Gomphrenin-Based Decarboxylated and Acylated Pigments from *Basella alba* L. Fruit Extracts Impair Survival of Colorectal Cancer Cells but Not Normal Cells – *In Vitro* Study

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SUPPLEMENTARY MATERIALS

Table S1. High-resolution mass spectrometric data obtained by the Orbitrap system for the novel decarboxylated gomphrenins and their fragmentation ions.

Figure S1. Image of cultivated *B. alba* plant in a greenhouse with ripening fruits containing gomphrenin-based pigments.

Figure S2. Detected primary MS^n fragmentation ions of 17-decarboxy-gomphrenin (**2**), 2-decarboxy-gomphrenin (**3**) and 2,17-bidecarboxy-gomphrenin (**4**) (Table S1).

Figure S3. Detected secondary MS^n fragmentation ions of 17-decarboxy-gomphrenin (**2**), 2-decarboxy-gomphrenin (**3**) and 2,17-bidecarboxy-gomphrenin (**4**) (Table S1).

Table S1. High-resolution mass spectrometric data obtained by the Orbitrap system for the novel decarboxylated gomphrenins and their fragmentation ions.

Compound	*$[M+H]^+$ molecular formula*	*$[M+H]^+$ observed*	*$[M+H]^+$ predicted*	*Error (mDa)*	*Error (ppm)*
2-Decarboxy-gomphrenin (**3**)	$C_{23}H_{27}N_2O_{11}$	507.1613	507.1609	0.4	0.79
	$C_{17}H_{17}N_2O_6$	345.1087	345.1081	0.6	1.74
	$C_{16}H_{15}N_2O_4$	299.1030	299.1026	0.4	1.34
	$C_{15}H_{15}N_2O_2$	255.1131	255.1128	0.3	1.18
	$C_{13}H_{12}NO_2$	214.0864	214.0863	0.1	0.47
	$C_9H_{10}NO_2$	164.0708	164.0706	0.2	1.22
	$C_8H_{10}NO_2$	152.0709	152.0706	0.3	1.97
	$C_8H_8NO_2$	150.0552	150.0550	0.2	1.33
	C_8H_6NO	132.0446	132.0444	0.2	1.51
	$C_6H_6NO_2$	124.0394	124.0393	0.1	0.81
	C_7H_8N	106.0653	106.0651	0.2	1.89
	$C_4H_4NO_2$	98.0238	98.0237	0.1	1.02
	C_5H_6N	80.0496	80.0495	0.1	1.25
	C_3H_6N	56.0496	56.0495	0.1	1.78
17-Decarboxy-gomphrenin (**2**)	$C_{23}H_{27}N_2O_{11}$	507.1616	507.1609	0.7	1.38
	$C_{17}H_{17}N_2O_6$	345.1087	345.1081	0.6	1.74
	$C_{16}H_{15}N_2O_4$	299.1032	299.1026	0.6	2.01
	$C_{15}H_{15}N_2O_2$	255.1133	255.1128	0.5	1.96
	$C_9H_8NO_3$	178.0501	178.0499	0.2	1.12
	$C_9H_8NO_2$	162.0552	162.0550	0.2	1.23
	$C_8H_8NO_2$	150.0552	150.0550	0.2	1.33
	C_8H_6NO	132.0447	132.0444	0.3	2.27
	C_7H_8N	106.0653	106.0651	0.2	1.89
	C_6H_8N	94.0653	94.0651	0.2	2.13
	C_5H_6N	80.0497	80.0495	0.2	2.50
	C_3H_6N	56.0497	56.0495	0.2	3.57
2,17-Bidecarboxy-gomphrenin (**4**)	$C_{22}H_{27}N_2O_9$	463.1719	463.1711	0.8	1.73
	$C_{16}H_{17}N_2O_4$	301.1191	301.1183	0.8	2.66
	$C_{15}H_{15}N_2O_2$	255.1134	255.1128	0.6	2.35
	$C_{13}H_{12}NO_2$	214.0868	214.0863	0.5	2.34
	$C_9H_{10}NO_2$	164.0710	164.0706	0.4	2.44
	$C_8H_{10}NO_2$	152.0710	152.0706	0.4	2.63
	$C_8H_8NO_2$	150.0551	150.0550	0.1	0.67
	C_8H_6NO	132.0447	132.0444	0.3	2.27
	C_7H_8N	106.0654	106.0651	0.3	2.83
	$C_4H_6NO_2$	100.0395	100.0393	0.2	2.00
	C_5H_6N	80.0497	80.0495	0.2	2.50
	C_3H_6N	56.0497	56.0495	0.2	3.57

