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Supporting Information

Antibacterial β-cyclodextrin derivatives inspired by the antimicrobial peptide polymyxin in order to better understand the role of single hydrophobic chain tail in selective anti-bacterial activity

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Table of contents

Table 1. Antibacterial activity of the β-CD derivatives.

				MIC （μM）				
β-CD				Gram-positive		Gram-negative		
	R1	R2	ΣClogP	*S. aureus*	*E. faecalis*	*E. coli*	*P. aeruginosa*	*S.* Typhimurium
noAcβ-CD								
21	H	H	-27.2	>102	>102	>102	>102	>102
12	C6H13	H	-24.5	50	99	>99	99	>99
13	C8H17	H	-23.5	49	>98	>98	>98	>98
14	C10H21	H	-22.4	12	49	97	49	>97
15	C12H25	H	-21.3	24	96	24	48	96
16	C14H29	H	-20.3	24	24	12	12	95
17	C16H33	H	-19.2	6	12	12	12	94
18	C17H35	H	-18.7	11	11	11	11	45
19	C18H37	H	-18.2	11	11	11	11	45
20	C22H45	H	-16.0	>76	>76	>76	>76	>76
Acβ-CDs								
27	H	Ac	-19.9	>83	>83	>83	>83	>83
22	C8H17	Ac	-16.4	20	81	20	20	20
23	C10H21	Ac	-15.3	10	40	5	10	10
24	C12H25	Ac	-14.3	5	20	5	5	9
25	C16H33	Ac	-12.1	20	10	10	10	39
26	C22H45	Ac	-8.4	72	38	36	36	72
polymyxins B				25	194	3	6	3

Table 2. Hemolytic activity of the β-CD derivatives.

β-CD				Hemolytic activity
	R1	R2	ΣClogP	50 μM
noAcβ-CD				
21	H	H	-27.2	0.2
12	C6H13	H	-24.5	4.8
13	C8H17	H	-23.5	4.9
14	C10H21	H	-22.4	13.1
15	C12H25	H	-21.3	6.2
16	C14H29	H	-20.3	5.1
17	C16H33	H	-19.2	5.4
18	C17H35	H	-18.7	5.1
19	C18H37	H	-18.2	9.9
20	C22H45	H	-16.0	48.4
Acβ-CD				
27	H	Ac	-19.9	4.8
22	C8H17	Ac	-16.4	43.4
23	C10H21	Ac	-15.3	63.8
24	C12H25	Ac	-14.3	96.8
25	C16H33	Ac	-12.1	99.1
26	C22H45	Ac	-8.4	67.9
polymyxins B				0.8

NMR and MS spectra