

Only Leaf (73)	Negative mode Common (239)	Only LP2 (81)
Paraxanthine	1,5-anhydroglucitol	3-Methoxy-19-norpregna-1,3,4(10)-tri-en-20-one
erythrose	Ergofylline	1-O-Phosphogentitol
1-[[[5-amino-2-furanyl(methylene)amino]-2,4-imidazolidinedione	Theobromine	D-Xylofuranose
Succinylacetone	Levonorgestrel	MPICD11043108
[+/-]-2-Hydroxyglutaric acid	Nicorandil	2-AMINO-4,6-DINITROTOLUENE
1-Deoxy-L-mannitol	4-Nitrophenol	(2S,4S)-4-Amino-2-hydroxy-2-methylpentanedioic acid
2-amino-2,3,7-trideoxy-D-xylo-hept-6-ulosonic acid	Metronidazole	DDO7S0000
3,5-di-tert-butyl-4-hydroxybenzyl alcohol	N-Acetyl-L-histidine	3-(methoxycarbonyl)amino)-2,2,3-trimethylbutanoic acid
nifediazene	D-(-)-Fructose	3(2Z)-[Hydroxy(2R,3R)-3-(hydroxymethyl)methyl]-2-oxiranylmethyl(methylene)amino]-L-alanine
fenamole	L-Tyrosine methyl ester	2-isopropylmaleic acid
1,5-Anhydro-D-erythro-hexo-2,3-diulose	Acetone peroxide	alpha-Aminoalpic acid
Ethyl 2,4-dioxohexanoate	2,2-Methyl-2-methyl-4-ethyl-6-tert-butylphenol	N-glycyl-beta-D-glucosamine
UP0783700	(+)-[6]-Gingerol	beta-D-Ethyl glucuronide
7-Cyano-7-deazaguanine	4-Methoxy-3,4a,5-trimethyl-4,4a,5,6,7,8a,9-octahydronaphtho[2,3-b]furan	cis-4-Octenedioic acid
N-Formyl-L-glutamic acid	2,3,4,5-Tetrahydroxypentanal	MPIC00056163
PE5118-310	Methylglutamic acid	1,1-Diethyl-3-oxo-2-triazanolate
6-(Hydroxymethyl)-2,4(1H,3H)-pteridinedione	1,5-Anhydro-D-Fructose	4-Oxoprolinone
8-(3,4-Dihydroxyphenyl)-5-hydroxy-7-methoxy-6H-[1,3]dioxolo[4,5-h]chromen-6-one	Pyrophosphoric Acid	Suberic acid
(E)-Nitrofurazone	2-Deoxypentose	Aminoparathion
Carbendazim	Alcholine	alpha-Ketoglutaric acid
2-amino-3-oxoadipic acid	Elagic acid	1-Hydroxy-1-(4-methoxyphenyl)-4-methyl-3-pentanone
4-Hydroxy-2-oxoglutaric acid	Isopropylmalic acid	Undecanedioic acid
(2R)-2,5-Dihydroxypropanoic acid	6-Deoxy-D-arabino-hexos-2-ulose	DL-Malic acid
CYS660000	Procarbazine	2-[(2E)-5-(1,3-Dimethyl-2-oxirany)-3-methyl-2-penten-1-yl]-1,3,5-benzenetriol
6-[[1(R,2S)-1,2-Dihydroxypropyl]-3,4-dihydro-2,4-pteridinediol	threonic acid	deoxyuridine
RVS40000	5-(-)-Willardine	Prostaglandin B1
mifuradone	Arabic acid	8-Hydroxy-7-methylguanine
SL3650000	Xylitol	Arabinosylphosphoribine
MFCD00041500	1,4,9-Trihydroxy-9-methyl-5,8,10-trioxo-5,8,9,10-tetrahydro-2-phenanthrenecarboxylic acid	MFCD00488630
Tocotrienol	Erythritol	1,7-Dihydroxy-6,6-dimethyl-3,5,5a,6,7,8,9a,9b-octahydronaphtho[1,2-c]furan-9(H)-one
NP-018716	Succinic acid	Methyl thiolbutyrate
Nicotinic acid	6-Hydroxycaproic acid	ETS956200
3-tert-Butyladipic acid	3,4-Dihydroxyphenylglycol	(4R)-4-Hydroxy-5-oxo-L-norvaline
