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Supporting Information

A New Class of Selective Low-Molecular-Weight Gelators Based on Salts of Diaminotriazinecarboxylic Acids

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CRYSTAL AND MOLECULAR STRUCTURE OF

C22 H28 N5 Na O4 S2 COMPOUND (JIW903)

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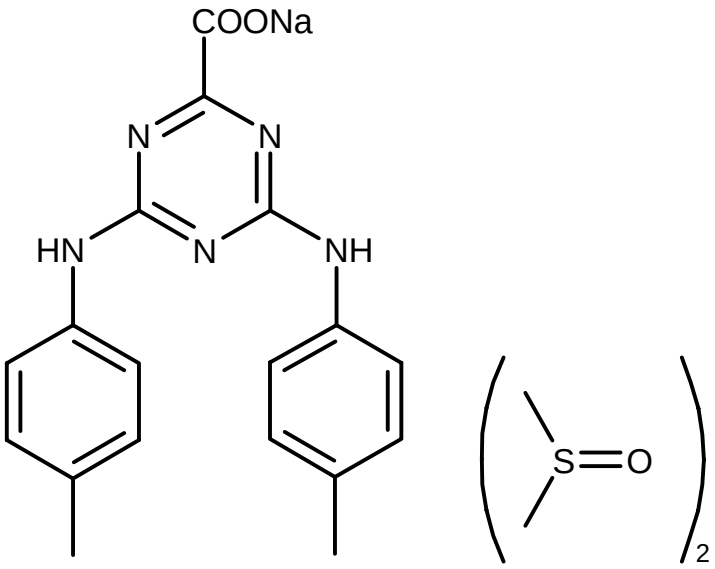


Structure solved and refined in the Laboratory of X-Ray Diffraction, Université de Montréal by Dr. Thierry Maris

Table 1. Crystal data and structure refinement for C22 H28 N5 Na O4 S2.

Identification code	JIW903
Empirical formula	C22 H28 N5 Na O4 S2
Formula weight	513.60
Temperature	100(2)K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	P21/c
Unit cell dimensions	a = 15.8524(3) Å α = 90° b = 10.4636(2) Å β = 105.0208(9)° c = 15.8729(3) Å γ = 90°
Volume	2542.93(8)Å^3
Z	4
Density (calculated)	1.342 g/cm^3
Absorption coefficient	2.384 mm^{-1}
F(000)	1080
Crystal size	0.22 x 0.07 x 0.07 mm
Theta range for data collection	2.89 to 68.05°
Index ranges	$-19 \leq h \leq 18$, $-12 \leq k \leq 11$, $-18 \leq \ell \leq 18$
Reflections collected	31713
Independent reflections	4580 [R_{int} = 0.037]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.6600 and 0.5600
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4580 / 0 / 314
Goodness-of-fit on F^2	1.003
Final R indices [I>2sigma(I)]	R_1 = 0.0401, wR_2 = 0.0996
R indices (all data)	R_1 = 0.0636, wR_2 = 0.1089
Extinction coefficient	0.00029(10)
Largest diff. peak and hole	0.288 and -0.378 e/Å^3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for C22 H28 N5 Na O4 S2.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U_{eq}
C(1)	5433(1)	9753(2)	2217(1)	19(1)
C(2)	4435(1)	9599(2)	2026(1)	18(1)
C(3)	3264(1)	8446(2)	2144(1)	19(1)
C(4)	3069(1)	10358(2)	1473(1)	19(1)
C(5)	2094(1)	6960(2)	2278(1)	20(1)
C(6)	1884(1)	5692(2)	2063(2)	23(1)
C(7)	1028(2)	5278(3)	1940(2)	27(1)
C(8)	368(2)	6110(3)	2009(2)	27(1)
C(9)	594(2)	7362(3)	2246(2)	28(1)
N(6)	2577(1)	11323(2)	1037(1)	22(1)
C(10)	1450(1)	7791(3)	2392(2)	25(1)
C(11)	-571(2)	5677(3)	1826(2)	36(1)
C(12)	1668(1)	11549(2)	836(1)	22(1)
C(13)	1059(2)	10720(3)	1014(2)	29(1)
C(14)	179(2)	11066(3)	800(2)	33(1)
C(15)	-112(2)	12219(3)	400(2)	28(1)
C(16)	506(2)	13023(3)	213(2)	31(1)
C(17)	1381(2)	12711(3)	428(2)	28(1)
N(5)	2973(1)	7346(2)	2400(1)	20(1)
C(18)	-1068(2)	12563(3)	165(2)	38(1)
C(20)	3484(2)	8858(3)	5562(2)	32(1)
C(21)	3427(2)	6573(3)	4748(2)	33(1)
C(30)	6043(2)	8601(3)	6299(2)	34(1)
C(31)	7219(2)	6763(3)	6333(2)	39(1)
N(1)	4150(1)	8532(2)	2314(1)	19(1)
N(2)	3946(1)	10552(2)	1600(1)	18(1)
N(3)	2700(1)	9340(2)	1732(1)	20(1)
Na(1)	5250(1)	7549(1)	3553(1)	21(1)
O(1)	5891(1)	8947(2)	2702(1)	23(1)
O(2)	5688(1)	10701(2)	1858(1)	22(1)
O(20)	4451(1)	8398(2)	4474(1)	27(1)
O(30)	6464(1)	7938(2)	4857(1)	25(1)
S(20)	3528(1)	8230(1)	4527(1)	25(1)
S(30)	6221(1)	7325(1)	5628(1)	25(1)

Table 3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for C22 H28 N5 Na O4 S2.

	x	y	z	U_{eq}
H(6)	2314	5122	2001	28
H(7)	895	4423	1809	33
H(9)	163	7930	2308	33
H(6A)	2868	11901	849	27
H(10)	1590	8630	2564	30
H(11A)	-628	4845	1563	53
H(11B)	-938	6271	1436	53
H(11C)	-743	5641	2362	53
H(13)	1235	9935	1275	35
H(14)	-224	10505	930	39
H(16)	327	13796	-65	37
H(17)	1783	13278	301	33
H(5)	3365	6815	2669	24
H(18A)	-1147	13399	-93	57
H(18B)	-1276	12559	682	57
H(18C)	-1391	11950	-244	57
H(20A)	3930	8464	6014	48
H(20B)	2922	8682	5657	48
H(20C)	3578	9765	5570	48
H(21A)	3475	6078	4254	50
H(21B)	2869	6420	4861	50
H(21C)	3883	6331	5250	50
H(30A)	6567	9099	6484	51
H(30B)	5888	8261	6800	51
H(30C)	5578	9132	5974	51
H(31A)	7449	6085	6050	58
H(31B)	7112	6449	6864	58
H(31C)	7633	7451	6463	58

