

Effects of water deficit and heat stress on *Nicotiana Langsdorffii* metabolomic pattern modified by insertion of *rolD* gene from *Agrobacterium rhizogenes*.

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Table S1: Metabolites identified by untargeted metabolomic analysis at levels 2 and 3. Diagnostic fragments are in bold.

Retention time (min)	Mass	Formula	Name	Fragments	Error (ppm)	ID Level
16,43	468.21310 (M - H)	C ₂₅ H ₃₁ N ₃ O ₆	Dicaffeoyl spermidine	332.16077, 306.18170, 289.15533, 135.04524, 264.17065	-1,9	2
22,09	783,32617 (M - H)	C ₃₄ H ₅₆ O ₂₀	Menthenetriol glucoside + ketoglutaric acid + octanoic acid	739.33136, 652.68506, 491.28287, 287.14825, 215.12827, 143.10721	-3,1	2
14,95	250,07155 (M - H)	C ₁₂ H ₁₃ NO ₅	Phenylacetylaspartic acid	132.03020, 232.06131	-2,18	2
9,88	315,07129 (M - H)	C ₁₃ H ₁₆ O ₉	Glucopyranosyloxyhydroxybenzoic acid	153.01921, 109.02940, 165.01924, 225.03976	-2,36	2
14,39	373.11310 (M - H)	C ₁₆ H ₂₂ O ₁₀	Secologanate	358.08963, 211.06085 , 196.03746, 179.07130, 153.0557, 304.91241, 265.07080, 195.02966, 180.04237, 139.04002	-3,1	2
9,65	367.12387 (M - H)	C ₁₄ H ₂₄ O ₁₁	Acetyl methyl glucuronic acid + gamma hydroxyvaleric acid	349.11319, 323.09775, 249.06126, 231.05061	-3,5	2

15,06	472,2439 (M-H)	C ₂₃ H ₄₀ NO ₇ P	LysoPE (18:4; 0:0)	381.17514, 350.20694, 308.19662, 186.16068, 121.02934, 137.06053, 266.08671	-5,32	2
13,23	372.12909 (M + FA - H) 326.12372 (M - H)	C ₁₅ H ₂₁ NO ₇	Phenylalanine glucopyranose	304.91229, 236.09235, 179.05600, 161.04530	-2,4	2
13,03	381,13959	C ₁₅ H ₂₆ O ₁₁	Acetylmethyl glucuronic acid- hydroxy methyl pentanoic acid	249.06136, 231.05087 , 206.06825	-2,4	2
16,09	385,11325	C ₁₇ H ₂₂ O ₁₀	Acetyl methyl glucuronic acid hydroxy acetophenone	267.07184, 249.06114	-2,3	2
11,20	399,13171	C ₁₅ H ₂₈ O ₁₀ S	Propyl -glucopyranosyl-2-tio- glucopyranoside	136,99147	-3,3	2
33,37	433,23569	C ₂₁ H ₃₉ O ₇ P	PA (18:2/0:0)	152.99603, 171.00659	-0,5	2
10,70	395,02789	C ₁₃ H ₁₆ O ₁₂ S	Periodic leaf movement factor, PLMF 3 (Glucopyranosyloxyhydroxyb enzoic acid sulfate)	351.03842, 377.01718, 241.00220, 153.01930, 241.00194, 253.02708, 109.02946	-3,3	2
14,05	504.17111 (M + FA - H) 458.16510 (M - H)	C ₂₀ H ₂₉ NO ₁₁	Cinnamide diglucoside	357.10263, 311.09732, 293.08664, 251.07672, 221.06549, 191.05542, 161.04521	-3,6	2
18,42	461.23703 (M + FA - H) 415.23175 (M - H)	C ₂₁ H ₃₆ O ₈	Sesquiterpenoid		-4,7	3
22,44	485,13596	C ₂₄ H ₂₆ N ₂ O ₇ S	Caffeoyl-indole-3-acetyl methionine	467.12592, 441.14661, 423.13562, 349.08429, 305.09497 , 232.09683, 190.03238	-5,8	2

