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Phenolics profile and antioxidant activities of in vitro propagules and field-raised plant organs of *Curculigo latifolia*

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Supplementary Material

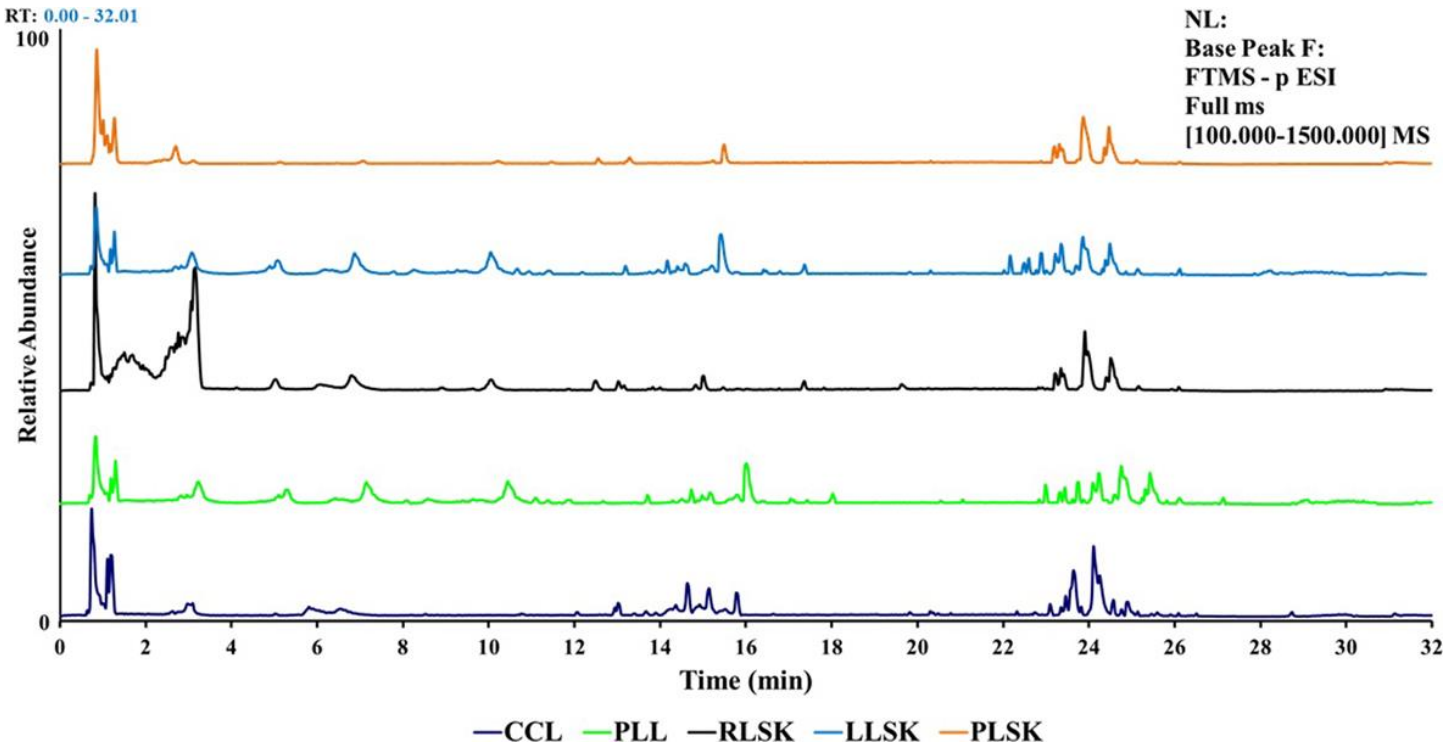

Figure S1. UHPLC-Q-Orbitrap HRMS chromatogram of 70% ethanol extract from callus of *C. latifolia* (CCL), plantlet leaf of *C. latifolia* (PLL), rhizome of *C. latifolia* originated from Sinjai-Puncak (RLSK), leaf of *C. latifolia* originated from Sinjai-Puncak (LLSK), and petiole of *C. latifolia* originated from Sinjai-Puncak (PLSK) of *C. latifolia*.

Table S1. Compounds identified in 70% ethanol extract from callus of *C. latifolia* (CCL), plantlet leaf of *C. latifolia* (PLL), rhizome of *C. latifolia* originated from Sinjai-Puncak (RLSK), leaf of *C. latifolia* originated from Sinjai-Puncak (LLSK), and petiole of *C. latifolia* originated from Sinjai-Puncak (PLSK) of *C. latifolia*.

