

name	category	cas_number	mol_formula	mol_weight	synonym
Tizanidine D4	deuteriumlabeledcom	1188331-19-2	C9H4D4ClN5S	257.74	5-Chloro-N-(4,5-dihydro-1H-imidazol-2-yl-d4)-2,1,3-benzothiadiazol-4-amine
17 β estradiol D4	deuteriumlabeledcom	66789-03-5	C18H20O2D4	276.41	Dihydrofolliculin-d4; (17 β)-Estra-1,3,5(10)-triene-3,17-diol-d4; 3,17-Epidihydroxyestratriene-d4;
5 Hydroxy methyl tolterodine tartrate D14	deuteriumlabeledcom	NA	C22H17NO2D14 .C4H6O6	505.66	2-[(1S)-3-[Bis(1-methylethyl)amino]-1-phenylpropyl]-4-methyl-phenol D14-Tartrate; (S)-Tolterodine D14-Tartrate
Acamprosate calcium salt D3	deuteriumlabeledcom	1225580-94-8	C5H7D3NO4SCa1/ 2	203.26	Calcium Acetylhomotaurinate-d3
Aripiprazole D8	deuteriumlabeledcom	1089115-06-9	C23H19Cl2N3O2D8	456.44	7-[4-[4-(2,3-Dichlorophenyl)-1-piperazinyl-d8]butoxy]-3,4-dihydro-2(1H)-quinolinone; 7-[4-[4-(2,3-Dichlorophenyl)-1-piperazinyl-d8]butoxy]-3,4-dihydrocarbostyryl; Abilify-d8; Abilitat-d8; Aripiprazole-d8

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Carvedilol D5	deuteriumlabeledcom	929106-58-1	C24H21N2O4D5	411.51	1-(9H-Carbazol-4-yloxy)-3-[[2-(2-methoxyphenoxy)ethyl]amino]-2-propanol-d5; Artist-d5; BM 14190; Cadilan-d5; Carca-d5; Cardivas-d5; Carloc-d5; Carvas-d5; Carvedilol-d5; Carvediol-d5; Coreg-d5; DQ 2466-d5; Dilatrend-d5; Dimitone-d5; Eucardic-d5; Korvasan-d5; Kredex-d5; Querto-d5; SKF 105517-d5; Talliton-d5;
Darifenacin hydrobromide D4	deuteriumlabeledcom	1261394-25-5	C28H27D4BrN2O2	511.48	(3R)-1-[2-(2,3-Dihydro-5-benzofuranyl)ethyl]- α - α -diphenyl-3-pyrrolidineacetamide-d4 Hydrobromide; ent-Darifenacin-d4 Hydrobromide
Desloratadine D5	deuteriumlabeledcom	1020719-34-9	C19H14D5ClN2	315.85	8-Chloro-6,11-dihydro-11-(4-piperidinylidene)-5H-benzo[5,6]cyclohepta[1,2-b]pyridine-2,3,4,5,5-d5; Aeriuss-d5; Allex-d5; Azomyr-d5; Clarinex-d5; Descarboethoxyloratadine-d5; NSC 675447-d5; Neoclarityn-d5; Opulis-d5; Sch 34117-d5

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Docetaxel D9	deuteriumlabeledcom	940867-25-4	C43H44NO14D9	816.93	(α R, β S)- β -[[[(1,1-Dimethylethoxy-d9)carbonyl]amino]- α -hydroxybenzenepropanoic Acid (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(Acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl Ester ; Docetaxol-d9; N-Debenzoyl-N-(tert-butoxycarbonyl-d9)-10-deacetyltaxol; RP 56976-d9; Taxotere-d9;
Fluoxetine hydrochloride D5	deuteriumlabeledcom	1173020-43-3	C17H13F3N0D5.HCl	350.82	N-Methyl- γ -[4-(trifluoromethyl)phenoxy](benzene-d5)propanamine Hydrochloride; (+/-)-N-Methyl-3-(phenyl-d5)-3-[4-(trifluoromethyl)phenoxy]propylamine Hydrochloride; Adofen-d5; Affectine-d5; Alzac 20-d5; Ansilan-d5; Deproxin-d5; Digassim-d5; Zepax-d5

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Irbesartan D4	deuteriumlabeledcom	1216883-23-6	C ₂₅ H ₂₄ N ₆ O ₄	432.55	2-Butyl-3-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-1,3-diazaspiro[4.4]non-1-en-4-one; BMS-186295-d4; SR-47436-d4; Aprovel-d4; Avapro-d4;
Levonorgestrel D6	deuteriumlabeledcom	NA	C ₂₁ H ₂₂ O ₂ D ₆	318.49	17-Ethynyl-18-methyl-19-nortestosterone; (17 α)-13-Ethyl-17-hydroxy-18,19-dinorpregn-4-en-20-yn-3-one d6;
Norgestrel D6	deuteriumlabeledcom	NA	C ₂₁ H ₂₂ D ₆ O ₂	318.49	(17 α)-(+/)-13-Ethyl-17-hydroxy-18,19-dinorpregn-4-en-20-yn-3-one-d6; (+/-)-13-Ethyl-17 α -ethynyl-17-hydroxygon-4-en-3-one-d6; (+/-)-Norgestrel-d6; DL-Norgestrel-d6; FH 122A-d6; Methylnorethindrone-d6; Monovar-d6; Neogest-d6; Ovrette-d6; Postinor-d6; SH 70850-d6; SH 850-d6; Wy 3707-d6;

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Memantine hydrochloride 13C2D6	deuteriumlabeledcom	41100-52-1	C ₁₀ H ₁₆ NCI D6 13C2	187.32	3,5-(Dimethyl-13C2d6)tricyclo[3.3.1.1 ^{3,7}]decan-1-amine Hydrochloride; 3,5-(Dimethyl-13C2d6)-1-adamantanamine; 1-Amino-3,5-(dimethyl-13C2d6)adamantane Hydrochloride;
Naproxen 13CD3	deuteriumlabeledcom	1216704-11-8	C ₁₃ H ₁₁ O ₃ 13C D3	234.27	rac 6-Methoxy- α -(methyl-13C,d3)-2-naphthaleneacetic Acid
N Desmethyl rosiglitazone D4	deuteriumlabeledcom	1215407-67-2	C ₁₇ H ₁₃ D ₄ N ₃ O ₃ S	347.42	5-[[4-[2-(2-Pyridinylamino)ethoxy]phenyl]methyl]-2,4-thiazolidinedione-d4; SB 237216-d4;
NDesmethyl sildenafil D8	deuteriumlabeledcompounds		C ₂₁ H ₂₀ N ₆ O ₄ SD8	468.61	5-[2-Ethoxy-5-(1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one-d8; Desmethylsildenafil-d8
Nebivolol D4	deuteriumlabeledcom	1219407-55-2	C ₂₂ H ₂₂ D ₄ NO ₄ F ₂ Cl	445.89	α , α' -[Iminobis(methylene)]bis[6-fluoro-3,4-dihydro-2H-1-benzopyran-2-methanol]-d4; α , α' -(Iminodimethylene)bis[6-fluoro-2-chromanmethanol]-d4; dl-Nebivolol-d4; Narbivolol-d4

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Nicotinic acid D4	deuteriumlabeledcom	66148-15-0	C6D4HNO2	127.14	3-Pyridinecarboxylic Acid-d4; 3-Carboxylpyridine-d4; 3-Carboxypyridine-d4; Akotin-d4; Apelagrin-d4; Niacin-d4; Niacor-d4; Niaspan-d4; Nicacid-d4; Pelonin-d4; Vitamin B3-d4; Vitamin B5-d4; Wampocap-d4; β -Pyridinecarboxylic Acid-d4;
Olmesartan D4	deuteriumlabeledcom	1420880-41-6	C24H22N6O3D4	450.54	4-(1-Hydroxy-1-methylethyl)-2-propyl-1-[[2'-(1H-tetazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-1H-imidazole-5-carboxylic Acid-d4; CS 088-d4; RNH 6270-d4
Pioglitazone D4	deuteriumlabeledcom	1134163-31-7	C19H16N2O3SD4	360.47	5-[[4-[2-(5-Ethyl-2-pyridinyl)ethoxy-d4]phenyl]methyl]-2,4-thiazolidinedione; AD-4833-d4; Actos-d4; U-72107A-d4
Pranlukast D4	deuteriumlabeledcom	NA	C27H19N5O4D4	485.54	N-{4-Oxo-2-(1H-tetrazol-5-yl)-4H-1-benzopyran-8-yl}-4-(4-phenylbutoxy)benzamide-d4; ONO-1078-d4

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Pravastatin sodium D9	deuteriumlabeledcom	NA	C23H26D9NaO7	455.57	(β R, δ R, 1S, 2S, 6S, 8S, 8aR)-1,2,6,7,8,8a-Hexahydro- β , δ , 6-trihydroxy-2-methyl-8-[[2S]-2-methyl-1-oxobutoxy]-1-naphthaleneheptanoic Acid Sodium Salt D9;
Ramipril D5	deuteriumlabeledcom	1132661-86-9	C23H27N2O5D5	421.55	(2S,3aS,6aS)-1-[(2S)-2-[[1S]-1-(Ethoxycarbonyl)-3-(phenyl-d5)propyl]amino]-1-oxopropyl]octahydrocyclopenta[b]pyrrole-2-carboxylic Acid; Altace-d5; Cardace-d5; Delix-d5; HOE-498-d5; Pramace-d5; Ramace-d5; Unipril-d5
Sibutramine D3 HCl	deuteriumlabeledcom	NA	C17H24Cl2ND3	319.33	1-(4-Chlorophenyl)-N,N-di(methyl-d3)- α -(2-methylpropyl)-cyclobutanemethanamine D3
Simvastatin lactone D3	deuteriumlabeledcom	NA	C25H38O5	418.56	[3S-[3 α ,5 β ,5a α ,6 α (2S*,4S*),6 α ,9a α ,10S*]]-2,2-Dimethyl-butanoic Acid 10-Chloro-6-[2-[4-[[1,1-dimethylethyl)dimethylsilyl]oxy]tetrahydro-6-oxo-2H-pyran-2-yl]ethyl]-3,4,5,5a,6,7-hexahydro-2-hydroxy-7-methyl-2H-3,9a-methano-1-benzoxepin-5-yl Ester D3

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Sodium estrone sulfate D4	deuteriumlabeledcom	438-67-5	C18D4H17NaO5S	376.44	Estra-1,3,5(10)-trien-17-one 3-(Sulfooxy) Sodium Salt; Estrone Sulfate Sodium Salt; Conestoral; Estrone Sodium Sulfate; Morestin; NSC 18313; Sodium Estrone-3-sulfate;
Tolterodine hydrochloride D14	deuteriumlabeledcom	1246816-99-8	C22H18D14ClNO	376.03	rac 2-[3-[Bis(1-methylethyl)amino]-1-phenylpropyl]-4-methylphenol-d14 Hydrochloride; R-(+)-N,N-Diisopropyl-3-(2-hydroxy-5-methylphenyl)-3-phenylpropylamine-d14 Hydrochloride; PNU-20058E-d14; Detrol-d14; Detrusitol-d14; R-(+)-Toltaridine-d14 Hydrochloride; Tolterodine-d14 Hydrochloride
Trospium chloride D8	deuteriumlabeledcom	NA	C25H22D8ClNO3	435.96	(1 α ,3 β ,5 α)-3-[(2-Hydroxy-2,2-diphenylacetyl)oxy]-spiro[8-azoniabicyclo[3.2.1]octane-8,1'-pyrrolidinium]-d8 Chloride; Azoniaspiro-d8; Keptan-d8; Relaspium-d8; Sanctura-d8; Spasmex-d8; Spasmo 3-d8

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Amlodipine maleate D4	deuteriumlabeledcom	NA	C ₂₀ H ₂₁ CIN ₂ O ₅ D ₄ .C	528.97	2-[(2-Aminoethoxy)methyl]-4-(2-chlorophenyl)-3-ethoxycarbonyl-5-methoxycarbonyl)-6-methyl-1,4-dihydropyridine-d4 Maleic Acid Salt;
Metformin D6	deuteriumlabeledcom	1185166-01-1	C ₄ H ₆ D ₆ CIN ₅	171.66	N,N-Dimethylimidodicarbonimidic Diamide-d6, Hydrochloride; Diabetosan-d6; Diabex-d6, Glucophage-d6; Metiguanide-d6
Donepezil hydrochloride D7	deuteriumlabeledcom	1261394-20-0	C ₂₄ H ₂₂ D ₇ NO ₃ · HC	422.99	2,3-Dihydro-5,6-dimethoxy-2-[[1-(phenylmethyl)-4-piperidinyl]methyl]-1H-inden-1-one-d7 Hydrochloride; Aricept-d7; Aricept D-d7
Etodolac D4	deuteriumlabeledcom	NA	C ₁₇ H ₁₇ D ₄ NO ₃	291.38	1,8-(Diethyl-d3)-1,3,4,9-tetrahydropyrano[3,4-b]indole-1-acetic Acid;(RS)-Etodolic Acid-d4; (+/-)-Etodolac-d4;
Clopidogrel hydrogen sulfate D3	deuteriumlabeledcom	NA	C ₁₆ H ₁₃ D ₃ CINO ₂ S.H ₂ S	422.93	(±)-Methyl-d3 2-(2-Chlorophenyl)-2-(6,7-dihydro-4H-thieno[3,2-c]pyridin-5-yl)acetate Hydrogen Sulfate; (±)-Clopidogrel-d3 Bisulfate; Clopidogrel-d3 Hemisulfate; Iscover-d3 ; Myogrel-d3 ; Plavix-d3 ; SR 25990C-d3 ; Stroka-d3

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D-[1-13C] Glucosamine HCl	deuteriumlabeledcom	84247-63-2	C6H13NO5 . HCl	180.16 36.46	2-Amino-2-deoxy-D-glucose-1-13C Hydrochloride
Ropinirole HCl D7	deuteriumlabeledcom	1261396-31-9	C16H18D7ClN2O	303.87	4-[2-(Dipropyl-d7-amino)ethyl]-1,3-dihydro-2H-indol-2-one Hydrochloride; 4-[2-(Di-n-propyl-d7-amino)ethyl]-2(3H)-indolone Hydrochloride; SKF-101468A-d7; Requip-d7
Raloxifene HCl D4	deuteriumlabeledcom	1188263-47-9	C28H23D4NO4S.HCl	514.08	[6-Hydroxy-2-(4-hydroxyphenyl)-benzo[b]thien-3-yl][4-[2-(1-piperidinyloxy)ethoxy]phenyl]methanone-d4 Hydrochloride; Keoxifene-d4; LY-139481-d4; Evista-d4

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Spirolactone D3	deuteriumlabeledcom	52-01-7	C24H29O4SD3	419.60	(7 α ,7 α)-7-(Acetylthio-d3)-17-hydroxy-3-oxopregn-4-one-21-carboxylic Acid γ -Lactone; 7 α -Acetylthio-d3-3-oxo-17 α -pregn-4-ene-21,17-carbolactone; SC-9420; Adactone; S-((2'R,7R,8R,9S,10R,13S,14S)-10,13-Dimethyl-3,5'-dioxo-1,2,3,4',5',6,7,8,9,10,11,12,13,14,15,16-hexadecahydro-3'H-spiro[cyclopenta[a]phenanthrene-17,2'-furan]-7-yl) ethanethioate-d3
Ethinyl estradiol D4	deuteriumlabeledcom	NA	C20H20O2D4	300.44	(17 α)-19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol-d4; 17 α -Ethinylestradiol-d4; Amenoron-d4; Eticylol-d4; Eticyclin-d4; Etivex-d4; Feminone-d4; Gynolett-d4; Kolpolyn-d4; Lynoral-d4; Oradiol-d4; Orestralyn-d4; Primogyn C-d4;
Valsartan D9	deuteriumlabeledcom	1089736-73-1	C24H20N5O3D9	444.52	N-(1-Oxopentyl)-N-[[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-L-valine-d9; CGP 48933-d9; Diovan-d9; Nisis-d9; Tareg-d9; Valsartan-d9;

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Imatinib - D4	deuteriumlabeledcom	NA	C29H27D4N7O	497.63	4-[(4-Methyl-1-piperazinyl-2,2,3,3,5,5,6,6-d8)methyl]-N-[4-methyl-3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]benzamide; CGP 57148-d4; Genfatinib-d4
Hydrochlorothiazide 13C 15N2 D2	deuteriumlabeledcom	NA	C6H6ClNO4S2 15N2 13C D2	302.73	6-Chloro-3,4-dihydro-2H-1,2,4-benzothiadiazine-13C,15N2,d2-sulfonamide 1,1-Dioxide; Aquarius-13C,15N2,d2; Bremil-13C,15N2,d2; Cidrex-13C,15N2,d2; Dihydrochlorothiazide-13C,15N2,d2; Dichlotride-13C,15N2,d2; Diurizid-13C,15N2,d2; Drenol-13C,15N2,d2; Hydrochlortiazid-13C,15N2,d2; Hydrex-13C,15N2,d2; Oretic-13C,15N2,d2; Pantemon-13C,15N2,d2; Thiuretic-13C,15N2,d2;
Desmethyl Imatinib D4	deuteriumlabeledcom	NA	C28H25D4N7O	483.61	4-[[4-[[[4-Methyl-3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]phenyl]amino]carbonyl]phenyl]methyl]-1-piperazinecarboxylic Acid 1,1-Dimethylethyl Ester D4;

