1 Chemical characterization, pathway enrichments and bioactive potentials of

2 catechin-producing endophytic fungi isolated from tea leaves

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Supplementary data

S.No.	Name of Compound	Retention time (min)	Relative area (%)	Chemical formula	M.W.
1	Propanoate	5.28	0.14	C ₃ H ₆ O ₂	74.08
2	Butanoic acid	8.63	1.12	$C_4H_8O_2$	88.11
3	Butane	11.92	0.23	C_4H_{10}	58.12
4	Decane	12.42	0.07	C ₁₀ H ₂₂	142.28
5	Propanoic acid	12.53	0.75	$C_3H_6O_2$	74.08
6	Undecane	13.88	0.09	$C_{11}H_{24}$	156.31
7	2-Methyl-pyridine	16.50	0.10	C ₆ H ₇ N	93.13
8	Pantoyl lactone	16.52	0.06	$C_{6}H_{10}O_{3}$	130.14
9	Dodecane	17.05	0.15	C ₁₂ H ₂₆	170.33
10	Pentanoic acid	18.06	0.32	$C_5H_{10}O_2$	102.13
11	Glycerol	19.22	0.15	$C_3H_8O_3$	92.09
12	2-methylpyran-4-one	19.52	0.16	C ₆ H ₆ O ₂	110.11
13	Butanedioic acid	20.41	2.51	C4H6O4	118.09
14	Pentadecane	20.65	0.09	$C_{15}H_{32}$	212.41
15	Benzaldehvde	22.09	0.07	C7H60	106.12
16	1-Dodecene	22.67	1.33	C12H24	168.32
17	Tetradecane	22.87	0.25	$C_{14}H_{30}$	198.39
18	Pentanedioic acid	22.94	0.07	$C_{5}H_{8}O_{4}$	132.11
19	Methylmaleic acid	23.43	0.19	C ₅ H ₆ O ₄	130.10
20	3-ketobutvrate	23.98	0.24	C ₄ H ₆ O ₃	102.09
21	Octanoic acid	24.17	0.11	$C_8H_{16}O_2$	144.21
22	Phenol	25.80	0.83	C ₆ H ₆ O	94.11
23	L-Proline	25.98	0.11	C ₅ H ₉ NO ₂	115.13
24	4-Pyrimidinamine	26.40	0.08	C ₄ H ₅ N ₃	95.10
25	Acetic acid	27.12	1.07	$C_2H_4O_2$	60.05
26	1-Dodecanol	27.26	0.26	C ₁₂ H ₂₆ O	186.33
27	4-Hydroxyphenylethanol	27.30	2.84	$C_8H_{10}O_2$	138.16
28	Hexadecen-1-ol	27.91	1.71	C ₁₆ H ₃₂ O	240.42
29	Phloroglucinol	28.05	0.16	$C_6H_6O_3$	126.11
30	Hexadecane	28.06	0.29	C ₁₆ H ₃₄	226.44
31	Heptadecane	28.07	0.27	C ₁₇ H ₃₆	240.47
32	Benzoic acid	28.68	1.61	$C_7H_6O_2$	122.12
33	Benzeneacetic acid	28.98	3.30	$C_8H_8O_2$	136.15
34	Dodecanoic acid	29.27	0.08	$C_{12}H_{24}O_{2}$	200.32
35	L-Threonic acid	29.91	0.11	$C_4H_8O_5$	136.10
36	11,14-Eicosadienoic acid	30.45	0.12	C ₂₀ H ₃₆ O ₂	308.50
37	Phosphorin	30.76	0.05	C ₅ H ₅ P	96.07
38	Glutaconic acid	31.06	0.23	C ₅ H ₆ O ₄	130.10
39	Nonanedioic acid	31.31	0.05	C ₉ H ₁₆ O ₄	188.22

Table S1. Compounds identified in CSPL6. The corresponding chromatogram is in Fig. 3B.

