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Supplementary Material

Effects of legacy metabolites from previous ecosystems on the environmental metabolomics of the brine of Lake Vida, East Antarctica

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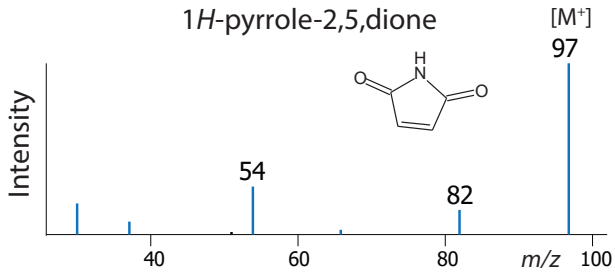
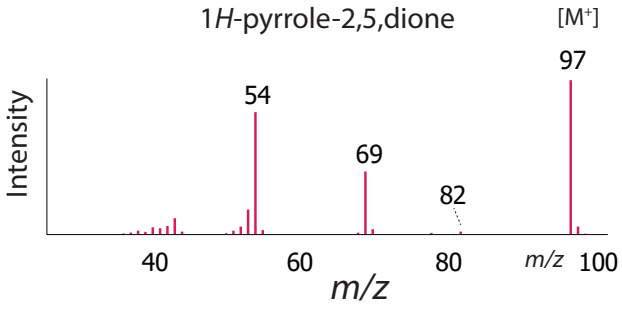
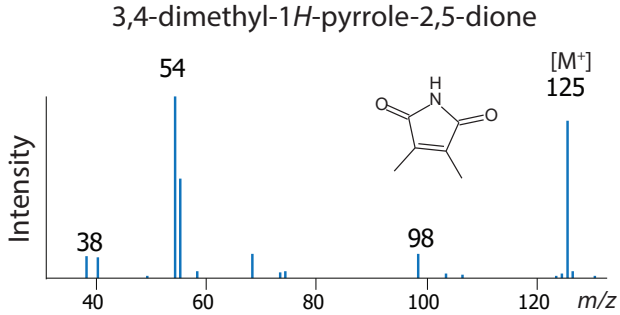
Mass Spectra Interpretation

Mass spectra of compounds discussed in this study is present in the **left column** of Figure S1 to S4. All mass spectra of paleometabolites were retrieved from the GC×GC-TOF-MS data. Each mass spectra was obtained from the ChromaTOF software, a mass spectral processing tool of the Leco's software package, which utilizes the "Peak True" deconvolution algorithm to subtract peaks from background noise.

Comparisons were made to mass spectra of compounds obtained from the NIST Chemistry WebBook, the Wiley Database, and various literature shown in the **right column** of Figure S1 to S4. For spectra that were obtained from the literature, we plotted the relative abundances of fragment ions to the base peak ions (only those that are reported in the studies) against those relative abundances in the mass spectra of our study. R^2 values were generated to show how well the compounds and their fragmentation patterns are correlated.



