

Table S1 List of candidate compounds

Number	Molecular formula	Name	CAS number	SMILES	Ownership of medicinal materials
comp001	C7H7NO2	Trigonelline	535-83-1	<chem>C[N+]1=CC=CC(=C1)C(=O)[O-]</chem>	Leonurus
comp002	C7H13NO2	Stachydrine	471-87-4	<chem>C[N+]1(CCCC1C(=O)[O-])C</chem>	Leonurus
comp003	C14H21N3O5	Leonurine	24697-74-3	<chem>COC1=CC(=CC(=C1O)OC)C(=O)OCCCCN=C(N)N</chem>	Leonurus
comp004	C21H20O12	Isoquercitrin	482-35-9	<chem>C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)OC4C(C(C(C(O4)CO)O)O)O)O</chem>	fried Toosendan
comp005*	C30H38O11	Toosendanin/Isotoosendanin	58812-37-6	<chem>CC(=O)OC1CC(C23COC(C1(C2CC(C4(C3C(=O)C(C5(C46C(O6)CC5C7=COC=C7)C)OC(=O)C)C)O)C)O)O</chem>	fried Toosendan
comp006*	C30H38O11	Toosendanin/Isotoosendanin	97871-44-8	<chem>CC(=O)OC1CC(C23COC(C1(C2CC(C4(C3C(=O)C(C5(C4C(=O)CC5C6=COC=C6)C)OC(=O)C)C)O)C)O)O</chem>	fried Toosendan
comp007	C31H40O7	MeliatooseninP	1355997-08-8	<chem>CC=C(C)C(=O)OC1CC(C2(COC3C2C1(C(C4(C3OC5C4=C(CC5C6=COC=C6)C)C)CC=O)C)C)O</chem>	fried Toosendan
comp008	C33H44O9	1-DeacetylrimbolinB	76689-98-0	<chem>CC=C(C)C(=O)OC1C2C3C(CO2)(C(CC(C3(C4(C1(C5=C(C(CC5OC(C4)O)C6=COC=C6)C)C)C)O)OC(=O)C)C</chem>	fried Toosendan
comp009	C33H42O9	1-O-tigloyl-1-O-debenzoylchinal	/	/	fried Toosendan
comp010	C15H22O	α -Cyperone	473-08-5	<chem>CC1=C2CC(CCC2(CCC1=O)C)C(=C)C</chem>	Cyperus
comp011	C27H30O15	Vicenin-II	23666-13-9	<chem>C1=CC(=CC=C1C2=CC(=O)C3=C(C(=C(C=C3O2)C4C(C(C(C(O4)CO)O)O)O)O)C5C(C(C(C(O5)CO)O)O)O)O)O</chem>	Bergamot
comp012	C11H10O4	6,7-Dimethoxy-2-	120-08-1	<chem>COC1=C(C=C2C(=C1)C=CC(=O)O2)OC</chem>	Bergamot

		benzopyrone			
comp013	C28H34O15	Hesperidin	520-26-3	<chem>CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=CC(=C4C(=O)CC(OC4=C3)C5=CC(=C(C=C5)OC)O)O)O)O)O)O)O</chem>	Bergamot
comp014	C15H12O5	Naringenin	67604-48-2、 480-41-1	<chem>C1C(OC2=CC(=CC(=C2C1=O)O)O)C3=CC=C(C=C3)O</chem>	Bergamot
comp015	C16H14O6	Hesperetin	520-33-2	<chem>COC1=C(C=C(C=C1)C2CC(=O)C3=C(C=C(C=C3O2)O)O)O</chem>	Bergamot
comp016	C26H30O8	Limonin	1180-71-8	<chem>CC1(C2CC(=O)C3(C(C24COC(=O)CC4O1)CC(C5(C36C(O6)C(=O)OC5C7=COC=C7)C)C)C</chem>	Bergamot
comp017	C16H18O9	Neochlorogenic acid	906-33-2	<chem>C1C(C(C(CC1(C(=O)O)O)OC(=O)C=CC2=CC(=C(C=C2)O)O)O)O</chem>	Artemisia argyi leaf / Hawthorn
comp018	C16H18O9	Chlorogenic acid	327-97-9	<chem>C1C(C(C(CC1(C(=O)O)O)OC(=O)C=CC2=CC(=C(C=C2)O)O)O)O</chem>	Artemisia argyi leaf / Hawthorn
comp019	C16H18O9	Cryptochlorogeni c acid	905-99-7、 87099-73-8	<chem>C1C(C(C(CC1(C(=O)O)O)O)OC(=O)C=CC2=C(C=C(C=C2)O)O)O</chem>	Artemisia argyi leaf / Hawthorn
comp020	C15H14O6	Catechin	154-23-4	<chem>C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O</chem>	Hawthorn
comp021	C21H20O12	Hyperoside	482-36-0	<chem>C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)OC4C(C(C(C(O4)CO)O)O)O)O)O</chem>	Hawthorn
comp022	C30H48O3	Betulinic acid	472-15-1	<chem>CC(=C)C1CCC2(C1C3CCC4C5(CCC(C(C5CC(C4(C3CC2)C)C)C)O)C)C(=O)O</chem>	Hawthorn
comp023	C30H48O3	Oleanolic acid	508-02-1	<chem>CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)O)C)C)C2C1)C)C(=O)O)C</chem>	Hawthorn
comp024	C27H32O14	Naringin	10236-47-2	<chem>CC1C(C(C(C(O1)OC2C(C(C(OC2OC3=CC(=C4C(=O)CC(OC4=C3)C5=CC=C(C=C5)O)O)O)CO</chem>	Artemisia argyi leaf

