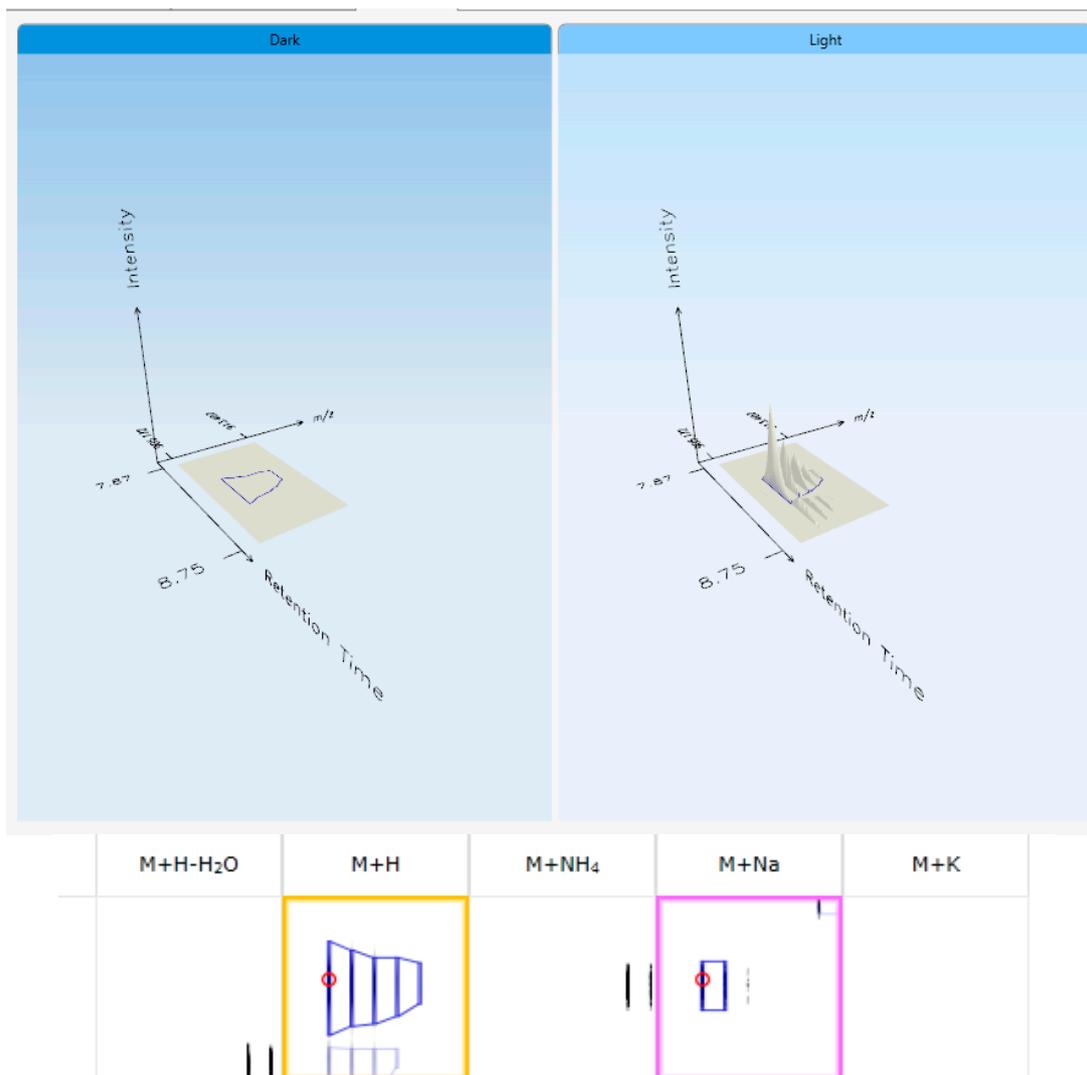


Supplementary Information



(A)

METLIN Metabolites

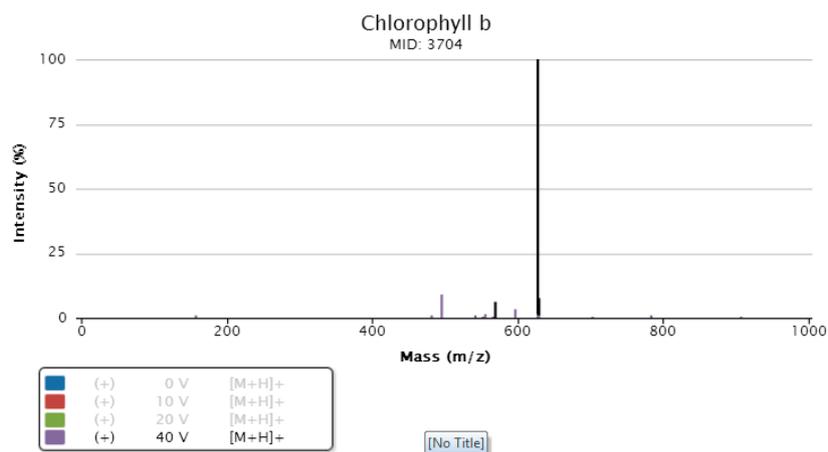
Mass 907.5210 with 5 ppm mass accuracy

[Change Query](#)

Total: 1 Metabolite

METLIN ID	MASS	Δ ppm	NAME	MS/MS	STRUCTURE
3704	[M+H] ⁺ m/z 907.5219 M 906.5146	0	Chlorophyll b Formula: C ₅₅ H ₇₀ MgN ₄ O ₆ CAS: 519-62-0	View	

Figure S1. Cont.



(B)

Figure S1. The statistical identification of metabolic alterations was followed by a review of the measurements using 3D montage and adducts deconvolution (A) and a search on local or online databases (e.g., METLIN, (B)) for structural identification. In this example, a database search lead to a putative structure of a chlorophyll *b*, which was detected only in broccoli sprouts grown in light conditions (A).