

Table S1

ID	Species	Putative identification	Retention time (min)	Elemental formula	experimental m/z (-)	ESI (-) main adduct	experimental m/z (+)	ESI (+) main adduct	mass error (-). (ppm)	Fragments (-)
1	<i>A. lusitanicum</i>	Sinapic acid derivative	4.60	C <sub>19</sub> H <sub>34</sub> O <sub>9</sub>	451.216	[M+HCOOH-H] <sup>+</sup>	429.207	[M+Na] <sup>+</sup>	3.882	De Sorricellis et al., 2024
2	<i>A. lusitanicum</i>	Benzylalcohol O-(O-pentosyl-hexoside)	5.08	C <sub>18</sub> H <sub>26</sub> O <sub>10</sub>	447.149	[M+HCOOH-H] <sup>+</sup>	425.14	[M+Na] <sup>+</sup>	1.208	De Sorricellis et al., 2024
3	<i>A. lusitanicum</i>	Sinapic acid hexose	5.16	C <sub>17</sub> H <sub>22</sub> O <sub>10</sub>	431.192	[M+HCOOH-H] <sup>+</sup>	409.182	[M+Na] <sup>+</sup>	- 171.64 7	De Sorricellis et al., 2024
4	<i>A. lusitanicum</i>	Sinapic acid hexoside	5.35	C <sub>17</sub> H <sub>22</sub> O <sub>10</sub>	385.112	[M-H] <sup>+</sup>	409.107	[M+Na] <sup>+</sup>	1.465	De Sorricellis et al., 2024
5	<i>A. lusitanicum</i>	UI	5.38	-	433.206	[M-H] <sup>+</sup>	411.19	[M+Na] <sup>+</sup>	-	De Sorricellis et al., 2024
6	<i>A. lusitanicum</i>	UI	5.58	-	433.207	[M+HCOOH-H] <sup>+</sup>	411.199	[M+Na] <sup>+</sup>	-	De Sorricellis et al., 2024
7	<i>A. lusitanicum</i>	Kaempferol-O-(O-hexosyl-hexosyl-desoxyhexoside)	5.74	C <sub>33</sub> H <sub>40</sub> O <sub>20</sub>	755.203	[M-H] <sup>+</sup>	757.218	[M+H] <sup>+</sup>	-0.581	De Sorricellis et al., 2024
8	<i>A. lusitanicum</i>	Phenylethyl primeveroside	5.96	C <sub>19</sub> H <sub>28</sub> O <sub>10</sub>	461.165	[M+HCOOH-H] <sup>+</sup>	439.154	[M+Na] <sup>+</sup>	-0.646	De Sorricellis et al., 2024
9	<i>A. lusitanicum</i>	Kaempferol-O-desoxyhexoside derivative	6.28	-	729.189	[M-H] <sup>+</sup>	-	-	-	De Sorricellis et al., 2024
10	<i>A. lusitanicum</i>	UI	6.39	-	551.270	[M+HCOOH-H] <sup>+</sup>	529.263	[M+Na] <sup>+</sup>	-	De Sorricellis et al., 2024
11	<i>A. lusitanicum</i>	UI	6.65	-	553.289	[M+HCOOH-H] <sup>+</sup>	531.279	[M+Na] <sup>+</sup>	-	De Sorricellis et al., 2024
12	<i>A. lusitanicum</i>	UI	6.73	-	553.286	[M+HCOOH-H] <sup>+</sup>	531.279	[M+Na] <sup>+</sup>	-	De Sorricellis et al., 2024
13	<i>A. lusitanicum</i>	Saponin class IV4 + 2 hexoses + 1 desoxyhexose	7.06	C <sub>45</sub> H <sub>74</sub> O <sub>19</sub>	963.483	[M+HCOOH-H] <sup>+</sup>	941.47	[M+Na] <sup>+</sup>	-3.114	De Sorricellis et al., 2024
14	<i>A. lusitanicum</i>	Saponin class IV4 + 2 hexoses + 1 desoxyhexose	7.13	C <sub>45</sub> H <sub>74</sub> O <sub>19</sub>	963.481	[M+HCOOH-H] <sup>+</sup>	941.47	[M+Na] <sup>+</sup>	-1.451	De Sorricellis et al., 2024

