

name	category	cas_number	mol_formula	mol_weight	synonym
3-OH Desloratidine	metabolites	119410-08-1	C ₁₉ H ₁₉ ClN ₂ O	326.82	8-Chloro-6,11-dihydro-11-(4-piperidinylidene)-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-3-ol; 3-Hydroxydesloratadine; Sch 45581;
Amlodipine metabolite	metabolites	113994-45-9	C ₂₀ H ₂₀ ClNO ₇	421.82	2-[(2-Amiethoxy)methyl]-4-(2-chlorophenyl)-3-ethoxycarbonyl-5-methoxycarbonyl)-6-methyl-1,4-dihydropyridine
Desvenlafexine succinate	metabolites	386750-22-7	C ₁₆ H ₂₅ N ₂ O ₂ .C ₄ H ₆ O ₄ .H ₂ O	263.38	4-[2-(Dimethylami)-1-(1-hydroxycyclohexyl)ethyl]phel Succinate;
Glycoursodeoxycholic acid	metabolites	64480-66-6	C ₂₆ H ₄₃ NO ₅	449.62	N-[(3.alpha.,5.beta.,7.beta.)-3,7-dihydroxy-24-oxocholan-24-yl]Glycine
Hydroxy Pioglitazone (MIV)	metabolites	146062-44-4	C ₁₉ H ₂₀ N ₂ O ₄ S	372.45	5-[[4-[2-[5-(2-Hydroxyethyl)-2-pyridinyl]ethoxy]phenyl]methyl]-2,4-thiazolidinedione;
4-Hydroxyphenyl Carvedilol	metabolites	142227-49-4	C ₂₄ H ₂₆ N ₂ O ₅	422.49	3-[2-[[3-(9H-Carbazol-4-yloxy)-2-hydroxypropyl]ami]ethoxy]-4-methoxyphel; 5-Hydroxycarvedilol; BM 140830;
N-Desmethyl Sildenafil	metabolites	139755-82-1	C ₂₁ H ₂₈ N ₆ O ₄ S	460.55	5-[2-Ethoxy-5-(1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one; Desmethylsildenafil; UK 103320;
Dihydroartemisinin	metabolites	71939-50-9	C ₁₅ H ₂₄ O ₅	284.35	(3R,5aS,6R,8aS,9R,10S,12R,12aR)-Decahydro-3,6,9-trimethyl- 3,12-epoxy-12H-pyra[4,3-j]-1,2-benzodioxepin-10-ol; β - Dihydroartemisinin;

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Simvastatin hydroxy Acid Ammonium Salt	metabolites	139893-43-9	C ₂₅ H ₄₃ NO ₆	453.61	(β R, δ R,1S,2S,6R,8S,8aR)-8-(2,2-Dimethyl-1-oxobutoxy)-1,2,6,7,8,8a-hexahydro- β , δ -dihydroxy-2,6-dimethyl-1-naphthaleneheptaic Acid Ammonium Salt;
Hydroxy Bupropion	metabolites	357399-43-0	C ₁₃ H ₁₈ ClNO ₂ .HCl	292.2	2-Hydroxy-2-(3'-chlorophenyl)-3,5,5-trimethylmorpholine; 2-(3-Chlorophenyl)-3,5,5-trimethyl-2-morpholil;
9-Hydroxy Risperidone	metabolites	130049-85-3	C ₁₃ H ₁₈ ClNO ₂ .HCl	426.48	(9R)-3-[2-[4-(6-Fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]ethyl]-6,7,8,9-tetrahydro-9-hydroxy-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one;
Clopidogrel carboxylic acid HCL	metabolites	144750-42-5	C ₁₃ H ₁₈ ClNO ₂ .HCl	344.31	(S)- α -(2-Chlorophenyl)-6,7-dihydrothie[3,2-c]pyridine-5(4H)-acetic Acid Hydrochloride; SR 26334 Hydrochloride;
Desacetyl Diltiazem	metabolites	42399-40-6	C ₂₀ H ₂₄ N ₂ O ₃ S	372.48	2S-cis)-5-[(Dimethylami)ethyl]-2,3-dihydro-3-hydroxy-2-(4-methoxyphenyl)-1,5-benzothiazepin-4(5H)-one;
3-Ketodesogestrel	metabolites	NA	C ₂₂ H ₂₈ O ₂	324.46	(8S,9S,10R,13S,14S,17R)-13-ethyl-17-ethynyl-17-hydroxy-11-methylidene-2,6,7,8,9,10,12,14,15,16-decahydro-1H-cyclopenta[a]phenanthren-3-one;
Benazeprilat	metabolites	86541-78-8	C ₂₂ H ₂₄ N ₂ O ₅	396.44	(3S)-3-[[[(1S)-1-Carboxy-3-phenylpropyl]ami]-2,3,4,5-tetrahydro-2-oxo-1H-1-benzazepine-1-acetic Acid-d5;

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Paliperidone N-oxide	metabolites	761460-08-6	C23H27FN4O4	442.48	3-[2-[4-(6-Fluoro-1,2-benzisoxazol-3-yl)-1-oxido-1-piperidinyl]ethyl]-6,7,8,9-tetrahydro-9-hydroxy-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one;
5-Hydroxy methyl Tolterodine,	metabolites	207679-81-0	C22H31NO2	341.49	3-[(1R)-3-[Bis(1-methylethyl)ami]-1-phenylpropyl]-4-hydroxybenzenemethal;
Trandolaprilat	metabolites	87679-71-8	C22H30N2O5	402.5	[2S-[1[R*(R*)],2 α ,3 α ,7 α]]-Octahydro-1-[2-[[1-(methoxycarbonyl)-3-phenylpropyl]ami]-1-oxopropyl]-1H-indole-2-carboxylic Acid;
N-Desmethyl Olanzapine	metabolites	161696-76-0	C16H18N4S	298.40	2-methyl-4-(1-piperazinyl)-10H-Thie[2,3-b][1,5]benzodiazepine
O-Desmethyl Tramadol	metabolites	80456-81-1	C15H23NO2.HCl	285.81	3-[(rel-1R,2R)2-[(Dimethylami)methyl]-1-hydroxycyclohexyl]phel Hydrochloride;
Thio Sildenafil	metabolites	479073-79-5	C22H30N6O3S	490.64	5-[2-Ethoxy-5-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidine-7-thione;
Clopidogrel carboxylic acid	metabolites	144457-28-3	C15H14ClNO2S	307.8	rac-2-(2-Chlorophenyl)-2-(6,7-dihydro-4H-thie[3,2-c]pyridin-5-yl)acetic Acid Hydrochloride;
Desacetyl Rifampicin	metabolites	16783-99-6	C15H14ClNO2S	780.92	25-O-Deacetyl-3-[(E)-[(4-methyl-1-piperazinyl)imi]methyl]rifamycin;

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Fenofibrate	metabolites	49562-28-9	C ₂₀ H ₂₁ ClO ₄	360.83	2-[4-(4-Chlorobenzoyl)phexy]-2-methyl-propaic Acid 1-Methylethyl Ester; LF 178; Lipanthyl; Lipantil; Lipidil Supra; Lipirex; Lipoclar
Hydroxy Itraconazole	metabolites	112559-91-8	C ₃₅ H ₃₈ Cl ₂ N ₈ O ₅	721.64	4-[4-[4-[4-[[2-(2,4-Dichlorophenyl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]-1-piperazinyl]phenyl]-2,4-dihydro-2-(2-hydroxy-1-methylpropyl)-3H-1,2,4-triazol-3-one;
O-Desmethyl Venlafaxine Succinate Hydrate	metabolites	386750-22-7	C ₁₆ H ₂₅ N ₂ O ₂ .C ₄ H ₆ O ₄ .H ₂ O	399.48	butanedioic acid;4-[2-(dimethylami)-1-(1-hydroxycyclohexyl)ethyl]phel;hydrate
Misoprostol Acid	metabolites	66792-31-2	C ₂₁ H ₃₆ O ₅	368.51	(11 α ,13E)-11,16-Dihydroxy-16-methyl-9-oxo-prost-13-en-1-oic Acid; Misoprostol Free Acid;
Enalaprilat	metabolites	76420-72-9	C ₁₈ H ₂₄ N ₂ O ₅	348.39	Enalapril Impurity C
N-Desethyl Oxybutynin	metabolites	80976-67-6	C ₁₈ H ₂₄ N ₂ O ₅	365.89	α -Cyclohexyl- α -hydroxybenzeneacetic Acid 4-(Ethylami)-2-butynyl Ester Hydrochloride Salt;
N-Desmethyl Diltiazem	metabolites	130606-60-9	C ₂₁ H ₂₄ N ₂ O ₄ S.HCl	436.96	(2S-cis)-3-(Acetyloxy)-2,3-dihydro-2-(4-methoxyphenyl)-5-[2-(methylami)ethyl]-1,5-benzothiazepin-4(5H)-one Mohydrochloride;

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Norfluoxetine HCl	metabolites	56296-78-7	C ₂₁ H ₂₄ N ₂ O ₄ S.HCl	331.76	γ -[4-(Trifluoromethyl)phenoxy]benzenepropanamine Hydrochloride; (+/-)- γ -[4-(Trifluoromethyl)phenoxy]benzenepropanamine Hydrochloride
Aceylated Flupirtine	metabolites	57226-68-3	C ₁₄ H ₁₅ FN ₄ O	274.3	ethyl N-[2-ami-6-[(4-fluorophenyl)methylamino]pyridin-3-yl]carbamate
Lovastatin OH Sodium salt	metabolites	75225-50-2	C ₂₄ H ₃₇ O ₆ · Na	444.54	Lovastatin Sodium Salt; MB 530B; Mevinilic Acid; Lovastatin EP Impurity B
Atorvastatin Lactone	metabolites	125995-03-1	C ₃₃ H ₃₃ FN ₂ O ₄	540.62	5-(4-Fluorophenyl)-2-(1-methylethyl)-N,4-diphenyl-1-[2-[(2R,4R)-tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl]ethyl]-1H-pyrrole-3-carboxamide;
Ramiprilat	metabolites	87269-97-4	C ₂₁ H ₂₈ N ₂ O ₅	388.20	(2S,3aS,6aS)-1-[(2S)-2-[[[(1S)-1-Carboxy-3-phenylpropyl]amino]-1-oxopropyl]octahydrocyclopenta[b]pyrrole-2-carboxylic Acid;
Tauroursodeoxycholic acid	metabolites	35807-85-3	C ₂₁ H ₂₈ N ₂ O ₅	499.72	2-[[[(3 α ,5 β ,6 α)-3,6-Dihydroxy-24-oxocholan-24-yl]amino]ethanesulfonic Acid;
Prasugrel active metabolite acetate salt	metabolites	204204-98-8 free	C ₂₁ H ₂₈ N ₂ O ₅	409.47	Prasugrel active metabolite ,R138727

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O-Hydroxy Atorvastatin Calcium Salt	metabolites	265989-47-7	C ₆₆ H ₆₈ CaF ₂ N ₄ O ₁₂	1187.34	(β R, δ R)-2-(4-Fluorophenyl)- β , δ -dihydroxy-4-[[[(2-hydroxyphenyl)ami]carbonyl]-5-(1-methylethyl)-3-phenyl-1H-pyrrole-1-heptaic Acid Calcium Salt (21)
3,5-Xylenol	metabolites	108-68-9	C ₈ H ₁₀ O	122.167	3,5-dimethylphel
P-Hydroxy Atorvastatin Calcium Salt	metabolites	265989-44-4	C ₆₆ H ₆₈ CaF ₂ N ₄ O ₁₂	1187.34	(β R, δ R)-2-(4-Fluorophenyl)- β , δ -dihydroxy-4-[[[(4-hydroxyphenyl)ami]carbonyl]-5-(1-methylethyl)-3-phenyl-1H-pyrrole-1-heptaic Acid Hemicalcium Salt;
N-N-Didesmethyl Venlafaxine	metabolites	93413-77-5	C ₁₅ H ₂₃ NO ₂	249.35	1-[2-Ami-1-(4-methoxyphenyl)ethyl]cyclohexal; 1-[2-Ami-1-(p-methoxyphenyl)ethyl]cyclohexal;
Erythro-Hydroxy Bupropion HCl	metabolites	292055-72-2	C ₁₃ H ₂₀ ClNO.HCl	278.22	(α S)-3-Chloro- α -[(1R)-1-[(1,1-dimethylethyl)ami]ethyl]-benzenemethal Hydrochloride;
Threo-Hydroxy Bupropion HCl	metabolites	153365-82-3	C ₁₃ H ₂₀ ClNO.HCl	278.22	rac threo-2-(tert-Butylami)-1-(3-chlorophenyl)propan-1-ol Hydrochloride
5-OH Omeprazole	metabolites	92340-57-3	C ₁₇ H ₁₉ N ₃ O ₄ S	361.42	4-Methoxy-6-[[[(5-methoxy-1H-benzimidazol-2-yl)sulfinyl]methyl]-5-methyl-3-pyridinemethal;
O-Desmethyl Dextromethorphan Dextro Impurity B	metabolites	1426173-22-9	C ₁₇ H ₂₃ NO	257.377	Dextrorphan; Dextrorphanum;D-3-Hydroxy-N-methylmorphinan; Levorphan d-form; Destrorfa [DCIT]
Nor-Trimebutine mono-desmethyl HCl	metabolites	294882-33-0	C ₂₁ H ₂₈ ClNO ₅	409.9	3,4,5-Trimethoxybenzoic Acid 2-(Methylami)-2-phenylbutyl Ester Hydrochloride

