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### Supplementary Material

#### **Spatial resolution of shell microchemistry for tracking dispersing pelagic mussels in a large open embayment in northern New Zealand**

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**Table S1.** Site pairs that had non-significant differences in microchemistry feature identified by the *post hoc* pairwise PERMANOVA of mean relative concentration of 12 elements measured in the reference mussel shell cultured among 22 sites in BoP for each of the three different sampling period iterations (i.e. Retrieval #1, Retrieval #2 and Retrieval #1+#2).

Sampling period	Site pairs	Distance (km)	Region	Environmental condition	Pseudo- <i>F</i>	<i>R</i> <sup>2</sup>	Adjusted <i>P</i>
<b>Retrieval #1</b>	S2 v. S6	24	OP-OH	Open coast – Runoff	0.64	0.04	0.64
	S2 v. ESA	8	OP-FA	Open coast – Offshore	2.65	0.13	0.05
	S5 v. WSA	5	OH-FA	Runoff – Offshore	1.38	0.08	0.22
	S6 v. ESA	17	OH-FA	Runoff – Offshore	1.41	0.07	0.24
	WF v. MF	5	FA	Offshore	1.91	0.10	0.13
<b>Mean</b>	<b>3.3%</b>	<b>11.8</b>					
<b>Retrieval #2</b>	S4 v. S6	12	OP-OH	Open coast – Runoff	1.28	0.07	0.25
	S12 v. S13	6	TH-PI	Volcanic – Runoff – Open coast	1.09	0.06	0.37
	S12 v. S14	12	TH-PI	Volcanic – Runoff – Open coast	1.28	0.07	0.26
	S12 v. S16	24	TH-PI	Volcanic – Runoff – Open coast	1.01	0.05	0.38
	S12 v. S17	30	TH-PI	Volcanic – Runoff – Open coast	1.94	0.10	0.12
	S13 v. S14	6	PI	Open coast	1.63	0.08	0.16
	S13 v. S16	18	PI	Open coast	1.96	0.10	0.16
	S14 v. S16	12	PI	Open coast	1.91	0.10	0.12
	S14 v. S17	18	PI	Open coast	2.41	0.12	0.07
	S15 v. S16	6	PI	Open coast	1.73	0.09	0.18
	S16 v. S17	6	PI	Open coast	1.10	0.06	0.33
<b>Mean</b>	<b>4.8%</b>	<b>13.6</b>					
<b>Retrieval #1 + #2 combined</b>	S2 v. S6	24	OP-OH	Open coast – Runoff	2.02	0.05	0.09
	S6 v. S8	12	OH-TH	Volcanic – Runoff	2.06	0.05	0.06
	S8 v. S10	12	TH	Volcanic- Runoff	2.20	0.07	0.06
	S11 v. S13	12	TH-PI	Volcanic – Runoff – Open coast	1.57	0.05	0.20
	S11 v. S14	18	TH-PI	Volcanic – Runoff – Open coast	1.52	0.05	0.20
	S12 v. S14	12	TH-PI	Volcanic – Runoff – Open coast	2.64	0.09	0.06
	S13 v. S14	6	PI	Open coast	1.59	0.04	0.20
	S13 v. S16	18	PI	Open coast	0.91	0.02	0.41
	S13 v. S17	24	PI	Open coast	1.95	0.05	0.14
	S13 v. WSA	43	PI-FA	Open coast – Offshore	2.03	0.05	0.11
	MF v. WF	5	FA	Offshore	1.76	0.05	0.15
<b>Mean</b>	<b>4.8%</b>	<b>16.9</b>					

WF, West Farm; MF, Mid Farm; EF, East Farm; WSA, West Spat Collection Area; ESA, East Spat Collection Area; S1–S17, S1 to S17; OP, Ōpōtiki region; OH, Ōhiwa region; TH, Thornton region; PI, Pikowai region; FA, Farm region.

