

Table 15. Parameters of XEVO UPLC-MS/MS analysis.

Targeted phenolics UPLC-US-MS/MS method details - According to Vrhovsek et al 2012. and Pál et al. 2019, with modifications:			
Preparation:	Homogenized leaf samples (0.2 g fresh weight) were weighted into 2 ml eppendorf tubes and immediately spiked with 20 ng [2H₆](+)-cis,trans-abscisic acid (OlChemIm s.r.o. Olomouc, Czech Republic) serving as internal standard. Samples were extracted two times with 2x1 ml methanol:water (2:1 v/v%) solution by vigorous vortex mixing and shaking in a MiniG 1600 instrument (SPEX SamplePrep.; Metuchen, NJ, USA) in cryo-cooled rack at 1250 RPM for 3 min. After centrifugation at 16000 g (at 4°C for 10 min), supernatants were pooled and the methanol-water sample solution was liquid-liquid partitioned by adding 1 ml of n-hexane to remove carotenoids and fats. Afterwards, centrifugation at 10000 g (at 4°C for 10 min) was addressed to collect the methanol:water phase that was finally filtered through 0.22 µm PTFE syringe filters prior to analysis.		
UPLC:	Waters Acquity I-class		
Column:	Waters HSS T3 column (1.8 µm, 100 mm × 2.1 mm) at 40°C		
inj vol.:	2 µl	Autosampler temperature:	10 °C

Gradient conditions			
A: Water (0.1 v/v% formic acid)		B: Acetonitrile (0.1 v/v% formic acid)	
Time (min)	Flow rate (ml/min)	A%	B%
0	0.4	95	5
3	0.4	80	20
4.3	0.4	80	20
9	0.4	55	45
11	0.4	0	100
13	0.4	0	100
13.01	0.4	95	5
15	0.4	95	5

Detector 1:	PDA - 210-700 nm; 20 scans/sec
Detector 2:	Xevo TQ-XS with Unispray source
Resolution:	Unit mass (+/- 0.8 Da)
Impactor voltage:	2 kV
Polarity:	UniSpray Positive
Desolvation temperature:	550°C
Nebulizer gas:	6.5 bar N ₂
Desolvation gas flow:	1000 L/h N ₂
Cone gas flow:	450 L/h N ₂
Collision gas flow:	0.15 ml/min Argon 5.0

Component name	Unispray Impactor voltage polarity	quant. MS/MS transition	RT (min)	Cone voltage (V)	Collision ennergy (eV)	Solvent calibration (if reference standard was not available, relative quantitation against indicated compound)
[2H6](+)-cis,trans-abscisic acid Internal standard	negative	269.1 > 159.1	7.13	20	10	external
4-hydroxybenzoic acid (pHBA NEG)	negative	137 > 93	2.84	20	12	external
caffeic acid neg	negative	179 > 135	3.23	20	17	external
ferulic acid neg	negative	193 > 134	4.55 and 4.68	20	14	external
jasmonic-acid-LE/ILE SUM	negative	322.2 > 130.1	9.93	25	22	external
kaempferol-3-O-glucoside	positive	449 > 287	5.54	18	20	kaempferol-3-O-rutinoside
robinin isomer	positive	741 > 287	3.91	22	38	robinin
abscisic acid	negative	263.1 > 153	7.18	20	10	external
chlorogenic acid	negative	353 > 191.1	2.84	36	22	external - REMARK - Component evaluated by PDA at 325+/- 30nm
cryptochlorogenic acid	negative	353 > 173	2.93	34	14	external - REMARK - Component evaluated by PDA at 325+/- 30nm
fraxin	positive	369 > 207	3.09	32	20	external
gallic acid	positive	169 > 79	1.41	28	22	external
IAA - Indole3AA - AUXIN	positive	176.1 > 130.1	6.05	25	14	external
jasmonic acid	negative	209.12 > 58.9	8.3	22	12	external
kaempferol-3-O-rutinoside	positive	595 > 287	5.14	18	20	external
naringenin	negative	271 > 150.9	8.23	46	18	external
neochlorogenic acid	negative	353 > 191	2.24	26	18	external
p-coumaric acid neg	negative	163 > 93	4.04	20	26	external
phaseic acid	negative	279.12 > 139	5.24	25	12	external
phloridzin	negative	435 > 273	6.21	32	16	external - REMARK - Component evaluated by PDA at 325+/- 30nm
quercetin	positive	303 > 153	7.41	50	34	external
quercetin NEG	negative	301 > 150.95	7.41	42	24	external
quercetin-3-O-glucoside	positive	465 > 303	4.56	18	12	quercetin-3-o-glucoronide
rutin and/or its isomers or Quercetin 3-O-glucosyl-rhamnosyl-glucoside SUM	negative	609.1 > 300.1	4.28	90	38	external

salicylic acid neg	negative	137 > 93	5.81	20	12	external
sinapic acid	negative	223 > 208	4.67	14	10	external
syringic acid	positive	197 > 182	3.35	22	14	external
vanillic acid	positive	169 > 93	3.28	18	14	external

