Supporting information for

Identifying the source organisms producing paralytic

shellfish toxins in a subtropical bay in the South China Sea

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The following supporting information appendix consists of

nine pages, including

three figures and seven tables.

1. SUPPLEMENTARY FIGURES



Figure S1. The description of high-throughput sequencing samples in Daya Bay in

2017 and 2018.



Figure S2. The combinatorial graph of paralytic shellfish toxin contents in phytoplankton (pmol L⁻¹) and the abundance of related potential toxigenic algal species producing paralytic shellfish toxins identified based on microscopic examination (cells L⁻¹) and high throughput sequencing (%) in Daya Bay in 2017 and 2018, respectively (Inverted square and triangles represented the total paralytic shellfish toxin contents in phytoplankton samples collected in 2017 and 2018. The blue and azure colors represent the *A. tamarense* species complex and *A. minutum* as potential algal species producing paralytic shellfish toxins as identified by microscopic examination, respectively. The stacked bar and stacked bar with twill show the relative abundance of the *A. pacificum* species complex (group IV) and *A. minutum* determined by high throughput sequencing in 2017 and 2018, respectively. The bubble charts show the cell densities of the *A. tamarense* species complex and *A. minutum*, with circles for the 2017 data, and hexagons for the 2018 data).



Figure S3. The composition of main phytoplankton (genus) and *Alexandrium* species indicated by relative abundance using high-throughput sequencing at S7 station of Daya Bay in 2018.

 Table S1 Concentrations and compositions of paralytic shellfish toxins detected in phytoplankton samples in Daya Bay

	Samula site						Toxin co	omposition (p	omol L ⁻¹)					
	Sample site	C1	C2	GTX1	GTX1	dcGTX3	GTX5	dcGTX2	GTX3	GTX2	NEO	dcSTX	STX	Total
	S1	0.85	5.39	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.25
	S2	0.67	4.68	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	5.35
	S 3	0.76	5.43	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.19
	S4	0.39	1.87	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.26
	S5	0.33	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.44
	S 6	0.00	0.16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.16
August	S 7	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2017	S 8	0.00	0.31	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.31
	S9	0.00	0.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.40
	S10	0.00	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.14
	S11	0.10	0.16	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.26
	S12	0.00	0.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.13
	S13	0.07	0.15	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.23
	S14	0.00	0.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.12
	S1	0.54	4.40	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.94
T	S 3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2018	S 6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2010	S 7	1.41	2.76	0.00	0.00	0.96	0.00	0.00	0.00	0.00	0.00	0.00	0.00	5.13
	Z1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	Z2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

					T	oxin con	position (n	mol g ⁻¹)						Toxicity
Shellfish species	C1	C2	GTX4	GTX1	dcGTX3	GTX5	dcGTX2	GTX3	GTX2	NEO	dcSTX	STX	Total	(μg STX _{eq} 100g ⁻¹)
					August	t 2017								
Clausinella isabellina	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Chlamys nobilis	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.01
Turritella bacillum	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ruditapes philippinesis	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.01
Atrina pectinata	0.00	0.02	0.44	0.24	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.70	20.79
Scapharca broughtonii	0.42	14.48	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	14.92	5.89
Perna viridis	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
Scapharca subcrenata	0.02	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.01
Ostrea rivularis	0.19	0.16	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.02	0.39	0.92
					January	2018								
Chlamys nobilis	0.14	0.24	0.00	0.00	0.02	2.42	0.01	0.00	0.00	0.00	0.58	0.00	3.40	16.81
Perna viridis	0.03	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.26
Ostrea rivularis	0.17	0.05	0.00	0.00	0.03	0.89	0.00	0.00	0.00	0.00	0.00	0.00	1.14	2.44

Table S2 Concentration and composition of paralytic shellfish toxins detected in different species shellfish samples collected from Daya Bay

Table S3 Concentration and composition of paralytic shellfish toxins in different tissues of the scallop samples collected from Daya Bay at the
two sampling times

Toxin composition (nmol g ⁻¹)										Toxicity				
Tissues	C1	C2	GTX4	GTX1	dcGTX3	GTX5	dcGTX2	GTX3	GTX2	NEO	dcSTX	STX	Total	(μg STX _{eq} 100g ⁻ 1)
August 2017														
Whole tissue	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.01
Adductor muscle	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
Visceral mass	0.35	0.16	0.00	0.00	0.05	5.97	0.11	0.06	0.66	0.00	0.00	0.00	7.36	25.11
Gonad	0.03	0.01	0.00	0.00	0.03	0.00	0.06	0.00	0.00	0.00	0.00	0.00	0.13	0.76
Mantle	0.01	0.01	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.04	0.37
					Janu	ary 2018	3							
Whole tissue	0.14	0.24	0.00	0.00	0.02	2.42	0.01	0.00	0.00	0.00	0.58	0.00	3.40	16.81
Adductor muscle	0.08	0.06	0.00	0.00	0.00	0.00	0.04	0.00	0.00	0.02	0.19	0.00	0.40	4.66
Visceral mass	6.31	1.97	0.82	0.14	0.04	2.00	0.08	0.10	0.19	0.13	1.00	0.07	12.84	66.91
Gonad	0.46	0.16	0.07	0.00	0.12	0.03	0.09	0.14	0.34	0.08	0.23	0.06	1.77	37.97
Mantle	0.49	0.18	0.00	0.00	0.05	0.03	0.27	0.00	0.00	0.01	0.24	0.00	1.26	7.38