15	<i>A. lusitanicum</i>	Saponin class V3 + 3 hexoses + 3 desoxyhexoses	7.42	C <sub>62</sub> H <sub>102</sub> O <sub>32</sub>	678.325	[2M-H] <sup>+</sup>	1381.656	[M+Na] <sup>+</sup>	-23.588	De Sorricellis et al., 2024
16	<i>A. lusitanicum</i>	Saponin class IV4 + 2 hexoses + 1 desoxyhexose + acetyl group	7.60	C <sub>47</sub> H <sub>76</sub> O <sub>20</sub>	1005.492	[M+HCOOH-H] <sup>+</sup>	983.483	[M+Na] <sup>+</sup>	-1.989	De Sorricellis et al., 2024
17	<i>A. lusitanicum</i>	Saponin class IV4 + 2 hexoses + 1 desoxyhexose	7.65	C <sub>47</sub> H <sub>76</sub> O <sub>20</sub>	1005.492	[M+HCOOH-H] <sup>+</sup>	983.483	[M+Na] <sup>+</sup>	-1.989	De Sorricellis et al., 2024
18	<i>A. lusitanicum</i>	UI saponin	8.33	-	1241.580	[M+HCOOH-H] <sup>+</sup>	1219.561	[M+Na] <sup>+</sup>	-	De Sorricellis et al., 2024
19	<i>A. lusitanicum</i>	Saponin class IV3 + 2 hexoses + 2 desoxyhexoses + 1 pentose	8.44	C <sub>56</sub> H <sub>92</sub> O <sub>26</sub>	1225.592	[M+HCOOH-H] <sup>+</sup>	1203.575	[M+Na] <sup>+</sup>	-7.343	De Sorricellis et al., 2024
20	<i>A. lusitanicum</i>	Saponin class IV3 + 2 hexoses + 2 desoxyhexoses	8.46	C <sub>51</sub> H <sub>84</sub> O <sub>22</sub>	1093.545	[M+HCOOH-H] <sup>+</sup>	1071.536	[M+Na] <sup>+</sup>	-1.554	De Sorricellis et al., 2024
21	<i>A. lusitanicum</i>	Saponin class IV3 + 2 hexoses + 3 desoxyhexoses	8.52	C <sub>57</sub> H <sub>94</sub> O <sub>26</sub>	1193.598	[M-H] <sup>+</sup>	1217.597	[M+Na] <sup>+</sup>	-2.513	De Sorricellis et al., 2024
22	<i>A. lusitanicum</i>	Saponin class IV3 + 2 hexoses + 1 desoxyhexose + 1 pentose	8.55	C <sub>50</sub> H <sub>82</sub> O <sub>22</sub>	1079.531	[M+HCOOH-H] <sup>+</sup>	1057.522	[M+Na] <sup>+</sup>	-3.705	De Sorricellis et al., 2024
23	<i>A. lusitanicum</i>	Saponin class IV3 + 2 hexoses + 1 desoxyhexoses	8.65	C <sub>45</sub> H <sub>74</sub> O <sub>18</sub>	947.487	[M+HCOOH-H] <sup>+</sup>	925.479	[M+Na] <sup>+</sup>	-1.785	De Sorricellis et al., 2024
24	<i>A. lusitanicum</i>	Saponin class III3 + 1 pentose + 1 hexose + 3 desoxyhexoses	8.76	C <sub>56</sub> H <sub>90</sub> O <sub>25</sub>	1207.573	[M+HCOOH-H] <sup>+</sup>	1185.564	[M+Na] <sup>+</sup>	0.816	De Sorricellis et al., 2024
25	<i>A. lusitanicum</i>	Saponin class IV3 + 2 hexoses + 3 desoxyhexoses + acetyl group	9.41	C <sub>59</sub> H <sub>96</sub> O <sub>27</sub>	1281.611	[M+HCOOH-H] <sup>+</sup>	1259.59	[M+Na] <sup>+</sup>	-0.039	De Sorricellis et al., 2024
26	<i>S. pratensis</i>	Protocatechuic acid 4-O-β-hexoside	3.41	C <sub>13</sub> H <sub>16</sub> O <sub>9</sub>	315.0716	[M-H] <sup>+</sup>	339.1044	[M+Na] <sup>+</sup>	0.00	152.0115; 108.0222
27	<i>S. pratensis</i>	UI	3.69		435.1145	[M+HCOOH-H] <sup>+</sup>	413.1060	[M+Na] <sup>+</sup>	-	389.1100; 227.0574; 209.0459; 165.0558; 141.0191
28	<i>S. pratensis</i>	Neochlorogenic acid	3.96	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub>	353.0877	[M-H] <sup>+</sup>	377.0838	[M+Na] <sup>+</sup>	-1.13	191.0566; 179.0365; 135.0465
29	<i>S. pratensis</i>	Esculetin	4.20	C <sub>15</sub> H <sub>16</sub> O <sub>9</sub>	339.0719	[M-H] <sup>+</sup>	341.0855	[M+H] <sup>+</sup>	-0.88	177.0185; 133.0301
30	<i>S. pratensis</i>	Eucommicin A	4.22	C <sub>32</sub> H <sub>36</sub> O <sub>18</sub>	707.1833	[M-H] <sup>+</sup>	731.1789	[M+Na] <sup>+</sup>	-1.41	191.06
31	<i>S. pratensis</i>	8-epiLoganic acid	4.28	C <sub>16</sub> H <sub>24</sub> O <sub>10</sub>	375.1291	[M-H] <sup>+</sup>	399.1259	[M+Na] <sup>+</sup>	1.87	213.0777; 169.0873; 151.0768; 125.0611; 113.0245