2-O-ETHYL ASCORBIC ACID	D-Glucono-delta lactone	cloacinine
fenoxycarb	4-amino-2-hydroxyamino-6-nitrotoluene	14,18-Dihydroxy-12-oxo-9,13,15-octadecatrienoic acid
Diphylline	Ethylmalonic acid	Corchorfatty acid F
Ethyl myristate	5-acetamido-6-formamido-3-methyluracil	ser-asp
Oxalosuccinic acid	Glutaric acid	cis-6-Dodecan-4-alide
NBN	1-(4,7-Dimethylpyrazolo[5,1-c][1,2,4]triazin-3-yl)ethan-1-one	butanethiol
acetic acid geranyl ester	triacetic acid	Isonicotinylglycine
2-Oxo-4-hydroxy-5-aminovalerate	4-Methyleneglutaric acid	Acetylhistamine
MFCD00376633	3-Deoxy-5-aminosalicylic acid	Artemisinol
3-(2-Thienyl)-DL-alanine	6-Amino-9H-purine-9-propanoic acid	3,7,9-Trihydroxy-6H-[1]benzofuro[3,2-c]chromen-6-one
Botrydial	D-Glucopyranuronic acid	2,3-Dihydrothiophene
(10E,15Z)-9,12,13-Trihydroxy-10,15-octadecadienoic acid	beta-D-Xylopyranose	coenzyme Q1
D-Sucrose	2,5-di-tert-butylhydroquinone	11-Deoxocourbutacin I
Pyrazinemethanethiol	D-Naladonic acid	1S,1S-DHOMD
2-Amino-5-[[[4,5-dihydroxy-2-cyclopenten-1-yl]amino)methyl]-4H-pyrrolo[2,3-d]pyrimidin-4-on	AMPA	TU4153400
N-(Ketocaproyl)-L-homosierine lactone	17970000	(6Z)-3,6,10-Trimethyl-3a,5a,8,10,11,11a-hexahydrocycloclad[2]furan-2,5(3H,4H)-dione
TU1100000	OM1220000	Palmitic acid
Furan-2-ylmethanethiol	(+/-)-3-Laudanosine	(2a)-Trehalose
Phenazopyridine	DL-Mevalonic acid	Quilicic Acid
1,4-Bis(2-ethoxyethyl) sulfosuccinate	2-Ethylglutaric acid	12-HSA
MFCD00712375	1,1,7-Triethylsulfuric acid	epigallocatechin gallate
6-Methyl-7,8-dihydroimidazo[1,5-c]pyrimidine-5(6H)-thione	shrimp shell	Propargylgenistein A2
N-formylmaleamic acid	Aselaic acid	13(S)-HOTIE
isobornide dinitrate	Diosdorb	ethionamide 5-oxide
P-D-ribosufuranosylxanthine	1-Deoxypentitol	MFCD00213847
L-dihydroquinacapsin	Lumazine	(4Z)-9,11-Dihydroxy-1,1,4,7a-tetramethyl-10-[(3-methylbutanoyl)-1,1a,2,3,6,7,7a,8,13a,13b-decahydrocyclopropa[9,10]cyclodeca[1,2-b]chromene-12-carbaldehyde
5-Chloro-3-fluoro-1,2-benzenediol	Metirosine	Matairesinol
NP-003039	8B5100000	Asiatic acid
5-allyl propenethioate	2-cyclopenten-1-one, 4-hydroxy-3-methyl-2-(2-pentenyl)-	8-Methyl-8-azabicyclo[3.2.1]oct-3-yl [(3S)-1,2-dithiolane-3-carboxylate
MEIQX	Vitamin C	4-Hydroxypropylserine
2,4-Dibromophenol	N-Acetyl-6-oxo-L-norleucine	Histidylglycine
Carbamazote	4-Amino(carboxymethyl)-5-oxoprolinone	Penityl isothiocyanate
(R)-ACPA	cis-2-Carboxycyclohexenyl-acetic acid	calcicaflo
Chlorambucil	Methional	UNIK-V9Q7UJUZ15U
felbamate	5-Dinitroglutacal	(1R,5S,6R,7R,9S,11S,12S,13S,14S)-3-Amino-14-methyl-8,10-dioxo-2,4-diazatetracyclo[7.3.1.1"7,11"-0"1,6"]tetradec-2-ene-5,9,12,13,14-pentol
