

*Supplementary Materials*

# Phytochemical Compound Screening to Identify Novel Small Molecules Against Dengue Virus: A Docking and Dynamics Study

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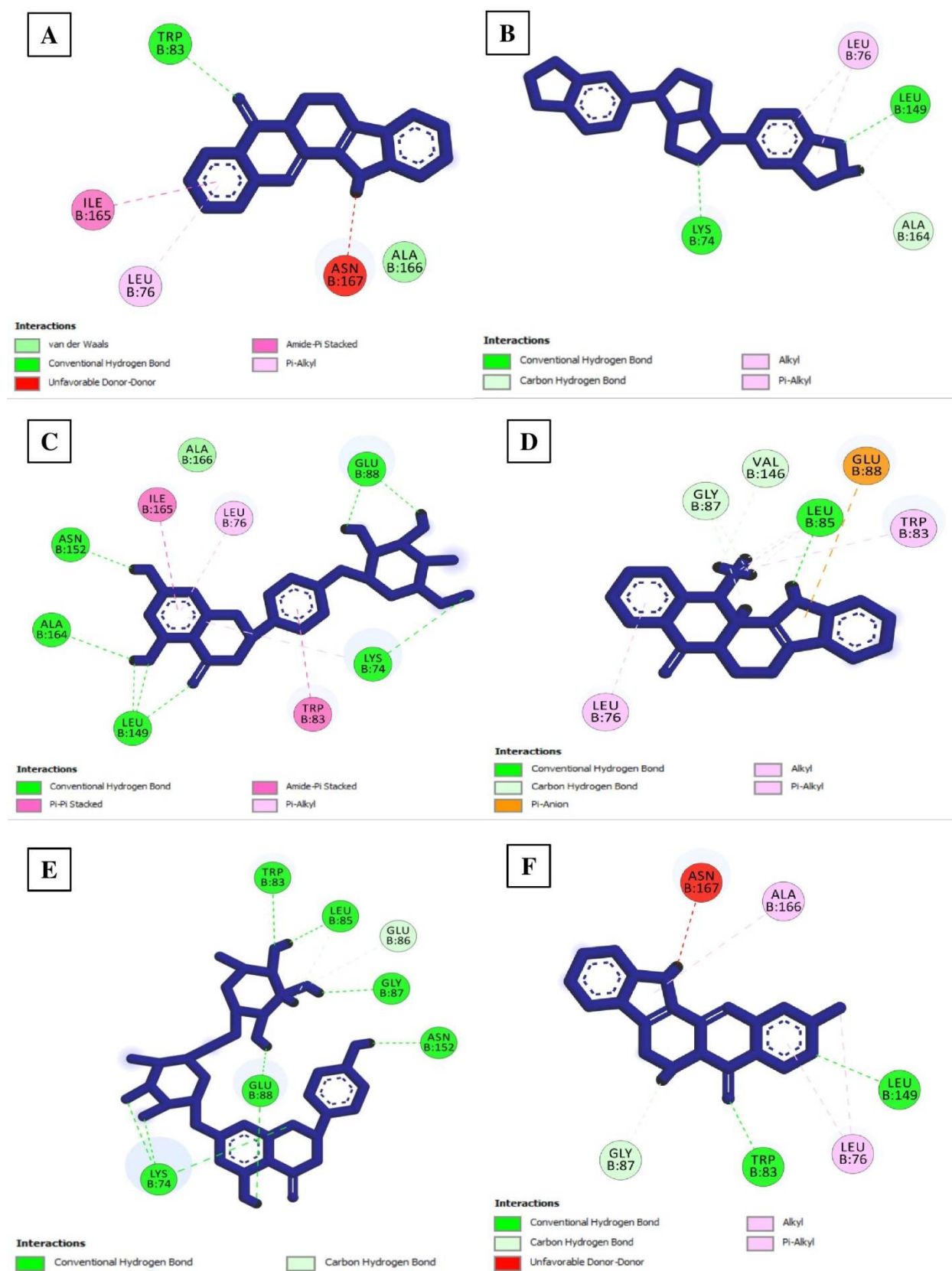
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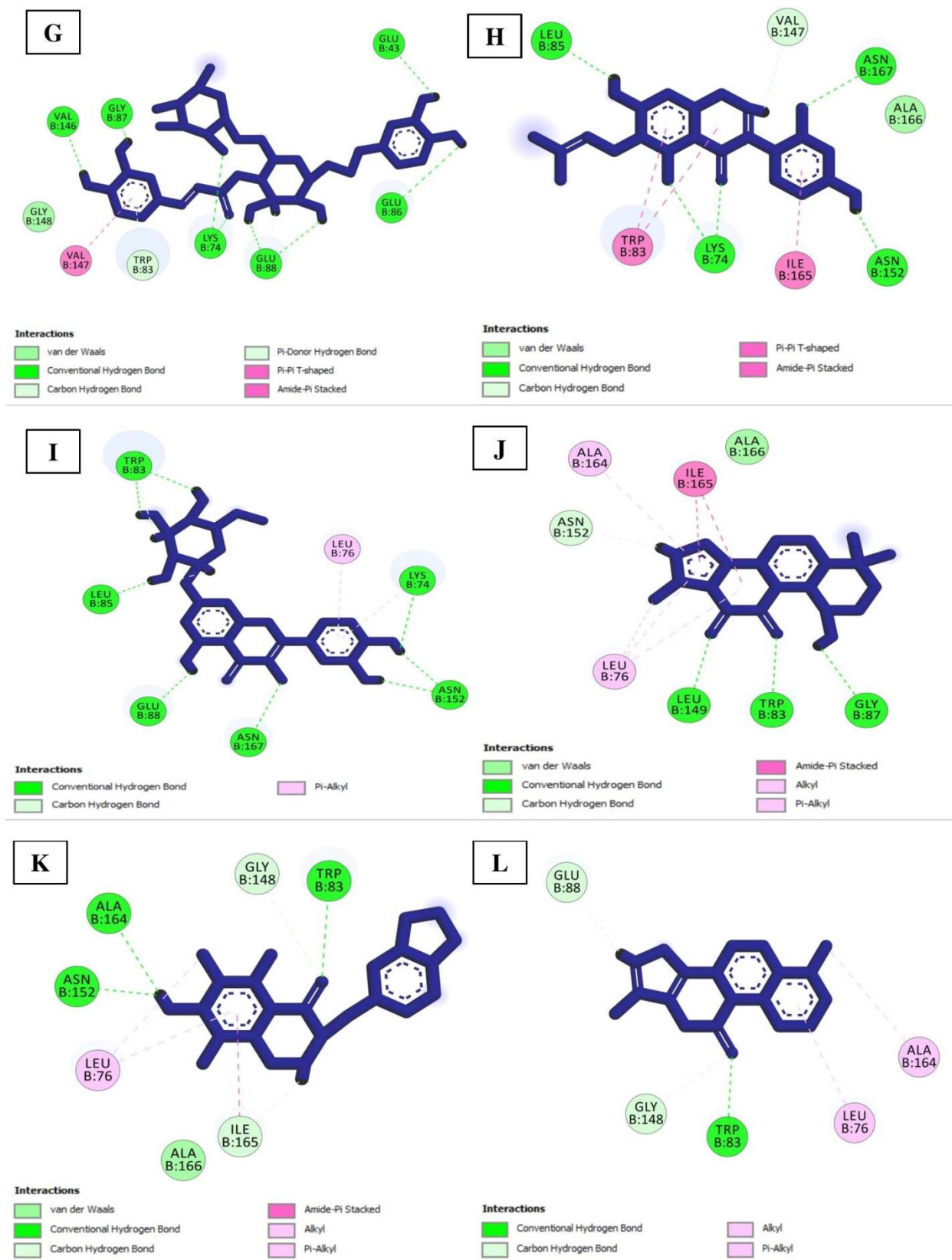
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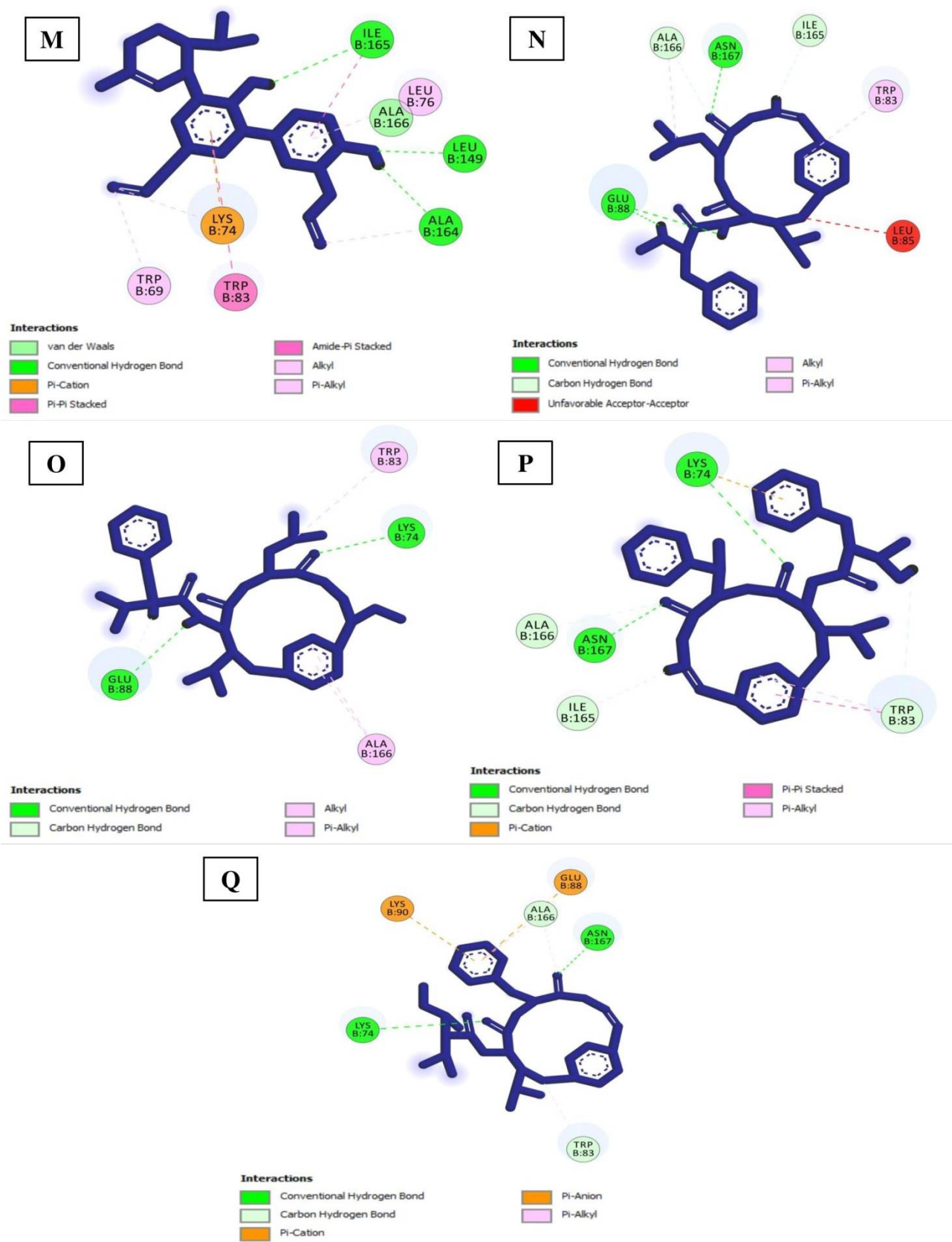
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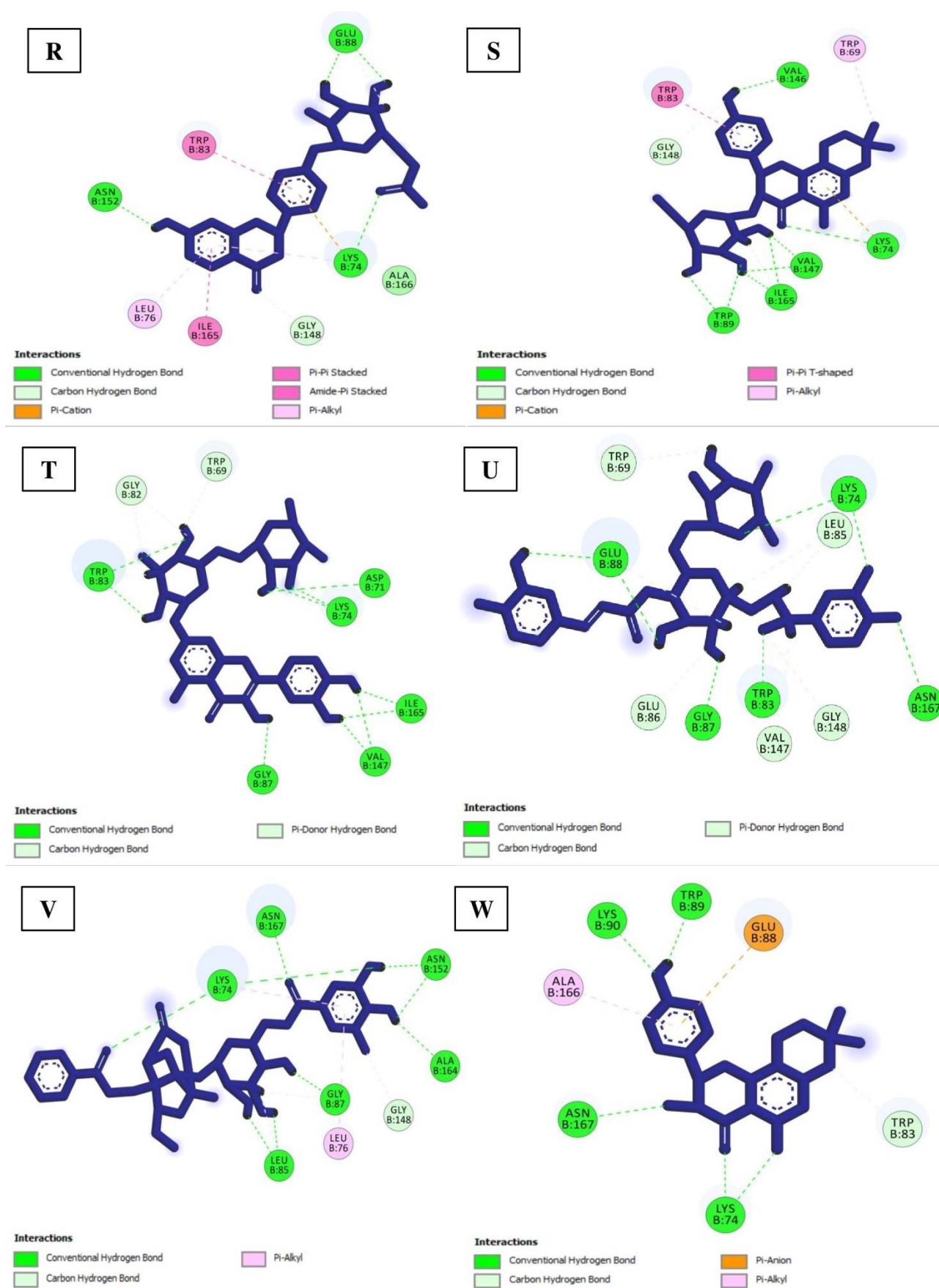
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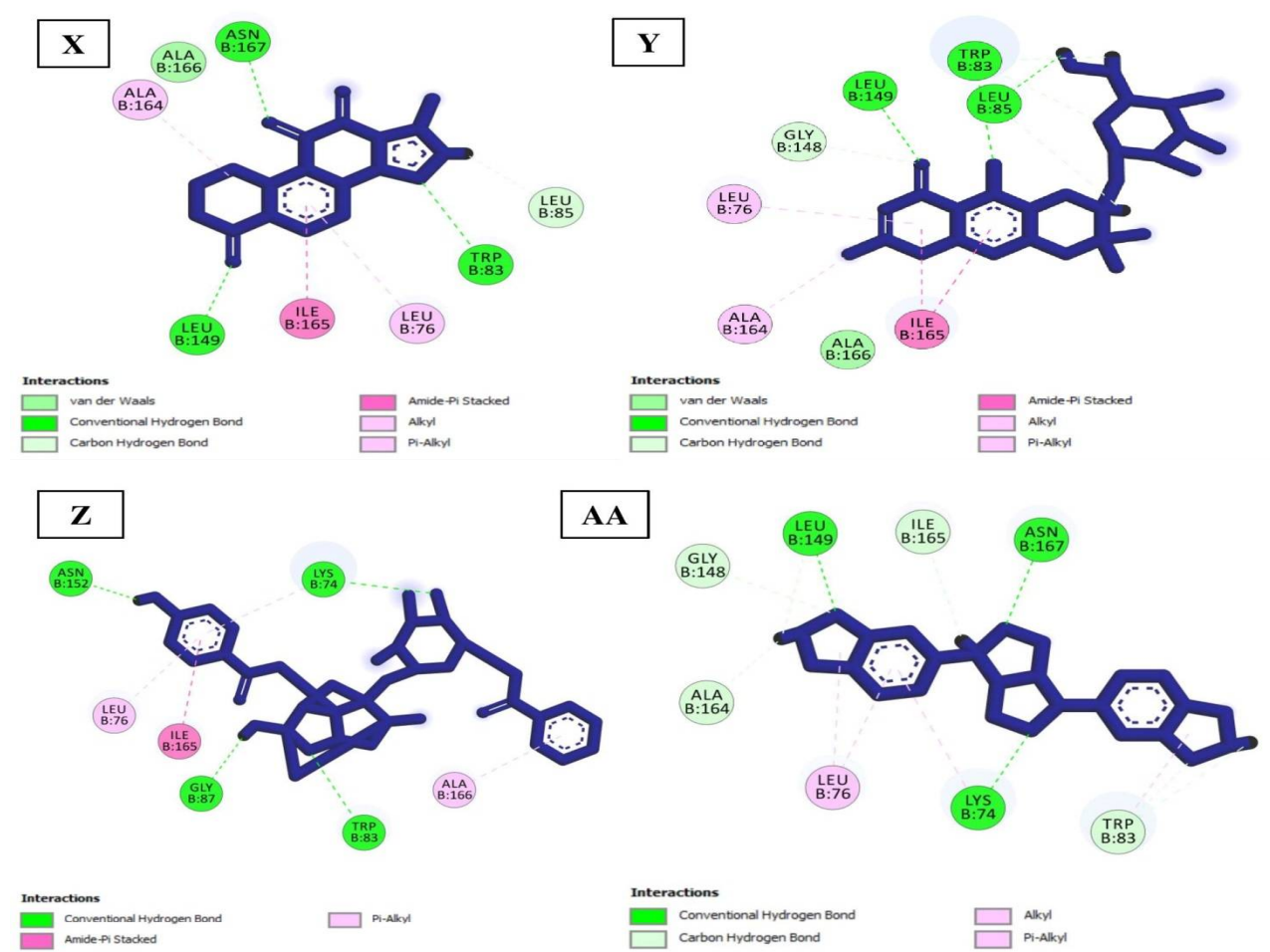












