Supplementary Tables

Table S1 The top 10 differential metabolites of *C. deserticola* by comparison of inflorescence and succulent stem in three ecotypes groups using VIP (⩾1) and Fold Change (fold change⩾2 or fold change⩽0.5)

Index	Compounds	Class	Inflorescence			Succulent stem			VIP	Fold Change	Type
A1 vs A2 (Saline-alkali land)			HM1-1	HM2-1	HM3-1	HM1-2	HM2-2	HM3-2			
CdM267	Cyanidin 3-O-rutinoside (Keracyanin)	Anthocyanins	-	-	-	1.28E+08	2.56E+08	2.87E+05	2.51681463	1.42E+07	up
CdM584	Icariin (kaempferol 3,7-O-diglucoside 8-prenyl derivative)	Flavonol	-	-	-	1.73E+07	1.15E+07	5.70E+06	2.50496261	1.28E+06	up
CdM350	Homovanillic acid	Hydroxycinnamoyl derivatives	-	-	-	7.69E+06	5.28E+06	2.87E+06	2.43612955	5.87E+05	up
CdM411	Chlorogenic acid methyl ester	Quinate and its derivatives	-	-	-	4.02E+06	4.17E+06	3.86E+06	2.41898013	4.46E+05	up
CdM357	Rosinidin O-hexoside	Anthocyanins	-	-	-	1.06E+06	3.10E+06	5.14E+06	2.37353296	3.44E+05	up
CdM365	N', N''-di-p-coumaroylspermidine	Phenolamides	1.11E+07	1.09E+07	1.07E+07	-	-	-	2.51009205	8.26E-07	down
CdM424	8-C-hexosyl-luteolin O-hexoside	Flavone C-glycosides	3.35E+07	2.99E+07	2.62E+07	-	-	-	2.5982196	3.01E-07	down
CdM330	Caffeic acid	Hydroxycinnamoyl derivatives	1.21E+06	6.38E+07	3.25E+07	-	-	-	2.51405008	2.77E-07	down
CdM504	Isorhamnetin O-hexoside	Flavonol	3.17E+07	4.17E+07	5.17E+07	-	-	-	2.62602235	2.16E-07	down

CdM482	Isorhamnetin 5-O-hexoside	Flavonol	3.11E+07	4.21E+07	5.30E+07	-	-	-	2.62644662	2.14E-07	down
B1 vs B2 (Grassland)			HM4-1	HM5-1	HM6-1	HM4-2	HM5-2	HM6-2			
CdM30	L-(+)-Arginine	Amino acids	-	-	-	5.26E+06	5.83E+05	1.37E+06	2.51E+00	2.67E+05	up
CdM1040	Adipic acid	Organic acids	-	-	-	3.47E+05	2.43E+05	2.52E+06	2.41E+00	1.15E+05	up
CdM199	N-Methylnicotinamide	Nicotinic acid derivatives	-	-	-	6.32E+05	9.81E+05	5.06E+05	2.43E+00	7.85E+04	up
CdM328	4-Hydroxybenzoic acid	Organic acids	-	-	-	6.75E+05	9.01E+05	4.48E+05	2.42E+00	7.50E+04	up
CdM1109	Dihydromyricetin	Flavonol	-	-	-	8.42E+05	6.41E+05	2.54E+04	2.29E+00	5.59E+04	up
CdM357	Rosinidin O-hexoside	Anthocyanins	5.29E+06	5.27E+06	5.25E+06	-	-	-	2.64E+00	1.71E-06	down
CdM330	Caffeic acid	Hydroxycinnamoyl derivatives	7.87E+06	9.64E+06	1.14E+07	-	-	-	2.70E+00	9.34E-07	down
CdM504	Isorhamnetin O-hexoside	Flavonol	2.90E+04	5.87E+07	7.37E+04	-	-	-	2.29E+00	4.59E-07	down
CdM396	Selgin 5-O-hexoside	Flavone	1.99E+07	3.93E+07	4.32E+05	-	-	-	2.64E+00	4.53E-07	down
CdM482	Isorhamnetin 5-O-hexoside	Flavonol	2.99E+07	5.97E+07	7.84E+04	-	-	-	2.58E+00	3.01E-07	down
C1 vs C2 (Sandy land)			HM26-1	HM27-1	HM28-1	HM26-2	HM27-2	HM28-2			
CdM458	O-Feruloyl 4-hydroxylcoumarin	Coumarins	-	-	-	5.73E+07	3.86E+07	1.54E+07	2.39E+00	4.12E+06	up
CdM1054	Syringin	Hydroxycinnamoyl derivatives	-	-	-	8.74E+06	9.76E+06	1.59E+07	2.31E+00	1.27E+06	up