CCL

No.	RT[min]	Adduct ion	Formula	Tentative identification	Expected *m/z*	Experimental *m/z*	Accuracy (ppm)	Fragment MS and MS/MS	Chemical type
1	0.87	$[M - H]^-$	$C_{23}H_{26}O_{10}$	Orchioside B	461.153	461.157	-8.674	443.134; 433.150; 371.113	Phenolic glycosides
2	0.90	$[M - H]^-$	$C_{17}H_{14}O_5$	1,1-bis(3,4-dihydroxyphenyl)-1-(2-furan)-methane	297.084	297.082	6.732	281.045; 269.081	Phenolic
3	1.33	$[M + H]^+$	$C_8H_8O_3$	Vanillin	153.047	153.047	0.000	150.981; 137.018; 136.015; 129.113	Phenolic
4	2.33	$[M + H]^+$	$C_{23}H_{24}O_{11}$	Crassifoside I	477.132	477.137	-10.479	457.114; 445.114; 387.108	Phenolic
5	3.29	$[M - H]^-$	$C_{13}H_{18}O_7$	Orcinol glucoside	285.105	285.105	0.000	285.105	Phenolic glycosides
6	7.49	$[M + H]^+$	$C_{23}H_{26}O_{11}$	Nyasicoside	479.148	479.152	-8.348	479.152	Phenolic
7	13.62	$[M - H]^-$	$C_{24}H_{23}O_{13}$	Pelargonidin 3-*O*-(6-*O*-malonyl-beta-*D*-glucoside)	518.114	518.116	-3.860	285.170; 257.175; 243.159	Flavonoid
8	14.02	$[M + H]^+$	$C_{24}H_{23}O_{13}$	Pelargonidin 3-*O*-(6-*O*-malonyl-beta-*D*-glucoside)	520.114	520.114	0.000	433.113; 271.061	Flavonoid
9	14.57	$[M - H]^-$	$C_{22}H_{26}O_{11}$	Orchioside A	465.148	465.149	-2.150	449.108; 447.129; 435.129	Phenolic glycosides
10	14.81	$[M + H]^+$	$C_{21}H_{24}O_{11}$	Curculigoside B	453.132	453.130	4.414	290.271; 276.244	Phenolic glycosides
11	15.07	$[M + H]^+$	$C_{22}H_{26}O_{11}$	Orchioside A	467.148	467.148	0.000	350.143; 213.143	Phenolic glycosides
12	15.44	$[M + H]^+$	$C_{50}H_{42}O_9$	Sarmentosumin D	787.283	787.281	2.540	769.279; 759.295; 691.232	Flavanone
13	15.97	$[M - H]^-$	$C_{23}H_{24}O_{11}$	Crassifoside I	475.132	475.129	6.314	457.114; 445.114; 387.108	Phenolic
14	16.31	$[M + H]^+$	$C_{27}H_{44}O_7$	Ecdysterone	481.309	481.304	10.388	473.333; 467.106; 454.833; 451.750	Sterol
15	17.59	$[M - H]^-$	$C_{22}H_{26}O_{12}$	Curculigoside C	481.142	481.140	4.157	463.124; 453.140; 451.124	Phenolic glycosides
16	17.91	$[M + H]^+$	$C_{28}H_{22}O_{11}$	Theanaphthoquinone	535.116	535.116	0.000	517.112; 507.128; 477.118	Quinones
17	19.61	$[M - H]^-$	$C_{32}H_{40}O_7$	Longirostrerone A	535.277	535.276	1.868	535.277	Azaphilones
18	19.75	$[M + H]^+$	$C_{26}H_{38}O_{16}$	Pothobanoside C	607.216	607.214	3.294	607.214	Hemiterpene glucoside
19	20.09	$[M - H]^-$	$C_{14}H_{20}O_7$	Salidroside	299.121	299.123	-6.686	299.123	Glucoside
20	21.65	$[M - H]^-$	$C_{22}H_{24}O_{10}$	Neosakuranin	447.137	447.135	4.473	447.135	Chalcone glycoside
21	21.98	$[M - H]^-$	$C_{21}H_{18}O_{12}$	Breviscapin	461.080	461.081	-2.169	285.040; 267.029; 257.045; 243.029	Glucuronates
22	22.10	$[M - H]^-$	$C_{23}H_{26}O_{11}$	Nyasicoside	477.148	477.144	8.383	459.129; 449.145; 447.129	Phenolic
23	22.41	$[M + H]^+$	$C_{32}H_{40}O_7$	Longirostrerone A	537.277	537.275	3.722	537.275	Azaphilones
24	25.67	$[M + H]^+$	$C_{27}H_{38}O_{14}$	Laciniatoside V	587.226	587.223	5.109	569.222; 407.170; 393.154; 343.175	Iridoid glucoside
25	26.04	$[M - H]^-$	$C_{30}H_{20}O_8$	Emodin Dianthrone	507.116	507.116	0.000	491.077; 467.077; 441.097; 425.066	Glycosides
26	27.27	$[M + H]^+$	$C_{36}H_{70}O_2$	3-methoxy-5-acetyl-31-tritriacontene	535.538	535.537	1.867	535.537	-
27	30.92	$[M + H]^+$	$C_{41}H_{68}O_{13}$	Curculigosaponin C	769.466	769.466	0.000	606.413; 474.370	Cycloartane triterpene

