Supporting Information

Synthesis, X-ray crystal structures, and preliminary anti-proliferative activities of new s-triazine-hydroxybenzylidene hydrazone derivatives

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X-Ray data for compounds **4f, 5b,** and **5f**

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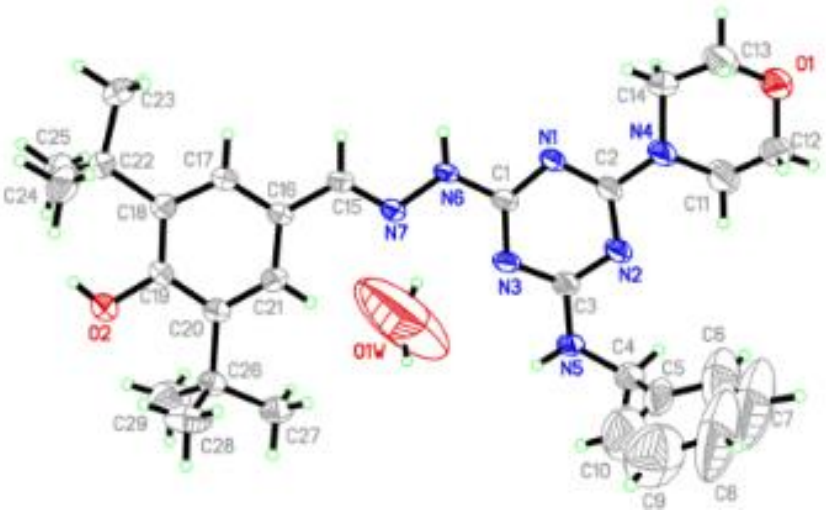

Figure S1 ORTEPs diagram of the titled compound **4f**. Displacement ellipsoids are plotted at the 40% probability level for non-H atoms.

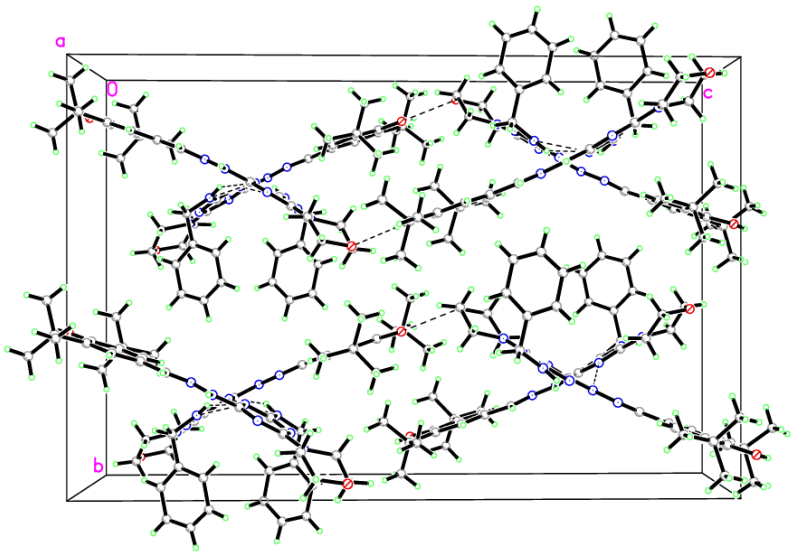

Figure S2 Molecular packing of compound **4f** showing the hydrogen bonds, which are drawn as dashed lines.

Table S1 Experimental details for compound **4f**

Crystal data	**4f**
Chemical formula	$C_{29}H_{40}N_7O_2$
Mr	518.68
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	293
a, *b*, *c* (Å)	10.4467 (5), 20.033 (1), 30.3531 (16)
α, *β*, *γ* (°)	90.00, 91.768 (2), 90.00
V (Å3)	6349.2 (6)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	0.07
Crystal size (mm)	0.57 × 0.41 × 0.06
Tmin, Tmax	0.673, 0.832
No. of measured, independent and observed [I > 2σ(I)] reflections	68185, 5607 and 2874
R_{int}	0.191
R[F^2 > 2σ(F^2)], wR(F^2), S	0.101, 0.312, 1.04
No. of reflections	5607
No. of parameters	353
No. of restraints	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.67, −0.38 (e $Å^{-3}$)
CCDC no.	1567719