40	Hydrocinnamic acid	31.75	0.12	$C_9H_{10}O_2$	150.17
41	Azelaic acid	32.59	0.11	C ₉ H ₁₆ O ₄	188.22
42	1-Nonadecene	32.60	1.27	C ₁₉ H ₃₈	266.50
43	Carbamic acid	33.89	0.05	CH ₃ NO ₂	61.04
44	D-Mannopyranose	33.97	0.08	C ₆ H ₁₂ O ₆	180.16
45	13-cis-Retinoic acid	34.42	0.21	$C_{20}H_{28}O_2$	300.44
46	α-D-Glucopyranoside	34.88	0.13	C ₆ H ₁₁ O ₆ -	179.15
47	3-Hydroxyanthranilic acid	34.93	0.07	C ₇ H ₇ NO ₃	153.14
48	Methylglutaconic acid	35.27	0.26	$C_6H_8O_4$	144.13
49	Cinnamic acid	35.67	0.12	$C_9H_8O_2$	148.16
50	n-Pentadecanoic acid	35.84	0.06	$C_{15}H_{30}O_2$	242.40
51	2-Undecenoic acid	35.94	0.32	$C_{11}H_{20}O_2$	184.28
52	10-Undecenoic acid	35.94	0.27	$C_{11}H_{20}O_2$	184.28
53	D-(+)-trehalose	35.967	0.06	$C_{12}H_{22}O_{11}$	342.30
54	2-Quinolinecarboxylic acid	36.71	0.50	$C_{10}H_7NO_2$	173.17
55	Heneicosane	36.98	0.15	$C_{21}H_{44}$	296.57
56	Palmitelaidic acid	37.41	0.50	$C_{16}H_{30}O_2$	254.41
57	Hexadecanoic acid	37.91	4.44	$C_{16}H_{32}O_2$	256.42
58	Trinexapac-ethyl	38.67	0.06	$C_{13}H_{16}O_5$	252.26
59	2-Hydroxy-5-nitrobenzyl alcohol	39.42	0.18	$C_7H_7NO_4$	169.13
60	D-Galactopyranose	39.73	0.29	$C_{6}H_{12}O_{6}$	180.16
61	1,2,4-Triazole	40.05	0.06	$C_2H_3N_3$	69.07
62	1-Docosene	40.74	0.47	$C_{22}H_{44}$	308.59
63	Glycine	40.87	0.91	$C_2H_5NO_2$	75.07
64	9,12-Octadecadienoic acid	40.96	0.09	$C_{18}H_{32}O_2$	280.40
65	11-cis-Octadecenoic acid	41.21	0.11	$C_{18}H_{34}O_2$	282.50
66	3-methylvaleric acid	41.27	0.08	$C_6H_{12}O_2$	116.16
67	Camphoric acid	41.32	0.13	$C_{10}H_{16}O_4$	200.23
68	Octadecanoic acid	41.63	2.12	$C_{18}H_{36}O_2$	284.48
69	Tetratriacontane	41.66	0.08	$C_{34}H_{70}$	478.92
70	2,5-Piperazinedione	42.13	0.05	$C_4H_6N_2O_2$	114.10
71	Tetradecanoic acid	42.98	0.78	$C_{14}H_{28}O_2$	228.37
72	Octacosanol	44.29	0.29	C ₂₈ H ₅₈ O	410.76
73	Uridine	45.13	0.18	$C_{9}H_{12}N_{2}O_{6}$	244.20
74	Linolenic acid	45.68	0.07	$C_{18}H_{30}\overline{O_2}$	278.43
75	5α-Androstan-17-one	45.95	0.09	C ₁₉ H ₃₀ O	274.40
76	1-Methyladenosine	47.44	0.78	$C_{11}H_{15}N_5O_4$	281.27
77	Pregn-4-ene-3,20-dione	47.94	0.14	$C_{21}H_{30}O_2$	316.46
78	2-Amino-1-phenylethanol	49.79	0.12	C ₈ H ₁₁ NO	137.18
79	Benzeneethanamine	49.79	0.16	$C_8H_{11}N$	121.18

