Fig. S1 The representative image of Ziqin and Kuqin

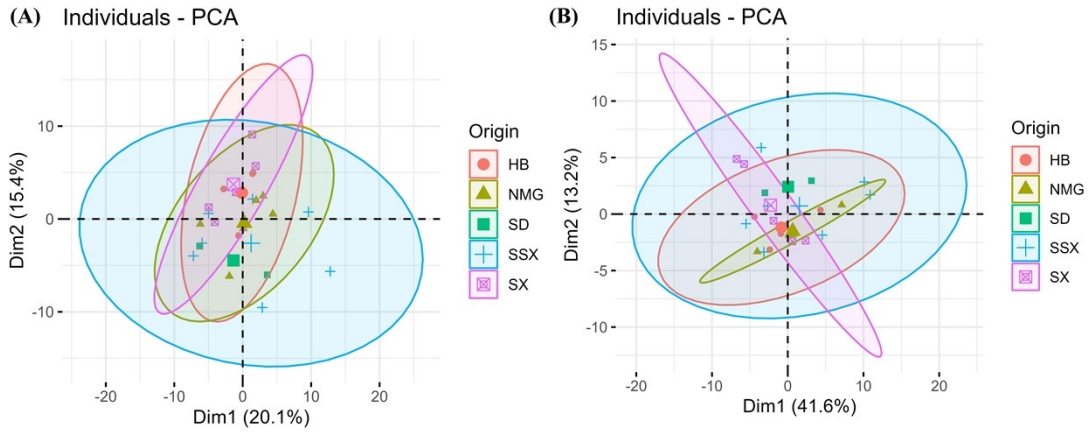

Fig. S2 The PCA score of different geographical origins of SR samples based on non-volatile compounds (A) and volatile compounds (B)

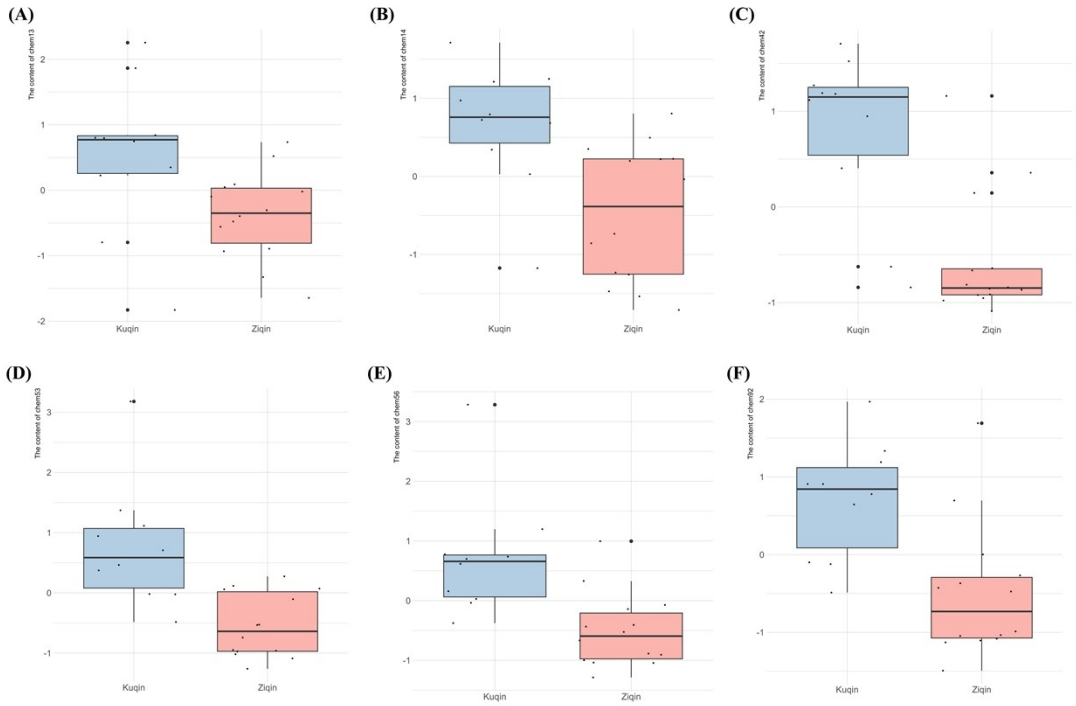

Fig. S3 The content of markers in different growth stages of SR samples: chem13 (A), chem14 (B), chem42 (C), chem53 (D), chem56 (E), chem92 (F)

