

A1-A2

ID	Metabolite 代谢物	Metab ID	KEGG Path	KEGG Path 通路	KEGG Compound	Library ID
neg_2188	11beta,17beta,11beta, 17beta-metab_65	-	-	-	C18075	HMDB006
pos_24	Dinotefur 呋虫胺	metab_15	-	-	C18509	HMDB024
pos_5200	Trigonellin 葫芦巴碱	metab_44	map00760	Nicotinate 烟酸和烟酰胺	C01004	HMDB000
neg_1611	(S)-2-Acet (S) -2- metab_59	map01100	Metabolic 代谢途径	C06006	HMDB000	
pos_59	6-beta-D-6-beta-D-吡 metab_48	-	-	-	-	HMDB003
neg_423	5,7-Dihydro 5,7-二羟基 metab_87	-	-	-	-	LMPK1211

A1-A3

neg_2188	11beta,17	11β	17β	metab_65	-	-	-	C18075	HMDB006
pos_24	Dinotefur	呋虫胺	metab_15	-	-	-	-	C18509	HMDB024
pos_3484	Tebuconazole	戊唑醇	metab_26	-	-	-	-	C18489	HMDB025
pos_3444	Trifloxystrobin	-	metab_25	-	-	-	-	C18562	-
pos_2420	Methylcellulose	甲基纤维素	metab_15	-	-	-	-	-	HMDB002
pos_128	6-O-Gallic	6-邻没食子	metab_30	-	-	-	-	-	HMDB003
pos_109	Indoleacrylate	吲哚乙酸	metab_10	-	-	-	-	-	HMDB000
pos_325	L-2-Amino	L-2-氨基	metab_23	map00660	C5-Branch	C5支化二	C00651	HMDB002	
pos_3653	Octadecanoic	十八碳-2	metab_27	-	-	-	-	-	HMDB024
pos_57	Glycitin	黄豆黄甙	metab_47	map00940	Isoflavonoid	异黄酮生物	C16195	HMDB000	
pos_6	Neocarlinone	新卡诺赛酮	metab_48	-	-	-	C10109	HMDB003	
pos_478	Isoorientin	异东方素2	metab_39	-	-	-	-	HMDB003	
pos_4327	13-Hydroxy	13-羟基-5	metab_34	-	-	-	-	HMDB003	
pos_233	Kaempferol	-	metab_14	-	-	-	-	HMDB003	
neg_349	Kaempferol	山奈酚3-7	metab_79	-	-	-	-	HMDB030	
pos_4426	N-succinyl	n-琥珀酰	metab_35	-	-	-	-	HMDB025	
pos_1934	Trans-cinnamic	-	metab_10	-	-	-	C04164	HMDB030	
pos_5152	Pipelicolic	胡椒酸	metab_43	map01100	Metabolic	代谢途径	C00408	HMDB000	
pos_1048	(+)-Syringic	-	metab_54	-	-	-	C10890	-	
pos_4333	Kaempferol	山奈酚3-7	metab_34	map00940	Flavone	ar 黄酮和黄	C12634	HMDB030	
neg_4073	Lampranthen	兰普兰廷	metab_10	map00940	Flavone	ar 黄酮和黄	C12634	HMDB030	
neg_2147	Perilloside	紫苏甙A	metab_65	-	-	-	-	HMDB003	
pos_59	6-beta-D-6	β-D-吡	metab_48	-	-	-	-	HMDB003	
neg_423	5,7-Dihydro	5,7-二羟基	metab_87	-	-	-	-	LMPK1211	
pos_1063	Scoparin	2 东莨菪碱2	metab_71	-	-	-	-	HMDB003	
pos_1088	(7'R)-(+)-l	-	metab_98	-	-	-	-	HMDB003	
neg_55	(+)-Lyoniric	(+) -利	metab_99	-	-	-	-	HMDB004	

A2-A3

pos_32	Pisumionone 皮苏米奥酮	metab_23	-	-	-	HMDB003
pos_3444	Trifloxystrobin -	metab_25	-	-	C18562	-
pos_2420	Methylcellulose 甲基纤维素	metab_15	-	-	-	HMDB002
pos_6	Neocarlinone 新卡诺赛酮	metab_48	-	-	C10109	HMDB003
pos_478	Isoorientin 异东方素2	metab_39	-	-	-	HMDB003
pos_233	Kaempferol -	metab_14	-	-	-	HMDB003
neg_349	Kaempferol 山奈酚3-7 metab_79	-	-	-	-	HMDB030