Table 4. Anisotropic parameters ($Å^2$ x 10^3) for C22 H28 N5 Na O4 S2.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
C(1)	17(1)	22(2)	17(1)	-4(1)	4(1)	-2(1)
C(2)	20(1)	21(2)	13(1)	-3(1)	3(1)	-1(1)
C(3)	16(1)	24(2)	15(1)	-1(1)	3(1)	-1(1)
C(4)	20(1)	24(2)	14(1)	0(1)	2(1)	0(1)
C(5)	18(1)	25(2)	15(1)	3(1)	3(1)	-2(1)
C(6)	23(1)	22(2)	23(1)	3(1)	4(1)	1(1)
C(7)	29(1)	25(2)	27(1)	2(1)	5(1)	-7(1)
C(8)	21(1)	36(2)	22(1)	7(1)	1(1)	-5(1)
C(9)	20(1)	32(2)	32(1)	4(1)	8(1)	1(1)
N(6)	18(1)	21(1)	27(1)	6(1)	5(1)	2(1)
C(10)	22(1)	25(2)	28(1)	2(1)	7(1)	-2(1)
C(11)	24(1)	45(2)	36(2)	6(1)	5(1)	-11(1)
C(12)	18(1)	29(2)	18(1)	1(1)	1(1)	4(1)
C(13)	22(1)	34(2)	31(1)	9(1)	3(1)	3(1)
C(14)	21(1)	45(2)	31(1)	7(1)	5(1)	1(1)
C(15)	21(1)	40(2)	21(1)	1(1)	2(1)	8(1)
C(16)	27(1)	36(2)	28(1)	5(1)	3(1)	11(1)
C(17)	25(1)	29(2)	29(1)	8(1)	6(1)	5(1)
N(5)	15(1)	22(1)	22(1)	4(1)	3(1)	0(1)
C(18)	26(1)	55(2)	31(1)	1(1)	3(1)	9(1)
C(20)	37(2)	32(2)	29(1)	-2(1)	13(1)	2(1)
C(21)	40(2)	32(2)	34(2)	-1(1)	19(1)	-3(1)
C(30)	46(2)	35(2)	21(1)	0(1)	9(1)	-1(1)
C(31)	33(1)	46(2)	35(2)	13(1)	4(1)	4(1)
N(1)	16(1)	21(1)	18(1)	1(1)	3(1)	-2(1)
N(2)	16(1)	20(1)	18(1)	-2(1)	3(1)	0(1)
N(3)	16(1)	21(1)	21(1)	2(1)	3(1)	1(1)
Na(1)	19(1)	24(1)	18(1)	0(1)	3(1)	1(1)
O(1)	17(1)	25(1)	26(1)	4(1)	3(1)	1(1)
O(2)	17(1)	24(1)	25(1)	1(1)	5(1)	-2(1)
O(20)	29(1)	29(1)	26(1)	-1(1)	12(1)	0(1)
O(30)	28(1)	30(1)	18(1)	-1(1)	7(1)	1(1)
S(20)	27(1)	29(1)	21(1)	1(1)	8(1)	3(1)
S(30)	25(1)	26(1)	21(1)	1(1)	4(1)	0(1)

Table 5. Bond lengths [Å] and angles [°] for C22 H28 N5 Na O4 S2

C(1)-O(1)	1.242(3)	C(10)-C(5)-N(5)	122.4(2)
C(1)-O(2)	1.262(3)	C(6)-C(5)-N(5)	118.1(2)
C(1)-C(2)	1.541(3)	C(7)-C(6)-C(5)	119.8(2)
C(2)-N(1)	1.329(3)	C(6)-C(7)-C(8)	121.5(3)
C(2)-N(2)	1.335(3)	C(9)-C(8)-C(7)	117.8(2)
C(3)-N(3)	1.341(3)	C(9)-C(8)-C(11)	120.7(2)
C(3)-N(5)	1.341(3)	C(7)-C(8)-C(11)	121.5(3)
C(3)-N(1)	1.362(3)	C(8)-C(9)-C(10)	121.6(2)
C(4)-N(3)	1.331(3)	C(4)-N(6)-C(12)	131.4(2)
C(4)-N(6)	1.352(3)	C(5)-C(10)-C(9)	119.7(2)
C(4)-N(2)	1.367(3)	C(13)-C(12)-C(17)	118.8(2)
C(5)-C(10)	1.388(3)	C(13)-C(12)-N(6)	125.0(2)
C(5)-C(6)	1.389(3)	C(17)-C(12)-N(6)	116.1(2)
C(5)-N(5)	1.415(3)	C(12)-C(13)-C(14)	119.6(2)
C(6)-C(7)	1.388(3)	C(15)-C(14)-C(13)	122.1(2)
C(7)-C(8)	1.389(4)	C(16)-C(15)-C(14)	117.3(2)
C(8)-C(9)	1.384(4)	C(16)-C(15)-C(18)	121.7(2)
C(8)-C(11)	1.509(3)	C(14)-C(15)-C(18)	121.0(2)
C(9)-C(10)	1.390(3)	C(17)-C(16)-C(15)	121.8(3)
N(6)-C(12)	1.413(3)	C(16)-C(17)-C(12)	120.4(2)
C(12)-C(13)	1.380(3)	C(3)-N(5)-C(5)	127.43(19)
C(12)-C(17)	1.397(3)	C(2)-N(1)-C(3)	114.33(19)
C(13)-C(14)	1.395(3)	C(2)-N(1)-Na(1)	112.82(13)
C(14)-C(15)	1.385(4)	C(3)-N(1)-Na(1)	127.24(15)
C(15)-C(16)	1.381(4)	C(2)-N(2)-C(4)	113.44(19)
C(15)-C(18)	1.508(3)	C(2)-N(2)-Na(1)#1	115.61(14)
C(16)-C(17)	1.379(3)	C(4)-N(2)-Na(1)#1	129.51(15)
C(20)-S(20)	1.787(2)	C(4)-N(3)-C(3)	114.73(19)
C(21)-S(20)	1.784(3)	O(20)-Na(1)-O(1)	119.92(7)
C(30)-S(30)	1.774(3)	O(20)-Na(1)-O(2)#2	94.41(6)
C(31)-S(30)	1.785(2)	O(1)-Na(1)-O(2)#2	131.10(6)
N(1)-Na(1)	2.4880(19)	O(20)-Na(1)-O(30)	81.08(6)
N(2)-Na(1)#1	2.492(2)	O(1)-Na(1)-O(30)	91.14(6)
Na(1)-O(20)	2.3433(18)	O(2)#2-Na(1)-O(30)	130.39(7)
Na(1)-O(1)	2.3895(18)	O(20)-Na(1)-N(1)	87.40(6)
Na(1)-O(2)#2	2.4243(18)	O(1)-Na(1)-N(1)	67.28(6)
Na(1)-O(30)	2.4670(17)	O(2)#2-Na(1)-N(1)	82.03(6)
Na(1)-N(2)#2	2.492(2)	O(30)-Na(1)-N(1)	146.07(7)
O(2)-Na(1)#1	2.4243(18)	O(20)-Na(1)-N(2)#2	138.73(7)
O(20)-S(20)	1.4962(16)	O(1)-Na(1)-N(2)#2	98.91(6)
O(30)-S(30)	1.5176(17)	O(2)#2-Na(1)-N(2)#2	66.32(6)
		O(30)-Na(1)-N(2)#2	84.98(6)
O(1)-C(1)-O(2)	127.5(2)	N(1)-Na(1)-N(2)#2	122.75(7)
O(1)-C(1)-C(2)	117.2(2)	C(1)-O(1)-Na(1)	120.01(14)
O(2)-C(1)-C(2)	115.32(19)	C(1)-O(2)-Na(1)#1	120.13(14)
N(1)-C(2)-N(2)	126.7(2)	O(20)-S(20)-C(21)	105.35(11)
N(1)-C(2)-C(1)	116.37(19)	O(20)-S(20)-C(20)	106.22(11)
N(2)-C(2)-C(1)	116.9(2)	C(21)-S(20)-C(20)	98.57(13)
N(3)-C(3)-N(5)	120.52(19)	O(30)-S(30)-C(30)	106.24(11)
N(3)-C(3)-N(1)	125.0(2)	O(30)-S(30)-C(31)	105.99(11)
N(5)-C(3)-N(1)	114.5(2)	C(30)-S(30)-C(31)	97.21(13)
N(3)-C(4)-N(6)	120.9(2)	O(30)-S(30)-Na(1)	46.14(6)
N(3)-C(4)-N(2)	125.8(2)	C(30)-S(30)-Na(1)	116.41(9)
N(6)-C(4)-N(2)	113.3(2)	C(31)-S(30)-Na(1)	139.99(10)
C(10)-C(5)-C(6)	119.5(2)		