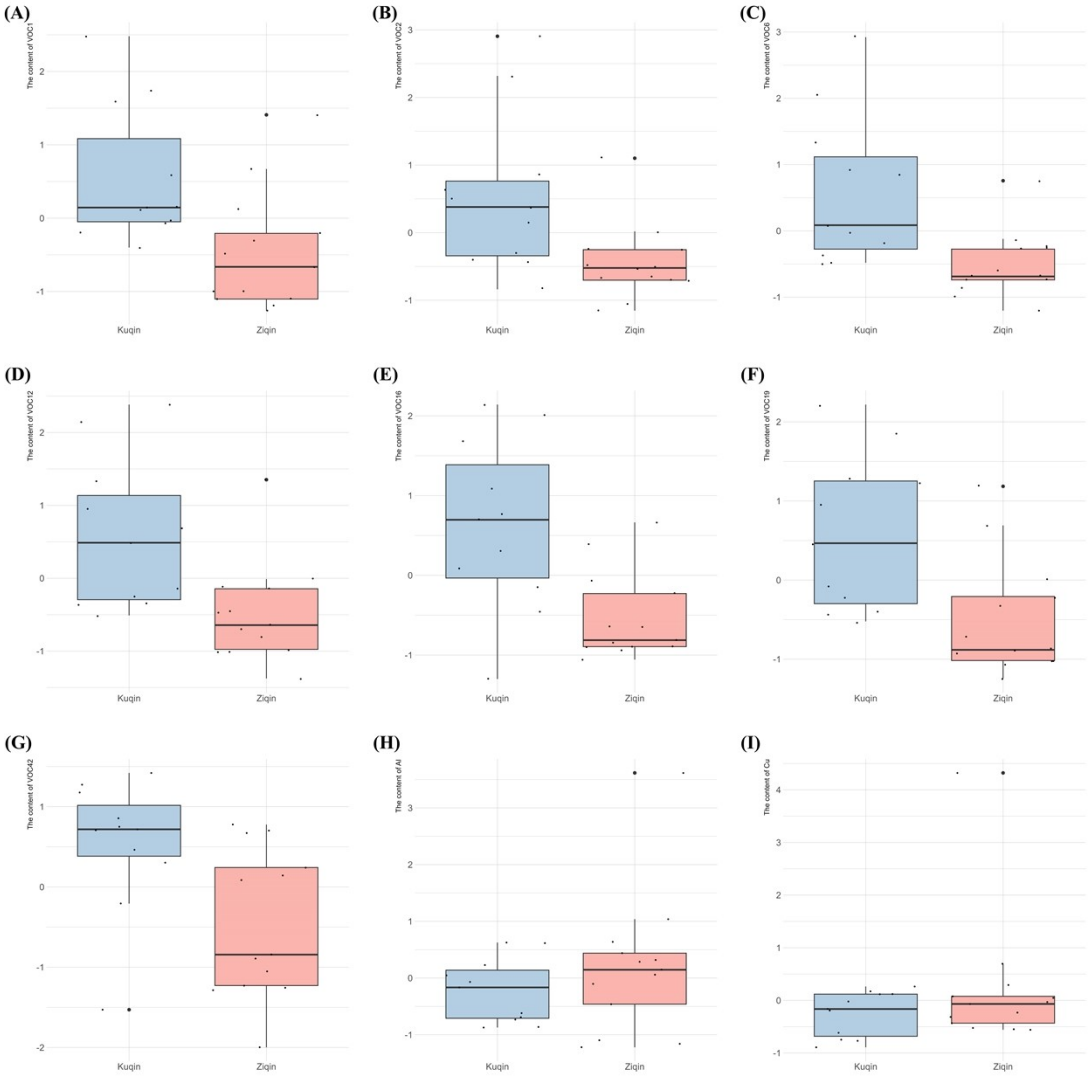

Fig. S4 The content of markers in different growth stages of SR samples: VOC1 (A), VOC2 (B), VOC6 (C), VOC12 (D), VOC16 (E), VOC19 (F), VOC42 (G), Al (H), Cu (I)

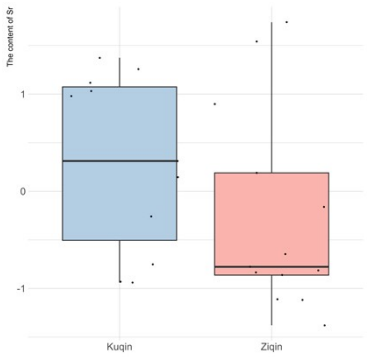

Fig. S5 The content of Sr in different growth stages of SR samples

Table S1 Information of 13 batches of Ziqin samples and 11 batches of Kuqin samples

NO.	Sample ID	Specification	Morphological characteristics	Region
1	Kuqin-1	Kuqin	hollow interior	Hebei
2	Kuqin-2	Kuqin	hollow interior	Hebei
3	Kuqin-3	Kuqin	hollow interior	Neimenggu
4	Kuqin-4	Kuqin	hollow interior	Neimenggu
5	Kuqin-5	Kuqin	hollow interior	Neimenggu
6	Kuqin-6	Kuqin	hollow interior	Shandong
7	Kuqin-7	Kuqin	hollow interior	Shaanxi
8	Kuqin-8	Kuqin	hollow interior	Shaanxi
9	Kuqin-9	Kuqin	hollow interior	Shaanxi
10	Kuqin-10	Kuqin	hollow interior	Shanxi
11	Kuqin-11	Kuqin	hollow interior	Shanxi
12	Ziqin-1	Ziqin	compact interior	Hebei
13	Ziqin-2	Ziqin	compact interior	Hebei
14	Ziqin-3	Ziqin	compact interior	Neimenggu
15	Ziqin-4	Ziqin	compact interior	Neimenggu
16	Ziqin-5	Ziqin	compact interior	Neimenggu
17	Ziqin-6	Ziqin	compact interior	Shandong
18	Ziqin-7	Ziqin	compact interior	Shaanxi
19	Ziqin-8	Ziqin	compact interior	Shaanxi
20	Ziqin-9	Ziqin	compact interior	Shaanxi
21	Ziqin-10	Ziqin	compact interior	Shaanxi
22	Ziqin-11	Ziqin	compact interior	Shanxi

