Supporting Information

Mimicking an Antimicrobial Peptide Polymyxin B by Use of Cyclodextrin

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Syntheses of polyamino cyclodextrin (CD) derivatives 1-3 and polybenzylamino derivatives 4-6

Octaamino γ-CD derivatives **3** were synthesized as follows. Lyophilized octakis(6-*O*-*p*-tosyl)-γ-CD (986 mg, 1.98 x 10^{-4} mol)[7] was reacted with sodium azide (1.02 g, 1.56x10^{-4} mol) in DMF (10 mL) at 60 °C for 1 day. After addition of water (10 mL) the solution was concentrated in vacuo and poured into water (100 mL). The precipitate was collected by centrifugation (3000 rpm, 10 min) and lyophilized, giving octaazido derivative (421 mg, 72.2%). The azido (298 mg, 2.02x10^{-4} mol) in 1,4-dioxane/CH_3OH (5:1, 36ml) was reacted with triphenylphosphine (1.28 g, 4.90x10^{-3} mol) in argon atmosphere for 1 d. After addition of 28% aq. NH_3 (10 mL) followed by addition of d HCl to pH 4, the solution was washed with benzene (100 mL x 3) and lyophilized, giving a crude product (321 mg). The preparation was performed twice. The crude (465 mg) was dissolved in water (1.2 mL) and applied to gel filtration chromatography (Sephadex LH-20, Pharmacia) to give an octaamino derivative **3** (162 mg). The hexa- and heptaamino derivatives **1** and **2** were prepared similarly from the corresponding poly-6-*O*-sulfonyl-CD.[7]

The octa-benzylamino derivative **6** was prepared as follows. Lyophilized octakis(6-*O*-*p*-tosyl)-γ-CD (150 mg, 5.93 x 10^{-5} mol)[7] was reacted with benzylamine (24 ml) at 90 °C for 45 h. The solution was concentrated in vacuo, to which water (1 mL)

was added. On neutralization by 1 M aq. HCl the precipitate was observed and it was removed by filtration. The filtrate was applied to gel filtration chromatography (Sephadex LH-20, Pharmacia) to give **6** (23.6 mg, 17.3 %). Its low yield was because most of the **6** was eluted with benzylamine on the chromatography. It may be due to complex formation of benzylamine by CD molecule. The hexa- and hepta-benzylamino derivatives **4** and **5** were prepared similarly.