Table S2 Selected geometric parameters (Å, °) **4f**

O1—C12	1.419 (6)	N4—C2	1.345 (7)
O1—C13	1.404 (7)	N4—C11	1.508 (10)
O2—C19	1.368 (5)	N4—C14	1.463 (7)
N1—C2	1.347 (6)	N5—C4	1.440 (7)
N1—C1	1.326 (6)	N5—C3	1.336 (5)
N2—C3	1.330 (6)	N6—N7	1.382 (5)
N2—C2	1.337 (5)	N6—C1	1.369 (6)
N3—C1	1.332 (5)	N7—C15	1.270 (6)
N3—C3	1.351 (6)		
C12—O1—C13	110.9 (4)	N2—C2—N4	115.7 (5)
C1—N1—C2	112.9 (3)	N1—C2—N4	118.3 (4)
C2—N2—C3	114.4 (4)	N2—C3—N3	125.7 (4)
C1—N3—C3	113.0 (4)	N3—C3—N5	116.2 (4)
C2—N4—C14	124.0 (5)	N2—C3—N5	118.0 (4)
C2—N4—C11	120.8 (5)	N5—C4—C5	114.1 (5)
C11—N4—C14	112.3 (5)	N4—C11—C12	112.4 (7)
C3—N5—C4	122.8 (4)	O1—C12—C11	113.9 (6)
N7—N6—C1	119.8 (3)	O1—C13—C14	116.9 (6)
N6—N7—C15	115.8 (3)	N4—C14—C13	110.9 (6)
N1—C1—N6	114.3 (4)	N7—C15—C16	122.9 (4)
N3—C1—N6	118.0 (4)	O2—C19—C20	114.9 (4)
N1—C1—N3	127.8 (4)	O2—C19—C18	122.2 (4)
N1—C2—N2	126.0 (4)		

Table S3 Hydrogen-bond geometry (Å, °) **4f**

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···O1^{i}	0.8200	2.2600	2.830 (5)	127.00
N5—H5A···N3^{ii}	0.8600	2.2000	2.969 (5)	149.00
N6—H6C···N1^{iii}	0.8600	2.3300	3.079 (5)	145.00
C11—H11A···N2	0.9700	2.3300	2.730 (9)	104.00
C24—H24C···O2	0.9600	2.4900	3.122 (6)	123.00
C25—H25B···O2	0.9600	2.4400	3.099 (6)	126.00
C28—H28A···O2	0.9600	2.3500	2.973 (7)	122.00
C29—H29A···O2	0.9600	2.2500	2.881 (6)	122.00

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

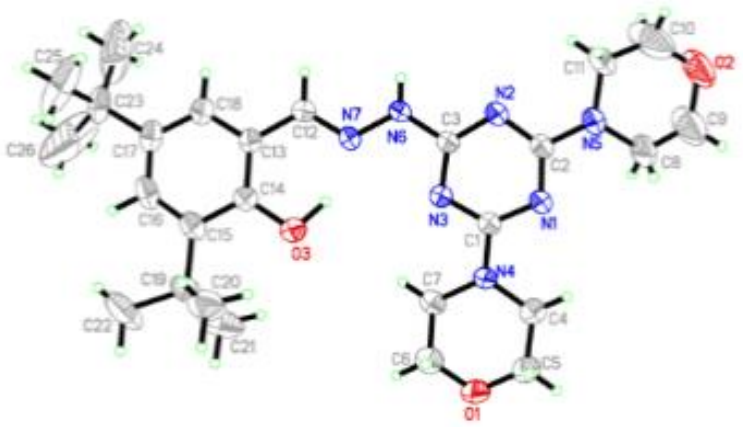

Figure S3 ORTEPs diagram of the titled compound **5b**. Displacement ellipsoids are plotted at the 40% probability level for non-H atoms.

