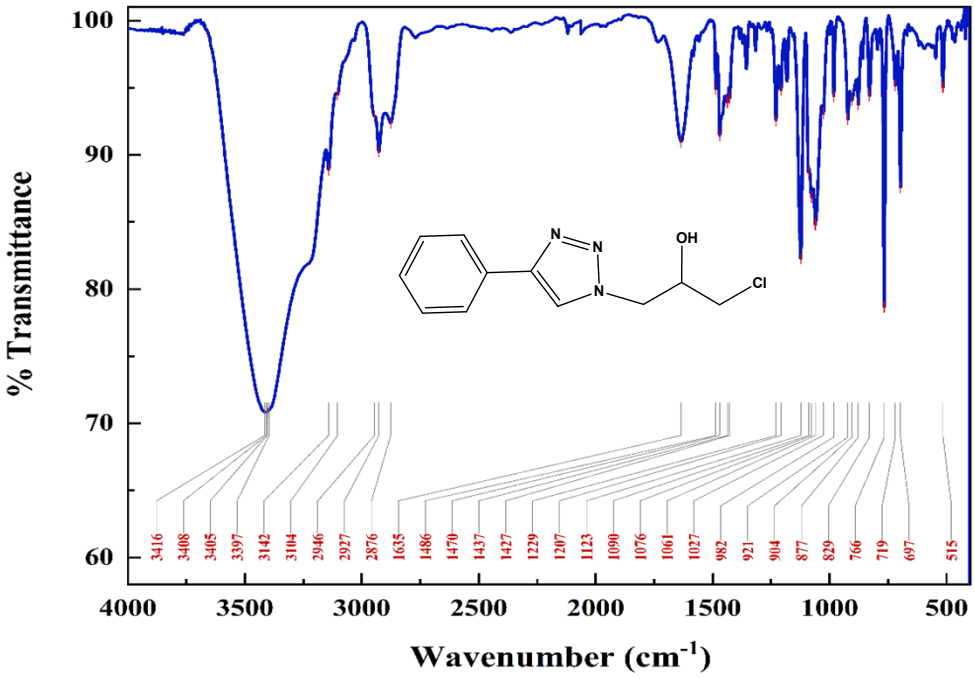


Fig. S18: The FT-IR spectrum of synthesized **T2** on KBr disk

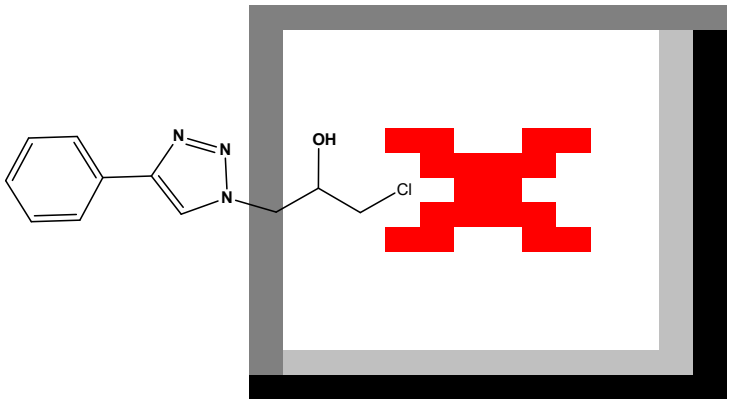


Fig. S19: ^{1}H-NMR spectrum of the **T2** in $CDCl_3$ solution.

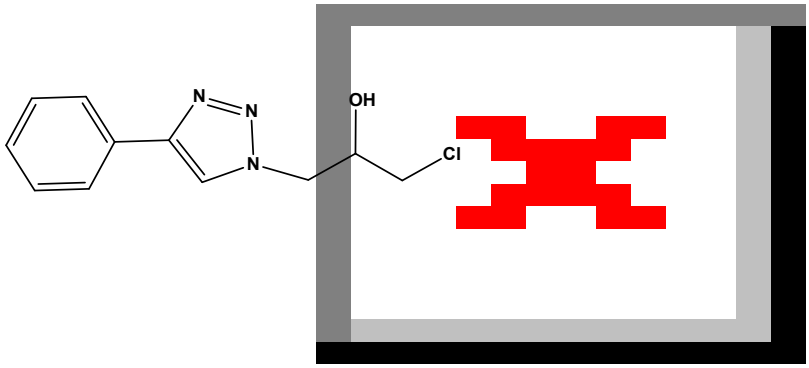


Fig. S20: ^{13}C-NMR spectrum of the **T2** in $CDCl_3$ solution.

