Supplementary Material: Multi-Toxin Quantitative Analysis of Paralytic Shellfish Toxins and Tetrodotoxins in Bivalve Mollusks with Ultra-Performance Hydrophilic Interaction LC-MS/MS— An In-House Validation Study
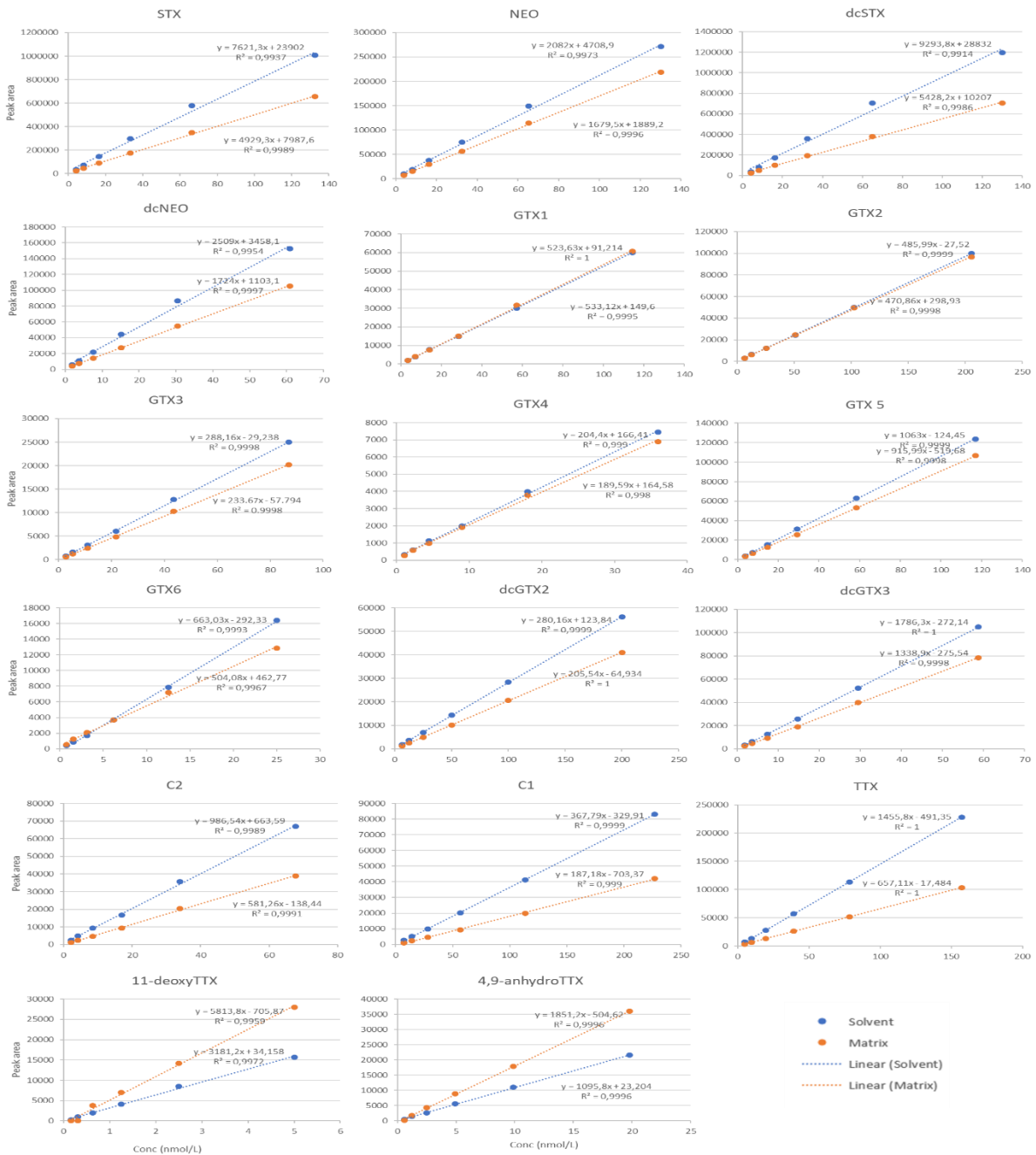

Figure S1. Comparison of the slopes in matrix matched calibration curves and the calibration curves in solvent for each of the toxins, showing matrix effects as distinct signal suppression for STX, NEO, dcSTX, dcNEO, GTX3, GTX6, dcGTX2, dcGTX3, C1, C2 and TTX; low signal suppression for GTX2, GTX4 and GTX5; signal enhancement for 4,9-anhydroTTX, 11-anhydroTTX and no matrix effect for GTX1.
