

Supplementary Information for

A strategic screening approach to identify transformation products of organic micropollutants formed in natural waters

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Post-acquisition data processing

Post-acquisition data processing was carried out for the identification of target compounds and the structural characterization of non-target and unknown polar compounds. Data obtained with LC-ESI-QToF/MS were processed with the PeakView software (AB Sciex), which incorporates tools to display, filter, and process data-dependent MSⁿ acquisition (IDA), along with XIC Manager and MS Library tools. XIC Manager and the MS library were used for rapid screening and identification of target compounds and for other compounds not included a priori in the analytical method (considered as non-target compounds in this study). The library of accurate mass information from AB Sciex was utilized, which includes approx. 3000 compounds (mainly pesticides and pharmaceuticals). In addition to this, a new library database containing both ToF MS and MS/MS spectra of 65 target compounds (see Table S1) was made at CE (-)35±15 eV and used for confirming the detected parent compounds in this study.

Confirmation of target analytes was based on the retention time, the accurate mass measurement of the molecular ion (mass error), the isotopic pattern and by automatic MS/MS library search. For the positive identification of the target compounds with the automatic search, the following values were selected: retention time ± 0.5 min, isotope score >90%, library score >70%, mass error <5 ppm and mass error score >90%. The default threshold for the XIC (extracted ion chromatogram) was 1000 cps, S/N <5 and peaks >500 counts. For the identification of non-target analytes included in the commercial library the same criteria were used, except for the retention time. The confirmation of non-target analytes and structural characterization of unknown analytes (analytes not included in the MS/MS libraries) was performed using the PeakView software and the Formula Finder tool and based on the accurate mass measurement (mass error <5 ppm), elemental composition assignment, isotopic pattern distribution, ring and double bonds (RDB) factor and MS/MS spectrum interpretation. This data processing includes the matching of the experimental MS/MS spectrum with a list of theoretical fragment masses which was performed by applying a mass tolerance threshold lower than 20 ppm.

List of target analytes

Table S1. Summary of target analytes used for confirmation of the presence of parent compounds.

Target analyte	Classification	Molecular formula	CAS #	Molecular weight	logK _{ow} ^a
Positive					
3,4 Dichloro Aniline	transferases enzyme	C6H5Cl2N	95-76-1	160.9799	2.35
Ametryn	methylthiotriazine herbicide	C9H17N5S	834-12-8	227.1205	2.60
Asulam	herbicide	C8H10N2O4S	3337-71-1	230.0361	0.08
Atenolol	beta-blocker	C14H22N2O3	29122-68-7	266.1630	0.43
Atorvastatin	statins	C33H35FN2O5	134523-00-5	558.2530	5.39
Atrazine	triazine herbicide	C8H14ClN5	1912-24-9	215.0938	2.20
Bromacil	herbicide	C9H13BrN2O2	314-40-9	260.0160	2.51
Caffeine	stimulant	C8H10N4O2	58-08-2	194.0804	-0.55
Carbamazepine	anticonvulsant	C15H12N2O	298-46-4	236.0950	2.77
Carbofuran	carbamate pesticide	C12H15NO3	1563-66-2	221.1052	2.05
Citalopram	antidepressant	C20H21FN2O	59729-33-8	324.1638	3.76
Clopyralid	herbicide	C6H3Cl2NO2	1702-17-6	190.9541	2.23
Codeine	opioid pain relief	C18H21NO3	76-57-3	299.1521	1.34
DEET	insect repellent	C12H17NO	134-62-3	191.1310	2.50
Desethyl Atrazine	Personal Herbicides	C6H10N5Cl	6190-65-4	187.0625	1.54
Desisopropyl Atrazine	triazine herbicide	C5H8ClN5	1007-28-9	173.0468	1.12
Desmethyl Citalopram	antidepressant	C19H19FN2O	144010-85-5	346.1248	3.38
Desmethyldiazepam	anticonvulsant	C15H11ClN2O	1088-11-5	270.0560	3.21
Diazinon	organophosphate insecticide	C12H21N2O3PS	333-41-5	304.1011	4.19
Dichlorvos	organophosphate insecticide	C4H7Cl2O4P	62-73-7	219.9459	1.37
Diuron	herbicide	C9H10Cl2N2O	330-54-1	232.0170	2.53
Fenamiphos	insecticide	C13H22NO3PS	22224-92-6	303.1058	3.31
Fluometuron	herbicide	C10H11F3N2O	2164-17-2	232.0823	2.20
Fluoxetine	antidepressant	C17H18F3NO	54910-89-3	309.1340	4.17
Fluroxypyr	herbicide	C7H5Cl2FN2O3	69377-81-7	253.9661	1.59
Gabapentin	anticonvulsant	C9H17NO2	60142-96-3	171.1259	-1.27
Hexazinone	herbicide	C12H20N4O2	51235-04-2	252.1586	1.37
Imazapic	herbicide	C14H17N3O3	104098-48-8	275.1270	1.83
Imazethapyr	pesticide	C15H19N3O3	81335-77-5	289.1426	2.28
Imidacloprid	insecticide	C9H10ClN5O2	138261-41-3	255.0523	-0.59
Iopromide	X-ray contrast agent	C18H24I3N3O8	73334-07-3	790.8698	-0.44
Malathion	organophosphate insecticide	C10H19O6PS2	121-75-5	330.0361	1.86
Methiocarb	insecticide	C11H15NO2S	2032-65-7	225.0823	3.13
Methomyl	carbamate insecticide	C5H10N2O2S	16752-77-5	162.0463	0.72
Metolachlor	herbicide	C15H22ClNO2	51218-45-2	283.1339	3.45
Metribuzin	herbicide	C8H14N4OS	21087-64-9	214.0888	1.96
Metsulfuron-Methyl	sulfonylurea herbicide	C14H15N5O6S	74223-64-6	381.0743	1.84
Naproxen	anti-inflammatory drug	C14H14O3	22204-53-1	230.0943	2.99
Paracetamol	aniline analgesics	C8H9NO2	103-90-2	151.0633	0.91
Picloram	herbicide	C6H3Cl3N2O2	6607	239.9260	2.00

Prometryn	triazine pesticide	C10H19N5S	7287-19-6	241.1361	3.01
Propiconazole	triazole fungicide	C15H17Cl2N3O2	60207-90-1	341.0698	4.33
Propoxur	carbamate insecticide	C11H15NO3	114-26-1	209.1052	2.09
Simazine	triazine herbicide	C7H12ClN5	122-34-9	201.0781	1.78
Tebuconazole	fungicide	C16H22ClN3O	107534-96-3	307.1451	3.69
Tebuthiuron	herbicide	C9H16N4OS	34014-18-1	228.1045	1.35
Temazepam	psychoactive drug	C16H13ClN2O2	846-50-4	300.0666	2.79
Terbuthylazine-desethyl	herbicide	C7H12ClN5	5915-41-3	201.0781	1.82
Terbuthylazine	pesticide	C9H16ClN5	30125-63-4	229.1094	2.48
Terbutryn	herbicide	C10H19N5S	886-50-0	241.1361	2.88
Tramadol	opioid pain relief	C16H25NO2	27203-92-5	263.1885	2.45
Venlafaxine	antidepressant	C17H27NO2	93413-69-5	277.2042	2.74
Negative					
2,4-D	herbicide	C8H6Cl2O3	94-75-7	219.9694	2.50
2,4,5-T	herbicide	C8H5Cl3O3	93-76-5	253.9304	3.11
Acesulfame	artificial sweetener	C4H5NO4S	33665-90-6	162.9939	-0.55
Bromoxynil	nitrile herbicide	C7H3Br2NO	1689-84-5	274.8581	3.06
Dicamba	herbicide	C8H6Cl2O3	1918-00-9	219.9694	2.68
Furosemide	diuretic	C12H11ClN2O5S	54-31-9	330.0077	1.75
Haloxyfop	phenoxy herbicide	C15H11ClF3NO4	69806-34-4	361.0329	4.22
Hydrochlorothiazide	diuretic	C7H8ClN3O4S2	58-93-5	296.9645	-0.58
Ibuprofen	anti-inflammatory drug	C13H18O2	15687-27-1	206.1307	3.84
MCPA	herbicide	C9H9ClO3	94-74-6	200.0240	2.41
Mecoprop	herbicide	C10H11ClO3	7085-19-0	214.0397	2.98
Triclopyr	herbicide	C7H4Cl3NO3	55335-06-3	254.9257	2.70
Triclosan	consumer product	C12H7Cl3O2	3380-34-5	287.9512	4.98

^a logK_{OW} values were obtained from <http://www.chemicalize.com> on January 26, 2017.

Detection of target analytes in the studied river

Acetaminophen from fyris_u

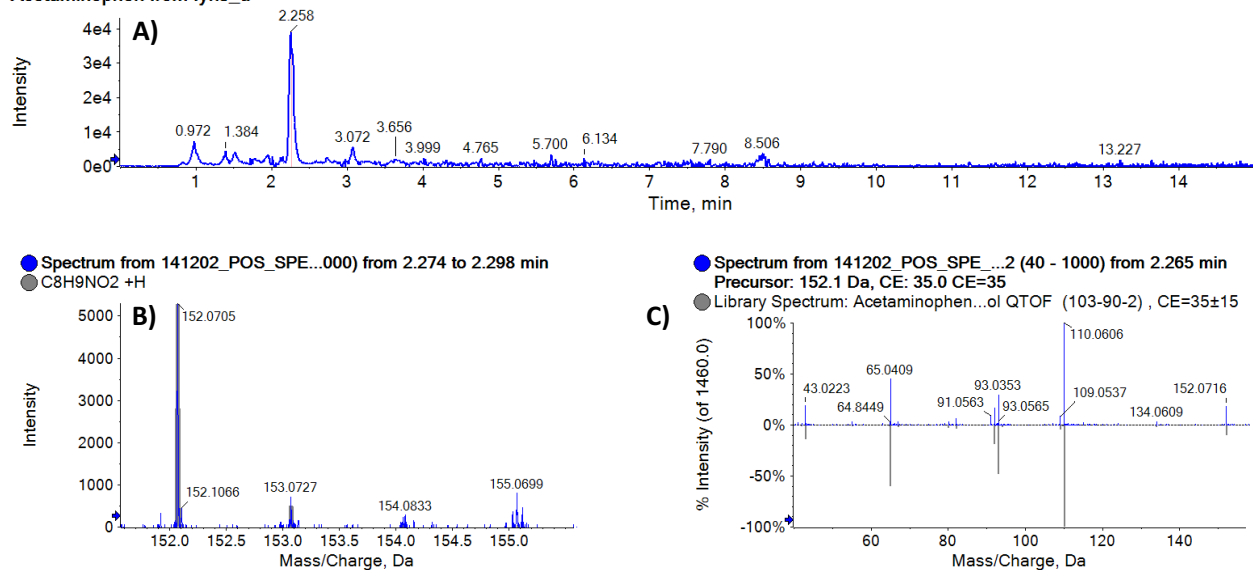


Figure S1. Detection of acetaminophen in river FY (RT = 2.26 min): A) extracted ion chromatogram, B) HR-MS spectra of the molecular ion with its isotope pattern, and C) comparison between the detected fragments of the precursor ion of 152.0705 and the HR-MS/MS spectra recorded in the library.

Carbamazepine from fyris_u

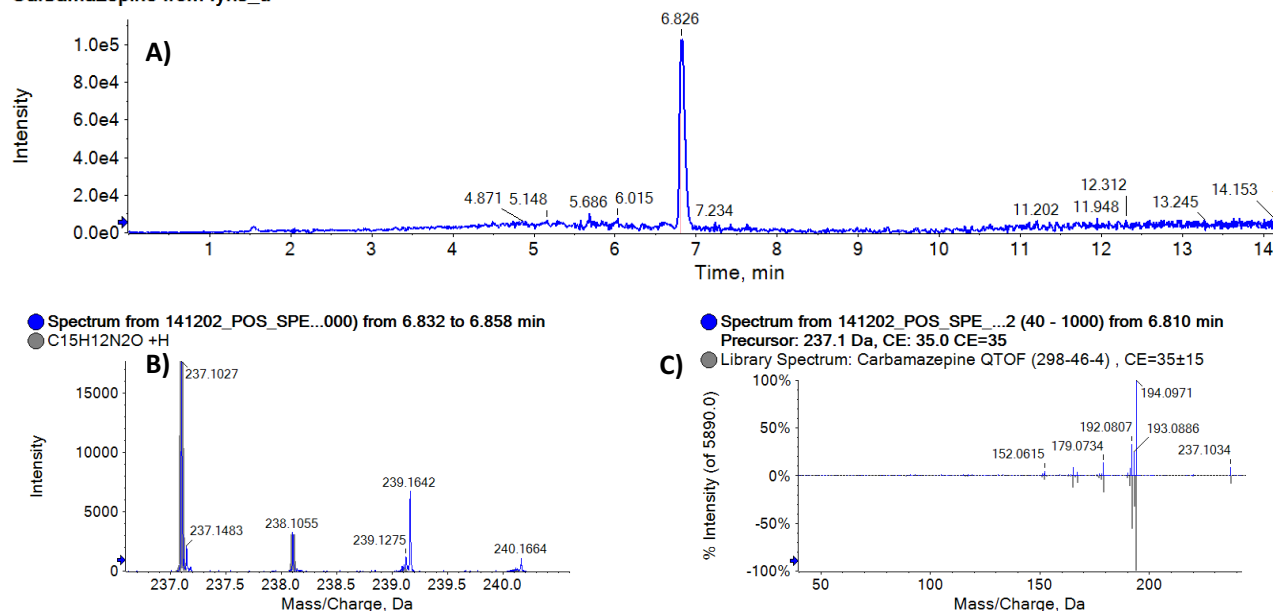


Figure S2. Detection of carbamazepine in river FY (RT = 6.83 min): A) extracted ion chromatogram, B) HR-MS spectra of the molecular ion with its isotope pattern, and C) comparison between the detected fragments of the precursor ion of 237.1027 and the HR-MS/MS spectra recorded in the library.

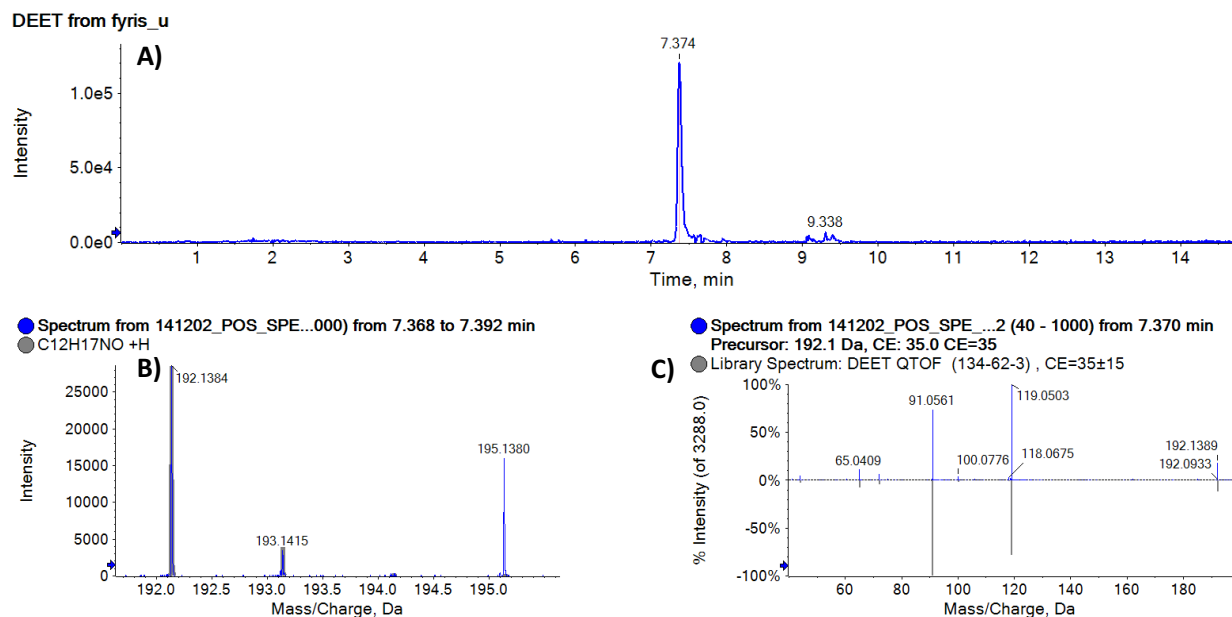


Figure S3. Detection of DEET in river FY (RT = 7.37 min): A) extracted ion chromatogram, B) HR-MS spectra of the molecular ion with its isotope pattern, and C) comparison between the detected fragments of the precursor ion of 192.1384 and the HR-MS/MS spectra recorded in the library.

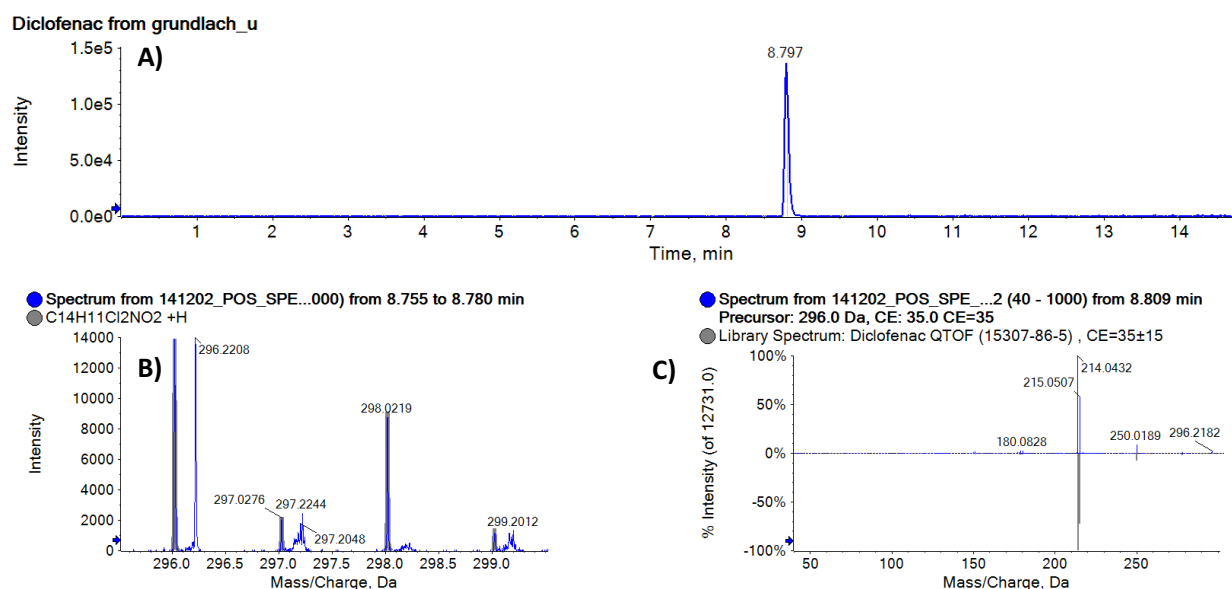


Figure S4. Detection of diclofenac in river GR (RT = 8.80 min): A) extracted ion chromatogram, B) HR-MS spectra of the molecular ion with its isotope pattern, and C) comparison between the detected fragments of the precursor ion of 296.0240 and the HR-MS/MS spectra recorded in the library.

Furosemide QTOF from fysis_u

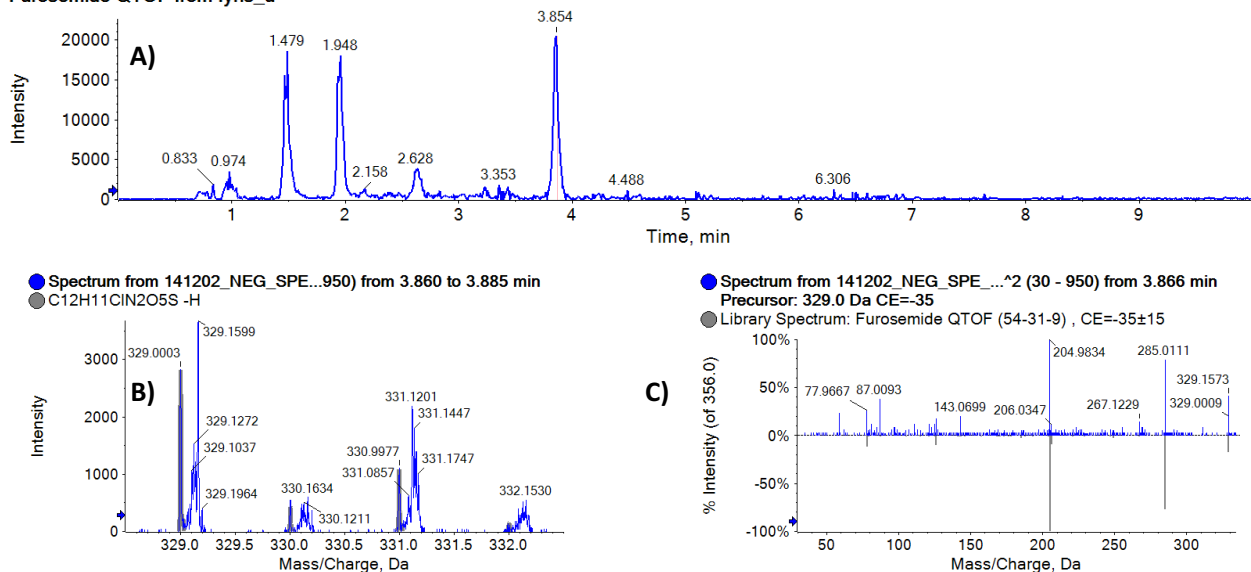


Figure S5. Detection of furosemide in river FY (RT = 3.85 min): A) extracted ion chromatogram, B) HR-MS spectra of the molecular ion with its isotope pattern, and C) comparison between the detected fragments of the precursor ion of 329.0003 and the HR-MS/MS spectra recorded in the library.

Gabapentin from fysis_u

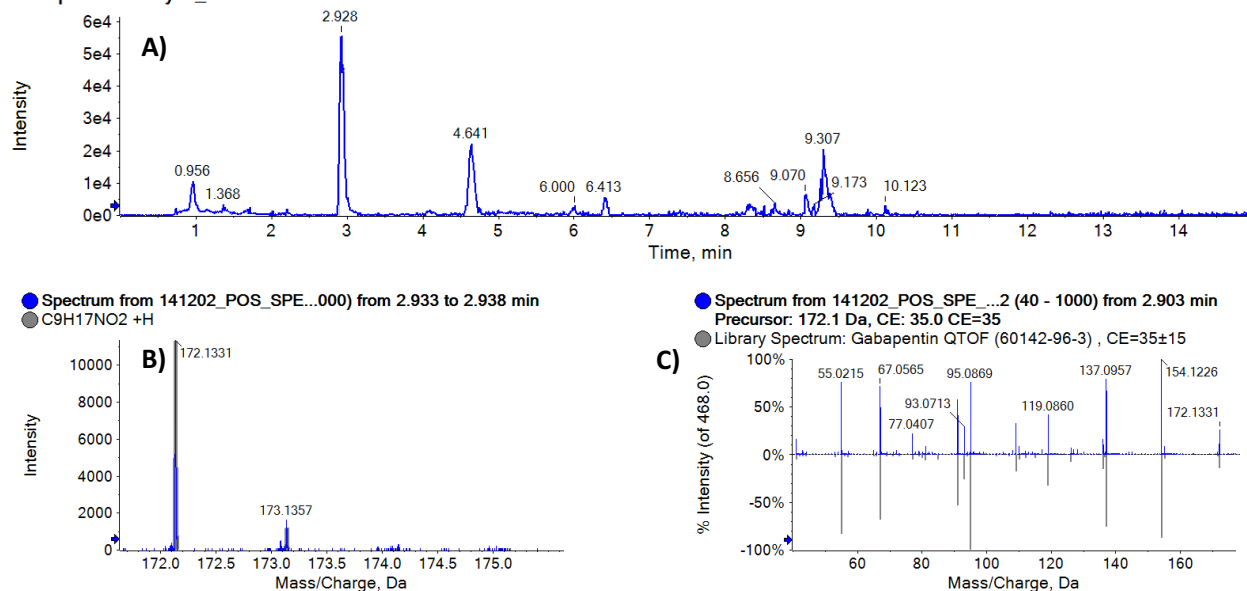


Figure S6. Detection of gabapentin in river FY (RT = 2.93 min): A) extracted ion chromatogram, B) HR-MS spectra of the molecular ion with its isotope pattern, and C) comparison between the detected fragments of the precursor ion of 172.1331 and the HR-MS/MS spectra recorded in the library.

Hydrochlorothiazide from fyris_u

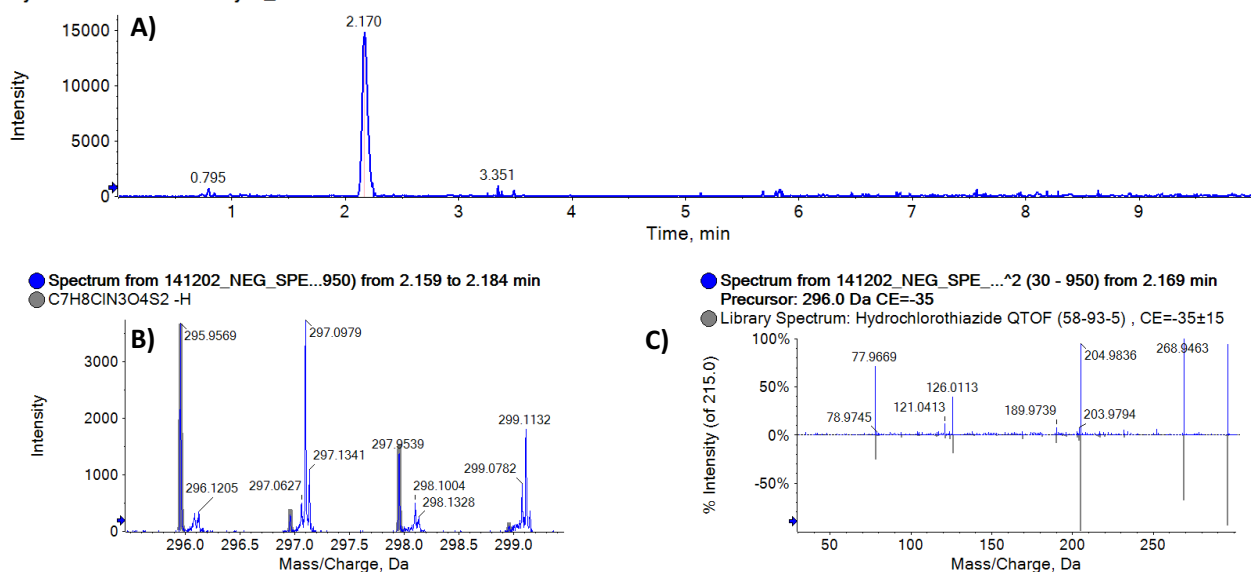


Figure S7. Detection of hydrochlorothiazide in river FY (RT = 2.17 min): A) extracted ion chromatogram, B) HR-MS spectra of the molecular ion with its isotope pattern, and C) comparison between the detected fragments of the precursor ion of 295.9569 and the HR-MS/MS spectra recorded in the library.

Sulfamethoxazole from grundlach_u

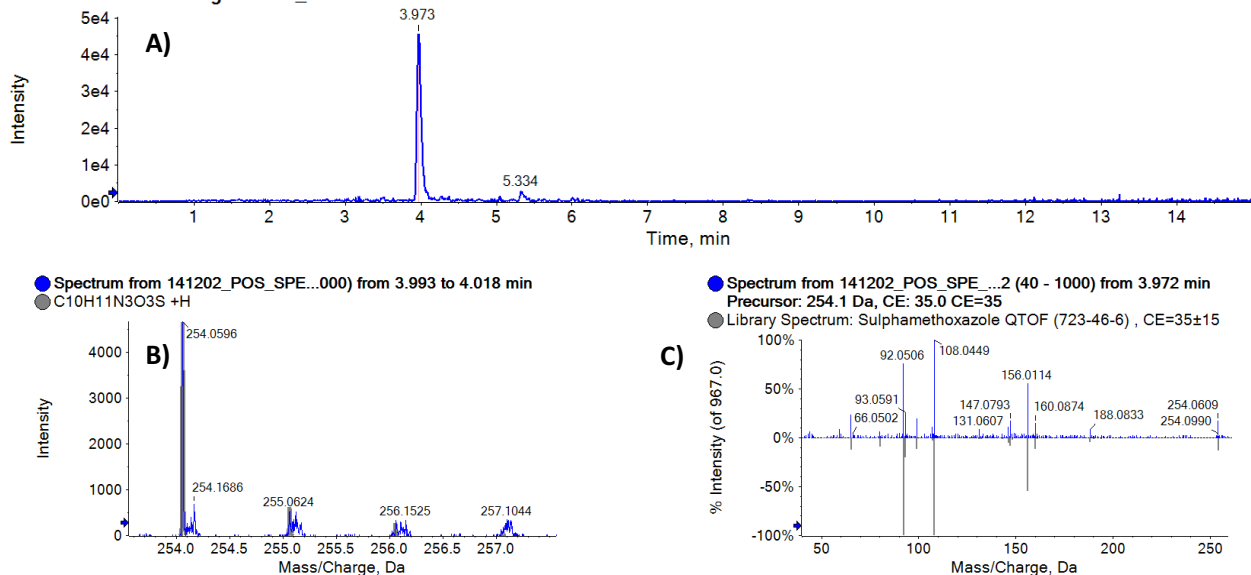


Figure S8. Detection of sulfamethoxazole in river GR (RT = 3.97 min): A) extracted ion chromatogram, B) HR-MS spectra of the molecular ion with its isotope pattern, and C) comparison between the detected fragments of the precursor ion of 254.0596 and the HR-MS/MS spectra recorded in the library.