**Figure S1.** 2D representation of the selected compounds against Dengue Virus NS2B/NS3 Protease (PDB: 2FOM). (A) Rutaecarpine, (B) Sesamin, (C) Choerospondin, (D) Evodiamine, (E) Narirutin, (F) Angustidine, (G) Forsythoside A, (H) Luteone, (I) Quercimeritrin, (J) Hydroxytanshinone, (K) Methylophiopogonanone A, (L) Tanshinlactone, (M) Piperitylthonokiol, (N) Sanjoinine B, (O) Sanjoinine D, (P) Scutianine D, (Q) Scutianine C, (R) 6''-O-Acetyllicquiritin, (S) Phellodendroside, (T) Quercetin-7-O-Rutinoside, (U) (S)-Suspensaside, (V) Paeonidanin B, (W) Phellamuretin, (X) Nortanshinone, (Y) Sec-O-Glucosylhamaudol, (Z) Benzoyloxypaeoniflorin, and (AA) Asarinin.

**Table S1.** Selected plants, their compounds and CID of each compound.

no	Name	Compounds	CID	Reference
1.	Asarum sieboldii (45)	Methylpluviatilol	5320622	
		Pluviatilol	70695727	
		Epipinoresinol	637584	
		Sesamin	72307	
		Piperitol	10247670	
		Methyleugenol	7127	
		(±)-car-3-ene-2,5-dione	181910	
		-N-isobutyl-2,4,8,10-dodecatetraenamide	57404464	
		Myristicin	4276	
		Safrole	5144	
		Asarinol A	46174001	
		Asarinol B	46174002	
		Asarinol C	21631051	
		(+)-Asarinol D	21631052	
		3-Caren-2-one	13901618	
		m-Cymene	10812	
		p-Cymene	7463	
		p-Cymen-7-ol	325	1
		2,3-Dehydro-1,8-cineol	523035	1
		Fenchone	14525	1
		Myrcenol	10975	1
		Phellandral	89488	1
		Sabinyol acetate	94266	1
		Terpinen-4-yl acetate	20960	1
		Calarene	28481	1
		Alpha-Guaiene	5317844	2
		Beta-Guaiene	6949	2
		Isoledene	530426	3
		Sativene	11830550	
		3',4'-Dimethoxycinnamaldehyde	5375268	
		3,5-Dimethoxytoluene	77844	
		2,3,5-Trimethoxytoluene	170114	
		Asaricin	4276	
		Alpha-Asarone	636822	
		Beta-Asarone	5281758	
		Croweacin	5316141	
		Elemicin	10248	
		(E)-Isocroweacin	14601153	
		Methyl kakuol	13672435	
		3,4-Methylene-dioxypropiofenone	95682	
		Asarinin	11869417	
		Asatone	431129	
		Tetradecane	12389	
		1-Tridecene	17095	
2.	Scutellaria baicalensis	Acetophenone	7410	4
		l-phenyl-1	11062753	

3.	(30)	(E)-4-phenyl-3-buten-2-one	129825247	5
		3-butanedione	6409633	
		palmitic acid	985	
		oleic acid	445639	
		b-carotene	5280489	
		benzyl alcohol	244	
		b-sitosterol	222284	
		Benzoic acid	243	
		Lutein	5281243	
		Baicalin	64982	
		Baicalein	5281605	
		Wogonoside	3084961	
		Wogonin	5281703	
		Tenaxin-I	159029	
		Viscidulin III	5271991	
		Viscidulin I	5320471	
		Viscidulin II	5322059	
		Baicalein-7-O-D-glucoside	5320313	
		Norwogonin	5281674	
		Chrysin	5281607	
		Chrysin-8-C- $\beta$ -D-glucopyranoside	44257620	
		Skullcapflavone II	124211	
		Salvigenin	161271	
		Oroxylin A	5320315	
		Oroxylin A-7-O-glucuronide	14655551	
		Eriodictyol	440735	
		5-Hydroxy-7,8-dimethoxyflavone	188316	
		Dihydrobaicalin	14135325	
		Dihydrooroxylin A	5316733	
		Eriodictyol	440735	
	Cinnamomum cassia	endo-borneol	1201518	
		(-)- $\alpha$ -terpineol	443162	
		$\beta$ -bisabolene	10104370	
		$\alpha$ -bisabolol	1616126	
		curcumene	92139	
		$\delta$ -cadinene	12306054	
		espatulenol	522266	
		caryophyllene oxide	1742210	
		$\alpha$ -muurolene	12306049	
		$\alpha$ -cadinol	6431302	
		coniferaldehyde	5280536	
		cinnamylalcohol	5315892	
		2-methoxycinnamaldehyde	641298	
		20-methoxycinnamaldehyde	641298	
		benzyl benzoate	2345	
		2-hydroxybenzaldehyde	6998	
		3-phenylpropanol	31234	
		Benzaldehyde	240	
		phenylethyl alcohol	6054	
		benzenepropanal	7707	



1-terpineol	11468	6
cis- $\beta$ -terpineol	8748	6
caryophyllene	5281515	6
eugenol	3314	6
cinnamyl acetate	5282110	6
linalool	6549	7
camphene	6616	7
$\beta$ -pinene	440967	7
camphor	2537	7
geranyl acetate	1549026	7
copaene	19725	7
1-(1,5-dimethyl-4-hexenyl)-4-methylbenzene	92139	7
Cedrene	521207	7
$\alpha$ -calacorene	528708	7
isolekene	530426	7
cis-cinnamaldehyde	6428995	7
trans-cinnamaldehyde	637511	7
ethyl cinnamate	637758	7
benzene,1,3-dimethyl	7929	7
styrene	7501	7
1,3-pentanediol,2,2,4-trimethyl	71330332	7
Decanal	8175	7
dodecane, 2,6,10-trimethyl	6430052	7
coumarin	323	7
cinnzeylanol	44559448	8
anhydrocinnzeylanol	73099741	8
cinnzeylanone	101693755	8
Anhydrocinnzeylanine	131752069	8
cinnassiol A	46173967	9
cinnassiol B	71448932	9
cinnassiol C	75144796	9
cinnassiol E	139031772	9
cinnacasol	102421920	9
perseanol	21672106	10
cinnassiol D1	139031768	10
D1 glucoside	131751606	10
D2 glucoside	131751607	10
D4 glucoside	131751659	10
trans-caryophyllene	5281515	11
germacrene D	5317570	11
cinnamaldehyde	637511	11
cis-2-methoxycinnamic acid	1622530	11
o-methoxycinnamaldehyde	641298	11
2,2,4,6,6-pentamethylheptane	26058	11
2,5,9-trimethyldecane	522020	11
2-ethyl-5-propylphenol	522454	11
3,4-dimethoxyphenethyl alcohol	81911	11
2,5-dimethylundecane	28452	11
2-hydroxycinnamic acid	637540	12
2-hydroxycinnamaldehyde	5318169	12

	4-methoxycinnamaldehyde	641294	12
	cinnamic acid	444539	12
	cinnacasolide A	70692598	13
	cinnacasolide B	70692599	13
	cinnacasolide C	70694646	13
	rosavin	9823887	13
	dihydromelilotoside	5316728	13
	methyl dihydromelilotoside	46881368	13
	cinnacasside A	25214691	14
	cinnacasside C	25214689	14
	cinnacasside B	102035893	15
	picrasmalignan A	122395445	16
	(-)-syringaresinol	11604108	16
	(+)-isolariciresinol	160521	16
	(-)-secoisolariciresinol	65373	16
	Lawsonicin	70698092	16
	5-methoxylariciresinol	44559567	16
	(+)-5,5 -dimethoxylariciresinol	14157882	16
	(1→6)-β-d-glucopyranoside	476541	17
	(-)-lyoniresinol 3α-O-β-d-glucopyranoside	10483388	17
	5R-methyl-3-heptatriacontyl-2(5H)-furanone	129882098	18
	Echinatin	6442675	
	Glycyrin	480787	
	Glycyrol	5320083	
	Isoangustone A	21591148	
	Isoglycyrol	124050	
	7-O-methyluteone	441251	
	Glyasperin D	480860	
	Dehydroglyasperin D	10109594	
	Gancaonin I	480777	
	Semilicoisoflavone B	5481948	
4.	Kumatakenin	5318869	19
	Licoricone	5319013	
	Angustone A	15664151	
	Licoflavonol	5481964	
	Topazolin	5481965	
	Licoisoflavone A	5281789	
	Wighteone	5281814	
	Allolicoisoflavone B	10383349	
	Lupiwighteone	5317480	
	Licoarylcoumarin	10090416	
	Isolicoflavonol	5318585	
	Formononetin	5280378	
	Genkwanin	5281617	
	Glycy coumarin	5317756	
	Isoglabrone	102597283	19
	Glyurallin A	15818598	
	11b-hydroxy-11b,1-dihydromedicarpin	44437741	
	Kaempferol 3-O-methyl ether	5280862	
	Glycyrrhiza-isoflavone C	10546844	

