

CAS	Name	Formula	SMILES
553-86-6	2-coumarone	C8H6O2	<chem>c1cccc2CC(=O)Oc12</chem>
91-64-5	coumarin	C9H6O2	<chem>c1cc2OC(=O)C=Cc2cc1</chem>
939-19-5	3-hydroxycoumarin	C9H6O3	<chem>c12OC(=O)C(O)=Cc1cccc2</chem>
1076-38-6	4-hydroxycoumarin	C9H6O3	<chem>c1ccc2C(O)=CC(=O)Oc2c1</chem>
93-35-6	umbelliferone; 7-hydroxycoumarin	C9H6O3	<chem>c1cc(O)cc2OC=CC(=O)c12</chem>
305-01-1	eculetin; 6,7-dihydroxycoumarin	C9H6O4	<chem>c1c(O)c(O)cc2OC(=O)C=Cc12</chem>
119-84-6	dihydrocoumarin	C9H8O2	<chem>O=C(Oc(c(ccc1)C2)c1)C2</chem>
7400-08-0	4-coumaric acid	C9H8O3	<chem>C(\C(O)=O)=C/c1ccc(cc1)O</chem>
119179-66-7	6-chloro-7-hydroxy-4-(trifluoromethyl)coumarin	C10H4ClF3O3	<chem>O=C1C=C(C(F)(F)F)c2cc(Cl)c(O)cc2o1</chem>
575-03-1	7-hydroxy-4-(trifluoromethyl)coumarin	C10H5F3O3	<chem>O=C1C=C(C(F)(F)F)c2ccc(O)cc2o1</chem>
53518-15-3	7-amino-4-(trifluoromethyl)coumarin	C10H6F3NO2	<chem>O=C1C=C(C(F)(F)F)c2ccc(N)cc2O1</chem>
531-81-7	coumarin-3-carboxylic acid	C10H6O4	<chem>O=C1C(=C2c(cccc2)O1)C(=O)O</chem>
6174-86-3	3-chloro-4-methyl-7-hydroxycoumarin	C10H7ClO3	<chem>c1c(cc2c(c1)\C(=C(/C(O2)=O)\Cl)\C)O</chem>
92-48-8	6-methylcoumarin	C10H8O2	<chem>c1cc(C)cc2C=CC(=O)Oc12</chem>
531-59-9	7-methoxycoumarin; herniarin	C10H8O3	<chem>c1c(OC)ccc2C=CC(=O)Oc12</chem>
2445-83-2	7-methylcoumarin	C10H8O3	<chem>COc1cccc2C=CC(=O)Oc12</chem>
92-61-5	scopoletin; 7-hydroxy-6-methoxycoumarin	C10H8O4	<chem>c1c(OC)c(O)cc2OC(=O)C=Cc12</chem>
26093-31-2	7-amino-4-methylcoumarin	C10H9NO2	<chem>O=C1C=C(C)c2ccc(N)cc2O1</chem>
	coumarin deriv., T-4604-007	C11H6N2O3	<chem>c1cccc2C(c3nocn3)=CC(=O)Oc12</chem>
	coumarin deriv., T-4604-011	C11H8N2O3	<chem>c1cccc2C(C3=NOCN3)=CC(=O)Oc12</chem>
779-30-6	3-acetamidocoumarin	C11H9NO3	<chem>c1cccc2c1OC(=O)C(=C2)NC(=O)C</chem>
487-06-9	limettin; 5,7-dimethoxycoumarin	C11H10O4	<chem>COc1cc(OC)cc2OC(=O)C=Cc12</chem>
	coumarin deriv., T-4604-008	C12H8N2O3	<chem>c1cccc2C(c3noc(C)n3)=CC(=O)Oc12</chem>
	coumarin deriv., T-4604-004	C12H10ClNO4	<chem>c1cccc2C(C(CCO)=NO)=C(Cl)C(=O)Oc12</chem>
53518-14-2	coumarin 152	C12H10F3NO2	<chem>O=C1C=C(C(F)(F)F)c2ccc(N(C)C)cc2O1</chem>
	coumarin deriv., T-4604-012	C12H10N2O3	<chem>c1cccc2C(C3=NOC(C)N3)=CC(=O)Oc12</chem>
	coumarin deriv., T-4604-005	C12H10N2O4	<chem>c1cccc2C(C(N)=NOC(=O)C)=CC(=O)Oc12</chem>
6093-71-6	7-hydroxycoumarin-3-carboxylic acid ethyl ester	C12H10O5	<chem>c1cc(O)cc2OC(=O)C(C(=O)OCC)=Cc12</chem>
952-23-8	3,6-diaminoacridine monohydrochloride; proflavine monohydrochloride	C13H12ClN3	<chem>Nc3ccc2cc1ccc([N+])cc1nc2c3.[Cl-]</chem>
531-73-7	3,6-diaminoacridine dihydrochloride; proflavine dihydrochloride	C13H13Cl2N3	<chem>[N+]c3ccc2cc1ccc([N+])cc1nc2c3.[Cl-].[Cl-]</chem>
553-30-0	proflavine sulfate	C13H13N3O4S	<chem>c1c([N+])ccc2cc3ccc([N+])cc3nc12.[O-]S(=O)(=O)[O-]</chem>
84-60-6	2,6-dihydroxy-9,10-anthraquinone; anthraflavic acid	C14H8O4	<chem>c1c(O)ccc2C(=O)c3cc(O)ccc3C(=O)c12</chem>
82-29-1	flavopurpurin; Mordant Red 4	C14H8O5	<chem>c1c(O)ccc2C(=O)c3c(O)c(O)cc(c3C(=O)c12)</chem>
1150-37-4	2,3-dihydro-5,7-dimethoxycyclopentenone[2,3-c]coumarin; cyclopenta(c)	C14H12O5	<chem>c1c(OC)cc(OC)c2c1OC(=O)C3=C2C(=O)CC3</chem>
1146-71-0	5,7-dimethoxycyclopentene[c]coumarin; cyclopenta(c)(1)benzopyran-4(1H)	C14H14O4	<chem>c1c(OC)cc(OC)c2c1OC(=O)C3=C2CCC3</chem>
321-54-0	Coroxon; Coumaphos oxygen analogue	C14H16ClO6P	<chem>c12OC(=O)C(Cl)=C(C)c1ccc(OP(=O)(OCC)OCC)c2</chem>
56-72-4	Coumaphos; Co-Ral; thiophosphoric acid, O,O-diethyl-O-(3-chloro-4-met	C14H16ClO5PS	<chem>S=P(OCC)(OCC)Oc1ccc2C(C)=C(Cl)C(=O)Oc2c1</chem>
37681-00-8	coumazoline	C14H16N2O	<chem>CCC=2OC=1C=CC=CC=1C=2CC=3NCCN=3</chem>
	flavone, 6-NO2, 8-NO2, 4'-NO2	C15H7N3O8	<chem>c1c(N(=O)=O)cc(N(=O)=O)c2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12</chem>
	flavone, 5-NO2, 6-OH, 7-NO2, 4'-NO2	C15H7N3O9	<chem>O=N(=O)c1c(O)c(N(=O)=O)cc2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12</chem>
	flavone, 6-NO2, 7-OH, 8-NO2, 4'-NO2	C15H7N3O9	<chem>c1c(N(=O)=O)c(O)c(N(=O)=O)c2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12</chem>
	flavonoid deriv., 4063-093	C15H7N3O9	<chem>O1C(c2ccc(N(=O)=O)cc2)=CC(=O)c3cc(N(=O)=O)c(O)c(N(=O)=O)c13</chem>
	flavonoid deriv., 4063-105	C15H7N3O9	<chem>O1C(c2ccc(N(=O)=O)cc2)=CC(=O)c3c(N(=O)=O)c(O)c(N(=O)=O)cc13</chem>
	flavone, 6-NO2, 4'-NO2	C15H8N2O6	<chem>c1c(N(=O)=O)ccc2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12</chem>