32	<i>S. pratensis</i>	Chlorogenic acid	4.63	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub>	353.0887	[M-H] <sup>-</sup>	377.0834	[M+Na] <sup>+</sup>	-3.97	191.06
33	<i>S. pratensis</i>	Oleoside	4.74	C <sub>16</sub> H <sub>22</sub> O <sub>11</sub>	389.1089	[M-H] <sup>-</sup>	-	-	-1.28	345.1196; 209.0459; 183.0653; 165.0558; 121.0653
34	<i>S. pratensis</i>	Caffeoyl quinic acid isomer	4.80	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub>	353.0875	[M-H] <sup>-</sup>	377.0836	[M+Na] <sup>+</sup>	-0.57	191.0566; 179.0338; 173.0463; 135.0441
35	<i>S. pratensis</i>	Swertiamarin	4.90	C <sub>16</sub> H <sub>22</sub> O <sub>10</sub>	419.1187	[M+HCOOH-H] <sup>-</sup>	397.1110	[M+Na] <sup>+</sup>	0.72	373.1129; 355.1029; 193.0505; 179.0557; 161.0469; 149.0610; 141.0191; 119.0359; 113.0245; 101.0241; 89.0237
36	<i>S. pratensis</i>	Luteolin-C-hexosyl-O-hexoside	5.12	C <sub>27</sub> H <sub>30</sub> O <sub>16</sub>	609.1457	[M-H] <sup>-</sup>	611.1613	[M+H] <sup>+</sup>	-0.16	447.0943; 357.0610; 313.0364; 299.0557; 285.0418
37	<i>S. pratensis</i>	Gentiopicroside	5.32	C <sub>16</sub> H <sub>20</sub> O <sub>9</sub>	401.1083	[M+HCOOH-H] <sup>-</sup>	379.1000	[M+Na] <sup>+</sup>	0.25	355.1029; 193.0505; 179.0557; 161.0469; 149.0610; 119.0359; 101.0241; 89.0237
38	<i>S. pratensis</i>	Sweroside	5.41	C <sub>16</sub> H <sub>22</sub> O <sub>9</sub>	403.1238	[M+HCOOH-H] <sup>-</sup>	381.1157	[M+Na] <sup>+</sup>	0.50	357.1190; 195.0662; 179.0557; 161.0469; 151.0768; 125.0245; 119.0359; 113.0245
39	<i>S. pratensis</i>	Apigenin-C-hexosyl-O-hexoside	5.58	C <sub>27</sub> H <sub>30</sub> O <sub>15</sub>	593.1515	[M-H] <sup>-</sup>	595.1666	[M+H] <sup>+</sup>	-1.52	431.0982; 311.0552; 297.0417; 283.0619; 269.0463
40	<i>S. pratensis</i>	Luteolin-C-hexosyl-O-(caffeoyl)hexoside	5.74	C <sub>36</sub> H <sub>36</sub> O <sub>19</sub>	771.1782	[M-H] <sup>-</sup>	773.1932	[M+H] <sup>+</sup>	-1.17	447.0943; 357.0610; 327.0514; 299.0557; 285.0418; 179.0392; 161.0235
41	<i>S. pratensis</i>	Apigenin-C-hexosyl-O-(caffeoyl)hexoside	6.13	C <sub>36</sub> H <sub>36</sub> O <sub>18</sub>	755.1823	[M-H] <sup>-</sup>	757.1973	[M+H] <sup>+</sup>	1.06	431.0982; 341.0671; 311.0552; 283.0619; 179.0392; 161.0235
42	<i>S. pratensis</i>	Dicaffeoyl quinic acid	6.96	C <sub>25</sub> H <sub>24</sub> O <sub>12</sub>	515.1199	[M-H] <sup>-</sup>	-	-	-1.75	353.0887; 191.0566; 179.0463
43	<i>S. pratensis</i>	Dicaffeoyl quinic acid	7.24	C <sub>25</sub> H <sub>24</sub> O <sub>12</sub>	515.1188	[M-H] <sup>-</sup>	-	-	0.39	353.0887; 191.0566; 179.0365; 173.0463; 135.0465
44	<i>S. pratensis</i>	Akebia saponin D or Palustroside III	8.81	C <sub>47</sub> H <sub>76</sub> O <sub>18</sub>	973.4997	[M+HCOOH-H] <sup>-</sup>	951.4901	[M+Na] <sup>+</sup> <sub>+</sub>	1.13	927.5005; 603.3918; 573.3791; 323.0957; 179.0557
45	<i>S. pratensis</i>	Akebia saponin D or Palustroside III isomer	9.53	C <sub>47</sub> H <sub>76</sub> O <sub>18</sub>	927.4968	[M-H] <sup>-</sup>	951.4901	[M+Na] <sup>+</sup> <sub>+</sub>	-1.62	603.3918; 323.0957; 179.0611
46	<i>S. pratensis</i>	4'-O-Acetyl-akebia saponin D or acetyl-palustroside III	9.97	C <sub>49</sub> H <sub>78</sub> O <sub>19</sub>	1015.5114	[M+HCOOH-H] <sup>-</sup>	993.5025	[M+Na] <sup>+</sup>	2.07	969.5089; 645.4037; 627.3903; 323.0994
47	<i>D. superbus</i>	UI	2.58		349.0769	[M+HCOOH-H] <sup>-</sup>	327.0689	[M+Na] <sup>+</sup>	-	303.072; 141.0206; 111.0095

