Supplementary Table 1 Structures of metabolites isolated from *Psoralea corylifolia* L.

Category	No.	Metabolite	Formula	Molecular weight	Reference
Coumarins	1	psoralen	$C_{11}H_6O_3$	186.0317	(Khatune et al., 2004)
	2	isopsoralen	$C_{11}H_6O_3$	186.0317	
	3	8-methoxy psoralen	$C_{12}H_8O_4$	216.0423	(Ji and Xu, 1995)
	4	5-methoxy psoralen	$C_{12}H_8O_4$	216.0423	(Kulikov et al., 2022)
	5	bakuchicin	$C_{11}H_6O_3$	186.0317	(Khatune et al., 2004)
	6	psoralenoside	$C_{17}H_{18}O_9$	366.0951	(Qiao et al., 2006)
	7	isopsoralenoside	$C_{17}H_{18}O_9$	366.0951	
	8	psoralidin	$C_{20}H_{16}O_5$	336.0998	(Khatune et al., 2004)
	9	isopsoralidin	$C_{20}H_{16}O_5$	336.3	(Khastgir et al., 1961)
	10	corylidin	$C_{20}H_{16}O_7$	368.0896	(Gupta et al., 1977)
	11	psoralidin-2′,3′-oxide	$C_{24}H_{20}O_8$	436.4	(Gupta et al., 1980)
	12	3″,4″-dehydroisopsoralidin	$C_{20}H_{14}O_5$	334.33	(Yang et al., 2024)
	13	bvacoumestan A	$C_{20}H_{16}O_6$	352.0947	(Gupta et al., 1990)
	14	bvacoumestan B	$C_{20}H_{16}O_6$	352.0947	
	15	bavacoumestan C	$C_{20}H_{16}O_7$	368.3	(Chai, 2020)
	16	epi-bavacoumestan C	$C_{20}H_{16}O_7$	368.3	(Zhu et al., 2019)
	17	3″-methoxy-bavacoumestan C	$C_{21}H_{18}O_7$	382.3	(Lin et al., 2018)
	18	bavacoumestan D	$C_{20}H_{16}O_5$	336.3	(Chai, 2020)
	19	bavacoumestan E	$C_{21}H_{18}O_5$	350.37	(Zhu et al., 2019)
	20	neopsoralen	$C_{17}H_8O_5$	293.0372	(Peng et al., 1996)
	21	(E)-5-methoxy-8,8-dimethyl-3-[2-methyl-pent-3-en-2-yl-6-phenylpyrano[3,2-g] chromen-2(8H)-one	$C_{27}H_{28}O_4$	416.52	(Srinivasan and Sarada, 2012)
	22	7,2′,4′-trihydroxy-3-aryl-coumarin	$C_{15}H_{10}O_5$	270.0528	(Limper et al., 2013)
	23	psoracoumestan	$C_{20}H_{14}O_5$	334.3	
	24	pyranocoumarin	$C_{20}H_{18}O_4$	322.4	(Srinivasan and Sarada, 2012)
	25	4,5′,8-trioxsalen	$C_{14}H_{12}O_3$	228.2	(Zhang et al., 2017)
	26	sophoracoumestan A	$C_{20}H_{14}O_5$	334.0841	(Gupta et al., 1990)
	27	6-hydroxy-7-prenyl-coumarin	$C_{14}H_{14}O_3$	230.26	(Zhao, 2023)
	28	bavacoumestan F	$C_{20}H_{14}O_6$	350.33	(Xu et al., 2022)
	29	bavacoumestan G	$C_{22}H_{20}O_7$	396.40	
	30	bavacoumestan H	$C_{20}H_{16}O_7$	368.34	
	31	bavacoumestan I	$C_{20}H_{16}O_7$	368.34	
	32	bavacoumestan J	$C_{20}H_{16}O_6$	352.34	

	33	bavacoumestan K	$C_{20}H_{18}O_8$	386.36	(Yang et al., 2024)
	34	bavacoumestan L	$C_{20}H_{14}O_5$	334.33	
	35	coumesterol	$C_{15}H_8O_5$	268.22	
	36	3′-methoxycoumestrol	$C_{16}H_{10}O_6$	298.25	
Flavonoids	37	astragalin	$C_{21}H_{20}O_{11}$	446.0849	(Ji and Xu, 1995)