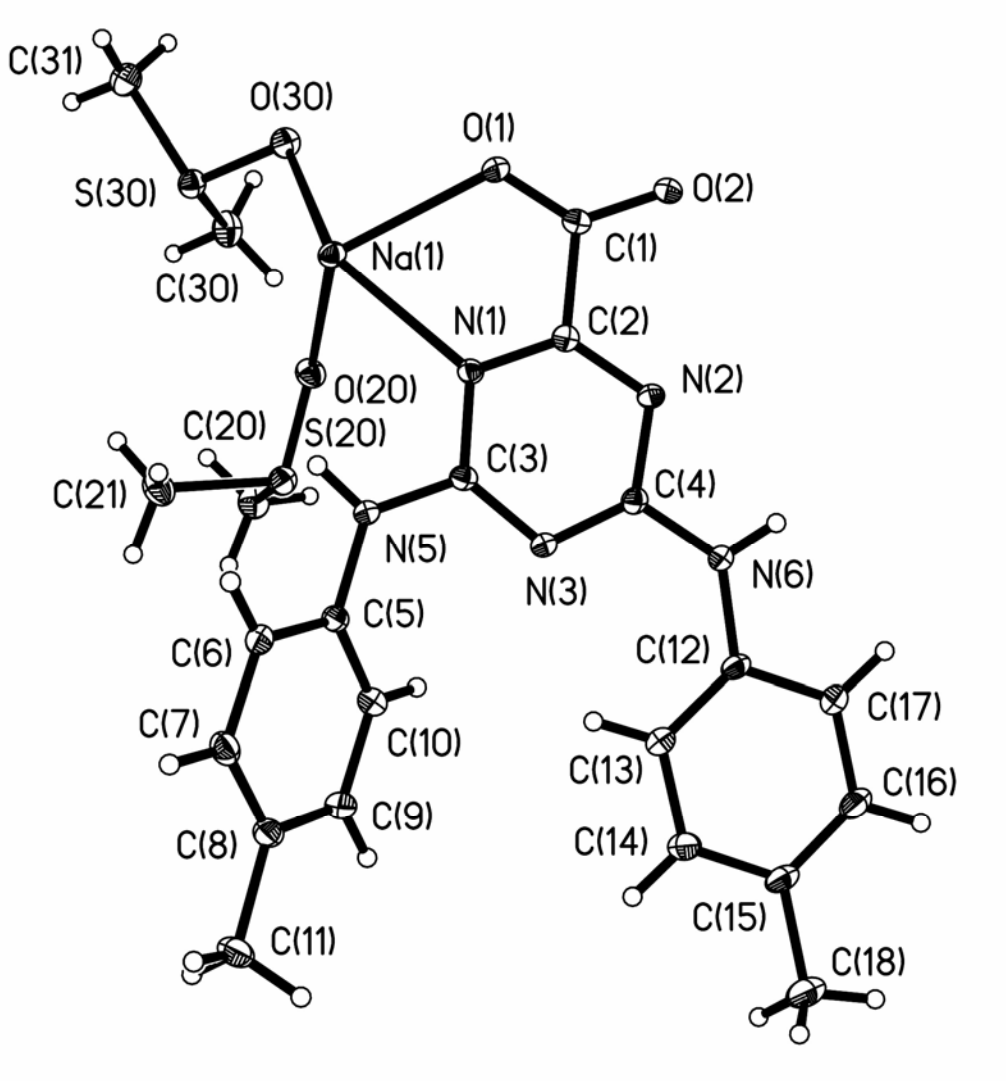
Symmetry transformations: #1 -x+1,y+1/2,-z+1/2 #2 -x+1,y-1/2,-z+1/2

Table 6. Torsion angles [°] for C22 H28 N5 Na O4 S2.