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N-Desmethyl Trimebutine HCL	metabolites	84333-59-5	C21H27NO5.HCl	409.91	3,4,5-Trimethoxybenzoic Acid 2-(Methylami)- 2-phenylbutyl Ester Hydrochloride; N- Modesmethyltrimebutine Hydrochloride;
Losartan carboxylic acid	metabolites	124750-92-1	C22H21ClN6O2	436.90	2-Butyl-4-chloro-1-[[2'-(1H-tetrazol-5-yl)[1,1'- biphenyl]-4-yl]methyl]-1H-imidazole-5- carboxylic Acid;
Prednisone	metabolites	53-03-2	C21H26O5	358.43	17,21-Dihydroxypregna-1,4-diene-3,11,20- trione; 1,2-Dehydrocortisone;
Norverapamil HCl	metabolites	67812-42-4	C26H37ClN2O4	477.03	α -[3-[[2-(3,4- Dimethoxyphenyl)ethyl]ami]propyl]-3,4- dimethoxy- α -(1-methylethyl)- benzeneacetonitrile; Verapamil EP Impurity J HCl;
N- desethylamodiaqui ne	metabolites	37672-04-2	C18H18ClN3O	327.81	4-[(7-Chloro-4-quinyl)ami]-2- [(ethylami)methyl]phenyl Hydrochloride; Modesethylamodiaquine Hydrochloride;
Prasugrel metabolite derivative HCl(trans R- 138727MP)	metabolites	929211-64-3	C27H28FN05S.HCl	534.03	4-[(7-Chloro-4-quinyl)ami]-2- [(ethylami)methyl]phenyl Hydrochloride; Modesethylamodiaquine Hydrochloride;

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N-Desmethyl Galanthamine	metabolites	41303-74-6	C ₁₆ H ₁₉ NO ₃	273.33	(4aS,6R,8aS)-4a,5,9,10,11,12-Hexahydro-3-methoxy-6H-benzofuro[3a,3,2-ef][2]benzazepin-6-ol; (-)-N-Demethylgalanthamine;
Dehydrodeoxy Donepezil	metabolites	120013-45-8	C ₂₄ H ₂₉ NO ₂ .HCl	399.7	4-[(5,6-Dimethoxy-1H-inden-2-yl)methyl]-1-(phenylmethyl)piperidine;1-Benzyl-4-(5,6-dimethoxy-1H-2-indenylmethyl)piperidine
N-Desmethyl Zolmitriptan	metabolites	139264-35-0	C ₁₅ H ₁₉ N ₃ O ₂	273.33	(4S)-4-[[3-[2-(Methylamino)ethyl]-1H-indol-5-yl]methyl-2-oxazolidine; 183C91; Zolmitriptan USP Related Compound A
Desacetyl Rifabutine	metabolites	100324-63-8	C ₄₄ H ₆₀ N ₄ O ₁₀	804.97	25-O-Deacetyl-1',4-didehydro-1-deoxy-1,4-dihydro-5'-(2-methylpropyl)-1-oxorifamycin XIV;
N-desethylamodiaquine	metabolites	37672-04-1	C ₁₈ H ₁₈ ClN ₃ O	327.81	4-[(7-Chloro-4-quinolyl)amino]-2-[(ethylamino)methyl]phenyl Hydrochloride; Modesethylamodiaquine Hydrochloride;
Doxorubicinol	metabolites	25316-40-9	C ₂₇ H ₃₁ NO ₁₁	545.55	[8S-[8 α ,8(R*),10 α]]-10-[(3-Amino-2,3,6-trideoxy- α -L-lyxo-hexopyranosyl)oxy]-8-(1,2-dihydroxyethyl)-7,8,9,10-tetrahydro-6,8,11-trihydroxy-1-methoxy-5,12-naphthacenedione;
o-Hydroxy Atorvastatin Dihydrate Mosodium salt	metabolites	1421760-64-6	C ₃₃ H ₃₈ FN ₂ NaO ₈	632.65	(β R, δ R)-2-(4-Fluorophenyl)- β , δ -dihydroxy-4-[[[(2-hydroxyphenyl)amino]carbonyl]-5-(1-methylethyl)-3-phenyl-1H-pyrrole-1-heptaic Acid Dihydrate Mosodium Salt;

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Montelukast acid	metabolites	158966-92-8	C ₃₅ H ₃₅ ClNNaO ₃ S	608.17	1-[1-[[[(1R)-1-[3-[(1E)-2-(7-Chloro-2-quiliny)ethenyl]phenyl]-3-[2-(1-hydroxy-1-methylethyl)phenyl]propyl]thio]methyl]cyclopropaneacetic Acid Sodium Salt;
Rabeprazole Sulfone	metabolites	117976-47-3	C ₁₈ H ₂₁ N ₃ O ₄ S	375.44	2-[[[4-(3-Methoxypropoxy)-3-methyl-2-pyridinyl]methyl]sulfonyl]-1H-benzimidazole
Rabeprazole Sulfide	metabolites	117977-21-6	C ₁₈ H ₂₁ N ₃ O ₂ S	343.44	2-[[[3-Methyl-4-(3-methoxypropoxy)-2-pyridyl]methyl]thio]-1H-benzimidazole;
2-Pyridyl Acetic Acid	metabolites	54363-97-2	C ₇ H ₇ NO ₂	137.14	2-Pyridineacetic acid
2-Pyridyl Acetic Acid HCl	metabolites	16179-97-8	C ₇ H ₇ NO ₂ .HCl	173.59	2-Pyridineacetic acid hydrochloride
Olmesartan Acid	metabolites	144689-24-7	C ₂₄ H ₂₆ N ₆ O ₃	446.50	4-(1-Hydroxy-1-methylethyl)-2-propyl-1-[[2'-(1H-tetazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-1H-imidazole-5-carboxylic Acid; CS 088;
Prasugrel Metabolite (R-95913, Mixture of Diastereomers)	metabolites	150322-38-6	C ₁₈ H ₁₈ FN ₂ O ₂ S	331.41	2-[1-[2-Cyclopropyl-1-(2-fluorophenyl)-2-oxoethyl]-4-(methylthio)-3-piperidinylidene]acetic Acid;
(R)-Propionyl Carnitine	metabolites	17298-37-2	C ₁₀ H ₁₉ NO ₄	217.265	3-propyloxy-4-(trimethylazaniumyl)butaate
Modafinil Acid	metabolites	63547-24-0	C ₁₅ H ₁₄ O ₃ S	274.3	2-[(Diphenylmethyl)sulfinyl]acetamide; (±)-Modafinil; 2-(Benzhydrylsulfinyl)acetamide;

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Hydroxy Bupropion HCL	metabolites	357399-43-0	C13H18ClNO2.HCl	292.20	2-(3-chlorophenyl)-3,5,5-trimethyl-2-morpholil
Desmethyl Sertraline	metabolites	87857-41-8	C16H15Cl2N	292.203	(1S,4S)-4-(3,4-dichlorophenyl)-1,2,3,4-tetrahydronaphthalen-1-amine
9-Trans Retinoic Acid	metabolites	5300-03-8	C20H28O	284.45	9-Trans Retinoic Acid
Perindoprilat	metabolites	95153-31-4	C17H28N2O5	340.42	(2S,3aS,7aS)-1-[(2S)-2-[[[(1S)-1-Carboxybutyl]ami]-1-oxopropyl]octahydro-1H-indole-2-carboxylic Acid; [2S-[1[R*(R*)],2 α ,3a β ,7a β]]-1-[2-[(1-Carboxybutyl)ami]-1-oxopropyl]octahydro-1H-indole-2-carboxylic Acid;
6-Methoxysalicylic Acid	metabolites	3147-64-6	CH3OC6H3(OH)CO2H	168.15	2-Hydroxy-6-methoxybenzoic acid
Hydroxy hydrocinnamic Acid	metabolites	501-52-0	C9H10O3	166.17	3-(4-hydroxyphenyl)propaic acid
N-Methyl Pregabalin	metabolites	1155843-61-0	C9H19NO2	173.25	(3S)-5-methyl-3-(methylamimethyl)hexaic acid
D-L-Mevalonic Acid Dicyclohexylammo nium Salt	metabolites	1215802-31-5	C18H35NO4	329.47	3,5-Dihydroxy-3-(methyl) Pentaic Acid Dicyclohexylammonium Salt; Hiochic Acid Dicyclohexylammonium Salt;

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Alpha -Hydroxy Metoprolol	metabolites	110458-46-3	C ₁₅ H ₂₅ N ₄ O ₄	283.37	4-[2-Hydroxy-3-[(1-methylethyl)ami]propoxy]- α -(methoxymethyl)-benzenemethan- ol; H 119/66; α -Hydroxymetoprolol;
6-OH Taxol	metabolites	153212-75-0	C ₄₇ H ₅₁ N ₄ O ₁₅	869.9	6 α -hydroxy Taxol
Desbutyl Dronedarone	metabolites	197431-02-0	C ₂₇ H ₃₇ ClN ₂ O ₅ S	537.11	N-[2-Butyl-3-[4-[3- (butylami)propoxy]benzoyl]-5-benzofuranyl]- methanesulfonamide Hydrochloride; SR 35021;
N-Butyl Dronedarone	metabolites	NA	C ₂₇ H ₃₇ ClN ₂ O ₅ S	537.11	N-[2-Butyl-3-[4-[3- (butylami)propoxy]benzoyl]-5-benzofuranyl]- methanesulfonamide Hydrochloride;
Des Methyl Rizatriptan	metabolites	144034-84-4	C ₁₄ H ₁₇ N ₅	255.325	N-methyl-2-[5-(1,2,4-triazol-1-ylmethyl)-1H- indol-3-yl]ethanamine
Rosuvastatin Lactone	metabolites	503610-43-3	C ₂₂ H ₂₆ FN ₃ O ₅ S	463.52	N-[4-(4-Fluorophenyl)-6-(1-methylethyl)-5- [(1E)-2-[(2S,4R)-tetrahydro-4-hydroxy-6-oxo- 2H-pyran-2-yl]ethenyl]-2-pyrimidinyl]-N- methyl-methanesulfonamide;
trans-Hydroxy Glimepiride	metabolites	600177-94-4	C ₂₄ H ₃₄ N ₄ O ₆ S	506.61	3-Ethyl-2,5-dihydro-N-[2-[4-[[[trans-4- (hydroxymethyl)cyclohexyl]ami]carbonyl]ami]su lfonyl]phenyl]ethyl]-4-methyl-2-oxo-1H- pyrrole-1-carboxamide;
1-Alpha-25(OH) ₂ Vitamin D ₂	metabolites	60133-18-8	C ₂₈ H ₄₄ O ₃	428.65	(1R,3S,5Z)-4-Methylene-5-[(2E)-2- [(1R,3aS,7aR)-octahydro-1-[(1R,2E)-5-hydroxy- 1,4,5-trimethyl-2-hexen-1-yl]-7a-methyl-4H- inden-4-ylidene]ethylidene]-1,3- cyclohexanediol;

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10,11-Dihydro-10-Hydroxy Carbamazepine	metabolites	29331-92-8	C15H14N2O2	254.29	10,11-Dihydro-10-hydroxy-5H-dibenz[b,f]azepine-5-carboxamide; 10-Hydroxy-10,11-dihydrocarbamazepine;
(3R)-3-Hydroxy Quinidine	metabolites	53467-23-5	C20H24N2O3	340.43	(3 α ,8 α ,9R)-6'-methoxycinchonan-3,9-diol; (3R)-Hydroxyquinine
N-Monodesmethyl Rizatriptan Benzoate	metabolites	144034-84-4	C14H17N5 . C7H6O2	377.45	N-Methyl-5-(1H-1,2,4-triazol-1-ylmethyl)-1H-indole-3-ethanamine
Lovastatin OH Ammonium salt	metabolites	77550-67-5	C24H41NO6	439.58	Lovastatin Sodium Salt; MB 530B; Mevilinic Acid; Lovastatin EP Impurity B
Pitavastatin Lactone	metabolites	141750-63-2	C25H22FNO3	403.46	(4R,6S)-6-[(E)-2-[2-cyclopropyl-4-(4-fluorophenyl)quin-3-yl]ethenyl]-4-hydroxyoxan-2-one
(3S)-3-Hydroxy Quinidine	metabolites	53467-23-5	C20H24N2O3	340.43	(9S)-6'-Methoxy-Cinchonan-3,9-diol; (3S)-Hydroxyquinidine; 3-Hydroxyquinidine;
17-Beta-Estradiol	metabolites	50-28-2	C18H24O2	272.38	Dihydrofolliculin; (17 β)-Estra-1,3,5(10)-triene-3,17-diol; 3,17-Epidihydroxyestratriene; Cimara;
Keto Pioglitazone M-III	metabolites	146062-45-5	C19H18N2O4S	370.42	5-[[4-[2-(5-Acetyl-2-pyridinyl)ethoxy]phenyl]methyl]-2,4thiazolidinedione; Keto-Pioglitazone (M-III);

name	category	cas_number	mol_formula	mol_weight	synonym
N-Desmethyl Ivabradine HCL	metabolites	1246638-08-3	C ₂₆ H ₃₄ N ₂ O ₅ . HCl	491.03	3-[3-[[[(7S)-3,4-Dimethoxybicyclo[4.2.0]octa-1,3,5-trien-7-yl]methyl]ami]propyl]-1,3,4,5-tetrahydro-7,8-dimethoxy-2H-3-benzazepin-2-one;
Dexmethyl phenidate HCl	metabolites	19262-68-1	C ₁₄ H ₂₀ ClNO ₂	269.769	methyl (2R)-2-phenyl-2-[(2R)-piperidin-2-yl]acetate;hydrochloride
2-OH Desipramine	metabolites	1977-15-7	C ₁₈ H ₂₂ N ₂ O	282.39	10,11-Dihydro-5-[3-(methylami)propyl]-5H-dibenz[b,f]azepin-2-ol;
SN 38	metabolites	86639-52-3	C ₂₂ H ₂₀ N ₂ O ₅	392.4	(4S)-4,11-Diethyl-4,9-dihydroxy-1H-pyra[3',4'6,7]indolizi[1,2-b]quiline-3,14(4H,12H)dione;
N-desmethyl Imatinib	metabolites	404844-02-6	C ₂₈ H ₂₉ N ₇ O	479.58	N-[4-Methyl-3-[[4-(3-pyridinyl)-2-pyrimidinyl]ami]phenyl]-4-(1-piperazinylmethyl)-benzamide; N-Desmethyl Gleevec; CGP-74588;
4-Hydroxy Propranolol Sulphate Potassium Salt	metabolites	1261395-42-9	C ₁₆ H ₂₀ NO ₆ S.K	393.50	1-[(4-Methoxy-1-naphthalenyl)oxy]-3-[(1-methylethyl)ami]-2-propal; 1-(Isopropylami)-3-[(4-methoxy-1-naphthyl)oxy]-2-propal
7-Hydroxy Methotrexate	metabolites	5939-37-7	C ₂₀ H ₂₂ N ₈ O ₆	470.44	7-Hydroxy Amethopterin, 4-Ami-7-hydroxy-10-methylpteroylglutamic Acid;
17-Desacetyl Norgestimate	metabolites	74183-54-3	C ₂₁ H ₂₉ N ₂ O ₂	327.46	(8R,9S,10R,13S,14S,17R,Z)-13-Ethyl-17-ethynyl-17-hydroxy-6,7,8,9,10,11,12,13,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3(2H)-one