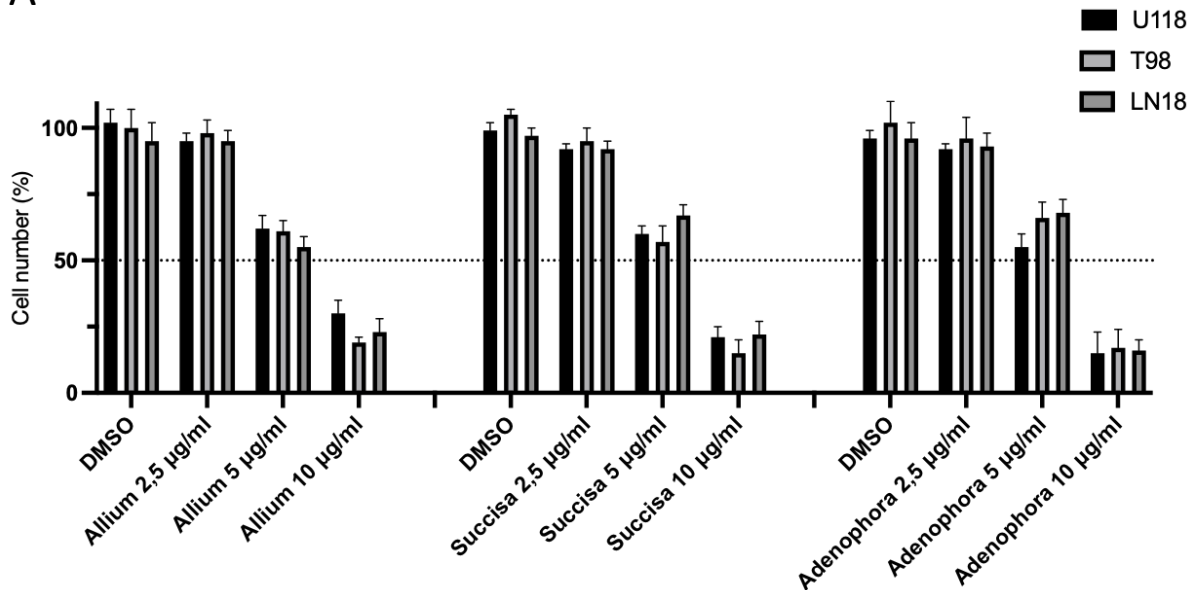
48	<i>D. superbus</i>	UI	2.90		309.1195	[M+HCOOH-H] <sup>+</sup>	287.1102	[M+Na] <sup>+</sup>	-	174.9536; 146.9610
49	<i>D. superbus</i>	UI	3.57		291.1080	[M-H] <sup>+</sup>	315.1053	[M+Na] <sup>+</sup>	-	161.0457; 113.0240; 101.0217
50	<i>D. superbus</i>	UI	3.49		499.1656	[M+HCOOH-H] <sup>+</sup>	477.1580	[M+Na] <sup>+</sup>	-	453.1626; 263.0778; 221.0660; 179.0569; 161.0457; 143.0352
51	<i>D. superbus</i>	UI	3.60		337.1133	[M+HCOOH-H] <sup>+</sup>	315.1049	[M+Na] <sup>+</sup>	-	291.1070; 161.8907; 243.8793; 225.8662; 207.8649; 189.0770; 161.0431; 101.0237
52	<i>D. superbus</i>	UI	3.95		453.1605	[M-H] <sup>+</sup>	477.1578	[M+Na] <sup>+</sup>	-	291.1070; 189.0770; 179.0569; 161.0431; 143.0328; 119.0353; 113.0240; 101.0237; 89.0255
53	<i>D. superbus</i>	UI	4.44		447.1863	[M+HCOOH-H] <sup>+</sup>	425.1777	[M+Na] <sup>+</sup>	-	401.1791; 249.0975; 239.1277; 221.1178; 153.0923
54	<i>D. superbus</i>	Tetrahydroxy-flavone-C-hexoside-O-hexoside (luteolin)	5.13	C <sub>27</sub> H <sub>30</sub> O <sub>16</sub>	609.1469	[M-H] <sup>+</sup>	611.1613	[M+H] <sup>+</sup>	-2.13	447.0967; 357.0603; 327.0511; 313.0363; 299.0557; 285.0420
55	<i>D. superbus</i>	Tetrahydroxy-flavone-C-(deoxyhexosyl)hexoside-O-hexoside (luteolin)	5.13	C <sub>33</sub> H <sub>40</sub> O <sub>20</sub>	801.2114	[M+HCOOH-H] <sup>+</sup>	757.2191	[M+H] <sup>+</sup>	-3.12	593.1556; 473.1092; 429.0804; 369.0630; 357.0641; 339.0550; 327.0511; 309.0406; 298.0479; 285.0420
56	<i>D. superbus</i>	Trihydroxy-flavone-C-(deoxyhexosyl)hexoside-O-hexoside (apigenin)	5.57	C <sub>33</sub> H <sub>40</sub> O <sub>19</sub>	739.2106	[M-H] <sup>+</sup>	741.2238	[M+H] <sup>+</sup>	-2.71	577.1600; 413.0885; 293.0447
57	<i>D. superbus</i>	Trihydroxy-flavone derivative (apigenin)	5.78	C <sub>28</sub> H <sub>32</sub> O <sub>16</sub>	623.1624	[M-H] <sup>+</sup>	647.1552	[M+Na] <sup>+</sup>	-1.93	461.1047; 445.0737; 341.0628; 327.0511; 298.0479; 269.0466
58	<i>D. superbus</i>	Tetrahydroxy-flavone derivative (luteolin)	5.86	C <sub>41</sub> H <sub>46</sub> O <sub>23</sub>	905.2353	[M-H] <sup>+</sup>	907.2501	[M+H] <sup>+</sup>	-0.11	593.1508; 473.1069; 429.0814; 357.0590; 339.0481; 327.0497; 309.0396; 285.0380
59	<i>D. superbus</i>	Tetrahydroxy-flavone derivative (luteolin)	6.25	C <sub>43</sub> H <sub>48</sub> O <sub>23</sub>	931.2508	[M-H] <sup>+</sup>	933.2654	[M+H] <sup>+</sup>	0.00	593.1508; 473.1069; 429.0814; 357.0590; 339.0481; 327.0497; 309.0396; 285.0380
60	<i>D. superbus</i>	UI	6.40		565.1918	[M+HCOOH-H] <sup>+</sup>	543.1840	[M+Na] <sup>+</sup>	-	339.1266; 327.1214
61	<i>D. superbus</i>	UI	6.59		1195.5383	[M+HCOOH-H] <sup>+</sup>	1173.5278	[M+Na] <sup>+</sup>	-	1149.537; 969.473; 663.277; 485.146; 439.321
62	<i>D. superbus</i>	Akebonoic acid + 2 hexose derivative	6.61	C <sub>47</sub> H <sub>74</sub> O <sub>19</sub>	987.4818	[M-H] <sup>+</sup>	1011.4756	[M+Na] <sup>+</sup>	-1.76	663.3770; 439.3196