	flavone, 8-NO <sub>2</sub> , 4'-NO <sub>2</sub>	C15H <sub>8</sub> N <sub>2</sub> O <sub>6</sub>	c1ccc(N(=O)=O)c2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12
	flavone, 5-OH, 6-NO <sub>2</sub> , 4'-NO <sub>2</sub>	C15H <sub>8</sub> N <sub>2</sub> O <sub>7</sub>	Oc1c(N(=O)=O)ccc2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12
	flavone, 5-OH, 8-NO <sub>2</sub> , 4'-NO <sub>2</sub>	C15H <sub>8</sub> N <sub>2</sub> O <sub>7</sub>	Oc1ccc(N(=O)=O)c2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12
	flavone, 6-NO <sub>2</sub> , 7-OH, 4'-NO <sub>2</sub>	C15H <sub>8</sub> N <sub>2</sub> O <sub>7</sub>	c1c(N(=O)=O)c(O)cc2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12
	flavone, 6-OH, 8-NO <sub>2</sub> , 4'-NO <sub>2</sub>	C15H <sub>8</sub> N <sub>2</sub> O <sub>7</sub>	c1c(O)cc(N(=O)=O)c2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12
	flavone, 7-OH, 8-NO <sub>2</sub> , 4'-NO <sub>2</sub>	C15H <sub>8</sub> N <sub>2</sub> O <sub>7</sub>	c1cc(O)c(N(=O)=O)c2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12
479-13-0	coumestrol	C15H <sub>8</sub> O <sub>5</sub>	Oc1ccc2c3C(=O)Oc4cc(O)ccc4c3oc2c1
10420-73-2	6-chloroflavone	C15H <sub>9</sub> ClO <sub>2</sub>	O=C1C3=C(OC(=C1)c2cccc2)C=CC(=C3)Cl
	flavone, 4'-NO <sub>2</sub>	C15H <sub>9</sub> NO <sub>4</sub>	c1cccc2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12
	flavone, 6-OH, 4'-NO <sub>2</sub>	C15H <sub>9</sub> NO <sub>5</sub>	c1c(O)ccc2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12
	flavone, 7-OH, 4'-NO <sub>2</sub>	C15H <sub>9</sub> NO <sub>5</sub>	c1cc(O)cc2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12
	flavone, 5-OH, 7-OH, 4'-NO <sub>2</sub>	C15H <sub>9</sub> NO <sub>6</sub>	Oc1cc(O)cc2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12
525-82-6	flavone	C15H <sub>10</sub> O <sub>2</sub>	c1ccc2C(=O)C=C(c3cccc3)Oc2c1
577-85-5	3-hydroxyflavone	C15H <sub>10</sub> O <sub>3</sub>	C/1(=C(/Oc2c(C1=O)cccc2)\c1cccc1)\O
491-78-1	5-hydroxyflavone	C15H <sub>10</sub> O <sub>3</sub>	c12c(C(C=C(O1)c1cccc1)=O)c(ccc2)O
6515-36-2	7-hydroxyflavanone	C15H <sub>10</sub> O <sub>3</sub>	c1cc(O)cc2OC(=CC(=O)c12)c3cccc3
6665-86-7	7-hydroxyflavone	C15H <sub>10</sub> O <sub>3</sub>	c1cc(O)cc2OC(c3cccc3)=CC(=O)c12
13057-72-2	7-hydroxyisoflavone	C15H <sub>10</sub> O <sub>3</sub>	Oc1ccc2C(=O)C(c3cccc3)=COc2c1
	flavone, 4'-OH	C15H <sub>10</sub> O <sub>3</sub>	c1cccc2OC(c3ccc(O)cc3)=CC(=O)c12
	flavone, 7-OH	C15H <sub>10</sub> O <sub>3</sub>	c1cc(O)cc2OC(c3cccc3)=CC(=O)c12
4143-64-0	3',4'-dihydroxyflavone	C15H <sub>10</sub> O <sub>4</sub>	c12c(C(\C=C(/O1)\c1cc(c(cc1)O)O)=O)cccc2