name	category	cas_number	mol_formula	mol_weight	synonym
Pilocarpic Acid Sodium Salt (mixture of diastereomers)	metabolites	92598-79-3	C ₁₁ H ₁₇ N ₂ O ₃ . Na	248.25	[S-(R*,S*)]- α -Ethyl- β -(hydroxymethyl)-1-methyl-1H-Imidazole-5-butaic Acid Mosodium Salt; Sodium Pilocarpate;
14 (R) Hydroxy Clarithromycin	metabolites	116836-41-0	C ₃₈ H ₆₉ N ₁₄ O	763.95	3R,4S,5S,6R,7R,9R,11R,12R,13S,14R)-6-[(2S,3R,4S,6R)-4-(dimethylami)-3-hydroxy-6-methyloxan-2-yl]oxy-14-ethyl-12,13,14-trihydroxy-4-[(2R,4R,5S,6S)-5-hydroxy-4-methoxy-4,6-dimethyloxan-2-yl]oxy-7-methoxy-3,5,7,9,11,13-hexamethyl-oxacyclotetradecane-2,10-dione
Prothionamide Sulfoxide	metabolites	62178-61-4	C ₉ H ₁₂ N ₂ OS	196.27	2-Propyl- α -sulfinyl-4-pyridinemethanamine; 2-Propyl-4-pyridinecarbothioamide S-Oxide; 2-Propylthioisonicotinamide S-Oxide
Ethionamide Sulfoxide	metabolites	536-28-7	C ₈ H ₁₀ N ₂ OS	182.25	2-Ethyl-4-pyridinecarbothioamide S-Oxide; 2-Ethylthioisonicotinamide S-Oxide; Ethionamide-S-oxide;
Butylated Hydroxy Toluene	metabolites	128-37-0	C ₁₅ H ₂₄ O	220.35	2,6-Di-tert-butyl-4-methylphel, 2,6-Di-tert-butyl-p-cresol, BHT,

name	category	cas_number	mol_formula	mol_weight	synonym
10-deacetyl Baccatin	metabolites	32981-86-5	C ₂₉ H ₃₆ O ₁₀	544.59	(2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(Acetyloxy)-12-(benzoyloxy)-1,2a,3,4,4a,6,9,10,11,12,12a,12b-dodecahydro-4,6,9,11-tetrahydroxy-4a,8,13,13-tetramethyl-7,11-metha-5H-cyclodeca[3,4]benz[1,2-b]oxet-5-one;
Trans-Hydroxy Glimepiride	metabolites	600177-94-4	C ₂₄ H ₃₄ N ₄ O ₆ S	506.61	3-Ethyl-2,5-dihydro-N-[2-[4-[[[trans-4-(hydroxymethyl)cyclohexyl]ami]carbonyl]ami]sulfonyl]phenyl]ethyl]-4-methyl-2-oxo-1H-pyrrole-1-carboxamide;
5-Hydroxy Propafenone	metabolites	86384-10-3	C ₂₁ H ₂₈ ClNO ₄	393.90	1-[5-Hydroxy-2-[2-hydroxy-3-(propylami)propoxy]phenyl]-3-phenyl-1-propane Hydrochloride; GPV 129;
6-Beta Hydroxy norgestrel	metabolites	55555-97-0	C ₂₁ H ₂₈ O ₃	328.46	6 β -Hydroxy Levorgestrel 17-Acetate
4- hydroxy propafene	metabolites	102059-10-9	C ₂₁ H ₂₈ ClNO ₄	393.90	1-[4-Hydroxy-2-[2-hydroxy-3-(propylami)propoxy]phenyl]-3-phenyl-1-propane Hydrochloride
N-Desmethyl Dapoxetine	metabolites	119357-18-5	C ₂₀ H ₂₂ ClNO	327.85	N-Methyl- α -[2-(1-naphthalenyloxy)ethyl]benzenemethanamine Hydrochloride;
Moacetyl Dapsone	metabolites	565-20-8	C ₁₄ H ₁₄ N ₂ O ₃ S	290.34	N-[4-[(4-Amiphenyl)sulfonyl]phenyl]-acetamide; Acetyldapsone; MADDS; Moacetyldapsone;

name	category	cas_number	mol_formula	mol_weight	synonym
Oseltamavir Acid	metabolites	187227-45-8	C ₁₄ H ₂₄ N ₂ O ₄	284.35	(3R,4R,5S)-4-(Acetylami)-5-ami-3-(1-ethylpropoxy)-1-cyclohexence-1-carboxylic Acid; Oseltamivir Carboxylic Acid;
Dehydro Rifaximin	metabolites	80621-76-7	C ₄₃ H ₄₉ N ₃ O ₁₁	783	Synmyn[2S(2R*,16Z,18E,20R*,21R*,22S*,23S*,24S*,25R*,26S*,27R*,28E)]-25-(Acetyloxy)-5,21,23-trihydroxy-27-methoxy-2,4,11,16,20,22,24,26-octamethyl-6H-27-(epoxypentadeca[1,11,13]trienitrilo)benzofuro[4,5-e]pyrido[1,2-a]benzimidazole-1,6,15(2H)-trione;
N-Desmethyl Rosiglitazone	metabolites	257892-31-2	C ₁₇ H ₁₇ N ₃ O ₃ S	343.4	5-[[4-[2-(2-Pyridinylami)ethoxy]phenyl]methyl]-2,4-thiazolidinedione; SB 237216;
Fosinoprilat	metabolites	95399-71-6	C ₂₃ H ₃₄ N ₂ O ₅ P	435.5	(4S)-4-Cyclohexyl-1-[[hydroxy(4-phenylbutyl)phosphinyl]acetyl]-L-proline; trans-4-Cyclohexyl-1-[[hydroxy(4-phenylbutyl)phosphinyl]acetyl]-L-proline;
Desmethyl Mebeverine Acid	metabolites	586357-02-0	C ₁₅ H ₂₃ N ₃ O ₃	265.36	4-[Ethyl[2-(4-hydroxyphenyl)-1-methylethyl]ami]butaic Acid;
Demethyl Tadalafil	metabolites	171596-36-4	C ₂₁ H ₁₇ N ₃ O ₄	375.384	(6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydropyrazi[1',2'-1,6]pyrido[3,4-b]indole-1,4-dione;
Hydroxy Iloperidone P88	metabolites	133454-55-4	C ₂₄ H ₂₉ FN ₂ O ₄	428.5	4-[3-[4-(6-Fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]propoxy]-3-methoxy-α-methylbenzenemethal; P 88; P 88-8991;

name	category	cas_number	mol_formula	mol_weight	synonym
Phenol Metabolite of Bosentan	metabolites	147536-97-8	C ₂₆ H ₂₇ N ₅ O ₆ S	537.59	4-(1,1-Dimethylethyl)-N-[6-(2-hydroxyethoxy)-5-(2-hydroxyphexy)[2,2'-bipyrimidin]-4-yl]benzenesulfonamide;
Dehydro Aripiprazole	metabolites	129722-25-4	C ₂₃ H ₂₅ N ₃ O ₂ Cl ₂	446.37	OPC 14857; DM 14857; 7-[4-[4-(2,3-Dichlorophenyl)-1-piperazinyl]butoxy]-2(1H)-quinoline;
Cefpodoxime Acid	metabolites	80210-62-4	C ₁₅ H ₁₇ N ₅ O ₆ S ₂	427.46	(6R,7R)-7-[[[(2Z)-2-(2-Ami-4-thiazolyl)-2-(methoxyimi)acetyl]ami]-3-(methoxymethyl)-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic Acid;
Ranelic Acid	metabolites	135459-87-9	C ₁₂ H ₁₀ N ₂ O ₈ S	342.29	5-[Bis(carboxymethyl)ami]-2-carboxy-4-cya-3-thiopheneacetic Acid;
Des-Methyl Frovatriptan	metabolites	147009-08-3	C ₁₄ H ₁₉ N ₃ O	245.326	(6R)-6-ami-6,7,8,9-tetrahydro-5H-carbazole-3-carboxamide;methane
N-Desmethyl Rosuvastatin Na Salt	metabolites	371775-74-5	C ₂₁ H ₂₄ FN ₃ O ₆ S.2Na	511.47	(E)-7-[4-(4-Fluorophenyl)-6-isopropyl-2-mesylamipyrimidin-5-yl]-(3R,5S)-dihydroxyhept-6-eic Acid Disodium Salt Mohydrate;
Pyridostigmine Metabolite	metabolites	155-97-5	C ₆ H ₈ NO. Br	110.14 79.90	(1-methylpyridin-1-ium-3-yl) N,N-dimethylcarbamate
Dehydro Nifedipine	metabolites	67035-22-7	C ₁₇ H ₁₆ N ₂ O ₆	344.32	2,6-Dimethyl-4-(2-nitrophenyl)-3,5-pyridinedicarboxylic Acid 3,5-Dimethyl Ester;

name	category	cas_number	mol_formula	mol_weight	synonym
Desmethyl Bosentan	metabolites	253688-61-8	C ₂₆ H ₂₇ N ₅ O ₆ S	537.6	4-(1,1-Dimethylethyl)-N-[6-(2-hydroxyethoxy)-5-(2-hydroxyphoxy)[2,2'-bipyrimidin]-4-yl]benzenesulfonamide;
Dehydro Lercanidipine	metabolites	887769-34-8	C ₃₆ H ₃₉ N ₃ O ₆ .HCl	645	2,6-Dimethyl-4-(3-nitrophenyl)-3,5-pyridinedicarboxylic Acid 3-[2-[(3,3-Diphenylpropyl)methylami]-1,1-dimethylethyl] 5-Methyl Ester;
Deschloro Atovaquone	metabolites	92458-44-1	C ₂₂ H ₂₀ O ₃	332.39	trans-2-Hydroxy-3-(4-phenylcyclohexyl)-1,4-naphthalenedione;
Eicosapentaeic Acid	metabolites	10417-94-4	C ₂₀ H ₃₀ O ₂	302.45	5Z,8Z,11Z,14Z,17Z)-5,8,11,14,17-Eicosapentaeic Acid; (all-Z)-5,8,11,14,17-Eicosapentaeic Acid;
4-Hydroxy Thalidomide	metabolites	5054-59-1	C ₁₃ H ₁₀ N ₂ O ₅	274.232	2-(2,6-dioxopiperidin-3-yl)-4-hydroxyisoindole-1,3-dione
4-Hydroxy Propranolol HCL	metabolites	14133-90-5	C ₁₆ H ₂₁ N ₃ O ₃ .HCl	311.80	4-[2-Hydroxy-3-[(1-methylethyl)ami]propoxy]-1-naphthalel Hydrochloride
N-Desmethyl Mifepristone	metabolites	104004-96-8	C ₂₈ H ₃₃ N ₂ O ₂	415.57	(11β,17β)-17-Hydroxy-11-[4-(methylami)phenyl]-17-(1-propyn-1-yl)-estra-4,9-dien-3-one; N-Desmethyl-RU 486; RU 42633;
N desmethyl Enzalutamide	metabolites	1242137-16-1	C ₂₀ H ₁₄ F ₄ N ₄ O ₂ S	450.41	4-[3-[4-Cya-3-(trifluoromethyl)phenyl]-5,5-dimethyl-4-oxo-2-thioxo-1-imidazolidinyl]-2-fluorobenzamide

name	category	cas_number	mol_formula	mol_weight	synonym
Desmethyl Lacosamide	metabolites	175481-38-6	C ₂₀ H ₁₄ F ₄ N ₄ O ₂ S	236.27	(2R)-2-(Acetylamino)-3-hydroxy-N-(phenylmethyl)propanamide; N-Acetyl-D-Serine Benzyl Amide;
Hydroxy Mifepristone	metabolites	105012-15-5	C ₂₀ H ₁₄ F ₄ N ₄ O ₂ S	445.61	(11β,17β)-11-[4-(Dimethylamino)phenyl]-17-hydroxy-17-(3-hydroxy-1-propyn-1-yl)-estra-4,9-dien-3-one; RU 42698;
3-Hydroxy Thalidomide	metabolites	5054-59-1	C ₁₃ H ₁₀ N ₂ O ₅	274.24	cis-5-Hydroxy-3-phthalimidoglutarimide; 2-(5-Hydroxy-2,6-dioxo-3-piperidinyl)-1H-Isoindole-1,3(2H)-dione;
N-Hydroxy Thalidomide	metabolites	126663-38-5	C ₁₃ H ₁₀ N ₂ O ₅	274.24	2-(1-hydroxy-2,6-dioxopiperidin-3-yl)isoindole-1,3-dione
N-Desmethyl Loperamide	metabolites	66164-07-6	C ₂₈ H ₃₁ ClN ₂ O ₂	463.01	4-(4-Chlorophenyl)-4-hydroxy-N-methyl-α,α-diphenyl-1-piperidinebutanamide; R 20905;
Amoxicillin Diketopiperazine	metabolites	94659-47-9	C ₁₆ H ₁₉ N ₃ O ₅ S	365.41	2-[5-(4-Hydroxyphenyl)-3,6-dioxo-2-piperazinyl]-5,5-dimethyl-4-thiazolidinecarboxylic Acid;
3-hydroxy-N- Methyl Pyridinium	metabolites	4685-07-8	C ₆ H ₈ NO ⁺	110.134	1-(2,4-Dinitrophenyl)-3,4-dimethyl-pyridinium Chloride
Curcumin Sulphate	metabolites	339286-19-0	C ₂₁ H ₂₀ O ₉ S	448.44	(1E,6E)-1-(4-Hydroxy-3-methoxyphenyl)-7-[3-methoxy-4-(sulfooxy)phenyl]-1,6-heptadiene-3,5-dione Tetrabutylammonium Salt;
4-Methylamino Antipyrine	metabolites	519-98-2	C ₂₁ H ₂₀ O ₉ S	217.27	N-(2,3-Dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)acetamide; 4-(N-Acetylamino)antipyrine

