Synthesis, characterization and evaluation of the substituent effect on the amoebicide activity of new hydrazones derivatives

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Supplementary information

Collection data details, bond distances and bond angles for compound 1 (*E)-1-((5-(4-nitrophenyl)furan-2-yl)methylene)-2-phenylhydrazine*

Table S1. Crystal data and structure refinement for b24.

Identification code	shelx	
Empirical formula	C17 H13 N3 O3	
Formula weight	307.30	
Temperature	130(2) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 12.9041(3) Å	α= 90°.
	b = 12.7877(3) Å	β= 90°.
	c = 17.6929(4) Å	γ = 90°.
Volume	2919.57(12) $Å^3$	
Z	8	
Density (calculated)	1.398 Mg/m^3	
Absorption coefficient	0.813 mm^{-1}	
F(000)	1280	
Crystal size	0.5142 x 0.4634 x 0.3295 mm^3	
Theta range for data collection	4.999 to 72.854°.	
Index ranges	-15<=h<=15, -11<=k<=15, -21<=l<=20	
Reflections collected	19665	
Independent reflections	2894 [R(int) = 0.0318]	
Completeness to theta = 67.684°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2894 / 1 / 212	
Goodness-of-fit on F^2	1.058	
Final R indices [I>2sigma(I)]	R1 = 0.0401, wR2 = 0.1020	
R indices (all data)	R1 = 0.0497, wR2 = 0.1095	

Extinction coefficient	0.00039(7)
Largest diff. peak and hole	0.217 and -0.214 e.Å^{-3}

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for b24. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9860(1)	1533(1)	3391(1)	32(1)
C(2)	10799(1)	1803(1)	3050(1)	36(1)
C(3)	10822(1)	2134(1)	2308(1)	39(1)
C(4)	9916(1)	2199(1)	1892(1)	43(1)
C(5)	8985(1)	1916(1)	2227(1)	44(1)
C(6)	8947(1)	1579(1)	2971(1)	37(1)
C(7)	9098(1)	965(1)	5254(1)	33(1)
C(8)	8227(1)	856(1)	5755(1)	31(1)
C(9)	8186(1)	645(1)	6507(1)	36(1)
C(10)	7129(1)	612(1)	6707(1)	36(1)
C(11)	6578(1)	803(1)	6067(1)	32(1)
C(12)	5483(1)	907(1)	5908(1)	32(1)
C(13)	4760(1)	647(1)	6461(1)	41(1)
C(14)	3712(1)	767(1)	6327(1)	44(1)
C(15)	3396(1)	1134(1)	5630(1)	38(1)
C(16)	4090(1)	1373(1)	5062(1)	37(1)
C(17)	5136(1)	1266(1)	5204(1)	35(1)
O(1)	7248(1)	953(1)	5470(1)	31(1)
O(2)	2018(1)	1518(1)	4838(1)	54(1)
O(3)	1683(1)	1169(1)	6011(1)	63(1)
N(1)	9878(1)	1231(1)	4143(1)	34(1)
N(2)	8985(1)	1132(1)	4543(1)	32(1)
N(3)	2294(1)	1279(1)	5486(1)	45(1)

Table S3. Bond lengths [Å] and angles [°] for b24.

C(1)-N(1)	1.385(2)
C(1)-C(6)	1.394(2)
C(1)-C(2)	1.396(2)
C(2)-C(3)	1.381(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.384(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.387(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.386(2)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-N(2)	1.285(2)
C(7)-C(8)	1.438(2)
C(7)-H(7)	0.9500
C(8)-C(9)	1.357(2)
C(8)-O(1)	1.3656(16)
C(9)-C(10)	1.410(2)
C(9)-H(9)	0.9500
C(10)-C(11)	1.358(2)
C(10)-H(10)	0.9500
C(11)-O(1)	1.3784(17)
C(11)-C(12)	1.448(2)
C(12)-C(13)	1.392(2)
C(12)-C(17)	1.401(2)
C(13)-C(14)	1.382(2)
C(13)-H(13)	0.9500
C(14)-C(15)	1.381(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.379(2)
C(15)-N(3)	1.4572(19)
C(16)-C(17)	1.380(2)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500

O(2)-N(3)	1.238(2)
O(3)-N(3)	1.227(2)
N(1)-N(2)	1.3580(17)
N(1)-H(1F)	0.935(15)

