

Group1	Name	Pubchem CID
REFJWTPEDVJJIY-UHFFFAOYS/	Quercetin-7-olate	46906036
REFJWTPEDVJJIY-UHFFFAOYS/	Quercetin	5280343
QIQXTHQIDYTRH-UHFFFAOYS,	Stearic acid	5281
ODKSFYDXXFIFQN-UHFFFAOYS	2-Azaniumyl-5-(diaminomethylideneamino)	59119146
KZNIHFPLKGYRTM-UHFFFAOYS	Apigenin-7-olate	25200950
KZNIHFPLKGYRTM-UHFFFAOYS	Apigenin	5280443
HFDVRLIODXPAHB-UHFFFAOYS	1-Tetradecene	14260
DANYIYRPLHHOCZ-UHFFFAOYS	Acacetin	5280442
TZBJGXHYKVUXJN-UHFFFAOYS	Genistein(1-)	25201420
TZBJGXHYKVUXJN-UHFFFAOYS	Genistein	5280961
JVXZRQGOGOXCEC-UHFFFAOY	Scutellarein	5281697
QAIPRVGONGVQAS-DUXPYHPU	Caffeic acid	689043
OYHQOLUKZRVURQ-HZJYTTRN	Linoleic acid	5280450
AWUBJLRYWHOLFW-WZUFQYTHSA-N		
CXMXRPHRNRROMY-UHFFFAO\	Sebacic acid	5192
GYHFUZHODSMOHU-UHFFFAO\	Nonanal	31289
KEMQGTRYUADPNZ-UHFFFAOY	Heptadecanoic acid	10465
QZZGJDVWFLFXDLK-UHFFFAOY!	Tetracosanoic acid	11197
RJWUMFHQJJBOD-UHFFFAOY	2-Methylheptadecane	15265
UKMSUNONTOPOIO-UHFFFAOY	Docosanoic acid	8215
VKOBVWXKNCXXDE-UHFFFAO\	Arachidic acid	10467
WQEPLUUGTLDZJY-UHFFFAOY!	Pentadecanoic acid	13849
RECUKUPTGUEGMW-UHFFFAO\	Carvacrol	10364
ZFMSMUAANRZJFM-UHFFFAOY!	Estragole	8815
YXOLAZRVSSWPPT-UHFFFAOY	Morin	5281670
IPCSVZSSVZVIGE-UHFFFAOYS/	Palmitic acid	985
FXNFHKRTJBSTCS-UHFFFAOYS	Baicalein	5281605
RTIXKCRFFJGDFG-UHFFFAOYS	7-Hydroxy-4-oxo-2-phenylchromen-5-olate	25200543
RTIXKCRFFJGDFG-UHFFFAOYS	Chrysin	5281607
FTVWIRXFELQLPI-UHFFFAOYS/	Naringenin	932
DLPRXTUOPLIHNV-FOCLMDBB	3-Octadecenoic acid	5282751
DTOSIQBPPRVQHS-IUQGRGSQ!	9,12,15-Octadecatrienoic acid	5282822
FIKTURVKRGQNQD-VHEBQXMU	trans-2-Icosenoic acid	6438157
FLIACVVOZYBSBS-UHFFFAOYS,	Methyl palmitate	8181
FUGDHQXYVPQGLJ-UHFFFAOY	Cyclotetradecanone	77153
GEHPRJRWZDWFBJ-FOCLMDBE	2-Heptadecenoic acid	5282747
IEDKVDCIEARIIU-UHFFFAOYSA-	2-Nonadecanone	69423
IGGUPRCHHJZPBS-UHFFFAOYS	Nonacosane	12409
JESIHYIJKKUWIS-UHFFFAOYSA,	1-(4-Methylphenyl)ethanol	10817
JZQKTMZYLNHNFPL-BLHCBFLLS/	2,4-Decadienal	5283349
NDJKXXJCMXVBWU-UHFFFAOY!	Heptadecane	12398
NHKDEMRRYWOJOF-UHFFFAO\	Octadecanoic acid, hexacosyl ester	3085149
OIPHBJBKSAKTTI-IVZWYUIFSA-I	(E,E,E)-N-(2-Methylpropyl)hexadeca-2,6,8-	5281152
OSOIQJGOYGSIMF-UHFFFAOYS	Cyclopentadecanone	10409
OYHQOLUKZRVURQ-AVQMFFA!	Linoelaidic acid	5282457