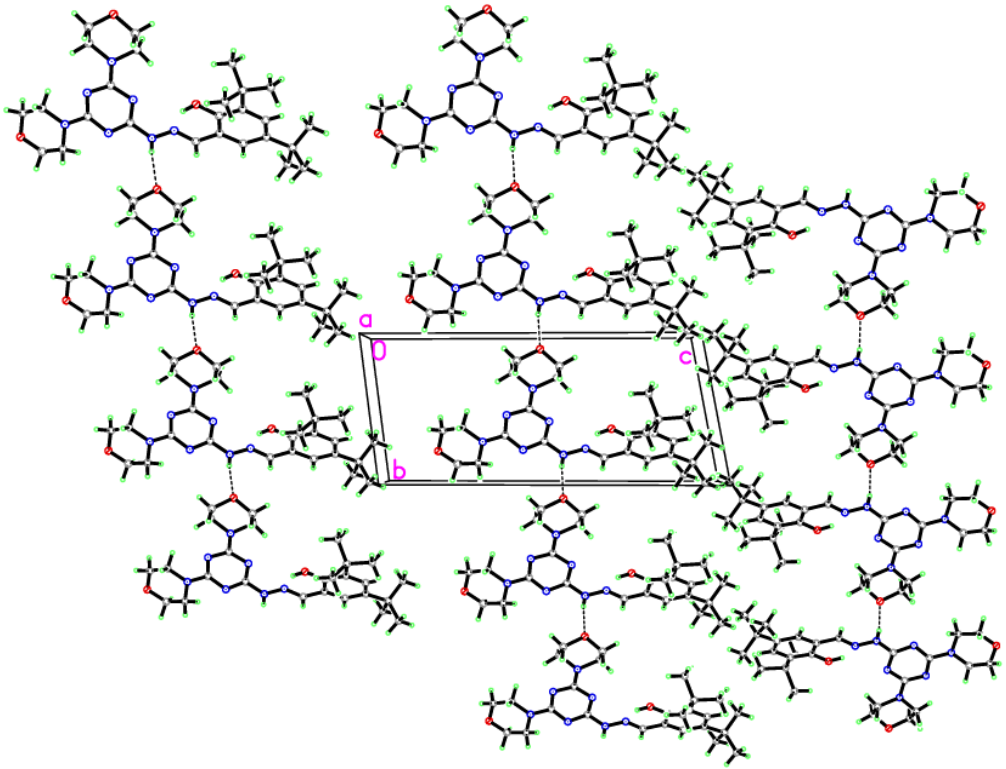

Figure S4 Molecular packing of compound **5b** showing the hydrogen bonds, which are drawn as dashed lines.

Table S4 Experimental details for compound **5b**

Crystal data	**5b**
Chemical formula	$C_{26}H_{39}N_7O_3$
Mr	497.64
Crystal system, space group	Triclinic, *P*-1
Temperature (K)	293
a, *b*, *c* (Å)	8.9822 (13), 9.1626 (13), 18.917 (3)
α, *β*, *γ* (°)	80.068 (4), 85.686 (5), 67.012 (4)
V (Å3)	1411.7 (3)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.08
Crystal size (mm)	0.37 × 0.34 × 0.12
Tmin, Tmax	0.771, 0.925
No. of measured, independent and observed [I > 2σ(I)] reflections	29134, 4968 and 2617
R_{int}	0.111
R[F^2 > 2σ(F^2)], wR(F^2), S	0.081, 0.248, 1.01
No. of reflections	4968
No. of parameters	371
No. of restraints	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.37, −0.31 (e $Å^{-3}$)
CCDC no.	1567728

Table S5 Selected geometric parameters (Å, °) **5b**

O1—C5	1.416 (5)	N3—C3	1.323 (5)
O1—C6	1.420 (5)	N4—C4	1.459 (6)
O2—C9	1.382 (8)	N4—C7	1.456 (5)
O2—C10	1.338 (9)	N4—C1	1.349 (5)
O3—C14	1.365 (5)	N5—C8	1.419 (8)
N1—C2	1.345 (5)	N5—C11	1.446 (6)
N1—C1	1.335 (5)	N5—C2	1.356 (5)
N2—C2	1.338 (5)	N6—C3	1.359 (5)
N2—C3	1.334 (4)	N6—N7	1.348 (4)
N3—C1	1.341 (5)	N7—C12	1.270 (5)
C5—O1—C6	111.3 (3)	N2—C2—N5	117.7 (4)
C9—O2—C10	114.4 (5)	N1—C2—N5	116.2 (3)
C1—N1—C2	114.0 (3)	N3—C3—N6	116.3 (3)
C2—N2—C3	112.6 (3)	N2—C3—N6	115.7 (3)
C1—N3—C3	113.3 (3)	N2—C3—N3	128.0 (3)
C1—N4—C4	122.4 (3)	N4—C4—C5	111.3 (4)
C1—N4—C7	121.8 (3)	O1—C5—C4	113.6 (4)
C4—N4—C7	113.8 (3)	O1—C6—C7	113.5 (4)
C2—N5—C8	122.3 (4)	N4—C7—C6	111.3 (4)
C2—N5—C11	122.1 (3)	N5—C8—C9	122.7 (7)
C8—N5—C11	115.6 (4)	O2—C9—C8	120.8 (6)
N7—N6—C3	119.2 (3)	O2—C10—C11	129.4 (9)
N6—N7—C12	121.5 (4)	N5—C11—C10	114.4 (5)
N1—C1—N3	125.8 (4)	N7—C12—C13	120.4 (4)
N1—C1—N4	117.7 (3)	O3—C14—C13	120.5 (3)
N3—C1—N4	116.5 (3)	O3—C14—C15	118.8 (3)
N1—C2—N2	126.2 (3)		