S No	Compound Namo	Retention time	Relative area	Relative area Molecular	
5.110.	Compound Name	(min)	(%)	formula	IVI. VV .
1	2-Propenoic acid	5.17	0.29	$C_3H_4O_2$	72.06
2	Propanoate	5.35	0.83	$C_3H_6O_2$	74.08
3	L-(+)-Lactic acid	7.64	0.07	$C_3H_6O_3$	90.08
4	2,3-Butanediol	7.83	0.11	$C_4H_{10}O_2$	90.12
5	Butanoic acid	8.33	4.75	$C_4H_8O_2$	88.11
6	Propanoic acid	12.62	7.50	$C_3H_6O_2$	74.08
7	Butane	16.38	5.40	$C_{4}H_{10}$	58.12
8	n-octene	16.46	0.18	C_8H_{16}	112.21
9	1-Dodecene	16.80	0.26	$C_{12}H_{24}$	168.32
10	Dodecane	17.05	0.07	$C_{12}H_{26}$	170.33
11	Pentanoic acid	18.03	1.42	$C_{5}H_{10}O_{2}$	102.13
12	5-Nonanol	18.09	0.28	$C_9H_{20}O$	144.25
13	Ethyl succinate	18.45	0.05	C ₆ H ₈ O ₄ -2	144.12
14	Glycerol	19.24	0.31	$C_3H_8O_3$	92.09
15	3-Pyridinecarboxylic acid	19.79	0.32	C ₆ H ₅ NO ₂	123.11
16	1,3-Dioxolane	19.92	0.14	$C_3H_6O_2$	74.08
17	Benzeneacetic acid	19.96	4.54	$C_8H_8O_2$	136.15
18	Valproic acid	20.27	0.34	$C_8H_{16}O_2$	144.21
19	Butanedioic acid	20.51	8.15	$C_4H_6O_4$	118.09
20	Benzaldehyde	22.10	0.13	C_7H_6O	106.12
21	1-Tridecene	22.67	0.91	$C_{13}H_{26}$	182.35
22	Tetradecane	22.87	0.13	$C_{14}H_{30}$	198.39
23	Pentanedioic acid	22.95	0.16	$C_5H_8O_4$	132.11
24	D-Isoleucine	23.83	0.15	$C_6H_{13}NO_2$	131.17
25	3-ketobutyrate	23.99	0.23	$C_4H_6O_3$	102.09
26	4H-Pyran-4-one	24.89	0.60	$C_5H_4O_2$	96.08
27	Gly-leu	25.11	0.08	$C_8H_{16}N_2O_3$	188.22
28	Phenol	25.81	0.87	C ₆ H ₆ O	94.11
29	4-Pyrimidinamine	26.41	0.05	$C_4H_5N_3$	95.10
30	Acetic acid	27.13	1.37	$C_2H_4O_2$	60.05
31	1-Dodecanol	27.26	0.23	$C_{12}H_{26}O$	186.33
32	4-Hydroxyphenylethanol	27.30	2.59	$C_8H_{10}O_2$	138.16
33	1-Hexadecene	27.92	1.23	$C_{16}H_{32}$	224.42
34	Hexadecane	28.07	0.15	$C_{16}H_{34}$	226.44
35	6-Amino-1-hexanol	28.33	0.14	C ₆ H ₁₅ NO	117.19
36	Heptanedioic acid	28.43	0.05	$C_7H_{12}O_4$	160.17
37	Benzoic acid	28.68	1.30	$C_7H_6O_2$	122.12
38	Dodecanoic acid	29.27	0.07	C ₁₂ H ₂₄ O ₂	200.32
39	Ala-Thr	29.43	0.10	$C_7 H_{14} N_2 O_4$	190.20
40	Octanedioic acid	30.33	0.11	$C_8H_{14}O_4$	174.19
41	Azelaic acid	32.58	0.24	$C_9H_{16}O_4$	188.22
42	1-Nonadecene	32.61	1.23	$C_{19}H_{38}$	266.50
43	Octadecane	32.74	0.13	$C_{18}H_{38}$	254.49

Table S2. Compounds identified in CSPL5b. The corresponding chromatogram is in Fig. 3C.

44	N-Acetyl-L-phenylalanine	32.85	0.09	$C_{11}H_{13}NO_3$	207.23
45	3-(2-Hydroxyethyl)indole	33.45	0.34	C ₁₀ H ₁₁ NO	161.20
46	Tetradecanoic acid	33.74	0.17	$C_{14}H_{28}O_2$	228.37
47	Hydrocinnamic acid	34.25	0.11	$C_9H_{10}O_2$	150.17
48	3-Hydroxyanthranilic acid	34.93	0.08	C ₇ H ₇ NO ₃	153.14
49	2,5-Piperazinedione	36.12	0.05	$C_4H_6N_2O_2$	114.10
50	4-Aminobenzoic acid	36.83	0.20	C ₇ H ₇ NO ₂	137.14
51	Indole-3-carboxylic acid	36.92	0.12	C ₉ H ₇ NO ₂	161.16
52	Heneicosane	36.97	0.08	$C_{21}H_{44}$	296.57
53	Eicosane	36.97	0.08	$C_{20}H_{42}$	282.55
54	2-Mercaptobenzothiazole	37.32	0.38	C ₇ H ₅ NS ₂	167.25
55	Hexadecanoic acid	37.88	3.07	C ₁₆ H ₃₂ O ₂	256.42
56	Methyl stearate	39.42	0.15	C ₁₉ H ₃₈ O ₂	298.50
57	1-Docosene	40.73	0.45	$C_{22}H_{44}$	308.59
58	9,12-Octadecadienoic acid	40.95	0.09	$C_{18}H_{32}O_2$	280.40
59	Androst-2-en-17-amine	41.04	0.13	$C_{19}H_{31}N$	273.50
60	trans-9-Octadecenoic acid	41.06	0.32	$C_{18}H_{34}O_2$	282.46
61	Octadecanoic acid	41.59	1.87	$C_{18}H_{36}O_2$	284.48
62	Mannopyranose	44.26	0.24	$C_{6}H_{12}O_{6}$	180.16
63	Octacosanol	44.28	0.36	C ₂₈ H ₅₈ O	410.76
64	Uridine	45.11	0.28	$C_9H_{12}N_2O_6$	244.20
65	2'-Deoxyadenosine	47.22	0.06	C ₁₀ H ₁₃ N ₅ O ₃	251.24
66	1-Methyladenosine	47.45	1.61	C ₁₁ H ₁₅ N ₅ O ₄	281.27