CdM357	Rosinidin O-hexoside	Anthocyanins	-	-	-	3.12E+06	5.60E+06	8.07E+06	2.24E+00	6.22E+05	up
CdM403	3-(4-Hydroxyphenyl)propionic acid	Hydroxycinnamoyl derivatives	-	-	-	3.01E+06	2.87E+06	4.17E+06	2.20E+00	3.72E+05	up
CdM350	Homovanillic acid	Hydroxycinnamoyl derivatives	-	-	-	2.15E+06	9.81E+05	4.88E+06	2.17E+00	2.97E+05	up
CdM1186	Chrysoeriol O-rhamnosyl-O-glucuronic acid	Flavone	6.07E+06	2.02E+04	1.29E+06	-	-	-	2.00E+00	3.66E-06	down
CdM407	C-hexosyl-apigenin O-caffeoylhexoside	Flavone C-glycosides	2.82E+06	3.50E+06	4.18E+06	-	-	-	2.21E+00	2.57E-06	down
CdM529	Selgin O-malonylhexoside	Flavone	8.22E+06	4.11E+06	4.94E+03	-	-	-	1.96E+00	2.19E-06	down
CdM504	Isorhamnetin O-hexoside	Flavonol	1.93E+07	9.65E+06	7.75E+03	-	-	-	2.02E+00	9.32E-07	down
CdM424	8-C-hexosyl-luteolin O-hexoside	Flavone C-glycosides	7.23E+07	1.79E+04	3.62E+07	-	-	-	2.13E+00	2.49E-07	down

Note: VIP: variable importance in the projection value; "-": not detected; A1: Inflorescence in saline-alkali land, A2: Succulent stem in saline-alkali land, B1: Inflorescence in grassland, B2: Succulent stem in grassland, C1: Inflorescence in sandy land, and C2: Succulent stem in sandy land.

Table S2 Information of potential targets

Rank	Diseases	PDB ID	Uniport ID	Gene name	Protein name	Positive Drug	Score of Protein Drug (Kcal.moL^{-1})	Degree
1	Atherosclerosis	3DEI	P42574	*CASP3*	Caspase-3	RXB（(1S)-2-oxo-1-phenyl-2-[(1,3,4-trioxo-1,2,3,4-tetrahydroisoquinolin-5-yl)amino]ethyl acetate）	-7.5	39
2	Atherosclerosis	3I4A	O94760	*DDAH1*	N(G),N(G)-dimethylarginine dimethylaminohydrolase 1	LN5（N5-(1-iminopropyl)-L-ornithine）	-5.2	12
3	Atherosclerosis	3TL5	P48736	*PIK3CG*	Phosphatidylinositol 4,5-Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform	980（(2S)-1-(4-{[2-(2-aminopyrimidin-5-yl)-7-methyl-4-(morpholin-4-yl)thieno[3,2-d]pyrimidin-6-yl]methyl}piperazin-1-yl)-2-hydroxypropan-1-one）	-8.3	26
4	Osteoporosis	1ZW5	P14324	*FDPS*	Farnesyl pyrophosphate synthase	ZOL（zoledronic acid）	-6.2	85
5	Osteoporosis	2VF6	P14324	*FDPS*	Farnesyl pyrophosphate synthase	M0N (MINODRONATE)	-7.2	85
6	Osteoporosis	3KWZ	P43235	*CTSK*	Cathepsin K	4-(3-piperidin-1-ylpropyl)-6-[3-(trifluoromethyl)phenyl]pyrimidine-2-carbonitrile（KWZ）	-6.6	94
7	Osteoporosis	4X6H	P43235	*CTSK*	Cathepsin K	4-amino-3-fluoro-N-(1-{[(2Z)-2-iminoethyl]carbamoyl}cyclohexyl)benzamide	-7.4	94
8	Alzheimer	4AU8	Q00535	*CDK5*	Cyclin-dependent-like kinase 5	Z3R（4-(1,3-benzothiazol-2-yl)thiophene-2-sulfonamide）	-8.5	14
9	Alzheimer	1UNL	Q00535	*CDK5*	Cyclin-dependent-like kinase 5	RRC（R-ROSCOVITINE）	-8.4	14