108238-41-1	3,6-dihydroxyflavone	C15H <sub>10</sub> O <sub>4</sub>	c1c(O)ccc2OC(=C(O)C(=O)c12)c3cccc3
38183-03-8	7,8-dihydroxyflavone	C15H <sub>10</sub> O <sub>4</sub>	c12OC(c3cccc3)=CC(=O)c1ccc(O)c2O
	flavone, 5-OH, 3'-OH	C15H <sub>10</sub> O <sub>4</sub>	Oc1cccc2OC(c3cc(O)ccc3)=CC(=O)c12
	flavone, 5-OH, 4'-OH	C15H <sub>10</sub> O <sub>4</sub>	Oc1cccc2OC(c3ccc(O)cc3)=CC(=O)c12
480-40-0	flavone, 5-OH, 7-OH; chrysin	C15H <sub>10</sub> O <sub>4</sub>	Oc1cc(O)cc2OC(=CC(=O)c12)c3cccc3
548-58-3	flavone, 5-OH, 8-OH	C15H <sub>10</sub> O <sub>4</sub>	c12Oc(c3cccc3)=CC(=O)c1c(O)ccc2O
	flavone, 6-OH, 3'-OH	C15H <sub>10</sub> O <sub>4</sub>	c1c(O)ccc2OC(c3cc(O)ccc3)=CC(=O)c12
	flavone, 7-OH, 3'-OH	C15H <sub>10</sub> O <sub>4</sub>	c1cc(O)cc2OC(c3cc(O)ccc3)=CC(=O)c12
486-66-8	flavone, 7-OH, 4'-OH; diadzein	C15H <sub>10</sub> O <sub>4</sub>	c1cc(O)ccc1C1=COc2cc(O)ccc2c1=O
	flavone, 7-OH, 8-OH	C15H <sub>10</sub> O <sub>4</sub>	c1cc(O)c(O)c2OC(c3cccc3)=CC(=O)c12
548-83-4	3,5,7-trihydroxyflavone; galangin	C15H <sub>10</sub> O <sub>5</sub>	Oc1cc(O)cc2OC(=C(O)C(=O)c12)c3cccc3
491-67-8	5,6,7-trihydroxyflavone; baicalein	C15H <sub>10</sub> O <sub>5</sub>	Oc1c(O)c(O)c2C(=O)C=C(c3cccc3)Oc2c1
520-36-5	5,7,4'-trihydroxyflavone; apigenin	C15H <sub>10</sub> O <sub>5</sub>	Oc1cc(O)cc2OC(=CC(=O)c12)c3ccc(O)cc3
446-72-0	5,7,4'-trihydroxyisoflavone; genistein	C15H <sub>10</sub> O <sub>5</sub>	Oc1ccc(cc1)C3=COc2cc(O)cc(O)c2C3=O
4443-09-8	5,7,8-trihydroxyflavone; norwogonin	C15H <sub>10</sub> O <sub>5</sub>	c12Oc(c3cccc3)=CC(=O)c1c(O)cc(O)c2O
	flavone, 3-OH, 5-OH, 7-OH	C15H <sub>10</sub> O <sub>5</sub>	Oc1cc(O)cc2OC(c3cccc3)=C(O)C(=O)c12
	flavone, 5-OH, 7-OH, 4'-OH	C15H <sub>10</sub> O <sub>5</sub>	Oc1cc(O)cc2OC(c3ccc(O)cc3)=CC(=O)c12
	flavone, 7-OH, 8-OH, 3'-OH	C15H <sub>10</sub> O <sub>5</sub>	c1cc(O)c(O)c2OC(c3cc(O)ccc3)=CC(=O)c12
3440-24-2	3',4',7,8-tetrahydroxyflavone	C15H <sub>10</sub> O <sub>6</sub>	c12c(C(\C=C(/O1)\c1cc(c(cc1)O)O)=O)ccc(c2O)O
520-18-3	flavone, 3-OH, 5-OH, 7-OH, 4'-OH; kaempferol	C15H <sub>10</sub> O <sub>6</sub>	Oc1cc(O)cc2OC(=C(O)C(=O)c12)c3ccc(O)cc3
528-48-3	flavone, 3-OH, 7-OH, 3'-OH, 4'-OH; fisetin	C15H <sub>10</sub> O <sub>6</sub>	c1cc(O)cc2OC(=C(O)C(=O)c12)c3cc(O)c(O)cc3
491-70-3	flavone, 5-OH, 7-OH, 3'-OH, 4'-OH; luteolin	C15H <sub>10</sub> O <sub>6</sub>	Oc1cc(O)cc2OC(=CC(=O)c12)c3cc(O)c(O)cc3
480-16-0	flavone, 3-OH, 5-OH, 7-OH, 2'-OH, 4'-OH; morin	C15H <sub>10</sub> O <sub>7</sub>	Oc1cc(O)cc2OC(=C(O)C(=O)c12)c3c(O)cc(O)cc3
117-39-5	flavone, 3-OH, 5-OH, 7-OH, 3'-OH, 4'-OH; quercetin	C15H <sub>10</sub> O <sub>7</sub>	Oc1cc(O)cc2OC(=C(O)C(=O)c12)c3cc(O)c(O)cc3