19,59	483.20779 (M + FA - H) 437.20227 (M - H)	C ₁₉ H ₃₄ O ₁₁	Caprylic acid + xylopyranosyl glucopyranoside	293,08746	-4,04	2
26,24	552.24249 (M + FA - H) 506.23688 (M - H)	C ₂₆ H ₃₇ NO ₉	Octahydro-quinolizine- Glucopyranosyl-hydroxy- methoxy-cinnamoyl	362.12244, 200.07079, 305.15894, 260.09140, 117.03468	-2,28	2
13,61	491.13986 (M + FA - H) 445.13428 (M - H)	C ₁₉ H ₂₆ O ₁₂	Benzoic acid difructofuranose dianhydrhyde	323.09787, 305.08676, 263.07663, 221.06628, 179.05598	-3	2
19,94	555,22815	C ₂₉ H ₄₀ O ₁₅	Menthenetriol diglucoside	509.22238, 491.21146, 431.19080, 389.18036, 365.10730, 305.15964 , 347.17001 , 233.13889, 161.04529, 179.05534, 143.03474	-2,3	2
22,06	649.30432 (M + 2FA - 2H) 1207.60474 (M - H)	C ₅₈ H ₉₆ O ₂₆	Diosgenin + 3glucoses + 1 dehydroxyglucose + 1 methyldehydroxyglucose (Methyldichotomin)	626.30121 (-46), 603.29865 (-46), 1061.54749 (-146)	-5,8	2
18,04	645.25842 (M + FA - H) 599.25323 (M - H)	C ₂₅ H ₄₄ O ₁₆	Menthenetriol diglucoside + glycerol + galactose	581.24353, 305.15909 , 497.22095, 455.13800, 347.16897 , 275.07568, 233.13835, 215.12788, 161.04489, 179.05542	-4,7	2
26,62	653.26202 (M + FA - H) 607.25720 (M - H)	C ₂₇ H ₄₄ O ₁₅	Acylcsucrose (S4:15)	627.54944, 565.24677 , 56077814, 495.20340, 481.18893 , 477.19397, 463.17798	-5,8	2

18,26	645.25812 (M + FA - H) 599.25323 (M - H)	C ₂₅ H ₄₄ O ₁₆	Menthenetriol diglucoside + carboxyethylglucose	581.24353, 275.07599, 539.23181, 497.22095, 455.13800, 389.17941, 347.16898, 305.15884, 161.04489, 215.12823, 143.10721, 233.13835	-3,1	2
27,16	721.36536 (M + FA - H) 675.35974 (M - H)	C ₃₃ H ₅₆ O ₁₄	Diglucopyranosyl linolenylglycerol (C18:3)	415.14557, 397.13477, 235.08237	0,2	2
33,01	723.38110 (M + FA - H) 677.37512 (M - H)	C ₃₃ H ₅₇ O ₁₄	Acylsucrose (S3:21)	593.31763, 551.27081 , 533.26013	-0,38	2
35,08	751.44861 (M + FA - H) 705.44324 (M - H)	C ₃₆ H ₆₆ O ₁₃	Dirhamnolipid C24:0 (C8:0, C16:0)	561.32794, 543.31775	0,2	2
35,58	765.42755 (M + FA - H) 719.42200 (M - H)	C ₃₆ H ₆₄ O ₁₄	Acylsucrose (S3:24)	593.31781, 575.30658, 467.21338 , 449.20279	-0,4	2
33,54	773.43237 (M + FA - H) 727.42731 (M - H)	C ₃₈ H ₆₄ O ₁₃	Dirhamnolipid C25:3 (C18:3, C7:0)	583.31195, 565.30157, 277.21729	-0,144	2
34,42	775.44818 (M + FA - H) 729.44269 (M - H)	C ₃₈ H ₆₆ O ₁₃	Dirhamnolipid C25:2 (C18:2, C7:0)	585.32806, 567.31610, 279.23318	-0,5	2
37,25	807.43829 (M + FA - H) 761.43182 (M - H)	C ₃₈ H ₆₆ O ₁₅	Acylsucrose S4:26	719.42218, 635.32861, 593.31799 , 467.21503, 575.30829 , 449.20309, 621.34656	-1,4	2
15,79	470.22781 (M - H)	C ₂₃ H ₃₈ O ₇ NP	LysoPE (18:4; 0:0)	334.17599, 291.17035, 121.02929, 137.06046, 169.13408, 180.06590, 237.12361, 249.12352	-7,3	3
19,01	579.20538 (M - H)	C ₂₈ H ₃₆ O ₁₃	Syringaresinol O-beta-D- glucoside	417,15314	-5,06	2
21,50	569.26837 (M + 2FA - 2H) 1047.53406 (M-H)	C ₅₁ H ₈₄ O ₂₂	Diosgenin + 3glucoses + 1 hydroxyglucose (methylprotodioscin)	546.26544 (-46) 523.26245 (-92)	-4,48	2

