

Supporting Information for
Polymeric membrane potentiometric antibiotic sensors using
computer-aided screening of supramolecular macrocyclic carriers

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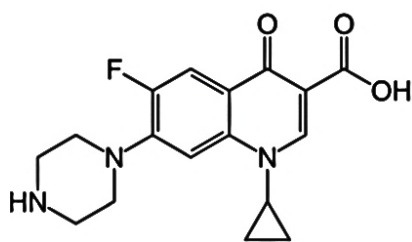
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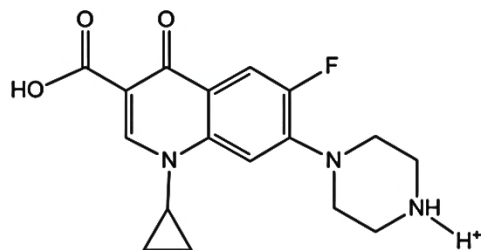
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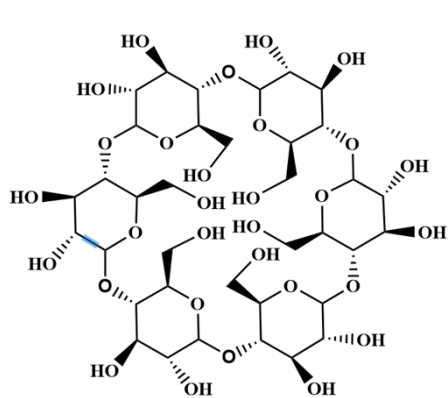
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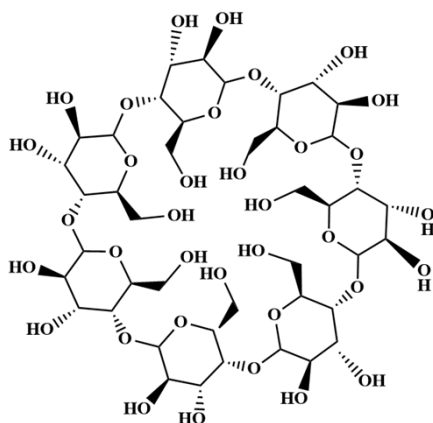
Neutral CIP



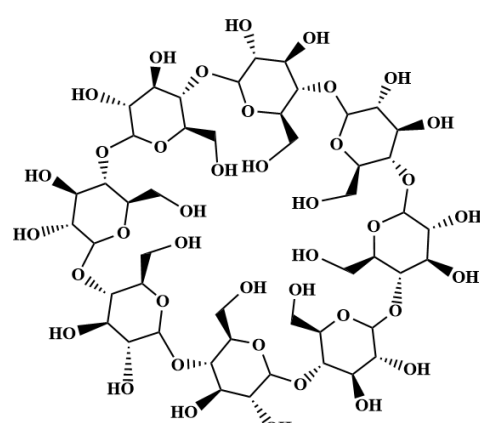
Protonated CIP



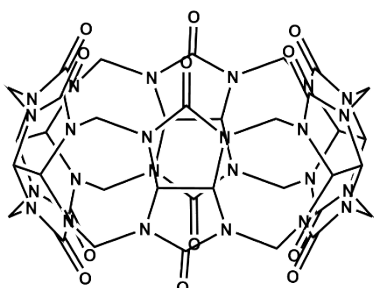
α -CD



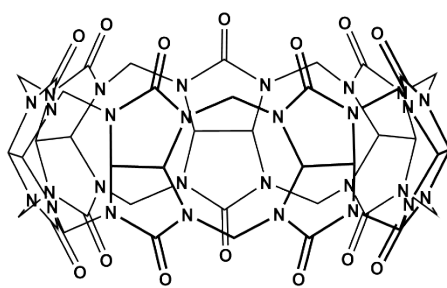
β -CD



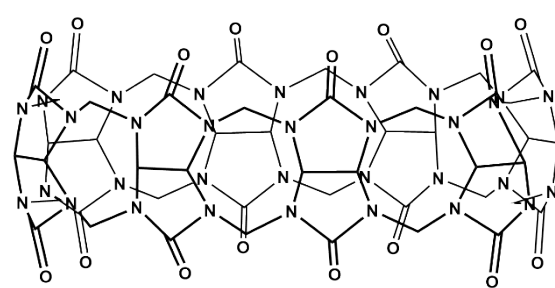
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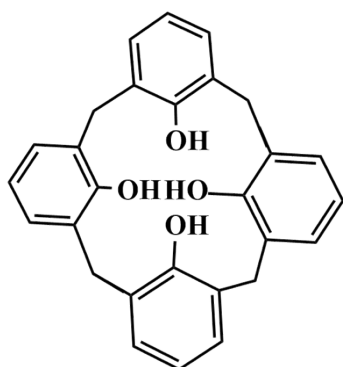
CB[6]