	flavone, 3-OH, 5-OH, 7-OH, 3'-OH, 5'-OH	C15H10O7	Oc1cc(O)cc2OC(c3cc(O)cc(O)c3)=C(O)C(=O)c12
	flavone, 7-OH, 8-OH, 3'-OH, 4'-OH, 5'-OH	C15H10O7	c1cc(O)c(O)c2OC(c3cc(O)c(O)c3)=CC(=O)c12
529-44-2	flavone, 3-OH, 5-OH, 7-OH, 3'-OH, 4'-OH, 5'-OH; myricetin	C15H10O8	Oc1cc(O)cc2OC(=C(O)C(=O)c12)c3cc(O)c(O)c(O)c3
	flavone, 4'-NH2	C15H11NO2	c1cccc2OC(c3ccc(N)cc3)=CC(=O)c12
	flavone, 6-OH, 4'-NH2	C15H11NO3	c1c(O)ccc2OC(c3ccc(N)cc3)=CC(=O)c12
	flavone, 7-OH, 4'-NH2	C15H11NO3	c1cc(O)cc2OC(c3ccc(N)cc3)=CC(=O)c12
	flavone, 5-OH, 7-OH, 4'-NH2	C15H11NO4	Oc1cc(O)cc2OC(c3ccc(N)cc3)=CC(=O)c12
	4',6-dichloroflavan	C15H12Cl2O	c1c(Cl)ccc2OC(c3ccc(Cl)cc3)CCc12
	flavone, 6-NH2, 3'-NH2	C15H12N2O2	c1c(N)ccc2OC(c3cc(N)ccc3)=CC(=O)c12
	flavone, 6-NH2, 4'-NH2	C15H12N2O2	c1c(N)ccc2OC(c3ccc(N)cc3)=CC(=O)c12
	flavone, 8-NH2, 4'-NH2	C15H12N2O2	c1ccc(N)c2OC(c3ccc(N)cc3)=CC(=O)c12
	flavone, 5-OH, 6-NH2, 4'-NH2	C15H12N2O3	Oc1c(N)ccc2OC(c3ccc(N)cc3)=CC(=O)c12
	flavone, 5-OH, 8-NH2, 4'-NH2	C15H12N2O3	Oc1ccc(N)c2OC(c3ccc(N)cc3)=CC(=O)c12
	flavone, 6-NH2, 7-OH, 3'-NH2	C15H12N2O3	c1c(N)c(O)cc2OC(c3cc(N)ccc3)=CC(=O)c12
	flavone, 6-NH2, 7-OH, 4'-NH2	C15H12N2O3	c1c(N)c(O)cc2OC(c3ccc(N)cc3)=CC(=O)c12
	flavone, 6-OH, 8-NH2, 4'-NH2	C15H12N2O3	c1c(O)cc(N)c2OC(c3ccc(N)cc3)=CC(=O)c12
	flavone, 7-OH, 8-NH2, 4'-NH2	C15H12N2O3	c1cc(O)c(N)c2OC(c3ccc(N)cc3)=CC(=O)c12
6515-37-3	4'-hydroxyflavanone	C15H12O3	c1cccc2OC(CC(=O)c12)c3ccc(O)cc3
480-41-1	5,7,4'-trihydroxyflavanone; naringenin	C15H12O5	Oc1cc(O)c2C(=O)CC(c3ccc(O)cc3)Oc2c1
	flavone, 6-NH2, 8-NH2, 4'-NH2	C15H13N3O2	c1c(N)cc(N)c2OC(c3ccc(N)cc3)=CC(=O)c12
	flavone, 5-NH2, 6-OH, 7-NH2, 3'-NH2	C15H13N3O3	Nc1c(O)c(N)cc2OC(c3cc(N)ccc3)=CC(=O)c12
	flavone, 5-NH2, 6-OH, 7-NH2, 4'-NH2	C15H13N3O3	Nc1c(O)c(N)cc2OC(c3ccc(N)cc3)=CC(=O)c12
	flavone, 6-NH2, 7-OH, 8-NH2, 4'-NH2	C15H13N3O3	c1c(N)c(O)c(N)c2OC(c3ccc(N)cc3)=CC(=O)c12
	flavan	C15H14O	c1cccc2OC(CC12)c3ccccc3
	isoflavan	C15H14O	c1cccc2OCC(Cc12)c3ccccc3
94105-90-5	Equol; 4',7-dihydroxyflavone; see also CAS 66036-38-2	C15H14O3	c1cc(O)cc2OCC(c3ccc(O)cc3)Cc12
17874-34-9	4,6-dimethyl-8-tert-butylcoumarin	C15H18O2	CC(C)(C)c1cc(C)cc2C(C)=CC(=O)Oc12
	flavone, 3-COOH, 4'-Br	C16H9BrO4	c1cccc2OC(c3ccc(Br)cc3)=C(C(=O)O)C(=O)c12
	flavone, 3-COOH, 4'-NO2	C16H9NO6	c1cccc2OC(c3ccc(N(=O)=O)cc3)=C(C(=O)O)C(=O)c12
	flavone, 3-COOH, 5-OH, 7-OH, 4'-NO2	C16H9NO8	Oc1cc(O)cc2OC(c3ccc(N(=O)=O)cc3)=C(C(=O)O)C(=O)c12
	coumarin deriv., T-4604-016	C16H10N2O4S	c1cccc2C(C3=NOS(=O)N3c4ccccc4)=CC(=O)Oc12
	flavone, 5-OCH3, 8-NO2, 4'-NO2	C16H10N2O7	COc1ccc(N(=O)=O)c2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12
	flavone, 6-OCH3, 8-NO2, 4'-NO2	C16H10N2O7	c1c(OC)cc(N(=O)=O)c2OC(c3ccc(N(=O)=O)cc3)=CC(=O)c12
	flavone, 3-COOH, 4'-OH	C16H10O5	c1cccc2OC(c3ccc(O)cc3)=C(C(=O)O)C(=O)c12
	coumarin deriv., T-4604-001	C16H11ClN2O3	c1cccc2C(C(Nc3ccccc3)=NO)=C(Cl)C(=O)Oc12
	coumarin deriv., T-4604-006	C16H12N2O2	c1cccc2C(C=NNc3ccccc3)=CC(=O)Oc12
29976-75-8	6-methylflavone	C16H12O2	O=C1C3=C(OC(=C1)c2ccccc2)C=CC(=C3)C
26964-24-9	6-methoxyflavone	C16H12O3	O=C1C3=C(OC(=C1)c2ccccc2)C=CC(=C3)OC
22395-22-8	7-methoxyflavone	C16H12O3	O=C1C3=C(OC(=C1)c2ccccc2)C=C(OC)C=C3
29550-13-8	5,6-dihydroxy-7-methoxyflavone; baicalein-7-methyl ether	C16H12O5	c12c(C(\C=C(/O1)\c1ccccc1)=O)c(c(c2)OC)O
480-44-4	acacetin; 5,7-dihydroxy-4'-methoxyflavone	C16H12O5	Oc1cc(O)cc2oc(c3ccc(OC)cc3)=CC(=O)c12
	flavone, 5-OH, 7-OCH3, 4'-OH	C16H12O5	Oc1cc(OC)cc2OC(c3ccc(O)cc3)=CC(=O)c12
	flavone, 5-OCH3, 8-NH2, 4'-NH2	C16H14N2O3	COc1ccc(N)c2OC(c3ccc(N)cc3)=CC(=O)c12
	flavone, 6-OCH3, 8-NH2, 3'-NH2	C16H14N2O3	c1c(OC)cc(N)c2OC(c3cc(N)ccc3)=CC(=O)c12
	flavone, 6-OCH3, 8-NH2, 4'-NH2	C16H14N2O3	c1c(OC)cc(N)c2OC(c3ccc(N)cc3)=CC(=O)c12

