Table S2. Molecular ion transitions (Q1> Q3) and wavelengths used for the detection of palytoxin and its analogues (ovatoxins, ostreocins, mascarenotoxins)

Analogs	Q1 (*m/z*)	Q3 (*m/z*, fragment A)	UV detection λ (nm)	References
PlTX	1340.2 $[M+2H]^{2+}$ 1331.2 $[M+2H-H_2O]^{2+}$ 887.5 $[M+3H-H_2O]^{3+}$	327.2	233, 263	[31, 93]
42-OH-PlTX	1348.2 $[M+2H]^{2+}$ 1339.2 $[M+2H-H_2O]^{2+}$ 899.7 $[M+3H]^{3+}$	327.2	233, 263	[94, 95]
Ovatoxin-a	1324.3 $[M+2H]^{2+}$ 1315.2 $[M+2H-H_2O]^{2+}$ 876.8 $[M+3H-H_2O]^{3+}$	327.2	233, 263	[31, 40]
Ovatoxin-b	1346.3 $[M+2H]^{2+}$ 1337.3 $[M+2H-H_2O]^{2+}$ 891.5 $[M+3H-H_2O]^{3+}$	371.2	233, 263	[33, 40]
Ovatoxin-c	1354.3 $[M+2H]^{2+}$ 1345.3 $[M+2H-H_2O]^{2+}$ 896.8 $[M+3H-H_2O]^{3+}$	371.2	233, 263	[33, 40]
Ovatoxin-d	1332.3 $[M+2H]^{2+}$ 1323.2 $[M+2H-H_2O]^{2+}$ 882.2 $[M+3H-H_2O]^{3+}$	327.2	233, 263	[33, 40]
Ovatoxin-e	1332.3 $[M+2H]^{2+}$ 1323.2 $[M+2H-H_2O]^{2+}$ 882.2 $[M+3H-H_2O]^{3+}$	343.2	233, 263	[33, 40]
Ovatoxin-f	1338.3 $[M+2H]^{2+}$ 1329.3 $[M+2H-H_2O]^{2+}$ 886.2 $[M+3H-H_2O]^{3+}$	327.2	233, 263	[34, 40]
Ovatoxin-g	1316.3 $[M+2H]^{2+}$ 1307.2 $[M+2H-H_2O]^{2+}$ 871.5 $[M+3H-H_2O]^{3+}$	327.2	233, 263	[35]
Ovatoxin-h	1317.3 $[M+2H]^{2+}$ 1308.3 $[M+2H-H_2O]^{2+}$ 872.2 $[M+3H-H_2O]^{3+}$	327.2	233, 263	[36]
Ovatoxin-i	1345.3 $[M+2H]^{2+}$ 1336.3 $[M+2H-H_2O]^{2+}$ 890.8 $[M+3H-H_2O]^{3+}$	327.2	233, 263	[40]
Ovatoxin-j1/j2	1353.3 $[M+2H]^{2+}$ 1344.3 $[M+2H-H_2O]^{2+}$ 896.2 $[M+3H-H_2O]^{3+}$	327.2	233, 263	[40]
Ovatoxin-k	1361.3 $[M+2H]^{2+}$ 1352.2 $[M+2H-H_2O]^{2+}$ 901.5 $[M+3H-H_2O]^{3+}$	327.2	233, 263	[40]
Ostreocin-D	1329.2 $[M+H+Na]^{2+}$ 1318.2 $[M+2H]^{2+}$ 893.3 $[M+H+2Na]^{3+}$	313.2	233, 263	[44]
Ostreocin-B	1337.2 $[M+H+Na]^{2+}$ 1326.2 $[M+2H]^{2+}$ 898.7 $[M+H+2Na]^{3+}$	313.2	233, 263	[47, 80]
Ostreocin-A	1337.2 $[M+H+Na]^{2+}$ 1326.2 $[M+2H]^{2+}$ 898.7 $[M+H+2Na]^{3+}$	313.2	233, 263	[46]
Ostreocin-E1	1320.2 $[M+H+Na]^{2+}$ 1309.2 $[M+2H]^{2+}$ 887.3 $[M+H+2Na]^{3+}$	313.2	233, 263	[46]
Mascarenotoxin-A	1295.5 836.9 606.3	327.2	233, 263	[96, 97]
Mascarenotoxin-B	1304.3 864.9 836.2	327.2	233, 263	[96]
Mascarenotoxin-C	1326.3 $[M+H+Na]^{2+}$ 1315.3 $[M+2H]^{2+}$ 877 $[M+3H]^{3+}$	327.2	233, 263	[97]