23	Ziqin-12	Ziqin	compact interior	Shanxi
24	Ziqin-13	Ziqin	compact interior	Shanxi

Table S2 The linear relationship of inorganic elements

Inorganic elements	Equation	R^2
Cd	Y=21989.11X+13.62	1.000
Al	Y=45450.28X+6134.19	0.995
V	Y=54419.35X+28407.2	1.000
Cr	Y=50970.35X+20965.63	1.000
Mn	Y=80490.29X+3666.51	1.000
Fe	Y=1664.8X+62479.49	0.996
Ni	Y=12229.4X+499.09	1.000
Cu	Y=14031.78X+734.71	0.999
Zn	Y=9718.58X+4255.9	0.998
As	Y=7399.67X+721.07	1.000
Se	Y=634.39X+343.5	1.000
Sr	Y=82785.06X+1073.34	1.000
Co	Y=61222.9X+176.78	1.000
Ba	Y=16487.9X+253.84	0.998
Pb	Y=93876.13X+403.12	1.000
Bi	Y=143889.32X+93.91	0.999

Table S3 The detailed information of non-volatile compounds in SR samples

ID	RT/ min	*m/z*	Compound Name	Ionization mode	Formula	MS^2 fragment
chem1	19.3	285.0638	Prunetin	$[M+H]^+$	$C_{16}H_{12}O_5$	179.0418, 252.0311, 270.0409, 271.0441, 285.0635
chem2	19.4	255.0546	Daidzein	$[M+H]^+$	$C_{15}H_{10}O_4$	103.0502, 129.0284, 153.0121, 181.0577, 209.0511, 255.0543
chem3	16.8	285.0633	5-O-Methylgenistein	$[M+H]^+$	$C_{16}H_{12}O_5$	179.0415, 252.0308, 270.0404, 271.0439, 285.0627
chem4	17.4	331.0669	Tricin	$[M+H]^+$	$C_{17}H_{14}O_7$	108.0200, 154.0256, 197.0365, 270.0408, 283.0480, 287.0426, 316.0435, 331.0668, 333.0722
chem5	0.8	365.0886	Tetramethylscutellarein	$[M+Na]^+$	$C_{19}H_{18}O_6$	185.0337, 203.0433, 365.0886
chem6	11.0	303.0357	Tricetin	$[M+H]^+$	$C_{15}H_{10}O_7$	95.0082, 149.0163, 153.0110, 167.0260, 179.0340, 201.0450, 207.0191, 257.0323, 303.0357
chem7	14.8	255.0540	Chrysin	$[M+H]^+$	$C_{15}H_{10}O_4$	103.0550, 153.0117, 255.0535
chem8	17.9	271.0487	Genistein	$[M+H]^+$	$C_{15}H_{10}O_5$	119.0443, 145.0226, 153.0121
chem9	18.2	323.0385	Tectorigenin	$[M+Na]^+$	$C_{16}H_{12}O_6$	137.0231, 286.0343, 324.0425
chem10	17.8	315.0728	Velutin	$[M+H]^+$	$C_{17}H_{14}O_6$	153.0475, 300.0226, 315.0725
chem11	11.2	195.0924	Caffeine	$[M+H]^+$	$C_8H_{10}N_4O_2$	91.0512, 116.0511, 123.0260
chem12	13.9	287.0423	Kaempferol	$[M+H]^+$	$C_{15}H_{10}O_6$	121.0271, 153.0118, 213.0530, 287.0423
chem13	17.7	269.0650	Columbianetin	$[M+Na]^+$	$C_{14}H_{14}O_4$	137.0230, 226.0530, 227.0563, 254.0465

chem14	19.5	285.0635	Physcion	$[M+H]^+$	$C_{16}H_{12}O_5$	167.9984, 179.0490, 242.0469, 270.0407, 271.0440
chem15	15.5	257.0695	(2R)-5-Methoxy-2-methyl-2,3,8,9-tetrahydrofuro[2,3-h]chromen-4-one	$[M+Na]^+$	$C_{13}H_{14}O_4$	103.0497, 153.0122
chem16	22.2	425.1936	6-[(1E,3E,5E,7Z)-8-[(2S,3R,4R,5R)-3,4-Dihydroxy-2,4,5-trimethyloxolan-2-yl]-7-methylocta-1,3,5,7-tetraenyl]-4-methoxy-5-methylpyran-2-one	$[M+Na]^+$	$C_{23}H_{30}O_6$	116.0475, 425.1936, 426.1971
chem17	18.5	301.0575	Fallacinol	$[M+H]^+$	$C_{16}H_{12}O_6$	167.9984, 286.0347, 301.0575
chem18	22.4	473.3213	(3R,5S,7R,9S,10S,12S,13R,17R)-17-((2R)-4-(3-(Hydroxymethyl)oxetan-2-yl)butan-2-yl)-10,13-dimethylhexadecahydro-1H-cyclopenta[a]phenanthrene-3,7,12-triol	$[M+Na]^+$	$C_{27}H_{46}O_5$	471.3198, 473.3213, 474.3247