520-33-2	4'-methoxy-5,7,3'-trihydroxyflavanone; hesperetine coumarin deriv., T-4604-003	C16H14O6	<chem>c1(O)cc(O)cc2c1C(=O)CC(c1cc(O)c(OC)cc1)O2</chem>
15776-59-7	3-[2-(diethylamino)ethyl]-7-hydroxy-4-methylcoumarin hydrochloride coumarin deriv., T-4604-009 coumarin deriv., T-4604-015 flavone, 3-COOCH3, 4'-Br flavone, 3-COOCH3, 4'-NO2 flavone, 3-COOH, 6-OCH3, 4'-NO2 flavone, 3-COOH, 7-OCH3, 4'-NO2 coumarin deriv., T-4604-013 flavone, 3-COCH3, 4'-OH flavone, 3-COOH, 4'-OCH3 flavone, 3-COOH, 7-OCH3, 4'-OH coumarin deriv., T-4604-002 flavone, 3-COOCH3, 4'-NH2	C16H17ClN2O3 C16H22ClNO3 C17H10N2O3 C17H10N2O3S C17H11BrO4 C17H11NO6 C17H11NO7 C17H11NO7 C17H12N2O3 C17H12O5 C17H12O5 C17H12O6 C17H13ClN2O3 C17H13NO4	<chem>c1cccc2C(C(NC3CCCC3)=NO)=C(Cl)C(=O)Oc12</chem> <chem>c1cc(O)cc2OC(=O)C(CC[N+](CC)CC)=C(C)c12.[Cl-]</chem> <chem>c1cccc2C(c3noc(c4cccc4)n3)=CC(=O)Oc12</chem> <chem>c1cccc2C(C3=NOC(=S)N3c4cccc4)=CC(=O)Oc12</chem> <chem>c1cccc2OC(c3ccc(Br)cc3)=C(C(=O)OC)C(=O)c12</chem> <chem>c1cccc2OC(c3ccc(N(=O)=O)cc3)=C(C(=O)OC)C(=O)c12</chem> <chem>c1c(OC)ccc2OC(c3ccc(N(=O)=O)cc3)=C(C(=O)O)C(=O)c12</chem> <chem>c1cc(OC)cc2OC(c3ccc(N(=O)=O)cc3)=C(C(=O)O)C(=O)c12</chem> <chem>c1cccc2C(C3=NOCN3c4cccc4)=CC(=O)Oc12</chem> <chem>c1cccc2OC(c3ccc(O)cc3)=C(C(=O)OC)C(=O)c12</chem> <chem>c1cccc2OC(c3ccc(OC)cc3)=C(C(=O)O)C(=O)c12</chem> <chem>c1cc(OC)cc2OC(c3ccc(O)cc3)=C(C(=O)O)C(=O)c12</chem> <chem>c1cccc2C(C(Nc3ccc(C)cc3)=NO)=C(Cl)C(=O)Oc12</chem> <chem>c1cccc2OC(c3ccc(N)cc3)=C(C(=O)OC)C(=O)c12</chem>
15301-97-0	xylocoumarol	C17H14O3	<chem>O/C2=C(\C=1/C=C(/C)C=C(C)C=1)C(=O)OC=3C=CC=CC2=3</chem>
1157-39-7	4',7-dimethoxyisoflavone flavone, 3'-OCH3, 5'-OCH3	C17H14O4 C17H14O4	<chem>c12c(C(=O)/C(=C/O1)/c1ccc(cc1)OC)ccc(c2)OC</chem> <chem>c1cccc2OC(c3cc(OC)cc(OC)c3)=CC(=O)c12</chem>
117-52-2	Coumafuryl flavone, 3'-OCH3, 4'-OH, 5'-OCH3 flavone, 6-OH, 3'-OCH3, 4'-OH, 5'-OCH3 flavone, 7-OH, 3'-OCH3, 4'-OH, 5'-OCH3	C17H14O5 C17H14O6 C17H14O6 C17H14O6	<chem>O=C1C(C(CC(C)=O)C2=CC=CO2)=C(O)C(C=CC=C3)=C3O1</chem> <chem>c1cccc2OC(c3cc(OC)c(O)c(OC)c3)=CC(=O)c12</chem> <chem>c1c(O)ccc2OC(c3cc(OC)c(O)c(OC)c3)=CC(=O)c12</chem> <chem>c1cc(O)cc2OC(c3cc(OC)c(O)c(OC)c3)=CC(=O)c12</chem>
34334-69-5	6,7-dimethoxy-3',4',5-trihydroxyflavone flavone, 3-OH, 5-OH, 7-OH, 3'-OCH3, 5'-OCH3	C17H14O7 C17H14O7	<chem>c12c(C(\C=C(/O1)\c1cc(c(cc1)O)O)=O)c(c(c2)OC)OC)O</chem> <chem>Oc1cc(O)cc2OC(c3cc(OC)cc(OC)c3)=C(O)C(=O)c12</chem>
83-88-5	(-)-riboflavin coumarin deriv., T-4604-010 coumarin deriv., T-4604-017 coumarin deriv., T-4604-018 flavone, 3-COOCH3, 6-OCH3, 4'-NO2 flavone, 3-COOCH3, 7-OCH3, 4'-NO2 coumarin deriv., T-4604-014 flavone, 3-COOCH3, 4'-OCH3 flavone, 3-COOCH3, 6-OCH3, 4'-OH flavone, 3-COOCH3, 7-OCH3, 4'-OH flavone, 3-COOH, 3'-OCH3, 4'-OCH3 flavone, 3-COOH, 3'-OCH3, 5'-OCH3	C17H20N4O6 C18H12N2O4 C18H12N2O4 C18H13NO5 C18H13NO7 C18H13NO7 C18H14N2O3 C18H14O5 C18H14O6 C18H14O6 C18H14O6 C18H14O6 C18H16O2 C18H16O3 C18H16O5 C18H16O5 C18H16O5 C18H16O6 C18H16O6 C18H16O6	<chem>Cc1c(C)cc2N=C3C(=O)NC(=O)N=C3N(CC(O)C(O)C(O)CO)c2c1</chem> <chem>c1cccc2C(c3noc(c4ccc(OC)cc4)n3)=CC(=O)Oc12</chem> <chem>c1cccc2C(C3=NC(c4ccc(OC)cc4)=NO3)=CC(=O)Oc12</chem> <chem>c1cccc2C(C3OC(c4ccc(OC)cc4)=NO3)=CC(=O)Oc12</chem> <chem>c1c(OC)ccc2OC(c3ccc(N(=O)=O)cc3)=C(C(=O)OC)C(=O)c12</chem> <chem>c1cc(OC)cc2OC(c3ccc(N(=O)=O)cc3)=C(C(=O)OC)C(=O)c12</chem> <chem>c1cccc2C(C3=NOC(C)N3c4cccc4)=CC(=O)Oc12</chem> <chem>c1cccc2OC(c3ccc(OC)cc3)=C(C(=O)OC)C(=O)c12</chem> <chem>c1c(OC)ccc2OC(c3ccc(O)cc3)=C(C(=O)OC)C(=O)c12</chem> <chem>c1cc(OC)cc2OC(c3ccc(O)cc3)=C(C(=O)OC)C(=O)c12</chem> <chem>c1cccc2OC(c3cc(OC)c(OC)cc3)=C(C(=O)O)C(=O)c12</chem> <chem>c1cccc2OC(c3cc(OC)cc(OC)c3)=C(C(=O)O)C(=O)c12</chem> <chem>c1cccc2oC(=O)C(C(CC)c3ccccc3)=Cc12</chem> <chem>c1cc(OC(C)C)cc2OC=C(c3ccccc3)C(=O)c12</chem>
435-97-2	Phenprocoumon	C18H16O5	<chem>c12c(C(\C=C(/O1)\c1cc(c(cc1)OC)OC)=O)ccc(c2)OC</chem>
35212-22-7	lpriflavone	C18H16O5	<chem>O1C(c2cc(OC)c(OC)c(OC)c2)=CC(=O)c3ccccc13</chem>
22395-24-0	3',4',7-trimethoxyflavone	C18H16O5	<chem>O1C(c2cc(OC)c(OC)c(OC)c2)=CC(=O)c3ccccc13</chem>
973-67-1	5,6,7-trimethoxyflavone flavonoid deriv., 4063-029 flavonoid deriv., 4063-048 flavone, 6-OH, 3'-OCH3, 4'-OCH3, 5'-OCH3 flavone, 7-OH, 3'-OCH3, 4'-OCH3, 5'-OCH3	C18H16O5 C18H16O6 C18H16O6 C18H16O6	<chem>c1c(O)ccc2OC(c3cc(OC)c(OC)c(OC)c3)=CC(=O)c12</chem> <chem>c1cc(O)cc2OC(c3cc(OC)c(OC)c(OC)c3)=CC(=O)c12</chem> <chem>c12c(C(\C=C(/O1)\c1cc(c(cc1)OC)O)=O)c(c(c2)OC)OC)O</chem>
855-96-9	3',5-dihydroxy-4',6,7-trimethoxyflavone	C18H16O7	