Mode	KEGG Con	KEGG Con	KEGG Pat	KEGG Pat	HMDB Su	HMDB Cla	M/Z	Adducts
neg	-	-	-	-	Lipids and Steroids a		349.2022	M+FA-H
pos	-	-	-	-	Organic ni	Organonit	203.1138	M+H, 2M-
pos	-	-	Metabolis	Metabolis	Alkaloids z	Not Availa	138.0549	M+H
neg	-	-	Metabolis	Global anc	Organic a	Keto acids	351.1297	2M+Hac-I
pos	-	-	-	-	Phenylpro	Flavonoid	477.1388	M+H, M+
neg	-	-	-	-	Phenylpro	Flavonoid	475.1246	M+Cl, M+
neg	-	-	-	-	Lipids and Steroids a		349.2022	M+FA-H
pos	-	-	-	-	Organic ni	Organonit	203.1138	M+H, 2M-
pos	-	-	-	-	Benzenoic Benzene a		308.1521	M+H
pos	-	-	-	-	-	-	409.1367	M+H
pos	-	-	-	-	Organic o: Organoox		722.3563	M+ACN+I
pos	-	-	-	-	Benzenoic Benzene a		512.1583	M+H, M+
pos	-	-	-	-	Organohe	Indoles an	188.0705	M+H, M+
pos	-	-	Metabolis	Carbohyd	Organic a	Carboxylic	124.0395	M+H-2H2
pos	-	-	-	-	Not Availa	Not Availa	275.2003	M+H-2H2
pos	-	-	Metabolis	Biosynthes	Phenylpro	Isoflavono	447.1282	M+H-2H2
pos	-	-	-	-	Phenylpro	Flavonoid	581.15	M+H, M+
pos	-	-	-	-	Lignans, n Lignan gly		787.2077	M+H, M+
pos	-	-	-	-	Lipids and Prenol lipi		480.2225	M+NH4
pos	-	-	-	-	Phenylpro	Flavonoid	581.1499	M+H-H2C
neg	-	-	-	-	Phenylpro	Flavonoid	579.1358	M-H, M+C
pos	-	-	-	-	Organic o: Organoox		616.2597	M+CH3OH
pos	-	-	-	-	Phenylpro	Cinnamic i	621.2153	2M+H
pos	-	-	Metabolis	Global anc	Organic a	Carboxylic	130.0863	M+H
pos	-	-	-	-	-	-	598.2493	M+NH4, M
pos	-	-	Metabolis	Biosynthes	Phenylpro	Flavonoid	611.1605	M+H
neg	-	-	Metabolis	Biosynthes	Phenylpro	Flavonoid	609.1464	M-H
neg	-	-	-	-	Lipids and Prenol lipi		673.3443	2M+FA-H
pos	-	-	-	-	Phenylpro	Flavonoid	477.1388	M+H, M+
neg	-	-	-	-	Phenylpro	Flavonoid	475.1246	M+Cl, M+
pos	-	-	-	-	Phenylpro	Flavonoid	625.1757	M+H, M+
pos	-	-	-	-	Lignans, n Lignan gly		600.2648	M+NH4, M
neg	-	-	-	-	Lignans, n Lignan gly		581.2244	M-H, M+C
pos	-	-	-	-	Lipids and Prenol lipi		427.1936	M+Na, M-
pos	-	-	-	-	-	-	409.1367	M+H
pos	-	-	-	-	Organic o: Organoox		722.3563	M+ACN+I
pos	-	-	-	-	Phenylpro	Flavonoid	581.15	M+H, M+
pos	-	-	-	-	Lignans, n Lignan gly		787.2077	M+H, M+
pos	-	-	-	-	Phenylpro	Flavonoid	581.1499	M+H-H2C
neg	-	-	-	-	Phenylpro	Flavonoid	579.1358	M-H, M+C