name	category	cas_number	mol_formula	mol_weight	synonym
N-Desmethyl Rosuvastatin calcium Salt	metabolites	371775-74-5 (acid)	C ₂₁ H ₂₄ FN ₃ O ₆ S ₁ /2Ca	485.53	(E)-7-[4-(4-Fluorophenyl)-6-isopropyl-2-mesylamipyrimidin-5-yl]-(3R,5S)-dihydroxyhept-6-enoic Acid Disodium Salt Monohydrate;
Deacetyl Colchicine	metabolites	3476-50-4	C ₂₀ H ₂₃ NO ₅	357.4	7-ami-1,2,3,10-tetramethoxy-6,7-dihydrobenzo[a]heptalen-9(5H)-one;
Daurubicinol	metabolites	54193-28-1	C ₂₇ H ₃₁ NO ₁₀	529.55	(8S,10S)-10-[(3-Ami-2,3,6-trideoxy- α -L-lyxo-hexopyrasyloxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-[1-hydroxyethyl]-1-methoxy-5,12-naphthacenedione Hydrochloride;
6-Hydroxy Testosterone	metabolites	62-99-7	C ₁₉ H ₂₈ O ₃	304.43	(6R,8R,9S,10R,13S,14S,17S)-6,17-dihydroxy-10,13-dimethyl-1,2,6,7,8,9,11,12,14,15,16,17-dodecahydrocyclopenta[a]phenanthren-3-one
Tetrahydro curcumin	metabolites	36062-04-1	C ₂₁ H ₂₄ O ₆	372.41	1,7-Bis(4-hydroxy-3-methoxyphenyl)-3,5-heptanedione; HZIV 81-2; NSC 687845; Sabiwhite; Tetrahydrodiferuloylmethane
Octahydro Curcumin	metabolites	36062-07-4	C ₂₁ H ₂₈ O ₆	376.44	1,7-Bis(4-hydroxy-3-methoxyphenyl)-3,5-heptanediol
3-Keto norgestimate	metabolites	18290-31-8	C ₂₃ H ₃₀ O ₃	354.48	(8R,9S,10R,13S,14S,17R,Z)-13-Ethyl-17-ethynyl-17-hydroxy-6,7,8,9,10,11,12,13,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3(2H)-one
Docosaheptaenoic Acid ethyl ester	metabolites	73310-11-9	C ₂₄ H ₃₆ O ₂	356.55	(all-Z)-4,7,10,13,16,19-Docosaheptaenoic Acid Ethyl Ester; Cervonic Acid Ethyl Ester; Ethyl (all-Z)-4,7,10,13,16,19-Docosaheptaenoate;

name	category	cas_number	mol_formula	mol_weight	synonym
Eicosapentaenoic Acid Ethyl Ester	metabolites	86227-47-6	C ₂₂ H ₃₄ O ₂	330.50	Ethyl Eicosapentaeate; Timdonic Acid Ethyl Ester; cis-Eicosapentaeic Acid Ethyl Ester;
Docosahexaenoic Acid	metabolites	6217-54-5	C ₂₂ H ₃₂ O ₂	328.49	(all-Z)-4,7,10,13,16,19-Docosahexaenic Acid; DHA; Cervonic Acid; Doconexent; Maril D 50TG; Ropufa 60; AlgaMac 3050
6-O-Desmethyl Donepezil	metabolites	120013-56-1	C ₂₃ H ₂₇ NO ₃	365.48	1-Benzyl-4-[(6-hydroxy-5-methoxy-1-oxo-indan-2-yl)methyl]piperidine; 2,3-Dihydro-6-hydroxy-5-methoxy-2-[[1-(phenylmethyl)-4-piperidinyl]methyl]-1H-inden-1-one;
Desbutyl Lumefrantine	metabolites	355841-11-1	C ₂₆ H ₂₄ Cl ₃ NO	472.83	(Z)-Desbutyl-benflumetol; (9Z)- α -[(Butylami)methyl]-2,7-dichloro-9-[(4-chlorophenyl)methylene]-9H-fluorene-4-methal
Fingolimod Phosphate HCl	metabolites	1348803-59-7	C ₂₆ H ₂₄ Cl ₃ NO	423.92	rac FTY720 Phosphate; 1,3-Propanediol, 2-ami-2-[2-(4-octylphenyl)ethyl]-, 1-(dihydrogen phosphate) hydrochloride; 2-Ami-2-[2-(4-octylphenyl)ethyl]-1,3-propanediol 1-(Dihydrogen Phosphate);
Dehydro Lacidipine	metabolites	130996-24-6	C ₂₆ H ₃₁ NO ₆	453.54	E)-4-[2-[3-(1,1-Dimethylethoxy)-3-oxo-1-prphenyl]-2,6-dimethyl-3,5 -pyridinedicarboxylic Acid Diethyl Ester; GR 510922qopenyl];
Desmethyl Mirtazapine	metabolites	61337-68-6	C ₁₆ H ₁₇ N ₃ .HCl	251.3	1,2,3,4,10,14b-hexahydro-pyrazi[2,1-a]pyrido[2,3-c][2]benzapine N-demethylmirtazapine;

name	category	cas_number	mol_formula	mol_weight	synonym
Fingolimod Phosphate	metabolites	402615-91-2	C ₁₉ H ₃₄ N ₅ O ₅ P	387.45	2-ami-2-(hydroxymethyl)-4-(4-octylphenyl)butyl dihydrogen phosphate
Carbamazepine 10,11-epoxide	metabolites	36507-30-9	C ₁₅ H ₁₂ N ₂ O ₂	252.27	1a,10b-Dihydro-6H-dibenzo[b,f]oxire[d]azepine-6-carboxamide; 10,11-Dihydro-10,11-epoxycarbamazepine;
1-Methoxy Decane	metabolites	68989-91-3	C ₁₁ H ₂₄ O	172.31	-methoxy-; Decyl methyl ether;
4-oxo-Retinoic acid	metabolites	38030-57-8	C ₂₀ H ₂₆ O ₃	314.42	4-Ketoretiic acid; 4-oxo-Tretiin; All-trans-4-oxoretiic acid;
Mebeverine Alcohol	metabolites	14367-47-6	C ₁₆ H ₂₇ N ₂ O ₂	265.4	4-[Ethyl[2-(4-methoxyphenyl)-1-methylethyl]ami]-1-butyl; 4-[Ethyl[2-(p-methoxy- α -phenyl)-1-methylethyl]ami]-1-butyl;
9-Cis-Retinoic Acid	metabolites	5300-03-8	C ₂₀ H ₂₈ O ₂	300.42	(2E,4E,6Z,8E)-3,7-Dimethyl-9-(2,6,6-trimethylcyclohex-1-enyl)na-2,4,6,8-tetraeic Acid; 9-cis-Tretiin;
Docosahexoic acid Ester	metabolites	2566-90-7	C ₂₃ H ₃₄ O ₂	342.51	methyl (4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaeate
Doxorubicine	metabolites	25316-40-9	C ₂₁ H ₁₈ O ₉	414.36	(8S,10S)-7,8,9,10-tetrahydro-6,8,10,11-tetrahydroxy-8-(2-hydroxyacetyl)-1-methoxy-5,12-naphthacenedione; Adriamycin Aglycone;
4-Oxo Alitritonin	metabolites	71748-58-8	C ₂₀ H ₂₆ O ₃	314.425	(2Z,4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethyl-3-oxocyclohexen-1-yl)na-2,4,6,8-tetraeic acid
N-Desmethyl Asenapine	metabolites	128915-56-0	C ₁₆ H ₁₅ Cl ₂ NO	308.202	Desmethyl asenapine

name	category	cas_number	mol_formula	mol_weight	synonym
Desmethyl Mebeverine Alcohol	metabolites	155172-67-1	C ₁₅ H ₂₅ NO ₂	251.37	4-[2-[Ethyl(4-hydroxybutyl)ami]propyl]phel
4-OXO-Isotritonine	metabolites	71748-58-8	C ₂₀ H ₂₆ O ₃	314.425	(2Z,4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethyl-3-oxocyclohexen-1-yl)na-2,4,6,8-tetraic acid
Mebeverine Acid	metabolites	475203-77-1	C ₁₆ H ₂₅ NO ₃	279.38	4-[ethyl-[1-(4-methoxyphenyl)propan-2-yl]ami]butaic acid
DM-3411 (metabolite of brexpiprazole)	metabolites	913611-97-9	C ₂₅ H ₂₇ N ₃ O ₃ S	449.56	4-(4-{4-[(2-oxo-1,2-dihydroquinolin-7-yl)oxy]butyl}piperazin-1-yl)-1H-1-benzothiophen-1-ium-1-olate;
Dihydrodiol Ibrutinib	metabolites	1654820-87-7	C ₂₅ H ₂₆ N ₆ O ₄	474.51	1-[3-[4-Ami-3-(4-phexyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl]piperidin-1-yl]-2,3-dihydroxypropan-1-one;
Desmethyl Selegeline	metabolites	18913-84-3	C ₁₂ H ₁₅ N	173.259	1-phenyl-N-prop-2-ynylpropan-2-amine
Moxifloxacin-n- sulfphate	metabolites	234080-64-9	C ₂₁ H ₂₄ FN ₃ O ₇ S	481.49	7-[(4aS,7aS)-1-sulfo-3,4,4a,5,7,7a-hexahydro-2H-pyrrolo[3,4-b]pyridin-6-yl]-1-cyclopropyl-6-fluoro-8-methoxy-4-oxoquinoline-3-carboxylic acid
3- Alpha-Hydroxy Tibolone	metabolites	100239-44-9	C ₂₁ H ₃₀ O ₂	314.46	(3R,7R,8R,9S,13S,14S,17R)-17-ethynyl-7,13-dimethyl-2,3,4,6,7,8,9,11,12,14,15,16-dodecahydro-1H-cyclopenta[a]phenanthrene-3,17-diol;

name	category	cas_number	mol_formula	mol_weight	synonym
5-Hydroxy Saxagliptin	metabolites	841302-24-7	C ₁₈ H ₂₅ N ₃ O ₃	331.42	(1S,3S,5S)-2-[(2S)-2-ami-2-(3,5-dihydroxytricyclo[3.3.1.1 ^{3,7}]dec-1-yl)acetyl]-2-Azabicyclo[3.1.0]hexane-3-carbonitrile; BMS 510849;
4-Hydroxy-N-Desmethyl - Tamoxifen	metabolites	125618-41-9	C ₃₀ H ₃₅ NO ₄	473.6	4-[(E/Z)-1-[4-[N-Boc-2-(methylami)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]phel
Doxorubicinolone	metabolites	24385-10-2	C ₂₁ H ₂₀ O ₉	416.39	(8S,10S)-8-[(1S)-1,2-Dihydroxyethyl]-7,8,9,10-tetrahydro-6,8,10,11-tetrahydroxy-1-methoxy-5,12-naphthacenedione;
(+)- β - Dihyrotetrabenazine	metabolites	924854-60-4	C ₁₉ H ₂₉ NO ₃	319.44	(2S,3R,11bR)-1,3,4,6,7,11b-Hexahydro-9,10-dimethoxy-3-(2-methylpropyl)-2H-benzo[a]quilizin-2-ol; (2S,3R,11bR)-Dihyrotetrabe
(+)- α - Dihyrotetrabenazine	metabolites	85081-18-1	C ₁₉ H ₂₉ NO ₃	319.43	(2R,3R,11bR)-1,3,4,6,7,11b-Hexahydro-9,10-dimethoxy-3-(2-methylpropyl)-2H-benzo[a]quilizin-2-ol;
Hydroxy Ropinirole	metabolites	NA	C ₁₆ H ₂₄ N ₂ O ₂	276.37	4-(2-(dipropylami)ethyl)-1-hydroxyindolin-2-one
Abiraterone Acetate	metabolites	154229-18-2	C ₂₆ H ₃₃ N ₂ O ₂	391.55	(3 β)-17-(3-Pyridinyl)androsta-5,16-dien-3-ol Acetate (Ester);

name	category	cas_number	mol_formula	mol_weight	synonym
Abiraterone Sulphate	metabolites	NA	C ₂₄ H ₃₁ N ₄ O ₄ S	429.57	[(8R,9S,10R,13S,14S)-10,13-dimethyl-17-pyridin-3-yl-2,3,4,7,8,9,11,12,14,15-decahydro-1H-cyclopenta[a]phenanthren-3-yl] hydrogen sulfate
Tazarotenic Acid	metabolites	118292-41-4	C ₁₉ H ₁₇ N ₂ O ₂ S	323.41	6-[2-(3,4-Dihydro-4,4-dimethyl-2H-1-benzothiopyran-6-yl)ethynyl]-3-pyridinecarboxylic Acid;
Tazarotenic Acid Methyl Ester	metabolites	1332579-70-0	C ₂₀ H ₁₉ N ₂ O ₂ S	337.43	6-[2-(3,4-Dihydro-4,4-dimethyl-2H-1-benzothiopyran-6-yl)ethynyl]-,3-Pyridinecarboxylic Acid Methyl Ester
Lurasidone metabolite 14283	metabolites	186204-32-0	C ₂₈ H ₃₆ N ₄ O ₃ S	508.69	
6 Beta Naltrexol	metabolites	49625-89-0	C ₂₀ H ₂₅ N ₄ O ₄	343.42	Naltrexol;6b-Naltrexo;6-Naltrexol;a-Naltrexol;6-β-Naltrexol HCl;6-Hydroxynaltrexone;6b-Hydroxynaltrexone;
Didemethyl clomipramine	metabolites	62724-32-7	C ₁₇ H ₁₉ ClN ₂	286.8	3-Chloro-10,11-dihydro-5H-dibenz[b,f]azepine-5-propanamine
11-O-Sulphate Asenapine	metabolites	1399103-21-9	C ₁₇ H ₁₆ ClNO ₅ S	381.83064	Asenapine O-sulfate;Asenapine 11-Hydroxysulfate
Lurasidone metabolite 14326	metabolites	186204-33-1	C ₂₈ H ₃₆ N ₄ O ₃ S	508.69	5 α /6 α -Hydroxy Lurasidone;Lurasidone metabolite 14326;
17 beta estradiol sulphate sodium salt	metabolites	4999-79-5	C ₁₈ H ₂₃ NaO ₅ S	374.43	2-((8R,9S,13S,14S,17S)-17-Hydroxy-13-methyl-3-oxido-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-4-yl)acetate

