

Metabolomic insights into marine phytoplankton diversity

Rémy Marcellin-Gros ^{1,2}, Gwenaël Piganeau ^{2,*} and Didier Stien ^{1,*}

¹ Sorbonne Université, CNRS, Laboratoire de Biodiversité et Biotechnologie Microbiennes, LBBM, Observatoire Océanologique, 66650 Banyuls-sur-Mer, France

² Sorbonne Université, CNRS, Biologie Intégrative des Organismes Marins, BIOM, Observatoire Océanologique, 66650 Banyuls-sur-Mer, France

* Correspondence: gwenael.piganeau@obs-banyuls.fr; Tel.: +33-468887343 (G.P.). didier.stien@cnrs.fr; Tel.: +33-430192476 (D.S.)

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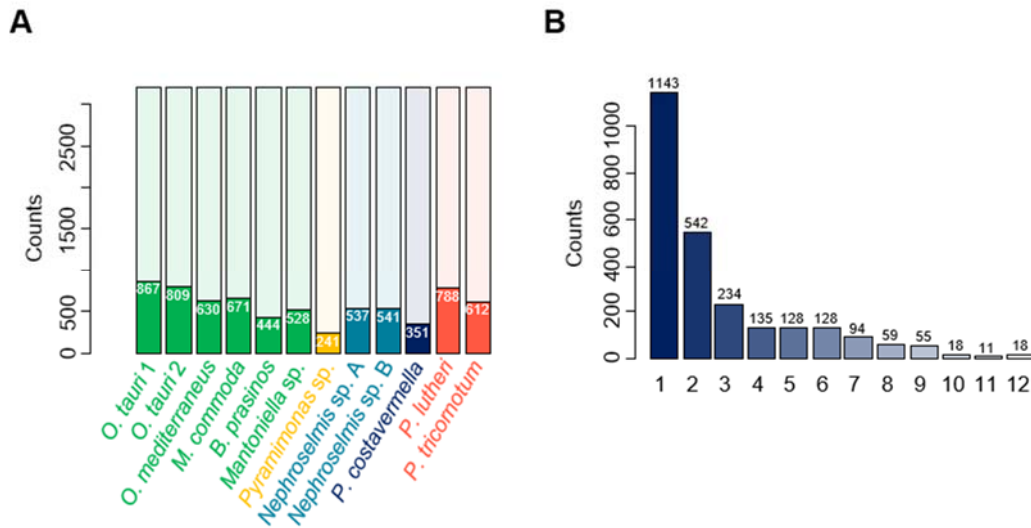


Figure S1. Stacked histogram of detected compounds (bottom bars, intense colors) among total detected compounds (upper bars, blurred colors) in the twelve strains of algae (A). Histogram of counts of shared compounds between different strains (abscise axis indicates the number of strains sharing the same compound). Most of compounds (1143) are uniquely detected in one strain (1) while only few compounds (18) are detected in every alga (12) (B).

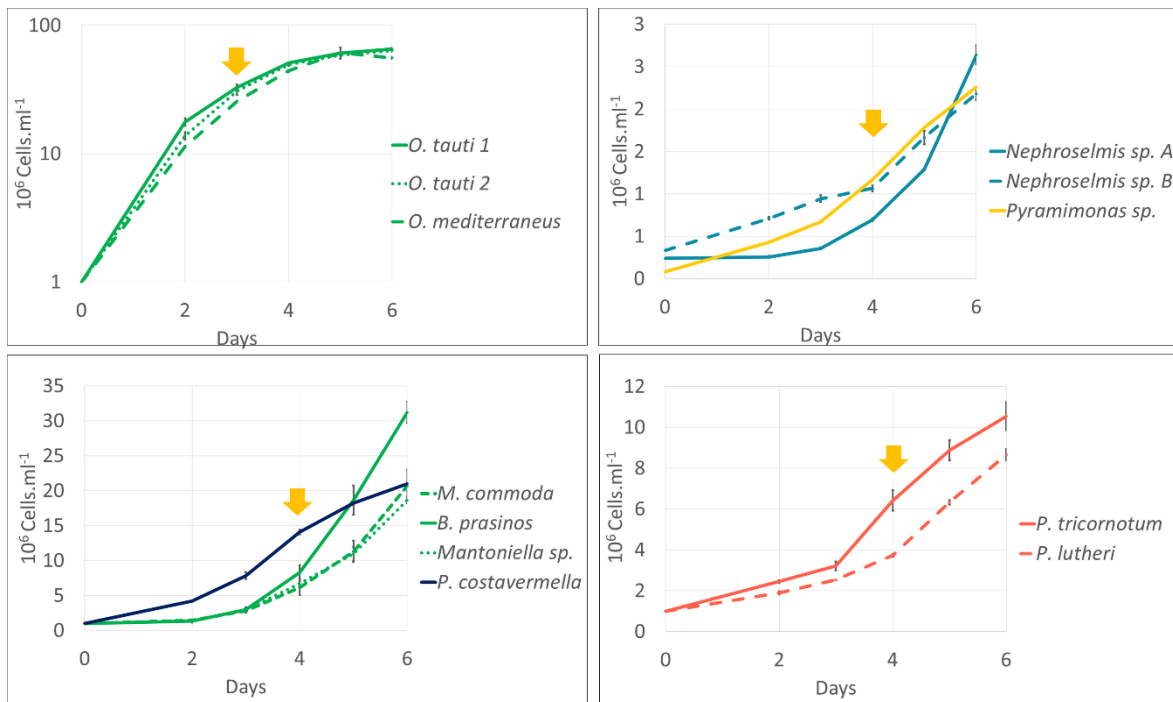


Figure S2. Microalgae concentration growth curves over time. Yellow arrows: metabolite extraction was performed at 3 days post-inoculation for *Ostreococcus* species and 4 days post inoculation for the others.

Table S1. Algal and bacterial concentration (cells.ml⁻¹) at sampling day for the twelve algae species. RCC for Roscoff Culture Collection numbers for strain identification.

Species	RCC number	Algal cell concentration (Cells.ml ⁻¹) mean ± sd	Bacterial cell concentration (Cells.ml ⁻¹) mean ± sd	Bacteria proportion (%)	Sampling day post inoculation
<i>O. tauri</i> 1	6850	32×10 ⁶ ± 1.7×10 ⁶	2.6×10 ⁴ ± 0.2×10 ⁴	0.07	3
<i>O. tauri</i> 2	4221	30×10 ⁶ ± 2.1×10 ⁶	6.1×10 ⁴ ± 0.6×10 ⁴	0.2	3
<i>O. mediterraneus</i>	2590	25×10 ⁶ ± 0.1×10 ⁶	5.6×10 ⁴ ± 0.8×10 ³	0.2	3
<i>B. prasinos</i>	4222	8.3×10 ⁶ ± 0.9×10 ⁶	5.0×10 ⁵ ± 0.7×10 ⁵	5.7	4
<i>M. commoda</i>	827	2.8×10 ⁶ ± 0.3×10 ⁶	2.7×10 ⁶ ± 0.3×10 ⁶	49	4
<i>Mantoniella</i> sp.	6849	2.9×10 ⁶ ± 0.1×10 ⁶	2.5×10 ⁶ ± 1.9×10 ⁶	46	4
<i>Pyramimonas</i> sp.	6848	6.7×10 ⁵ ± 0.3×10 ⁵	6.2×10 ⁵ ± 1.7×10 ⁵	48	4
<i>Nephroselmis</i> sp. A	6846	3.5×10 ⁵ ± 0.1×10 ⁵	3.3×10 ⁶ ± 0.2×10 ⁶	90	4
<i>Nephroselmis</i> sp. B	6847	9.4×10 ⁵ ± 0.4×10 ⁵	8.4×10 ⁵ ± 0.4×10 ⁴	8.2	4
<i>P. costavermella</i>	4223	14×10 ⁶ ± 0.3×10 ⁶	1.5×10 ⁶ ± 1.3×10 ⁶	9.7	4
<i>P. lutheri</i>	6852	2.5×10 ⁶ ± 0.3×10 ⁴	3.5×10 ⁶ ± 0.2×10 ⁶	58	4
<i>P. tricorutum</i>	6851	3.2×10 ⁶ ± 0.2×10 ⁶	0.4×10 ⁵ ± 0.9×10 ⁴	1.4	4

Phaeo_3 #2318 RT: 8.98 AV: 1 NL: 7.20E+007
T: FTMS + c ESI d Full ms2 793.4862@hcd30.00 [55.0000-825.0000]