10	Alzheimer	3ION	O15530	*PDPK1*	3-phosphoinositide-dependent protein kinase 1	8H1（2-(5-{[(2S)-2-amino-3-phenylpropyl]oxy}pyridin-3-yl)-8,9-dimethoxybenzo[c][2,7]naphthyridin-4-amine）	-9.7	12
11	Parkinson	3PO7	P27338	*MAOB*	Amine oxidase [flavin-containing] B	Zonisamide	-7.3	10
12	Ventricular tachycardia	4GQS	P33261	*CYP2C19*	Cytochrome P450 2C19	0XV（4-hydroxy-3,5-dimethylphenyl)(2-methyl-1-benzofuran-3-yl)methanone）	-9.6	3
13	Vascular disease	4BZR	P12821	*ACE*	Angiotensin-converting enzyme	K26 （N-ACETYL-L-ILE-L-TYR-(R)-1-AMINO-2-(4-HYDROXYPHENYL)ETHYLPHOSPHONIC ACID）	-8.5	51
14	Myocardial injury	5D3F	P63104	*YWHAZ*	14-3-3 protein zeta/delta	FSC（fusicoccin）	-7.3	31
15	Rectal Cancer	3E5A	O14965	*AURKA*	Aurora kinase A	VX69CYCLOPROPANECARBOXYLIC ACID {4-[4-(4-METHYL-PIPERAZIN-1-YL)-6-(5-METHYL-2H-PYRAZOL-3-YLAMINO)-PYRIMIDIN-2-YLSULFANYL]-PHENYL}-AMIDE)	-9.8	2

Note: The smaller the score, the better the docking.

Table S3 The results of the docking of the main active components in the succulent stems of *C. deserticola* with disease targets.

No.	Compounds	Binding energy (Kcal·moL^{-1})(PDB ID)
1	2'-O-Acetylpoliumoside	-7.2(3KWZ), -7.8(4X6H), -10(4BZR), -7.5(5D3F)
2	2′-Acetylacteoside	-8(3DEI), -8.5(3TL5), -6.3(1ZW5), -7.1(3KWZ), -8.5 (4BZR)
3	6-Deoxycatalpol	-6.1(3I4A), -8.5(1ZW5), -8.4(2VF6)
4	8-Hydroxygeraniol-1-O-β-D-glucopyranoside	-6.2(3I4A), -8.3(3PO7), -7.5(1ZW5), -7.4(2VF6)
5	8-Epiloganic acid	-8.1(1ZW5), -7.8(2VF6)
6	8-Epideoxyloganic acid	-7.7(1ZW5), -7.5(2VF6)
7	Adoxosidic acid	-7.6(1ZW5), -7.3(2VF6)
8	Antirrhide	-7.2(1ZW5), -7.4(2VF6)
9	Arenarioside	-8.7(3DEI), -6.8(1ZW5), -7.1(3KWZ), -7.8(4X6H), -10.1(4BZR), -7.8(5D3F)
10	Bartsioside	-6.5(3I4A), -8.4(1ZW5), -8.1(2VF6)
11	Betulalbuside A	-7.6(1ZW5), -7.4(2VF6)
12	Campneoside I	-6.7(3KWZ), -9.1(4BZR), -7.3(5D3F)
13	Campneoside II	-7.3(3KWZ), -7.8(4X6H), -9.1(4BZR), -7.4(5D3F)
14	Cistanoside A	-7.8(3DEI), -7.6(4X6H), -10.3(4BZR)
15	Cistanoside F	-9(1ZW5), -8.2(2VF6), -8.6(4BZR)
16	Cistanoside I	-8.9(1ZW5), -8.1(2VF6)
17	Cistanoside K	-8.7(3TL5), -8.4(1UNL), -7.1(3KWZ), -7.6(4X6H), -9(4BZR)
18	Cistanosinenside A	-8.1(3DEI), -6.6(3KWZ), -7.9(4X6H), -9.5(4BZR)
19	Cistanosinensose A1A2	-7(3KWZ), -7.8(4X6H), -9.5(4BZR)
20	CistansinensideB	-8.2(3DEI), -6.8(3KWZ), -10.4(4BZR), -7.3(5D3F)
21	Cistantubulose A1A2	-7.1(1ZW5), -6.6(3KWZ), -7.5(4X6H), -9.9(4BZR)
22	Cistantubuloside A	-7.1(3KWZ), -8.1(4X6H), -10.6(4BZR), -7.4(5D3F)
23	Cistantubuloside B1	-8.5(3TL5), -7.2(3KWZ), -7.9(4X6H), -9.4(4BZR), -8.4(5D3F)
24	Cistantubuloside C1	-7.6(4X6H), -10.1(4BZR)

