

Supplementary Materials: A complete survey of glycoalkaloids using LC-FTICR-MS and IRMPD in a commercial variety and a local landrace of eggplant (*Solanum melongena* L.) and their anticholinesterase and antioxidant activities

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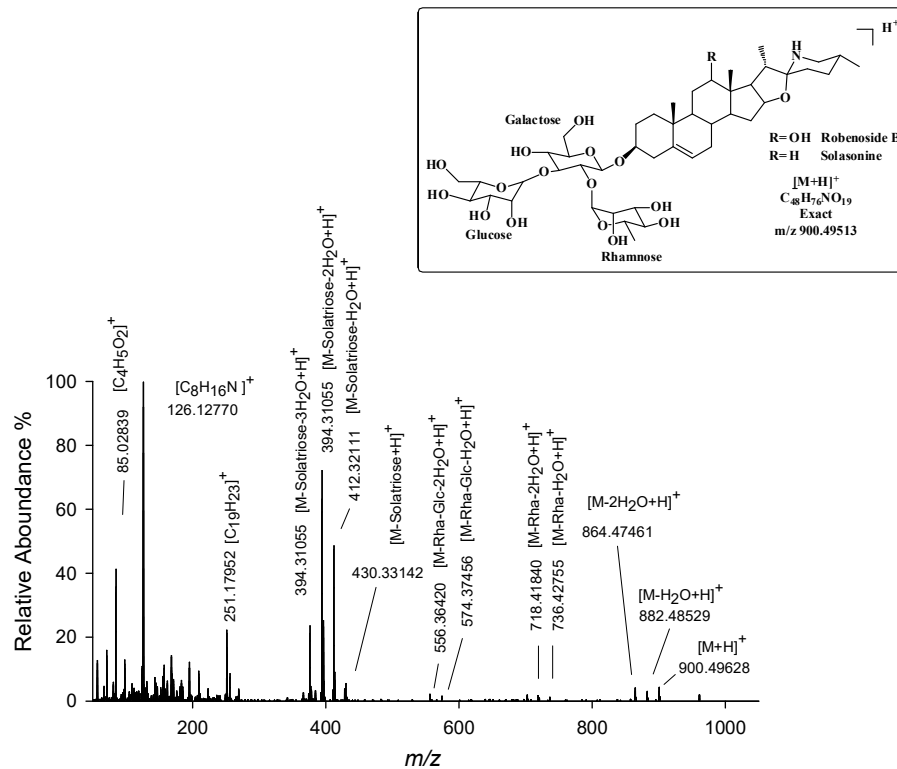


Figure S1. High-resolution IRMPD FTICR mass spectrum of the protonated Robenoside B at m/z 900. Following transfer to the ICR cell, precursor ion populations were photon-irradiated for 290 ms at 100% laser power.