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Risedronic acid D4	deuteriumlabeledcom	1035438-80-2	C7H7NO7P2D4	287.14	[1-Hydroxy-2-(3-pyridinyl)ethylidene]bis phosphonic Acid-d4; Actonel-d4; NE 58095-d4
Pramipexole D5	deuteriumlabeledcom	NA	C10H12D5N3S	216.36	4,5,6,7-Tetrahydro-N6-propyl-d5-2,6-benzothiazole diamine Dihydrochloride
Ezetimibe D4	deuteriumlabeledcom	1093659-90-5	C24H17D4F2NO3	413.46	(3R,4S)-1-(4-Fluorophenyl)-3-[(3S)-3-(4-fluorophenyl)-3-hydroxypropyl]-4-(4-hydroxyphenyl)-2-azetidinone-d4

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Lisinopril D5	deuteriumlabeledcom	1356905-39-9	C21H26N3O5D5	410.53	(S)-1-[N2-(1-Carboxy-3-phenyl-d5-propyl)-L-lysyl]-L-proline; Acerbon-d5; Alapril-d5; Amicor-d5; Carace-d5; Cipral-d5; Cipril-d5; Coric-d5; Diroton-d5; Inopril-d5; Irumed-d5; Laaven-d5; Linopril-d5; Linvas-d5; Lipril-d5; Lisipril-d5; Lisitec-d5; Lisopril-d5; Lisoril-d5; Lispril-d5; Listril-d5; Lizinopril-d5; Lizonoton-d5; Longes-d5; Loril-d5; MK 521-d5; MK 522-d5; N-(1(S)-Carboxy-3-phenyl-d5-propyl)-L-lysyl-L-proline; N2-[(S)-1-Carboxy-3-phenyl-d5-propyl]-L-lysyl-L-proline; Nanopril-d5; Noperten-d5; Novatec-d5; Optimon-d5; Presiten-d5; Prinil-d5; Prinivil-d5; Prinivil-d5; Skopryl-d5; Tensopril-d5; Tensyn-d5; Vitopril-d5; Vivatec-d5; Zestril-d5
Isradipine D6	deuteriumlabeledcom	NA	C19H15N3O5D6	377.42	4-(4-Benzofurazanyl)-1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic Acid Methyl-d6 1-Methylethyl Ester; Isrodipine-D6

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Trimetazidine D8 2HCl	deuteriumlabeledcom	1219908-67-4	C14H16D8Cl2N2O3	347.31	1-[(2,3,4-Trimethoxy-phenyl)methyl]piperazine-d8 Dihydrochloride; 1-(2,3,4-Trimethoxy-benzyl)piperazine-d8 Dihydrochloride; Kyurinett-d8; Vastarel-d8 F; Yoshimilon-d8;
4-Hydroxy Propranolol HCL D7	deuteriumlabeledcom	1219908-86-7	C16H14D7NO3.HCl	318.85	4-[2-Hydroxy-3-[(1-methylethyl-d7)amino]propoxy]-1-naphthalenol Hydrochloride
Lacidipine 13C8	deuteriumlabeledcom	1261432-01-2	C18H33NO6 13C8	463.48	(E)-4-[2-[3-(1,1-Dimethylethoxy)-3-oxo-1-propenyl]phenyl]-1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic Acid Diethyl Ester-13C8; GR-43659X-13C8
Salmeterol D3	deuteriumlabeledcom	497063-94-2	C25H34D3NO4	418.59	4-Hydroxy- α 1[[[6-(4-phenylbutoxy)hexyl]amino]methyl]-1,3-benzenedimethanol-d3; GR-33343X-d3;

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Omeprazole 13CD3	deuteriumlabeledcom	1261395-28-1	C ₁₆ H ₁₆ N ₃ O ₃ S D ₃ 13C	349.42	6-Methoxy-2-[[[4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole-13C,D3; 5-Methoxy-2-[[[4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole-13C,D3; (±)-Omeprazole-13C,D3; Antra-13C,D3; Gastrogard-13C,D3; Gastroloc-13C,D3; Losec-13C,D3; Mepral-13C,D3; Mopral-13C,D3; Omepral-13C,D3; Prilosec-13C,D3; Zoltum-13C,D3
Ramiprilat D5 (not in solid form)	deuteriumlabeledcom	1132661-86-9	C ₂₁ H ₂₃ N ₂ O ₅ D ₅	393.49	(2S,3aS,6aS)-1-[(2S)-2-[[[1S]-1-(Ethoxycarbonyl)-3-(phenyl-d ₅)propyl]amino]-1-oxopropyl]octahydrocyclopenta[b]pyrrole-2-carboxylic Acid; Altace-d ₅ ; Cardace-d ₅ ; Delix-d ₅ ; HOE-498-d ₅ ; Pramace-d ₅ ; Ramace-d ₅ ; Unipril-d ₅

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Rasagiline mesylate 13C3	deuteriumlabeledcom	1391052-18-8	C9 13C3 H13N.CH3S	270.32	(1R)-2,3-Dihydro-N-2-propyn-1-yl-1H-inden-1-amine-13C3 Mesylate; (R)-2,3-Dihydro-N-2-Propynyl-1-indenamine-13C3 Mesylate; Agilect-13C3 ; Azilect-13C3 Mesylate; TVP-1012-13C3 Mesyalte
Alendronic Acid D6	deuteriumlabeledcom	1035437-39-8	C4H7D6NO7P2	255.13	P,P'-(4-Amino-1-hydroxybutylidene)bisphosphonic Acid-d6; 4-Amino-1-hydroxybutane-1,1-diphosphonate-d6; 4-Amino-1-hydroxybutane-1,1-diphosphonic Acid-d6; 4-Amino-1-hydroxybutane-1,1-diyldiphosphonic Acid-d6; 4-Amino-1-hydroxybutylidene-1,1-bis(phosphonic acid)-d6; ABDP-d6; BPH 1-d6
Quetiapine D4	deuteriumlabeledcom	NA	C21H21D4N3O2S.1/2C4H4O4	445.22	2-[2-(4-Dibenzo[b,f][1,4]thiazepin-11-yl-1-piperazinyl)ethoxy]ethanol-d4 (2E)-2-Butenedioate;
Oseltamivir acid 13C D3	deuteriumlabeledcom	NA	C13H21N2O4 13C D	288.36	(3R,4R,5S)-4-Acetylamino-5-amino-3-(1-ethylpropoxy)-1-cyclohexene-1-carboxylic Acid-13C,d3

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Metronidazole Hydrochloride D4	deuteriumlabeledcom	1261397-74-3	C6H5D4N3O3 · HCl	211.63	2-Methyl-5-nitro-1H-imidazole-1-(ethanol-d4); Anagiardil-d4; Arilin-d4; Bayer 5360-d4; Cimetrol 500LPCI-d4; Clont-d4; Deflamon-d4; Dentamet Gel-d4; Efloran-d4; Elyzol-d4; Entizol-d4; Flagesol-d4; Flagil-d4; 1-(2-Hydroxyethyl-d4)-2-methyl-5-nitroimidazole; NSC 50364-d4; NSC 69587-d4; Nidazole-d4
Exemestane D2	deuteriumlabeledcom	NA	C20H22D2O2	298.42	6-Methyleneandrosta-1,4-diene-3,17-dione-19-d2 FCE 24304-19-d2
Famotidine 13C	deuteriumlabeledcom	NA	C713C1H15N7O2S 3	338.44	3-[[[2-[(Aminoiminomethyl)amino]-4-thiazolyl]methyl]thio]-N-(aminosulfonyl)propanimidamide-13C; N-(Aminosulfonyl)-3-[[[2-[(diaminomethylene)amino]-4-thiazolyl]methyl] thio]propanimidamide-13C

name	category	cas_number	mol_formula	mol_weight	synonym
Lercanidipine 13CD3	deuteriumlabeledcom	NA	C35H39CIN3O6D3 13C	652.19	1,4-Dihydro-2,6-dimethyl-4-(3-nitrophenyl)-3,5-pyridinedicarboxylic Acid 2-[(3,3-Diphenylpropyl)(methyl-13Cd3)amino]-1,1-dimethylethyl Methyl Ester Hydrochloride;
Pramipexole D3	deuteriumlabeledcom	NA	C10H14D3N3S	214.34	4,5,6,7-Tetrahydro-N6-(propyl-d3)-2,6-benzothiazole-diamine Dihydrochloride
Celecoxib D7	deuteriumlabeledcom	544686-21-7	C17H7D7F3N3O2S	388.37	4-[5-[4-(Methyl-d3)phenyl-2,3,5,6-d4]-3-(trifluoromethyl)-1H-pyrazol-1-yl]-benzenesulfonamide; Celebra-d7; Celecox-d7; Celebex-d7; SC 58635-d7; YM 177-d7
Galantamine D3 HBr	deuteriumlabeledcom	NA	C17H18D3NO3.HBr	371.29	4aS,6R,8aS)-4a,5,9,10,11,12-Hexahydro-3-methoxy-11-methyl-6H-benzofuro[3a,3,2,-ef][2]benzazepin-6-ol D3; BRN 0093736 D3; Galantamin D3;
Lapatinib 13C 2H7	deuteriumlabeledcom	NA	C29H26CIFN4O4S	589.09	N-[3-Chloro-4-[(3-fluorophenyl)methoxy]phenyl]-6-[5-[[[2-(methylsulfonyl)ethyl-d7]amino]methyl]-2-furanyl]-4-quinazolinamine Bis(4-methylbenzenesulfonate)



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name	category	cas_number	mol_formula	mol_weight	synonym
Dipyridamole D20	deuteriumlabeledcom	1189983-52-5	C ₂₄ H ₂₀ D ₂₀ N ₈ O ₄	524.75	2,2',2'',2'''-[(4,8-Di-1-piperidinyl-d20-pyrimido[5,4-d]pyrimidine-2,6-diyl)dinitrilo]tetrakis-ethanol; NSC-515776-d20; RA-8-d20; Anginal-d20; Cardoxin-d20; Cleridium-d20; Dipyridan-d20; Natyl-d20; Peridamol-d20; Persantine-d20

name	category	cas_number	mol_formula	mol_weight	synonym
Pantoprazole D3	deuteriumlabeledcom	922727-37-5	C16H12D3F2N3O4S	386.39	6-(difluoromethoxy)-2-[[[3-methoxy-4-(methoxy-d3)-2-pyridinyl]methyl]sulfinyl]-1H-Benzimidazole; 5-(difluoromethoxy)-2-[[[(3,4-dimethoxy-d3-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole; (±)-Pantoprazole-d3; 2-[[[(3,4-Dimethoxy-d3-pyridin-2-yl)methyl]sulfinyl]-5-difluoromethoxy-1H-benzimidazole; 5-(Difluoromethoxy)-2-[[[(3,4-dimethoxy-d3-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole; 5-(Difluoromethoxy)-2-[[[(3,4-dimethoxy-d3-2-pyridyl)methyl]sulfinyl]-1H-benzimidazole; BY 1023-d3; Pantocid-d3; Pantozol-d3; Protium-d3

name	category	cas_number	mol_formula	mol_weight	synonym
Ketoconazole D3	deuteriumlabeledcom	1217766-70-5	C ₂₆ H ₂₅ D ₃ Cl ₂ N ₄ O ₄	534.45	rel-1-[4-[4-[[[(2R,4S)-2-(2,4-dichlorophenyl)-2-(1H-imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]-1-piperazinyl]ethanone-d ₃ ; cis-1-Acetyl-d ₃ -4-[4-[[2-(2,4-dichlorophenyl)-2-(1H-imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]piperazine; (+/-)-Ketoconazole-d ₃ ; Brizoral-d ₃ ; Fungarest-d ₃ ; Fungoral-d ₃ ; Ketoderm-d ₃ ; Ketoisdin-d ₃ ; Ketozoral-d ₃ ; Nizoral-d ₃ ; Nizral-d ₃ ; Onofin K-d ₃ ; Orifungal M-d ₃ ; Panfungol-d ₃
Lovastatin D3 Ammonium salt	deuteriumlabeledcom	1002345-93-8	C ₂₄ H ₃₃ D ₃ O ₅	407.55	(2S)-2-(Methyl-d ₃)butanoic Acid (1S,3R,7S,8S,8aR)-1,2,3,7,8,8a-Hexahydro-3,7-dimethyl-8-[2-[(2R,4R)-tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl]ethyl]-1-naphthalenyl Ester; MK-803-d ₃ ; Lovalip-d ₃ ; Lovastatin Lactone-d ₃ ; Mevacor-d ₃ ; Mevinacor-d ₃

name	category	cas_number	mol_formula	mol_weight	synonym
Quinapril D5 (wax form)	deuteriumlabeledcom	1279034-23-9	C ₂₅ H ₂₅ D ₅ N ₂ O ₅	443.55	(3S)-2-[(2S)-2-[[[(1S)-1-Carboxy-(3-phenyl-d5)propyl]amino]-1-oxopropyl]-1,2,3,4-tetrahydro-3-isoquinolinecarboxylic Acid; Accuprin-d5
Betahistine D3	deuteriumlabeledcom	244094-70-0	C ₈ H ₁₁ D ₃ Cl ₂ N ₂	212.13	N-(Methyl-d3)-2-pyridineethanamine; 2-[β-(Methyl-d3)aminoethyl]pyridine; 2-[2-(Methyl-d3)aminoethyl]pyridine; Betahistine; N-(Methyl-d3)-N-[2-(pyridin-2-yl)ethyl]amine; NSC 42617-d3; Y-G 14-d3; [2-(2-Pyridyl)ethyl](methyl-d3)amine
Varenicline 13C2 15N2	deuteriumlabeledcom	NA	13C ₂ C ₁₁ H ₁₃ 15N ₂ N	215.26	7,8,9,10-Tetrahydro-6,10-methano-6H-pyrazino[2,3-h][3]benzazepine-13C 15N2 Dihydrochloride
Clopidogrel Carboxylic Acid D4 HCl	deuteriumlabeledcom	NA	C ₁₅ H ₁₀ CINO ₂ SD ₄ . HCl	348.29	(S)-α-(2-Chlorophenyl)-6,7-dihydrothieno[3,2-c]pyridine-5(4H)-acetic Acid D4 Hydrochloride; SR 26334 D4 Hydrochloride
Acetyl salicylic acid D4	deuteriumlabeledcom	97781-16-3	C ₉ H ₄ O ₄ D ₄	184.19	2-Acetoxybenzoic-3,4,5,6-d4 Acid; Acetylsalicylic Acid-d4; Acylpyrin-d4; Angettes-d4; Aspro-d4; Aspirin-d4

name	category	cas_number	mol_formula	mol_weight	synonym
3-Keto Desogestrel D6	deuteriumlabeledcom	NA	C22H22O2D6	330.50	(17 α)-13-Ethyl-17-hydroxy-11-methylene-18,19-dinorpregn-4-en-20-yn-3-one-d6; 3-Ketodesogestrel-d6; 3-Oxodesogestrel-d6
Teriflunomide metabolite D4	deuteriumlabeledcom	NA	C12H5D4F3N2O2	274.23	N-(4-Trifluoromethylphenyl)-2-cyano-3-hydroxycrotonamide-d4, 2-Cyano-3-hydroxy-N-[4-(trifluoromethyl)phenyl]-2-beuteamide-d4, LEF-M-d4;
Dienogest D5	deuteriumlabeledcom	65928-58-7 unlabeled	C20H20NO2D5	316.46	(17 α)-17-Hydroxy-3-oxo-19-norpregna-4,9-diene-21-nitrile-d5;
Gestodene D6	deuteriumlabeledcom	NA	C21H20O2D6	316.48	(17 α)-13-Ethyl-17-hydroxy-18,19-dinorpregna-4,15-dien-20-yn-3-one-d6
Nicotinuric Acid D4	deuteriumlabeledcom	1216737-36-8	C8H4N2O3D4	184.19	N-[(3-Pyridinyl-d4)carbonyl]glycine; N-(Nicotinoyl)-d4-glycine; 2-(Nicotinylamino-d4)acetic Acid; NSC 71273-d4; (Nicotinoyl-d4)glycine; (Nicotinyl-d4)glycine

name	category	cas_number	mol_formula	mol_weight	synonym
Rabeprazole D4	deuteriumlabeledcom	934295-48-4	C18H16N3NaO3SD4	385.46	2-[[[4-(3-methoxypropoxy)-3-methyl-2-pyridinyl]methyl]sulfinyl]-1H-benzimidazole-4,5,6,7-d4; (±)-Rabeprazole-d4; 2-[[[3-Methyl-4-(3-methoxypropoxy)-2-pyridinyl]methyl]sulfinyl]-1H-benzimidazole-d4; 2-[[[3-Methyl-4-(3-methoxypropoxy)-2-pyridyl]methyl]sulfinyl]-1H-benzimidazole-d4; 2-[[[4-(3-Methoxypropoxy)-3-methyl-2-pyridyl]methyl]sulfinyl]benzimidazole-d4; 2-[[[4-(3-Methoxypropoxy)-3-methylpyridin-2-yl]methyl]sulfinyl]-1H-benzimidazole;-d4 Rabeprazole-d4; LY 307640-d4; Newprazole-d4; Pariets-d4; Rabeloc-d4; Rabemax-d4; Rabiral-d4
Atovaquone D4	deuteriumlabeledcom	NA	C22H15ClO3D4	370.86	2-[trans-4-(4-Chlorophenyl)cyclohexyl-d4]-3-hydroxy-1,4-naphthalenedione; 566C80-d4; Wellvone-d4;