nitroisocaproic acid	Pyrene	CUS774000
(2a,3b,19a)-2,3,19-Trihydroxyclean-12-en-28-oic acid	NP-002089	2'-Deoxycytidine
Oxaburimamide	1-(Propylsulfanyl)-1-(propylsulfanyl)propane	Aciclovir
alpha-Glucoheptitol	4-Acetamido-2-amino-6-nitrotoluene	N-Acetylcytidine
isomaid	2-Oxo-5-pentyltetrahydro-3-furancarboxylic acid	Valproic acid
-	N-Acetyl-D-glucosamine	L-3-hydroxykynurenine
-	4-hydroxyamino-2,6-dinitrotoluene	9-(beta-D-Arabinofuranosyl)-2-imino-3,7,8,9-tetrahydro-2H-purin-6-ol
-	Naipiricin	asn-val
-	Methylmalonic acid	Homocysteine thiolactone
-	(1S,3R,4S)-3,4-Dihydrocyclohexanecarboxylic acid	Ethyl 3-(furfurylthio)propionate
-	N-Acetylneuraminic acid	2-Monocaprin
-	Acetylglutamide	Methyl 9-oxononanoate
-	N-Undecanoylglycine	Fungin
-	Citic acid	-
-	2-Methyltetrahydrothiophen-3-one	-
-	Glucosheptonic Acid	-
-	Kinetin	-
-	N-(Carboxymethyl)serine	-
-	N-Acetyl-L-aspartic acid	-
-	Mentyl	-
-	(3-Hydroxy-3,4,5,6-tetrahydro-1H-cyclopenta[c]furan-4-yl)acetic acid	-
-	2,4-Dimethylthiazole	-
-	mycinose	-
-	2,4,5-Trimethyl-1,3-thiazole	-
-	Ventafaxine	-
-	Troxactabine	-
-	2,4-di-tert-Butylphenol	-
-	4-Nitroazomino)-1-(3-pyridinyl)-1-butanone	-
-	Glu-Gly	-
-	N.pl.-Methyl-L-histidine	-
-	Butyl isothiocyanate	-
-	1-(6-Azido-5-deoxy-beta-D-ribofuranosyl)-4-hydroxy-2(1H)-pyrimidinone	-
-	Aspartyl-L-proline	-
-	APM	-
-	antiscapin	-
-	2,6-Dideoxy-3-O-methyl-L-arabino-hexopyranose	-
-	Lycocommune	-
-	Sarin	-
-	(1S,11S)-DHQME	-
-	Hex-2-ulose	-
-	2-Deoxy-scyllo-inosamine	-
-	Dodecyl sulfate	-
-	Egumined	-
-	2,4-DIMETHYL-5-VINYLTIAZOLE	-
-	4-Dodecylbenzenesulfonic acid	-
-	Thio-ThiP	-
-	5-Allyl-L-cysteine	-
-	Rosardine	-
-	Etilevodopa	-
-	Ethyl 2-(methylthio)propanoate	-
-	Estroene	-
-	Cytidine	-
-	3-(5-oxoisoxazolin-4-yl)-L-alanine	-
-	3-(1-Piperazinyl)benzothiazole	-
-	(+/-)-Camphoric acid	-
-	2-thiazolylethylamine	-
-	3,4-dihydroxyglutamic acid	-
-	Rondazole	-
-	propylthiouacil	-
-	Cori thiazoline	-
-	NXB480000	-
-	Isulfuraphate	-
-	Estradiol Diopropionate	-
-	NP-019547	-
-	Phenylmethylsulfonyl fluoride	-
-	Dodecanedioic acid	-
-	Butylparaben	-
-	N-(6-Amino-5-nitro-4-pyrimidinyl)pentofuranosylamine	-
-	(2S,3R,5S)-3-(2-Aminoethoxy)-7-oxo-4-oxa-1-azabicyclo[3.2.0]heptane-2-carboxylic acid	-
-	Quinquepic acid	-
-	benthiocarb	-
-	Proxiphylline	-
-	Tetrahydrothiophene	-
-	N-(Carboxymethyl)-P-alanine	-
-	methyl thioacetate	-
-	N-methyl-2-oxoglutaramic acid	-
-	Ser-Glu	-
-	Nitraldozone	-
-	OA-6129-D	-
-	2-Deoxyhexopyranose	-
-	N-Hydroxy-metIQX	-
-	Diethyl (2R,3R)-2-hydroxy-3-methylsuccinate	-
-	(3aS,6S,6aR)-3,3,3a,6-Tetrahydroxytetrahydrofuro[3,2-b]furan-2(3H)-one [non-preferred name]	-