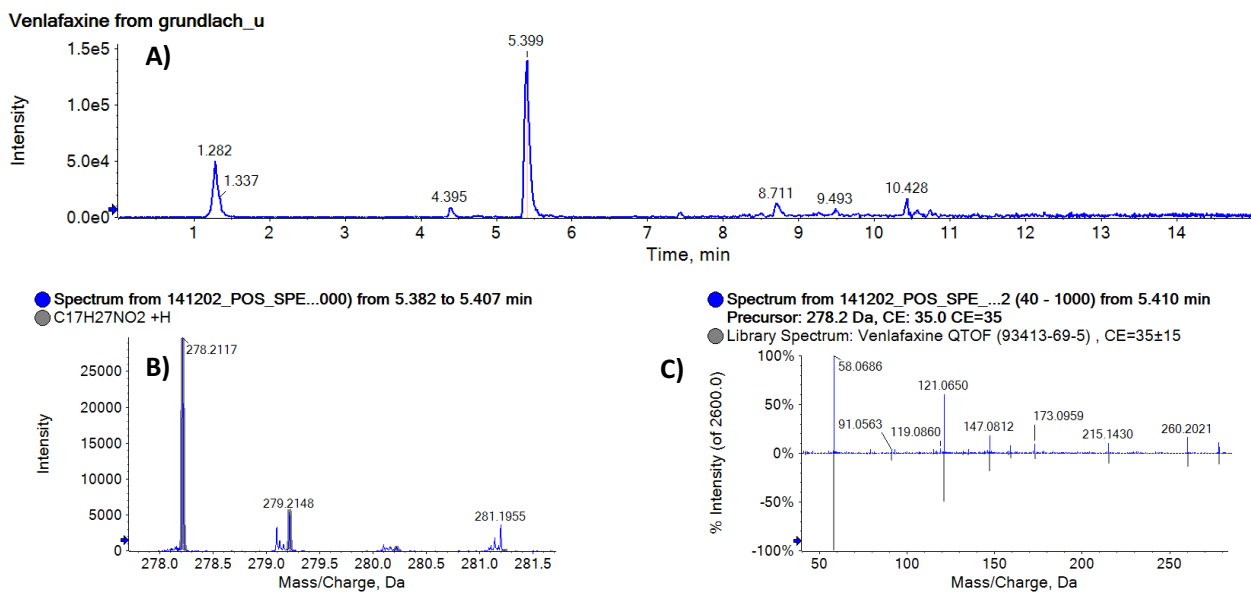


Figure S9. Detection of venlafaxine in river GR (RT = 5.40 min): A) extracted ion chromatogram, B) HR-MS spectra of the molecular ion with its isotope pattern, and C) comparison between the detected fragments of the precursor ion of 278.2117 and the HR-MS/MS spectra recorded in the library.

Structural elucidation of TP benzamide identified and confirmed in river GR

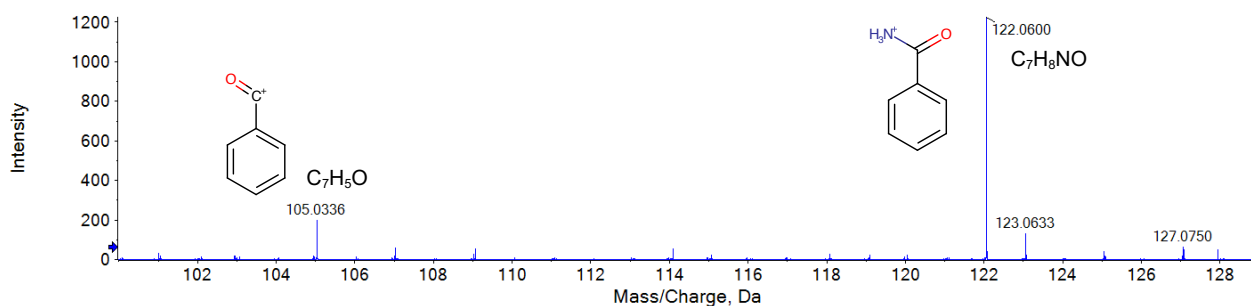


Figure S10. HR-MS/MS spectra of benzamide detected in river GR. The fragment structure was proposed by MetFrag.

Table S2. Complete list of transformation products (TPs) predicted from the EAWAG-BBD Pathway Prediction System for the parent compounds and used for TP screening in the study.

Predicted transformation product	SMILES	Molecular formula	Exact mass
8-Hydroxyquinoline_TP1	<chem>OC1=CC=C2C=CC=NC2=C1O</chem>	C9H7NO2	161.0477
8-Hydroxyquinoline_TP2	<chem>[O-]C(=O)C=Cc1cccnc1C([O-])=O</chem>	C9H7NO4	193.0375
8-Hydroxyquinoline_TP3	<chem>Oc1cc(C=CC([O-])=O)c(nc1O)C([O-])=O</chem>	C9H7NO6	225.0273
8-Hydroxyquinoline_TP4	<chem>OC(CC([O-])=O)c1cccnc1C([O-])=O</chem>	C9H9NO5	211.0481
8-Hydroxyquinoline_TP5	<chem>[O-]C(=O)CCc1cccnc1C([O-])=O</chem>	C9H9NO4	195.0532
acetaminophen_TP1	<chem>Nc1ccc(O)cc1</chem>	C6H7NO	109.0528
acetaminophen_TP2	<chem>Oc1ccc(O)cc1</chem>	C6H6O2	110.0368
acetaminophen_TP3	<chem>[O-]C(=O)CC(=O)C=CC([O-])=O</chem>	C6H6O5	158.0215
bezafibrate_TP4	<chem>CC(C)Oc1ccc(CCNC(=O)c2ccc(Cl)cc2)cc1</chem>	C7H6ClNO	155.0138
bezafibrate_TP1	<chem>[O-]C(=O)c1ccc(Cl)cc1</chem>	C18H20ClNO2	317.1183
bezafibrate_TP2	<chem>CC(C)(Oc1ccc(CCN)cc1)C([O-])=O</chem>	C7H5ClO2	155.9978
bezafibrate_TP3	<chem>NC(=O)c1ccc(Cl)cc1</chem>	C12H17NO3	223.1208
bezafibrate_TP5	<chem>CC(C)(Oc1ccc(CC=O)cc1)C([O-])=O</chem>	C12H14O4	222.0892
bezafibrate_TP6	<chem>CC(C)(Oc1ccc(CCNC(=O)c2ccccc2)cc1)C([O-])=O</chem>	C19H21NO4	327.1471
bezafibrate_TP7	<chem>CC(CC([O-])=O)Oc1ccc(CCNC(=O)c2ccc(Cl)cc2)cc1</chem>	C19H20ClNO4	361.1081
bezafibrate_TP8	<chem>Oc1ccc(CCNC(=O)c2ccc(Cl)cc2)cc1</chem>	C15H14ClNO2	275.0713
bezafibrate_TP9	<chem>CC(C)Oc1ccc(CCN)cc1</chem>	C11H17NO	179.1310
bezafibrate_TP10	<chem>CC(C)Oc1ccc(CCNC(=O)c2ccccc2)cc1</chem>	C18H21NO2	283.1572
bezafibrate_TP11	<chem>CC(C)Oc1ccc(CC=O)cc1</chem>	C11H14O2	178.0994
bezafibrate_TP12	<chem>CC(C)(Oc1ccc(CCN)c(O)c1O)C([O-])=O</chem>	C12H17NO5	255.1107
bezafibrate_TP13	<chem>CC(CC([O-])=O)Oc1ccc(CCN)cc1</chem>	C12H17NO3	223.1208
bezafibrate_TP14	<chem>CC(C)(Oc1ccc(CCN)cc1)C([O-])=O</chem>	C12H17NO3	223.1208
bezafibrate_TP15	<chem>CC(CO)(Oc1ccc(CCNC(=O)c2ccccc2)cc1)C([O-])=O</chem>	C19H21NO5	343.1420
bezafibrate_TP16	<chem>CC(CC([O-])=O)Oc1ccc(CCNC(=O)c2ccccc2)cc1</chem>	C19H21NO4	327.1471
bezafibrate_TP17	<chem>CC(C)Oc1ccc(CC([O-])=O)cc1</chem>	C11H14O3	194.0943
bezafibrate_TP18	<chem>[O-]C(=O)c1ccccc1</chem>	C7H6O2	122.0368
bezafibrate_TP19	<chem>Oc1ccc(cc1)C([O-])=O</chem>	C7H6O3	138.0317
bezafibrate_TP20	<chem>NC(=O)c1ccccc1</chem>	C7H7NO	121.0528
bezafibrate_TP21	<chem>Oc1ccc(CC=O)cc1</chem>	C8H8O2	136.0524
bezafibrate_TP22	<chem>Oc1ccc(CCNC(=O)c2ccccc2)cc1</chem>	C15H15NO2	241.1103
bezafibrate_TP23	<chem>Oc1ccc(Cl)cc1O</chem>	C6H5ClO2	143.9978
bezafibrate_TP24	<chem>NCCc1ccc(O)cc1</chem>	C8H11NO	137.0841
bezafibrate_TP25	<chem>[O-]C(=O)C=CC(Cl)=CC([O-])=O</chem>	C6H5ClO4	175.9876
bezafibrate_TP26	<chem>[O-]C(=O)C(=O)CC(Cl)=C</chem>	C5H5ClO3	147.9927
bezafibrate_TP27	<chem>[O-]C(=O)C(=O)CC=CCl</chem>	C5H5ClO3	147.9927
bezafibrate_TP28	<chem>Oc1ccccc1O</chem>	C6H6O2	110.0368
bezafibrate_TP29	<chem>Oc1ccc(cc1O)C([O-])=O</chem>	C7H6O4	154.0266
bezafibrate_TP30	<chem>Oc1cccc(C([O-])=O)c1O</chem>	C7H6O4	154.0266
bezafibrate_TP31	<chem>[O-]C(=O)CC=CCC([O-])=O</chem>	C6H8O4	144.0423
bezafibrate_TP32	<chem>[O-]C(=O)C1=CCCC=C1</chem>	C7H8O2	124.0524
bezafibrate_TP33	<chem>CC(C)(OC(=CC=C(CCN)C([O-])=O)C([O-])=O)C([O-])=O</chem>	C12H17NO7	287.1005
bezafibrate_TP34	<chem>NCCC(C=CC([O-])=O)C(=O)C([O-])=O</chem>	C8H11NO5	201.0637

bezafibrate_TP35	CC(C)(O)C([O-])=O	C4H9O3	105.0552
bezafibrate_TP36	CC(CC([O-])=O)Oc1ccc(CCN)c(O)c1O	C12H17NO5	255.1107
bezafibrate_TP37	CC(C)(Oc1ccc(CC=O)c(O)c1O)C([O-])=O	C12H14O6	254.0790
bezafibrate_TP38	CC(C)(Oc1ccc(CC([O-])=O)cc1)C([O-])=O	C12H14O5	238.0841
bezafibrate_TP39	CC(=O)CC([O-])=O	C4H6O3	102.0317
bezafibrate_TP40	CC(CC([O-])=O)Oc1ccc(CC=O)cc1	C12H14O4	222.0892
bezafibrate_TP41	CC(C)(Oc1ccc(CC([O-])=O)c(O)c1O)C([O-])=O	C12H14O7	270.0740
bezafibrate_TP42	CC(C)(Oc1ccc(cc1)C(O)C([O-])=O)C([O-])=O	C12H14O6	254.0790
bezafibrate_TP43	CC(CC([O-])=O)Oc1ccc(CC([O-])=O)cc1	C12H14O5	238.0841
bezafibrate_TP44	CC(Oc1ccc(CCN(C(=O)c2ccccc2)cc1)(C=O)C([O-])=O	C19H19NO5	341.1263
bezafibrate_TP45	CC(CO)(Oc1ccc(CCN)cc1)C([O-])=O	C12H17NO4	239.1158
bezafibrate_TP46	CC(CO)(Oc1ccc(CC=O)cc1)C([O-])=O	C12H14O5	238.0841
bicalutamide_TP1	C[C@](O)(CS(=O)(=O)c1ccc(F)cc1)C(=O)Nc1ccc(C([O-])=O)c(c1)C(F)(F)F	C18H15F4NO6S	449.0556
bicalutamide_TP2	Oc1cc(C#N)c(cc1O)C(F)(F)F	C8H4F3NO2	203.0194
bicalutamide_TP3	C[C@](O)(CS(=O)(=O)c1ccc(F)cc1)C(N)=O	C8H4F3NO2	203.0194
bicalutamide_TP4	C[C@](O)(CS(=O)(=O)c1ccc(F)cc1)C([O-])=O	C10H11FO5S	262.0311
bicalutamide_TP5	Nc1ccc(C#N)c(c1)C(F)(F)F	C8H5F3N2	186.0405
bicalutamide_TP6	C[C@](O)(CS(=O)(=O)c1ccc(F)cc1)C(=O)Nc1ccc(O)c(c1)C(F)(F)F	C17H15F4NO5S	421.0607
bicalutamide_TP7	Oc1ccc(C#N)c(c1O)C(F)(F)F	C8H4F3NO2	203.0194
bicalutamide_TP8	Nc1ccc(C([O-])=O)c(c1)C(F)(F)F	C8H6F3NO2	205.0351
bicalutamide_TP9	C[C@](O)(CS(=O)(=O)c1ccc(F)c(O)c1O)C([O-])=O	C10H11FO7S	294.0210
bicalutamide_TP10	C[C@H](O)(CS(=O)(=O)c1ccc(F)cc1	C9H11FO3S	218.0413
bicalutamide_TP11	Oc1cc(C([O-])=O)c(cc1O)C(F)(F)F	C8H5F3O4	222.0140
bicalutamide_TP12	[O-]C(=O)C(=O)CC(=CC#N)C(F)(F)F	C7H4F3NO3	207.0143
bicalutamide_TP13	Nc1ccc(O)c(c1)C(F)(F)F	C7H6F3NO	177.0401
bicalutamide_TP14	[O-]C(=O)C(=O)CC(=CC(F)(F)F)C#N	C7H4F3NO3	207.0143
bicalutamide_TP15	Oc1cc(O)c(cc1O)C(F)(F)F	C7H5F3O3	194.0191
bicalutamide_TP16	[O-]C(=O)C=CC(C#N)=C(C([O-])=O)C(F)(F)F	C8H4F3NO4	235.0092
bicalutamide_TP17	Oc1ccc(C([O-])=O)c(c1O)C(F)(F)F	C8H5F3O4	222.0140
bicalutamide_TP18	[O-]C(=O)C(=O)CC=CC#N	C6H5NO3	139.0269
bicalutamide_TP19	[O-]C(=O)C(=O)C(C(=C)C#N)C(F)(F)F	C7H4F3NO3	207.0143
bicalutamide_TP20	Oc1ccc(O)c(c1O)C(F)(F)F	C7H5F3O3	194.0191
bicalutamide_TP21	OC(C=CC([O-])=O)=C(C([O-])=O)C(F)(F)F	C7H5F3O5	226.0089
bicalutamide_TP22	OC(=C)C(C(=O)C([O-])=O)C(F)(F)F	C6H5F3O4	198.0140
bicalutamide_TP23	CC(C#N)C(C(=O)C([O-])=O)C(F)(F)F	C7H6F3NO3	209.0300
bicalutamide_TP24	[O-]C(=O)C(=O)CC(F)(F)F	C4H3F3O3	156.0034
bicalutamide_TP25	[O-]C(=O)C(=O)CCCC#N	C6H7NO3	141.0426
bicalutamide_TP26	[O-]C(=O)C(=C)C(C(=O)C([O-])=O)C(F)(F)F	C7H5F3O5	226.0089
bicalutamide_TP27	[O-]C(=O)C=CCC(=O)C([O-])=O	C6H6O5	158.0215
bicalutamide_TP28	[O-]C(=O)C=CC(C([O-])=O)=C(C([O-])=O)C(F)(F)F	C8H5F3O6	254.0038
bicalutamide_TP29	[O-]C(=O)C=CC(C#N)C(C([O-])=O)C(F)(F)F	C8H6F3NO4	237.0249
bicalutamide_TP30	[O-]C(=O)CCC(C#N)=C(C([O-])=O)C(F)(F)F	C8H6F3NO4	237.0249
bicalutamide_TP31	OC(CC(=O)C([O-])=O)=CC(F)(F)F	C6H5F3O4	198.0140
bicalutamide_TP32	[O-]C(=O)C(=O)CC(CC(F)(F)F)C#N	C7H6F3NO3	209.0300
bicalutamide_TP33	FC(F)(F)CC(=O)C#N	C4H2F3NO	137.0088
bicalutamide_TP34	Oc1ccc(O)c(c1)C(F)(F)F	C7H5F3O2	178.0242

bicalutamide_TP35	[O-]C(=O)C(=O)CC(CC#N)C(F)(F)F	C7H6F3NO3	209.0300
bicalutamide_TP36	[O-]C(=O)C(=O)CC(=CC(F)(F)F)C([O-])=O	C7H5F3O5	226.0089
bicalutamide_TP37	FC(F)(F)C(=O)CC#N	C4H2F3NO	137.0088
bicalutamide_TP38	[O-]C(=O)C=C(CC(=O)C([O-])=O)C(F)(F)F	C7H5F3O5	226.0089
bicalutamide_TP39	CC(=O)CS(=O)(=O)c1ccc(F)cc1	C9H9FO3S	216.0256
bicalutamide_TP40	C[C@H](O)CS(=O)(=O)c1ccc(F)c(O)c1O	C9H11FO5S	250.0311
bicalutamide_TP41	C[C@](O)(CS(=O)(=O)C(=CC=C(F)C([O-])=O)C([O-])=O)C([O-])=O	C10H11FO9S	326.0108
bisoprolol_TP1	CC(C)OCCOCc1ccc(OCC(O)CN)cc1	C15H25NO4	283.1784
bisoprolol_TP2	CC(C)OCCOCc1ccc(OCC(O)C=O)cc1	C15H22O5	282.1467
bisoprolol_TP3	CC(C)NCC(=O)COc1ccc(COCCOC(C)C)cc1	C18H29NO4	323.2097
bisoprolol_TP4	CC(C)OCCOCc1ccc(O)cc1	C12H18O3	210.1256
bisoprolol_TP5	CC(C)NCC(O)C=O	C6H13NO2	131.0946
bisoprolol_TP6	CC(C)OCCO	C5H12O2	104.0837
bisoprolol_TP7	CC(C)NCC(O)COc1ccc(C=O)cc1	C13H19NO3	237.1365
bisoprolol_TP8	CC(C)NCC(O)COc1ccc(CO)cc1	C13H21NO3	239.1521
bisoprolol_TP9	CC(C)OCC=O	C5H10O2	102.0681
bisoprolol_TP10	CC(C)NCC(O)COc1ccc(COCC=O)cc1	C15H23NO4	281.1627
bisoprolol_TP11	CC(C)NCC(O)COc1ccc(COCCO)cc1	C15H25NO4	283.1784
bisoprolol_TP12	CC(C)NC(O)CCOc1ccc(COCCOC(C)C)cc1	C15H25NO4	283.1784
bisoprolol_TP13	CC(C)OCCOCc1ccc(OCC(=O)CN)cc1	C15H23NO4	281.1627
bisoprolol_TP14	NCC(O)COc1ccc(COCCO)cc1	C12H19NO4	241.1314
bisoprolol_TP15	NCC(O)COc1ccc(COCC=O)cc1	C12H17NO4	239.1158
bisoprolol_TP16	NCC(O)COc1ccc(CO)cc1	C10H15NO3	197.1052
bisoprolol_TP17	NCC(O)COc1ccc(C=O)cc1	C10H13NO3	195.0895
bisoprolol_TP18	CC(C)OCCOCc1ccc(OCCC(N)O)cc1	C15H25NO4	283.1784
bisoprolol_TP19	CC(C)OCCOCc1ccc(OCC(O)C([O-])=O)cc1	C15H22O6	298.1416
bisoprolol_TP20	CC(C)NCC(=O)COc1ccc(COCC=O)cc1	C15H21NO4	279.1471
bisoprolol_TP21	CC(C)OCCOCc1ccc(OCC(=O)C=O)cc1	C15H20O5	280.1311
bisoprolol_TP22	CC(C)NCC(=O)C=O	C6H11NO2	129.0790
bisoprolol_TP23	Oc1ccc(COCC=O)cc1	C9H10O3	166.0630
bisoprolol_TP24	CC(C)NCC(=O)COc1ccc(COCCO)cc1	C15H23NO4	281.1627
bisoprolol_TP25	OCCOCc1ccc(O)cc1	C9H12O3	168.0786
bisoprolol_TP26	CC(C)NCC(O)C([O-])=O	C6H13NO3	147.0895
bisoprolol_TP27	CC(C)NCC(=O)COc1ccc(C=O)cc1	C13H17NO3	235.1208
bisoprolol_TP28	Oc1ccc(C=O)cc1	C7H6O2	122.0368
bisoprolol_TP29	OCCOCc1ccc(OCC(O)C=O)cc1	C12H16O5	240.0998
bisoprolol_TP30	CC(C)NC(O)CCOc1ccc(COCCO)cc1	C15H25NO4	283.1784
bisoprolol_TP31	OCc1ccc(O)cc1	C7H8O2	124.0524
bisoprolol_TP32	CC(C)NCC(=O)COc1ccc(CO)cc1	C13H19NO3	237.1365
bisoprolol_TP33	OCc1ccc(OCC(O)C=O)cc1	C10H12O4	196.0736
bisoprolol_TP34	CC(C)NC(O)CCOc1ccc(CO)cc1	C13H21NO3	239.1521
bisoprolol_TP35	CC(C)NCC(O)COc1ccc(cc1)C([O-])=O	C13H19NO4	253.1314
bisoprolol_TP36	CC(C)NCC(O)COc1ccc(COCC([O-])=O)cc1	C15H23NO5	297.1576
bisoprolol_TP37	CC(C)OCCOCc1ccc(OCCC=O)cc1	C15H22O4	266.1518
bisoprolol_TP38	NCC(O)COc1ccc(COCC([O-])=O)cc1	C12H17NO5	255.1107
bisoprolol_TP39	NCC(=O)COc1ccc(COCCO)cc1	C12H17NO4	239.1158

bisoprolol_TP40	<chem>NCC(=O)COc1ccc(CO)cc1</chem>	C10H13NO3	195.0895
bisoprolol_TP41	<chem>NCC(=O)COc1ccc(C=O)cc1</chem>	C10H11NO3	193.0739
bisoprolol_TP42	<chem>NCC(=O)COc1ccc(COCC=O)cc1</chem>	C12H15NO4	237.1001
bisoprolol_TP43	<chem>CC(C)OCCOCc1ccc(OCC(=O)C([O-])=O)cc1</chem>	C15H20O6	296.1260
bisoprolol_TP44	<chem>OCCOCc1ccc(OCC(O)C([O-])=O)cc1</chem>	C12H16O6	256.0947
bisoprolol_TP45	<chem>OCc1ccc(OCC(O)C([O-])=O)cc1</chem>	C10H12O5	212.0685
bisoprolol_TP46	<chem>OC(COc1ccc(C=O)cc1)C([O-])=O</chem>	C10H10O5	210.0528
bisoprolol_TP47	<chem>OC(COc1ccc(COCC=O)cc1)C([O-])=O</chem>	C12H14O6	254.0790
bisoprolol_TP48	<chem>CC(C)NCC(=O)COc1ccc(COCC([O-])=O)cc1</chem>	C15H21NO5	295.1420
bisoprolol_TP49	<chem>NC(O)CCOc1ccc(COCCO)cc1</chem>	C12H19NO4	241.1314
bisoprolol_TP50	<chem>CC(C)NCC(=O)C([O-])=O</chem>	C6H11NO3	145.0739
bisoprolol_TP51	<chem>NCC(O)COc1ccc(cc1)C([O-])=O</chem>	C10H13NO4	211.0845
bisoprolol_TP52	<chem>Oc1ccc(COCC([O-])=O)cc1</chem>	C9H10O4	182.0579
bisoprolol_TP53	<chem>OCCOCc1ccc(OCC(=O)C=O)cc1</chem>	C12H14O5	238.0841
bisoprolol_TP54	<chem>CC(C)NC(O)CC([O-])=O</chem>	C6H13NO3	147.0895
bisoprolol_TP55	<chem>CC(C)NCC(=O)COc1ccc(cc1)C([O-])=O</chem>	C13H17NO4	251.1158
bisoprolol_TP56	<chem>OCCOCc1ccc(OCCC=O)cc1</chem>	C12H16O4	224.1049
bisoprolol_TP57	<chem>NC(O)CCOc1ccc(CO)cc1</chem>	C10H15NO3	197.1052
bisoprolol_TP58	<chem>OCc1ccc(OCC(=O)C=O)cc1</chem>	C10H10O4	194.0579
bisoprolol_TP59	<chem>OCc1ccc(OCCC=O)cc1</chem>	C10H12O3	180.0786
bisoprolol_TP60	<chem>OC(COc1ccc(cc1)C([O-])=O)C=O</chem>	C10H10O5	210.0528
bisoprolol_TP61	<chem>CC(C)NC(O)CCOc1ccc(cc1)C([O-])=O</chem>	C13H19NO4	253.1314
bisoprolol_TP62	<chem>OC(COc1ccc(COCC([O-])=O)cc1)C=O</chem>	C12H14O6	254.0790
bisoprolol_TP63	<chem>CC(C)NC(O)CCOc1ccc(COCC([O-])=O)cc1</chem>	C15H23NO5	297.1576
bisoprolol_TP64	<chem>CC(C)OCCOCc1ccc(OCCC([O-])=O)cc1</chem>	C15H22O5	282.1467
cetirizine_TP1	<chem>[O-]C(=O)COCCNCCN(CC=O)C(c1ccccc1)c1ccc(Cl)cc1</chem>	C21H25ClN2O4	404.1503
cetirizine_TP2	<chem>[O-]C(=O)COCCN(CCNC(c1ccccc1)c1ccc(Cl)cc1)CC=O</chem>	C21H25ClN2O4	404.1503
cetirizine_TP3	<chem>[O-]C(=O)COCCN1CCNCC1</chem>	C8H16N2O3	188.1161
cetirizine_TP4	<chem>Clc1ccc(cc1)C(=O)c1ccccc1</chem>	C13H9ClO	216.0342
cetirizine_TP5	<chem>OCCN1CCN(CC1)C(c1ccccc1)c1ccc(Cl)cc1</chem>	C19H23ClN2O	330.1499
cetirizine_TP6	<chem>Clc1ccc(cc1)C(N1CCNCC1)c1ccccc1</chem>	C17H19ClN2	286.1237
cetirizine_TP7	<chem>[O-]C(=O)COCCN1CCN(CC1)C(c1ccccc1)c1ccccc1</chem>	C21H26N2O3	354.1943
cetirizine_TP8	<chem>Clc1ccc(cc1)C(N1CCN(CC=O)CC1)c1ccccc1</chem>	C19H21ClN2O	328.1342
cetirizine_TP9	<chem>NCCN(CC=O)C(c1ccccc1)c1ccc(Cl)cc1</chem>	C17H19ClN2O	302.1186
cetirizine_TP10	<chem>Clc1ccc(cc1)C(NCCNCC=O)c1ccccc1</chem>	C17H19ClN2O	302.1186
cetirizine_TP11	<chem>C1CN(CCN1)C(c1ccccc1)c1ccccc1</chem>	C17H20N2	252.1626
cetirizine_TP12	<chem>Oc1cccc(C(N2CCNCC2)c2ccc(Cl)cc2)c1O</chem>	C17H19ClN2O2	318.1135
cetirizine_TP13	<chem>[O-]C(=O)COCCNCCN(CC([O-])=O)C(c1ccccc1)c1ccc(Cl)cc1</chem>	C21H25ClN2O5	420.1452
cetirizine_TP14	<chem>[O-]C(=O)COCCN(CCNC(c1ccccc1)c1ccc(Cl)cc1)CC([O-])=O</chem>	C21H25ClN2O5	420.1452
cetirizine_TP15	<chem>OCCN1CCNCC1</chem>	C6H14N2O	130.1106
cetirizine_TP16	<chem>O=CCN1CCNCC1</chem>	C6H12N2O	128.0950
cetirizine_TP17	<chem>[O-]C(=O)COCCNCCNCC=O</chem>	C8H16N2O4	204.1110
cetirizine_TP18	<chem>NCCN(CCOCC([O-])=O)CC=O</chem>	C8H16N2O4	204.1110
cetirizine_TP19	<chem>O=C(c1ccccc1)c1ccccc1</chem>	C13H10O	182.0732
cetirizine_TP20	<chem>Oc1cccc(C(=O)c2ccc(Cl)cc2)c1O</chem>	C13H9ClO3	248.0240
cetirizine_TP21	<chem>NCCN(CCO)CC=O</chem>	C6H14N2O2	146.1055