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Diltiazem HCl D4	deuteriumlabeledcom	1217769-52-2	C ₂₂ H ₂₂ N ₂ O ₄ SD ₄	455.01	(2S,cis)-3-(Acetyloxy)-5-[(2-dimethylamino-d ₄)ethyl]-2,3-dihydro-2-(4-methoxyphenyl)-1,5-benzothiazepin-4(5H)-one Hydrochloride; CRD-401-d ₄ ; Adizem-d ₄ ; Altiazem-d ₄ ; Dilzem-d ₄ ; Masdil-d ₄ ; Zilden-d ₄
Entacapone D10	deuteriumlabeledcom	1185241-19-3	C ₁₄ H ₅ N ₃ O ₅ D ₁₀	315.35	(2E)-2-Cyano-3-(3,4-dihydroxy-5-nitrophenyl)-N,N-di-(ethyl-d ₅)-2-propenamide; OR-611-d ₁₀ ; Comtan-d ₁₀ ; Comtess-d ₁₀
Artesunate D4	deuteriumlabeledcom	1316753-15-7	C ₁₉ H ₂₄ O ₈ D ₄	388.44	Butanedioic Acid Mono(3R,5aS,6R,8aS,9R,10R,12R,12aR)-decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-yl] Ester-d ₄ ; Artesunic Acid-d ₄
Ambrisentan D10	deuteriumlabeledcom	1046116-27-1	C ₂₂ H ₁₂ N ₂ O ₄ D ₁₀	388.48	(α S)- α -[(4,6-dimethyl-2-pyrimidinyl)oxy]- β -methoxy- β -(phenyl-2,3,4,5,6-d ₅)benzene-2,3,4,5,6-d ₅ -propanoic Acid

name	category	cas_number	mol_formula	mol_weight	synonym
Atazanavir D6	deuteriumlabeledcom	1092540-50-5	C38H46D6N6O7	710.89	(3S,8S,9S,12S)-,12-Bis(1,1-dimethylethyl)-8-hydroxy-4,11-dioxo-9-(phenylmethyl)-6-[[4-(2-pyridinyl)phenyl]methyl]-2,5,6,10,13-Pentaazatetradecanedioic Acid 14- di(methyl-d3) Ester
Rabeprazole Sodium 13C D3	deuteriumlabeledcom	1261392-48-6 free base	C17H17N3NaO3S 13	385.43	2-[[[4-(3-Methoxypropoxy)-3-methyl-2-pyridinyl]methyl]sulfinyl]-1H-benzimidazole-13CD3, Sodium Salt
Bosentan 13C2 D4	deuteriumlabeledcom	150726-52-6 unlabeled	C2513C2H25D4N5O	557.62	4-(1,1-Dimethylethyl)-N-[6-(2-hydroxyethoxy-13C2, d4)-5-(2-methoxyphenoxy)[2,2'-bipyrimidin]-4-yl]benzenesulfonamide; p-tert-Butyl-N-[6-(2-hydroxyethoxy-13C2, d4)-5-(o-methoxyphenoxy) -2-(2-pyrimidinyl)-4-pyrimidinyl]benzenesulfonamide; Actelion-13C2, d4; Ro 47-0203-13C2, d4; Ro 47-0203/039-13C2, d4; Tracleer-13C2, d4

name	category	cas_number	mol_formula	mol_weight	synonym
Artemether 13C D3	deuteriumlabeledcom	71963-77-4 unlabeled	C15H23O5 13C D3	302.39	(3R,5aS,6R,8aS,9R,10S,12R,12aR)-Decahydro-10-methoxy-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-3C, d3; Decahydro-10-methoxy-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-3C, d3; Artemos-3C, d3; Artenam-3C, d3; Artesaph-3C, d3; Artesian-3C, d3; Dihydroartemisinin Methyl Ether-3C, d3; Falcidol-3C, d3; Gvither-3C, d3; Larither-3C, d3; Malartem-3C, d3; SM 224-3C, d3; β -Artemether-3C, d3; β -Dihydroartemisinin Methyl Ether-3C, d3

name	category	cas_number	mol_formula	mol_weight	synonym
Isoniazid D4	deuteriumlabeledcom	774596-24-6	C6H3N3OD4	141.17	4-(Pyridine-d4)carboxylic Acid Hydrazide; Isonicotinic Acid-d4 Hydrazide; 4-(Hydrazinocarbonyl)pyridine-d4; 4-(Pyridine-d4)carbonylhydrazine; 4-(Pyridine-d4)carboxylic Hydrazide; 4-(Pyridyl-d4)carbonylhydrazide; 5015 R.P.-d4; Armazid-d4; Armazide-d4; Atcotibine-d4; Isonizide-d4; Isotebezid-d4; Isozide-d4; Robisellin-d4; Sauterazid-d4; Zinadon-d4; Zonazide-d4; Tubazid-d4
N-Desethyl Amodiaquine DiHCl D5	deuteriumlabeledcom	NA	C18H15D5Cl3N3O	405.76	4-[(7-Chloro-4-quinoliny)amino]-2-[(ethyl-d5-amino)methyl]phenol Dihydrochloride; Monodesethylamodiaquine-d5 Dihydrochloride; Desethylamodiaquine-d5 Dihydrochloride

name	category	cas_number	mol_formula	mol_weight	synonym
Amodiaquine-D10	deuteriumlabeledcom	1189449-70-4	C20H12CIN3OD10	365.92	4-[(7-Chloro-4-quinolinyl)amino]-2-[[diethylamino-d10)methyl]phenol; 4-[(7-Chloro-4-quinolyl)amino]- α -(diethylamino-d10)-o-cresol; Camochin-d10; Camoquin-d10; Camoquinal-d10; Camoquine-d10; Flavoquine-d10; Miaquin-d10; NSC 13453-10; SN-10751-d10
Candesartan D4	deuteriumlabeledcom	1346604-70-3	C24H16D4N6O3	444.49	2-Ethoxy-1-[[2'-(1H-tetrazol-5-yl)[1-(phenyl-d4)-1'-phenyl]-4-yl]methyl]-1H-benzimidazole-7-carboxylic Acid; CV-11974-d4; Candesartan M1-d4; 3-[[2'-(1H-Tetrazol-5-yl)[1-(phenyl-d4)-1'-phenyl]-4-yl]methyl]-2-ethoxy-3H-benzimidazole-4-carboxylic Acid
Ziprasidone D8	deuteriumlabeledcom	1126745-58-1	C21H13CIN4OSD8	420.99	5-[2-[4-(1,2-Benzisothiazol-3yl)-1-(piperaziny-d8)]ethyl]-6-chloro-1,3-dihydro-2H-indol-2-one
Hydrochlorothiazid e 13C6	deuteriumlabeledcom	1261396-79-5	C1H8CIN3O4S2 13C	303.69	6-Chloro-3,4-dihydro-2H-1,2,4-benzothiadiazine-13C6-sulfonamide 1,1-Dioxide; Aquarius-13C6; Bremil-13C6

name	category	cas_number	mol_formula	mol_weight	synonym
Telmisartan 13CD3	deuteriumlabeledcom	1261396-33-1	C32H27N4O2 13C D3	518.63	4'-[(1,4'-Dimethyl-2'-propyl[2,6'-bi-H-benzimidazol]-1'-yl)methyl][1,1'-biphenyl]-2-carboxylic Acid-13CD3; 4'-[[4-Methyl-6-(1-methyl-2-benzimidazolyl)-2-propyl-1-benzimidazolyl] methyl]-2-biphenylcarboxylic Acid-13CD3; BIBR 277-13CD3; BIBR 277SE-13CD3; Micardis-13CD3; Pritor-13CD3
Quinine D3	deuteriumlabeledcom	NA	C20H21N2O2D3	327.44	(8 α ,9R)-6'-(Methoxy-d3)cinchonan-9-ol; (-)-Quinine-d3; (8S,9R)-Quinine-d3; (R)-(-)-Quinine-d3; 6'-Methoxycinchonidine-d3; Chinine-d3; NSC 192949-d3
Nor-Trimebutine mono-desmethyl-d5 HCl	deuteriumlabeledcom	NA	C21H22NO5D5 . HC	378.48 36.46	3,4,5-Trimethoxybenzoic Acid 2-(N-Benzylmethylamino)-2-phenylbutyl-d5 Ester; N-Benzyl N-Monodesmethyltrimebutine-d5;
Losartan D4	deuteriumlabeledcom	1030937-27-9	C22H19CIN6OD4	426.93	2-Butyl-4-chloro-1-[[2'-(1H-tetrazol-5yl)[1,1'-biphenyl-d4]-4-yl]methyl]-1H-imidazole-5-methanol; Cozaar-d4

name	category	cas_number	mol_formula	mol_weight	synonym
Tramadol D6 HCl	deuteriumlabeledcom	1109217-84-6	C16H19D6NO2 · HC	305.87	cis-(+/-)-2-[(Dimethylamino)methyl]-1-(3-methoxyphenyl)cyclohexanol Hydrochloride; Amadol-d6; Contramal-d6; Crispin-d6
Nisoldipine D6	deuteriumlabeledcom	NA	C20H18N2O6D6	394.46	1,4-Dihydro-2,6-dimethyl-4-(2-nitrophenyl)-3,5-pyridinedicarboxylic Acid Methyl 2-methylpropyl Ester-d6
Simvastatin D6	deuteriumlabeledcom	1002347-71-8	C25H32D6O5	424.61	2,2-(Dimethyl-d6)butanoic Acid(1S,3R,7S,8S,8aR)-1,2,3,7,8,8a-hexahydro -3,7-dimethyl-8-[2-[(2R,4R)-tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl]ethyl] -1-naphthalenyl Ester; (+)-Simvastatin-d6; Cholestat-d6; Lipex-d6; Novo-Simvastatin-d6; Simvotin-d6; Sinvacor-d6; Statin-d6; Zocor-d6; Zorced-d6
Ibandronate Sodium 13C D3	deuteriumlabeledcom	1261395-45-2	C8H19NNaO7P2 D3	345.22	[1-Hydroxy-3-(methylpentylamino)propylidene-13CD3]bisphosphonic Acid Sodium Salt

name	category	cas_number	mol_formula	mol_weight	synonym
Linezolid D8	deuteriumlabeledcom	1032182-14-1	C16H12D8FN3O4	345.40	N-[[[(5S)-3-[3-Fluoro-4-(4-morpholinyl)phenyl]-2-oxo-5-oxazolidinyl]methyl]-acetamide-d8; Linospan-d8
Mesalazine-d3	deuteriumlabeledcom	1309283-32-6	C7H4NO3D3	156.16	5-Amino-2-hydroxybenzoic Acid-d3; 5-Aminosalicylic Acid-d3; 5-Aminosalicylic Acid-d3; Mesalamine-d3
N-Acetyl Mesalamine D3	deuteriumlabeledcom	93968-79-7	C9H6NO4D3	198.19	5-(Acetylamino-d3)-2-hydroxybenzoic Acid; 3-Carboxyparacetamol-d3; 5-Acetamidosalicylic Acid-d3; CJ 46A-d3; N-Acetylmescalamine-d3; N-(Acetyl-d3)-5-aminosalicylic Acid
13C6 Prasugrel metabolie derivative HCl(trans R-138727MP)	deuteriumlabeledcom	NA	C21H28FN05S 13C6	539.99	(2E)-2-[1-[2-Cyclopropyl-1-(2-fluorophenyl)-2-oxoethyl]-4-[[2-(3-methoxyphenyl)-2-oxoethyl]thio]-3-piperidinylidene]acetic Acid Hydrochloride
Primidone D5	deuteriumlabeledcom	73738-06-4	C12H9N2O2D5	223.29	5-(Ethyl-d5)dihydro-5-phenyl-4,6(1H,5H)-pyrimidinedione; Liskantin-d5; Mylepsinum-d5; Mysoline-d5; Resimatil-d5; Sertan-d5

name	category	cas_number	mol_formula	mol_weight	synonym
Pyrazinamide D3	deuteriumlabeledcom	1432059-16-9	C5H2N3OD3	126.13	Pirazinecarboxamide-,d3; Pyrazinoic Acid Amide-d3; Piralidina-d3 Zinamide-d3
D6 Montelukast Sodium Salt	deuteriumlabeledcom	151767-02-1 unlabeled	C35H29ClNO3SNa D6	614.20	1-[1-[[[(1R)-1-[3-[(1E)-2-(7-Chloro-2-quinolinyl)ethenyl]phenyl]-3-[2-(1-hydroxy-1-methylethyl-d6)phenyl]propyl]thio]methyl]cyclopropane acetic Acid Sodium Salt; MK-476-d6; Singulair
Cefditoren 13C D3	deuteriumlabeledcom	104145-95-1 unlabeled	C18H15N6O5S3 13C D3	510.58	(6R,7R)-7-[[[(2Z)-(2-Amino-4-thiazolyl)methoxyimino-13Cd3)acetyl]amino]-3-[(1Z)-2-(4-methyl-5-thiazolyl)ethenyl]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic Acid
Budesonide D8	deuteriumlabeledcom	1105542-94-6	C25H26D8O6	438.58	(11 β ,16 α)-16,17-[Butylidenebis(oxy)]-11,21-dihydroxypregna-1,4-diene-3,20-dione; Bidien; Budenofalk; Budesomide; Budeson; Cortivent; Entocort; Micronyl; Nebuampul; Preferid; Pulmicort; Respules; Rhinocort; Rhinocort Aqua; S 1320; Spirocort; Turbuhaler

name	category	cas_number	mol_formula	mol_weight	synonym
O-Desmethyl Venlafaxine-d10	deuteriumlabeledcom	NA	C16H15D10NO2	273.44	1-Cyclohexen-1-yl-4-methoxy-N,N-(dimethyl-d10)benzeneethanamine; 4-[1-(cyclohex-1-en-1-yl)-2-[(dimethyl-d6)amino]ethyl]phenol;
Vardenafil-d5 HCl	deuteriumlabeledcom	1189685-70-8 free base	C23H27N6O4SD5	493.64	1-[[3-(1,4-Dihydro-5-methyl-4-oxo-7-propylimidazo[5,1-f][1,2,4]triazin-2-yl)-4-ethoxyphenyl]sulfonyl]-4-(ethyl-d5)-piperazine; Levitra-d5; Nuviva-d5;
Oxcarbazepine-d4	deuteriumlabeledcom	1020719-71-4	C15H8N2O2D4	256.30	10,11-Dihydro-10-oxo-5H-dibenz[b,f]azepine-5-carboxamide-d4; Aurene-d4; GP 47680-d4; Oxacarbazepine-d4; Oxecarb-d4; Oxetol-d4; Trileptal-d4;
10,11-Dihydro-10-Hydroxy Carbamazepine-d4	deuteriumlabeledcom	1020719-39-4	C15H10N2O2D4	258.31	10,11-Dihydro-10-hydroxy-5H-dibenz[b,f]azepine-5-carboxamide-D4; 10-Hydroxy-10,11-dihydrocarbamazepine-D4; BIA 2-005-D4; GP 47779-D4; Licarbazepine-D4

name	category	cas_number	mol_formula	mol_weight	synonym
Modafinil D5	deuteriumlabeledcom	1133712-38-5	C15H10NO2SD5	278.39	2-[(Diphenylmethyl-d5)sulfinyl]acetamide; (±)-Modafinil-d5; 2-(Benzhydrylsulfinyl)acetamide-d5; CEP 1538-d5; CRC 40476-d5; CRL 40476-d5; DEP 1538-d5; Modaphonil-d5; Modiodal-d5; Provigil-d5
Desacetyl Diltiazem HCl D4	deuteriumlabeledcom	NA	C20H20N2O3SD4.H	412.94	(2S,3S)-5-[2-(Dimethylamino)ethyl-d4]-2,3-dihydro-3-hydroxy-2-(4-methoxyphenyl)-1,5-benzothiazepin-4(5H)-one Monohydrochloride; (2S-cis)-5-[2-(Dimethylamino)ethyl-d4]-2,3-dihydro-3-hydroxy-2-(4-methoxyphenyl)-1,5-benzothiazepin-4(5H)-one Monohydrochloride; Deacetyldiltiazem-d4 Hydrochloride
Desmethyl Diltiazem D4	deuteriumlabeledcom	NA	C21H20N2O4SD4.H	440.98	(2S-cis)-3-(Acetyloxy)-2,3-dihydro-2-(4-methoxyphenyl)-5-[2-(methylamino-d4)ethyl]-1,5-benzothiazepin-4(5H)-one-d4 Monohydrochloride; N-Demethyldiltiazem-d4
Gabapentin HCl D6	deuteriumlabeledcom	1432061-73-8	C9H11NO2D6 . HCl	213.74	1-(Aminomethyl)cyclohexane-d6-acetic Acid Hydrochloride