FOLLOWING COMPOUNDS HAVE BEEN SURVEYED BUT NOT DETECTED IN PEPPER SAMPLES ABOVE LIMIT OF QUANTIFICATION						
luteolin-7-O-glucoside	negative	447 > 285	4.57	46	24	external
apigenin	negative	269 > 117	8.31	42	34	external
apigenin-7-O-glucoside	positive	433 > 271	5.79	24	20	apigenin
1,3-dicaffeoylquinic acid	negative	515 > 353	3.45	34	20	not calibrated
1,5-dicaffeoylquinic acid	negative	515 > 191	5.22	26	28	not calibrated
2,4-dihydroxybenzoic acid	positive	153 > 109	3.29	24	14	external
2,5-dihydroxybenzoic acid	positive	153 > 109	2.89	26	16	external
2,6-dihydroxybenzoic acid	positive	153 > 109	3.59	26	14	external
3,4-dihydroxybenzoic acid	positive	153 > 81	2.12	24	20	external
3,5-dihydroxybenzoic acid	positive	153 > 109	2.11	26	14	external
3-hydroxybenzaldehyde	positive	123 > 95	4	20	10	external
4-hydroxycoumarin	positive	163 > 91	6.04	42	18	not calibrated
4-hydroxystilbene	negative	195 > 93	10.7	44	26	not calibrated
4-methylumbelliferone	positive	177 > 121	5.87	34	20	external
6-methoxyflavone	positive	253 > 108	10.64	16	38	not calibrated
acetovanillone	positive	167 > 43	4.59	20	12	external
aesculetin	positive	179 > 133	3.49	34	22	external
alpha-viniferin	negative	677 > 437	8.65	48	30	external
ampelopsin D + quadrangularin A	negative	453 > 359	6.74	42	18	not calibrated
ampelopsin H + vaticanol C-like isomer	negative	905 > 811	8.03	52	30	not calibrated
anthranilic acid	positive	138 > 65	3.96	14	26	not calibrated
apiin	positive	565 > 271	5.45	26	30	external
astringin	negative	405 > 243	3.57	36	20	external
baicalein	positive	271 > 123	8.8	46	32	external
benzoic acid	negative	121 > 77	5.51	22	12	external
caffeic acid + catechin condensation product	negative	451 > 341	5.53	34	18	not calibrated

caftaric acid	negative	311 > 149	2.31	18	10	external
catechin gallate	negative	441 > 289	4.36	34	18	external
catechol	negative	109 > 81	2.88	36	12	external
catechin	negative	289 > 203	2.83	32	20	external
chrysin	negative	253 > 143	10.19	44	30	external
cinnamic acid	positive	131 > 103	7.57	40	12	external
cis-e-viniferin	negative	453 > 347	7.97	48	22	external
cis-gm-viniferin	negative	453 > 347	8.5	46	20	external
cis-piceid	negative	389 > 227	5.94	28	20	external
cis-resveratrol	negative	227 > 185	7.55	40	22	external
coniferyl alcohol	positive	163 > 131	4.04	12	10	external
coniferyl aldehyde	negative	179 > 119	5.71	22	14	not calibrated
daidzein	negative	255 > 199	6.95	30	24	external
daphnetin	positive	179 > 123	3.24	36	22	external
dihydro kaempferol	negative	287 > 259	6.12	20	14	external
dihydro-phaseic acid	negative	281.14 > 237.2	3.56	25	12	external
E-cis-miyabenol	negative	679 > 345	8.28	54	30	not calibrated
ellagic acid	negative	301 > 145	4.36	52	34	external
epicatechin gallate	negative	441 > 289	4.33	34	18	external
epicatechin	negative	289 > 203	3.31	34	20	external
epigallocatechin	negative	305 > 125	2.56	32	22	external
epigallocatechin gallate	negative	457 > 169	3.42	32	16	external
eriodictyol	negative	289 > 153	7.29	30	24	external
esculin	positive	341 > 179	2.42	24	18	external
eupatorin-5-methylether	positive	359 > 329	8.9	12	18	not calibrated
fertaric acid	negative	325 > 193	3.15	20	16	external
galangin	positive	271 > 153	6.08	48	32	external
galocatechin	negative	305 > 125	1.98	32	26	external
galocatechin gallate	negative	457 > 169	3.59	26	20	external
hesperetin	positive	303 > 153	8.52	32	26	external
hesperidin	positive	611 > 449	5.89	18	10	external
isohopeaphenol	negative	905 > 359	7.61	48	38	not calibrated
isorhamnetin	positive	317 > 302	8.72	44	26	external

