

NCBI name	molecular formula	monoisotopic mass of precursor ion	CAS number	NCBI CID
1,2-naphthoquinone-4-sulfonate	C ₁₀ H ₆ O ₅ S	236.9863	521-24-4 (Na-salt)	10637
trinitroresorcinol	C ₆ H ₃ N ₃ O ₈	243.9847	82-71-3	6721
2-hydroxy-5-methoxybenzophenon	C ₁₄ H ₁₂ O ₃	227.0713	14770-96-8	26881
2-naphthylamine-4,8-disulfonic acid	C ₁₀ H ₉ NO ₆ S ₂	301.9798	131-27-1	8563
thiodipropionic acid	C ₆ H ₁₀ O ₄ S	177.0221	111-17-1	8096
m-nitrobenzoic acid	C ₇ H ₅ NO ₄	166.0145	121-92-6	8497
4-(aminomethyl)benzoic acid	C ₈ H ₉ NO ₂	150.0560	56-91-7	65526
chloroxine	C ₉ H ₅ Cl ₂ NO	211.9675	773-76-2	2722
acarbose	C ₂₅ H ₄₃ NO ₁₈	644.2407	56180-94-0	441184
acediasulfone	C ₁₄ H ₁₄ N ₂ O ₄ S	305.0601	80-03-5	66451
acemetacin	C ₂₁ H ₁₈ ClNO ₆	414.0749	53164-05-9	1981
acetosulfam	C ₄ H ₅ NO ₄ S	161.9866	33665-90-6	36573
acetylcysteine	C ₅ H ₉ NO ₃ S	162.0230	616-91-1	12035
acetylmethionine	C ₇ H ₁₃ NO ₃ S	190.0543	1115-47-5	6180
acetylsalicylic acid	C ₉ H ₈ O ₄	179.0349	50-78-2	2244
galactaric acid	C ₆ H ₁₀ O ₈	209.0302	526-99-8	607
acitretin	C ₂₁ H ₂₆ O ₃	325.1809	55079-83-9	5284513
aconitic acid	C ₆ H ₆ O ₆	173.0091	585-84-2	309
allobarbital	C ₁₀ H ₁₂ N ₂ O ₃	207.0775	52-43-7	5842
enallypropymal	C ₁₁ H ₁₆ N ₂ O ₃	223.1088	1861-21-8	95636
allylbutylbarbituric acid	C ₁₁ H ₁₆ N ₂ O ₃	223.1088	3146-66-5	48522
amobarbital	C ₁₁ H ₁₈ N ₂ O ₃	225.1244	57-43-2	2164
allylpropymal	C ₁₀ H ₁₄ N ₂ O ₃	209.0931	77-02-1	6464
aristolochic acid I	C ₁₇ H ₁₁ NO ₇	340.0462	61117-05-3	2236
ascorbic acid	C ₆ H ₈ O ₆	175.0248	50-81-7	5785
aspartic acid	C ₄ H ₇ NO ₄	132.0302	617-45-8	424
atorvastatin	C ₃₃ H ₃₅ FN ₂ O ₅	557.2457	134523-00-5	60823
barbital	C ₈ H ₁₂ N ₂ O ₃	183.0775	57-44-3	8943
barbituric acid	C ₄ H ₄ N ₂ O ₃	127.0149	67-52-7	6211
bendroflumethiazide	C ₁₅ H ₁₄ F ₃ N ₃ O ₄ S ₂	420.0305	73-48-3	2315
benzbromarone	C ₁₇ H ₁₂ Br ₂ O ₃	420.9080	3562-84-3	2333
benzoic acid	C ₇ H ₆ O ₂	121.0295	65-85-0	243
brallobarbital	C ₁₀ H ₁₁ BrN ₂ O ₃	284.9880	561-86-4	68416
bromisovalum	C ₆ H ₁₁ BrN ₂ O ₂	220.9931	496-67-3	2447
buclosamide	C ₁₁ H ₁₄ ClNO ₂	226.0640	575-74-6	68466
bumadizone	C ₁₉ H ₂₂ N ₂ O ₃	325.1557	3583-64-0	19161
butalbital	C ₁₁ H ₁₆ N ₂ O ₃	223.1088	77-26-9	2481
secbutobarbital	C ₁₀ H ₁₆ N ₂ O ₃	211.1088	125-40-6	2479
butobarbital	C ₁₀ H ₁₆ N ₂ O ₃	211.1088	77-28-1	6473
captopril	C ₉ H ₁₅ NO ₃ S	216.0699	62571-86-2	44093