	38	3,5,3′,4′-tetrahydroxy-7-methoxyflavone-3′-o-α-l-xylopyranosyl(1→3)-o-α-larabinopyranosyl(1→4)-o-β-d-galactopyranoside	$C_{32}H_{38}O_{20}$	742.1956	(Yadava and Verma, 2005)
	39	corylifol C	$C_{21}H_{18}O_5$	338.1154	(Yin et al., 2004)
	40	coryfolia D	$C_{20}H_{16}O_5$	336.0998	(Yang et al., 2009)
	41	5,4′-dihydroxy-6,7-[(1′S,2′R)-1′-hydroxy-2′-(1-hydroxy-1-methylethyl)-furano]-flavonol	$C_{20}H_{18}O_8$	386.36	(Xu et al., 2021a)
	42	neoschaftoside	$C_{26}H_{28}O_{14}$	564.50	(He et al., 2021)
	43	4′-methoxyflavone	$C_{16}H_{12}O_3$	252.0786	(Rajendra Prasad et al., 2004)
	44	bavachin	$C_{19}H_{19}O_4$	324.1362	(Bhalla et al., 1968)
	45	bavachinin	$C_{20}H_{21}O_4$	338.1518	
	46	isobavachin	$C_{20}H_{19}O_4$	324.1362	
	47	6-prenylnaringenin	$C_{20}H_{20}O_5$	340.1311	(Matsuda et al., 2007)
	48	3′-hydroxyl isobavachin	$C_{20}H_{20}O_5$	340.38	(Yin et al., 2004)
	49	2(R,S)-4′-hydroxy-6,7-[2-(1-methoxy-1-methylethyl)-furano]-flavanone	$C_{21}H_{20}O_5$	352.1307	(Ma et al., 2016)
	50	brosimacutin E	$C_{20}H_{20}O_5$	340.38	(Takashima and Ohsaki, 2002)
	51	chromenoflavanone	$C_{20}H_{18}O_4$	322.1205	(Krishnamurti and Parthasarathi, 1981)
	52	bakuflavanone	$C_{20}H_{20}O_5$	340.10	(Cui et al., 2015)
	53	(2S)-7-methoxy-6-(2-hydroxy-3-methylbut-3-en-1-yl)-2-(4-hydroxyphenyl) chroman-4-one	$C_{21}H_{22}O_5$	354.40	(Zhu et al., 2019)
	54	corylifol F	$C_{17}H_{14}O_5$	298.2	(Du et al., 2019)
	55	corylifol H	$C_{20}H_{18}O_5$	338.36	(Liu et al., 2021)
	56	1″-methoxy-6,7-furanflavanone	$C_{21}H_{22}O_6$	370.40	(Zhu et al., 2019)
	57	2(*S*)-4′-hydroxy-7-methoxy-6- (1″, 2″-epoxy-3″-hydroxy dimethyl) flavanone	$C_{21}H_{22}O_6$	370.40	
	58	2(S)-4'-hydroxy-6-methoxy-	$C_{21}H_{20}O_5$	352.39	(Zhao, 2023)

59	7-(2"-carbanyl-3"-methybult-3"enyl)-flavanone (2S)-7,4′-dihydroxyl-6-(2″,3″-epoxy-3″-methylbutyl)-flavanone	$C_{20}H_{20}O_5$	340.38	(Liu et al., 2018)
60	(2*S*) -4′-hydroxyl-7-hydroxymethylene-6-(2″, 3″-epoxy-3″-methylbutyl) -flavanone	$C_{21}H_{22}O_5$	354.40	(Zhu et al., 2019)
61	2(S)-6-methoxy-7-hydroxymethylene-4′-hydroxyl-flavanone	$C_{17}H_{16}O_5$	300.31	(Lin et al., 2018)
62	bavachinone A	$C_{20}H_{18}O_5$	338.36	(Li, 2019)
63	bavachinone B	$C_{20}H_{16}O_5$	336.34	
64	bavachinone C	$C_{20}H_{18}O_5$	338.36	
65	bavachinone D	$C_{17}H_{12}O_4$	280.28	
66	bavachinone E	$C_{20}H_{18}O_6$	354.36	
67	bavachinone F	$C_{20}H_{18}O_5$	338.36	(Xu et al., 2022)
68	bavachinone G	$C_{20}H_{18}O_5$	338.36	
69	bavachinone H	$C_{21}H_{22}O_5$	354.40	
70	bavachinone I	$C_{17}H_{16}O_6$	316.31	
71	bavachinone J	$C_{21}H_{24}O_7$	388.42	
72	furano-(2″,3″:7,6)-4′-hydroxyflavanone	$C_{17}H_{12}O_4$	280.28	