Table S6 Hydrogen-bond geometry (Å, °) **5b**

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H1N6···O1^{i}	0.79 (4)	2.19 (4)	2.963 (4)	169 (4)
O3—H1O3···N7	0.98 (6)	1.64 (6)	2.548 (4)	153 (5)
C4—H4B···N1	0.9700	2.3800	2.755 (6)	102.00
C7—H7A···N3	0.9700	2.3300	2.729 (6)	104.00
C20—H20B···O3	0.9600	2.3200	2.962 (6)	124.00
C21—H21C···O3	0.9600	2.3600	2.979 (6)	122.00

Symmetry code: (i) x−1, y+1, z.

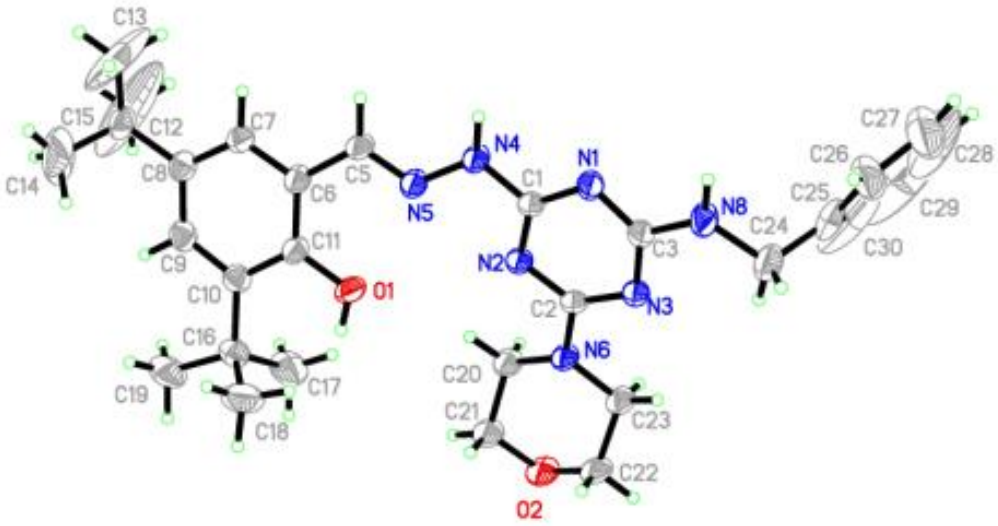

Figure S5 ORTEPs diagram of the titled compound **5f**. Displacement ellipsoids are plotted at the 40% probability level for non-H atoms.