chem19	0.7	175.1111	L-Arginine	$[M+H]^+$	$C_6H_{14}N_4O_2$	112.0870, 130.0922, 175.1111
chem20	1.6	268.0918	Adenosine	$[M+H]^+$	$C_{10}H_{13}N_5O_4$	119.0300, 136.0556, 268.0918
chem21	23	685.4002	Acetylcimigenol arabinoside	$[M+Na]^+$	$C_{37}H_{58}O_{10}$	685.4002, 686.4038
chem22	24.6	455.3124	Gitogenin	$[M+Na]^+$	$C_{27}H_{44}O_4$	455.3118, 456.3150, 457.3276
chem23	14.4	257.0697	Trihydroxychalcone	$[M+H]^+$	$C_{15}H_{12}O_4$	165.0626, 193.0565, 197.0504, 211.0760, 239.0597, 240.0625
chem24	21.1	300.2755	D-Sphingosine	$[M+H]^+$	$C_{18}H_{37}NO_2$	93.0690, 95.0815, 97.0967, 110.0960, 264.2681
chem25	15.5	287.0788	Sakuranetin	$[M+H]^+$	$C_{16}H_{14}O_5$	167.0268
chem26	14.5	289.0578	Eriodictyol	$[M+H]^+$	$C_{15}H_{12}O_6$	89.0400, 153.0119, 154.0152, 179.0300
chem27	25.5	284.2811	Stearamide	$[M+H]^+$	$C_{18}H_{37}NO$	284.2816, 285.2852
chem28	9.8	289.0565	Norfludiazepam	$[M+H]^+$	$C_{15}H_{10}ClFN_2O$	153.0105, 271.0570
chem29	12.9	301.0571	Diosmetin	$[M+H]^+$	$C_{16}H_{12}O_6$	286.0344, 287.0376, 301.0572, 302.0604
chem30	24.1	413.3034	2-Methyl-2-(3-pentadecylphenoxy)propanoic acid	$[M+Na]^+$	$C_{25}H_{42}O_3$	327.2610, 413.3034, 414.3065
chem31	17.9	303.0715	Piperazine-1,4-bisethanesulfonic acid	$[M+H]^+$	$C_8H_{18}N_2O_6S_2$	127.0020, 167.9987, 183.0214, 184.0246, 301.0584
chem32	9.4	305.0507	Haemoventosine	$[M+H]^+$	$C_{15}H_{12}O_7$	123.0381, 153.0108, 191.0247, 241.0379, 287.0406
chem33	15.9	317.0515	Pinoquercetin	$[M+H]^+$	$C_{16}H_{12}O_7$	302.0291, 317.0515, 318.0548
chem34	18.3	271.0488	Emodin	$[M+H]^+$	$C_{15}H_{10}O_5$	95.0120, 103.0503, 123.0028, 141.0180,

						169.0063, 225.0452, 253.0389, 271.0487
chem35	18.9	313.0933	Dehydrocurvularin	$[M+Na]^+$	$C_{16}H_{18}O_5$	105.0295, 123.0118, 181.0056, 255.0650, 283.0476, 298.0828, 313.0930
chem36	11.2	303.0720	Sternbin	$[M+H]^+$	$C_{16}H_{14}O_6$	167.0261, 168.0295
chem37	18.3	361.0761	α-Hydrojuglone 4-glucoside	$[M+Na]^+$	$C_{16}H_{18}O_8$	232.0372, 303.0528, 331.0306, 361.0761, 362.0795
chem38	1.9	284.0861	Guanosine	$[M+H]^+$	$C_{10}H_{13}N_5O_5$	110.0306, 135.0245, 152.0502, 153.0523, 284.0861
chem39	17.3	287.0789	Peucedanol	$[M+Na]^+$	$C_{14}H_{16}O_5$	103.0494, 140.0048, 167.9985, 183.0210, 287.0789, 288.0824
chem40	21.4	365.1185	(7E,13E)-9,15-Dihydroxy-4,10,16-trimethyl-1,5,11-trioxacyclohexadeca-7,13-diene-2,6,12-trione	$[M+Na]^+$	$C_{16}H_{22}O_8$	105.0288, 106.0321, 107.0343, 163.0679, 165.0736, 365.1185, 366.1219
chem41	11.5	465.0805	Sorafenib	$[M+H]^+$	$C_{28}H_{24}ClF_3N_4O_6S$	163.1240, 289.0568, 303.0633, 465.0805, 466.0836
chem42	14.0	339.0923	Vanilloloside	$[M+Na]^+$	$C_{14}H_{20}O_8$	105.0700, 177.0470, 178.0576, 339.0923
chem43	5.7	205.0872	L-Tryptophane	$[M+H]^+$	$C_{11}H_{12}N_2O_2$	91.0498, 115.0491, 118.0597, 119.0631, 143.0661, 146.0530, 170.0518
chem44	11.2	539.1133	Isochlorogenic acid A	$[M+Na]^+$	$C_{25}H_{24}O_{12}$	121.0239, 335.0523, 377.0687, 387.0826, 421.0425, 539.1133, 540.1280