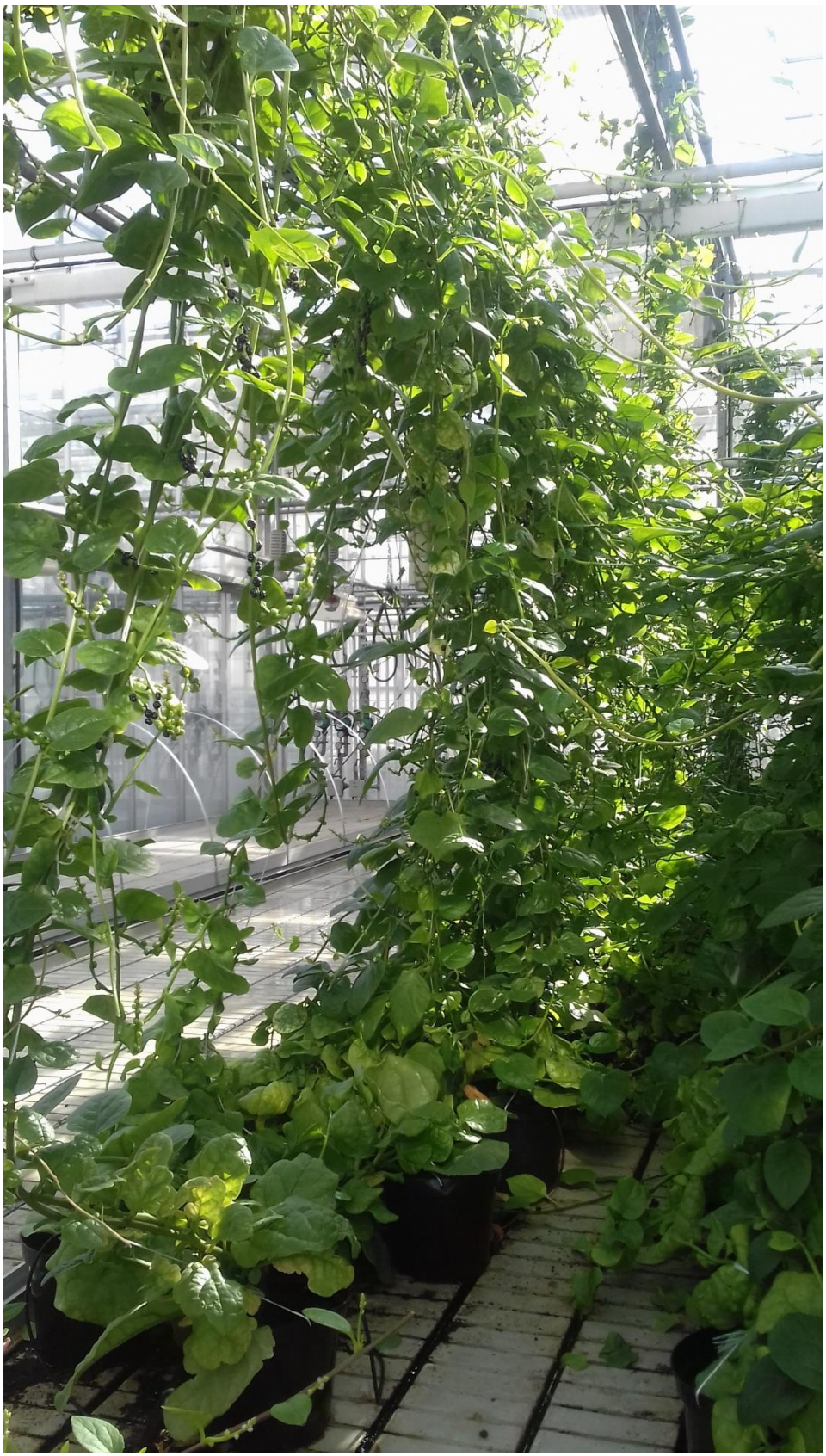
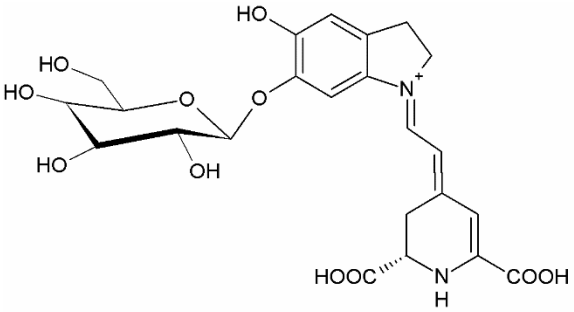
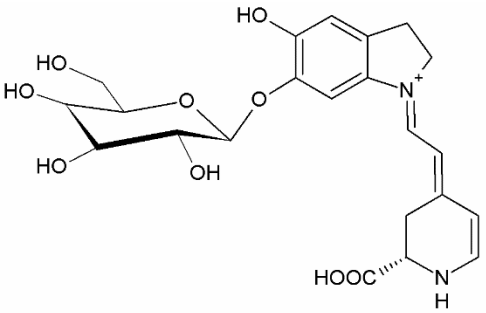