63	<i>D. superbus</i>	Tetrahydroxy-flavone derivative (luteolin)	6.94	C <sub>41</sub> H <sub>46</sub> O <sub>23</sub>	951.2431	[M+HCOOH-H] <sup>+</sup>	907.2502	[M+H] <sup>+</sup>	-2.62	905.2375; 743.1837; 579.1136; 473.1048; 441.0736; 357.0641; 327.0511; 309.0406; 298.0514; 285.0420
64	<i>D. superbus</i>	Tetrahydroxy-flavone derivative (luteolin)	7.55	C <sub>44</sub> H <sub>52</sub> O <sub>25</sub>	979.2747	[M+HCOOH-H] <sup>+</sup>	935.2810	[M+H] <sup>+</sup>	-2.83	933.2717; 771.2173; 607.1489; 575.1409; 473.1092; 411.0694; 357.0603; 327.0511; 309.0406; 298.0443; 285.0385
65	<i>D. superbus</i>	Tetrahydroxy-flavone-C-deoxyhexose-O-hexoside derivative (luteolin)	7.58	C <sub>43</sub> H <sub>50</sub> O <sub>23</sub>	979.2736	[M+HCOOH-H] <sup>+</sup>	935.2813	[M+H] <sup>+</sup>	-1.74	933.2717; 771.2173; 607.1489; 575.1409; 473.1092; 411.0694; 369.0591; 357.0603; 339.0512; 327.0511; 309.0406; 298.0443; 285.0385
66	<i>D. superbus</i>	Tetrahydroxyflavone-C-(feruloyl+deoxyhexosyl)hexoside-O-hexoside	7.65	C <sub>43</sub> H <sub>48</sub> O <sub>23</sub>	931.2538	[M-H] <sup>+</sup>	933.2620	[M+H] <sup>+</sup>	0.59	298.0443; 285.0316; 193.0516; 309.0406; 473.1092; 575.1409; 593.151; 605.133; 769.201; 931.253
67	<i>D. superbus</i>	Trihydroxy-flavone derivative (apigenin)	7.95	C <sub>43</sub> H <sub>50</sub> O <sub>22</sub>	963.2808	[M+HCOOH-H] <sup>+</sup>	919.2868	[M+H] <sup>+</sup>	-3.94	917.2724; 755.2221; 591.1535; 559.1449; 457.1141; 395.072; 293.0447; 269.0433; 195.0645
68	<i>D. superbus</i>	Gypsogenic acid + 5 hexose	8.22	C <sub>60</sub> H <sub>96</sub> O <sub>30</sub>	1295.5931	[M-H] <sup>+</sup>	1319.5860	[M+Na] <sup>+</sup>	-1.81	1115.5347; 647.3813; 485.1463; 467.1407; 423.3257; 383.1207; 221.0691; 179.0569; 161.0431
69	<i>D. superbus</i>	Tetrahydroxy-flavone derivative (luteolin)	8.49	C <sub>53</sub> H <sub>60</sub> O <sub>26</sub>	1111.3313	[M-H] <sup>+</sup>	1113.3430	[M+H] <sup>+</sup>	-1.63	771.2173; 607.1489; 575.1458; 473.1092; 411.0694; 357.0680; 327.0511; 309.0406; 298.0479; 285.0479
70	<i>D. superbus</i>	Gypsogenic acid + 5 hexose	8.64	C <sub>60</sub> H <sub>96</sub> O <sub>30</sub>	1295.5927	[M-H] <sup>+</sup>	1319.5790	[M+Na] <sup>+</sup>	-1.45	1115.5415; 647.3813; 485.1463; 467.1452; 423.3257; 383.1167; 221.0630; 179.0542
71	<i>D. superbus</i>	Gypsogenic acid + 4 hexoses	8.80	C <sub>54</sub> H <sub>86</sub> O <sub>25</sub>	1179.5459	[M+HCOOH-H] <sup>+</sup>	1157.5350	[M+Na] <sup>+</sup>	-2.00	1133.5435; 971.4943; 953.4749; 647.3813; 485.1508; 423.3300
72	<i>D. superbus</i>	Gypsogenic acid + 3 hexoses	8.95	C <sub>48</sub> H <sub>76</sub> O <sub>20</sub>	971.4882	[M-H] <sup>+</sup>	995.4840	[M+Na] <sup>+</sup>	-3.11	647.3813; 423.3257
73	<i>D. superbus</i>	Gypsogenic acid + 3 hexoses + 1 pentose	9.26	C <sub>53</sub> H <sub>84</sub> O <sub>24</sub>	1149.5324	[M+HCOOH-H] <sup>+</sup>	1127.5220	[M+Na] <sup>+</sup>	3.49	1103.5295; 923.4627; 701.3907; 617.3733; 503.3363; 423.3300; 305.0849
74	<i>D. superbus</i>	Polygalacic acid + 3 hexoses	9.52	C <sub>48</sub> H <sub>78</sub> O <sub>21</sub>	989.4984	[M-H] <sup>+</sup>	1013.4920	[M+Na] <sup>+</sup>	-2.73	503.336; 485.3312; 457.3329; 441.3381