name	category	cas_number	mol_formula	mol_weight	synonym
Amantadine D6	deuteriumlabeledcom	1219805-53-4	C10H11ND6	157.29	Tricyclo[3.3.1.1 ^{3,7}]decan-d15-1-amine Hydrochloride; EXP-105-1-d6; NSC-83653-d6
Estradiol D4	deuteriumlabeledcom	66789-03-5	C18H20O2D4	276.41	Dihydrofolliculin-d4; (17 β)-Estra-1,3,5(10)-triene-3,17-diol-d4; 3,17-Epidihydroxyestratriene-d4; Cimara-d4; Estrace-d4; Estraderm-d4; Estradot-d4; Estring-d4; Estrofem-d4; Estrogel-d4; Evorel-d4; Ethinyl Estradiol Impurity D (EP)-d4
Bupropion D9 HCl	deuteriumlabeledcom	1189725-26-5	C ₁₃ H ₉ ClNOD ₉ .HCl	285.26	1-(3-Chlorophenyl)-2-[(1,1-dimethylethyl-d9)amino]-1-propanone Hydrochloride; (\pm)-Bupropion-d9 Hydrochloride; Amfebutamon-d9 Hydrochloride; Amfebutamone-d9 Hydrochloride; Aplenzin-d9 Hydrochloride; Bupropion-d9 SR Hydrochloride; Elontril-d9 Hydrochloride; α -(tert-Butylamino-d9)-m-chloropropiophenone Hydrochloride

name	category	cas_number	mol_formula	mol_weight	synonym
Gemfibrozil D6	deuteriumlabeledcom	1184986-45-5	C15H16O3D6	256.37	5-(2,5-Dimethylphenoxy)-2,2-(dimethyl-d6)-pentanoic Acid; 2,2-(Dimethyl-d6)-5-(2,5-xylyloxy)valeric Acid; Cl-7-d6; Decrelip-d6; Genlip-d6; Gevilon-d6; Lipozid-d6; Lopid-d6
Estrone D4	deuteriumlabeledcom	53866-34-5	C18H18O2D4	274.40	3-Hydroxyestra-1,3,5(10)-trien-17-one-d4; (+)-Estrone-d4; 1,3,5(10)-Estratrien-3-ol-17-one-d4; 3-Hydroxy-17-keto-estra-1,3,5-triene-d4; Aquacrine-d4; Crinovaryl-d4; Cristallovor-d4; Crystogen-d4; WAY 164397-d4; Wynestron-d4
Dextromethorphan D3	deuteriumlabeledcom	524713-56-2	C18H22D3NO.HBr	355.33	(9 α ,13 α ,14 α)-3-Methoxy-17-(methyl-d3)morphinan; (+)-3-Methoxy-N-(methyl-d3)morphinan; d-3-Methoxy-N-(methyl-d3)morphinan
Alvimopan D7	deuteriumlabeledcom	170098-43-8 unlabeled	C25H25D7N2O4	431.57	rac-N-[2-[[4-(3-Hydroxyphenyl)-3,4-dimethyl-1-piperidinyl]methyl]-1-oxo-3-(phenyl)propyl]glycine-d7 Hydrate; ADL 8-2698-d7 Hydrate; LY 246736-d7 ; Entereg-d7 ;

name	category	cas_number	mol_formula	mol_weight	synonym
Cinacalcet HCl D3	deuteriumlabeledcom	1185097-33-9	C22H19F3ND3.HCl	396.90	α -(Methyl-d3)-N-[3-[3-(trifluoromethyl)phenyl)propyl]-1-naphthalenemethanamine Hydrochloride; N-(3-(3-(trifluoromethyl)phenyl)propyl)-1-(1-naphthyl)ethylamine-d3 Hydrochloride
Fluticasone Propionate D-5	deuteriumlabeledcom	1093258-28-6	C25H26F3O5SD5	505.60	(6 α ,11 β ,16 α ,17 α)-Androsta-1,4-diene-17-carbothioic acid, 6,9-difluoro-11-hydroxy-16-methyl-3-oxo-17-(1-oxopropoxy-2,2,3,3,3-d5)-S-(fluoromethyl) Ester; (6 α ,11 β ,16 α ,17 α)-6,9-Difluoro-11-hydroxy-16-methyl-3-oxo-17-(1-oxopropoxy-d5)androsta-1,4-diene-17-carbothioic Acid S-(Fluoromethyl) Ester; Atemur Mite-d5; CCI 18781-d5; Cutivate-d5; Flixonase-d5; Flonase-d5; Flovent-d5; Flutide-d5; Flutide N-d5; Flutivate-d5; Zofluf-d5

name	category	cas_number	mol_formula	mol_weight	synonym
Fluoxetine D4 Oxalate	deuteriumlabeledcom	NA	C19H16D4F3NO5	403.39	N-Methyl- γ -[4-(trifluoromethyl)phenoxy](benzene-d4)propanamine Hydrochloride; (+/-)-N-Methyl-3-(phenyl-d5)-3-[4-(trifluoromethyl)phenoxy]propylamine Hydrochloride; Adofen-d4; Affectine-d4
Paracetamol D4	deuteriumlabeledcom	NA	C8H5D4NO2	155.19	N-(4-Hydroxyphenyl)acetamide-d4; 4'-Hydroxyacetanilide-d4; 4-Acetamidophenol-d4; N-Acetyl-4-aminophenol-d4; APAP-d4; Acamol-d4; Acenol-d4; Paracetamol-d4; Paracetamole-d4; Parageniol-d4; Paralend4; Paramol-d4; Paraspem-d4; Valadol-d4; Valgesic-d4; Vermidon-d4
Salicylic Acid D6	deuteriumlabeledcom	NA	C7D6O3	144.16	2-Hydroxybenzoic Acid-d6; 2-Carboxyphenol-d6; 2-Hydroxybenzenecarboxylic Acid-d6; 2-Hydroxybenzoic Acid-d4; o-Carboxyphenol-d6; o-Hydroxybenzoic Acid-d6;

name	category	cas_number	mol_formula	mol_weight	synonym
N-Desethyl Oxybutynin D5 HCL	deuteriumlabeledcom	NA	C20H22NO3D5.HCl	370.93	α -Cyclohexyl- α -hydroxybenzeneacetic Acid 4-[(Ethyl-d5)amino]-2-butynyl Ester Hydrochloride Salt;
Progesterone D9	deuteriumlabeledcom	15775-74-3	C21H21O2D9	323.53	Pregn-4-ene-3,20-dione-d9; Δ 4-Pregnene- 3,20-dione-d9; Agolutin-d9; Bio-luton-d9; CIDR-d9; Corlutin-d9; Corlutina-d9; Corluvite-d9; Gestone-d9; Progestan-d9; Progestasert-d9; Progestogel-d9; Progesterone-2,2,4,6,6,17a,21,21,21-d9;
Metoprolol D7 HCL	deuteriumlabeledcom	NA	C15H19NO3CID7	310.87	4-[2-Hydroxy-3-[(1- methylethyl)amino]propoxy- d7]benzeneacetic Acid Ethyl Ester; [p-[2- Hydroxy-3-(isopropylamino)propoxy- d7]phenyl]acetic Acid Ethyl Ester; Ethyl 4- [2-Hydroxy-3-(isopropylamino)propoxy- d7]phenylacetate
Solifenacin D5 HCL	deuteriumlabeledcom	1426174-05-1	C23H22D5ClN2O2	403.96	(1S)-3,4-Dihydro-1-phenyl-d5-2(1H)- isoquinolinecarboxylic Acid (3R)-1- Azabicyclo-[2.2.2]oct-3-yl Ester Hydrochloride;

name	category	cas_number	mol_formula	mol_weight	synonym
O-Desmethyltramadol Hydrochloride D6	deuteriumlabeledcom	1261393-87-6	C ₁₅ H ₁₇ D ₆ NO ₂ · HC	291.85	3-[(rel-1R,2R)2-[(Di(methyl-d ₃)amino)methyl]-1-hydroxycyclohexyl]phenol Hydrochloride; 2-[(rel-1R, 2R)(Di(methyl-d ₃)amino)methyl]-1-(m-hydroxyphenyl)cyclohexanol Hydrochloride
Tenofovir D6 base	deuteriumlabeledcom	NA	C ₉ H ₈ D ₆ N ₅ O ₄ P	293.25	[(1R)-2(6-Amino-9H-purin-9-yl)-1-methylethoxy-d ₅]methyl]phosphonic Acid; (R)-9-(2-Phosphonomethoxypropyl)adenine-d ₆ ; (R)-PMPA-d ₅ ; GS-1278-d ₆ ;
Capecitabine D11	deuteriumlabeledcom	1132662-08-8	C ₁₅ H ₁₁ FN ₃ O ₆ D ₁₁	370.42	5'-Deoxy-5-fluoro-N-[(pentyl-d ₁₁ -oxy)carbonyl]cytidine; [1-(5-Deoxy-β-D-ribofuranosyl)-5-fluoro-1,2-dihydro-2-oxo-4-pyrimidinyl] carbamic Acid Pentyl Ester; Capecitabine-d ₁₁ ; Capecytabine-d ₁₁ ; Capiibine-d ₁₁ ; Captabin-d ₁₁ ; Ro 09-1978-d ₁₁ ; Ro 09-1978/000-d ₁₁ ; Xeloda-d ₁₁ ;

name	category	cas_number	mol_formula	mol_weight	synonym
Aprepitant D4	deuteriumlabeledcom	1133387-60-6	C23H17F7N4O3D4	538.46	5-[[[(2R,3S)-2-[(1R)-1-[3,5-Bis(trifluoromethyl)phenyl]ethoxy]-3-(4-fluorophenyl-d4)-4-morpholinyl]methyl]-1,2-dihydro-3H-1,2,4-triazol-3-one; Emend-d4; L 754030-d4; MK 0869-d4; MK 869-d4; ONO 7436-d4;
(Hydroxy bupropion D6)	deuteriumlabeledcom	1216893-18-3	C13H12ClNO2D6	261.78	2-Hydroxy-2-(3'-chlorophenyl)-3,5,5-trimethylmorpholine-d6
Lacosamide D3	deuteriumlabeledcom	1217689-95-6	C13H15N2O3D3	253.32	(2R)-2-(Acetylamino)-3-(methoxy-d3)-N-(phenylmethyl)propanamide; (2R)-2-(Acetamido-d3)-N-benzyl-3-methoxypropanamide; ADD 243037-d3; Erlosamide-d3; Harkoseride-d3; Lacosamide-d3; SPM 927-d3; Vimpat-d3;
Ethambutol-D4 Dihydrochloride	deuteriumlabeledcom	1129526-19-7	C10H22D4Cl2N2O2	281.26	(S,S)-2,2'-(1,2-Ethanediyldiimino)-bis-1-butanol-d4 Dihydrochloride; Dexambutol-d4; Ebutol-d4; Etibi-d4; Etapiam-d4; Myambutol-d4; Mycobutol-d4; Sural-d4; Tibutol-d4; EMB-d4

name	category	cas_number	mol_formula	mol_weight	synonym
Gliclazide-D4	deuteriumlabeledcom	1185039-30-8	C15H17D4N3O3S	327.43	N-[[[(Hexahydrocyclopenta[c]pyrrol-2(1H)-yl]amino]carbonyl]-4-methyl-(benzene-d4)sulfonamide; Diamicron-d4; Glimicron-d4; Nordialex-d4; S-1702-d4;
Pregabalin-D4	deuteriumlabeledcom	NA	C8H13NO2D4	163.23	(3S)-3-(Aminomethyl)-5-methylhexanoic-d4 Acid; (S)-(+)-3-(Aminomethyl)-5-methylhexanoic-d4 Acid; (S)-3-(Ammoniomethyl)-5-methylhexanoate-d4; CI 1008-d4; Lyrica-d4; PD 144723-d4
Vitamin d2- D6	deuteriumlabeledcom	1311259-89-8	C28H38OD6	402.69	3β,5Z,7E,22E)-9,10-Secoergosta-5,7,10(19),22-tetraen-3-ol-d6; Calciferol-d6; Ercalciol-d6; Ergosterol-d6 Irradiated; Ergocalciferol-d6; Oleovitamin D2-d6; Radiostol-d6; Radsterin-d6; (+)-Vitamin D2-d6; Viosterol-d6; Vio D-d6; Vitavel-D-d6;

name	category	cas_number	mol_formula	mol_weight	synonym
Bromocriptine-13C-d3 Mesylate	deuteriumlabeledcom	NA	C31 13CH37BrN5O5	754.73	2-Bromo-ergocryptine; (5' α)-2-Bromo-12'-hydroxy-2'-(1-methylethyl)-5'-(2-methylpropyl)ergotaman-3',6',18-trione; 8H-Oxazolo[3,2-a]pyrrolo[2,1-c]pyrazine-ergotaman-3',6',18-trione Deriv 13CD3.; Indolo[4,3-fg]quinoline-ergotaman-3',6',18-trione Deriv13CD3.; (+)-Bromocriptine; 2-Bromo- α -ergocryptine 13CD3;
Levodopa D3	deuteriumlabeledcom	NA	C9H8NO4D3	200.21	3-Hydroxytyrosine; 3-Hydroxy-L-tyrosine; (-)-3-(3,4-Dihydroxyphenyl)-L-alanineD3; BendopaD3; DeadopD3
(S)-(-)Carbidopa-D3	deuteriumlabeledcom	NA	C10H11N2O4D3	229.25	(α S)- α -Hydrazino-3,4-dihydroxy- α -methylbenzenepropanoic Acid; (-)-L- α -Hydrazino-3,4-dihydroxy- α -methylhydrocinamic Acid D3; (S)-CarbidopaD3;
Buspirone-D8 HCL	deuteriumlabeledcom	NA	C21H23D8N5O2.HC	429.96	
5-Fluorouracil-15N2	deuteriumlabeledcom	NA	C4H3F15N2O2	132.10	5-Fluoro-2,4(1H,3H)pyrimidinedione-15N2; 2,4-Dihydroxy-5 -fluoropyrimidine-15N2;

name	category	cas_number	mol_formula	mol_weight	synonym
Naloxone-d5 HCl	deuteriumlabeledcom	NA	C19H16NO4D5.HCl	368.83	5 α)-4,5-Epoxy-3,14-dihydroxy-17-(2-propenyl-d5)morphinan-6-one Hydrochloride; 17-Allyl-4,5 α -epoxy-3,14-dihydroxymorphinan-6-one-d5 Hydrochloride
Ibuprofen -d3	deuteriumlabeledcom	121662-14-4	C13H15D3O2	209.30	2-(4-Isobutylphenyl)propionic Acid-D3
fenspiride D5	deuteriumlabeledcom	NA	C15H15N2O2D5	265.37	8-[2-(Phenyl-d5)ethyl]-1-oxa-3,8-diazaspiro[4.5]decan-2-one Hydrochloride; Decaspir-d5;
Valganciclovir-d5 HCl	deuteriumlabeledcom	NA	C14H17N6O5D5 . HCl	395.86	2-[(2-Amino-1,6-dihydro-6-oxo-9H-purin-9-yl)methoxy]-3-hydroxypropyl-d5 Ester L-Valine Hydrochloride; RS 079070-194-d5; Ro 107-9070/194-d5; Valcyte-d5; (S)-Valganciclovir-d5 Hydrochloride
Moxifloxacin HCL D4	deuteriumlabeledcom	NA	C21H20FN3O4D4 . HCl	441.93	1-Cyclopropyl-6-fluoro-1,4-dihydro-8-methoxy-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-3-quinolinecarboxylic Acid-D4Hydrochloride;

name	category	cas_number	mol_formula	mol_weight	synonym
Methyl Diethyldithio Carbamate D10 (liquid form)	deuteriumlabeledcom	686-07-7 unlabeled	C6H13NS2	173.36	N,N-Diethylcarbamodithioic Acid Methyl-d10 Ester; Diethyldithiocarbamic Acid Methyl-d10 Ester; Diethyldithiocarbamate Methyl-d10 Ester;
25-Desacetyl Rifampicin D4	deuteriumlabeledcom	NA	C41H52N4O11D4	784.95	3-[(1-Piperazinylimino-d4)methyl]rifamycin; 3-(Piperazino-d4)iminomethyl Rifamycin SV; 4-N-Demethylrifampicin-d4; AF/AP-d4; Demethylrifampicin-d4; N-Demethylrifampicin-d4
Curcumin D6	deuteriumlabeledcom	1246833-26-0	C21H14O6D6	374.43	(1E,6E)-1,7-Bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione-d6; (E,E)-1,7-Bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione-d6; C Yellow 15-d6; C.I. 75300-d6; Curcuma-d6; Curcumine-d6; Diferuloylmethane-d6; Haidr-d6; Halad-d6; Haldar-d6; Ukon-d6;
Ranolazine-D8	deuteriumlabeledcom	NA	C24H25N3O4D8	435.59	N-(2,6-Dimethylphenyl)-4-[2-hydroxy-3-(2-methoxy-d8-phenoxy)propyl]-1-piperazineacetamide; RS 43285-d3; RS 43285-193-d8