22,59	409.20578 (M + FA - H) 363.20068 (M - H)	C ₁₇ H ₃₂ O ₈	Allylglucose + caprylic acid	220.31882, 143.10709	-4,8	2
21,02	642.29803 (M + 2FA - 2H) 1193.59351 (M - H)	C ₅₇ H ₉₄ O ₂₆	Diosgenin + 3 glucoses + 2 dehydroxyglucose (Dichotomin)	619.29651 (-46), 596.29382 (-46), 523.26288 (-146), 1031.53821, 450.23441, 1047.53345, 901.47559, 1029.52332, 883.46600, 755.41864 , 737.40845	-3,05	2
22,92	1175,58032	C ₅₇ H ₉₂ O ₂₅	Diosgenin + 2 glucoses + 3 hydroxyglucoses	1029.52246 (-146), 883.46417 (-146), 737.40668 (-146), 557.34369 (-180), 865.45385, 806.02380, 766.13739, 719.39764, 671.37610, 653.36548, 575.35547 , 599.04858, 509.32275	-4,4	2
26,06	575.30457 (M+FA-H) 529.29895 (M-H)	C ₂₈ H ₄₂ O ₆ N ₄	Bisdihydrocaffeoylspermine	511.28836, 407.19012, 293.21066, 253.09164, 275.20032	-6,7	2
20,23	553,21173	C ₂₃ H ₃₈ O ₁₅	Menthenetriol diglucoside	509.22156, 389.17978, 347.16946 , 305.15915, 263.07602, 233.13853, 161.04503, 179.05545	-3,7	3
21,34	435,09119	C ₂₀ H ₂₀ O ₁₁	Glucopyranosyl hydroxybenzoyl dihydroxybenzoic acid	297.06003 , 315.07043 , 152.01093, 179.03415	-6,5	2
12,27	312.09442 (M + FA - H) 266.08936 (M - H)	C ₁₀ H ₁₃ N ₅ O ₄	Adenosine	242.94350, 134.04739	-0,44	2
35,55	277,2171	C ₁₈ H ₃₀ O ₂	Linolenic acid	259.20651, 233.22757	-0,7	2
22,43	312,12228	C ₁₈ H ₁₉ NO ₄	Feruloyltyramine	297.09930, 270.11288, 242.94244, 178.05029 , 148.05272, 135.04482	-5,9	2