75	<i>D. superbus</i>	Gypsogenic acid hexose derivative	9.63	C <sub>48</sub> H <sub>77</sub> O <sub>20</sub>	1039.4749	[M+HCOOH-H <sup>+</sup> ] <sup>-</sup>	995.4770	[M+H <sup>+</sup> ] <sup>+</sup>	0.10	993.4719; 971.4943; 729.3781; 507.3112; 485.1508; 323.0954; 179.0542
76	<i>D. superbus</i>	Gypsogenic acid + 3 hexoses	9.64	C <sub>48</sub> H <sub>76</sub> O <sub>20</sub>	971.4881	[M-H <sup>+</sup> ] <sup>-</sup>	995.4811	[M+H <sup>+</sup> ] <sup>+</sup>	-2.99	485.33
77	<i>D. superbus</i>	Polygalacic acid + 2 hexoses	9.79	C <sub>42</sub> H <sub>68</sub> O <sub>16</sub>	827.4449	[M-H <sup>+</sup> ] <sup>-</sup>	851.4390	[M+Na <sup>+</sup> ] <sup>+</sup>	-2.42	503.3363; 485.3267; 457.3373; 441.3381
78	<i>D. superbus</i>	Gypsogenic acid + 2 hexoses	9.96	C <sub>42</sub> H <sub>66</sub> O <sub>15</sub>	809.4349	[M-H <sup>+</sup> ] <sup>-</sup>	833.4270	[M+Na <sup>+</sup> ] <sup>+</sup>	-3.21	485.33
79	<i>D. superbus</i>	Gypsogenic acid derivative	10.31	C <sub>48</sub> H <sub>76</sub> O <sub>20</sub>	1017.4923	[M+HCOOH-H <sup>+</sup> ] <sup>-</sup>	995.4770	[M+Na <sup>+</sup> ] <sup>+</sup>	-1.69	971.4879; 791.4225; 569.3491; 485.3267; 305.0884; 179.0569
80	<i>D. superbus</i>	UI	11.43		1699.7247	[M-H <sup>+</sup> ] <sup>-</sup>	1723.7180	[M+Na <sup>+</sup> ] <sup>+</sup>	-	955.46