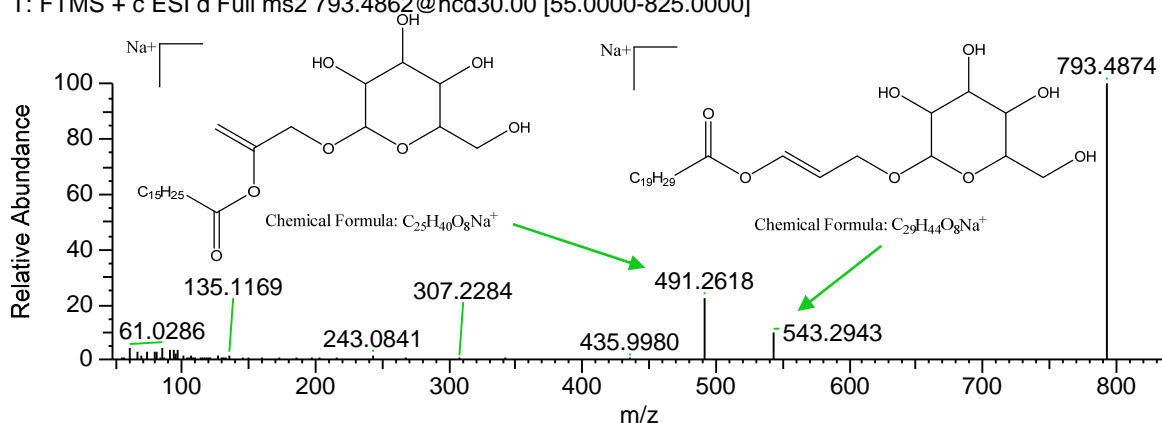


Figure S3. Compound M3629 – *m/z* 793.4874 – [M+Na]⁺ – *t_R* = 8.976 min – C₄₅H₇₀O₁₀ – MGDG 20:5/16:3

4222_2 #2865 RT: 11.13 AV: 1 NL: 2.91E+006
T: FTMS + c ESI d Full ms2 832.5256@hcd30.00 [57.6667-865.0000]

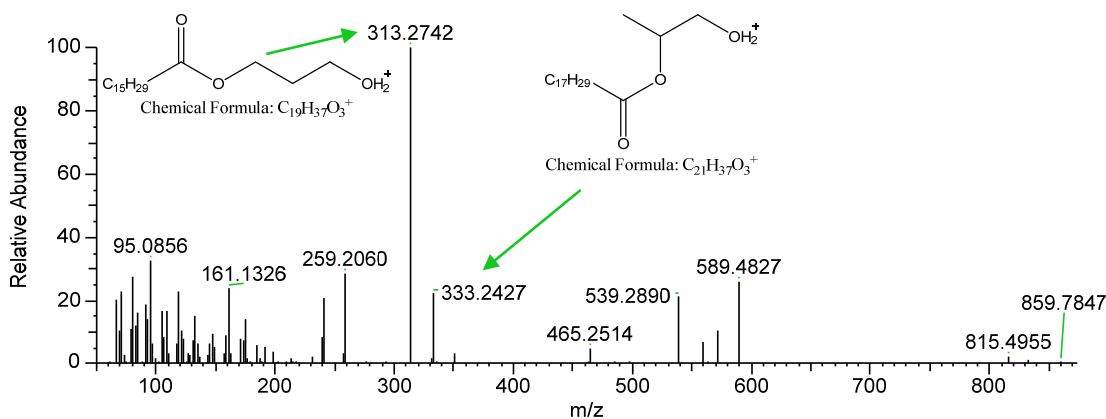


Figure S4. Compound M5273 – *m/z* 815.4985 – [M+H]⁺ – *t_R* = 9.167 min – C₄₃H₇₄SO₁₂ – SQDG 16:0/18:4

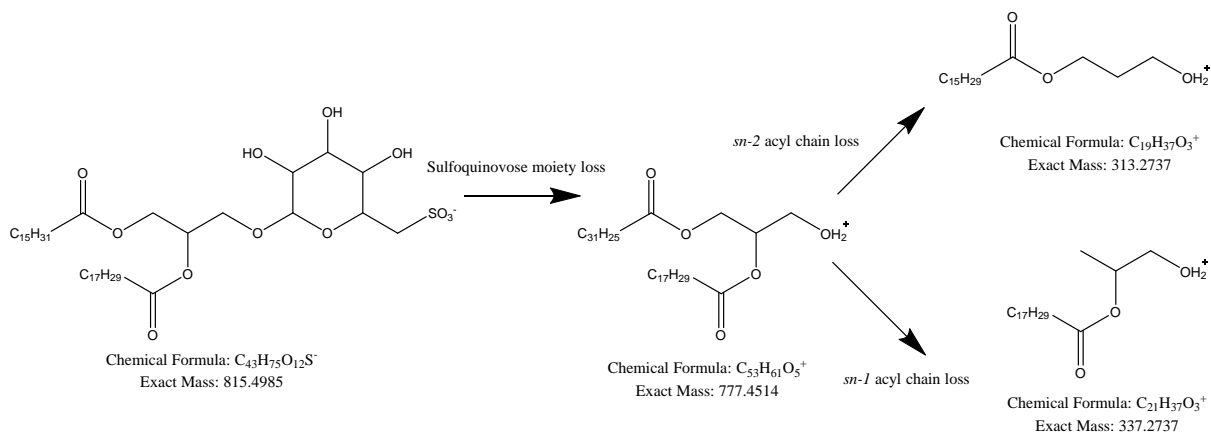


Figure S5. Fragmentation pathway proposed for SQDGs

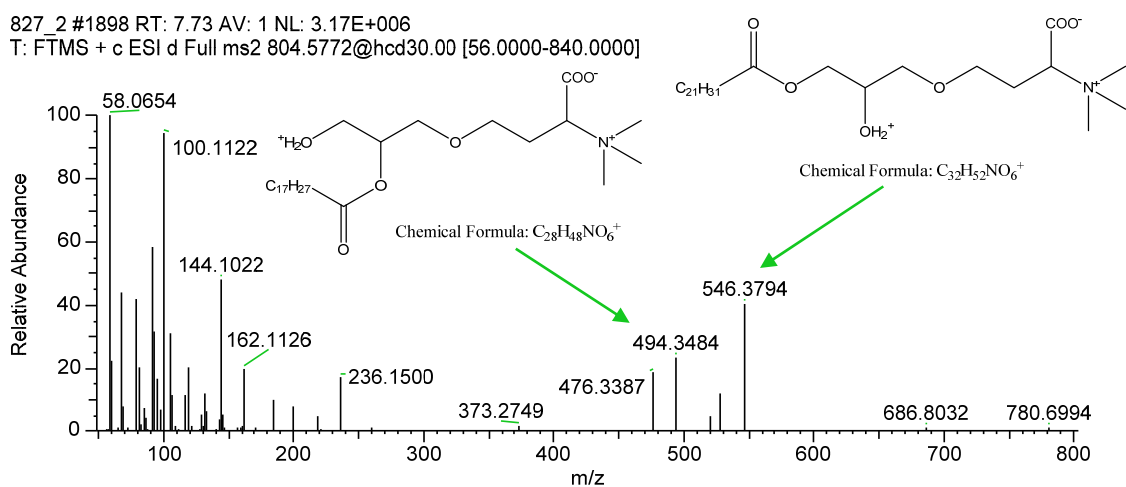


Figure S6. Compound M2531 – m/z 804.578 – $[M+H]^+$ – t_r = 8.976 min – $C_{50}H_{77}NO_7$ – DGTS 22:6/18:4

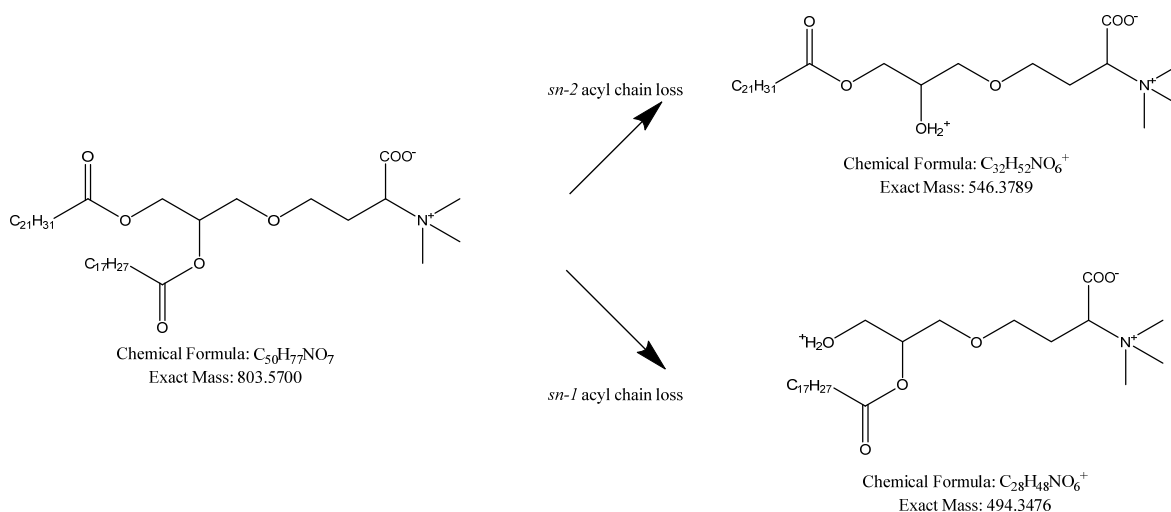


Figure S7. Fragmentation pathway proposed for DGTSs (Fragmentation pattern of the DGTAs are similar)

Pav_3 #2312 RT: 9.10 AV: 1 NL: 1.85E+006
T: FTMS + c ESI d Full ms2 774.5884@hcd30.00 [54.0000-810.0000]