12,72	372,09241	C ₁₆ H ₂₃ NO ₉	Acetyl methyl glucuronic acid isonicotinic acid	249.06108, 231.05063	-3,2	2
36,65	279,23283	C ₁₈ H ₃₂ O ₂	Linoleic acid	261,22223	-0,4	2
16,57	403.15964 (M + FA - H) 357.15430 (M - H)	C ₁₇ H ₂₆ O ₈	Sesquiterpenoid	161,04518	-3,3	3
14,64	447.14957 (M + FA - H) 401.14401 (M - H)	C ₁₅ H ₂₆ O ₁₀	Benzylalcohol hexose-pentose	269.10226, 293.08694, 356.13223, 233.06602, 161.04523, 277.09036, 251.09190, 262.06754	-3,2	2
14,11	451.21786 (M + FA - H) 405.21252 (M - H)	C ₁₉ H ₃₄ O ₉	Megastigmenetetrol- glucopyranoside (Sesquiterpenoid)	340.12256, 243.16002, 225.14966, 179.05597, 167.10770, 149.09705, 143.03485	-1,1	2
28,01	474,26242	C ₂₃ H ₄₂ NO ₇ P	LysoPE (18:3/0:0)	277.21722, 233.22748, 259.20682	-0,4	2
26,30	623,23627	C ₃₆ H ₃₆ N ₂ O ₈	Grossamide	486.15283, 460.17346, 445.14996, 297.11136, 283.09583, 268.07312, 471.12894, 427.13953, 352.08035	-5,8	2
32,28	651.41113 (M + FA - H) 605.40533 (M - H)	C ₃₆ H ₅₈ O ₈	Saponin		-0,92	3
28,14	638,33118	C ₂₉ H ₅₄ NO ₁₂ P	LysoPE (18:2/0:0) + hexose	476.27805, 518.28864, 279.23279	-0,05	2
34,03	637,43188	C ₃₆ H ₆₂ O ₉	Saponin		-0,35	3
42,19	673.46729 (M + FA)	C ₃₈ H ₆₄ O ₆	Feruloyloxyfatty acid (C28:0)		-0,5	3

31,03	695.35022 (M + FA - H) 649.34393 (M - H)	C ₃₁ H ₅₄ O ₁₄	Acylsucrose (S3:19)	565.28619 , 551.27069, 523.23926	-0,23	2
31,29	823.46887 (M - H)	C ₄₄ H ₇₂ O ₁₂ S	SQDG 35:6	805.46167, 585.24005, 567.22925, 415.14474, 397.13489, 661.41632 (- 162), 643.40631 (-180), 187.09793	1,69	2
32,12	735.34393 (M + FA - H)	C ₃₃ H ₅₄ O ₁₅	Acylsucrose (S4:21)		-0,223	2
32,75	737.36023 (M + FA - H) 691.35449 (M - H)	C ₃₃ H ₅₆ O ₁₅	Acylsucrose (S4:21)	649.34418 , 607.29761, 565.25488 , 523.932, 481.19174	-0,223	2
33,47	751.37561 (M + FA - H) 705.37012 (M - H)	C ₃₄ H ₅₈ O ₁₅	Acylsucrose (S4:22)	663.35950, 607.29712 , 555.28638, 537.25513, 481.19266 , 450.04047, 579.26575	-0,2	2
34,12	583.31543 (M - H)	C ₂₇ H ₅₂ O ₁₁ S	Deoxysulfoquinovosylmonoac yl glycerol	522.35614, 299.04395 , 225.00765 , 297.27969	-0,55	2
34,74	765.39105 (M + FA - H) 719.38678	C ₃₅ H ₆₀ O ₁₅	Acylsucrose (S4:23)	677.37555, 635.32880, 593.28906 , 551.27112 , 566.47937, 548.46857	-0,48	2
35,53	779.40680 (M + FA - H) 733.40088 (M - H)	C ₃₆ H ₆₂ O ₁₅	Tetraacylsucrose (S4:24)	691.39069 , 607.29718, 565.28638 , 481.19226 , 439.18195	-0,9	2
41,51	837,48236	C ₄₅ H ₇₄ O ₁₂ S	SQDG 36:6 (C:18/C:18)	778.50342, 579.28290, 559.25781, 537.27264 , 481.71002, 413.66330	0,1	2
23,30	327,21603	C ₁₈ H ₃₂ O ₅	Trihydroxyoctadecadienoic	171.10214 , 211.13322, 229.14371 , 239.12776, 273.18454, 291.19528, 309.20554, 153.09113, 127.11237, 193.15909, 247.20549, 273.18460	-4,6	2