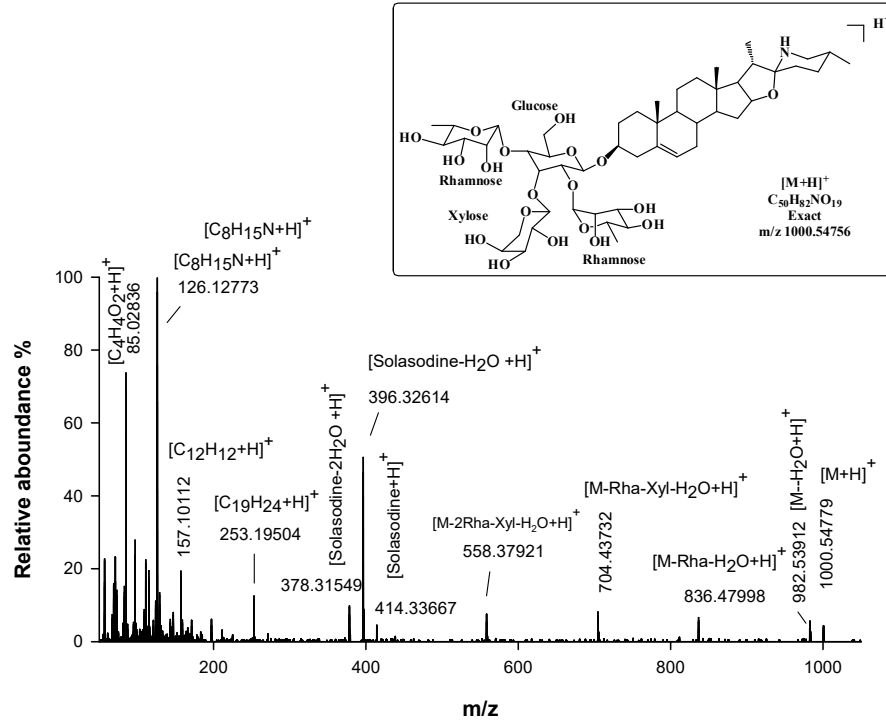


Figure S2. High-resolution IRMPD FTICR mass spectrum of the protonated arudonine at m/z 1000. Following transfer to the ICR cell, precursor ion populations were photon-irradiated for 290 ms at 100% laser power.

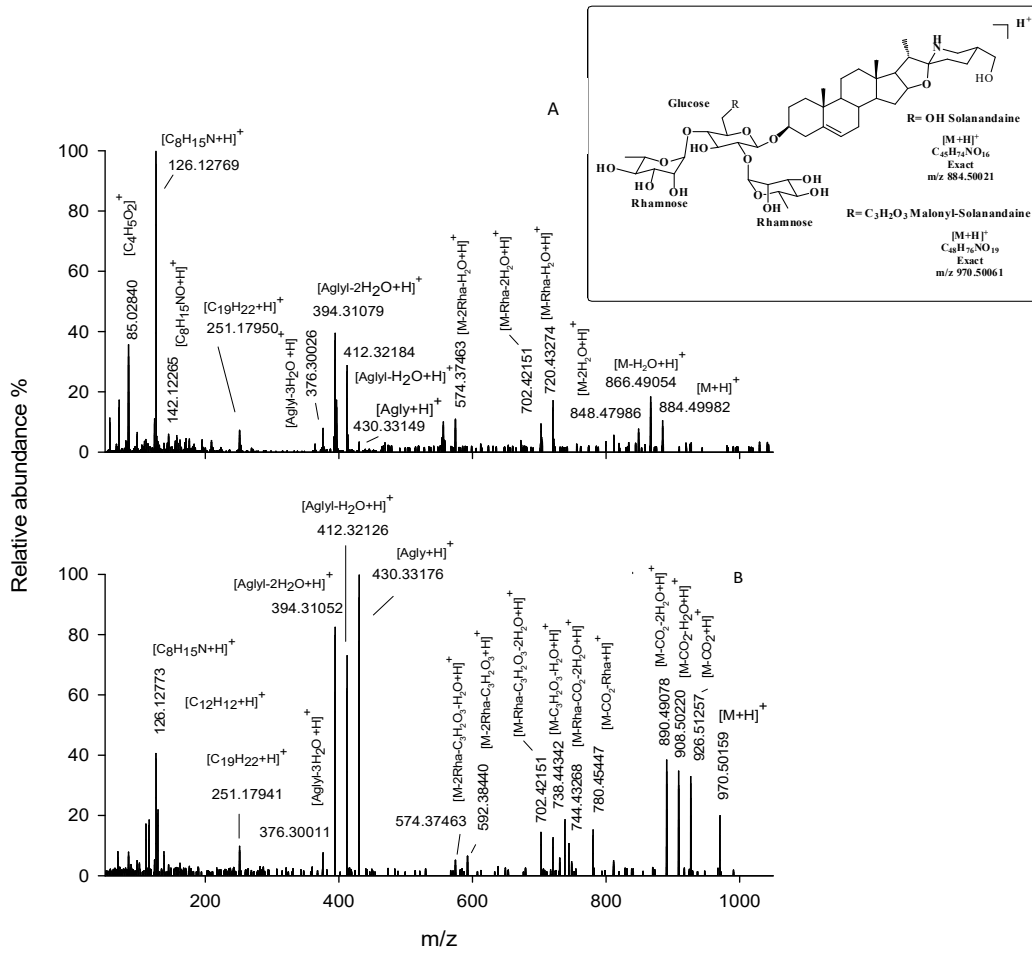


Figure S3. High-resolution IRMPD FTICR mass spectra of the protonated solanandaine (A) at m/z 884 and malonyl-solanandaine (B) at m/z 970. Following transfer to the ICR cell, precursor ion populations were photon-irradiated for 290 ms at 100% laser power.