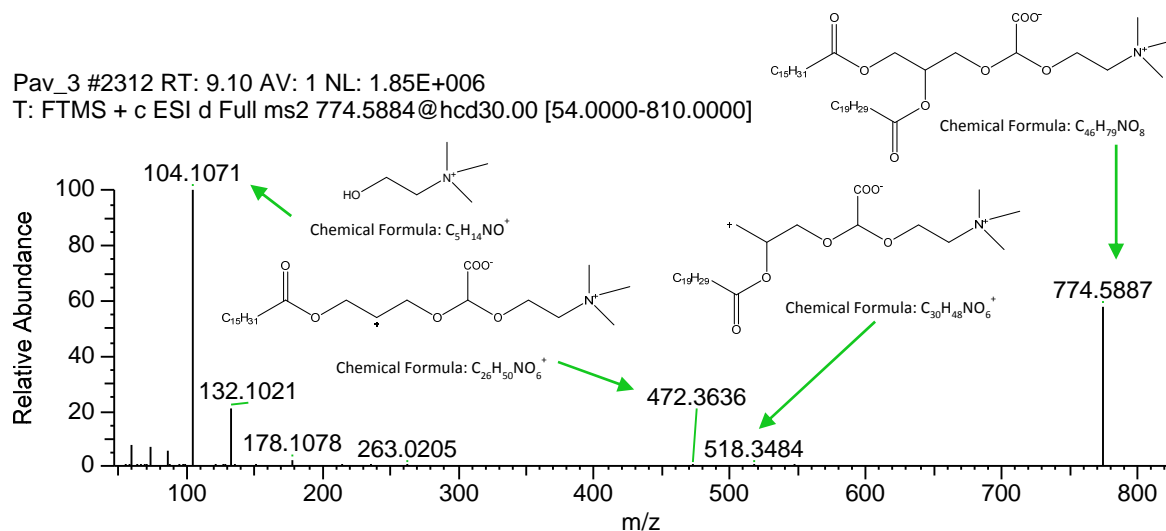


Figure S8. Compound M3834 – m/z 774.5888 – $[M+H]^+$ – $t_R = 9.167$ min – $C_{46}H_{79}NO_8$ – DGCC 16:0/20:5

4222_2 #3557 RT: 13.53 AV: 1 NL: 2.12E+007
T: FTMS + c ESI d Full ms2 932.4946@hcd30.00 [64.6667-970.0000]

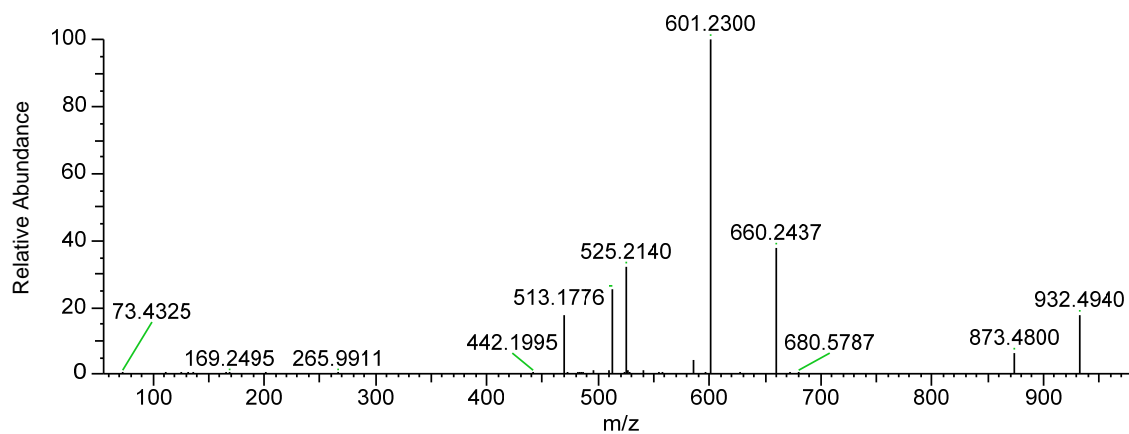


Figure S9. Compound M6284 – m/z 932.4940 – $[M]^+$ – $t_R = 13.397$ min – $C_{56}H_{68}MgN_4O_7$ – Chlorophyll a derivative 1

A551_1 #3984 RT: 15.03 AV: 1 NL: 3.43E+007
T: FTMS + c ESI d Full ms2 952.5202@hcd30.00 [66.0000-990.0000]

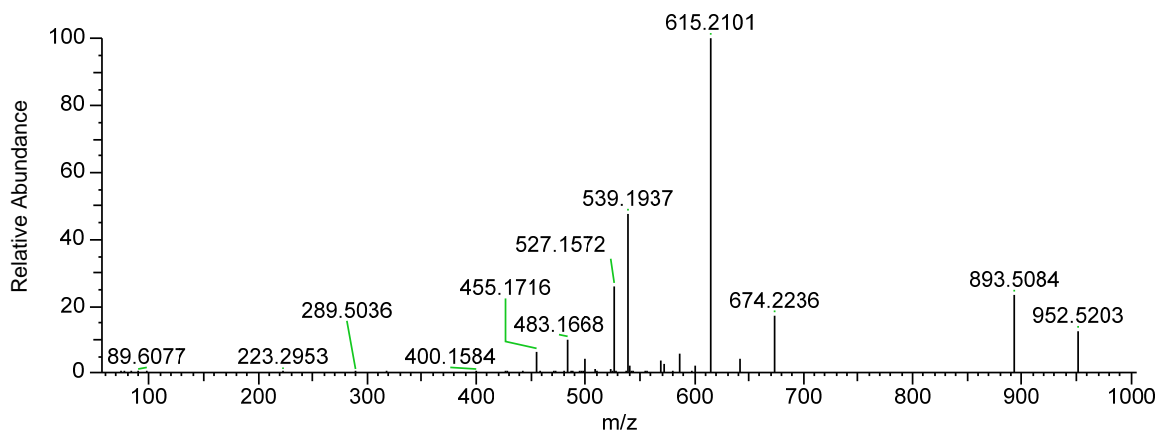


Figure S10. Compound M6982 – m/z 952.5200 – $[M]^+$ – $t_R = 15.072$ min – $C_{56}H_{72}MgN_4O_8$ – Chlorophyll a derivative 2

4222_2 #4311 RT: 16.20 AV: 1 NL: 2.33E+006
T: FTMS + c ESI d Full ms2 938.5413@hcd30.00 [65.0000-975.0000]

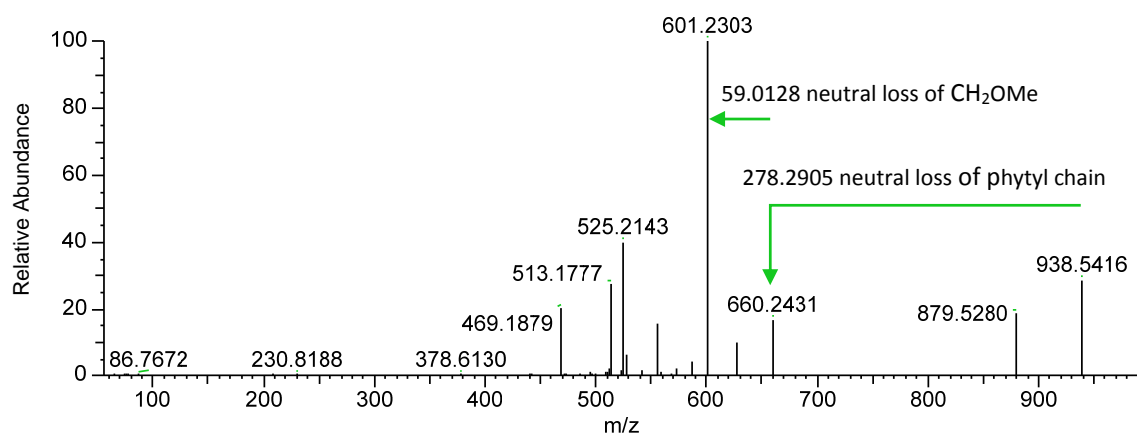


Figure S11. Compound M7441 – m/z 938.5412 – $[M]^+$ – $t_R = 16.286$ min – $C_{56}H_{74}MgN_4O_7$ – Chlorophyll a derivative 3