23,13	1113.52881 (M + FA - H) 1067.52161 (M - H)	C ₅₀ H ₈₄ O ₂₄	Nicotianoside III	921.46710 (-146), 903.45825, 757.39960, 613.35699, 775.40753 (- 146), 629.35046 (-146), 467.29852 (- 146), 575.31903 , 595.34308	-4,4	2
28,87	476,27701	C ₂₃ H ₄₄ NO ₇ P	LysoPE (18:2/0:0)	279.23212, 261.22208	-2,6	2
25,71	609.26501 (M - H)	C ₂₇ H ₄₇ O ₁₃ P	PA (18:4;0:0) + glucose	563.26831, 467.21176, 447.21265 (- 162), 429.20215 (-180), 293.21054, 315.04654, 275.20016, 241.01062, 235.16841, 265.21635, 244.75534	-5,15	2
14,05	172,09782	C ₈ H ₁₅ NO ₃	Acetyl-leucine	130,08746	-0,56	2
7,14	203,08176	C ₁₁ H ₁₂ N ₂ O ₂	Tryptophan	159.09236, 186.05562, 142.06607, 116.05032	-4,09	2
12,54	249,12405	C ₁₃ H ₁₈ N ₂ O ₃	Caffeoylputrescine	207.11348, 135.04503	-1,6	2
11,56	192,0667	C ₁₀ H ₁₁ NO ₃	Benzoylalanine	146.93811, 131.47552, 102.73841, 74.02512, 66.10155	0,43	2
11,92	215,13998	C ₁₀ H ₂₀ N ₂ O ₃	Valyl valine	197.12953, 128.03546, 169.13451, 141.10333, 127.05141, 84.04576, 66.10163	-0,63	2
13,23	321,14499	C ₁₆ H ₂₂ N ₂ O ₅	Acetyl-tyrosil valine	277,15555	-1,88	2
14,39	373,11261	C ₁₆ H ₂₂ O ₁₀	Propyl gallate glucoside	358.08932, 304.91312, 328.13907, 211.06067, 195.02950, 153.05544, 180.04230, 179.07085, 196.03738	-3,77	2
13,77	343,09238	C ₁₅ H ₂₀ O ₉	Dihydroxyacetophenone glucoside	328.08023, 299.10422, 275.07788, 181.05101, 166.02739, 234.04906	-3	2