Metabolite Set	Total	Hits	Expect	P value	Holm P	FDR
Saturated Fatty Acids	38	9	0.0103	6.6E-25	4.82E-22	4.82E-22
Hydrocarbons	52	6	0.0142	6.17E-15	4.5E-12	2.26E-12
Alkanes	42	5	0.0114	1.05E-12	7.62E-10	2.55E-10
Organic dicarboxylic acids	23	3	0.00626	3.37E-8	2.45E-5	6.15E-6
Unsaturated Fatty Acids	267	4	0.0727	9.64E-7	7.01E-4	1.33E-4
Straight chain Fatty Acids	6	2	0.00163	1.09E-6	7.92E-4	1.33E-4
Dicarboxylic acids	140	3	0.0381	8.32E-6	0.00603	8.69E-4
Pyridoxines	2	1	5.45E-4	5.45E-4	0.394	0.0442
Tyrosols	2	1	5.45E-4	5.45E-4	0.394	0.0442
Phenols	3	1	8.17E-4	8.17E-4	0.59	0.0498
Aminopyrimidines	3	1	8.17E-4	8.17E-4	0.59	0.0498
Benzenetriols	3	1	8.17E-4	8.17E-4	0.59	0.0498
Cinnamic acids	4	1	0.00109	0.00109	0.783	0.0569
Biopterins	4	1	0.00109	0.00109	0.783	0.0569
Hydroxybenzoic acids	6	1	0.00163	0.00163	1.0	0.0746
Pyrimidine ribonucleosides	6	1	0.00163	0.00163	1.0	0.0746
Purine ribonucleosides	8	1	0.00218	0.00218	1.0	0.0808
Quinoline carboxylic acids	8	1	0.00218	0.00218	1.0	0.0808
Disaccharides	9	1	0.00245	0.00245	1.0	0.0808
TCA acids	9	1	0.00245	0.00245	1.0	0.0808
Phenethylamines	9	1	0.00245	0.00245	1.0	0.0808
Benzyl alcohols	9	1	0.00245	0.00245	1.0	0.0808
Hydroxy Fatty Acids	274	2	0.0746	0.0026	1.0	0.0808
Amino acids	277	2	0.0754	0.00265	1.0	0.0808
Sugar alcohols	12	1	0.00327	0.00326	1.0	0.0954
Phenylacetic acids	15	1	0.00408	0.00408	1.0	0.115
Monosaccharides	18	1	0.0049	0.00489	1.0	0.132
Phenylpropanoic acids	23	1	0.00626	0.00625	1.0	0.163
Benzoic acids	24	1	0.00654	0.00652	1.0	0.164
Fatty alcohols	452	2	0.123	0.00686	1.0	0.167
Oxo Fatty Acids	43	1	0.0117	0.0116	1.0	0.275
Retinoids	70	1	0.0191	0.0189	1.0	0.431
C21 steroids	148	1	0.0403	0.0395	1.0	0.861
Oxo Fatty Acids	150	1	0.0408	0.04	1.0	0.861
Branched Fatty Acids	372	1	0.101	0.0964	1.0	1.0

Phytochemical sub-classes identified in CSPL6. Data corresponds to Fig. 4A. Color shade (red to white) indicates a high to low level of abundance.