cetirizine_TP22	[O-]C(=O)C(=O)C(C=C)C(=O)c1ccc(Cl)cc1	C12H9ClO4	252.0189
cetirizine_TP23	Oc1cccc(C(=O)c2cccc2)c1O	C13H10O3	214.0630
cetirizine_TP24	[O-]C(=O)C(=O)c1ccc(Cl)cc1	C8H5ClO3	183.9927
cetirizine_TP25	OCCNCCN(CC=O)C(c1cccc1)c1ccc(Cl)cc1	C19H23ClN2O2	346.1448
cetirizine_TP26	OCCN(CCNC(c1cccc1)c1ccc(Cl)cc1)CC=O	C19H23ClN2O2	346.1448
cetirizine_TP27	OCCN1CCN(CC1)C(c1ccc(Cl)cc1)c1cccc(O)c1O	C19H23ClN2O3	362.1397
cetirizine_TP28	OCCN1CCN(CC1)C(c1cccc1)c1cccc1	C19H24N2O	296.1889
cetirizine_TP29	CC(O)N1CCN(CC1)C(c1cccc1)c1ccc(Cl)cc1	C19H23ClN2O	330.1499
cetirizine_TP30	Clc1ccc(cc1)C(N1CCN(CC=O)CC1)c1cccc1	C19H21ClN2O	328.1342
cetirizine_TP31	Clc1ccc(cc1)C(N1CCNCC1)c1cccc1	C17H19ClN2	286.1237
cetirizine_TP32	OCCNCCN(CC=O)C(c1cccc1)c1ccc(Cl)cc1	C19H23ClN2O2	346.1448
cetirizine_TP33	Oc1cccc(C(=O)c2ccc(Cl)cc2)c1O	C13H9ClO3	248.0240
cetirizine_TP34	O=C(c1cccc1)c1cccc1	C13H10O	182.0732
cetirizine_TP35	Oc1cccc(C(NCCNCC=O)c2ccc(Cl)cc2)c1O	C17H19ClN2O3	334.1084
cetirizine_TP36	NCCN(CC=O)C(c1ccc(Cl)cc1)c1cccc(O)c1O	C17H19ClN2O3	334.1084
cetirizine_TP37	[O-]C(=O)C(=O)C(C=C)C(N1CCNCC1)c1ccc(Cl)cc1	C16H19ClN2O3	322.1084
cetirizine_TP38	[O-]C(=O)C(N1CCNCC1)c1ccc(Cl)cc1	C12H15ClN2O2	254.0822
cetirizine_TP39	Oc1cccc(C(N2CCNCC2)c2cccc2)c1O	C17H20N2O2	284.1525
cetirizine_TP40	O=CCNCCNC(c1cccc1)c1cccc1	C17H20N2O	268.1576
cetirizine_TP41	NCCN(CC=O)C(c1cccc1)c1cccc1	C17H20N2O	268.1576
cetirizine_TP42	[O-]C(=O)CNCCNC(c1cccc1)c1ccc(Cl)cc1	C17H19ClN2O2	318.1135
cetirizine_TP43	NCCN(CC([O-])=O)C(c1cccc1)c1ccc(Cl)cc1	C17H19ClN2O2	318.1135
cetirizine_TP44	OCCNCCN(CC([O-])=O)C(c1cccc1)c1ccc(Cl)cc1	C19H23ClN2O3	362.1397
cetirizine_TP45	[O-]C(=O)COCCNCCNC(c1cccc1)c1ccc(Cl)cc1	C19H23ClN2O3	362.1397
cetirizine_TP46	[O-]C(=O)CNCCNCCOCC([O-])=O	C8H16N2O5	220.1059
cetirizine_TP47	[O-]C(=O)CN(CC=O)C(c1cccc1)c1ccc(Cl)cc1	C17H16ClNO3	317.0819
cetirizine_TP48	[O-]C(=O)CNC(c1cccc1)c1ccc(Cl)cc1	C15H14ClNO2	275.0713
cetirizine_TP49	[O-]C(=O)COCCNCC=O	C6H11NO4	161.0688
cetirizine_TP50	[O-]C(=O)COCCNCCN(CC([O-])=O)C(c1cccc1)c1cccc1	C21H26N2O5	386.1842
cetirizine_TP51	[O-]C(=O)CN(CCNC=O)C(c1cccc1)c1ccc(Cl)cc1	C19H21ClN2O3	360.1241
cetirizine_TP52	[O-]C(=O)CNCCOCC([O-])=O	C6H11NO5	177.0637
cetirizine_TP53	Clc1ccc(cc1)C(NCC=O)c1cccc1	C15H14ClNO	259.0764
cetirizine_TP54	NC(c1cccc1)c1ccc(Cl)cc1	C13H12ClN	217.0658
cetirizine_TP55	[O-]C(=O)COCCN(CC=O)CC([O-])=O	C8H13NO6	219.0743
cetirizine_TP56	NCCN(CCOCC([O-])=O)CC([O-])=O	C8H16N2O5	220.1059
cetirizine_TP57	OCCN(CCNC(c1cccc1)c1ccc(Cl)cc1)CC([O-])=O	C19H23ClN2O3	362.1397
cetirizine_TP58	[O-]C(=O)CN(CCNC(c1cccc1)c1ccc(Cl)cc1)CC=O	C19H21ClN2O3	360.1241
cetirizine_TP59	[O-]C(=O)COCCN(CCNC(c1cccc1)c1cccc1)CC([O-])=O	C21H26N2O5	386.1842
cetirizine_TP60	[O-]C(=O)CN1CCNCC1	C6H12N2O2	144.0899
cetirizine_TP61	OCCNCCNCC=O	C6H14N2O2	146.1055
cetirizine_TP62	CC(O)N1CCNCC1	C6H14N2O	130.1106
cetirizine_TP63	[O-]C(=O)CN1CCN(CC1)C(c1cccc1)c1ccc(Cl)cc1	C19H21ClN2O2	344.1292
cetirizine_TP64	Oc1cccc(C(N2CCN(CC=O)CC2)c2ccc(Cl)cc2)c1O	C19H21ClN2O3	360.1241
cetirizine_TP65	OCCNCCN(CC=O)C(c1ccc(Cl)cc1)c1cccc(O)c1O	C19H23ClN2O4	378.1346
cetirizine_TP66	OCCN(CCNC(c1ccc(Cl)cc1)c1cccc(O)c1O)CC=O	C19H23ClN2O4	378.1346
cetirizine_TP67	OCCN1CCN(CC1)C(C(C=C)C(=O)C([O-])=O)c1ccc(Cl)cc1	C18H23ClN2O4	366.1346

cetirizine_TP68	<chem>OCCN1CCN(CC1)C(C([O-])=O)c1ccc(Cl)cc1</chem>	C14H19ClN2O3	298.1084
cetirizine_TP69	<chem>OCCN1CCN(CC1)C(c1ccccc1)c1ccc(O)c1O</chem>	C19H24N2O3	328.1787
cetirizine_TP70	<chem>CC(O)N1CCN(CC1)C(c1ccc(Cl)cc1)c1ccc(O)c1O</chem>	C19H23ClN2O3	362.1397
cetirizine_TP71	<chem>OCCNCCN(CC=O)C(c1ccccc1)c1ccccc1</chem>	C19H24N2O2	312.1838
cetirizine_TP72	<chem>OCCN(CCNC(c1ccccc1)c1ccccc1)CC=O</chem>	C19H24N2O2	312.1838
cetirizine_TP73	<chem>O=CCN1CCN(CC1)C(c1ccccc1)c1ccccc1</chem>	C19H22N2O	294.1732
cetirizine_TP74	<chem>CC(O)N1CCN(CC1)C(c1ccccc1)c1ccccc1</chem>	C19H24N2O	296.1889
cycloheximide_TP1	<chem>C[C@H]1C[C@H](C)C(=O)[C@@H](C1)C(=O)CC1CC(=O)NC(=O)C1</chem>	C15H21NO4	279.1471
cycloheximide_TP2	<chem>C[C@H]1C[C@H](C)C(=O)[C@@H](C1)[C@H](O)CC(CC(N)=O)CC([O-])=O</chem>	C15H25NO5	299.1733
cycloheximide_TP3	<chem>C[C@H]1C[C@H](C)C(=O)OC(C1)[C@H](O)CC1CC(=O)NC(=O)C1</chem>	C15H23NO5	297.1576
cycloheximide_TP4	<chem>C[C@H](CC(O)[C@H](O)CC1CC(=O)NC(=O)C1)[C@H](C)C([O-])=O</chem>	C15H25NO6	315.1682
cycloheximide_TP5	<chem>C[C@H]1C[C@H](C)C(=O)OC(C1)C(=O)CC1CC(=O)NC(=O)C1</chem>	C15H21NO5	295.1420
cycloheximide_TP6	<chem>C[C@H]1C[C@H](C)C(=O)OC(C1)[C@H](O)CC(CC(N)=O)CC([O-])=O</chem>	C15H25NO6	315.1682
cycloheximide_TP7	<chem>C[C@H]1C[C@H](C)C(=O)[C@@H](C1)[C@H](O)CC(CC([O-])=O)C([O-])=O</chem>	C15H24O6	300.1573
cycloheximide_TP8	<chem>C[C@H](CCC(=O)CC1CC(=O)NC(=O)C1)[C@H](C)C([O-])=O</chem>	C15H23NO5	297.1576
cycloheximide_TP9	<chem>C[C@H]1C[C@H](C)C(=O)[C@@H](C1)C(=O)CC(CC(N)=O)CC([O-])=O</chem>	C15H23NO5	297.1576
cycloheximide_TP10	<chem>C[C@@H]1CCC(=O)[C@@H](C)C1</chem>	C8H14O	126.1045
cycloheximide_TP11	<chem>C[C@H]1C[C@H](CO)C(=O)[C@@H](C1)C(=O)CC1CC(=O)NC(=O)C1</chem>	C15H21NO5	295.1420
cycloheximide_TP12	<chem>[O-]C(=O)CC1CC(=O)NC(=O)C1</chem>	C7H9NO4	171.0532
cycloheximide_TP13	<chem>C[C@H]1C[C@H](CO)C[C@@H](C(=O)CC2CC(=O)NC(=O)C2)C1=O</chem>	C15H21NO5	295.1420
cycloheximide_TP14	<chem>C[C@H]1C[C@@H](C[C@@H](C(=O)CC2CC(=O)NC(=O)C2)C1=O)C=O</chem>	C15H19NO5	293.1263
cycloheximide_TP15	<chem>C[C@@H](C[C@H](CO)CCC(=O)CC1CC(=O)NC(=O)C1)C([O-])=O</chem>	C15H23NO6	313.1525
cycloheximide_TP16	<chem>C[C@H]1C[C@H](C=O)C(=O)[C@@H](C1)C(=O)CC1CC(=O)NC(=O)C1</chem>	C15H19NO5	293.1263
cycloheximide_TP17	<chem>C[C@H]1C[C@H](CO)CCC1=O</chem>	C8H14O2	142.0994
cycloheximide_TP18	<chem>C[C@H](CCC(=O)CC1CC(=O)NC(=O)C1)[C@H](CO)C([O-])=O</chem>	C15H23NO6	313.1525
cycloheximide_TP19	<chem>C[C@@H]1CCC(=O)[C@@H](CO)C1</chem>	C8H14O2	142.0994
cycloheximide_TP20	<chem>OC1(CC([O-])=O)CC(=O)NC(=O)C1</chem>	C7H9NO5	187.0481
cycloheximide_TP21	<chem>C[C@@H]1CCC(=O)OC(C)C1</chem>	C8H14O2	142.0994
cycloheximide_TP22	<chem>C[C@H]1C[C@H](CO)C[C@@H](C(=O)CC(CC(N)=O)CC([O-])=O)C1=O</chem>	C15H23NO6	313.1525
cycloheximide_TP23	<chem>C[C@H]1C[C@H](CO)C(=O)[C@@H](C1)C(=O)CC(CC(N)=O)CC([O-])=O</chem>	C15H23NO6	313.1525
cycloheximide_TP24	<chem>NC(=O)CC(CC([O-])=O)CC([O-])=O</chem>	C7H11NO5	189.0637
cycloheximide_TP25	<chem>C[C@H](CCC(=O)CC(CC(N)=O)CC([O-])=O)C[C@H](C)C([O-])=O</chem>	C15H25NO6	315.1682
cycloheximide_TP26	<chem>C[C@H]1C[C@H](C)C(=O)[C@@H](C1)C(=O)CC(CC([O-])=O)CC([O-])=O</chem>	C15H22O6	298.1416
cycloheximide_TP27	<chem>C[C@H](CCC(=O)CC1CC(=O)NC(=O)C1)C([O-])=O</chem>	C12H17NO5	255.1107
cycloheximide_TP28	<chem>C[C@H]1C[C@H](C)C(=O)OC(C1)[C@H](O)CC(CC([O-])=O)CC([O-])=O</chem>	C15H24O7	316.1522
cycloheximide_TP29	<chem>C[C@H]1C[C@H](C)C(=O)OC(C1)C(=O)CC(CC(N)=O)CC([O-])=O</chem>	C15H23NO6	313.1525
cycloheximide_TP30	<chem>C[C@@H](C[C@H](C)C([O-])=O)CC(O)C(=O)CC1CC(=O)NC(=O)C1</chem>	C15H23NO6	313.1525
cycloheximide_TP31	<chem>C[C@@H](C[C@H](C)C([O-])=O)CC(O)[C@H](O)CC(CC(N)=O)CC([O-])=O</chem>	C15H27NO7	333.1788
cycloheximide_TP32	<chem>C[C@H](CC(O)[C@H](O)CC1CC(=O)NC(=O)C1)C([O-])=O</chem>	C12H19NO6	273.1212
diclofenac_TP1	<chem>Nc1c(Cl)cccc1Cl</chem>	C6H5Cl2N	160.9799

diclofenac_TP2	<chem>Oc1cccc(CC([O-])=O)c1O</chem>	C8H8O4	168.0423
diclofenac_TP3	<chem>[O-]C(=O)Cc1cccc1Nc1cccc1Cl</chem>	C14H12ClNO2	261.0557
diclofenac_TP4	<chem>Oc1cccc(Cl)c1O</chem>	C6H5ClO2	143.9978
diclofenac_TP5	<chem>Nc1cccc1CC([O-])=O</chem>	C8H9NO2	151.0633
diclofenac_TP6	<chem>[O-]C(=O)Cc1cccc1Nc1cccc1</chem>	C14H13NO2	227.0946
diclofenac_TP7	<chem>Nc1cccc1Cl</chem>	C6H6ClN	127.0189
diclofenac_TP8	<chem>[O-]C(=O)CC(C=C)C(=O)C([O-])=O</chem>	C7H8O5	172.0372
diclofenac_TP9	<chem>Nc1c(Cl)cc(O)c(O)c1Cl</chem>	C6H5Cl2NO2	192.9697
diclofenac_TP10	<chem>Oc1cc(Cl)c(O)c(Cl)c1O</chem>	C6H4Cl2O3	193.9537
diclofenac_TP11	<chem>Nc1ccc(O)c(O)c1Cl</chem>	C6H6ClNO2	159.0087
diclofenac_TP12	<chem>Nc1cc(O)c(O)cc1Cl</chem>	C6H6ClNO2	159.0087
diclofenac_TP13	<chem>[O-]C(=O)C=C(Cl)C(=N)C(Cl)C([O-])=O</chem>	C6H5Cl2NO4	224.9596
diclofenac_TP14	<chem>CCC(CC([O-])=O)C(=O)C([O-])=O</chem>	C7H10O5	174.0528
diclofenac_TP15	<chem>Nc1cccc1</chem>	C6H7N	93.0578
diclofenac_TP16	<chem>Oc1ccc(CC([O-])=O)c(Nc2cccc2)c1</chem>	C14H13NO3	243.0895
diclofenac_TP17	<chem>[O-]C(=O)C=C\C=C(Cl)C([O-])=O</chem>	C6H5ClO4	175.9876
emodin_TP1	<chem>Cc1cc2C(=O)c3cc(O)cc(O)c3C(=O)c2c(O)c1O</chem>	C15H10O6	286.0477
emodin_TP2	<chem>OCc1cc(O)c2C(=O)c3c(O)cc(O)cc3C(=O)c2c1</chem>	C15H10O6	286.0477
emodin_TP3	<chem>Cc1cc(O)c(C([O-])=O)c(c1)C(=O)c1cc(O)cc(O)c1O</chem>	C15H12O7	304.0583
emodin_TP4	<chem>CC(C=C1C(=O)C(=O)c2c(O)cc(O)cc2C1=O)=C(O)C([O-])=O</chem>	C15H10O8	318.0376
emodin_TP5	<chem>Cc1cc(C(=O)c2cc(O)cc(O)c2C([O-])=O)c(O)c(O)c1O</chem>	C15H12O8	320.0532
emodin_TP6	<chem>Oc1cc(O)c2C(=O)c3c(O)cc(C=O)cc3C(=O)c2c1</chem>	C15H8O6	284.0321
emodin_TP7	<chem>OCc1cc(O)c(C([O-])=O)c(c1)C(=O)c1cc(O)cc(O)c1O</chem>	C15H12O8	320.0532
emodin_TP8	<chem>Cc1cc(O)c(C([O-])=O)c(c1)C(=O)C([O-])=O</chem>	C10H8O6	224.0321
emodin_TP9	<chem>Cc1cc(O)c(C([O-])=O)c(c1)C([O-])=O</chem>	C9H8O5	196.0372
emodin_TP10	<chem>OCc1cc(O)c(C([O-])=O)c(c1)C(=O)C([O-])=O</chem>	C10H8O7	240.0270
emodin_TP11	<chem>Cc1cc(O)c(O)c(c1)C(=O)C([O-])=O</chem>	C9H8O5	196.0372
emodin_TP12	<chem>Oc1cc(O)c(O)c(c1)C(=O)c1cc(C=O)cc(O)c1C([O-])=O</chem>	C15H10O8	318.0376
emodin_TP13	<chem>Oc1cc(O)c2C(=O)c3c(O)cc(cc3C(=O)c2c1)C([O-])=O</chem>	C15H8O7	300.0270
emodin_TP14	<chem>Cc1cc(C(=O)c2cccc(O)c2C([O-])=O)c(O)c(O)c1O</chem>	C15H12O7	304.0583
emodin_TP15	<chem>Cc1c(O)cc(O)c(C(=O)c2cc(O)cc(O)c2C([O-])=O)c1O</chem>	C15H12O8	320.0532
emodin_TP16	<chem>CC(C=C(C([O-])=O)C(=O)c1cc(O)cc(O)c1C([O-])=O)=C(O)C([O-])=O</chem>	C15H12O10	352.0430
emodin_TP17	<chem>CC(=CC(=C(O)C([O-])=O)C(=O)c1cc(O)cc(O)c1C([O-])=O)C([O-])=O</chem>	C15H12O10	352.0430
emodin_TP18	<chem>Cc1cc(C(=O)c2cc(O)cc(O)c2O)c(O)c(O)c1O</chem>	C14H12O7	292.0583
emodin_TP19	<chem>CC(C=C1C(=O)C(=O)c2c(O)cc(O)cc2C1=O)C(=O)C([O-])=O</chem>	C15H10O8	318.0376
fexofenadine_TP1	<chem>CC(C)C([O-])=O)c1ccc(cc1)C(O)CCC=O</chem>	C14H18O4	250.1205
fexofenadine_TP2	<chem>OC(C1CCNCC1)(c1cccc1)c1cccc1</chem>	C18H21NO	267.1623
fexofenadine_TP3	<chem>CC(C)C([O-])=O)c1ccc(cc1)C(O)CCCNCCC(CC=O)C(O)(c1cccc1)c1cccc1</chem>	C32H39NO5	517.2828
fexofenadine_TP4	<chem>CC(C)c1ccc(cc1)C(O)CCCN1CCC(CC1)C(O)(c1cccc1)c1cccc1</chem>	C31H39NO2	457.2981
fexofenadine_TP5	<chem>CC(C)C([O-])=O)c1ccc(cc1)C(=O)CCCN1CCC(CC1)C(O)(c1cccc1)c1cccc1</chem>	C32H37NO4	499.2723
fexofenadine_TP6	<chem>CC(CC([O-])=O)c1ccc(cc1)C(O)CCCN1CCC(CC1)C(O)(c1cccc1)c1ccc1</chem>	C32H39NO4	501.2879
fexofenadine_TP7	<chem>CC(=CC([O-])=O)c1ccc(cc1)C(O)CCCN1CCC(CC1)C(O)(c1cccc1)c1cccc1</chem>	C32H37NO4	499.2723
fexofenadine_TP8	<chem>CC(CC([O-])=O)c1ccc(cc1)C(=O)CCCN1CCC(CC1)C(O)(c1cccc1)c1cccc1</chem>	C32H37NO4	499.2723

fexofenadine_TP9	CC(C)(C([O-])=O)c1ccc(cc1)C(=O)CCCN1CCC(O)(CC1)C(O)(c1ccccc1)c1ccccc1	C32H37NO5	515.2672
fexofenadine_TP10	CC(CC([O-])=O)c1ccc(cc1)C(O)CCCNCCC(CC=O)C(O)(c1ccccc1)c1ccccc1	C32H39NO5	517.2828
fexofenadine_TP11	CC(C)c1ccc(cc1)C(=O)CCCN1CCC(CC1)C(O)(c1ccccc1)c1ccccc1	C31H37NO2	455.2824
fexofenadine_TP12	CC(C)(C([O-])=O)c1ccc(cc1)C(=O)CCCNCCC(CC=O)C(O)(c1ccccc1)c1ccccc1	C32H37NO5	515.2672
fexofenadine_TP13	CC(C)c1ccc(cc1)C(O)CCCNCCC(CC=O)C(O)(c1ccccc1)c1ccccc1	C31H39NO3	473.2930
fexofenadine_TP14	CC(C)(C([O-])=O)c1ccc(cc1)C(O)CCCNCCC(CC([O-])=O)C(O)(c1ccccc1)c1ccccc1	C32H39NO6	533.2777
fexofenadine_TP15	CC(CC([O-])=O)c1ccc(cc1)C(O)CCC=O	C14H18O4	250.1205
fexofenadine_TP16	CC(C)(C([O-])=O)c1ccc(cc1)C(=O)CCC=O	C14H16O4	248.1049
fexofenadine_TP17	CC(C)c1ccc(cc1)C(O)CCC=O	C13H18O2	206.1307
fexofenadine_TP18	OC(c1ccccc1)(c1ccccc1)C1(O)CCNCCC1	C18H21NO2	283.1572
fexofenadine_TP19	CC(C)(C([O-])=O)c1ccc(cc1)C(O)CCC([O-])=O	C14H18O5	266.1154
fexofenadine_TP20	NCCC(CC=O)C(O)(c1ccccc1)c1ccccc1	C18H21NO2	283.1572
fexofenadine_TP21	NCCC(CC([O-])=O)C(O)(c1ccccc1)c1ccccc1	C18H21NO3	299.1521
fexofenadine_TP22	CC(C)c1ccc(cc1)C(O)CCC([O-])=O	C13H18O3	222.1256
fexofenadine_TP23	CC(C)(C([O-])=O)c1ccc(cc1)C(=O)CCC([O-])=O	C14H16O5	264.0998
fexofenadine_TP24	CC(CC([O-])=O)c1ccc(cc1)C(O)CCC([O-])=O	C14H18O5	266.1154
fexofenadine_TP25	NCCC(O)(CC=O)C(O)(c1ccccc1)c1ccccc1	C18H21NO3	299.1521
fexofenadine_TP26	OC(C(CC=O)CC([O-])=O)(c1ccccc1)c1ccccc1	C18H18O4	298.1205
fexofenadine_TP27	CC(C)(C([O-])=O)c1ccc(cc1)C(O)CCCN	C14H21NO3	251.1521
fexofenadine_TP28	CC(C)c1ccc(cc1)C(O)CCCNCCC(CC([O-])=O)C(O)(c1ccccc1)c1ccccc1	C31H39NO4	489.2879
fexofenadine_TP29	CC(C)c1ccc(cc1)C(=O)CCC=O	C13H16O2	204.1150
fexofenadine_TP30	CC(C)(C([O-])=O)c1ccc(cc1)C(=O)CCCNCCC(CC([O-])=O)C(O)(c1ccccc1)c1ccccc1	C32H37NO6	531.2621
fexofenadine_TP31	CC(CC([O-])=O)c1ccc(cc1)C(=O)CCC=O	C14H16O4	248.1049
fexofenadine_TP32	CC(=CC([O-])=O)c1ccc(cc1)C(O)CCC=O	C14H16O4	248.1049
fexofenadine_TP33	CC(C)c1ccc(cc1)C(=O)CCCNCCC(CC=O)C(O)(c1ccccc1)c1ccccc1	C31H37NO3	471.2773
fexofenadine_TP34	CC(C)(O)c1ccc(cc1)C(=O)CCCN1CCC(CC1)C(O)(c1ccccc1)c1ccccc1	C31H37NO3	471.2773
fexofenadine_TP35	CC(CC([O-])=O)c1ccc(cc1)C(O)CCCNCCC(CC([O-])=O)C(O)(c1ccccc1)c1ccccc1	C32H39NO6	533.2777
fexofenadine_TP36	CC(C)c1ccc(cc1)C(=O)CCCN1CCC(O)(CC1)C(O)(c1ccccc1)c1ccccc1	C31H37NO3	471.2773
fexofenadine_TP37	CC(CC([O-])=O)c1ccc(cc1)C(=O)CCCN1CCC(O)(CC1)C(O)(c1ccccc1)c1ccccc1	C32H37NO5	515.2672
fexofenadine_TP38	CC(C)(C([O-])=O)c1ccc(cc1)C(=O)CCCNCCC(O)(CC=O)C(O)(c1ccccc1)c1ccccc1	C32H37NO6	531.2621
fexofenadine_TP39	CC(CC([O-])=O)c1ccc(cc1)C(=O)CCCNCCC(CC=O)C(O)(c1ccccc1)c1ccccc1	C32H37NO5	515.2672
fexofenadine_TP40	CC(=CC([O-])=O)c1ccc(cc1)C(=O)CCCN1CCC(CC1)C(O)(c1ccccc1)c1ccccc1	C32H35NO4	497.2566
fexofenadine_TP41	CC(=CC([O-])=O)c1ccc(cc1)C(O)CCCNCCC(CC=O)C(O)(c1ccccc1)c1ccccc1	C32H37NO5	515.2672
fexofenadine_TP42	CC(O)(CC([O-])=O)c1ccc(cc1)C(O)CCCN1CCC(CC1)C(O)(c1ccccc1)c1ccccc1	C32H39NO5	517.2828
flufenamic acid_TP1	Oc1ccc(cc1O)C(F)(F)F	C7H5F3O2	178.0242
flufenamic acid_TP2	Nc1ccccc1C([O-])=O	C7H7NO2	137.0477
flufenamic acid_TP3	Nc1cccc(c1)C(F)(F)F	C7H6F3N	161.0452
flufenamic acid_TP4	Oc1cccc(c1O)C(F)(F)F	C7H5F3O2	178.0242
flufenamic acid_TP5	[O-]C(=O)C(=O)C(C=C)C(F)(F)F	C6H5F3O3	182.0191
flufenamic acid_TP6	[O-]C(=O)C1CC(=O)CCC1=N	C7H9NO3	155.0582

