

SUPPLEMENTAL DATA

Table S1. The information of all compounds in RRL.

ID	Name	OB	DL
M01	chrysophanol-8-o-beta-d-glucopyranoside	59.31	0.03
M02	indoxyl	48.11	0.03
M03	quinazolinone	16.27	0.19
M04	rhodionin	55.79	0.02
M05	rutin	32.45	0.03
M06	α -pinene	44.66	0.03
M07	camphene	41.42	0.02
M08	sabinene	22.70	0.04
M09	cis-coumaric acid	75.28	0.10
M10	β -myrcene	57.80	0.09
M11	α -terpinene	20.18	0.08
M12	limonene	41.42	0.02
M13	β -phellandrene	40.56	0.06
M14	γ -terpinene	19.10	0.67
M15	styrene	8.89	0.02
M16	n-pentanol	42.37	0.24
M17	6-methyl-5-hepten-2-one	51.08	0.05
M18	trans-2-octenal	36.91	0.75
M19	picein	73.43	0.44
M20	β -thujone	17.55	0.78
M21	cis-linalool oxide	4.54	0.85
M22	trans-linalool oxide	66.02	0.48
M23	isomenthone	20.95	0.07
M24	n-decanal	101.44	0.26
M25	benzaldehyde	50.99	0.26
M26	isopinocampone	34.23	0.03
M27	pinocarvone	17.11	0.78
M28	linalool	17.18	0.78
M29	bornyl acetate	81.72	0.04
M30	rosavin	48.08	0.03
M31	β -caryophyllene	12.11	0.14
M32	neomenthol	4.07	0.75
M33	myrtenal	23.11	0.02
M34	menthol	20.88	0.54
M35	trans-pinocarveol	18.21	0.04
M36	α -terpineol	3.20	0.68
M37	geranyl formate	56.44	0.02
M38	carvone	27.37	0.05
M39	geranial	2.42	0.77
M40	geranyl acetate	17.80	0.80

M41	trans-p-coumaric acid	59.94	0.04
M42	myrtenol	46.20	0.05
M43	nerol	35.05	0.04
M44	cis-carveol	55.71	0.01
M45	benzyl alcohol	45.20	0.04
M46	cinnamaldehyde	40.56	0.02
M47	carvacrol	25.21	0.02
M48	cinnamyl alcohol	43.93	0.01
M49	decanoic acid	75.12	0.00
M50	acetovanillone	29.62	0.02
M51	benzyl benzoate	21.14	0.01
M52	kaempferol	10.40	0.20
M53	cinnamic alcohol	18.86	0.02
M54	salidroside	32.90	0.01
M55	β -sitosterol	38.18	0.04
M56	glucobrassicin	7.56	0.19
M57	cinnamyl acetate	75.28	0.04
M58	gallic acid	73.43	0.03
M59	beta-sitosterol, glucoside	69.69	0.04
M60	p-cymene	69.61	0.24
M61	n-nonanol	68.88	0.08
M62	benzyl, glucoside	63.88	0.05
M63	trans-ocimene	59.94	0.04
M64	quercetin,3-o-rutinoside	58.27	0.08
M65	trans-p-coumaric,acid	55.82	0.03
M66	caffeic acid	55.45	0.03
M67	tyrosol	53.99	0.06
M68	1,4-p-menthadien-7-ol	51.39	0.02
M69	indigo	49.79	0.06
M70	gallocatechin, gallate	49.57	0.06
M71	3-carene	48.54	0.04
M72	cuminy acetate	46.34	0.01
M73	neoglucobrassicin	45.52	0.01
M74	geraniol	45.22	0.04
M75	gallic acid ethyl ester	45.17	0.02
M76	umbelliferone	44.26	0.03
M77	perilla aldehyde	43.09	0.03
M78	cyrtophylin	42.94	0.03
M79	benzyl-o-beta-d-glucopyranoside	42.77	0.04
M80	arbutin	42.11	0.03
M81	rosiridin	41.23	0.06
M82	n-hexanol	40.34	0.26
M83	perilla alcohol	39.34	0.02
M84	rhodioloside	38.77	0.03
M85	betulin	38.24	0.03
M86	n-decanol	36.11	0.07