Isoliquiritigenin	638278	
Isoglycycoumarin	14187587	
Genistein	5280961	
Kumatakenin B	5318869	
Luteone	5281797	
Licocoumarone	503731	
Uralenol	5315126	
Glicoricone	10361658	
Pratensein	5281803	
Dehydroglyasperin C	480775	
Homobutein	6438092	
Kaempferol	5280863	
Gancaonin L	14604077	
Licoisoflavanone	392443	19
biochanin A	5280373	
Liquiritigenin	114829	
Licoflavone A	5319000	
Glyasperin C	480859	
Daidzein	5281708	
1-methoxyphaseollin	10247433	
Isolupalbigenin	26238934	
6,8-diprenylgenistein	480783	
2'-hydroxyisolupalbigenin	14237659	
Isoderrone	14237660	
Licoricidin	480865	
Glicophenone	10021298	
Licoisoflavone B	5481234	
Vicenin-2	442664	
Isoviolanthin	101422758	
Liquiritin apioside	10076238	
Liquiritin	503737	
Ononin	442813	
Isoliquiritin	5318591	
Glycyroside	101939210	
Sophoraflavone B	5491513	
Daidzin	107971	
Glycyrrhizic acid	14982	20
lignoceric acid	11197	20
methoxyfolicifolinol	480872	20
docosanol	12620	20
betulinic acid	64971	20
docosyl caffeate	5316952	20
neoglycyrol	5320083	20
gancaonin H	5481949	20
3R-vestitol	439310	20
Licoarylcoumarin	10090416	20
7,2',4'-trihydroxy-5-methoxy-3-arylcoumarin	25015742	20
Isoliquiritigenin	638278	20
Glycyrin	480787	20
isoliquiritin apioside	6442433	20

		hedysarimcoumestan B	11558452	20
		AH-1	132525571	
		astragaloside I	13996685	
		Astragaloside-II	71306915	
		Astragaloside III	441905	
		Astragaloside IV	13943297	
		Astragaloside V	71448939	
		Astragaloside VI	71448940	
		Astragaloside VII	14241100	
		Isoastragaloside I	60148697	
		Isoastragaloside II	60148655	
		Azukisaponin V methyl ester	101683319	
		Malonylastragaloside	50917280	
		astramembrannin II	132492418	
5.	Astragalus membranaceus	brachyoside B	100927164	
	(30)	cyclocanthoside E	21633193	21
		astramembranoside A	24795974	
		astramembranoside B	24796110	
		Astragalan	103026223	
		Kaempferol	5280863	
		Isorhamnetin	5281654	
		Rhamnocitrin	5320946	
		kumatakenin	5318869	
		rhamnocitrin-3-glucoside	44259544	
		quercetin-3-glucoside	5280804	
		Formononetin	5280378	
		Calycosin	5280448	
		2'-hydroxy-3',4',7-trimethoxyisoflavone	44257240	
		3,9,10-trimethoxypterocarpan	15689655	
		Astragalus polysaccharides (APS)	2782115	
		Berberine	2353	
		Berberrubine	72703	
		Berberastine	442180	
		Bis-[4-(dimethylamino)phenyl]methanone	282874	
		Evodiamine	442088	
		Palmatine	19009	
		Tetrahydropalmatine	5417	
		Tetrahydroberberine	34458	
6.	Phellodendron amurense	Phellodendrine	3081405	22
	(70)	Magnocurarine	53266	
		Magnoflorine	73337	
		Y-Fagarine	107936	
		Canthin-6-one	97176	
		4-methoxy-N-methyl-2-quinolone	182073	
		Oxypalmatine	10926678	
		Candicine	23135	
		Lotusine	5274587	
		(-)-Oblongine	157128	
		Tetrahydrojatrorrhizine	185605	22
		Menisperine	161487	

(+) N-methylcorydine	52949574
N-methylflindersine	72819
Litcubine	85243417
Tetrahydropalmatine	5417
Xanthoplanine	14262868
N-methylphoebine	101731569
Columbamine	72310
Epiberberine	160876
Pteleine	159650
Noroxyhydrastinine	89047
Chilenine	11025386
Rutecarpine	65752
Skimmianine	6760
Tembetarine	167718
Tetramethyl-O-scutellarin	96118
γ-hydroxybutenolide	16221764
Armepavine	442169
Demethyleneberberine	363209
8-oxoberberine	12039004
8-oxoepiberberine	12799036
Oxyberberine	11066
Oxypalmatine	10926678
Kihadanin B	156766
Niloticin	14021529
Obaculactone or limonin	179651
Obacunone or Obacunoic acid	119041
Rutaevin	441805
Coniferin	5280372
Vanilloloside	44577222
Herculin	5318023
Ferulic acid	445858
Quinic acid	6508
Neochlorogenic acid	5280633
3-O-feruloylquinic acid	9799386
Chlorogenic acid	1794427
Methyl 3-O-feruloylquininate	24813764
Methyl 5-O-feruloylquininate	102004731
Sanleng acid	5321100
(+/-)-lyoniresinol	10483388
Amurensin	5318156
Quercetin	5280343
Phellamurin	193876
Phellatin	44258781
Phellavin	5320517
Phellodendroside	101316827
Icariside-1	5745470
Phellamuretin	7092536
Isovaleric acid	10430
7-Dehydrostigmasterol	12303924
Syringin	5316860



		Daucosterol	5742590	
		$\alpha$ -Pinene	6654	
		Sabinene	18818	
		$\beta$ -Myrcene	31253	
		d-Limonene	440917	
		(Z)- $\beta$ -Ocimene	5320250	
		(E)- $\beta$ -Ocimene	5281553	
7.	Mentha arvensis	3-Octanol	11527	
	(15)	l-Menthone	26447	23
		Isomenthone	6986	
		Menthyl acetate	27867	
		Neomenthol	19243	
		Caryophyllene	5281515	
		l-Menthol	16666	
		$\alpha$ -Terpineol	17100	
		Piperitone	6987	
		5-O-caffeoyl quinic acid	5280633	24
		chlorogenic acid methyl ester	6476139	24
		quercetin	5280343	24
		quercitrin	5280459	24
		isoquercitrin	5280804	24
		rutin	5280805	24
		saikosaponin D	107793	24
		saikosaponin A	167928	24
8.	Bupleurum falcatum	saikosaponin C	131801344	24
	(20)	2,2,4-trimethyl-3-penten-1-ol	79926	25
		2,3-dimethyl-3-buten-2-ol	82652	25
		2,3-dimethyl-pentane	11260	25
		9-octadecenoic acid (z)	6439696	25
		octadecanoic acid	5281	25
		nonanedioic acid	2266	25
		octanedioic acid	10457	25
		6-O-acetyl-saikosaponin d	21637630	25
		Palbinone	9841735	
		13-Methyl tetradecanoic acid	151014	
		Peonin (peonidin-3,5-diglucoside)	44256843	
		Albiflorin	24868421	
		Albiflorin R1	5317181	
		Benzoylpaeoniflorin	21631106	
		8-Debenzoylpaeoniflorin	71452333	
9.	Paeonia lactiflora	Paeonidanin B	102417825	
	(45)	Paeonidanin A	44253993	26
		Paeonidanin C	46883513	
		Paeoniflorigenone	70698143	
		Paeoniflorin	442534	
		Paeonilactone A	10081437	
		Paeonilactone B	10375422	
		Paeonilactone C	10471123	
		Pyrethrin I	5281045	
		Pyrethrin II	5281555	

		$\beta$ -Sitosterol	521199	
		Casuariin	14035442	
		Casuarictin	73644	
		5-Desgalloylstachyurin	10417809	
		1-O-galloyl- $\beta$ -D-glucose	124021	
		3-O-Galloylquinic acid	442988	
		4-O-Galloylquinic acid	475263	
		Pedunculagin	442688	
		1,2,3,4,6-Pentagalloylglucose	65238	
		Strictinin	73330	
		Tellimagrandin I	442690	
		1,3,6-Trigalloyl- $\beta$ -D-glucose	452707	
		1,2,3-Tri-O-galloyl- $\beta$ -D-glucose	13270010	
		Benzoic acid	243	
		Phenol (Carbolic acid)	996	
		p-hydroxybenzoic acid	135	
		gallic acid	370	
		methylgallate	7428	
		paeonol	11092	
		paeonoside	442924	
		(+)-catechin	9064	
		Paeoniflorin	442534	27
		Oxypaeoniflorin	21631105	
		Benzoyloxypaeoniflorin	21631107	
		Galloylpaeoniflorin	46882879	
		betulinic acid	64971	
		hederagenin	73299	
		oleanolic acid	10494	
		Atractylenolide I	5321018	28
		Atractylenolide II	14448070	28
		Atractylenolide III	155948	28
		Atractylone	3080635	28
		Hinesol	10878761	28
		$\beta$ -Eudesmol	91714393	28
		Atractylodin	5321047	28
		Stigmasterol	5280794	28
		coumarin osthol	10228	29
	Atractylodes lancea	atractylochromene	10244247	29
		Kudtdiol	26471785	29
10.		atractyloside A	71307451	29
	(30)	atractyloside B	71448952	29
		pterocarpol	12314741	29
		eudesma-4(14),7(11)-dien-8-one	13986100	29
		(+) eudesma-4(14),7(11)-dien-8-one	13986100	29
		atractylenolide IV	132510447	29
		atractyloside C	71448953	29
		atractyloside D	71448954	29
		atractyloside E	71448955	29
		atractyloside G	71448957	29
		atractyloside I	10929902	29

11.	Cimicifuga dahurica (25)	atractyloside F	71448956	29
		heterolupeol	604983	29
		Atractylodinol	10012964	29
		Acetylactylodinol	5315531	29
		1,3-di-O-caffeoylquinic acid	6474640	29
		Osthol	10228	29
		5-hydroxymethyl furaldehyde	237332	29
		L-phenylalanine	6140	29
		diethyl phthalate	6781	29
		Geniposide	107848	30
		24-O-acetylhydroshengmanol	157168	30
		prim-O-glucosylcimifugin	14034912	30
		acerinol	73347277	30
		cimigenol	16020000	30
		Cimiracemoside C	15541911	31
		Cimigenoside	16088242	31
		25-O-Acetylcimigenol	46881255	31
		25-Anhydrocimigenol	15967434	31
		23-epi-26-Deoxyactein	21668683	31
		Actein	10032468	31
		Cimicifugic acid A	6449879	31
		Cimicifugic acid B	6449880	31
		Cimicifugic acid D	11742743	31
		Cimicifugamide	5318530	31
		Visnagin	6716	31
		2-Isoferuloyl piscidic acid	6450179	32
		Ferulic acid 4-O- $\beta$ -D-glucopyranoside	13916049	32
		Caffeic acid 3-O- $\beta$ -D-glucopyranoside	5281759	32
		Shomaside A	46209783	32
		Caffeic ester glucoside	5281761	32
		Caffeic methyl ester	689075	32
		Carboxymethyl isoferulate	16729361	32
		3, 4-Dimethoxycinnamic acid	717531	32
		2-Feruloyl piscidic acid	10002902	32
		(E)-3-(3-Methyl-2-butenylidene)-2-indolinone	5319526	32
		(Z)-3-(3-Methyl-2-butenylidene)-2-indolinone	5249879	32
12.	Cnidium officinale (08)	6-(1-oxopentyl)-salicylic acid methyl ester	134612870	33
		Falcarindiol	5281148	33
		conifenyl ferulate	6441913	33
		ferulic aldehyde	5280536	33
		senkyunolide C	642374	33
		(E)-3-methoxy-1-(3-methoxyphenyl)propane	15418925	33
		Coniferol	1549095	33
13.	Angelica dahurica (30)	p-hydroxyphenol	785	33
		Isoimperatorin	68081	34
		imperatorin	10212	34
		bergapten	2355	34
		osthenol	5320318	34
		xanthotoxin	4114	34
		dehydrogeijerin	620900	34

	phellopterin	98608	34
	7-demethylsuberosin	5316525	34
	Alloimperatorin	69502	34
	Xanthotoxol	65090	34
	Isooxypeucedanin	625383	34
	Alloisoimperatorin	5317436	34
	5-hydroxy-8-methoxypsoralen	5385192	34
	oxypeucedanin methanolate	483514	34
	pabulenol	3009225	34
	byakangelicin	10211	34
	marmesin	334704	34
	(+) -decursinol	442127	34
	Heraclenol	73253	34
	oxypeucedanin hydrate	17536	34
	marmesinin	216283	34
	ulopterol	176475	34
	uracil	1174	34
	oxypeucedanin	160544	35
	byakangelicol	3055167	35
	isopimpinellin	68079	35
	pimpinellin	4825	35
	scopoletin	5280460	35
	1-Phenylpropane-1,2-dione	11363	36
	(S)-cathinone	25203656	36
	(1R,2S)-norephedrine	10297	36
	(2S,4S,5R)-2,4-dimethyl-5-phenyl oxazolidine	130754154	36
	(1R,2S)-ephedrine	6922965	36
	(1R,2S)-N-methylephedrine	6918907	36
	(1S,2S)-norpseudoephedrine	6918945	36
	(1S,2S)-pseudoephedrine	7028	36
	(1S,2S)-N-methylpseudoephedrine	7059595	36
	proanthocyanidin A4	13556387	36
	catechin	9064	37
	epicatechin	72276	37
	gallocatechin	65084	37
	epigallocatechin	72277	37
	Ephedradine A	126326	37
	Ephedradine B	156055	38
	Ephedradine C	558490	38
	Ephedradine D	100996000	38
	Feruloylhistamine	10401784	38
	L(+)-Pseudoephedrine	7028	38
	D(-)Norephedrine	62943	38
	D(-)Methylephedrine	3041454	38
	Ephedroxane	161171	38
	2, 3, 4-Trimethyl-5-phenyloxazolidine	5322112	38
	Hordenine	68313	38
	Maokonine	54704413	38
	Tetramethylpyrazine	14296	38
	N-methylbenzylamine	7669	38

14.

Ephedra sinica

(55)

		Herbacetin	5280544	38
		Herbacetin 7-methyl ether	44259958	38
		Pollenitin	44259965	38
		Herbacetin 7-O-glucoside	5318021	
		Kaempferol 3-O-rhamnoside 7-O-glucoside	554033	
		Herbacetin 7-O-neohesperidoside	102444811	
		Kaempferol-3-O-glucoside-7-O-rhamnoside	14035324	
		Dihydroquercetin	439533	
		Naringenin	932	
		Hesperidin	10621	
		(-)-epicatechin	72276	
		(-)-epiafzelechin	443639	
		Afzelechin	442154	
		Leucocyanidin	71629	
		Symplocoside	44257110	
		Tricin	5281702	
		Apigenin	5280443	38
		3-Methoxyherbacetin	5319442	
		Swertisin	124034	
		Isovitexin-2''-O-rhamnoside	23844078	
		Leucodelphinidin	3081374	
		Ephedrannin A	21676348	
		Ephedrannin B	25051177	
		Sesquipinsapol B	101767126	
		Ethyl caprylate	7799	
		Sitosterol	222284	
		Trans-cinnamic acid	444539	
		Physcion	10639	
		Rhein	10168	
		Panaxadione	25233029	
		20(S)-protopanaxatriol	11468733	
		3-keto-20(S)-protopanaxatriol	44198762	
		ginsenoside Rg2	21599924	
		ginsenoside Rd	24721561	
		phenethyl alcohol- xylopyranosyl(1→6)glucopyra-		
		noside	131129	39
		panaxoside A	441923	39
		Panaxoside Re	58774156	39
		protopanaxadiol	9920281	39
		panacon	6325774	39
		panaxadiol	73498	39
		panaxol	328778	39
		ginsenoside R0	11815492	40
		ginsenoside Rb-1	9898279	
		ginsenoside Rb-2	6917976	
		ginsenoside Rc	12855889	
		ginsenoside Rd	24721561	
		ginsenoside Rf	441922	
		ginsenoside Rg-1	441923	
		ginsenoside Rg-2	21599924	

15.

