Supplementary data

Diethylenetriamine-Driven Assembly of a Dimeric Cadmium Bromide Hybrid and an Organic Bromide Salt: Structural, Vibrational, Optical, in Silico study and Biological Insights

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Table S.1: Crystallographic data and structure refinement for $(C_4H_{16}N_3)[CdBr_5]\cdot H_2O$ and $(C_4H_{16}N_3)Br_3$.

Empirical formula	$(C_4H_{16}N_3)[CdBr_5]\cdot H_2O$	$(C_4H_{16}N_3)Br_3$
Formula weight (g/mol)	636.16	345.93
Crystal system	Monoclinic	Monoclinic
Space groupe	$P2_1/c$	$P2_1/c$
a (Å)	10.3311(3)	6.2138(5)
b (Å)	10.4970(2)	19.5497(16)
c (Å)	14.6429(3)	8.9715(9)
β (°)	110.462(3)	93.211(8)
V (Å^3)	1487.76(7)	1088.13(17)
Z	4	4
Crystal size (mm^3)	0.32 × 0.23 × 0.12	0.47 × 0.38 × 0.22
Color	colorless	colorless
Shape	block-shaped	block-shaped
T (K)	100.0(2)	150.00(10)
Calculated density	2.840	2.112
λ (MoKα) (Å)	0.71073 Å	0.71073 Å
Absorption correction	multi-scan	multi-scan
Measured reflexions	17601	13441
Independant reflexions	3886	2221
Reflexions [I >2σ (I)]	3444	1977
Domain of θ (°)	$2.4 \leq \theta \leq 31.2$	$3.1 \leq \theta \leq 26.4$
T_{min} et T_{max}	0.087, 1.000	0.009, 0.085
Index range	$-14 \leq h \leq 14$	$-7 \leq h \leq 7$
	$-15 \leq k \leq 15$	$-24 \leq k \leq 24$
	$-16 \leq l \leq 20$	$-11 \leq l \leq 11$
Number of Parameters	132	94
R_1	0.041	0.036
wR_2	0.105	0.088
Goof	1.061	1.026

Table S.2: Geometric parameters (Å, °) of DETCdBr and DETBr.

DETCdBr			
Cd1—Br1	2.7422 (6)	Br1—Cd1—Br2	93.389 (17)
Cd1—Br2	2.7559 (5)	Br1—Cd1—Br2^{i}	171.367 (19)
Cd1—Br2^{i}	2.8462 (6)	Br1—Cd1—Br3	85.307 (16)
Cd1—Br3	2.8438 (5)	Br1—Cd1—Br4	92.753 (17)
Cd1—Br4	2.7590 (5)	Br1—Cd1—Br5	93.528 (17)
Cd1—Br5	2.7579 (5)	Br2—Cd1—Br2^{i}	83.462 (16)
O1—H1F	0.86	Br2—Cd1—Br3	91.367 (16)
O1—H1G	0.87	Br2—Cd1—Br4	173.543 (19)
N3—C4	1.482 (6)	Br2—Cd1—Br5	92.142 (16)
N1—C1	1.482 (6)	Br3—Cd1—Br2^{i}	86.730 (16)
N2—C2	1.503 (6)	Br4—Cd1—Br2^{i}	90.732 (17)
N2—C3	1.488 (6)	Br4—Cd1—Br3	91.118 (16)
C1—C2	1.524 (7)	Br5—Cd1—Br2^{i}	94.619 (17)
C3—C4	1.517 (7)	Br5—Cd1—Br3	176.362 (18)
		Br5—Cd1—Br4	85.491 (16)
		Cd1—Br2—Cd1^{i}	96.538 (16)
		H1F—O1—H1G	109.5
		C3—N2—C2	112.4 (4)
		N2—C2—C1	113.3 (4)
		N2—C3—C4	108.4 (4)
		N3—C4—C3	110.6 (4)
DETBr			
N1—C1	1.483 (6)	C3—N2—C2	114.2 (3)
N2—C2	1.501 (5)	N2—C2—C1	111.8 (3)
N2—C3	1.488 (5)	N2—C3—C4	109.1 (3)
C1—C2	1.503 (6)	N3—C4—C3	110.1 (4)
C3—C4	1.515 (6)	N1—C1—C2	113.8 (3)

Table S.3: Hydrogen bonding geometry (Å, ◦) of DETCdBr.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1F···Br2	0.87	2.82	3.432 (4)	129
O1—H1F···Br3	0.87	2.72	3.385 (4)	135
O1—H1G···Br4^{ii}	0.87	2.47	3.330 (4)	171
N3—H00C···Br1^{iii}	0.91	2.39	3.287 (4)	167
N3—H00A···Br2^{iv}	0.91	2.65	3.441 (4)	146
N3—H00B···Br4^{v}	0.91	2.60	3.282 (4)	132
N1—H1A···Br3^{i}	0.91	2.56	3.325 (5)	143
N1—H1C···Br4^{vi}	0.91	2.44	3.343 (4)	170
N1—H1B···O1^{vii}	0.91	1.82	2.721 (6)	168
N2—H2A···Br3^{v}	0.91	2.46	3.299 (4)	154
N2—H2B···Br5	0.91	2.39	3.226 (4)	152
C4—H4B···O1i	0.99	2.48	3.303 (6)	141

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*, −*y*+1/2, *z*+1/2; (iii) −*x*, *y*+1/2, −*z*+1/2; (iv) *x*, −*y*+3/2, *z*−1/2; (v) *x*, *y*+1, *z*; (vi) *x*, −*y*+3/2, *z*+1/2; (vii) −*x*+1, *y*+1/2, −*z*+3/2.

