Supplementary materials

From Structure to Function: 2-Chloro-5-nitrobenzoic Acid Derivatives as Potential Next-Generation Antibacterials

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2. Results

2.1 Synthesis and structural characterization

Table S1. Selected geometric parameters of hydrogen bonds (Å, ◦) in compound **1**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)	Symmetry transformations for acceptor
O(5)-H(5A)...O(2)	0.82	1.83	2.648(3)	176.9	x+1,y,z+1
N(2)-H(2A)...O(1)	0.89	1.87	2.721(3)	159.0	x+1,y,z+1
N(2)-H(2B)...O(5)	0.89	2.03	2.827(3)	149.2	-x+1,-y,-z+2

Table S2. Bond distances (Å) and bond angles (◦) in the metal coordination cores of compound **2.**

K(1)-O(1W)	2.726(6)	K(1)-O(3)#3	2.881(5)
K(1)-O(1)#1	2.761(6)	K(1)-O(2)#2	3.321(5)
K(1)-O(1)	2.770(6)	K(1)-Cl(1)	3.523(3)
K(1)-O(1W)#1	2.801(6)	K(1)-Cl(1)#1	3.583(3)
K(1)-O(1)#2	2.850(4)		
O(1W)-K(1)-O(1)#1	169.54(13)	O(1)#1-K(1)-O(3)#3	119.36(19)
O(1W)-K(1)-O(1)	84.13(16)	O(1)-K(1)-O(3)#3	108.02(17)
O(1)#1-K(1)-O(1)	95.48(14)	O(1W)#1-K(1)-O(3)#3	81.45(17)
O(1W)-K(1)-O(1W)#1	95.59(15)	O(1)#2-K(1)-O(3)#3	151.67(18)
O(1)#1-K(1)-O(1W)#1	82.91(16)	O(1W)-K(1)-O(2)#2	69.66(14)
O(1)-K(1)-O(1W)#1	169.69(13)	O(1)#1-K(1)-O(2)#2	101.67(15)
O(1W)-K(1)-O(1)#2	85.74(16)	O(1)-K(1)-O(2)#2	118.54(13)
O(1)#1-K(1)-O(1)#2	83.83(14)	O(1W)#1-K(1)-O(2)#2	52.31(13)

O(1)-K(1)-O(1)#2	83.66(14)	O(1)#2-K(1)-O(2)#2	41.49(13)
O(1W)#1-K(1)-O(1)#2	86.03(16)	O(3)#3-K(1)-O(2)#2	113.05(16)
O(1W)-K(1)-O(3)#3	70.42(18)		

Symmetry transformations used to generate equivalent atoms: #1 x+1,y,z #2 x+1/2,-y+1/2,-z+2 #3 x+1,y+1,z

Table S3. Band assignments (cm^{-1}) of vibrational modes observed in ATR-FTIR spectra of tested compounds

	$v_{as}COO^-$	v_sCOO^-	*vC=O*	*vC-O*	*vC-N*	vNH_2^+	δNH_2^+	*vO-H*	*vC-H arom*	$v_{as}NO_2$	v_sNO_2	*v(C-Cl)*
2Cl5NBH	-	-	1685	1250	-	-	-	-	3105	1528	1346	727
1	1584	1403	-	-	1076	bands 3100-2300	1584	-	3104	1516	1347	733
2	1596	1401	-	-	-	-	-	3438, 3219	3104	1521	1340	742

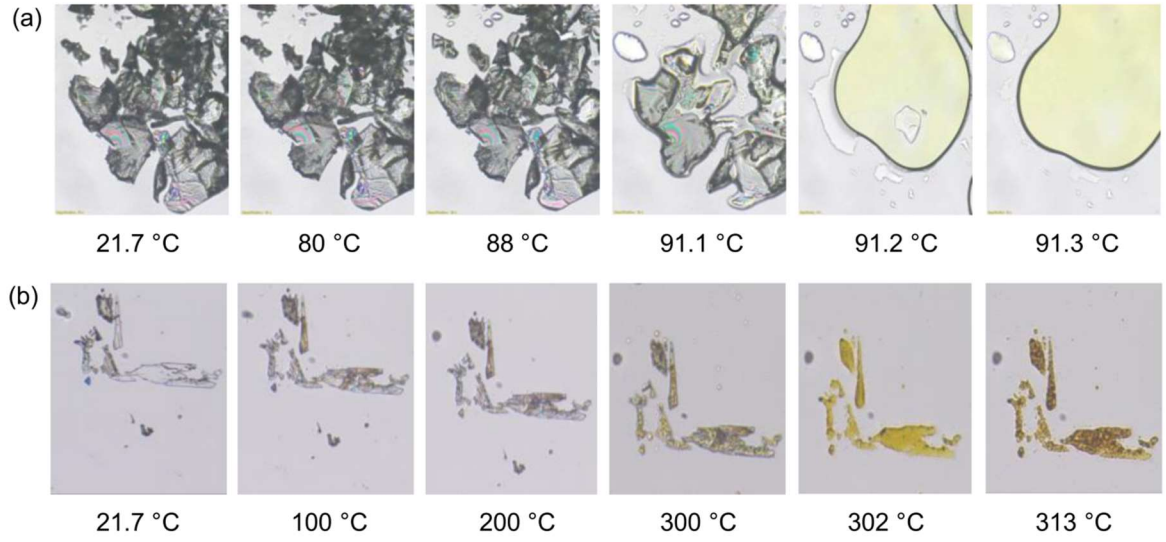


Figure S1. Optical micrographs of compounds **1** and **2** showing melting (a) and thermal degradation (b), respectively