PLL

No.	RT[min]	Adduct ion	Formula	Tentative identification	Expected *m/z*	Experimental *m/z*	Accuracy (ppm)	Fragment MS and MS/MS	Chemical type
1	0.92	$[M + H]^+$	$C_{17}H_{14}O_5$	1,1-bis(3,4-dihydroxyphenyl)-1-(2-furan)-methane	299.084	299.087	-10.031	166.072	Phenolic
2	8.46	$[M + H]^+$	$C_{21}H_{24}O_{11}$	Curculigoside B	453.132	453.135	-6.621	290.271; 276.244	Phenolic glycosides
3	10.08	$[M + H]^+$	$C_8H_8O_3$	Vanillin	153.047	153.047	0.000	150.981; 137.018; 136.015; 129.113	Phenolic
4	12.35	$[M + H]^+$	$C_{15}H_{26}O_3$	Capitulatin B	255.188	255.189	-3.919	255.189	Eudesman
5	13.41	$[M + H]^+$	$C_{24}H_{28}O_{11}$	(1S,2R)-*O*-methylnyasicoside	493.163	493.161	4.055	373.055	Norlignan glycosides
6	14.14	$[M + H]^+$	$C_{16}H_{17}NO_4$	Lycorine	288.116	288.116	0.000	270.113; 252.102; 240.102; 216.102	Alkaloid
7	15.07	$[M – H]^–$	$C_{22}H_{26}O_{11}$	Orchioside A	465.148	465.150	-4.300	449.108; 447.129; 435.129	Phenolic glycosides
8	15.30	$[M + H]^+$	$C_{18}H_{18}O_6$	(1R,2R)-crassifogenin-D	331.110	331.112	-6.040	331.190; 249.112; 167.033	Norlignan glycosides
9	15.54	$[M – H]^–$	$C_{23}H_{26}O_{10}$	Orchioside B	461.153	461.149	8.674	443.134; 433.150; 371.113	Phenolic glycosides
10	17.87	$[M + H]^+$	$C_{22}H_{24}O_{10}$	Neosakuranin	449.137	449.137	0.000	449.137	Chalcone glycoside
11	19.27	$[M – H]^–$	$C_{16}H_{17}NO_4$	Lycorine	286.116	286.116	0.000	270.076; 268.097; 258.076; 256.097	Alkaloid
12	19.97	$[M + H]^+$	$C_{27}H_{44}O_7$	Ecdysterone	481.309	481.307	4.155	473.333; 467.106; 454.833; 451.750	Steroid
13	20.43	$[M + H]^+$	$C_{26}H_{38}O_{16}$	Pothobanoside C	607.216	607.213	4.941	607.213	Hemiterpene glucoside
14	20.65	$[M – H]^–$	$C_{20}H_{28}Cl_2O_{12}$	Curculigine A	529.096	529.099	-5.670	529.099	Phenolic glycosides
15	21.24	$[M + H]^+$	$C_{13}H_{18}O_7$	Orcinol glucoside	287.105	287.105	0.000	269.100; 256.121; 254.993; 251.093; 237.020	Phenolic glycosides
16	21.70	$[M + H]^+$	$C_{30}H_{48}O_5$	Asiatic acid	489.350	489.355	-10.218	453.336; 407.331; 330.222	Pentacyclic triterpene
17	22.10	$[M – H]^–$	$C_{23}H_{26}O_{11}$	Nyasicoside	477.148	477.144	8.383	459.129; 449.145; 447.129	Phenolic
18	23.37	$[M + H]^+$	$C_{22}H_{26}O_{11}$	Orchioside A	467.148	467.149	-2.141	350.143; 213.143	Phenolic glycosides
19	23.49	$[M – H]^–$	$C_{21}H_{22}O_{10}$	Prunin	433.121	433.118	6.926	273.076; 179.034	Flavanone glycoside
20	23.99	$[M – H]^–$	$C_{21}H_{18}O_{12}$	Breviscapin	461.080	461.084	-8.675	285.040; 267.029; 257.045; 243.029	Glucuronates
21	24.02	$[M + H]^+$	$C_{22}H_{26}O_{12}$	Curculigoside C	483.142	483.138	8.279	465.139; 421.112	Phenolic glycosides
22	24.12	$[M – H]^–$	$C_{21}H_{24}O_{11}$	Curculigoside B	451.132	451.129	6.650	433.114; 423.129	Phenolic glycosides
23	25.60	$[M – H]^–$	$C_{30}H_{20}O_8$	Emodin dianthrone	507.116	507.121	-9.860	254.058	Glycosides
24	25.67	$[M + H]^+$	$C_{27}H_{38}O_{14}$	Laciniatoside V	587.226	587.222	6.812	569.222; 407.170; 393.154; 343.175	Iridoid glucoside
25	27.01	$[M + H]^+$	$C_{36}H_{70}O_2$	3-methoxy-5-acetyl-31-tritriacontene	535.538	535.543	-9.336	535.543	-
26	30.92	$[M + H]^+$	$C_{41}H_{68}O_{13}$	Curculigosaponin C	769.466	769.466	0.000	606.413; 474.370	Cycloartane triterpene
27	31.20	$[M – H]^–$	$C_8H_8Cl_2O_2$	2,4-dichloro-5-methoxy-3-methylphenol	204.990	204.991	-4.878	176.987; 174.972; 154.990; 150.972	Phenolic