N(1)-C(1)-C(6)	122.55(13)
N(1)-C(1)-C(2)	117.93(13)
C(6)-C(1)-C(2)	119.52(14)
C(3)-C(2)-C(1)	120.34(14)
C(3)-C(2)-H(2)	119.8
C(1)-C(2)-H(2)	119.8
C(2)-C(3)-C(4)	120.40(15)
C(2)-C(3)-H(3)	119.8
C(4)-C(3)-H(3)	119.8
C(3)-C(4)-C(5)	119.22(16)
C(3)-C(4)-H(4)	120.4
C(5)-C(4)-H(4)	120.4
C(6)-C(5)-C(4)	121.21(15)
C(6)-C(5)-H(5)	119.4
C(4)-C(5)-H(5)	119.4
C(5)-C(6)-C(1)	119.29(14)
C(5)-C(6)-H(6)	120.4
C(1)-C(6)-H(6)	120.4
N(2)-C(7)-C(8)	122.12(14)
N(2)-C(7)-H(7)	118.9
C(8)-C(7)-H(7)	118.9
C(9)-C(8)-O(1)	110.14(13)
C(9)-C(8)-C(7)	130.77(13)
O(1)-C(8)-C(7)	119.07(13)
C(8)-C(9)-C(10)	106.80(13)
C(8)-C(9)-H(9)	126.6
C(10)-C(9)-H(9)	126.6
C(11)-C(10)-C(9)	106.95(14)
C(11)-C(10)-H(10)	126.5
C(9)-C(10)-H(10)	126.5
C(10)-C(11)-O(1)	109.59(13)

C(10)-C(11)-C(12)	133.60(14)
O(1)-C(11)-C(12)	116.77(13)
C(13)-C(12)-C(17)	119.30(14)
C(13)-C(12)-C(11)	119.68(14)
C(17)-C(12)-C(11)	121.02(14)
C(14)-C(13)-C(12)	120.54(16)
C(14)-C(13)-H(13)	119.7
C(12)-C(13)-H(13)	119.7
C(15)-C(14)-C(13)	118.68(16)
C(15)-C(14)-H(14)	120.7
C(13)-C(14)-H(14)	120.7
C(16)-C(15)-C(14)	122.30(14)
C(16)-C(15)-N(3)	118.53(16)
C(14)-C(15)-N(3)	119.17(15)
C(15)-C(16)-C(17)	118.68(16)
C(15)-C(16)-H(16)	120.7
C(17)-C(16)-H(16)	120.7
C(16)-C(17)-C(12)	120.48(15)
C(16)-C(17)-H(17)	119.8
C(12)-C(17)-H(17)	119.8
C(8)-O(1)-C(11)	106.51(11)
N(2)-N(1)-C(1)	120.76(12)
N(2)-N(1)-H(1F)	118.2(12)
C(1)-N(1)-H(1F)	118.5(12)
C(7)-N(2)-N(1)	115.43(12)
O(3)-N(3)-O(2)	123.01(14)
O(3)-N(3)-C(15)	118.71(16)
O(2)-N(3)-C(15)	118.28(15)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2$x 10^3)for b24. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	26(1)	27(1)	41(1)	-2(1)	-1(1)	2(1)
C(2)	25(1)	38(1)	45(1)	1(1)	-1(1)	1(1)
C(3)	31(1)	39(1)	47(1)	2(1)	5(1)	1(1)
C(4)	42(1)	45(1)	42(1)	6(1)	-2(1)	2(1)
C(5)	34(1)	48(1)	50(1)	5(1)	-9(1)	1(1)
C(6)	26(1)	37(1)	47(1)	1(1)	-2(1)	-1(1)
C(7)	24(1)	33(1)	42(1)	-4(1)	-2(1)	0(1)
C(8)	21(1)	30(1)	41(1)	-5(1)	-3(1)	1(1)
C(9)	26(1)	42(1)	40(1)	-3(1)	-4(1)	1(1)
C(10)	29(1)	42(1)	37(1)	-3(1)	1(1)	0(1)
C(11)	26(1)	32(1)	37(1)	-6(1)	3(1)	-2(1)
C(12)	25(1)	32(1)	40(1)	-9(1)	0(1)	-1(1)
C(13)	29(1)	56(1)	37(1)	-8(1)	-1(1)	-1(1)
C(14)	28(1)	61(1)	44(1)	-15(1)	6(1)	-3(1)
C(15)	21(1)	39(1)	53(1)	-18(1)	-4(1)	2(1)
C(16)	32(1)	32(1)	47(1)	-7(1)	-6(1)	2(1)
C(17)	28(1)	33(1)	43(1)	-3(1)	1(1)	0(1)
O(1)	23(1)	35(1)	36(1)	-3(1)	0(1)	1(1)
O(2)	33(1)	55(1)	73(1)	-7(1)	-16(1)	3(1)
O(3)	25(1)	92(1)	73(1)	-34(1)	4(1)	1(1)
N(1)	20(1)	42(1)	40(1)	0(1)	0(1)	0(1)
N(2)	23(1)	32(1)	42(1)	-2(1)	2(1)	0(1)
N(3)	26(1)	47(1)	62(1)	-22(1)	-5(1)	1(1)

Table S5. Hydrogen bonds for b24 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1F)...O(2)#1	0.935(15)	2.120(15)	3.0456(17)	170.2(17)

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z