73	abyssinone I	$C_{20}H_{18}O_4$	322.36	
74	2*S*-abyssinone II	$C_{20}H_{20}O_4$	324.38	
75	3′-hydroxylbavachin	$C_{20}H_{20}O_5$	340.38	
76	(2*S*)-7-methoxy-6- (2-hydroxy-3-methylbut-3-en-1-yl)-2-(4-hydroxyphenyl) chroman-4-one	$C_{21}H_{22}O_5$	354.40	(Yang et al., 2024)
77	(2*S*)-6-[(2″*R*)-2″,3″-dihydroxy-3″-methylbutyl]-2-(4-hydroxyphenyl)-7-methoxyflavanone	$C_{21}H_{24}O_6$	372.42	
78	brosimacutin D	$C_{20}H_{20}O_5$	340.4	(Liu, 2019)
79	brosimacutin E	$C_{20}H_{20}O_5$	340.4	
80	bavadin	$C_{27}H_{30}O_{13}$	562.1686	(Yang and Qin, 2006)
81	8-geranyldaidzein	$C_{24}H_{24}O_4$	376.45	(Liu et al., 2021)
82	bavaisoflavone A	$C_{17}H_{10}O_4$	278.26	
83	bavaisoflavone B	$C_{20}H_{14}O_4$	318.33	
84	bavaisoflavone C	$C_{20}H_{16}O_5$	336.34	
85	bavaisoflavone D	$C_{21}H_{18}O_5$	350.37	
86	bavaisoflavone E	$C_{20}H_{18}O_6$	354.36	
87	bavaisoflavone F	$C_{20}H_{18}O_5$	338.36	
88	bavaisoflavone G	$C_{20}H_{18}O_5$	338.36	
89	bavaisoflavone H	$C_{23}H_{24}O_7$	412.44	(Xu et al., 2022)
90	bavaisoflavone I	$C_{25}H_{28}O_6$	424.49	
91	bavaisoflavone J	$C_{25}H_{26}O_6$	422.48	
92	bavaisoflavone K	$C_{25}H_{26}O_5$	406.48	
93	bavaisoflavone L	$C_{25}H_{26}O_6$	422.48	
94	bavaisoflavone M	$C_{25}H_{26}O_6$	422.48	
95	bavaisoflavone N	$C_{25}H_{24}O_5$	404.46	
96	bavaisoflavone O	$C_{25}H_{24}O_5$	404.46	
97	bavaisoflavone P	$C_{25}H_{26}O_5$	406.48	

98	corylifol A	$C_{25}H_{26}O_4$	390.1831	(Yin et al., 2004)
99	corylifols D	$C_{20}H_{18}O_5$	338.36	(Song et al., 2013)
100	corylifols E	$C_{20}H_{18}O_6$	354.1103	
101	corylifol G	$C_{25}H_{26}O_5$	406.4	(Du et al., 2019)
102	neobavaisoflavone	$C_{20}H_{18}O_4$	322.4	(Li, 2019)
103	isoneobavaisoflavone	$C_{20}H_{18}O_4$	322.4	(Yin et al., 2004)
104	corylin	$C_{20}H_{16}O_4$	320.3	(Liu, 2019)
105	genistein	$C_{15}H_{10}O_5$	270.0528	(Hsu et al., 2001)
106	daidzein	$C_{15}H_{10}O_4$	254.0579	
107	biochanin A	$C_{16}H_{11}O_5$	284.0685	
108	8-prenyldaidzein	$C_{20}H_{18}O_4$	322.1205	(Qiu et al., 2010)
109	bakuisoflavone	$C_{20}H_{18}O_5$	338.10	(Cui et al., 2015)
110	erythrinin A	$C_{20}H_{16}O_4$	320.1049	(Yin et al., 2004)
111	hydroxypsoralenol A	$C_{20}H_{18}O_5$	338.10	(Suri et al., 1978)
112	hydroxypsoralenol B	$C_{20}H_{18}O_6$	354.36	
113	psoralenol	$C_{20}H_{18}O_5$	338.1154	
114	neocorylin	$C_{25}H_{24}O_4$	322.1205	(Choi et al., 2008)
115	myrsininone A	$C_{25}H_{26}O_5$	406.48	(Limper et al., 2013)
116	wighteone	$C_{20}H_{18}O_5$	338.1154	
117	isowighteone	$C_{20}H_{18}O_5$	338.1154	
118	3′-hydroxydaidzein	$C_{15}H_{10}O_5$	270.24	