RLSK

No.	RT[min]	Adduct ion	Formula	Tentative identification	Expected *m/z*	Experimental *m/z*	Accuracy (ppm)	Fragment MS and MS/MS	Chemical type
1	0.914	$[M – H]^–$	$C_{17}H_{14}O_5$	1,1-bis(3,4-dihydroxyphenyl)-1-(2-furan)-methane	297.082	297.084	-6.732	281.045; 271.061; 269.081	Phenolic
2	0.930	$[M + H]^+$	$C_{16}H_{17}NO_4$	Lycorine	288.116	288.116	0.000	270.113; 252.102; 240.102; 216.102	Alkaloid

3	1.334	$[M + H]^+$	$C_8H_8O_3$	Vanillin	153.047	153.046	6.534	150.981; 137.018; 136.015; 129.113	Phenolic
4	1.453	$[M – H]^–$	$C_8H_8Cl_2O_2$	2,4-dichloro-5-methoxy-3-methylphenol	204.989	204.990	-4.878	176.987; 174.972; 154.990; 150.972	Phenolic
5	2.335	$[M + H]^+$	$C_{23}H_{24}O_{11}$	Crassifoside I	477.131	477.136	-10.479	457.114; 445.114; 387.108	Phenolic
6	2.783	$[M + H]^+$	$C_{16}H_{17}NO_4$	Lycorine	288.115	288.116	-3.471	270.113; 252.102; 240.102; 216.102	Alkaloid
7	3.118	$[M + H]^+$	$C_{13}H_{18}O_7$	Orcinol glucoside	287.107	287.105	6.966	269.100; 256.121; 254.993; 251.093; 237.020	Phenolic glycosides
8	5. 832	$[M – H]^–$	$C_{23}H_{28}O_{12}$	Curculigine	495.158	495.158	0.000	315.148; 161.109	Chlorophenols glucosides
9	6.376	$[M + H]^+$	$C_{21}H_{24}O_{11}$	Curculigoside B	453.132	453.132	0.000	290.271; 276.244	Phenolic glycosides
10	14.135	$[M + H]^+$	$C_{22}H_{26}O_{11}$	Orchioside A	467.153	467.148	10.703	305.144; 291.144	Phenolic glycosides
11	14.575	$[M – H]^–$	$C_{22}H_{26}O_{11}$	Orchioside A	465.147	465.149	-4.300	449.108; 447.129; 435.129	Phenolic glycosides
12	14.021	$[M + H]^+$	$C_{24}H_{23}O_{13}$	Pelargonidin 3-*O*-(6-*O*-malonyl-beta-*D*-glucoside)	520.113	520.114	-1.923	433.113; 271.061	Flavonoid
13	22.102	$[M + H]^+$	$C_{23}H_{26}O_{11}$	Nyasicoside	479.147	479.151	-8.348	479.152	Phenolic
14	24.027	$[M + H]^+$	$C_{22}H_{26}O_{12}$	Curculigoside C	483.142	483.137	10.349	465.139; 421.112	Phenolic glycosides
15	24.680	$[M – H]^–$	$C_{21}H_{24}O_{11}$	Curculigoside B	451.128	451.132	-8.867	433.114; 423.129	Phenolic glycosides
16	24.680	$[M – H]^–$	$C_{23}H_{26}O_{10}$	Orchioside B	461.157	461.153	8.674	443.134; 433.150; 371.113	Phenolic glycosides
17	30.887	$[M – H]^–$	$C_{41}H_{68}O_{13}$	Curculigosaponin C	767.464	767.466	-2.606	693.421; 659.416	Cycloartane