25	Cistantubuloside C2	-8.1(3DEI), -7(3KWZ), -7.7(4X6H), -10(4BZR)
26	Coniferin	-7.4(1ZW5)
27	Crenatoside	-8.4(3DEI), -7.4(3KWZ), -8.7(4X6H), -9.9(4BZR), -7.9(5D3F)
28	Dehydrodiconiferyl alcohol 4-O-β-D-glucopyranoside	-8.2(3DEI), -7(1ZW5), -7.5(3KWZ), -8.3(4X6H)
29	Dehydrodiconiferyl alcohol γ′-O-β-D-glucopyranoside	-8.7(3DEI), -6.8(3KWZ), -8(4X6H), -7.8(5D3F)
30	Epimeridinoside A	-8.6(3TL5), -8(4X6H), -9.4(4BZR)
31	Eucommin A	/
32	Eutigoside A	-7.9(1ZW5), -7.1(3KWZ), -7.7(4X6H), -7.9(2VF6), -9.1(4BZR), -7.7(5D3F)
33	Geniposidc	-7.6(1ZW5)
34	Gluroside	-6.4(3I4A), -8.8(1ZW5), -8.7(2VF6)
35	Inosine	-6.7(3I4A), -7.6(1ZW5), -7.8(2VF6)
36	Iseucommin A	-8.6(3DEI)
37	Isocistanoside C	-8.7(3DEI), -9.1(3TL5), -8.5(1UNL), -7.5(1ZW5), -7.1(3KWZ), -7.9(4X6H), -9.4(4BZR)
38	Isosyringalide-3′-α-L-rhamnopyranoside	-8.8(3DEI), -7.3(1ZW5), -6.9(3KWZ), -7.8(4X6H), -8.6(4BZR), -7.8(5D3F)
39	Kankanol	-6.3(1ZW5)
40	Kankanose	-8.1(3DEI), -7.7(1ZW5), -6.6(3KWZ), -7.7(4X6H), -9.2(4BZR)
41	Kankanoside D	-6.3(3I4A), -7.8(3PO7), -7.6(1ZW5), -7.4(2VF6)
42	Kankanoside E	-6(3I4A), -7.8(3PO7), -7.6(1ZW5), -7.3(2VF6)
43	Kankanoside F	-8.4(3DEI), -7.8(1ZW5), -7(3KWZ), -8.3(4X6H), -9.5(zyme), -9.4(4BZR)
44	Kankanoside G	-7.4(1ZW5), -7.1(3KWZ), -7.8(4X6H), -8.7(4BZR)
45	Kankanoside H1	-7.7(4X6H), -9.6(4BZR), -7.3(5D3F)
46	Kankanoside I	-8.4(3DEI), -7.3(3KWZ), -7.6(4X6H), -10.5(4BZR), -7.3(5D3F)
47	Kankanoside J1J2	-8.8(3DEI), -8.4(1UNL), -7(3KWZ), -7.9(4X6H), -9.4(4BZR)
48	Kankanoside K1K2	-6.9(3KWZ), -8.2(4X6H), -9.7(4BZR), -7.4(5D3F)
49	Kankanoside L	-7.6(1ZW5), -7.3(2VF6)
50	Kankanoside M	-7.5(1ZW5), -7.4(2VF6)