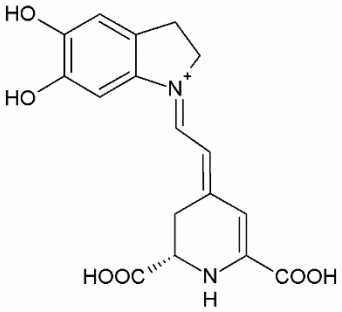
Figure S1. Image of cultivated *B. alba* plant in a greenhouse with ripening fruits containing gomphrenin-based pigments.



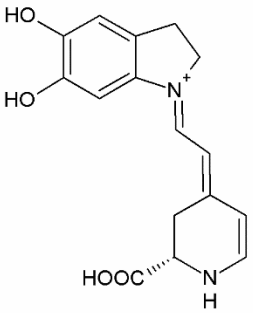
Monoisotopic Mass: 507.1609 Da
Molecular Formula: $C_{23}H_{27}N_2O_{11}$



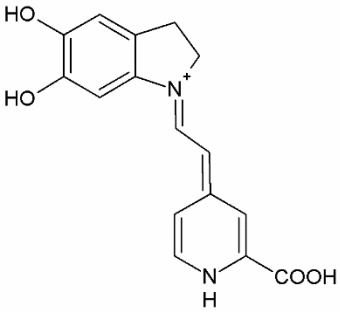
Monoisotopic Mass: 463.1711 Da
Molecular Formula: $C_{22}H_{27}N_2O_9$



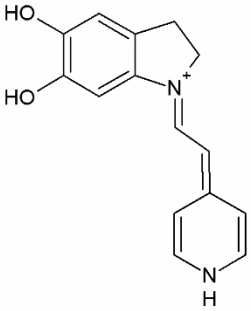
Monoisotopic Mass: 345.1081 Da
Molecular Formula: $C_{17}H_{17}N_2O_6$



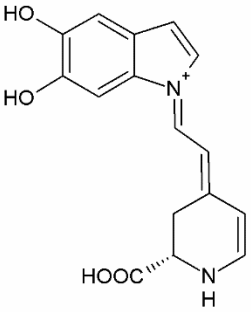
Monoisotopic Mass: 301.1183 Da
Molecular Formula: $C_{16}H_{17}N_2O_4$



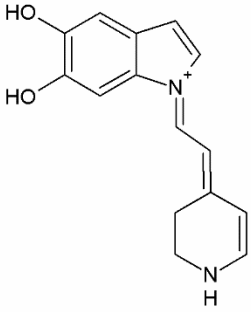
Monoisotopic Mass: 299.1026 Da
Molecular Formula: $C_{16}H_{15}N_2O_4$



