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Synthetic modifications of the antibiotic peptide gramicidin S : conformational and biological aspects

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**Synthetic Modifications
of the Antibiotic Peptide
Gramicidin S**
Conformational and Biological Aspects

PROEFSCHRIFT

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List of abbreviations

Å	Ångstrom	ESI	electron spray ionization
AA	amino acid	Et	ethyl
Ac	acetyl	<i>et al.</i>	<i>et alii</i> (and others)
ACN	acetonitrile	EtOAc	ethyl acetate
Ada	adamantyl	Fmoc	9H-fluoren-9-ylmethoxycarbonyl
aq.	aqueous	g	gram(s)
Ar	aromatic	GC	gas chromatography
<i>B. cereus</i>	<i>Bacillus cereus</i>	GS	gramicidin S
<i>B. brevis</i>	<i>Bacillus brevis</i>	h	hour(s)
<i>B. subtilis</i>	<i>Bacillus subtilis</i>	HATU	2-(1 <i>H</i> -7-azabenzotriazol-1-yl)- 1,1,3,3-tetramethyl uranium
BHA	benzylhydramine		hexafluorophosphate
Bn	benzyl		methanaminium
Boc	<i>tert</i> -butoxycarbonyl	HBTU	O-Benzotriazole- <i>N,N,N',N'</i> - tetramethyl-uronium-hexafluoro- phosphate
br	broad		2-(6-chloro-1 <i>H</i> -benzotriazole-1- yl)-1,1,3,3-tetramethyl-aminium
Bu	butyl		hexafluorophosphate
calcd.	calculated	HCTU	1-hydroxy-benzotriazole
cat.	catalytic		4-(4-hydroxymethyl-3-methoxy- phenoxy)- butyric acid
CAP	cationic antimicrobial peptide	HOBt	high performance liquid
CD	circular dichroism	HMPB	chromatography
COSY	correlation spectroscopy		high resolution mass spectroscopy
C _q	quaternary carbon atom	HPLC	heteronuclear single quantum
cROESY	compensated rotational nuclear Overhauser effect spectroscopy		coherence spectroscopy
CSA	camphorsulfonic acid	HRMS	hertz
CVFF	Consistent Valence Force Field	HSQC	hemolytic concentration at which 50% of human red blood cells are lysed
d	doublet		<i>id est.</i> (in other words)
δ	chemical shift	Hz	infrared
Δ	change	HC ₅₀	isopropyl
DCE	1,2-dichloroethane		coupling constant
DCM	dichloromethane	<i>i. e.</i>	liter(s)
dd	doublet of doublet	IR	leucine (one letter abbreviation)
ddd	double double doublet	isoprop	liquid chromatography mass
ddt	double double triplet	<i>J</i>	spectroscopy
DEAD	diethyl azodicarboxylate	L	lipopolysaccharide
DG	distance geometry	Leu (L)	lysine (one letter abbreviation)
DiPEA	<i>N,N</i> -diisopropyl- <i>N</i> -ethylamine	LC/MS	multiplet
DNA	deoxyribonucleic acid		morpholino amino acid
DMAP	<i>N,N</i> -dimethylaminopyridine	LPS	mass/charge ratio
DMF	<i>N,N</i> -dimethylformamide	Lys (K)	4-methylbenzyl-hydramine
DQF	Double-Quantum Filtered	m	methyl
DMSO	dimethylsulfoxide	MAA	
dt	double triplet	<i>m/z</i>	
<i>E. coli</i>	<i>Escherichia coli</i>	MBHA	
<i>E. faecalis</i>	<i>Enterococcus faecalis</i>	Me	
<i>e.g.</i>	<i>exempli gratia</i> (for example)		
eq	(molar) equivalents		

MeOH	methanol	RP	reversed phase
MIC	minimal inhibitory concentration	rt	room temperature
MS	mass spectrometry	RT	retention time
MRSA	methicilin resistant <i>Staphylococcus aureus</i>	s	singlet
		sat.	saturated
MW	molecular weight	<i>S.aureus</i>	<i>Staphylococcus aureus</i>
NMP	<i>N</i> -methyl-2-pyrrolidone	<i>S. epidermidis</i>	<i>Staphylococcus epidermidis</i>
NMR	nuclear magnetic resonance	SAA	sugar amino acid
NOE	nuclear Overhauser effect	sext	sextet
Orn (O)	ornithine (one letter abbreviation)	SPPS	solid-phase peptide synthesis
ORD	optical rotary dispersion	t	triplet
<i>P. aeruginosa</i>	<i>Pseudomonas aeruginosa</i>	TBAF	tetra n-butylammonium fluoride
PE	light petroleum ether	TBDPS	t-butylidiphenylsilyl
Phe (F)	phenylalanine (one letter abbreviation)	THF	tetrahydrofuran
		Tf	triflate
Ph	phenyl	TFA	trifluoroacetic acid
ppb	parts per billion	TFE	trifluoroethanol
ppm	parts per million	TIS	triisoproylsilane
Pro (P)	proline (one letter abbreviation)	TMS	trimethylsilyl
pyBOP	benzotriazol-1-yl-oxy-tris-pyrrolidinophosphonium hexafluorophosphate	Ts	tosyl
		TLC	thin-layer chromatography
q	quartet	TOCSY	totally correlated spectroscopy
ROE	rotational nuclear Overhauser effect	Tyr (Y)	tyrosine (one letter abbreviation)
		UV	ultraviolet
r.o.s.	recovery of starting material	v/v	volume ratio
		Valine (V)	valine (one letter abbreviation)