51	Kankanoside O	-6.1(3I4A), -8.1(3PO7), -7.7(1ZW5), -7.4(2VF6)
52	Kankanoside P	-5.4(3I4A), -7.9(3PO7), -7.7(1ZW5), -7.5(2VF6)
53	Leonuride	-8.3(1ZW5), -7.6(2VF6)
54	Mussaenosidic acid	-8.2(1ZW5), -7.9(2VF6)
55	Ononin	-8.7(3DEI), -9.8(4AU8), -7.9(3PO7), -6.7(3KWZ), -8.1(4X6H)
56	Osmanthuside B	-8.8(3DEI), -8.4(1UNL), -6.5(1ZW5), -7.7(3KWZ), -7.7(4X6H), -7.4(5D3F), -8.8(4BZR), -7.4(5D3F)
57	Pheliposide	-7.9(1ZW5), -7.6(2VF6)
58	Phelypaeside	-7.8(1ZW5), -7.6(2VF6)
59	Plantainoside C	-8.5(3DEI), -8.7(3TL5), -8.5(4AU8), -9(1UNL), -7.6(1ZW5), -7.1(3KWZ), -7.6(4X6H), -9.9 (4BZR)
60	Rhodioloside	-6.7(3I4A), -7.9(3PO7), -8.3(1ZW5), -8.2(2VF6)
61	Salasides A	-8.8(3DEI), -8.7(3TL5), -9(1UNL), -9.7(3ION), -9.1(1ZW5), -7.4(3KWZ), -8(4X6H), -9.4 (2VF6), -9.7(4BZR), -8.6(5D3F)
62	Salasides B	-8.3(3DEI), -9(1ZW5), -7.9(3KWZ), -7.8(4X6H), -9.3(2VF6), -8.8(4BZR), -7.3(5D3F)
63	Salsaside C1C2	-8.6(3DEI), -8.6(3TL5), -8.5(1UNL), -8.6(1ZW5), -7.2(3KWZ), -8.4(4X6H), -9.3(2VF6), -9.6(4BZR), -7.9(5D3F)
64	Salsaside E	-8.3(3DEI), -6.8(3KWZ), -7.8(4X6H), -8.7(4BZR)
65	Salsaside F	-8.1(3DEI), -9.1(3TL5), -9.2(1c3s), -8.5(1UNL), -6.6(1ZW5), -6.6(3KWZ), -9.5(4BZR), -7.3(5D3F)
66	Sinapaldehyde glucoside	-7.2(1ZW5)
67	Syringalide A-3′-α-L-rhamnopyranoside	-8.5(1UNL), -7.7(1ZW5), -7.2(3KWZ), -7.7(4X6H), -9.3(4BZR), -9.6(4GQS)
68	Wiedemanninoside C	-8.5(3DEI), -9.4(1c3s), -7.1(3KWZ), -7.8(4X6H), -9.4(4BZR), -7.3(5D3F)
69	Beta-Sitosterol	-9.4(3DEI), -8.5(1UNL), -7.5(1ZW5), -10.5(3E5A), -8.8(4BZR), -10.5(4GQS), -7.7(5D3F)
70	Tubuloside A	-8(3DEI), -6.8(3KWZ), -7.9(4X6H), -9.7(4BZR), -7.5(5D3F)
71	Tubuloside B	-7.1(3KWZ), -7.5(4X6H), -8.6(4BZR)
72	Tubuloside C	-7.7(4X6H)
73	Tubuloside E	-8.8(3DEI), -9.3(4BZR), -7.4(5D3F)

