

C₆₀ Secondary Ion Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

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Table of Contents

Figure S-1: Schematic drawing of the C ₆₀ SIMS source that has been coupled to a 12 T FT-ICR MS.....	S-2
Figure S-2: C ₆₀ SIMS FT-ICR MS of ~5 pmol gramicidin S.	S-3
Table S-1: Sequence identification/annotation and performance metrics for CID MS/MS of gramicidin S (see Fig. 3 in main text).....	S-4

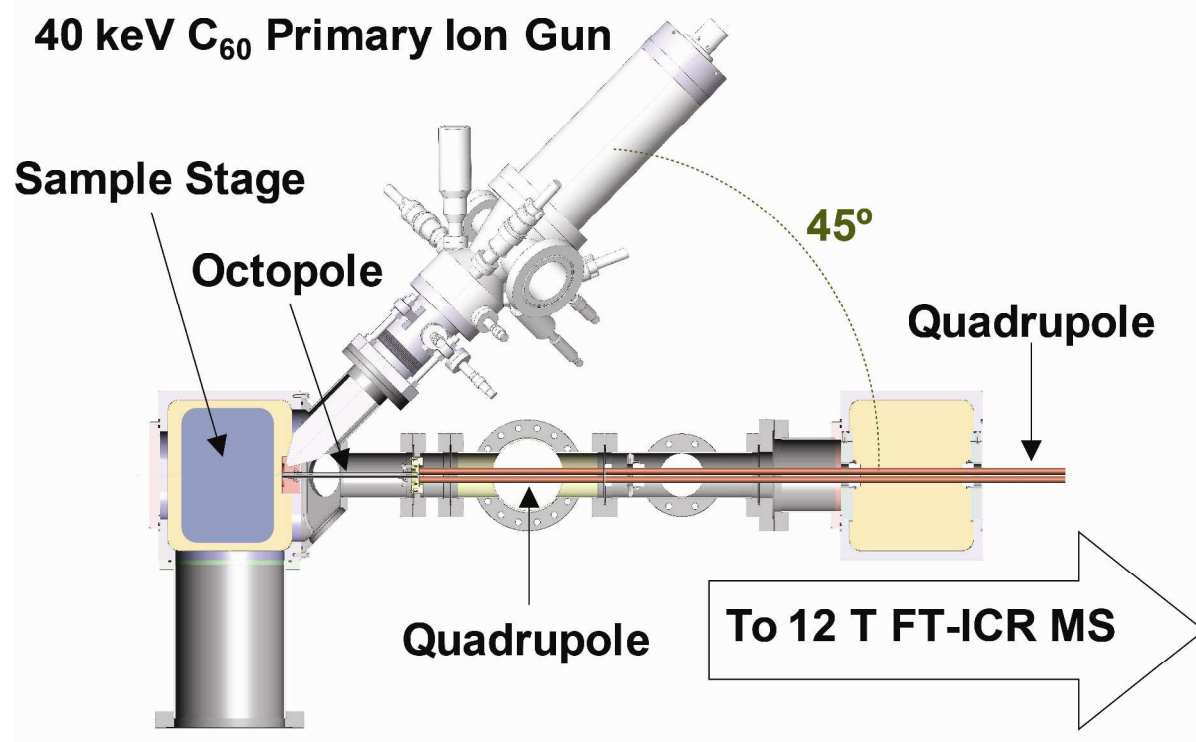


Figure S-1: Schematic drawing of the C₆₀ SIMS source that has been coupled to a 12 T FT-ICR MS.