119	3′-methoxydaidzein	$C_{16}H_{12}O_5$	284.27	(Yang et al., 2024)
120	4′,7-dihydroxy-3′,5′-diprenyl-isoflavone	$C_{25}H_{26}O_4$	390.48	
121	corylinal	$C_{16}H_{10}O_5$	282.0528	(Wei et al., 2019)
122	4′,7-dihydroxy-3′-(6″ β-hydroxy-3″,7″-dimethyl-,2″,7″-dibutenyl)-geranylisoflavone	$C_{25}H_{26}O_5$	406.48	(Lin et al., 2018)
123	4′,7-dihydroxy-3′-(7″-hydroxy-7″-methyl-2″,5″-dibutenyl)-geranylisoflavone	$C_{25}H_{26}O_5$	406.48	
124	daidzin	$C_{20}H_{18}O_9$	416.1107	(Qiu et al., 2010)
125	corylinin	$C_{25}H_{26}O_4$	390.5	(Ruan et al., 2007)
126	7-*O*-methylcorylifol A	$C_{26}H_{28}O_4$	404.51	(Chen et al., 2017)
127	7-*O*-isoprenylcorylifol A	$C_{30}H_{34}O_4$	458.60	
128	7-*O*-isoprenylneobavaisoflavone	$C_{25}H_{26}O_4$	390.48	
129	5,7,4'-trihydroxyflavone	$C_{15}H_{10}O_5$	270.0528	(Liu et al., 2008)
130	7-methoxybakuchiol	$C_{21}H_{20}O_5$	352.39	(Suri et al., 1978)
131	3″-acetoxy-7-methoxybakuchiol	$C_{23}H_{22}O_6$	394.42	
132	3″,7-acetoxybakuchiol	$C_{25}H_{25}O_7$	437.47	
133	corylisoflavone A	$C_{18}H_{18}O_6$	330.34	(Dong et al., 2015)
134	bavarigenin-4″-O-β-d-	$C_{27}H_{30}O_{12}$	561.1976	(Shi et al.,

	glucopyranoside			2024)
135	bavarigenin-4″-O-β-d-glucopyranoside-4′-O-β-d-fucopyranoside	$C_{33}H_{40}O_{16}$	705.2367	
136	daidzein-3′-carboxylic acid	$C_{16}H_{10}O_6$	297.0413	
137	bavachalcone	$C_{20}H_{20}O_4$	324.40	(Bhalla et al.,
138	isobavachalcone	$C_{20}H_{20}O_4$	324.40	1968)
139	neobavachalcone	$C_{17}H_{14}O_6$	314.0790	(Gupta et al., 1977)
140	isoneobavachalcone	$C_{17}H_{14}O_5$	314.0790	(Bhalla et al., 1968)
141	bavachromanol	$C_{20}H_{20}O_5$	340.4	(Suri et al., 1980)
142	corylifol B	$C_{20}H_{20}O_5$	340.4	(Yin et al., 2004)
143	bavachromene	$C_{20}H_{18}O_4$	322.1205	(Lee et al.,
144	isobavachromene	$C_{20}H_{18}O_4$	322.1205	2005)
145	brosimacutin G	$C_{20}H_{20}O_6$	356.4	(Yin et al., 2004)
146	bakuchalcone	$C_{20}H_{20}O_5$	340.4	
147	psorachalcone A	$C_{20}H_{20}O_5$	340.38	(Yu, 2005)
148	psorachalcone B	$C_{20}H_{20}O_5$	340.38	
149	psorachalcone C	$C_{21}H_{24}O_7$	388.42	(Xu et al., 2022)
150	psorachromene	$C_{20}H_{18}O_4$	322.36	
151	4,2′-dihydroxy-2″-(1‴-methylethyl)-2″3″-dihydro-(4″,5″,3′,4′) furano chalk one	$C_{20}H_{20}O_4$	324.1362	(Agarwal et al., 2006)
152	4′-*O*-methylbavachalcone	$C_{21}H_{22}O_4$	338.40	
153	xanthoangelol	$C_{25}H_{28}O_4$	392.1988	(Limper et al., 2013)
154	kanzonol B	$C_{25}H_{24}O_4$	388.46	
155	licoagrochalcone A	$C_{20}H_{20}O_4$	324.38	
156	lespecyrtin B_3	$C_{20}H_{20}O_5$	340.38	