flufenamic acid_TP7	[O-]C(=O)C(=O)CC(=C)C(F)(F)F	C6H5F3O3	182.0191
flufenamic acid_TP8	[O-]C(=O)C(=O)CC=CC(F)(F)F	C6H5F3O3	182.0191
flufenamic acid_TP9	[O-]C(=O)C(=O)CCCC(F)(F)F	C6H7F3O3	184.0347
flufenamic acid_TP10	CC(CC(=O)C([O-])=O)C(F)(F)F	C6H7F3O3	184.0347
flufenamic acid_TP11	[O-]C(=O)C=CC=CC([O-])=O	C6H6O4	142.0266
flufenamic acid_TP12	[O-]C(=O)C1COC(=O)CCC1=N	C7H9NO4	171.0532
flufenamic acid_TP13	[O-]C(=O)C1CC(=O)CCC1=O	C7H8O4	156.0423
flufenamic acid_TP14	CCC(C(=O)C([O-])=O)C(F)(F)F	C6H7F3O3	184.0347
gabapentin_TP1	[O-]C(=O)CC1(CCCCC1)C=O	C9H14O3	170.0943
gabapentin_TP2	[O-]C(=O)CC1(CCCCC1)C([O-])=O	C9H14O4	186.0892
gabapentin_TP3	OC(C([O-])=O)C1(CCCCC1)C([O-])=O	C9H14O5	202.0841
gabapentin_TP4	OC1CCC(CC([O-])=O)(CC1)C([O-])=O	C9H14O5	202.0841
gabapentin_TP5	OC1CCCC(CC([O-])=O)(C1)C([O-])=O	C9H14O5	202.0841
gabapentin_TP6	OC1CCCCC1(CC([O-])=O)C([O-])=O	C9H14O5	202.0841
gemifibrozil_TP1	Cc1ccc(C)c(O)c1	C8H10O	122.0732
gemifibrozil_TP2	CC(C)(CCC=O)C([O-])=O	C7H12O3	144.0786
gemifibrozil_TP3	Cc1ccc(CO)cc1OCCCC(C)(C)C([O-])=O	C15H22O4	266.1518
gemifibrozil_TP4	Cc1ccc(CO)c(OCCCC(C)(C)C([O-])=O)c1	C15H22O4	266.1518
gemifibrozil_TP5	Cc1ccc(C)c(OCC(O)CC(C)(C)C([O-])=O)c1	C15H22O4	266.1518
gemifibrozil_TP6	CC(CCCOc1cc(C)ccc1C)CC([O-])=O	C15H22O3	250.1569
gemifibrozil_TP7	Cc1ccc(CC(CC([O-])=O)C([O-])=O)cc1OCCCC(C)(C)C([O-])=O	C19H26O7	366.1679
gemifibrozil_TP8	Cc1ccc(C)c(O)c1O	C8H10O2	138.0681
gemifibrozil_TP9	Cc1ccc(CO)cc1O	C8H10O2	138.0681
gemifibrozil_TP10	Cc1ccc(CO)c(O)c1	C8H10O2	138.0681
gemifibrozil_TP11	Cc1ccc(CC(CC([O-])=O)C([O-])=O)cc1O	C12H14O5	238.0841
gemifibrozil_TP12	CC(C)(CCC([O-])=O)C([O-])=O	C7H12O4	160.0736
gemifibrozil_TP13	Cc1ccc(C=O)cc1OCCCC(C)(C)C([O-])=O	C15H20O4	264.1362
gemifibrozil_TP14	CC(CCCOc1cc(CO)ccc1C)CC([O-])=O	C15H22O4	266.1518
gemifibrozil_TP15	Cc1ccc(C=O)c(OCCCC(C)(C)C([O-])=O)c1	C15H20O4	264.1362
gemifibrozil_TP16	CC(CCCOc1cc(C)ccc1CO)CC([O-])=O	C15H22O4	266.1518
gemifibrozil_TP17	CC(C)(CCCOc1cc(CC(CC([O-])=O)C([O-])=O)ccc1CO)C([O-])=O	C19H26O8	382.1628
gemifibrozil_TP18	Cc1ccc(CC(CC([O-])=O)C([O-])=O)cc1OCC(O)CC(C)(C)C([O-])=O	C19H26O8	382.1628
gemifibrozil_TP19	CC(CC(O)COc1cc(C)ccc1C)CC([O-])=O	C15H22O4	266.1518
gemifibrozil_TP20	CC(C)(CC(O)C=O)C([O-])=O	C7H12O4	160.0736
gemifibrozil_TP21	Cc1ccc(C)c(OCC(=O)CC(C)(C)C([O-])=O)c1	C15H20O4	264.1362
gemifibrozil_TP22	CC(CCCOc1cc(C)ccc1C)=CC([O-])=O	C15H20O3	248.1412
gemifibrozil_TP23	CC(CCCOc1cc(CC(CC([O-])=O)C([O-])=O)ccc1C)CC([O-])=O	C19H26O7	366.1679
gemifibrozil_TP24	Cc1ccc(CC(C(O)C([O-])=O)C([O-])=O)cc1OCCCC(C)(C)C([O-])=O	C19H26O8	382.1628
gemifibrozil_TP25	Cc1ccc(cc1OCCCC(C)(C)C([O-])=O)C(O)C(CC([O-])=O)C([O-])=O	C19H26O8	382.1628
gemifibrozil_TP26	Cc1ccc(C=C(CC([O-])=O)C([O-])=O)cc1OCCCC(C)(C)C([O-])=O	C19H24O7	364.1522
gemifibrozil_TP27	Cc1ccc(CCC(C([O-])=O)C([O-])=O)cc1OCCCC(C)(C)C([O-])=O	C19H26O7	366.1679
gemifibrozil_TP28	CC(C=C)C(=O)C([O-])=O	C6H8O3	128.0473
gemifibrozil_TP29	Cc1ccc(C=O)cc1O	C8H8O2	136.0524
gemifibrozil_TP30	Cc1ccc(C=O)c(O)c1	C8H8O2	136.0524
gemifibrozil_TP31	OCc1ccc(CC(CC([O-])=O)C([O-])=O)cc1O	C12H14O6	254.0790
gemifibrozil_TP32	Cc1ccc(CC(CC([O-])=O)C([O-])=O)c(O)c1O	C12H14O6	254.0790

gemifibrozil_TP33	Cc1ccc(CC(C(O)C([O-])=O)C([O-])=O)cc1O	C12H14O6	254.0790
gemifibrozil_TP34	Cc1ccc(cc1O)C(O)C(CC([O-])=O)C([O-])=O	C12H14O6	254.0790
gemifibrozil_TP35	Cc1ccc(C=C(CC([O-])=O)C([O-])=O)cc1O	C12H12O5	236.0685
gemifibrozil_TP36	Cc1ccc(CCC(C([O-])=O)C([O-])=O)cc1O	C12H14O5	238.0841
gemifibrozil_TP37	CC(CCC([O-])=O)CC([O-])=O	C7H12O4	160.0736
gemifibrozil_TP38	Cc1ccc(cc1OCCCC(C)C)C([O-])=O)C([O-])=O	C15H20O5	280.1311
gemifibrozil_TP39	CC(CCCOc1cc(C=O)ccc1C)CC([O-])=O	C15H20O4	264.1362
gemifibrozil_TP40	CC(CCCOc1cc(CO)ccc1C)=CC([O-])=O	C15H20O4	264.1362
gemifibrozil_TP41	CC(CCC=O)CC([O-])=O	C7H12O3	144.0786
gemifibrozil_TP42	CC(C)(CCCOc1cc(CCC(C([O-])=O)C([O-])=O)ccc1CO)C([O-])=O	C19H26O8	382.1628
gemifibrozil_TP43	CC(C)(CCCOc1cc(C=C(CC([O-])=O)C([O-])=O)ccc1CO)C([O-])=O	C19H24O8	380.1471
gemifibrozil_TP44	CC(CCCOc1cc(C(C(C([O-])=O)C([O-])=O)ccc1CO)CC([O-])=O	C19H26O8	382.1628
gemifibrozil_TP45	CC(C)(CCCOc1cc(C(C(C([O-])=O)C([O-])=O)ccc1C=O)C([O-])=O	C19H24O8	380.1471
gemifibrozil_TP46	CC(CCCOc1cc(C)ccc1CO)=CC([O-])=O	C15H20O4	264.1362
gemifibrozil_TP47	CC(CCCOc1cc(C)ccc1C=O)CC([O-])=O	C15H20O4	264.1362
gemifibrozil_TP48	Cc1ccc(C([O-])=O)c(OCCCC(C)C)C([O-])=O)c1	C15H20O5	280.1311
gemifibrozil_TP49	Cc1ccc(C)c(OCC(=O)C(O)C(C)C([O-])=O)c1	C15H20O5	280.1311
gemifibrozil_TP50	Cc1ccc(CO)cc1OCC(=O)CC(C)C([O-])=O	C15H20O5	280.1311
gemifibrozil_TP51	Cc1ccc(CO)c(OCC(=O)CC(C)C)C([O-])=O)c1	C15H20O5	280.1311
gemifibrozil_TP52	CC(C)(CC(=O)C=O)C([O-])=O	C7H10O4	158.0579
gemifibrozil_TP53	CC(CC([O-])=O)CC(=O)COc1cc(C)ccc1C	C15H20O4	264.1362
gemifibrozil_TP54	CC(C)(CC(O)C([O-])=O)C([O-])=O	C7H12O5	176.0685
gemifibrozil_TP55	Cc1ccc(CC(CC([O-])=O)C([O-])=O)cc1OCC(=O)CC(C)C([O-])=O	C19H24O8	380.1471
gemifibrozil_TP56	CC(CC(O)C=O)CC([O-])=O	C7H12O4	160.0736
gemifibrozil_TP57	CC(CC(O)COc1cc(C)ccc1C)=CC([O-])=O	C15H20O4	264.1362
gemifibrozil_TP58	Cc1ccc(CCC(C([O-])=O)C([O-])=O)cc1OCC(O)CC(C)C([O-])=O	C19H26O8	382.1628
gemifibrozil_TP59	CC(CC(O)COc1cc(C(C(C([O-])=O)C([O-])=O)ccc1C)CC([O-])=O	C19H26O8	382.1628
gemifibrozil_TP60	Cc1ccc(C=C(CC([O-])=O)C([O-])=O)cc1OCC(O)CC(C)C([O-])=O	C19H24O8	380.1471
gemifibrozil_TP61	CC(CCCOc1cc(C=C(CC([O-])=O)C([O-])=O)ccc1C)CC([O-])=O	C19H24O7	364.1522
gemifibrozil_TP62	CC(CCCOc1cc(CCC(C([O-])=O)C([O-])=O)ccc1C)CC([O-])=O	C19H26O7	366.1679
gemifibrozil_TP63	CC(CCCOc1cc(C(C(C([O-])=O)C([O-])=O)ccc1C)=CC([O-])=O	C19H24O7	364.1522
gemifibrozil_TP64	Cc1ccc(C)c(OCCCC(C)C)C([O-])=O)c1	C15H22O4	266.1518
gemifibrozil_TP65	CC(CCC=O)=CC([O-])=O	C7H10O3	142.0630
gemifibrozil_TP66	Cc1ccc(cc1OCCCC(C)C)C([O-])=O)C(O)CC(C([O-])=O)C([O-])=O	C19H26O8	382.1628
gemifibrozil_TP67	Cc1ccc(CC(O)(CC([O-])=O)C([O-])=O)cc1OCCCC(C)C([O-])=O	C19H26O8	382.1628
gemifibrozil_TP68	Cc1ccc(cc1OCCCC(C)C)C([O-])=O)C(=O)C(CC([O-])=O)C([O-])=O	C19H24O8	380.1471
gemifibrozil_TP69	CC(CCCOc1cc(ccc1C)C(O)C(CC([O-])=O)C([O-])=O)CC([O-])=O	C19H26O8	382.1628
gemifibrozil_TP70	Cc1ccc(CC(C([O-])=O)C(=O)C([O-])=O)cc1OCCCC(C)C([O-])=O	C19H24O8	380.1471
gemifibrozil_TP71	Cc1ccc(C=C(C(O)C([O-])=O)C([O-])=O)cc1OCCCC(C)C([O-])=O	C19H24O8	380.1471
gemifibrozil_TP72	CC(CCCOc1cc(C(C(O)C([O-])=O)C([O-])=O)ccc1C)CC([O-])=O	C19H26O8	382.1628
heptaminol_TP1	CC(=O)CCCC(C)C(O)	C8H16O2	144.1150
heptaminol_TP2	CC(=O)C(O)CCC(C)C(O)	C8H16O3	160.1099
heptaminol_TP3	CC(=O)CCC(O)C(C)C(O)	C8H16O3	160.1099
heptaminol_TP4	CC(=O)CCCC(C)(O)CO	C8H16O3	160.1099
heptaminol_TP5	CC(C)(O)CCCC(=O)CO	C8H16O3	160.1099
heptaminol_TP6	CC(C)(O)CCCC(=O)C=O	C8H14O3	158.0943

heptaminol_TP7	<chem>CC(=O)CCCC(C)(O)C=O</chem>	C8H14O3	158.0943
heptaminol_TP8	<chem>CC(=O)CCC(=O)C(C)(C)O</chem>	C8H14O3	158.0943
heptaminol_TP9	<chem>CC(=O)C(=O)CCC(C)(C)O</chem>	C8H14O3	158.0943
hydrochlorothiazide_TP1	<chem>[O-]S(=O)(=O)c1cc2c(NCNS2(=O)=O)cc1Cl</chem>	C7H7ClN2O5S2	297.9485
hydrochlorothiazide_TP2	<chem>NS(=O)(=O)c1ccc2NCNS(=O)(=O)c2c1</chem>	C7H9N3O4S2	263.0034
hydrochlorothiazide_TP3	<chem>Nc1cc(Cl)c(cc1S(=O)(=O)NC=O)S(N)(=O)=O</chem>	C7H8ClN3O5S2	312.9594
hydrochlorothiazide_TP4	<chem>NCNc1cc(Cl)c(cc1S([O-])(=O)=O)S(N)(=O)=O</chem>	C7H10ClN3O5S2	314.9750
hydrochlorothiazide_TP5	<chem>NCNc1cc(Cl)c(cc1O)S(N)(=O)=O</chem>	C7H10ClN3O3S	251.0131
hydrochlorothiazide_TP6	<chem>NS(=O)(=O)c1cc(c(NC=O)cc1Cl)S([O-])(=O)=O</chem>	C7H7ClN2O6S2	313.9434
hydrochlorothiazide_TP7	<chem>NCNc1cc(Cl)c(c(O)c1O)S(N)(=O)=O</chem>	C7H10ClN3O4S	267.0081
hydrochlorothiazide_TP8	<chem>Nc1cc(Cl)c(cc1S([O-])(=O)=O)S(N)(=O)=O</chem>	C6H7ClN2O5S2	285.9485
hydrochlorothiazide_TP9	<chem>NCNc1ccc(cc1S([O-])(=O)=O)S(N)(=O)=O</chem>	C7H11N3O5S2	281.0140
hydrochlorothiazide_TP10	<chem>NCNc1cc(Cl)c(cc1S([O-])(=O)=O)S([O-])(=O)=O</chem>	C7H9ClN2O6S2	315.9591
hydrochlorothiazide_TP11	<chem>Nc1ccc(cc1S(=O)(=O)NC=O)S(N)(=O)=O</chem>	C7H9N3O5S2	278.9984
hydrochlorothiazide_TP12	<chem>Nc1cc(Cl)c(cc1S(=O)(=O)NC=O)S([O-])(=O)=O</chem>	C7H7ClN2O6S2	313.9434
hydrochlorothiazide_TP13	<chem>[O-]S(=O)(=O)c1ccc2NCNS(=O)(=O)c2c1</chem>	C7H8N2O5S2	263.9875
hydrochlorothiazide_TP14	<chem>Oc1cc2c(NCNS2(=O)=O)cc1Cl</chem>	C7H7ClN2O3S	233.9866
hydrochlorothiazide_TP15	<chem>Oc1c(O)c2c(NCNS2(=O)=O)cc1Cl</chem>	C7H7ClN2O4S	249.9815
hydrochlorothiazide_TP16	<chem>Nc1cc(Cl)c(O)c(O)c1S(=O)(=O)NC=O</chem>	C7H7ClN2O5S	265.9764
hydrochlorothiazide_TP17	<chem>[O-]C(=O)C(Cl)=CC1=C(C([O-])=O)S(=O)(=O)NCN1</chem>	C7H7ClN2O6S	281.9713
hydrochlorothiazide_TP18	<chem>Oc1ccc2NCNS(=O)(=O)c2c1O</chem>	C7H8N2O4S	216.0205
hydrochlorothiazide_TP19	<chem>NCNc1cc(Cl)c(O)c(O)c1S([O-])(=O)=O</chem>	C7H9ClN2O5S	267.9921
hydrochlorothiazide_TP20	<chem>Nc1cc(Cl)c(O)cc1S(=O)(=O)NC=O</chem>	C7H7ClN2O4S	249.9815
hydrochlorothiazide_TP21	<chem>Oc1ccc2NCNS(=O)(=O)c2c1</chem>	C7H8N2O3S	200.0256
hydrochlorothiazide_TP22	<chem>Oc1cc2NCNS(=O)(=O)c2cc1O</chem>	C7H8N2O4S	216.0205
hydrochlorothiazide_TP23	<chem>NCNc1cc(Cl)c(O)cc1S([O-])(=O)=O</chem>	C7H9ClN2O4S	251.9972
hydrochlorothiazide_TP24	<chem>Oc1cc(Cl)c(cc1S(=O)(=O)NC=O)S([O-])(=O)=O</chem>	C7H6ClNO7S2	314.9274
hydrochlorothiazide_TP25	<chem>Nc1ccc(cc1S(=O)(=O)NC=O)S([O-])(=O)=O</chem>	C7H8N2O6S2	279.9824
hydrochlorothiazide_TP26	<chem>NCNc1ccc(cc1S([O-])(=O)=O)S([O-])(=O)=O</chem>	C7H10N2O6S2	281.9980
hydrochlorothiazide_TP27	<chem>Oc1c(O)c(cc(c1Cl)S([O-])(=O)=O)S([O-])(=O)=O</chem>	C6H5ClO8S2	303.9114
hydrochlorothiazide_TP28	<chem>Nc1cc(Cl)c(cc1S([O-])(=O)=O)S([O-])(=O)=O</chem>	C6H6ClNO6S2	286.9325
hydrochlorothiazide_TP29	<chem>Nc1ccc(cc1S([O-])(=O)=O)S(N)(=O)=O</chem>	C6H8N2O5S2	251.9875
hydrochlorothiazide_TP30	<chem>NCNc1cc(Cl)c(c(O)c1O)S([O-])(=O)=O</chem>	C7H9ClN2O5S	267.9921
hydrochlorothiazide_TP31	<chem>[O-]S(=O)(=O)c1cc(c(NC=O)cc1Cl)S([O-])(=O)=O</chem>	C7H6ClNO7S2	314.9274
hydrochlorothiazide_TP32	<chem>NCNc1ccc(c(O)c1O)S(N)(=O)=O</chem>	C7H11N3O4S	233.0470
hydrochlorothiazide_TP33	<chem>NCNc1cc(Cl)c(cc1O)S([O-])(=O)=O</chem>	C7H9ClN2O4S	251.9972
hydrochlorothiazide_TP34	<chem>NS(=O)(=O)c1ccc(NC=O)c(c1)S([O-])(=O)=O</chem>	C7H8N2O6S2	279.9824
hydrochlorothiazide_TP35	<chem>NCNc1ccc(cc1O)S(N)(=O)=O</chem>	C7H11N3O3S	217.0521
hydrochlorothiazide_TP36	<chem>Nc1cc(Cl)c(c(O)c1O)S(N)(=O)=O</chem>	C6H7ClN2O4S	237.9815
hydrochlorothiazide_TP37	<chem>Nc1cc(Cl)c(cc1O)S(N)(=O)=O</chem>	C6H7ClN2O3S	221.9866
hydrochlorothiazide_TP38	<chem>NS(=O)(=O)c1c(Cl)cc(NC=O)c(O)c1O</chem>	C7H7ClN2O5S	265.9764
hydrochlorothiazide_TP39	<chem>NS(=O)(=O)c1cc(O)c(NC=O)cc1Cl</chem>	C7H7ClN2O4S	249.9815
hydrochlorothiazide_TP40	<chem>NCNc1cc(O)c(cc1O)S(N)(=O)=O</chem>	C7H11N3O4S	233.0470
hydroxyphenyl diphenyl phosphate_TP1	<chem>Oc1ccc(OP(=O)(Oc2ccccc2)Oc2ccccc2)cc1O</chem>	C18H15O6P	358.0606
hydroxyphenyl diphenyl phosphate_TP2	<chem>Oc1ccc(OP([O-])(=O)Oc2ccccc2)cc1</chem>	C12H11O5P	266.0344

hydroxyphenyl diphenyl phosphate_TP3	<chem>Oc1ccc(O)cc1</chem>	C6H6O2	110.0368
hydroxyphenyl diphenyl phosphate_TP4	<chem>Oc1ccccc1</chem>	C6H6O	94.0419
hydroxyphenyl diphenyl phosphate_TP5	<chem>[O-]P(=O)(Oc1ccccc1)Oc1ccccc1</chem>	C12H11O4P	250.0395
hydroxyphenyl diphenyl phosphate_TP6	<chem>[O-]P([O-])(=O)Oc1ccccc1</chem>	C6H7O4P	174.0082
hydroxyphenyl diphenyl phosphate_TP7	<chem>Oc1ccc(O)c(O)c1</chem>	C6H6O3	126.0317
hydroxyphenyl diphenyl phosphate_TP8	<chem>Oc1ccc(OP([O-])([O-])=O)cc1</chem>	C6H7O5P	190.0031
hydroxyphenyl diphenyl phosphate_TP9	<chem>[O-]C(=O)CC(=O)C=CC([O-])=O</chem>	C6H6O5	158.0215
hydroxyphenyl diphenyl phosphate_TP10	<chem>Oc1ccc(cc1)C([O-])=O</chem>	C7H6O3	138.0317
hydroxyphenyl diphenyl phosphate_TP11	<chem>Oc1ccccc1O</chem>	C6H6O2	110.0368
hydroxyphenyl diphenyl phosphate_TP12	<chem>Oc1ccc(OP([O-])(=O)Oc2ccccc2)cc1O</chem>	C12H11O6P	282.0293
hydroxyphenyl diphenyl phosphate_TP13	<chem>[O-]C(=O)C(=O)CC(=C)OP(=O)(Oc1ccccc1)Oc1ccccc1</chem>	C17H15O7P	362.0555
hydroxyphenyl diphenyl phosphate_TP14	<chem>[O-]C(=O)C=CC(OP(=O)(Oc1ccccc1)Oc1ccccc1)=CC([O-])=O</chem>	C18H15O8P	390.0505
hydroxyphenyl diphenyl phosphate_TP15	<chem>[O-]C(=O)CC(OP(=O)(Oc1ccccc1)Oc1ccccc1)C=CC([O-])=O</chem>	C18H17O8P	392.0661
hydroxyphenyl diphenyl phosphate_TP16	<chem>[O-]C(=O)CCC(OP(=O)(Oc1ccccc1)Oc1ccccc1)=CC([O-])=O</chem>	C18H17O8P	392.0661
hydroxyphenyl diphenyl phosphate_TP17	<chem>CC(=O)OP(=O)(Oc1ccccc1)Oc1ccccc1</chem>	C14H13O5P	292.0501
hydroxyphenyl diphenyl phosphate_TP18	<chem>CC(CC(=O)C([O-])=O)OP(=O)(Oc1ccccc1)Oc1ccccc1</chem>	C17H17O7P	364.0712
hydroxyphenyl diphenyl phosphate_TP19	<chem>[O-]C(=O)C(=O)CC(=C)OP([O-])(=O)Oc1ccccc1</chem>	C11H11O7P	286.0242
hydroxyphenyl diphenyl phosphate_TP20	<chem>[O-]C(=O)C=CC(OP([O-])(=O)Oc1ccccc1)=CC([O-])=O</chem>	C12H11O8P	314.0192
hydroxyphenyl diphenyl phosphate_TP21	<chem>CC(=O)CC(=O)C([O-])=O</chem>	C5H6O4	130.0266
hydroxyphenyl diphenyl phosphate_TP22	<chem>Oc1ccc(OP([O-])([O-])=O)cc1O</chem>	C6H7O6P	205.9980
hydroxyphenyl diphenyl phosphate_TP23	<chem>OC(C=CC([O-])=O)=CC([O-])=O</chem>	C6H6O5	158.0215
hydroxyphenyl diphenyl phosphate_TP24	<chem>[O-]C(=O)C=CC=CC([O-])=O</chem>	C6H6O4	142.0266
hydroxyphenyl diphenyl phosphate_TP25	<chem>Oc1ccc(cc1O)C([O-])=O</chem>	C7H6O4	154.0266
hydroxyphenyl diphenyl phosphate_TP26	<chem>[O-]C(=O)c1ccccc1</chem>	C7H6O2	122.0368
hydroxyphenyl diphenyl phosphate_TP27	<chem>[O-]C(=O)CCC(=O)CC([O-])=O</chem>	C6H8O5	160.0372
lamotrigine_TP1	<chem>Nc1nnc(c(N)n1)-c1c(O)c(O)cc(Cl)c1Cl</chem>	C9H7Cl2N5O2	286.9977
lamotrigine_TP2	<chem>Nc1nnc(c(N)n1)-c1ccccc1Cl</chem>	C9H8ClN5	221.0468
lamotrigine_TP3	<chem>Nc1nnc(c(N)n1)-c1cccc(Cl)c1</chem>	C9H8ClN5	221.0468
lamotrigine_TP4	<chem>Nc1nnc(c(N)n1)-c1cc(O)c(O)c(Cl)c1Cl</chem>	C9H7Cl2N5O2	286.9977
lamotrigine_TP5	<chem>Nc1nnc(C=C(Cl)C(Cl)C(=O)C([O-])=O)c(N)n1</chem>	C8H7Cl2N5O3	290.9926
lamotrigine_TP6	<chem>Nc1nnc(C=CC([O-])=O)C(Cl)=C(Cl)C([O-])=O)c(N)n1</chem>	C9H7Cl2N5O4	318.9875
lamotrigine_TP7	<chem>Nc1nnc(c(N)n1)-c1cc(O)c(O)c(Cl)c1</chem>	C9H8ClN5O2	253.0367
lamotrigine_TP8	<chem>Nc1nnc(c(N)n1)-c1cc(O)c(O)cc1Cl</chem>	C9H8ClN5O2	253.0367
lamotrigine_TP9	<chem>Nc1nnc(c(N)n1)-c1ccc(O)c(O)c1Cl</chem>	C9H8ClN5O2	253.0367
lamotrigine_TP10	<chem>Nc1nnc(c(N)n1)-c1ccccc1</chem>	C9H9N5	187.0858