**Table S2.** Percentage correct reclassification successes for the site-specific quadratic discriminant analysis models comparing the microchemistry feature of *in situ* cultured green-lipped mussel shells across the BoP during Retrieval #1 and #2 and the suite of elements included in the discriminant models that contribute to those successes at each site.

Regions	Sites	Different site-scale model establishing and cross-validation approaches						
		LOOCV					Retrieval #1 samples	Retrieval #2 samples
		QDA-S- All	QDA-S- Lost	QDA-S- Ret1	QDA-S- Ret2	QDA-S- Half	QDA-S-Ret2	QDA-S-Ret1
Classification success (%) of the Quadratic discriminant analysis model at each site								
<b>FA</b>	<b>EF</b>	65.0	65.0	80.0	90.0	25.0	70.0	70.0
	<b>ESA</b>	75.0	75.0	80.0	80.0	70.0	0.0	0.0
	<b>MF</b>	52.6	52.6	44.4	60.0	60.0	60.0	60.0
	<b>WF</b>	70.0	70.0	70.0	80.0	28.6	0.0	0.0
	<b>WSA</b>	77.8	77.8	62.5	70.0	33.3	0.0	0.0
<b>OP</b>	<b>S1</b>	70.0	70.0	70.0	30.0	73.3	70.0	70.0
	<b>S2</b>	50.0	50.0	60.0	70.0	50.0	0.0	0.0
	<b>S3</b>	50.0	60.0	70.0	40.0	63.6	50.0	50.0
	<b>S4</b>	20.0	-	-	50.0	-	-	-
<b>OH</b>	<b>S5</b>	35.0	35.0	60.0	70.0	36.4	10.0	50.0
	<b>S6</b>	50.0	50.0	80.0	70.0	25.0	0.0	0.0
	<b>S7</b>	65.0	65.0	80.0	80.0	33.3	0.0	0.0
<b>TH</b>	<b>S8</b>	50.0	50.0	70.0	30.0	44.4	0.0	0.0
	<b>S9</b>	75.0	75.0	70.0	50.0	50.0	0.0	60.0
	<b>S10</b>	30.0	-	-	60.0	-	-	-
	<b>S11</b>	30.0	-	-	70.0	-	-	-
	<b>S12</b>	10.0	-	-	30.0	-	-	-
<b>PI</b>	<b>S13</b>	65.0	65.0	100.0	70.0	44.4	0.0	0.0
	<b>S14</b>	50.0	55.0	80.0	50.0	0.0	0.0	0.0
	<b>S15</b>	75.0	75.0	70.0	80.0	40.0	0.0	30.0
	<b>S16</b>	65.0	65.0	90.0	60.0	30.0	0.0	0.0
	<b>S17</b>	65.0	65.0	90.0	50.0	58.3	0.0	0.0
<b>Overall</b>		<b>57.4</b>	<b>62.2</b>	<b>74.0</b>	<b>60.9</b>	<b>45.3</b>	<b>11.8</b>	<b>21.7</b>
Suite of elements selected for inclusion in the discriminate models		<sup>7</sup> Li <sup>59</sup> Co <sup>60</sup> Ni <sup>138</sup> Ba <sup>139</sup> La <sup>238</sup> U	<sup>7</sup> Li <sup>59</sup> Co <sup>60</sup> Ni <sup>138</sup> Ba <sup>139</sup> La <sup>238</sup> U	<sup>7</sup> Li <sup>59</sup> Co <sup>138</sup> Ba <sup>139</sup> La	<sup>59</sup> Co <sup>60</sup> Ni <sup>138</sup> Ba <sup>139</sup> La	<sup>7</sup> Li <sup>59</sup> Co <sup>66</sup> Zn <sup>208</sup> Pb	<sup>7</sup> Li <sup>59</sup> Co <sup>138</sup> Ba <sup>139</sup> La	<sup>59</sup> Co <sup>60</sup> Ni <sup>138</sup> Ba <sup>139</sup> La
<b>Multi-class AUC</b>		<b>0.99</b>	<b>0.95</b>	<b>0.96</b>	<b>0.95</b>	<b>0.86</b>	<b>0.64</b>	<b>0.65</b>

Retrieval #2 samples and QDA-S-Lost did not contain samples from sites S4, 10, 11 and 12.