name	category	cas_number	mol_formula	mol_weight	synonym
17 beta 8,9 dehydro estradiol	metabolites	23392-54-3	C ₁₈ H ₂₂ O ₂	270.37	(17β)-Estra-1,3,5(10),8-tetraene-3,17-diol; Estra-1,3,5(10),8-tetraene-3,17β - diol; 17β - 8,9-Dehydroestradiol; 17β -8-Dehydroestradiol;
17 beta 8,9 Dehydro estradiol Na sulphate	metabolites	61612-83-7	C ₁₈ H ₂₁ NaO ₅ S	372.41	(17β)-Estra-1,3,5(10),8-tetraene-3,17-diol; Estra-1,3,5(10),8-tetraene-3,17β - diol; 17β - 8,9-Dehydroestradiol; 17β -8-Dehydroestradiol;
8,9 dehydroestrone	metabolites	474-87-3	C ₁₈ H ₂₀ O ₂	268.35	3-Hydroxyestra-1,3,5(10),8-tetraen-17-one; Δ 8-Dehydroestrone; Δ8-Isoequilin; 8,9- Dehydroestrone;
8,9 dehydroestrone sulphate sodium salt	metabolites	61612-83-7	C ₁₈ H ₁₉ O ₅ SNa	370.4	3-(Sulfooxy)-estra-1,3,5(10),8-tetraen-17-one Sodium Salt;Δ8,9-Dehydroestrone Sodium Sulfate;
Betamethasone 17 propionate	metabolites	5534-13-4	C ₂₅ H ₃₃ FO ₆	448.52	(11β,16β)-9-Fluoro-11,21-dihydroxy-16- methyl-17-(1-oxopropoxy)pregna-1,4-diene- 3,20-dione; Betamethasone 17α -Propionate;
17 beta Dihydroequilin	metabolites	3563-27-7	C ₁₈ H ₂₂ O ₂	270.37	(17β)-Estra-1,3,5(10),7-tetraene-3,17-diol; Estra-1,3,5(10),7-tetraene-3,17β -diol; 7- Dehydroestradiol; NSC 12170; β - Dihydroequilin;
Olsalazine o sulphide	metabolites	NA	C ₁₄ H ₁₀ N ₂ O ₉ S	382.3	5-[(2E)-2-(3-carboxy-4-oxocyclohexa-2,5-dien- 1-ylidene)hydrazinyl]-2-sulfooxybenzoic acid
Beclomethasone 21 propionate	metabolites	69224-79-9	C ₂₅ H ₃₃ ClO ₆	464.98	(11β,16β)-9-Chloro-11,17-dihydroxy-16- methyl-21-(1-oxopropoxy)-pregna-1,4-diene- 3,20-dione;

name	category	cas_number	mol_formula	mol_weight	synonym
Roflumilast N oxide	metabolites	292135-78-5	C ₁₇ H ₁₄ Cl ₂ F ₂ N ₂ O ₄	419.2	3-(Cyclopropylmethoxy)-N-(3,5-dichloro-1-oxido-4-pyridinyl)-4-(difluoromethoxy)benzamide;
Desethoxy hydroxy Ticagrelor	metabolites	NA	C ₂₁ H ₂₄ F ₂ N ₆ O ₃ S	478.52	(3aR,4S,6R,6aS)-6-[7-[[[(1R,2S)-2-(3,4-Difluorophenyl)cyclopropyl]ami]-5-(propylthio)-3H-1,2,3-triazolo[4,5-d]pyrimidin-3-yl]tetrahydro-2,2-dimethyl-4H-cyclopenta-1,3-dioxol-4-ol
Betamethasone 21 propionate	metabolites	75883-07-7	C ₂₅ H ₃₃ FO ₆	448.52	(11β,16β)-9-Fluoro-11,17-dihydroxy-16-methyl-21-(1-oxopropoxy)pregna-1,4-diene-3,20-dione;
Sofosbuvir metabolite GS331007	metabolites	863329-66-2	C ₁₀ H ₁₃ FN ₂ O ₅	260.22	(2S)-Isopropyl 2-((((2R,3R,4R,5R)-5-(2,4-Dioxo-3,4-dihydropyrimidin-1(2H)-yl)-4-fluoro-3-hydroxy-4-methyltetrahydrofuran-2
4 hydroxy methyl ambrisentan	metabolites	1106685-66-8	C ₂₂ H ₂₂ N ₂ O ₅	394.42	(αS)-α-[[4-(Hydroxymethyl)-6-methyl-2-pyrimidinyl]oxy]-β-methoxy-β-phenylbenzenepropionic Acid
Abiraterone N oxide	metabolites	NA	C ₂₄ H ₃₁ NO ₂	365.52	
Sofosbuvir metabolite GS 566500	metabolites	1233335-78-8	C ₁₃ H ₁₉ FN ₃ O ₉ P	411.28	(S)-2-(((S)-(((2R,3R,4R,5R)-5-(2,4-Dioxo-3,4-dihydropyrimidin-1(2H)-yl)-4-fluoro-3-hydroxy-4-methyltetrahydrofuran-2-yl)methoxy)(phoxy)phosphoryl)ami)propionic

name	category	cas_number	mol_formula	mol_weight	synonym
Desmethyl clomipramine	metabolites	NA	C ₁₈ H ₂₂ Cl ₂ N ₂	337.29	3-(2-chloro-5,6-dihydrobenzo[b][1]benzazepin-11-yl)-N-methylpropan-1-amine;hydrochloride
Albendazole sulfoxide	metabolites	54029-12-8	C ₁₂ H ₁₅ N ₃ O ₃ S	281.33	Albendazole Oxide, Ricobendazole, RS-8852, Albendazole Impurity B (EP), Albendazole EP Impurity B;Albendazole EP Impurity B ;
Carboxylic acid Enzalutamide metabolite	metabolites	1242137-15-0	C ₂₀ H ₁₃ F ₄ N ₃ O ₃ S	451.39	4-[3-[4-Cya-3-(trifluoromethyl)phenyl]-5,5-dimethyl-4-oxo-2-thioxo-1-imidazolidinyl]-2-fluoro-benzoic Acid
Decladisyl Azithromycin	metabolites	117693-41-1	C ₃₀ H ₅₈ N ₂ O ₉	590.79	(2R,3S,4R,5R,8R,10R,11R,12S,13S,14R)-2-Ethyl-3,4,10,13-tetrahydroxy-3,5,6,8,10,12,14-heptamethyl-11-[[3,4,6-trideoxy-3-(dimethylami)-β-D-xylo-hexopyrasyl]oxy]-1-oxa-6-azacyclopentadecan-15-one;
O-desmethyl Gefitinib	metabolites	847949-49-9	C ₂₁ H ₂₂ ClFN ₄ O ₃	432.88	4-[(3-Chloro-4-fluorophenyl)ami]-6-[3-(4-morpholinyl)propoxy]-7-quinazolil;
Clozapine N oxide	metabolites	34233-69-7	C ₁₈ H ₁₉ ClN ₄ O	342.82	8-Chloro-11-(4-methyl-1-piperazinyl)-5H-dibenzo[b,e][1,4]diazepine N-Oxide, C
Chlorpromazine N- Oxide	metabolites	1672-76-0	C ₁₇ H ₁₉ ClN ₂ OS	334.86	3-(2-chlorophethiazin-10-yl)-N,N-dimethylpropan-1-amine oxide
Chlorpromazine Sulfoxide	metabolites	969-99-3	C ₁₇ H ₁₉ ClN ₂ OS	334.86	2-Chloro-N,N-dimethyl-10H-Phethiazine-10-propanamine 5-Oxide; 2-Chloro-10-[3-(dimethylami)propyl]phethiazine 5-Oxide;
Albendazole sulfone	metabolites	75184-71-3	C ₁₂ H ₁₅ N ₃ O ₄ S	297.33	N-[6-(Propylsulfonyl)-1H-benzimidazol-2-yl]carbamic Acid Methyl Ester;

name	category	cas_number	mol_formula	mol_weight	synonym
Desmethyl prochlorperazine	metabolites	49780-18-9	C ₂₇ H ₃₀ ClN ₃ O ₈ S	592.06	2-Chloro-10-[3-(1-piperazinyl)propyl]-10H-phethiazine Dimaleate;
N desmethyl erythromycin	metabolites	992-62-1	C ₃₆ H ₆₅ NO ₁₃	719.9	Des-N-methylerythromycin; Demethylerythromycin; USP Clarithromycin Impurity R; Erythromycin EP Impurity B
Zolimitriptan N Oxide	metabolites	251451-30-6	C ₁₆ H ₂₁ N ₃ O ₃	303.362	N,N-dimethyl-2-[5-[(2-oxo-1,3-oxazolidin-4-yl)methyl]-1H-indol-3-yl]ethanamine oxide
Demethyl chlorpromazine HCl	metabolites	3953-65-9	C ₁₆ H ₁₈ Cl ₂ N ₂ S	341.30	2-Chloro-N-methyl-10H-phethiazine-10-propanamine Hydrochloride;
N desmethyl clozapine	metabolites	6104-71-8	C ₁₇ H ₁₇ ClN ₄	312.8	8-Chloro-11-(1-piperazinyl)-5H-dibenzo[b,e][1,4]diazepine
3-OH Anagrelide HCl	metabolites	733043-41-9	C ₁₀ H ₇ Cl ₂ N ₃ O ₂ HCl	308.55	6,7-Dichloro-1,5-dihydro-3-hydroxyimidazo[2,1-b]quinazolin-2(3H)-one HCL;
Dihydrotestosteron e	metabolites	521-18-6	C ₁₉ H ₃₀ O ₂	290.44	(5S,8R,9S,10S,13S,14S,17S)-17-hydroxy-10,13-dimethyl-1,2,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydrocyclopenta[a]phenanthren-3-one
Macitenatan metabolite ACT- 132577	metabolites	1103522-45-7	C ₁₆ H ₁₄ Br ₂ N ₆ O ₄ S	546.19	N-[5-(4-Bromophenyl)-6-[2-[(5-bromo-2-pyrimidinyl)oxy]ethoxy]-4-pyrimidinyl]-sulfamide, ACT-132577
4-OH Alverine HCl salt	metabolites	142047-93-6	C ₂₀ H ₂₇ NO HCl	333.89	4-(3-(ethyl(3-phenylpropyl)ami)propyl)phel

name	category	cas_number	mol_formula	mol_weight	synonym
3-OH methyl Tolcapone	metabolites	134612-80-9	C15H13NO5	287.3	
N-desmethyl Regorafenib- n- oxide M5 metabolite	metabolites	835621-12-0	C20H13ClF4N4O4	484.79	4-[4-[[[4-Chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]-3-fluorophenyl]-2-pyridinecarboxamide 1-Oxide
Regorafenib- n- oxide M2 metabolite	metabolites	835621-11-9	C21H15ClF4N4O4	498.81	4-[4-[[[4-Chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]-3-fluorophenyl]-N-methyl-2-pyridinecarboxamide 1-Oxide
Dasatinib N oxide/Dasatinib M5 metabolite	metabolites	910297-52-8	C22H26ClN7O3S	504.00	N-[2-Chloro-6-methylphenyl]-2-[[6-[4-(2-hydroxyethyl)-1-piperazinyl]-2-methyl-4-pyrimidinyl]amino]-5-thiazolecarboxamide N-Oxide;
Desmethyl Nefopam	metabolites	46868-19-3	C16H17NO. HCl	275.77	3,4,5,6-Tetrahydro-1-phenyl-1H-2,5-benzoxazocine; N-Desmethylnefopam; rnefopam;
E- 10- hydroxynortriptylin e	metabolites	1156-99-6	C19H21NO	279.38	(5Z)-10,11-Dihydro-5-[3-(methylamino)propylidene]-5H-dibenzo[a,d]cyclohepten-10-ol; (Z)-10-Hydroxyrtriptyline; 10-Hydroxy-(Z)-rtriptyline;
Lamotrigine N2 Oxide	metabolites	136565-76-9	C9H7Cl2N5O	272.09	6-(2,3-Dichlorophenyl)-1,2,4-triazine-3,5-diamine 2-Oxide;

name	category	cas_number	mol_formula	mol_weight	synonym
(S)-Empagliflozin	metabolites	864070-44-0	C ₂₃ H ₂₇ ClO ₇	450.91	(1S)-1,5-anhydro-1-(4-chloro-3-{4-[(3S)-tetrahydrofuran-3-yloxy]benzyl}phenyl)-D-glucitol-1-chloro-4-(glucopyras-1-yl)-2-(4-(tetrahydrofuran-3-yloxy)benzyl)benzene
Daunorubicin HCl	metabolites	23541-50-6	C ₂₇ H ₂₉ NO ₁₀ .HCl	563.98	(8S,10S)-10-[(3-Ami-2,3,6-trideoxy- α -L-lyxohexopyrasyl)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-[1-hydroxyethyl]-1-methoxy-5,12-naphthacenedione Hydrochloride;
7 hydroxy chlorpromazine	metabolites	2095-62-7	C ₁₇ H ₁₉ ClN ₂ OS	334.86	8-Chloro-10-[3-(dimethylamipropyl)-10H-phethiazin-3-ol];
N1 acetyl triethelene tetramine	metabolites	141998-21-2	C ₈ H ₂₀ N ₄ O	188.27	N-Acetyl-triethylenetetramine
nor Doxepin hydrochloride	metabolites	2887-91-4	C ₁₈ H ₁₉ NO.HCL	301.81	3-(Dibenz[b,e]oxepin-11(6H)-ylidene)-N-methyl-1-propanamine; Δ 11(6H), γ -[3-(Methylami)propylidene]dibenz[b,e]oxepine Hydrochloride
nor Doxepin	metabolites	1225-56-5	C ₁₈ H ₁₉ NO	265.356	(3E)-3-(6H-benzo[c][1]benzoxepin-11-ylidene)-N-methylpropan-1-amine
Macitentan metabolite 373898	metabolites	1433875-14-9	C ₁₅ H ₁₇ BrN ₄ O ₅ S	445.29	2-[[5-(4-Bromophenyl)-6-[[[(propylami)sulfonyl]ami]-4-pyrimidinyl]oxy]-acetic Acid;