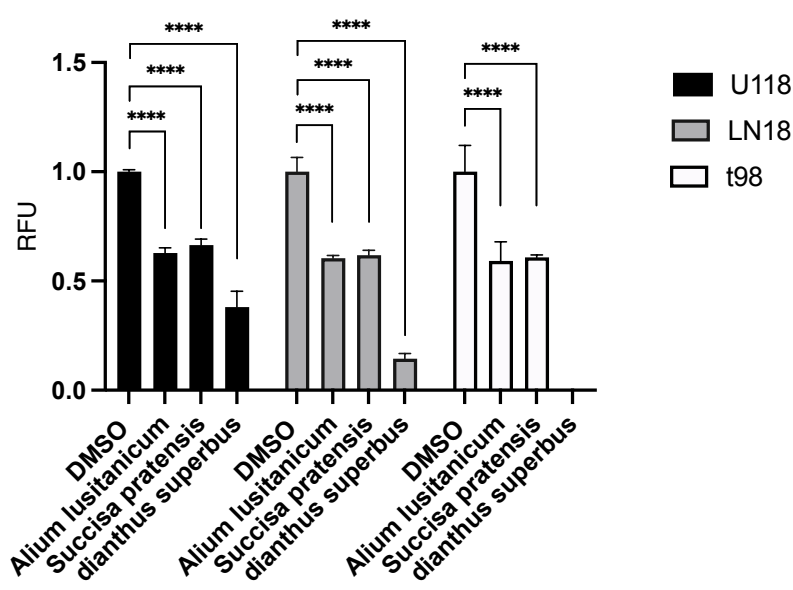
Figure S1

A

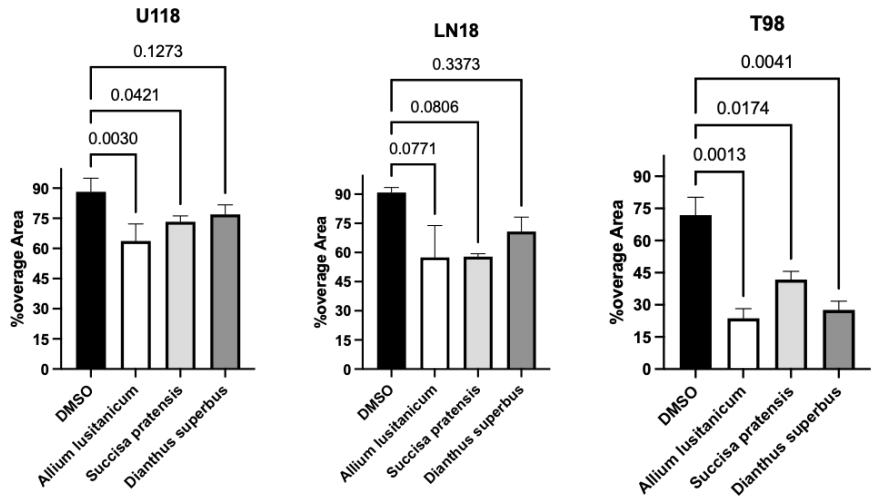
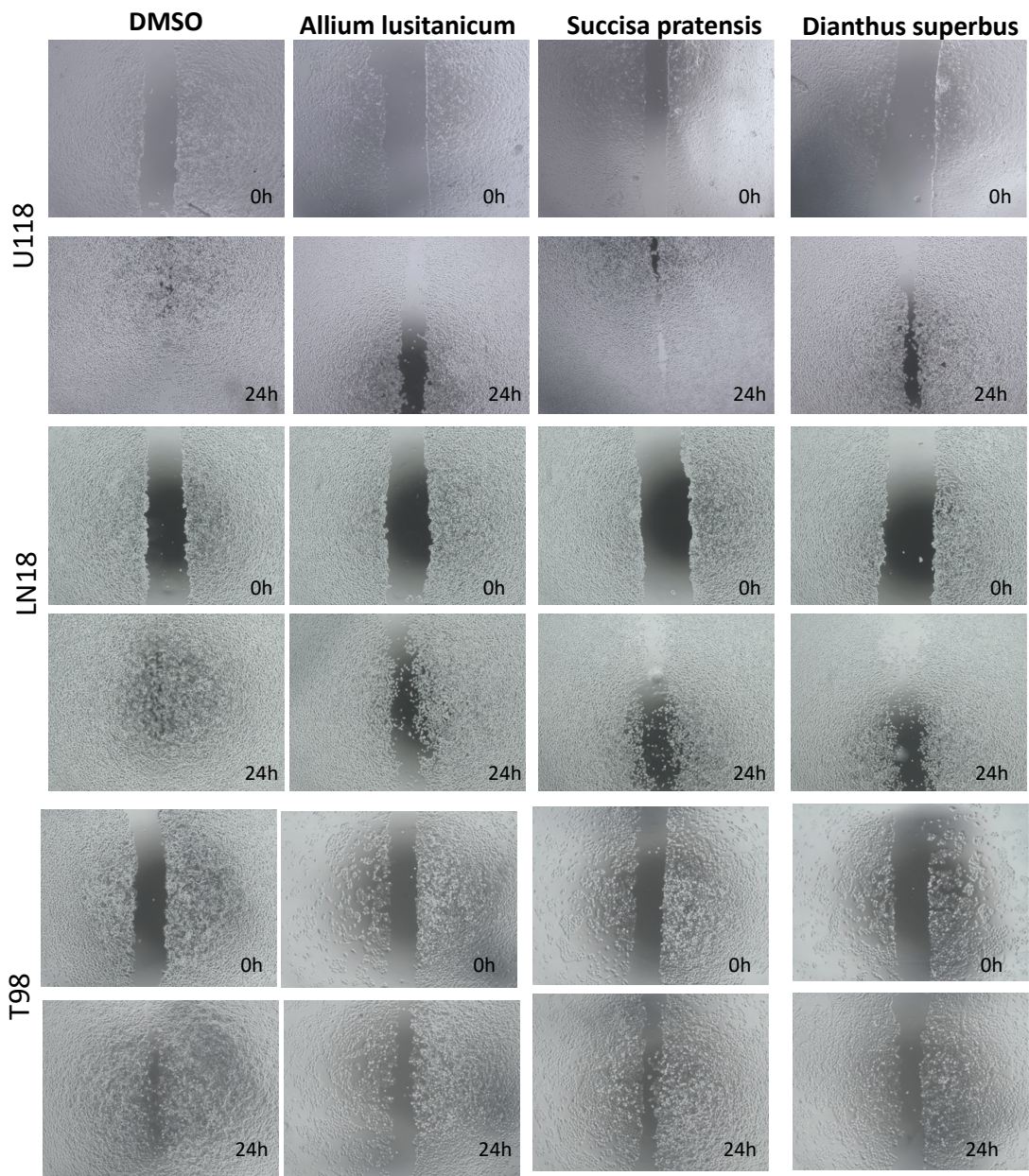


B

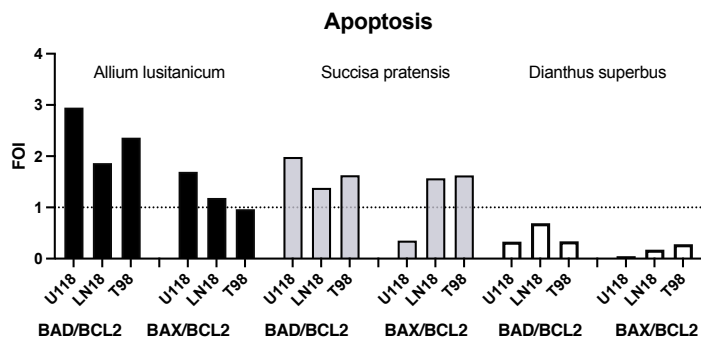
Cell proliferation



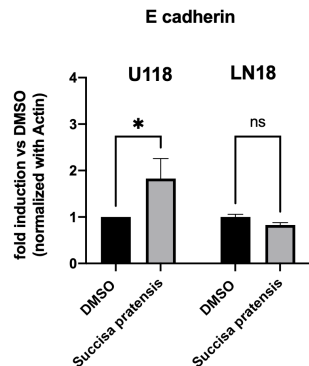
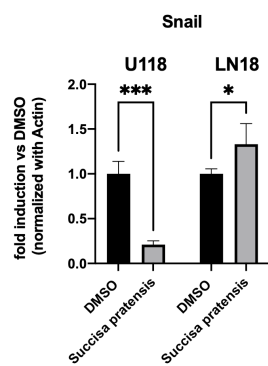
C