M87	pentadecanoic acid	34.19	0.01
M88	hexanal	33.87	0.03
M89	phenylethyl alcohol	33.62	0.02
M90	4-methoxy-cinnamyl-O-b -D-glucopyranoside	33.19	0.01
M91	cumin alcohol	33.02	0.02
M92	cinnamyl-(6-O-b -xylopyranosyl)-O-b-glucopyranoside	33.01	0.02
M93	quercetin	32.68	0.02
M94	cis-cou-maric acid	32.63	0.01
M95	indirubin	31.88	0.02
M96	p-tyrosol	30.59	0.02
M97	rosarin	30.44	0.09
M98	octadecyl acetate	30.09	0.02
M99	lupenone	29.57	0.02
M100	octanoic acid	29.47	0.02
M101	coumarin	29.26	0.05
M102	santene	28.16	0.04
M103	dodecanoic acid	27.15	0.02
M104	indican	26.15	0.02
M105	n-nonanal	25.61	0.06
M106	n-octanal	24.53	0.04
M107	lupeol	23.20	0.01
M108	trans-2-Nonenal	22.60	0.14
M109	n-octanol	22.23	0.56
M110	quercetin 3-O-rhamnopyranosyl	21.14	0.01
M111	hexadecanoic acid	20.59	0.01
M112	phenylpropenoids rosin	20.55	0.02
M113	2-heptanone	19.30	0.10
M114	scopoletin	18.46	0.03
M115	dodecanol	16.87	0.01
M116	skimmin	16.40	0.02
M117	cuminyl aldehyde	16.15	0.15
M118	b-phellandrene	11.62	0.57
M119	2-pentyl furan	11.61	0.58
M120	hexanoic acid	11.61	0.58
M121	cis-ocimene	10.94	0.21
M122	4-hydroxycinnamyl-O-b -D-glucopyranoside	10.84	0.23
M123	kaemperol-3-O-beta-D-glucopyranoside-7-alpha-O-L-rhamnoside	8.50	0.42
M124	terpinolene	7.01	0.20
M125	rhodiogidin	4.67	0.28
M126	tricyclene	3.20	0.68
M127	heptanal	3.20	0.68

Table S2. The target genes of the potential active compound in RRL.

Target ID	Target name	Gene symbol
T01	Gamma-aminobutyric-acid receptor subunit alpha-3	GABRA3
T02	Glutamate receptor 2	GRIA2
T03	Estrogen receptor beta	ESR2
T04	Sodium channel protein type 5 subunit alpha	SCN5A
T05	Acetylcholinesterase	ACHE
T06	Neuronal acetylcholine receptor subunit alpha-7	CHRNA7
T07	Muscarinic acetylcholine receptor M3	CHRM3
T08	Tyrosine-protein phosphatase non-receptor type 1	PTPN1
T09	Nitric-oxide synthase, endothelial	NOS3
T10	Glycogen synthase kinase-3 beta	GSK3B
T11	Gamma-aminobutyric-acid receptor subunit alpha-1	GABRA1
T12	Androgen receptor	AR
T13	Mitogen-activated protein kinase 14	MAPK14
T14	Proto-oncogene serine/threonine-protein kinase Pim-1	PIM1
T15	Carbonic anhydrase 2	CA2
T16	Beta-2 adrenergic receptor	ADRB2
T17	Prothrombin	F2
T18	Dipeptidyl peptidase 4	DPP4
T19	Retinoic acid receptor RXR-alpha	RXRA
T20	Peroxisome proliferator-activated receptor gamma	PPARG
T21	cAMP-dependent protein kinase catalytic subunit alpha	PRKACA
T22	Prostaglandin G/H synthase 1	PTGS1
T23	cGMP-inhibited 3', 5'-cyclic phosphodiesterase A	PDE3A
T24	Nitric oxide synthase, inducible	NOS2
T25	Phosphatidylinositol-4, 5-bisphosphate 3-kinase catalytic subunit gamma isoform	PIK3CG
T26	Prostaglandin G/H synthase 2	PTGS2
T27	Serine/threonine-protein kinase Chk1	CHEK1
T28	Cyclin-A2	CCNA2
T29	Estrogen receptor	ESR1
T30	Cell division protein kinase 2	CDK2
T31	Heat shock protein HSP 90-alpha	HSP90AA1
T32	Trypsin-1	PRSS1
T33	Amine oxidase [flavin-containing] B	MAOB
T34	Nuclear receptor coactivator 2	NCOA2
T35	Gamma-aminobutyric-acid receptor subunit alpha-2	GABRA2
T36	Chymotrypsinogen B	CTRB1
T37	Amine oxidase [flavin-containing] A	MAOA
T38	Alcohol dehydrogenase 1C	ADH1C
T39	Alcohol dehydrogenase 1B	ADH1B
T40	Alcohol dehydrogenase 1A	ADH1A
T41	Lysozyme	LYZ