Panax ginseng

(30)



16.	Zingiber officinale (45)	ginsenoside Rg-3	9918693	41
		ginsenoside Rh-1	12855920	
		ginsenoside Rh-2	119307	
		panacene	181799	
		$\beta$ -elemene	6918391	
		citric acid	311	
		fumaric acid	444972	
		ketoglutaric acid	51	
		choline	305	
		[6]-gingerol	442793	
		[6]-shogaol	5281794	
		[4]-gingerol	5317596	
		[7]-gingerol	11472344	
		[8]-gingerol	168114	
		[10]-gingerol	168115	
		[6]-Paradol	94378	
		[7]- paradol	13733135	
		[8]- paradol	213821	
		[10]- paradol	51352076	
		methyl [6]-paradol	85807832	
		[4]- shogaol	9794897	
		[8]- shogaol	6442560	
		[10]- shogaol	6442612	
		[12]-shogaol	9975813	
		[6]-isoshogaol	11694761	
		[6]- gingerdione	162952	
		[8]- gingerdione	14440537	
		[10]- gingerdione	14440539	
		[12]- gingerdione	86251913	
		citral/ geranial	638011	42
		borneol	64685	
		bisabolene	3033866	
		Gingerdiol	11369949	
		1-dehydrogingerdione	9796015	
		5-acetoxy [6] gingerdiol	101419545	
		Ar-curcumene	92139	
		$\beta$ -bisabolene	10104370	
		(-) $\beta$ -sesquiphellandrene	519764	
		6-methyl-5-hepten-2-one	9862	
		$\alpha$ -phellandrene	7460	
		$\beta$ -phellandrene	11142	
		limonene	22311	
		citronellol	8842	
		neral	643779	
		geraniol	637566	
		bornyl acetate	6448	
		2 undecanone	8163	
		citronellyl acetate	9017	
		$\alpha$ -copaene	70678558	
		geranyl acetate	1549026	

		eucalyptol/ 1,8-cineole	2758	
		isobornyl formate	23623868	43
		$\alpha$ -zingiberene	521253	43
		$\alpha$ farnesene	5281516	43
17.	Poria cocos (43)	dehydroeburicoic acid	15250826	44
		3-epi-dehydrotumulosic acid	10005581	44
		dehydrotrametenolic acid	15250826	44
		pachymic acid	5484385	44
		eburicoic acid	73402	44
		trametenolic acid	12309443	44
		$\alpha$ -amyrin acetate	71597151	44
		adenosine	60961	44
		16 $\alpha$ -Hydroxytrametenolic acid	132285301	45
		3-O-Acetyl-16 $\alpha$ -hydroxytrametenolic acid	15226712	45
		3-O-Acetyl-16 $\alpha$ -hydroxydehydrotrametenolic acid	15226714	45
		Dehydrotrametenonic acid	44424826	45
		Dehydroeburiconic acid	11431307	45
		Dehydropachymic acid	15226717	45
		3-epi-Dehydropachymic acid	15226716	45
		Tumulosic acid	12314446	45
		Dehydrotumulosic acid	15225964	45
		3-epi-Dehydrotumulosic acid	10005581	45
		15 $\alpha$ -Hydroxydehydrotumulosic acid	16736459	45
		Polyporenic acid C	9805290	45
		6 $\alpha$ -Hydroxypolyporenic acid C	101280198	
		29-Hydroxypolyporenic acid C	139585448	
		25-Hydroxy-3-epi-tumulosic acid	46882675	
		5 $\alpha$ -8 $\alpha$ -Peroxydehydrotumulosic acid	16736654	
		Poricoic acid B	5471852	
		16-Deoxyporicoic acid B	16736458	
		Poricoic acid E	15225966	
		Poricoic acid BM	15225967	
		Poricoic acid G	5471966	
		Poricoic acid GM	44556812	
		Poricoic acid A	5471851	
		Poricoic acid C	56668247	45
		Poricoic acid D	44424827	
		Poricoic acid F	101928114	
		Poricoic acid H	10918099	
		Poricoic acid CM	16736060	
		Poricoic acid DM	44424830	
		Poricoic acid HM	44556877	
		6,7-Dehydroporicoic acid H	44556878	
		25-Hydroxyporicoic acid C	44556811	
		25-Hydroxyporicoic acid H	16736865	
		26-Hydroxyporicoic acid DM	44556810	
		25-Methoxyporicoic acid A	46882628	
18.	Paeonia suffruticosa	Mudanpioside F	21631108	46
		Procyanidin B6	474540	

(60)	Oxypaeoniflorin	21631105	
	Procyanidin B6	474540	
	Mudanpioside E	86278277	
	(p)-Catechin	107957	
	Apiopaeonoside	127509	
	Methyl gallate	7428	
	Paeonolide	442923	
	1,3,6-Tri-O-galloyl-b-D-glucose	452707	
	Suffruticoside A	9986231	
	Suffruticoside B	10258205	
	Suffruticoside C	10258206	
	Suffruticoside D	5321547	
	Tetragalloyl glucose	102012877	
	Suffruticoside A	9986231	
	Suffruticoside B	10258205	
	Suffruticoside C	10258206	
	Suffruticoside D	5321547	
	Quercetin 7-O-glucoside	5381351	
	Galloylpaeoniflorin	46882879	
	Albiflorin	24868421	
	1,2,3,4,6-Penta-O-galloyol-beta-D glucose	65238	
	Mudanpioside H	71457654	
	Hexagalloyl glucose	54036807	
	Galloyloxypaeoniflorin	3036133	
	Benzoyloxypaeoniflorin	21631107	
	Quercetin 3-O-rhamnosylglucoside	5491657	
	Mudanpioside C	21631098	
	Benzoylpaeoniflorin	21631106	
	Mudanpioside B	21631102	
	hederagenin	73299	47
	chrysoeriol	5280666	47
	trans-ε-viniferin	5281728	47
	trans-resveratrol	445154	47
	stigmaterol	5280794	47
	β-daucosterol	5742590	47
	quinic acid	6508	48
	galloylquinic acid	129650210	48
	kaempferol 3,7-di-O-glucoside	6325460	48
	isorhamnetin 3,7-di-O-glucoside	5323537	48
	galloyl glucose	124021	48
	pentagalloylglucose	65238	48
	hexagalloylglucose	129630523	48
	heptagalloylglucose	25202629	48
	Paeonisuffrone	10104180	49
	Paeonisuffral	101050848	49
	Deoxypaeonisuffrone	10035257	49
	mudanpioside A	21631101	49
	mudanpioside D	21631103	49
	α-benzoyloxypaeoniflorin	102597515	49
	β-benzoyloxypaeoniflorin	21631107	49

		oxypaeonidanin	71457653	49
		9-epi-oxypaeonidanin	71450490	49
		trigalloyl-glucose	440308	49
		(-)-Epigallocatechin gallate	65064	49
		uridine	6029	49
		thymidine	5789	49
		paeoniflorigenone	70698143	49
		Honokiol	72303	
		pinoresinol	73399	
		salicylic acid	338	
		p-hydroxy-cinnamic acid	637542	
		songorine	71456946	
		karakoline	441742	
		Aconitine	245005	
		Mesaconitine	441747	
		Hypaconitine	441737	
		Talatizamine	441761	
		Isotalatizidine	3084020	
		Neoline	120682	
		Fuziline	14163819	
		Isodelphinine	102146471	
	Aconitum carmichaelii	Benzoylmesaconine	24832659	50
	Debeaux	Senbusine A	158048	50
		Senbusine C	14163819	50
		Hokbusine A	24832661	50
	(65)	Benzoylaconine	20055771	50
		Benzoylhypaconine	78358526	51
		Neojiangyouaconitine	78358553	
		Aldohypaconitine	5317220	
		Deoxyaconitine	21598997	
		Beiwutine	21627927	
		Aconifine	441705	
		Aconine	20054813	
		Yunaconitine	155569	
		Chasmanine	20055812	
		Foresticine	154723942	
		N-deethylaconine	101552717	
		Beiwutinine	101552718	
		Hypaconine	101671038	
		Mesaconine	76189547	
		Oxonitine	6708531	
		Guiwuline	70688216	
		Bullatine B	120682	
		Penduline	179472	
		Ignavine	71448929	
		Delgradine	139075130	51
		14-O-Anisoylneoline	12068477	
		14-O-Acetyneoline	14312993	
		Foresaconitine	20055981	
		Crassicauline A	157539	

	Hetisine	431673	
	Songoramine	14526618	
	12-Epinapelline	3133561	
	Aconicarchamine A	102484827	
	Aconicarchamine B	102484828	
	Napelline	441749	
	Carmichaeline A	102144179	
	Yokonoside	3085046	
	Higenamine	114840	
	Salsolinol	91588	
	Fuzitine	72201752	
	Oleracein E	21574476	
	16beta-Hydroxycardiopetaline	102511299	
	Columbianine	101457306	
	Aconitamide	15944660	
	6''-O-Acetyllicquiritin	101051311	
	Liquiritigenin	114829	
	Isoliquiritigenin	638278	
	Liquiritin	503737	
	Gracillin	159861	
	Glyceryl monopalmitate	3084463	
	Fuzinoside	102339571	
20.	Danshensu	11600642	52
	protocatechuic aldehyde	8768	
	lithospermic acid	6441498	
	tanshinone IIB	9926694	
	dihydrotanshinone I	11425923	
	tanshinone I	114917	
	miltiradiene	20837867	
	isoquercitrin	5280804	
	salvianolic acid A	5281793	
	salvianolic acid B	11629084	
(60)	salvianolic acid C	13991590	53
	salvianolic acid D	75412558	
	salvianolic acid E	86278266	
	salvianolic acid G	11530200	
	methyl rosmarinate	6479915	
	dimethyl lithospermate	70688393	
	lithospermic acid B	6451084	
	ursolic acid	64945	
	tigogenin	99516	
	tanshinone IIA	164676	
	tanshinone VI	149138	
	cryptotanshinone	160254	
	isotanshinone I	623940	
	isotanshinone II	44425166	
	isotanshinone IIB	184102	
	isocryptotanshinone	626608	
	hydroxytanshinone IIA	5318349	
	methyl tanshinonate	14610613	



		danshenxinkun A	149138	
		danshenxinkun B	5320113	
		danshenxinkun C	5320114	
		danshenxinkun D	127172	
		dihydroisotanshinone I	89406	
		neocryptotanshinone	389888	
		deoxyneocryptotanshinone	15690458	
		salviol	13966146	
		nortanshinone	10062187	
		Tanshindiol A	16730071	
		Tanshindiol B	5321620	
		Tanshindiol C	126072	
		Miltirone	160142	
		1,2-Dihydrotanshinquinone	105119	
		Ferruginol	442027	
		4-methylenemiltirone	14609851	53
		Tanshinlactone	5321617	
		danshinspiroketallactone	5316298	
		Epidanshenspiroketallactone	102004791	
		cryptoacetalide	46896125	
		miltiodiol	11011966	
		miltipolone	10086184	
		norsalvioxide	14139391	
		2-isopropyl-8-methylphenanthrene-3,4-dione	135872	
		Dihydrotanshinone	5316743	
		Neosalvianen	11472648	
		Salvianen	11186248	
		Salviadione	135442608	54
		Lithospermic acid B	6451084	
		Dihydrotanshinone I	11425923	
		Cryptotanshinone	160254	
		Tanshinone IIA	164676	
		Hesperidin	10621	55
		Naringin	442428	55
		Neohesperidin	442439	55
		Naringenin	932	55
		Hesperetin	72281	55
21.	Citrus unshiu	<i>p</i> -coumaric acid	637542	56
	(25)	sinapic acid	637775	56
		protocatechuic acid	72	56
		<i>p</i> -hydroxybenzoic acid	135	56
		vanillic acid	8468	56
		narirutin	442431	56
		Nobiletin (3',4',5,6,7,8-hexamethoxyflavone)	72344	57
		kaempferol 3-O-rutinoside	5318767	57
		limocitrin 3-glucoside	44259988	57
		didymin (4'-methoxyl naringenin 7- O-rutinoside)	16760075	57
		naringenin 7-Orutinoside		
		Hesperetin-7-O-glucoside	85704	57
		Prunin	20111686	58