604-59-1	flavone, 7-OH, 8-OH, 3'-OCH3, 4'-OCH3, 5'-OCH3	C18H16O7	c1cc(O)c(O)c2OC(c3cc(OC)c(OC)c(OC)c3)=CC(=O)c12
6051-87-2	alpha-naphthoflavone	C19H12O2	O(c(c(C(=O)C=1)ccc2cccc3)c23)C1c(cccc4)c4
66-76-2	beta-naphthoflavone	C19H12O2	O=C2C=C(Oc3ccc1ccccc1c23)c4cccc4
37470-13-6	dicoumarol	C19H12O6	O=C1Oc2ccccc2C(O)=C1CC3=C(O)c4cccc4OC3=O
81-82-3	flavodic acid	C19H14O8	O=C1C=C(OC2=CC(=CC(OCC(=O)O)=C12)OCC(=O)O)C3=CC=CC=C3
152-72-7	Coumachlor	C19H15ClO4	CC(=O)CC(c1ccc(Cl)cc1)C3=C(O)c2ccccc2OC3=O
5836-29-3	Acenocoumarol	C19H15NO6	O=C1Oc2ccccc2C(O)=C1C(CC(=O)C)c3ccc(cc3)N(=O)=O
	Coumatetralyl	C19H16O3	OC3=C(C1CCc2ccccc12)C(=O)Oc4cccc34
	flavone, 3-COOCH3, 3'-OCH3, 4'-OCH3	C19H16O6	c1cccc2OC(c3cc(OC)c(OC)cc3)=C(C(=O)OC)C(=O)c12
	flavone, 3-COOCH3, 3'-OCH3, 5'-OCH3	C19H16O6	c1cccc2OC(c3cc(OC)cc(OC)c3)=C(C(=O)OC)C(=O)c12
	flavone, 3-COOH, 3'-OCH3, 4'-OCH3, 5'-OCH3	C19H16O7	c1cccc2OC(c3cc(OC)c(OC)c(OC)c3)=C(C(=O)O)C(=O)c12
855-97-0	flavone, 7-OCOCH3, 3'-OCH3, 4'-OH, 5'-OCH3	C19H16O7	c1cc(OC(=O)C)cc2OC(c3cc(OC)c(O)c(OC)c3)=CC(=O)c12
	3',4',5,7-tetramethoxyflavone; luteolin tetramethyl ether	C19H18O6	COc1cc(OC)cc2OC(=CC(=O)c12)c3cc(OC)c(OC)cc3
	flavone, 6-OCH3, 3'-OCH3, 4'-OCH3, 5'-OCH3	C19H18O6	c1c(OC)ccc2OC(c3cc(OC)c(OC)c(OC)c3)=CC(=O)c12
	flavone, 7-OCH3, 3'-OCH3, 4'-OCH3, 5'-OCH3	C19H18O6	c1cc(OC)cc2OC(c3cc(OC)c(OC)c(OC)c3)=CC(=O)c12
	flavone, 3-COOCH3, 6-OCH3, 4'-NH-COCH3	C20H17NO6	c1c(OC)ccc2OC(c3ccc(NC(=O)C)cc3)=C(C(=O)OC)C(=O)c12
	flavone, 3-COOCH3, 7-OCH3, 4'-NH-COCH3	C20H17NO6	c1cc(OC)cc2OC(c3ccc(NC(=O)C)cc3)=C(C(=O)OC)C(=O)c12
518-20-7	Pyranocoumarin	C20H18O4	c1ccc2OC(=O)C(C(c4cccc4)C3)=C(OC3(C)OC)c2c1
	flavone, 3-COOCH3, 3'-OCH3, 4'-OCH3, 5'-OCH3	C20H18O7	c1cccc2OC(c3cc(OC)c(OC)c(OC)c3)=C(C(=O)OC)C(=O)c12
4366-18-1	coumetarol	C21H16O7	O=C2OC1=CC=CC=C1C(O)=C2[C@]([H])(CO)C4=C(O)C=3C=CC=CC=3O
35838-63-2	clocoumarol	C21H21ClO3	O/C1=C(/C(=O)OC=2C=CC=CC1=2)[C@]([H])(CCC)C3=CC=C(C=C3)CC[C
478-01-3	nobiletin; 5,6,7,8,3',4'-hexamethoxyflavone	C21H22O8	COc1c(OC)c(OC)c(OC)c2OC(c3cc(OC)c(OC)cc3)=CC(=O)c12
15686-60-9	flavamine	C21H23NO2	O=C2C=1C=C(C=CC=1O/C=C2/C)C3=CC=CC=C3)CN(CC)CC
	flavone, 6-OH, 4'-O-Si(CH3)2-C(CH3)3	C21H24O4Si	c1c(O)ccc2OC(c3ccc(O[Si](C)(C)C(C)C)cc3)=CC(=O)c12