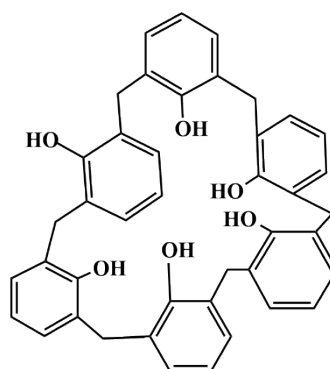
CB[7]



CB[8]



calix [4] arene



calix [6] arene

Fig. S1. Chemical structures of 8 organic carriers and CIP.

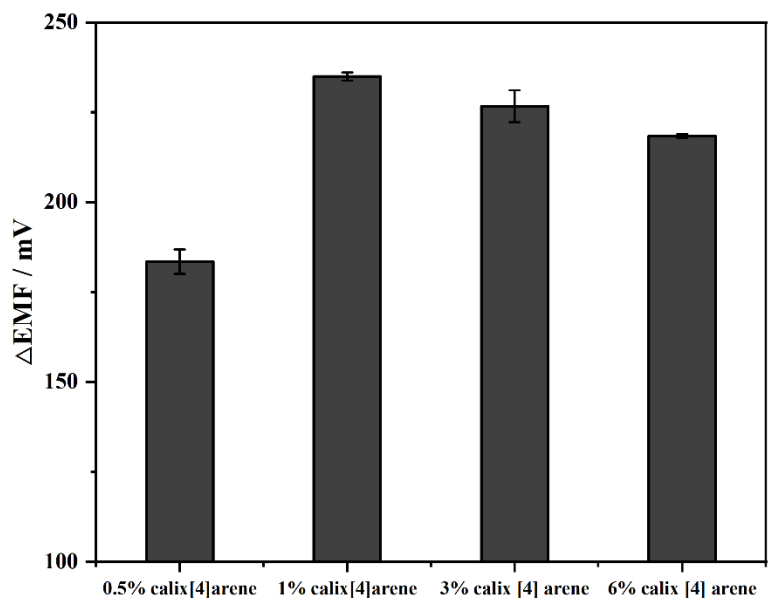


Fig. S2. Effect of the amount of the carrier calix [4] arene on the potential response.

Table S1. Docking and binding sites between CIP and supramolecular macrocyclic carriers.

Receptor	center x	center y	center z	size x	size y	size z
α-CD	-1	0	0	15	15	15
β-CD	0	0	0	15	15	15
γ-CD	1	0	0	15	15	15
CB[6]	-3	1	0	15	15	15
CB[7]	-2	1	1	15	15	15
CB[8]	-4	-1	0	16	16	16.5
calix [4] arene	-2	0	0	15	15	15
calix [6] arene	0	0	0	15	15	15

Table S2. Non-covalent interactions between 8 carriers and neutral CIP and corresponding bond lengths.

Creatinine complex	Interaction	Category	Type	Bond length(Å)	
Calix[4]arene-neutral CIP	benzene...cyclopropane	Hydrophobic	Pi-Alkyl	3.75	
	benzene...cyclopropane	Hydrophobic	Pi-Alkyl	4.03	
	benzene...cyclopropane	Hydrophobic	Pi-Alkyl	4.36	
	benzene...cyclopropane	Hydrophobic	Pi-Alkyl	4.10	
	calix[4]arene...cyclopropane	Hydrophobic	Alkyl	3.05	
	Calix[6]arene-neutral CIP	benzene...benzene	Hydrophobic	Pi-Pi T-shaped	5.32
		benzene...cyclopropane	Hydrophobic	Pi-Alkyl	5.44
β-CD-neutral CIP	C...O-H26	Hydrogen Bond	Conventional Hydrogen Bond	3.58	
	H128...O-C	Hydrogen Bond	Conventional Hydrogen Bond	1.90	
	H153...F	Hydrogen bond	Hydrogen /Halogen Bond	2.85	
	H108...O-C	Hydrogen Bond	Carbon Hydrogen Bond	2.52	
	H152...F-C	Hydrogen Bond	Carbon Hydrogen Bond	2.74	
	H156...O=C	Hydrogen Bond	Carbon Hydrogen Bond	2.80	
	H161...O=C	Hydrogen Bond	Carbon Hydrogen Bond	2.71	
	H164...O=C	Hydrogen Bond	Carbon Hydrogen Bond	2.49	
	CB[7]-neutral CIP	C=O...H26	Hydrogen Bond	Conventional Hydrogen Bond	3.06
C=O...H26		Hydrogen Bond	Conventional Hydrogen Bond	1.97	
C=O...C		Hydrogen Bond	Carbon Hydrogen Bond	3.51	

