

**Supplementary Table 2:** Molecular weight, detected ion mass by qTOF and optimized MRM (multiple reaction monitoring) conditions for the identified polyphenol compounds in Navelina sweet orange pulps by HPLC-ESI-MS/MS.

| Compound                      | MW     | [M-H] <sup>-</sup> | Quantification |        | Confirmation |        |
|-------------------------------|--------|--------------------|----------------|--------|--------------|--------|
|                               |        |                    | MS/MS          | CE (V) | MS/MS        | CE (V) |
| Benzoic acid                  | 122.12 | 121.0304           | 121>77         | 8      | 121>59       | 4      |
| Phloroglucinol                | 126.11 | 125.0265           | 125>57         | 20     | 125>125      | 0      |
| Hydroxybenzoic acid           | 138.12 | 137.0256           | 137>93         | 40     | 137>119      | 40     |
| Protocatechuic acid           | 154.12 | 153.0215           | 153>109        | 16     | 153>62       | 40     |
| p-Coumaric acid               | 164.16 | 163.0774           | 163>119        | 16     | 163>93       | 36     |
| Gallic Acid                   | 170.12 | 169.0137           | 169>125        | 12     | 169>79       | 24     |
| Caffeic acid                  | 180.16 | 179.0344           | 179>135        | 16     | 179>107      | 24     |
| Ferulic acid                  | 194.18 | 193.052            | 193>134        | 12     | 193>178      | 12     |
| Apigenin                      | 270.24 | 269.0452           | 269>117        | 44     | 269>151      | 28     |
| Naringenin                    | 272.25 | 271.0619           | 271>151        | 20     | 271>119      | 32     |
| Kaempferol                    | 286.24 | 285.0403           | 285>239        | 28     | 285>117      | 56     |
| Eriodictyol                   | 288.25 | 287.0793           | 287>151        | 12     | 271>135      | 28     |
| Disomletin                    | 300.26 | 299.0565           | 299>284        | 20     | 299>256      | 36     |
| Quercetin                     | 302.24 | 301.0100           | 301>151        | 20     | 301>179      | 20     |
| Hesperetin                    | 302.28 | 301.0525           | 301>164        | 28     | 301>286      | 16     |
| Protocatechuic acid glucoside | 316.26 | 315.0737           | 315>153        | 10     | 315>109      | 20     |
| hGallic acid O-glucoside      | 332.26 | 341.0896           | 331>169        | 12     | 331>125      | 12     |
| Caffeic acid O-glucoside      | 342.30 | 341.0896           | 341>179        | 20     | 341>323      | 10     |
| Chlorogenic acid              | 354.31 | 353.0905           | 353>191        | 16     | 353>85       | 16     |
| Feruloylquinnic acid          | 368.34 | 367.1062           | 367>193        | 40     | 367>161      | 40     |
| Phloridzin                    | 436.41 | 435.1331           | 435>273        | 10     | 435>167      | 40     |
| Kaempferol-3-O-glucoside      | 448.38 | 447.0974           | 447>284        | 28     | 447>255      | 40     |
| Eriodictyol-7-O-glucoside     | 450.39 | 449.1084           | 449>287        | 12     | 449>151      | 36     |
| Hyperoside                    | 464.38 | 463.0917           | 463>300        | 32     | 463>271      | 48     |
| Isorhamnetin-3-O-glucoside    | 478.40 | 477.1014           | 477>314        | 32     | 477>285      | 40     |
| Myricetin-3-O-glucoside       | 480.38 | 479.0841           | 479>317        | 20     | 479>461      | 10     |
| Narirutin                     | 580.53 | 579.1762           | 579>271        | 40     | 579>151      | 48     |
| Naringin                      | 580.53 | 579.1762           | 579>271        | 40     | 579>151      | 48     |
| Kaempferol-3-O-rutinoside     | 594.52 | 593.1560           | 593>353        | 32     | 593>255      | 60     |
| Didymin                       | 594.56 | 593.1963           | 593>285        | 20     |              |        |
| Eriocitrin                    | 596.53 | 595.1705           | 595>287        | 20     |              |        |
| Neoeriocitrin                 | 596.53 | 595.1711           | 595>287        | 20     |              |        |
| Rutin                         | 610.52 | 609.1508           | 609>300        | 40     | 609>271      | 60     |
| Hesperidin                    | 610.56 | 609.1869           | 609>301        | 20     | 609>286      | 52     |

Abbreviations: MW, molecular weight; CE, collision energy; Ms>Ms transitions.