LLSK

No.	RT[min]	Adduct ion	Formula	Tentative identification	Expected *m/z*	Experimental *m/z*	Accuracy (ppm)	Fragment MS and MS/MS	Chemical type
1	0.876	$[M + H]^+$	$C_{18}H_{18}O_6$	(1R,2R)-crassifogenin-D	331.113	331.110	9.060	315.086; 313.107; 303.122	Norlignan
2	0.888	$[M – H]^–$	$C_{17}H_{14}O_5$	1,1-bis(3,4-dihydroxyphenyl)-1-(2-furan)-methane	297.082	297.084	-6.732	281.045; 271.061; 269.081	Phenolic
3	1.332	$[M + H]^+$	$C_8H_8O_3$	Vanillin	153.047	153.047	0.000	150.981; 137.018; 136.015; 129.113	Phenolic
4	7.886	$[M + H]^+$	$C_{21}H_{24}O_{11}$	Curculigoside B	453.136	453.132	8.827	290.271; 276.244	Phenolic glycosides
5	14.025	$[M + H]^+$	$C_{24}H_{23}O_{13}$	Pelargonidin 3-*O*-(6-*O*-malonyl-beta-*D*-glucoside)	520.113	520.113	0.000	433.113; 271.061	Flavonoid
6	14.863	$[M – H]^–$	$C_{17}H_{14}O_5$	Sinensigenin B	297.084	297.084	0.000	295.173; 190.152	Norlignan
7	15.965	$[M – H]^–$	$C_{23}H_{24}O_{11}$	Crassifoside I	475.131	475.129	4.209	457.114; 445.114; 387.108	Phenolic
8	24.564	$[M – H]^–$	$C_{23}H_{26}O_{10}$	Orchioside B	461.157	461.153	8.674	443.134; 433.150; 371.113	Phenolic glycosides
9	20.657	$[M – H]^–$	$C_{20}H_{28}Cl_2O_{12}$	Curculigine A	529.096	529.099	-5.670	529.099	Phenolic glycosides
10	24.585	$[M – H]^–$	$C_{21}H_{24}O_{11}$	Curculigoside B	451.128	451.132	-8.867	433.114; 423.129	Phenolic glycosides
11	25.183	$[M – H]^–$	$C_{22}H_{26}O_{11}$	Orchioside A	465.144	465.148	-8.599	449.108; 447.129; 435.129	Phenolic glycosides
12	25.658	$[M – H]^–$	$C_{35}H_{60}O_6$	3-*O*-*B*-*D*-glucopyranosyl sitosterol	575.441	575.439	3.476	559.400; 547.400; 477.322	Sitosterol
13	25.931	$[M – H]^–$	$C_{47}H_{78}O_{17}$	Curculigosaponin H	913.526	913.524	2.189	895.506; 883.506; 781.474; 767.458	Cycloartane
14	31.436	$[M – H]^–$	$C_8H_8Cl_2O_2$	2,4-dichloro-5-methoxy-3-methylphenol	204.992	204.990	9.756	176.987; 174.972; 154.990; 150.972	Phenolic

PLSK

No.	RT[min]	Adduct ion	Formula	Tentative identification	Expected *m/z*	Experimental *m/z*	Accuracy (ppm)	Fragment MS and MS/MS	Chemical type
1	0.850	$[M – H]^–$	$C_{23}H_{24}O_{11}$	Crassifoside I	475.128	475.132	-8.419	457.114; 445.114; 387.108	Phenolic

