McLean Group Collision Cross Section Database
MALDI Generated Data
Natural Products

Biomolecular Class	Name	species	m/z (Da)	Ω (Å^2)	σ
cyclic peptide	valinomycin	[M+H]+	1111.6	271.9	1.4
cyclic peptide	valinomycin	[M+Na]+	1133.6	269.7	0.8
cyclic peptide	valinomycin	[M+K]+	1149.6	274.5	0.6
cyclic peptide	phleomycin	[M+H]+	1427.7	275.7	1.3
cyclic peptide	phleomycin	[M+Na]+	1448.4	276.7	1.2
cyclic peptide	phleomycin	[M+Cu]+	1489.5	276.8	2.7
cyclic peptide	cyclosporin	[M+H]+	1202.6	296.6	1.2
cyclic peptide	cyclosporin	[M+Na]+	1224.8	289.9	1.2
cyclic peptide	polymyxin	[M+H]+	1187.6	283.9	1.1
cyclic peptide	polymyxin	[M+Na]+	1225.7	279.4	0.9
cyclic peptide	polymyxin	[M+K]+	1241.7	284.4	4.9
cyclic peptide	actinomycin	[M+H]+	1255.6	280.1	1.9
cyclic peptide	actinomycin	[M+Na]+	1277.6	284.2	0.7
cyclic peptide	actinomycin	[M+K]+	1293.6	280.8	4.1
cyclic peptide	bacitracin	[M+H]+	1422.8	301.2	0.8
cyclic peptide	bacitracin	[M+Na]+	1444.7	305.3	1.0
cyclic peptide	bacitracin	[M+K]+	1460.7	303.6	2.3
cyclic peptide	thiostrepton	[M+H]+	1664.5	310.0	1.6

cyclic peptide	thiostrepton	[M+Na]+	1686.5	315.5	1.0
cyclic peptide	thiostrepton	[M+K]+	1702.5	314.8	3.0
cyclic peptide	vancomycin	[M+H]+	1448.4	299.4	0.9
cyclic peptide	vancomycin	[M+Na]+	1470.4	296.0	3.7
cyclic peptide	vancomycin	[M+K]+	1486.4	299.4	3.8
cyclic peptide	ampicillin	[M+Na]+	372.1	110.1	1.3
cyclic peptide	siamycin I	[M+Na]+	2185.8	373.2	0.8
cyclic peptide	siamycin I	[M+K]+	2201.8	375.2	1.7
polyether antibiotics	monensin	[M+Na]+	694.4	183.9	0.5
polyether antibiotics	monensin	[M+K]+	709.3	183.8	1.0
macrolide	amphotericin	[M-H_2O+H]+	905.9	235.0	4.3
macrolide	amphotericin	[M+H]+	924.4	236.1	2.8
macrolide	amphotericin	[M-H2O+Na]+	928.8	236.2	3.9
macrolide	amphotericin	[M-H2O+K]+	947.1	241.9	1.5
macrolide	nystatin	[M-H2O+Na]+	930.8	234.6	4.5
macrolide	nystatin	[M+Na]+	948.7	241.5	2.1
macrolide	josamycin	[M+H]+	828.2	241.4	1.2
macrolide	josamycin	[M+Na]+	850.2	239.6	0.8
macrolide	josamycin	[M+K]+	865.6	241.8	1.5
macrolide	tylosin	[M+H]+	916.7	239.3	1.3
macrolide	tylosin	[M+Na]+	938.6	226.2	2.3
macrolide	erythromycin	[M+H]+	735.4	191.6	1.0
macrolide	erythromycin	[M+Na]+	757.3	196.0	0.7
macrolide	erythromycin	[M+K]+	773.1	195.1	0.7
macrolide	brefeldin	[M+Na]+	303.0	107.0	1.3
macrolide	isoapoptolidin	[M+Na]+	1152.1	260.0	0.7
macrolide	isoapoptolidin	[M+K]+	1168.6	259.4	2.5
macrolide	rifampacin	[M+H]+	823.4	206.1	2.4

macrolide	rifampacin	[M+Na]+	846.4	216.7	1.1
macrolide	rifampacin	[M+K]+	862.6	214.3	1.2
aromatic polyketide	tetracyclin	[M+H]+	443.1	132.4	1.3
aromatic polyketide	tetracyclin	[M+Na]+	465.2	133.3	1.7
aromatic polyketide	doxorubicin	[M+H]+	544.8	156.9	0.8
aromatic polyketide	doxorubicin	[M+Na]+	566.8	159.4	0.9
aminoglycoside antibiotic	everninomycin	[M-HCl+H]+	1563.5	294.4	0.7
aminoglycoside antibiotic	everninomycin	[M+Na]+	1621.5	303.6	0.7
aminoglycoside antibiotic	apramycin	[M+H]+	540.9	156.5	1.4
aminoglycoside antibiotic	apramycin	[M+Na]+	563.0	152.4	4.6
aminoglycoside antibiotic	apramycin	[M+K]+	576.9	160.5	3.9
aminoglycoside antibiotic	kanamycin	[M+H]+	486.1	133.1	1.9
aminoglycoside antibiotic	kanamycin	[M+Na]+	508.4	136.5	1.0
aminoglycoside antibiotic	neomycin	[M+H]+	615.9	164.3	0.9
aminoglycoside antibiotic	neomycin	[M+Na]+	638.2	164.3	1.3
other	antimycin	[M+H]+	551.0	171.7	2.3
other	antimycin	[M+Na]+	571.8	169.5	0.8
other	antimycin	[M+K]+	587.7	172.7	2.7
other	capsaicin	[M+H]+	307.3	119.0	1.4
other	capsaicin	[M+Na]+	329.4	114.2	3.2
other	lincomycin	[M+H]+	408.0	134.6	0.5
other	lincomycin	[M+Na]+	429.9	133.5	0.7
other	lincomycin	[M+K]+	441.9	140.2	0.9