lamotrigine_TP11	<chem>Nc1nnc(c(N)n1)-c1cc(Cl)cc(O)c1O</chem>	C9H8ClN5O2	253.0367
lamotrigine_TP12	<chem>Nc1nnc(c(N)n1)-c1c(Cl)ccc(O)c1O</chem>	C9H8ClN5O2	253.0367
lamotrigine_TP13	<chem>Nc1nnc(C(C([O-])=O)=C(Cl)C(Cl)=CC([O-])=O)c(N)n1</chem>	C9H7Cl2N5O4	318.9875
lamotrigine_TP14	<chem>Nc1nnc(C([O-])=O)c(N)n1</chem>	C4H5N5O2	155.0443
lamotrigine_TP15	<chem>[O-]C(=O)C(=O)CC(Cl)=CCl</chem>	C5H4Cl2O3	181.9537
lamotrigine_TP16	<chem>[O-]C(=O)C(=O)CC(Cl)CCl</chem>	C5H6Cl2O3	183.9694
lamotrigine_TP17	<chem>Nc1cnnc(N)n1</chem>	C3H5N5	111.0545
lamotrigine_TP18	<chem>[O-]C(=O)C(=O)CC=CCl</chem>	C5H5ClO3	147.9927
lamotrigine_TP19	<chem>[O-]C(=O)C(=O)CC(Cl)=C</chem>	C5H5ClO3	147.9927
lamotrigine_TP20	<chem>Nc1nnc(C=C(Cl)C(Cl)=CC([O-])=O)c(N)n1</chem>	C8H7Cl2N5O2	274.9977
lamotrigine_TP21	<chem>Nc1nnc(C(C(Cl)C(Cl)=CC([O-])=O)C([O-])=O)c(N)n1</chem>	C9H9Cl2N5O4	321.0032
lamotrigine_TP22	<chem>Nc1nnc(C(C([O-])=O)=C(Cl)C(Cl)CC([O-])=O)c(N)n1</chem>	C9H9Cl2N5O4	321.0032
lamotrigine_TP23	<chem>Nc1nnc(CC([O-])=O)c(N)n1</chem>	C5H7N5O2	169.0600
lamotrigine_TP24	<chem>Nc1nnc(C(C([O-])=O)=C(Cl)C=CC([O-])=O)c(N)n1</chem>	C9H8ClN5O4	285.0265
lamotrigine_TP25	<chem>Nc1nnc(C(=CC(Cl)=CC([O-])=O)C([O-])=O)c(N)n1</chem>	C9H8ClN5O4	285.0265
lamotrigine_TP26	<chem>Nc1nnc(c(N)n1)-c1cccc(O)c1O</chem>	C9H9N5O2	219.0756
lamotrigine_TP27	<chem>Nc1nnc(C(=C)C(Cl)C(=O)C([O-])=O)c(N)n1</chem>	C8H8ClN5O3	257.0316
lamotrigine_TP28	<chem>Nc1nnc(C(C=CC([O-])=O)=C(Cl)C([O-])=O)c(N)n1</chem>	C9H8ClN5O4	285.0265
lamotrigine_TP29	<chem>Nc1nnc(C(CC(=O)C([O-])=O)=CCl)c(N)n1</chem>	C8H8ClN5O3	257.0316
lamotrigine_TP30	<chem>Nc1nnc(c(N)n1)-c1ccc(O)c(O)c1</chem>	C9H9N5O2	219.0756
lamotrigine_TP31	<chem>Nc1nnc(C(=CC([O-])=O)C(Cl)=CC([O-])=O)c(N)n1</chem>	C9H8ClN5O4	285.0265
lamotrigine_TP32	<chem>Nc1nnc(C(=CC([O-])=O)C=C(Cl)C([O-])=O)c(N)n1</chem>	C9H8ClN5O4	285.0265
lamotrigine_TP33	<chem>Nc1nnc(C(CC([O-])=O)C(Cl)=C(Cl)C([O-])=O)c(N)n1</chem>	C9H9Cl2N5O4	321.0032
lamotrigine_TP34	<chem>Nc1nnc(C=C(Cl)CC(=O)C([O-])=O)c(N)n1</chem>	C8H8ClN5O3	257.0316
lamotrigine_TP35	<chem>Nc1nnc(C(=CC([O-])=O)C(Cl)C(Cl)C([O-])=O)c(N)n1</chem>	C9H9Cl2N5O4	321.0032
lamotrigine_TP36	<chem>Nc1nnc(C=CC(Cl)C(=O)C([O-])=O)c(N)n1</chem>	C8H8ClN5O3	257.0316
lamotrigine_TP37	<chem>Nc1nnc(CC(Cl)=O)c(N)n1</chem>	C5H6ClN5O	187.0261
lamotrigine_TP38	<chem>Nc1nnc(CC(Cl)C(Cl)C(=O)C([O-])=O)c(N)n1</chem>	C8H9Cl2N5O3	293.0082
losartan_TP1	<chem>O=Cc1ccc(cc1)-c1cccc1-c1nn[nH]n1</chem>	C14H10N4O	250.0855
losartan_TP2	<chem>CCCCc1nc(Cl)c(C=O)n1Cc1ccc(cc1)-c1cccc1-c1nn[nH]n1</chem>	C22H21ClN6O	420.1465
losartan_TP3	<chem>CCCCc1nc(Cl)c(CO)[nH]1</chem>	C8H13ClN2O	188.0716
losartan_TP4	<chem>CCCCc1ncc(CO)n1Cc1ccc(cc1)-c1cccc1-c1nn[nH]n1</chem>	C22H24N6O	388.2012
losartan_TP5	<chem>CCCCc1nc(Cl)c(CO)n1Cc1ccc(c(O)c1O)-c1cccc1-c1nn[nH]n1</chem>	C22H23ClN6O3	454.1520
losartan_TP6	<chem>CCCCc1nc(Cl)c(CO)n1Cc1ccc(cc1)-c1c(O)c(O)ccc1-c1nn[nH]n1</chem>	C22H23ClN6O3	454.1520
losartan_TP7	<chem>[O-]C(=O)C(=O)CC=Cc1nn[nH]n1</chem>	C6H6N4O3	182.0440
losartan_TP8	<chem>CCCCc1nc(Cl)c(CO)n1Cc1ccc(cc1)C([O-])=O</chem>	C16H19ClN2O3	322.1084
losartan_TP9	<chem>CCCCc1nc(Cl)c(CO)n1CC(=CC=C(C([O-])=O)c1cccc1-c1nn[nH]n1)C([O-])=O</chem>	C22H23ClN6O5	486.1418
losartan_TP10	<chem>CCCCc1nc(Cl)c(C=O)n1Cc1ccc(cc1)-c1c(O)c(O)ccc1-c1nn[nH]n1</chem>	C22H21ClN6O3	452.1364
losartan_TP11	<chem>[O-]C(=O)c1cccc1-c1nn[nH]n1</chem>	C8H6N4O2	190.0491
losartan_TP12	<chem>CCCCc1ncc(CO)n1Cc1ccc(cc1)-c1c(O)c(O)ccc1-c1nn[nH]n1</chem>	C22H24N6O3	420.1910
losartan_TP13	<chem>CCCCc1nc(Cl)c(CO)n1CC(C=C)C(=O)C([O-])=O</chem>	C14H19ClN2O4	314.1033
losartan_TP14	<chem>CCCCc1ncc(CO)n1Cc1ccc(c(O)c1O)-c1cccc1-c1nn[nH]n1</chem>	C22H24N6O3	420.1910
losartan_TP15	<chem>CCCCc1nc(Cl)c(C=O)n1Cc1ccc(c(O)c1O)-c1cccc1-c1nn[nH]n1</chem>	C22H21ClN6O3	452.1364
losartan_TP16	<chem>Oc1ccc(-c2nn[nH]n2)c(c1O)-c1ccc(C=O)cc1</chem>	C14H10N4O3	282.0753
losartan_TP17	<chem>CCCCc1ncc(C=O)n1Cc1ccc(cc1)-c1cccc1-c1nn[nH]n1</chem>	C22H22N6O	386.1855
losartan_TP18	<chem>CCCCc1ncc(CO)[nH]1</chem>	C8H14N2O	154.1106

losartan_TP19	<chem>Oc1c(C=O)ccc(c1O)-c1ccccc1-c1nn[nH]n1</chem>	C14H10N4O3	282.0753
losartan_TP20	<chem>CCCCc1nc(Cl)c(C([O-])=O)n1Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1</chem>	C22H21ClN6O2	436.1415
losartan_TP21	<chem>CCCCc1nc(Cl)c(C=O)[nH]1</chem>	C8H11ClN2O	186.0560
losartan_TP22	<chem>[O-]C(=O)c1ccc(cc1)-c1ccccc1-c1nn[nH]n1</chem>	C14H10N4O2	266.0804
losartan_TP23	<chem>Oc1ccc(cc1O)-c1ccccc1-c1nn[nH]n1</chem>	C13H10N4O2	254.0804
losartan_TP24	<chem>c1ccc(cc1)-c1ccccc1-c1nn[nH]n1</chem>	C13H10N4	222.0905
losartan_TP25	<chem>CCCCc1nc(Cl)c([nH]1)C([O-])=O</chem>	C8H11ClN2O2	202.0509
losartan_TP26	<chem>Oc1c(O)c(ccc1C([O-])=O)-c1ccccc1-c1nn[nH]n1</chem>	C14H10N4O4	298.0702
losartan_TP27	<chem>CCCCc1nc(Cl)cn1Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1</chem>	C21H21ClN6	392.1516
losartan_TP28	<chem>Oc1ccc(-c2nn[nH]n2)c(-c2ccc(cc2)C([O-])=O)c1O</chem>	C14H10N4O4	298.0702
losartan_TP29	<chem>CCCCc1ncc(C([O-])=O)n1Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1</chem>	C22H22N6O2	402.1804
losartan_TP30	<chem>CCCCc1nc(Cl)c(C([O-])=O)n1Cc1ccc(c(O)c1O)-c1ccccc1-c1nn[nH]n1</chem>	C22H21ClN6O4	468.1313
losartan_TP31	<chem>CCCCc1ncc(C=O)[nH]1</chem>	C8H12N2O	152.0950
losartan_TP32	<chem>[O-]C(=O)C(=O)C(C=C)C=O</chem>	C6H6O4	142.0266
losartan_TP33	<chem>CCCCc1ncc(C=O)n1Cc1ccc(c(O)c1O)-c1ccccc1-c1nn[nH]n1</chem>	C22H22N6O3	418.1753
losartan_TP34	<chem>[O-]C(=O)C(C=O)=CC=C(C([O-])=O)c1ccccc1-c1nn[nH]n1</chem>	C14H10N4O5	314.0651
losartan_TP35	<chem>CCCCc1nc(Cl)c(C=O)n1CC(C=C)C(=O)C([O-])=O</chem>	C14H17ClN2O4	312.0877
losartan_TP36	<chem>CCCCc1nc(Cl)c(CO)n1CCC(=O)C([O-])=O</chem>	C12H17ClN2O4	288.0877
losartan_TP37	<chem>[O-]C(=O)c1ccc(C=O)cc1</chem>	C8H6O3	150.0317
losartan_TP38	<chem>CCCCc1nc(Cl)c(CO)n1CC(CC)C(=O)C([O-])=O</chem>	C14H21ClN2O4	316.1190
losartan_TP39	<chem>CCCCc1nc(Cl)c(C([O-])=O)n1Cc1ccc(cc1)-c1c(O)c(O)ccc1-c1nn[nH]n1</chem>	C22H21ClN6O4	468.1313
losartan_TP40	<chem>CCCCc1ncc(CO)n1CC(C=C)C(=O)C([O-])=O</chem>	C14H20N2O4	280.1423
losartan_TP41	<chem>Oc1cccc(-c2nn[nH]n2)c1O</chem>	C7H6N4O2	178.0491
losartan_TP42	<chem>CCCCc1ncc(C=O)n1Cc1ccc(cc1)-c1c(O)c(O)ccc1-c1nn[nH]n1</chem>	C22H22N6O3	418.1753
losartan_TP43	<chem>CCCCc1ncc(CO)n1CC(=CC=C(C([O-])=O)c1ccccc1-c1nn[nH]n1)C([O-])=O</chem>	C22H24N6O5	452.1808
losartan_TP44	<chem>Oc1ccc(-c2nn[nH]n2)c(C([O-])=O)c1O</chem>	C8H6N4O4	222.0389
losartan_TP45	<chem>Oc1ccc(C([O-])=O)c(-c2nn[nH]n2)c1O</chem>	C8H6N4O4	222.0389
losartan_TP46	<chem>Oc1cc(C([O-])=O)c(cc1O)-c1nn[nH]n1</chem>	C8H6N4O4	222.0389
losartan_TP47	<chem>CCCCc1nc(Cl)c(C=O)n1CC(=CC=C(C([O-])=O)c1ccccc1-c1nn[nH]n1)C([O-])=O</chem>	C22H21ClN6O5	484.1262
losartan_TP48	<chem>CCCCc1nc(Cl)c(CO)n1CC(=CC=Cc1ccccc1-c1nn[nH]n1)C([O-])=O</chem>	C21H23ClN6O3	442.1520
losartan_TP49	<chem>CCCCc1nc(Cl)c(CO)n1CC(CC=C(C([O-])=O)c1ccccc1-c1nn[nH]n1)C([O-])=O</chem>	C22H25ClN6O5	488.1575
losartan_TP50	<chem>CCCCc1nc(Cl)c(CO)n1CC(=CCC(C([O-])=O)c1ccccc1-c1nn[nH]n1)C([O-])=O</chem>	C22H25ClN6O5	488.1575
losartan_TP51	<chem>CCCCc1ncc(CO)n1Cc1ccc(cc1)C([O-])=O</chem>	C16H20N2O3	288.1474
losartan_TP52	<chem>CCCCc1nc(Cl)c(CO)n1Cc1ccc(O)c(O)c1</chem>	C15H19ClN2O3	310.1084
losartan_TP53	<chem>CCCCc1nc(Cl)c(C=O)n1Cc1ccc(cc1)C([O-])=O</chem>	C16H17ClN2O3	320.0928
losartan_TP54	<chem>CCCCc1nc(Cl)c(CO)n1Cc1ccc(C([O-])=O)c(O)c1O</chem>	C16H19ClN2O5	354.0982
losartan_TP55	<chem>CCCCc1nc(Cl)c(CO)n1Cc1ccccc1</chem>	C15H19ClN2O	278.1186
losartan_TP56	<chem>[O-]C(=O)C(=O)CCCC1nn[nH]n1</chem>	C6H8N4O3	184.0596
metamfepramone_TP1	<chem>CNC(C)C(=O)c1ccccc1</chem>	C10H13NO	163.0997
metamfepramone_TP2	<chem>CC(=O)C(=O)c1ccccc1</chem>	C9H8O2	148.0524
metamfepramone_TP3	<chem>CC(N)C(=O)c1ccccc1</chem>	C9H11NO	149.0841
metamfepramone_TP4	<chem>OCC(=O)C(=O)c1ccccc1</chem>	C9H8O3	164.0473
metamfepramone_TP5	<chem>O=CC(=O)C(=O)c1ccccc1</chem>	C9H6O3	162.0317

metoprolol_TP1	COCCc1ccc(OCC(O)CN)cc1	C12H19NO3	225.1365
metoprolol_TP2	CC(C)NCC(O)COc1ccc(CCO)cc1	C14H23NO3	253.1678
metoprolol_TP3	COCCc1ccc(OCC(=O)CNC(C)C)cc1	C15H23NO3	265.1678
metoprolol_TP4	COCCc1ccc(OCC(O)C=O)cc1	C12H16O4	224.1049
metoprolol_TP5	COCCc1ccc(O)cc1	C9H12O2	152.0837
metoprolol_TP6	CC(C)NCC(O)C=O	C6H13NO2	131.0946
metoprolol_TP7	CC(C)NCC(O)COc1ccc(CC=O)cc1	C14H21NO3	251.1521
metoprolol_TP8	COCCc1ccc(OCCC(O)NC(C)C)cc1	C15H25NO3	267.1834
metoprolol_TP9	COCCc1ccc(OCCC=O)cc1	C12H16O3	208.1099
metoprolol_TP10	CC(C)NCC(O)COc1ccc(CC([O-])=O)cc1	C14H21NO4	267.1471
metoprolol_TP11	Oc1ccc(CC=O)cc1	C8H8O2	136.0524
metoprolol_TP12	CC(C)NCC(O)C([O-])=O	C6H13NO3	147.0895
metoprolol_TP13	CC(C)NCC(=O)COc1ccc(CC=O)cc1	C14H19NO3	249.1365
metoprolol_TP14	CC(C)NCC(=O)C=O	C6H11NO2	129.0790
metoprolol_TP15	COCC(O)c1ccc(O)cc1	C9H12O3	168.0786
metoprolol_TP16	OCCc1ccc(O)cc1	C8H10O2	138.0681
metoprolol_TP17	NCC(O)COc1ccc(CC=O)cc1	C11H15NO3	209.1052
metoprolol_TP18	COCCc1ccc(OCC(O)C([O-])=O)cc1	C12H16O5	240.0998
metoprolol_TP19	COCCc1ccc(OCC(=O)C=O)cc1	C12H14O4	222.0892
metoprolol_TP20	COCCc1ccc(OCC(=O)CN)cc1	C12H17NO3	223.1208
metoprolol_TP21	OCCc1ccc(OCC(O)C=O)cc1	C11H14O4	210.0892
metoprolol_TP22	CC(C)NCC(=O)COc1ccc(CCO)cc1	C14H21NO3	251.1521
metoprolol_TP23	CC(C)NC(O)CCOc1ccc(CCO)cc1	C14H23NO3	253.1678
metoprolol_TP24	NCC(O)COc1ccc(CCO)cc1	C11H17NO3	211.1208
metoprolol_TP25	COCCc1ccc(OCCC(N)O)cc1	C12H19NO3	225.1365
metoprolol_TP26	NC(O)CCOc1ccc(CCO)cc1	C11H17NO3	211.1208
metoprolol_TP27	OCCc1ccc(OCCC=O)cc1	C11H14O3	194.0943
metoprolol_TP28	OCCc1ccc(OCC(=O)C=O)cc1	C11H12O4	208.0736
metoprolol_TP29	NCC(=O)COc1ccc(CCO)cc1	C11H15NO3	209.1052
metoprolol_TP30	NCC(=O)COc1ccc(CC=O)cc1	C11H13NO3	207.0895
metoprolol_TP31	OCCc1ccc(OCC(O)C([O-])=O)cc1	C11H14O5	226.0841
metoprolol_TP32	COCCc1ccc(OCC(=O)C([O-])=O)cc1	C12H14O5	238.0841
metoprolol_TP33	OC(COc1ccc(CC=O)cc1)C([O-])=O	C11H12O5	224.0685
metoprolol_TP34	OC(C=O)c1ccc(O)cc1	C8H8O3	152.0473
metoprolol_TP35	COCC(=O)c1ccc(O)cc1	C9H10O3	166.0630
metoprolol_TP36	OCC(O)c1ccc(O)cc1	C8H10O3	154.0630
metoprolol_TP37	NCC(O)COc1ccc(CC([O-])=O)cc1	C11H15NO4	225.1001
metoprolol_TP38	CC(C)NCC(=O)C([O-])=O	C6H11NO3	145.0739
metoprolol_TP39	CC(C)NCC(=O)COc1ccc(CC([O-])=O)cc1	C14H19NO4	265.1314
metoprolol_TP40	CC(C)NC(O)CC([O-])=O	C6H13NO3	147.0895
metoprolol_TP41	Oc1ccc(CC([O-])=O)cc1	C8H8O3	152.0473
metoprolol_TP42	OC(COc1ccc(CC([O-])=O)cc1)C=O	C11H12O5	224.0685
metoprolol_TP43	CC(C)NC(O)CCOc1ccc(CC([O-])=O)cc1	C14H21NO4	267.1471
metoprolol_TP44	COCCc1ccc(OCCC([O-])=O)cc1	C12H16O4	224.1049
minoxidil_TP1	Nc1cc(NCCCCC=O)nc(=N)n1O	C9H15N5O2	225.1226
minoxidil_TP2	Nc1cc(NCCCCC([O-])=O)nc(=N)n1O	C9H15N5O3	241.1175

minoxidil_TP3	[O-]C(=O)CCCC=O	C5H8O3	116.0473
minoxidil_TP4	Nc1cc(N)n(O)c(=N)n1	C4H7N5O	141.0651
minoxidil_TP5	Nc1cc(NCCC([O-])=O)nc(=N)n1O	C7H11N5O3	213.0862
oxprenolol_TP1	NCC(O)COc1ccccc1OCC=C	C12H17NO3	223.1208
oxprenolol_TP2	OC(COc1ccccc1OCC=C)C=O	C12H14O4	222.0892
oxprenolol_TP3	CC(C)NCC(=O)COc1ccccc1OCC=C	C15H21NO3	263.1521
oxprenolol_TP4	Oc1ccccc1OCC=C	C9H10O2	150.0681
oxprenolol_TP5	CC(C)NCC(O)C=O	C6H13NO2	131.0946
oxprenolol_TP6	CC(C)NCC(O)COc1ccccc1O	C12H19NO3	225.1365
oxprenolol_TP7	CC(C)NCC(O)COc1ccccc1OCC1CO1	C15H23NO4	281.1627
oxprenolol_TP8	CCCOc1ccccc1OCC(O)CNC(C)C	C15H25NO3	267.1834
oxprenolol_TP9	CC(C)NC(O)CCOc1ccccc1OCC=C	C15H23NO3	265.1678
oxprenolol_TP10	NCC(=O)COc1ccccc1OCC=C	C12H15NO3	221.1052
oxprenolol_TP11	NCC(O)COc1ccccc1OCC1CO1	C12H17NO4	239.1158
oxprenolol_TP12	NCC(O)COc1ccccc1O	C9H13NO3	183.0895
oxprenolol_TP13	CCCOc1ccccc1OCC(O)CN	C12H19NO3	225.1365
oxprenolol_TP14	NC(O)CCOc1ccccc1OCC=C	C12H17NO3	223.1208
oxprenolol_TP15	OC(COc1ccccc1OCC=C)C([O-])=O	C12H14O5	238.0841
oxprenolol_TP16	CC(C)NCC(=O)COc1ccccc1O	C12H17NO3	223.1208
oxprenolol_TP17	C=CCOc1ccccc1OCC(=O)C=O	C12H12O4	220.0736
oxprenolol_TP18	CC(C)NCC(=O)C=O	C6H11NO2	129.0790
oxprenolol_TP19	CCCOc1ccccc1OCC(=O)CNC(C)C	C15H23NO3	265.1678
oxprenolol_TP20	CC(C)NC(O)CCOc1ccccc1OCC1CO1	C15H23NO4	281.1627
oxprenolol_TP21	CC(C)NCC(=O)COc1ccccc1OCC1CO1	C15H21NO4	279.1471
oxprenolol_TP22	CC(C)NCC(O)COc1ccccc1OCC(O)CO	C15H25NO5	299.1733
oxprenolol_TP23	CCCOc1ccccc1OCC(O)C=O	C12H16O4	224.1049
oxprenolol_TP24	CCCOc1ccccc1O	C9H12O2	152.0837
oxprenolol_TP25	CCCOc1ccccc1OCCC(O)NC(C)C	C15H25NO3	267.1834
oxprenolol_TP26	C=CCOc1ccccc1OCCC=O	C12H14O3	206.0943
oxprenolol_TP27	CCCOc1ccccc1OCCC(N)O	C12H19NO3	225.1365
oxprenolol_TP28	CCCOc1ccccc1OCC(=O)CN	C12H17NO3	223.1208
oxprenolol_TP29	Oc1ccccc1O	C6H6O2	110.0368
oxprenolol_TP30	Oc1ccccc1OCC1CO1	C9H10O3	166.0630
oxprenolol_TP31	NC(O)CCOc1ccccc1O	C9H13NO3	183.0895
oxprenolol_TP32	NC(O)CCOc1ccccc1OCC1CO1	C12H17NO4	239.1158
oxprenolol_TP33	OC(COc1ccccc1OCC1CO1)C=O	C12H14O5	238.0841
oxprenolol_TP34	NCC(=O)COc1ccccc1O	C9H11NO3	181.0739
oxprenolol_TP35	NCC(O)COc1ccccc1OCC(O)CO	C12H19NO5	257.1263
oxprenolol_TP36	NCC(=O)COc1ccccc1OCC1CO1	C12H15NO4	237.1001
oxprenolol_TP37	OC(COc1ccccc1OCC1CO1)C([O-])=O	C12H14O6	254.0790
oxprenolol_TP38	[O-]C(=O)C(=O)COc1ccccc1OCC=C	C12H12O5	236.0685
oxprenolol_TP39	OC(COc1ccccc1O)C([O-])=O	C9H10O5	198.0528
oxprenolol_TP40	CCCOc1ccccc1OCC(O)C([O-])=O	C12H16O5	240.0998
oxprenolol_TP41	CCCOc1ccccc1OCC(=O)C=O	C12H14O4	222.0892
oxprenolol_TP42	CC(C)NCC(=O)C([O-])=O	C6H11NO3	145.0739
oxprenolol_TP43	Oc1ccccc1OCC(=O)C=O	C9H8O4	180.0423

oxprenolol_TP44	<chem>O=CC(=O)COc1ccccc1OCC1CO1</chem>	C12H12O5	236.0685
oxprenolol_TP45	<chem>CC(C)NCC(=O)COc1ccccc1OCC(O)CO</chem>	C15H23NO5	297.1576
oxprenolol_TP46	<chem>CC(O)COc1ccccc1O</chem>	C9H12O3	168.0786
oxprenolol_TP47	<chem>OCC(O)COc1ccccc1O</chem>	C9H12O4	184.0736
oxprenolol_TP48	<chem>[O-]C(=O)C(=O)CC=C</chem>	C5H6O3	114.0317
oxprenolol_TP49	<chem>[O-]C(=O)C=CC=CC([O-])=O</chem>	C6H6O4	142.0266
oxprenolol_TP50	<chem>Oc1ccccc1OCCC=O</chem>	C9H10O3	166.0630
oxprenolol_TP51	<chem>CC(C)NC(O)CCOc1ccccc1OCC(O)CO</chem>	C15H25NO5	299.1733
oxprenolol_TP52	<chem>CC(C)NCC(O)COc1ccccc1OCC(O)C=O</chem>	C15H23NO5	297.1576
oxprenolol_TP53	<chem>CC(C)NCC(O)COc1ccccc1OCC(=O)CO</chem>	C15H23NO5	297.1576
oxprenolol_TP54	<chem>OCC(O)COc1ccccc1OCC(O)C=O</chem>	C12H16O6	256.0947
oxprenolol_TP55	<chem>OC(COc1ccccc1O)C=O</chem>	C9H10O4	182.0579
oxprenolol_TP56	<chem>O=CCCOc1ccccc1OCC1CO1</chem>	C12H14O4	222.0892
oxprenolol_TP57	<chem>CC(C)NC(O)CCOc1ccccc1O</chem>	C12H19NO3	225.1365
oxprenolol_TP58	<chem>CC(C)NCC(O)C([O-])=O</chem>	C6H13NO3	147.0895
oxprenolol_TP59	<chem>CCCOc1ccccc1OCCC=O</chem>	C12H16O3	208.1099
oxprenolol_TP60	<chem>[O-]C(=O)CCOc1ccccc1OCC=C</chem>	C12H14O4	222.0892
pentoxifylline_TP1	<chem>CC(=O)CCCCn1c(=O)n(C)c2nc[nH]c2c1=O</chem>	C12H16N4O3	264.1222
pentoxifylline_TP2	<chem>CC(=O)CCCC=O</chem>	C6H10O2	114.0681
pentoxifylline_TP3	<chem>Cn1cnc2n(C)c(=O)[nH]c(=O)c12</chem>	C7H8N4O2	180.0647
pentoxifylline_TP4	<chem>CC(=O)CCCCn1c(=O)n(C)c2[nH]c(=O)n(C)c2c1=O</chem>	C13H18N4O4	294.1328
pentoxifylline_TP5	<chem>Cn1c2nc[nH]c2c(=O)n(CCCCC(=O)CO)c1=O</chem>	C12H16N4O4	280.1172
pentoxifylline_TP6	<chem>CC(=O)CCCCn1c(=O)n(C)c2[nH]c(=O)[nH]c2c1=O</chem>	C12H16N4O4	280.1172
pentoxifylline_TP7	<chem>CC(=O)C(O)CCCn1c(=O)n(C)c2nc[nH]c2c1=O</chem>	C12H16N4O4	280.1172
pentoxifylline_TP8	<chem>CC(=O)CCC(O)Cn1c(=O)n(C)c2nc[nH]c2c1=O</chem>	C12H16N4O4	280.1172
pentoxifylline_TP9	<chem>Cn1c2nc[nH]c2c(=O)[nH]c1=O</chem>	C6H6N4O2	166.0491
pentoxifylline_TP10	<chem>CC(=O)CCCC([O-])=O</chem>	C6H10O3	130.0630
pentoxifylline_TP11	<chem>Cn1cnc2[nH]c(=O)[nH]c(=O)c12</chem>	C6H6N4O2	166.0491
pentoxifylline_TP12	<chem>Cn1c2c([nH]c1=O)n(C)c(=O)[nH]c2=O</chem>	C7H8N4O3	196.0596
pentoxifylline_TP13	<chem>Cn1c2c([nH]c1=O)n(C)c(=O)n(CCCCC(=O)CO)c2=O</chem>	C13H18N4O5	310.1277
pentoxifylline_TP14	<chem>CC(=O)C(O)CCCn1c(=O)n(C)c2[nH]c(=O)n(C)c2c1=O</chem>	C13H18N4O5	310.1277
pentoxifylline_TP15	<chem>CC(=O)CCC(O)Cn1c(=O)n(C)c2[nH]c(=O)n(C)c2c1=O</chem>	C13H18N4O5	310.1277
pentoxifylline_TP16	<chem>CC(=O)CCCC(O)n1c(=O)n(C)c2[nH]c(=O)n(C)c2c1=O</chem>	C13H18N4O5	310.1277
pentoxifylline_TP17	<chem>CC(=O)CCC(=O)Cn1c(=O)n(C)c2[nH]c(=O)n(C)c2c1=O</chem>	C13H16N4O5	308.1121
pentoxifylline_TP18	<chem>CC(=O)C(=O)CCCn1c(=O)n(C)c2[nH]c(=O)n(C)c2c1=O</chem>	C13H16N4O5	308.1121
pentoxifylline_TP19	<chem>Cn1c2c([nH]c1=O)n(C)c(=O)n(CCCCC(=O)C=O)c2=O</chem>	C13H16N4O5	308.1121
pentoxifylline_TP20	<chem>Cn1c2c([nH]c1=O)[nH]c(=O)[nH]c2=O</chem>	C6H6N4O3	182.0440
pentoxifylline_TP21	<chem>CC(=O)CCC(O)C=O</chem>	C6H10O3	130.0630
pentoxifylline_TP22	<chem>CC(=O)C(O)CCC=O</chem>	C6H10O3	130.0630
pentoxifylline_TP23	<chem>CC(=O)CC([O-])=O</chem>	C4H6O3	102.0317
pentoxifylline_TP24	<chem>OCC(=O)CCCC=O</chem>	C6H10O3	130.0630
pentoxifylline_TP25	<chem>O=c1[nH]c2nc[nH]c2c(=O)[nH]1</chem>	C5H4N4O2	152.0334
pentoxifylline_TP26	<chem>CC(=O)CCC(=O)Cn1c(=O)n(C)c2nc[nH]c2c1=O</chem>	C13H14N4O5	306.0964
pentoxifylline_TP27	<chem>CC(=O)CCCC(O)n1c(=O)n(C)c2nc[nH]c2c1=O</chem>	C12H16N4O4	280.1172
pentoxifylline_TP28	<chem>Cn1c2[nH]c(=O)[nH]c2c(=O)[nH]c1=O</chem>	C6H6N4O3	182.0440
pentoxifylline_TP29	<chem>CC(=O)C(=O)CCCn1c(=O)n(C)c2nc[nH]c2c1=O</chem>	C12H14N4O4	278.1015