Formula	Retention	RSD	Fragment	Theoretical	Mass Error	CAS ID	HMDB Sub	A1_1
C19H28O	6.2266	0.000789	0	86.5	0.522345	1816-85-9	Androstan	6.7885
C7H14N4	3.0924	0.001754	55.3	0	-0.33431	165252-7	Guanidine	6.2941
C7H7NO2	1.1117	0.005763	83.2	0	-0.23569	535-83-1	Not Availa	7.286
C6H10O4	4.7048	0.00529	0	72.7	0.001796	113919-0	Short-cha	6.7886
C23H24O	4.88	0.003903	0	82.3	-0.71474	74198-15	Flavonoid	7.1039
C22H22O	5.3159	0.0059	0	53	-0.05838	163350-2	Flavonoid	6.5607
C19H28O	6.2266	0.000789	0	86.5	0.522345	1816-85-9	Androstan	6.7885
C7H14N4	3.0924	0.001754	55.3	0	-0.33431	165252-7	Guanidine	6.2941
C16H22Cl	6.4132	0.005072	87.2	0	-0.97679	107534-9	Phenylbut	6.9271
C20H19F3	6.4688	0.002826	93.7	0	-0.55591	141517-2	-	7.1012
C29H54O	6.4053	0.009595	0	58	-0.9905	9004-67-1	Carbohydi	6.2293
C19H26O	4.7604	0.00073	0	49.5	-5.53591	115731-1	Benzoic ac	6.5649
C11H9NO	3.2279	0.005582	0	33.7	-0.39579	29953-71	Indoles	6.5996
C6H9NO4	1.39	0.006666	0	51.3	1.031405	16804-57	Amino aci	6.3913
C18H30O	6.16	0.004959	0	54.2	-0.81296	-	Not Availa	7.1496
C22H22O	4.9197	0.001688	0	79.6	-0.92369	40246-10	Isoflavono	6.6309
C26H28O	4.1158	0.00155	0	63	-0.16672	83151-89	Flavonoid	7.6972
C37H38O	4.6329	0.00382	0	64	-0.41768	220948-7	Not Availa	6.6391
C24H30O	4.275	0.008355	0	62.4	-0.67085	112471-0	Sesquiterp	6.4598
C26H28O	3.8061	0.00331	0	65.5	-0.27104	99816-59	Flavonoid	6.8761
C26H28O	4.3468	0.011928	0	86.9	0.366326	-	Flavonoid	6.7656
C22H37N	3.949	0.005004	0	56.2	6.46485	-	Carbohydi	6.6074
C15H18O	3.941	0.006581	0	64.2	-4.02622	-	Cinnamic	6.4593
C6H11NO	1.3342	0.009516	67.1	0	0.540494	3105-95-1	Amino aci	7.1539
C28H36O	4.7924	0.014163	78.5	0	-0.23006	7374-79-1	-	6.7083
C27H30O	4.2511	0.003904	45.3	0	-0.31047	-	Flavonoid	6.6672
C27H30O	4.7441	0.005683	0	83.5	0.510407	32074-65	Flavonoid	6.4958
C16H26O	6.1248	0.008167	0	49.5	0.305988	-	Terpene g	6.8983
C23H24O	4.88	0.003903	0	82.3	-0.71474	74198-15	Flavonoid	7.1039
C22H22O	5.3159	0.0059	0	53	-0.05838	163350-2	Flavonoid	6.5607
C28H32O	4.6567	0.001383	0	71.6	-1.00941	124902-1	Flavonoid	7.4722
C28H38O	4.3307	0.005558	84.1	0	-0.47633	87585-32	Not Availa	7.2962
C28H38O	4.8147	0.00695	0	52.2	0.6708	-	Not Availa	6.5548
C19H32O	3.4405	0.008697	0	72.3	-0.62723	371113-0	Terpene g	6.7516
C20H19F3	6.4688	0.002826	93.7	0	-0.55591	141517-2	-	7.1012
C29H54O	6.4053	0.009595	0	58	-0.9905	9004-67-1	Carbohydi	6.2293
C26H28O	4.1158	0.00155	0	63	-0.16672	83151-89	Flavonoid	7.6972
C37H38O	4.6329	0.00382	0	64	-0.41768	220948-7	Not Availa	6.6391
C26H28O	3.8061	0.00331	0	65.5	-0.27104	99816-59	Flavonoid	6.8761
C26H28O	4.3468	0.011928	0	86.9	0.366326	-	Flavonoid	6.7656