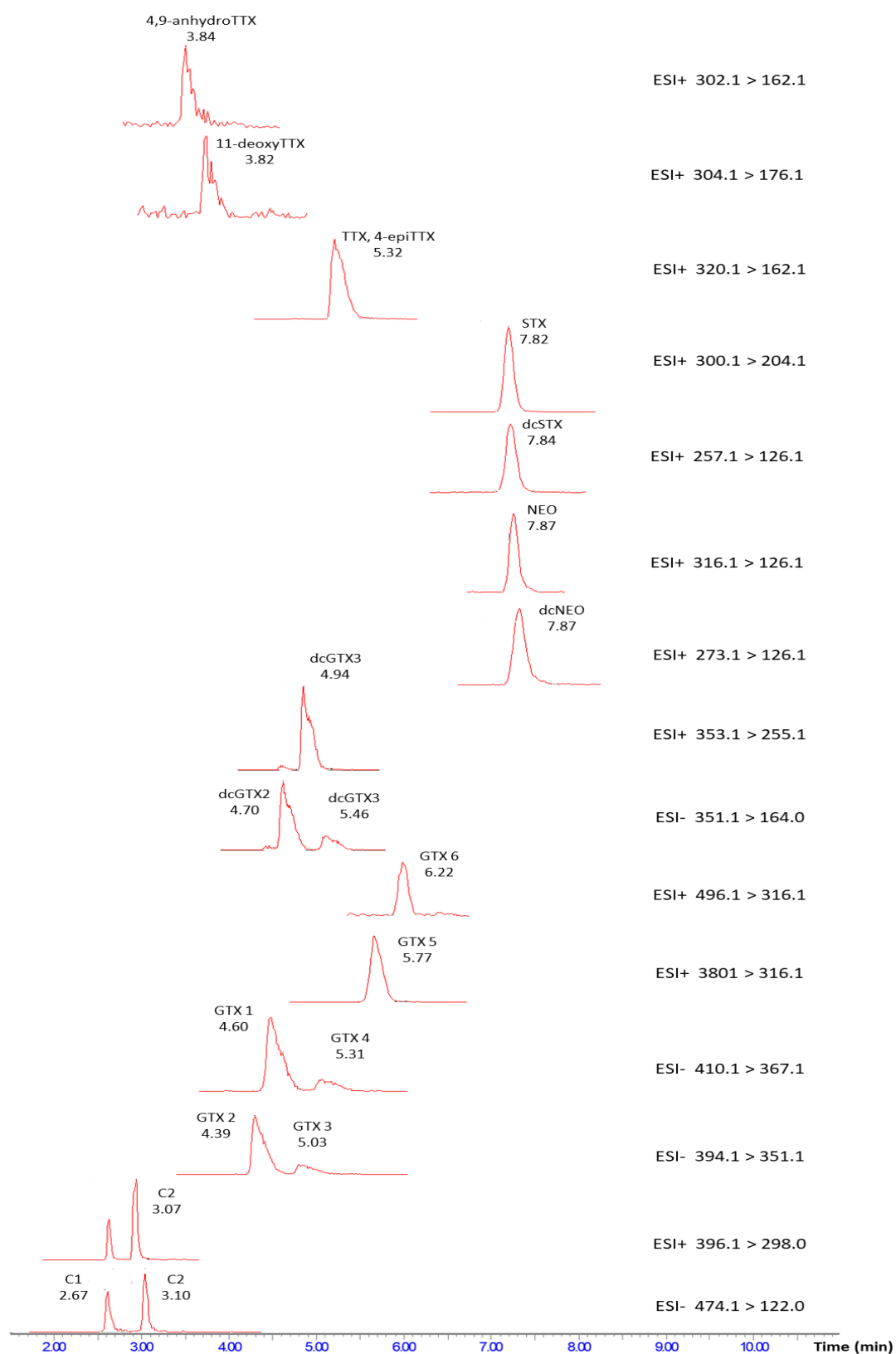
Figure S2. Full MRM transitions of each toxins at mid-level concentration spiked in blue mussel matrix.