name	category	cas_number	mol_formula	mol_weight	synonym
Ranolazine-D8 2HCL (piperazine- D8)	deuteriumlabeledcom	NA	C24H25N3O4D8.2H	508.51	N-(2,6-Dimethylphenyl)-4-[2-hydroxy-3-(2-methoxy-d8-phenoxy)propyl]-1-piperazineacetamide; RS 43285-d8; RS 43285-193-d8
Equilin D4	deuteriumlabeledcom	285979-79-5	C18D4H16O2	272.37	1,3,5,7-Estratetraen-3-ol-17-one-d4; 3-Hydroxyestra-1,3,5(10),7-tetraen-17-one-d4; 7-Dehydroestrone-d4; NSC 10971-d4;
Salicylic Acid D4	deuteriumlabeledcom	78646-17-0	C7H2D4O3	142.15	2-Hydroxybenzoic Acid-d4; 2-Carboxyphenol-d4; 2-Hydroxybenzenecarboxylic Acid-d4; 2-Hydroxybenzoic Acid-d4; o-Carboxyphenol-d4; o-Hydroxybenzoic Acid-d4; Rutranex-d4; Saligel-d4; Salonil-d4; Salvona Nanosal-d4; Stri-Dex-d4; Trans-Ver-Sal-d4; Verrugon-d4;
carbamazepine- epoxide-D10	deuteriumlabeledcom	1219804-16-6	C15H2N2OD10	246.33	1a,10b-Dihydro-6H-dibenzo[b,f]oxireno[d]azepine-6-carboxamide-d10

name	category	cas_number	mol_formula	mol_weight	synonym
4,6-Pregnadien - Acetate -D3 Megestrol Acetate	deuteriumlabeledcom	162462-72-8	C22H25O3D5	347.51	17-(Acetyloxy)-6-(methyl-d3)-pregna-4,6-diene-3,20-dione; BDH 1298-d3; DMAP-d3; MGA-d3; Magestin-d3; Maygace-d3; Megace-d3; Megeron-d3; Megestat-d3; Magestryl Acetate-d3; Ovarid-d3
Lovastatin-d3 Hydroxy Acid Sodium Salt	deuteriumlabeledcom	1217528-38-5	C24H33D3O5	407.55	Lovastatin-d3 Sodium Salt; MB 530B-d3
Eplerenone-d3	deuteriumlabeledcom	NA	C24H27O6D3	417.52	(7 α ,11 α ,17 α)-9,11-Epoxy-17-hydroxy-3-oxopregn-4-ene-7,21-dicarboxylic Acid; γ -Lactone 7-(Methyl-d3) Ester; CGP 30083-d3; Epoxymexrenone-d3; Inspra-d3; SC-66110-d3;
Rivastigmine D6 Tartrate	deuteriumlabeledcom	194930-00-2	C14H16D6N2O2 · C4H6O6	406.46	N-Ethyl-N-methylcarbamic Acid 3-[(1S)-1-(Dimethylamino)ethyl]phenyl Ester-d6 (2R,3R)-2,3-Dihydroxybutanedioate

name	category	cas_number	mol_formula	mol_weight	synonym
Riluzole-13C-15N2	deuteriumlabeledcom	1215552-03-6	C7H5F3OS 13C 15N2	237.18	6-(Trifluoromethoxy)-2-benzothiazolamine-13C,15N2; 6-(Trifluoromethoxy)-2-amino-benzothiazole-13C,15N2; 2-Amino-6-(trifluoromethoxy)benzothiazole-13C,15N2; PK-26124-13C,15N2; RP-54274-13C,15N2; Rilutek-13C,15N2
Quinidine D3	deuteriumlabeledcom	1267657-68-0	C20H21D3N2O2	327.44	(9S)-6'-Methoxycinchonan-9-ol-d3; (+)-Quinidine-d3; (8R,9S)-Quinidine-d3; Chinidin-d3; Cin-quin-d3; Conchinin-d3; Conchicine-d3; Conquinine-d3; Kinidin-d3; Pitayin-d3; Pitayine-d3; β -Quinidine-d3; β -Quinine-d3
Triamterene D5	deuteriumlabeledcom	1189922-23-3	C12H6D5N7	258.29	6-(Phenyl-d5)-2,4,7-pteridinetriamine; 2,4,7-Triamino-6-(phenyl-d5)pteridine; 6-(Phenyl-d5)-2,4,7-triaminopteridine; Ademin-d5; Ademine-d5; Diren-d5; Ditak-d5; Diurene-d5; NSC 77625-d5; Noridil-d5; Pterofen-d5; Pterophene-d5; Triteren-d5; Urocaudal-d5
Duloxetine D3 HCl	deuteriumlabeledcom	NA	C18H16NOSD3 . HC	336.90	N-Methyl- γ -(1-naphthalenyloxy)-,2-thiophenepropanamine Ethanedioate-d3

name	category	cas_number	mol_formula	mol_weight	synonym
Duloxetine D3 Oxalate	deuteriumlabeledcom	116817-77-7 unlabeled	C18H16D3NOS·C2H	390.47	N-Methyl- γ -(1-naphthalenyloxy)-,2-thiophenepropanamine Ethanedioate-d3
Febuxostat D9	deuteriumlabeledcom	1246819-50-0	C16H7D9N2O3S	325.45	2-[3-Cyano-4-(2-methylpropoxy-d9)phenyl]-4-methyl-5-thiazolecarboxylic Acid; 2-(3-Cyano-4-isobutyloxyphenyl-d9)-4-methyl-5-thiazolecarboxylic Acid
Atenolol-D7	deuteriumlabeledcom	1202864-50-3	C14H15D7N2O3	273.38	4-[2-Hydroxy-3-[(1-methylethyl-d7)amino]propoxyl]benzeneacetamide; 2-[p-[2-Hydroxy-3-(isopropylamino-d7)propoxy]phenyl]acetamide; (RS)-Atenolol-d7; (+/-)-Atenolol-d7; ICI-66082-d7; Atehexal-d7; Atenol-d7; Cuxanorm-d7; Myocord-d7; Normalol-d7; Normiten-d7; Uniloc-d7; Vericordin-d7; Wesipin-d7; Xaten-d7; dl-Atenolol-d7
Nicotine-D4	deuteriumlabeledcom	350818-69-8	C10H10N2D4	166.26	3-(1-Methyl-2-pyrrolidinyl)pyridine-2,4,5,6-d4; (\pm)-Nicotine-d4; (\pm)-3-(1-Methyl-2-pyrrolidinyl)pyridine-d4; (R,S)-Nicotine-d4; (\pm)-Nicotine-d4; 1-Methyl-2-(3-pyridyl)pyrrolidine-d4; DL-Nicotine-d4

name	category	cas_number	mol_formula	mol_weight	synonym
Cotinine-D4	deuteriumlabeledcom	350818-68-7	C10H8D4N2O	180.24	(+/-)-1-(Methyl-d4)-5-(2-pyridinyl)-2-pyrrolidinone; (+/-)-Cotinine-d4
Phenytoin D10	deuteriumlabeledcom	65854-97-9	C15H2N2O2D10	262.34	5,5-(Diphenyl-d10)-2,4-imidazolidinedione; Aleviatin-d10; DPH-d10; Denyl-d10; Di-Hydan-d10; Di-Lan-d10; Dihycon-d10; Dilabid-d10; Dintoina-d10; Diphantoin-d10; Diphedan-d10; Diphenat-d10; Diphenylan-d10; Phenytoin-d10; Phenytoine-d10; Sodanton-d10; Zentropil-d10
Lidocaine-D10 HCL	deuteriumlabeledcom	1189959-13-4	C14H12D10N2O.H Cl	280.86	2-(Diethyl-d10-amino)-N-(2,6-dimethylphenyl)acetamide Hydrochloride; Basicaina-d10; Batixim-d10; Dynexan-d10; Heweneural-d10; Licain-d10
Lansoprazole-D4	deuteriumlabeledcom	934294-22-1	C16H10F3N3O2SD4	373.39	2-[[[3-Methyl-4-(2,2,2-trifluoroethoxy)-2-pyridinyl]methyl]sulfinyl]-1H-benzimidazole-d4; A-65006-d4; AG-1749-d4; Agopton-d4; Lansox-d4; Lanzor-d4; Limpidex-d4; Ogast-d4; Prevacid-d4

name	category	cas_number	mol_formula	mol_weight	synonym
Caffeine-D3	deuteriumlabeledcom	26351-04-2	C ₈ H ₇ N ₄ O ₂ D3	197.21	artificial Almond Oil-d5; Benzaldehyde FFC-d5; Benzenecarbonal-d5; Benzenecarboxaldehyde-d5; Benzoic Acid Aldehyde-d5; Benzoic Aldehyde-d5; NSC 7917-d5; Phenylformaldehyde-d5; Phenylmethanal-d5
Cortisol-D4	deuteriumlabeledcom	73565-87-4	C ₂₁ H ₂₆ D ₄ O ₅	366.49	(11 β)-11,17,21-Trihydroxy-pregn-4-ene-3,20-dione-d4; Pregn-4-ene-3,20-dione-d4; 11 β -Hydroxycortisone-d4; 17-Hydroxycorticosterone-d4; Acticort-d4; Dermacort-d4; Hydrocortal-d4
4-Phenylbutyric-d11 Acid	deuteriumlabeledcom	358730-86-6	C ₁₀ HD ₁₁ O ₂	175.27	Benzene-d ₅ -butanoic-d ₆ Acid
Levothyroxine-D3	deuteriumlabeledcom	NA	C ₁₅ H ₉ D ₃ Cl ₄ NO ₄	816.34	O-(4-Hydroxy-3,5-diiodophenyl)-3,5-diiodo-L-tyrosine; (-)-Thyroxine D3; 3,3',5,5'-Tetraiodo-L-thyronine D3;
Felodipine D5	deuteriumlabeledcom	1242281-38-4	C ₁₈ H ₁₄ Cl ₂ NO ₄ D ₅	389.29	(2,3-Dichlorophenyl)-1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic Acid Ethyl Methyl-d ₅ ; Feloday-D5

name	category	cas_number	mol_formula	mol_weight	synonym
Dutasteride 13C6	deuteriumlabeledcom	1217685-27-2	C21H30F6N2O2 13C6	534.48	(4aR,4bS,6aS,7S,9aS,9bS,11aR)-N-[2,5-Bis(trifluoromethyl)phenyl]-2,4a,4b,5,6,6a,7,8,9,9a,9b,10,11,11a-tetradecahydro-4a,6a-dimethyl-2-oxo-1H-indeno[5,4-f]quinoline-7-carboxamide-13C6; (5 α ,17 β)-N-[2,5-Bis(trifluoromethyl)phenyl]-3-oxo-4-azaandrost-1-ene-17-carboxamide-13C6; Avodart-13C6; Avolve-13C6; GG 745-13C6; GI 198745-13C6; Veltride-13C6
Pregabalin-D10	deuteriumlabeledcom	NA	C8H7NO2D10	169.29	(Aminomethyl)-5-methylhexanoic-D10; rac-PD-144723-D10;
Desipramine-D4 HCL	deuteriumlabeledcom	NA	C18H19D4ClN2	306.87	0,11-Dihydro-N-methyl-5H-dibenz[b,f]azepine-5-propanamine-d4; G-35020-d4; JB-8181-d4; NSc-114901-d4; Norpramin-d4; Nortimil-d4; Pertofran-d4; Pertofrane-d4; Petylyl-d4;
Propafenone-D7 HCL	deuteriumlabeledcom	1219799-06-0	C21H20NO3D7.HCl	384.95	1-[2-[2-Hydroxy-3-(propylamino)propoxy-d7]phenyl]-3-phenyl-1-propanone Hydrochloride; 2'-[2-Hydroxy-3-(propylamino)propoxy-d7]-3-phenylpropiophenone Hydrochloride

name	category	cas_number	mol_formula	mol_weight	synonym
simvastatin-d6 Hydroxy Acid Sodium Salt	deuteriumlabeledcom	NA	C ₂₅ H ₃₃ O ₆ D ₆ . Na	464.61	[1S-[1 α (β S*, δ S*),2 α ,6 α ,8 β ,8 α]]-8-(2,2-Dimethyl-1-oxobutoxy)-1,2,6,7,8,8a-hexahydro- β , δ -dihydroxy-2,6-dimethyl-1-naphthaleneheptanoic Acid Monosodium Salt
Hydroxy pioglitazone D4M4	deuteriumlabeledcom	1188263-49-1	C ₁₉ H ₁₆ N ₂ O ₄ SD ₄	376.47	5-[[4-[2-[5-(1-Hydroxyethyl)-2-pyridinyl]ethoxy]phenyl]methyl]-2,4-thiazolidinedione-d4
Famotidine 13CD3	deuteriumlabeledcom	1185241-48-8	C ₇ H ₁₂ N ₇ O ₂ S ₃ 13C	341.45	3-[[[2-[(Aminoiminomethyl)amino]-4-thiazolyl]methyl]thio]-N-(aminosulfonyl)propanimidamide-13C ₃ ; N-(Aminosulfonyl)-3-[[[2-[(diaminomethylene)amino]-4-thiazolyl]methyl] thio]propanimidamide-13C ₃ ; Amfamox-13C ₃ ; Antodine-13C ₃ ; Famodin-13C ₃ ; Famosan-13C ₃ ; Ganor-13C ₃ ; Lecedil-13C ₃ ; Mosul-13C ₃ ; Motiax-13C ₃ ; Ulfamid-13C ₃

name	category	cas_number	mol_formula	mol_weight	synonym
Topiramate D12	deuteriumlabeledcom	1279037-95-4	C12H9D12NO8S	351.44	2,3:4,5-Bis-O-(1-methylethylidene)- β -D-fuctopyranose-d12 1-Sulfamate; Epitoma-d12; Epitomax-d12; McN 4853-d12; RWJ 17021-d12; TPM-d12; Topamac-d12; Topamax-d12; Topimax-d12; Topina-d12; Topomax-d12
Metaxalone D6	deuteriumlabeledcom	1189944-95-3	C12H9NO3D6	227.29	5-[(3,5-Dimethylphenoxy)methyl]oxazolidin-2-one-d6; AHR-438-d6; Skelaxin-d6
Pitavastatin D4 Calcium Salt	deuteriumlabeledcom	NA	C25H19D4FNNaO4	447.47	(3R,5S,6E)-7-[2-Cyclopropyl-4-(4-fluorophenyl)-3-quinolinyl]-3,5-dihydroxy-6-heptenoic Acid-d4 Calcium Salt; Flovas-d4; Livalo-d4; NK 104-d4; NK 104 (acid)-d4; Pitava-d4; Pitava 1-d4; Pitavastatin-d4 Hemicalcium
Proguanil D6	deuteriumlabeledcom	NA	C11H11D6Cl2N5	296.24	N-(4-Chlorophenyl-d6)-N'-(1-methylethyl)-imidodicarbonimidic Diamide Hydrochloride; 1-(p-Chlorophenyl-d6)-5-isopropylbiguanide Hydrochloride; Bigumal-d6;

name	category	cas_number	mol_formula	mol_weight	synonym
1-Alpha Hydroxy vitamin D2-D6	deuteriumlabeledcom	216244-04-1	C28H38O2D6	418.69	(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-d3; (1 α ,3 β ,5Z,7E,22E)-9,10-Secoergosta- 5,7,10(19),22-tetraene-1,3,25-triol-d3; 1,25-Dihydroxycalciferol-d3; 1,25- Dihydroxyergocalciferol-d3; Ercalcitriol-d3;
Vitamin D3-D6	deuteriumlabeledcom	NA	C27H38D6O	390.67	(3 β ,5Z,7E)-9,10-Secocholesta-5,7,10(19)- trien-3-ol-d6; Cholecalciferol-d6; DuphafraL D3 1000-d6
Ivabradine D6 HCL	deuteriumlabeledcom	148870-59-1 unlabeled free base	C27H30N2O5D6 . HCl	511.08	3-[3-[[[(7S)-3,4- Dimethoxybicyclo[4.2.0]octa-1,3,5-trien-7- yl]methyl]methylamino]propyl]-1,3,4,5- tetrahydro-7,8-dimethoxy-2H-3- benzazepin-2-one-d6 Hydrochloride

name	category	cas_number	mol_formula	mol_weight	synonym
Acetazolamide D3	deuteriumlabeledcom	1189904-01-5	C4H3N4O3S2D3	225.26	N-[5-Aminosulfonyl]-1,3,4-thiadiazol-2-yl]acetamide-d3; 5-Acetamido-1,3,4-thiadiazole-2-sulfonamide-d3; Acetamox-d3; Atenezol-d3; Defiltran-d3; Diamox-d3; Didoc-d3
Drosperinone D4	deuteriumlabeledcom	NA	C24H26D4O3	370.52	6 β ,7 β ,15 β ,16 β -Dimethylene-3-oxo-4-androstene-[17(β -1')-spiro-5']perhydrofuran-2'-one-d4; Dihydrospirorenone-d4; Drospirenona-d4
Itraconazole D3	deuteriumlabeledcom	1217512-35-0	C35H35Cl2N8O4D3	708.67	(+/-)-4-[4-[4-[4-[[2R,4S)-(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-(1-methyl-d3-propyl)-3H-1,2,4-triazol-3-one; Itrizole-d3; Oriconazole-d3; R-51211-d3; Sporamelt-d3; Sporanox-d3; Triasporin-d3;