2	0.882	$[M - H]^-$	$C_{17}H_{14}O_5$	1,1-bis(3,4-dihydroxyphenyl)-1-(2-furan)-methane	297.082	297.084	-6.732	281.045; 271.061; 269.081	Phenolic
3	1.442	$[M - H]^-$	$C_8H_8Cl_2O_2$	2,4-dichloro-5-methoxy-3-methylphenol	204.990	204.990	0.000	176.987; 174.972; 154.990; 150.972	Phenolic
4	3.142	$[M + H]^+$	$C_{16}H_{17}NO_4$	Lycorine	288.116	288.116	0.000	270.113; 252.102; 240.102; 216.102	Alkaloid
5	3.295	$[M - H]^-$	$C_{13}H_{18}O_7$	Orcinol glucoside	285.105	285.105	0.000	285.105	Phenolic glycosides
6	3.684	$[M - H]^-$	$C_{22}H_{26}O_{11}$	Orchioside A	465.150	465.148	4.300	449.108; 447.129; 435.129	Phenolic glycosides
7	6.378	$[M + H]^+$	$C_{21}H_{24}O_{11}$	Curculigoside B	453.133	453.132	2.207	290.271; 276.244	Phenolic glycosides
8	19.012	$[M - H]^-$	$C_{16}H_{17}NO_4$	Lycorine	286.118	286.116	6.990	270.076; 268.097; 258.076; 256.097	Alkaloid
9	23.292	$[M - H]^-$	$C_{42}H_{70}O_{13}$	Curculigosaponin G	781.475	781.482	-8.957	749.448; 635.416	Cycloartane
10	24.591	$[M - H]^-$	$C_{23}H_{26}O_{10}$	Orchioside B	461.157	461.153	8.674	443.134; 433.150; 371.113	Phenolic glycosides
11	24.627	$[M - H]^-$	$C_{21}H_{24}O_{11}$	Curculigoside B	451.129	451.132	-6.650	433.114; 423.129	Phenolic glycosides
12	25.944	$[M - H]^-$	$C_{47}H_{78}O_{17}$	Curculigosaponin H	913.524	913.524	0.000	895.506; 883.506; 781.474; 767.458	Cycloartane
13	29.206	$[M - H]^-$	$C_{35}H_{60}O_6$	3-*O*-*B*-*D*-glucopyranosyl sitosterol	575.434	575.439	-8.689	559.400; 547.400; 477.322	Sitosterol
14	30.893	$[M - H]^-$	$C_{41}H_{68}O_{13}$	Curculigosaponin C	767.466	767.466	0.000	693.421; 659.416	Cycloartane
15	31.027	$[M - H]^-$	$C_8H_8Cl_2O_2$	2,4-dichloro-5-methoxy-3-methylphenol	204.992	204.990	9.756	176.987; 174.972; 154.990; 150.972	Phenolic