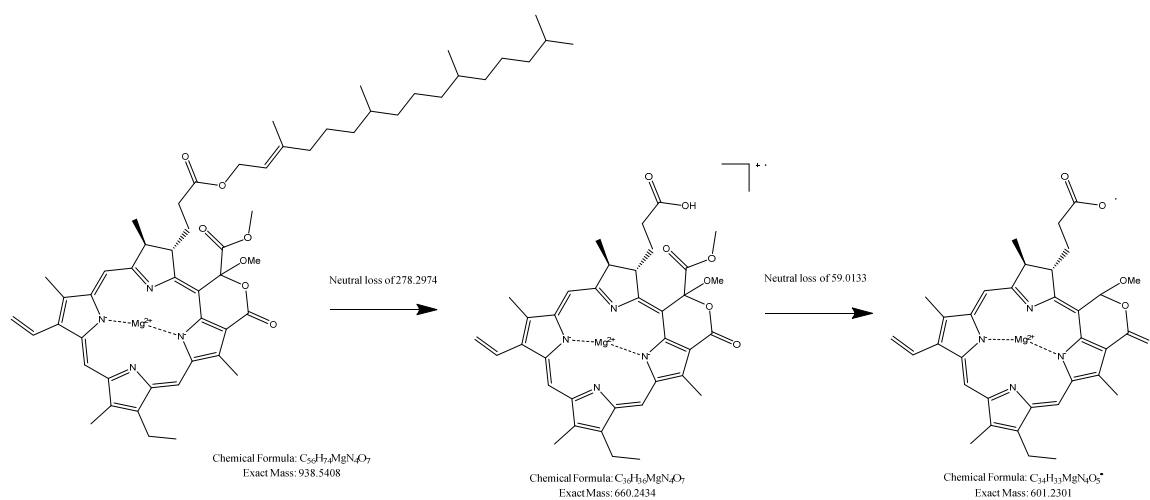


Figure S12. Proposed fragmentation pathway for Compound M7441

ML_2 #4294 RT: 16.05 AV: 1 NL: 3.12E+007
T: FTMS + c ESI d Full ms2 871.5740@hcd30.00 [60.3333-905.0000]

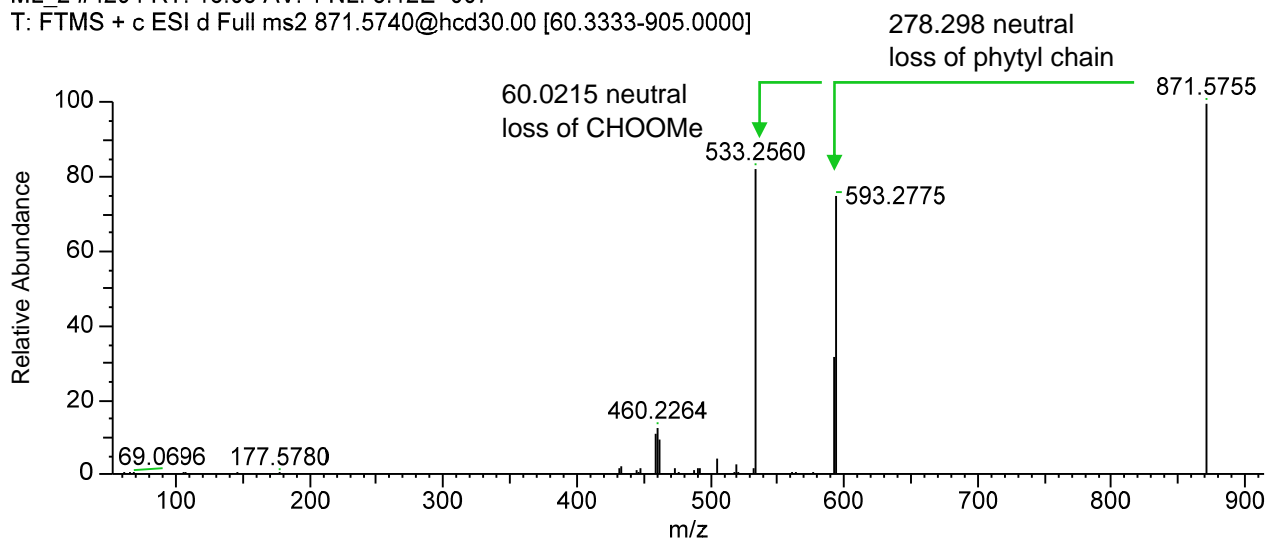


Figure S13. Compound 7354 – m/z 871.5740 – $[M+H]^+$ – $t_r = 16.096$ min – $C_{55}H_{74}N_4O_5$ – Pheophytin a isomer 1

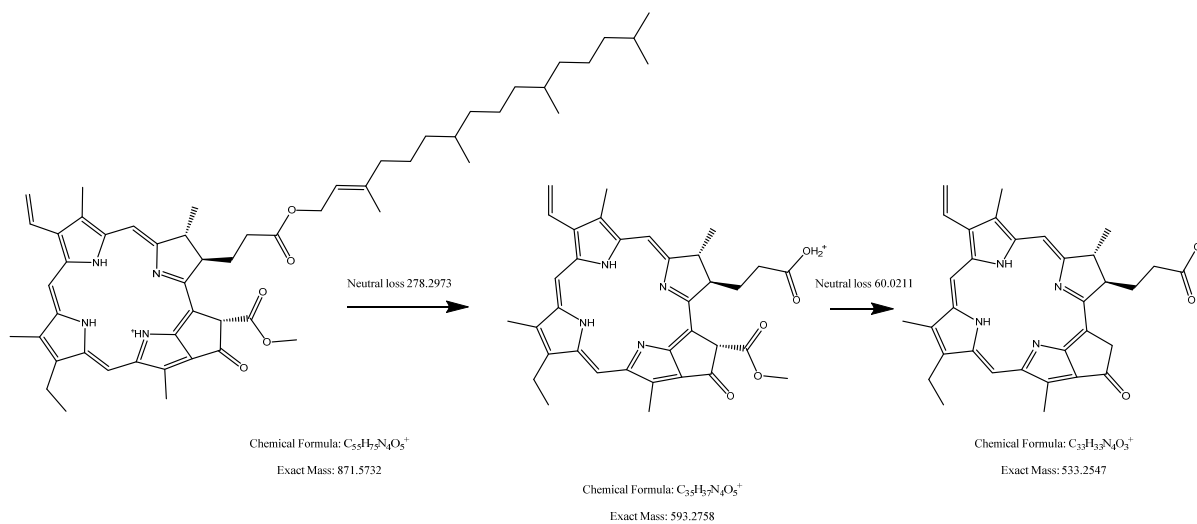


Figure S14. Proposed fragmentation pathway for Compound M7354

ML_2 #4294 RT: 16.05 AV: 1 NL: 3.12E+007
 T: FTMS + c ESI d Full ms2 871.5740@hcd30.00 [60.3333-905.0000]

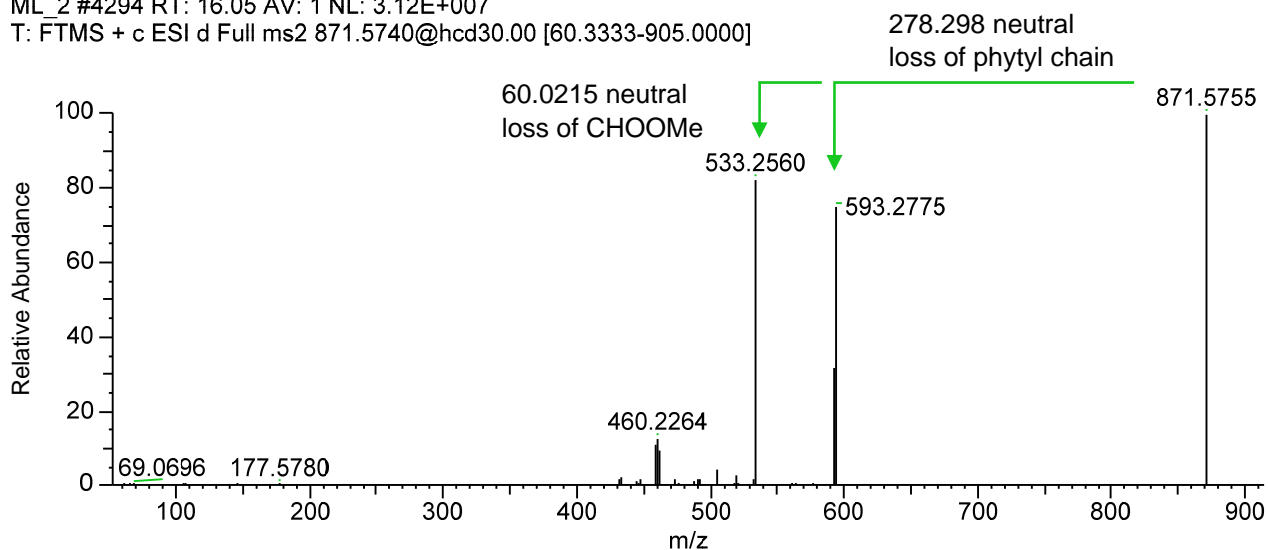


Figure S15. Compound 7377 – m/z 871.5740 – $[M+H]^+$ – $t_r = 16.169$ min – $C_{55}H_{74}N_4O_5$ – Pheophytin a isomer 2

4222_2 #3323 RT: 12.71 AV: 1 NL: 2.22E+007
 T: FTMS + c ESI d Full ms2 887.5696@hcd30.00 [61.6667-925.0000] - H₂O

