| **Peak number** | ***t*R/min** | **Molecular formula** | **Accurate** | **Calculated** | **Error (ppm)** | **Identified compounds** |
| --- | --- | --- | --- | --- | --- | --- |
|  | 0.824 | C6H12O6 | 180.06339 | 180.0629 | −2.48 | D-(+)-Glucose |
|  | 1.018 | C4H6O5 | 134.02152 | 134.0211 | −2.92 | DL-Malic acid |
|  | 1.229 | C6H6O3 | 126.03169 | 126.0312 | −4 | Pyrogallol |
|  | 2.201 | C9H17NO5 | 219.11067 | 219.1102 | −2.14 | Pantothenic acid |
|  | 3.265 | C8H8O3 | 152.04734 | 152.047 | −2.3 | 2-Anisic acid |
|  | 4.062 | C7H6O3 | 138.03169 | 138.0313 | −3.07 | Salicylic acid |
|  | 5.626 | C15H14O6 | 290.07904 | 290.0787 | −1.33 | Catechin |
|  | 5.72 | C6H10O4 | 146.05791 | 146.0576 | −2.4 | Adipic acid |
|  | 5.763 | C8H8O4 | 168.04226 | 168.0419 | −2.36 | Vanillic acid |
|  | 6.578 | C7H6O2 | 122.03678 | 122.0365 | −2.45 | Benzoic acid |
|  | 8.569 | C8H8O3 | 152.04734 | 152.047 | −2.15 | Vanillin |
|  | 9.315 | C10H10O4 | 194.05791 | 194.0575 | −2.29 | Ferulic acid |
|  | 10.946 | C15H12O7 | 304.0583 | 304.0576 | −2.21 | Dihydrorobinetin |
|  | 10.953 | C6H6O3 | 126.03169 | 126.0309 | −5.95 | Phloroglucinol |
|  | 4.049 | C11H12N2O2 | 204.08988 | 204.0894 | −2.25 | D-(+)-Tryptophan |
|  | 11.272 | C21H20O10 | 432.10565 | 432.1049 | −1.85 | Isovitexin |
|  | 11.275 | C21H20O12 | 464.09548 | 464.0949 | −1.25 | Quercetin-3-O-glucoside |
|  | 12.071 | C9H8O2 | 148.05243 | 148.0521 | −2.07 | trans-Cinnamic acid |
|  | 12.774 | C21H20O11 | 448.10056 | 448.0998 | −1.67 | Isoorientin |
|  | 12.895 | C15H12O6 | 288.06339 | 288.0629 | −1.64 | Fustin |
|  | 13.052 | C9H10O2 | 150.06808 | 150.0678 | −2.18 | Hydrocinnamic acid |
|  | 15.655 | C8H11NO | 137.08406 | 137.0837 | −2.6 | Tyramine |
|  | 15.736 | C15H10O7 | 302.04265 | 302.042 | −2.3 | Robinetin |
|  | 15.751 | C15H10O6 | 286.04774 | 286.0472 | −2.06 | Luteolin |
|  | 17.106 | C9H16O4 | 188.10486 | 188.1044 | −2.64 | Azelaic acid |
|  | 17.631 | C15H10O5 | 270.05282 | 270.0525 | −1.36 | Genistein |
|  | 21.755 | C16H30O4 | 286.21441 | 286.2139 | −1.63 | Hexadecanedioic acid |
|  | 38.385 | C30H46O4 | 470.33961 | 470.3389 | −1.43 | 18-β-Glycyrrhetinic acid |
|  | 40.138 | C30H48O3 | 456.36035 | 456.3597 | −1.36 | Ursolic acid |
|  | 41.117 | C30H48O3 | 456.36035 | 456.36 | −0.83 | Oleanolic acid |
|  | 0.753 | C6H14N4O2 | 174.11168 | 174.11157 | −0.58 | L-(+)-Arginine |
|  | 1.118 | C9H11NO3 | 181.07389 | 181.07368 | −1.17 | L-Tyrosine |
|  | 9.58 | C10H10O2 | 162.06808 | 162.0679 | −1.1 | Methyl cinnamate |
|  | 11.63 | C9H7NO | 145.05276 | 145.05256 | −1.41 | 8-Hydroxyquinoline |
|  | 11.787 | C21H20O10 | 432.10565 | 432.10494 | −1.64 | Vitexin |
|  | 13.668 | C10H16O | 152.12012 | 152.12 | −0.75 | Citral |
|  | 16.6 | C20H17NO4 | 335.11576 | 335.11495 | −2.42 | Berberine |
|  | 17.966 | C16H12O7 | 316.0583 | 316.05771 | −1.89 | Rhamnetin |
|  | 43.089 | C29H48O2 | 428.36543 | 428.36437 | −2.48 | Stigmastane-3,6-dione |