name	category	cas_number	mol_formula	mol_weight	synonym
Levocetirizine D4	deuteriumlabeledcom	NA	C21H21ClN2O3D4	465.84	2-[2-[4-[(R)-(4-Chlorophenyl)phenylmethyl]-1-piperazinyl]ethoxy-d4]acetic Acid Dihydrochloride; (-)-Cetirizine-d4 Dihydrochloride; ;
Rivastigmine D6 Oxalate	deuteriumlabeledcom	194929-99-2 free base	C14H16D6N2O2 · C2H2O4	346.41	N-Ethyl-N-methylcarbamic Acid 3-[(1S)-1-(Dimethylamino)ethyl]phenyl Ester-d6 (2R,3R)-2,3-Dihydroxybutanedioate;
Finasteride D9	deuteriumlabeledcom	1131342-85-2	C23H27N2O2D9	381.61	(5 α ,17 β)-N-(1,1-Dimethylethyl-d9)-3-oxo-4-azaandrost-1-ene-17-carboxamide; MK-906-d9; Proscar-d9; Prostide-d9; Finastid-d9;
Fesoterodine-d7 HCl	deuteriumlabeledcom	NA	C26H30NO3D7 · HCl	455.09	2-Methylpropanoic Acid 2-[rac-3-[Bis(1-methylethyl-d7)amino]-1-phenylpropyl] -4-(hydroxymethyl)phenyl Ester (2E)-2-Butenedioate; SMP 8272-d7; SPM 907-d7;
Meloxicam D3	deuteriumlabeledcom	942047-63-4	C14H10N3O4S2D3	354.42	4-Hydroxy-2-(methyl-d3)-N-(5-methyl-2-thiazolyl)-2H-1,2-benzothiazine -3-carboxamide 1,1,-Dioxide; Metacam-d3; Mobic-d3; Mobicox-d3; Movalis-d3; Movatec-d3; Parocin-d3

name	category	cas_number	mol_formula	mol_weight	synonym
N-Desethylamodiaquine D5	deuteriumlabeledcom	1173023-19-2	C18H13D5ClN3O	332.83	4-[(7-Chloro-4-quinolinyl)amino]-2-[(ethyl-d5-amino)methyl]phenol; Monodesethylamodiaquine-d5; Desethylamodiaquine-d5;
Citalopram Oxalate D6	deuteriumlabeledcom	1246819-94-2	C20H15D6FN2O·C2	420.47	1-[3-(Dimethylamino-d6)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbonitrile Oxalate Salt;
Flecainide Acetate D4	deuteriumlabeledcom	1276197-21-7	C17H16D4F6N2O3·CH3CO2H	478.42	N-(2-Piperidinylmethyl)-2,5-bis(2,2,2-trifluoroethoxy)benzamide Monoacetate D4; (±)-Flecainide Acetate D4; 2,5-Bis(2,2,2-trifluoroethoxy)-N-(2-piperidylmethyl)benzamide Acetate D4;
Prednisolone D6	deuteriumlabeledcom	NA	C21H22O5D6	366.48	(11β)-11,17,21-Trihydroxy-pregna-1,4-diene-3,20-dione-d6; Metacortandralone-d6; Delta F-d6; Hydrocortisone-d6;
warfarin D5	deuteriumlabeledcom	75472-93-4	C19H11D5O4	313.36	4-Hydroxy-3-(3-oxo-1-phenyl-d5-butyl)-2H-1-benzopyran-2-one; 3-(α-Acetylbenzyl)-4-hydroxy-coumarin-d5; Warf compound 42-d5; Rodex-d5; Sakarat X-d5; Warfotox-d5;

name	category	cas_number	mol_formula	mol_weight	synonym
Donepezil D4 HCL	deuteriumlabeledcom	NA	C24H26D4ClNO3	419.98	2,3-Dihydro-5,6-dimethoxy-2-[[1-(phenylmethyl)-4-piperidinyl]methyl]-1H-inden-1-one-d4 Hydrochloride; Aricept-d4; Aricept D-d4;
Megestrol D5	deuteriumlabeledcom	NA	C22H25O3D5	347.51	17-Hydroxy-6-(methyl-d5)-pregna-4,6-diene-3,20-dione; 6-(Methyl-d3)megestrol;
Norfluoxetine D5 HCL	deuteriumlabeledcom	1185132-92-6	C16H11D5F3NO · H	336.80	γ -[4-(Trifluoromethyl)phenoxy]benzenepropanamine-d5 Hydrochloride; (+/-)- γ -[4-(Trifluoromethyl)phenoxy]benzenepropanamine-d5 Hydrochloride; Desmethylfluoxetine-d5 Hydrochloride
Roflumilast-D4	deuteriumlabeledcom	1398065-69-4	C17H10Cl2F2N2O3 D4	407.24	3-(Cyclopropyl-d4)methoxy-N-(3,5-dichloro-4-pyridinyl)-4-(difluoromethoxy)benzamide; B 9302-107-d4; BY 217-d4; BYK 20869-d4; Daxas-d4

name	category	cas_number	mol_formula	mol_weight	synonym
Letrozole D4	deuteriumlabeledcom	1133712-96-5	C17H7N5D4	289.33	4,4'-(1H-1,2,4-Triazol-1-ylmethylene)bisbenzotrile-d4; 4-[1-(4-Cyanophenyl)-1-(1,2,4-triazol-1-yl)methyl]benzotrile-d4; CGS 20267-d4; Femara-d4; Lerazole-d4; Letrazole-d4
Fexofenadine D10	deuteriumlabeledcom	NA	C32H29NO4D10	511.72	4-[1-Hydroxy-4-[4-(hydroxydiphenyl-d10-methyl)-1-piperidiny]butyl]- α , α -dimethylbenzeneacetic Acid Hydrochloride; Carboxyterfenadine-d10 Hydrochloride; Terfenadinecarboxylate-d10 Hydrochloride; Alernex-d10; Allegra-d10; Feksine-d10; Fexadyne-d10; Fexo-d10; Fexofen-d10; MDL 16455A-d10; Telfast-d10; Telfast BD-d10; Vivafeks-d10;
Clopidogrel-d4 Hydrogensulfate	deuteriumlabeledcom	1219274-96-0	C15H10ClNO2SD4. HCl	348.29	α -(2-Chlorophenyl-d4)-6,7-dihydro-thieno[3,2-c]pyridine-5(4H)-acetic Acid Methyl Ester Sulfate; (+/-)-Clopidogrel-d4 Bisulfate

name	category	cas_number	mol_formula	mol_weight	synonym
Benzaldehyde D5	deuteriumlabeledcom	14132-51-5	C ₇ H ₅ O	111.15	Artificial Almond Oil-d5; Benzaldehyde FFC-d5; Benzenecarbonal-d5; Benzenecarboxaldehyde-d5; Benzoic Acid Aldehyde-d5; Benzoic Aldehyde-d5; NSC 7917-d5; Phenylformaldehyde-d5; Phenylmethanal-d5
Oseltamavir D3	deuteriumlabeledcom	NA	C ₁₆ H ₂₅ N ₂ O ₄ D ₃	315.43	(3R,4R,5S)-4-(Acetylamino-d3)-5-amino-3-(1-ethylpropoxy)-1-cyclohexene-1-carboxylic Acid; Oseltamivir-d3 Carboxylic Acid
Diflunisal-d3	deuteriumlabeledcom	NA	C ₁₃ H ₅ F ₂ O ₃ D ₃	253.22	2',4'-Difluoro-4-hydroxy-[1,1'-biphenyl]-3-carboxylic Acid-d3; 2',4'-Difluoro-4-hydroxy- biphenyl-3-carboxylic Acid-d3; 5-(2,4-Difluorophenyl)salicylic Acid-d3; Adomal-d3; Difludol-d3; Diflusinal-d3; Dolisal-d3; Doloban-d3; Dolobid-d3; Dolobis-d3; Flovacil-d3; Fluniget-d3; Fluodonil-d3; Flustar-d3; MK 647-d3
Norgestimate D6	deuteriumlabeledcom	1263194-12-2	C ₂₃ H ₂₅ N ₃ O ₃ D ₆	375.54	(17 α)-17-(Acetyloxy)-13-ethyl-18,19-dinorpregn-4-en-20-yn-3-one 3-Oxime-d6; Dexnorgestrel Acetime-d6; D-138-d6; ORF-10131-d6

name	category	cas_number	mol_formula	mol_weight	synonym
Colchicine D6	deuteriumlabeledcom	1217651-73-4	C22H19D6NO6	405.47	N-[(7S)-5,6,7,9-Tetrahydro-1,2,3,10-tetramethoxy-9-oxobenzo[a]heptalen-7-yl]acetamide-d6; (-)-Colchicine-d6; Colchineos-d6; Colchisol-d6; Colcin-d6; Colsaloid-d6; Condylon-d6; NSC 757-d6
Docosahexanoic Acid Ethyl Ester-d5	deuteriumlabeledcom	159146-01-7	C24H31O2D5	361.58	Cervonic acid d5; Efalex D5
Sitagliptin D4	deuteriumlabeledcom	NA	C16H11F6N5OD4 . H	447.80	7-[(3R)-3-Amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-5,6,7,8-tetrahydro-3-(trifluoromethyl)-1,2,4-triazolo[4,3-a]pyrazine-d4 Phosphate; Januvia-d4; MK 0431-d4;
Eicosapentaenoic Acid Ethyl Ester-d5	deuteriumlabeledcom	1392217-44-5	C22H29O2D5	335.55	(5Z,8Z,11Z,14Z,17Z)-5,8,11,14,17-Eicosapentaenoic Acid Ethyl-d5 Ester; (all-Z)-5,8,11,14,17-Eicosapentaenoic Acid Ethyl-d5 Ester; Epadel-d5; Ethyl-d5 Eicosapentaenoate; Timnodonic Acid Ethyl-d5 Ester; cis-Eicosapentaenoic Acid Ethyl-d5 Ester

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Pimozide D4	deuteriumlabeledcom	2062-78-4 unlabeled	C28H25F2N3OD4	465.58	7-[(3R)-3-Amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-5,6,7,8-tetrahydro-3-(trifluoromethyl)-1,2,4-triazolo[4,3-a]pyrazine-d4 Phosphate; Januvia-d4; MK 0431-d4;
M1 Metabolite of Glimepiride D4	deuteriumlabeledcom	NA	C24H30N4O5SD4	494.65	3-(Ethyl-d4)-2,5-dihydro-N-[2-[4-[[[[[trans-4-(hydroxymethyl)cyclohexyl]amino]carbonyl]amino]sulfonyl]phenyl]ethyl]-4-methyl-2-oxo-1H-pyrrole-1-carboxamide;
Efavirenz 13C6	deuteriumlabeledcom	1261394-62-0	C8H9CIF3NO2 13C6	321.63	6-Chloro-4-(2-cyclopropyl-d5-ethynyl)-1,4-dihydro-4-(trifluoromethyl)-2H-3,1-benzoxazin-2-one; DMP 266-13C6; L 743726-13C6;
Aliskiren Hemifumarate 13C2 D6	deuteriumlabeledcom	1261398-71-3 free base	C2813C2H47D6N3O	617.82	α S, γ S, δ S, ζ S)- δ -Amino-N-(3-amino-2,2-dimethyl-3-oxopropyl)- γ -hydroxy-4-methoxy-3-(3-methoxypropoxy)- α ,z-bis(1-methylethyl)benzeneoctanamide-13C2d6 Hydrochloride; CGP 60536-13C2d6
Zidovudine 13C D3	deuteriumlabeledcom	325484-33-1	C9H10N5O4 13C D3	271.25	AZT-13Cd3; Retrovis-13Cd3; Timazid-13Cd3; NSC 602670-13Cd3;

name	category	cas_number	mol_formula	mol_weight	synonym
Mycophenolate Mofetil D4 Oxalate	deuteriumlabeledcom	1132748-21-0 free base	C23H27D4NO7 · C2	527.55	(4E)-6-(1,3-Dihydro-4-hydroxy-6-methoxy-7-methyl-3-oxo-5-isobenzofuranyl)-4-hexenoic Acid-d4 4-methyl-2-(4-morpholinyl)ethyl Ester; Mycophenolic Acid-d4-2-(4-Morpholinyl)ethyl Ester; RS 61443-d4; TM-MMF-d4;
Rifabutin D6	deuteriumlabeledcom	72559-06-9 unlabeled	C46H56D6N4O11	853.04	'4-Didehydro-1-deoxy-1,4-dihydro-5'-(2-methylpropyl)-1-oxorifamycin XIV-d6; Ansatipine-d6; Ansamycin-d6
Phenylephrine HCL D3	deuteriumlabeledcom	NA	C9H10D3NO2 · HCl	206.68	(±)-3-Hydroxy-α - [(methylamino)methyl]benzenemethanol-d3 Hydrochloride, ; (±)-m-Hydroxy-α - [(methylamino)methyl]benzyl Alcohol-d3 Hydrochloride; (±)-Phenylephrine Hydrochloride-d3; 1-(3-Hydroxyphenyl)-2-methylaminoethanol-d3 Hydrochloride; DL-Phenylephrine-d3 Hydrochloride; NSC 14029-d3

name	category	cas_number	mol_formula	mol_weight	synonym
Betamethasone Dipropionate D5	deuteriumlabeledcom	NA	C28H32D5FO7	509.61	(11 β ,16 β)-9-Fluoro-11-hydroxy-16-methyl-17,21-bis(1-oxopropoxy)-pregna-1,4-diene-3,20-dione-d5; Betamethasone 17,21-Dipropionate-d5;
Mirtazapine DIHCL D4	deuteriumlabeledcom	85650-52-8 unlabeled free base	C17H15D4N3.2HCl	342.29	1,2,3,4,10,14b-Hexahydro-2-methyl-pyrazino[2,1-a]pyrido[2,3-c][2]benzazepine-d4; Org-3770-d4; Remeron-d4; Zispin-d4;
Phenoxybenzamine HCL D7	deuteriumlabeledcom	1261393-48-9	C18H15D7ClNO · HCl	347.33	N-(2-Chloroethyl)-N-(1-methyl-2-phenoxyethyl)benzenemethanamine-d7 Hydrochloride; N-2-Phenoxyisopropyl-N-benzyl- β -chloroethylamine-d7 Hydrochloride; Dibenzylamine-d7 Chloride; Dibenzylamine-d7 Hydrochloride;
Cyclobenzaprine-d3 HCl(N-methyl-d3)	deuteriumlabeledcom	1184983-42-3	C20H19D3ClN	314.87	3-(5H-Dibenzo[a,d]cyclohepten-5-ylidene)-N-methyl-N-(methyl-d3)-1-propanamine Hydrochloride; Flexeril-d3; Flexiban-d3
Albuterol D3	deuteriumlabeledcom	NA	C13H18NO3D3	242.33	α 1-[[[(1,1-Dimethylethyl)amino]methyl]-4-hydroxy-1,3-benzenedimethanol-d3; Salbutamol-d3

name	category	cas_number	mol_formula	mol_weight	synonym
Guaifenesin D3	deuteriumlabeledcom	1189924-85-3	C10H11O4D3	201.24	3-(o-Methoxyphenoxy)-1,2-propanediol-d3, Guaiacol Glyceryl Ether-D3; Robitussin-d3
Emtricitabine 15N D3	deuteriumlabeledcom	143491-57-0 unlabeled	C8H7FN2O3S 15N D3	251.26	Amino-5-fluoro-1-[(2R,5S)-2-hydroxymethyl)-1,3-oxathiolan-5-yl]-2-(1H-pyrimidinone-D315N2; (-)-2',3'-Dideoxy-5-fluoro-3'-thiacytidine-D315N2; (-)-2'-Deoxy-5-fluoro-3'-thiacytidine-D3,15N2
Nilutamide D6	deuteriumlabeledcom	1189477-66-4	C12H4D6F3N3O4	323.26	5,5-(Dimethyl-d6)-3-[4-nitro-3-(trifluoromethyl)phenyl]-2,4-imidazolidinedion; 1-(3-Trifluoromethyl-4-nitrophenyl)-4,4-(dimethyl-d6)imidazoline-2,5-dione; Anandron-d6; Nilandron-d6; Nilandrone-d6; RU 23908-d6; RU 23908-10-d6
Bicalutamide D4	deuteriumlabeledcom	1185035-71-5	C18H114F4N2O4S	434.37	N-[4-Cyano-3-trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methylpropanamide-d4; ICI-176334-d4; Casodex-d4