name	category	cas_number	mol_formula	mol_weight	synonym
Calcifedol	metabolites	19356-17-3	C ₂₇ H ₄₄ O ₂	400.64	3β,5Z,7E)-9,10-Secocholesta-5,7,10(19)-triene-3,25-diol; 25-Hydroxycholecalciferol; 25-Hydroxyvitamin D;
N,N-Diethyldithiocarbamate	metabolites	1470-61-7	C ₅ H ₁₀ AgNS ₂	256.14	Carbamic acid, diethyldithio-, sodium salt, trihydrate (8Cl) ;Carbamodithioic acid, diethyl-, sodium salt, trihydrate (9Cl)
Diethyl dithiocarbamate	metabolites	392-74-5	C ₅ H ₁₀ NS ₂	148.262	Carbamodithioic acid, diethyl-, ion(1-);
3,4-Dimethoxybenzoic acid	metabolites	93-07-2	C ₉ H ₁₀ O ₄	182.175	Benzoic acid, 3,4-dimethoxy-; Dimethylprotocatechuic acid;
15 OH Lubiprostone	metabolites	475992-30-4	C ₂₀ H ₃₄ F ₂ O ₅	392.48	7-[(1R,2R,3R)-2-(4,4-difluoro-3-hydroxyoctyl)-3-hydroxy-5-oxocyclopentyl]heptaic acid
Desethyl sacubitril	metabolites	149709-44-4	C ₂₂ H ₂₅ NO ₅	383.44	[S-(R*,S*)]- γ -[(3-Carboxy-1-oxopropyl)ami]-α -methyl-[1,1'-Biphenyl]-4-pentaic Acid; (2R,4S)-4-[(3-Carboxy-1-oxopropyl)ami]-4-[(p-phenylphenyl)methyl]-2-methylbutaic Acid;
17 beta exemestane	metabolites	122370-91-6	C ₂₀ H ₂₆ O ₂	298.42	17 β -Hydroxy-6-methyleneandrosta-1,4-dien-3-one ;
3-OH Methyl Mefenamic acid	metabolites	5129-20-4	C ₁₅ H ₁₅ NO ₃	257.29	2-[[3-(Hydroxymethyl)-2-methylphenyl]ami]-benzoic Acid; N-(α 3-Hydroxy-2,3-xylyl)-anthranilic Acid;

name	category	cas_number	mol_formula	mol_weight	synonym
3 Carboxy Mefenamic acid	metabolites	190379-82-9	C ₁₅ H ₁₃ NO ₄	271.27	3-[(2-Carboxyphenyl)ami]-2-methylbenzoic Acid;
Sarpogrelate metabolite	metabolites	125926-17-2	C ₂₄ H ₃₁ NO ₆	429.513	4-[1-(dimethylami)-3-[2-[2-(3-methoxyphenyl)ethyl]phexy]propan-2-yl]oxy-4-oxobutaic acid
7-desmethyl agomelatine	metabolites	152302-45-9	C ₁₄ H ₁₅ NO ₂	229.27	N-[2-(7-Hydroxy-1-naphthalenyl)ethyl]acetamide; O-Demethylagomelatine; S 21517;
N-Desmethyl Tamoxifen HCl	metabolites	15917-65-4	C ₂₅ H ₂₈ ClNO	393.95	(Z)-2-[4-(1,2-Diphenyl-1-butenyl)phexy]-N-methylethanamine Hydrochloride;N-Demethyltamoxifen Hydrochloride;
N desmeThyl ulipristal	metabolites	159681-67-1	C ₂₉ H ₃₅ NO ₄	461.59	(11β)-17-Hydroxy-11-[4-(methylami)phenyl]-19-rpregna-4,9-diene-3,20-dione;
N,N-Didesmethyl Ulipristal	metabolites	244206-52-8	C ₂₈ H ₃₃ NO ₄	459.57	(11β)-11-(4-Amiphenyl)-17-hydroxy-19-rpregna-4,9-diene-3,20-dione;
M12 METABOLITE OF OLAPARIB	metabolites	NA	C ₂₄ H ₂₄ FN ₄ O ₄	452.47	N-(2-(Cyclopropanecarboxamido)ethyl)-2-fluoro-N-(2-hydroxyethyl)-5-((4-oxo-3,4-dihydrophthalazin-1-yl)methyl)benzamide
M15 METABOLITE OF OLAPARIB	metabolites	NA	C ₂₄ H ₂₃ FN ₄ O ₄	450.46	4-((3-(4-(Cyclopropanecarbonyl)piperazine-1-carbonyl)-4-fluorophenyl)(hydroxy)methyl)phthalazin-1(2H)-one

name	category	cas_number	mol_formula	mol_weight	synonym
M18 METABOLITE OF OLAPARIB	metabolites	763113-22-0	C ₂₄ H ₂₃ FN ₄ O ₃	434.46	4-[(3-{[4-(cyclopropylcarbonyl)piperazin-1-yl]carbonyl}-4-fluorophenyl)methyl]phthalazin-1(2H)-one
5 carboxy pirfenidione	metabolites	77837-08-2	C ₁₂ H ₉ N ₃ O ₃	215.20	1,6-Dihydro-6-oxo-1-phenyl-3-pyridinecarboxylic Acid; 6-Oxo-1-phenyl-1,6-dihydropyridine-3-carboxylic Acid;
N1 N10 diacetyl Triethelyne tetramine	metabolites	141998-22-3	C ₁₀ H ₂₂ N ₄ O ₂	230.31	N,N'-[1,2-Ethanediy]bis(imi-2,1-ethanediy)]bisacetamide; N1,N10-Diacetyltriethylenetetramine;
N-Deshydroxyethyl Dasatinib/Dasatini b metabolite M4	metabolites	910297-51-7	C ₂₀ H ₂₂ ClN ₇ OS	443.95	N-(2-Chloro-6-methylphenyl)-2-[[2-methyl-6-(1-piperazinyl)-4-pyrimidinyl]ami]-5-thiazolecarboxamide;
O-Desmethyl Apremilast	metabolites	1384441-38-6	C ₂₀ H ₂₀ N ₂ O ₇ S	432.45	N-[2-[(1S)-1-(3-ethoxy-4-hydroxyphenyl)-2-methylsulfonylethyl]-1,3-dioxoisindol-4-yl]acetamide
O-Acetyl Silodosin	metabolites	160970-86-5	C ₂₇ H ₃₄ F ₃ N ₃ O ₅	537.57	(R)-1-[3-(Acetyloxy)propyl]-2,3-dihydro-5-[2-[[2-[2-(2,2,2-trifluoroethoxy)phexy]ethyl]ami]propyl]-1H-Indole-7-carboxamide
3-Demethyl Colchicine	metabolites	7336-33-6	C ₂₁ H ₂₃ N ₃ O ₆	385.42	N-[(7S)-5,6,7,9-Tetrahydro-3-hydroxy-1,2,10-trimethoxy-9-oxobenzo[a]heptalen-7-yl]-acetamide; O3-Demethylcolchicine;
N desmethyl atomoxetine	metabolites	1189961-95-2	C ₁₆ H ₁₉ NO	241.34	3-(2-methylphexy)-3-phenylpropan-1-amine;

name	category	cas_number	mol_formula	mol_weight	synonym
4 OH atomoxetine	metabolites	435293-66-6	C ₁₇ H ₂₁ NO ₂	271.35	3-Methyl-4-[(1R)-3-(methylamino)-1-phenylpropoxy]phenol; Atomoxetine 4-Hydroxy Impurity
Dasatinib Carboxylic Acid Ethyl Ester/Dasatinib metabolite M6	metabolites	910297-62-0	C ₂₄ H ₂₈ ClN ₇ O ₃ S	530.04	4-[6-[[5-[[2-chloro-6-methylphenyl]amino]carbonyl]-2-thiazolyl]amino]-2-methyl-4-pyrimidinyl]-1-piperazineacetic Acid Ethyl Ester
N desmethyl Riociguat	metabolites	625115-52-8	C ₁₉ H ₁₇ FN ₈ O ₂	408.4	[4,6-Diamino-2-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-5-pyrimidinyl]-, methyl ester carbamic acid;
Rotigotine Sulfate	metabolites	128478-69-3	C ₁₉ H ₂₅ NO ₄ S ₂	395.54	(6S)-5,6,7,8-tetrahydro-6-[propyl[2-(2-thienyl)ethyl]amino]-1-naphthalene-1-sulfate (Hydrogen Sulfate);
N-despropyl Rotigotine sulfate	metabolites	1196459-54-7	C ₁₆ H ₁₉ NO ₄ S ₂	353.46	(6S)-5,6,7,8-Tetrahydro-6-[2-(2-thienyl)ethyl]amino]-1-naphthalene-1-sulfate (Hydrogen sulfate)
N-desethienylethyl rotigotine sulfate	metabolites	154714-31-5	C ₁₆ H ₁₉ NO ₄ S ₂	285.36	(S)-5,6,7,8-Tetrahydro-6-(propylamino)-1-naphthalene-1-sulfate (Hydrogen Sulfate Ester)
Rivastigmine metabolite	metabolites	1217706-31-4	C ₁₀ H ₁₅ NO	165.23	Ethylmethylcarbamate 3-[(1S)-1-(dimethylamino)ethyl]phenyl Ester; Ethylmethylcarbamate 3-[1-(dimethylamino)ethyl]phenyl Ester, (S)-;

name	category	cas_number	mol_formula	mol_weight	synonym
N-oxide Abiraterone SO4	metabolites	NA	C ₂₄ H ₃₁ N ₅ O ₅ S	445.57	[(8R,9S,10R,13S,14S)-10,13-dimethyl-17-(1-oxidopyridin-1-ium-3-yl)-2,3,4,7,8,9,11,12,14,15-decahydro-1H-cyclopenta[a]phenanthren-3-yl] hydrogen
Acetyl Isoniazid	metabolites	1078-38-2	C ₈ H ₉ N ₃ O ₂	179.18	2-Acetylhydrazide-4-pyridinecarboxylic Acid; 1-Acetyl-2-isonicotiylhydrazine; Acetylisoniazide;
Albuterol sulphate	metabolites	51022-70-9	C ₁₃ H ₂₁ N ₆ O ₆ S	319.37	α 1-[[[(1,1-Dimethylethyl)am]methyl]-4-hydroxy-1,3-benzenedimethal Sulfate; Aerolin; Albuterol Hemisulfate;
6-Hydroxy Chlorzoxazone	metabolites	1750-45-4	C ₇ H ₄ ClNO ₃	185.6	5-Chloro-6-hydroxy-2(3H)-benzoxazolone; 6-Hydroxychlorzoxazone; NSC 24955;
Tapentadol O sulphate	metabolites	1300037-87-9	C ₁₄ H ₂₃ N ₄ O ₄ S	301.4	[3-[(2R,3R)-1-(dimethylamino)-2-methylpentan-3-yl]phenyl] hydrogen sulfate
N-desethyl Sunitinib	metabolites	356068-97-8	C ₂₀ H ₂₃ FN ₄ O ₂	370.42	N-[2-(Ethylamino)ethyl]-5-[(Z)-(5-fluoro-1,2-dihydro-2-oxo-3H-indol-3-ylidene)methyl]-2,4-dimethyl-1H-pyrrole-3-carboxamide;
Escitalopram N oxide	metabolites	917482-45-2	C ₂₀ H ₂₁ FN ₂ O ₂	340.4	(1S)-1-[3-(Dimethyloxidoamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile ;
Pravastatin Lactone	metabolites	85956-22-5	C ₂₃ H ₃₄ O ₆	406.51	(2S)-2-Methylbutaioic Acid (1S,3S,7S,8S,8aR)-1,2,3,7,8,8a-Hexahydro-3-hydroxy-7-methyl-8-[2-[(2R,4R)-tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl]ethyl]-1-naphthalenyl Ester; R 414;

name	category	cas_number	mol_formula	mol_weight	synonym
3 Alpha hydroxy Pravastatin	metabolites	81093-43-8	C ₂₃ H ₃₅ O ₇	423.51	(β R, δ R,1S,2R,3S,8S,8aR)-1,2,3,7,8,8a-Hexahydro- β , δ ,3-trihydroxy-2-methyl-8-[(2S)-2-methyl-1-oxobutoxy]-1-naphthaleneheptaic Acid
Olanzapine N oxide	metabolites	174794-02-6	C ₁₇ H ₂₀ N ₄ OS	328.43	2-Methyl-4-(4-methyl-4-oxido-1-piperazinyl)-10H-thie[2,3-b][1,5]benzodiazepine;
3',4'- DIHYDROXYPHEN YL ACETONE	metabolites	2503-44-8	C ₉ H ₁₀ O ₃	166.17	1-(3,4-Dihydroxyphenyl)-2-propane; 1-(3',4'-Dihydroxyphenyl)-2-propane; 1-(3,4-Dihydroxyphenyl)-2-propane;
Abiraterone O sulphate	metabolites	NA	C ₂₄ H ₃₁ N ₄ O ₄ S	429.575	[(8R,9S,10R,13S,14S)-10,13-dimethyl-17-pyridin-3-yl-2,3,4,7,8,9,11,12,14,15-decahydro-1H-cyclopenta[a]phenanthren-3-yl] hydrogen sulfate
DexLansoprazole sulfone	metabolites	131926-99-3	C ₁₆ H ₁₄ F ₃ N ₃ O ₃ S	385.36	Lansoprazole sulfone
5-OH Lansoprazole	metabolites	131926-98-2	C ₁₆ H ₁₄ F ₃ N ₃ O ₂ S	369.36	2-[[[3-Methyl-4-(2,2,2-trifluoroethoxy)-2-pyridinyl]methyl]thio]-1H-benzimidazol-6-ol;
Conjugated Taurine obeticholic acid	metabolites	NA	C ₂₈ H ₄₈ NNaO ₆ S	549.74	2-[[[(4R)-4-[(3R,5S,7R,8R,9S,10S,13R,14S,17R)-3,7-dihydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]pentayl]ami]ethanesulfonic acid