isorhamnetin-3-O-glucoside	positive	479 > 317	5.78	16	14	isorhamnetin-3-rutinoside
isorhamnetin-3-rutinoside	positive	625 > 317	5.42	18	20	external
isorhapontin	negative	419 > 241	4.74	30	36	external
kaempferol	negative	285 > 187.1	8.59	50	26	external
kaempferol-3-O-glucuronide	positive	463 > 287	5.5	18	16	external
laricitrin	positive	333 > 318	7.5	44	26	external
luteolin	positive	287 > 135	7.43	52	32	external
luteolin-8-C-glucoside	positive	449 > 329	3.88	36	30	luteolin
m-coumaric acid	positive	165 > 147	4.76	18	12	external
m-coumaric acid neg	negative	163 > 93	4.76	20	26	external
methyl gallate	positive	183 > 124	2.94	32	22	external
morin	positive	303 > 153	6.81	38	32	external
Myricetin	negative	317 > 150.9	6.3	20	24	external
myricitrin	positive	465 > 319	4.3	14	10	not calibrated
o-coumaric acid	positive	165 > 103	5.78	18	16	external
o-coumaric acid neg	negative	163 > 93	5.76	20	26	external
pallidol	negative	453 > 359	6.07	32	14	external
p-coumaric acid	positive	165 > 91	4.04	16	24	external
phloretin	negative	273 > 167	8.29	32	18	external
picetannol	negative	243 > 159	5.01	40	28	external
procyanidin A2	negative	575 > 285	4.7	42	30	external
procyanidin B1	negative	577 > 289	2.49	32	26	external
procyanidin B2 + B4	negative	577 > 289	3.06	30	24	external
procyanidin B3	negative	577 > 289	2.72	34	22	external
pterostilbene	negative	255 > 240	10.6	40	18	external
quercetin-3,4'-diglucoside	positive	627 > 303	3.62	18	32	quercetin-3-o-glucuronide
quercetin-3-Glc-Ara	positive	597 > 303	4.07	20	22	not calibrated
quercetin-3-O-galactoside	positive	465 > 303	4.25	18	12	quercetin-3-o-glucuronide
quercetin-3-O-glucose-6'-acetate	positive	507 > 303	5.74	20	16	not calibrated
quercetin-3-O-glucuronide	positive	479 > 303	4.51	20	18	external
quercetin-3-O-rhamnoside	positive	449 > 303	5.61	16	10	quercetin-3-o-glucuronide
quercetin-3-sulfate	negative	381 > 301	4.55	24	18	not calibrated
quercetin-4'-O-glucoside	positive	465 > 303	5.7	18	12	quercetin-3-o-glucuronide

rhamnetin	positive	317 > 123.01	9.54	48	42	external
robinin	positive	741 > 287	3.81	22	38	external
rosmarinic acid	negative	359 > 161	6.11	30	18	external
sakuranetin	negative	287 > 119	10.24	32	30	external
salicin	positive	309 > 185	2.28	38	16	not calibrated
scopoletin	positive	193 > 133	4.53	34	20	external
sinapyl alcohol	negative	193 > 161	4.11	14	10	external
sinensetin	positive	373 > 343	9.91	8	28	not calibrated
syringaldehyde	positive	183 > 123	4.38	20	12	external
syringetin	positive	347 > 153	8.57	40	28	external
syringetin-3-O-glucoside + syringetin-3-O-galactoside	positive	509 > 347	5.8	16	14	not calibrated
taxifolin	negative	303 > 125	4.76	20	20	external
trans-coutaric acid	negative	295 > 163	2.88	20	12	external
trans-e-viniferin	negative	453 > 347	8.13	52	22	external
trans-gm-viniferin	negative	453 > 347	8.65	48	22	external
trans-piceid	negative	389 > 227	4.25	28	18	external
trans-resveratrol	negative	227 > 185	6.59	38	18	external
trilobatin	negative	435 > 273	6.74	36	18	not calibrated
umbelliferone	positive	163 > 107	4.41	32	20	external
vanillin	positive	153 > 93	4.07	20	16	external
Z-miyabenol C	negative	679 > 345	8.91	54	36	not calibrated

Gradient conditions			
Eluent 'A': Water with 0.1 % (v/v) formic acid; eluent 'B': acetonitrile with 0.1 % (v/v) formic acid			
Time (min)	Flow rate (ml/min)	A%	B%
0.0	0.4	95	5
0.5	0.4	95	5
8.0	0.4	82	18
12.0	0.4	60	40
15.0	0.4	20	80
16.0	0.4	0	100
18.0	0.4	0	100
19.0	0.4	95	5
22.0	0.4	95	5