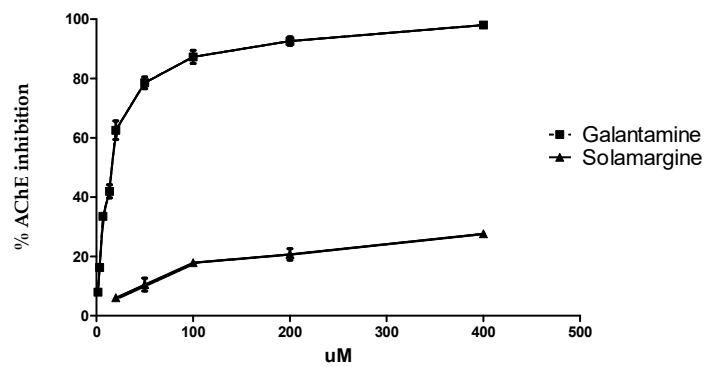


Figure S4. Inhibition of Acetylcholinesterase (AChE) enzyme by Galantamine and Solamargine.

Table S1. IRMPD FTICR MS product ions obtained from glycoalkaloids and malonyl glycoalkaloid and identified in *S. melongena* pulp by high resolution LC-ESI-IRMPD-FTICR MS.

Compound	Chemical formula as protonated molecule, [M+H] ⁺	Precursor Ion Accurate m/z	Main IRMPD MS/MS product ions (accurate m/z) ^a and mass error (ppm) ^b
1)	[C ₄₅ H ₇₂ NO ₁₆] ⁺	882.48419	864.47543 (C ₄₅ H ₇₀ NO ₁₅ ⁺ , 1.6), 718.41730 (C ₃₉ H ₆₀ NO ₁₁ ⁺ , 0.7), 572.35901 (C ₃₃ H ₅₀ NO ₇ ⁺ , 1.5), 428.31628 (C ₂₇ H ₄₂ NO ₃ ⁺ , 0.8), 410.30557 (C ₂₇ H ₄₀ NO ₂ ⁺ , 0.5), 392.29504 (C ₂₇ H ₃₈ NO ⁺ , 0.6), 374.28439 (C ₂₇ H ₃₆ N ⁺ , 0.4), 267.17441 (C ₁₉ H ₂₃ O ⁺ , 0.2), 126.12770 (C ₈ H ₁₆ N ⁺ , -0.2)
2)	[C ₄₅ H ₇₂ NO ₁₅] ⁺	866.49005	720.43188 (C ₃₉ H ₆₂ NO ₁₁ ⁺ , 0.2), 574.37402 (C ₃₃ H ₅₂ NO ₇ ⁺ , 0.3), 412.31111 (C ₂₇ H ₄₂ NO ₂ ⁺ , 0.2), 394.31052 (C ₂₇ H ₄₀ NO ⁺ , 0.1), 182.15393 (C ₁₁ H ₂₀ NO ⁺ , -0.05), 157.10114 (C ₁₂ H ₁₃ ⁺ , -0.3), 85.02840 (C ₄ H ₅ O ₂ ⁺ , -0.1)
3)	[C ₄₅ H ₇₂ NO ₁₅] ⁺	866.48950	848.48059 (C ₄₅ H ₇₀ NO ₁₄ ⁺ , 1.5), 720.43060 (C ₃₉ H ₆₂ NO ₁₁ ⁺ , -1.6), 702.42242 (C ₃₉ H ₆₀ NO ₁₀ ⁺ , -1.4), 574.37469 (C ₃₃ H ₅₂ NO ₇ ⁺ , 1.1), 558.37952 (C ₃₃ H ₅₀ NO ₆ ⁺ , 1.1), 556.36407 (C ₃₃ H ₅₀ NO ₆ ⁺ , 1.4), 412.32129 (C ₂₇ H ₄₂ NO ₂ ⁺ , 0.7), 396.32632 (C ₂₇ H ₄₂ NO ⁺ , 0.6), 394.31067 (C ₂₇ H ₄₀ NO ⁺ , 0.6), 376.30002 (C ₂₇ H ₃₈ N ⁺ , -1.0)