pentoxifylline_TP30	<chem>CC(=O)CCC(O)Cn1c(=O)n(C)c2[nH]c(=O)[nH]c2c1=O</chem>	C12H16N4O5	296.1121
pentoxifylline_TP31	<chem>CC(=O)C(O)CCCN1c(=O)n(C)c2[nH]c(=O)[nH]c2c1=O</chem>	C12H16N4O5	296.1121
pentoxifylline_TP32	<chem>Cn1c2[nH]c(=O)[nH]c2c(=O)n(CCCCC(=O)CO)c1=O</chem>	C12H16N4O5	296.1121
pentoxifylline_TP33	<chem>Cn1c2nc[nH]c2c(=O)n(CCCCC(=O)C=O)c1=O</chem>	C12H14N4O4	278.1015
phenazone_TP1	<chem>Cc1cc(=O)n(-c2cccc(O)c2O)n1C</chem>	C11H12N2O3	220.0848
phenazone_TP2	<chem>Cn1c(CO)cc(=O)n1-c1cccc1</chem>	C11H12N2O2	204.0899
phenazone_TP3	<chem>Cc1cc(=O)n(C([O-])=O)n1C</chem>	C6H8N2O3	156.0535
phenazone_TP4	<chem>[O-]C(=O)C(=O)CC=C</chem>	C5H6O3	114.0317
phenazone_TP5	<chem>Cn1c(CO)cc(=O)n1-c1cccc(O)c1O</chem>	C11H12N2O4	236.0797
phenazone_TP6	<chem>Cn1c(C=O)cc(=O)n1-c1cccc1</chem>	C11H10N2O2	202.0742
phenazone_TP7	<chem>Cn1c(CO)cc(=O)n1C([O-])=O</chem>	C6H8N2O4	172.0484
phenazone_TP8	<chem>Cn1c(C=O)cc(=O)n1-c1cccc(O)c1O</chem>	C11H10N2O4	234.0641
phenazone_TP9	<chem>Cn1c(cc(=O)n1-c1cccc1)C([O-])=O</chem>	C11H10N2O3	218.0691
phenazone_TP10	<chem>Cn1c(cc(=O)n1C([O-])=O)C([O-])=O</chem>	C6H6N2O5	186.0277
phenprobamate_TP1	<chem>O=CCCc1cccc1</chem>	C9H10O	134.0732
phenprobamate_TP2	<chem>OC(COC(O)=N)Cc1cccc1</chem>	C10H13NO3	195.0895
phenprobamate_TP3	<chem>[O-]C(=O)CCc1cccc1</chem>	C9H10O2	150.0681
phenprobamate_TP4	<chem>OC(Cc1cccc1)C=O</chem>	C9H10O2	150.0681
phenprobamate_TP5	<chem>OC(=N)OCC(=O)Cc1cccc1</chem>	C10H11NO3	193.0739
phenprobamate_TP6	<chem>[O-]C(=O)c1cccc1</chem>	C7H6O2	122.0368
phenprobamate_TP7	<chem>OC(Cc1cccc1)C([O-])=O</chem>	C9H10O3	166.0630
phenprobamate_TP8	<chem>O=CC(=O)Cc1cccc1</chem>	C9H8O2	148.0524
phenprobamate_TP9	<chem>OC(C(=O)COC(O)=N)c1cccc1</chem>	C10H11NO4	209.0688
pyroquilon_TP1	<chem>OC1CN2c3c1cccc3CCC2=O</chem>	C11H11NO2	189.0790
pyroquilon_TP2	<chem>[O-]C(=O)CCc1cccc2CCNc12</chem>	C11H13NO2	191.0946
pyroquilon_TP3	<chem>O=C1CN2c3c1cccc3CCC2=O</chem>	C11H9NO2	187.0633
pyroquilon_TP4	<chem>OC1CNc2c1cccc2CCC([O-])=O</chem>	C11H13NO3	207.0895
pyroquilon_TP5	<chem>OC1Cc2cccc3CCC(=O)N1c23</chem>	C11H11NO2	189.0790
pyroquilon_TP6	<chem>Nc1c(CCC([O-])=O)cccc1CC=O</chem>	C11H13NO3	207.0895
pyroquilon_TP7	<chem>[O-]C(=O)c1cccc2CCNc12</chem>	C9H9NO2	163.0633
pyroquilon_TP8	<chem>O=C1CCc2cccc3C(=O)OCN1c23</chem>	C11H9NO3	203.0582
pyroquilon_TP9	<chem>[O-]C(=O)CCc1cccc2C(=O)CNc12</chem>	C11H11NO3	205.0739
pyroquilon_TP10	<chem>Nc1c(CCC([O-])=O)cccc1C(O)C=O</chem>	C11H13NO4	223.0845
pyroquilon_TP11	<chem>OC1CNc2c1cccc2C([O-])=O</chem>	C9H9NO3	179.0582
pyroquilon_TP12	<chem>OC1Cc2cccc(CCC([O-])=O)c2N1</chem>	C11H13NO3	207.0895
pyroquilon_TP13	<chem>O=CCc1cccc2CCC(=O)Nc12</chem>	C11H11NO2	189.0790
pyroquilon_TP14	<chem>Nc1c(CCC([O-])=O)cccc1CC([O-])=O</chem>	C11H13NO4	223.0845
pyroquilon_TP15	<chem>Oc1cc2CCNc2c(C([O-])=O)c1O</chem>	C9H9NO4	195.0532
pyroquilon_TP16	<chem>Oc1cc(C([O-])=O)c2NCCc2c1O</chem>	C9H9NO4	195.0532
pyroquilon_TP17	<chem>Oc1ccc2CCNc2c1O</chem>	C8H9NO2	151.0633
pyroquilon_TP18	<chem>Nc1c(CC=O)cccc1C([O-])=O</chem>	C9H9NO3	179.0582
sotalol_TP1	<chem>CC(C)NCC(O)c1ccc(NS(C)(=O)=O)c(O)c1O</chem>	C12H20N2O5S	304.1093
sotalol_TP2	<chem>CS(=O)(=O)Nc1ccc(cc1)C(O)CN</chem>	C9H14N2O3S	230.0725
sotalol_TP3	<chem>CC(C)NCC(=O)c1ccc(NS(C)(=O)=O)cc1</chem>	C12H18N2O3S	270.1038
sotalol_TP4	<chem>CS(=O)(=O)Nc1ccc(cc1)C(O)C=O</chem>	C9H11NO4S	229.0409
sotalol_TP5	<chem>CC(C)NCC(O)c1ccc(N)cc1</chem>	C11H18N2O	194.1419

sotalol_TP6	<chem>CC(C)NC(O)Cc1ccc(NS(C)(=O)=O)cc1</chem>	C12H20N2O3S	272.1195
sotalol_TP7	<chem>CS(=O)(=O)Nc1ccc(CC=O)cc1</chem>	C9H11NO3S	213.0460
sotalol_TP8	<chem>CC(C)NC(O)Cc1ccc(N)cc1</chem>	C11H18N2O	194.1419
sotalol_TP9	<chem>CC(C)NCC(O)c1ccc(O)c(O)c1</chem>	C11H17NO3	211.1208
sotalol_TP10	<chem>CC(C)NCC(=O)c1ccc(N)cc1</chem>	C11H16N2O	192.1263
sotalol_TP11	<chem>Nc1ccc(cc1)C(O)C=O</chem>	C8H9NO2	151.0633
sotalol_TP12	<chem>NCC(O)c1ccc(N)cc1</chem>	C8H12N2O	152.0950
sotalol_TP13	<chem>CS(=O)(=O)Nc1ccc(cc1)C(O)C([O-])=O</chem>	C9H11NO5S	245.0358
sotalol_TP14	<chem>CS(=O)(=O)Nc1ccc(cc1)C(=O)C=O</chem>	C9H9NO4S	227.0252
sotalol_TP15	<chem>CS(=O)(=O)Nc1ccc(cc1)C(=O)CN</chem>	C9H12N2O3S	228.0569
sotalol_TP16	<chem>CS(=O)(=O)Nc1ccc(CC(N)O)cc1</chem>	C9H14N2O3S	230.0725
sotalol_TP17	<chem>CS(=O)(=O)Nc1ccc(C(O)C=O)c(O)c1O</chem>	C9H11NO6S	261.0307
sotalol_TP18	<chem>CC(C)NCC(=O)c1ccc(NS(C)(=O)=O)c(O)c1O</chem>	C12H18N2O5S	302.0936
sotalol_TP19	<chem>CS(=O)(=O)Nc1ccc(C(O)CN)c(O)c1O</chem>	C9H14N2O5S	262.0623
sotalol_TP20	<chem>CC(C)NCC(O)C(C=C)C(=O)C([O-])=O</chem>	C10H17NO4	215.1158
sotalol_TP21	<chem>CC(C)NC(O)Cc1ccc(NS(C)(=O)=O)c(O)c1O</chem>	C12H20N2O5S	304.1093
sotalol_TP22	<chem>CC(C)NCC(O)c1ccc(N)c(O)c1O</chem>	C11H18N2O3	226.1317
sotalol_TP23	<chem>CC(C)NCC(O)C=CCC(=O)C([O-])=O</chem>	C10H17NO4	215.1158
sotalol_TP24	<chem>CC(C)NC(O)Cc1ccc(N)c(O)c1O</chem>	C11H18N2O3	226.1317
sotalol_TP25	<chem>Nc1ccc(C(O)C=O)c(O)c1O</chem>	C8H9NO4	183.0532
sotalol_TP26	<chem>CS(=O)(=O)Nc1ccc(CC=O)c(O)c1O</chem>	C9H11NO5S	245.0358
sotalol_TP27	<chem>CC(C)NCC(O)CC(=O)C([O-])=O</chem>	C8H15NO4	189.1001
sotalol_TP28	<chem>CC(C)NCC([O-])=O</chem>	C5H11NO2	117.0790
sotalol_TP29	<chem>[O-]C(=O)C(=O)CC=C</chem>	C5H6O3	114.0317
sotalol_TP30	<chem>CCC(C(O)CNC(C)C)C(=O)C([O-])=O</chem>	C10H19NO4	217.1314
sotalol_TP31	<chem>NCC(O)c1ccc(N)c(O)c1O</chem>	C8H12N2O3	184.0848
sotalol_TP32	<chem>CC(C)NC(O)CC(C=C)C(=O)C([O-])=O</chem>	C10H17NO4	215.1158
sotalol_TP33	<chem>OC(C=O)C(C=C)C(=O)C([O-])=O</chem>	C7H8O5	172.0372
sotalol_TP34	<chem>NCC(O)C(C=C)C(=O)C([O-])=O</chem>	C7H11NO4	173.0688
sotalol_TP35	<chem>CS(=O)(=O)Nc1ccc(CC(N)O)c(O)c1O</chem>	C9H14N2O5S	262.0623
sotalol_TP36	<chem>CC(C)NCC(=O)c1ccc(N)c(O)c1O</chem>	C11H16N2O3	224.1161
sotalol_TP37	<chem>CC(C)NCC(=O)C(C=C)C(=O)C([O-])=O</chem>	C10H15NO4	213.1001
sotalol_TP38	<chem>CS(=O)(=O)Nc1ccc(C(=O)CN)c(O)c1O</chem>	C9H12N2O5S	260.0467
sotalol_TP39	<chem>CS(=O)(=O)Nc1ccc(C(=O)C=O)c(O)c1O</chem>	C9H9NO6S	259.0151
sotalol_TP40	<chem>CS(=O)(=O)Nc1ccc(C(O)C([O-])=O)c(O)c1O</chem>	C9H11NO7S	277.0256
sotalol_TP41	<chem>CS(=O)(=O)Nc1ccc(cc1)C(=O)C([O-])=O</chem>	C9H9NO5S	243.0201
sotalol_TP42	<chem>NC(O)Cc1ccc(N)cc1</chem>	C8H12N2O	152.0950
sotalol_TP43	<chem>NCC(=O)c1ccc(N)cc1</chem>	C8H10N2O	150.0793
sotalol_TP44	<chem>Nc1ccc(cc1)C(O)C([O-])=O</chem>	C8H9NO3	167.0582
sotalol_TP45	<chem>Nc1ccc(cc1)C(=O)C=O</chem>	C8H7NO2	149.0477
sotalol_TP46	<chem>NCC(O)c1ccc(O)c(O)c1</chem>	C8H11NO3	169.0739
sotalol_TP47	<chem>CC(C)NCC(=O)c1ccc(O)c(O)c1</chem>	C11H15NO3	209.1052
sotalol_TP48	<chem>OC(C=O)c1ccc(O)c(O)c1</chem>	C8H8O4	168.0423
sotalol_TP49	<chem>CC(C)NCC(O)C(C=CC([O-])=O)=CC([O-])=O</chem>	C11H17NO5	243.1107
sotalol_TP50	<chem>CC(C)NCC(O)C(=C)CC(=O)C([O-])=O</chem>	C10H17NO4	215.1158
sotalol_TP51	<chem>CC(C)NC(O)Cc1ccc(O)c(O)c1</chem>	C11H17NO3	211.1208

sotalol_TP52	<chem>Nc1ccc(CC=O)cc1</chem>	C8H9NO	135.0684
sotalol_TP53	<chem>CS(=O)(=O)Nc1ccc(CC([O-])=O)cc1</chem>	C9H11NO4S	229.0409
sulfamethoxazole_TP1	<chem>Cc1cc(N)no1</chem>	C4H6N2O	98.0480
sulfamethoxazole_TP2	<chem>Nc1ccc(cc1)S([O-])(=O)=O</chem>	C6H7NO3S	173.0147
sulfamethoxazole_TP3	<chem>Nc1cc(CO)on1</chem>	C4H6N2O2	114.0429
sulfamethoxazole_TP4	<chem>Oc1ccc(cc1)S([O-])(=O)=O</chem>	C6H6O4S	173.9987
sulfamethoxazole_TP5	<chem>Nc1cc(C=O)on1</chem>	C4H4N2O2	112.0273
sulfamethoxazole_TP6	<chem>Oc1ccc(O)cc1</chem>	C6H6O2	110.0368
sulfamethoxazole_TP7	<chem>Oc1ccc(cc1O)S([O-])(=O)=O</chem>	C6H6O5S	189.9936
sulfamethoxazole_TP8	<chem>Oc1ccc(O)c(O)c1</chem>	C6H6O3	126.0317
sulfapyridine_TP1	<chem>Nc1ccc(c(O)c1O)S(=O)(=O)Nc1cccn1</chem>	C11H11N3O4S	281.0470
sulfapyridine_TP2	<chem>Nc1cccn1</chem>	C5H6N2	94.0531
sulfapyridine_TP3	<chem>Nc1ccc(cc1)S([O-])(=O)=O</chem>	C6H7NO3S	173.0147
sulfapyridine_TP4	<chem>Nc1ccc(cc1)S(=O)(=O)Nc1ccc(O)c(O)n1</chem>	C11H11N3O4S	281.0470
sulfapyridine_TP5	<chem>[O-]C(=O)C(=O)CC=CS(=O)(=O)Nc1cccn1</chem>	C10H10N2O5S	270.0310
sulfapyridine_TP6	<chem>Nc1ccc(c(O)c1O)S([O-])(=O)=O</chem>	C6H7NO5S	205.0045
sulfapyridine_TP7	<chem>Oc1ccc(cc1)S([O-])(=O)=O</chem>	C6H6O4S	173.9987
sulfapyridine_TP8	<chem>Nc1ccc(O)c(O)n1</chem>	C5H6N2O2	126.0429
sulfapyridine_TP9	<chem>Nc1ccc(cc1)S(=O)(=O)NC(C=CC([O-])=O)=NC([O-])=O</chem>	C11H11N3O6S	313.0369
sulfapyridine_TP10	<chem>[O-]C(=O)C(=O)CCCS(=O)(=O)Nc1cccn1</chem>	C10H12N2O5S	272.0467
sulfapyridine_TP11	<chem>[O-]C(=O)CS(=O)(=O)Nc1cccn1</chem>	C7H8N2O4S	216.0205
sulfapyridine_TP12	<chem>[O-]C(=O)C(=O)CC=CS([O-])(=O)=O</chem>	C5H6O6S	193.9885
sulfapyridine_TP13	<chem>NC(C=C)C(=O)C([O-])=O</chem>	C5H7NO3	129.0426
sulfapyridine_TP14	<chem>Oc1ccc(c(O)c1O)S([O-])(=O)=O</chem>	C6H6O6S	205.9885
sulfapyridine_TP15	<chem>Oc1ccc(O)cc1</chem>	C6H6O2	110.0368
sulfapyridine_TP16	<chem>Oc1ccc(cc1O)S([O-])(=O)=O</chem>	C6H6O5S	189.9936
sulfapyridine_TP17	<chem>Oc1ccc(O)c(O)c1</chem>	C6H6O3	126.0317
sulfapyridine_TP18	<chem>NC(C=CC([O-])=O)=NC([O-])=O</chem>	C5H6N2O4	158.0328
sulfapyridine_TP19	<chem>Nc1ccc(cc1)S(=O)(=O)NC(=NC([O-])=O)C(O)CC([O-])=O</chem>	C11H13N3O7S	331.0474
sulfapyridine_TP20	<chem>Nc1ccc(cc1)S(=O)(=O)NC(CCC([O-])=O)=NC([O-])=O</chem>	C11H13N3O6S	315.0525
sulpiride_TP1	<chem>COc1ccc(cc1C(=O)NCCC1CCCN1)S(N)(=O)=O</chem>	C13H19N3O4S	313.1096
sulpiride_TP2	<chem>CCNC(CCC=O)CNC(=O)c1cc(ccc1OC)S(N)(=O)=O</chem>	C15H23N3O5S	357.1358
sulpiride_TP3	<chem>CCNCCCC(=O)CNC(=O)c1cc(ccc1OC)S(N)(=O)=O</chem>	C15H23N3O5S	357.1358
sulpiride_TP4	<chem>CCN1CCCC1CNC(=O)c1cc(ccc1O)S(N)(=O)=O</chem>	C14H21N3O4S	327.1253
sulpiride_TP5	<chem>COc1ccc(cc1C([O-])=O)S(N)(=O)=O</chem>	C8H9NO5S	231.0201
sulpiride_TP6	<chem>CCN1CCCC1CN</chem>	C7H16N2	128.1313
sulpiride_TP7	<chem>CCN1CCCC1CNC(=O)c1cc(ccc1OC)S([O-])(=O)=O</chem>	C15H22N2O5S	342.1249
sulpiride_TP8	<chem>COc1ccc(cc1C(N)=O)S(N)(=O)=O</chem>	C8H10N2O4S	230.0361
sulpiride_TP9	<chem>CCN1CCCC1C=O</chem>	C7H13NO	127.0997
sulpiride_TP10	<chem>COc1ccc(cc1C(=O)NCCC(=O)CCCN)S(N)(=O)=O</chem>	C13H19N3O5S	329.1045
sulpiride_TP11	<chem>NS(=O)(=O)c1ccc(O)c(c1)C(=O)NCCC1CCCN1</chem>	C12H17N3O4S	299.0940
sulpiride_TP12	<chem>COc1ccc(cc1C(=O)NCCC1CCCN1)S([O-])(=O)=O</chem>	C13H18N2O5S	314.0936
sulpiride_TP13	<chem>NCCC1CCCN1</chem>	C5H12N2	100.1000
sulpiride_TP14	<chem>O=CC1CCCN1</chem>	C5H9NO	99.0684
sulpiride_TP15	<chem>COc1ccc(cc1C(=O)NCCC(N)CCC=O)S(N)(=O)=O</chem>	C13H19N3O5S	329.1045
sulpiride_TP16	<chem>CCNC(CCC([O-])=O)CNC(=O)c1cc(ccc1OC)S(N)(=O)=O</chem>	C15H23N3O6S	373.1308

sulpiride_TP17	CCNCCCC(=O)CNC(=O)c1cc(ccc1O)S(N)(=O)=O	C14H21N3O5S	343.1202
sulpiride_TP18	CCNCCCC(=O)CN	C7H16N2O	144.1263
sulpiride_TP19	CCNCCCC(=O)CNC(=O)c1cc(ccc1OC)S([O-])(=O)=O	C15H22N2O6S	358.1199
sulpiride_TP20	CCNCCCC(=O)C=O	C7H13NO2	143.0946
sulpiride_TP21	CCNC(CCC=O)CNC(=O)c1cc(ccc1O)S(N)(=O)=O	C14H21N3O5S	343.1202
sulpiride_TP22	CCN1CCCC1CNC(=O)c1cc(ccc1O)S([O-])(=O)=O	C14H20N2O5S	328.1093
sulpiride_TP23	CCNC(CN)CCC=O	C7H16N2O	144.1263
sulpiride_TP24	CCN1CCCC1CNC(=O)c1cc(O)c(O)cc1OC	C15H22N2O4	294.1580
sulpiride_TP25	CCN1CCCC1CNC(=O)c1cc(O)ccc1OC	C15H22N2O3	278.1630
sulpiride_TP26	CCN1CCCC1CNC(=O)c1c(O)c(O)ccc1OC	C15H22N2O4	294.1580
sulpiride_TP27	CCNC(CCC=O)CNC(=O)c1cc(ccc1OC)S([O-])(=O)=O	C15H22N2O6S	358.1199
sulpiride_TP28	COc1ccc(O)cc1C([O-])=O	C8H8O4	168.0423
sulpiride_TP29	COc1ccc(O)c(O)c1C([O-])=O	C8H8O5	184.0372
sulpiride_TP30	COc1cc(O)c(O)cc1C([O-])=O	C8H8O5	184.0372
sulpiride_TP31	COc1ccc(cc1C(=O)NCC(N)CCC([O-])=O)S(N)(=O)=O	C13H19N3O6S	345.0995
sulpiride_TP32	[O-]C(=O)C1CCCN1	C5H9NO2	115.0633
sulpiride_TP33	COc1ccc(cc1C(N)=O)S([O-])(=O)=O	C8H9NO5S	231.0201
sulpiride_TP34	COc1ccc(cc1C([O-])=O)S([O-])(=O)=O	C8H8O6S	232.0042
sulpiride_TP35	NS(=O)(=O)c1ccc(O)c(c1)C([O-])=O	C7H7NO5S	217.0045
sulpiride_TP36	NCC(N)CCC=O	C5H12N2O	116.0950
sulpiride_TP37	NC(=O)c1cc(ccc1O)S(N)(=O)=O	C7H8N2O4S	216.0205
sulpiride_TP38	COc1cc(O)c(O)cc1C(=O)NCC1CCCN1	C13H18N2O4	266.1267
sulpiride_TP39	NCCCC(=O)CN	C5H12N2O	116.0950
sulpiride_TP40	COc1ccc(cc1C(=O)NCC(N)CCC=O)S([O-])(=O)=O	C13H18N2O6S	330.0886
sulpiride_TP41	COc1ccc(O)cc1C(=O)NCC1CCCN1	C13H18N2O3	250.1317
sulpiride_TP42	NCCCC(=O)C=O	C5H9NO2	115.0633
sulpiride_TP43	COc1ccc(O)c(O)c1C(=O)NCC1CCCN1	C13H18N2O4	266.1267
sulpiride_TP44	Oc1ccc(cc1C(=O)NCC1CCCN1)S([O-])(=O)=O	C12H16N2O5S	300.0780
sulpiride_TP45	NC(CCC=O)CNC(=O)c1cc(ccc1O)S(N)(=O)=O	C12H17N3O5S	315.0889
sulpiride_TP46	COc1ccc(cc1C(=O)NCC(=O)CCCN)S([O-])(=O)=O	C13H18N2O6S	330.0886
sulpiride_TP47	NCCCC(=O)CNC(=O)c1cc(ccc1O)S(N)(=O)=O	C12H17N3O5S	315.0889
sulpiride_TP48	COc1ccc(cc1C(=O)NCC(=O)CCC=O)S(N)(=O)=O	C13H16N2O6S	328.0729
sulpiride_TP49	CCNC(CNC(=O)c1cc(ccc1OC)S(N)(=O)=O)C([O-])=O	C13H19N3O6S	345.0995
sulpiride_TP50	CCNC(CCC([O-])=O)CNC(=O)c1cc(ccc1O)S(N)(=O)=O	C14H21N3O6S	359.1151
sulpiride_TP51	COc1ccc(cc1C(=O)NCC(=O)CCC([O-])=O)S(N)(=O)=O	C13H16N2O7S	344.0678
sulpiride_TP52	CCNC(CN)CCC([O-])=O	C7H16N2O2	160.1212
sulpiride_TP53	CCNC(CCC([O-])=O)C=O	C7H13NO3	159.0895
sulpiride_TP54	CCNC(CCC([O-])=O)CNC(=O)c1cc(ccc1OC)S([O-])(=O)=O	C15H22N2O7S	374.1148
sulpiride_TP55	NS(=O)(=O)c1ccc(O)c(c1)C(=O)NCC(=O)CCC=O	C12H14N2O6S	314.0573
sulpiride_TP56	NCC(=O)CCC=O	C5H9NO2	115.0633
sulpiride_TP57	COc1ccc(cc1C(=O)NCC(=O)CCC=O)S([O-])(=O)=O	C13H15N07S	329.0569
sulpiride_TP58	CCNCCCC(=O)CNC(=O)c1cc(ccc1O)S([O-])(=O)=O	C14H20N2O6S	344.1042
sulpiride_TP59	CCNCCCC(=O)CNC(=O)c1cc(O)c(O)cc1OC	C15H22N2O5	310.1529
sulpiride_TP60	CCNCCCC(=O)CNC(=O)c1cc(O)ccc1OC	C15H22N2O4	294.1580
sulpiride_TP61	CCNCCCC(=O)C([O-])=O	C7H13NO3	159.0895
sulpiride_TP62	CCNCCCC(=O)CNC(=O)c1c(O)c(O)ccc1OC	C15H22N2O5	310.1529