T42	Trypsin-3	PRSS3
T43	Gamma-aminobutyric-acid receptor subunit alpha-6	GABRA6
T44	Muscarinic acetylcholine receptor M1	CHRM1
T45	Ig gamma-1 chain C region	IGHG1
T46	Muscarinic acetylcholine receptor M2	CHRM2
T47	Gamma-aminobutyric-acid receptor subunit alpha-4	GABRA4
T48	Gamma-aminobutyric-acid receptor subunit alpha-5	GABRA5
T49	D(1A) dopamine receptor	DRD1
T50	Neuronal acetylcholine receptor subunit alpha-2	CHRNA2
T51	Alpha-1B adrenergic receptor	ADRA1B
T52	Sodium-dependent noradrenaline transporter	SLC6A2
T53	Potassium voltage-gated channel subfamily H member 2	KCNH2
T54	Cholinesterase	CHEI
T55	Beta-1 adrenergic receptor	ADRB1
T56	Alpha-2C adrenergic receptor	ADRA2C
T57	Alpha-1A adrenergic receptor	ADRA1A
T58	Sodium-dependent dopamine transporter	SLC6A3
T59	Alpha-2B adrenergic receptor	ADRA2B
T60	Alpha-2A adrenergic receptor	ADRA2A
T61	Sodium-dependent serotonin transporter	SLC6A4
T62	Progesterone receptor	PGR

Table S3. GlueGO information of targets.

Term	GO Processes	Count	Genes	P-Value
GO:0071880	adenylate cyclase-activating adrenergic receptor signaling pathway	6	ADRB1, ADRA2A, ADRA1B, ADRA1A, ADRA2C, ADRA2B	2.54E-10
GO:0007267	cell-cell signaling	6	ADRB1, ADRA2A, ADRA1B, ADRA1A, ADRA2C, ADRA2B	1.67E-07
GO:0007271	synaptic transmission, cholinergic	4	CHRM3, CHRM2, CHRNA7, CHRNA2	8.24E-05
GO:0006940	regulation of smooth muscle contraction	3	ADRB2, CHRM2, ADRA2C	8.25E-05
GO:0045987	positive regulation of smooth muscle contraction	3	CHRM3, ADRA1B, ADRA1A	1.37E-04
GO:0055117	regulation of cardiac muscle contraction	2	ADRA1B, ADRA1A	7.54E-03
GO:0019371	cyclooxygenase pathway	2	PTGS2, PTGS1	7.54E-03
GO:0001994	norepinephrine-epinephrine vasoconstriction involved in regulation of systemic arterial blood pressure	2	ADRA1B, ADRA1A	1.13E-02
GO:0007263	nitric oxide mediated signal transduction	2	NOS3, NOS2	1.13E-02
GO:0045909	positive regulation of vasodilation	2	NOS3, NOS2	1.13E-02
GO:0006809	nitric oxide biosynthetic process	2	NOS3, NOS2	1.13E-02
GO:0031284	positive regulation of guanylate cyclase activity	2	NOS3, NOS2	1.13E-02
GO:0045776	negative regulation of blood pressure	2	NOS3, NOS2	1.50E-02
GO:0007197	adenylate cyclase-inhibiting G-protein coupled acetylcholine receptor signaling pathway	2	CHRM3, CHRM2	1.87E-02
GO:0007207	phospholipase C-activating G-protein coupled acetylcholine receptor signaling pathway	2	CHRM3, CHRM2	1.87E-02
GO:0006351	transcription, DNA-templated	6	PGR, AR, NCOA2, RXRA, ESR1, ESR2	2.12E-02
GO:0006954	inflammatory response	3	PTGS2, PTGS1, NOS2	2.62E-02
GO:0045907	positive regulation of vasoconstriction	2	ADRA1B, ADRA1A	3.71E-02
GO:0008217	regulation of blood pressure	2	PTGS2, PTGS1	5.16E-02
GO:0007204	positive regulation of cytosolic calcium ion concentration	2	ADRA1B, ADRA1A	5.16E-02
GO:0006979	response to oxidative stress	2	PTGS2, PTGS1	7.99E-02