O(1)-C(1)-C(2)-N(1)	-7.7(3)	C(2)-N(1)-Na(1)-O(20)	102.58(15)
O(2)-C(1)-C(2)-N(1)	172.59(19)	C(3)-N(1)-Na(1)-O(20)	-49.20(19)
O(1)-C(1)-C(2)-N(2)	171.6(2)	C(2)-N(1)-Na(1)-O(1)	-21.49(14)
O(2)-C(1)-C(2)-N(2)	-8.2(3)	C(3)-N(1)-Na(1)-O(1)	-173.3(2)
C(10)-C(5)-C(6)-C(7)	1.7(3)	C(2)-N(1)-Na(1)-O(2)#2	-162.59(15)
N(5)-C(5)-C(6)-C(7)	179.9(2)	C(3)-N(1)-Na(1)-O(2)#2	45.63(19)
C(5)-C(6)-C(7)-C(8)	1.4(4)	C(2)-N(1)-Na(1)-O(30)	32.8(2)
C(6)-C(7)-C(8)-C(9)	-3.0(4)	C(3)-N(1)-Na(1)-O(30)	-118.99(19)
C(6)-C(7)-C(8)-C(11)	176.5(2)	C(2)-N(1)-Na(1)-N(2)#2	-107.50(15)
C(7)-C(8)-C(9)-C(10)	1.4(4)	C(3)-N(1)-Na(1)-N(2)#2	100.72(19)
C(11)-C(8)-C(9)-C(10)	-178.0(2)	C(2)-N(1)-Na(1)-S(30)	83.92(18)
N(3)-C(4)-N(6)-C(12)	6.2(4)	C(3)-N(1)-Na(1)-S(30)	-67.9(2)
N(2)-C(4)-N(6)-C(12)	-174.2(2)	O(2)-C(1)-O(1)-Na(1)	165.62(18)
C(6)-C(5)-C(10)-C(9)	-3.2(3)	C(2)-C(1)-O(1)-Na(1)	-14.1(3)
N(5)-C(5)-C(10)-C(9)	178.7(2)	O(20)-Na(1)-O(1)-C(1)	-53.72(18)
C(8)-C(9)-C(10)-C(5)	1.6(4)	O(2)#2-Na(1)-O(1)-C(1)	74.59(19)
C(4)-N(6)-C(12)-C(13)	-4.7(4)	O(30)-Na(1)-O(1)-C(1)	-134.07(17)
C(4)-N(6)-C(12)-C(17)	175.1(2)	N(1)-Na(1)-O(1)-C(1)	18.97(16)
C(17)-C(12)-C(13)-C(14)	-1.2(4)	N(2)#2-Na(1)-O(1)-C(1)	140.84(17)
N(6)-C(12)-C(13)-C(14)	178.6(2)	S(30)-Na(1)-O(1)-C(1)	-129.84(16)
C(12)-C(13)-C(14)-C(15)	0.8(4)	O(1)-C(1)-O(2)-Na(1)#1	-155.17(19)
C(13)-C(14)-C(15)-C(16)	0.3(4)	C(2)-C(1)-O(2)-Na(1)#1	24.5(2)
C(13)-C(14)-C(15)-C(18)	179.2(2)	O(1)-Na(1)-O(20)-S(20)	121.18(13)
C(14)-C(15)-C(16)-C(17)	-1.2(4)	O(2)#2-Na(1)-O(20)-S(20)	-22.44(14)
C(18)-C(15)-C(16)-C(17)	179.9(2)	O(30)-Na(1)-O(20)-S(20)	-152.67(14)
C(15)-C(16)-C(17)-C(12)	0.9(4)	N(1)-Na(1)-O(20)-S(20)	59.36(14)
C(13)-C(12)-C(17)-C(16)	0.3(4)	N(2)#2-Na(1)-O(20)-S(20)	-80.93(16)
N(6)-C(12)-C(17)-C(16)	-179.4(2)	S(30)-Na(1)-O(20)-S(20)	-130.31(14)
N(3)-C(3)-N(5)-C(5)	1.0(3)	O(20)-Na(1)-O(30)-S(30)	51.37(9)
N(1)-C(3)-N(5)-C(5)	-177.0(2)	O(1)-Na(1)-O(30)-S(30)	171.49(9)
C(10)-C(5)-N(5)-C(3)	-41.8(3)	O(2)#2-Na(1)-O(30)-S(30)	-36.83(13)
C(6)-C(5)-N(5)-C(3)	140.1(2)	N(1)-Na(1)-O(30)-S(30)	122.98(12)
N(2)-C(2)-N(1)-C(3)	-0.2(3)	N(2)#2-Na(1)-O(30)-S(30)	-89.66(10)
C(1)-C(2)-N(1)-C(3)	178.99(18)	Na(1)-O(20)-S(20)-C(21)	61.50(16)
N(2)-C(2)-N(1)-Na(1)	-155.77(18)	Na(1)-O(20)-S(20)-C(20)	165.43(14)
C(1)-C(2)-N(1)-Na(1)	23.4(2)	Na(1)-O(30)-S(30)-C(30)	-111.25(11)
N(3)-C(3)-N(1)-C(2)	-0.7(3)	Na(1)-O(30)-S(30)-C(31)	146.07(12)
N(5)-C(3)-N(1)-C(2)	177.26(19)	O(20)-Na(1)-S(30)-O(30)	-122.09(11)
N(3)-C(3)-N(1)-Na(1)	150.69(17)	O(1)-Na(1)-S(30)-O(30)	-9.57(10)
N(5)-C(3)-N(1)-Na(1)	-31.3(3)	O(2)#2-Na(1)-S(30)-O(30)	151.29(11)
N(1)-C(2)-N(2)-C(4)	0.6(3)	N(1)-Na(1)-S(30)-O(30)	-101.54(15)
C(1)-C(2)-N(2)-C(4)	-178.60(18)	N(2)#2-Na(1)-S(30)-O(30)	88.07(10)
N(1)-C(2)-N(2)-Na(1)#1	168.19(17)	O(20)-Na(1)-S(30)-C(30)	-34.62(11)
C(1)-C(2)-N(2)-Na(1)#1	-11.0(2)	O(1)-Na(1)-S(30)-C(30)	77.90(12)
N(3)-C(4)-N(2)-C(2)	-0.1(3)	O(2)#2-Na(1)-S(30)-C(30)	-121.24(11)
N(6)-C(4)-N(2)-C(2)	-179.70(19)	O(30)-Na(1)-S(30)-C(30)	87.47(14)
N(3)-C(4)-N(2)-Na(1)#1	-165.62(17)	N(1)-Na(1)-S(30)-C(30)	-14.07(16)
N(6)-C(4)-N(2)-Na(1)#1	14.8(3)	N(2)#2-Na(1)-S(30)-C(30)	175.54(11)
N(6)-C(4)-N(3)-C(3)	178.9(2)	O(20)-Na(1)-S(30)-C(31)	-178.67(16)
N(2)-C(4)-N(3)-C(3)	-0.6(3)	O(1)-Na(1)-S(30)-C(31)	-66.15(17)
N(5)-C(3)-N(3)-C(4)	-176.8(2)	N(2)#2-Na(1)-S(30)-C(31)	31.49(16)
N(1)-C(3)-N(3)-C(4)	1.1(3)		

Symmetry transformations used to generate equivalent atoms:

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



Thermal ellipsoid view of the C22 H28 N5 Na O4 S2 compound with the numbering scheme adopted. Ellipsoids are drawn at the 30% probability level. Hydrogen atoms are represented by a sphere of arbitrary size.