WF, West Farm; MF, Mid Farm; EF, East Farm; WSA, West Spat Collection Area; ESA, East Spat Collection Area; S1–S17, S1 to S17).

**Table S3.** Percentage of reclassification success for the regional quadratic discriminant analysis model comparing the microchemistry features of *in situ* cultured green-lipped mussel shells across the BoP during Retrieval #1 and #2 and the suite of elements included in the discriminant models that contribute to those successes at each site.

Regions	Different region-scale model establishing and cross-validation approaches						
	QDA-R-All	QDA-R-Lost	LOOCV			R1 samples	R2 samples
QDA-R-Ret1			QDA-R-Ret2	QDA-R-Half	QDA-R-Ret2	QDA-R-Ret1	
Classification success (%) of the Quadratic discriminant analysis model at each site							
<b>FA</b>	86.6	87.6	89.4	80.0	78.3	29.8	42.0
<b>OP</b>	80.0	81.7	70.0	87.5	76.3	30.0	53.3
<b>OH</b>	56.7	63.3	83.3	60.0	57.1	40.0	53.3
<b>TH</b>	52.9	52.5	75.0	74.0	35.5	15.0	30.0
<b>PI</b>	80.0	90.0	98.0	82.0	81.6	14.0	18.0
<b>Overall</b>	<b>73.3</b>	<b>79.3</b>	<b>85.9</b>	<b>77.7</b>	<b>68.3</b>	<b>25.4</b>	<b>37.8</b>
Suite of elements included in the discriminate models	<sup>7</sup> Li	<sup>7</sup> Li	<sup>7</sup> Li	<sup>7</sup> Li	<sup>7</sup> Li	<sup>7</sup> Li	<sup>7</sup> Li
	<sup>59</sup> Co	<sup>59</sup> Co	<sup>59</sup> Co	<sup>59</sup> Co	<sup>59</sup> Co	<sup>59</sup> Co	<sup>59</sup> Co
	<sup>63</sup> Cu	<sup>63</sup> Cu	<sup>138</sup> Ba	<sup>60</sup> Ni	<sup>60</sup> Ni	<sup>138</sup> Ba	<sup>60</sup> Ni
	<sup>88</sup> Sr	<sup>88</sup> Sr	<sup>139</sup> La	<sup>138</sup> Ba	<sup>138</sup> Ba	<sup>139</sup> La	<sup>138</sup> Ba
	<sup>138</sup> Ba	<sup>138</sup> Ba	<sup>140</sup> Ce	<sup>139</sup> La	<sup>139</sup> La	<sup>140</sup> Ce	<sup>139</sup> La
	<sup>139</sup> La	<sup>139</sup> La	<sup>208</sup> Pb	<sup>208</sup> Pb	<sup>140</sup> Ce	<sup>208</sup> Pb	<sup>208</sup> Pb
	<sup>140</sup> Ce	<sup>140</sup> Ce			<sup>208</sup> Pb		
	<sup>208</sup> Pb	<sup>208</sup> Pb					
<b>Multi-class AUC</b>	<b>0.91</b>	<b>0.93</b>	<b>0.96</b>	<b>0.93</b>	<b>0.87</b>	<b>0.64</b>	<b>0.74</b>

Retrieval #2 samples and QDA-R-Lost did not contain samples from sites S4, 10, 11 and 12.

OP, Ōpōtiki region; OH, Ōhiwa region; TH, Thornton region; PI, Pikowai region; FA, Farm region.