				<chem>O)O)O)O)O</chem>	
comp025	C25H24O12	Isochlorogenic acid B	14534-61-3	<chem>C1C(C(C(CC1(C(=O)O)O)OC(=O)C=CC2=CC(=C(C=C2)O)O)OC(=O)C=CC3=CC(=C(C=C3)O)O)O</chem>	Artemisia argyi leaf
comp026	C25H24O12	Isochlorogenic acid A	89919-62-0	<chem>C1C(C(C(CC1(C(=O)O)O)OC(=O)C=CC2=CC(=C(C=C2)O)O)O)OC(=O)C=CC3=CC(=C(C=C3)O)O</chem>	Artemisia argyi leaf
comp027	C25H24O12	Isochlorogenic acid C	89886-30-6	<chem>C1C(C(C(CC1(C(=O)O)O)OC(=O)C=CC2=CC(=C(C=C2)O)O)OC(=O)C=CC3=CC(=C(C=C3)O)O)O</chem>	Artemisia argyi leaf
comp028	C18H16O8	Centaureidin	17313-52-9	<chem>COC1=C(C=C(C=C1)C2=C(C(=O)C3=C(O2)C=C(C(=C3O)OC)O)OC)O</chem>	Artemisia argyi leaf
comp029	C17H14O7	Jaceosidin	18085-97-7	<chem>COC1=C(C=CC(=C1)C2=CC(=O)C3=C(O2)C=C(C(=C3O)OC)O)O</chem>	Artemisia argyi leaf
comp030	C18H16O8	Chrysosplenol D	14965-20-9	<chem>COC1=C(C(=C2C(=C1)OC(=C(C2=O)OC)C3=CC(=C(C=C3)O)O)O)OC</chem>	Artemisia argyi leaf
comp031	C18H16O7	Eupatilin	22368-21-4	<chem>COC1=C(C=C(C=C1)C2=CC(=O)C3=C(O2)C=C(C(=C3O)OC)O)OC</chem>	Artemisia argyi leaf
comp032	C19H18O8	Vitexicarpin	479-91-4	<chem>COC1=C(C=C(C=C1)C2=C(C(=O)C3=C(C(=C(C=C3O2)OC)OC)O)OC)O</chem>	Artemisia argyi leaf
comp033	C20H23NO4	Tetrahydrojatrorhizine	27313-86-6	<chem>COC1=C(C2=C(CC3C4=CC(=C(C=C4CCN3C2)O)OC)C=C1)OC</chem>	vinegar Corydalis
comp034	C21H25NO4	Rotundine	483-14-7	<chem>COC1=C(C2=C(CC3C4=CC(=C(C=C4CCN3C2)OC)OC)C=C1)OC</chem>	vinegar Corydalis
comp035	C21H25NO4	Tetrahydropalmatine	2934-97-6	<chem>COC1=C(C2=C(CC3C4=CC(=C(C=C4CCN3C2)OC)OC)C=C1)OC</chem>	vinegar Corydalis
comp036	C20H19NO5	Protopine	130-86-9	<chem>CN1CCC2=CC3=C(C=C2C(=O)CC4=C(C1)C5=C(C(=C4)OCO5)OCO3</chem>	vinegar Corydalis
comp037	C21H25NO4	Coryphenanthrine	66190-61-2	<chem>COC(C1=C(C=C(OC)C(OC)=C2)C2=CC=C1C(=C(C=C2)O)OC)O</chem>	vinegar