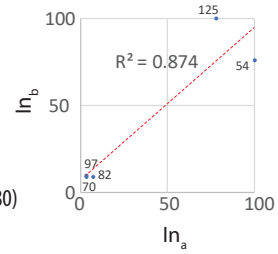


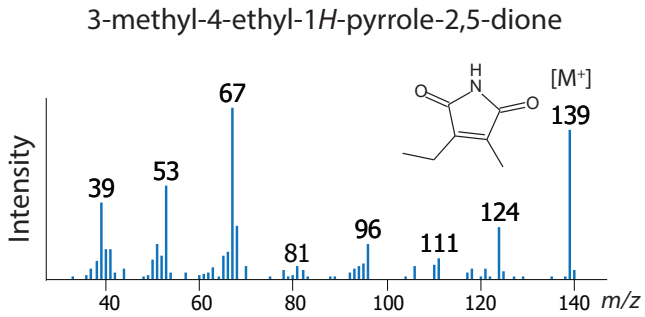


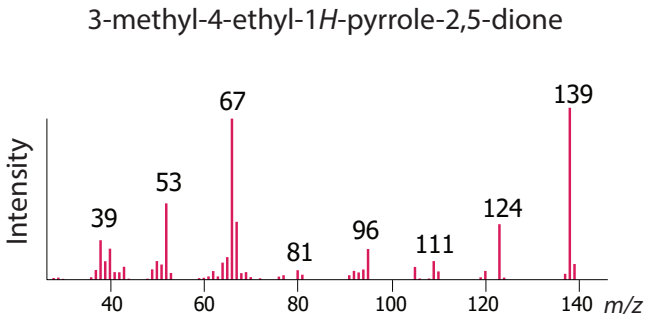
3,4-dimethyl-1*H*-pyrrole-2,5-dione

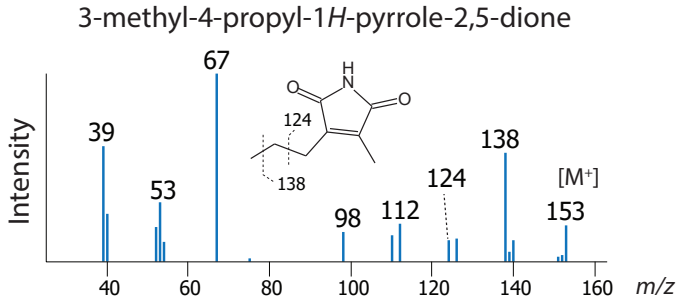
m/z	In_a	In_b
54	100%	76%
70	3.0%	8.6%
82	7.0%	8.6%
97	3.0%	9.5%
125	78%	100%

In_a : relative intensity(%) in Martin et al. (1980)
In_b : relative intensity(%) in this study









No authentic standard available

Figure S1: Mass spectra of maleimides (1H-pyrrole-2,5,diones) from this study (**left**) compared to library spectra of authentic standards (**right**).