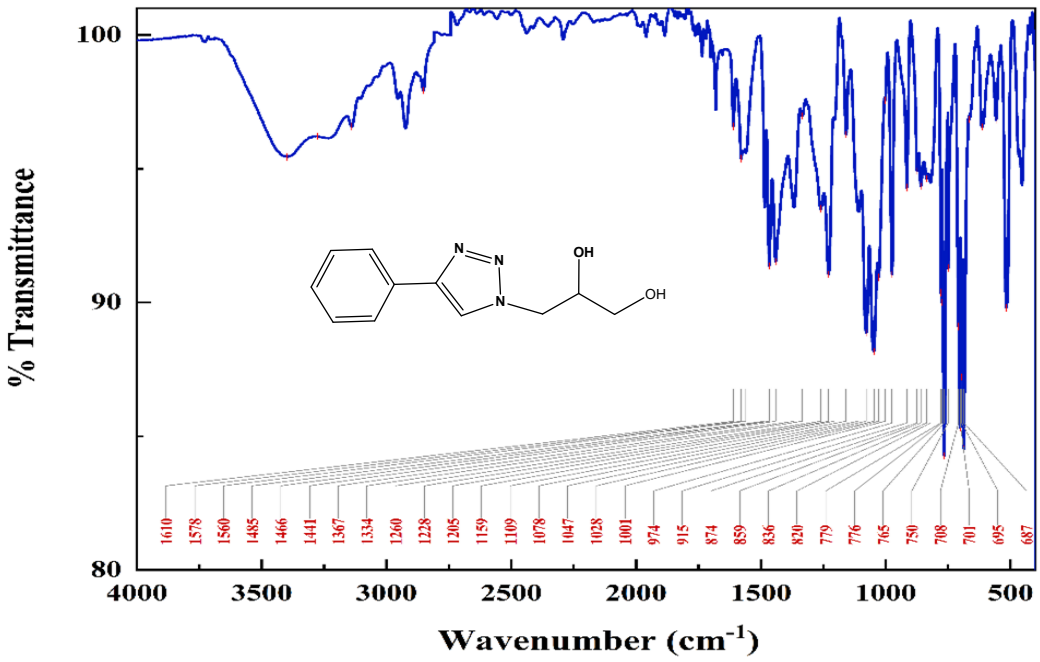


Fig. S21: The FT-IR spectrum of **T3** on KBr disk

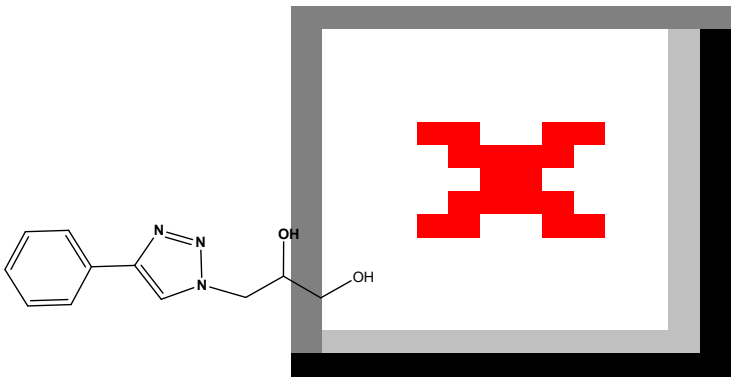


Fig. S22: ^{1}H-NMR spectrum of the **T3** in $CDCl_3$ solution.