2.2 Computational study

Table S4. Intermolecular interactions for compounds **1** and **2** derived from Hirshfeld surface analysis (*d_norm* surfaces)

Interaction category	Contact Types Included	Compound 1 (%)	Compound 2 (%)
Hydrogen bonding	O-H	37.4	30
	N-H	0.2	0.9
	Cl-H	13.3	4.3
	K-H	0	2.3
	total	**50.90%**	**38%**
van der Waals + π	H-H	26.8	12.8
	C-H	9.2	4.1
	C-C	2.8	6.7
	C-N	1.3	1.3
	O-C	3.3	3.7

	O-O	1.2	2.1
	total	**44.60%**	**30.70%**
Halogen contacts	Cl-Cl	0	0.5
	Cl-O	3	9
	Cl-N	0	0.1
	Cl-C	0	2.7
	total	**3.00%**	**12.30%**
Metal coordination contacts	K-Cl	0	1.8
	K-O	0	15.9
	K-C	0	0.7
	total	**0**	**18.40%**

All percentage values correspond to distinct interaction types; overlapping or duplicate contacts that could contribute to multiple categories have been omitted to ensure clear and independent representation of each interaction.

4. Materials and Methods

4.2 Assessment of antibacterial activity

4.2.2 Inhibition zone measurement

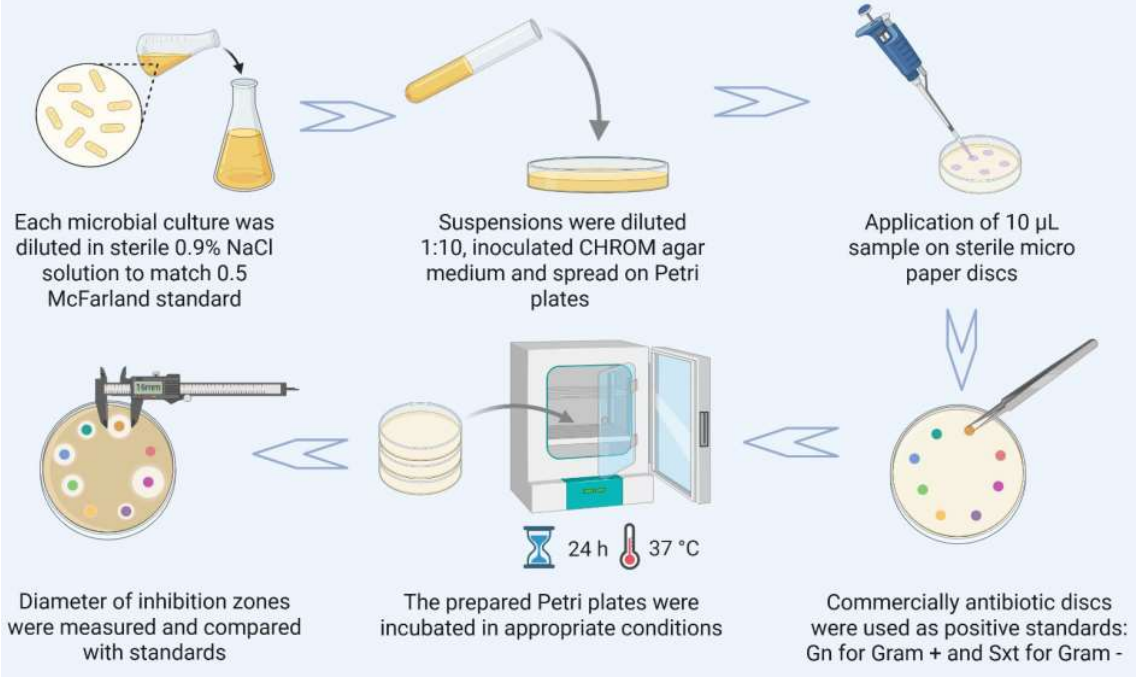


Figure S2. Main steps involved in the disk diffusion test for antibacterial activity evaluation