A1_2	A1_3	A2_1	A2_2	A2_3	A3_1	A3_2	A3_3	D1_1
6.7128	6.9929	7.4712	7.5426	7.6294	7.58	7.6108	7.8248	5.7827
5.9443	6.4398	6.8452	7.0926	7.1165	6.9683	7.1693	7.2428	4.5784
7.4369	7.3955	7.0724	7.1367	7.2589	7.1309	7.2705	7.2176	6.5324
6.7752	7.1022	6.4644	6.4934	6.5497	6.4346	6.5709	6.7398	6.884
7.1453	7.0237	6.8033	6.9022	6.8852	6.7873	6.7977	6.9395	3.0542
6.5714	6.4367	6.2965	6.3251	6.3306	6.2951	6.2949	6.3966	2.632
6.7128	6.9929	7.4712	7.5426	7.6294	7.58	7.6108	7.8248	5.7827
5.9443	6.4398	6.8452	7.0926	7.1165	6.9683	7.1693	7.2428	4.5784
6.8931	7.2264	7.2096	7.11	7.4369	7.8041	7.8237	7.9128	4.9255
6.9687	7.3391	7.5195	7.302	7.6127	7.9647	7.9862	8.0443	3.7884
6.0977	6.3337	6.534	6.3585	6.6993	7.0765	7.021	6.9975	4.822
6.6252	6.5502	6.477	6.4252	6.4828	6.3953	6.3615	6.3131	2.9037
6.5406	6.566	6.4092	6.4217	6.3831	6.3304	6.3289	6.2734	7.3025
6.396	6.4226	6.3243	6.356	6.3415	6.305	6.3056	6.2932	6.5217
7.2334	7.1578	7.0952	7.0741	7.0988	7.0752	7.0556	7.0468	5.4551
6.6343	6.5276	6.4944	6.5245	6.5272	6.4798	6.4802	6.4864	6.376
7.8298	7.552	7.6523	7.8316	7.7984	7.345	7.2667	6.7431	6.237
6.7631	6.6093	6.5623	6.8785	6.8211	6.2277	6.1855	5.6503	5.5567
6.4635	6.4018	6.4147	6.5429	6.3278	6.2533	6.2658	6.0867	3.7439
7.0255	6.7875	6.8056	6.9983	6.9188	6.445	6.4175	5.9665	5.1068
6.9266	6.6001	6.6873	6.8317	6.7843	6.3795	6.3397	5.8737	5.36
6.6218	6.5635	6.548	6.5311	6.642	6.4174	6.4031	6.3112	3.7077
6.41	6.3775	6.4116	6.3702	6.4478	6.3293	6.2976	6.2865	3.5556
7.2936	6.8964	6.9735	7.1339	6.8693	6.8308	6.7564	6.6214	6.3738
6.8515	6.7495	6.6201	6.6339	6.8449	6.5901	6.5922	6.5132	3.5452
6.8407	7.1266	6.5616	6.9032	6.845	6.2659	6.5589	6.1456	2.9154
6.6643	6.9344	6.4172	6.726	6.6655	6.1636	6.4342	6.0473	4.4825
7.0084	6.9999	6.7811	6.7604	6.8515	6.8265	6.7784	6.8846	1.9962
7.1453	7.0237	6.8033	6.9022	6.8852	6.7873	6.7977	6.9395	3.0542
6.5714	6.4367	6.2965	6.3251	6.3306	6.2951	6.2949	6.3966	2.632
7.4535	7.5552	7.2042	7.4151	7.3705	7.2112	7.2498	7.3361	5.9941
7.3532	7.3255	7.1356	7.1079	7.388	7.1307	7.0977	7.0837	4.0959
6.6301	6.5917	6.3705	6.3316	6.634	6.373	6.3357	6.344	4.2694
6.7542	6.7914	6.608	6.4609	6.6818	6.8411	6.9074	7.045	6.4288
6.9687	7.3391	7.5195	7.302	7.6127	7.9647	7.9862	8.0443	3.7884
6.0977	6.3337	6.534	6.3585	6.6993	7.0765	7.021	6.9975	4.822
7.8298	7.552	7.6523	7.8316	7.7984	7.345	7.2667	6.7431	6.237
6.7631	6.6093	6.5623	6.8785	6.8211	6.2277	6.1855	5.6503	5.5567
7.0255	6.7875	6.8056	6.9983	6.9188	6.445	6.4175	5.9665	5.1068
6.9266	6.6001	6.6873	6.8317	6.7843	6.3795	6.3397	5.8737	5.36