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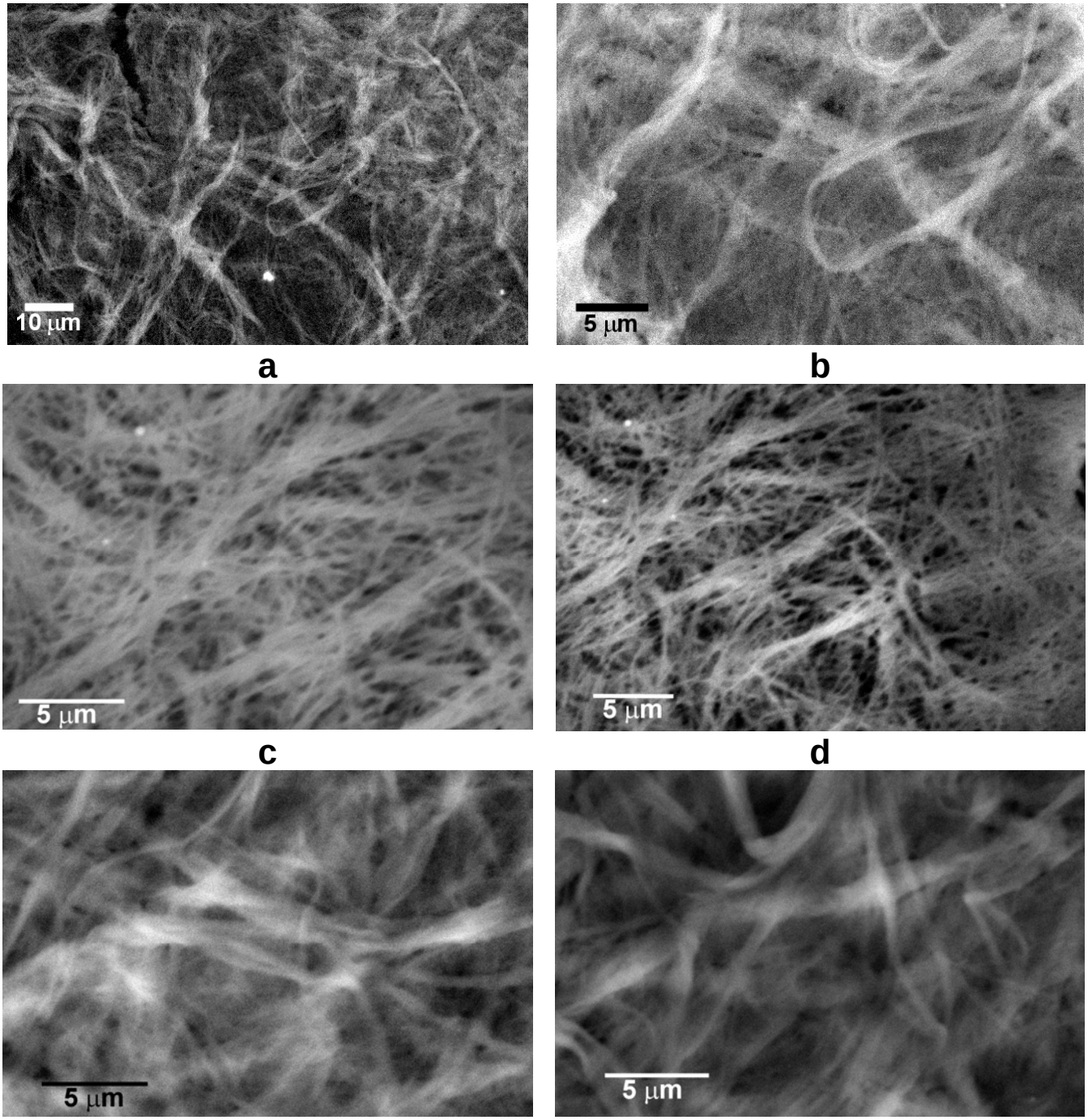

10 μm
a
5 μm
b
5 μm
c
5 μm
d
5 μm
e
5 μm
f

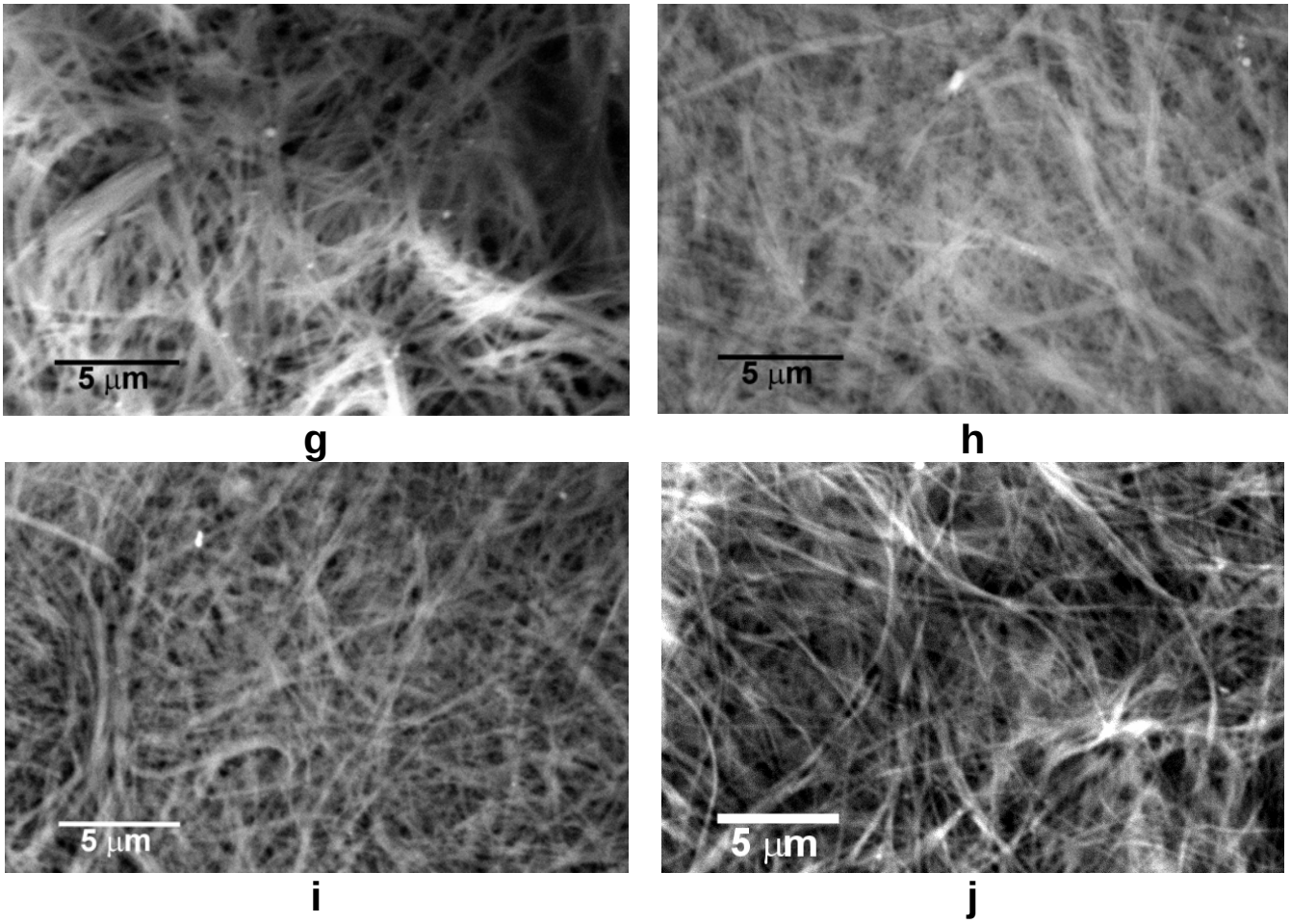
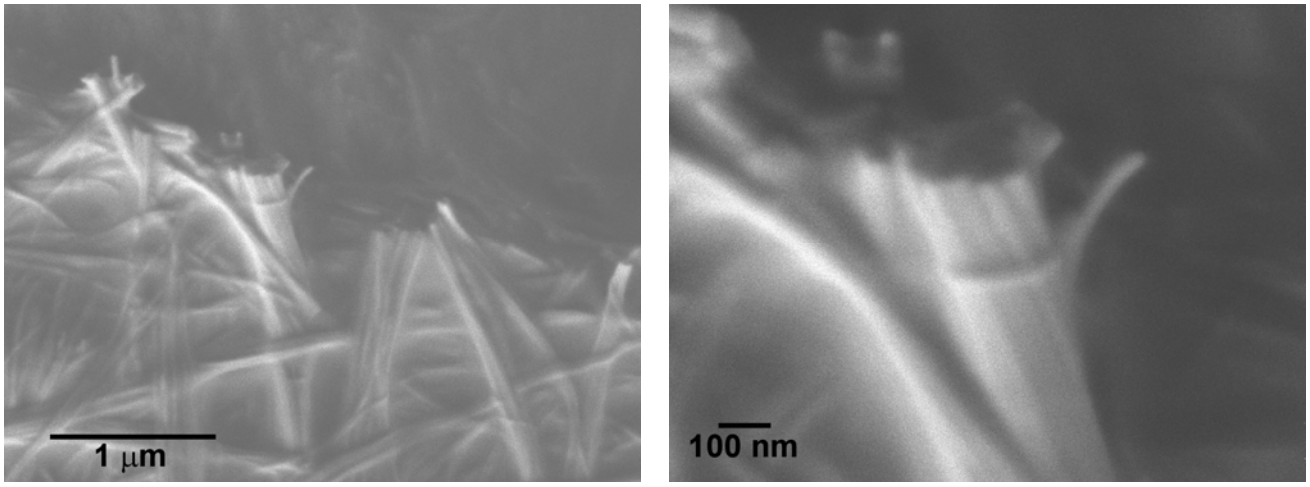