γ-CD- neutral CIP	C=O...benzene	Hydrogen Bond	Pi-Donor Hydrogen Bond	3.29
	C-O...F	Hydrogen bond Halogen bond	Hydrogen/Hal ogen Bond	3.21
	H158...O=C	Hydrogen Bond	Carbon Hydrogen Bond	2.46
	C-O...benzene	Hydrogen Bond	Pi-Donor Hydrogen Bond	3.42
α-CD- neutral CIP	C-O...benzene	Hydrogen Bond	Pi-Donor Hydrogen Bond	3.94
	C-O...H26	Hydrogen Bond	Conventional Hydrogen Bond	2.70
	H149...O=C	Hydrogen Bond	Conventional Hydrogen Bond	2.83
	H122...O-C	Hydrogen Bond	Carbon Hydrogen Bond	2.86
CB[8]-neutral CIP	C=O...C	Hydrogen Bond	Carbon Hydrogen Bond	3.71
	C=O...F	Halogen Bond	Halogen Bond	3.20
CB[6]-neutral CIP	C=O...H26	Hydrogen Bond	Conventional Hydrogen Bond	2.74
	C=O...O-H26	Hydrogen Bond	Conventional Hydrogen Bond	3.03
	C=O...C	Hydrogen Bond	Carbon Hydrogen Bond	3.80
	C=O... benzene	Hydrogen Bond	Pi-Donor Hydrogen Bond	3.45

Table S3. Non-covalent interactions between 8 carriers and protonated CIP and

corresponding bond lengths.

Creatinine complex	Interaction	Category	Type	Bond length(Å)
Calix[4]arene-protonated CIP	benzene...benzene	Hydrophobic	Pi-Pi Stacked	4.92
	benzene...piperazine	Hydrophobic	Pi-Pi Stacked	4.29
	calix[4]arene...cyclopropane	Hydrophobic	Alkyl	3.01
	benzene...cyclopropane	Hydrophobic	Pi-Alkyl	3.72
	benzene...cyclopropane	Hydrophobic	Pi-Alkyl	4.34
	benzene...cyclopropane	Hydrophobic	Pi-Alkyl	3.96
	benzene...cyclopropane	Hydrophobic	Pi-Alkyl	4.13
Calix[6]arene-protonated CIP	benzene...benzene	Hydrophobic	Pi-Pi Stacked	4.33
	benzene...piperazine	Hydrophobic	Pi-Pi Stacked	5.30
	benzene...piperazine	Hydrophobic	Pi-Pi T-shaped	5.80
	benzene...cyclopropane	Hydrophobic	Pi-Alkyl	5.29
	C...H42-O	Hydrogen bond	Carbon hydrogen bond	3.71
β-CD-protonated CIP	H129...F	Hydrogen bond Halogen bond	Hydrogen/Halogen bond	2.69
	H152...C=O	Hydrogen bond	Conventional hydrogen bond	2.98
	C...O-H170	Hydrogen bond	Carbon hydrogen bond	3.53
	H152...O=C	Hydrogen bond	Carbon hydrogen bond	2.60
	H165...F-C	Hydrogen bond	Carbon hydrogen bond	2.41
H167...F-C	Hydrogen bond	Carbon hydrogen bond	2.20	

CB[7]- protonated CIP	C=O...H27	Hydrogen Bond	Conventional hydrogen bond	2.83
	C=O...H27	Hydrogen bond	Conventional hydrogen bond	1.94
	C=O...O=C	Hydrogen bond	Conventional hydrogen bond	2.86
	C=O...O=C	Hydrogen bond	Conventional hydrogen bond	3.05
	C=O...benzene	Hydrogen bond	Pi-Donor hydrogen bond	3.92
γ-CD- protonated CIP	H147...O=C	Hydrogen bond	Conventional hydrogen bond	2.83
	H185O...C	Hydrogen bond	Carbon hydrogen bond	3.50
α-CD- protonated CIP	H142O...H16	Hydrogen bond	Conventional hydrogen bond	1.99
	H111-O...C	Hydrogen bond	Carbon hydrogen bond	3.44
	H95...F-C	Hydrogen bond	Carbon hydrogen bond	2.43
CB[8]- protonated CIP	C=O...C	Hydrogen bond	Carbon hydrogen bond	3.4
	C=O...H27	Hydrogen bond	Conventional hydrogen bond	2.6
CB[6]- protonated CIP	C=O...C	Hydrogen bond	Carbon hydrogen bond	3.53
	H27...O=C	Hydrogen bond	Conventional hydrogen bond	3.03