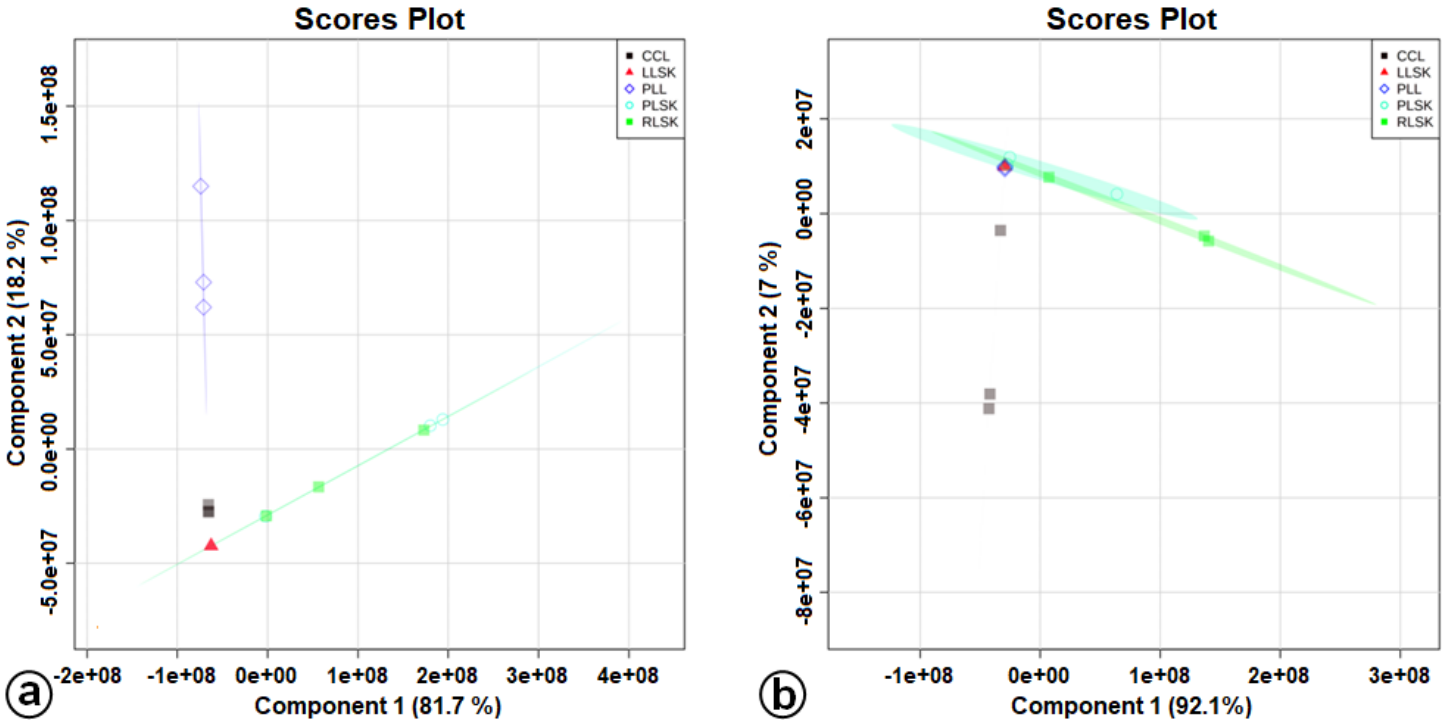

Figure S2. Supervised PLS-DA score plot showing separation of clusters for *in vitro* propagules and original plant organs based on bioactive metabolites at positive (a) and negative (b) modes generated by the UHPLC-Q-Orbitrap HRMS analysis.

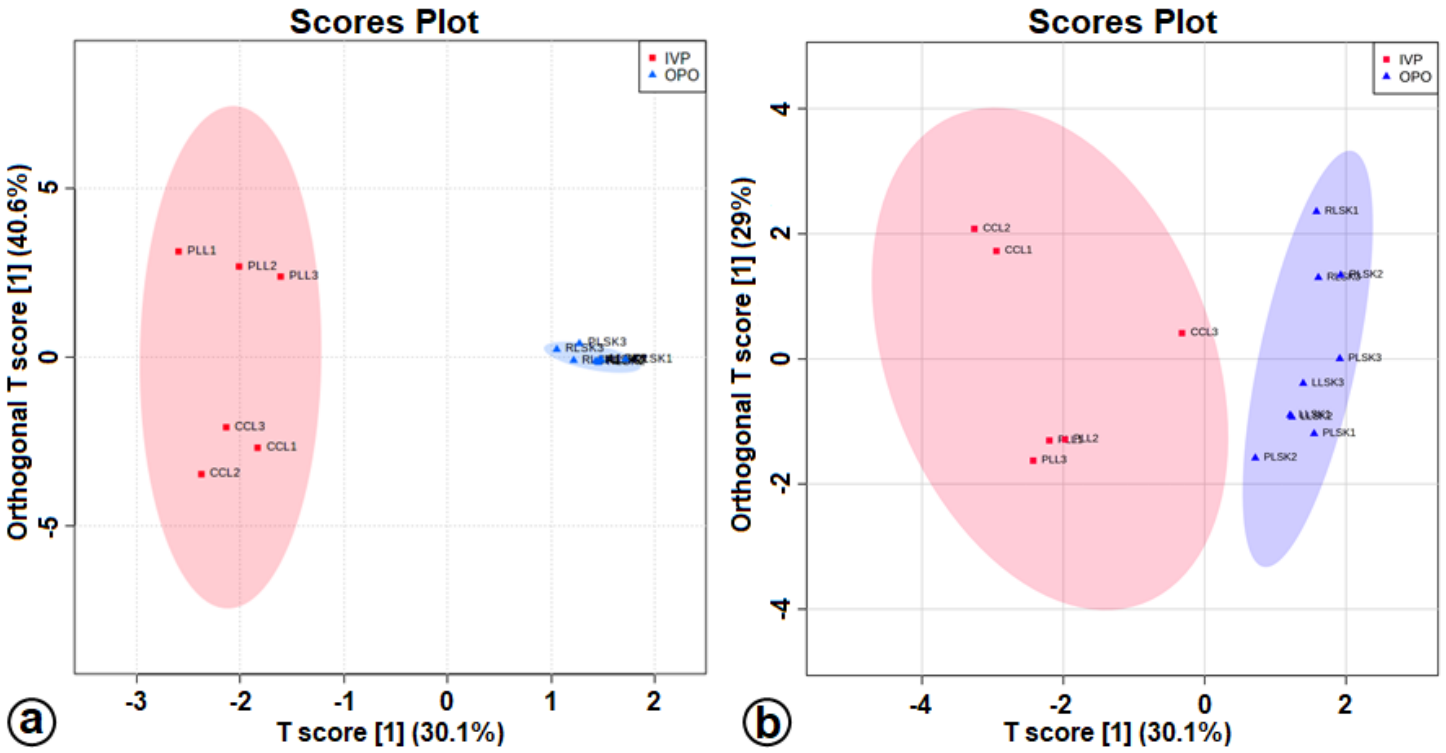

Figure S3. The OPLS-DA score plot at positive (a) and negative (b) modes for the separation of *in vitro* propagules and original plant organs of *C. latifolia*.