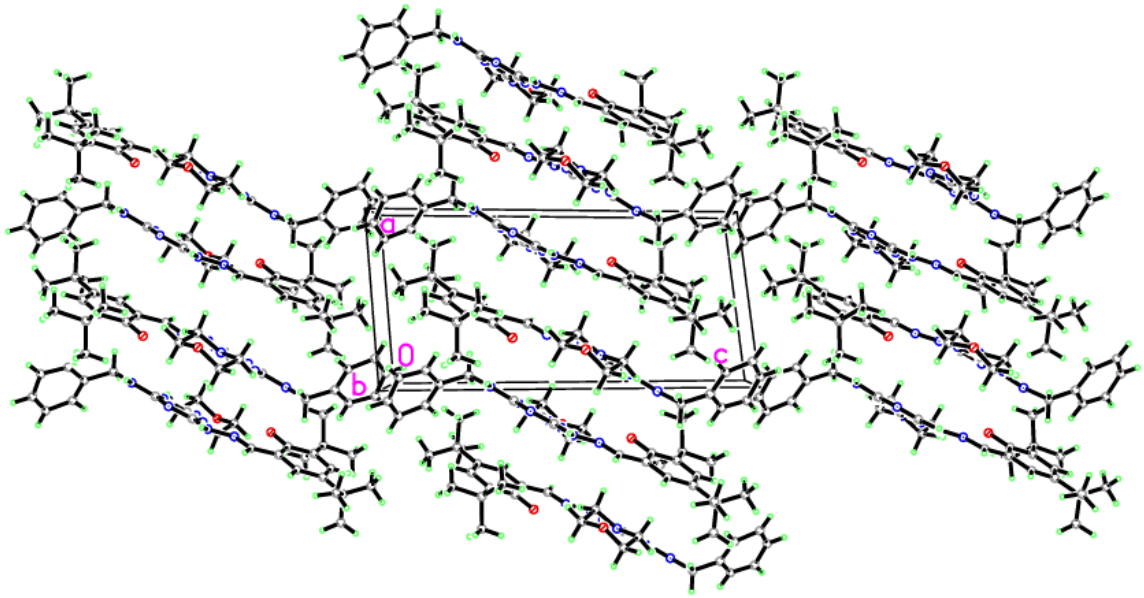

Figure S6 Molecular packing of compound **5f** showing the hydrogen bonds, which are drawn as dashed lines

Table S7 Experimental details for compound **5f**.

Crystal data	**5f**
Chemical formula	$C_{29}H_{38}N_7O_2$
Mr	516.66
Crystal system, space group	Triclinic, *P*-1
Temperature (K)	296
a, *b*, *c* (Å)	8.9020 (6), 9.8891 (6), 18.2177 (12)
α, *β*, *γ* (°)	104.724 (2), 90.723 (3), 109.037 (2)
V (Å3)	1458.23 (16)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.08
Crystal size (mm)	0.39 × 0.26 × 0.19
Tmin, Tmax	0.971, 0.986
No. of measured, independent and observed [I > 2σ(I)] reflections	45390, 5141 and 2959
R_{int}	0.109
R[F^2 > 2σ(F^2)], wR(F^2), S	0.080, 0.251, 1.03
No. of reflections	5141
No. of parameters	354
No. of restraints	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.63, −0.30 (e $Å^{-3}$)
CCDC no.	1567725

Table S8 Selected geometric parameters (Å, °) **5f**

O1—C11	1.357 (5)	N4—N5	1.359 (5)
O2—C21	1.436 (5)	N4—C1	1.374 (6)
O2—C22	1.431 (5)	N5—C5	1.267 (5)
N1—C1	1.329 (5)	N6—C2	1.356 (5)
N1—C3	1.333 (5)	N6—C20	1.447 (5)
N2—C1	1.331 (5)	N6—C23	1.462 (5)
N2—C2	1.342 (5)	N8—C3	1.346 (5)
N3—C2	1.336 (5)	N8—C24	1.457 (7)
N3—C3	1.349 (5)		
C21—O2—C22	110.6 (3)	N2—C2—N3	126.2 (3)
C1—N1—C3	112.6 (3)	N2—C2—N6	115.8 (3)
C1—N2—C2	113.2 (3)	N1—C3—N8	116.1 (4)
C2—N3—C3	113.1 (3)	N3—C3—N8	116.9 (4)
N5—N4—C1	116.3 (3)	N1—C3—N3	127.1 (3)
N4—N5—C5	123.5 (3)	N5—C5—C6	118.5 (4)
C2—N6—C20	121.1 (3)	O1—C11—C10	119.2 (3)
C2—N6—C23	121.9 (3)	O1—C11—C6	120.6 (3)
C20—N6—C23	114.1 (3)	N6—C20—C21	110.7 (4)
C3—N8—C24	125.8 (4)	O2—C21—C20	110.9 (3)
N1—C1—N4	116.5 (3)	O2—C22—C23	111.3 (4)
N2—C1—N4	115.8 (3)	N6—C23—C22	109.9 (3)
N1—C1—N2	127.8 (4)	N8—C24—C25	111.8 (5)
N3—C2—N6	117.9 (3)		

Table S9 Hydrogen-bond geometry (Å, °) **5f**

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H1N4···O2^{i}	0.91 (5)	1.93 (5)	2.842 (5)	174 (5)
C17—H17C···O1	0.9800	2.3100	2.977 (6)	125.00
C18—H18B···O1	0.9800	2.3300	2.964 (6)	122.00
C20—H20B···N2	0.9900	2.2900	2.702 (5)	104.00
C23—H23A···N3	0.9900	2.3800	2.760 (5)	102.00
C24—H24A···N3	0.9900	2.3900	2.809 (6)	105.00

Symmetry code: (i) x, y+1, z.