

Article Supplementary Information

A reliable and fast two-step solid-phase extraction methodology for the obtention of anthocyanin-rich extracts from different sources

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Table S1. LC-MS identification of main polyphenols (non-anthocyanins) in the different full extracts on negative mode. N.D. stands for “not determined”.

| Extract | R _t (min) | [M-H] (m/z) | Main fragment ions | λ _{max} (nm) | Tentative identification |
|-------------------------|----------------------|----------------|---------------------------------------|-----------------------|---|
| cornflower | 8.19 | 627.18 | 465.18, 303.19 | 276, 332 | Taxifolin-O-dihexoside |
| | 9.38 | 191.1 | 126.92 | 292, 312 | Quinic acid isomer 1 |
| | 10.12 | 727.32 | 627.19, 465.25, 447.29, 285.15 | 280, 324 | Kaempferol derivative |
| | 11.3 | 191.08 | 126.91 | 280, 312 | Quinic acid isomer 2 |
| | 12.8 | 607.27 | 445.19, 431.21, 269 | 268, 320 | Apigenin-O-hexoside-O-glucuronide isomer 1 |
| | 13.07 | 607.22 | 445.14, 431.19, 269.11 | 276, 308 | Apigenin-O-hexoside-O-glucuronide isomer 2 |
| | 18.34 | 693.23 | 649.23, 473.19, 445.35, 269.2 | 268, 320 | Apigenin-O-glucuronide-O-(malonylhexoside) |
| | 22.94 | 445.15 | 269.04 | 268, 336 | Apigenin-O-glucuronide |
| wild pansy | 9.74 | 609.33 | 301.35 | 288, 334 | Quercetin-3-O-rutinoside isomer 1 |
| | 10.69 | 593.28 | 285.17 | 288, 334 | Kaempferol-3-O-rutinoside |
| | 10.87 | 627.28 | 465.38 | 288, 334 | Taxifolin-O-dihexoside |
| | 13.06 | 625.32 | 317.09 | 265, 352 | Myricetin-3-O-rutinoside |
| | 13.45 | 755.45 | 609.28 | 252, 353 | Quercetin-3-O-(6-O-rhamnosylglucoside)-7-O-rhamnoside |
| | 14.23 | 785.45 | 639.30, 315.04 | 268, 300 | Isorhamnetin-3-(2-rhamnosyl)-O-diglucoside |
| | 16.26 | 609.36 | 301 | 264, 348 | Quercetin-3-O-rutinoside isomer 2 |
| | 17 | 769.44 | 623.27, 605.3, 503.37, 357.13, 315.14 | 269, 336 | Isorhamnetin-3-O-(2,6-di-O-rhamnosyl-glucoside) |
| butterfly pea flower | 10.57 | 722.62 | 641.48, 560.40 | 288, 356, 376 | N. D |
| | 13.36 | 755.37 | 609.29, 301.13 | 267, 356 | Quercetin-3-O-(6-O-rhamnosylglucoside)-7-O-rhamnoside |
| | 14.73 | 609.29 | | 266, 356 | Quercetin-3-O-rutinoside |
| | 15.22 | 898.57 | 876.41, 795.39 | 288, 376 | N. D |
| | 15.59 | 739.4 | 593.24, 285.17 | 264, 348 | Kaempferol 3-(2G-rhamnosylrutinoside) |