4)	[C ₄₅ H ₇₄ NO ₁₆] ⁺	884.50055	866.49023 (C ₄₅ H ₇₂ NO ₁₅ ⁺ , 0.6), 412.32104 (C ₂₇ H ₄₂ NO ₂ ⁺ , 0.08), 394.31076 (C ₂₇ H ₄₀ NO ⁺ , 0.6), 271.20560 (C ₁₉ H ₂₇ O ⁺ , -0.2), 253.19504 (C ₁₉ H ₂₅ ⁺ , -0.15), 157.10112 (C ₁₂ H ₁₃ ⁺ , -0.4), 85.02837 (C ₄ H ₅ O ₂ ⁺ , -0.4)
5)	[C ₄₅ H ₇₄ NO ₁₆] ⁺	884.49982	866.50575 (C ₄₅ H ₇₂ NO ₁₅ ⁺ , 1.0), 720.43368 (C ₃₉ H ₆₂ NO ₁₁ ⁺ , 2.7), 430.33249 (C ₂₇ H ₄₄ NO ₃ ⁺ , 2.1), 412.32184 (2.0), 394.311116 (C ₂₇ H ₄₀ NO ⁺ , 1.8), 376.00063 (C ₂₇ H ₃₈ N ⁺ , 1.9), 364.26401 (C ₂₅ H ₃₄ NO ⁺ , 1.4), 251.17964 (C ₁₉ H ₂₃ ⁺ , 0.8), 126.12769 (C ₈ H ₁₆ N ⁺ , -0.3)
6)	[C ₄₅ H ₇₄ NO ₁₆] ⁺	884.50000	866.50500 (C ₄₅ H ₇₂ NO ₁₅ ⁺ , 0.1), 720.43324 (C ₃₉ H ₆₂ NO ₁₁ , 2.1), 558.37856 (C ₃₃ H ₅₂ NO ₆ , -0.6), 414.33592 (C ₂₇ H ₄₄ NO ₂ , -1.7), 396.32658 (C ₂₇ H ₄₂ NO, 1.2), 253.19576 (C ₁₉ H ₂₅ , 2.7), 157.10123 (C ₁₂ H ₁₃ , 0.3), 126.12772 (C ₈ H ₁₆ N, 1.4), 85.02845 (C ₄ H ₅ O ₂ , 0.5)
7)	[C ₄₅ H ₇₄ NO ₁₇] ⁺	900.49607	882.48529 (C ₄₅ H ₇₂ NO ₁₆ , 0.8), 864.47461 (C ₄₅ H ₇₀ NO ₁₅ , 0.7), 736.42755(), 718.41640 (C ₃₉ H ₆₀ NO ₁₁ , 0.4), 574.37456 (C ₃₃ H ₅₂ NO ₆ , 1.3), 556.36420 (C ₃₃ H ₅₀ NO ₅ , 1.7), 430.33142 (C ₂₇ H ₄₄ NO ₃ , -0.8), 412.32111 (C ₂₇ H ₄₂ NO ₂ , 0.2), 394.31055 (C ₂₇ H ₄₀ NO, 0.3), 376.26370 (C ₂₆ H ₃₄ NO, 0.6), 251.17952 (C ₁₉ H ₂₃ , 0.4), 126.12770 (C ₈ H ₁₆ N, 0.04), 85.02839 (C ₄ H ₅ O ₂ , -0.02)