name	category	cas_number	mol_formula	mol_weight	synonym
3OH 7DESMETHYL AGOMELATINE	metabolites	166527-00-0	C ₁₄ H ₁₅ NO ₃	245.27	N-[2-(3,7-dihydroxy-1-naphthalenyl)ethyl]acetamide; Agomelatine 7-Desmethyl-3-Hydroxy Impurity
N-Desmethyl Ulipristal Acetate	metabolites	159681-66-0	C ₂₉ H ₃₅ NO ₄	461.59	(11 β)-17-(Acetyloxy)-11-[4-(methylami)phenyl]-19-rpregna-4,9-diene-3,20-dione; CDB 3877; N-Modemethyl CDB 2914;
N,N-Didesmethyl Ulipristal Acetate	metabolites	NA	C ₂₈ H ₃₃ NO ₄	459.57	(11 β)-17-(Acetyloxy)-11-(4-amiphenyl)-19-rpregna-4,9-diene-3,20-dione
Dapoxetine N- Oxide HCl	metabolites	1346603-24-4	C ₂₁ H ₂₃ NO ₂ . HCl	357.88	(α S)-N,N-Dimethyl-N-oxido- α -[2-(1-naphthalenyloxy)ethyl]benzenemethanamine;
Axitinib sulfoxide (M12)	metabolites	1347304-18-0	C ₂₂ H ₁₈ N ₄ O ₂ S	402.47	N-Methyl-2-[[3-[(1E)-2-(2-pyridinyl)ethenyl]-1H-indazol-6-yl]sulfinyl]-benzamide
Nefopam N oxide	metabolites	66091-32-5	C ₁₇ H ₁₉ NO ₂	269.34	3,4,5,6-Tetrahydro-5-methyl-1-phenyl-1H-2,5-benzoxazocine 5-Oxide;
3 OH N propagyl 1 aminoindan	metabolites	NA	C ₁₂ H ₁₃ NO	187.24	(1S)-N-prop-2-ynyl-2,3-dihydro-1H-inden-1-amine
3 OH 1 aminoindan	metabolites	NA	C ₉ H ₁₁ NO	149.19	
3 Hydroxy Pilocarpine	metabolites	936031-05-9	C ₁₁ H ₁₆ N ₂ O ₃	224.26	(3S,4R)-3-ethyl-3-hydroxy-4-[(3-methylimidazol-4-yl)methyl]oxolan-2-one

name	category	cas_number	mol_formula	mol_weight	synonym
N acetylated Amantadine	metabolites	880-52-4	C ₁₂ H ₁₉ NO	193.29	1-Acetamidoadamantane; 1-Acetamidotricyclo[3.3.1.1(3,7)]decane; 1-Acetylamidadamantane; N-(1-Adamanthyl)acetamide;
Ranolazine N-Oxide	metabolites	N/A	C ₂₄ H ₃₃ N ₃ O ₅	443.54	1-(2-((2,6-dimethylphenyl)ami)-2-oxoethyl)-4-(2-hydroxy-3-(2-methoxyphexy)propyl)piperazine 1-oxide
Ranolazine Bis N-oxide	metabolites	1246816-00-1	C ₂₄ H ₃₃ N ₃ O ₆	459.54	N-(2,6-Dimethylphenyl)-4-[2-hydroxy-3-(2-methoxyphexy)propyl]-1-piperazineacetamide 1,4-Dioxide;
Dasatinib carboxylic acid	metabolites	910297-53-9	C ₂₂ H ₂₄ ClN ₇ O ₃ S	501.99	4-[6-[[5-[(2-Chloro-6-methylphenyl)ami]carbonyl]-2-thiazolyl]ami]-2-methyl-4-pyrimidinyl]-1-piperazineacetic Acid;
Rosuvastatin Keto Acid	metabolites	1346747-49-6	C ₂₂ H ₂₆ FN ₃ O ₆ S	479.52	(3R,6E)-7-[4-(4-Fluorophenyl)-6-(1-methylethyl)-2-[methyl(methylsulfonyl)ami]-5-pyrimidinyl]-3-hydroxy-5-oxo-6-hepteic Acid;
25 hydroxy vitamin D2	metabolites	21343-40-8	C ₂₈ H ₄₄ O ₂	412.65	(1S,3Z)-4-Methylene-3-[(2E)-2-[(1R,3aS,7aR)-octahydro-1-[(1R,2E,4S)-5-hydroxy-1,4,5-trimethyl-2-hexenyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]cyclohexal;
Dasatinib metabolite M21	metabolites	NA	C ₂₂ H ₂₅ N ₇ O ₂ S	451.55	
Isocitric acid	metabolites	1637-73-6 (anhydrous)	C ₆ H ₅ NaO ₇ · XH ₂ O	258.07	1-hydroxypropane-1,2,3-tricarboxylic acid

name	category	cas_number	mol_formula	mol_weight	synonym
7-HYDROXY PROPRANOLOL	metabolites	81907-81-5	C ₁₆ H ₂₁ N ₃ O ₃	275.34	8-[2-Hydroxy-3-[(1-methylethyl)ami]propoxy]-2-naphthalel; (+/-)-8-[2-Hydroxy-3-[(1-methylethyl)ami]propoxy]-2-naphthalel;
5-HYDROXY PROPRANOLOL	metabolites	81907-82-6	C ₁₆ H ₂₁ N ₃ O ₃	275.34	5'-Hydroxypropralol;5-Hydroxy Propralol;1-(5-Hydroxy-1-naphthoxy)-3-(isopropylami)-2-propal;
M1 Metabolite of Nintedanib	metabolites	656247-17-5	C ₃₀ H ₃₁ N ₅ O ₄	525.61	3-(((4-N-methyl-2-(4-methylpiperazin-1-yl)acetamido)phenyl)ami)(phenyl)methylene)-2-oxoindoline-6-carboxylicacid;
5 oxo fluvastatin	metabolites	NA	C ₂₄ H ₂₃ F ₃ N ₄ O ₄	408.43	E)-(+/-)-7-[3-(4-Fluorophenyl)-1-(methylethyl)-1H-indol-2-yl]-3-hydroxy-5-oxo-6-hepteic Acid;
4 hydroxy diclofenac	metabolites	64118-84-9	C ₁₄ H ₁₁ Cl ₂ N ₃ O ₃	312.15	2-[(2,6-Dichloro-4-hydroxyphenyl)ami]benzeneacetic Acid; 4'-Hydroxydiclofenac
N desmethyl thiothixene	metabolites	NA	C ₂₂ H ₂₇ N ₃ O ₂ S ₂	429.60	NA
Thiothixene Sulfoxide	metabolites	NA	C ₂₃ H ₂₉ N ₃ O ₃ S ₂	459.62	NA
Liothyronine sulfate	metabolites	31135-55-4	C ₁₅ H ₁₂ I ₃ N ₃ O ₇ S	731.04	Triiodothyronine Sulfate; 3,5-Diiodo-O-[3-iodo-4-(sulfooxy)phenyl]-L-tyrosine;
7- Alpha thiomethyl Spironolactone	metabolites	38753-77-4	C ₂₃ H ₃₂ O ₃ S	388.56	17 α -Hydroxy-7 α -(methylthio)-3-oxo-pregn-4-ene-21-carboxylic Acid γ -Lactone;SC 26519; 7 α -Thiomethylspiro lactone; 7 α -Thiomethyl-SL;

name	category	cas_number	mol_formula	mol_weight	synonym
6- β -Hydroxy-7- α -thiomethyl Spirolactone	metabolites	42219-60-3	C ₂₃ H ₃₂ O ₄ S	404.56	(6 β ,7 α ,17 α)-6,17-Dihydroxy-7-(methylthio)-3-oxo-pregn-4-ene-21-carboxylic Acid γ -Lactone
7 hydroxy quetiapine	metabolites	139079-39-3	C ₂₁ H ₂₅ N ₃ O ₃ S	399.51	11-[4-[2-(2-Hydroxyethoxy)ethyl]-1-piperazinyl]dibenzo[b,f][1,4]thiazepin-7-ol;
Selexipag Metabolite - ACT 333679	metabolites	475085-57-5	C ₂₅ H ₂₉ N ₃ O ₃	419.53	2-[4-[(5,6-Diphenyl-2-pyrazinyl)(1-methylethyl)ami]butoxy]-acetic Acid; [4-[(5,6-Diphenylpyrazinyl)(1-methylethyl)ami]butoxy]-acetic Acid;
6-hydroxy etodolac	metabolites	101901-06-8	C ₁₇ H ₂₁ NO ₄	303.35	1,8-Diethyl-1,3,4,9-tetrahydro-6-hydroxypyra[3,4-b]indole-1-acetic Acid;
6-Hydroxybenzbromarone	metabolites	152831-00-0	C ₁₇ H ₁₂ Br ₂ O ₄	440.08	(3,5-Dibromo-4-hydroxyphenyl)(2-ethyl-6-hydroxy-3-benzofuranyl)methane;(3,5-Dibromo-4-hydroxyphenyl)(2-ethyl-6-hydroxybenzofuran-3-yl)methane
Quetiapine Sulfoxide	metabolites	329216-63-9	C ₂₁ H ₂₅ N ₃ O ₃ S	399.51	2-[2-[4-(5-Oxidodibenzo[b,f][1,4]thiazepin-11-yl)-1-piperazinyl]ethoxy]ethal;Quetiapine S-Oxide; Quetiapine EP Impurity S;
Lenvatinib N-Oxide	metabolites	1788901-86-9	C ₂₁ H ₁₉ ClN ₄ O ₅	442.85	4-[3-Chloro-4-[[[(cyclopropylami)carbonyl]ami]phexyl]-7-methoxy-6-quilinecarboxamide 1-Oxide; Lenvatinib Metabolite M3

name	category	cas_number	mol_formula	mol_weight	synonym
O-Demethyl Lenvatinib	metabolites	C20H17ClN4O4	C20H17ClN4O4	412.83	4-[3-Chloro-4- [[[(cyclopropylamino)carbonyl]amino]phenoxy]-7- hydroxy-6-quinolinecarboxamide; Lenvatinib M2
Norcyclobenzaprine	metabolites	303-50-4	C19H19N	261.36	N-Methyl-5H-dibenzo[a,d]cycloheptene-Δ ⁵ , γ - propylamine; 3-(5H-Dibenzo[a,d]cyclohepten- 5-ylidene)-N-methyl-1-propanamine;
Chlorpromazine N- oxide	metabolites	1672-76-0	C17H19ClN2OS	334.86	3-(2-chlorophethiazine-10-yl)-N,N- dimethylpropan-1-amine oxide
Sulphoxy chlorpromazine	metabolites	NA	C17H19ClN2OS	334.86	2-Chloro-N,N-dimethyl-10H-Phethiazine-10- propanamine 5-Oxide; 2-Chloro-10-[3- (dimethylamino)propyl]phethiazine 5-Oxide; NSC 17470;
Desmethyl tacrolimus	metabolites	132172-14-6	C43H67NO12	790.01	13-Desmethyl FK 506
Phloroglucinol Sulphate	metabolites	72630-02-5	C ₆ H ₉ NO ₆ S	223.2	3,5-Dihydroxyphenyl Hydrogen Sulfate, Ammonia Salt
5-(4-cyaphoxy)-2- hydroxyl benzoic acid (AN8323)	metabolites	613-94-5	C14H10BN ₃ O3	251.048	4-[(1-hydroxy-3H-2,1-benzoxaborol-5- yl)oxy]benzonitrile
3-Hydroxy Fampridine	metabolites	52334-53-9	C5H6N2O	110.116	4-amipyridin-3-ol
3-Hydroxy Fampridine Sulfate	metabolites	NA	C5H6N2O4S	190.177	(4-amipyridin-3-yl)oxidanesulfonic acid

name	category	cas_number	mol_formula	mol_weight	synonym
Linacotide Metabolite	metabolites	851199-59-2	C ₅₉ H ₇₉ N ₁₅ O ₂₁ S ₆	1526.74	L-Cysteinyl-L-cysteinyl-L- α -glutamyl-L-tyrosyl-L-cysteinyl-L-cysteinyl-L-asparaginyl-L-prolyl-L-alanyl-L-cysteinyl-L-threonylglycyl-L-cysteinyl-L-tyrosine Cyclic (1→6),(2→10),(5→13)-Tris(disulfide);
Tizaxonide	metabolites	173903-47-4	C ₁₀ H ₇ N ₃ O ₄ S	265.24	2-hydroxy-N-(5-nitro-1,3-thiazol-2-yl)benzamide
RO 64-1056 (Bosentan metabolite	metabolites	253688-62-9	C ₂₆ H ₂₇ N ₅ O ₇ S	553.587	4-(1-hydroxy-2-methylpropan-2-yl)-N-[6-(2-hydroxyethoxy)-5-(2-hydroxyphexy)-2-(pyrimidin-2-yl)pyrimidin-4-yl]benzene-1-sulfonamide
Dasatinib M24	metabolites	910297-58-4	C ₂₂ H ₂₆ ClN ₇ O ₃ S	504	NA
4-methoxy Moxonidine	metabolites	75439-01-9	C ₁₀ H ₁₅ N ₅ O ₂	237.26	N-(4,5-Dihydro-1H-imidazol-2-yl)-4,6-dimethoxy-2-methyl-5-pyrimidinamine
Promethazine N- Oxide	metabolites	81480-39-9	C ₁₇ H ₂₀ N ₂ OS	300.42	N,N, α -Trimethyl-10H-phethiazine-10-ethanamine N-Oxide
Promethazine Sufone	metabolites	13754-56-8	C ₁₇ H ₂₀ N ₂ O ₂ S	316.42	N,N, α -Trimethyl-5,5-dioxide-10H-phethiazine-10-ethanamine; 10-[2-(dimethylami)propyl]-5,5-dioxidephethiazine;
7- hydroxyfluphenazin e	metabolites	33098-48-5	C ₂₂ H ₂₆ F ₃ N ₃ O ₂ S	453.52	0-[3-[4-(2-Hydroxyethyl)-1-piperazinyl]propyl]-8-(trifluoromethyl)-10H-phethiazin-3-ol;