| | | | | | |
|--------------|-------|---------|--------------------------------|---------------|--|
| | 17.39 | 593.38 | | 300, 356 | Kaempferol 3-neohesperidoside |
| | 22.15 | 795.57 | 714.55, 612.49, | 292, 380 | N. D |
| | 23.02 | 971.62 | 949.41, 868.33, 714.44 | 292, 376 | N. D |
| | 25.13 | 714.57 | 612.49, 397.17 | 296, 380 | N. D |
| | 31.33 | 868.58 | 766.54, 685.5, 612.48, 307.21 | 292, 356 | N. D |
| | 7.95 | 789.38 | 627.26, 447.33, 285.03 | 280, 376 | Kaempferol derivative |
| | 8.88 | 1097.66 | 935.29, 773.38, 663.32, 447.24 | 280, 304 | Kaempferol-3-(hydroxycoumaroyl)-O-sophoroside-7-O- sophoroside |
| | 9.53 | 1155.43 | 993.35, 787.39, 607.09, 463.39 | 296, 324 | N. D |
| purple | 12.28 | 935.41 | 773.3, 447.32, 285.02 | 286, 312 | Kaempferol-3-(hydroxycoumaroyl)-sophoroside-7-glucoside |
| cabbage | 13.09 | 965.34 | 803.3, 447.2, 285.09 | 281, 324 | Kaempferol-3-(hydroxyferuloyl)-O-sophoroside-7-O-glucoside |
| | 13.33 | 995.39 | 833.28, 447.35, 285.01 | 278, 328 | Kaempferol-3-(hydroxysinapoyl)-O-sophoroside-7-O-glucoside |
| | 15.1 | 833.43 | 671.34, 447.21, 285.17 | 288, 320 | Kaempferol derivative |
| | 19.46 | 947.40 | | 284, 324 | Kaempferol-3-feruloyldigluconide-7-glucoside |
| | 6.97 | 197.11 | 178.9, 135.03, 122.99, 72.84 | 280, 320 | Salvianic acid A |
| | 7.21 | 359.24 | 196.94, 179.05 | 279, 292 | Rosmarinic acid |
| | 7.39 | 428.37 | 345.12, 248.02, 164.94 | 296, 380 | N. D |
| | 7.65 | 433.39 | | 288 | Naringenin-O-hexoside |
| | 7.84 | 437.36 | 275.06, 164.93 | 276, 306 | N. D |
| | 8.2 | 311.13 | 178.91, 149.01, 135.48 | 328 | Caftaric acid |
| | 8.55 | 197.02 | 179.04 | 280, 326 | Salvianic acid A |
| | 8.99 | 521.32 | 341.16, 197.06 | 280, 322 | N. D |
| purple basil | 9.22 | 465.22 | 303.13, 285.15, 124.91 | 284, 328 | Taxifolin-O-hexoside |
| | 9.63 | 935.42 | 773.27, 447.26, 285.08 | 280, 312, 376 | Kaempferol-3-(hydroxycoumaroyl)-sophoroside-7-glucoside |
| | 10.01 | 465.3 | 303.15, 285.13, 124.88 | 295, 320 | Taxifolin-O-hexoside |
| | 10.3 | 711.28 | | 268, 296 | Quercetin-malonyl-glucoside |
| | 10.56 | 193.04 | | 298, 324 | Ferulic acid |
| | 13.03 | 951.29 | 789.24, 481.19, 345.20, 315.07 | 296, 306 | Isorhamnetin derivative |
| | 14.47 | 595.35 | 445.18, 300.07 | 276, 380 | N. D |
| | 16.11 | 597.38 | 311.15, 267.07 | 296, 328, 380 | N. D |
| | 22.07 | 717.47 | 519.28, 339.24 | 288, 332 | Salvianolic acid E |
| | 23.23 | 359.27 | 197.03, 179.02 | 288, 328 | Rosmarinic acid |
| | 6.62 | 311.19 | | 258, 301, 368 | Caftaric acid |
| | 7.38 | 164.04 | 146.91, 102.92 | 296 | N. D |
| | 7.68 | 341.25 | 178.97, 161.04 | 296 | Caffeic acid 3-glucoside |
| | 8.22 | 311.1 | 179.04, 149.02, 135.04 | 328 | Caftaric acid |
| purple sweet | 8.94 | 521.39 | 341.19, 197.06 | 268, 289 | N. D |
| potato | 9.24 | 465.25 | 303.04 | 288, 322 | Taxifolin-O-hexoside |
| | 10.06 | 305.13 | 225.04 | 300, 320, 380 | Gallocatechin |
| | 12.48 | 917.32 | 755.26, 593.25, 447.27, 285.14 | 296, 320 | Kaempferol-3-O-rutinoside-7-O-sophoroside |
| | 13.09 | 951.37 | 481.13, 345.23, 315.08 | 304, 376 | Isorhamnetin derivative |
| | 16.19 | 609.34 | 301.06 | 297, 332 | Quercetin-3-O-rutinoside |
| | 23.43 | 359.18 | 197.03, 179.01 | 290, 328 | Rosmarinic acid |

Table S2. Cumulative amount of anthocyanins after 40 BV of water applied in each resin. The results are present % \pm SD of the TAC determined for the full extracts (n=3-8).