chem45	23.9	457.3272	Nakijiquinone H	$[M+H]^+$	$C_{26}H_{40}N_4O_3$	135.1172, 457.3270, 458.3300, 459.3478
chem46	19.7	345.0820	Lysionotin	$[M+H]^+$	$C_{18}H_{16}O_7$	133.0651, 182.9936, 228.0486, 287.0561, 315.0361
chem47	21	267.1592	Tributyl phosphate	$[M+H]^+$	$C_{12}H_{27}O_4P$	80.9702, 98.9798, 123.0019, 211.1093
chem48	13.8	463.1022	Rutarin	$[M+K]^+$	$C_{20}H_{24}O_{10}$	163.1236, 301.0572, 302.0606, 303.0631, 463.1022, 464.1058
chem49	17.3	463.1005	Kaempferol 3-glucuronoside	$[M+H]^+$	$C_{21}H_{18}O_{12}$	113.0221, 285.0628, 287.0920, 288.0824, 463.1005, 464.1054
chem50	6.7	271.1040	Alloimperatorin	$[M+H]^+$	$C_{16}H_{14}O_4$	93.0655, 111.0077, 133.0650, 271.1000
chem51	6.9	341.0698	Antibiotic AGI-B4	$[M+Na]^+$	$C_{16}H_{14}O_7$	133.0870, 163.0309, 165.0859, 179.0248, 341.0698, 342.0716
chem52	0.8	527.1334	NCGC00384944-01	$[M+Na]^+$	$C_{21}H_{28}O_{14}$	432.0935, 527.1334, 528.1368
chem53	19.7	449.1032	Quercitrin	$[M+H]^+$	$C_{21}H_{20}O_{11}$	229.0651, 269.0330, 325.0584, 449.1021, 450.1065
chem54	22.7	398.2125	(Z)-7-((Butyl(methyl)ammonio)methyl)-2-(2,5-dimethoxybenzylidene)-3-oxo-2,3-dihydrobenzofuran-6-olate	$[M+H]^+$	$C_{23}H_{27}NO_5$	149.0159, 239.0731, 398.2125, 399.2160
chem55	19.1	361.0759	3-p-Coumaroylquinic acid	$[M+Na]^+$	$C_{16}H_{18}O_8$	303.0531, 313.0208, 331.0303, 361.0759, 362.0791
chem56	12.9	303.0724	Hesperetin	$[M+H]^+$	$C_{16}H_{14}O_6$	86.0970, 153.0180, 167.9980, 183.0210, 284.3310, 286.0343,

						287.0431, 301.0570, 302.0600
chem57	6.7	295.0877	7-Acetoxy-2-methylisoflavone	$[M+H]^+$	$C_{18}H_{14}O_4$	97.0237, 133.0500
chem58	12.8	305.0518	2',3,5,6',7-Pentahydroxyflavanone	$[M+H]^+$	$C_{15}H_{12}O_7$	153.0115, 154.0151, 213.0540, 259.0626
chem59	18.2	269.0321	Galangin	$[M-H]^-$	$C_{15}H_{10}O_5$	101.0351, 136.9825, 138.9970, 141.0642, 167.0422, 169.0577, 171.0368, 195.0448, 197.0510, 198.0544, 223.0291, 239.0230, 269.0321, 270.0354
chem60	23.4	279.2186	9-Octadecynoic acid	$[M-H]^-$	$C_{18}H_{32}O_2$	96.9217, 279.2185, 280.2221, 281.2370
chem61	20.0	313.2228	Dronabinol	$[M-H]^-$	$C_{21}H_{30}O_2$	96.9558, 99.9250, 116.9227, 183.0034, 184.1329, 197.1304, 314.2268
chem62	23.7	265.1347	Lauryl sulfate	$[M-H]^-$	$C_{12}H_{26}O_4S$	96.9559
chem63	17.6	257.0328	Norlichexanthone	$[M-H]^-$	$C_{14}H_{10}O_5$	185.0517, 242.0371
chem64	20.1	194.0727	Acridone	$[M-H]^-$	$C_{13}H_9NO$	194.0726, 195.0760, 196.0779
chem65	25.0	311.1526	Triptophenolide	$[M-H]^-$	$C_{20}H_{24}O_3$	119.0460, 183.0030, 197.0179, 311.1526, 312.1558, 313.1509
chem66	6.7	323.1179	Isobavachin	$[M-H]^-$	$C_{20}H_{20}O_4$	119.0189, 183.0018, 323.1179, 324.1218
chem67	15.7	283.0474	Genkwanin	$[M-H]^-$	$C_{16}H_{12}O_5$	109.9956, 165.9827, 239.0226, 268.0244
chem68	5.7	203.0716	Tryptophan	$[M-H]^-$	$C_{11}H_{12}N_2O_2$	116.0445, 142.0587
chem69	9.0	207.0197	2-Naphthalenesulfonic acid	$[M-H]^-$	$C_{10}H_8O_3S$	108.0164, 120.0086, 164.0022, 192.0070

chem70	18.6	299.0414	Hematein	$[M-H]^-$	$C_{16}H_{12}O_6$	136.9815, 212.0373, 284.0184, 299.0414, 300.0449
chem71	14.7	287.0418	6,7,3',4'-Tetrahydroxyflavanone	$[M-H]^-$	$C_{15}H_{12}O_6$	125.0184, 133.0231, 162.0199, 177.0550, 259.0457
chem72	11.3	161.0166	Umbelliferone	$[M-H]^-$	$C_9H_6O_3$	105.0293, 117.0350, 133.0232, 134.0269, 161.0163, 162.0177
chem73	8.2	577.1294	Procyanidin B1	$[M-H]^-$	$C_{30}H_{26}O_{12}$	289.0464, 576.1265, 577.1294, 578.1326
chem74	23.6	379.2150	6,18,19-Trihydroxytrachyloban-2-one	$[M+FA-H]^-$	$C_{20}H_{30}O_4$	124.0323, 267.1365, 333.2117
chem75	11.1	301.0203	Delphinidin	$[M-2H]^{2-}$	$C_{15}H_{11}O_7$	107.0085, 121.0236, 124.0105, 150.9962
chem76	4.1	315.0552	Pannaric acid	$[M-H]^-$	$C_{16}H_{12}O_7$	108.0155, 109.0227, 110.0264, 315.0552, 316.0581
chem77	17.0	313.0199	Porphyrilic acid	$[M-H]^-$	$C_{16}H_{10}O_7$	197.0610, 225.0296, 269.0323, 270.0357, 313.0199, 314.0234
chem78	12.5	187.0883	Azelaic acid	$[M-H]^-$	$C_9H_{16}O_4$	95.0448, 123.0278, 125.0910, 187.0883
chem79	19.1	315.1654	Hannokinol	$[M-H]^-$	$C_{19}H_{24}O_4$	172.0028, 187.1247, 315.1654, 316.1688
chem80	8.0	179.0297	Caffeic acid	$[M-H]^-$	$C_9H_8O_4$	90.0360, 108.0449, 134.0307, 135.0358, 137.0406
chem81	8.9	153.0116	2,3-Dihydroxybenzoic acid	$[M-H]^-$	$C_7H_6O_4$	91.0148, 108.0216, 109.0238, 153.0116, 154.0145
chem82	22.3	387.1365	Divaricatic acid	$[M-H]^-$	$C_{21}H_{24}O_7$	133.0629, 387.1365, 388.1396
chem83	0.7	173.0953	N-Acetylornithine	$[M-H]^-$	$C_7H_{14}N_2O_3$	128.9527, 131.0758
chem84	9.5	177.0105	Daphnetin	$[M-H]^-$	$C_9H_6O_4$	92.0221, 106.0289, 121.0235, 132.0218,

