**Supplementary Table S1**. Identification of phenolic compounds in Japanese knotweed in negative ionization with HPLC-MS and $MS^2$/$MS^3$

| Phenolic group | λ (nm) | $[M-H]^-$ (*m*/*z*) | $MS^2$ (*m*/*z*) | $MS^3$ (*m*/*z*) |
|---|---|---|---|---|
| **Hydroxybenzoic acids derivatives** | | | | |
| Gallic acid | 271 | 169 | 125 | |
| Galloylhexoside 1 | 276 | 331 | 169 | |
| Galloylhexoside 2 | 276 | 331 | 169 | |
| **Hydroxycinnamic acid derivatives** | | | | |
| 3-Feruloylquinic acid | 320 | 367 | 193,134 | 149 |
| 3-Caffeoylquinic acid | 234, 326 | 353 | 191, 179, 135 | 173, 127, 85 |
| 3-*p*-Coumaroylquinic acid | 312 | 337 | 163 | |
| 4-Caffeoylquinic acid | 234, 328 | 353 | 173, 179 | |
| 4-*p*-Coumaroylquinic acid | 312 | 337 | 173, 163, 155, 137, 191 | |
| 5-*p*-Coumaroylquinic acid 1 | 312 | 337 | 191,173,163 | |
| 5-*p*-Coumaroylquinic acid 2 | 311 | 337 | 191,163,173 | |
| 5-Caffeoylquinic acid 1 | 234,328 | 353 | 191,179,135 | 173,127,85 |
| 5-Caffeoylquinic acid 2 | 234,328 | 353 | 191,179,135 | |
| *cis*-Coutaric acid | 310 | 295 | 163 | |
| Dicaffeoylquinic acid 1 | 334 | 515 | 353 | 191 |
| Dicaffeoylquinic acid 2 | 333 | 515 | 353 | 191 |
| Caffeic acid hexoside | 330 | 341 | 179 | |
| *p*-Coumaric acid hexoside | 311 | 325 | 163 | |
| Caftaric acid 1 | 328 | 311 | 149,179 | |
| Caftaric acid 2 | 328 | 311 | 149,179 | |
| Ferulic acid pentoside | 290,310 | 325 | 163 | |
| *trans*-Coutaric acid | 310 | 295 | 163 | |
| *p*-Coumaric acid | 310 | 163 | 119 | |
| **Flavanols** | | | | |
| Epicatechin | 234,279 | 289 | 245 | |
| Catechin hexoside | 235,280 | 451 | 289 | |
| Catechin gallate | 235,280 | 441 | 289 | |
| Procyanidin dimer 1 | 278 | 577 | 425,451,407,289 | |
| Procyanidin dimer 2 | 278 | 577 | 425,451,407,289 | |
| Procyanidin dimer 3 | 279 | 577 | 425,407,289 | |
| Procyanidin tetramer 1 | 234,278 | 1153 | 1135, 1027, 983, 865, 863, 577 | |
| Procyanidin tetramer 2 | 234,278 | 1153 | 1135, 1027, 983, 865, 863, 695,577, | |
| Procyanidin tetramer 3 | 234,278 | 1153 | 1027, 983, 865, 577, 575 | |
| Procyanidin tetramer 4 | 234,278 | 1153 | 1135, 1027, 983, 865, 863, 577 | |
| Procyanidin trimer 1 | 234,278 | 865 | 577,407,289 | |
| Procyanidin trimer 2 | 234,278 | 865 | 577,425,407,289 | |
| Procyanidin trimer 3 | 235,280 | 865 | 577,425,407,289 | |
| Procyanidin trimer 4 | 236,279 | 865 | 577,425,289 | |
| Procyanidin trimer 5 | 234,280 | 865 | 577,407,289 | |
| Procyanidin trimer 6 | 235,279 | 865 | 577,425,407,289 | |
| Procyanidin trimer 7 | 234,280 | 865 | 577,425,407,289 | |
| **Flavones** | | | | |
| Apigenin hexoside | 268,334 | 431 | 269 | |
| **Flavonols** | | | | |
| Isorhamnetin hexoside | 255,352 | 477 | 315 | |
| Kaempferol hexoside | 266,346 | 447 | 285 | |
| Kaempferol-3-rhamnoside | 266, 347 | 431 | 285 | |
| Kaempferol-3-rutinoside | 264,345 | 593 | 285 | |
| Quercetin-3-xyloside | 356,255 | 433 | 301 | |
| Quercetin-3-arabinofuranoside | 355,255 | 433 | 301 | |
| Quercetin acetyl hexoside | 255,355 | 505 | 463 | 301 |
| Quercetin dihexoside | 255,356 | 625 | 301 | |
| Quercetin-3-arabinopyranoside | 256, 352 | 433 | 301 | |
| Quercetin-3-galactoside | 256,356 | 463 | 301 | |
| Quercetin-3-glucoside | 255,355 | 463 | 301 | |

| Phenolic group | λ (nm) | [M-H]⁻ (*m*/*z*) | MS² (*m*/*z*) | MS³ (*m*/*z*) |
|---|---|---|---|---|
| Quercetin-3-rhamnoside | 266,356 | 447 | 301 | |
| Quercetin-3-rutinoside | 255,355 | 609 | 301 | |
| Myricetin-3-rhamnoside | 261, 349 | 463 | 317 | |
| **Quinones** | | | | |
| Emodin hexoside | 282,450 | 431 | 269 | |
| **Stilbenes** | | | | |
| Astringin | 331,305 | 405 | 243,225,199 | |
| *cis*-Resveratroloside | 311 | 389 | 227,371,209 | |
| Piceatannol hexoside 1 | 324,290,306 | 405 | 243 | |
| Piceatannol hexoside 2 | 324,290,306 | 405 | 243 | |
| *trans*-Resveratroloside | 311 | 389 | 227 | |
| *trans*-Piceid 1 | 318,306,229 | 389 | 227,185 | |
| *trans*-Piceid 2 | 318,306,229 | 389 | 227,185 | |