74	Salidroside	-7.6(1ZW5), -7.5(2VF6)
75	Daucosterol	-9.3(3DEI), -9.8(3ION), -7.3(3KWZ), -8.2(4X6H), -9.8(3E5A), -7.4(5D3F)
76	Cistanoside C	-8.5(3DEI), -6.3(1ZW5), -7(3KWZ), -7.6(4X6H), -9.2(4BZR)
77	Cistanoside D	-8.6(3DEI), -6.8(3KWZ), -7.6(4X6H), -9.2(4BZR)
78	2-(3,4-Dihydroxyphenyl)ethyl 3-O,6-O-bis(a-L-rhamnopyranosyl)-4-O-[(E)-3-(3,4-dihydroxyphenyl)propenoyl-β-D-glucopyranosid	-8.1(3DEI), -7.7(3KWZ), -7.9(4X6H), -8.9(4BZR), -7.8(5D3F)
79	Geniposidic acid	-6.5(3I4A), -7(1ZW5), -7.9(2VF6),
80	Acteoside	-8.2(3DEI), -8.8(3TL5), -8.6(1UNL), -8.1(1ZW5), -7.3(3KWZ), -7.6(4X6H), -9.3(4BZR), -9.6(4GQS), -7.4(5D3F)
81	Decaffeoylacteoside	-8.8(1ZW5), -6.8(3KWZ), -7.6(4X6H), -8.4(2VF6)
82	Panaxytriol	-7.4(3PO7)
83	Cistanoside E	-8.7(1ZW5), -7.4(3KWZ), -8.5(2VF6)
84	CistanosideG	-5.5(3I4A), -8.6(1ZW5), -8.2(2VF6)
85	Cistanoside H	-8(1ZW5)
86	Echinacoside	-8.2(3DEI), -7(3KWZ), -8(4X6H), -10.4(4BZR)
87	Daucosterol	-8.9(3DEI), -8.5(3TL5), -6.9(3KWZ), -7.5(4X6H), -8.6(4BZR), -7.8(5D3F)
88	Isoacteoside	-8.3(3DEI), -7.1(3KWZ), -8.5(4X6H), -8.8(4BZR), -7.6(5D3F)

Note: Atherosclerosis: 3DEI, 3I4A, 3TL5; Alzheimer disease: 4AU8, 1UNL, 3ION; Parkinson: 3PO7; Osteoporosis: 1ZW5, 3KWZ, 4X6H, 2VF6; Rectal cancer: 3E5A; Vascular diseases: 4BZR; Ventricular tachycardia: 4GQS; Myocardial injury: 5D3F; This table only shows results that are better than the positive drug ligand scores.

Table S4 The results of the docking of the main active ingredients with the inflammatory target in the inflorescence of *C. deserticola*.

Disease	Targets	Compounds	Binding energy (Kcal·moL^{-1})
Inflammation	6KBA	Chrysoeriol	-8.6
		Cynaroside	-8.2
		Hesperetin	-8.2
		Homoeriodictyol	-8.3
	7AWC	Chrysoeriol	-7.1
		Cynaroside	-7.5
		Hesperetin	-7.0
		Homoeriodictyol	-7.3

Supplementary Figures

Figure S1 OPLS-DA score map and Permutation tests of inflorescence and Succulent stem in three ecotypes. (a) OPLS-DA score map. High predictability (Q^2) of the OPLS-DA models was observed in the comparison between inflorescence versus Succulent stem in saline–alkali land (Q^2 =0.996), grassland (Q^2=0.997), and sandy land (Q^2= 0.997). (b) Permutation tests of PLS-DA models, the permutation tests were carried out with 200 random permutations. The red dots and blue dots respectively represent R^2 and Q^2 of the model after Y replacement. If R^2 and Q^2 are both smaller than R^2 and Q^2 of the original model, that is, the corresponding points do not exceed the corresponding line, which indicates that the model is meaningful.

A1: Inflorescence in saline-alkali land, A2: Succulent stem in saline-alkali land, B1: Inflorescence in grassland, B2: Succulent stem in grassland, C1: Inflorescence in sandy land, and C2: Succulent stem in sandy land.