20,53	381.164492 (M + FA - H) 305.15997 (M - H)	C ₁₄ H ₂₆ O ₇	Glucopyranosyloxyoctanone	207.05090, 143.10780 (-162)	-1,62	2
13,91	386.14432 (M - H + FA) 340.13922 (M - H)	C ₁₆ H ₂₂ NO ₇	Acetyltyramine glucoside	178,08691	-2,8	2
13,23	329,08661	C ₁₄ H ₁₈ O ₉	Trihydroxyacetophenone glucopyranoside	167.03474, 311.1601	-1,9	2
15,67	321,15408	C ₁₄ H ₂₆ O ₈	Octanoic acid glucoside	311.83716, 303.14395, 159.10197, 141.09163	-2,6	2
14,82	192,06606	C ₁₀ H ₁₁ NO ₃	Phenylacetyl glycine	74,0251	-2,8	2
11,99	340,13943	C ₁₆ H ₂₃ NO ₇	Acetyl-hydroxy phenethylamine glucopyranose	178.08711, 161.04544, 143.03485, 125.02441, 101.02449	-2,19	2
15,65	399.09238 (M + FA - H) 353.08685 (M - H)	C ₁₆ H ₁₈ O ₉	3CQA	191,03455	-2,7	1
15,87	461.16623 (M + FA - H) 415.16101 (M - H)	C ₁₉ H ₂₈ O ₁₀	Phenylethanol apiofuranosyl glucopyranoside	311.09796, 293.08740, 191.05603, 161.04555, 149.04562, 131.03503, 113.02453	-4	2
32,28	481,25677	C ₂₂ H ₄₃ O ₉ P	PG (16:1/0:0)	253.21730, 245.04327, 152.99620	-0.8	2
32,09	431,22028	C ₂₁ H ₃₇ O ₇ P	PA(18:3/0:0)	152.99603, 363.21521, 171.00633	-0,309	2
19,32	483.20621 (M + FA - H) 437.20065 (M - H)	C ₁₉ H ₃₄ O ₁₁	Octanoic acid + dyhydroxymethylene butanoyl beta glucopyranoside	403.69440, 293.08636, 191.05574, 149.04539, 131.03494, 125.02441, 101.02441, 89.02454	-4,99	2
18,66	513.21667 (M - H + FA) 467.21097 (M - H)	C ₂₀ H ₃₆ O ₁₂	Sucrose octanoate	323.09671, 305.08640	-5,2	2

18,04	675.25775 (M + FA - H) 599.25262 (M - H)	C ₂₅ H ₄₃ O ₁₆	Octenediol - diglucose - xylose	305.15884, 581.24194, 539.23181, 497.22095, 455.13800, 389.17941, 347.16898, 275.07568, 233.13835, 161.04489	-4,05	2
30,08	577,26654	C ₂₇ H ₄₆ O ₁₁ S	SQMGC18:3	299.04263, 225.00653, 277.21597	-3,925	2
17,65	245,09212	C ₁₃ H ₁₄ N ₂ O ₃	Acetyl tryptophan	203.08199, 186.05530, 159.09239, 142.06580, 116.05039	-4,2	2
22,81	597.23712 (M + FA - H) 551.23236	C ₂₅ H ₄₂ O ₁₆	Triacylsucrose (S3:12)	536.29572, 509.22107 , 467.17386 , 311.22119, 425.16483, 407.15314	-4,8	2
22,97	597.23712 (M + FA - H) 551.23236	C ₂₅ H ₄₂ O ₁₆	Triacylsucrose (S3:12)	536.29572, 509.22107 , 467.17386 , 311.22119, 425.16483, 407.15314	-4,8	2
34,28	409,23572	C ₁₉ H ₃₉ O ₇ P	LPA(0:0/16:0)	152.99606, 369.90182, 340.20300, 171.00641	-0,107	2
27,92	653.30243 (M + AF - H) 607.29736 (M-H)	C ₂₈ H ₄₈ O ₁₄	Triacylsucrose (S3:16)	523.23962, 509.22409 , 491.21301, 425.16415, 407.15527, 319.07587, 439.18204, 396.82724, 323.09824	-0,089	2
15,35	321,15442	C ₁₄ H ₂₆ O ₈	Octanoic acid glucoside	303.14401, 159.10231, 141.09180, 119.03476, 101.02428	-3,35	2
28,30	681.29718 (M + FA - H) 635.29163 (M - H)	C ₃₀ H ₄₉ O ₁₇	Tetraacylsucrose (S4:17)	593.28168, 551.23468 , 509.22233 , 471.75043, 399.14078, 491.21207, 467.31448	-0,32	2