	Sinensetin	92794	58
	Tangeretin	145659	58
	$\gamma$ -terpinene	68077	58
	2- $\beta$ -pinene	7461	59
	1-methyl-2-isopropylbenzene	6654	59
	L-limonene	10703	59
	$\beta$ -ocimene	439250	59
		5281553	59
	geniposidic acid	443354	
	chlorogenic acid	1794427	
	genipin-1- $\beta$ -gentiobioside	14179128	
	geniposide	107848	
	genipin	442424	
	crocin-1	5281233	
	crocin-2	9940690	
	jasminoside I	102596097	
	gardenoside	24721095	
	gardaloside	11631807	
	5, 7, 3', 4', 5'-pentamethoxyflavone	16044716	
	shikimic acid	8742	
	1, 2, 4-benzenetriol	10787	
	3, 4-dimethoxy-benzoic acid	86584921	60
22.	dibutyl phthalate	3026	
	diisobutyl phthalate	6782	
	$\alpha$ -gardiol	101936008	
	$\beta$ -gardiol	57340454	
	genameside C	11692460	
	deacetylasperulosidic acid	12315350	
		10742	
	syringic acid	8655	
	syringaldehyde	8468	
	vanillic acid	129848169	
	3-hydroxy-vanillic acid	69505	
	3, 4, 5-trimethoxy-phenol	31244	
	4-methoxy-benzaldehyde	129848159	
	7-hydroxy-5-methoxy-chromone	5496475	
	5, 7, 3'-trihydroxy-6, 4', 5'-trimethoxyflavone		
	3beta,23- dihydroxyurs-12-en-28-oic acid	14136881	
	emodin	3220	
	physcion	10639	
	stearic acid	5281	
	Gardenal	4763	
	Geniposide	107848	
	6- $\alpha$ -hydroxy geniposide	6325021	60
	Feretoside	442433	
	genipin-1- $\beta$ -gentiobioside	14179128	
	shanzhiside	11948668	
	lamalbidic acid	101434718	
	picrocrocinic acid	5320582	
	jasminoside A	98050833	

		epijasminoside A	76551288	
		jasminoside R	71552546	
		jasminoside S	71552547	
		jasminoside T	71552548	
		chikusetsusaponin IVa methyl ester	637855	
		chikusetsusaponin IVa butyl ester	44566502	
		protocatechuic acid	72	
		genipin-gentiobioside	3082301	
		7alpha-hydroxy sitosterol	146158661	
		jasminosides R	71552546	
		z-3-hexenyl tiglate	5352469	
		trans-beta-ocimene	5281553	
		genipin 1-O-beta-D-gentiobioside	3082301	
		scandoside methyl ester	442433	
		deacetylasperulosidic acid methyl ester	6325021	
		10-O-succinoylgeniposide	44255239	60
		6'-O-acetylgeniposide	44253991	
		10-O-acetylgeniposide	6324916	
		Jasminodiols	24896698	
		jasminoside H	102596096	
		jasminoside I	102596097	
		imperatorin	10212	
		isoimperatorin	68081	
		crocetin	5281232	
		sudan III	62331	
		crocin-3	10461942	
		methyl 5-O-caffeoyl-3-O-sinapoylquinat	11671431	
		ethyl 5-O-caffeoyl-3-O-sinapoylquinat	11699888	
		methyl 5-O-caffeoyl-4-O-sinapoylquinat	11635556	
		ethyl 5-O-caffeoyl-4-O-sinapoylquinat	11512664	
		methyl 3,5-di-O-caffeoyl-4-O-(3-hydroxy-3-methyl) glutaroylquinat	11693219	60
		Ixoroside	44566558	
		8-epiapodantheroside	11372643	
		gardenate A	10611205	
		2-hydroxyethylgardenamide A	10825707	
		Jasminoside F	10807517	
		β-amyrin	225687	61
		β-amyrin acetate	345510	61
		uvaol	92802	61
		gentiopicroside	88708	62
		6beta-hydroxyswertiajaposide A	11153922	62
		Gelidoside	46174003	62
23.		Trifloroside	101688128	62
		Scabraside	159134	62
		Durvillonol	634965	63
		masilinic acid	73659	63
		urjinolic acid	146156259	63
		3beta-erythrodiol	101761	63
		corosolic acid	6918774	63

	pygenic acid C	69049736	63
	chiratenol	14831162	63
24.	Magnolol	72300	64
	Honokiol	72303	
	O-methylhonokiol	155160	
	Piperitylmagnolol	11732171	
	Dipiperitylmagnolol	101612410	
	Piperitylhonokiol	13337242	
	Bornylmagnolol	13337239	
	Eudesmagnolol	14587417	
	Eudeshonokiol A	14587421	
	Eudeshonokiol B	21726646	
	Clovanemagnolol	10323149	
	Caryolanemagnolol	21726647	
	Magnolignan A	5319201	
	Magnolignan B	5319202	
	Magnolignan C	5319203	
	Magnolignan D	5319204	
	Magnolignan A-2-O-beta-D-glucopyranoside	71720154	
	Randainal/Magnaldehyde B	5320888	
	Randaiol	13337243	
	Magnatriol B	5319191	
	Magnaldehyde D	5319189	
	Magnaldehyde E	5319190	
	4'-methoxymagnaldehyde B	23657448	
	4'-methoxymagnaldehyde E	23657447	
Magnolignan E	15714551		
Coumanolignan	24796112		
Magnaldehyde C	5319188		
4'-methoxymagnaldehyde	23634517		
Manglieside D	102473624		
Magnolignan F	5319207		
Magnolignan I	373768		
Isomagnolol	159137		
Obovatol	100771		
Eudesobovatol A	442837		
Eudesobovatol B	10346031		
Obovatal	6439677		
Magnolignan G	15714552		
Magnolignan H	373767		
Icariside E5	91884923		
Lariciresinol	332427		
(+)-Syringaresinol	443023		
Pinoresinol-4-O-beta-D-glucopyranoside	486614		
Magnoloside A	21629882		
Magnoloside B	14018784		
Magnoloside C	14018786		
Magnoloside D	131676053		
Crassifolioside	102193658		
Acteoside	5281800		

Tachioside	11962143	
Syringaldehyde	8655	
Sinapic aldehyde	5280802	
Isosyringinoside	57399043	
Erigeside C	14132346	
Coniferaldehyde	5280536	
Coniferyl alcohol	1549095	
p-Coumaric acid	637542	
Caffeic acid methyl ester	689075	
Coniferin	5280372	
Magnolianone	16739270	
O-methyleugenol	7127	
Chavicol	68148	
p-Hydroxybenzaldehyde	126	
Loliolide	100332	
Blumenol A	5280462	
Blumenol B	14135402	
S-(+)-dehydrovomifoliol	688492	
Grasshopper ketone	13922639	
(S)-tembetarine	167718	
Reticuline	439653	
Magnoflorine	73337	
(+)-Laurifoline	12305611	
(+)-Menisperine	30358	
(+)-Xanthoplanine	5315336	64
Asimilobine	160875	
Lysicamine	122691	
Roemerine	119204	
Anonaine	160597	
Anolobine	164710	
Liriodenine	10144	
Nornantenine	3084228	
Anaxagoreine	13891860	
N-nornuciferine	12313579	
10-demethylcryptaustoline	100969440	
N-methylisosalsoline	40091	
N-Feruloylputrescine(trans)	92339985	
Indole-3-aldehyde	10256	
Betaine	247	
Limonene	22311	
Caryophyllene	5281515	
Caryophyllene epoxide	14350	
β-eudesmol	91457	64
γ-eudesmol	6432005	
Cryptomeridiol	165258	
β-sitostenone	60123241	
Stigmasta- 4,22-dien- 3-one	6442194	
Hyperoside	5281643	
Afzelin	5316673	
Choerospondin	157745	

25.	Ophiopogon japonicus (30)	Isorhamnetin- 3-O- $\beta$ -D-glucoside	5318645	65
		Choerospondin	157745	
		Ethyl palmitate (Ethyl hexadecanoate)	12366	
		Ethyl stearate (Ethyl octadecanoate)	8122	
		Arachidic acid (Icosanoic acid)	10467	
		1-hexacosanol (hexacosan-1-ol)	68171	
		Palmitone (hentriacontan-16-one)	94741	
		Nonacosylic acid (Nonacosanoic acid)	20245	
		glycoside C	44566500	
		nolinospiroside F	86289919	
		ophiopogonin B	46173857	
		ophiopogonin D	46173859	
		ophiopogonin A	46173858	
		diosgenin	99474	
		ophiopogonin C'	4483248	
		ophiopogonin D'	10033524	
		ophiopogonin P	102195415	
		ophiopogonin Q	71522132	
		sprengerinin A	102081298	
		cixiophiopogon A	102004869	
		ophiopo japonin C	146160153	
		ophiopogonin R	71523896	
		ophiopogonin S	71523897	
		prazerigenin A	13833781	
		methylophiopogonone B	23259413	65
		ophiopogonone B	14826840	65
		methylophiopogonone A	10065830	65
		6-aldehydo-isoophiopogonone A	5317207	65
		ophiopogonone A	10087732	65
		ophiopogonone C	11142766	65
		ophiopogonanone E	5316797	65
		methylophiopogonanone B	46886723	65
		methylophiopogonanone A	5319741	65
		ophiopogonanone A	9996586	65
		ophiopogonanone C	10871974	65
		Cryptomeridiol	165258	66
		Pennogenin	12314056	66
		Sprengerinin C	44583957	66
26.	Perilla frutescens L. (200)	3-Epicorosolic acid	15917998	67
		3-Epimaslinic acid	25564831	
		Augustic acid	15560128	
		Corosolic acid	6918774	
		Hyptadienic acid	14605533	
		Pomolic acid	382831	
		Tormentic acid	73193	
		Triacylglycerol	11146	
		Pentadecanoic acid	13849	
		Stearic acid	5281	
		$\beta$ -Cholesterol	6665	

Docosanol	12620
Eicosanol	12404
Heneicosanol	85014
Heptacosanol	74822
Hexacosanol	68171
Octacosanol	68406
Tetracosanol	10472
Triacontanol	68972
Tricosanol	18431
$\beta$ -Tocopherol	6857447
$\gamma$ -Tocopherol	92729
$\delta$ -Tocopherol	92094
Rosmarinic acid methyl ester	3012090
Apigenin 7-O-glucuronide	5319484
Apigenin 7-O-diglucuronide	126843388
Cimidahurinine	5315870
Chrysoeriol	5280666
Luteolin 7-O-diglucuronide	146036993
Luteolin 7-O-glucoside	5280637
Luteolin 7-O-glucuronide	5280601
Luteolin-5-O-glucoside	5317471
Scutellarein	5281697
Chrysotenenin	197081
Cyanin	441688
Malonylshisonin	11972402
Shisonin	5282068
(E,E)- $\alpha$ -Farnesene	5281516
(Z)-3-Hexenyl acetate	5363388
(Z,E)- $\alpha$ -Farnesene	5362889
1,10-Decanediol	37153
1,2-Benzenedicarboxylic acid	1017
1,6-Cyclodecadiene	5365639
10-Undecyn-1-ol	76015
1-Cyclohexene-1-methanol	317542
1-Octen-3-ol	18827
2,2-Dimethylpentane	11542
2,4,6-Triisopropylphenol	82158
2,4-Hexadienal	637564
2-Acetyl-5-methyl furan	14514
2-Acetylfuran	14505
2-Butylamine	24874
2-Cyclopentenone	13588
2-Ethyladamantane	139758
2-Hexanoylfuran	61738
2-Hexenal	5281168
2-Hydroxypyridine	8871
2-Isopropylidene-3-methylhexa-3,5-dienal	5368460
2-Methoxy-3-propenyl-phenol	74069607
2-Methyl-2-cyclopentenone	14266
2-Methylcyclopentanone	14265

2-Nonyne	140536
3,5-Diethyl-toluene	16302
3-Octanol	11527
4,4-Dimethyl-2-cyclopenten-1-one	140955
4-Tert-pentylphenol	6643
Acetophenone	7410
Acetyl eugenol	7136
a-Cubebene	86609
Alloaromadendrene	91354
All-trans-squalene	638072
Anisole	7519
Apiol	10659
Asarone	636822
a-Terpinyl acetate	111037
Benzene acetaldehyde	998
Bornyl acetate	6448
Cadina-3,9-diene	10657
Calarene	28481
Camphane	92108
Carvone	7439
Caryophyllene	5281515
Caryophyllene oxide	1742210
cis-Asarone	5281758
cis-Geraniol	643820
cis-Lanceol	6536796
cis-Nerolidol	5320128
cis-Ocimene	5320250
cis-Verbenol	164888
Cosmene	5368451
Cuminaldehyde	326
Curlone	196216
Cycloheptane	9265
Cyclohexanone	7967
Decane	15600
Dihydrocarveol	12072
Dihydrocarveol acetate	30248
Dodecane	8182
Egomaketone	42978
Elemicin	10248
Elixene	94254
Elsholtziaketone	521240
Eremophilene	12309744
Eucalyptol	2758
Farnesol	445070
Furfuryl alcohol	7361
Geraniol	637566
Germacrene D	5317570
Germacrene D-4-ol	5352847
Heneicosane	12403
Hexadecane	11006



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Hexahydrofarnesyl acetone	10408
Humulene epoxide II	10704181
Isobornyl acetate	247573
Isocaryophyllene	5281522
Isoegomaketone	5318556
Isoelemicin	5318557
Isoeugenol	853433
Isolimonene	521268
Isomenthone	6986
Isopulegone	34645
Limonene oxide	91496
Limonene oxide, trans	8029780
Linalool oxide trans	6432254
Linalyl oxide cis	6428573
Longifolene	289151
Longipinocarvone	535296

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Massoia lactone	39914
Menthol	1254
Menthone	26447
Methyl chavicol	8815
Methyl eugenol	7127
Methyl geranate	5365910
Methyl isoeugenol	7128
Methyl thymyl ether	14104
M-Mentha-6,8-diene	102625
Naginata ketone	564412
Nerol acetate	1549025
n-Heptadecane	12398
Nonacosane	12409
Nonane	8141
n-Tricosane	12534
Octacosane	12408
Patchoulane	29408
p-Cymene	7463
Pentacosane	12406
Perilla ketone	68381
Perillaldehyde	16441
Perillene	68316

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Perillic acid	1256
Perillyl alcohol	10819
Piperitenone	381152
p-Menth-1-en-4-ol	11230
p-Menth-1-en-8-ol	17100
p-Mentha-3,8-diene	521851
Pulegone	442495
Phytol	5280435
Phytone	10408
Sabinene	18818
Santolina triene	519872
Spathulenol	92231