name	category	cas_number	mol_formula	mol_weight	synonym
Rosuvastatin D6 calcium salt	deuteriumlabeledcom	NA	C22H21FN3O6SD6.	506.61	7-[4-(4-Fluorophenyl)-6-(1-methylethyl-d6)-2-[methyl(methylsulfonyl)amino]-5-pyrimidinyl]-3,5-dihydroxy-6-heptenoic Acid Sodium Salt;
Acyclovir-D4	deuteriumlabeledcom	1185179-33-2	C8H7N5O3D4	229.23	2-Amino-1,9-dihydro-9-[(2-hydroxyethoxy-d4)methyl]-6H-Purin-6-one; 9-[(2-Hydroxyethoxy-d4)methyl]guanine; Acycloguanosine-d4; Acicloftal-d4; Cargosil-d4; Gerpevir-d4; Herpevir-d4; Zovirax-d4; Zyclir-d4;
Cephalexin D5	deuteriumlabeledcom	NA	C16H12N3O4SD5	352.43	(6R,7R)-7-[[[(2R)-2-Amino-2-(phenyl-d5)acetyl]amino]-3-methyl-8-oxo -5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic Acid Hydrate; Alcephin-d5; Alsporin-d5; Cefablan-d5; Cefadal-d5; Cefadin-d5; Taicelexin-d5; Tepaxin-d5;
Prasugrel-d4 Metabolite(R-95913, Mixture of Diastereomers)	deuteriumlabeledcom	NA	C18H14FNO2SD4	335.44	5-[2-(Cyclopropyl-d5)-1-(2-fluorophenyl)-2-oxoethyl]-5,6,7,7a-tetrahydrothieno[3,2-c]pyridin-2(4H)-one; R 95913-d4;

name	category	cas_number	mol_formula	mol_weight	synonym
Fluindione D4	deuteriumlabeledcom	1246820-41-6	C15H5FO2D4	244.26	2-(4-Fluorophenyl)-1H-indene-1,3(2H)-dione-d4; 2-(p-Fluorophenyl)-1,3-indandione-d4; LM 123-d4; Previscan-d4
Eletriptan D5 HCL	deuteriumlabeledcom	NA	C22H21D5N2O2S.H	423.98	3-[[[(2R)-1-Methyl-2-pyrrolidiny]methyl]-5-[2-(phenylsulfonyl)ethyl]-1H-indole-d5; UK-116044-d5; Relpax-d5;
Repaglinide D5	deuteriumlabeledcom	1217709-85-7	C27H31N2O4 D5	NA	2-(Ethoxy-d5)-4-[2-[[[(1S)-3-methyl-1-[2-(1-piperidiny]phenyl]butyl]amino]-2-oxoethyl]benzoic Acid; AG-EE-623-d5; Novonorm-d5; Prandin-d5;
Atorvastatin D5	deuteriumlabeledcom	222412-82-0	C33H29FN2O5D5.1/	582.69	(β R, δ R)-2-(4-Fluorophenyl)-β, δ -dihydroxy-5-(1-methylethyl)-3-(phenyl-d5)-4-[(phenylamino)carbonyl]-1H-pyrrole-1-heptanoic Acid Calcium Salt (2:1); Atorvastatin-d5 Hemicalcium
P-OH-Atorvastatin-D5	deuteriumlabeledcom	265989-45-5	C33H29FN2O6D5.1/	598.58	3R,5R)-tert-Butyl 7-(2-(4-Fluorophenyl)-4-((4-hydroxyphenyl)carbamoyl)-5-isopropyl-3-phenyl-d5-1H-pyrrol-1-yl)-3,5-dihydroxyheptanoate

name	category	cas_number	mol_formula	mol_weight	synonym
Acitretin D3	deuteriumlabeledcom	1185241-03-5	C21H23O3D3	329.46	(all-E)-9-(4-Methoxy-2,3,6-trimethylphenyl)-3,7-dimethyl-2,4,6,8-nonatetraenoic Acid-d3; Neotigason-d3; Soriatane-d3
Imuthiol D10	deuteriumlabeledcom	1261395-23-6	C5H10NS2 · Na	181.32	N,N-Diethyl-carbamodithioic Acid-d10 Sodium Salt; Diethyldithio-carbamic Acid-d10 Sodium Salt; Dithiocarb-d10; Dithiocarb-d10 sodium; Ditiocarb-d10 sodium; Imuthiol-d10; Kupral-d10; Soxinol ESL-d10; Thiocarb-d10
Silodosin DiHCL D6	deuteriumlabeledcom	1261392-62-4	C25H26D6F3N3O4 · H	574.49	2,3-Dihydro-1-(3-hydroxypropyl-d6)-5-[(2R)-2-[[2-[2-(2,2,2-trifluoroethoxy)phenoxy]ethyl]amino]propyl]-1H-indole-7-carboxamide; (R)-1-(3-Hydroxypropyl-d6)-5-[2- [[2-[2-(2,2,2-trifluoroethoxy)phenoxy]ethyl]amino]propyl]indoline-7-carboxamide; KAD 3213-d6; KMD 3213-d6; Urief-d6;
Oseltamavir HCL D5	deuteriumlabeledcom	NA	C16H23D5N2O4 · H	353.90	(3R,4R,5S)-4-(Acetylamino-d5)-5-amino-3-(1-ethylpropoxy)-1-cyclohexene-1-carboxylic Acid Ethyl Ester Phosphate; Ro 64-0796/002-d5; Tamiflu-d5;

name	category	cas_number	mol_formula	mol_weight	synonym
Mycophenolic Acid 13C D3	deuteriumlabeledcom	1261432-16-9	C16H17O6 13C D3	324.35	(4E)-6-(1,3-Dihydro-4-hydroxy-6-methoxy-13C ₃ -7-methyl-3-oxo-5-isobenzofuranyl)-4-methyl-4-hexenoic Acid;
5-Azacytidine - 15N4	deuteriumlabeledcom	NA	C8H1215N4O5	248.18	Azacidine-15N ₄ ; 4-Amino-1-β-D-ribofuranosyl-1,3,5-triazin-2(1H)-one-15N ₄ ; 5-AC-15N ₄ ; 5-AZC-15N ₄ ; 5-AZCR-15N ₄ ; 5-AzaC-15N ₄ ; Antibiotic U 18496-15N ₄ ; Azacytidine-15N ₄ ; Ladakamycin-15N ₄ ; Ledakamycin-15N ₄ ; Mylosar-15N ₄ ; NSC 102816-15N ₄ ; NSC 103-627-15N ₄ ; U 18496-15N ₄ ; Vidaza-15N ₄
lloperidone 13CD3	deuteriumlabeledcom	NA	C23H24FN2O4 13C	430.50	1-[4-[3-[4-(6-Fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]propoxy]-3-(methoxy-13C ₃)phenyl]ethanone; HP 87313C-d3
Fampridine D4	deuteriumlabeledcom	45498-20-2	C5H2N2D4	98.14	4-Pyridinamine-d ₄ ; 4-Aminopyridine-d ₄ ; 4-Pyridinylamine-d ₄ ; 4-Pyridylamine-d ₄ ; 4AP-d ₄ ; Ampyra-d ₄ ; Avitrol-d ₄ ; EL 970-d ₄ ; Fampridine-d ₄ ; NSC 15041-d ₄ ; Neurelan-d ₄ ; Phillips 1861-d ₄ ; Pyridine-4-ylamine-d ₄ ; VMI 10-3-d ₄ ; p-Aminopyridine-d ₄ ; γ-Aminopyridine-d ₄

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Penicillamine D3 Acetate	deuteriumlabeledcom	NA	C5H8NO2SD3.C2H4	212.28	3-Mercapto-L-valine D3; (+)-Penicillamine D3; (R)-Penicillamine D3; L-Penicillamine D3; NSC 241261 D3;
Milnacipran D5 HCl	deuteriumlabeledcom	NA	C15H17N2OD5 . HC	287.85	(1R,2S)-rel-2-(Amino-methyl)-N,N-diethyl-1-phenylcyclopropanecarboxamide-d5, Monohydrochloride; F-2207-d5; Dalcipran-d5;
Amoxicillin -D4	deuteriumlabeledcom	26787-78-0 unlabeled	C16H15N3O5SD4	369.44	(2S,5R,6R)-6-[[[(2R)-2-Amino-2-(4-hydroxyphenyl)acetyl]amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic Acid-d4; AMPC-d4; Amoxycillin-d4; Helvamox-d4;Pasetocin-d4; Penimox-d4; Zamocillin-d4
Flupritine D4 HCl	deuteriumlabeledcom	NA	C15H13FN4O2D4.H	344.81	N-[2-Amino-6-[[[(4-fluorophenyl)methyl]amino]-3-pyridinyl]carbamic Acid Ethyl Ester Hydrochloride; 2-Amino-6-[(p-fluorobenzyl)amino]-3-pyridinecarbamic Acid Ethyl Ester Hydrochlorite;

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Propranolol-d7 HCL	deuteriumlabeledcom	NA	C16H14D7NO2.HCl	302.85	2R)-1-[(1-Methylethyl-d7)amino]-3-(1-naphthalenyloxy)-2-propanol Hydrochloride; (+)-1-(Isopropyl-d7)amino-3-(1-naphthyloxy)-2-propanol Hydrochloride; (+)-Anapriline-d7; (+)-Propranolol-d7 Hydrochloride
Paroxetine Oxalate D6	deuteriumlabeledcom	1435728-63-4 free base	C19H14D6FNO3 · C	425.44	3S-trans)-3-[(1,3-Benzodioxol-5-yloxy)methyl]-4-(4-fluorophenyl)piperidine D6Hydrochloride; Aropax D6; Deroxat D6;
Ramelteon -D3	deuteriumlabeledcom	1185146-24-0	C ₁₆ H ₁₈ D ₃ NO ₂	262.36	rac N-[[1,6,7,8-Tetrahydro-2H-indeno[5,4-b]furan-8-yl]ethyl]propanamide-d3; rac TAK-375-d3; rac Rozerem-d3
O-Hydroxy Atorvastatin D5	deuteriumlabeledcom	265989-47-7	C33H29FN2O6D5.1/	598.58	3S,5S)-tert-Butyl 7-(2-(4-Fluorophenyl)-4-((4-hydroxyphenyl)carbamoyl)-5-isopropyl-3-phenyl-d5-1H-pyrrol-1-yl)-3,5-dihydroxyheptanoate

name	category	cas_number	mol_formula	mol_weight	synonym
Abacavir D4	deuteriumlabeledcom	1217731-56-0	C14H14N6OD4	290.36	(1S,4R)-4-[2-Amino-6-(cyclopropylamino-d4)-9H-purin-9-yl]-2-cyclopentene-1-methanol;(1S-cis)-4-[2-Amino-6-(cyclopropylamino-d4)-9H-purin-9-yl]-2-cyclopentene-1-methanol; 1592U89-d4; ABC-d4; Abacavir Stable Isotope
Loteprednol Etabonate D5	deuteriumlabeledcom	82034-46-6 unlabeled	C24H26D5ClO7	471.98	11 β ,17 α)-17-[(Ethoxycarbonyl)oxy]-11-hydroxy-3-oxo-androsta-1,4-diene-17-carboxylic Acid-d5 Chloromethyl Ester; CDDD-5604-d5
Everolimus D4	deuteriumlabeledcom	1338452-54-2	C53H79NO14D4	962.27	40-O-(2-Hydroxyethyl-d4)rapamycin; 42-O-(2-Hydroxy)ethyl-d4 Rapamycin; Afinitor-d4; Certican-d4; RAD-d4; RAD 001-d4; SDZ-RAD-d4; XIENCE V-d4
Piroxicam D3	deuteriumlabeledcom	942047-64-5	C15H10N3O4SD3	334.36	4-Hydroxy-2-(methyl-d3)-N-2-pyridinyl-2H-1,2-benzothiazine-3-carboxamide 1,1-Dioxide; Artroxicom-d3; Baxo-d3; Bruxicom-d3; CHF 1251-d3; CP 16171-d3; Caliment-d3; Roxicom-d3; Roxiden-d3; Sasulen-d3; Solocalm-d3

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Tetrabenazine D7	deuteriumlabeledcom	NA	C19H20NO3D7	324.47	(3R,11bR)-rel-1,3,4,6,7,11b-Hexahydro-9,10-dimethoxy-3-(2-methylpropyl)-2H-benzo[a]quinolizin-2-one-d7; cis-2-Oxo-3-(isobutyl)-9,10-dimethoxy-1,2,3,4,6,7-hexahydro -11bH-benzo[a]quinolizine-d7
Simvastatin-d6 Hydroxy Acid Ammonium Salt	deuteriumlabeledcom	NA	C25H34D6O6 · NH3	459.65	(β R, δ R,1S,2S,6R,8S,8aR)-8-[2,2-(Dimethyl-d6)-1-oxobutoxy]-1,2,6,7,8,8a-hexahydro- β , δ -dihydroxy-2,6-dimethyl-1-naphthaleneheptanoic Acid Ammonium Salt; Simvastatin-d6 Acid Ammonium Salt; Simvastatin-d6 Ammonium Salt; Simvastatin-d6 Carboxylic Acid Ammonium Salt
Hydroxy Chloroquine D4-O-Sulfate	deuteriumlabeledcom	NA	C18H21NaD4ClN3O	441.94	2-[[4-[(7-Chloro-4-quinolinyl)amino]pentyl]ethylamino]ethanol-d4 1-(Hydrogen Sulfate); 2-[[4-[(7-Chloro-4-quinolyl)amino]pentyl]ethylamino]ethanol-d4 Sulfate
Fingolimod-D4 HCl	deuteriumlabeledcom	NA	C19H29D4NO2.HCl	347.96	2-amino-2-[2-(4-octylphenyl)ethyl]propane-1,3-diol D4

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Bumetanide-D5	deuteriumlabeledcom	1216739-35-3	C17H15D5N2O5S	369.45	3-(Aminosulfonyl)-5-[(butyl-d5)amino]-4-phenoxy-benzoic Acid; 3-[(Butyl-d5)amino]-4-phenoxy-5-sulfamoylbenzoic Acid; Bufenox-d5; Bumex-d5; Burinex-d5; Fordiuran-d5; Lixil-d5; Lunetoron-d5; PF 1593-d5; Ro 10-6338-d5
Testosterone-D4	deuteriumlabeledcom	638163-36-7	C19H24D4O2	292.44	Androderm D4; Testoderm D4; SustanonD4
Nevirapine D4	deuteriumlabeledcom	129618-40-2 unlabeled	C15H10N4O D4	270.33	1-Cyclopropyl-5,11-dihydro-4-methyl-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one-d3; BI-RG 587-d4;Viramune-d4;
Asenapine HCl-13CD3 (-20 product)	deuteriumlabeledcom	1261392-55-5	C16H13CINO 13C D3·HCl	326.24	(3aR,12bR)-rel-5-Chloro-2,3,3a,12b-tetrahydro-2-(methyl-13C,d3)-1H-dibenz[2,3:6,7]oxepino[4,5-c]pyrrole; trans-5-Chloro-2,3,3a,12b-tetrahydro-2-(methyl-13C,d3) -1H-dibenz[2,3:6,7]oxepino[4,5-c]pyrrole;
N-(+)-Desmethylnasapine HCl-13C6	deuteriumlabeledcom	1261393-91-2 free base	C10H14CINO 13C6	314.13	(3aR,12bR)-rel-5-Chloro-2,3,3a,12b-tetrahydro-1H-dibenz[2,3:6,7]oxepino[4,5-c]pyrrole-13C6Hydrochloride

name	category	cas_number	mol_formula	mol_weight	synonym
Isosorbide-13C6 5-Mononitrate	deuteriumlabeledcom	1217604-00-6	13C6 H9NO6	197.07	1,4:3,6-Dianhydro-D-glucitol-13C6 5-Nitrate; 6-Nitrooxyhexahydro-furo[3,2-b]furan-3-ol-13C6; Isosorbide-13C6 5-Nitrate; Corangin-13C6; Elan-13C6; Elantan-13C6; Imdur-13C6; Monocedocard-13C6; Monoclair-13C6; Monosorb-13C6; Pentacard-13C6
Toresamide D7	deuteriumlabeledcom	1189375-06-1	C16H13N4O3SD7	355.47	N-[[[(1-Methylethyl-d7)amino]carbonyl]-4-[(3-methylphenyl)amino]-3-pyridinesulfonamide; AC-4464-d7; BM-02015-d7; JDL-464-d7; Demadex-d7; Luplac-d7; Toradiur-d7; Torem-d7; Torasemide-d7; Unat-d7
Fingolimod Phosphate D4	deuteriumlabeledcom	402615-91-2 unlabeled	C19H30NO5PD4	391.45	2-Amino-2-[2-(4-octylphenyl)ethyl]-1,3-propanediol 1-(Dihydrogen Phosphate) D4; 2-Amino-2-[2-(4-octylphenyl)ethyl]-1,3-propanediol Mono(dihydrogen phosphate) Ester D4

name	category	cas_number	mol_formula	mol_weight	synonym
25- dihydroxy vitamin D2 D6	deuteriumlabeledcom	1262843-46-8	C28H38D6O3	434.68	(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]cyclohexanol-d6; (3 β ,5Z,7E,22E)-9,10-Secoergosta- 5,7,10(19),22-tetraene-3,25-diol-d6; 25- Hydroxycalciferol-d6; 25- Hydroxyergocalciferol-d6; Ercalcidiol-d6
5-Hydroxy Propafenone D5	deuteriumlabeledcom	1215370-87-8	C21H22D5NO4.HCl	398.94	1-[5-Hydroxy-2-[2-hydroxy-3- (propylamino)propoxy]phenyl]-3-phenyl-1- propanone- d5 Hydrochloride
Bisoprolol D5 hemifumarate	deuteriumlabeledcom	NA	C18H26NO4D5.1/2	388.52	1-[4-[[2-(1- Methylethoxy)ethoxy]methyl]phenoxy]-3- [(1-methylethyl)amino]-2-propanol-d5 (2E)-2-butenedioate (2:1) (salt)
Formoterol-d3	deuteriumlabeledcom	NA	C19H21N2O4D3	347.43	D,L-N-[2-Hydroxy-5-[1-hydroxy-2-[[1-[(4- methoxyphenyl)methyl-d3]ethyl]amino] ethyl]phenyl]formamide;