157	(1- [2, 4-dihydroxy-3- (3-methylbut-2-enyl)phenyl] -3- (4-hydroxyphenyl)propan- 1-one)	$C_{20}H_{22}O_4$	326.39	
158	(*E*)-1-(6-hydroxybenzofuran-5-yl) -3-(4-hydroxyphenyl)prop-2-en-1-one	$C_{17}H_{12}O_4$	280.28	(Yang et al., 2024)
159	(*E*) -1- (4-hydroxybenzofuran-5-yl) -3-(4-hydroxyphenyl)prop-2-en-1-one	$C_{17}H_{12}O_4$	280.28	
160	[3′, 4′-(3-hydroxy-2, 2-dimethyldihydropyrano)-2′, 4-dihydroxychalcone	$C_{20}H_{20}O_5$	340.38	
161	1-(3,4-dihydro-5-hydroxy-2,2-dimethyl-2*H*-1-benzopyran-8-yl) -3- (4-hydroxyphenyl) -2-propen-1-one	$C_{20}H_{20}O_4$	324.38	
162	artonin ZA	$C_{20}H_{18}O_4$	332.36	(Du et al.,

				2019)
163	4,2',3'-trihydroxy-4'-(2"β-hydroxy-3"-methybult-3"-enyl) chalcone	$C_{20}H_{20}O_5$	340.38	
164	4,2',3'-trihydroxy-4'-(2"α-hydroxy-3"-methybult-3"-enyl) chalcone	$C_{20}H_{20}O_5$	340.38	
165	4,2'-dihydroxy-4'-methoxy-5'-(2"β-hydroxy-3"-methybult-3"-enyl) chalcone	$C_{21}H_{20}O_5$	354.40	
166	4,2',4'-trihydroxy-3'-(2"α-3"-dihydroxy-3"-dimethybult) chalcone	$C_{20}H_{22}O_6$	358.39	
167	4,2',4'-trihydroxy-3'-(2"β-3"-dihydroxy-3"-dimethybult) chalcone	$C_{20}H_{22}O_6$	358.39	(Zhao, 2023)
168	4-hydroxy-3',4'-(2"α-3"-hydroxy-3"-dimethybult) furano-chalcone	$C_{20}H_{20}O_5$	340.38	
169	4,2',3'-trihydroxy-4'-methoxy-5'-(2"β-hydroxy-3"-methoxy-3"-dimethybult) chalcone	$C_{22}H_{26}O_6$	386.44	
170	4,2',3'-trihydroxy-4'-prenyl-chalcone	$C_{20}H_{20}O_4$	324.38	
171	4,2′-dihydroxy-4′-methoxy-5′-(3″,3″dimethylallyl) chalkone	$C_{21}H_{22}O_4$	354.40	(Gao et al., 2021)
172	bavaisoflavanol	$C_{20}H_{22}O_6$	358.39	(Xu et al., 2022)
173	6-(γ,γ-dimethylallyl)-4′-hydroxy-7-methoxy-(2R,3R)-dihydroflavonol	$C_{21}H_{22}O_5$	353.1400	(Shi et al., 2024)
174	coryaurone A	$C_{20}H_{18}O_6$	354.36	
175	(2*Z*) -2- [(4′-hydroxyphenyl) -methylene] -6-hydroxy-7-prenyl-3(2*H*) -benzofurane	$C_{20}H_{18}O_4$	322.36	
176	7,2′,5′-trihydroxy-8-prenylaurone	$C_{20}H_{18}O_5$	338.36	
177	licoagroaurone	$C_{20}H_{18}O_5$	338.36	
178	damaurone C	$C_{21}H_{18}O_5$	350.37	
179	damaurone D	$C_{20}H_{18}O_4$	322.36	
180	(*Z*)-2-(4-methoxybenzylidene)- 7, 7-dimethyl-7, 8-dihydro-2*H*-furo[2, 3-*f*]chromene-3, 9-dione	$C_{22}H_{20}O_5$	364.40	(Zhao et al., 2021)
181	(*Z*) -4, 6-dimethoxy-7, 4′-dihydroxyaurone	$C_{17}H_{14}O_6$	314.29	
182	rugaurone B	$C_{16}H_{12}O_5$	284.27	
183	6,7,3′,4′-tetrahydroxyaurone	$C_{15}H_{10}O_6$	286.24	
184	(2*Z*) -2- [(3′, 4′-dihydroxyphenyl) -methylene] -6-methoxy-7-prenyl-3(*2H*) -benzofurane	$C_{21}H_{20}O_5$	352.39	
185	(2*Z*) -2- [(4′-hydroxyphenyl) -methylene] -6-methoxy-7-	$C_{21}H_{20}O_4$	336.39	

		prenyl-3 (2*H*)-benzofurane			