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		Terpinen-4-ol	11230	
		Terpinolene	11463	
		Thujyl alcohol	10550	
		trans-Nerolidol	5284507	
		trans-Shisool	519954	
		Triacontane	12535	
		Tridecane	12388	
		Valencene	9855795	
		Valeric acid, pent-2-en-4-ynyl ester	5353036	
		Viridiflorene	10910653	
		Viridiflorol	11996452	
		$\alpha$ -Bulnesene	520826	
		$\alpha$ -Cadinol	10398656	
		$\alpha$ -Caryophyllene	5281520	
		$\alpha$ -Citral	638011	
		$\alpha$ -Copaene	70678558	
		$\alpha$ -Farnesene	5281516	
		$\alpha$ -Fenchene	12309839	
		$\alpha$ -Patchoulene	521710	
		$\alpha$ -Santalol	5281531	
		$\beta$ -Cubebene	93081	
		$\beta$ -Bourbonene	324224	
		$\beta$ -Cadinene	10657	
		$\beta$ -Cyclocitral	9895	
		$\beta$ -Elemene	6918391	
		$\beta$ -Farnesene	5281517	
		$\beta$ -Guaiene	6949	
		$\beta$ -Gurjunene	6450812	
		$\beta$ -Ionone	638014	
		$\beta$ -Pinene	14896	
		$\beta$ -Selinene	442393	
		$\beta$ -Phellandrene	11142	
		$\beta$ -Terpinene	66841	
		$\gamma$ -Pyronene	578237	
		$\delta$ -Cadinene	441005	
		$\delta$ -Elemene	12309449	67
		Methyl- $\alpha$ -D-fructofuranoside	6325664	68
		Methyl- $\beta$ -D-fructofuranoside	128889	68
		3,5-Di-O-caffeoylquinic acid	6474310	68
		Pimaric acid	220338	69
		(-)-Kaur-16-en-19-oic acid	73062	69
		Falcarindiol	5281148	69
		17-Hydroxy-ent-kaur-15-en-19-oic acid	169654	69
		Alpha-mono palmitin	14900	69
		Kaurenoic acid	73062	70
		Continentalic acid	10086296	70
		Neomangiferin	6918448	
		Mangiferin	5281647	
		Isomangiferin	5318597	71
		Vitexin	5280441	

		Isosakuranetin	160481	
		Macrostemonoside J	101669618	
		Asparagosome G	3042722	
		Tomatoside A	426059	
		Timosaponin BII	44575945	
		Officinalisinin-I	441889	
		Timosaponin D	132545772	
		Filicinoside-A	190854	
		Timosaponin F	101005526	
		Anemarrhenasaponin I	101672279	
		Anemarrhenasaponin II	101672380	
		Anemarrhenasaponin III	101672280	
		F-gitonin	44559009	
		Timosaponin AIV	154572708	
		Timosaponin AIII	15953793	
		Desgalactotigonin	162401	
		Timosaponin AI	71767755	
		cis-hinokiresinol	5281830	
		monomethyl-cis-hinokiresinol	5319736	
		Foliamangiferoside A	46206548	
		2,6,4'-trihydroxy-4- methoxybenzophenone	10467773	
		Phytosphingosine	122121	
		Dimethisterone	6607	
		Macrostemonoside F	192523	72
		Platycodin D	162859	72
		Platycoside A	50900942	72
		Platycodin D2	53317652	72
		Polygalacin D2	53325781	72
		Platycodin D3	70698293	72
		trans-Hinokiresinol	12310493	72
		Isosarsasapogenin	91439	73
		Markogenin	12304414	73
		Neogitogenin	12304409	73
		Sarsasapogenin	92095	73
		Diosgenin	99474	73
		Arctigenin	64981	74
		Arctiin	100528	74
		Trachelogenin	452855	74
		Lappaol F	73425459	74
		Diartigenin	16215736	74
		Methyl palmitate	8181	75
		Methyl linoleate	5284421	75
		Methyl oleate	5364509	75
		Hexanal	6184	
		Benzeneacetaldehyde	998	
		cis-Sabinene hydrate	101629835	
		trans-Sabinene hydrate	12315151	76
		cis-Verbenol	164888	
		trans-Verbenol	89664	
		cis-Chrysanthanol	527032	

		Verbenone	29025	
		Chrysanthenyl acetate	162747	
		Lavandulyl acetate	30247	
		Silphiperfol-5-ene	91747334	
		Germacrene D	5317570	
		Zingiberene	92776	
		Germacrene D 4-ol	5352847	
		Neophytadiene	10446	
		Hexadecanoic acid	985	
		Phytol	5280435	
		Nonacosane	12409	
		Hentriacontane	12410	
		Dotriacontane	11008	
		Tritriacontane	12411	
		Isolariciresinol	160521	77
		isolariciresinol 9-O-beta-D-glucopyranoside	85210374	77
		pinoresinol-4-O-beta-D glucoside	486614	77
		dehydrodiconiferyl alcohol 4-O-b-D-glucopyranoside	5316442	77
		neo-olivil	9976812	77
		medioresinol	181681	77
		americanol A	637304	77
		pinoresinol	73399	77
	Pinellia ternate	burselignan	11631864	77
		L-Ephedrine	9294	78
31.		Inosine	135398641	78
	(75)	Cytidine	6175	78
		Pedatisectine B	190	78
		8-Octadecenoic acid	5282758	78
		Pentadecanoic acid	13849	78
		9-Hexadecenoic acid	5282745	78
		Hexadecanoic acid	985	78
		Heptadecanoic acid	10465	78
		7-Hexadecenoic acid	543268	78
		Octadecanoic acid	5281	78
		9-Oxo-nonanoic acid	75704	78
		11-Eicosenoic acid	5282768	
		Eicosanoic acid	10467	
		10,13-Eicosadienoic acid	72444876	
		Docosanoic acid	8215	
		Pinellic acid	9858729	
		Succinic acid	1110	
		3-Methyleicosane	98417	78
		3-Decyne	75425	
		2-Methyldecane	23415	
		Octadecane	11635	
		2,6,10-Trimethyltetradecane	85785	
		2,5-Dimethyltetradecane	41836	
		Vinylcyclohexane	12757	
		1-Octene	8125	

	6-Methyl-2-heptanone	13572	
	3-Nonanone	61235	
	Cis-4-decenal	5362620	
	2-Undecanone	8163	
	9-Heptadecanol	136435	
	Anethole	637563	
	Citronellal	7794	
	Aromandendrene	91354	
	Farnesane	19773	
	$\beta$ -Patchoulene	101731	
	$\alpha$ -Elemol	92138	
	1-Methyl-4-(1-methylethenyl)-cyclohexene	6453304	
	Dibutyl phthalate	3026	
	2,6-Di-tert-butyl-4-methylphenol	31404	
	2-Pentylfuran	19602	
	Furfural	7362	
	2,4-Dimethyl furan	19462	
	Anisic acid	7478	
	Pulegone	442495	
	Isopulegol	170833	
	3-Nonyne	140649	
	2-Methylnonane	13379	
	3,4-Dihydroxycinnamyl alcohol	5282096	
	Sachaliside 1	14048613	
	Stigmast-4-en-3-one	5484202	
	Cycloartenol	92110	
	Protocatechuic aldehyde	8768	
	Shogaol	5281794	78
	Gingerol	442793	
	Erythritol	222285	
	Melissane	182192	
	Nonacosane	12409	
	Homogentisic acid	780	
	Benzene-1,4-diol	785	
	Benzene-1,2-diol	289	
	Monogalactosyldiacylglycerol	90657729	
	Soyacerebroside I	11104507	
	Soyacerebroside II	15599558	
	N-acetylglutamate	70914	
	Platycoside A	50900942	
	Platycoside B	101937508	
	Platycoside C	101937509	
	Platycoside D	100974704	
	Platycoside E	70698202	
32.	Platycodon grandifloras	Platycoside G1	70698289 79
	(55)	Platycoside F	101048500
		Platycoside G2	102217526
		Platycoside G3	70698263
		Platycoside H	11665339
		Platycoside I	11622299

Platycoside J	11528185	
Platycoside K	102004765	
Platycoside L	11556931	
Platycoside M-1	101403595	
Platycoside M-2	101403596	
Platycoside M-3	101403597	
Platycodin A	46173910	
Platycodin C	46173919	
Platycodin D	162859	
Deapioplatycodin D	70698266	
Platycodin D2	53317652	
Deapioplatycodin D2	50900942	
Platycodin J	102052427	
Platycodin K	102052428	
Platycodin L	102052429	
3-O- $\beta$ -D-glucopyranosylplatycodigenin	102185205	
Polygalacin D	46173909	
20-O-acetylPolygalacin D	53321792	
30-O-acetylPolygalacin D	53321793	
Polygalacin D2	53325781	
30-O-acetylPolygalacin D2	53321794	
Platyconic acid A	70698300	
Platyconic acid B lactone	50900852	
Deapioplatyconic acid B lactone	50900941	79
Platycogenic acid A	20056221	
Platyconic acid B	101495504	
Platyconic acid C	102052424	
Platyconic acid D	102052425	
Platyconic acid E	102052426	
Platycogenic acid B	69570716	
Platycogenic acid C	69569686	
Platyconin	90659256	
(2R, 3R) taxifolin	439533	79
quercetin-7-O-glucoside	5282160	79
quercetin-7-O-rutinoside	101764560	79
luteolin-7-O-glucoside	5280637	79
apigenin-7-O-glucoside	12304093	79
p-hydroxybenzoic acid	135	79
2,3-dihydroxybenzoic acid	19	79
2-hydroxy4-methoxybenzoic acid	75231	79
homovanillic acid	1738	79
spinasterol	5281331	79
botulin	49895112	79
$\delta$ -7-stigmastenone-3	5748344	79
Apigenin	5280443	79
Luteolin	5280445	79
Platycoside	101403597	79
Flavoplatycoside	10416329	79
3,4-dimethoxycinnamic acid	717531	79
Isoferulic acid	736186	79

33.	(45)	Rehmannia glutinosa	m-coumaric acid	637541	79
			p-coumaric acid	637542	80
			$\alpha$ -resorcylic acid	7424	80
			Chlorogenic acid	1794427	80
			Lobetyolin	53486204	80
			Lobetyolinin	5459227	80
			Iobetyol	5807986	80
			Betulin	72326	80
			$\beta$ -sitosterol	521199	80
			Inulin	24763	80
			Grandoside	10341593	80
			Lariciresinol	332427	81
			hierochin D	85382912	81
			yemuoside 1	195850	81
			darendoside B	21668724	81
			decaffeoyl acteoside	13889681	81
			jionoside B <sub>1</sub>	5281782	81
			<a href="#">catalpol</a>	91520	81
			ajugol	6325127	81
			6-O-vanilloylajugol	14396664	81
			6-O-E-feruloylajugol	6325178	81
			Rehmapicroside	21637711	81
			Rehmapicrogenin	15693863	82
			hydroferulic acid	14340	82
			aucubin	91458	82
			isoacteoside	6476333	82
			acteoside	5281800	82
			ethyl $\beta$ -D-fructofuranoside	138113708	82
			eleutheroside C	9859136	82
			mannitol	6251	82
			raffinose	439242	82
			stachyose	439531	82
			glutinolic acid	53248310	82
			paulownin	3084131	82
			monopalmitin	14900	82
			pinellic acid	9858729	82
			jio-cerebroside	10169092	82
			aeginetic acid 5-O-beta-D-quinovoside	53248311	83
			aeginetoyl ajugol 5"-O-beta-D-quinovoside	101790066	83
			rehmaionoside A	10023290	83
			dihydroxy-beta-ionone	15693868	83
			rehmaglutin D	5320906	83
			ajugoside	9865184	83
			martynoside	5319292	84
			leucosceptoside A	10394343	84
			5-hydroxymethyl furfural	237332	84
			Tyrosol	10393	84
			Isomartynoside	91895373	84
			purpureaside C	11953944	84
			jionoside A1	6325450	84

	ferulic acid methyl ester	5357283	85
	coniferin	5280372	85
	leonoside F	57325811	85
	echinacoside	5281771	85
	diincarvilone A	60155233	85
	pterolactam	181561	85
	3-indolecarboxylic acid	69867	85
	Ledebouriellol	5318962	86
	Hamaudol	164722	
	sec-O-glucosylhamaudol	10478277	
	Divaricatol	9974111	
	Cimifugin	441960	
	prim -O – glucosylcimifugin	14034912	
	5-O-methylvisamminol	441970	
	4'-O-β-D-glucosyl-5-O-methylvisamminol	21670038	
	Norcimifugin	46240156	
	undulatoside A	5321494	
	wogonin	5281703	
	bergapten	2355	
	byakangelicin	10211	
	deltoid	906525	
	imperatorin	10212	
	isoimperatorin	68081	
	isobergapten	68082	
	marmesin	334704	
	nodakenetin	26305	
Saposhnikovia divaricate	oxypeucedanin hydrate	17536	
	phellopterin	98608	
	psoralen	6199	
	xanthotoxin	4114	
(45)	5-hydroxy-8-methoxypsoralen	5385192	
	Nodakenin	73191	
	Xanthoarnol	11482406	
	Fraxidin	3083616	
	Isofraxidin	5318565	
	Scopoletin	5280460	
	Umbelliferone	5281426	
	Anomalin	10251869	
	Decursinol	442127	
	decursinol angelate	776123	
	praeruptorin B	5319259	
	praeruptorin F	51668830	
	cis-3', 4'-diseneciokhellactone	1119128	
	(-)-cis-khellactone	455821	
	(3'S)-hydroxydeltoid	455821	
	Panaxynol	5281149	
	Falcarindiol	5281148	
	(9Z)-1-methoxy9-heptadecene-4,6-diyn-3-ol	146026404	
	Marmesinin		
	tectochrysin	216283	



		glyceryl monooleate	5281954	
		8'-epicleomiscosin A	5283468	
35.	Glycyrrhiza uralensis (30)		11200016	86
		lignoceric acid	11197	
		licorisoflavan A	196831	
		methoxyficifolinol	480872	
		docosanol	12620	
		betulinic acid	64971	
		licoricidin	480865	
		kumatakenin	5318869	
		docosyl caffeate	5316952	
		neoglycyrol	5320083	
		gancaonin H	5481949	
		isoglycyrol	124050	
		liquiritigenin	114829	
		lupiwighteone	5317480	
		3R-vestitol	439310	
		Echinatin	6442675	87
		Glycycoumarin	5317756	
		Licoarylcoumarin	10090416	
		7,2',4'-trihydroxy-5-methoxy-3-arylcoumarin	25015742	
		Glicoricone		
		Isoliquiritigenin	10361658	
		Formononetin	638278	
		Licoricone	5280378	
		Glycyrin	5319013	
		formononetin-7-O- $\beta$ -D-glucoside	480787	
		liquiritin	101350244	
		isoliquiritin apioside	503737	
		glycyrrhizic acid	6442433	
		liquiritin apioside	14982	
		hedysarimcoumestan B	10076238	
			11558452	
36.	Ziziphus jujuba (70)	Mauritine A	11353668	
		Mucronine D	5373023	
		Amphibine H	51029223	
		Nummularine A	131750852	
		Nummularine B	51017057	
		sativanine-B	5281595	
		frangulanine	5281587	
		sativanine F	102156891	
		coclaurine	160487	88
		isoboldine	133323	
		norisoboldine	14539911	
		asimilobine	160875	
		sanjoinenine	14729078	
		amphibine-D	5318120	
		sanjoinine-B	14729076	
		sanjoinine-D	44566617	
		sanjoinine-F	14729081	

