

Supplementary materials

Paralytic Shellfish Poisoning (PSP) Toxins in Bivalve Molluscs from Southern Italy Analysed by Liquid Chromatography Coupled with High-Resolution Mass Spectrometry (UHPLC-HRMS/MS)

Pasquale Gallo, Sara Lambiase, Ida Duro, Mauro Esposito and Angela Pepe

Table S1: Stock standard aqueous solutions of the PSP toxins studied.

PSP Toxin	Certified concentration ($\mu\text{g mL}^{-1}$)	Volume (μL)	Solvent (μL)	Total Volume (μL)	Final Concentration ($\mu\text{g mL}^{-1}$)
STX	9.84	125	305	1000	1.23
dc-STX	21.39	50			1.07
GTX 1	23.51	50			1.18
GTX 4	7.40				0.37
GTX 1 / 4 (sum)	30.91				1.55
GTX 2	40.53	25			1.01
GTX 3	17.18				0.43
GTX 2 / 3 (sum)	57.71				1.44
GTX 5	21.11	50			1.06
GTX 6	5.21	200			1.04
NEO	20.00	50			1.00
dc-NEO	10.14	100			1.01
dc-GTX 2	35.24	25			0.88
dc-GTX 3	10.35				0.26
dc-GTX 2 / 3 (sum)	45.58				1.14
C 1	53.87	20			1.08
C 2	16.10				0.32
C 1 / 2 (sum)	69.97				1.40

Table S2: Working standard solutions containing the PSP toxins studied.

	Working standard solutions					
	1	2	3	4	5	6
Mobile phase B (μL)	1200	1200	1200	1200	1200	1200
Stock standard solution (μL)	5	10	20	50	100	200
Blank matrix solution (μL)	295	290	280	250	200	100
GTX 1 (μg mL⁻¹)	0.0039	0.0078	0.0156	0.039	0.078	0.156
GTX 4 (μg mL⁻¹)	0.0012	0.0024	0.0048	0.012	0.024	0.048
NEO (μg mL⁻¹)	0.0033	0.0066	0.0132	0.033	0.066	0.132
GTX 2 (μg mL⁻¹)	0.0034	0.0068	0.0136	0.034	0.068	0.136
GTX 3 (μg mL⁻¹)	0.0014	0.0028	0.0056	0.014	0.028	0.056
STX (μg mL⁻¹)	0.0041	0.0082	0.0164	0.041	0.082	0.164
dc-STX (μg mL⁻¹)	0.0036	0.0072	0.0144	0.036	0.072	0.144
GTX 5 (μg mL⁻¹)	0.0035	0.0070	0.0140	0.035	0.070	0.140
dc-GTX 2 (μg mL⁻¹)	0.0029	0.0058	0.0116	0.029	0.058	0.116
dc-GTX 3 (μg mL⁻¹)	0.0009	0.0018	0.0036	0.009	0.018	0.036
dc-NEO (μg mL⁻¹)	0.0034	0.0068	0.0136	0.034	0.068	0.136
C 1 / 2 (μg mL⁻¹)	0.0047	0.0094	0.0188	0.047	0.094	0.188
GTX 6 (μg mL⁻¹)	0.0035	0.0070	0.0140	0.035	0.070	0.140

Table S3: UHPLC gradient elution program for PSP toxins analysis.

Time (min)	Flow rate (mL min⁻¹)	Mobile phase A (%)	Mobile phase B (%)
0.0	0.5	36	64
8.0	0.5	36	64
8.1	0.5	30	70
9.0	0.5	30	70
9.1	0.7	80	20
19.0	0.7	80	20
19.5	0.5	36	64
25.0	0.5	36	64

Mobile phase A: water containing 3.6 mM formic acid and 0.2 mM ammonium formate.

Mobile phase B: Acetonitrile-Water (95/5 v/v) containing 3.6 mM formic acid and 0.2 mM ammonium formate.

Table S4: Toxicity equivalent factors (TEFs) proposed by the EFSA Panel, to be applied on a molar basis.

Toxin	TEF	Molecular weight (g mol⁻¹)
STX	1.0	372.2
NEO	1.0	315.1
GTX 1	1.0	411.4
GTX 2	0.4	395.4
GTX 3	0.6	395.4
GTX 4	0.7	411.4
GTX 5	0.1	379.35
GTX 6	0.1	395.35
dc-STX	1.0	329.2
dc-NEO	0.4	345.2
dc-GTX 2	0.2	352.3
dc-GTX 3	0.4	352.3
C1 / 2	0.1	476.05