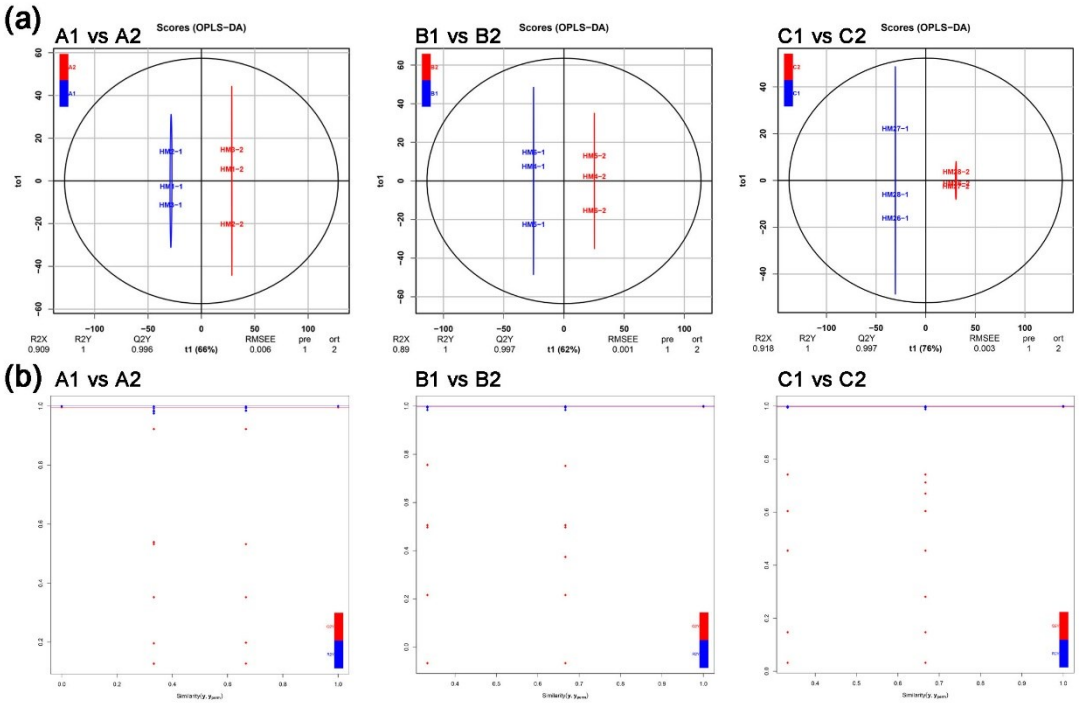

Figure S2 OPLS-DA score map and Permutation tests of differential metabolites related to salt-alkali stress. (a) and (b) OPLS-DA score map and permutation tests plot. High predictability (Q^2) of the OPLS-DA models was observed in the comparison between saline–alkali land versus grassland of inflorescence (Q^2 =0.997) and Succulent stem (Q^2= 0.991). (c) and (d) OPLS-DA score map and permutation tests plot. High predictability (Q^2) of the OPLS-DA models was observed in the comparison between sandy land versus saline–alkali land of inflorescence (Q^2=0.988) and Succulent stem (Q^2= 0.995). Permutation tests of PLS-DA models, the permutation tests were carried out with 200 random permutations. The red dots and blue dots respectively represent R^2 and Q^2 of the model after Y replacement. If R^2 and Q^2 are both smaller than R^2 and Q^2 of the original model, that is, the corresponding points do not exceed the corresponding line, which indicates that the model is meaningful.
A1: Inflorescence in saline-alkali land, A2: Succulent stem in saline-alkali land, B1: Inflorescence in grassland, B2: Succulent stem in grassland, C1: Inflorescence in sandy land, and C2: Succulent stem in sandy land.

