

# An Experimental Study of the Solvent-Dependent Self-assembly/Disassembly and Conformer Preferences of Gramicidin A

*Liuxi Chen, Shu-Hua Chen and David H. Russell*

Laboratory for Biological Mass Spectrometry

Department of Chemistry, Texas A&M University, College Station, TX 77843

## Supporting information:

1. Figure S1. Expanded view of the ESI mass spectrum of the as received Fluka gramicidin sample.
2. Figure S2. H/D exchange data (plot of deuterium content vs. incubation time in deuteriated ( $\text{CH}_3\text{OD}$ )) for GA.
3. Figure S3. The fitting parameters of H/D exchange rates by Equation 2.

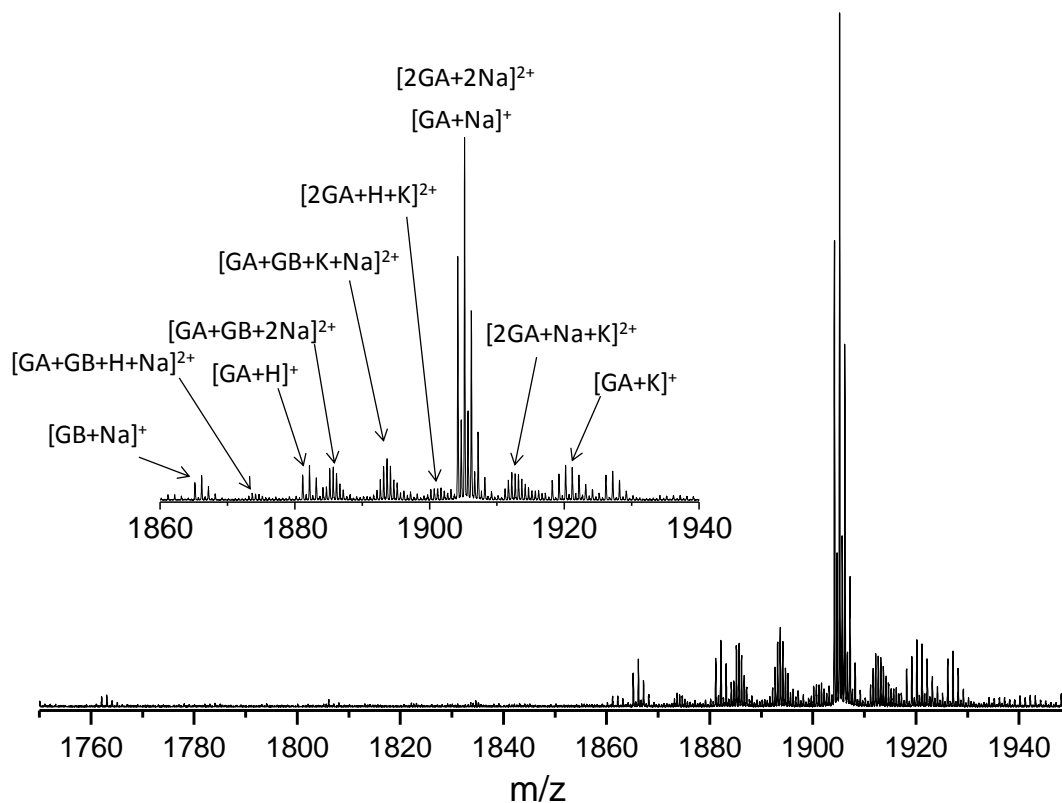


Figure S1. Expanded view of the ESI mass spectrum of the ‘as received’ Fluka gramicidin sample, which is a mixture containing gramicidins A, B, C and D. The spectrum contains signals for gramicidin A and gramicidin B, as well as signals that correspond to dimer ions composed of GA/GB; however, the signals are widely separated from the GA dimer and do not interfere with either the mass or ion mobility measurements. No signals for gramicidin C and D were observed.

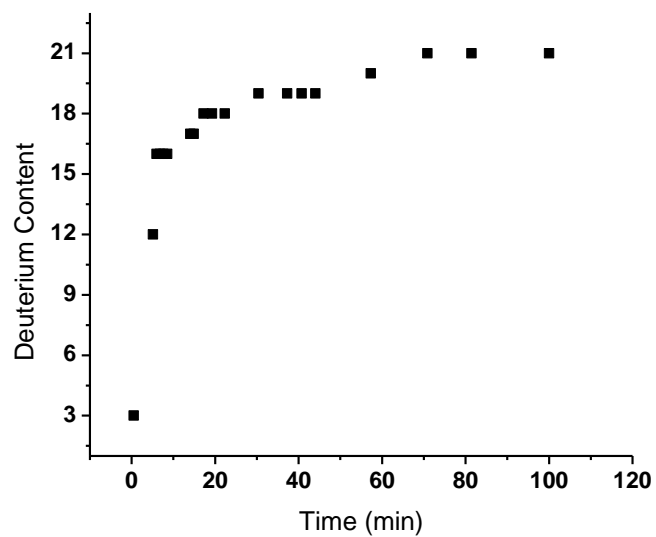
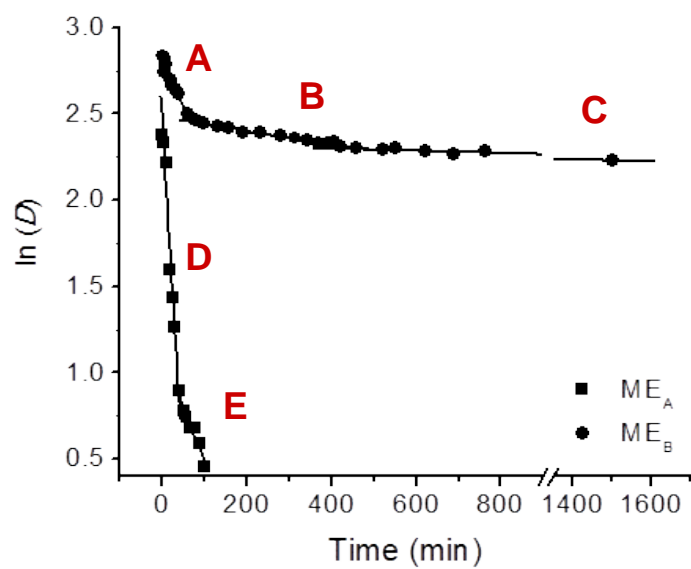


Figure S2. H/D exchange data (plot of deuterium content vs. incubation time in deuteriated ( $\text{CH}_3\text{OD}$ )) for GA. The data shows that all 21 exchangeable hydrogen atoms are exchanged for deuteriums during the 2 hr incubation.



Group		$k_{\text{ex}}^i \text{ (min}^{-1}\text{)}$	$\ln(H_{\text{tot}}^i)$	$R^2$
$\text{ME}_A$	D	$4.1 \times 10^{-2}$	2.5	0.9660
	E	$6.4 \times 10^{-3}$	1.1	0.9472
$\text{ME}_B$	A	$5.5 \times 10^{-3}$	2.8	0.9452
	B	$4.0 \times 10^{-4}$	2.4	0.9817
	C	$6.3 \times 10^{-5}$	2.3	0.8968

Figure S3. The fitting parameters of H/D exchange rates by Equation 2.  $H_{\text{tot}}^i$  is the total number of exchangeable hydrogens,  $k_{\text{ex}}^i$  is the HDX rate constant, and  $t$  is the incubation time.