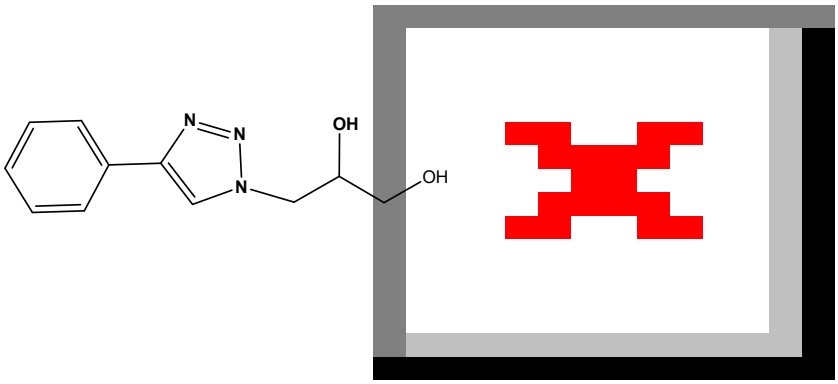


Fig. S23: ^{13}C-NMR spectrum of the **T3** in $CDCl_3$ solution.

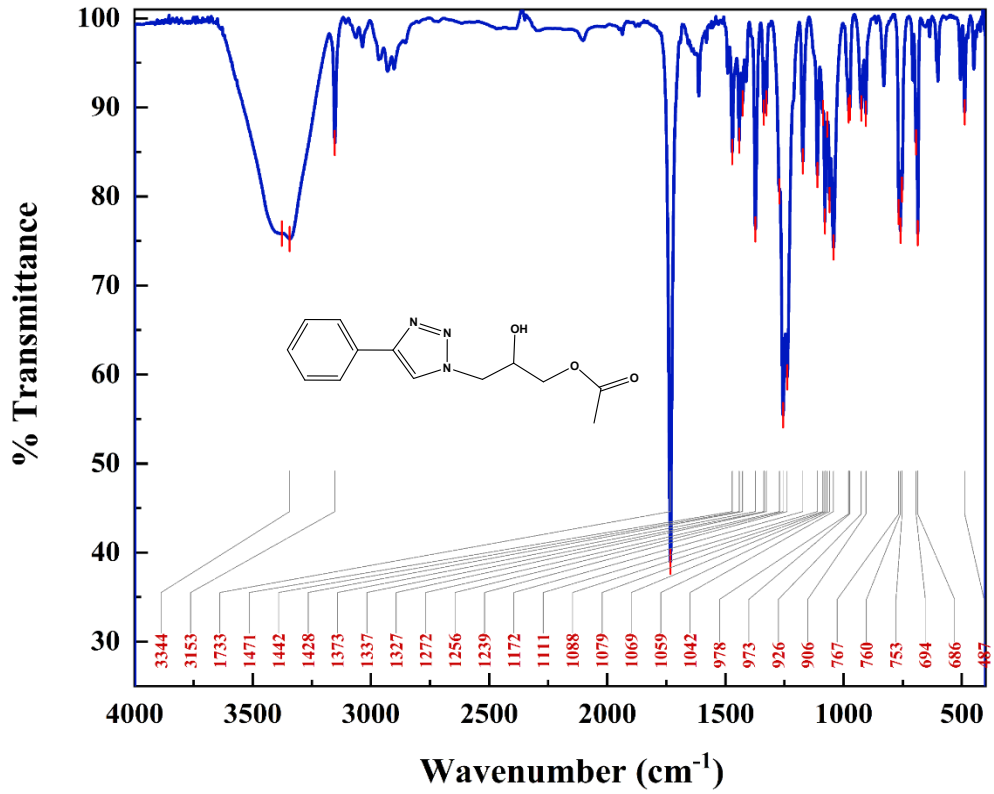


Fig. S24: The FT-IR spectrum of synthesized **T4** on KBr disk

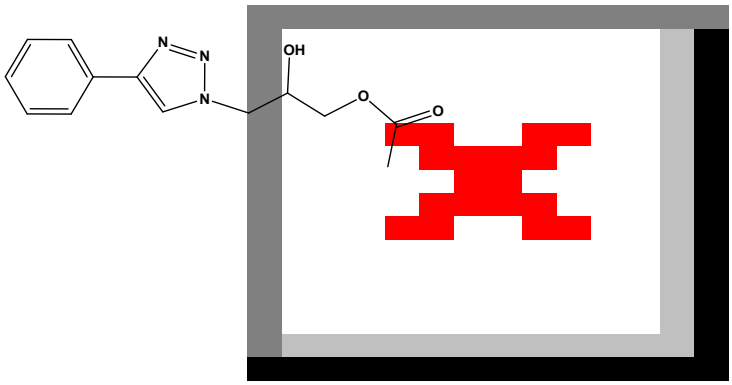


Fig. S25: ^{1}H-NMR spectrum of the **T4** in $CDCl_3$ solution.