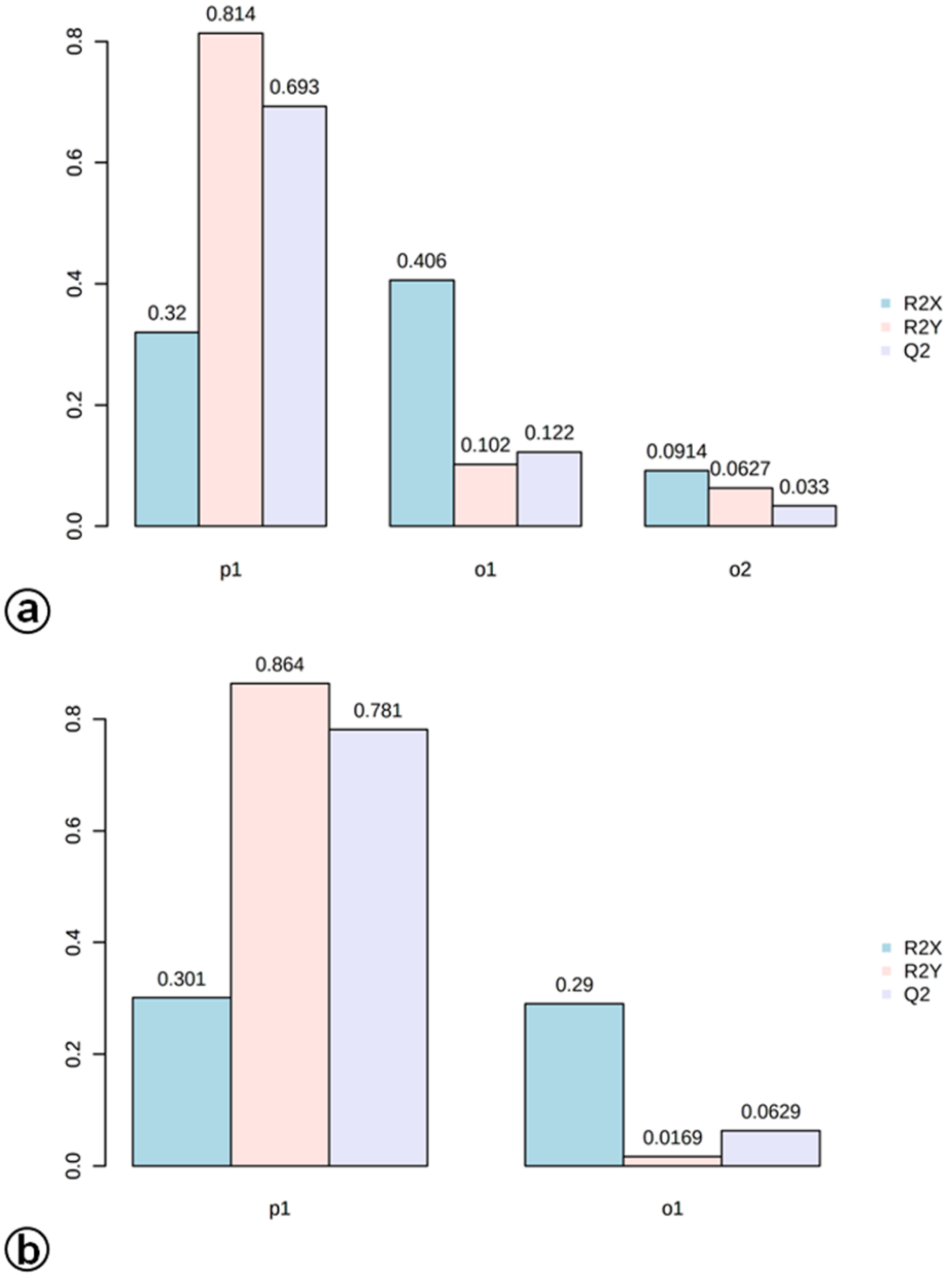

Figure S4. The OPLS-DA model shows the level of goodness-of-fit (R^2) and predictability level (Q^2) at positive (a) and negative (b) modes.