sulpiride_TP63	CCN1CCCC1CNC(=O)c1cc(O)c(O)cc1O	C14H20N2O4	280.1423
sulpiride_TP64	CCN1CCCC1CNC(=O)c1c(O)ccc(O)c1O	C14H20N2O4	280.1423
sulpiride_TP65	CCN1CCCC1CNC(=O)c1cc(O)ccc1O	C14H20N2O3	264.1474
sulpiride_TP66	CCN1CCCC1C([O-])=O	C7H13NO2	143.0946
sulpiride_TP67	Oc1ccc(cc1C([O-])=O)S([O-])(=O)=O	C7H6O6S	217.9885
sulpiride_TP68	NC(=O)c1cc(ccc1O)S([O-])(=O)=O	C7H7NO5S	217.0045
sulpiride_TP69	NS(=O)(=O)c1ccc(O)c(O)c1	C6H7NO4S	189.0096
sulpiride_TP70	NS(=O)(=O)c1ccc(O)cc1	C6H7NO3S	173.0147
sulpiride_TP71	CCNC(CCC=O)CNC(=O)c1cc(ccc1O)S([O-])(=O)=O	C14H20N2O6S	344.1042
sulpiride_TP72	CCN1CCCC1CNC(=O)C(C(=C)OC)C(=O)C([O-])=O	C14H22N2O5	298.1529
sulpiride_TP73	CCN1CCCC1CNC(=O)C(C([O-])=O)=C(OC)C=CC([O-])=O	C15H22N2O6	326.1478
sulpiride_TP74	CCNC(CCC=O)CNC(=O)c1c(O)c(O)ccc1OC	C15H22N2O5	310.1529
sulpiride_TP75	CCNC(CCC=O)CNC(=O)c1cc(O)ccc1OC	C15H22N2O4	294.1580
sulpiride_TP76	COc1ccc(O)c(O)c1C(N)=O	C8H9NO4	183.0532
sulpiride_TP77	COc1ccc(O)cc1C(N)=O	C8H9NO3	167.0582
sulpiride_TP78	COc1cc(O)c(O)cc1C(N)=O	C8H9NO4	183.0532
sulpiride_TP79	CCN1CCCC1CNC(=O)C=C(CC(=O)C([O-])=O)OC	C14H22N2O5	298.1529
sulpiride_TP80	CCN1CCCC1CNC(=O)C(=CC([O-])=O)C(OC)=CC([O-])=O	C15H22N2O6	326.1478
sulpiride_TP81	CCNC(CCC=O)CNC(=O)c1cc(O)c(O)cc1OC	C15H22N2O5	310.1529
sulpiride_TP82	CCNC(CCC=O)C([O-])=O	C7H13NO3	159.0895
telmisartan_TP1	CCCc1nc2c(C)cc(cc2n1Cc1ccc(c(O)c1O)-c1ccccc1C([O-])=O)-c1nc2ccccc2n1C	C33H30N4O4	546.2267
telmisartan_TP2	CCCc1nc2c(C)cc(cc2[nH]1)-c1nc2ccccc2n1C	C19H20N4	304.1688
telmisartan_TP3	CCCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1c(O)c(O)ccc1C([O-])=O)-c1nc2ccccc2n1C	C33H30N4O4	546.2267
telmisartan_TP4	CCCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1ccccc1C([O-])=O)-c1nc2ccccc2[nH]1	C32H28N4O2	500.2212
telmisartan_TP5	CCCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1cccc(O)c1O)-c1nc2ccccc2n1C	C32H30N4O2	502.2369
telmisartan_TP6	[O-]C(=O)c1ccccc1-c1ccc(C=O)cc1	C14H10O3	226.0630
telmisartan_TP7	CCCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1ccccc1C([O-])=O)-c1nc2c(O)c(O)ccc2n1C	C33H30N4O4	546.2267
telmisartan_TP8	CCCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1ccccc1C([O-])=O)-c1nc2ccc(O)c(O)c2n1C	C33H30N4O4	546.2267
telmisartan_TP9	CCCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1ccccc1C([O-])=O)-c1nc(C=CC([O-])=O)c(C([O-])=O)n1C	C33H30N4O6	578.2165
telmisartan_TP10	CCCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1ccccc1C([O-])=O)-c1nc(C([O-])=O)c(C=CC([O-])=O)n1C	C33H30N4O6	578.2165
telmisartan_TP11	CCCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1ccccc1C([O-])=O)-c1nc2ccc(O)c(O)c2[nH]1	C32H28N4O4	532.2111
telmisartan_TP12	CCCc1nc2c(C)cc(cc2[nH]1)-c1nc2ccc(O)c(O)c2n1C	C19H20N4O2	336.1586
telmisartan_TP13	CCCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1ccccc1C([O-])=O)-c1nc2c(O)c(O)ccc2[nH]1	C32H28N4O4	532.2111
telmisartan_TP14	Oc1ccc(c1O)-c1ccc(C=O)cc1	C13H10O3	214.0630
telmisartan_TP15	CCCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1cccc(O)c1O)-c1nc2ccccc2[nH]1	C31H28N4O2	488.2212
telmisartan_TP16	CCCc1nc2c(C)cc(cc2[nH]1)-c1nc2c(O)c(O)ccc2n1C	C19H20N4O2	336.1586
telmisartan_TP17	CCCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)C([O-])=O)-c1nc2ccccc2n1C	C27H26N4O2	438.2056
telmisartan_TP18	[O-]C(=O)c1ccc(cc1)-c1ccccc1C([O-])=O	C14H10O4	242.0579
telmisartan_TP19	CCCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1c(O)c(O)ccc1C([O-])=O)-c1nc2ccccc2[nH]1	C32H28N4O4	532.2111
telmisartan_TP20	CCCc1nc2c(C)cc(cc2[nH]1)-c1nc2ccccc2[nH]1	C18H18N4	290.1531
telmisartan_TP21	[O-]C(=O)C=CCC(=O)C([O-])=O	C6H6O5	158.0215

telmisartan_TP22	Oc1ccc(C([O-])=O)c(c1O)-c1ccc(C=O)cc1	C14H10O5	258.0528
telmisartan_TP23	Oc1c(O)c(ccc1C=O)-c1ccccc1C([O-])=O	C14H10O5	258.0528
telmisartan_TP24	CCc1nc2c(C)cc(cc2n1Cc1ccc(c(O)c1O)-c1ccccc1C([O-])=O)-c1nc2ccccc2[nH]1	C32H28N4O4	532.2111
telmisartan_TP25	CCc1nc2c(C)cc(cc2n1CC(=CC=C(C([O-])=O)c1ccccc1C([O-])=O)C([O-])=O)-c1nc2ccccc2n1C	C33H30N4O6	578.2165
telmisartan_TP26	[O-]C(=O)c1ccccc1C([O-])=O	C8H6O4	166.0266
telmisartan_TP27	CCc1nc2c(C)cc(cc2n1CC(C=C)C(=O)C([O-])=O)-c1nc2ccccc2n1C	C25H26N4O3	430.2005
telmisartan_TP28	CCc1nc2c(C)cc(cc2n1CCC(=O)C([O-])=O)-c1nc2ccccc2n1C	C23H24N4O3	404.1848
telmisartan_TP29	CCc1nc2c(C)cc(cc2n1CC(C)C(=O)C([O-])=O)-c1nc2ccccc2n1C	C25H28N4O3	432.2161
telmisartan_TP30	Oc1ccc(C([O-])=O)c(C([O-])=O)c1O	C8H6O6	198.0164
telmisartan_TP31	CCc1nc2c(C)cc(cc2n1CC(C=C)C(=O)C([O-])=O)-c1nc2ccccc2[nH]1	C24H24N4O3	416.1848
telmisartan_TP32	Oc1cc(C([O-])=O)c(cc1O)C([O-])=O	C8H6O6	198.0164
telmisartan_TP33	[O-]C(=O)C(=O)C(C=C)C=O	C6H6O4	142.0266
telmisartan_TP34	CCc1nc2c(C)cc(cc2n1CC(=CCC(C([O-])=O)c1ccccc1C([O-])=O)C([O-])=O)-c1nc2ccccc2n1C	C33H32N4O6	580.2322
telmisartan_TP35	CCc1nc2c(C)cc(cc2n1CC(=CC=Cc1ccccc1C([O-])=O)C([O-])=O)-c1nc2ccccc2n1C	C32H30N4O4	534.2267
telmisartan_TP36	CCc1nc2c(C)cc(cc2n1CC(CC=C(C([O-])=O)c1ccccc1C([O-])=O)C([O-])=O)-c1nc2ccccc2n1C	C33H32N4O6	580.2322
telmisartan_TP37	CCc1nc2c(C)cc(cc2n1CC(=CC=C(C([O-])=O)c1ccccc1C([O-])=O)C([O-])=O)-c1nc2ccccc2[nH]1	C32H28N4O6	564.2009
telmisartan_TP38	[O-]C(=O)C(C=O)=CC=C(C([O-])=O)c1ccccc1C([O-])=O	C14H10O7	290.0427
telmisartan_TP39	[O-]C(=O)CCCC(=O)C([O-])=O	C6H8O5	160.0372
telmisartan_TP40	CCc1nc2c(CO)cc(cc2[nH]1)-c1nc2ccccc2[nH]1	C18H18N4O	306.1481
telmisartan_TP41	Oc1c(O)c(ccc1C([O-])=O)-c1ccccc1C([O-])=O	C14H10O6	274.0477
telmisartan_TP42	Oc1ccc(C([O-])=O)c(c1O)-c1ccc(cc1)C([O-])=O	C14H10O6	274.0477
telmisartan_TP43	CCC(O)c1nc2c(C)cc(cc2[nH]1)-c1nc2ccccc2[nH]1	C18H18N4O	306.1481
telmisartan_TP44	[O-]C(=O)c1ccc(C=O)cc1	C8H6O3	150.0317
telmisartan_TP45	Oc1ccc(cc1O)-c1ccccc1C([O-])=O	C13H10O4	230.0579
telmisartan_TP46	CCc1nc2c(C)cc(cc2[nH]1)-c1nc2c(O)c(O)ccc2[nH]1	C18H18N4O2	322.1430
telmisartan_TP47	CCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)C([O-])=O)-c1nc2ccccc2[nH]1	C26H24N4O2	424.1899
telmisartan_TP48	CCc1nc2c(C)cc(cc2n1Cc1ccccc1)-c1nc2ccccc2n1C	C26H26N4	394.2157
telmisartan_TP49	Oc1cccc(c1O)-c1ccc(cc1)C([O-])=O	C13H10O4	230.0579
telmisartan_TP50	CCc1nc2c(C)cc(cc2n1Cc1ccc(C([O-])=O)c(O)c1O)-c1nc2ccccc2n1C	C27H26N4O4	470.1954
telmisartan_TP51	CCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)C([O-])=O)-c1nc2c(O)c(O)ccc2n1C	C27H26N4O4	470.1954
telmisartan_TP52	CCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)C([O-])=O)-c1nc2ccc(O)c(O)c2n1C	C27H26N4O4	470.1954
telmisartan_TP53	CCc1nc2c(C)cc(cc2n1Cc1ccc(O)c(O)c1)-c1nc2ccccc2n1C	C26H26N4O2	426.2056
telmisartan_TP54	CCc1nc2c(C)cc(cc2[nH]1)-c1nc2ccc(O)c(O)c2[nH]1	C18H18N4O2	322.1430
telmisartan_TP55	CCc1nc2c(C)cc(cc2[nH]1)-c1nc(C([O-])=O)C(C=CC([O-])=O)n1C	C19H20N4O4	368.1485
telmisartan_TP56	CCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1ccccc1C([O-])=O)-c1nc(C([O-])=O)C(C=CC([O-])=O)[nH]1	C32H28N4O6	564.2009
telmisartan_TP57	CCc1nc2c(C)cc(cc2[nH]1)-c1nc(C=CC([O-])=O)c(C([O-])=O)n1C	C19H20N4O4	368.1485
telmisartan_TP58	CCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1ccccc1C([O-])=O)-c1nc(C=CC([O-])=O)c([nH]1)C([O-])=O	C32H28N4O6	564.2009
telmisartan_TP59	CCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1cccc(O)c1O)-c1nc(C([O-])=O)C(C=CC([O-])=O)n1C	C32H30N4O6	566.2165
telmisartan_TP60	CCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1ccccc1C([O-])=O)-c1nc(C([O-])=O)c(C(O)CC([O-])=O)n1C	C33H32N4O7	596.2271
telmisartan_TP61	CCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1ccccc1C([O-])=O)-c1nc(C([O-])=O)c(CCC([O-])=O)n1C	C33H32N4O6	580.2322

telmisartan_TP62	CCc1nc2c(C)cc(cc2n1Cc1ccc(c(O)c1O)-c1cccc1C([O-])=O)-c1nc(C([O-])=O)c(C=CC([O-])=O)n1C	C33H30N4O8	610.2064
telmisartan_TP63	CCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1c(O)c(O)ccc1C([O-])=O)-c1nc(C([O-])=O)c(C=CC([O-])=O)n1C	C33H30N4O8	610.2064
telmisartan_TP64	CCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1cccc1C([O-])=O)-c1nc(C(O)CC([O-])=O)c(C([O-])=O)n1C	C33H32N4O7	596.2271
telmisartan_TP65	CCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1cccc1C([O-])=O)-c1nc(CCC([O-])=O)c(C([O-])=O)n1C	C33H32N4O6	580.2322
telmisartan_TP66	CCc1nc2c(C)cc(cc2n1Cc1ccc(c(O)c1O)-c1cccc1C([O-])=O)-c1nc(C=CC([O-])=O)c(C([O-])=O)n1C	C33H30N4O8	610.2064
telmisartan_TP67	CCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1c(O)c(O)ccc1C([O-])=O)-c1nc(C=CC([O-])=O)c(C([O-])=O)n1C	C33H30N4O8	610.2064
telmisartan_TP68	CCc1nc2c(C)cc(cc2n1Cc1ccc(cc1)-c1cccc(O)c1O)-c1nc(C=CC([O-])=O)c(C([O-])=O)n1C	C32H30N4O6	566.2165
terbutryn_TP1	CCNc1nc(O)nc(NC(C)(C)C)n1	C9H17N5O	211.1433
terbutryn_TP2	CSc1nc(N)nc(NC(C)(C)C)n1	C8H15N5S	213.1048
terbutryn_TP3	CC(C)(C)Nc1nc(N)nc(O)n1	C7H13N5O	183.1120
terbutryn_TP4	CCNc1nc(O)nc(O)n1	C5H8N4O2	156.0647
terbutryn_TP5	CC(C)(C)Nc1nc(O)nc(O)n1	C7H12N4O2	184.0960
terbutryn_TP6	CC(C)(C)Nc1nc(N)nc(S)n1	C7H13N5S	199.0892
terbutryn_TP7	CS(=O)c1nc(N)nc(NC(C)(C)C)n1	C8H15N5OS	229.0997
terbutryn_TP8	Nc1nc(O)nc(O)n1	C3H4N4O2	128.0334
terbutryn_TP9	Oc1nc(O)nc(O)n1	C3H3N3O3	129.0174
terbutryn_TP10	CC(C)(C)Nc1nc(N)nc(n1)S([O-])=O	C7H13N5O2S	231.0790
terbutryn_TP11	CC(C)(C)Nc1nc(N)nc(n1)S(C)(=O)=O	C8H15N5O2S	245.0946
terbutryn_TP12	CC(C)(C)Nc1nc(N)nc(n1)S([O-])(=O)=O	C7H13N5O3S	247.0739
torasemide_TP1	Cc1cccc(Nc2ccncc2S(=O)(=O)NC(N)=O)c1	C13H14N4O3S	306.0787
torasemide_TP2	CC(C)NC(=O)NS(=O)(=O)c1cnccc1Nc1cccc(CO)c1	C16H20N4O4S	364.1205
torasemide_TP3	Cc1cccc(Nc2ccncc2S(N)(=O)=O)c1	C12H13N3O2S	263.0728
torasemide_TP4	Cc1cccc(Nc2ccncc2S([O-])(=O)=O)c1	C12H12N2O3S	264.0569
torasemide_TP5	Cc1cccc(Nc2c(O)c(O)nc2S([O-])(=O)=O)c1	C12H12N2O5S	296.0467
torasemide_TP6	Cc1cccc(Nc2ccncc2O)c1	C12H12N2O	200.0950
torasemide_TP7	Cc1cc(O)c(O)c(Nc2ccncc2S([O-])(=O)=O)c1	C12H12N2O5S	296.0467
torasemide_TP8	Cc1cc(Nc2ccncc2S([O-])(=O)=O)cc(O)c1O	C12H12N2O5S	296.0467
torasemide_TP9	OCc1cccc(Nc2ccncc2S([O-])(=O)=O)c1	C12H12N2O4S	280.0518
torasemide_TP10	Cc1cc(O)c(O)c(Nc2ccncc2S(N)(=O)=O)c1	C12H13N3O4S	295.0627
torasemide_TP11	Cc1cccc(Nc2c(O)c(O)nc2S(N)(=O)=O)c1	C12H13N3O4S	295.0627
torasemide_TP12	Cc1cc(Nc2ccncc2S(N)(=O)=O)cc(O)c1O	C12H13N3O4S	295.0627
torasemide_TP13	NS(=O)(=O)c1cnccc1Nc1cccc(CO)c1	C12H13N3O3S	279.0678
torasemide_TP14	NC(=O)NS(=O)(=O)c1cnccc1Nc1cccc(CO)c1	C13H14N4O4S	322.0736
torasemide_TP15	CC(C)NC(=O)NS(=O)(=O)c1cnccc1Nc1cccc(C=O)c1	C16H18N4O4S	362.1049
torasemide_TP16	CC(C)NC(=O)NS(=O)(=O)c1cnccc1Nc1cccc(c1)C([O-])=O	C16H18N4O5S	378.0998
torasemide_TP17	NC(=O)NS(=O)(=O)c1cnccc1Nc1cccc(C=O)c1	C13H12N4O4S	320.0579
torasemide_TP18	NS(=O)(=O)c1cnc(O)c(O)c1Nc1cccc(CO)c1	C12H13N3O5S	311.0576
torasemide_TP19	NS(=O)(=O)c1cnccc1Nc1cc(CO)cc(O)c1O	C12H13N3O5S	311.0576
torasemide_TP20	NS(=O)(=O)c1cnccc1Nc1cc(O)c(O)c(CO)c1	C12H13N3O5S	311.0576
torasemide_TP21	NS(=O)(=O)c1cnccc1Nc1cccc(C=O)c1	C12H11N3O3S	277.0521
torasemide_TP22	CC=CC(Nc1cncc1S(N)(=O)=O)=CC([O-])=O)C([O-])=O	C12H13N3O6S	327.0525
torasemide_TP23	CC(C=CNc1ccncc1S(N)(=O)=O)C(=O)C([O-])=O	C11H13N3O5S	299.0576
torasemide_TP24	NS(=O)(=O)c1cnccc1NC(=C)CC(=O)C([O-])=O	C10H11N3O5S	285.0419

torasemide_TP25	<chem>Cc1cccc(NC(C([O-])=O)C(=CNC([O-])=O)S(N)(=O)=O)c1</chem>	C12H15N3O6S	329.0682
torasemide_TP26	<chem>OCc1cc(Nc2ccncc2S([O-])(=O)=O)cc(O)c1O</chem>	C12H12N2O6S	312.0416
torasemide_TP27	<chem>NS(=O)(=O)c1cnccc1NC([O-])=O</chem>	C6H7N3O4S	217.0157
torasemide_TP28	<chem>OCc1cc(O)c(O)c(Nc2ccncc2S([O-])(=O)=O)c1</chem>	C12H12N2O6S	312.0416
torasemide_TP29	<chem>CC(=C)CC(=O)C([O-])=O</chem>	C6H8O3	128.0473
torasemide_TP30	<chem>OCc1cccc(Nc2c(O)c(O)nc2S([O-])(=O)=O)c1</chem>	C12H12N2O6S	312.0416
torasemide_TP31	<chem>[O-]S(=O)(=O)c1cnccc1Nc1cccc(C=O)c1</chem>	C12H10N2O4S	278.0361
torasemide_TP32	<chem>CC(=CC(Nc1ccncc1S([O-])(=O)=O)=CC([O-])=O)C([O-])=O</chem>	C12H12N2O7S	328.0365
torasemide_TP33	<chem>CC(C=CNc1ccncc1S([O-])(=O)=O)C(=O)C([O-])=O</chem>	C11H12N2O6S	300.0416
torasemide_TP34	<chem>[O-]C(=O)C(=O)CC(=C)Nc1ccncc1S([O-])(=O)=O</chem>	C10H10N2O6S	286.0260
torasemide_TP35	<chem>[O-]C(=O)Nc1ccncc1S([O-])(=O)=O</chem>	C6H6N2O5S	217.9997
torasemide_TP36	<chem>OCc1cccc(Nc2ccncc2O)c1</chem>	C12H12N2O2	216.0899
torasemide_TP37	<chem>Cc1cc(Nc2ccncc2O)cc(O)c1O</chem>	C12H12N2O3	232.0848
torasemide_TP38	<chem>Cc1cc(O)c(O)c(Nc2ccncc2O)c1</chem>	C12H12N2O3	232.0848
torasemide_TP39	<chem>Cc1cccc(Nc2c(O)cnc(O)c2O)c1</chem>	C12H12N2O3	232.0848
torasemide_TP40	<chem>Cc1cccc(NC(C([O-])=O)C(=CNC([O-])=O)S([O-])(=O)=O)c1</chem>	C12H14N2O7S	330.0522
tramadol_TP1	<chem>CNC[C@H]1CCCC[C@]1(O)c1cccc(OC)c1</chem>	C15H23NO2	249.1729
tramadol_TP2	<chem>COc1cccc(c1)[C@@]1(O)CCCC[C@@H]1C=O</chem>	C14H18O3	234.1256
tramadol_TP3	<chem>CN(C)C[C@H]1CCCC[C@]1(O)c1cccc(O)c1</chem>	C15H23NO2	249.1729
tramadol_TP4	<chem>COc1cccc(c1)[C@@]1(O)CCCCC1(O)CN(C)C</chem>	C16H25NO3	279.1834
tramadol_TP5	<chem>COc1cccc(c1)[C@@]1(O)CCCC[C@@H]1C([O-])=O</chem>	C14H18O4	250.1205
tramadol_TP6	<chem>COc1cccc(c1)[C@@]1(O)CCCC[C@@H]1CN</chem>	C14H21NO2	235.1572
tramadol_TP7	<chem>CN(C)C[C@H]1CCCC[C@]1(O)c1cccc(O)c1O</chem>	C15H23NO3	265.1678
tramadol_TP8	<chem>CNC[C@H]1CCCC[C@]1(O)c1cccc(O)c1</chem>	C14H21NO2	235.1572
tramadol_TP9	<chem>Oc1cccc(c1)[C@@]1(O)CCCC[C@@H]1C=O</chem>	C13H16O3	220.1099
tramadol_TP10	<chem>CNCC1(O)CCCC[C@]1(O)c1cccc(OC)c1</chem>	C15H23NO3	265.1678
tramadol_TP11	<chem>COc1cccc(c1)[C@@]1(O)CCCCC1(O)C=O</chem>	C14H18O4	250.1205
tramadol_TP12	<chem>CN(C)C[C@H]1CCCC[C@]1(O)c1cc(O)ccc1O</chem>	C15H23NO3	265.1678
tramadol_TP13	<chem>CN(C)CC1(O)CCCC[C@]1(O)c1cccc(O)c1</chem>	C15H23NO3	265.1678
tramadol_TP14	<chem>CN(C)C[C@H]1CCCC[C@]1(O)c1ccc(O)c(O)c1</chem>	C15H23NO3	265.1678
tramadol_TP15	<chem>COc1cccc(c1)[C@@]1(O)CCCCC1C(O)N(C)C</chem>	C16H25NO3	279.1834
tramadol_TP16	<chem>COc1cccc(c1)[C@@]1(O)CCCCC1C=O</chem>	C14H18O3	234.1256
tramadol_TP17	<chem>Oc1ccc(cc1O)[C@@]1(O)CCCC[C@@H]1C=O</chem>	C13H16O4	236.1049
tramadol_TP18	<chem>CN(C)C[C@H]1CCCC[C@]1(O)C=CCC(=O)C([O-])=O</chem>	C14H23NO4	269.1627
tramadol_TP19	<chem>CN(C)C[C@H]1CCCC[C@]1(O)C(=C)CC(=O)C([O-])=O</chem>	C14H23NO4	269.1627
tramadol_TP20	<chem>CN(C)C(O)C1CCCC[C@]1(O)c1cccc(O)c1</chem>	C15H23NO3	265.1678
tramadol_TP21	<chem>Oc1cccc(c1)[C@@]1(O)CCCCC1(O)C=O</chem>	C13H16O4	236.1049
tramadol_TP22	<chem>CN(C)CC1(O)CCCC[C@]1(O)c1cccc(O)c1O</chem>	C15H23NO4	281.1627
tramadol_TP23	<chem>CN(C)CC1(O)CCCC[C@]1(O)c1ccc(O)c(O)c1</chem>	C15H23NO4	281.1627
tramadol_TP24	<chem>CN(C)CC1(O)CCCC[C@]1(O)c1cc(O)ccc1O</chem>	C15H23NO4	281.1627
tramadol_TP25	<chem>CN(C)C[C@H]1CCCC[C@]1(O)C(=O)CC(=O)C=CC([O-])=O</chem>	C15H23NO5	297.1576
tramadol_TP26	<chem>CNC[C@H]1CCCC[C@]1(O)c1ccc(O)c(O)c1</chem>	C14H21NO3	251.1521
tramadol_TP27	<chem>Oc1ccc(O)c(c1)[C@@]1(O)CCCC[C@@H]1C=O</chem>	C13H16O4	236.1049
tramadol_TP28	<chem>CNCC1(O)CCCC[C@]1(O)c1cccc(O)c1</chem>	C14H21NO3	251.1521
tramadol_TP29	<chem>COc1cccc(c1)[C@@]1(O)CCCCC1(O)C([O-])=O</chem>	C14H18O5	266.1154
tramadol_TP30	<chem>CNC(O)C1CCCC[C@]1(O)c1cccc(OC)c1</chem>	C15H23NO3	265.1678

tramadol_TP31	CNC[C@H]1CCCC[C@]1(O)c1cc(O)ccc1O	C14H21NO3	251.1521
tramadol_TP32	CN(C)C[C@H]1CCCC[C@]1(O)C([O-])=O	C10H19NO3	201.1365
tramadol_TP33	CN(C)C[C@H]1CCCC[C@]1(O)C(C=C)C(=O)C([O-])=O	C14H23NO4	269.1627
tramadol_TP34	Oc1cccc(c1O)[C@@]1(O)CCCC[C@@H]1C=O	C13H16O4	236.1049
tramadol_TP35	COc1cccc(c1)[C@@]1(O)CCCC1(O)CN	C14H21NO3	251.1521
tramadol_TP36	CNC[C@H]1CCCC[C@]1(O)c1cccc(O)c1O	C14H21NO3	251.1521
tramadol_TP37	Oc1cccc(c1)[C@@]1(O)CCCC[C@@H]1C([O-])=O	C13H16O4	236.1049
tramadol_TP38	NC[C@H]1CCCC[C@]1(O)c1cccc(O)c1	C13H19NO2	221.1416
tramadol_TP39	COc1cccc(c1)C(=O)CCCCC([O-])=O	C14H18O4	250.1205
tramadol_TP40	COc1cccc(c1)[C@@]1(O)CCCC(O)[C@@H]1C([O-])=O	C14H18O5	266.1154
tramadol_TP41	COc1cccc(c1)[C@@]1(O)CCC(O)C[C@@H]1C([O-])=O	C14H18O5	266.1154
trenbolone_TP1	C[C@]12C=CC3=C4CCOC(=O)C=C4CC[C@H]3[C@@H]1CC[C@@H]2O	C18H22O3	286.1569
trenbolone_TP2	C[C@]12C=CC3=C4CCC(=O)C=C4CC[C@H]3[C@@H]1CCC2=O	C18H20O2	268.1463
trenbolone_TP3	C[C@]12C=CC3[C@@H](CCC4=CC(=O)CCC34)[C@@H]1CC[C@@H]2O	C18H24O2	272.1776
trenbolone_TP4	C[C@]12CCC3=C4CCC(=O)C=C4CC[C@H]3[C@@H]1CC[C@@H]2O	C18H24O2	272.1776
trenbolone_TP5	C[C@]12C=CC3=C4CCC(=O)CC4CC[C@H]3[C@@H]1CC[C@@H]2O	C18H24O2	272.1776
trenbolone_TP6	C[C@]12C=CC3=C4CCC(=O)OCC4CC[C@H]3[C@@H]1CC[C@@H]2O	C18H24O3	288.1725
trenbolone_TP7	C[C@]12CCC3=C4CCC(=O)CC4CC[C@H]3[C@@H]1CC[C@@H]2O	C18H26O2	274.1933
trenbolone_TP8	C[C@]12C=CC3[C@@H](CCC4CC(=O)CCC34)[C@@H]1CC[C@@H]2O	C18H26O2	274.1933
trenbolone_TP9	C[C@]12CCC3[C@@H](CCC4=CC(=O)CCC34)[C@@H]1CC[C@@H]2O	C18H26O2	274.1933
trenbolone_TP10	C[C@]12C=CC3=C4CCC(=O)CC4CC[C@H]3[C@@H]1CCC2=O	C18H22O2	270.1620
trenbolone_TP11	C[C@]12CCC3=C4CCC(=O)C=C4CC[C@H]3[C@@H]1CCC2=O	C18H22O2	270.1620
trenbolone_TP12	C[C@]12C=CC3[C@@H](CCC4=CC(=O)CCC34)[C@@H]1CCC2=O	C18H22O2	270.1620
trenbolone_TP13	CC12OC(=O)CC[C@H]1[C@@H]1CCC3=CC(=O)CCC3=C1C=C2	C18H20O3	284.1412
trenbolone_TP14	C[C@]12CCC3=C4CCOC(=O)C=C4CC[C@H]3[C@@H]1CC[C@@H]2O	C18H24O3	288.1725
trenbolone_TP15	C[C@]12C=CC3[C@@H](CCC4=CC(=O)OCCC34)[C@@H]1CC[C@@H]2O	C18H24O3	288.1725
trenbolone_TP16	C[C@]12C=CC3=C4CCOC(=O)CC4(O)CC[C@H]3[C@@H]1CC[C@@H]2O	C18H24O4	304.1675
trenbolone_TP17	C[C@]12C=CC3=C4CCOC(=O)C=C4CC[C@H]3[C@@H]1CCC2=O	C18H20O3	284.1412
trenbolone_TP18	C[C@]12C=CC3=C(CCO)C(CC[C@H]3[C@@H]1CC[C@@H]2O)=CC([O-])=O	C18H24O4	304.1675
trenbolone_TP19	C[C@]12C=CC3=C4CCOC(=O)CC4CC[C@H]3[C@@H]1CC[C@@H]2O	C18H24O3	288.1725
trenbolone_TP20	C[C@]12C=CC3=C(CCO)C(CC([O-])=O)CC[C@H]3[C@@H]1CC[C@@H]2O	C18H26O4	306.1831
trenbolone_TP21	C[C@]12C=CC3=C4CCOC(=O)CC4CC[C@H]3[C@@H]1CCC2=O	C18H22O3	286.1569
trenbolone_TP22	C[C@]12C=CC3=C(CC=O)C(CC[C@H]3[C@@H]1CC[C@@H]2O)=CC([O-])=O	C18H22O4	302.1518
trenbolone_TP23	C[C@]12C=CC3=C(CCO)C(CC[C@H]3[C@@H]1CCC2=O)=CC([O-])=O	C18H22O4	302.1518
trenbolone_TP24	C[C@]12C=CC3=C(CCO)C(O)(CC([O-])=O)CC[C@H]3[C@@H]1CC[C@@H]2O	C18H26O5	322.1780
trenbolone_TP25	C[C@]12[C@@H](CCC1=O)[C@@H]1CCC3=CC(=O)OCCC3=C1CC2O	C18H22O4	302.1518
trenbolone_TP26	C[C@]12C=CC3[C@@H](CCC4CC(=O)OCCC34)[C@@H]1CC[C@@H]2O	C18H26O3	290.1882
trenbolone_TP27	C[C@]12C=CC3=C4CCOC(=O)CC4(O)CC[C@H]3[C@@H]1CCC2=O	C18H22O4	302.1518