	186	bakuchiol	$C_{18}H_{24}O$	256.1827	(Mehta et al., 1966)
	187	bisbakuchiols A	$C_{36}H_{46}O_4$	542.3396	(Wu et al., 2007)
	188	bisbakuchiols B	$C_{36}H_{46}O_4$	542.3396	
	189	bisbakuchiols C	$C_{36}H_{48}O_3$	528.78	(Wu et al., 2008)
	190	2,3-epoxybakuchiol	$C_{18}H_{24}O_2$	272.39	
	191	delta(1),3-hydroxybakuchiol	$C_{18}H_{24}O_2$	272.1776	(Huang et al., 2014)
	192	delta (3),2-hydroxybakuchiol	$C_{18}H_{24}O_2$	272.1776	
	193	corylifolin	$C_{13}H_{16}O$	188.1201	(Sun et al., 1998)
	194	psoracorylifol A	$C_{18}H_{24}O_3$	288.1725	
	195	psoracorylifol B	$C_{18}H_{24}O_3$	288.1725	(Yin et al., 2006)
	196	psoracorylifol C	$C_{18}H_{24}O_3$	288.1725	
	197	psoracorylifol D	$C_{18}H_{24}O_2$	272.1776	
	198	psoracorylifol E	$C_{18}H_{24}O_2$	272.1776	
	199	psoracorylifol F	$C_{18}H_{24}O_2$	272.1776	(Xiao et al., 2012)
	200	psoralen ether	$C_{23}H_{30}O$	324.51	
	201	psoracorylifol G	$C_{19}H_{26}O$	270.42	(Yang et al., 2022)
	202	psoracorylifol H	$C_{18}H_{24}O_3$	288.1725	
	203	7α,8α,12α-psoracorylifol A	$C_{19}H_{26}O_3$	302.41	
	204	7α,8α,12β-psoracorylifol A	$C_{19}H_{26}O_3$	302.41	(Zhao, 2023)
	205	7α,8β,12α-psoracorylifol A	$C_{19}H_{26}O_3$	302.41	
	206	(12′S)-bisbakuchiol C	$C_{36}H_{48}O_3$	528.3603	(Wu et al., 2008)
	207	12,13-dihydro-12,13-dihydroxybakuchiol	$C_{18}H_{26}O_3$	290.40	
Meroterpenes	208	delta(1),3-bakuchiol	$C_{18}H_{22}O$	254.37	
	209	12,13-dihydro-13-hydroxybakuchiol	$C_{18}H_{26}O_2$	274.1933	
	210	15-demetyl-12,13-dihydro-13-ketobakuchiol	$C_{17}H_{22}O_2$	258.36	(Huang et al., 2014)
	211	delta(10)-12,13-dihydro-12(R)-methoxyisobakuchiol	$C_{19}H_{26}O_2$	286.1933	
	212	delta(10)-12,13-dihydro-12(S)-methoxyisobakuchiol	$C_{19}H_{26}O_2$	286.1933	
	213	delta(11)-12-hydroxy-12-dimethyl bakuchiol	$C_{18}H_{24}O_2$	272.39	(Lin et al., 2018)
	214	13-methoxyisobakuchiol	$C_{19}H_{26}O_2$	286.1933	(Huang et al.,
	215	13-ethoxyisobakuchiol	$C_{20}H_{28}O_2$	300.2089	2014b)
	216	13-hydroxyisobakuchiol	$C_{18}H_{24}O_2$	272.39	
	217	8*α*-hydroxy-cyclobakuchiol C	$C_{18}H_{26}O_3$	290.1882	(Yang et al., 2024)
	218	8-ketone-cyclobakuchiol C	$C_{18}H_{24}O_3$	288.1725	
	219	7*α*,8*β*-hydroxy-12*β*-cyclobakuchiol C	$C_{18}H_{26}O_3$	290.1882	
	220	12*α*-psoracorylifol F	$C_{18}H_{24}O_2$	272.1776	(Xiu et al., 2021)
	221	7*β*,8*α*-hydroxy-12*β*-psoracorylifol F	$C_{18}H_{24}O_2$	272.1776	
	222	psoracorylifether	$C_{23}H_{30}O$	322.49	(Yang et al., 2022)
	223	12R,13-diolbakuchiol	$C_{18}H_{26}O_3$	290.40	
	224	12S,13-diolbakuchiol	$C_{18}H_{26}O_3$	290.40	(Liu, 2019)