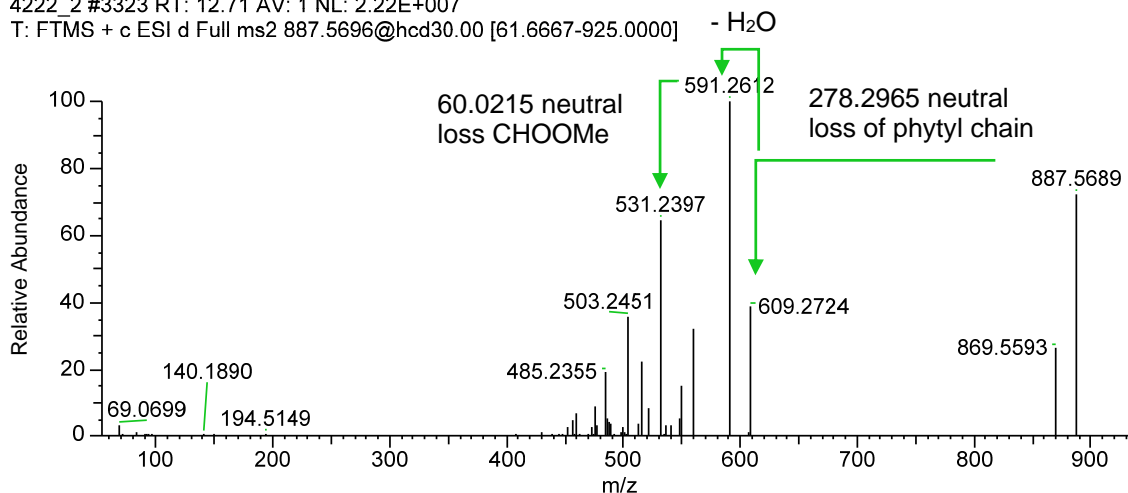


Figure S16. Compound M5963 – m/z 887.5688 – $[M+H]^+$ – $t_r = 12.658$ min – $C_{55}H_{74}N_4O_6$ – Hydroxy-pheophytin isomer 1

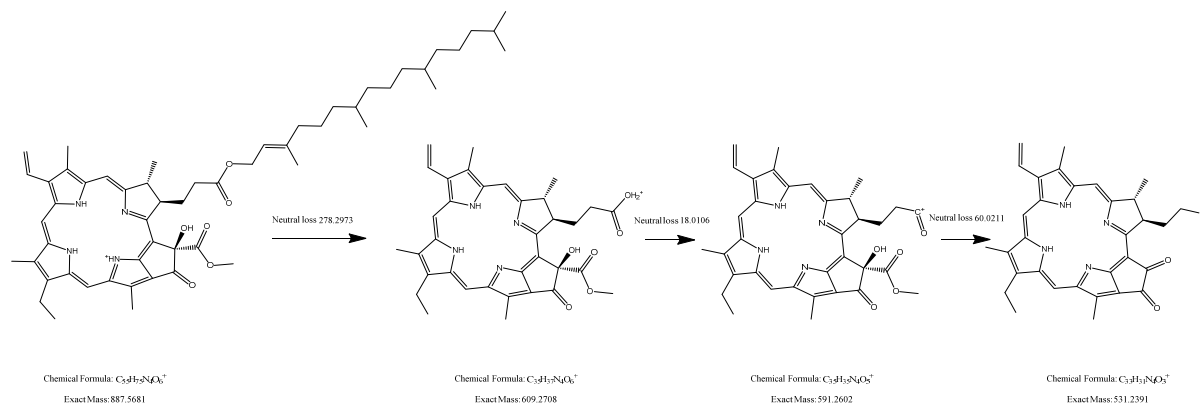


Figure S17. Proposed fragmentation pathway for Compound M5963

4222_2 #3323 RT: 12.71 AV: 1 NL: 2.22E+007
T: FTMS + c ESI d Full ms2 887.5696@hcd30.00 [61.6667-925.0000]

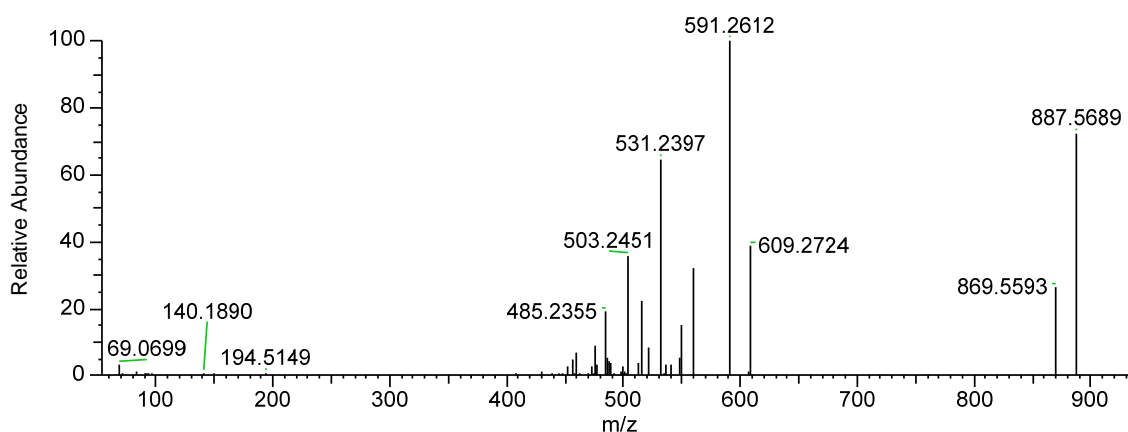


Figure S18. Compound M6021 – m/z 887.5688 – $[M+H]^+$ – $t_r = 12.779$ min – $C_{55}H_{74}N_4O_6$ – Hydroxy-pheophytin isomer 2

B521_3 #3719 RT: 14.21 AV: 1 NL: 7.71E+006
T: FTMS + c ESI d Full ms2 887.5689@hcd30.00 [61.6667-925.0000]

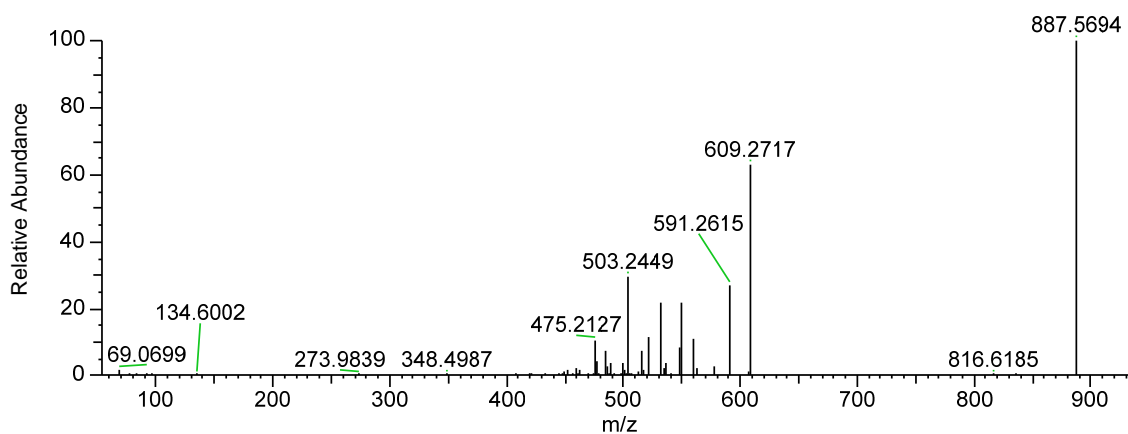


Figure S19. Compound M6695 – m/z 887.5688 – $[M+H]^+$ – $t_r = 14.279$ min – $C_{55}H_{74}N_4O_6$ – Hydroxy-pheophytin isomer 3

4222_2 #3781 RT: 14.32 AV: 1 NL: 1.12E+007
T: FTMS + c ESI d Full ms2 887.5694@hcd30.00 [61.6667-925.0000]

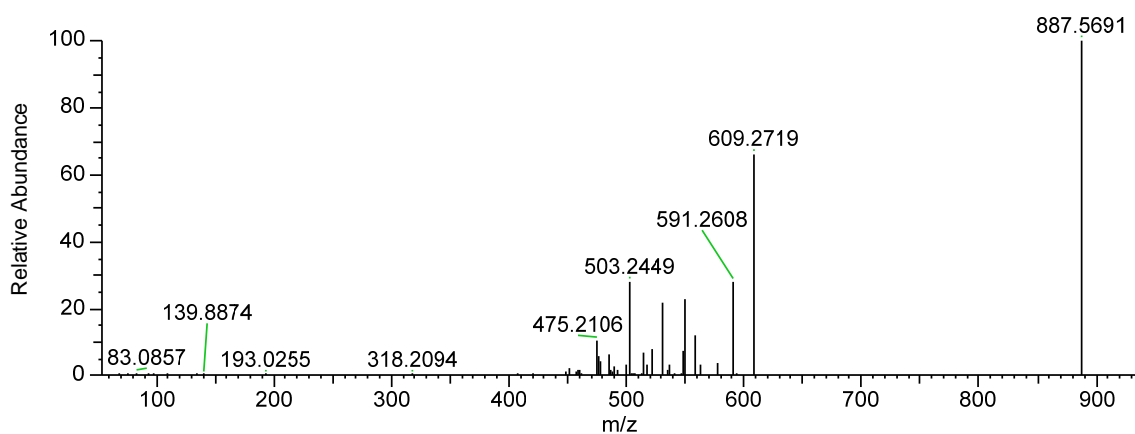


Figure S20. Compound M6726 – m/z 887.5688 – $[M+H]^+$ – $t_r = 14.396$ min – $C_{55}H_{74}N_4O_6$ – Hydroxy-pheophytin isomer 4