	flavone, 7-OH, 4'-O-Si(CH3)2-C(CH3)3	C21H24O4Si	c1cc(O)cc2OC(c3ccc(O[Si](C)(C)C(C)C)cc3)=CC(=O)c12
	flavone, 5-OH, 4'-OCH2-C6H5	C22H16O4	Oc1cccc2OC(c3ccc(OCc4cccc4)cc3)=CC(=O)c12
	flavone, 7-OH, 4'-OCH2-C6H5	C22H16O4	c1cc(O)cc2OC(c3ccc(OCc4cccc4)cc3)=CC(=O)c12
548-00-5	ethyl-biscoumacetate	C22H16O8	c1cccc2C(O)=C(C(=O)Oc12)C(C(=O)OCC)C3=C(O)c4cccc4OC3=O
17692-56-7	moxicoumone	C22H30N2O6	O=C3/C=C(/C)C=2C(=CC(OCCN1CCOCC1)=CC=2O3)OCCN4CCOCC4
	flavone, 6-OH, 3'-OCH3, 4'-O-Si(CH3)2-C(CH3)3, 5'-OCH3	C23H28O6Si	c1c(O)ccc2OC(c3cc(OC)c(O[Si](C)(C)C(C)C)c(OC)c3)=CC(=O)c12
	flavone, 7-OH, 3'-OCH3, 4'-O-Si(CH3)2-C(CH3)3, 5'-OCH3	C23H28O6Si	c1cc(O)cc2OC(c3cc(OC)c(O[Si](C)(C)C(C)C)c(OC)c3)=CC(=O)c12
	flavone, 7-OH, 8-OH, 3'-OCH3, 4'-O-Si(CH3)2-C(CH3)3, 5'-OCH3	C23H28O7Si	c1cc(O)c(O)c2OC(c3cc(OC)c(O[Si](C)(C)C(C)C)c(OC)c3)=CC(=O)c12
	flavone, 3-COOCH3, 4'-OCH2-C6H5	C24H18O5	c1cccc2OC(c3ccc(OCc4cccc4)cc3)=C(C(=O)OC)C(=O)c12
62507-01-1	3'-benzyloxy-5,7-dihydroxy-3,4'-dimethoxyflavone	C24H20O7	c12c(C(\C=C(/O1)c1cc(c(cc1)OC)OCc1cccc1)\OC)=O)c(cc(c2)O)O
15301-69-6	flavoxate	C24H25NO4	O=C2C=1C=CC=C(C=1O/C=C2/C)C3=CC=CC=C3)C(=O)OCCN4CCCC4
3717-88-2	Flavoxate hydrochloride	C24H26ClNO4	c1cccc1C2=C(C)C(=O)c3cccc(c3O2)C(=O)OCC4CC[N+](C)C4.[Cl-]
	flavone, 3-COOCH3, 6-OCH3, 4'-OCH2-C6H5	C25H20O6	c1c(OC)ccc2OC(c3ccc(OCc4cccc4)cc3)=C(C(=O)OC)C(=O)c12
	flavone, 3-COOCH3, 7-OCH3, 4'-OCH2-C6H5	C25H20O6	c1cc(OC)cc2OC(c3ccc(OCc4cccc4)cc3)=C(C(=O)OC)C(=O)c12
	flavone, 7-OCOCH3, 3'-OCH3, 4'-O-Si(CH3)2-C(CH3)3, 5'-OCH3	C25H30O7Si	c1cc(OC(=O)C)cc2OC(c3cc(OC)c(O[Si](C)(C)C(C)C)c(OC)c3)=CC(=O)c12
	flavone, 7-OCOCH3, 8-OCOCH3, 3'-OCH3, 4'-O-Si(CH3)2-C(CH3)3, 5'-OCH3	C27H32O9Si	c1cc(OC(=O)C)c(OC(=O)C)c2OC(c3cc(OC)c(O[Si](C)(C)C(C)C)c(OC)c3)=
70321-32-3	alpha-tetrahydroflavanthrone	C28H16N2O2	c1cccc2c(O)c3ccc4Nc5c6cccc6c(O)c8(c5c7c4c3c(c12)nc7cc8)
4670-05-7	theaflavine	C29H24O12	Oc1cc(O)cc2O[C@]([H])([C@]([H])(O)Cc12)C3C=C(O)C(=O)c4c(O)c(O)cc(c4C=
56073-10-0	Brodifacoum; Talon; 3-(3-(4'-bromo-(1,1'-biphenyl)-4-yl)-1,2,3,4-tetrahydr	C31H23BrO3	c1cc(Br)ccc1c(cc2)ccc2C3Cc4cccc4C(C5=C(O)c6cccc6OC5(=O))C3
	flavone, 3-COOCH3, 5-OCH2-C6H5, 7-OCH2-C6H5, 4'-NO2	C31H23NO8	c4cccc4COc1cc(OCc4cccc4)cc2OC(c3ccc(N(=O)O)cc3)=C(C(=O)OC)C(=
56073-07-5	Difenacoum	C31H24O3	O=C1Oc2ccccc2C(O)=C1C3c4cccc4CC(c5ccc(c6cccc6)cc5)C3