Table 2S UPLC gradient conditions

Detector parameters	
Detector 1:	PDA - 220-600 nm; 20 scans/s at 2.4 nm resolution
Detector 2:	Vion IMS QTOF MS with ESI ion source
Resolution:	> 40 000 (calculated for leucine enkephalin)
Capillary voltage:	0.5 kV
Polarity:	negative and positive
Source temperature:	120°C
Desolvation temperature:	550°C
Nebulizer gas:	6.5 bar N ₂
Cone gas voltage:	30 V
Desolvation gas flow:	1000 L/h N ₂
Cone gas flow:	150 L/h N ₂
Collision gas flow:	0.15 ml/min Ar 5.0
IMS:	ON
MS scan:	m/z 90 – 2000
MS scan time:	0.4 s
Lock mass:	ON
MS/MS scan:	m/z 50 – 2000
MS/MS collision energy:	individually optimized
MS ^E low collision energy:	6.0 eV
MS ^E high collision energy ramp:	20.0-30.0 eV

Table 3S. ESI-IMS-QTOF-MS parameters applied during the study.

Table 4S. Compounds measured by GCxGC TOF/MS (ISTD: amount calculated using ribitol as the internal standard; <LOQ: below the quantitation limit; RSD: relative standard deviation).

No.	Compound	Note
	Amino acids	
1	L-Valine	RSD > 30%
2	L-Alanine	RSD > 30%
3	Glycine	<LOQ
4	L-Leucine	<LOQ
5	L-Proline	RSD > 30%
6	L-Isoleucine	
7	L-Serine	
8	L-Threonine	
9	L-Aspartic acid	
10	β -Alanine	<LOQ
11	L-Hydroxyproline, (E)-	<LOQ
12	L-Methionine	<LOQ
13	L-5-Oxoproline	RSD > 30%
14	γ -Aminobutyric acid (GABA)	
15	Phenylalanine	
16	Asparagine	<LOQ
17	L-Lysine	<LOQ
18	Tyrosine	<LOQ
19	L-Glutamic acid (ISTD)	
20	Alanylglycine (ISTD)	
21	L-Ornithine	<LOQ
	Organic acids	
22	α -Ketoglutaric acid	
23	Succinic acid	RSD > 30%
24	Fumaric acid	
25	Aconitic acid, (E)-	<LOQ
26	Citric acid	
27	Malic acid (ISTD)	
28	Ribonic acid (ISTD)	
	Sugars and sugar alcohols	
29	Maltose	
30	Galactose (ISTD)	
31	Sucrose (ISTD)	
32	D-Mannose	RSD > 30%
33	D-Glucose	
34	D-Ribose	<LOQ
35	Inosose	RSD > 30%
36	Glucose-6-phosphate	
37	D-Mannitol	<LOQ
38	D-Pinitol (ISTD)	

39	Myo-Inositol	
	Polyamines	
40	Putrescine	<LOQ
41	Spermidine	

Table 5S. Amount of different phenolic compounds in *C. roseus* plants grown either at control (NL) or reduced light (LL) conditions separated according to the flower colour (Red: ‘Red’; Pink: ‘Rose’; White: ‘Polka Dot’).