Table S.4: Hydrogen bonding geometry (Å, ◦) of DETBr.

D—H···*A*	*D*—H	*H*···*A*	*D*···*A*	*D*—H···*A*
N1—H1C···Br1	0.91	2.47	3.203 (3)	138
N1—H1A···Br1^{i}	0.91	2.36	3.250 (3)	168
N1—H1B···Br3^{ii}	0.91	2.42	3.310 (4)	167
N2—H2A···Br1^{i}	0.91	2.65	3.286 (4)	127
N2—H2A···Br2	0.91	2.66	3.305 (3)	129
N2—H2B···Br3	0.91	2.39	3.257 (3)	159
N3—H3B···Br2^{iii}	0.91	2.58	3.453 (4)	162
N3—H3A···Br2^{iv}	0.91	2.50	3.372 (4)	161

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

Table S.5: Global Reactivity Descriptors of DETBr and DETCdBr Calculated from HOMO–LUMO Energies.

Parameter	**DETBr**	**DETCdBr**
HOMO (eV)	−22.03	−17.018
LUMO (eV)	−13.65	−13.714
Energy Gap, Eg (eV, FMO)	8.378	3.304
Optical Band Gap (eV)	~6.08	~2.85
Dipole Moment (D)	13.54	60.89
SCF Energy (eV)	−2190.9	−3233.53
Chemical Potential, μ (eV)	−17.84	−15.37
Electronegativity, χ (eV)	17.84	15.37
Chemical Hardness, η (eV)	4.19	1.65
Softness, S (eV^{-1})	0.239	0.605
Electrophilicity Index, ω (eV)	38.0	71.5

Table S.6: Predicted Physicochemical and ADME Properties of DETBr and DETCdBr.

Parameter	Property	DETBr	DETCdBr
Physicochemical	Molecular Weight (g/mol)	345.93	636.16
	TPSA	71.89	162.24
Lipophilicity	Consensus Log P	-4.75	-10.58
Water Solubility	Ali Log S (Class)	-1.92 (Very soluble)	-5.70 (Moderately soluble)
Pharmacokinetics	GI Absorption	Low	Low
	BBB Permeant	No	No
	P-gp Substrate	Yes	Yes

Drug-likeness	Lipinski Violations	0	2 (MW > 500, TPSA > 140)
	Veber Violations	0	1 (TPSA > 140)
	Bioavailability Score	0.55	0.11
Synthesis	Synthetic Accessibility	1.42	4.17

Table S.7: Molecular Docking Interactions of Acarbose, DETBr, and DETCdBr with α-Amylase (PDB ID: 4W93).

Ligand	Ligand Sites	Receptor Sites	Type of Interaction	Distance (Å)	Binding Energy (kcal/mol)	Total Binding Energy (kcal/mol)
Acarbose	O16	THR A163	H-donor	2.81	-2.6	**-8.32**
	O54	ASP A300 (OD1)	H-donor	2.95	-0.9	
	O61	ASP A300 (OD2)	H-donor	3.03	-1.0	
	O21	GLN A63 (NE2)	H-acceptor	3.00	-2.1	
	C9	TRP A59 (6-ring)	H–π	4.25	-0.6	
	O38	TRP A59 (5-ring)	H–π	3.62	-2.4	
DETBr	N4	ASP A300 (OD2)	H-donor	2.83	-9.5	**-4.84**
	N9	ASP A197 (OD1)	H-donor	3.13	-2.6	
	N9	ASP A197 (OD2)	H-donor	3.08	-14.0	
	C18	ASP A197 (OD1)	H-donor	3.37	-2.1	
	N4	ASP A300 (OD2)	Ionic	2.83	-5.8	
	N9	ASP A197	Ionic	3.13	-3.7	

		(OD1)				
	N9	ASP A197 (OD2)	Ionic	3.08	-4.0	
DETCdBr	N11	ASP A356 (OD2)	H-donor	2.94	-12.2	**-5.43**
	C20	ASP A356 (OD2)	H-donor	3.45	-0.7	
	Br3	ASN A298 (ND2)	H-acceptor	3.77	-0.6	
	Br5	ALA A307 (N)	H-acceptor	3.59	-1.0	
	Br6	HIS A305 (NE2)	H-acceptor	4.47	-1.0	
	Br6	ASP A300 (OD1)	Ionic	3.23	-3.1	
	Br6	ASP A300 (OD2)	Ionic	3.66	-1.4	
	N11	ASP A356 (OD2)	Ionic	2.94	-4.9	