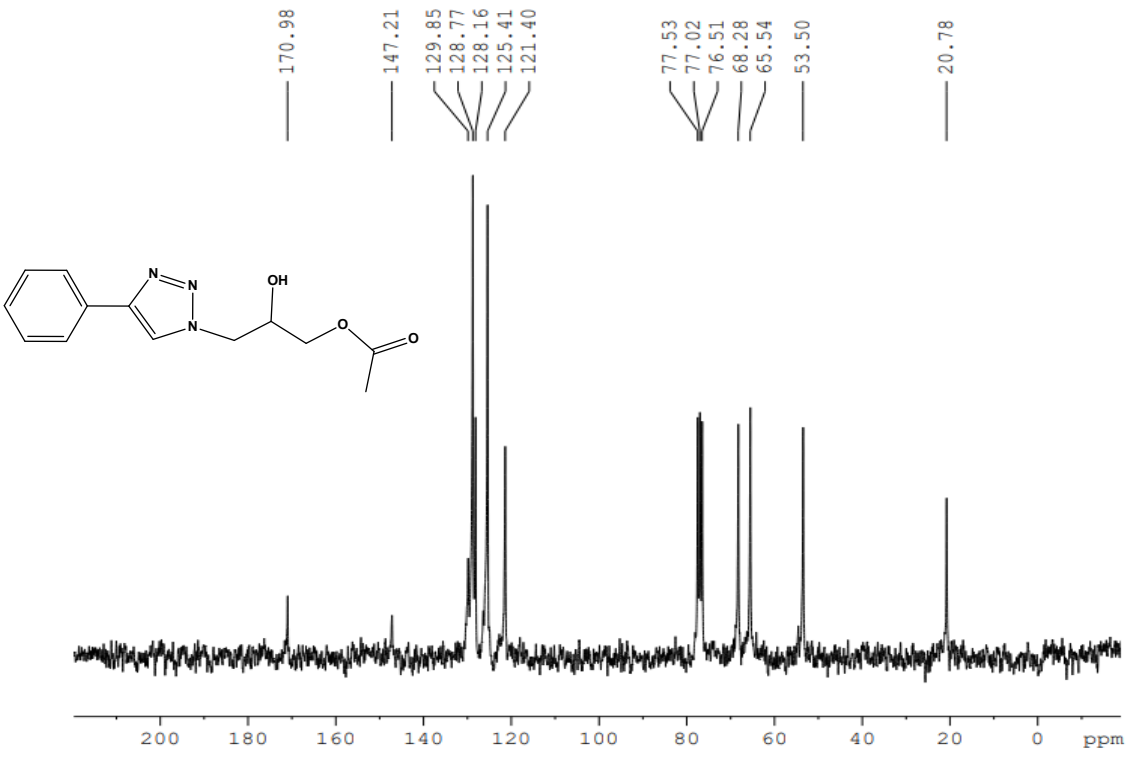
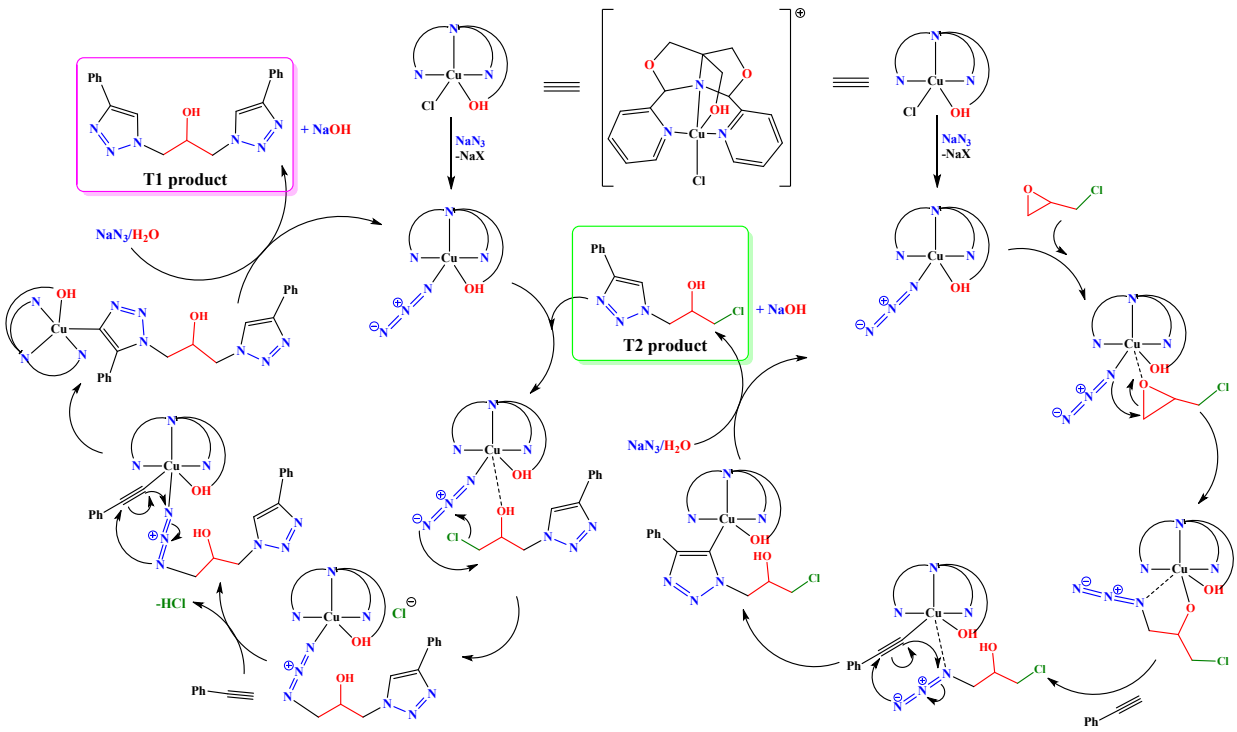