PCBKWKNYISJGPJ-BUHFOSPR	3-Hexadecenoic acid	5312418
RSLTVQQROJUNCD-ALCCZGGF	5-Cyclopentadecene-1-one	5316264
SECPZKHBENQXJG-BQYQJAHW	9-Hexadecenoic acid	5282745
SEKHAGCBKYMSBO-UHFFFAOY	5,9-Dimethyl-8-decenoic acid	21612893
UOURIOWCMYPGGF-UHFFFAO\	3-Acetyl-2,6-dihydroxy-4-methoxybenzalde	610933
XOEMDGMZEQVND-XXRVVYS	5-Cyclotetradecen-1-one	5316269
YCOZIPAWZNQLMR-UHFFFAOY!	Pentadecane	12391
ZQPPMHVWECSIRJ-MDZDMXLP	Elaidic acid	637517
BKIMMITUMNQMOS-UHFFFAOY	Nonane	8141
OLOOJGVNMBJLLR-UHFFFAOY!	Imperatorin	10212
PAYRUJLWNCNPSJ-UHFFFAOY!	Aniline	6115
RRAFCDWBNXTKKO-UHFFFAO\	Eugenol	3314

GLZPCOQZEFWAFX-JXMROGB\ Geraniol	637566
WPYMKLBDIGXBTP-UHFFFAOY\ Hydron;benzoate	20144841
WWZKQHOCKIZLMA-UHFFFAOY Octanoic acid	379
BPYKTIZUTYGOLE-IFADSCNNS\ Bilirubin	5280352
OFYPDAKTVZXXPC-UHFFFAOY\ 5,7,2'-Trihydroxyflavone	5322064
SECPZKHBENQXJG-FPLPWBNI Palmitoleic acid	445638
TUNFSRHWOTWDNC-UHFFFAO Myristic acid	11005
XHEFDIBZLJXQHF-UHFFFAOYS\ Fisetin	5281614
LNTHITQWFMADLM-UHFFFAOY\ Gallic acid	370
ZQPPMHVWECSIRJ-KTKRTIGZS Oleic acid	445639
VFLDPWHFBUODDF-FCXRPNKF Curcumin	969516
ZIUSSTSXXLLKKK-KOBPDAPS, (1E,4Z,6E)-5-Hydroxy-1,7-bis(4-hydroxy-3-NGSWKAQJJWESNS-ZZXKWVIF 4-Hydroxycinnamic acid	5281767
CKDRPCYJCDMPFO-UHFFFAOY 8a-Hydroxy-1,8-dimethyl-5-methylidene-5a	75144776
CPGCVOVWHCWVTP-UHFFFAO Nonacosan-10-ol	25240035
CXENHBSYCFKJS-VDQVFBMK\ alpha-Farnesene	5281516
DAGYDJHSDMRWJX-UHFFFAOY Nonacosane-6,8-diol	130335
DJJQWLWXJHJPIH-UHFFFAOYS 4-(7-Hydroxy-4H-chromen-3-yl)benzene-1,;	101040114
DTHUVZQMVMVXNB-LVSIQRNO [(4S,5R,6S)-5,6-Dihydroxy-5,6-dihydro-4H-FCXRFTLSXMRXTM-LBPRGKRZ\ (2S)-4',5,7-Trihydroxy-6-methoxyflavanone	45098905
FCXRFTLSXMRXTM-UHFFFAOY\ 5,7,4'-Trihydroxy-6-methoxyflavanone	46893290
FFRFJIZJLZXEJX-PORYWJCVSA-N	5322074
FPDSMLMTMDHJQT-UHFFFAOY Hydroxymuscovopyridine A	184938
FUZZWVXGSFPDMH-UHFFFAOY Hexanoic acid	8892
GYHKMDWFVHCCRA-UHFFFAO` 2-(2,4-Dihydroxyphenyl)-6-hydroxybenzofu	15480861
HFPZCAJZSCWRBC-UHFFFAOY P-Cymene	7463
HJFYFYWETUVIHT-UHFFFAOYS Tetrahydrodemethoxydiferuloylmethane	9906039
IGWDEVSBEKYORK-UHFFFAOY Isoimperatorin	68081
IMNKABOILQOFDL-UHFFFAOYS, 3-Methyl-16-azabicyclo[10.3.1]hexadeca-11	5319970
