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Synthesis, Crystal Structure and Bioactivities of *N*-(5-(4-chlorobenzyl)−1,3,5-Triazinan−2-Ylidene)Nitramide

Yao-Guo Qin [1,2], Zhao-Kai Yang [2], Jia Fan [1,*], Xin Jiang [1], Xin-Ling Yang [2,*] and Ju-Lian Chen [1,*]

[1] State Key Laboratory for Biology of Plant Diseases and Insect Pests, Institute of Plant Protection, Chinese Academy of Agricultural Sciences, Beijing 100193, China; qinyg1018@163.com (Y-G.Q.); 18911895763@163.com (X.J.)

[2] Department of Applied Chemistry, College of Science, China Agricultural University, Beijing 100193, China; yangzhaokai@cau.edu.cn

* Correspondence: jfan@ippcaas.cn (J.F.); yangxl@cau.edu.cn (X-L.Y.); chenjulian@caas.cn (J-L.C.)

Table S1. Bond Lengths for Compound **1**.

Bond	Distance (Å)	Bond	Distance (Å)
Cl(1)—C(8)	1.7538(15)	N(4)—N(5)	1.3405(17)
O(1)—N(5)	1.2459(17)	N(4)—C(1)	1.3707(19)
O(2)—N(5)	1.2500(16)	C(4)—C(5)	1.506(2)
N(1)—C(2)	1.4476(18)	C(5)—C(6)	1.390(2)
N(1)—C(3)	1.4453(19)	C(5)—C(10)	1.396(2)
N(1)—C(4)	1.4757(18)	C(6)—C(7)	1.388(2)
N(2)—C(1)	1.3310(19)	C(7)—C(8)	1.380(2)
N(2)—C(2)	1.4743(19)	C(8)—C(9)	1.387(2)
N(3)—C(1)	1.3277(19)	C(9)—C(10)	1.390(2)
N(3)—C(3)	1.472(2)		

Table S2. Bond angles for Compound **1**.

Angle	(°)	Angle	(°)
C(2)—N(1)—C(4)	112.61(11)	N(1)—C(3)—N(3)	111.35(12)
C(3)—N(1)—C(2)	108.67(12)	N(1)—C(4)—C(5)	111.81(12)
C(3)—N(1)—C(4)	113.44(12)	C(6)—C(5)—C(4)	119.62(14)
C(1)—N(2)—C(2)	123.18(13)	C(6)—C(5)—C(10)	118.68(14)
C(1)—N(3)—C(3)	119.53(13)	C(10)—C(5)—C(4)	121.70(13)
N(5)—N(4)—C(1)	119.53(12)	C(7)—C(6)—C(5)	121.47(15)
O(1)—N(5)—O(2)	121.48(12)	C(8)—C(7)—C(6)	118.35(14)
O(1)—N(5)—N(4)	114.46(12)	C(7)—C(8)—Cl(1)	118.41(12)
O(2)—N(5)—N(4)	124.06(13)	C(7)—C(8)—C(9)	122.04(14)
N(2)—C(1)—N(4)	112.72(13)	C(9)—C(8)—Cl(1)	119.55(13)
N(3)—C(1)—N(2)	119.06(14)	C(8)—C(9)—C(10)	118.62(15)
N(3)—C(1)—N(4)	128.22(14)	C(9)—C(10)—C(5)	120.81(14)
N(1)—C(2)—N(2)	111.42(12)		

Table S3. Torsion angles for Compound **1**.

Torsion	(°)	Torsion	(°)
Cl(1)-C(8)-C(9)-C(10)	−178.93(12)	C(3)-N(1)-C(4)-C(5)	−58.12(16)
N(1)-C(4)-C(5)-C(6)	138.98(14)	C(3)-N(3)-C(1)-N(2)	2.5(2)
N(1)-C(4)-C(5)-C(10)	−40.97(19)	C(3)-N(3)-C(1)-N(4)	−177.22(14)

N(5)-N(4)-C(1)-N(2)	−178.25(12)	C(4)-N(1)-C(2)-N(2)	77.23(15)
N(5)-N(4)-C(1)-N(3)	1.4(2)	C(4)-N(1)-C(3)-N(3)	−67.62(16)
C(1)-N(2)-C(2)-N(1)	18.05(19)	C(4)-C(5)-C(6)-C(7)	−179.65(14)
C(1)-N(3)-C(3)-N(1)	−35.90(18)	C(4)-C(5)-C(10)-C(9)	178.31(14)
C(1)-N(4)-N(5)-O(1)	175.90(12)	C(5)-C(6)-C(7)-C(8)	1.2(2)
C(1)-N(4)-N(5)-O(2)	−3.4(2)	C(6)-C(5)-C(10)-C(9)	−1.6(2)
C(2)-N(1)-C(3)-N(3)	58.45(15)	C(6)-C(7)-C(8)-Cl(1)	177.65(12)
C(2)-N(1)-C(4)-C(5)	177.92(12)	C(6)-C(7)-C(8)-C(9)	−1.5(2)
C(2)-N(2)-C(1)-N(3)	6.7(2)	C(7)-C(8)-C(9)-C(10)	0.2(2)
C(2)-N(2)-C(1)-N(4)	−173.60(13)	C(8)-C(9)-C(10)-C(5)	1.4(2)
C(3)-N(1)-C(2)-N(2)	−49.32(15)	C(10)-C(5)-C(6)-C(7)	0.3(2)