(104.00	Metabolite Set	Total	Hits	Expect	P value	Holm P	FDR
	Saturated Fatty Acids	38	8	0.00939	3.7E-22	2.71E-19	2.71E-19
	Alkanes	42	4	0.0104	3.66E-10	2.67E-7	1.34E-7
	Hydrocarbons	52	4	0.0128	8.83E-10	6.44E-7	2.15E-7
	Organic dicarboxylic acids	23	3	0.00568	2.5E-8	1.82E-5	4.57E-6
	Straight chain Fatty Acids	6	2	0.00148	8.97E-7	6.52E-4	1.31E-4
	Unsaturated aliphatic hydrocarbons	12	2	0.00297	3.94E-6	0.00286	4.8E-4
	Tyrosols	2	1	4.94E-4	4.94E-4	0.358	0.0493
	Dicarboxylic acids	140	2	0.0346	5.7E-4	0.412	0.0493
	Phenols	3	1	7.41E-4	7.41E-4	0.536	0.0493
	Aminopyrimidines	3	1	7.41E-4	7.41E-4	0.536	0.0493
	Benzenetriols	3	1	7.41E-4	7.41E-4	0.536	0.0493
	Indolecarboxylic acids	4	1	9.88E-4	9.88E-4	0.711	0.0602
	Purine deoxyribonucleosides	5	1	0.00124	0.00123	0.888	0.0645
	Medium-chain keto acids	5	1	0.00124	0.00123	0.888	0.0645
	Hydroxybenzoic acids	6	1	0.00148	0.00148	1.0	0.0677
	Pyrimidine ribonucleosides	6	1	0.00148	0.00148	1.0	0.0677
	Aminobenzoic acids	7	1	0.00173	0.00173	1.0	0.0743
	Purine ribonucleosides	8	1	0.00198	0.00198	1.0	0.0784
	Unsaturated Fatty Acids	267	2	0.066	0.00204	1.0	0.0784
	TCA acids	9	1	0.00222	0.00222	1.0	0.0812
	Sugar alcohols	12	1	0.00297	0.00296	1.0	0.103
	Pyridinecarboxylic acids	14	1	0.00346	0.00345	1.0	0.113
	Phenylacetic acids	15	1	0.00371	0.0037	1.0	0.113
	Indoles	15	1	0.00371	0.0037	1.0	0.113
	Monosaccharides	18	1	0.00445	0.00444	1.0	0.13
	Dipeptides	416	2	0.103	0.00484	1.0	0.136
	Phenylpropanoic acids	23	1	0.00568	0.00567	1.0	0.148
	Fatty alcohols	452	2	0.112	0.00568	1.0	0.148
	Benzoic acids	24	1	0.00593	0.00591	1.0	0.149
	Branched Fatty Acids	38	1	0.00939	0.00935	1.0	0.228
	Oxo Fatty Acids	43	1	0.0106	0.0106	1.0	0.249
	Fatty acid esters	133	1	0.0329	0.0323	1.0	0.739
	Oxo Fatty Acids	150	1	0.0371	0.0364	1.0	0.806
	Amino acids	277	1	0.0685	0.0662	1.0	1.0
	Unsaturated Fatty Acids	911	1	0.225	0.202	1.0	1.0
	Wax monoesters	949	1	0.235	0.21	1.0	1.0

Table S4. Phytochemical sub-classes identified in CSPL5b. Data corresponds to Fig. 4B. Color shade (red to white) indicates a high to low level of abundance.