Jubanine-A	101316794	
Jubanine-B	101316795	
Scutianine-C	45268911	
Scutianine-D	45267179	
Jubanine-C	131752168	
Zizyphine-A	6324833	
6'''- sinapoylspinosin	101616450	88
6'''-feruloylspinosin	21597353	88
6'''-pcoumaroylspinosin	5316122	88
jujuboside A	51346169	88
jujuboside B	24721031	88
jujuboside A1	177396	88
jujuboside B1	73156987	88
jujuboside C	71448946	88
acetyljujuboside B	73093046	88
protojujuboside A	71448943	88
protojujuboside B	71448944	88
protojujuboside B1	71448945	88
Puerarin	5281807	88
6'''-feruloylisospinosin	10795344	88
Isospinosin	11801844	88
Kaempferol 3-O-robinobioside	15944778	88
Kaempferol 3-O-rutinoside	5318767	88
colubrinic acid	21672700	88
alphitolic acid	12305768	88
zizyberenalic acid	15958448	88
betulinic acid	64971	88
3-O-( <i>cis-p</i> -coumaroyl)-alphitolic acid	5316118	89
3-beta-O-( <i>trans-p</i> -coumaroyl)maslinic acid	14335962	89
pomonic acid	12314449	89
2-oxopomolic acid	44593379	89
benthamic acid	3838010	89
terminic acid	132568257	89
traumatic acid	5283028	89
( <i>Z</i> )-4-oxotetradec-5-enoic acid	132568256	89
Magnoflorine	73337	89
Franganine	45270592	
Spinosyn	155692	
3beta,6beta-stigmast-4-en-3,6-diol	146156493	
Maslinic acid	73659	
Ceanothic acid	161352	
Vitexin	5280441	
Oleamide	5283387	
Ent-epicatechinoceanothic acid A	132967447	90
Lupeol	259846	
2-alpha-hydroxyursolic acid	6918774	
Ziziphin	441957	
Squalene	638072	
epiceanothic acid	23631167	
ceanothenic acid	71451218	

		zizyberanolic acid	21672700	
		ursonic acid	9890209	
		apigenin triacetate	18721	
		daidzein diacetate	10359753	
		daidzein dimethyl ether	136419	
		daidzin	107971	
		puerarin	5281807	
		daidzein	5281708	
		formononetin	5280378	
		puerarol	44257531	
	Pueraria lobata	3'-Hydroxypuerarin	5748205	
		3'-Methoxydaidzein	5319422	
37.		3'-methoxydaidzin	10527347	91
	(50)	3'-methoxypuerarin	5319485	
		6''-O-D-Xylosylpuerarin	101776119	
		biochanin A	5280373	
		4'-Methoxypuerarin	5319486	
		3'-Methoxypuerarin	5319485	
		mirificin	21676217	
		ononin	442813	
		puerarin-4'-O-glucoside	44257212	
		irisolidone	5281781	
		kaikasaponin I	102120183	
		soyasaponin I	122097	91
		astragaloside VIII	124491170	91
		azukisaponin I	14103656	91
		baptisiasaponin I	102317160	91
		genistein	5280961	91
		genistin	5281377	91
		glycitein	5317750	91
		glycitin	187808	91
		kaikasaponin II	101538997	91
		kaikasaponin III	188384	91
		kakkalide	5490351	91
		kakkasaponin I	100945993	91
		kakkasaponin II	102500447	91
		kakkasaponin III	102500448	91
		luteolin	5280445	91
		phaseoside IV	101679107	92
		soyasaponin IV	24721354	92
		tectorigenin	5281811	92
		tectorigenin-7-O-xylosylglucoside	100968221	92
		nicotiflorin	5318767	92
		robinin	5281693	92
		beta-sitosterol palmitate	13747834	92
		lupeone	92158	92
		diisobutyl phthalate	6782	92
		bis(2-ethylhexyl) phthalate	8343	92
		sophoracoumestan A	14630492	92
		coumestrol	5281707	92

38.	Coix lacryma-jobi (15)	allantion	439714	92
		Sissotorin	73407546	92
		(6S,9R)-roseoside	9930064	92
		Coixenolide	46173943	93
		$\gamma$ -Tocopherol	14985	93
		Docosanol	12620	93
		4-Ketopinoresinol	44578390	93
		p-Hydroxy benzaldehyde	126	93
		Tangeretin	68077	93
		Naringenin	932	93
		Nobiletin	72344	93
		Neolignan	261166	93
		5-Amino-1-(quinolin-8-yl)-1,2,3-triazole-4-carbox- amide	26435789	94
		Pyridine	1049	94
		Propenamide	6579	94
39.	Rheum palmatum (22)	N-methoxy-N-methyl-3,4-dihydro-2H-thiopy- ran-6-carboxamide	24813996	94
		1,3-dioctanoin	150911	94
		tetradecanoic acid	11005	94
		aloe-emodin	10207	
		chrysophanol	10208	
		emodin	3220	
		emodin-6-O-beta-D-glucopyranoside	5317038	
		physcion	10639	
		physcion-8-O-beta-D-glucopyranoside	5319323	
		rhein	10168	
		rhein-8-O-beta-D-glucopyranoside	146156489	
		palmidin A	5320384	
		palmidin B	5320385	
		palmidin C	5320386	
		rheinoside A	13888123	95
		rheinoside C	13888128	
		sennidin C	5321255	
		sennoside A	73111	
		sennoside B	91440	
		sennoside C	46173829	
		sennoside D	46173830	
		rhapontigenin	5320954	
40.	Uncaria rhynchophylla (30)	gallic acid 3-O-beta-D-glucopyranoside	101683334	
		gallic acid 4-O-beta-D-glucopyranoside	10088114	
		coumaroyl-O-galloyl-glucose	146170723	
		Hirsutine	3037884	
		Hirsuteine	3037151	
		epi-allo-corynantheine	101603230	
		corynantheidine	3000341	96
		dihydrocorynantheine	3039336	
		akuammigine	1268096	
		yohimbine	8969	
		angustine	441983	

	angustoline	3084765	
	angustidine	3084770	
	corynoxine	44568160	
	18,19-dehydrocorynoxinic acid	24970642	
	Isorhynchophylline	3037048	
	Isocorynoxine	3037448	
	18,19-dehydrocorynoxinic acid B	24970641	
	cadambine	398038	
	3 Alpha-dihydrocadambine	162138	
	vincoside lactam	44567645	
	rhynchophine	11972452	
	strictosidine	161336	
	strictosamide	10345799	
	6beta-hydroxyursolic acid	20055642	
	uncarinic acid C	44583694	
	uncarinic acid D	44583694	
	uncarinic acid B	100967916	
	uncarinic acid E	10746421	
	trifolin	5282149	
	hyperin	5281643	
	cleomiscosin B	156875	
	cleomiscosin D	13965876	
	(+)-pinoresinol	73399	
	(+)-phillygenin	4166098	
	Phillyrin	101712	
	(+) epipinoresinol	637584	
	Pinoresinol	73399	
	8- hydroxypinoresinol	3010930	
	benzenebutanoic acid	4775	
	Arctigenin	64981	
	(-) dimethylmatairesinol	1286	
	Arctiin	100528	
	(-)- matairesinoside	486612	
	Olivil	5273570	
	(+) lariciresinol	332427	
41.	forsythialan A	44453412	97
	forsythialan B	44453332	
	(-)-egenine	189685	
	(-)-bicuculline	185838	
	Rutaecarpine	65752	
	p-hydroxyphenylacetic acid	127	
	suspenolic acid	10774324	
	Trans-nerolidol	5284507	
	2,4-di-tert-butylphenol	7311	
	estragole	8815	
	p-tyrosol	10393	
	hydroxytyrosol	82755	
	Sasanquin	5317538	
	tannic acid	16129778	
	esculetin	5281416	

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	cedrusin	11210164
	glochidioboside	24982202
	icaraside E4	21589939
	Isolariciresinol	160521
	(+)-isoolivil	5316262
Forsythiaside (forsythoside A)		5281773
	forsythoside D	24721571
	forsythoside E	69634125
	salidroside	159278
	forsythoside I	23958169
	calceolarioside A	5273566
	Suspensaside A	132550846
	R-suspensaside	102228838
	S-suspensaside	102228839
	forsythoside B	23928102
	forsythoside F	6442994
	forsythoside G	101231533
	forsythoside H	129449684
	calceolarioside B	5273567
	plantainoside A	5320625
	plantainoside B	9847922
	calceolarioside C	45360240
Wogonin-7-O-glucoside		51136398
	Hesperidin	10621
	Hyperin	5281643
	taraxasterol acetate	13889352
	nigaichigoside F1	16118969
	quadranside IV	10372074
	esculentic acid	9898760
	corosolic acid	6918774
	onjisaponin F	10701737
	arjunglucoside I	14658050
	arjunglucoside II	52951052
	hovenic acid	70698002
	alphitolic acid	12305768
	isobauerenyl acetate	181096
	Ocotillone	12313665
	garcinielliptone Q	102452579
	agatholic acid	101306703
	3- oxoanticopalic acid	13858184
	haplopappic acid	102117108
	dehydropinifolic acid	22568711
	adoxosidic acid	13892717
	Alpha-thujene	17868
	sabinene	18818
	$\gamma$ -terpinene	7461
	terpinolene	11463
	(+)-carene	442461
	$\alpha$ -ocimene	5320249
	terpinen-4-ol	11230

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		p-cymen-8-ol	14529	
		trans-carveol	94221	
		(-)-myrtenal	1201529	
		cornoside	11809239	
		rengyolone	10725564	
		forsythenside A	11797786	
		forsythenside B	10576163	
		Rengyoside B	11045420	
		(6S,9R)- roseoside	129316932	
		Rengyol	363707	
		Rengyoxide	14353410	
		rengyoside A	10958239	
		rengynic acid	54033324	
		Alisol A	15558616	
		Alisol B	15558620	
		Alisol C	46173914	
		Alisol E (epi-alisol A)	101297679	
		Alisol F	76310822	
		Alisol G ( 25-Anhydro-alisol A)	76314443	
		Alisol O	102004738	
		Alisol P	101840124	
		Alisol A 23-acetate	70690607	
		Alisol B 23-acetate	14036811	
		Alisol C 23-acetate	14036813	
		Alisol E 23-acetate	101661272	
42.	Alisma orientale	Alisol J 23-acetate	100936564	98
	(60)	Alisol K 23-acetate	100936565	
		Alisol L 23-acetate	100936566	
		Alisol M 23-acetate	70688546	
		Alisol N 23-acetate	100936567	
		Alisol A 24-acetate	76336194	
		Alismaketone A 23-acetate	11800363	
		Alismaketone B 23-acetate	100941986	
		Alismaketone C 23-acetate	100941987	
		Alismalactone 23-acetate	101701562	
		Alisolide	101840122	
		11-Deoxy-alisol B 23-acetate	101661275	
		11-Deoxy-alisol C 23-acetate	101664412	
		13 $\beta$ ,17 $\beta$ -Epoxy-alisol B	101664542	
		25-Anhydro-alisol A 11-acetate	5318945	
		25-Anhydro-alisol F	102004739	
		16-Oxo-alisol A	9983614	
		16,23-Oxido-alisol B	9847547	
		25-O-methyl-alisol A	102004721	
		Orientalol E	637282	
		Orientalol F	11020886	
		Orientalone	11727780	
		Sulfoorientalol B	5321551	
		Sulfoorientalol C	5321552	
		Sulfoorientalol D	146033487	

	Alismorientol A	16742799	
	Alismorientol B	16742798	
	Alismol	5318916	
	Alismoxide	10988340	
	Clovandiol	76319362	
	Germacrene D	5317570	
	Germacrene C	25244915	
	Oplopanone	10466745	
	Oriediterpenol	5320304	
	Oriediterpenoside	6325764	
	Robustaflavone	5281694	
	Amentoflavone	5281600	
	Calycosin	5280448	
	7-Hydroxy-coumarin	5281426	
	Emodin	3220	
	Falcalindiol	6436239	
	Isoimperatorin	68081	
	Seselin	68229	
	Dulcitol	11850	
	Stachyose	439531	
	Verbascose	441434	
	Manninotriose	5461026	
	Verbascotetraose	102273024	
	(+)-5-endo-hydroxycamphor	9543191	99
	protocatechuic acid methyl ester	287064	99
	betulabuside A	14484636	99
	hedychiol A	10105633	100
	pygmol	14167388	100
	dihydroyashabushiketol	10265808	100
	Tricyclene	79035	101
	o-Cymene	10703	101
	1,8-Cineole	2758	101
	(E)- $\beta$ -Ocimene	5281553	101
	$\alpha$ -Terpinolene	11463	101
	Camphor	2537	101
	2,6-Dimethyl-2,4,6-octatriene	5368821	101
	Terpinen-4-ol	11230	101
	Fenchyl acetate	107217	101
	Bornyl acetate	6448	101
	Bicycloelemene	56842786	101
	Dodecamethyl-cyclohexasiloxane	10911	101
	$\alpha$ -Cubebene	442359	101
	$\beta$ -Cubebene	93081	101
	Alpha-Gurjunene	15560276	
	Beta-Gurjunene	6450812	
	Aromadendrene	91354	
	$\gamma$ -Gurjunene	15560285	101
	Germacrene D	5317570	
	$\alpha$ -Amorphene	12306052	
	Beta-Selinene	442393	



