Supplementary Materials

Figure S1. PCA scores plot from analysis of mass spectra (70–590 m/z) from negative ion FT-ICR metabolic footprinting analyses of (●) unlabelled and ^13^C-labelled (●) seawater without algal cells (as controls, n = 6 each), and (■) unlabelled and (■) ^13^C-labelled cultures of *Alexandrium tamarense* (n = 6 each). Black triangles represent QC samples. The major separation along the PC1 axis corresponds to the differences between the metabolic footprints of seawater samples with vs. without algal cells present. Separation along PC2 corresponds to differences between the metabolic footprints of ^13^C-labelled vs. unlabelled *A. tamarense* cultures.
Figure S2. Stable isotope patterns observed in mass spectra collected from $^{13}$C-labeled cultures of *Alexandrium tamarense*. Signal intensity template presented in green, additional $^{13}$C labeled peaks in black and isotopic peaks observed in mass spectra of non-labeled *Alexandrium tamarense* samples in red. Despite the high sensitivity and mass accuracy of FT-ICR MS, a relatively high number of non-ideal SIPs were found (a–d); these arose because the signal intensity of partially or fully-labelled compound dropped below the detection level of the FTICR MS, which resulted in missing peaks across the SIP; a single $m/z$ peak resulted from two or more metabolites of similar mass, which resulted in an altered isotope intensity profile; some $m/z$ features were falsely assigned to a particular SIP in part because of the finite mass accuracy of the FT-ICR; or no all-$^{12}$C peak or $^{12}$C–$^{13}$C isotope peak pair could be located.
Figure S3. Stable isotope patterns modeled with six different labeling efficiencies (a) 1.1%, (b) 20%, (c) 40% (d) 60% (e) 80% and (f) 100% and four different numbers of $^{12}$C atoms in a particular empirical formula: $^{12}$C$_5$H$_h$N$_n$O$_o$P$_p$S$_s$ (black), $^{12}$C$_{10}$H$_h$N$_n$O$_o$P$_p$S$_s$ (blue), $^{12}$C$_{15}$H$_h$N$_n$O$_o$P$_p$S$_s$ (red) and $^{12}$C$_{20}$H$_h$N$_n$O$_o$P$_p$S$_s$ (green). As the labelling efficiency is varied the isotope intensity distribution will move, becoming left-shifted for label efficiencies less than 50% and right-shifted for label efficiencies greater than 50%.
**Figure S4.** Mass spectral characterization after solid-phase-extraction of the putatively annotated (based upon accurate mass measurement) myristic acid, (a) mass spectra for unlabelled fraction FM2 (top) and $^{13}$C-labelled FM2 (Orbitrap Velos), showing the isotopic pattern related to the original m/z 227.20143 signal. Both the monoisotopic signal and the SIP had their maximum intensities in the same FM2 fractions; (b) collision-induced fragmentation (CID) MS/MS spectra (Orbitrap, normalised collision energy of 30%) for the monoisotopic signal m/z 227 from the unlabelled FM2 fraction, overlaid with CID spectra for three of the SIP signals from the labelled FM2 fraction, all four SIP signals show a similar pattern of losses, as would be expected from isotopes; (c) CID MS/MS spectra (LTQ FT Ultra, normalised collision energy of 45%) for the monoisotopic signal m/z 227 from the unlabelled FM2 fraction, compared with that of an authentic myristic acid standard, while the signals in the standard constitute the main fragments in the sample, there is likely another, isomeric compound present.
Table S1. Stable isotope patterns located and annotated in mass spectra collected from $^{13}$C-labeled cultures of *Alexandrium tamarense*.

<table>
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<tr>
<th>m/z</th>
<th>Intensity (Figure S5)</th>
<th>ID SIP</th>
<th>Empirical formula (all-$^{12}$C containing peak)</th>
<th>Ion form</th>
<th>Mass error (ppm)</th>
<th>KEGG compound</th>
<th>r-value</th>
<th>p-value</th>
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<td>C$<em>{3}$H$</em>{4}$O</td>
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Table S1. Cont.