4223_2 #1948 RT: 7.74 AV: 1 NL: 8.44E+006
T: FTMS + c ESI d Full ms2 593.2761@hcd30.00 [50.0000-625.0000]

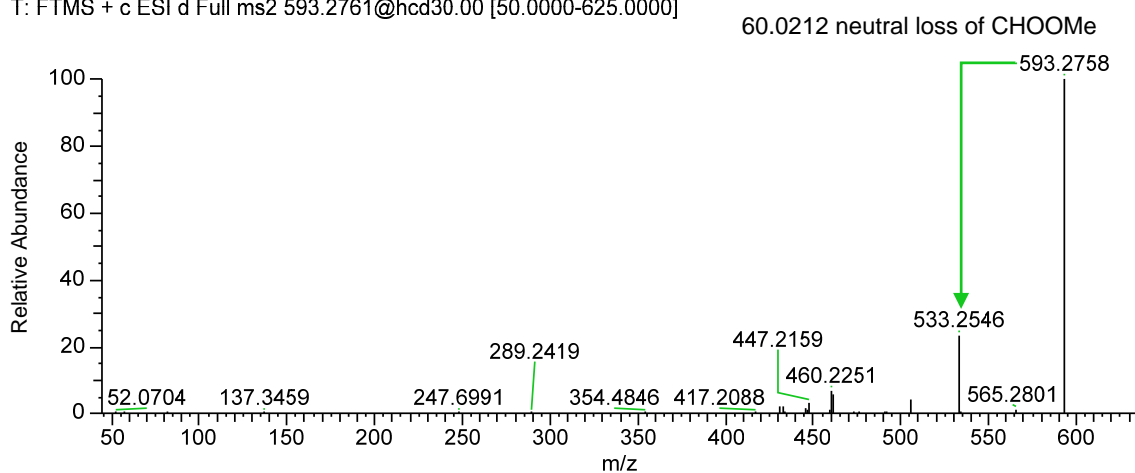


Figure S21. Compound M2385 – m/z 593.2763 – $[M+H]^+$ – $t_r = 7.626$ min – $C_{35}H_{36}N_4O_5$ – Pheophorbide a isomer 1

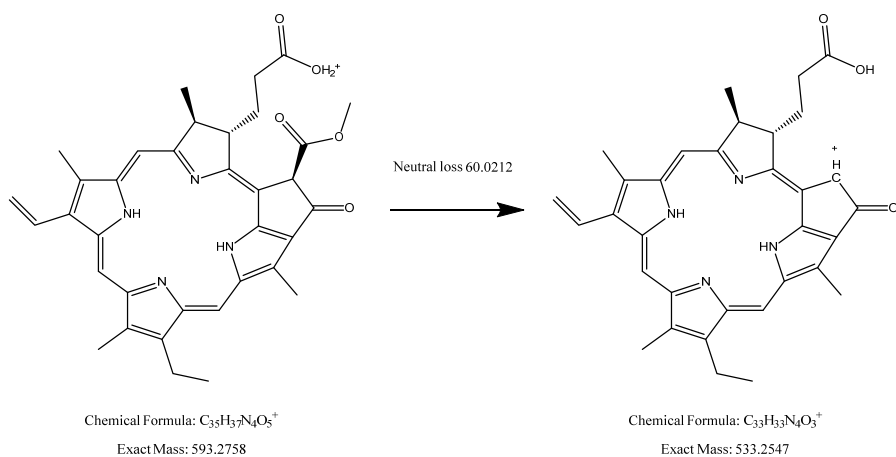


Figure S22. Proposed fragmentation pathway for Compound M2385

4223_3 #2038 RT: 8.10 AV: 1 NL: 5.43E+007
T: FTMS + c ESI d Full ms2 593.2763@hcd30.00 [50.0000-625.0000]

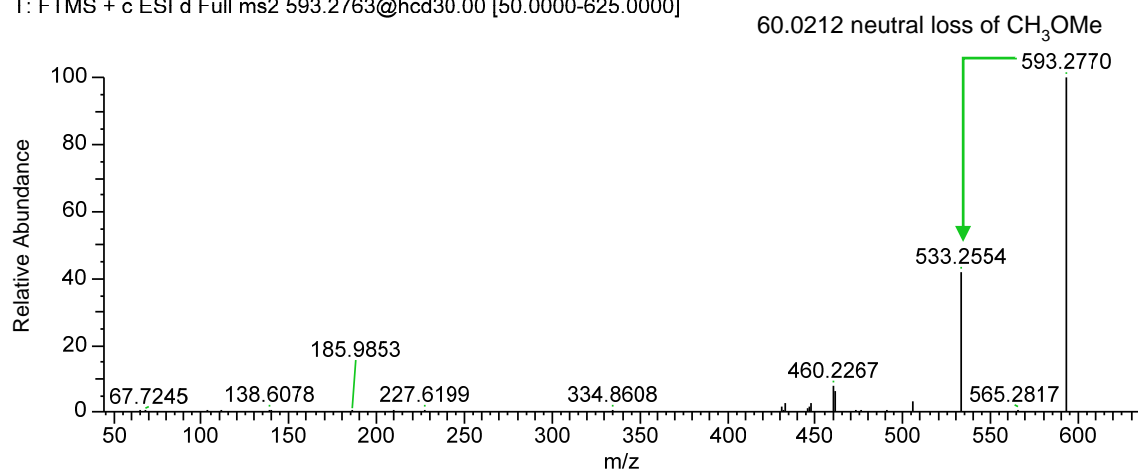


Figure S23. Compound M2789 – m/z 593.2763 – $[M+H]^+$ – t_R = 8.064 min – $C_{35}H_{36}N_4O_5$ – Pheophorbide a isomer 2

A551_2 #3561 RT: 13.70 AV: 1 NL: 2.01E+005
T: FTMS + c ESI d Full ms2 808.6011@hcd30.00 [56.0000-840.0000]

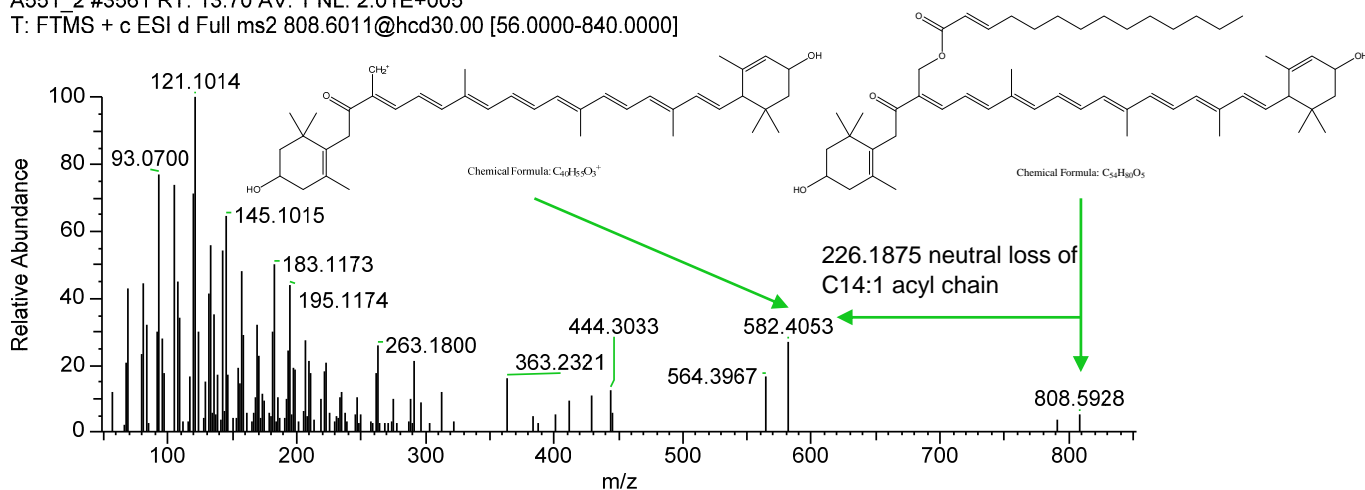


Figure S24. Compound M6441 – m/z 808.6011 – $[M]^+$ – $t_R = 13.721$ min – C₅₄H₈₀O₅ – Siphonaxanthin ester 14:1

A551_1 #2874 RT: 11.17 AV: 1 NL: 8.73E+005
T: FTMS + c ESI d Full ms2 807.5936@hcd30.00 [56.0000-840.0000]