						177.0105
chem85	1.3	138.0122	6-Hydroxynicotinic Acid	$[M-H]^-$	$C_6H_5NO_3$	94.0250, 95.0289, 138.0122
chem86	9.3	563.1118	Schaftoside	$[M-H]^-$	$C_{26}H_{28}O_{14}$	353.0489, 383.0578, 443.0759, 473.0848
chem87	10.1	479.0916	5,7,8,3′,4′-Pentahydroxyflavanone-7-O-glucuronide	$[M-H]^-$	$C_{21}H_{20}O_{13}$	166.9904, 181.0050, 285.0269, 303.0358
chem88	16.4	431.0757	Baicalein-7-O-glucoside	$[M-H]^-$	$C_{21}H_{20}O_{10}$	269.0311
chem89	19.4	313.1503	Dihydroxy-dimethoxyflavone	$[M-H]^-$	$C_{17}H_{14}O_6$	283.0094, 298.0323
chem90	13.3	639.1948	Luteolin-7-diglucuronide	$[M+H]^+$	$C_{30}H_{38}O_{15}$	177.0457, 339.0900
chem91	9.5	565.1283	Isoschaftoside	$[M+H]^+$	$C_{26}H_{28}O_{14}$	391.0648, 499.1008, 529.1100, 547.1189
chem92	11.1	465.0806	Carthamidin 7-O-glucuronide	$[M+H]^+$	$C_{21}H_{20}O_{12}$	147.0374, 169.0053, 289.0570
chem93	11.9	595.1357	Paniculatin	$[M+H]^+$	$C_{27}H_{30}O_{15}$	271.0465, 433.0911, 595.2249
chem94	12.2	417.0980	Chrysin 8-C-glucoside	$[M+H]^+$	$C_{21}H_{20}O_9$	267.0518, 297.0612, 381.0782, 399.0878, 417.0962
chem95	12.6	523.1191	5,2',6'-Trihydroxy-6,7,8-trimethoxyflavone 2'-O-*β*-D-glucoside	$[M+H]^+$	$C_{24}H_{26}O_{13}$	313.0194, 331.0301, 361.0740, 523.1166
chem96	13.5	287.0419	5,7,2',6'-Tetrahydroxyflavone	$[M+H]^+$	$C_{15}H_{10}O_6$	153.0104, 287.0402
chem97	13.4	303.0724	6-Methoxynaringe	$[M+H]^+$	$C_{16}H_{14}O_6$	107.0436, 123.0380, 133.0217, 167.0255,

			nin			229.0746, 257.0683, 285.0618, 303.0346
chem98	13.7	463.0647	Isoscutellarein 8-O-glucuronide	$[M+H]^+$	$C_{21}H_{18}O_{12}$	269.0308, 287.0406
chem99	12.3	417.0980	Chrysin 6-C-glucoside	$[M+H]^+$	$C_{21}H_{20}O_9$	267.0516, 297.0607, 381.0775, 399.0882, 417.0972
chem100	15.4	271.0484	Norwogonin	$[M+H]^+$	$C_{15}H_{10}O_5$	103.0494, 123.0018, 169.0051, 253.0379, 271.0470
chem101	14.2	289.0572	Carthamidin	$[M+H]^+$	$C_{15}H_{12}O_6$	153.0108
chem102	14.8	449.0863	Dihydrobaicalin	$[M+H]^+$	$C_{15}H_{12}O_5$	131.0427, 273.0623
chem103	15.9	431.0768	Chrysin 7-O-β-D-glucuronide	$[M+H]^+$	$C_{21}H_{18}O_{10}$	255.0529
chem104	17.6	331.0667	Viscidulin II	$[M+H]^+$	$C_{17}H_{14}O_7$	269.0322, 285.0257, 287.0419, 297.0261, 299.0400, 315.0356, 331.0663
chem105	19.3	345.0817	Skullcapflavone	$[M+H]^+$	$C_{18}H_{16}O_7$	165.0111, 181.0051, 197.0358, 283.0474, 301.0570, 311.0415, 315.0359, 329.0509, 345.0812
chem106	19.1	539.0723	8,8’-Bibaicalein	$[M+H]^+$	$C_{30}H_{18}O_{10}$	105.0291, 269.0327, 271.0478, 391.0272, 393.0421, 419.0209, 539.0727
chem107	19.5	315.0725	5,7-Dihydroxy-6,8-dimethoxy flavone	$[M+H]^+$	$C_{17}H_{14}O_6$	182.9845, 225.0457, 285.0269, 315.0723
chem108	13.7	447.0619	Baicalin	$[M+H]^+$	$C_{21}H_{18}O_{11}$	269.0329, 287.0424, 447.0726, 448.0757, 449.0778
chem109	14.9	447.0723	Glychionide A	$[M+H]^+$	$C_{21}H_{18}O_{11}$	241.0391, 269.0327, 285.0632