D



E



F

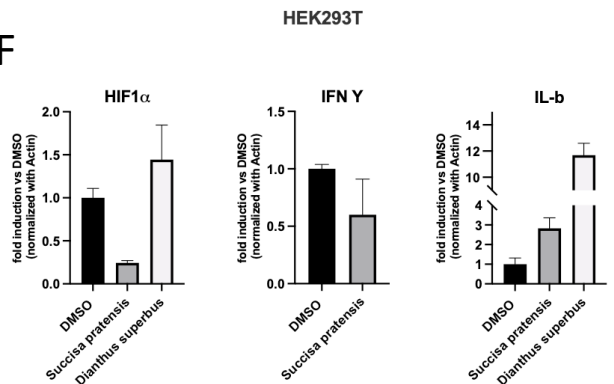
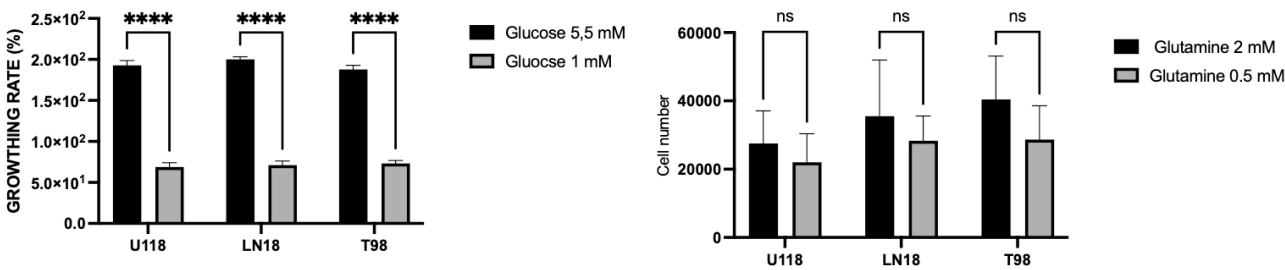


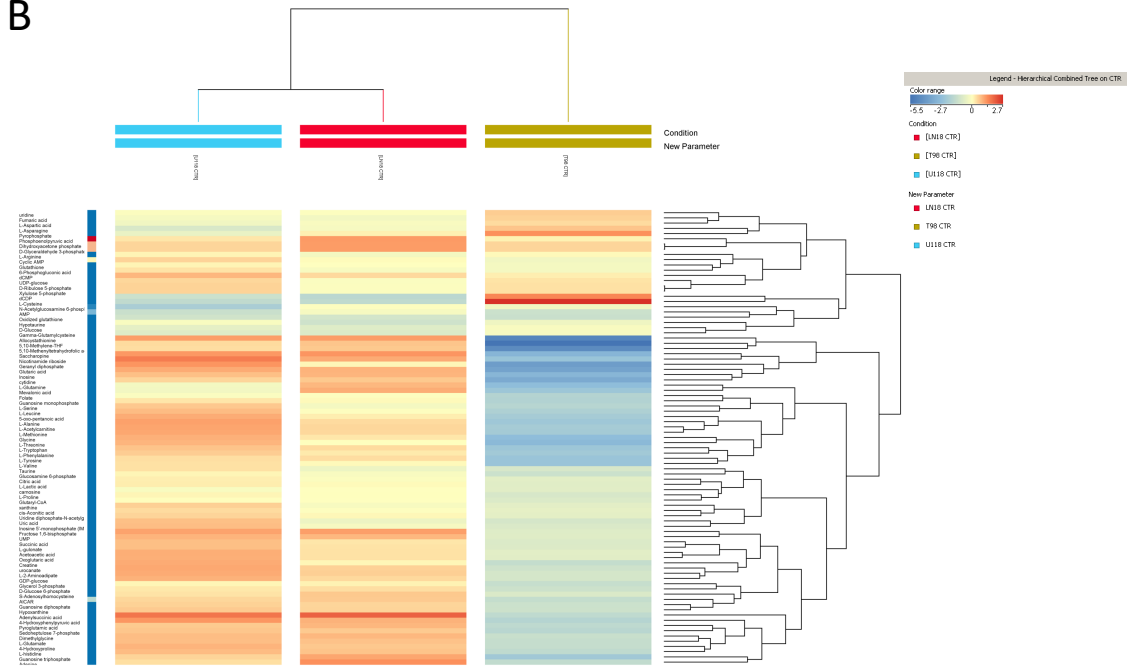


Figure S2

A



B



## SUPPLEMENTARY TABLES

**Supplementary Table S2. List of primers used for qPCR.**

Gene	Primer sequence Fw	Primer sequence Rw
$\beta$ -actin	CACCATTGGCAATGAGCGGTTC	AGGTCTTTGCGGATGTCCACG
HIF-1 $\alpha$	TGATTGCATCTCCATCTCCTACC	GACTCAAAGCGACAGATAACACG
IFN $\gamma$	GAGTGTGGAGACCATCAAGGAAG	TGCTTTGCGTTGGACATTCAAGTC
IL-18	GATAGCCAGCCTAGAGGTATGG	CCTTGATGTTATCAGGAGGATTCA
IL-1b	CCACAGACCTTCCAGGAGAATG	GTGCAGTTCAGTGATCGTACAGG
NFkB	GCAGCACTACTTCTTGACCACC	TCTGCTCCTGAGCATTGACGTC
E-CAD	GCTGAGCTGGACAGGGAGGA	ATGGGGGCGTTGTCATTAC
NRF2	CAGCGACGGAAAGAGTATGA	TGGGCAACCTGGGAGTAG
KEAP1	TTCTGGGGATCCATG	CTCCAAGGACGTAGATTCTC
GPX4	CGCAACGATGTTGCCTGGAAC TTT	AGGCTCGATGTCAATGGTCTGGAA
BAD	CCAACCTCTGGGCAGCACAGC	TTTGCCGCATCTGCGTTGCTGT
BAX	TCAGGATGCGTCCACCAAGAAG	TGTGTCCACGGCGGCAATCATC
BCL-2	ATCGCCCTGTGGATGACTGAGT	GCCAGGAGAAATCAAACAGAGGC
SOD-1	CTCACTCTCAGGAGACCATTGC	CCACAAGCCAAACGACTTCCAG
SOD-2	CTGGACAAACCTCAGCCCTAAC	AACCTGAGCCTTGGACACCAAC
Catalase	GTGCGGAGATTCAAACTGCCA	CGGCAATGTTCTCACACAGACG
SNAIL	GAAAGGCCTTCAACTGCAAA	TGACATCTGAGTGGGTCTGG