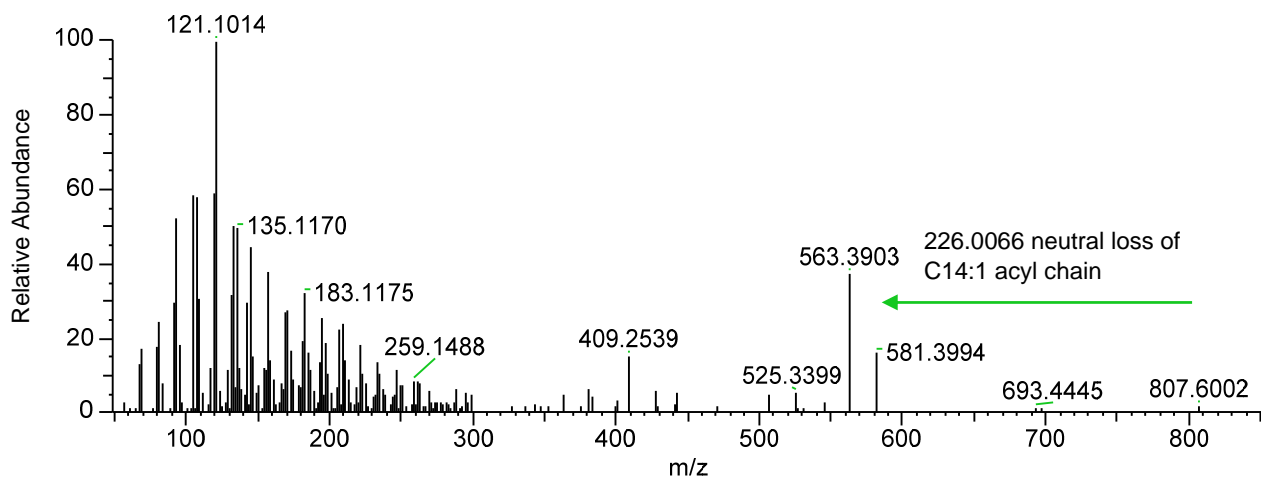


Figure S25. Compound M5328 – m/z 807.5936 – $[M+H]^+$ – $t_R = 11.231$ min – C₅₄H₈₀O₆ – Hydro-siphonaxanthin ester 14:1

A551_1 #2870 RT: 11.15 AV: 1 NL: 1.14E+006
 T: FTMS + c ESI d Full ms2 599.4097@hcd30.00 [50.0000-630.0000]

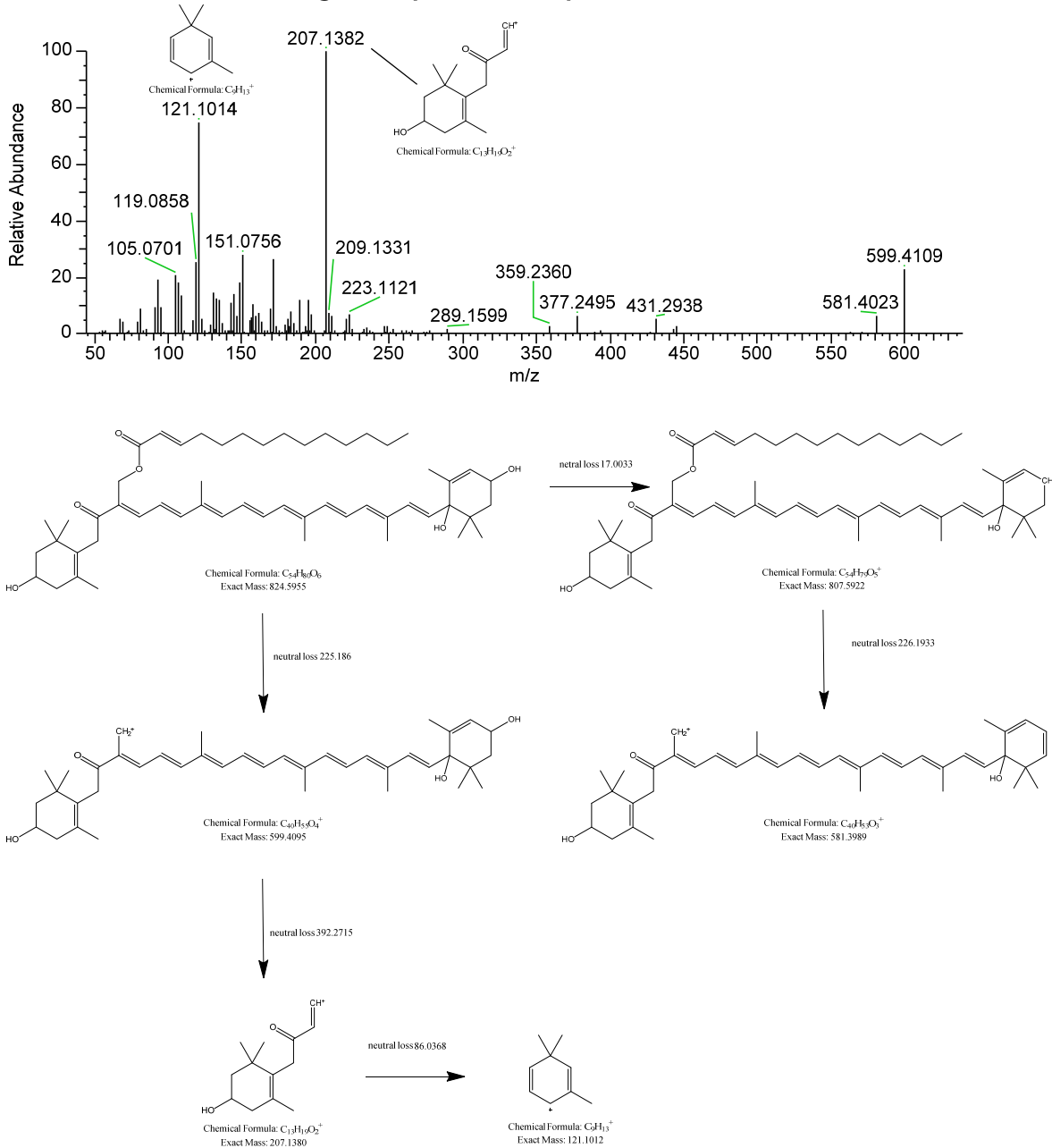


Figure S26. Mass spectra and fragmentation pattern of Siphonaxanthin

A553_3 #3242 RT: 12.11 AV: 1 NL: 1.05E+006
 T: FTMS + c ESI d Full ms2 803.5600@hcd30.00 [55.6667-835.0000]

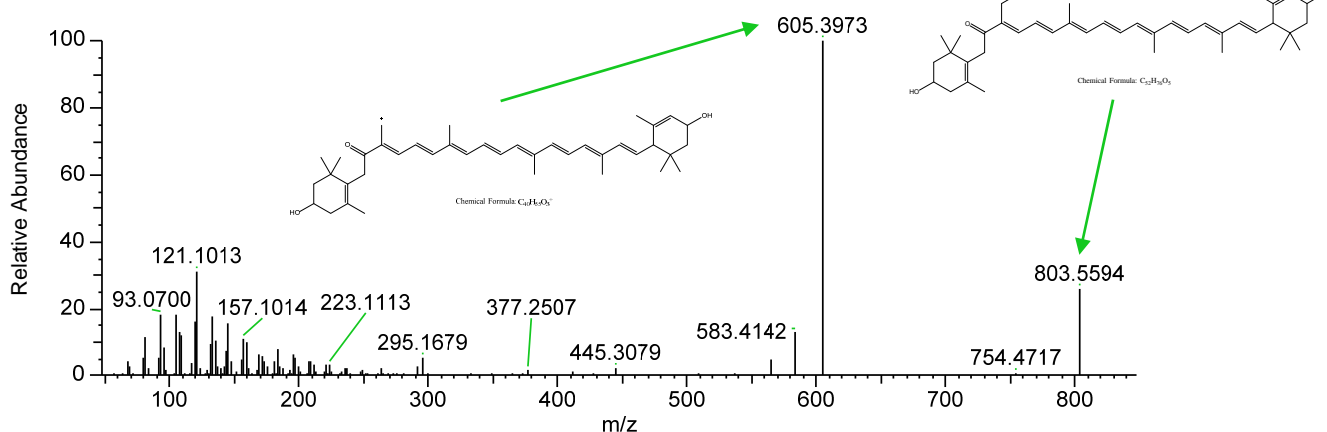


Figure S27. Compound M5763 – m/z 803.5596 – $[M+Na]^+$ – $t_R = 12.187$ min – C22H36O5 – Siphonein

4221_2 #1933 RT: 7.77 AV: 1 NL: 1.12E+006
 T: FTMS + c ESI d Full ms2 601.4246@hcd30.00 [50.0000-630.0000]

