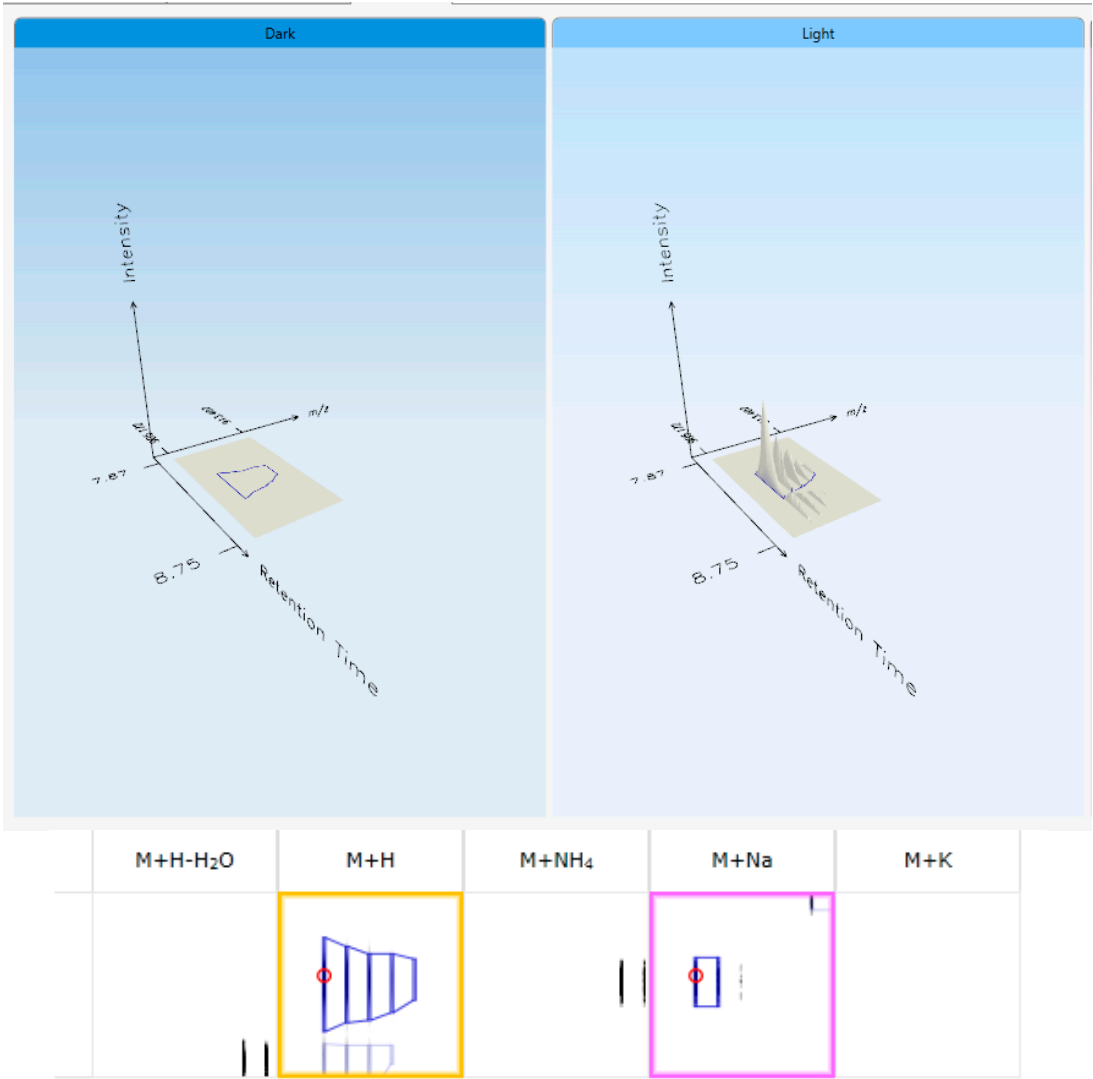


Supplementary Information



(A)

**METLIN**  
Metabolites

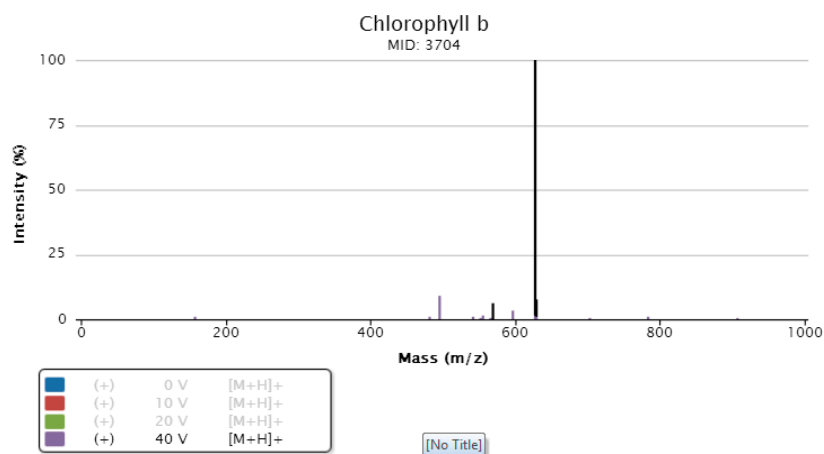
Mass 907.5210 with 5 ppm mass accuracy

Change Query

Total: 1 Metabolite

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

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**).