chem110	15.6	461.0872	Oroxylin A 7-O-*β*-D-glucoside	$[M+H]^+$	$C_{22}H_{19}O_{11}$	270.0405, 285.0633, 286.0665, 287.0689
chem111	16.8	461.0876	Wogonoside	$[M+H]^+$	$C_{22}H_{20}O_{11}$	179.0431, 270.0405, 271.0439, 285.0634, 286.0666, 287.0691
chem112	18.3	271.0488	Baicalein	$[M+H]^+$	$C_{15}H_{10}O_5$	123.0028, 169.0063, 225.0453, 253.0389
chem113	19.3	285.0635	Wogonin	$[M+H]^+$	$C_{16}H_{12}O_5$	179.0421, 252,0316, 270.0413, 271.0445, 285.0640
chem114	19.4	375.0916	Scullcapflavone II	$[M+H]^+$	$C_{19}H_{18}O_8$	121.0601, 169.0063, 197.0000, 327.0358, 345.0454
chem115	19.5	285.0637	Oroxylin A	$[M+H]^+$	$C_{16}H_{12}O_5$	140.0050, 167.9985, 242.0467, 270.0407, 271.0439

Table S4 The content of inorganic elements in different growth stages of SR samples

Growth stages	Cd/(mg/kg)	AI/(mg/kg)	V/(mg/kg)	Cr/(mg/kg)	Mn/(mg/kg)	Fe/(mg/kg)	Ni/(mg/kg)	Cu/(mg/kg)
KQ-1	0.04±0	915.47±54.5	2.37±0.15	2.87±0.15	37.54±2.7	862.63±65.2	1.91±0.11	14.54±0.79
KQ-5	0.02±0	1130.24±74.3	3.01±0.29	6.22±0.42	35.16±4.02	1288.82±107.71	3.22±0.53	8.8±1.12
TQ-9	0.05±0	3788.4±15.5	3.45±0.1	5.3±0.19	43.44±0.51	1279.47±4.5	4.29±0.06	12.25±0.12
TQ-11	0.31±0	7664.72±33.5	9.6±0.22	18.88±0.22	75.6±0.45	3663.85±23	10.3±0.1	41.69±0.31
TQ-1	0.02±0	2318.24±9.01	3.09±0.03	4.61±0.15	33.37±0.08	1000.69±1.35	2.73±0.04	11.71±0
TQ-2	0.15±0	1723.83±26	1.57±0.04	2.15±0.08	18.43±0.11	547.44±9.7	1.9±0.07	12.62±0.1
KQ-2	0.02±0	3150.89±16	4.12±0.15	8±0.17	39.97±0.03	1562.42±11.5	4.24±0.06	12.7±0.01
TQ-4	0.03±0	5619.07±11	5.82±0.13	9±0.32	48.37±0.97	2002.96±6	4.83±0.1	18.27±0.27
TQ-5	0.02±0	1534.25±34.38	4.4±0.06	6.96±0.17	47.95±1.03	1974.61±40.47	3.06±0.07	10.36±0.19
KQ-7	0.02±0	1294.78±54.68	3.71±0.2	5±0.16	40.65±2.85	1648.25±91.6	2.27±0.07	8.93±1.01
KQ-8	0.02±0	926.21±35.28	2.8±0.15	5.89±0.18	34.03±1.41	1243.44±39.65	2.57±0.07	8±0.31
TQ-13	0.03±0	2300.65±51.97	6.59±0.14	7.55±0.26	71.79±1.9	2948.75±97.2	3.5±0.15	12.52±0.39
TQ-14	0.01±0	575.37±41.86	1.64±0.12	3.62±0.18	21.48±1.2	795.18±46.93	5.69±0.33	10.96±0.61
KQ-3	0.02±0	2124.64±21.5	2.28±0.04	4.96±0.15	24.49±0.2	803.88±4.15	3.27±0.02	14.51±0.12
KQ-4	0.02±0	1191.34±67.4	3.67±0.2	5.67±0.64	40.24±1.46	1666.53±40.53	2.88±0.4	9.77±0.1
TQ-6	0.01±0	390.15±11.31	1.14±0.06	2.84±0.1	18.35±0.93	533.34±27.25	1.49±0.06	10.22±0.27
KQ-9	0.04±0	3167.54±	5.12±0	5.87±0.	46.7±0.	1854.32±3	3.23±0.	15.47±