Components detected above LoQ:		4-hydroxybenzoic acid (pHBA)	p-coumaric acid neg	gallic acid and its isomers	vanillic acid	IAA - Indole3AA	caffeic acid neg	ferulic acid 1 NEG 4.55 (trans isomer)	ferulic acid 2 NEG 4.68 (unknown cis isomer)	syringic acid	quercetin	fraxin	kaempferol-3-O-glucoside	quercetin-3-O-glucoside	kaempferol-3-O-rutinoside	Rutin and/or izomers or Quercetin 3-O-glucosyl-rhamnosyl-glucoside SUM	robinin isomer	salicylic acid	jasmonic acid	jasmonic-acid-LE/ILE SUM	sinapic acid (trans - and unknown cis isomer sum)	abscisic acid	Naringenin	phaseic acid	phloridzin	DAD325nm(+ /-30nm) - 2.18min - neochlorogenic acid	DAD325nm(+ /-30nm) - 2.77min - chlorogenic acid	DAD325nm(+ /-30nm) - 2.9min - cryptochlorogenic acid
		ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ng/g F.W.	ug/g F.W.	ug/g F.W.	ug/g F.W.
Red LL	Average	91.4	40.1	6.0	<LoQ	0.8	112.0	112.3	224.7	<LoQ	3.1	122.2	319.7	28.0	91.4	1163	5030	41.9	714.0	23.1	428	9.1	<LoQ	1.3	62.9	68.9	536.7	214.7
	SD	3.3	11.8	1.0	<LoQ	0.1	7.5	17.8	45.0	<LoQ	0.2	68.3	97.8	4.0	13.1	567	325	14.7	118.4	8.8	71	0.2	<LoQ	0.2	2.3	8.1	36.4	6.0
White LL	Average	92.5	56.0	4.9	<LoQ	1.4	102.6	78.1	135.3	<LoQ	2.2	62.2	101.1	109.0	47.3	1796	4400	33.1	703.0	29.5	448	11.7	0.7	1.4	38.1	83.0	598.0	213.7
	SD	0.2	11.0	0.1	<LoQ	0.2	7.7	1.9	40.7	<LoQ	0.5	20.4	21.9	76.9	3.9	1464	351	12.1	59.7	5.0	91	2.3	0.4	0.1	0.1	16.8	63.3	11.7
Pink LL	Average	93.1	39.2	4.6	<LoQ	1.1	70.4	71.3	82.9	<LoQ	3.2	71.7	125.5	76.2	107.8	5459	6223	17.3	292.3	9.6	266	9.1	<LoQ	1.9	53.2	90.3	538.0	220.0
	SD	0.4	17.3	0.7	<LoQ	0.6	25.3	33.8	25.7	<LoQ	0.8	13.7	39.9	57.0	73.9	5283	1452	3.4	122.3	7.1	106	1.3	<LoQ	0.6	14.8	37.7	45.6	17.5
Red NL	Average	102.5	70.8	6.9	<LoQ	1.0	160.3	104.9	240.7	<LoQ	12.4	224.0	329.7	486.0	87.3	6973	5667	32.6	506.0	26.6	403	21.6	<LoQ	3.6	92.9	101.9	671.3	268.0
	SD	7.0	23.0	0.6	<LoQ	0.1	43.5	34.3	40.5	<LoQ	4.7	25.2	51.6	133.4	13.8	1703	577	12.7	178.2	19.2	56	2.9	<LoQ	0.3	10.6	11.9	92.2	36.4
White NL	Average	104.7	57.0	6.2	<LoQ	1.1	114.0	107.1	221.0	<LoQ	11.2	216.3	452.0	724.3	153.3	15867	6327	29.1	431.0	27.9	364	16.7	0.7	2.8	101.1	113.9	683.7	278.3
	SD	6.0	16.4	0.1	<LoQ	0.2	11.5	25.9	33.2	<LoQ	0.9	52.5	197.6	403.4	43.4	3450	478	11.7	49.8	11.3	65	0.5	0.4	0.3	19.5	18.1	68.6	29.7
Pink NL	Average	88.2	53.3	11.3	<LoQ	0.9	153.7	293.7	781.7	<LoQ	9.7	624.0	596.7	594.3	146.0	17933	4890	87.8	808.0	53.3	955	13.8	0.7	2.9	141.3	90.2	649.7	233.3
	SD	5.3	14.6	1.8	<LoQ	0.2	19.9	39.6	129.6	<LoQ	3.0	65.6	119.7	305.8	14.7	4508	779	15.7	77.7	14.0	137	2.2	0.1	0.5	27.1	21.7	157.4	44.2
Cells marked with orange background and font indicate that the result was below Limit of Quantification (LoQ).																												

Table 6S. Abundance of certain non-dimeric vinca alkaloids and related compounds detected in *C. roseus* plants with different flower colours grown either at control (NL) or reduced light (LL) conditions. Mean of counts per second (cps) $\pm$ SD values, n=3. Different letters indicate statistically significant differences between the different colours within the same growth conditions at $p < 0.05$ level.

	Red NL	White NL	Pink NL	Red LL	White LL	Pink LL
19-S-vindolinine	24,556 $\pm$ 427 ^a	25,448 $\pm$ 966 ^a	24,387 $\pm$ 1,079 ^a	25,883 $\pm$ 858 ^a	25,443 $\pm$ 399 ^a	25,214 $\pm$ 480 ^a
Catharanthine	10,217 $\pm$ 466 ^{ab}	9,846 $\pm$ 509 ^{ab}	9,808 $\pm$ 585 ^{ab}	11,146 $\pm$ 111 ^a	9,008 $\pm$ 858 ^b	9,785 $\pm$ 647 ^{ab}
Deacetylvindoline	431 $\pm$ 21 ^a	231 $\pm$ 26 ^c	278 $\pm$ 43 ^{bc}	339 $\pm$ 39 ^b	222 $\pm$ 52 ^c	201 $\pm$ 35 ^c
Loganic acid	25,492 $\pm$ 1,424 ^a	26,285 $\pm$ 853 ^a	24,154 $\pm$ 1,797 ^a	18,810 $\pm$ 1,665 ^b	20,743 $\pm$ 1119 ^b	14,700 $\pm$ 1,240 ^c
Secologanin	51,754 $\pm$ 1,442 ^a	47,303 $\pm$ 670 ^b	46,156 $\pm$ 1,021 ^b	46,172 $\pm$ 1,983 ^b	40,077 $\pm$ 1491 ^c	41,644 $\pm$ 1750 ^c
Strictosidine	1,085 $\pm$ 167 ^a	708 $\pm$ 86 ^b	744 $\pm$ 231 ^b	1,154 $\pm$ 95 ^a	690 $\pm$ 108 ^b	565 $\pm$ 100 ^b
Vincadifformine	740 $\pm$ 35 ^b	243 $\pm$ 13 ^c	430 $\pm$ 10 ^c	937 $\pm$ 39 ^a	314 $\pm$ 41 ^d	403 $\pm$ 21 ^c
Vindoline	537 $\pm$ 8 ^{ab}	460 $\pm$ 10 ^{bcd}	519 $\pm$ 38 ^{abc}	578 $\pm$ 11 ^a	401 $\pm$ 78 ^d	426 $\pm$ 72 ^{cd}
Vindolinine	20,151 $\pm$ 405 ^{ab}	20,971 $\pm$ 276 ^a	19,801 $\pm$ 298 ^{bc}	19,004 $\pm$ 612 ^{cd}	18,872 $\pm$ 863 ^{cd}	17,944 $\pm$ 223 ^d

