Molecular Self Assembly: Solvent Guests Tune the Conformation of a Series of 2,6-Bis(2-anilinoethynyl)pyridine-Based Ureas

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Table S1. Crystallographic Data and Data Collections and Refinements Parameters for the investigated structures:

	L^1•2DMSO	**L^1•2DMSO•CH_3OH**	**L^1•3DMF**
Empirical formula	$C_{47}\ H_{51}\ N_7\ O_8\ S_2$	$C_{48}\ H_{55}\ N_7\ O_9\ S_2$	$C_{52}\ H_{60}\ N_{10}\ O_9$
Formula weight	906.07	938.11	969.10
Temperature	173(2) K	173(2) K	173(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Triclinic	Triclinic
Space group	$P2_1/c$	P-1	P-1
Unit cell dimensions	a = 14.7007(13) Å	a = 13.037(8) Å	a = 9.6860(14) Å
	b = 25.956(2) Å	b = 14.106(9) Å	b = 12.7435(18) Å
	c = 12.3794(11) Å	c = 14.707(9) Å	c = 20.683(3) Å
	α= 90°	α= 112.755(10)	α= 93.436(3)°
	β= 103.568(1)°	β= 103.142(10)°	β= 98.492(3)°
	γ = 90°.	γ = 92.983(11)°	γ = 95.516(3)°
Volume	4591.8(7) $Å^3$	2399(3) $Å^3$	2506.1(6) $Å^3$
Z	4	2	2
Density (calculated)	1.311 Mg/m^3	1.299 Mg/m^3	1.284 Mg/m^3
Absorption coefficient	0.177 mm^{-1}	0.173 mm^{-1}	0.090 mm^{-1}
F(000)	1912	992	1028
Crystal size	0.33 x 0.23 x 0.12 mm^3	0.38 x 0.22 x 0.05 mm^3	0.19 x 0.04 x 0.02 mm^3
Theta range for data collection	1.57 to 25.00°	1.58 to 24.00°.	1.00 to 25.00°.
Index ranges	-17<=h<=17, -30<=k<=30, -14<=l<=14	-14<=h<=14, -16<=k<=16, -16<=l<=16	-11<=h<=11, -15<=k<=15, -24<=l<=24

Reflections collected	44074	20819	24347
Independent reflections	8098 [R(int) = 0.0233]	7533 [R(int) = 0.0580]	8816 [R(int) = 0.0638]
Completeness to theta = 25.00°	100.0 %	99.9 %	99.8 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.9791 and 0.9439	0.9914 and 0.9370	0.9982 and 0.9832
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	8098 / 0 / 593	7533 / 6 / 666	8816 / 6 / 654
Goodness-of-fit on F^2	1.014	1.032	1.005
Final R indices [I>2sigma(I)]	R1 = 0.0473, wR2 = 0.1226	R1 = 0.0867, wR2 = 0.2233	R1 = 0.0698, wR2 = 0.1632
R indices (all data)	R1 = 0.0538, wR2 = 0.1290	R1 = 0.1382, wR2 = 0.2502	R1 = 0.1309, wR2 = 0.2028
Largest diff. peak and hole	0.748 and -0.613 e.Å^{-3}	0.609 and -0.759 e.Å^{-3}	0.499 and -0.270 e.Å^{-3}

	$L^2 \cdot H_2O \cdot 0.5DMSO$	$L^3 \cdot H_2O \cdot DMSO$ (I)	$L^3 \cdot H_2O \cdot DMSO$ (II)
Empirical formula	$C_{38}\ H_{26}\ F_6\ N_7\ O_{7.50}\ S_{0.50}$	$C_{41}\ H_{35}\ F_6\ N_5 O_6\ S$	$C_{41}\ H_{35}\ F_6\ N_5 O_6\ S$
Formula weight	830.69	839.80	839.80
Temperature	173(2) K	173(2) K	173(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Triclinic	Triclinic
Space group	*P*2/*n*	*P*-1	*P*-1
Unit cell dimensions	*a* = 14.8341(13) Å	*a* = 8.7292(10) Å	*a* = 9.533(2) Å
	b = 9.5759(9) Å	*b* = 13.3810(15) Å	*b* = 14.185(3) Å
	c = 29.903(3) Å	*c* = 17.3731(19) Å	*c* = 16.112(4) Å
	α = 90°	α= 84.395(2)°	α= 73.871(4)°
	β= 90.690(2)°	β= 78.492(2)°	β= 78.002(4)°
	γ = 90°	γ = 80.087(2)°	γ = 71.375(4)°
Volume	4247.3(7) $Å^3$	1954.6(4) $Å^3$	1966.3(7) $Å^3$
Z	4	2	2
Density (calculated)	1.299 Mg/m^3	1.427 Mg/m^3	1.418 Mg/m^3
Absorption coefficient	0.133 mm^{-1}	0.167 mm^{-1}	0.166 mm^{-1}
F(000)	1700	868	868
Crystal size	0.43 x 0.12 x 0.03 mm^3	0.33 x 0.12 x 0.03 mm^3	0.45 x 0.06 x 0.04 mm^3
Theta range for data collection	1.36 to 25.00°.	1.20 to 25.00°.	1.56 to 25.00°
Index ranges	-17<=h<=17, -11<=k<=11, -35<=l<=35	10<=h<=10, -15<=k<=15, -20<=l<=20	-11<=h<=11, -16<=k<=16, -19<=l<=19
Reflections collected	39732	19048	18895
Independent reflections	7464 [R(int) = 0.0439]	6884 [R(int) = 0.0204]	6893 [R(int) = 0.0428]