Figure S1. Additional variable-pressure scanning electron micrographs of the gel prepared by dissolving sodium 4,6-bis(phenylamino)-1,3,5-triazine-2-carboxylate (**6a**) in DMSO (3.0 mg/mL). Images were recorded at 27 ^{o}C and 30-50 Pa with an electron beam of 15-20 kV.



a **b**

Figure S2. Additional field-emission scanning electron micrographs of a xerogel formed by sodium 4,6-bis(phenylamino)-1,3,5-triazine-2-carboxylate (**6a**). The gel formed by a 3.0 mg/mL solution of salt **6a** in DMSO was dried under vacuum and observed uncoated with an electron beam of 1 kV.

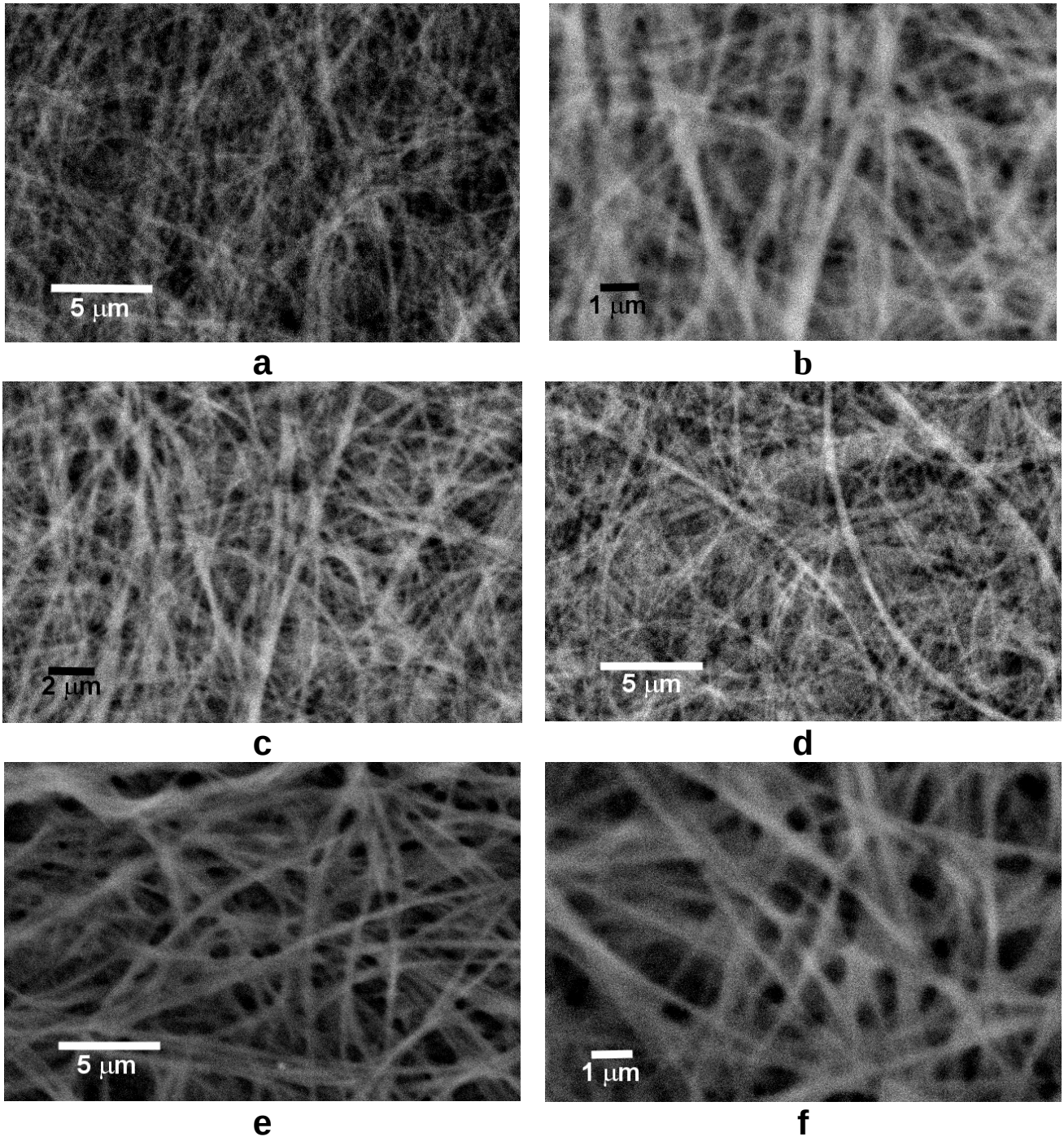
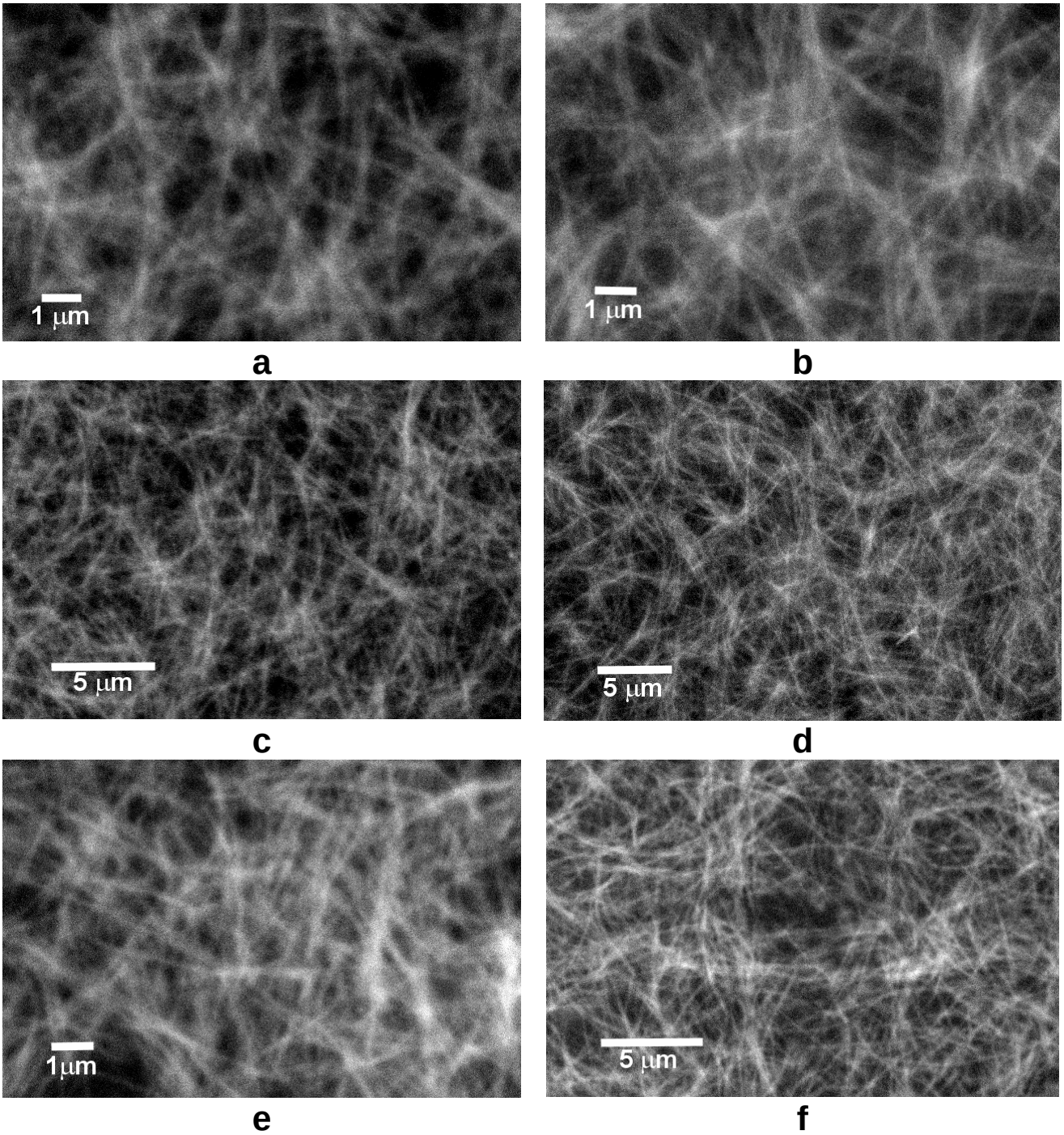