carbromal	C ₇ H ₁₃ BrN ₂ O ₂	235.0087	77-65-6	6488
carprofen	C ₁₅ H ₁₂ ClNO ₂	272.0483	53716-49-7	2581
cefuroxime	C ₁₆ H ₁₆ N ₄ O ₈ S	423.0616	55268-75-2	5479529
chloramphenicol	C ₁₁ H ₁₂ Cl ₂ N ₂ O ₅	321.0050	56-75-7	5959
chlorazepate	C ₁₆ H ₁₁ ClN ₂ O ₃	313.0385	23887-31-2	2809
chlorbromuron	C ₉ H ₁₀ BrClN ₂ O ₂	290.9541	13360-45-7	25912
chloramphenicol palmitate	C ₂₇ H ₄₂ Cl ₂ N ₂ O ₆	559.2347	530-43-8	10736
chlorpropamide	C ₁₀ H ₁₃ ClN ₂ O ₃ S	275.0262	94-20-2	2727
ciprofloxazin	C ₁₇ H ₁₈ FN ₃ O ₃	330.1259	85721-33-1	2764
creatine	C ₄ H ₉ N ₃ O ₂	130.0622	57-00-1	586
cyclobarbital	C ₁₂ H ₁₆ N ₂ O ₃	235.1088	52-31-3	5838
cyqualon	C ₂₂ H ₂₂ O ₅	365.1394	579-23-7	11366
cyclamate	C ₆ H ₁₃ NO ₃ S	178.0543	100-88-9	7533
cynarin	C ₂₅ H ₂₄ O ₁₂	515.1195	30964-13-7	5281769
dapsone	C ₁₂ H ₁₂ N ₂ O ₂ S	247.0546	80-08-0	2955
dicamba	C ₈ H ₆ Cl ₂ O ₃	218.9621	1918-00-9	3030
dichloroprop	C ₉ H ₈ Cl ₂ O ₃	232.9777	120-36-5	8427
diclofenac	C ₁₄ H ₁₁ Cl ₂ NO ₂	294.0094	15307-86-5	3033
diflunisal	C ₁₃ H ₈ F ₂ O ₃	249.0368	27494-42-4	3059
dinitrobenzoic acid	C ₇ H ₄ N ₂ O ₆	210.9996	99-34-3	7433
valproic acid	C ₈ H ₁₆ O ₂	143.1077	99-66-1	3121
enalapril	C ₂₀ H ₂₈ N ₂ O ₅	375.1925	75847-73-3	5388962
equilin sulfate	C ₁₈ H ₂₀ O ₅ S	347.0958	27540-07-4	27993
ezetimibe	C ₂₄ H ₂₁ F ₂ NO ₃	408.1416	163222-33-1	150311
fenoprofen	C ₁₅ H ₁₄ O ₃	241.0870	31879-05-7	3342

floxacin	C ₁₉ H ₁₇ ClFN ₃ O ₅ S	452.0488	5250-39-5	21319
flufenamic acid	C ₁₄ H ₁₀ F ₃ NO ₂	280.0590	530-78-9	3371
fluprofen	C ₁₅ H ₁₃ FO ₂	243.0826	17692-38-5	219068
flurbiprofen	C ₁₅ H ₁₃ FO ₂	243.0826	5104-49-4	3394
fructose	C ₆ H ₁₂ O ₆	179.0561	57-48-7	5984
furosemide	C ₁₂ H ₁₁ ClN ₂ O ₅ S	329.0004	54-31-9	3440
fusidic acid	C ₃₁ H ₄₆ O ₆	515.3378	6990-06-03	3000226
4-hydroxybutyric acid	C ₄ H ₈ O ₃	103.0400	30470-15-6	10413
gliboruride	C ₁₈ H ₂₆ N ₂ O ₄ S	365.1540	26944-48-9	33649
glucose	C ₆ H ₁₂ O ₆	179.0561	50-99-7	24749
glutethimide	C ₁₃ H ₁₅ NO ₂	216.1030	77-21-4	3487
guaifenesin	C ₁₀ H ₁₄ O ₄	197.0819	93-14-1	3516
heptabarbital	C ₁₃ H ₁₈ N ₂ O ₃	249.1244	509-86-4	10518
hesperidin	C ₂₈ H ₃₄ O ₁₅	609.1824	520-26-3	10621
hexachlorophene	C ₁₃ H ₆ Cl ₆ O ₂	402.8426	70-30-4	3598
hexobarbital	C ₁₂ H ₁₆ N ₂ O ₃	235.1088	56-29-1	3608
ibuprofen	C ₁₃ H ₁₈ O ₂	205.1234	15687-27-1	3672
indoprofen	C ₁₇ H ₁₅ NO ₃	280.0979	31842-01-0	3718