sampling	station	microscopic observat	tion (cell L ⁻¹)	high-throughput sequencing (percentage)			
time	station	A. tamarense species complex	A. minutum	A. tamarense IV	A. minutum		
	S 1	85	750	0.029%	0.253%		
	S2	0	583	-	-		
	S3	333	667	0.033%	0.073%		
	S4	0	972	-	-		
	S5	335	629	-	-		
	S 6	317	556	0.168%	0.687%		
2017	S 7	0	119	0.000%	0.029%		
2017	S 8	66	412	0.047%	0.919%		
	S9	169	211	0.004%	0.012%		
	S10	148	332	0.056%	0.262%		
	S11	0	62				
	S12	165	248	0.197%	1.917%		
	S13	0	157	0.000%	0.196%		
	S14	0	89	0.000%	1.24%		
	S1	370	833	0.238%	1.178%		
	S 3	-	-	0.687%	2.854%		
2010	S6	90	181	0.039%	0.429%		
2018	S 7	236	707	0.396%	5.580%		
	Z1	88	66	-	-		
	Z2	-	-	-	-		

Table S4 The abundance and species of related-PSTs producing algae based on microscope observation and high-throughput sequencing in Daya Bay in 2017 and 2018.

Notes: The table showed that cell density of related-PSTs producing algae were counted by microscopy and relative abundance restored by HTS. The symbol of "-" indicated that the numeric was absent.

Table S5 The sequences of isolated strains producing paralytic shellfish toxin by Sanger sequencing and Alexandrium-OTUs extracted from
HTS dataset.

A. tamarense- liked species_1	A. tamarense- liked species_2	A. minutum- liked species	OTU-137	OTU-477	OTU-729	OTU-792	OTU-993
TATTAAAGT	TATTAAAGT	TATTAAAGT	TATTAAAGT	TATTAAAGT	TATTAAAAT	TATTAAAGT	TATTAAAGT
TGTTGCGGT	TGTTGCGGT	TGTTGCGGT	TGTTGCGGT	TGTTGCGGT	TGTTGCGGT	TGTTGCGGT	TGTTGCGGT
TAAAAAGCT	TAAAAAGCT	TAAAAAGCT	TAAAAAGCT	TAAAAAGCT	TAAAAAGCT	TAAAAAGCT	TAAAAAGCT
CGTAGTTGG	CGTAGTTGG	CGTAGTTGG	CGTAGTTGG	CGTAGTTGG	CGTAGTTGG	CGTAGTTGG	CGTAGTTGG
ATTTCTGCT	ATTTCTGCT	ATTTCTGCT	ATTTCTGCT	ATTTCTGCT	ATTTCTGCT	ATTTCTGCT	GATTCTGCT
GAGGATGGC	GAGGATGGC	GAGGGTGGC	GAGGATGGC	TAGGGTGGC	GATGGTGGC	GAGGGTGGC	TTGGGTGGC
TGGTCCGCC	TGGTCCGCC	TGGTCCGCC	TGGTCCGCC	TGGTCCGCC	TGGTCCGCC	TGGTCCGCC	TGGTCTGCC
CTCTGGGTG	CTCTGGGTG	CTCTGGGTG	CTCTGGGTG	CTCTGGGTG	CTCTGGGTG	CTCTGGGTG	TTCTGGGTG
AGTATTTGG	AGTATTTGG	AGTATCTGG	AGTATTTGG	AGTATCTGG	GGTATCTGG	AGTATCTGG	AGTATCTGG
CACAGCCTG	CACAGCCTG	CACAGCCTG	CACAGCCTG	CACAGCCTA	CACAACCAC	CACAGCCTG	TTCAGCCTG
AGCATTTAT	AGCATTTAT	AGCATTTTT	AGCATTTAT	AGCTTTTTT	AGCACTTCC	AGCATTTTT	AGCATTTTC
CTTGAAAGC	CTTGAAAGC	CTTGAAAGC	CTTGAAAGC	TCAAAGGCA	CAAAAACAT	CTTGAAAGC	TTGAAAGCA
ACAACTGCA	ACAACTGCA	ACAACTGCA	ACAACTGCA	CAACTGCAC	AACTGCACT	ACAACTGCA	TAATTGCAC
CTTGACTGT	CTTGACTGT	CTTGACTGT	CTTGACTGT	TTGACTGTG	TGACTGTGT	CTTGACTGT	TTGACTGTG
GTGGTGTGT	GTGGTGTGT	GTGGTGTGG	GTGGTGTGT	TGGTGTGGT	GGTGTGGTA	GTGGTGTGG	TGGTGTGGT
TATTGAGAA	TATTGAGAA	TATTGAGAA	TATTGAGAA	TTTGAAAAC	TTGGGAAAT	TATTGAGAA	TTTGAGAAC
CATTTACTT	CATTTACTT	CCTTTACTT	CATTTACTT	CTTTACTTT	TTTACTTTG	CCTTTACTT	CTTTACTTT
TGAGGAAAT	TGAGGAAAT	TGAGGAAAT	TGAGGAAAT	GAGGAAATC	AGGAAATCA	TGAGGAAAT	GAGGAAATC
CAGAGTGTT	CAGAGTGTT	CAGAGTGTT	CAGAGTGTT	AGAGTGTTT	GAGTGTTTC	CAGAGTGTT	GGAGTGCTT
TCAAGCAGG	TCAAGCAGG	TCAAGCAGG	TCAAGCAGG	CAAGCAGGC	AAGCAGGC	TCAAGCAGG	CAAGCAGGC