| Resin | Cumulative amount of anthocyanins (%) | | | | | |
|---------------------|---------------------------------------|-----------------|------------------|-----------------|-----------------|------------------|
| | CF ¹ | WP ¹ | BPF ¹ | PC ¹ | PB ¹ | PSP ¹ |
| C18 Silica | 2.7 \pm 0.5 | 3.3 \pm 1.0 | 1.3 \pm 0.2 | 5.1 \pm 2.1 | 2.3 \pm 0.8 | 5.7 \pm 2.1 |
| Amberlite® XAD 7-HP | 45.4 \pm 2.2 | 46.6 \pm 4.7 | 64.7 \pm 5.8 | 55.5 \pm 8.7 | 52.6 \pm 1.9 | 49.6 \pm 6.0 |
| Toyopearl® HW-65S | 2.2 \pm 0.2 | 2.6 \pm 0.4 | 2.1 \pm 0.3 | 1.8 \pm 0.9 | 1.7 \pm 0.7 | 2.2 \pm 0.4 |
| Sephadex® LH-20 | 29.3 \pm 2.8 | 45.1 \pm 2.2 | 45.3 \pm 3.2 | 42.9 \pm 5.2 | 43.6 \pm 2.5 | 31.2 \pm 5.4 |
| Oasis® HLB | 1.6 \pm 0.7 | 1.5 \pm 0.3 | 1.3 \pm 0.2 | 2.3 \pm 0.2 | 2.2 \pm 1.0 | 1.3 \pm 0.1 |

¹ CF – cornflower; WP – wild pansy; BPF – butterfly pea flower; PC – purple cabbage; PB – purple basil; PSP – purple sweet potato;

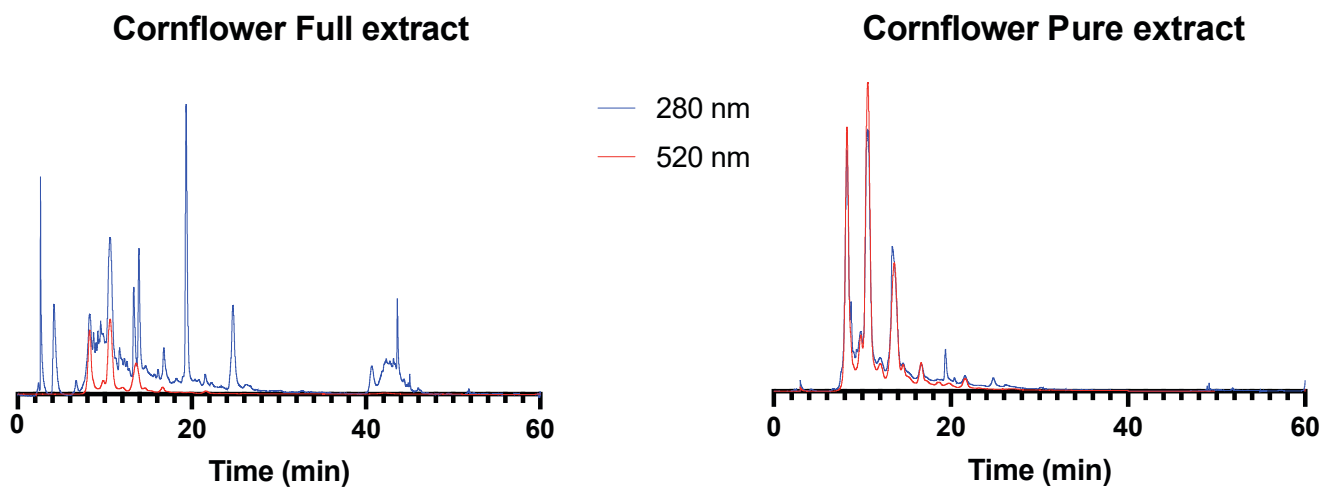


Figure S1. a) Purity of the cornflower anthocyanin extracts (full and after the application of the two-step purification) by superimposing the chromatograms obtained by UHPLC-PDA at 280 nm and 520 nm.