Table 7S. Results of two-way ANOVA produced with SPSS 16.0 software for the effects of the different treatments

Parameters	Source of variation	Sum of Squares	df	Mean Square	F	Significance
Fv/Fm	Colour	0.00122	2	0.00061	28.63214	1.56E-6
	Light	5.33E-05	1	5.33E-05	2.50213	0.131
	Colour x Light	1.72E-05	2	8.61E-06	0.403995	0.673
Y(II)	Colour	0.000406	2	0.000203	0.567058	0.577
	Light	0.002946	1	0.002946	8.238163	0.010
	Colour x Light	0.005148	2	0.002574	7.198359	0.005
Y(NPQ)	Colour	0.000545	2	0.000272	0.484931	0.623
	Light	0.003733	1	0.003733	6.644982	0.018
	Colour x Light	0.00372	2	0.00186	3.310864	0.059
Y(NO)	Colour	0.002423	2	0.001211	15.88483	1.06E-4
	Light	0.000436	1	0.000436	5.722118	0.027
	Colour x Light	1.13E-05	2	5.67E-06	0.074373	0.928
Salicylic acid	Colour	5702.201	2	2851.101	18.6035	2.1E-4
	Light	1634.014	1	1634.014	10.66198	0.006
	Colour x Light	1735.488	2	867.7439	5.662051	0.018
Jasmonic acid	Colour	485854.8	2	242927.4	20.0192	1.5E-4
	Light	636.0556	1	636.0556	0.052416	0.822
	Colour x Light	99674.11	2	49837.06	4.10698	0.043
Jasmonic-acid-LE/ILE SUM	Colour	1134.272	2	567.1359	4.033199	0.045
	Light	1040.592	1	1040.592	7.400194	0.018
	Colour x Light	846.1924	2	423.0962	3.008858	0.087
Absciscic acid	Colour	85.02204	2	42.51102	12.47273	0.001
	Light	245.8284	1	245.8284	72.12603	2.03E-6
	Colour x Light	20.06738	2	10.03369	2.943884	0.091
Phaseic acid	Colour	0.454444	2	0.227222	1.498168	0.262
	Light	11.045	1	11.045	72.82418	1.93E-6
	Colour x Light	1.09	2	0.545	3.593407	0.059
19-S-vindolinine	Colour	1282832	2	641415.9	0.75307	0.491
	Light	2309394	1	2309394	2.711401	0.125
	Colour x Light	1359079	2	679539.4	0.79783	0.472
3'4'-anhydrovinblastine	Colour	1.45E+0	2	72684787	11.35627	0.001
	Light	412189.1	1	412189.1	0.0644	0.803
	Colour x Light	88884.47	2	44442.23	0.006944	0.993
Catharanthine	Colour	4989063	2	2494531	5.025836	0.025
	Light	2377.402	1	2377.402	0.00479	0.945
	Colour x Light	2345446	2	1172723	2.362733	0.136
Deacetylvindoline	Colour	92573.94	2	46286.97	22.02047	9.64E-5
	Light	15707.72	1	15707.72	7.472759	0.018
	Colour x Light	5889.217	2	2944.609	1.400862	0.283
Loganic acid	Colour	5196974	2	25984874	9.003308	0.004
	Light	2.35E+0	1	2.35E+08	81.39932	1.08E-6
	Colour x Light	1214413	2	6072066	2.103865	0.164