Completeness to theta = 25.00°	99.7 %	99.8 %	99.7 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.9935 and 0.9128	0.9950 and 0.9471	0.9934 and 0.9292
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	7464 / 0 / 561	6884 / 0 / 648	6893 / 0 / 556
Goodness-of-fit on F^2	1.049	1.002	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0722, wR2 = 0.1943	R1 = 0.0569, wR2 = 0.1643	R1 = 0.0671, wR2 = 0.1623
R indices (all data)	R1 = 0.0963, wR2 = 0.2080	R1 = 0.0711, wR2 = 0.1820	R1 = 0.1144, wR2 = 0.1919
Largest diff. peak and hole	0.574 and -0.342 e.Å^{-3}	0.882 and -0.518 e.Å^{-3}	0.818 and -0.361 e.Å^{-3}

Table S2. Hydrogen bonding interactions in **L^1•2DMSO** [Å and °].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(5)-H(5N)···O(8)	0.81(3)	2.20(3)	2.935(3)	151(2)
N(6)-H(6N)···O(8)	0.85(3)	1.99(3)	2.790(3)	156(2)
N(3)-H(3N)···O(7)	0.83(3)	1.93(3)	2.757(2)	169(2)
N(2)-H(2N)···O(7)	0.80(3)	2.42(3)	3.122(2)	148(2)

Table S3. Hydrogen bonding interactions in **L^1•2DMSO•CH_3OH** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2N)...O(1S)	1.01(6)	2.41(6)	3.202(5)	135(4)
N(6)-H(6N)...O(2S)	1.06(5)	1.71(5)	2.767(6)	172(4)
O(1S)-H(1S)...N(1)	1.07(7)	1.69(7)	2.731(5)	163(6)
N(5)-H(5N)...O(2S)	1.15(6)	2.25(6)	3.229(6)	141(4)
N(3)-H(3N)...O(1S)	0.95(5)	1.84(5)	2.786(5)	174(4)

Table S4. Hydrogen bonding interactions of **L^1•3DMF** [Å and °].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(2)-H(2N)···O(1S)#1	0.86(4)	2.35(4)	3.137(4)	151(3)
N(3)-H(3N)···O(1S)#1	0.88(4)	2.02(4)	2.851(4)	159(4)
N(5)-H(5N)···O(2S)	0.84(3)	2.36(4)	3.052(4)	140(3)
N(6)-H(6N)···O(2S)	0.91(4)	1.93(4)	2.825(4)	168(3)

Symmetry transformations used to generate equivalent atoms: #1 x+1, y, z

Table S5. Hydrogen bonding interactions in **L^2•H_2O•0.5DMSO** [Å and °].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)

N(2)-H(2N)···O(1S)	0.91(4)	2.49(4)	3.229(4)	138(3)
N(3)-H(3N)···O(1S)	0.89(4)	1.92(4)	2.795(4)	167(3)
O(1S)-H(1S)···N(1)	0.75(5)	2.12(5)	2.867(4)	174(5)
O(1S)-H(2S)···O(4)#2	0.90(10)	1.92(10)	2.821(4)	177(9)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,y,-z+1/2 #2 -x+1,-y+1,-z

Table S6. Hydrogen bonding interactions of **L^3•H_2O•DMSO** (**I**) [Å and °]

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(5)-H(5N)···S(1S)#1	0.86(4)	2.92(4)	3.660(3)	145(3)
N(5)-H(5N)···O(1S)#1	0.86(4)	1.95(4)	2.783(3)	163(3)
O(5)-H(5B)···O(3)#1	0.71(5)	2.10(5)	2.804(3)	169(5)
O(5)-H(5A)···N(1)	0.77(4)	2.09(4)	2.809(3)	157(3)
N(3)-H(3N)···O(5)	0.89(3)	1.93(3)	2.799(3)	165(3)
N(4)-H(4N)···O(1S)#1	0.81(3)	2.33(3)	3.030(3)	147(2)
N(2)-H(2N)···O(5)	0.84(3)	2.28(3)	3.030(3)	148(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+1

Table S7. Hydrogen bonding interactions in **L^3•H_2O•DMSO (II)** [Å, °]

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(2)-H(2N)···O(5)	0.76(3)	2.35(4)	3.039(5)	150(3)
N(3)-H(3N)···O(5)	0.81(3)	2.04(4)	2.828(5)	165(3)