8)	[C ₄₈ H ₇₄ NO ₁₈] ⁺	952.48956	908.50000 (C ₄₇ H ₇₄ NO ₁₆ , -0.2), 890.48959 (C ₄₇ H ₇₂ NO ₁₅ , -0.2), 762.44232 (C ₄₁ H ₄₆ NO ₁₂ , 0.02), 720.43188 (C ₃₉ H ₆₂ NO ₁₁ , 0.2), 574.37378 (C ₃₃ H ₅₂ NO ₇ , -0.08), 412.32077 (C ₂₇ H ₄₂ NO ₂ , -0.5), 394.31030 (C ₂₇ H ₄₀ NO, -0.4), 162.12762 (C ₁₁ H ₁₆ N, -0.6), 85.02835 (C ₄ H ₅ O ₂ , -0.6)
9)	[C ₄₅ H ₇₄ NO ₁₅] ⁺	868.50641	850.49524 (C ₄₅ H ₇₂ NO ₁₄ ⁺ , 0.6), 704.44912 (C ₃₉ H ₆₂ NO ₁₀ ⁺ , 1.6), 414.33682 (C ₂₇ H ₄₄ NO ₂ ⁺ , 0.4), 396.32608 (C ₂₇ H ₄₂ NO ⁺ , -0.02), 378.31564 (C ₂₇ H ₄₀ N ⁺ , 0.3), 253.19507 (C ₁₉ H ₂₅ ⁺ , 0.03)
10)	[C ₄₅ H ₇₄ NO ₁₅] ⁺	868.50573	850.50995 (C ₄₅ H ₇₂ NO ₁₄ ⁺ , 1.6), 704.44910 (C ₃₉ H ₆₂ NO ₁₀ ⁺ , 1.6), 558.37844 (C ₃₃ H ₅₂ NO ₆ ⁺ , -0.8), 414.33688 (C ₂₇ H ₄₄ NO ₂ ⁺ , 0.5), 396.32617 (C ₂₇ H ₄₂ NO ⁺ , 0.2), 378.31558 (C ₂₇ H ₄₀ N ⁺ , 0.1), 271.2056 (C ₁₉ H ₂₇ O ⁺ , 0.2), 253.19508 (C ₁₉ H ₂₅ ⁺ , 0.02), 197.13243 (C ₁₅ H ₁₇ ⁺ , -0.2), 157.10110 (C ₁₂ H ₁₃ ⁺ , -0.5), 147.06511 (C ₆ H ₁₁ O ₄ ⁺ , -0.5), 143.08546 (C ₁₁ H ₁₁ ⁺ , -0.5), 126.12766 (C ₈ H ₁₆ N ⁺ , -0.6), 85.02835 (C ₄ H ₅ O ₂ ⁺ , -0.6)
11)	[C ₄₅ H ₆₈ NO ₁₅] ⁺	862.45864	716.39897 (C ₃₉ H ₅₈ NO ₁₁ ⁺ , -2.0), 570.34136 (C ₃₃ H ₄₈ NO ₇ ⁺ , -2.0), 408.28930 (C ₂₇ H ₃₈ NO ₂ ⁺ , -1.0), 390.27904 (C ₂₇ H ₃₆ NO ⁺ , -0.3), 376.26392 (C ₂₆ H ₃₄ NO ⁺ , 1.1)