name	category	cas_number	mol_formula	mol_weight	synonym
Fluphenazine Decanoate N- Oxide	metabolites	76005-64-6	C ₃₂ H ₄₄ F ₃ N ₃ O ₃ S	607.77	2-[4-[3-[2-(Trifluoromethyl)phethiazin-10-yl]propyl]-1-piperazinyl]ethyl Ester Decaic Acid N-Oxide 4-[3-[2-(trifluoromethyl)phethiazin-10-yl]propyl]-1-Piperazineethyl Decaate (Ester) N-oxide 2-[1-Oxido-4-[3-[2-(trifluoromethyl)-10H-phethiazin-10-yl]propyl]-1-piperazinyl]ethyl Ester Decaic Acid
Venetoclax M30	metabolites	NA	C ₄₅ H ₅₃ ClN ₇ O ₅ S	838.35	2-((1H-Pyrrolo[2,3-b]pyridin-5-yl)oxy)-N-((3-ami-4-(((tetrahydro-2H-pyran-4-yl)methyl)ami)phenyl)sulfonyl)-4-(4-((4'-chloro-5,5-dimethyl-3,4,5,6-tetrahydro-[1,1'-biphenyl]-2-yl)methyl)piperazin-1-
O-DESMETHYL DIHYDROTETRAB ENAZINE	metabolites	1065193-59-0	C ₁₈ H ₂₇ N ₃ O ₃	305.41	+) -9-O-DESMETHYL-DTBZ;2H-BENZO[A]QUILIZINE-2,9-DIOL, 1,3,4,6,7,11B-HEXAHYDRO-3-ISOBUTYL-10-METHOXY-;2H-BENZO[A]QUILIZINE-2,9-DIOL, 1,3,4,6,7,11B-HEXAHYDRO-10-METHOXY-3-(2-METHYLPROPYL)-;
N-Desmethyl- dextrorphan	metabolites	15676-23-0	C ₁₆ H ₂₁ NO	243.34	NA
Ethyl hydrogen fumarate/Monoeth yl fumarate	metabolites	2459-05-4	C ₆ H ₈ O ₄	144.126	(E)-4-ethoxy-4-oxobut-2-eic acid

name	category	cas_number	mol_formula	mol_weight	synonym
6 hydroxy paclitaxel	metabolites	153212-75-0	C ₄₇ H ₅₁ NO ₁₅	869.917	(α R, β S)- β -(Benzoylami)- α ,4-dihydroxybenzenepropaic Acid 6,12b-Bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-3,4,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-metha-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl Ester;
N desmethyl tapentadol	metabolites	1300037-83-5	C ₁₃ H ₂₁ NO	207.317	3-[(2R,3R)-2-methyl-1-(methylami)pentan-3-yl]phel
N-Hydroxymethyl aripiprazole	metabolites	NA	C ₂₄ -H ₂₉ -Cl ₂ -N ₃ -O ₃	478.4171	2(1H)-Quiline, 7-(4-(4-(2,3-dichlorophenyl)-1-piperazinyl)butoxy)-3,4-dihydro-1-(hydroxymethyl)-
Tenofovir Monophosphate	metabolites	206646-04-0	C ₉ H ₁₅ N ₅ O ₇ P ₂	367.2	Isohypophosphoric acid, [[(1R)-2-(6-ami-9H-purin-9-yl)-1-methylethoxy)methyl]- (9Cl);
Tenofovir Diphosphate	metabolites	166403-66-3	C ₉ H ₁₆ N ₅ O ₁₀ P ₃	447.173	[(2R)-1-(6-amipurin-9-yl)propan-2-yl]oxymethyl-[hydroxy(phosphooxy)phosphoryl]oxyphosphinic acid
4-O-Methyl Dopa	metabolites	555-30-6	C ₁₀ H ₁₃ NO ₄	211.217	(2S)-2-ami-3-(3-hydroxy-4-methoxyphenyl)propaic acid
Chlorhexidine acetate	metabolites	56-95-1	C ₂₂ H ₃₀ Cl ₂ N ₁₀ 2[CH ₃ COO	505.4526005	N,N''-Bis(4-chlorophenyl)-3,12-diimi-2,4,11,13-tetraazatetradecanediimidamide Diacetate; 1,1'-Hexamethylenebis[5-(p-chlorophenyl)-biguanide Diacetate;

name	category	cas_number	mol_formula	mol_weight	synonym
N desmethyl ranolazine	metabolites	172430-45-4	C ₂₃ H ₃₁ N ₃ O ₄	413.51	N-(2,6-Dimethylphenyl)-4-[2-hydroxy-3-(2-hydroxyphexy)propyl]-1-piperazineacetamide
Desmethyl Rivastigmine	metabolites	1230021-28-9	C ₁₃ H ₂₀ N ₂ O ₂	236.315	[3-[(1S)-1-(dimethylamino)ethyl]phenyl] N,N-dimethylcarbamate
N-Desmethyl Levofloxacin	metabolites	117707-40-1	C ₁₇ H ₁₈ FN ₃ O ₄	347.346	Levofloxacin related compound A;
Hydroxy celecoxib	metabolites	170571-00-3	C ₁₇ H ₁₄ F ₃ N ₃ O ₃ S	397.37	4-[5-[4-(Hydroxymethyl)phenyl]-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide
Tapentadol N- Oxide	metabolites	1346601-17-9	C ₁₄ H ₂₃ NO ₂	237.343	(2R,3R)-3-(3-hydroxyphenyl)-N,N,2-trimethylpentan-1-amine oxide
N-Desmethyl Toremifene HCl	metabolites	176671-73-1	C ₂₅ H ₂₇ Cl ₂ NO	428.39	2-[4-[(1Z)-4-Chloro-1,2-diphenyl-1-buten-1-yl]phexy]-N-methylethanamine Hydrochloride Salt;
4-Hydroxy Toremifene	metabolites	177748-22-0	C ₂₆ H ₂₈ ClNO ₂	421.96	4-[(1Z)-4-Chloro-1-[4-[2-(dimethylamino)ethoxy]phenyl]-2-phenyl-1-buten-1-yl]phel; (Z)-4-Hydroxytoremifene;
Toremifene N- Oxide	metabolites	163130-29-8	C ₂₆ H ₂₈ ClNO ₂	421.96	2-[4-[(1Z)-4-Chloro-1,2-diphenyl-1-butenyl]phexy]-N,N-dimethylethanamine N-Oxide;
6 hydroxy desloratidine	metabolites	119410-05-8	C ₁₉ H ₁₉ ClN ₂ O	326.82	8-Chloro-6,11-dihydro-11-(4-piperidinylidene)-5H-benzo[5,6]cyclohepta[1,2-b]pyridin-6-ol;

name	category	cas_number	mol_formula	mol_weight	synonym
N-Demethyl Ondansetron	metabolites	99614-14-9	C ₁₇ H ₁₇ N ₃ O	279.34	1,2,3,9-Tetrahydro-3-[(2-methyl-1H-imidazol-1-yl)methyl]-4H-carbazol-4-one; Desmethylandansetron;
1-Veratrylglycine	metabolites	32161-30-1	C ₁₁ H ₁₅ NO ₄	225.24	3-Methoxy-O-methyl-L-tyrosine; (S)-3,4-Dimethoxyphenylalanine; β -(3,4-Dimethoxyphenyl)-L-alanine;
Rac α -Methyl Dopa	metabolites	55-40-3	C ₁₀ H ₁₃ NO ₄	211.21	3-Hydroxy- α -methyltyrosine; 3-(3,4-Dihydroxyphenyl)-2-methylalanine;
N-Formyl Amlodipine	metabolites	93848-81-8	C ₂₁ H ₂₅ ClN ₂ O ₆	436.89	4-(2-Chlorophenyl)-2-[[2-(formylamino)ethoxy]methyl]-1,4-dihydro-6-methyl-,3,5-pyridinedicarboxylic Acid 3-ethyl 5-methyl Ester
Amlodipine Metabolite 5	metabolites	114018-75-6	C ₁₉ H ₁₈ ClNO ₇	407.81	Amlodipine Metabolite 5
N-(2-hydroxyethyl)- phthalamic acid	metabolites	58509-24-3	C ₁₀ H ₁₁ NO ₄	209.2	Amlodipine Impurity
Dehydro Amlodipine N- Oxide	metabolites	113994-41-5	C ₂₀ H ₂₃ ClN ₂ O ₆	422.86	Dehydro Amlodipine N-Oxide
Deschloro Amlodipine Maleate	metabolites	88150-53-2	C ₂₀ H ₂₆ N ₂ O ₅	374.44	3-ethyl 5-methyl 2-((2-amioethoxy)methyl)-6-methyl-4-phenyl-1,4-dihydropyridine-3,5-dicarboxylate

name	category	cas_number	mol_formula	mol_weight	synonym
Desmethoxy Curcumin	metabolites	24939-17-1	C ₂₀ H ₁₈ O ₅	338.35	(E,E)-1-(4-Hydroxy-3-methoxyphenyl)-7-(4-hydroxyphenyl)-1,6-heptadiene-3,5-dione;
Glargine Metabolite 2	metabolites	NA	C ₂₅₇ H ₃₉₈ N ₆₂ O ₇₃ S ₆	5649.53	glycylseryl(methyl)histidyl; leucylvalyl-a-glutamylalanyltyrosylleucyl(methyl)valyl; methylglycyl;
Glargine Metabolite 1	metabolites	NA	C ₂₆₁ H ₄₀₅ N ₆₃ O ₇₅ S ₆	5750.64	glycylseryl(methyl)histidyl; leucylvalyl-a-glutamylalanyltyrosylleucyl(methyl)valyl; methylglycyl;
Raloxifene N oxide	metabolites	195454-31-0	C ₂₈ H ₂₇ N ₅ O ₅ S	489.58	[6-Hydroxy-2-(4-hydroxyphenyl)benzo[b]thien-3-yl][4-[2-(1-oxido-1-piperidinyl)ethoxy]phenyl]methane;
4 Chloro aniline	metabolites	106-47-8	C ₆ H ₆ ClN; ClC ₆ H ₄ NH ₂	127.571	4-Chlorobenzenamine; P-Chloraniline;
3 hydroxy repaglinide (Mixture of Diastereomers)	metabolites	874908-14-2	C ₂₇ H ₃₆ N ₂ O ₅	468.59	2-Ethoxy-4-[2-[[1-[2-(3-hydroxy-1-piperidinyl)phenyl]-3-methylbutyl]ami]-2-oxoethyl]benzoic Acid;
9-Methoxy Guanine	metabolites	1202645-50-8	C ₇ H ₉ N ₅ O ₂	195.18	2-Ami-1,9-dihydro-9-(methoxymethyl)-6H-purin-6-one;
4'-Hydroxy Dasatinib /Dasatinib metabolite M20	metabolites	910297-57-3	C ₂₂ H ₂₆ ClN ₇ O ₃ S	504.00	N-(2-Chloro-4-hydroxy-6-methylphenyl)-2-[[6-[4-(2-hydroxyethyl)-1-piperazinyl]-2-methyl-4

name	category	cas_number	mol_formula	mol_weight	synonym
Roflumilast N-oxide	metabolites	292135-78-5	C ₁₇ H ₁₄ Cl ₂ F ₂ N ₂ O ₄	419.21	3-(Cyclopropylmethoxy)-N-(3,5-dichloro-1-oxido-4-pyridinyl)-4-(difluoromethoxy)benzamide;
Chloropromazine N-	metabolites	NA	C ₁₇ H ₁₉ ClN ₂ OS	334.86	3-(2-chlorophenothiazin-10-yl)-N,N-dimethylpropan-1-amine oxide
9-Methoxy Gunanin	metabolites	1202645-50-8	C ₇ H ₉ N ₅ O ₂	195.18	2-Amino-1,9-dihydro-9-(methoxymethyl)-6H-purin-6-one;
Brexpiprazole N-oxi	metabolites	NA	C ₂₅ H ₂₇ N ₃ O ₃ S	449.58	7-[4-(4-Benzo[b]thien-4-yl-1-oxido-1-piperazinyl)butoxy]-2(1H)-quinolinone; Brexpiprazole Impurity 3
N-Desmethyl chloro	metabolites	NA	C ₁₆ H ₁₇ ClN ₂ S	304.84	2-Chloro-N-methyl-10H-phenothiazine-10-propanamine Hydrochloride;
Des gly midodrine	metabolites	3600-87-1	C ₁₀ H ₁₅ NO ₃	197.23	1-(2',5'-Dimethoxyphenyl)-2-aminoethanol; α-(Aminomethyl)-2,5-dimethoxy-benzyl Alcohol;
Insulin Glargine Met	metabolites	NA	C ₂₅₁ H ₃₆₀ N ₆₃ O ₇₂ S ₆ .13C ₆ 15N	'5656.60	Insulin Glargine Metabolite 2 13C ₆ 15N
Insulin Glargine Met	metabolites	NA	C ₂₅₅ H ₃₆₇ N ₆₄ O ₇₄ S ₆ .13C ₆ 15N	'5757.70	Insulin Glargine Metabolite 1 13C ₆ 15N
6 hydroxy chloroxazone(VL/M-287-03(P))	metabolites	1750-45-4	C ₇ H ₄ ClNO ₃	185.56	5-Chloro-6-hydroxy-2(3H)-benzoxazolone; 6-Hydroxychloroxazone; NSC 24955;

name	category	cas_number	mol_formula	mol_weight	synonym
O-desethyl azilsarta	metabolites	1442400-68-1	C ₂₃ H ₁₆ N ₄ O ₅	428.39	2-Oxo-3-((2'-(5-oxo-4,5-dihydro-1,2,4-oxadiazol-3-yl)-[1,1'-biphenyl]-4-yl)methyl)-2,3-dihydro-1H-benzo[d]imidazole-4-carboxylic Acid
Oseltamivir acid sod	metabolites	187227-45-8	C ₁₄ H ₂₃ NaN ₂ O ₄	306.35	(3R,4R,5S)-4-(Acetylamino)-5-amino-3-(1-ethylpropoxy)-1-cyclohexence-1-carboxylic Acid sodium salt;
Beta Estradiol 3-Sulfate sodium salt	metabolites	4999-79-5	C ₁₈ H ₂₃ O ₅ SNa	374.43	1,3,5(10)-Estratriene-3,17 β -diol 3-sulfate, 3,17 β -Dihydroxy-1,3,5(10)-estratriene 3-sulfate