		23.01	.31	16	04	4.02	12	0.04
TQ-10	0.14±0.01	3184.82±48.5	3.67±0.16	8.32±0.35	77.44±0.56	1326.58±12.5	9.4±0.21	13.56±0.09
TQ-12	0.05±0	2653.44±38.87	15.7±0.57	15.12±0.7	137.31±5.44	6411.74±356.4	6.05±0.3	15.65±0.54
TQ-15	0.33±0	2070.42±2.5	2.11±0.04	2.67±0.03	30.55±0.16	693.42±1.95	1.76±0.06	18.25±0.15
TQ-3	0.02±0	2705.24±36	2.87±0.09	8.01±0.08	27.43±0.03	1006.96±6	4.88±0.14	14.26±0.06
TQ-7	0.01±0	478.38±21.47	1.46±0.05	2.77±0.15	21.02±0.96	620.1±22.13	2.78±0.12	10.15±0.42
TQ-8	0.02±0	2446.38±35.85	3.67±0.1	5.4±0.29	33.7±0.45	1355±17.09	2.79±0.04	14.05±0.2
KQ-6	0.04±0	1978.01±86.14	5.2±0.13	5.33±0.24	71.96±1.7	2089.86±79.31	2.44±0.08	14.88±0.43
KQ-10	0.03±0	2569.1±15	4.5±0.3	9.26±0.32	41.06±0.51	1571.44±8.5	4.25±0.2	13.63±0.2

Table S5 The content of inorganic elements in different growth stages of SR samples

Growth stages	Zn/(mg/kg)	As/(mg/kg)	Se/(mg/kg)	Sr/(mg/kg)	Co/(mg/kg)	Ba/(mg/kg)	Pb/(mg/kg)	Bi/(mg/kg)
KQ-1	18.89±1.09	0.28±0.02	0.08±0	49.8±2.88	0.35±0.02	108.52±7.59	0.65±0.05	0.02±0
KQ-5	16.81±1.66	0.56±0.07	0.14±0	100.64±9.39	0.44±0.04	96.85±10.25	0.66±0.05	0.02±0
TQ-9	23.44±0.16	0.55±0.01	0.21±0.02	56.39±0.27	0.52±0.01	78.27±0.21	1.22±0.04	0.03±0
TQ-11	37.8±0.36	1.07±0.03	0.37±0.01	42.8±0.13	1.67±0.02	100.22±0.28	4.09±0.09	0.06±0
TQ-1	22.18±0.04	0.7±0.01	0.13±0.01	95.67±1.17	0.5±0.01	95.11±0.15	0.88±0.01	0.05±0
TQ-2	21.05±0.26	0.31±0.01	0.06±0	25.29±0.53	0.29±0.01	68.38±1.2	0.83±0.02	0.03±0
KQ-2	23.47±0.14	0.85±0.01	0.29±0.01	127.86±1.65	0.7±0.01	137.48±4.55	1.21±0.02	0.03±0
TQ-4	25.27±0.4	1.12±0.02	0.15±0.01	38.39±0.1	0.66±0.53	55.12±0.2	1.8±0.04	0.04±0
TQ-5	20.2±0.53	0.78±0.01	0.45±0.01	150.59±1.9	0.65±0.01	151.17±3.55	1.27±0.01	0.02±0
KQ-7	21.62±0.9	0.58±0.02	0.13±0.02	129.89±6.14	0.53±0.02	147.24±7.45	0.92±0.04	0.03±0
KQ-8	16.46±0.59	0.52±0.02	0.11±0.01	93.84±1.94	0.39±0.01	90.38±3.99	0.74±0.04	0.04±0
TQ-13	22.57±0.78	1.21±0.05	0.16±0.01	77.44±2.38	0.96±0.04	162.36±5.39	1.5±0.05	0.02±0
TQ-14	26.28±1.39	0.32±0.01	0.06±0.01	54.12±3.19	0.26±0.01	51.88±2.45	0.67±0.03	0.01±0
KQ-3	24.17±0.16	0.48±0.01	0.12±0	57.49±0.72	0.43±0.01	68.94±0.25	0.85±0.01	0.03±0
KQ-4	21.77±0.62	0.63±0.02	0.14±0.02	133.37±2.1	0.55±0.02	147.27±2.39	0.83±0.13	0.04±0
TQ-6	25.87±0.9	0.22±0.01	0.05±0.01	52.93±1.3	0.2±0.01	59.41±2.62	0.47±0.02	0.01±0

KQ-9	26.41±0.11	1.09±0.01	0.22±0.01	143.84±3	0.84±0.02	178.72±3.9	1.36±0.02	0.11±0
TQ-10	30.94±0.12	0.33±0.01	0.17±0.01	42.58±0.61	0.89±0.03	71.07±0.56	1.08±0.02	0.18±0
TQ-12	27.13±0.95	1.91±0.1	0.4±0.04	158.68±4.39	2.22±0.07	249.94±6.83	2.5±0.08	0.07±0
TQ-15	34.2±0.12	0.4±0.01	0.07±0.01	31.96±0.52	0.37±0	93.3±0.15	1.25±0.03	0.03±0
TQ-3	25.16±0.06	0.57±0.01	0.1±0	54.83±0.6	0.55±0	73.86±0.44	0.99±0.01	0.03±0
TQ-7	18.37±0.69	0.27±0.01	0.06±0	61.79±2.01	0.23±0.01	66.87±2.32	0.46±0.02	0.01±0
TQ-8	25.61±0.34	2.2±0.06	0.58±0.03	124.5±1.75	0.63±0.01	129.93±4.08	1.38±0.04	0.04±0
KQ-6	22.02±1.01	0.68±0.01	0.12±0.01	50.23±2.37	0.67±0.03	134.26±6.68	1.37±0.02	0.02±0
KQ-10	26.7±0.18	0.97±0.03	0.33±0.02	138.99±1.6	0.72±0.02	150.49±1.5	1.34±0.05	0.04±0