-	NP-020283	-
-	2-Methyl-3-undecyl-1,4-naphthoquinone	-
-	desiccivir	-
-	lactide	-
-	dihydroxyphenylalanine	-
-	Trolox	-
-	(15Z)-9,12,13-Trihydroxy-15-octadecanoic acid	-
-	Ethyl malate	-
-	Hexenic acid	-
-	alpha-ketoadipic acid	-
-	3-Methylsulfolene	-
-	5-Acetyl-2,4-dimethylthiazole	-

+	Pentitolol	+
+	3 (2-Amino-4-pyrimidinyl)alanine	+
+	Cislozone	+
+	N-(4-Hydroxyhexanoyl)glycine	+
+	5,6,7,8-tetrahydropterin-6-carboxylic acid	+
+	2-methylcitric acid	+
+	Aminone	+
+	5-amino-5-deoxy-3-dehydrokinic acid	+
+	Misorbine	+
+	2,2'-Ethylidene-bis(4,6-di-tert-butylphenol)	+
+	Phlostonic acid	+
+	Pidotimid	+
+	(S)-(-)-Gottin	+
+	MFCD00037315	+
+	NP-011548	+
+	V51150000	+
+	1-(4-Methoxyphenyl)-3-pentanone	+
+	3-oxopimelic acid	+
+	Methyldopa	+
+	4-Hydroxy-L-threonine	+
+	NS180000	+
+	guamisin	+
+	MFCD00030936	+
+	N-Acetylglucosaminitol	+
+	Ureosuccinone A	+
+	D-(-)-Erythrose	+
+	2,4-Dihydroxy-6-[(2E,6E,10E)-3,7,11,15-tetramethyl-2,6,10,14-hexadecatetraen-1-yl]phenyl acetate	+
+	9,10-Dihydroxysebacic acid	+
+	2-Hydroxy-4-oxo-1,6-dihydro-3-pyridinecarboxylic acid	+
+	Sebacic acid	+
+	(E)-Furazolidone	+
+	(2E)-2-Cyano-N-(ethylcarbamoyl)-2-(methoxymino)acetamide	+
+	3-[(1Z)-5-Oxo-2-buten-2-yl]pentanedioic acid	+
+	Glycyl-4-hydroxyproline	+
+	MFCD00004231	+
+	Diethylpyrocarbonate	+
+	carglumatic acid	+
+	Juniperic acid	+
+	Glycylglycylglycine	+
+	6-(1-Hydroxyethyl)-3-(hydroxymethyl)-2,7-dioxabicyclo[4.1.0]hept-3-en-5-one	+
+	Glucuronamide	+
+	8-DEMETHYL MEHQ	+
+	1,3,4,5-Tetrahydrocyclohexanecarboxylic acid	+
+	glu-ter	+
+	mephensin	+
+	Azacitidine	+
+	Gualfenesin	+
+	5-[2-(3-Furyl)ethyl]-8a-(hydroxymethyl)-5,6-dimethyl-3,4,4a,5,6,7,8,8a-octahydro-1-naphthalenecarboxylic acid	+
+	2,5-Dimethyl-4-ethoxy-3(2H)-furanone	+
+	glu-asp	+
+	Hept-2-ulose	+
+	XT5075000	+
+	gamma-lactone A	+
+	Bufo-20,22-dienolide	+
+	Sulfolane	+
+	3-Thiomorpholinecarboxylic acid	+
+	protonamide	+
+	4,5-Dihydroxy-3-oxo-1-cyclohexene-1-carboxylic acid	+
+	fenfluramine	+
+	N21504000	+
+	2-Methoxy-5-nitrophenol	+
+	Diethyl tartrate	+
+	1,4,5-Trihydroxy-1-cyclohexanecarboxylic acid	+
+	Oxetic acid	+
+	2,3,4,5-tetrahydrodipicolinic acid	+
+	Sulfural	+
+	2-(Methylthio)ethanol	+
+	Alkyl isothiocyanate	+
+	Methyl bisnorbiotinyl ketone	+
+	(4R,5S,9S,10R,12S,13S)-1,5,9-Trimethyl-11,14,15,16-tetraoxatetracyclo[10.3.1.0 <sup>4,13</sup> -0 <sup>8,19</sup> ]hexadecan-10-ol	+
+	MF0100	+
+	5-Hydantoinpropionic acid	+
+	2-isobutylthiazole	+
+	(5S)-5-(Carboxymethyl)-L-proline	+
+	Etamidazole	+
+	1,3,4-Trihydroxy-5-oxocyclohexanecarboxylic acid	+