Monoisotopic Mass: 255.1128 Da
Molecular Formula: $C_{15}H_{15}N_2O_2$

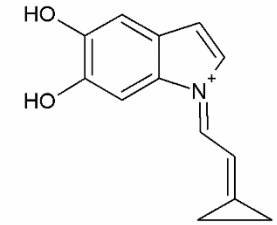


Monoisotopic Mass: 299.1026 Da
Molecular Formula: $C_{16}H_{15}N_2O_4$

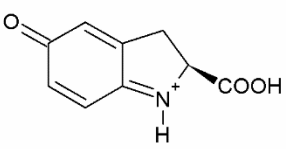


Monoisotopic Mass: 255.1128 Da
Molecular Formula: $C_{15}H_{15}N_2O_2$

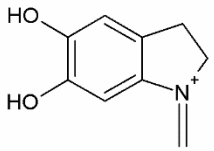
Figure S2. Detected primary MS^n fragmentation ions of 17-decarboxy-gomphrenin (**2**), 2-decarboxy-gomphrenin (**3**) and 2,17-bidecarboxy-gomphrenin (**4**) (Table S1).



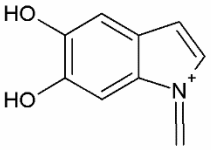
Monoisotopic Mass: 214.0863 Da
Molecular Formula: $C_{13}H_{12}NO_2$



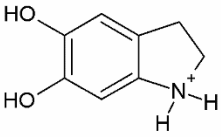
Monoisotopic Mass: 178.0499 Da
Molecular Formula: $C_9H_8NO_3$



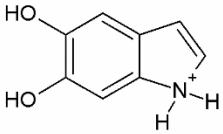
Monoisotopic Mass: 164.0706 Da
Molecular Formula: $C_9H_{10}NO_2$



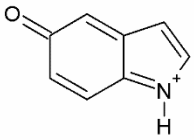
Monoisotopic Mass: 162.0550 Da
Molecular Formula: $C_9H_8NO_2$



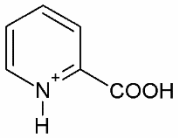
Monoisotopic Mass: 152.0706 Da
Molecular Formula: $C_8H_{10}NO_2$



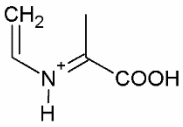
Monoisotopic Mass: 150.0550 Da
Molecular Formula: $C_8H_8NO_2$



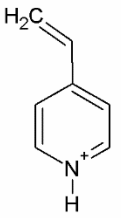
Monoisotopic Mass: 132.0444 Da
Molecular Formula: C_8H_6NO



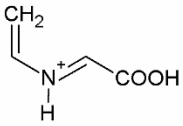
Monoisotopic Mass: 124.0393 Da
Molecular Formula: $C_6H_6NO_2$



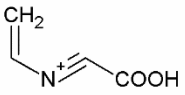
Monoisotopic Mass: 114.0550 Da
Molecular Formula: $C_5H_8NO_2$



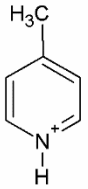
Monoisotopic Mass: 106.0651 Da
Molecular Formula: C_7H_8N



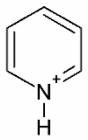
Monoisotopic Mass: 100.0393 Da
Molecular Formula: $C_4H_6NO_2$



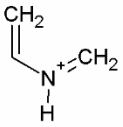
Monoisotopic Mass: 98.0237 Da
Molecular Formula: $C_4H_4NO_2$



Monoisotopic Mass: 94.0651 Da
Molecular Formula: C_6H_8N



Monoisotopic Mass: 80.0495 Da
Molecular Formula: C_5H_6N



Monoisotopic Mass: 56.0495 Da
Molecular Formula: C_3H_6N

Figure S3. Detected secondary MS^n fragmentation ions of 17-decarboxy-gomphrenin (**2**), 2-decarboxy-gomphrenin (**3**) and 2,17-bidecarboxy-gomphrenin (**4**) (Table S1).