				CCNC)=C3)=C3OC	Corydalis
comp038	C21H25NO4	Glaucine	475-81-0	CN1CCC2=CC(=C(C3=C2C1CC4=CC(=C(C=C43)OC)OC)OC)OC	vinegar Corydalis
comp039	C19H17NO4	Stylophine	7461-02-1	C1CN2CC3=C(CC2C4=CC5=C(C=C41)OCO5)C=CC6=C3OCO6	vinegar Corydalis
comp040	C20H19NO4	Columbamine	3621-36-1	COC1=C(C2=C[N+](C=C2C=C1)C4=CC(=C(C=C4CC3)OC)O)OC	vinegar Corydalis
comp041	C20H21NO4	Tetrahydroberberine	522-97-4、 5096-57-1	COC1=C(C2=C(CC3C4=CC5=C(C=C4CCN3C2)OCO5)C=C1)OC	vinegar Corydalis
comp042	C22H27NO4	Corydaline	518-69-4、 6018-35-5	CC1C2C3=CC(=C(C=C3CCN2CC4=C1C=CC(=C4OC)OC)OC)OC	vinegar Corydalis
comp043	C21H22NO4	Dehydrocorybulbine	59870-72-3	CC1=C2C=CC(=C(C2=C[N+](C=C1C4=CC(=C(C=C4CC3)O)OC)OC)OC	vinegar Corydalis
comp044	C21H22NO4	Palmatine	3486-67-7	COC1=C(C2=C[N+](C=C2C=C1)C4=CC(=C(C=C4CC3)OC)OC)OC	vinegar Corydalis
comp045	C22H24NO4	Dehydrocorydalin	30045-16-0	CC1=C2C=CC(=C(C2=C[N+](C=C1C4=CC(=C(C=C4CC3)OC)OC)OC)OC	vinegar Corydalis
comp046	C27H32O15	Neoeriocitrin	13241-32-2	CC1C(C(C(C(O1)OC2C(C(C(OC2OC3=CC(=C4C(=O)CC(OC4=C3)C5=CC(=C(C=C5)O)O)O)O)O)O)O)O	Green peel
comp047	C28H34O14	Poncirin	14941-08-3	CC1C(C(C(C(O1)OC2C(C(C(OC2OC3=CC(=C4C(=O)CC(OC4=C3)C5=CC(=C(C=C5)OC)O)C)O)O)O)O)O	Green peel
comp048	C20H20O7	Isosinensetin	17290-70-9	COC1=C(C=C(C=C1)C2=CC(=O)C3=C(O2)C(=C(C=C3OC)OC)OC)OC	Green peel
comp049	C21H22O9	Natsudaidain	35154-55-3	COC1=C(C=C(C=C1)C2=C(C(=O)C3=C(O2)C(=C(C=C3OC)OC)OC)OC)O)OC	Green peel
comp050	C20H20O7	Sinensetin	2306-27-6	COC1=C(C=C(C=C1)C2=CC(=O)C3=C(C(=C(C=C3O2)OC)OC)OC)OC	Green peel

comp051	C21H22O8	Nobiletin	478-01-3	<chem>COC1=C(C=C(C=C1)C2=CC(=O)C3=C(O2)C(=C(C(=C3OC)OC)OC)OC)OC</chem>	Green peel
comp052	C20H20O7	Tangeretin	481-53-8	<chem>COC1=CC=C(C=C1)C2=CC(=O)C3=C(O2)C(=C(C(=C3OC)OC)OC)OC</chem>	Green peel
comp053	C21H22O9	Gardenin A	21187-73-5	<chem>COC1=CC(=CC(=C1OC)OC)C2=CC(=O)C3=C(C(=C(C(=C3O2)OC)OC)OC)O</chem>	Green peel
comp054	C19H26O15	Galloylsucrose	1449244-58-9	<chem>C1=C(C=C(C(=C1O)O)O)C(=O)C2(C(C(C(C(O2)CO)O)O)OC3(C(C(C(O3)CO)O)O)O)CO</chem>	Radix
					Paeoniae
					Alba
comp055 [#]	C19H26O15	Galloylsucroseorisomer	115713-44-5	4': 055-1	Radix
				<chem>C1=C(C=C(C(=C1O)O)O)C(=O)OC2C(OC(C2O)(CO)OC3C(C(C(C(O3)CO)O)O)O)CO</chem>	Paeoniae
			115731-15-2	6': 055-2	Alba
comp056 [#]	C19H26O15	Galloylsucroseorisomer			
			115713-45-6	1': 056-1	Radix
				<chem>C1=C(C=C(C(=C1O)O)O)C(=O)OCC2C(C(C(O2)CO)O)O)OC3C(C(C(C(O3)CO)O)O)O</chem>	Paeoniae
comp057	C23H28O12	Oxypaeoniflorin	39011-91-1		Alba
comp058	C23H28O11	Albiflorin	39011-90-0		Radix
				<chem>C=CC=C4)OC5C(C(C(C(O5)CO)O)O)O</chem>	Paeoniae
					Alba
comp059	C23H28O11	Paeoniflorin	23180-57-6	<chem>CC12CC3(C4CC1(C4(C(O2)O3)COC(=O)C5=CC=CC=C5)OC6C(C(C(C(O6)CO)O)O)O)O</chem>	Radix
					Paeoniae

