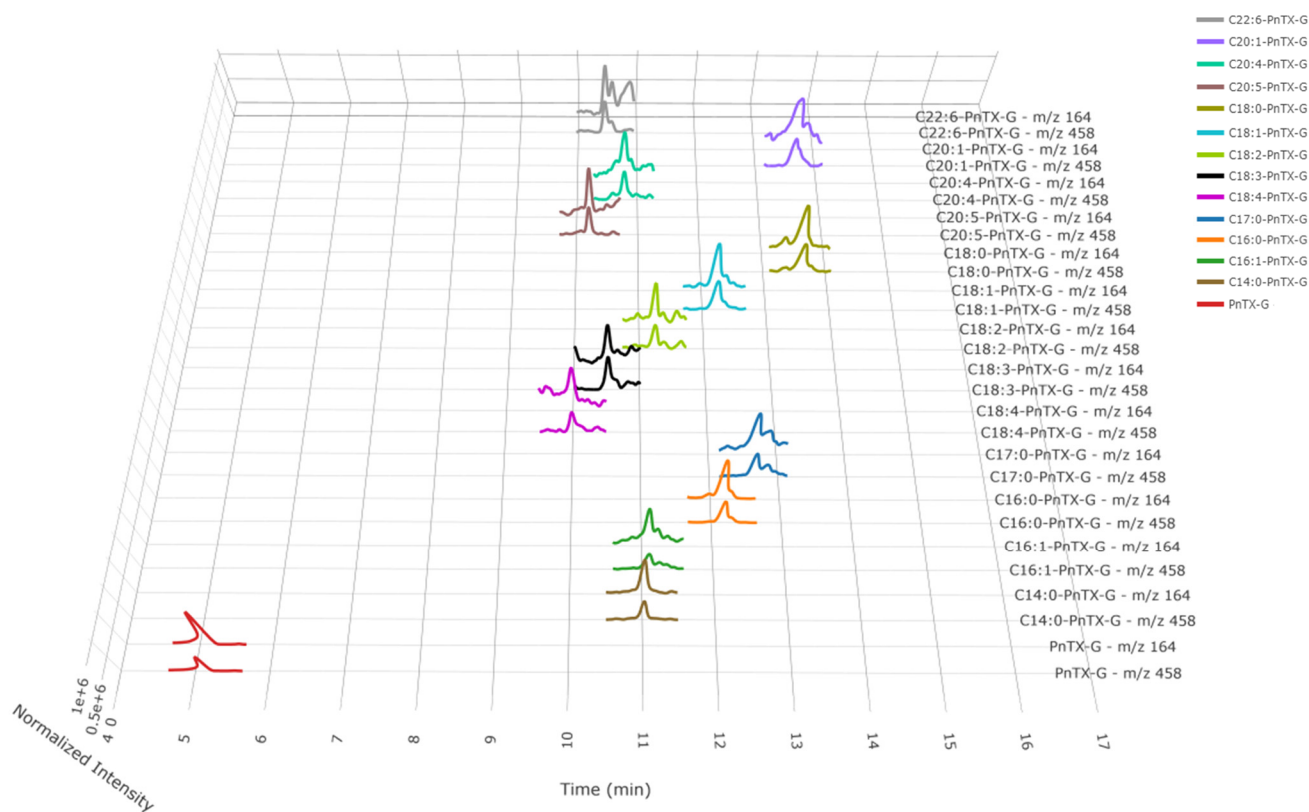
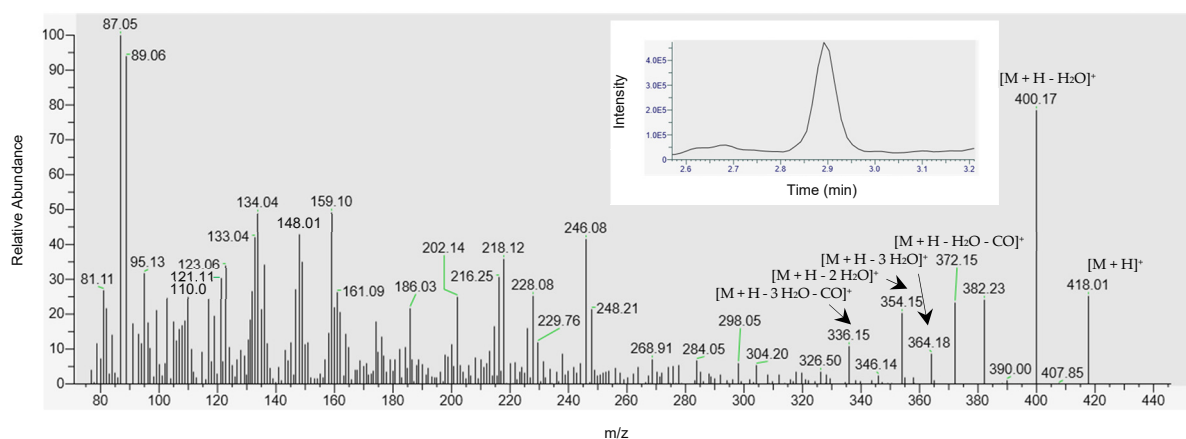