iobenzamic acid	C ₁₆ H ₁₃ I ₃ N ₂ O ₃	660.7987	3115-05-7	18377
iodamide	C ₁₂ H ₁₁ I ₃ N ₂ O ₄	626.7780	440-58-4	3723
iopanoic acid	C ₁₁ H ₁₂ I ₃ NO ₂	569.7929	96-83-3	3735
ketorolac	C ₁₅ H ₁₃ NO ₃	254.0822	74103-06-3	3826
lactose	C ₁₂ H ₂₂ O ₁₁	341.1089	63-42-3	6134
lifibrol	C ₂₁ H ₂₆ O ₄	341.1758	96609-16-4	57112
lisinopril	C ₂₁ H ₃₁ N ₃ O ₅	404.2190	83915-83-7	5362119
mecoprop	C ₁₀ H ₁₁ ClO ₃	213.0323	7085-19-0	7153
methacycline	C ₂₂ H ₂₂ N ₂ O ₈	441.1303	914-00-1	5281054
methital	C ₁₂ H ₂₀ N ₂ O ₂ S ₂	287.0893	467-43-6	3032307
methohexital	C ₁₄ H ₁₈ N ₂ O ₃	261.1244	151-83-7	9034
Mephobarbital	C ₁₃ H ₁₄ N ₂ O ₃	245.0931	115-38-8	8271
5-(p-methylphenyl)-5-phenylhydantoin	C ₁₆ H ₁₄ N ₂ O ₂	265.0982	51169-17-6	92334
monobenzene	C ₁₃ H ₁₂ O ₂	199.0764	103-16-2	7638
nalidixic acid	C ₁₂ H ₁₂ N ₂ O ₃	231.0775	389-08-2	4421
naphthoic acid	C ₁₁ H ₈ O ₂	171.0451	86-55-5	7123
naphthoresorcinol	C ₁₀ H ₈ O ₂	159.0451	132-86-5	8601
naphthaleneacetic acid	C ₁₂ H ₁₀ O ₂	185.0608	86-87-3	6862
nedocromil	C ₁₉ H ₁₇ NO ₇	370.0932	69049-73-6	50294
niclosamid	C ₁₃ H ₈ Cl ₂ N ₂ O ₄	324.9788	50-65-7	4477
nimesulide	C ₁₃ H ₁₂ N ₂ O ₅ S	307.0394	51803-78-2	4495
methylparaben	C ₈ H ₈ O ₃	151.0400	99-76-3	7456
ethylparaben	C ₉ H ₁₀ O ₃	165.0557	120-47-8	8434
propylparaben	C ₁₀ H ₁₂ O ₃	179.0713	94-13-3	7175
nitrofurantoin	C ₈ H ₆ N ₄ O ₅	237.0265	67-20-9	6604200
novobiocin	C ₃₁ H ₃₆ N ₂ O ₁₁	611.2246	303-81-1	4546
orotic acid	C ₅ H ₄ N ₂ O ₄	155.0098	65-86-1	967
pentobarbital	C ₁₁ H ₁₈ N ₂ O ₃	225.1244	76-74-4	4737
iodoaliphonic acid	C ₁₅ H ₁₂ I ₂ O ₃	492.8803	577-91-3	11350
phenobarbital	C ₁₂ H ₁₂ N ₂ O ₃	231.0775	50-06-6	4763
phenobutidil	C ₁₀ H ₉ I ₃ O ₃	556.7613	554-24-5	11127
phenolphthalol	C ₂₀ H ₁₈ O ₃	305.1183	81-92-5	66495
penicillin V	C ₁₆ H ₁₈ N ₂ O ₅ S	349.0863	87-08-1	6869
fentichlor	C ₁₂ H ₈ Cl ₂ O ₂ S	284.9549	97-24-5	7329
phenylpyruvic acid	C ₉ H ₈ O ₃	163.0400	156-06-9	997
p-sulfophenylhydrazine	C ₆ H ₈ N ₂ O ₃ S	187.0182	98-71-5	66825
phenyl salicylate	C ₁₃ H ₁₀ O ₃	213.0557	118-55-8	8361
phlorhizin	C ₂₁ H ₂₄ O ₁₀	435.1296	60-81-1	6072
phtalic acid	C ₈ H ₆ O ₄	165.0193	88-99-3	1017
picric acid	C ₆ H ₃ N ₃ O ₇	227.9898	88-89-1	6954
pimelic acid	C ₇ H ₁₂ O ₄	159.0662	111-16-0	385
pipemidic acid	C ₁₄ H ₁₇ N ₅ O ₃	302.1258	51940-44-4	4831
piperic acid	C ₁₂ H ₁₀ O ₄	217.0506	5285-18-7	5370536