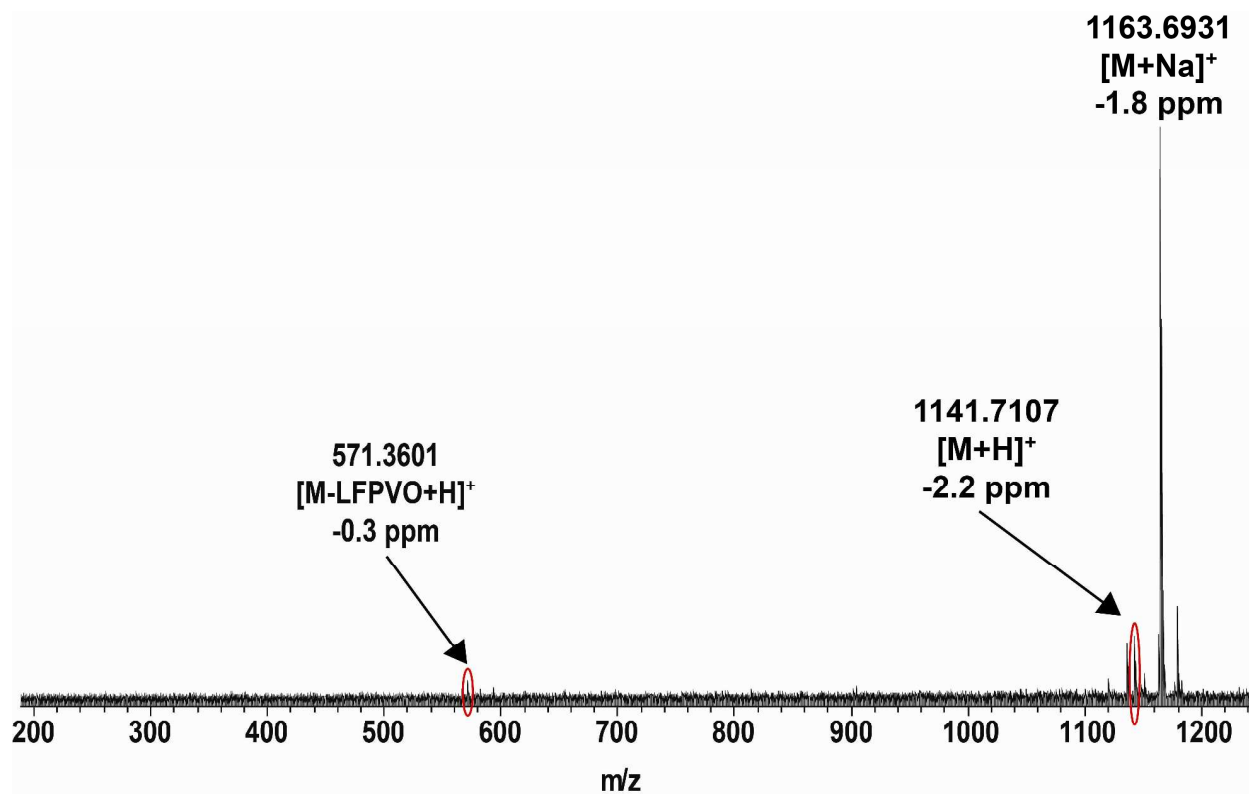


Figure S-2: C_{60} SIMS FT-ICR MS of ~5 pmol gramicidin S. The sodiated molecular ion dominates the mass spectrum and fragmentation is minimal. The ion at 571.3601 m/z is half of the cyclodecapeptide.

<u>Sequence</u>	<u>Annotation</u>	<u>Mass Resolving Power</u>	<u>External Calibration</u>		<u>Internal Calibration</u>	
			Measured Mass	MMA (ppm)	Measured Mass	MMA (ppm)
PVO	b _{3PF}	199,564	311.2077	-0.22	311.2077	-0.22
LFPV-CO	b _{4LO} -CO	152,268	429.2862	0.42	429.2863	0.66
LFPV	b _{4LO}	141,509	457.2808	-0.29	457.2809	-0.07
LFPVO	b _{5LO} *	109,941	571.3600	-0.43	571.3604	0.27
LFPVO-H ₂ O	b _{6LO} -H ₂ O	102,039	666.4329	-1.27	666.4336	-0.22
LFPVOF-H ₂ O	b _{7LO} -H ₂ O	78,030	813.5004	-2.16	813.5017	-0.57
LFPVOLF	b _{7LO}	64,985	831.5119	-0.99	831.5132	0.57
LFPVOLFPV	b _{9LO}	59,917	1027.6330	-0.84	1027.6354	1.49
LFPVOLFPVO	[M+H] ⁺	47,058	1141.7091	-3.61	1141.7122	-0.89

Table S-1: Sequence identification/annotation and performance metrics for CID MS/MS of gramicidin S (see Fig. 3 in main text). The spectrum was internally calibrated with respect to all ions indicated in the table. *The ion at 571.36 m/z is half of the cyclodecapeptide. Thus, it could be any of the following fragments: b_{5LO}, b_{5FL}, b_{5PF}, b_{5VP}, b_{5OV}, b_{5FL}, b_{5PF}, b_{5VP} or b_{5OV}. It is indicated here as b_{5LO} due to the identification of the other ions, where the cyclic peptide is broken at LO to form a decomposing linear ion.