IQGURDMZNWKPEW-VHYPUYL\ (3E,9E)-Undeca-3,9-dienoic acid	52914864
JSNRRGGBADWTMC-NTCAYCP\ beta-Farnesene	5281517
KVWWIYGFBYDJQC-GHMZBOCI Methyl (1R-trans)-3-oxo-2-pentylcyclopenta	1738124
KVWWIYGFBYDJQC-UHFFFAOY Methyl dihydrojasmonate	102861
MLOIFQIPYKRTPY-KZZDLZNXSA` (1E,6E)-1-(4-Hydroxy-3-methoxyphenyl)-7-	44629981
NDFKTBCGKNOHPJ-AATRIKPKS 2-Heptenal	5283316
PFIXJSCFTAVWBW-UHFFFAOY\ Curcolone	5316208
PUCHCUYBORIUSM-UHFFFAOY\ Methyl propyl disulfide	16592
PXPIJNMPDAFWSF-XBXARRHU\ (-)-(E)-1-(4-Hydroxyphenyl)-7-phenyl-6-hep	10039429
QATWTDKFCQHTAE-UHFFFAOYSA-N	
QBGSGZFGDIXJTOI-UHFFFAOYS\ 15-Azabicyclo[9.3.1]pentadeca-1(15),11,13	5320193
RZGFUGXQKMEMOO-BSANDHC 12-Hydroxyjasmonic acid	5497122
SSRDTRQCJGXMGY-PXNMLYILSA-N	
UAHWPYUMFXFYJY-UHFFFAOY Myrcene	31253
VFLDPWHFBUODDF-KYPMKJFL\ cis-Curcumin	24884282
VMDXHYHOJPKFEK-ADUATRDF Isofuranodiene	5317424
VSMOENVRRABVKN-UHFFFAOY 1-Octen-3-OL	18827
VZWGRQBCURJOMT-UHFFFAO` Dodecyl acetate	8205
WOLHVDCCOJEKFW-UHFFFAO` Methyl 2-(2-butyl-4-oxocyclopentyl)acetate	21862951
WXGBJURRRZPBDS-UHFFFAOYSA-N	
WYIDBNAGSMCMET-UHFFFAOY Anhydroglycinol	442667
XBGUIVFBMBVUEG-PFONDFGA\ (E)-gamma-Bisabolene	5352437
XCZTYQQNVNLGKI-LVUHIJSRSA` 2beta-[(Z)-5-Hydroxy-2-pentenyl]-3-oxocycl	101006119
XEKNCTZVXNUNGMI-UHFFFAOY Hydroxymuscovopyridine B	184939
XVOHELPNOXGRBQ-LXQMTTSM Furanodienon	6442374
YVBAUDVGOFCUSG-UHFFFAOY 2-Pentylfuran	19602
YZPIVPVXEUAVNR-UHFFFAOYS 16-Azabicyclo[10.3.1]hexadeca-1(16),12,14	5316410
ZLESWHXADLWJPV-YHYXMXQ\ 3,6,10-Trimethyl-4H,5H,6H,7H,8H,11H-cyc	13118283
ZNWNWEHQFXOPGK-UHFFFAO Sebacaldehyde	3016433

INVGWHRKADIJHF-UHFFFAOYS Sanguinarine	5154
GIKVSFNAEBQLGB-UHFFFAOYS 3',4',5',5',7-Pentamethoxyflavone	493376
MQBFFYQCZCKSBX-UHFFFAOY Gardenin A	261859
SBHXYTNGIZCORC-UHFFFAOYS (+/-)-Eriodictyol	11095
SBHXYTNGIZCORC-ZDUSSCGK Eriodictyol	440735
XLEYFDVVXLMULC-UHFFFAOYS 2',4',6'-Trihydroxyacetophenone	68073
QMVPMAAFGQKVCJ-UHFFFAOY Citronellol	8842
XPOJSWHIKCNLEQ-UHFFFAOYS Cryptopine	72616
BBFQZRXYIEMAW-UHFFFAOYS Aristolochic acid	2236
QAIPRVGONGVQAS-RQOWECA cis-Caffeic acid	1549111
QUCQEUCGKKTEBI-UHFFFAOYS Palmatine	19009
PVFGJHYLIHMCQD-UHFFFAOYS 7,3',4'-Trihydroxyflavone	5322065
YBHILYKTIRIUTE-UHFFFAOYSA- Berberine	2353

Group2	Overlap	p	adj-p	J	C