Figure S3. Variable-pressure scanning electron micrographs of the gel formed by dissolving sodium 4,6-bis[(4-methoxyphenyl)amino]-1,3,5-triazine-2-carboxylate (**6c**) in DMSO (3.0 mg/mL). Images were recorded at 27 ^{o}C and 30-50 Pa with an electron beam of 15-20 kV.


1 μm
a
1 μm
b
5 μm
c
5 μm
d
1μm
e
5 μm
f

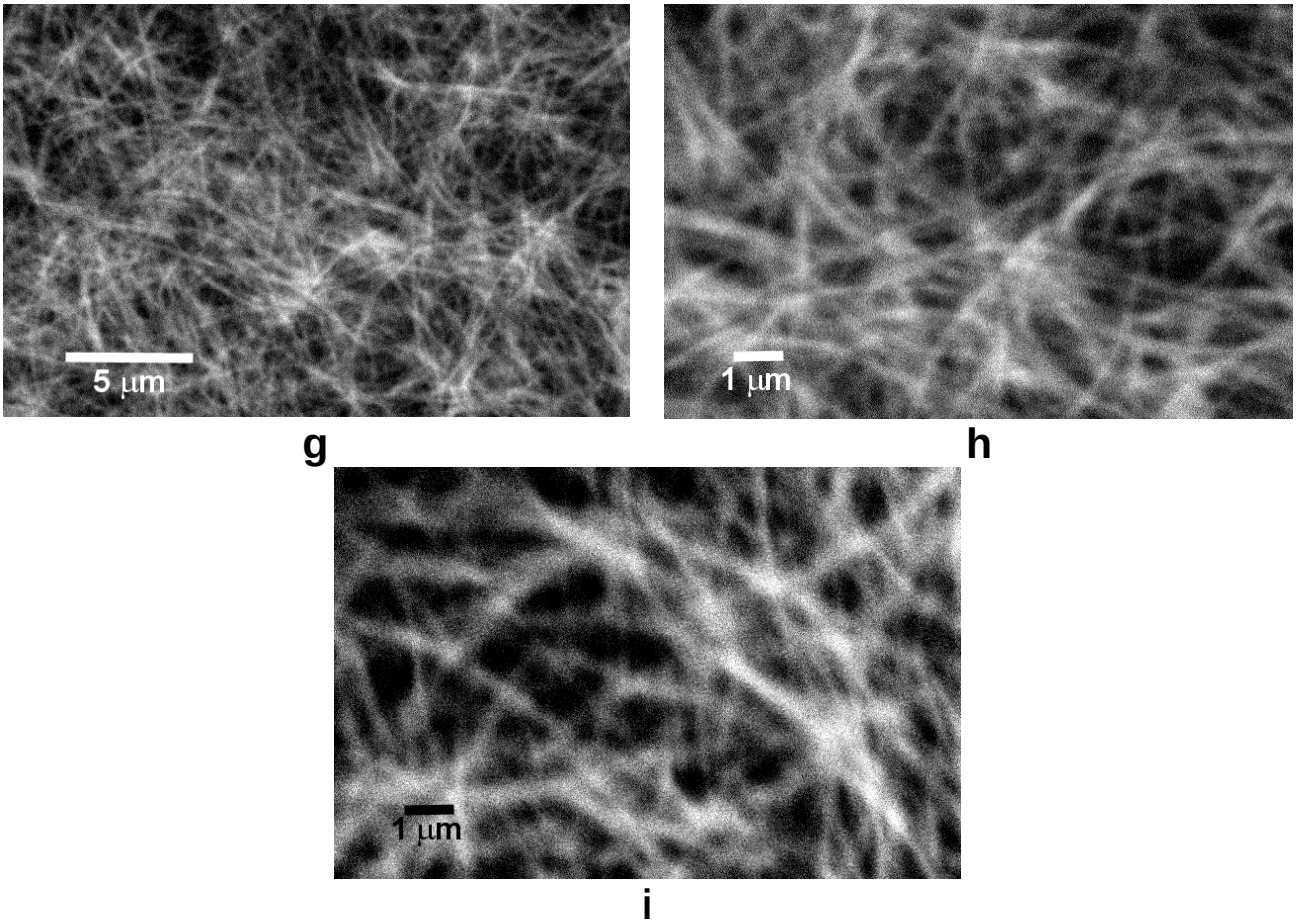
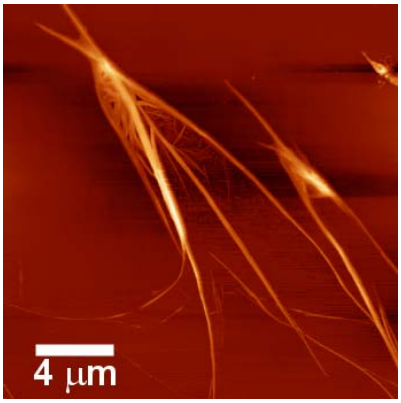
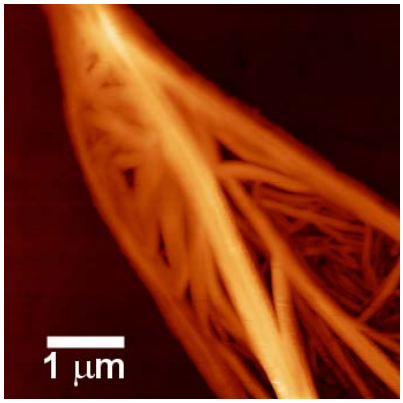