Fig. S26: ^{13}C-NMR spectrum of the **T4** in $CDCl_3$ solution.



Scheme S1: Proposed mechanism for the formation of **T1** and **T2** products in the presence of compound **3**

Table S1: Selected bond lengths (Å) and angles (°) for **T1**

Bond	Length/Å	Angles	deg/º	Angles	deg/º
C1–C2	1.3961 (19)	C2–C1–C6	118.66 (12)	N1–N2–N3	107.17 (11)
C1–C6	1.3968 (18)	C2–C1–C7	120.90 (12)	C8–N3–N2	110.92 (11)
C1–C7	1.4692 (18)	C6–C1–C7	120.40 (12)	C8–N3–C9	128.40 (12)
C2–C3	1.394 (2)	C3–C2–C1	120.38 (12)	N2–N3–C9	120.68 (11)
C3–C4	1.392 (2)	C4–C3–C2	120.56 (14)	N3–C8–C7	104.90 (12)
C4–C5	1.389 (2)	C5–C4–C3	119.34 (13)	N3–C9–C10	112.35 (11)
C5–C6	1.393 (2)	C4–C5–C6	120.20 (13)	O1–C10–O1i	85.6 (2)
C7–N1	1.3657 (17)	C5–C6–C1	120.85 (13)	O1–C10–C9i	114.48 (10)
C7–C8	1.3797 (18)	N1–C7–C8	107.97 (12)	O1–C10–C9	116.84 (10)
N1–N2	1.3181 (17)	N1–C7–C1	122.29 (12)		
N2–N3	1.3505 (17)	C8–C7–C1	129.70 (12)		
N3–C8	1.3474 (17)	N2–N1–C7	109.03 (11)		
N3–C9	1.4569 (17)	O1i–C10–C9	114.48 (10)		
C9–C10	1.5257 (17)	C9i–C10–C9	107.66 (15)		
C10–O1	1.351 (2)				

Symmetry code: (i) −x+1/2, −y+3/2, *z*.