trenbolone_TP28	CC(=O)OCCC1=C2C=C[C@]3(C)[C@@H](O)CC[C@H]3[C@@H]2C CC1=O	C18H24O4	304.1675
trenbolone_TP29	C[C@]12C=CC3C(CCO)C(CC[C@H]3[C@@H]1CC[C@H]2O)=CC([O-])=O	C18H26O4	306.1831
trenbolone_TP30	C[C@]12CCC3=C4CCOC(=O)CC4CC[C@H]3[C@@H]1CC[C@@H]2 O	C18H26O3	290.1882
trenbolone_TP31	C[C@]12C=CC3[C@@H](CCC4=CC(=O)OCCC34)[C@@H]1CCC2= O	C18H22O3	286.1569
trenbolone_TP32	C[C@]12C=CC3[C@@H](CCC4(O)CC(=O)OCCC34)[C@@H]1CC[C @@H]2O	C18H26O4	306.1831
trenbolone_TP33	C[C@]12CCC3=C(CCO)C(CC[C@H]3[C@@H]1CC[C@H]2O)=CC([O-])=O	C18H26O4	306.1831
trenbolone_TP34	C[C@]12CCC3=C4CCOC(=O)C=C4CC[C@H]3[C@@H]1CCC2=O	C18H22O3	286.1569
trenbolone_TP35	C[C@]12CCC3=C4CCOC(=O)CC4(O)CC[C@H]3[C@@H]1CC[C@@ H]2O	C18H26O4	306.1831
trenbolone_TP36	C[C@]12CCC3[C@@H](CCC4=CC(=O)OCCC34)[C@@H]1CC[C@@ H]2O	C18H26O3	290.1882
trenbolone_TP37	CC1(O)C=CC2=C3CCC(=O)C=C3CC[C@H]2[C@@H]1CCC([O-])=O	C18H22O4	302.1518
trenbolone_TP38	CC12OC(=O)CC[C@H]1[C@@H]1CCC3(O)CC(=O)CCC3=C1C=C2	C18H22O4	302.1518
trenbolone_TP39	CC12OC(=O)CC[C@H]1[C@@H]1CCC3=CC(=O)CCC3C1C=C2	C18H22O3	286.1569
trenbolone_TP40	CC12CCC3=C4CCC(=O)C=C4CC[C@H]3[C@@H]1CCC(=O)O2	C18H22O3	286.1569
trenbolone_TP41	CC12OC(=O)CC[C@H]1[C@@H]1CCC3CC(=O)CCC3=C1C=C2	C18H22O3	286.1569
trenbolone_TP42	C[C@]12CCC3[C@@H](CCC4=CC(=O)CCC34)[C@@H]1CCC2=O	C18H24O2	272.1776
trenbolone_TP43	C[C@]12C=CC3[C@@H](CCC4CC(=O)CCC34)[C@@H]1CCC2=O	C18H24O2	272.1776
trenbolone_TP44	C[C@]12CCC3=C4CCC(=O)CC4CC[C@H]3[C@@H]1CCC2=O	C18H24O2	272.1776
trenbolone_TP45	C[C@]12CCC(=O)[C@@H](CCc3cccc(O)c3)[C@@H]1CC[C@@H]2 O	C18H24O3	288.1725
trenbolone_TP46	C[C@]12CCC3[C@@H](CCC4CC(=O)CCC34)[C@@H]1CC[C@@H] 2O	C18H28O2	276.2089
trenbolone_TP47	C[C@]12C=CC3[C@@H](CCC4COC(=O)CCC34)[C@@H]1CC[C@@ H]2O	C18H26O3	290.1882
trenbolone_TP48	C[C@]12CCC3=C4CCC(=O)OCC4CC[C@H]3[C@@H]1CC[C@@H]2 O	C18H26O3	290.1882
trenbolone_TP49	C[C@]12C=CC3=C(CCC([O-])=O)C(CO)CC[C@H]3[C@@H]1CC[C@ @H]2O	C18H26O4	306.1831
trenbolone_TP50	C[C@]12C=CC3=C4CCC(=O)OCC4CC[C@H]3[C@@H]1CCC2=O	C18H22O3	286.1569
trihexyphenidyl_TP1	OC(CC=O)(C1CCCCC1)c1cccc1	C15H20O2	232.1463
trihexyphenidyl_TP2	C1CCNCC1	C5H11N	85.0891
trihexyphenidyl_TP3	OC(CCN1CCCCC1)(c1cccc1)C1(O)CCCCC1	C20H31NO2	317.2355
trihexyphenidyl_TP4	OC(CCNCCCCC=O)(C1CCCCC1)c1cccc1	C20H31NO2	317.2355
trihexyphenidyl_TP5	OC(CC([O-])=O)(C1CCCCC1)c1cccc1	C15H20O3	248.1412
trihexyphenidyl_TP6	OC(CC=O)(c1cccc1)C1(O)CCCCC1	C15H20O3	248.1412
trihexyphenidyl_TP7	NCCCCC=O	C5H11NO	101.0841
trihexyphenidyl_TP8	OC(CCNCCCCC=O)(c1cccc1)C1(O)CCCCC1	C20H31NO3	333.2304
trihexyphenidyl_TP9	OC(CCNCCCCC([O-])=O)(C1CCCCC1)c1cccc1	C20H31NO3	333.2304
trihexyphenidyl_TP10	OC1CCC(CC1)C(O)(CC([O-])=O)c1cccc1	C15H20O4	264.1362
trihexyphenidyl_TP11	OC(C([O-])=O)C(O)(C1CCCCC1)c1cccc1	C15H20O4	264.1362
trihexyphenidyl_TP12	O=C(C1CCCCC1)c1cccc1	C13H16O	188.1201
trihexyphenidyl_TP13	OC1CCCCC1C(O)(CC([O-])=O)c1cccc1	C15H20O4	264.1362
trihexyphenidyl_TP14	OC1CCCC(C1)C(O)(CC([O-])=O)c1cccc1	C15H20O4	264.1362
trihexyphenidyl_TP15	OC(CC([O-])=O)(c1cccc1)C1(O)CCCCC1	C15H20O4	264.1362
trihexyphenidyl_TP16	NCCCCC([O-])=O	C5H11NO2	117.0790
trihexyphenidyl_TP17	OC(CCNCCCCC([O-])=O)(c1cccc1)C1(O)CCCCC1	C20H31NO4	349.2253

trihexyphenidyl_TP18	[O-]C(=O)CCCC=O	C5H8O3	116.0473
trihexyphenidyl_TP19	NCCC(O)(C1CCCCC1)c1ccccc1	C15H23NO	233.1780
trihexyphenidyl_TP20	OC(CCNCCC([O-])=O)(C1CCCCC1)c1ccccc1	C18H27NO3	305.1991
valsartan_TP1	CCCCC(=O)N(CC(C)C)Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1	C23H29N5O	391.2372
valsartan_TP2	CCCCC(=O)N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)[C@H](C([O-])=O)C(C)(C)O	C24H29N5O4	451.2220
valsartan_TP3	CCCC(O)C(=O)N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)[C@@H](C(C)C)C([O-])=O	C24H29N5O4	451.2220
valsartan_TP4	CCCCC(=O)NCc1ccc(cc1)-c1ccccc1-c1nn[nH]n1	C19H21N5O	335.1746
valsartan_TP5	CC(C)C(=O)C([O-])=O	C5H8O3	116.0473
valsartan_TP6	CC(C)[C@H](N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C(=O)CCCCO)C([O-])=O	C24H29N5O4	451.2220
valsartan_TP7	CCCCC([O-])=O	C5H10O2	102.0681
valsartan_TP8	CC(C)[C@H](NCc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C([O-])=O	C19H21N5O2	351.1695
valsartan_TP9	CCCCC(=O)N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)CC(C)(C)O	C23H29N5O2	407.2321
valsartan_TP10	CC(C)CNCc1ccc(cc1)-c1ccccc1-c1nn[nH]n1	C18H21N5	307.1797
valsartan_TP11	CCCCC(=O)NCC(C)C	C9H19NO	157.1467
valsartan_TP12	O=Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1	C14H10N4O	250.0855
valsartan_TP13	CC(C)CN(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C(=O)CCCCO	C23H29N5O2	407.2321
valsartan_TP14	CCCC(O)C(=O)N(CC(C)C)Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1	C23H29N5O2	407.2321
valsartan_TP15	CCCC(O)C(=O)N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)[C@H](C([O-])=O)C(C)(C)O	C24H29N5O5	467.2169
valsartan_TP16	CC(C)(O)C(=O)C([O-])=O	C5H8O4	132.0423
valsartan_TP17	CCCCC(=O)N(CC([O-])=O)Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1	C21H23N5O3	393.1801
valsartan_TP18	CC(C)(O)[C@H](NCc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C([O-])=O	C19H21N5O3	367.1644
valsartan_TP19	CCCCC(=O)N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C(O)(C(C)C)C([O-])=O	C24H29N5O4	451.2220
valsartan_TP20	CC(C)(O)[C@H](N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C(=O)CCCCO)C([O-])=O	C24H29N5O5	467.2169
valsartan_TP21	CCCC(=O)C(=O)N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)[C@@H](C(C)C)C([O-])=O	C25H29N5O4	463.2220
valsartan_TP22	CC(C)[C@H](N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C(=O)CCCC=O)C([O-])=O	C24H27N5O4	449.2063
valsartan_TP23	CCCC(=O)C(=O)N(CC(C)C)Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1	C23H27N5O2	405.2165
valsartan_TP24	CC(C)CN(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C(=O)CCCC=O	C23H27N5O2	405.2165
valsartan_TP25	CCCC(O)C(=O)NCC(C)C	C9H19NO2	173.1416
valsartan_TP26	CCCC(O)C([O-])=O	C5H10O3	118.0630
valsartan_TP27	CC(C)CNC(=O)CCCCO	C9H19NO2	173.1416
valsartan_TP28	[O-]C(=O)c1ccc(cc1)-c1ccccc1-c1nn[nH]n1	C14H10N4O2	266.0804
valsartan_TP29	OCCCCC([O-])=O	C5H10O3	118.0630
valsartan_TP30	CCCCC(=O)NCC(C)(C)O	C9H19NO2	173.1416
valsartan_TP31	CCCCC(N)=O	C5H11NO	101.0841
valsartan_TP32	NCc1ccc(cc1)-c1ccccc1-c1nn[nH]n1	C14H13N5	251.1171
valsartan_TP33	CC(C)CNCc1ccc(cc1)-c1c(O)c(O)ccc1-c1nn[nH]n1	C18H21N5O2	339.1695
valsartan_TP34	CC(C)CNCc1ccc(cc1)c1O)-c1ccccc1-c1nn[nH]n1	C18H21N5O2	339.1695
valsartan_TP35	CC(C)(O)CNCc1ccc(cc1)-c1ccccc1-c1nn[nH]n1	C18H21N5O	323.1746
valsartan_TP36	CCCCC(=O)N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C(O)C(C)C	C23H29N5O2	407.2321
valsartan_TP37	CCCC(O)C(=O)N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)CC(C)(C)O	C23H29N5O3	423.2270
valsartan_TP38	CC(C)(O)CN(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C(=O)CCCCO	C23H29N5O3	423.2270
valsartan_TP39	CC(C)(O)[C@H](N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C(=O)CCCC=O)C([O-])=O	C24H27N5O5	465.2012

valsartan_TP40	<chem>CC(C)C(O)(N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C(=O)CCCCO)C([O-])=O</chem>	C24H29N5O5	467.2169
valsartan_TP41	<chem>CC(C)C(O)(NCc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C([O-])=O</chem>	C19H21N5O3	367.1644
valsartan_TP42	<chem>OCCCCC(=O)N(CC([O-])=O)Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1</chem>	C21H23N5O4	409.1750
valsartan_TP43	<chem>CC(C)(O)[C@H](NCc1ccc(cc1)-c1c(O)c(O)ccc1-c1nn[nH]n1)C([O-])=O</chem>	C19H21N5O5	399.1543
valsartan_TP44	<chem>CC(C)(O)[C@H](NCc1ccc(c(O)c1O)-c1ccccc1-c1nn[nH]n1)C([O-])=O</chem>	C19H21N5O5	399.1543
valsartan_TP45	<chem>CC(C)(O)[C@H](N)C([O-])=O</chem>	C5H11NO3	133.0739
valsartan_TP46	<chem>[O-]C(=O)CNCc1ccc(cc1)-c1ccccc1-c1nn[nH]n1</chem>	C16H15N5O2	309.1226
valsartan_TP47	<chem>OCCCCC(=O)NCc1ccc(cc1)-c1ccccc1-c1nn[nH]n1</chem>	C19H21N5O2	351.1695
valsartan_TP48	<chem>CCCC(O)C(=O)N(CC([O-])=O)Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1</chem>	C21H23N5O4	409.1750
valsartan_TP49	<chem>CCCC(O)C(=O)NCc1ccc(cc1)-c1ccccc1-c1nn[nH]n1</chem>	C19H21N5O2	351.1695
valsartan_TP50	<chem>CCCC(=O)C(=O)N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)[C@H](C([O-])=O)C(C)(C)O</chem>	C24H27N5O5	465.2012
valsartan_TP51	<chem>CCCC(O)C(=O)N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C(O)(C(C)C)C([O-])=O</chem>	C24H29N5O5	467.2169
valsartan_TP52	<chem>CC(C)[C@H](NCc1ccc(c(O)c1O)-c1ccccc1-c1nn[nH]n1)C([O-])=O</chem>	C19H21N5O4	383.1594
valsartan_TP53	<chem>CC(C)[C@H](NCc1ccc(cc1)-c1c(O)c(O)ccc1-c1nn[nH]n1)C([O-])=O</chem>	C19H21N5O4	383.1594
valsartan_TP54	<chem>CC(C)[C@H](N)C([O-])=O</chem>	C5H11NO2	117.0790
valsartan_TP55	<chem>CCCC(=O)C([O-])=O</chem>	C5H8O3	116.0473
valsartan_TP56	<chem>CCCC(O)C(N)=O</chem>	C5H11NO2	117.0790
valsartan_TP57	<chem>CCCC(=O)C(=O)NCc1ccc(cc1)-c1ccccc1-c1nn[nH]n1</chem>	C19H19N5O2	349.1539
valsartan_TP58	<chem>CCC(O)C(=O)C(=O)N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)[C@@H](C(C)C)C([O-])=O</chem>	C24H27N5O5	465.2012
valsartan_TP59	<chem>CC(C)[C@H](N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C(=O)C(=O)CCCCO)C([O-])=O</chem>	C24H27N5O5	465.2012
valsartan_TP60	<chem>NCc1ccc(c(O)c1O)-c1ccccc1-c1nn[nH]n1</chem>	C14H13N5O2	283.1069
valsartan_TP61	<chem>NCc1ccc(cc1)-c1c(O)c(O)ccc1-c1nn[nH]n1</chem>	C14H13N5O2	283.1069
valsartan_TP62	<chem>NC(=O)CCCCO</chem>	C5H11NO2	117.0790
valsartan_TP63	<chem>O=CCCCC(=O)NCc1ccc(cc1)-c1ccccc1-c1nn[nH]n1</chem>	C19H19N5O2	349.1539
valsartan_TP64	<chem>CC(C)[C@H](N(Cc1ccc(cc1)-c1ccccc1-c1nn[nH]n1)C(=O)CCCC([O-])=O)C([O-])=O</chem>	C24H27N5O5	465.2012
valsartan_TP65	<chem>Oc1c(C=O)ccc(c1O)-c1ccccc1-c1nn[nH]n1</chem>	C14H10N4O3	282.0753
valsartan_TP66	<chem>CC(C)[C@H](NCC(=CC=C(C([O-])=O)c1ccccc1-c1nn[nH]n1)C([O-])=O)C([O-])=O</chem>	C19H21N5O6	415.1492
valsartan_TP67	<chem>CC(C)[C@H](NCC(C=C)C(=O)C([O-])=O)C([O-])=O</chem>	C11H17NO5	243.1107
valsartan_TP68	<chem>[O-]C(=O)c1ccccc1-c1nn[nH]n1</chem>	C8H6N4O2	190.0491
valsartan_TP69	<chem>Oc1ccc(-c2nn[nH]n2)c(c1O)-c1ccc(C=O)cc1</chem>	C14H10N4O3	282.0753
valsartan_TP70	<chem>[O-]C(=O)C(=O)CC=Cc1nn[nH]n1</chem>	C6H6N4O3	182.0440
valsartan_TP71	<chem>CC(C)[C@H](NCc1ccc(cc1)C([O-])=O)C([O-])=O</chem>	C13H17NO4	251.1158
venlafaxine_TP1	<chem>CNCC(c1ccc(OC)cc1)C1(O)CCCCC1</chem>	C16H25NO2	263.1885
venlafaxine_TP2	<chem>COc1ccc(cc1)C(C=O)C1(O)CCCCC1</chem>	C15H20O3	248.1412
venlafaxine_TP3	<chem>COc1ccc(cc1)C(O)(CN(C)C)C1(O)CCCCC1</chem>	C17H27NO3	293.1991
venlafaxine_TP4	<chem>CN(C)CC(c1ccc(O)cc1)C1(O)CCCCC1</chem>	C16H25NO2	263.1885
venlafaxine_TP5	<chem>COc1ccc(cc1)C(CN)C1(O)CCCCC1</chem>	C15H23NO2	249.1729
venlafaxine_TP6	<chem>COc1ccc(cc1)C(C([O-])=O)C1(O)CCCCC1</chem>	C15H20O4	264.1362
venlafaxine_TP7	<chem>CNCC(O)(c1ccc(OC)cc1)C1(O)CCCCC1</chem>	C16H25NO3	279.1834
venlafaxine_TP8	<chem>COc1ccc(cc1)C(C(O)N(C)C)C1(O)CCCCC1</chem>	C17H27NO3	293.1991
venlafaxine_TP9	<chem>COc1ccc(cc1)C(O)(C=O)C1(O)CCCCC1</chem>	C15H20O4	264.1362
venlafaxine_TP10	<chem>CNCC(c1ccc(O)cc1)C1(O)CCCCC1</chem>	C15H23NO2	249.1729

venlafaxine_TP11	<chem>Oc1ccc(cc1)C(C=O)C1(O)CCCCC1</chem>	C14H18O3	234.1256
venlafaxine_TP12	<chem>CN(C)CC(O)(c1ccc(O)cc1)C1(O)CCCCC1</chem>	C16H25NO3	279.1834
venlafaxine_TP13	<chem>CN(C)CC(c1ccc(O)c(O)c1)C1(O)CCCCC1</chem>	C16H25NO3	279.1834
venlafaxine_TP14	<chem>CN(C)CC(C=CCC(=O)C([O-])=O)C1(O)CCCCC1</chem>	C15H25NO4	283.1784
venlafaxine_TP15	<chem>CN(C)CC(C(=C)CC(=O)C([O-])=O)C1(O)CCCCC1</chem>	C15H25NO4	283.1784
venlafaxine_TP16	<chem>Oc1ccc(cc1O)C(C=O)C1(O)CCCCC1</chem>	C14H18O4	250.1205
venlafaxine_TP17	<chem>CNCC(c1ccc(O)c(O)c1)C1(O)CCCCC1</chem>	C15H23NO3	265.1678
venlafaxine_TP18	<chem>CN(C)CC(O)(c1ccc(O)c(O)c1)C1(O)CCCCC1</chem>	C16H25NO4	295.1784
venlafaxine_TP19	<chem>CN(C)C(O)C(c1ccc(O)cc1)C1(O)CCCCC1</chem>	C16H25NO3	279.1834
venlafaxine_TP20	<chem>Oc1ccc(cc1)C(O)(C=O)C1(O)CCCCC1</chem>	C14H18O4	250.1205
venlafaxine_TP21	<chem>CNCC(O)(c1ccc(O)cc1)C1(O)CCCCC1</chem>	C15H23NO3	265.1678
venlafaxine_TP22	<chem>Oc1ccc(cc1)C(C([O-])=O)C1(O)CCCCC1</chem>	C14H18O4	250.1205
venlafaxine_TP23	<chem>NCC(c1ccc(O)cc1)C1(O)CCCCC1</chem>	C14H21NO2	235.1572
venlafaxine_TP24	<chem>COc1ccc(cc1)C(O)(C([O-])=O)C1(O)CCCCC1</chem>	C15H20O5	280.1311
venlafaxine_TP25	<chem>CNC(O)C(c1ccc(OC)cc1)C1(O)CCCCC1</chem>	C16H25NO3	279.1834
venlafaxine_TP26	<chem>O=C1CCCCC1</chem>	C6H10O	98.0732
venlafaxine_TP27	<chem>COc1ccc(CC([O-])=O)cc1</chem>	C9H10O3	166.0630
venlafaxine_TP28	<chem>COc1ccc(cc1)C(C([O-])=O)C1(O)CCC(O)CC1</chem>	C15H20O5	280.1311
venlafaxine_TP29	<chem>COc1ccc(cc1)C(O)(CN)C1(O)CCCCC1</chem>	C15H23NO3	265.1678
xipamide_TP1	<chem>Cc1cccc(C)c1NC(=O)c1cc(c(Cl)c(O)c1O)S(N)(=O)=O</chem>	C15H15ClN2O5S	370.0390
xipamide_TP2	<chem>Cc1cccc(C)c1NC(=O)c1cc(ccc1O)S(N)(=O)=O</chem>	C15H16N2O4S	320.0831
xipamide_TP3	<chem>Cc1cccc(CO)c1NC(=O)c1cc(c(Cl)cc1O)S(N)(=O)=O</chem>	C15H15ClN2O5S	370.0390
xipamide_TP4	<chem>Cc1cccc(C)c1NC(=O)c1cc(c(Cl)cc1O)S([O-])(=O)=O</chem>	C15H14ClNO5S	355.0281
xipamide_TP5	<chem>Cc1cccc(C)c1NC(=O)C(=CC(=C(Cl)C([O-])=O)S(N)(=O)=O)C([O-])=O</chem>	C15H15ClN2O7S	402.0289
xipamide_TP6	<chem>Cc1cccc(C)c1NC(=O)c1cc(cc(O)c1O)S(N)(=O)=O</chem>	C15H16N2O5S	336.0780
xipamide_TP7	<chem>Cc1cccc(CO)c1NC(=O)c1cc(ccc1O)S(N)(=O)=O</chem>	C15H16N2O5S	336.0780
xipamide_TP8	<chem>Cc1cccc(C)c1NC(=O)c1cc(c(Cl)c(O)c1O)S([O-])(=O)=O</chem>	C15H14ClNO6S	371.0230
xipamide_TP9	<chem>Cc1cccc(C=O)c1NC(=O)c1cc(c(Cl)cc1O)S(N)(=O)=O</chem>	C15H13ClN2O5S	368.0234
xipamide_TP10	<chem>Cc1cccc(C)c1NC(=O)c1cc(ccc1O)S([O-])(=O)=O</chem>	C15H15NO5S	321.0671
xipamide_TP11	<chem>Cc1cccc(CO)c1NC(=O)c1cc(c(Cl)cc1O)S([O-])(=O)=O</chem>	C15H14ClNO6S	371.0230
xipamide_TP12	<chem>Cc1cccc(C)c1NC(=O)c1cc(O)c(Cl)cc1O</chem>	C15H14ClNO3	291.0662
xipamide_TP13	<chem>Cc1cccc(C)c1NC(=O)c1c(O)cc(Cl)c(O)c1O</chem>	C15H14ClNO4	307.0611
xipamide_TP14	<chem>Cc1cccc(C)c1NC(=O)C(C([O-])=O)=C(O)C=C(Cl)C([O-])=O</chem>	C15H14ClNO6	339.0510
xipamide_TP15	<chem>Cc1cccc(C)c1NC(=O)c1c(O)ccc(O)c1O</chem>	C15H15NO4	273.1001
xipamide_TP16	<chem>Cc1cccc(CO)c1NC(=O)c1cc(O)c(Cl)cc1O</chem>	C15H14ClNO4	307.0611
xipamide_TP17	<chem>Cc1cccc(C)c1NC(=O)c1cc(O)ccc1O</chem>	C15H15NO3	257.1052
xipamide_TP18	<chem>Cc1cccc(C)c1NC(=O)c1cc(O)c(Cl)c(O)c1O</chem>	C15H14ClNO4	307.0611
xipamide_TP19	<chem>Cc1cccc(C=O)c1NC(=O)c1cc(c(Cl)cc1O)S([O-])(=O)=O</chem>	C15H12ClNO6S	369.0074
xipamide_TP20	<chem>Cc1cccc(CO)c1NC(=O)c1c(O)cc(Cl)c(O)c1O</chem>	C15H14ClNO5	323.0561
xipamide_TP21	<chem>Cc1cccc(C)c1NC(=O)c1cc(O)c(O)cc1O</chem>	C15H15NO4	273.1001
xipamide_TP22	<chem>Cc1cccc(CO)c1NC(=O)c1cc(ccc1O)S([O-])(=O)=O</chem>	C15H16NO6S	338.0698
xipamide_TP23	<chem>Cc1cccc(C)c1NC(=O)C=CC(=C(Cl)C([O-])=O)S(N)(=O)=O</chem>	C14H16ClN2O5S	359.0468
xipamide_TP24	<chem>Cc1cccc(C)c1N</chem>	C8H11N	121.0891
xipamide_TP25	<chem>NS(=O)(=O)C(C=C(C([O-])=O)C([O-])=O)=C(Cl)C([O-])=O</chem>	C7H9ClNO8S	301.9737
xipamide_TP26	<chem>Cc1cccc(C)c1NC(=O)C(CC(=C(Cl)C([O-])=O)S(N)(=O)=O)C([O-])=O</chem>	C15H19ClN2O7S	406.0602
xipamide_TP27	<chem>Cc1cccc(C)c1NC(=O)C(=CC(C(Cl)C([O-])=O)S(N)(=O)=O)C([O-])=O</chem>	C15H19ClN2O7S	406.0602

xipamide_TP28	<chem>Cc1cccc(C)c1NC(=O)C(=CC(=CC([O-])=O)S(N)(=O)=O)C([O-])=O</chem>	C15H18N2O7S	370.0835
xipamide_TP29	<chem>Cc1cccc(C)c1NC(=O)C(=CC(=C(Cl)C([O-])=O)S([O-])(=O)=O)C([O-])=O</chem>	C15H17ClNO8S	406.0363
xipamide_TP30	<chem>Cc1cccc(C)c1NC(=O)c1cc(cc(O)c1O)S([O-])(=O)=O</chem>	C15H16NO6S	338.0698
xipamide_TP31	<chem>Cc1cccc(C=O)c1NC(=O)c1cc(ccc1O)S(N)(=O)=O</chem>	C15H14N2O5S	334.0623
xipamide_TP32	<chem>Cc1cccc(C([O-])=O)c1NC(=O)c1cc(c(Cl)cc1O)S(N)(=O)=O</chem>	C15H14ClN2O6S	385.0261