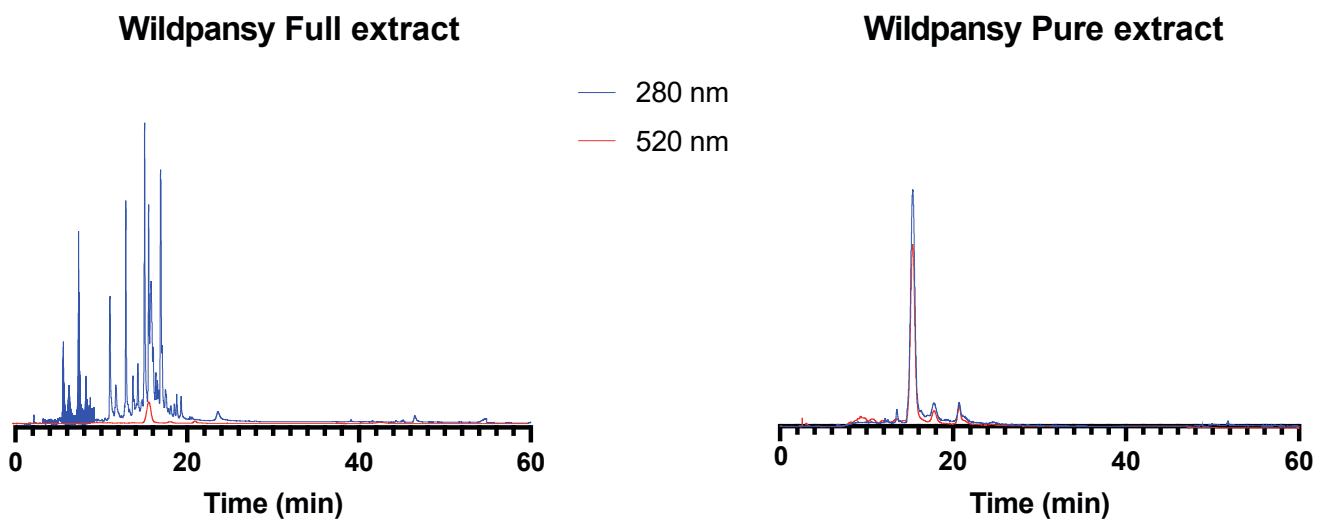
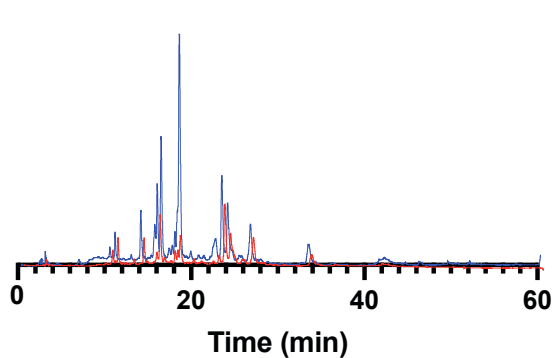


Figure S2. a) Purity of the wild pansy anthocyanin extracts (full and after the application of the two-step purification) by superimposing the chromatograms obtained by UHPLC-PDA at 280 nm and 520 nm.

Butterfly pea flower Full extract



Butterfly Pea flower extract Pure

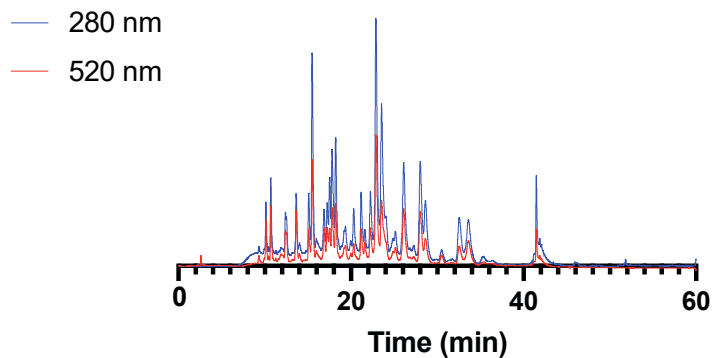
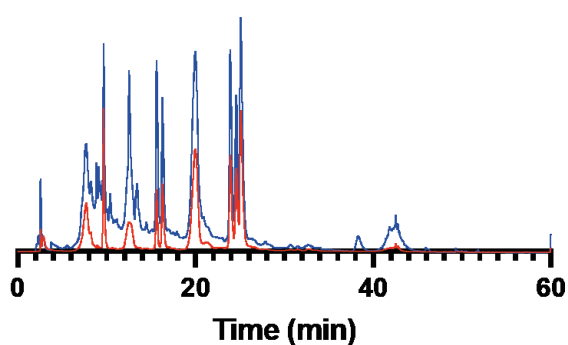


Figure S3. a) Purity of the butterfly pea flower anthocyanin extracts (full and after the application of the two-step purification) by superimposing the chromatograms obtained by UHPLC-PDA at 280 nm and 520 nm.