TGTTTGGCC	TGTTTGGCC	TGTTTGCCT	TGTTTGGCC	ATTTGCCTT	ATCCGCCTT	TGTTTGCCT	ATTAGCCGT
TTGAATACA	TTGAATACA	TGAATACAT	TTGAATACA	GAATACATT	GAATACATT	TGAATACAT	GAACACATT
TTAGCATGG	TTAGCATGG	TAGCATGGA	TTAGCATGG	AGCATGGAA	AGCATGGAA	TAGCATGGA	AGCATGGAA
AATAATAAT	AATAATAAT	ATAATATTA	AATAATAAT	TAATATTTT	TAATATTAT	ATAATATTA	TAATGCTGT
TAAGATCAT	TAAGATCAT	TAGGGCCTT	TAAGATCAT	AGGGCCTTG	AGGATCTTG	TAGGGCCTT	AGGGCGTTG
GATTCTTTT	GATTCTTTT	GGTTCTATT	GATTCTTTT	GTTCTATTT	GTTCTATTT	GGTTCTATT	GTTTTATTTT
TGTTGGTTT	TGTTGGTTT	TTGTTGGTT	TGTTGGTTT	TGTTGGTTT	TGTTGGTTT	TTGTTGGTT	GTTGGTTTT
CTAGAATTG	CTAGAATTG	TCTAGAACT	CTAGAATTG	CTAGAATTG	TTATAGCCG	TCTAGAACT	AGAATTATG
AGGTAATGA	AGGTAATGA	GAGGTAATG	AGGTAATGA	AGGTAATGA	AGGTAATGA	GAGGTAATG	GCAATGATT
TTAATAGGG	TTAATAGGG	ATTAATAGG	TTAATAGGG	TTGATAGGG	CAAATAGGG	ATTAATAGG	AATAGGGAT
ATAGTTGGG	ATAGTTGGG	GATAGTTGG	ATAGTTGGG	ATAGTTGGG	ATAGTTGGG	GATAGTTGG	AGTTGGGGG
GGCATTCGT	GGCATTCGT	GGGCATTCG	GGCATTCGT	GGCATTCGT	GGCATTCGT	GGGCATTCG	CATTCGTAT
ATTTGATTG	ATTTGATTG	TATTTAATT	ATTTGATTG	ATTTAATTG	ATTTAATTG	TATTTAATT	TTAATTGTC
TC	TC	GTC	TC	TC	TC	GTC	

Name	Species assigned	Query Cover	Percent Identity
A. tamarense-liked species_1_isolated in the Daya Bay	A. pacificum	100%	100%
A. tamarense-liked species_2_isolated in the Daya Bay	A. pacificum	100%	100%
A. minutum-liked species_isolated in the Daya Bay	A. minutum	99%	99.39%
OTU-137	A. pacificum	100%	100%
OTU-477	Alexandrium sp.	100%	96.01%
OTU-729	A. hiranoi	100%	99.66%
OTU-792	A. minutum	99%	99.39%
OTU-993	A. leei	100%	100%

Table S6 List of the 4 isolated strains and 5 OTUs from HTS data assigned to the species in genus *Alexandrium*.

Table S7 The Pearson Correlation Coefficient between the contents of paralytic shellfish toxins and the abundance of toxigenic algal species based on microscopic observation and high-throughput sequencing.

Method	Miaragaania abgarvation	High-throughput
Species	Microscopic observation	sequencing
A. tamarense species complex	0.294	0.322
A. minutum	0.724**	0.256
A. tamarense species complex + A. minutum	0.672**	0.264

Notes: The asterisk symbols (**) represent very significant difference (P < 0.01) between toxin content in phytoplankton and abundance of toxigenic algal species based on microscopic observation and high-throughput sequencing.