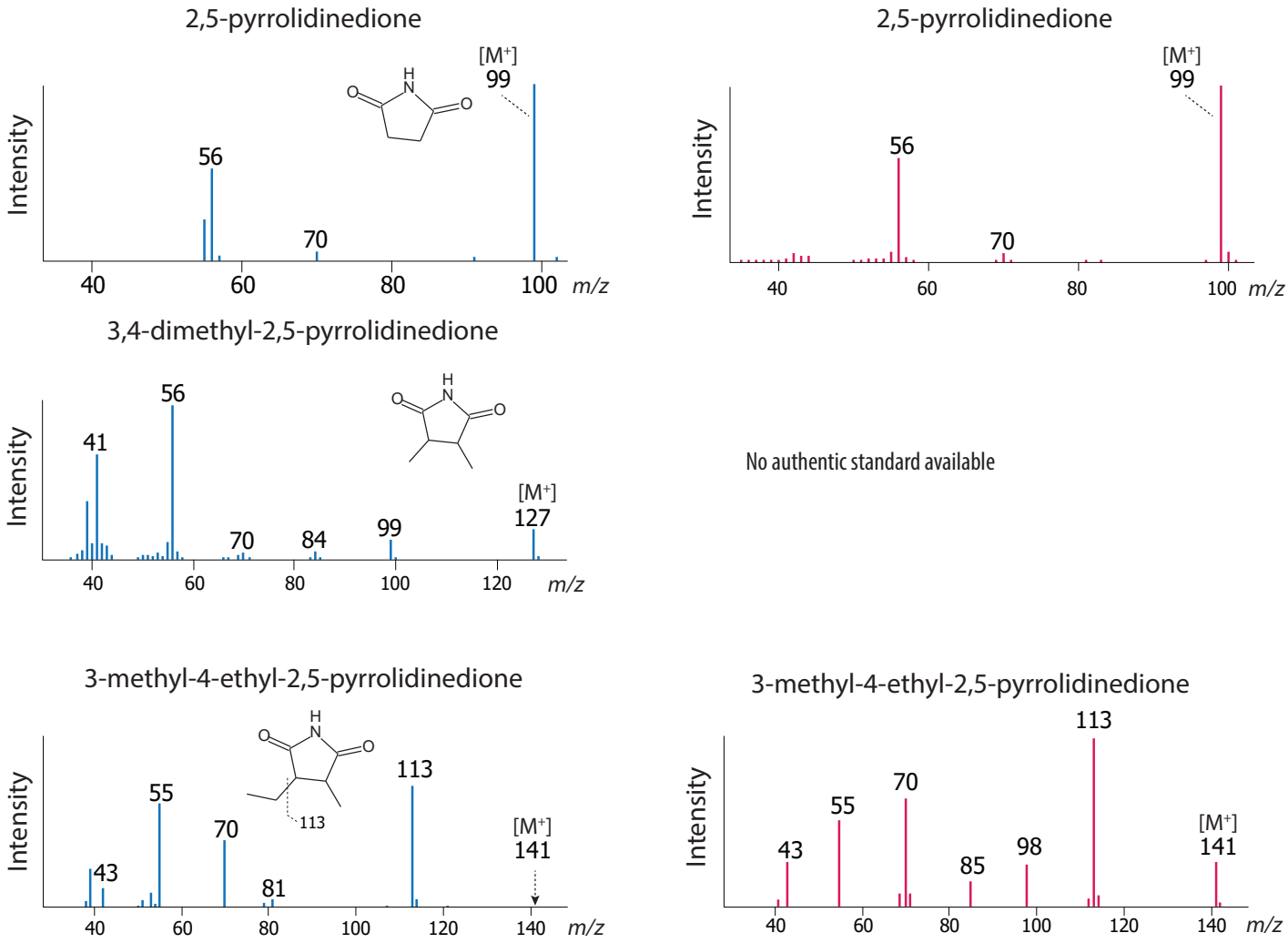


Figure S2: Mass spectra of succinimides (2,5-pyrrolidinedione) from this study (**left**) compared to library spectra of authentic standards (**right**).

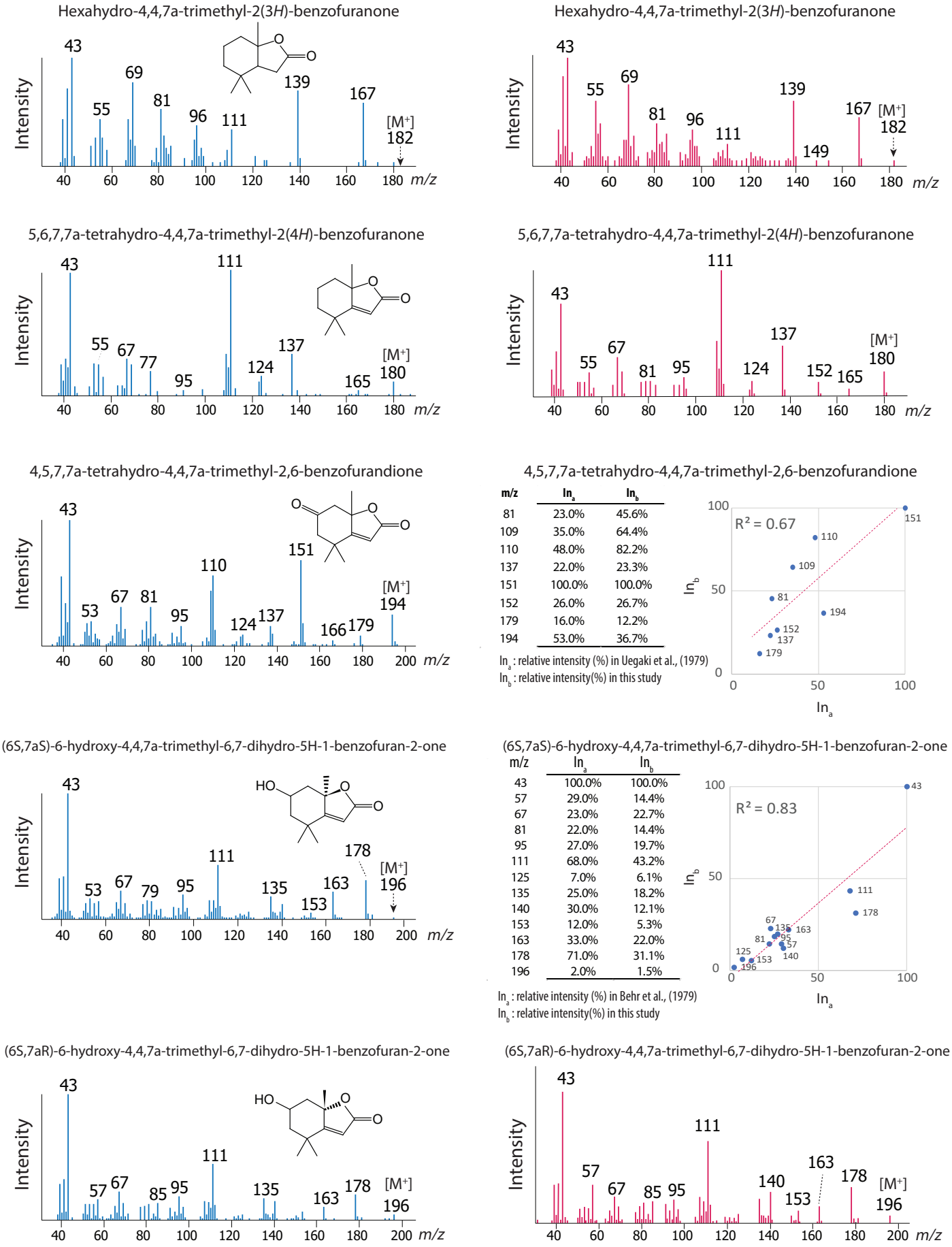


Figure S3: Mass spectra of carotenoid derivatives from this study (**left**) compared to library spectra of authentic standards (**right**).

