

Supporting Information

QSAR, Docking, and Molecular Dynamics Simulation Studies of Sigmacidins as Antimicrobials against *Streptococci*

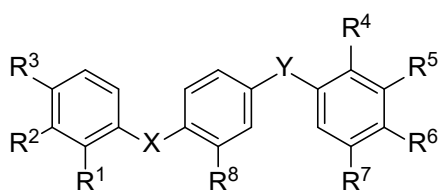
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
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Table S1. Chemical structures of the antimicrobials



Formular structure of **1–56**, except **cpd. 5** and **22**

Index	R ¹	R ²	R ³	R ⁴	R ⁵	R ⁶	R ⁷	R ⁸	X	Y
1	NH ₂	H	H	COOH	H	H	H	NO ₂	S	C(=O)
2	OCH ₃	H	H	COOH	H	H	H	NO ₂	S	C(=O)
3	H	Cl	Cl	COOH	H	H	H	NO ₂	S	C(=O)
4	H	H	H	COOH	H	H	H	NO ₂	NH	C(=O)
5										
6	NH ₂	H	H	H	COOH	H	H	NO ₂	S	C(O)NH
7	NH ₂	H	H	H	COOH	H	H	NO ₂	S	CH ₂ NH
8	H	NH ₂	H	COOH	H	H	H	NO ₂	S	C(=O)
9	H	H	NH ₂	COOH	H	H	H	NO ₂	S	C(=O)
10	NO ₂	H	CONEt ₂	COOH	H	H	H	NO ₂	S	C(=O)
11	H	H	H	COOH	H	H	H	NO ₂	CH ₂ N H	C(=O)
12	F	H	H	COOH	H	H	H	NO ₂	CH ₂ N H	C(=O)
13	H	CH ₃	H	COOH	H	H	H	NO ₂	NH	C(=O)
14	H	Cl	Cl	H	COOH	H	H	NO ₂	S	CH ₂ NH
15	H	Cl	Cl	H	COOH	H	H	NO ₂	S	C(O)NH
16	H	t-Bu	H	COOH	H	H	H	NO ₂	NH	C(=O)
17	F	H	H	COOH	H	H	H	NO ₂	S	C(=O)
18	H		H	COOH	H	H	H	NO ₂	S	C(=O)
19	NH ₂	H	H	H	H	COOH	H	NO ₂	S	C(O)NH
20	NH ₂	H	H	COOH	H	H	H	NO ₂	S	C(O)NH
21	CH ₃	H	CH ₃	COOH	H	H	H	NO ₂	S	C(=O)
22										
23	Cl	H	Cl	COOH	H	H	H	NO ₂	S	C(=O)
24	H		H	COOH	H	H	H	NO ₂	S	C(=O)
25	NH ₂	H	Cl	COOH	H	H	H	NO ₂	S	C(=O)
26	H	Cl	Cl	COOH	H	H	H	NO ₂	NH	C(=O)

27	NH ₂	H	H	COOH	H	H	H	NO ₂	S	CH ₂ NH
28	NH ₂	H	H	H	H	COOH	H	NO ₂	S	CH ₂ NH
29	H	AcNH	H	COOH	H	H	H	NO ₂	S	C(=O)
30	H	Cl	Cl	Cl	H	H	COOH	NO ₂	S	CH ₂ NH
31	H	Cl	Cl	OCH ₃	H	H	COOH	NO ₂	S	CH ₂ NH
32	H	Cl	Cl		H	H	COOH	NO ₂	S	CH ₂ NH
33	H	Cl	Cl	H	SO ₂ NH ₂	H	H	NO ₂	S	CH ₂ NH
34	H	Cl	Cl	CH ₃	H	H	COOH	NO ₂	S	CH ₂ NH
35	H	Cl	H	COOH	H	H	H	NO ₂	NH	C(=O)
36	H	Cl	Cl	Br	H	H	COOH	NO ₂	S	C(=O)
37	H	Cl	Cl	H	COOH	Cl	H	NO ₂	S	C(=O)
38	H	Cl	Cl	COOH	H	H	H	NO ₂	S	CH ₂ NH
39	H	Cl	Cl	COOH	H	H	H	H	S	C(=O)
40	H	Cl	Cl	COOH	H	H	Cl	NO ₂	S	CH ₂ NH
41	H	Cl	Cl	COOH	H	H	H	NO ₂	S	CH ₂
42	H	Cl	Cl	COOH	H	H	H	NH ₂	S	C(=O)
43	H	Cl	Cl	COOH	H	H	H	NMe ₂	S	C(=O)
44	H	Cl	Cl	COOH	H	H	Cl	NO ₂	S	C(=O)
45	H	Cl	Cl	COOH	H	Cl	H	NO ₂	S	C(=O)
46	H	Cl	Cl	COOH	H	H	CF ₃	NO ₂	S	C(=O)
47	H	Cl	Cl	COOH	H	Cl	H	NO ₂	S	CH ₂
48	H	Cl	Cl	COOH	H	H	CH ₃	NO ₂	S	CH ₂
49	H	Cl	Cl	COOH	H	H	OCH ₃	NO ₂	S	C(=O)
50	H	Cl	Cl	COOH	H	H	F	NO ₂	S	C(=O)
51	H	Cl	Cl	COOH	H	CF ₃	H	NO ₂	S	C(=O)
52	H	Cl	Cl	COOH	H	H	CF ₃	NO ₂	S	CH ₂
53	H	Cl	Cl	COOH	H	H	OCH ₃	NO ₂	S	CH ₂
54	H	Cl	Cl	COOH	H	H	Cl	NO ₂	S	CH ₂
55	H	Cl	Cl	COOH	H	H	F	NO ₂	S	C(=O)
56	H	Cl	Cl	COOH	H	CF ₃	H	NO ₂	S	C(=O)