Pathway Name	Match Status	р	-log(p)	Holm p	FDR	Impact
Biosynthesis of unsaturated fatty acids	4/22	2.2349E-4	3.6507	0.021455	0.021455	0.0
Butanoate metabolism	3/17	0.001686	2.7731	0.16017	0.080928	0.07143
Fatty acid biosynthesis	4/56	0.0080343	2.0951	0.75523	0.19366	0.01429
Glyoxylate and dicarboxylate metabolism	3/29	0.0080691	2.0932	0.75523	0.19366	0.09678
Phenylalanine metabolism	2/11	0.01066	1.9722	0.98072	0.20467	0.125
Sulfur metabolism	2/15	0.019633	1.707	1.0	0.31412	0.0
Propanoate metabolism	2/20	0.033971	1.4689	1.0	0.46588	0.04545
Synthesis and degradation of ketone bodies	1/4	0.058089	1.2359	1.0	0.61962	0.0
Linoleic acid metabolism	1/4	0.058089	1.2359	1.0	0.61962	0.66667
C5-Branched dibasic acid metabolism	1/6	0.085912	1.0659	1.0	0.82475	0.25
Aminoacyl-tRNA biosynthesis	2/46	0.14701	0.83264	1.0	1.0	0.07408
Vitamin B6 metabolism	1/11	0.15208	0.81793	1.0	1.0	0.14286
Nitrogen metabolism	1/12	0.16475	0.78317	1.0	1.0	0.0
Tyrosine metabolism	1/16	0.21366	0.67028	1.0	1.0	0.0
Cutin, suberine, and wax biosynthesis	1/18	0.23707	0.62512	1.0	1.0	0.07143
Citrate cycle (TCA cycle)	1/20	0.25982	0.58532	1.0	1.0	0.07143
Glycerolipid metabolism	1/21	0.27095	0.56711	1.0	1.0	0.03704
Alanine, aspartate and glutamate metabolism	1/22	0.28192	0.54987	1.0	1.0	0.0
Starch and sucrose metabolism	1/22	0.28192	0.54987	1.0	1.0	0.02857
Pyruvate metabolism	1/22	0.28192	0.54987	1.0	1.0	0.03448
Valine, leucine, and isoleucine biosynthesis	1/22	0.28192	0.54987	1.0	1.0	0.05
Thiamine metabolism	1/22	0.28192	0.54987	1.0	1.0	0.05263
Fatty acid elongation	1/23	0.29274	0.53352	1.0	1.0	0.0
Glycolysis / Gluconeogenesis	1/26	0.32425	0.48912	1.0	1.0	0.02941
Glutathione metabolism	1/26	0.32425	0.48912	1.0	1.0	0.0303
Galactose metabolism	1/27	0.33445	0.47566	1.0	1.0	0.0
Tryptophan metabolism	1/28	0.34451	0.4628	1.0	1.0	0.04348
alpha-Linolenic acid metabolism	1/28	0.34451	0.4628	1.0	1.0	0.08333
Cyanoamino acid metabolism	1/29	0.35442	0.45048	1.0	1.0	0.05
Glycine, serine and threonine metabolism	1/33	0.39265	0.40599	1.0	1.0	0.13514
Arginine and proline metabolism	1/34	0.40187	0.39592	1.0	1.0	0.05714
Valine, leucine and isoleucine degradation	1/37	0.42872	0.36783	1.0	1.0	0.0
Fatty acid degradation	1/37	0.42872	0.36783	1.0	1.0	0.02174
Pyrimidine metabolism	1/38	0.43741	0.35911	1.0	1.0	0.04

Table S5. Metabolic pathway impact for CSPL6. Data corresponds to Fig. 4D.

	Match				EDD	T
Pathway Name	Status	р	-log(p)	Holm p	FDK	Impact
Butanoate metabolism	3/17	9.1919E-4	3.0366	0.088242	0.088242	0.07143
Biosynthesis of unsaturated fatty acids	3/22	0.0020038	2.6982	0.19036	0.09618	0.0
Fatty acid biosynthesis	4/56	0.0037623	2.4245	0.35366	0.12039	0.01429
Sulfur metabolism	2/15	0.013311	1.8758	1.0	0.31947	0.0
Propanoate metabolism	2/20	0.023237	1.6338	1.0	0.44558	0.04545
Pyruvate metabolism	2/22	0.027849	1.5552	1.0	0.44558	0.06896
Glycolysis / Gluconeogenesis	2/26	0.038075	1.4194	1.0	0.45812	0.05882
Glyoxylate and dicarboxylate metabolism	2/29	0.046555	1.332	1.0	0.45812	0.03226
Synthesis and degradation of ketone bodies	1/4	0.047721	1.3213	1.0	0.45812	0.0
Linoleic acid metabolism	1/4	0.047721	1.3213	1.0	0.45812	0.66667
Phenylalanine metabolism	1/11	0.1261	0.89929	1.0	1.0	0.0
Nicotinate and nicotinamide metabolism	1/13	0.14735	0.83166	1.0	1.0	0.0
Tyrosine metabolism	1/16	0.17831	0.74883	1.0	1.0	0.0
Cutin, suberine and wax biosynthesis	1/18	0.19836	0.70255	1.0	1.0	0.07143
Citrate cycle (TCA cycle)	1/20	0.21794	0.66166	1.0	1.0	0.07143
Glycerolipid metabolism	1/21	0.22756	0.6429	1.0	1.0	0.03704
Alanine, aspartate and glutamate metabolism	1/22	0.23707	0.62512	1.0	1.0	0.0
Fatty acid elongation	1/23	0.24647	0.60823	1.0	1.0	0.0
Galactose metabolism	1/27	0.28299	0.54823	1.0	1.0	0.0
Folate biosynthesis	1/27	0.28299	0.54823	1.0	1.0	0.03448
Tryptophan metabolism	1/28	0.29185	0.53484	1.0	1.0	0.04348
Valine, leucine and isoleucine degradation	1/37	0.3671	0.43521	1.0	1.0	0.0
Fatty acid degradation	1/37	0.3671	0.43521	1.0	1.0	0.02174
Pyrimidine metabolism	1/38	0.37498	0.42599	1.0	1.0	0.04
Purine metabolism	1/63	0.54434	0.26413	1.0	1.0	0.01333

Table S6. Metabolic impact pathway for CSPL5b. Data corresponds to Fig. 4E.

