

Supporting Information

For

A One-step Polyphenol Removal Approach for Detection of Multiple Phytohormones from Grape Berry

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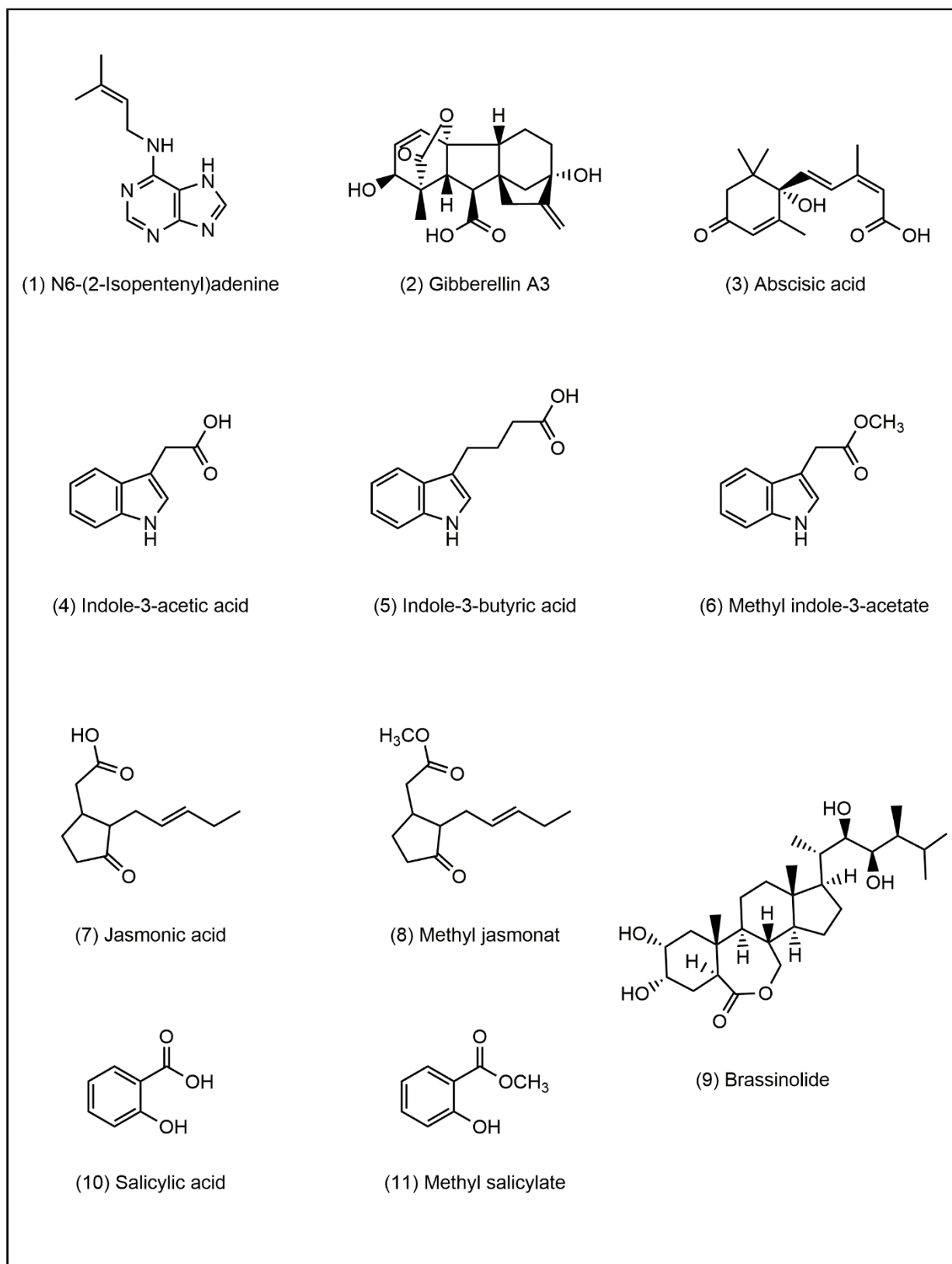


Figure S1: Chemical structures of IP, GA₃, SA, JA, IAA, IBA, MeIAA, MeSA, MeJA and BL as representative Phytohormones.

Table S1. The MRM parameters of 5 anthocyanins.

Analytes	Transition	Fragmentor	College Energy	Polarity
Cyanindin-glucoside	449>287	120	30	Positive
Delphinidin-glucoside	465>303	120	30	Positive
Malvidin-glucoside	493>331	120	30	Positive
Peonidin-glucoside	463>301	120	30	Positive
Petunidin-glucoside	479>317	120	30	Positive

Table S2. The MRM parameters of non-anthocyanin phenolics.