## Supplementary Materials



**Figure S1.** Detection of PnTX-G and 13 of its fatty acid esters by LC-MS/MS in the mussel sample collected in June (18 BM 122). Chromatogram created with R version 4.0.3, and with the Plotly package version 4.10.0 [49,51].



**Figure S2.** Product ion scan obtained from the precursor ion at m/z 418.2 (same as the protonated portimine-B  $[M + H]^+$ ) for the compound eluted at 2.9 min in sample 18 BM 150.

**Table S1.** Molecular formula and monoisotopic mass of the protonated PnTX-G esters  $[M + H]^+$  reported by McCarron et al. [17].

Fatty acid chain	Systematic name (Trivial name)	Ester molecular formula	Monoisotopic mass of the protonated molecule $[M + H]^+$
C14:0	Tetradecanoic (Myristic)	C <sub>56</sub> H <sub>89</sub> NO <sub>8</sub>	904.66664
C15:0	Pentadecanoic (Pentadecylic)	C <sub>57</sub> H <sub>91</sub> NO <sub>8</sub>	918.68229
C16:2	Hexadecadienoic	C <sub>58</sub> H <sub>89</sub> NO <sub>8</sub>	928.66664
C16:1	Hexadecaenoic	C <sub>58</sub> H <sub>91</sub> NO <sub>8</sub>	930.68229
C16:0	Hexadecanoic (Palmitic)	C <sub>58</sub> H <sub>93</sub> NO <sub>8</sub>	932.69794
C17:2	Heptadecadienoic	C <sub>59</sub> H <sub>91</sub> NO <sub>8</sub>	942.68229
C17:1	Heptadecaenoic	C <sub>59</sub> H <sub>93</sub> NO <sub>8</sub>	944.69794
C17:0	Heptadecanoic (Margaric)	C <sub>59</sub> H <sub>95</sub> NO <sub>8</sub>	946.71359
C18:4	Octadecatetraenoic	C <sub>60</sub> H <sub>89</sub> NO <sub>8</sub>	952.66664
C18:3	Octadecatrienoic	C <sub>60</sub> H <sub>91</sub> NO <sub>8</sub>	954.68229
C18:2	Octadecadienoic	C <sub>60</sub> H <sub>93</sub> NO <sub>8</sub>	956.69794
C18:1	Octadecaenoic	C <sub>60</sub> H <sub>95</sub> NO <sub>8</sub>	958.71359
C18:0	Octadecanoic (Stearic)	C <sub>60</sub> H <sub>97</sub> NO <sub>8</sub>	960.72924
C19:0	Nonadecanoic (Nonadecylic)	C <sub>61</sub> H <sub>99</sub> NO <sub>8</sub>	974.74489
C20:5	Eicosapentaenoic	C <sub>62</sub> H <sub>91</sub> NO <sub>8</sub>	978.68229
C20:4	Eicosatetraenoic	C <sub>62</sub> H <sub>93</sub> NO <sub>8</sub>	980.69794
C20:3	Eicosatrienoic	C <sub>62</sub> H <sub>95</sub> NO <sub>8</sub>	982.71359
C20:2	Eicosadienoic	C <sub>62</sub> H <sub>97</sub> NO <sub>8</sub>	984.72924
C20:1	Eicosenoic	C <sub>62</sub> H <sub>99</sub> NO <sub>8</sub>	986.74489
C22:6	Docosahexaenoic	C <sub>64</sub> H <sub>93</sub> NO <sub>8</sub>	1004.69794
C22:5	Docosapentaenoic	C <sub>64</sub> H <sub>95</sub> NO <sub>8</sub>	1006.71359
C22:4	Docosatetraenoic	C <sub>64</sub> H <sub>97</sub> NO <sub>8</sub>	1008.72924
C22:3	Docosatrienoic	C <sub>64</sub> H <sub>99</sub> NO <sub>8</sub>	1010.74489
C22:2	Docosadienoic	C <sub>64</sub> H <sub>101</sub> NO <sub>8</sub>	1012.76054
C24:6	Tetracosahexaenoic	C <sub>66</sub> H <sub>97</sub> NO <sub>8</sub>	1032.72924
C24:5	Tetracosapentaenoic	C <sub>66</sub> H <sub>99</sub> NO <sub>8</sub>	1034.74489