Table S7. Bioactivities of identified compounds. ▲ means increase; ▼ means decrease; • means no change.

CompoundsBioactivitiesRef	ferences
Palmitic acid $PLA_2 \lor$ (enzyme kinetic study)(Aparna	et al., 2012)
(hexadecanoic acid)	
Phenylacetic acid,Aux/IAAs ▼, TIR1/AFB ▼(Shimizu	ı-Mitao &
(Benzeneacetic acid) Kakimot	to, 2014)
Phytotoxin, Benzoic acid ▲ (Kawazu	ı, Zhang, &
Kanzaki	, 1996)
Antimicrobial activity (Kim et a	al., 2004)
Antifungal activity (Hwang,	Lim, Kim,
Lee, & N	Aoon, 2001;
Slininger	r, Burkhead,
& Schisl	er, 2004)
Myeloperoxidase $\mathbf{\nabla}$, PGE ₂ $\mathbf{\nabla}$, NF $\mathbf{\kappa}$ B $\mathbf{\nabla}$, COX-2 $\mathbf{\nabla}$, (K. M. K	Won et al.,
and mast cell activation V 2024)	
Succinic acid Antioxidant, protein SH groups $\mathbf{\nabla}$, ceruloplasmin $\mathbf{\Delta}$ (Bespyat	tykh,
(Butanedioic acid) Kokorina	a, & Domsk11,
	1 2012
Cardiomyocyte Akt ▲ (lang et	al., 2013)
Stearic acidLipid peroxidation ∇ , PPAR- $\gamma \triangle$, SOD \triangle , CAT \triangle (Zj. Water Stearing	ang, Liang,
(Octadecanoic acid)	& Yin, 2007)
$NF\kappa B \mathbf{\nabla} $ (Pan et a	ıl., 2010)
Tetradecanoic acidFree radical scavenging \blacktriangle , COX \lor (Henry, I)	Momin, Nair,
(myristic acid) & Dewit	t, 2002)
Scavenger receptor BI ▼, cholesteryl ester ▼, sterol (Loison,	Mendy,
27 hydroxylase ▲, 3-hydroxy-3-methyl glutaryl Sérougn	e, & Lutton,
coenzyme A reductase • 2002)	
Modulation ▼▲ of IL-1, TNF-α, IL-8, p38, JNK (Håverse	en,
kinases Danielss	on,
Fogelstra	and, &
Wiklund	, 2009)
Propionic acidLeptin mRNA expression \blacktriangle (S. a. H.(S. a. H.(S. a. H.)	Al-Lahham
(Propanoic acid) $et al., 20$	IU) Lallana at
Lipoprotein lipase \blacktriangle , INF- $\alpha \lor$, IL-4 \lor , IL-10 \lor , (S. a. Al-	-Lannam et
11-8 V, MIP-10 V, MIP-1p V, CCL5 V, and al., 2012)
T cell numbers \blacktriangle II 10 \bigstar and NPC111 \blacktriangledown (Haghiki	12 et al (2022)
$\begin{array}{c} 1 - ccn numbers \blacktriangle, 11 - 10 \clubsuit, and NFC1 1 \lor \\ \hline \\ Glucopeogenic enzymes \blacktriangledown \cdot AMDK \blacktriangle \\ \hline \\ \hline \\ (Voshid) \\ \hline \\ \end{array}$	a Ci al., 2022) a Ishii \Re
Gruconcogenie enzymes V, Alvir K A (105mula	a, 151111, & a 2019)
Butyrate (Butanoic $II_{-6} \bigvee II_{-16} \bigvee and II_{-10} \land$ (F. Wand	u, 20171
	gret al 2017)