12)	[C ₄₈ H ₇₆ NO ₁₉] ⁺	970.50130	926.51257 (C ₄₇ H ₇₆ NO ₁₇ ⁺ , -0.9), 908.50220 (C ₄₇ H ₇₆ NO ₁₇ ⁺ , -0.9), 890.49078 (C ₄₇ H ₇₂ NO ₁₅ ⁺ , 1.3), 780.45247 (C ₄₁ H ₆₆ NO ₁₃ ⁺ , -0.5), 744.43268 (C ₄₁ H ₆₂ NO ₁₁ ⁺ , 1.2), 702.42151 (C ₃₉ H ₆₀ NO ₁₀ ⁺ , 0.4), 430.33179 (C ₂₇ H ₄₄ NO ₃ ⁺ , 0.5), 412.32126 (C ₂₇ H ₄₂ NO ₂ ⁺ , 0.6), 394.31052 (C ₂₇ H ₄₀ NO ⁺ , 0.2), 376.30011 (C ₂₆ H ₃₄ NO ⁺ , 0.6), 251.17941 (C ₁₉ H ₂₃ ⁺ , 0.05), 126.12772 (C ₈ H ₁₆ N ⁺ , -0.02)
13)	[C ₄₈ H ₇₀ NO ₁₈] ⁺	948.45788	904.46846 (C ₄₇ H ₇₀ NO ₁₆ ⁺ , -0.5), 862.45704 (C ₄₅ H ₆₈ NO ₁₅ ⁺ , 1.5), 844.44654 (C ₄₅ H ₆₆ NO ₁₄ ⁺ , -1.5), 758.44888 (C ₄₁ H ₆₀ NO ₁₂ ⁺ , 2.0), 716.39987 (C ₃₉ H ₅₈ NO ₁₁ ⁺ , -0.8), 408.28955 (C ₂₇ H ₃₈ NO ₂ ⁺ , -0.4), 390.27852 (C ₂₇ H ₃₆ NO ⁺ , 1.8), 376.26380 (C ₂₆ H ₃₄ NO ⁺ , 0.8)
14)	[C ₅₀ H ₈₂ NO ₁₉] ⁺	1000.54779	982.53912 (C ₅₀ H ₈₀ NO ₁₈ ⁺ , 2.1), 836.47998 (C ₄₄ H ₇₀ NO ₁₄ ⁺ , 1.0), 704.43732 (C ₃₉ H ₆₂ NO ₁₀ ⁺ , 0.7), 558.37921 (C ₃₃ H ₅₂ NO ₁₀ ⁺ , 0.5), 414.33667 (C ₂₇ H ₄₄ NO ₂ ⁺ , 0.03), 396.32614 (C ₂₇ H ₄₂ NO ⁺ , 0.1), 378.31549 (C ₂₇ H ₄₀ N ⁺ , -0.1), 253.19504 (C ₁₉ H ₂₅ ⁺ , -0.1), 157.10112 (C ₁₂ H ₁₃ ⁺ , -0.3), 126.12766 (C ₈ H ₁₆ N ⁺ , -0.5)
15)	[C ₄₈ H ₇₆ NO ₁₈] ⁺	954.50584	910.51624 (C ₄₇ H ₇₆ NO ₁₆ ⁺ , 0.4), 892.50586 (C ₄₇ H ₇₄ NO ₁₅ ⁺ , 0.4), 764.45892 (C ₄₁ H ₆₆ NO ₁₂ ⁺ , 0.1), 746.44781 (C ₄₁ H ₆₄ NO ₁₁ ⁺ , 0.6), 722.44781 (C ₃₉ H ₆₄ NO ₁₁ ⁺ , 0.6), 576.38971 (C ₃₃ H ₅₄ NO ₇ ⁺ , 0.4), 558.37909 (C ₃₃ H ₅₂ NO ₆ ⁺ , 0.3), 414.33670 (C ₂₇ H ₄₄ NO ₂ ⁺ , 0.1), 396.32611 (C ₂₇ H ₄₂ NO ⁺ , 0.04), 378.31555 (C ₂₇ H ₄₀ NO ⁺ , 0.06), 271.20587 (C ₁₉ H ₂₇ O ⁺ , 0.8)
16)	[C ₄₈ H ₇₆ NO ₁₈] ⁺	954.50525	910.51751 (C ₄₇ H ₇₆ NO ₁₆ ⁺ , 1.8), 892.50543 (C ₄₇ H ₇₄ NO ₁₅ ⁺ , 0.1), 764.45806 (0.1), 746.44784 (C ₄₁ H ₆₆ NO ₁₂ ⁺ , 0.6), 722.44865 (C ₃₉ H ₆₄ NO ₁₁ ⁺ , 1.7), 576.38941 (C ₃₃ H ₅₄ NO ₇ ⁺ , -0.1), 558.37898 (C ₃₃ H ₅₂ NO ₆ ⁺ , 0.1), 414.33672 (C ₂₇ H ₄₄ NO ₂ ⁺ , 0.1), 396.32690 (C ₂₇ H ₄₂ NO ⁺ , 2.0), 378.31576 (C ₂₇ H ₄₀ NO ⁺ , 0.6), 253.19502 (C ₁₉ H ₂₇ ⁺ , -0.2)