C0038454	18	1.75E-16	1.80E-13	0.05505	0.18
C0038454	18	1.75E-16	1.80E-13	0.05505	0.18
C0038454	9	3.08E-12	3.17E-09	0.03475	0.3913
C0038454	9	7.55E-12	7.77E-09	0.03448	0.36
C0038454	12	3.82E-11	3.93E-08	0.0396	0.17143
C0038454	12	3.82E-11	3.93E-08	0.0396	0.17143
C0038454	8	4.19E-11	4.31E-08	0.03113	0.4
C0038454	9	1.76E-10	1.82E-07	0.03333	0.26471
C0038454	10	2.75E-10	2.83E-07	0.03521	0.20408
C0038454	10	2.75E-10	2.83E-07	0.03521	0.20408
C0038454	8	6.87E-10	7.07E-07	0.0303	0.2963
C0038454	9	1.73E-09	1.78E-06	0.03226	0.2093
C0038454	8	1.76E-09	1.81E-06	0.02996	0.26667
C0038454	7	2.20E-09	2.26E-06	0.02713	0.35
C0038454	7	2.20E-09	2.26E-06	0.02713	0.35
C0038454	7	2.20E-09	2.26E-06	0.02713	0.35
C0038454	7	2.20E-09	2.26E-06	0.02713	0.35
C0038454	7	2.20E-09	2.26E-06	0.02713	0.35
C0038454	7	2.20E-09	2.26E-06	0.02713	0.35
C0038454	7	2.20E-09	2.26E-06	0.02713	0.35
C0038454	7	2.20E-09	2.26E-06	0.02713	0.35
C0038454	7	2.20E-09	2.26E-06	0.02713	0.35
C0038454	7	2.20E-09	2.26E-06	0.02713	0.35
C0038454	7	4.74E-09	4.88E-06	0.02692	0.31818
C0038454	7	4.74E-09	4.88E-06	0.02692	0.31818
C0038454	8	8.54E-09	8.78E-06	0.0293	0.22222
C0038454	7	2.34E-08	2.41E-05	0.02642	0.25926
C0038454	8	2.56E-08	2.63E-05	0.02878	0.19512
C0038454	8	6.64E-08	6.83E-05	0.02827	0.17391
C0038454	8	6.64E-08	6.83E-05	0.02827	0.17391
C0038454	7	8.44E-08	8.69E-05	0.02593	0.21875
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	9.33E-08	9.61E-05	0.02317	0.3
C0038454	6	1.29E-07	1.33E-04	0.02308	0.28571
C0038454	6	1.29E-07	1.33E-04	0.02308	0.28571
C0038454	6	1.29E-07	1.33E-04	0.02308	0.28571
C0038454	6	1.29E-07	1.33E-04	0.02308	0.28571



C0038454	6	4.00E-06	4.11E-03	0.02182	0.16667
C0038454	5	4.11E-06	4.23E-03	0.01916	0.2381
C0038454	5	4.11E-06	4.23E-03	0.01916	0.2381
C0038454	5	4.11E-06	4.23E-03	0.01916	0.2381
C0038454	5	4.11E-06	4.23E-03	0.01916	0.2381
C0038454	5	4.11E-06	4.23E-03	0.01916	0.2381
C0038454	5	5.27E-06	5.42E-03	0.01908	0.22727
C0038454	5	5.27E-06	5.42E-03	0.01908	0.22727
C0038454	5	6.66E-06	6.86E-03	0.01901	0.21739
C0038454	5	6.66E-06	6.86E-03	0.01901	0.21739
C0038454	5	6.66E-06	6.86E-03	0.01901	0.21739
C0038454	5	8.34E-06	8.58E-03	0.01894	0.20833
C0038454	5	8.34E-06	8.58E-03	0.01894	0.20833