Purple Cabbage Full extract



Purple Cabbage Pure extract

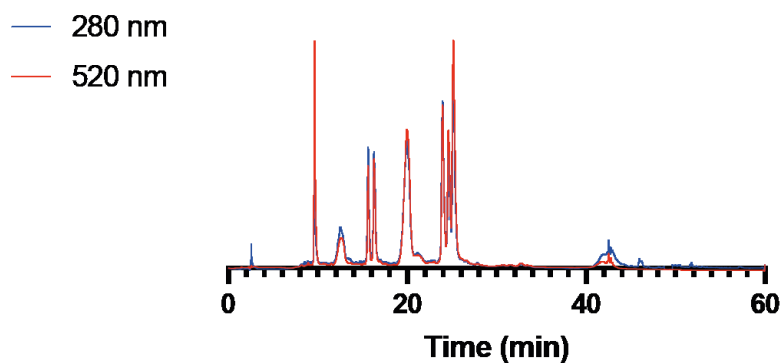
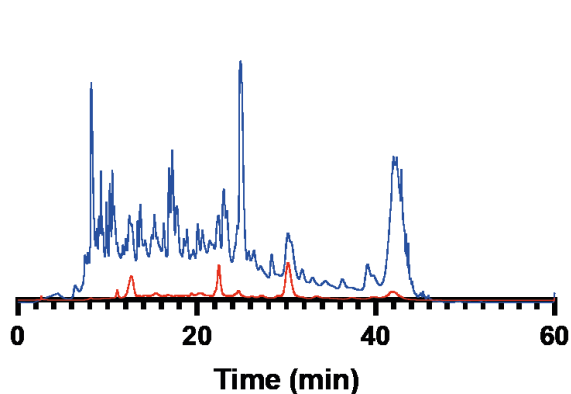


Figure S4. a) Purity of the purple cabbage anthocyanin extracts (full and after the application of the two-step purification) by superimposing the chromatograms obtained by UHPLC-PDA at 280 nm and 520 nm.

Purple Basil Full extract



Purple Basil Pure extract

— 280 nm
— 520 nm

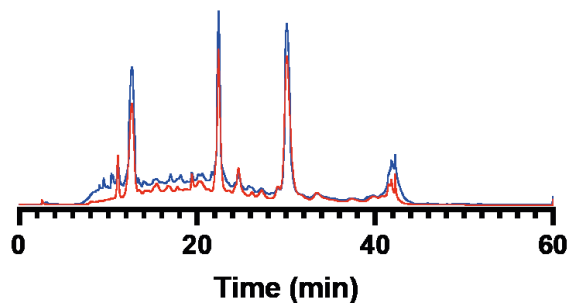
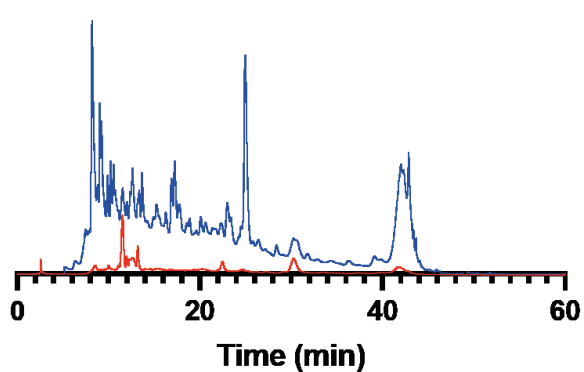


Figure S5. a) Purity of the purple basil anthocyanin extracts (full and after the application of the two-step purification) by superimposing the chromatograms obtained by UHPLC-PDA at 280 nm and 520 nm.

Purple Sweet Potato Full extract



Purple Sweet Potato Pure extract

— 280 nm
— 520 nm

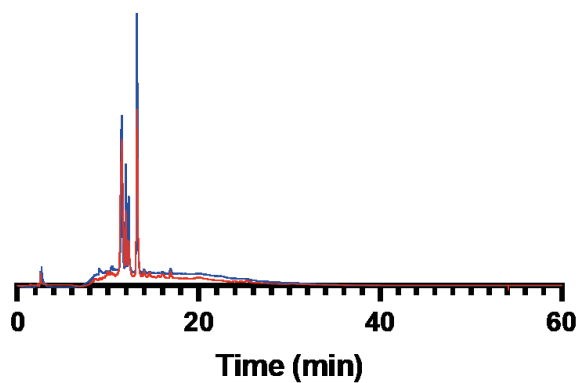


Figure S6. a) Purity of the purple sweet potato anthocyanin extracts (full and after the application of the two-step purification) by superimposing the chromatograms obtained by UHPLC-PDA at 280 nm and 520 nm.