17)	[C ₄₅ H ₇₄ NO ₁₆] ⁺	884.49939	866.48907 (C ₄₅ H ₇₂ NO ₁₅ ⁺ , -0.7), 848.47858 (C ₄₅ H ₇₀ NO ₁₄ ⁺ , -0.6), 720.43134 (C ₃₉ H ₆₂ NO ₁₁ ⁺ , -0.6), 574.37366 (C ₃₃ H ₅₂ NO ₇ ⁺ , -0.3), 430.33118 (C ₂₇ H ₄₄ NO ₃ ⁺ , -0.9), 412.32077 (C ₂₇ H ₄₂ NO ₂ ⁺ , -0.6), 394.31021 (C ₂₇ H ₄₀ NO ⁺ , -0.6), 376.29959 (C ₂₇ H ₃₈ N ⁺ , -0.7), 251.17924 (C ₁₉ H ₂₃ ⁺ , -0.7), 168.13818 (C ₁₀ H ₁₈ NO ⁺ , -0.6), 126.12765 (C ₈ H ₁₆ N ⁺ , -0.6)
18)	[C ₄₅ H ₇₄ NO ₁₆] ⁺	884.49994	866.48914 (C ₄₅ H ₇₂ NO ₁₅ ⁺ , -0.6), 720.43140 (C ₃₉ H ₆₂ NO ₁₁ ⁺ , -0.5), 430.33173 (C ₂₇ H ₄₄ NO ₃ ⁺ , 0.4), 412.32098 (C ₂₇ H ₄₂ NO ₂ ⁺ , -0.05), 394.31042 (C ₂₇ H ₄₀ NO ⁺ , -0.04), 376.29977 (C ₂₇ H ₃₈ N ⁺ , -0.3), 251.17937 (C ₁₉ H ₂₃ ⁺ , -0.2), 162.12770 (C ₁₁ H ₁₆ N ⁺ , -0.2), 126.12771 (C ₈ H ₁₆ N ⁺ , -0.1)
19)	[C ₄₅ H ₇₄ NO ₁₇] ⁺	900.49628	882.48529 (C ₄₅ H ₇₂ NO ₁₆ ⁺ , 0.8), 864.47461 (C ₄₅ H ₇₀ NO ₁₅ ⁺ , 0.7), 718.41699 (C ₃₉ H ₆₀ NO ₁₁ ⁺ , 1.2), 430.33124 (C ₂₇ H ₄₄ NO ₃ ⁺ , -0.8), 412.32111 (C ₂₇ H ₄₂ NO ₂ ⁺ , 0.2), 394.31055 (C ₂₇ H ₄₀ NO ⁺ , 0.3), 251.17952 (C ₁₉ H ₂₃ ⁺ , 0.4), 126.12773 (C ₈ H ₁₆ N ⁺ , 0.04), 85.02840 (C ₄ H ₅ O ₂ ⁺ , -0.02)

^a Mass error in part per million (ppm) = 10⁶ * (accurate mass-exact mass)/exact mass. ^b Significant signals with signal-to-noise ratio 5 or higher were taken into consideration.

Table S2. Fruit morphological traits of Mirabella and Bianca di Senise eggplants.

Traits and units	Eggplant genotype	
	Mirabella	Bianca di Senise
Color	dark purple	white with purple streaks
Length (cm)	11.1 ± 0.5	15.1 ± 0.4
Diameter at the middle (cm)	6.6 ± 0.5	8.4 ± 0.2
Fresh weight (g.)	152.6 ± 18	452.8 ± 54
Pulp dry matter (%)	11.5 ± 0.6	9.3 ± 0.3
Peel dry matter (%)	9.3 ± 0.1	7.0 ± 0.2