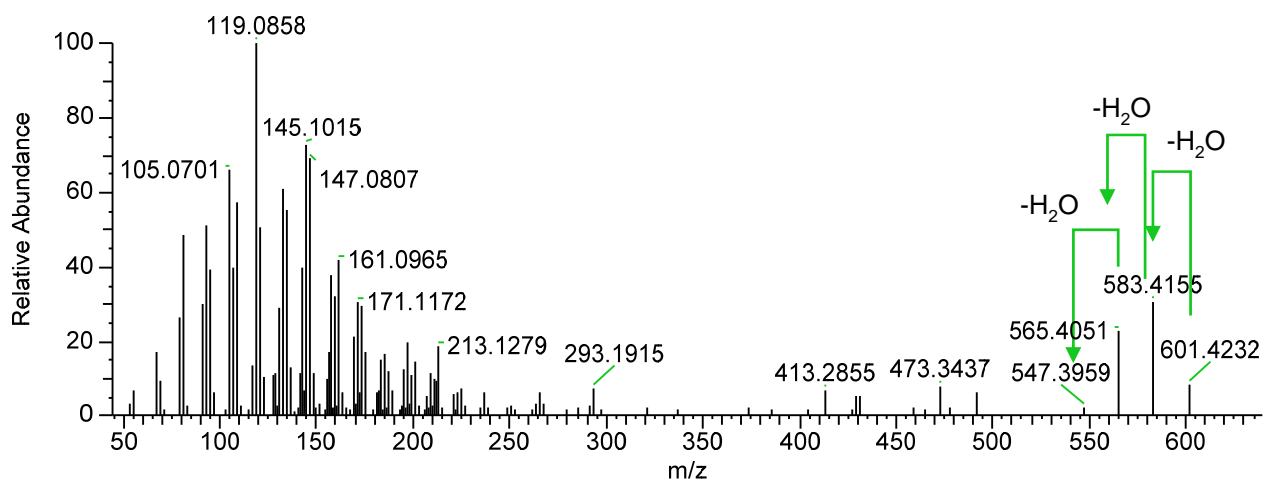


Figure S28. Compound M2546 – m/z 601.4246 – $[M+H]^+$ – $t_R = 7.787$ min – C40H56O4 – Prasinoxanthin

ML_2 #1714 RT: 7.06 AV: 1 NL: 6.43E+005
 T: FTMS + c ESI d Full ms2 600.4175@hcd30.00 [50.0000-630.0000]

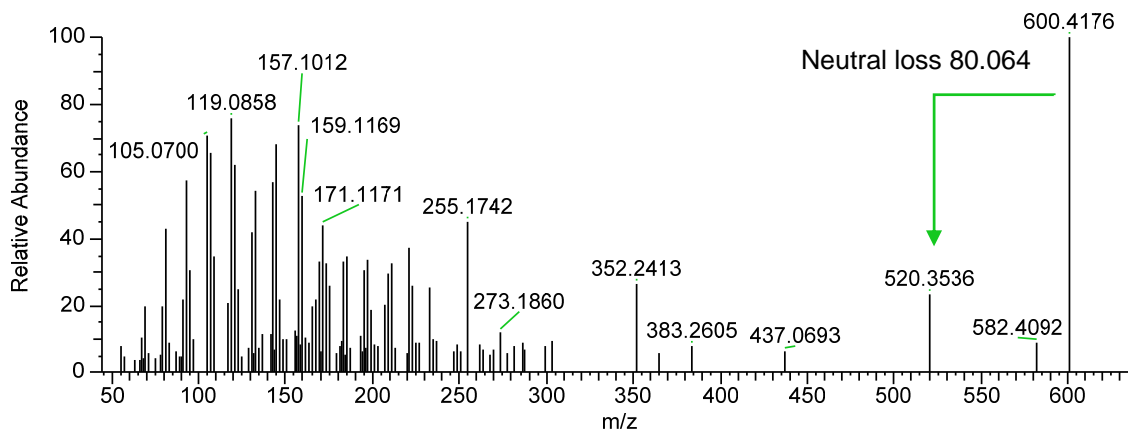
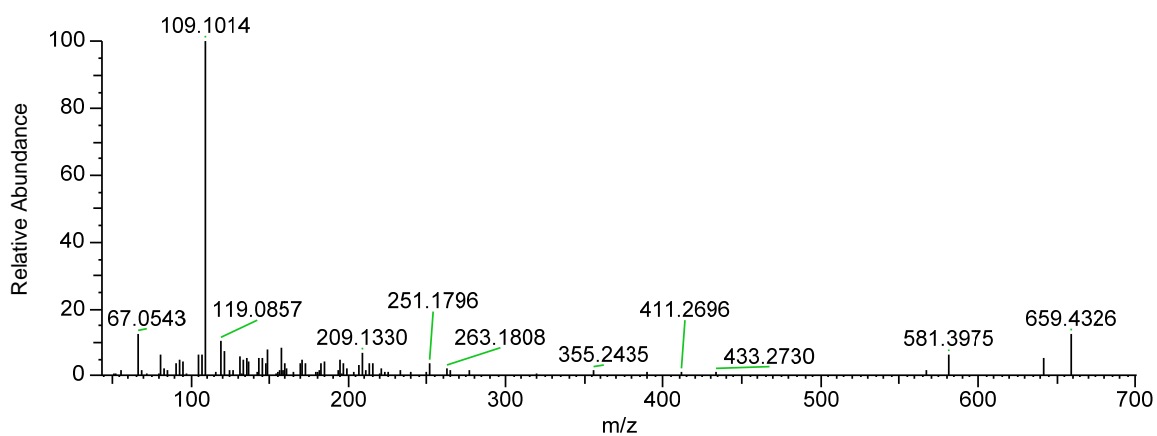


Figure S29. M1889 – m/z 600.4174 – $[M]^+$ – $t_R = 7.03$ min – $C_{40}H_{56}O_4$ – Violaxanthin

Pav_3 #1778 RT: 7.30 AV: 1 NL: 2.88E+005
T: FTMS + c ESI d Full ms2 659.4308@hcd30.00 [50.0000-690.0000]

A



Pav_3 #1807 RT: 7.39 AV: 1 NL: 8.62E+008
T: FTMS + c ESI Full lock ms [133.4000-2000.0000]

B

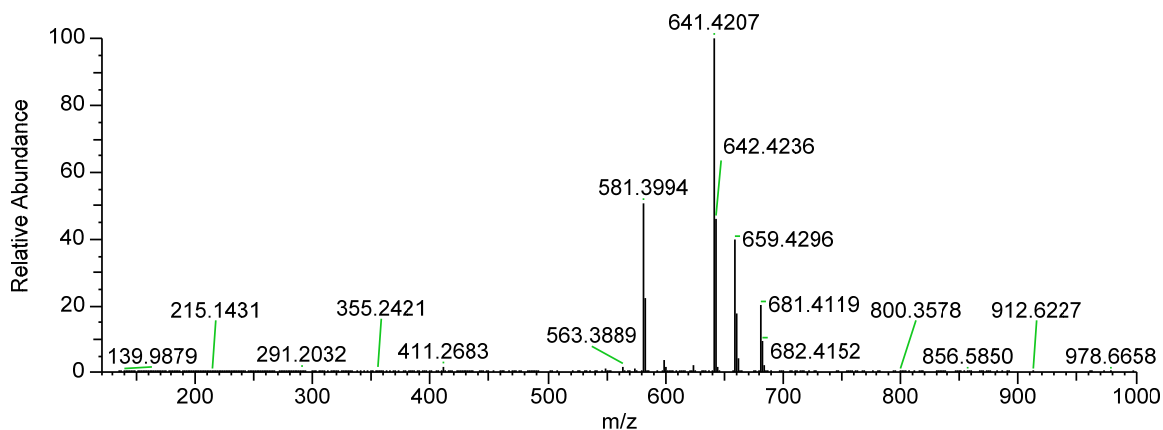


Figure S30. Compound M2211 – m/z 659.4307 – $[M+H]^+$ – $t_R = 7.391$ min – $C_{42}H_{58}O_6$ – Fucoxanthin. **A:** MS^2 , **B:** $MS1$

C1251_2 #3302 RT: 12.52 AV: 1 NL: 3.47E+006
T: FTMS + c ESI d Full ms2 534.4883@hcd30.00 [50.0000-565.0000]

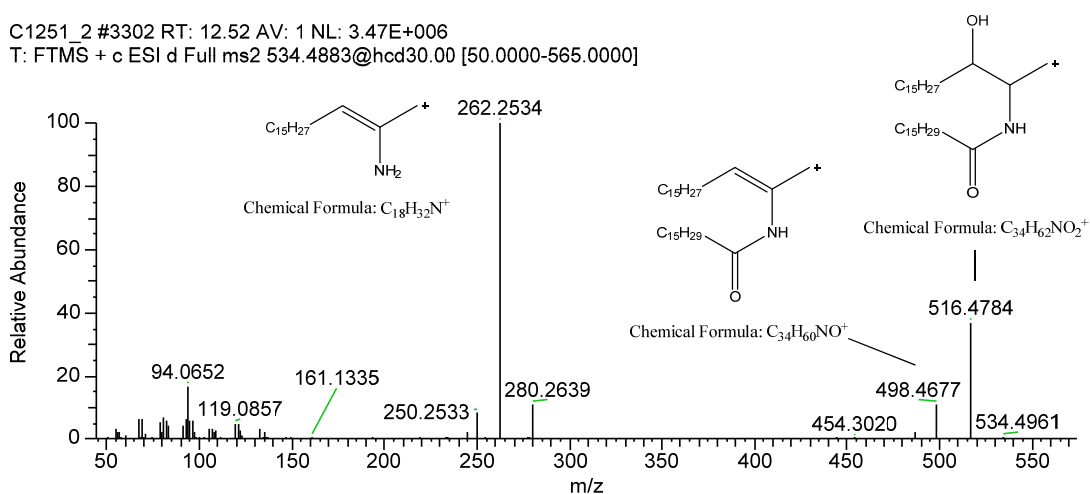


Figure S31. Compound M5935 – m/z 534.4882 – $[M+H]^+$ – $t_R = 12.589$ min – $C_{34}H_{63}NO_3$ – Cer(d18:2/16:1)