N(4)-H(4N)···O(1S)#1	0.74(4)	2.32(4)	2.950(4)	145(4)
N(5)-H(5N)···O(1S)#1	0.80(4)	2.02(4)	2.795(5)	163(4)
O(5)-H(5A)···N(1)	0.84(5)	2.04(5)	2.871(5)	172(5)
O(5)-H(5B)···O(3)#2	0.73(5)	2.07(6)	2.774(5)	163(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x+1,-y,-z+1

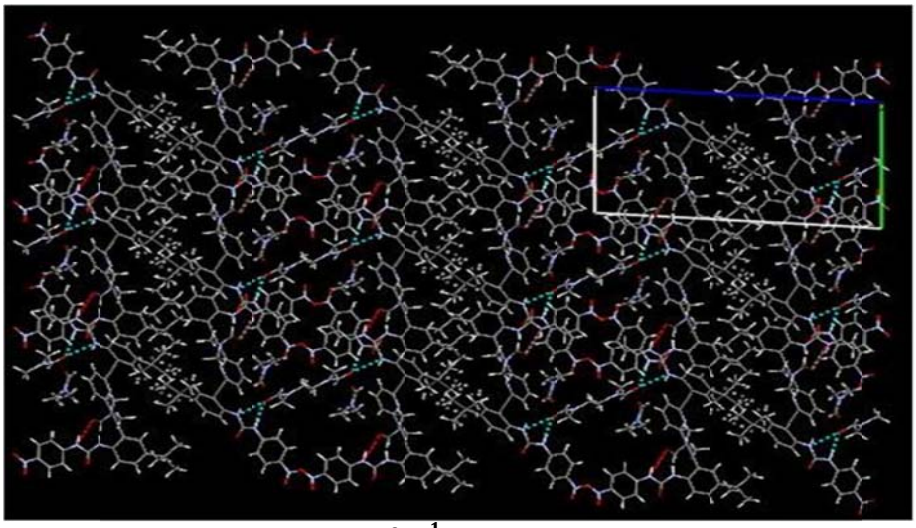

Figure S1. General packing diagram of **L^1•3DMF** viewed down the crystallographic *a*-axis showing the various hydrogen-bonding interactions.

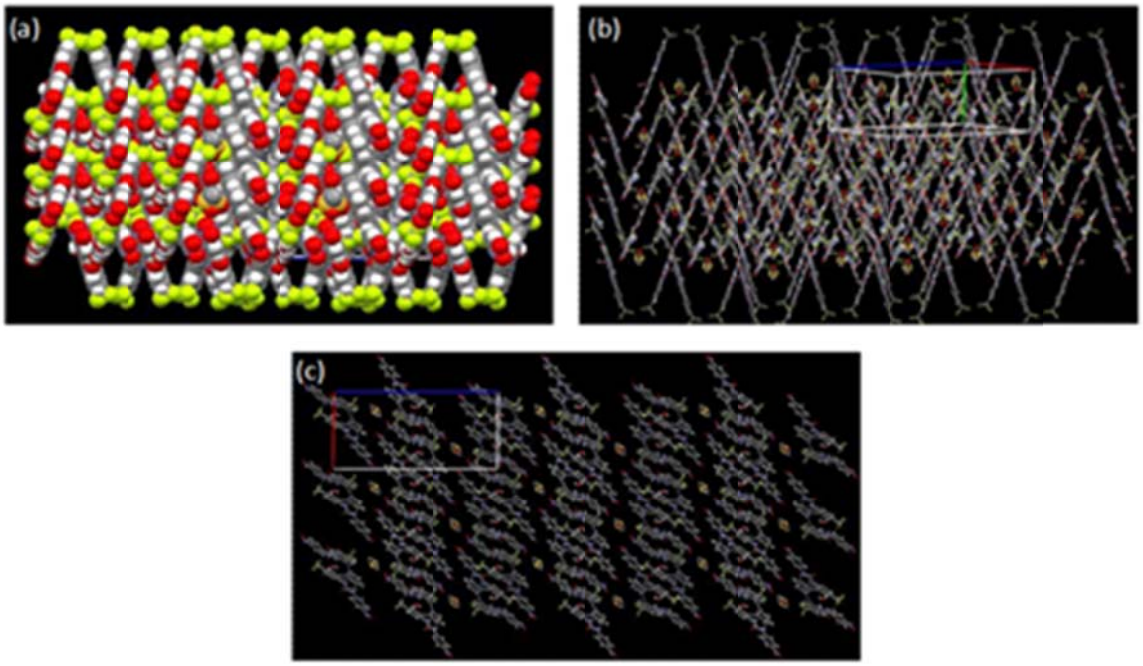

Figure S2. (a) Packing model of **L^2•H_2O•0.5DMSO** along the pseudo *c*-axis as a space-filling model (solvent water and DMSO molecules are omitted for clarity). (b) Packing model of **L^2•H_2O•0.5DMSO** and solvents along the pseudo *c*-axis and (c) *b*-axis.