Analytes	Transition	Fragmentor	Collision Energy	Polarity
Procyanin B1	449>287	120	30	Negative
Gallocatechin	465>303	120	30	Negative
Catechin	493>331	120	30	Negative
epicatechin	463>301	120	30	Negative
Procyanin C1	479>317	120	30	Negative
Epigallocatechin gallate	457>169	120	30	Negative
Epicatechin gallate	441>289	120	30	Negative
Chlorogenic acid	353>191	120	30	Negative
Caffeic acid	179>135	120	30	Negative
4-Hydroxycinnamic acid	163>119	120	30	Negative
Sinapic acid	223>149	120	30	Negative
Ferulic acid	193>134	120	30	Negative
Gallic acid	169>125	120	30	Negative
Protocatechuic acid	153>109	120	30	Negative
4-Hydroxybenzoic acid	137>93	120	30	Negative
Gentisic acid	153>109	120	30	Negative
Syringic acid	197>182	120	30	Negative
Vanillic acid	167>152	120	30	Negative
Myricetin-glucoside	479>316	120	30	Negative
Dihydroquercetin	303>125	120	30	Negative
Quercetin-glucuronide	477>301	120	30	Negative
Quercetin-glucoside	463>300	120	30	Negative
Dihydrokaempferol	287>259	120	30	Negative
Syringetin-glucoside	507>344	120	30	Negative
Isorhamnetin-glucoside	477>314	120	30	Negative
Quercetin-rhamnoside	447>300	120	30	Negative
Kaempferol-glucoside	447>255	120	30	Negative
Myricetin	317>151	120	30	Negative
Syringetin	345>315	120	30	Negative
Laricitrin	331>151	120	30	Negative
Isorhamnetin	315>300	120	30	Negative
Quercetin	301>151	120	30	Negative
Dihydromyricetin	319>193	120	30	Negative

Table S3. Abundance of anthocyanins and non-anthocyanin phenolics in sample solution using different elution solution.

Analytes	Abundance	
	Sample eluted by MeOH (0.1%FA)	Sample eluted by CH ₂ Cl ₂ (2.5% MeOH , 0.5%FA)
Cyanindin-glucoside	138930 ± 6183	nd
Delphinidin-glucoside	3302613 ± 104219	3340 ± 1280
Malvidin-glucoside	21929916 ± 1475216	52835 ± 918
Peonidin-glucoside	5301160 ± 296145	11545 ± 2382
Petunidin-glucoside	3133707 ± 218087	4439 ± 2080
Procyanin B1	15753 ± 416	nd
Gallocatechin	30743 ± 602	nd
Catechin	18687 ± 177	nd
epicatechin	3966 ± 83	nd
Caffeic acid	2797 ± 197	nd
Gallic acid	5635 ± 169	281 ± 63
Protocatechuic acid	10180 ± 344	1897 ± 273
Myricetin-glucoside	621727 ± 20892	1190 ± 730
Quercetin-glucuronide	245383 ± 7221	434 ± 246
Quercetin-glucoside	325262 ± 772	2562 ± 1938
Syringetin-glucoside	54013 ± 1238	6910 ± 3881
Isorhamnetin-glucoside	82956 ± 2927	11134 ± 6716
Quercetin-rhamnoside	6529 ± 159	260 ± 192
Kaempferol-glucoside	74814 ± 1177	1777 ± 1546
Myricetin	10107 ± 738	162 ± 75
Syringetin	14612 ± 1122	18319 ± 3529
Isorhamnetin	3187 ± 200	1749 ± 289
Quercetin	2440 ± 48	nd
Dihydromyricetin	1040 ± 22	nd

Table S4. The dMRM parameters of 11 hormones and internal standard.

Analytes	Transition	Fragmentor	College Energy	Retention Time (min)	Delta Retention Time (min)	Polarity
IP	204.13>136	99	16	2.4	0.6	Positive
GA ₃	345.1>239.1	162	12	3.37	0.5	Negative
SA	137>93	89	20	4.2	0.5	Negative
IAA	176.07>130	99	16	4.38	0.5	Positive
ABA	263.1>153	104	8	5.35	0.6	Negative
JA	209.12>59.1	118	12	6.48	0.5	Negative
IBA	204.1>186	94	12	6.61	0.4	Positive
MeIAA	190.1>130	84	24	6.94	0.5	Positive
MeSA	153.1>121	65	16	7.74	0.7	Positive
MeJA	225.15>151	95	12	9.46	0.7	Positive
BL	481.36>445.4	133	12	9.64	0.5	Positive
TPP	327>215	170	30	12.67	0.4	Positive

Table S5. Linearity, LODs and LOQs of IAA and IBA in dMRM mode.

Analytes	Equation of linear regression	R ²	Linear range (ng/ml)	LOD (ng/ml)	LOQ (ng/ml)
IAA	y=24.23x-0.0028	0.9998	0.5-250	0.16	0.5
IBA	y=18.44x+0.3598	0.9983	0.5-100	0.16	0.5