Table S4. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for Compound **1.**

Atom	x	y	z	U (eq)*
Cl1	291.6(8)	3228.0 (2)	5098.7(5)	27.24(13)
O1	9062(2)	620.8(4)	13220.5(13)	22.4(3)
O2	5889(2)	1038.4(4)	12081.4(13)	23.2(3)
N1	4840(2)	729.4(5)	6418.6(15)	15.5(3)
N2	7435(2)	212.5(5)	8275.4(15)	15.6(3)
N3	4681(2)	807.2(5)	9174.6(16)	16.8(3)
N4	8207(2)	456.7(5)	10768.5(14)	15.4(3)
N5	7660(2)	720.7(5)	12041.8(15)	16.5(3)
C1	6698(3)	509.0(6)	9426.5(17)	14.3(3)
C2	6274(3)	240.4(6)	6676.3(17)	16.7(3)
C3	3254(3)	786.7(6)	7653.4(18)	17.8(3)
C4	6379(3)	1209.6(6)	6212.9(18)	15.6(3)
C5	4850(3)	1710.3(6)	5888.6(18)	15.4(3)
C6	5598(3)	2196.7(6)	6582.4(19)	20.6(3)
C7	4235(3)	2666.9(6)	6321(2)	23.1(4)
C8	2073(3)	2640.2(6)	5371.8(19)	19.7(3)
C9	1264(3)	2163.9(6)	4652.1(19)	21.2(3)
C10	2684(3)	1700.4(6)	4904.6(19)	19.3(3)

* U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Table S5. Anisotropic displacement parameters ($Å^2 \times 10^3$) for Compound **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka\times b\times U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	27.8(2)	17.4(2)	36.7(3)	5.08(16)	3.52(18)	6.64(16)
O1	27.0(6)	24.3(6)	14.8(6)	−2.6(4)	−3.7(5)	3.7(5)
O2	28.2(6)	20.0(6)	21.8(6)	−1.3(5)	4.5(5)	11.3(5)
N1	15.3(6)	13.9(6)	17.1(7)	1.2(5)	0.2(5)	−0.3(5)
N2	15.8(6)	15.2(6)	15.2(7)	−0.7(5)	−1.3(5)	4.3(5)
N3	16.3(6)	20.0(7)	14.3(7)	0.2(5)	2.1(5)	5.1(5)
N4	18.3(6)	14.4(6)	13.3(6)	−2.2(5)	0.7(5)	3.1(5)
N5	19.6(6)	13.6(6)	16.4(7)	0.2(5)	2.8(5)	1.0(5)
C1	15.0(7)	11.2(7)	16.7(8)	1.6(5)	2.0(6)	−1.1(5)
C2	20.3(8)	13.7(7)	15.4(8)	−0.2(6)	−2.3(6)	1.2(6)
C3	13.1(7)	19.4(7)	20.5(8)	5.0(6)	−0.6(6)	−0.1(6)
C4	14.9(7)	14.6(7)	17.2(8)	0.9(6)	0.3(6)	−0.5(6)
C5	17.0(7)	15.3(7)	14.2(8)	2.5(6)	3.4(6)	0.1(6)
C6	18.9(8)	18.8(7)	23.3(9)	−2.0(6)	−2.9(6)	−0.9(6)
C7	25.4(8)	15.1(7)	28.7(9)	−3.1(6)	2.5(7)	−2.1(6)
C8	22.2(8)	14.9(7)	22.9(9)	4.9(6)	6.1(7)	4.7(6)
C9	21.6(8)	20.8(8)	20.6(9)	3.2(6)	−1.8(7)	1.4(6)

C10	21.4(8)	17.4(7)	18.2(8)	−0.7(6)	−2.9(6)	−0.4(6)

Table S6. Hydrogen atom coordinates (Å×10^4) and isotropic displacement parameters (Å^2×10^3) for Compound **1**.

Atom	x	y	z	U (eq)
H2	8630(30)	15(7)	8490(20)	19
H3	4320(30)	988(7)	9890(20)	20
H2A	7537	230	5961	20
H2B	5218	−71	6474	20
H3A	2123	484	7628	21
H3B	2296	1115	7498	21
H4A	7377	1147	5361	19
H4B	7477	1265	7142	19
H6	7043	2207	7236	25
H7	4767	2992	6776	28
H9	−197	2155	4014	25
H10	2184	1380	4412	23