	225	corypsoriol A	$C_{18}H_{24}O_2$	272.1776	(Yang et al.,
	226	corypsoriol B	$C_{18}H_{24}O_2$	272.1776	2024)

	227	corypsoriol C	$C_{18}H_{24}O_3$	288.1725	
	228	corypsoriol D	$C_{18}H_{22}O_3$	286.37	
	229	corypsoriol E	$C_{18}H_{22}O_3$	286.37	
	230	corypsoriol F	$C_{18}H_{24}O_4$	304.39	
	231	corypsoriol G	$C_{18}H_{24}O_4$	304.39	
	232	corypsoriol H	$C_{18}H_{24}O_2$	272.1776	
	233	corypsoriol I	$C_{19}H_{26}O_3$	302.41	
	234	corypsoriol J	$C_{19}H_{26}O_3$	302.41	
	235	corypsoriol K	$C_{19}H_{26}O_3$	302.41	
	236	corypsoriol L	$C_{19}H_{26}O_3$	302.41	
	237	corypsoriol M	$C_{19}H_{26}O_3$	302.41	
	238	corypsoriol N	$C_{19}H_{26}O_3$	302.41	
	239	cyclobakuchiol A	$C_{18}H_{24}O$	256.1827	(Huang et al., 2014)
	240	cyclobakuchiol B	$C_{18}H_{24}O$	256.1827	
	241	cyclobakuchiol C	$C_{18}H_{26}O_2$	274.1933	(Yin et al., 2007)
	242	bakuchiol ether A	$C_{29}H_{42}O_2$	422.65	(Xu et al., 2021)
	243	bakuchiol ether B	$C_{33}H_{50}O_2$	478.76	
	244	bakuchiol ether C	$C_{32}H_{46}O_2$	462.72	
	245	bisbakuchiol A	$C_{36}H_{46}O_4$	542.76	(Wu et al., 2007)
	246	bisbakuchiol B	$C_{36}H_{46}O_4$	542.76	
	247	bisbakuchiol D	$C_{36}H_{48}O_3$	528.78	
	248	bisbakuchiol E	$C_{36}H_{48}O_3$	528.78	
	249	bisbakuchiol F	$C_{36}H_{48}O_3$	528.78	
	250	bisbakuchiol G	$C_{36}H_{48}O_3$	528.78	(Xu et al., 2021)
	251	bisbakuchiol H	$C_{36}H_{46}O_4$	542.76	
	252	bisbakuchiol I	$C_{36}H_{46}O_4$	542.76	
	253	bisbakuchiol J	$C_{36}H_{48}O_4$	544.78	
	254	bisbakuchiol K	$C_{36}H_{48}O_4$	544.78	
	255	bisbakuchiol L	$C_{36}H_{48}O_4$	544.78	
	256	bisbakuchiol V	$C_{36}H_{48}O_4$	544.78	(Yang et al., 2022)
	257	bisbakuchiol M	$C_{36}H_{40}O_4$	536.71	
	258	bisbakuchiol N	$C_{36}H_{46}O_2$	510.76	
	259	bisbakuchiol O	$C_{36}H_{46}O_2$	510.76	
	260	bisbakuchiol P	$C_{36}H_{46}O_2$	510.76	(Xu et al., 2021)
	261	bisbakuchiol Q	$C_{36}H_{46}O_3$	526.76	
	262	bisbakuchiol R	$C_{37}H_{50}O_4$	558.80	
	263	bisbakuchiol S	$C_{37}H_{50}O_4$	558.80	
	264	bisbakuchiol T	$C_{36}H_{46}O_3$	526.76	
	265	bisbakuchiol U	$C_{36}H_{46}O_3$	526.76	
	266	12′*S*-bisbakuchiol C	$C_{36}H_{48}O_3$	528.78	(Yin et al., 2007)
Benzofurans	267	corylifonol	$C_{13}H_{14}O_4$	234.25	(Kuo and Lin, 1992)
	268	isocorylifonol	$C_{13}H_{14}O_4$	234.25	
	269	dihydrobutylcnideoside A	$C_{21}H_{28}O_9$	424.45	
	270	butylcnideoside A	$C_{21}H_{26}O_9$	422.43	
	271	methylcnidioside A	$C_{18}H_{20}O_9$	380.35	
	272	isopsoralenoside butyl ester	$C_{21}H_{26}O_9$	422.43	(He et al., 2021)
	273	isopsoralenoside methyl ester	$C_{18}H_{20}O_9$	380.35	
	274	dihydroisopsoralenoside butyl ester	$C_{21}H_{28}O_9$	424.45	