	and ABCG8	
	AKT \blacktriangle , and NF- κ B signaling \blacktriangle	(He et al., 2020)
	IL-22 \blacktriangle by CD4 ⁺ T cells and ILCs	(Yang et al., 2020)
Tryptophol (3-(2-	Anti-inflammatory properties, IFN- γ ▼, TNF-α ▼	(Schirmer et al., 2016)
Hydroxyethyl)indole)		
3-Hydroxyanthranilic	TNF-α ▼, IP-10 ▼, IL-8 ●, HO-1 ▼	(Krause et al., 2011)
acid	inhibits the PI3K/Akt/mTOR and NF-kB signaling	(K. Lee, Kwak, &
	pathways, IL-6 $\mathbf{\nabla}$, and TNF- $\mathbf{\alpha}$ $\mathbf{\nabla}$	Pyo, 2016)
Cinnamic acid	Obesity ▼, epididymal fat accumulation ▼, insulin	(A. G. Lee, Kang, Im,
	resistance ▼, glucose intolerance ▼, dyslipidemia ▼	& Pak, 2022)
	TNF- α $\mathbf{\nabla}$, and macrophage infiltration $\mathbf{\nabla}$	
	Reduced Ly6chigh monocytes, M1 adipose tissue	
	macrophages, and hypothalamus microglial activation	
	TNF- $\alpha \lor$, IL-6 \lor , MPO \lor , and TLR-4 \lor	(Rezaei et al., 2024)
Isotretinoin (13-cis-	Antimicrobial activity against Propionibacterium	(Raza et al., 2013)
Retinoic acid)	acnes	
Camphoric acid	Antifungal activity against Physalospora piricola	(Ma et al., 2014)
Phloroglucinol	Inhibits VEGF-dependent migration, EPCs, tumor	(YH. Kwon et al.,
	growth, angiogenesis, and CD45(-)/CD34(+)	2012)
	progenitor mobilization	
	iNOS $\mathbf{\nabla}$, and NF- κ B $\mathbf{\nabla}$	(Li, Khan, Qiu, & Li,
		2018)
	ROS ▼, NF-κB ▼, Bcl-2 ▼, MMP-2 ▼, VEGF ▼;	(Veena, Popavath,
	TNF- $\alpha \lor$, IL-6 \lor , IL-1 $\beta \lor$, and NO \lor	Kennedy, &
		Sakthivel, 2015)
Quinaldic acid (2-	Anti-microbial agent: $\mathbf{\nabla}$ Clostridium difficile and C.	(CH. Lee & Lee,
Quinolinecarboxylic	perfringens, C. difficile, and C. perfringens	2009)
acid)		
Valproate (Valproic	TNF- α $\mathbf{\nabla}$, leukocyte infiltration $\mathbf{\nabla}$, and MPO $\mathbf{\nabla}$	(Ximenes et al., 2013)
acid)	Inflammatory proteins $\mathbf{\nabla}$ (pNF κ B, iNOS, and COX-	(JY. Chen et al.,
	2), pro-apoptotic proteins $\mathbf{\nabla}$ (pAKT/AKT and pGSK-	2018)
	3β /GSK- 3β), and proinflammatory cytokines \checkmark	
	$(\text{TNF-}\alpha \text{ and IL-}1\beta)$	
Azelaic acid	IL-1 $\beta \vee$, IL-6 \vee , TNF- $\alpha \vee$, and NF- $\kappa B \vee$	(Mastrofrancesco et
		al., 2010)
	Antioxidant and free radical scavengers	(Passi et al., 1991;
		Spaggiari et al., 2023)

PLA₂= Phospholipase A₂; Aux= Auxin; IAA= Indole-3-acetic acid; TIR1= Transport inhibitor response 1; AFB= Auxin signaling F-box; PGE₂= Prostaglandin E₂; NF-κβ= Nuclear factor kappa beta; COX= Cyclooxygenase; PPAR- γ = peroxisome proliferator-activated receptor γ ; SOD= Superoxide dismutase; CAT= Catalase; IL= Interleukin; TNF- α = Tumor necrosis factor alpha; JNK= Jun N-terminal kinase; MIP= macrophage inflammatory protein; CCL5=;chemokine (C-C motif) ligand 5; CXCL10= C-X-C motif chemokine ligand 10; NPC111= Niemann-Pick C1-like 1; AMPK= AMP-activated protein kinase; ABCG5= ATP-binding cassette transporters G5; ABCG8= ATP-binding cassette transporters G8; ILCs= Innate lymphoid cells; IFN-γ= Interferon gamma; IP-10= interferon gamma-induced protein 10; HO-1= Heme oxygenase 1; PI3K= phosphoinositide-3-kinase; mTOR= mammalian target of rapamycin; MPO= Myeloperoxidase; TLR4= Toll-like receptor 4; iNOS= Inducible nitric oxide synthase; ROS= Reactive oxygen species; Bcl-2= B-cell lymphoma 2; MMP-2= matrix metalloproteinase-2; EPCs= endothelial progenitor cells; VEGF= vascular endothelial growth factor; NO= Nitric oxide; GSK-3= glycogen synthase kinase-3

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