					Alba
comp060	C30H32O15	Galloylpaeoniflorin	122965-41-7	CC12CC3(C4CC1(C4(C(O2)O3)COC(=O)C5=CC=CC=C5)OC6C(C(C(C(O6)COC(=O)C7=CC(=C(C(=C7)O)O)O)O)O)O	Radix Paeoniae Alba
comp061 ^s	C30H32O12	Benzoylpaeoniflorin	38642-49-8	CC12CC3(C4CC1(C4(C(O2)O3)COC(=O)C5=CC=CC=C5)OC6C(C(C(C(O6)COC(=O)C7=CC(=CC=C7)O)O)O)O	Radix Paeoniae Alba
comp062 ^s	C30H32O12	Benzoylpaeoniflorin isomer	38642-49-8	CC12CC3(C4CC1(C4(C(O2)O3)COC(=O)C5=CC=CC=C5)OC6C(C(C(C(O6)COC(=O)C7=CC(=CC=C7)O)O)O)O	Radix Paeoniae Alba
comp063	C27H44O7	β-Ecdysone	5289-74-7	CC12CCC3C(=CC(=O)C4C3(CC(C(C4)O)O)C)C1(CCC2C(C)(C(CCC(C)(C)O)O)O)O	Achyranthes bidentata
comp064	C27H44O7	25R-Inokosterone	19682-38-3	CC(CCC(C(C)(C1CCC2(C1(CCC3C2=CC(=O)C4C3(CC(C(C4)O)O)C)C)O)O)O)CO	Achyranthes bidentata
comp065	C27H44O7	25S-Inokosterone	19595-18-7	CC(CCC(C(C)(C1CCC2(C1(CCC3C2=CC(=O)C4C3(CC(C(C4)O)O)C)C)O)O)O)CO	Achyranthes bidentata
comp066	C48H76O19	Ginsenoside Ro	34367-04-9	CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)OC6C(C(C(C(O6)C(=O)O)O)O)OC7C(C(C(C(C(O7)CO)O)O)O)C)C2C1)C)C(=O)OC8C(C(C(C(C(O8)CO)O)O)O)C	Achyranthes bidentata
comp067	C47H74O18	Chikusetsusaponin IV	7518-22-1	CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)OC6C(C(C(C(O6)C(=O)O)OC7C(C(C(C(C(O7)CO)O)O)O)C)C2C1)C)C(=O)OC8C(C(C(C(O8)CO)O)O)O)C	Achyranthes bidentata
comp068	C47H74O18	Pseudoginsenoside Rt1	98474-74-9	CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(C5(C)C)OC6C(C(C(C(O6)C(=O)O)O)O)OC7C(C(C(C(C(O7)O)O)O)C)C2C1)C)C(=O)OC8C(C(C(C(O8)CO)O)O)O)C	Achyranthes bidentata
comp069	C47H70O20	Bidentatoside I	330808-27-0	O=C([CO]1(CCC(C)(C)C2)[CO]2([H])C3=CC[	Achyranthes