44.	(35)	Areca catechu	Epi-bicyclosquiphellandrene	91747125	102
			Cadina-1,4-diene	6427091	
			Bicyclogermacrene	13894537	
			Endo-1-bourbonanol	12301996	
			$\beta$ -Maaliene	101596917	
			Nerolidol	5284507	
			Spathulenol	92231	
			Caryophyllene oxide	1742210	
			Guaiol	227829	
			Beta-Himachalene	11586487	
			$\tau$ -Muurolol	51394521	
			Bulnesol	90785	
			Farnesol	445070	
			Farnesyl acetate	94403	
			Benzyl benzoate	2345	
			Benzyl salicylate	8363	
			Arecoline	2230	
			Arecaidine	10355	
			Arecolidine	5319882	
			methyl nicotinate	7151	
			ethyl nicotinate	69188	
			ethyl N-methylpiperidine-3-carboxylate	97981	
			isoguvacine	3765	
			homoarecoline	34167	
			isorhamnetin	5281654	
			chrysoeriol	5280666	
			liquiritigenin	114829	
			jacareubin	5281644	
			procyanidin A1	9872976	
			procyanidin B1	11250133	
			procyanidin B2	122738	
			arecatannin A1	13752000	
			arecatannin B1	14237657	
			arecatannin C1	9876038	
			arecatannin A2	16142155	
			arecatannin A3	16201011	
			arecatannin B2	71448962	
			ursonic acid	9890209	
			Arborinol	12305177	
			arborinol methyl ether	101600057	
			fernenol	12305178	
			arundoin	12308619	
			cycloartenol	92110	
			chrysophanol	10208	
			physcion	10639	
			p-hydroxybenzoic acid	135	
			epoxyconiferyl alcohol	57403796	
			isovanillic acid	12575	
			de-O-methylasiadiplodin	14562693	
			cyclo-(Leu-Tyr)	15550385	

45.	Cannabis sativa (90)	Cannabisol	102487751	103
		Cannabigerol	5315659	
		$\alpha$ -cadinyl-cannabigerolate	24862530	
		carmagerol	44586785	
		Sesquicannabigerol	54669855	
		Cannabichromene	30219	
		Cannabidiol	644019	
		cannabidiolic acid	160570	
		cannabidiol monomethyl ether	164905	
		(-)-cannabidivarin	11601669	
		cannabidivarinic acid	59444387	
		Cannabinodiol	11551346	
		cannabielsoic acid A	59444405	
		cannabielsoin	162113	
		cannabielsoic acid B	59444401	
		Cannabicyclol	30607	
		cannabicyclolic acid	71437560	
		8-hydroxycannabinolic acid A	44139742	
		8-hydroxycannabinol	44241652	
		Dehydrocannabifuran	59444381	
		Cannabifuran	9966466	
		cannabicitran	186149	
		cannabicooumaronone	625303	
		cannabiripsol	192007	
		Cannabimovone	46217279	
		cannflavin C	25141335	
		chrysoeriol	5280666	
		6-prenylapigenin	10382485	
		Docosanoic acid methyl ester	13584	
		acetyl stigmasterol	129671096	
		$\alpha$ -spinasterol	5315190	
		quebrachitol	151108	
		Isocannabispiradienone	101802953	
		Cannabinol	2543	
		Tetrahydrocannabivarin	93147	
		tetrahydrocannabinolic acid	98523	
		cannabinolic acid	3081990	
		cannabigerolic acid	6449999	
		cannabigerolic acid monomethyl ether	24739091	104
		cannabigerovarinic acid	59444383	
		cannabigerovarin	59444407	
		cannabichromevarin	6451726	
		cannabidivarin	11601669	
		cannabidiorcol	20586765	
		cannabicyclol	30607	
		Cannabinolic acid A	3081990	
		cannabinol methylether	628150	
		cannabivarin	622545	
		cannabichromanon	25105340	
		trigonelline	5570	

		muscarine	9308	
		neurine	10042	
		Piperidine	8082	
		Hordeine	68313	
		n-propylamine	7852	
		n-butylamine	8007	
		diethylamine	8021	
		pyrrolidine	31268	
		Cannabisativine	442846	
		Alanine	602	
		galacturonic acid	439215	
		erythritol	222285	
		galactitol	11850	
		ribitol	6912	
		Malonic acid	867	
		Phosphoric acid	1004	
		Pyroglutamic acid	7405	
		Quinic acid	6508	
		Behenic acid	633932	
		Sativic acid	92800	
		hexyl caproate	22873	
		campest-4-en-3-one	11988279	
		camphenhydrate	22155067	
		carvacrol	10364	
		carvone	7439	
		citronellol	8842	
		dihydrocarveyl acetate	30248	
		dihydrocarvone	24473	
		pinocarveol	102667	
		pinocarvone	121719	
		allo-aromadendrene	42608158	
		longifolene	289151	
		nerolidol	5284507	
		epi-beta-santalene	11106484	
		vomifoliol	5280462	
		dihydrovomifoliol	129317062	
		cannabispiradienone	90475437	
		beta-cannabispiranol	194174	
		cannabispirenone	10105874	
		cannabispirone	162936	
		canniprene	53439651	
		orientin	5281675	
		Carthamin	135565560	
		Safflor yellow A	71463725	
		Safflor yellow B	131751452	
		Saffloflavonesides A	101878345	
		Saffloflavonesides B	101878346	
46.		Safflomin A (Hydroxysafflor yellow A)	6443665	
	(35)	Tinctormine	42607657	
		Safflomin C	42607658	
				105

		Pecarhamin	101928647	
		Saffloquinoside A	45276863	
		Saffloquinoside B	101501319	
		Cartormin	131751684	
		Anhydrosafflor yellow B	102240413	
		Acacetin 7-O-alpha-L-rhamnopyranoside	44257896	
		Luteolin 7-O-beta-D-glucopyranoside	13093777	
		Acacetin	5280442	
		Isorhamnetin	5281654	
		Umbelliferone	5281426	
		Daphnoretin	5281406	
		N-feruloylserotonin	5969616	
		N-(p-coumaroyl)serotonin	5458879	
		Serotobenine	11725426	
		N-feruloyltryptamine	5458878	
		1-Tridecene-3,5,7,9,11-pentayne	441552	
		Sinapic acid	637775	
		Roseoside	9930064	
		Methylsyringin	131752679	
		Coniferyl alcohol	1549095	
		Sinapyl alcohol	5280507	
		Secoisolariciresinol	65373	
		Matairesinol	119205	
		Arctigenin	64981	
		Trachelogenin	452855	
		Guaiacol	460	106
		Phloroglucinol	359	106
		Phenylacetic acid	999	106
		Gentisic acid	3469	106
		Naringenin Chalcone	5280960	106
		Glycitein	5317750	106
		Delphinidin	68245	106
		Malvidin	159287	106
		Allo Ocimene	5368821	106
47.		Pinene-2-OL	22013424	106
	(20)	Linalyl Acetate	8294	106
		Elemicin	10248	106
		5-Hexene-2-one	7989	107
		Guaiol	227829	107
		Benzene-1-butylheptyl	20661	107
		Nootkatin	238797	107
		9,17-Octadecadienal	6431297	107
		Octadecanoic acid butyl ester	31278	107
		Tellimagrandin II	151590	
		Cornusiin A	16129730	
		Cornusiin B	16131156	
48.		Cornusiin C	16132407	108
		Gemin D	471119	
	(105)	Isoterchebin	442685	
		Tellimagrandin I	442690	

Cornusiin G	102061533
Cornusiin D	101826455
Zoomeric acid	445638
Nervonic acid	5281120
Lignoceric acid	11197
Phthalic anhydride	6811
Trans-9-Octadecenoic acid	637517
3, 5-Bis (1, 1-dimethylethyl)phenol	70825
4-Methyloctanoic acid	62089
2-Dibenzofuransulfonic acid	522803
Morrnionide	11228693
Cornuside	11228694
Loniceroside	179500
Kingiside	12304884
Sweroside	161036
Secoxyloganin	162868
8-epikingiside	12304886
Secologanoside	14136854
Cornin (Verbenalin)	73467
Hastatoside	92043450
Loganin	87691
Loganic acid	89640
7-O-methyl-morrnionide	127258930
7-O-ethyl-morrnionide	74399180
10-hydroxycornin	101637374
10-hydroxyhastatoside	100952769
Secologanin	161276
Arjunglucoside II	52951052
Linalyl propionate	61098
6, 10-Dimethyl-2-undecanone	95495
p-Menth-1-ene-7, 8-diol	110662
Cubebol	11276107
Tachioside	11962143
5-hydroxymethyl-2-furfural	237332
Glycidol	11164
3-Vinyl-1-cyclobutene	556371
1,3-Cyclohexadiene	11605
Methacrolein	6562
2-Vinylfuran	73881
1-Ethoxypropan-2-yl acetate	171378
Pyridine	1049
Pyrrole	8027
3-Pyrrolidinol	98210
3-Furaldehyde	10351
3-Furanmethanol	20449
Propargylamine	239041
Furfural	7362
2-Furanmethanol	7361
Cis-bicyclo[4.2.0]octane	643590
4-Cyclopentene-1,3-dione	70258

Cyclopent-4-ene-1,3-dione	70258	
1-Nonene	31285	
Pentanoic acid	7991	
2-Formylhistamine	541600	
2(5H)-Furanone	10341	
2-Cyclohexen-1-one	13594	
1-Methylpyrazol-3-amine	137254	
2H-Pyran-2-one	68154	
1H-Pyrrole-2-carboxaldehyde	13854	
4-Methyl-5H-furan-2-one	145832	
p-Cresol	2879	
2-Pentyne	12310	
Maltol	8369	
Benzyl nitrile	8794	
Dehydromevalonic lactone	557445	
E-7-Tetradecenol	5362726	
Creosol	7144	
Catechol	289	
5-Hydroxymethylfurfural	237332	
2-Coumaranone	68382	
4,6-Dioxadodecane	57645665	
1-Tridecene	17095	
Kessane	11310616	
Oxaceprol	65784	
2-Methoxy-4-vinylphenol	332	
1,2,3-Benzenetriol	1057	
1,2,4-Benzenetriol	10787	
3,4-Dimethyl-o-phenylenediamine	521077	
3,5-Dimethoxy-4-hydroxytoluene	240925	
4-Methoxycinnamaldehyde	641294	
D-Allose	439507	
1-Pentadecene	25913	
Pentadecane	12391	
Cyclotetradecane	67524	
Butyrovannillone	14035098	
Palmitoleic acid	445638	
Tridecanoic acid	12530	
1-Heptadecene	23217	109
9-Hexadecenoic acid	5282745	
5-Amino-2-thiocyanoacetophenone	284762	
Cyanoacetic acid, dodecyl ester	12606407	
1,5-Dodecadiene	5363382	
cis-1-Chloro-9-octadecene	5367784	
1-Nonadecene	29075	
1-Octadecene	8217	
Methyl 13-methyl-eicosanoate	85964992	
Tricosane	12534	
Oxacycloheptadecan-2-one	7984	
1-Docosene	74138	

49.	Eucommia ulmoides (55)	(-)-olivil	5273570	110
		Lariciresinol	332427	
		Balanophonin	23252258	
		vladinol D	70698172	
		(+)-cyclo-olivil	5316262	
		(+)-medioresinol	181681	
		(+)-pinoresinol	73399	
		(+)-syringaresinol	443023	
		(+)-epipinoresinol	637584	
		Arctiin	100528	
		citrusin B	131752580	
		threo-dihydroxydehydrodiconiferyl alcohol	5317204	
		hedyotol C	21636185	
		genipin	442424	
		aucubin	91458	
		geniposide	107848	
		geniposidic acid	443354	
		asperulosidic acid	11968867	
		asperulosidic acid ethyl ester	21580986	
		Ajugoside	9865184	
		Reptoside	44584096	
		eucommiol	154373	
		eucommioside II	6325167	
		1-deoxyeucommiol	5316559	
		Epieucommiol	101714787	
		ulmoidoside A	14540382	
		ulmoidoside B	14540384	
		asperuloside	84298	110
		ulmoside	11968295	
		eucomoside A	102382672	
		eucomoside B	23624546	
		eucomoside C	23625086	
		daphylloside	21602024	
		scandoside methyl ester	442433	
		loganin	87691	
		7-epi-loganin	10548420	
		artselaenin C	100930978	
		harpagide	10044294	
		catalpol	91520	
		avicularin	5490064	
		oroxylin A	5320315	
		licochalcone A	5318998	
		thunberginol C	10333412	
		C-veratrolylglycol	15765124	
		alternariol	5359485	
		salicifoliol	10955962	
		eucophenoside	102044905	
		Uvaol	92802	
		eleganoside A	101085911	
		borreriagenin	44583980	

50.	Foeniculum vulgare (55)	3-O-acetylerythrodil	118796402	111
		aplyolide D	10708956	
		Umbelliferone	5281426	
		Eriodictyol	440735	
		Homoeriodictyol	73635	
		Aromadendrol	122850	
		cyclo(Pro-Pro)	529063	
		Anisketone	31231	112
		Apiol	10659	
		4-Carene	530422	
		3-Carene	26049	
		Cathine	441457	
		2-Propyn-1-ol	7859	
		2,6-Dimethyl-2,4,6-octatriene	5368821	
		Sabinene hydrate	62367	
		Fenchyl acetate	107217	
		Dicyclopropyl carbinol	84336	
		Estragole	8815	
		<i>trans</i> -p-2,8-menthadien-1-ol	155626	
		1,4-Dimethoxybenzene	9016	
		<i>trans</i> -Anethole	637563	
		Allantoic acid	203	
		1-Undecanol	8184	
		Benzothiazole	7222	
		1,6-Hexanediol	12374	
		Mephnesin	4059	
		4-Fluorohistamine	541569	
		1-(3-Methoxyphenyl)-1-propanone	584765	
		1,5 dicaffeoylquinic acid	122685	113
		Hesperidin	10621	
		3- caffeoylquinic acid	102111217	
		4- caffeoylquinic acid	9798666	
		imperatorin	10212	
		psoralen	6199	
		bergapten	2355	
		xanthotoxin	4114	
		isopimpinellin	68079	
		Cuminal	326	
		cis-Anethole	1549040	
		p-Anisaldehyde	31244	
		2-methyl-3-oxoestran- 17-yl acetate	22212600	
		Vetivenene	529892	
		Anthracene	8418	
		2-Methoxy-4-ethylphenol	62465	
		1,2-Dimethoxy-4-methylbenzene	68126	
		Cedran-9-one	21723990	
		2,2-dimethyl-3-phenylpropanoate	6947002	
		3,3,6-Trimethyl-1-indanone	594538	
		o-Benzenedicarboxylic acid	1017	
		3,4-Dimethyl-1,5-cyclooctadiene	5365753	



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capric acid	2969
undecanoic acid	8180
pentadecadienoic acid	19047235
erucic acid	5281116
n-Hexacosane	12407
n-Heptacosane	11636
n-Octacosane	12408
n-Nonacosane	12409
n-Triacontane	12535
n-Dotriacontane	11008
n-Tetratriacontane	26519
n-Hexatriacontane	12412
n-Octatriacontane	23599
n-Tetracontane	20149

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