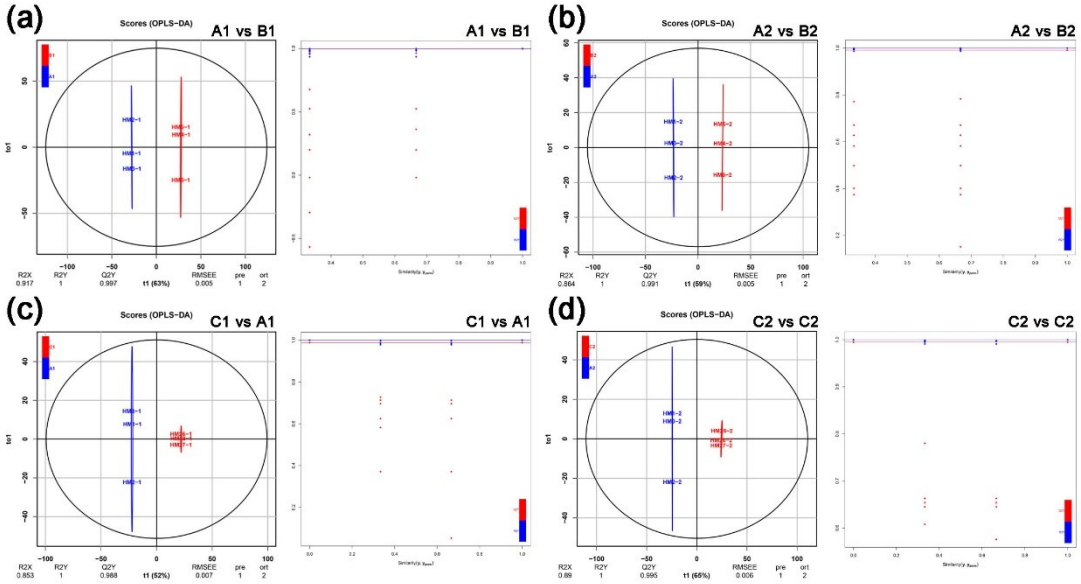

Figure S3 (a) Metabolites of each class content comparison pie chart of inflorescence and succulent stem samples in saline-alkali land. (b) Metabolites of each class content comparison pie chart of inflorescence and succulent stem samples in grassland. (c) Metabolites of each class content comparison pie chart of inflorescence and succulent stem samples in sandy land.

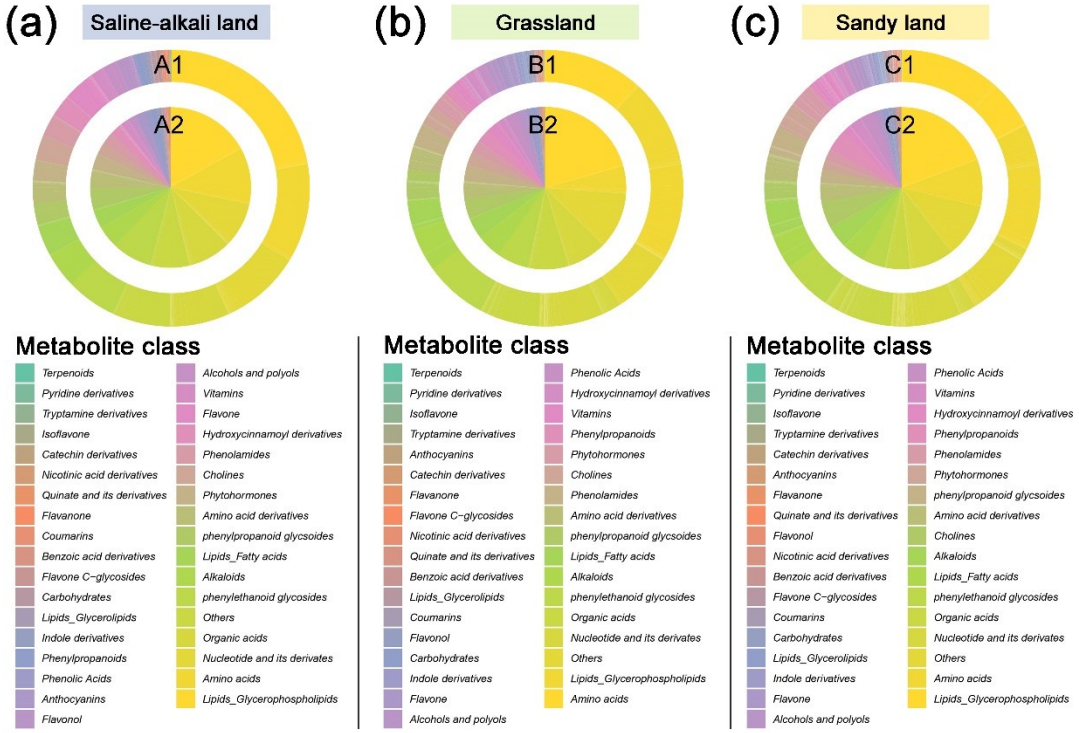

Figure S4 (a) Molecular docking analysis in the succulent stems of *Cistanche deserticola*: Predicted binding mode of important compounds with targets in three-dimensions (3D). 2'-acetylacteoside: vascular disease (4BZR) and atherosclerosis (3TL5); Acteoside: vascular disease (4BZR) and ventricular tachycardia (4GQS); Isoacteoside: vascular disease (4BZR) and osteoporosis (4X6H). (b) Molecular docking analysis in the inflorescence of *Cistanche deserticola*: Predicted binding mode of unique metabolites in inflorescence with important targets related to inflammation in three-dimensions (3D).