4.2.3 Bacterial cell viability evaluation

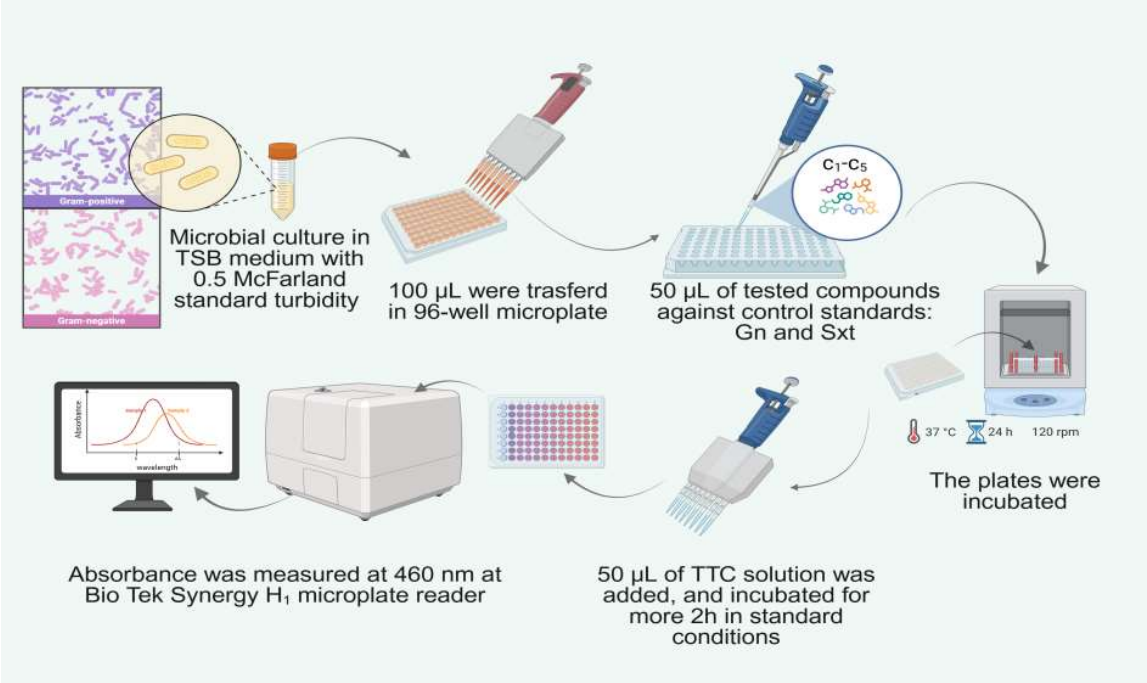


Figure S3. Sequential steps involved in the bacterial cell viability test

4.2.4 Biofilm inhibitory activity assessment

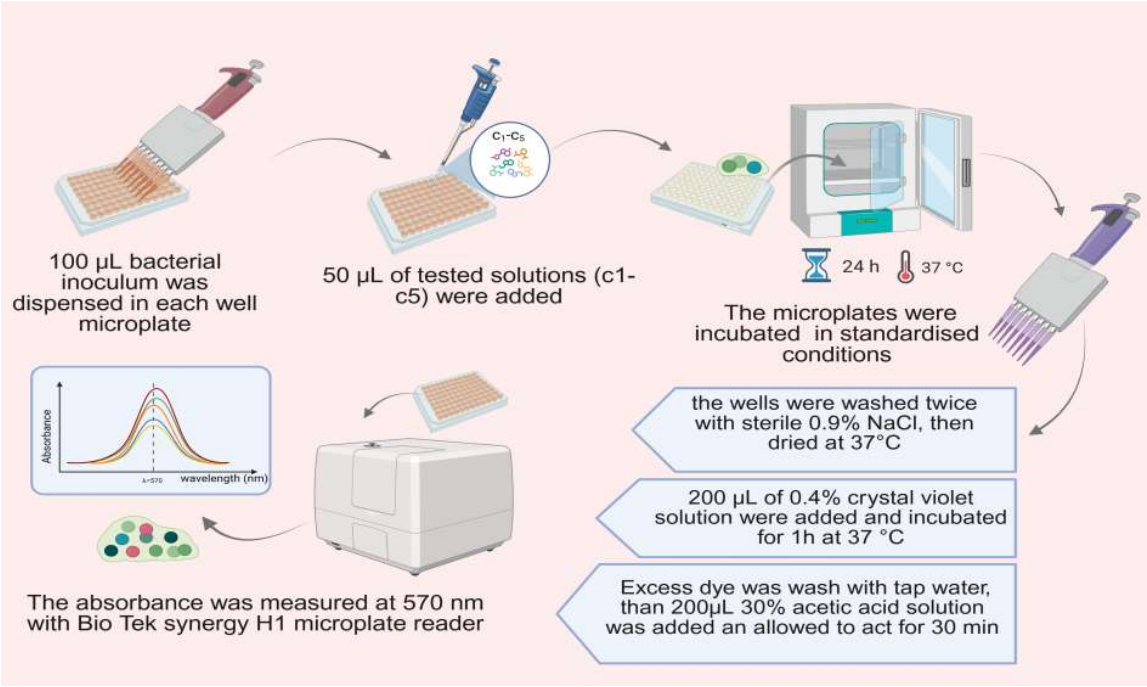


Figure S4. Experimental steps for evaluating the biofilm inhibitory activity of tested compounds