Secologanin	Colour	1.07E+0	2	53479411	16.72706	3.39E-4
	Light	1.5E+08	1	1.5E+08	46.90855	1.77E-5
	Colour x Light	5609332	2	2804666	0.877231	0.440
Strictosidine	Colour	789240.9	2	394620.5	13.2255	9.24E-4
	Light	8179.993	1	8179.993	0.274148	0.610
	Colour x Light	47627.75	2	23813.87	0.798109	0.472
Vinblastine	Colour	9271921	2	4635960	5.072325	0.025
	Light	37254.75	1	37254.75	0.040761	0.843
	Colour x Light	422094.9	2	211047.5	0.230913	0.797
Vincadifformine	Colour	1020554	2	510277.1	391.3637	1.19E-11
	Light	29277.9	1	29277.9	22.45507	4.81E-4
	Colour x Light	37651.41	2	18825.7	14.43862	6.4E-4
Vincristine	Colour	7992191	2	3996096	5.902236	0.016
	Light	140277.1	1	140277.1	0.207189	0.657
	Colour x Light	256278.5	2	128139.3	0.189262	0.829
Vindoline	Colour	50227.49	2	25113.74	7.722878	0.006
	Light	6033.905	1	6033.905	1.855522	0.198
	Colour x Light	14645.1	2	7322.55	2.251801	0.147
Vindolinine	Colour	3432510	2	1716255	4.582256	0.033
	Light	1302425	1	1302425	34.77367	7.29E-5
	Colour x Light	734271.7	2	367135.9	0.980222	0.403

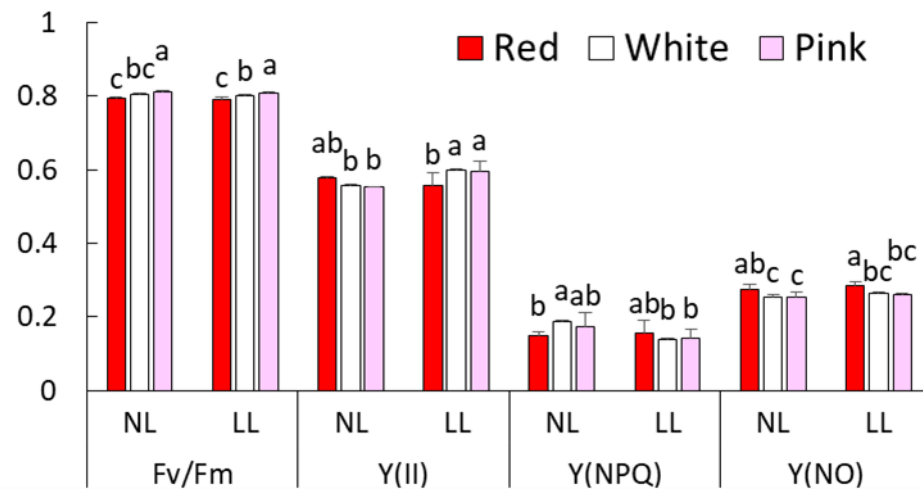


Fig. 1S. Chlorophyll-*a* fluorescence induction parameters in *C. roseus* plants grown either at control (NL) or reduced light (LL) conditions, separated according to the flower colour (Red: 'Red', Pink: 'Rose', White: 'Polka Dot' type). (Mean $\pm$ SD) Measurements were carried out at room temperature at steady-state level. Different letters on the top of the columns represent statistically significant differences at $p < 0.05$ levels.

Fig. 2S. Primary metabolites ($\mu\text{g g}^{-1}$ fresh mass) in *C. roseus* plants grown either at control full light (NL) or reduced light (LL) conditions, separated according to the flower colour (Red: 'Red', Pink: 'Rose', White: 'Polka Dot'). Values <LOQ were considered as 0. ISTD: amount was calculated using ribitol as the internal standard.

Components	Full light			Reduced light		
	Pink	White	Red	Pink	White	Red
L-Isoleucine	7.2	9.7	11.5	9.7	3.8	2.4
L-Serine	15.9	11.0	54.3	7.6	64.4	58.1
L-Threonine	22.0	21.1	22.9	25.0	31.8	35.3
Phenylalanine	8.1	13.7	12.7	11.1	3.3	0.0
L-Aspartic acid	199.4	142.0	149.4	238.6	43.6	5.8
L-Glutamic acid (ISTD)	9.0	9.5	7.0	5.0	2.1	2.2
Alanylglycine (ISTD)	2.6	2.3	2.7	0.4	0.2	0.0
GABA	134.5	54.6	140.9	87.8	51.2	40.5
alpha-Ketoglutaric acid	3364.4	2906.2	2599.0	2672.6	2478.3	1358.1
Fumaric acid	0.0	94.6	76.0	0.0	35.8	23.9
Citric acid	101.5	73.6	138.7	73.6	83.2	130.8
Malic acid (ISTD)	10.2	7.0	7.4	11.4	237.7	218.0
Ribonic acid (ISTD)	0.1	0.1	0.1	0.0	0.0	0.0
Sucrose (ISTD)	10.7	6.9	9.6	10.8	6.8	2.7
Maltose	52.8	44.8	60.6	39.0	51.5	54.2
Galactose (ISTD)	1.0	1.0	0.9	0.8	1.0	0.6
D-Glucose	957.1	1310.3	1087.7	1155.9	1561.3	1861.9
Glucose-6-phosphate	32.7	31.3	31.5	28.8	39.8	9.6
Myo-Inositol	665.4	0.0	542.2	599.2	1002.2	817.4
D-Pinitol (ISTD)	0.0	0.0	3.1	3.3	4.6	4.0
Spermidine	0.1	0.1	0.1	0.0	0.0	0.0