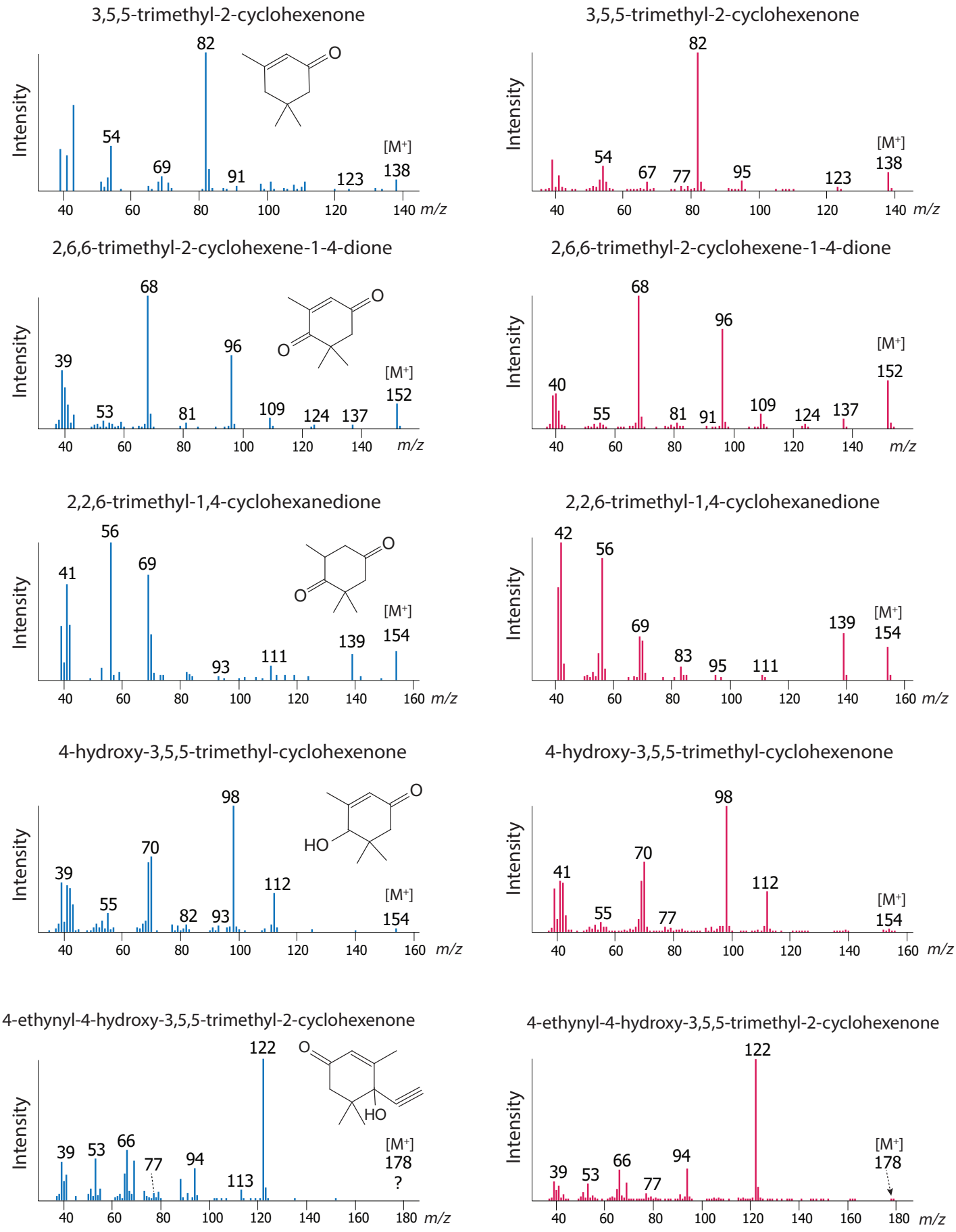
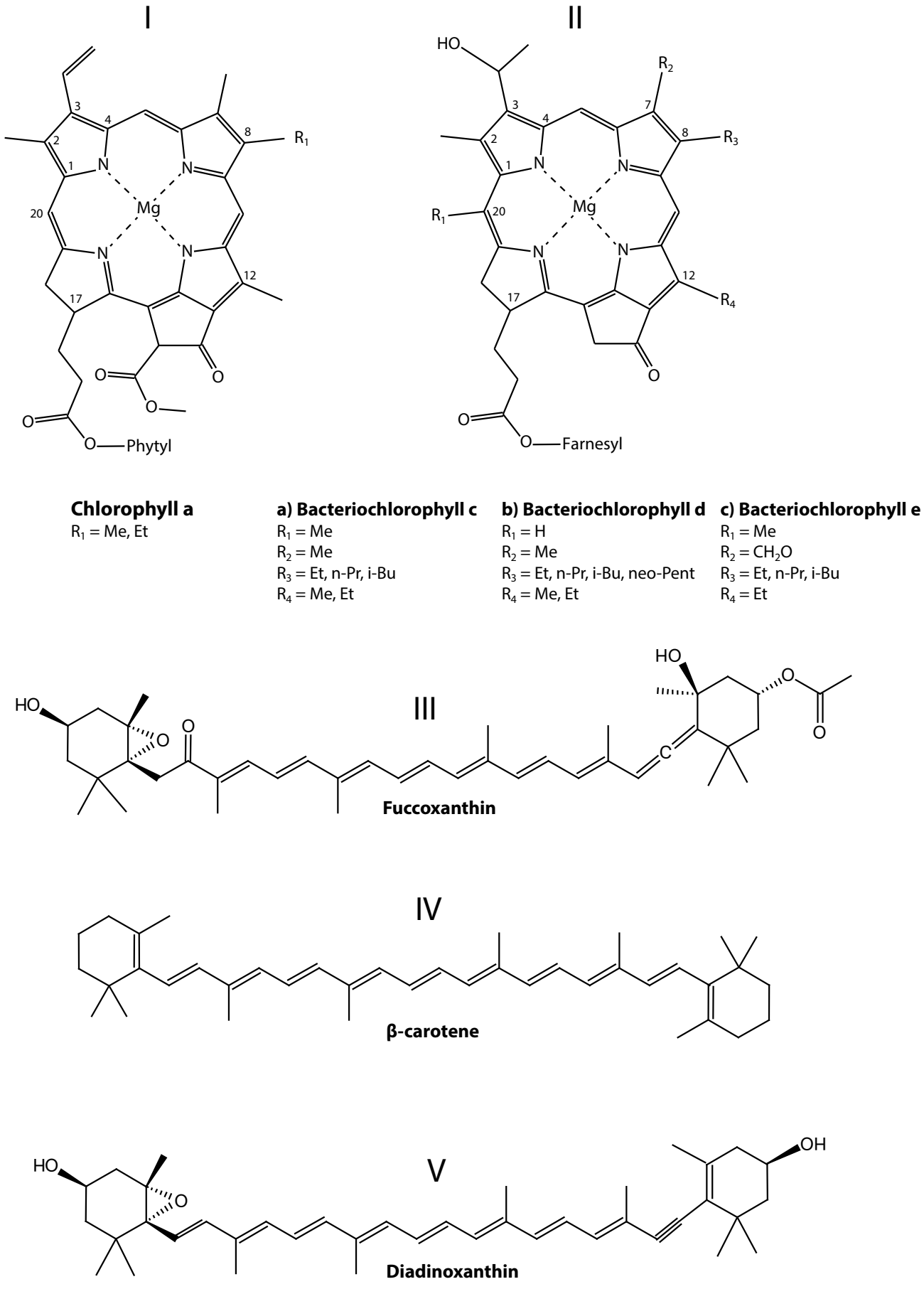


Figure S4: Mass spectra of carotenoid derivatives from this study (**left**) compared to library spectra of authentic standards (**right**).



Chlorophyll a
R_1 = Me, Et

a) Bacteriochlorophyll c
R_1 = Me
R_2 = Me
R_3 = Et, n-Pr, i-Bu
R_4 = Me, Et

b) Bacteriochlorophyll d
R_1 = H
R_2 = Me
R_3 = Et, n-Pr, i-Bu, neo-Pent
R_4 = Me, Et

c) Bacteriochlorophyll e
R_1 = Me
R_2 = CH_2O
R_3 = Et, n-Pr, i-Bu
R_4 = Et

Figure S5: Structures of photosynthetic pigments and carotenoids discussed in this study.

Work Cited

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