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<th>Ion form</th>
<th>Mass error (ppm)</th>
<th>KEGG compound</th>
<th>r-value</th>
<th>p-value</th>
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<td>Mass error (ppm)</td>
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<th>Mass error (ppm)</th>
<th>KEGG compound</th>
<th>r-value</th>
<th>p-value</th>
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<p>| m/z | Intensity  | ID SIP (Figure S5) | Empirical formula (all-^{13}C containing peak) | Ion form | Mass error (ppm) | Mass error value | Mass error value | Mass error value | Mass error value | KEGG compound          | r-value | p-value |
|-----|------------|--------------------|-----------------------------------------------|----------|------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------------|---------|---------|
| 471.25971 | 81347.33833 | 105                | C_{19}H_{26}N_{5}O_{7}                     | [M + Cl]^{-} | 1.29            | 0.51            | 0.93            | 1.15            | 0.8             | 0.5350                 | 0.92    | 0.0101  |
| 471.25971 | 81347.33833 | 105                | C_{12}H_{25}N_{2}O_{5}                     | [M + Cl]^{-} | 0.64            | 0.35            | 0.75            | 0.0182          | 0.085           | 0.5620                 | 0.75    | 0.0854  |
| 471.25971 | 81347.33833 | 105                | C_{23}H_{33}N_{2}O_{3}P_{3}                | [M + Cl]^{-} | 0.38            | 0.38            | 0.38            | 0.38            | 0.38            | 0.38                   | 0.75    | 0.0854  |
| 471.25971 | 81347.33833 | 105                | C_{20}H_{24}N_{6}O_{2}S_{2}               | [M + Cl]^{-} | −0.56           | −0.56           | −0.56           | −0.56           | −0.56           | −0.56                  | 0.89    | 0.0182  |
| 471.25971 | 81347.33833 | 105                | C_{13}H_{20}N_{6}O_{2}P_{2}               | [M − H]^{-} | 1.01            | 1.01            | 1.01            | 1.01            | 1.01            | 1.01                   | 0.89    | 0.0182  |
| 471.25971 | 81347.33833 | 105                | C_{20}H_{24}N_{6}O_{2}P_{4}               | [M − H]^{-} | 0.76            | 0.76            | 0.76            | 0.76            | 0.76            | 0.76                   | 0.89    | 0.0182  |
| 471.25971 | 81347.33833 | 105                | C_{19}H_{23}N_{2}O_{2}P_{2}               | [M − H]^{-} | 0.62            | 0.62            | 0.62            | 0.62            | 0.62            | 0.62                   | 0.89    | 0.0182  |
| 471.25971 | 81347.33833 | 105                | C_{19}H_{23}N_{2}O_{2}P_{4}               | [M − H]^{-} | −0.18           | −0.18           | −0.18           | −0.18           | −0.18           | −0.18                  | 0.89    | 0.0182  |
| 471.25971 | 81347.33833 | 105                | C_{23}H_{26}O_{6}                        | [M − H]^{-} | −0.53           | −0.53           | −0.53           | −0.53           | −0.53           | −0.53                  | 0.44    | 0.3875  |
| 471.25971 | 81347.33833 | 105                | C_{20}H_{25}N_{2}O_{4}                    | [M − H]^{-} | −1.17           | −1.17           | −1.17           | −1.17           | −1.17           | −1.17                  | 0.92    | 0.0101  |
| 465.35894 | 27617.706   | 106                | C_{20}H_{24}O_{6}                        | [M + Acetate]^{-} | 0.84          | 0.84            | 0.84            | 0.84            | 0.84            | 0.84                   | 0.69    | 0.0277  |
| 465.35894 | 27617.706   | 106                | C_{19}H_{20}O_{6}OS                      | [M + Acetate]^{-} | −0.63          | −0.63           | −0.63           | −0.63           | −0.63           | −0.63                  | 0.28    | 0.4349  |
| 465.35894 | 27617.706   | 106                | C_{20}H_{20}O_{6}                        | [M + Acetate]^{-} | 0.84            | 0.84            | 0.84            | 0.84            | 0.84            | 0.84                   | 0.44    | 0.2028  |
| 465.35894 | 27617.706   | 106                | C_{20}H_{20}N_{2}O_{4}                    | [M − H]^{-} | 0.19            | 0.19            | 0.19            | 0.19            | 0.19            | 0.19                   | 0.86    | 0.0012  |
| 465.35894 | 27617.706   | 106                | C_{20}H_{20}N_{2}O_{3}S                   | [M − H]^{-} | −0.63           | −0.63           | −0.63           | −0.63           | −0.63           | −0.63                  | 0.62    | 0.0583  |
| 465.35894 | 27617.706   | 106                | C_{12}H_{20}S_{2}                        | [M − H]^{-} | −1.03           | −1.03           | −1.03           | −1.03           | −1.03           | −1.03                  | 0.34    | 0.3428  |
| 475.42777 | 16099.36167 | 107                | C_{12}H_{20}O_{4}                        | [M + Acetate]^{-} | 1.44            | 1.44            | 1.44            | 1.44            | 1.44            | 1.44                   | −0.58   | 0.2262  |
| 475.42777 | 16099.36167 | 107                | C_{11}H_{20}O_{4}S_{3}                   | [M + Acetate]^{-} | 1.36            | 1.36            | 1.36            | 1.36            | 1.36            | 1.36                   | −0.35   | 0.5620  |
| 475.42777 | 16099.36167 | 107                | C_{12}H_{19}N_{2}O_{4}P_{2}              | [M + Acetate]^{-} | 1.18            | 1.18            | 1.18            | 1.18            | 1.18            | 1.18                   | 0.75    | 0.0854  |
| 475.42777 | 16099.36167 | 107                | C_{12}H_{20}O_{3}P_{2}                   | [M + Acetate]^{-} | 1.15            | 1.15            | 1.15            | 1.15            | 1.15            | 1.15                   | 0.89    | 0.0182  |
| 475.42777 | 16099.36167 | 107                | C_{12}H_{20}N_{2}O_{4}P_{3}              | [M + Acetate]^{-} | 0.93            | 0.93            | 0.93            | 0.93            | 0.93            | 0.93                   | −0.32   | 0.5350  |
| 475.42777 | 16099.36167 | 107                | C_{12}H_{20}N_{2}O_{4}P_{4}              | [M + Acetate]^{-} | 0.51            | 0.51            | 0.51            | 0.51            | 0.51            | 0.51                   | −0.91   | 0.0938  |</p>
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Figure S5. Stable isotope patterns located in mass spectra collected from $^{13}$C-labeled cultures of *Alexandrium tamarense*.
Figure S5. Cont.
Figure S5. Cont.
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Figure S5. Cont.
Figure S5. Cont.
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Figure S5. Cont.
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