Table S2: Hydrogen-bond geometry (Å, °) for **T1**

D–H···A	D–H	H···A	D···A	D–H···A
O1–H1···N1ii	0.84	2.54	3.264 (2)	146
O1–H1···N2ii	0.84	1.99	2.823 (2)	170

Symmetry code: (ii) x−1, y, z.

Table S3: Selected bond lengths (Å) and angles (°) for **T2**

Bond	Length/Å	Angle	deg/º	Angle	deg/º
C1–C2	1.397 (9)	C2–C1–C6	120.1 (5)	N10–C12–C13	110.3 (4)
C1–C6	1.398 (8)	C2–C1–H1A	119.9	N10–C12–H12A	109.6
C1–H1A	0.9500	C6–C1–H1A	119.9	C13–C12–H12A	109.6
C2–C3	1.373 (9)	C3–C2–C1	119.8 (6)	N10–C12–H12B	109.6
C2–H2A	0.9500	C3–C2–H2A	120.1	C13–C12–H12B	109.6
C3–C4	1.382 (9)	C1–C2–H2A	120.1	H12A–C12–H12B	108.1
C3–H3A	0.9500	C2–C3–C4	120.5 (6)	O14–C13–C15	113.9 (5)
C4–C5	1.378 (8)	C2–C3–H3A	119.8	O14–C13–C12	111.8 (5)
C4–H4A	0.9500	C4–C3–H3A	119.8	C15–C13–C12	109.7 (5)
C5–C6	1.399 (7)	C5–C4–C3	120.4 (6)	O14–C13–H13A	107.0
C5–H5A	0.9500	C5–C4–H4A	119.8	C15–C13–H13A	107.0
C6–C7	1.458 (8)	C3–C4–H4A	119.8	C12–C13–H13A	107.0
C7–N8	1.361 (6)	C4–C5–C6	120.2 (5)	C13–O14–H14A	109.5
C7–C11	1.368 (7)	C4–C5–H5A	119.9	C13–C15–Cl16	109.2 (4)
N8–N9	1.330 (7)	C6–C5–H5A	119.9	C13–C15–H15A	109.8
N9–N10	1.335 (6)	C1–C6–C5	119.0 (5)	Cl16–C15–H15A	109.8
N10–C11	1.343 (7)	C1–C6–C7	120.2 (5)	C13–C15–H15B	109.8
N10–C12	1.445 (7)	C5–C6–C7	120.8 (5)	Cl16–C15–H15B	109.8
C11–H11A	0.9500	N8–C7–C11	107.4 (5)	H15A–C15–H15B	108.3
C12–C13	1.535 (8)	N8–C7–C6	122.8 (5)		
C12–H12A	0.9900	C11–C7–C6	129.8 (5)		
C12–H12B	0.9900	N9–N8–C7	109.2 (4)		
C13–O14	1.395 (6)	N8–N9–N10	106.6 (4)		
C13–C15	1.493 (9)	N9–N10–C11	111.1 (4)		
C13–H13A	1.0000	N9–N10–C12	119.4 (5)		
O14–H14A	0.8400	C11–N10–C12	129.5 (4)		
C15–Cl16	1.820 (7)	N10–C11–C7	105.7 (4)		
C15–H15A	0.9900	N10–C11–H11A	127.2		
C15–H15B	0.9900	C7–C11–H11A	127.2		

Table S4: Hydrogen-bond geometry (Å, °) for **T2**

D–H···A	D–H	H···A	D···A	D–H···A
C11–H11A···N9^{i}	0.95	2.48	3.241 (7)	137
C11–H11A···O14^{ii}	0.95	2.55	3.107 (6)	117
O14–H14A···Cl16	0.84	2.67	3.096 (4)	113

Symmetry codes: (i) −x+1/2, y−1/2, z; (ii) −x+1/2, −y+1/2, z+1/2.