Table S1. Concentrations of the calibration standard solutions.

Calibration Standard Solutions	Calibration standard concentration (nmol/L)																
	dcGTX2	dcGTX3	dcSTX	GTX1	GTX4	GTX2	GTX3	NEO	STX	C1	C2	dcNEO	GTX5	GTX6	TTX	4,9-anhydroTTX	11-deoxyTTX
									nmol/L								
S1	200.20	58.80	130.00	114.40	36.00	205.20	87.00	130.20	132.60	226.80	67.80	60.80	116.98	25.00	157.20	5.00	19.80
S2	100.10	29.40	65.00	57.20	18.00	102.60	43.50	65.10	66.30	113.40	33.90	30.40	58.49	12.50	78.60	2.50	9.90
S3	50.05	14.70	32.50	28.60	9.00	51.30	21.75	32.55	33.15	56.70	16.95	15.20	29.25	6.25	39.30	1.25	4.95
S4	25.03	7.35	16.25	14.30	4.50	25.65	10.88	16.28	16.58	28.35	8.48	7.60	14.62	3.13	19.65	0.63	2.48
S5	12.51	3.68	8.13	7.15	2.25	12.83	5.44	8.14	8.29	14.18	4.24	3.80	7.31	1.56	9.83	0.32	1.24
S6	6.26	1.84	4.06	3.58	1.13	6.41	2.72	4.07	4.14	7.09	2.12	1.90	3.66	0.78	4.91	0.16	0.62

Calibration Standard Solutions	Calibration standard concentration as equivalent concentration of saxitoxin (µg STX eq/kg)																
	dcGTX2	dcGTX3	dcSTX	GTX1	GTX4	GTX2	GTX3	NEO	STX	C1	C2	dcNEO	GTX5	GTX6	TTX	4,9-anhydroTTX	11-deoxyTTX
									µg STX eq/kg							µg TTX eq/kg	
S1	272.56	120.08	671.53	941.16	207.32	649.00	412.74	821.02	793.69	21.56	64.46	167.90	88.75	19.77	100.33	30.31	119.23
S2	136.28	60.04	335.77	470.58	103.66	324.50	206.37	410.51	396.85	10.78	32.23	83.95	44.38	9.88	50.16	15.16	59.62
S3	68.14	30.02	167.88	235.29	51.83	162.25	103.19	205.25	198.42	5.39	16.12	41.97	22.19	4.94	25.08	7.58	29.81
S4	34.07	15.01	83.94	117.64	25.91	81.13	51.59	102.63	99.21	2.70	8.06	20.99	11.09	2.47	12.54	3.79	14.90
S5	17.03	7.50	41.97	58.82	12.96	40.56	25.80	51.31	49.61	1.35	4.03	10.49	5.55	1.24	6.27	1.89	7.45
S6	8.52	3.75	20.99	29.41	6.48	20.28	12.90	25.66	24.80	0.67	2.01	5.25	2.77	0.62	3.14	0.95	3.73