D1_2	D1_3	D2_1	D2_2	D2_3	D3_1	D3_2	D3_3	QC01
5.7376	6.0315	6.1028	5.747	5.9552	5.6715	5.7313	5.7049	7.2662
4.2636	3.8981	4.9793	5.9211	5.2662	4.833	5.031	4.9432	6.7581
6.4724	6.397	6.3151	6.5292	6.4435	6.4892	6.2253	6.3256	7.1484
6.7771	6.8797	6.8977	6.896	6.9412	6.8715	6.9831	6.9206	6.7392
3.0519	3.06	3.0371	3.037	3.064	3.0087	3.0288	3.0546	6.7546
2.6381	2.6186	2.632	2.6893	2.6277	2.605	2.6816	2.6494	6.2835
5.7376	6.0315	6.1028	5.747	5.9552	5.6715	5.7313	5.7049	7.2662
4.2636	3.8981	4.9793	5.9211	5.2662	4.833	5.031	4.9432	6.7581
4.0487	3.9728	5.1829	5.7153	5.7577	5.4108	5.0718	5.5022	7.3356
3.7089	3.717	4.0506	4.6982	5.1529	3.6657	3.6858	5.1412	7.4767
4.4245	5.1881	6.1418	4.7816	5.4418	4.4663	5.2013	4.6982	6.5726
2.5434	2.5515	2.5286	3.1218	3.3514	3.2495	2.7104	3.1166	6.2757
6.754	7.5662	7.4563	7.4653	7.174	7.319	7.4346	7.1225	7.0004
6.5154	6.3943	6.419	6.4762	6.4231	6.461	6.4737	6.4732	6.3843
5.0822	5.4357	5.4122	5.2188	5.5006	5.2497	5.327	5.2018	6.8758
6.3737	6.3818	6.3589	6.3587	6.3858	6.3305	6.3506	6.3764	6.367
6.023	6.2912	6.3783	6.205	6.433	6.2243	6.3275	6.211	7.4129
5.5544	5.5625	5.5396	5.5395	5.5666	5.5112	5.5313	5.5571	6.3721
4.0733	3.7496	3.7268	3.7266	3.7537	3.6984	3.7185	3.7443	6.137
4.5581	4.8952	5.3832	5.0671	5.4627	5.0386	5.2778	4.8984	6.5558
5.1082	5.3128	5.6465	5.3614	5.6846	5.4138	5.5226	5.3022	6.5074
3.7054	3.7134	3.6906	3.6904	3.7175	3.6622	3.746	3.7081	6.3088
3.5533	3.5614	3.5385	3.5383	3.9961	3.5101	3.5302	3.556	6.236
6.2662	6.4217	6.3705	6.3339	6.324	6.3774	6.2765	6.4086	6.8491
3.5429	4.1256	5.1265	3.528	3.5551	3.4997	4.1655	3.5456	6.5325
3.3535	3.6358	3.5921	2.8252	4.1641	3.1648	3.9217	6.175	6.5372
3.6639	4.678	4.7991	3.9788	4.6531	3.8872	4.0923	6.2326	6.4284
2.0022	3.8494	2.7341	3.9209	1.992	1.9695	2.0455	2.0135	6.7062
3.0519	3.06	3.0371	3.037	3.064	3.0087	3.0288	3.0546	6.7546
2.6381	2.6186	2.632	2.6893	2.6277	2.605	2.6816	2.6494	6.2835
5.9679	6.019	6.1669	5.9344	6.2128	6.1998	6.2104	6.1523	7.1838
4.2957	5.4444	5.8365	4.9803	5.0782	4.9053	5.6775	5.3548	7.0436
4.6006	5.1848	5.5166	4.9128	4.8258	4.7144	5.5062	5.2	6.3208
6.4265	6.4345	6.4117	6.4115	6.4386	6.3833	6.4034	6.4292	6.6537
3.7089	3.717	4.0506	4.6982	5.1529	3.6657	3.6858	5.1412	7.4767
4.4245	5.1881	6.1418	4.7816	5.4418	4.4663	5.2013	4.6982	6.5726
6.023	6.2912	6.3783	6.205	6.433	6.2243	6.3275	6.211	7.4129
5.5544	5.5625	5.5396	5.5395	5.5666	5.5112	5.5313	5.5571	6.3721
4.5581	4.8952	5.3832	5.0671	5.4627	5.0386	5.2778	4.8984	6.5558
5.1082	5.3128	5.6465	5.3614	5.6846	5.4138	5.5226	5.3022	6.5074

QC02	QC03
7.2669	7.2665
6.7585	6.757
7.1488	7.1443
6.7437	6.7423
6.7577	6.7574
6.2842	6.2883

7.2669	7.2665
6.7585	6.757
7.336	7.3396

7.4771	7.479
6.5796	6.5723
6.2763	6.2761
7.0008	7.0048
6.3845	6.3894
6.8761	6.8797

6.3683	6.367
7.4117	7.4129
6.3724	6.3751
6.1302	6.1316
6.5533	6.5558
6.5154	6.5172
6.3092	6.3053
6.2364	6.2411
6.8494	6.8421
6.5404	6.5283
6.5376	6.5345
6.429	6.4329
6.6993	6.7012
6.7577	6.7574
6.2842	6.2883
7.183	7.1826
7.0477	7.0436
6.3249	6.3267

6.6471	6.6535
7.4771	7.479
6.5796	6.5723
7.4117	7.4129
6.3724	6.3751
6.5533	6.5558
6.5154	6.5172