pirprofen	C ₁₃ H ₁₄ ClNO ₂	250.0640	31793-07-4	35935
pravastatin	C ₂₃ H ₃₆ O ₇	423.2388	81093-37-0	54687
propicillin	C ₁₈ H ₂₂ N ₂ O ₅ S	377.1176	551-27-9	65039
propionylprocainamide	C ₁₆ H ₂₅ N ₃ O ₂	290.1874	67635-46-5	197959
propofol	C ₁₂ H ₁₈ O	177.1284	2078-54-8	4943

propallylonal	$C_{10}H_{13}BrN_2O_3$	287.0036	545-93-7	11020
pyrithioxin	$C_{16}H_{20}N_2O_4S_2$	367.0791	1098-97-1	14190
pyrithydione	$C_9H_{13}NO_2$	166.0873	77-04-3	4994
pyromellitic acid	$C_{10}H_6O_8$	252.9989	89-05-4	6961
raffinose	$C_{18}H_{32}O_{16}$	503.1617	512-69-6	10542
ramipril	$C_{23}H_{32}N_2O_5$	415.2238	87333-19-5	5362129
repaglinide	$C_{27}H_{36}N_2O_4$	451.2602	135062-02-1	65981
saccharin	$C_7H_5NO_3S$	181.9917	81-07-2	5143
salicylamide	$C_7H_7NO_2$	136.0404	65-45-2	5147
salicylic acid	$C_7H_6O_3$	137.0244	69-72-7	338
salophen	$C_{15}H_{13}NO_4$	270.0771	118-57-0	1984
sebacic acid	$C_{10}H_{18}O_4$	201.1132	111-20-6	5192
secobarbital	$C_{12}H_{18}N_2O_3$	237.1244	76-73-3	5193
sorbitol	$C_6H_{14}O_6$	181.0717	50-70-4	5780
ouabain	$C_{29}H_{44}O_{12}$	583.2760	630-60-4	4605
guaiacolsulfonic acid	$C_7H_8O_5S$	203.0019	1321-14-8	159379
sulfathiourea	$C_7H_9N_3O_2S_2$	230.0063	515-49-1	3000579
thiamylal	$C_{12}H_{18}N_2O_2S$	253.1016	77-27-0	3032285
taurocholic acid	$C_{26}H_{45}NO_7S$	514.2843	81-24-3	6675
telmisartan	$C_{33}H_{30}N_4O_2$	513.2295	144701-48-4	65999
thioctic acid	$C_8H_{14}O_2S_2$	205.0362	62-46-4	6112
thiodiacetic acid	$C_4H_6O_4S$	148.9914	123-93-3	31277
thiopental	$C_{11}H_{18}N_2O_2S$	241.1016	76-75-5	3000715
thiosalicylic acid	$C_7H_6O_2S$	153.0015	147-93-3	5443
thymol blue	$C_{27}H_{30}O_5S$	465.1741	76-61-9	65565
tolmetin	$C_{15}H_{15}NO_3$	256.0979	26171-23-3	5509
topiramate	$C_{12}H_{21}NO_8S$	338.0915	97240-79-4	5284627
tranexamic acid	$C_8H_{15}NO_2$	156.1030	1197-18-8	5526
7-hydroxycoumarine	$C_9H_6O_3$	161.0244	93-35-6	5281426
ursodeoxycholic acid	$C_{24}H_{40}O_4$	391.2853	128-13-2	31401
valsartan	$C_{24}H_{29}N_5O_3$	434.2197	137862-53-4	60846
vinbarbital	$C_{11}H_{16}N_2O_3$	223.1088	125-42-8	5284636
tartaric acid	$C_4H_6O_6$	149.0091	87-69-4	875
xylitol	$C_5H_{12}O_5$	151.0611	87-99-0	6912
cinnamic acid	$C_9H_8O_2$	147.0451	621-82-9	444539
citric acid	$C_6H_8O_7$	191.0197	77-92-9	311
2-nitramidobenzoic acid	$C_7H_6N_2O_4$	181.0254		21544119