90035-08-8 Flocoumafen  
752-56-7 riboflavin tetrabutyrate  
4434-05-3 coumamycin

C33H25F3O4  
C33H44N4O10  
C55H59N5O20

O=C1Oc2ccccc2C(O)=C1C3c4ccccc4CC(c5ccc(OCc6ccc(C(F)(F)F)cc6)cc5)(  
c12N(CC(OC(=O)CCC)C(OC(=O)CCC)C(OC(=O)CCC)COC(=O)CCC)C3=NC  
OC=4C=3C=CC(O[C@]2([H])OC(C)(C)[C@]([H])(OC)[C@@]([H])(OC(=O)C=











C4=O  
2]

2  
=CC(=O)c12

:3)[C@@H]5[C@H](O)Cc6c(O)cc(O)cc6O5

=O)c12

C3

C(=O)NC(=O)C3=Nc1cc(C)c(C)c2

1NC(C)=CC=1][C@@]2(O)[H])=C(C)C=3OC(=O)C=4NC(=O)C5=CN/C(=C5/C)C(=O)N/C9=C\O)C=8C=CC(O[C@@]7([H])OC(C)(C)[C@@]([H])(OC)[C@]([H])(OC(=O)C=6NC(C)=CC=













=6)[C@]7(O)[H])=C(C)C=8OC9=O