	275	dihydroisopsoralenoside methyl ester	$C_{18}H_{22}O_9$	382.37	
Dimers	276	psocorylin A	$C_{39}H_{46}O_6$	610.79	(Xu et al., 2020)
	277	psocorylin B	$C_{38}H_{44}O_6$	596.76	

	278	psocorylin C	$C_{38}H_{44}O_6$	596.76	
	279	psocorylin D	$C_{38}H_{44}O_6$	596.76	
	280	psocorylin E	$C_{38}H_{44}O_6$	596.76	
	281	psocorylin F	$C_{38}H_{42}O_6$	594.75	
	282	psocorylin G	$C_{39}H_{44}O_6$	608.78	
	283	psocorylin H	$C_{39}H_{44}O_5$	592.78	
	284	psocorylin I	$C_{39}H_{44}O_6$	608.78	
	285	psocorylin J	$C_{39}H_{46}O_6$	610.79	
	286	psocorylin K	$C_{39}H_{46}O_7$	626.79	
	287	psocorylin L	$C_{39}H_{44}O_5$	592.78	
	288	psocorylin M	$C_{38}H_{44}O_6$	596.76	
	289	psocorylin N	$C_{38}H_{42}O_7$	610.75	
	290	psocorylin O	$C_{38}H_{42}O_7$	610.75	
	291	psocorylin P	$C_{38}H_{38}O_7$	606.72	
	292	psocorylin Q	$C_{38}H_{40}O_5$	576.73	
	293	psocorylin R	$C_{40}H_{40}O_8$	648.75	
	294	psocorylin S	$C_{40}H_{40}O_8$	648.75	
	295	psocorylin T	$C_{40}H_{38}O_9$	662.74	
	296	psocorylin U	$C_{40}H_{38}O_9$	662.74	(Xu et al., 2023)
	297	psocorylin V	$C_{40}H_{36}O_9$	660.72	
	298	psocorylin W	$C_{40}H_{36}O_9$	660.72	
	299	psocorylin X	$C_{40}H_{36}O_{10}$	676.72	
	300	psocorylin Y	$C_{39}H_{40}O_9$	652.74	
	301	psocorylin Z	$C_{41}H_{36}O_9$	672.73	
Other metabolites	302	uracil	$C_4H_4N_2O_2$	112.09	(Ruan and Kong, 2005)
	303	β-stigmasterol	$C_{29}H_{48}O$	412.70	(Tan, 2017)
	304	psoralester	$C_{22}H_{38}O_4$	366.54	(Tewari and Bhakuni, 2010)
	305	palmitic acid	$C_{16}H_{32}O_2$	256.43	
	306	stearic acid	$C_{18}H_{36}O_2$	284.48	(Tan, 2017)
	307	linoleic acid	$C_{18}H_{32}O_2$	280.45	
	308	pinitol	$C_7H_{14}O_6$	194.18	(Qiu et al., 2010)
	309	daucosterol	$C_{35}H_{60}O_6$	576.86	
	310	triacylglycerols	$C_{39}H_{74}O_6$	639.02	(Lu et al., 2019)
	311	glycerol diesters	$C_{27}H_{52}O_5$	456.71	
	312	glycerol monoesters	$C_{21}H_{44}O_3$	344.58	
	313	raffinose	$C_{11}H_{20}O_{10}$	312.27	
	314	methyl p-hydroxybenzoate	$C_8H_8O_3$	152.15	(Qiu et al., 2010)
	315	p-hydroxybenzaldehyde	$C_7H_6O_2$	122.12	(Peng et al., 1996)
	316	adenosine	$C_{10}H_{13}N_5O_4$	267.25	
	317	guanosine	$C_{10}H_{13}N_5O_5$	283.24	(He et al., 2021)
	318	1-ribitol-2, 3-dione-1, 2, 3, 4-tetrahydro-6, 7-dimethyl-quinoxaline	$C_{15}H_{20}N_2O_6$	324.33	
	319	glyinflain A	$C_{25}H_{28}O_5$	408.49	(Zhao et al., 2021)
	320	stigmasterol-3-*O*-*β*-*D*-glucopyranosyl-6′-*O*-palmitate	$C_{51}H_{88}O_7$	813.26	(Yang et al., 2022)
	321	*p*-hydroxybenzaldehyde	$C_7H_6O_2$	122.12	

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