

Peak	Class ^a	RT ^b (mins)	MW	Theoretical m/z	[M + H] ⁺ m/z	Mass error (mDa)	Formula	Tentative identification	Sample
1	PA	4.70	354.31	355.1024	354.0951	0.069	C ₁₆ H ₁₈ O ₉	Chlorogenic acid	YTL, MTL, NFP, FFP
2	PA	5.27	368.34	369.1180	368.1107	0.019	C ₁₇ H ₂₀ O ₉	5-Feruloylquinic acid	NFP, FFP
3	FL	6.46	302.24	303.0499	302.0427	-0.074	C ₁₅ H ₁₀ O ₇	Quercetin	YTL, NFP
4	FL	7.04	480.38	481.0977	480.0904	-0.007	C ₂₁ H ₂₀ O ₁₃	Myricetin-3-galactoside	YTL, MTL, NFP, FFP
5	PA	7.50	338.31	339.1074	338.1002	0.084	C ₁₆ H ₁₈ O ₈	3-p-Coumaroylquinic acid	NFP, FFP
6	AA	8.27	129.11	130.0499	129.0426	-	C ₅ H ₇ NO ₃	Pyroglutamic acid	YTL, MTL, NFP, FFP
7	FL	9.06	626.52	627.1556	626.1483	0.000	C ₂₇ H ₃₀ O ₁₇	Quercetin dihexoside	YTL, MTL, NFP, FFP
8	PA	10.17	516.45	517.1341	516.1268	0.003	C ₂₅ H ₂₄ O ₁₂	Dicaffeoylquinic acid 3	YTL, MTL, NFP, FFP
9	F3	13.32	458.37	459.0922	458.0849	0.029	C ₂₂ H ₁₈ O ₁₁	Epigallocatechin gallate	MTL
10	PA	15.16	516.45	517.1341	516.1268	0.035	C ₂₅ H ₂₄ O ₁₂	Dicaffeoylquinic acid 1	YTL, MTL, NFP, FFP
11	OA	16.59	90.08	91.0390	90.0317	-	C ₃ H ₆ O ₃	Lactic acid	NFP, FFP
12	PA	17.30	192.17	193.0707	192.0634	0.325	C ₇ H ₁₂ O ₆	Quinic acid	NFP, FFP
13	F3	17.94	290.27	291.0863	290.0790	0.023	C ₁₅ H ₁₄ O ₆	Epicatechin	YTL
14	PA	20.59	258.19	259.0561	258.0488	-0.003	C ₉ H ₁₀ N ₂ O ₇	Uronic acid	MTL, NFP, FFP
15	FL	22.33	726.63	727.2080	726.2007	-0.018	C ₃₂ H ₂₇ O ₁₄	Apigenin-6-C-glucosyl-8-C-arabinoside	FFP
16	PA	22.73	170.12	171.0288	170.0215	-0.144	C ₇ H ₆ O ₅	Gallic acid	NFP, FFP
17	PA	24.06	302.19	303.0135	302.0063	0.074	C ₁₄ H ₆ O ₈	Ellagic acid	NFP, FFP
18	PP	26.57	126.11	127.0390	126.0317	0.070	C ₆ H ₆ O ₃	Pyrogallol	NFP, FFP
19	PA	35.81	88.11	89.0597	88.0524	-	C ₄ H ₈ O ₂	Butyric acid	NFP, FFP
20	FL	37.54	464.38	465.1026	464.0955	0.003	C ₂₁ H ₂₀ O ₁₂	Quercetin-3-glucoside	YTL, MTL, FFP
21	F3	42.81	306.27	307.0812	306.0740	0.109	C ₁₅ H ₁₄ O ₇	Gallocatechin	MTL