28,01	679.28137 (M + FA - H) 633.27594 (M - H)	C ₃₀ H ₄₇ O ₁₇	Tetraacylsucrose (S4:17)	591.26581, 551.23230 , 509.22476 , 415.14536, 397.13455	-0,74	2
28,72	681.29718 (M + AF - H) 635.29163 (M - H)	C ₃₀ H ₅₀ O ₁₇ + CH ₂ O ₂	Tetraacylsucrose (S4:17)	593.28168, 551.23468, 509.22263, 399.14078, 491.21207	-3	2
15,98	353,11301	C ₁₃ H ₂₄ NO ₈ S	Homomethionine + quinic acid	309.12335, 191.05563	-5,5	2
30,42	709,32623	C ₃₁ H ₅₁ O ₁₅ + CH ₂ O ₂	Tetraacylsucrose (S4:19)	621.30927, 579.26245, 523.23724, 537.25281, 505.22699	-4.3	2
29,72	695.31165 (M + FA)	C ₃₀ H ₅₀ O ₁₅ + CH ₂ O ₂	Tetraacylsucrose (S4:18)	607.29517, 565.24805, 523.23773, 467.17517, 509.22223, 491.21164, 407.15445, 551.23254	-3.59	2
30,66	709,3277	C ₃₁ H ₅₁ O ₁₅ + CH ₂ O ₃	Tetraacylsucrose (S4:19)	621.30927, 523.23724, 537.25281, 565.25739, 421.17258	-1.6	2
27,33	721.36536 (M + AF - H) 675,35974 (M-H)	C ₃₃ H ₅₆ O ₁₄	Digalactopyranosyl lineoylglycerol (C18:3)	397,13483	0,016	2
33,01	723,38092	C ₃₃ H ₅₈ O ₁₄ + AF	Triacylsucrose (S3:21)	677.37500, 551.27081, 593.31763, 533.26019	0,33	2
22,47	453,13809	C ₂₁ H ₂₆ O ₁₁	Dihydroferulic acid glucuronide + methylfurane	435.12799, 371.09631, 353.08560, 331.10107, 249.06006	-4,7	2
41,73	787,46674	C ₄₁ H ₇₂ O ₁₂ S	SQDG 16:3 18:0	537.27368, 559.25854	-0,5	2
23,76	1007,46606	C ₄₇ H ₇₆ O ₂₃	Nicotianoside IV	963.47504, 903.45404, 921.46436, 775.40692, 757.39697	-4,36	2
26,98	1059.53882 (M + FA - H) 1013.53107 (M - H)	C ₅₁ H ₈₂ O ₂₀	Diosgenin tetraglicoside	868.47736, 722.41968, 576.35822	-0,866	2

19,51	1074.54419 (M - H + FA) 1028.53674 (M - H)	C ₅₁ H ₈₃ NO ₂₀	Solanidine tetraglycoside		-6,6	3
20,40	1119.63293 (M + FA - H)	C ₅₁ H ₉₅ NO ₂₂	Glykoalkaloid		-7,8	3
17,37	675.26807 (M + FA - H) 629.26263 (M - H)	C ₂₆ H ₄₅ O ₁₇	Sucrose + hexose octanoate	611.25220, 551.23083, 467.21072, 341.10675, 323.09659	-5,7	2
1,67	116.0709 (M + H)	C ₅ H ₉ NO ₂	Proline		-2.58	2
1,54	175.1192 (M + H)	C ₆ H ₁₄ N ₄ O ₂	Arginine	116.0706, 130.0961	1,71	2
1,7	132.1015 (M + H)	C ₆ H ₁₃ NO ₂	Leucine +Isoleucine	86.0967	3,02	2
1,7	166.0857 (M + H)	C ₉ H ₁₁ NO ₂	Phenylalanine	120.0804	3,34	2
1,65	182.0807 (M + H)	C ₉ H ₁₁ NO ₃	Tyrosine	165.0548, 136.0750	2,19	2
2,05	174.0527 (M-H)	C ₁₀ H ₉ NO ₂	3-Indole acetic acid	130.0639, 128.0485	1,14	2
14,28	265,14344 (M + H)	C ₁₅ H ₂₀ O ₄	Abscisic acid	247.1290, 187.1115	3.449	2