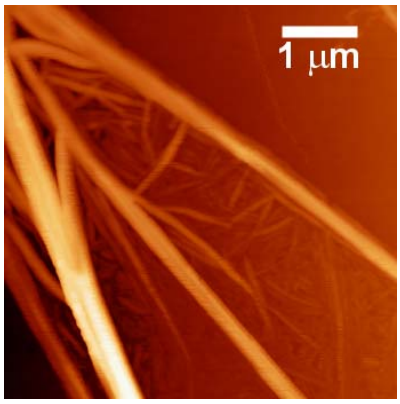
Figure S4. Variable-pressure scanning electron micrographs of a gel made by dissolving sodium 4,6-bis[(4-bromophenyl)amino]-1,3,5-triazine-2-carboxylate (**6e**) in DMSO (1.5 mg/mL). Images were recorded at 27 ^{o}C and 30-50 Pa with an electron beam of 15-20 kV.


4 μm

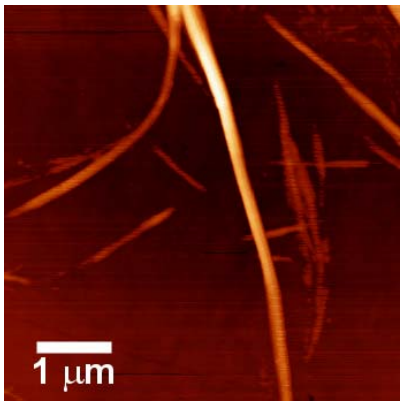
a


1 μm

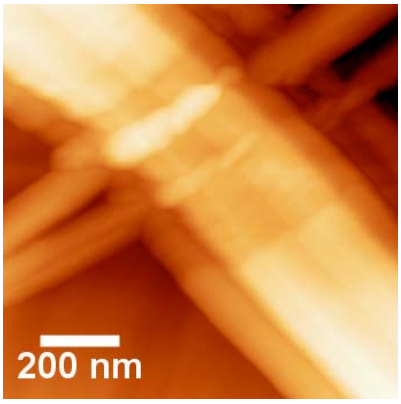
b

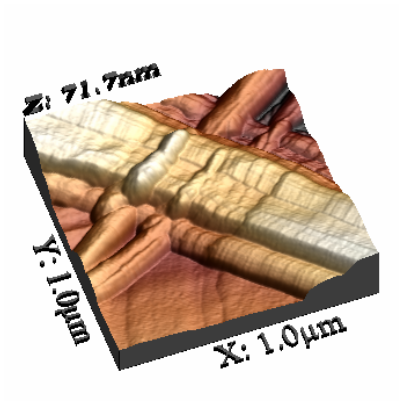

1 μm

c

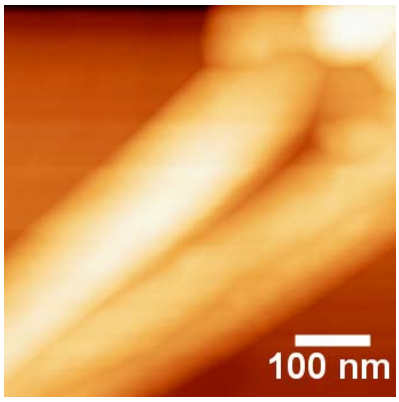

1 μm

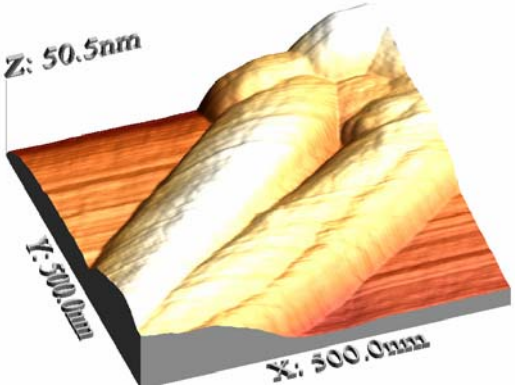
d


200 nm

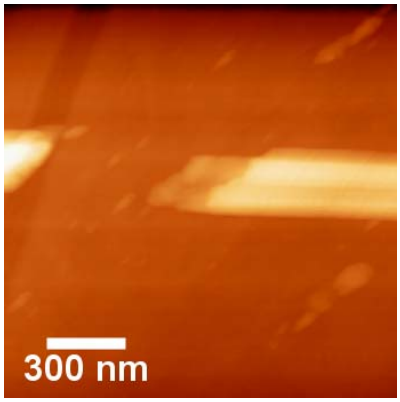

Z: 71.7nm
Y: 1.0μm
X: 1.0μm

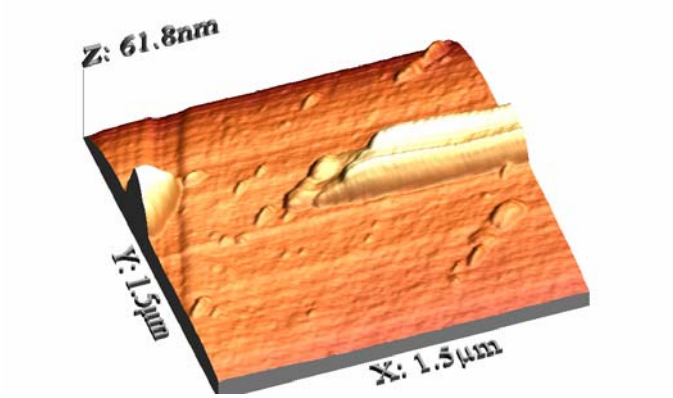
e


100 nm


Z: 50.5nm
Y: 500.0nm
X: 500.0nm

f





g

Figure S5. Additional tapping-mode atomic force micrographs of gel fibers spin-cast onto quartz from a 3.0 mg/mL solution of sodium 4,6-bis[(4-methylphenyl)amino)-1,3,5-triazine-2-carboxylate (**6b**) in DMSO. The images were recorded either in air or under vacuum (10^{-6} Torr). Three-dimensional perspectives are provided for some of the images.