lowest value  highest value

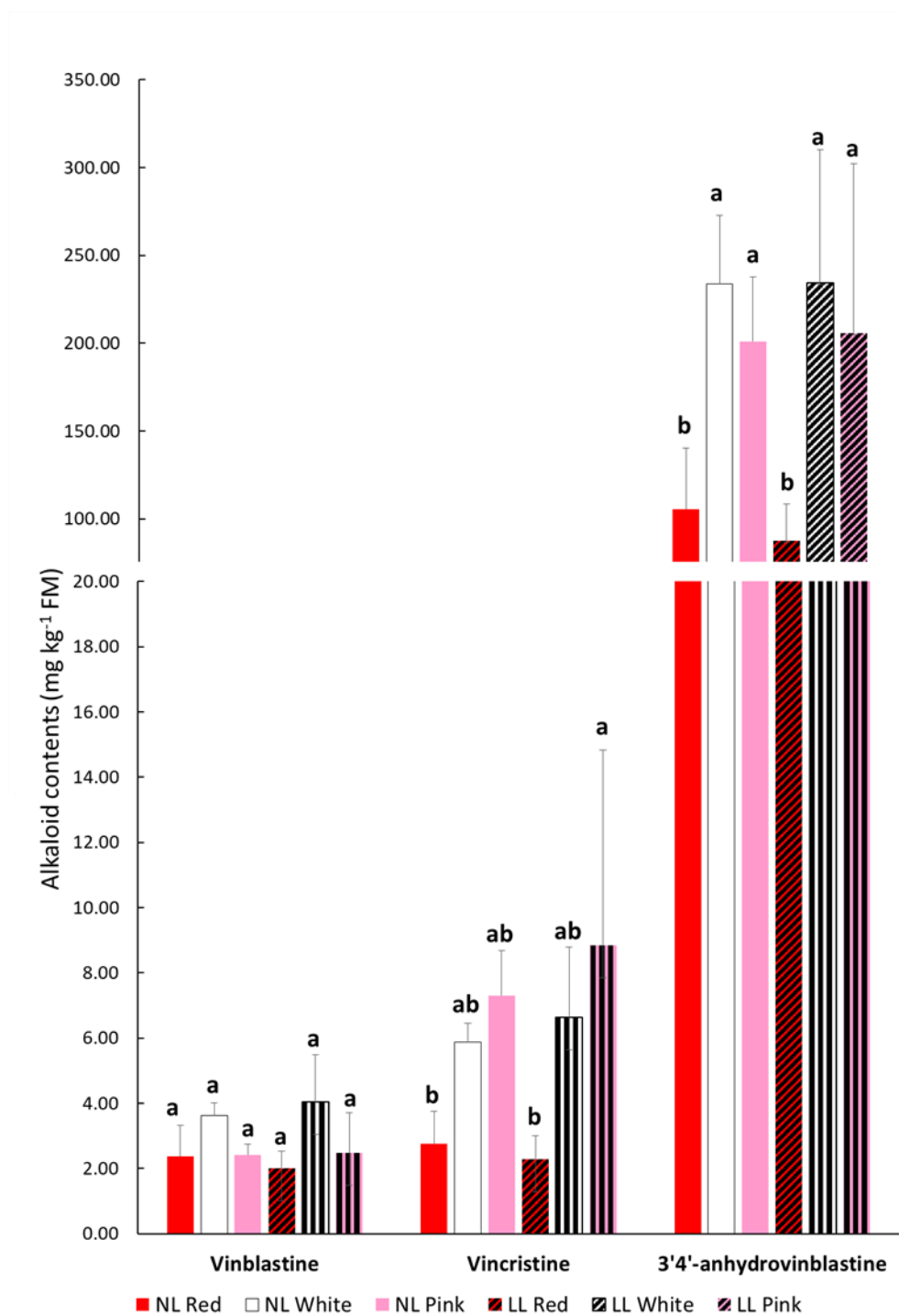


Fig. 3S. Concentration of dimeric vinca alkaloids in *C. roseus* plants grown either at control (NL, filled bars) or reduced light (LL stripped bars) conditions separated according to the flower colour (Red: 'Red', red bars; Pink: 'Rose', pink bars; White: 'Polka Dot', white bars). Mean $\pm$ SD; different letters indicate statistically significant differences between the treatments at $p < 0.05$ level.