Table S5: Selected bond lengths (Å) and angles (°) for **T4**

Bond	Length/Å	Angle	deg/º	Angle	deg/º
C1–C2	1.378 (6)	C2–C1–C6	120.7 (4)	N10–C12–C13	112.8 (3)
C1–C6	1.398 (5)	C2–C1–H1A	119.6	N10–C12–H12A	109.0
C1–H1A	0.9500	C6–C1–H1A	119.6	C13–C12–H12A	109.0
C2–C3	1.389 (8)	C1–C2–C3	120.3 (4)	N10–C12–H12B	109.0
C2–H2A	0.9500	C1–C2–H2A	119.9	C13–C12–H12B	109.0
C3–C4	1.381 (7)	C3–C2–H2A	119.9	H12A–C12–H12B	107.8
C3–H3A	0.9500	C4–C3–C2	119.4 (4)	O14–C13–C15	111.4 (3)
C4–C5	1.390 (6)	C4–C3–H3A	120.3	O14–C13–C12	106.6 (3)
C4–H4A	0.9500	C2–C3–H3A	120.3	C15–C13–C12	111.7 (3)
C5–C6	1.396 (5)	C3–C4–C5	121.0 (4)	O14–C13–H13A	109.0
C5–H5A	0.9500	C3–C4–H4A	119.5	C15–C13–H13A	109.0
C6–C7	1.463 (5)	C5–C4–H4A	119.5	C12–C13–H13A	109.0
C7–N8	1.372 (4)	C4–C5–C6	119.7 (4)	C13–O14–H14A	109.5
C7–C11	1.379 (5)	C4–C5–H5A	120.2	O16–C15–C13	105.8 (3)
N8–N9	1.311 (5)	C6–C5–H5A	120.2	O16–C15–H15A	110.6
N9–N10	1.354 (4)	C5–C6–C1	118.9 (4)	C13–C15–H15A	110.6
N10–C11	1.348 (5)	C5–C6–C7	120.5 (3)	O16–C15–H15B	110.6
N10–C12	1.457 (4)	C1–C6–C7	120.5 (3)	C13–C15–H15B	110.6
C11–H11A	0.9500	N8–C7–C11	107.8 (3)	H15A–C15–H15B	108.7
C12–C13	1.524 (5)	N8–C7–C6	121.9 (3)	C17–O16–C15	116.8 (3)
C12–H12A	0.9900	C11–C7–C6	130.3 (3)	O18–C17–O16	122.3 (4)
C12–H12B	0.9900	N9–N8–C7	109.1 (3)	O18–C17–C19	125.2 (4)
C13–O14	1.420 (5)	N8–N9–N10	107.3 (3)	O16–C17–C19	112.5 (3)
C13–C15	1.512 (4)	C11–N10–N9	110.8 (3)		
C13–H13A	1.0000	C11–N10–C12	128.8 (3)		
O14–H14A	0.8400	N9–N10–C12	120.3 (3)		
C15–O16	1.452 (4)	N10–C11–C7	105.0 (3)		
C15–H15A	0.9900	N10–C11–H11A	127.5		
C15–H15B	0.9900	C7–C11–H11A	127.5		
O16–C17	1.329 (4)	C17–C19–H19A	109.5		
C17–O18	1.200 (5)	C17–C19–H19B	109.5		
C17–C19	1.494 (5)	H19A–C19–H19B	109.5		
C19–H19A	0.9800	C17–C19–H19C	109.5		
C19–H19B	0.9800	H19A–C19–H19C	109.5		
C19–H19C	0.9800	H19B–C19–H19C	109.5		

Table S6: Hydrogen-bond geometry (Å, °) for **T4**

D–H···A	D–H	H···A	D···A	D–H···A
C11–H11A···O18i	0.95	2.42	3.174 (4)	136
C12–H12B···O18i	0.99	2.59	3.410 (5)	140
O14–H14A···N9ii	0.84	2.04	2.826 (4)	156
C15–H15B···N9	0.99	2.67	3.239 (4)	117

Symmetry codes: (i) x−1/2, −y+1, z+1/2; (ii) x+1/2, −y+1, z+1/2.