				COO]4([H])[COO](C)(CC[CO]5([H])[COO]4(C	bidentata
				C[COH](O[COO](O[COH](C(O)=O)[COH]6O)(	
				[H])[COO]7([H])[COO]6([H])OC(C(O)=O)(O)C	
				(OCC(O)=O)O7)C5(C)C)[CO]3(C)CC1)O[C	
				OOH]([COOH]([COOH](O)[COOH]8O)O)O[C	
				OOH]8CO	
comp070	C42H66O14	Chikusetsusaponi n IVa	51415-02-2	CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CCC(	Achyranthes
				C5(C)C)OC6C(C(C(C(O6)C(=O)O)O)O)C)C)	bidentata
				C2C1)C)C(=O)OC7C(C(C(C(O7)CO)O)O)O)C	
comp071	C10H17NO9S	Sinigrin	534-69-0	C=CCC(=NOS(=O)(=O)O)SC1C(C(C(C(O1)CO	fried Mustard
	2			)O)O)O	Seed
comp072	C12H18NO3	4-Hydroxybenzoyl choline	5094-31-5	C[N+](C)(C)CCOC(=O)C1=CC=C(C=C1)O	fried Mustard
					Seed
comp073	C16H24NO5	Sinapine	18696-26-9	C[N+](C)(C)CCOC(=O)C=CC1=CC(=C(C(=C1	fried Mustard
				)OC)O)OC	Seed
comp074	C11H12O5	Sinapicacid	530-59-6	COC1=CC(=CC(=C1O)OC)C=CC(=O)O	fried Mustard
					Seed
comp075	C9H13NO2	Synephrine	94-07-5	CNCC(C1=CC=C(C=C1)O)O	processed
					Evodia
					rutaecarpa
comp076	C19H13N3O	Evodianinine	878628-80-9	CN(C1=CC=CC=C1C2=O)C(N2C=C3)=C4C3=	processed
				C(C=CC=C5)C5=N4	Evodia
					rutaecarpa
comp077	C26H30O9	Rutaevin	33237-37-5	CC1(C2C(=O)C(C3(C(C24COC(=O)CC4O1)C	processed
				CC5(C36C(O6)C(=O)OC5C7=COC=C7)C)C)O)	Evodia
				C	rutaecarpa
comp078	C26H28O9	Evodol	22318-10-1	CC1(C2=C(C(=O)C3(C(C24COC(=O)CC4O1)C	processed
				CC5(C36C(O6)C(=O)OC5C7=COC=C7)C)C)O)	Evodia
				C	rutaecarpa

comp079	C19H17N3O	Evodiamine	518-17-2	CN1C2C3=C(CCN2C(=O)C4=CC=CC=C41)C5=CC=CC=C5N3	processed Evodia rutaecarpa
comp080	C18H13N3O	Rutaecarpine	84-26-4	C1CN2C(=NC3=CC=CC=C3C2=O)C4=C1C5=CC=CC=C5N4	processed Evodia rutaecarpa
comp081	C23H35NO	Dihydroevocarpin e	15266-35-0	CCCCCCCCCCCCC1=CC(=O)C2=CC=CC=C2N1C	processed Evodia rutaecarpa
comp082	C6H8O7	Citric acid	77-92-9	C(C(=O)O)C(CC(=O)O)(C(=O)O)O	/
comp083	C9H12N2O6	Uridine	58-96-8	C1=CN(C(=O)NC1=O)C2C(C(C(O2)CO)O)O	/
comp084	C7H6O5	Gallic acid	149-91-7	C1=C(C=C(C(=C1O)O)O)C(=O)O	/
comp085	C10H13N5O4	Adenosine	58-61-7	C1=NC(=C2C(=N1)N(C=N2)C3C(C(C(O3)CO)O)O)N	/
comp086	C10H13N5O5	Guanosine	118-00-3	C1=NC2=C(N1C3C(C(C(O3)CO)O)O)N=C(NC2=O)N	/
comp087	C30H26O12	Procyanidin B6	12798-58-2	C1C(C(OC2=C1C(=C(C(=C2)O)C3C(C(OC4=C(C(=CC(=C34)O)O)C5=CC(=C(C(=C5)O)O)O)O)C6=CC(=C(C(=C6)O)O)O	/
comp088	C26H28O14	Schaftoside	51938-32-0	C1C(C(C(C(O1)C2=C3C(=C(C(=C2O)C4C(C(C(C(O4)CO)O)O)O)C(=O)C=C(O3)C5=CC(=C(C(=C5)O)O)O)O	/
comp089	C27H30O16	Rutin	153-18-4	CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=C(O)C4=CC(=CC(=C4C3=O)O)O)C5=CC(=C(C(=C5)O)O)O)O)O)O)O	/
comp090	C27H30O16	Quercetin-3-O-β-D-glucosyl-(1→2)-α-L-rhamnoside	143016-74-4	O=C1C(O[COH])(O[COOH])(C[COH])(O[COH]2O)[COOH]2O[CO]([COOH])([COOH])(O[COOH]3O)O)([H])O[COOH]3CO=C(C4=CC(O)=C(O)C=C4)OC5=CC(O)=CC(O)=C15	/

comp091	C27H30O14	Apigenin-7-O-rut	552-57-8	CC1C(C(C(C(O1)OCC2C(C(C(C(O2)OC3=CC(/
		inosite		=C4C(=C3)OC(=CC4=O)C5=CC=C(C=C5)O)O
				)O)O)O)O)O)O

Note: *, # and \$ represent isomers.