name	category	cas_number	mol_formula	mol_weight	synonym
Indapamide D3	deuteriumlabeledcom	1217052-38-4	C16H13CIN3O3SD3	368.86	3-(Aminosulfonyl)-4-chloro-N-[2,3-dihydro-2-(methyl-d3)-1H-indol-1-yl]benzamide; (+/-)-4-Chloro-N-[2-(methyl-d3)-1-indolinyl]-3-sulfamoylbenzamide; Arifon-d3; Bajaten-d3; Damide-d3; Flubest-d3; Fludex-d3; Idamide-d3; Noranat-d3; Veroxil-d3; Tandix-d3; Tertensif-d3; Veroxil-d3
Ranelic Acid 13C4	deuteriumlabeledcom	NA	C8H6N2O8S 13C4.4	434.17	5-[Bis(carboxymethyl)amino]-2-carboxy-4-cyano-3-thiopheneacetic Acid 13C4;
Zolmitriptan D6	deuteriumlabeledcom	1217644-84-2	C16H15D6N3O2	293.39	(4S)-4-[[3-[2-(Dimethyl-d6-amino)ethyl]-1H-indol-5-yl]methyl-2-oxazolidinone; BW-311C90-d6; Zomig-d6
Ticagrelor D4	deuteriumlabeledcom	NA	C23H24F2N6O4SD4	526.59	(1S,2S,3R,5S)-3-[7-[[[(1R,2S)-2-(3,4-D1,2-Cyclopentane diolifluorophenyl)cyclopropyl]amino]-5-(propylthio-d4)-3H-1,2,3-triazolo[4,5-d]pyrimidin-3-yl]-5-(2-hydroxyethoxy)-1,2-cyclopentane diol; AR-C 126532XX-d4; AZD 6140-d4;

name	category	cas_number	mol_formula	mol_weight	synonym
Cholesterol D6	deuteriumlabeledcom	92543-08-3	C27H40D6O	392.70	Cholesterol-2,2,3,4,4,6-d6; (3 β)-Cholest-5-en-3-ol-d6; (3 β)-Cholest-5-en-3-ol-d6; (-)-Cholesterol-d6; 3 β -Hydroxycholest-5-ene-d6; 5:6-Cholesten-3 β -ol-d6; Cholest-5-en-3 β -ol-d6; Cholesterin-d6; Cholesteryl-d6 Alcohol; Dythol-d6; Lidinit-d6; Lidinite-d6; NSC 8798-d6; Provitamin D-d6; 5-Cholesten-3 β -ol-d6
Fluvastatin D6	deuteriumlabeledcom	93957-55-2	C24H19D6FNO4	416.48	(3R,5S,6E)-rel-7-[3-(4-Fluorophenyl)-1-(1-methylethyl-d6)-1H-indol-2-yl]-3,5-dihydroxy-6-heptenoic Acid Sodium Salt; Fluindostatin;-d6 XU 62-320-d6; Lescol-d6; Lipaxan-d6; Primexin-d6
Rac erythro dihydro bupropion D9	deuteriumlabeledcom	1217684-77-9	C13H11CINOD9 . HC	287.22	(α S)-rel-3-Chloro- α -[(1R)-1-[(1,1-dimethylethyl)amino]ethyl]benzenemethanol-d9; rac erythro-Hydroxybupropion-d9
Rac threo dihydro bupropion D9	deuteriumlabeledcom	1217815-08-1	C13H11CINOD9. HC	287.28	(α R)-rel-3-Chloro- α -[(1R)-1-[(1,1-dimethylethyl)amino]ethyl]benzenemethanol-d9; rac threo-Hydroxybupropion-d9

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4'-Hydroxyphenyl Carvedilol-d5	deuteriumlabeledcom	1261395-96-3	C24H21N2O5D5	427.52	S)-(+)-1-(9H-Carbazol-4-yloxy)-3-[[2-[2-methoxy-4-(phenylmethoxy)phenoxy]ethyl]amino]-2-propanol D5;
Cetirizine D8	deuteriumlabeledcom	NA	C21H17ClN2O3D8	469.87	[4-[(4-Chlorophenyl)-phenylmethyl]-1-piperazinyl-d8]ethoxy]acetic Acid;
Doxorubicin Trifluoroacetate salt 13CD3	deuteriumlabeledcom	23214-92-8 unlabeled free base	C2613CH28D3NO11	663.57	(8S,10S)-10-[(3-Amino-2,3,6-trideoxy- α -lyxo-hexopyranosyl13CD3)oxy]-7,8,9,10-tetrahydro-6,8,11-trihydroxy-8-(hydroxyacetyl)-1-methoxy-5,12-naphthacenedione Hydrochloride
Paricalcitol D6	deuteriumlabeledcom	131918-61-1 unlabeled	C27H38O3 D6	422.68	(1R,3R,5Z)-5-[(2E)-2-[(1R,3aS,7aR)-Octahydro-1-[(1R,2E,4S)-5-hydroxy-1,4,5-trimethyl-2-hexen-1-yl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-1,3-cyclohexanediol-d6; (1 α ,3 β ,7E,22E)-19-Nor-9,10-secoergosta-5,7,22-triene-1,3,25-triol-d6; 19-Nor-1,25-dihydroxyvitamin D2-d6; 1 α ,25-Dihydroxy-19-nor-vitamin D2-d6; Zemplar-d6

name	category	cas_number	mol_formula	mol_weight	synonym
Dronedarone D6 HCL	deuteriumlabeledcom	1329809-23-5	C31H39CIN2O5SD6	599.26	N-[2-Butyl-3-[4-[3-(dibutylamino)propoxy]benzoyl]-5-benzofuranyl]methanesulfonamide-d6 Hydrochloride; SR33589-d6 Hydrochloride; Multaq-d6 Hydrochloride
Dabigatran 13C6	deuteriumlabeledcom	1210608-88-0	C19H25N7O3 13C6	477.54	N-[[2-[[[4-(Aminoiminomethyl)phenyl]amino]methyl]-1-methyl-1H-benzimidazol-5-yl]carbonyl]-N-2-pyridinyl-β-alanine-13C6; BIBR 953-13C6; BIBR 953ZW-13C6
(+)-β-Dihyrotetrabenazine 13C2 D6	deuteriumlabeledcom	NA	C ₁₇ ¹³ C ₂ H ₂₃ D ₆ NO ₃	327.46	(2S,3R,11bR)-1,3,4,6,7,11b-Hexahydro-9,10-dimethoxy-3-(2-methylpropyl)-2H-benzo[a]quinolizin-2-ol-13C2D6; (2S,3R,11bR)-Dihyrotetrabe-13C2D6
N-Desbutyl Dronedarone D6 HCl (-20 product) not in powder form	deuteriumlabeledcom	1346598-70-6	C27H31CIN2O5SD6	543.16	N-[2-Butyl-3-[4-[3-(butylamino)propoxybenzoyl]-5-benzofuranyl]-methanesulfonamide-d6 Hydrochloride; SR 35021-d6;

name	category	cas_number	mol_formula	mol_weight	synonym
Citric Acid D4	deuteriumlabeledcom	147664-83-3	C6H4D4O7	196.15	2-Hydroxy-1,2,3-propanetricarboxylic-d4 Acid; Chemfill-d4; Citretten-d4; 2-Hydroxypropan-d4-1,2,3-tricarboxylic Acid; Citro-d4; E 330-d4; 3-Carboxy-3-hydroxypentane-d4-1,5-dioic Acid; Aciletten-d4; Celenex 3P6-d4
Tolvaptan D7	deuteriumlabeledcom	1246818-18-7	C26H18D7CIN2O3	455.98	N-[4-[(7-Chloro-2,3,4,5-tetrahydro-5-hydroxy-1H-1-benzazepin-1-yl)carbonyl]-3-methylphenyl]-2-methylbenzamide-d7; OPC 41061-d7
(+) - α - Dihydratetrabenazine 13C2 D6	deuteriumlabeledcom	NA	C17H23NO3D6 13C2	327.46	(2R,3R,11bR)-1,3,4,6,7,11b-Hexahydro-9,10-dimethoxy-3-(2-methylpropyl)-2H-benzo[a]quinolizin-2-ol-13C2D6; [2R-(2 α ,3 β ,11b β)]-1,3,4,6,7,11b-Hexahydro-9,10-dimethoxy-3-(2-methylpropyl)-2H-benzo[a]quinolizin-2-ol-13C2D6; (+)-(2R,3R,11bR)-Dihydratetrabenazine-13C2D6; (+)-DTBZ-13C2D6; (+)-Dihydratetrabenazine-13C2D6; (2R,3R,11bR)-DHTBZ-13C2D6

name	category	cas_number	mol_formula	mol_weight	synonym
Tacrolimus 13C D2	deuteriumlabeledcom	NA	C ₄₃ H ₆₇ N ₀₁₂ 13C D2	807.02	dvagraf-13C,D2; FR 900506-13C,D2; Fujimycin-13C,D2; L 679934-13C,D2; Prograf-13C,D2; Protopic-13C,D2; TacroBell-13C,D2
Saxagliptin-15N,D2 Hydrochloride	deuteriumlabeledcom	1309934-06-2	C ₁₈ H ₂₃ N ₂ O ₂ 15N D	354.88	(1S,3S,5S)-2-[(2S)-2-Amino-2-(3- hydroxytricyclo[3.3.1.1 ^{3,7}]dec-1-yl)acetyl]- 2-azabicyclo[3.1.0]hexane-3-carbonitrile- 15N,D2 Hydrochloride; BMS 477118- 15N,D2 Hydrochloride; BMS 477118-11- 15N,D2 Hydrochloride; Onglyza-15N,D2 Hydrochloride
(+)-cis-Sertraline D3 HCl	deuteriumlabeledcom	1217741-83-7	C ₁₇ H ₁₅ Cl ₃ N ₃	345.71	4-(3,4-Dichlorophenyl)-1,2,3,4-tetrahydro- N-methyl-1-naphthalenamine-d ₃ Hydrochloride
Abiraterone D4	deuteriumlabeledcom	NA	C ₂₄ H ₂₇ D ₄ NO	353.53	(3 β)-17-(3-Pyridinyl)androsta-5,16-dien- 3-ol-d ₄ ; CB 7598-d ₄
Losartan Carboxylic Acid D4	deuteriumlabeledcom	1246820-62-1	C ₂₂ H ₁₇ ClN ₆ O ₂ D4	440.89	2-Butyl-4-chloro-1-[[2'-(1H-tetrazol-5- yl)[1,1'-biphenyl]-4-yl)methyl]-1H- imidazole-5-carboxylic Acid-d ₄ ; EXP 3174- d ₄

name	category	cas_number	mol_formula	mol_weight	synonym
Miglitol D4 HCl	deuteriumlabeledcom	1346597-27-0	C8H13NO5D4.HCl	247.71	2R,3R,4R,5S)-1-(2-Hydroxyethyl-d4)-2-(hydroxymethyl)-3,4,5-piperidinetriol Hydrochloride; [2R-(2 α ,3 β ,4 α ,5 β)]-1-(2-Hydroxyethyl-d4)-2-(hydroxymethyl)-3,4,5-piperidinetriol Hydrochloride; BAY 1099-d4; BAY-m 1099-d4; Diastabol-d4; Glyset-d4; N-(2-Hydroxyethyl-d4)-1-deoxynojirimycin Hydrochloride; N-(2-Hydroxyethyl-4)moranoline Hydrochloride; Seibule-d4 Hydrochloride
Clozapine D4	deuteriumlabeledcom	204395-52-8	C18H15ClN4 D4	330.85	8-Chloro-11-(4-methyl-1-piperazinyl-2,2,6,6-d4)-5H-dibenzo[b,e][1,4]diazepine
Loperamide D6 HCL	deuteriumlabeledcom	1189574-93-3	C29H27D6ClN2O2.H	519.54	4-(4-Chlorophenyl)-4-hydroxy-N,N-(dimethyl-d6)- α , α -diphenyl-1-piperidinebutanamide Hydrochloride; Arret-d6; Blox-d6; Brek-d6; Dissenten-d6; Fortasec-d6; Imodium-d6; Imodium A-D-d6; Imosec-d6; Imosel-d6; Lopemid-d6; Lopemin-d6; Loperazine-d6; Loperyl-d6;

name	category	cas_number	mol_formula	mol_weight	synonym
Tamsulosin D4	deuteriumlabeledcom	1231943-97-7	C20H24D4N2O5S	412.54	[2-[[2-(Ethoxyphenoxy)ethyl]amino]propyl-d4]-2- methoxybenzenesulfonamide Hydrochloride; Omnic-d4; Pradif-d4; ; Yutanal-d4
Lenalidomide 13C5	deuteriumlabeledcom	1219332-91-8	C813C5H13N3O3	264.22	3-(4-Amino-1,3-dihydro-1-oxo-2H- isoindol-2-yl)-2,6-piperidinedione-13C5; 1-Oxo-2-(2,6-dioxopiperidin-3-yl)-4- aminoisoindoline-13C5; CC-5013-13C5
Rivaroxaban D4	deuteriumlabeledcom	1132681-38-9	C19H14D4CIN3O5S	439.91	5-Chloro-N-[[[(5S)-2-oxo-3-[4-(3-oxo-4- morpholinyl)phenyl-d4]-5- oxazolidinyl]methyl]-2- thiophenecarboxamide
Lopinavir D8	deuteriumlabeledcom	1322625-54-6	C37H40N4O5D8	636.87	(α S)-N-[(1S,3S,4S)-4-[[2-(2,6- Dimethylphenoxy)acetyl]amino]-3- hydroxy-5-phenyl-1- (phenylmethyl)pentyl]tetrahydro- α -(1- methylethyl)-2-oxo-1(2H)- pyrimidineacetamide- d8; A 157378.0-d8; ABT 378-d8; Aluviran-d8; Koletra-d8

name	category	cas_number	mol_formula	mol_weight	synonym
Lurasidone d8 HCl	deuteriumlabeledcom	NA	C28H29D8CIN4O2S	537.19	(3aR,4S,7R,7aS)-2-[[[(1R,2R)-2-[[4-(1,2-Benzisothiazol-3-yl)-1-piperazinyl]methyl]cyclohexyl]methyl]hexahydro-4,7-methano-1H-isoindole-1,3(2H)-dione-d8 Hydrochloride; Latuda-d8
Mosapride D5	deuteriumlabeledcom	1246820-66-5	C21H20CIFN3O3 D5	426.92	4-Amino-5-chloro-2-(ethoxy-d5)-N-[[4-(4-fluorophenyl)methyl]-2-morpholinyl]methyl]benzamide; Mosapid-d5; Mosid-MT-d5; Moza-d5
Nortriptyline D3 HCl	deuteriumlabeledcom	203784-52-5	C19H18D3N.HCl	302.86	3-(10,11-Dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)-N-(methyl-d3)-1-propanamine Hydrochloride; Acetexa-d3; Allegron-d3; Nortrilen-d3; Norzepine-d3; Pamelor-d3; Sensival-d3; Vividyl-d3
Amitriptyline-D6 Hcl	deuteriumlabeledcom	203645-63-0	C20H18D6CIN	319.91	3-(10,11-Dihydro-5H-dibenzo[a,d]cyclohepten-5-ylidene)-N,N-dimethyl-1-propanamine-d6 Hydrochloride; Adepril-d6; Amineurin-d6; Domical-d6; Elavil-d6; Endep-d6; Euplit-d6; Laroxyl-d6; Tryptanol-d6; Tryptizol-d6

name	category	cas_number	mol_formula	mol_weight	synonym
Posaconazole D5	deuteriumlabeledcom	NA	C37H37D5F2N8O4	705.81	2,5-Anhydro-1,3,4-trideoxy-2-C-(2,4-difluorophenyl)-4-[[4-[4-[4-[1-[(1S,2S)-1-ethyl-2-hydroxypropyl]-1,5-dihydro-5-oxo-4H-1,2,4-triazol-4-yl]phenyl]-1-piperazinyl]phenoxy]methyl]-1-(1H-1,2,4-triazol-1-yl)-D-threo-pentitol-d5;
Melphalan HCl D8	deuteriumlabeledcom	1217854-43-7	C13H10D8Cl2N2O2	349.71	4-[Bis(2-chloroethyl)amino]-L-phenylalanine-d8 Dihydrochloride; p-Di-(2-chloroethyl)amino-L-phenylalanine-d8 Dihydrochloride; L-Phenylalanine Mustard-d8 Dihydrochloride; Melfalan-d8 Dihydrochloride
Albendazole sulfoxide D3	deuteriumlabeledcom	NA	C12H12N3O3S D3	284.33	Albendazole Oxide-d3; Albendazole Impurity B (EP)-d3
Bezafibrate D6	deuteriumlabeledcom	1219802-74-0	C19H14D6ClNO4	367.87	2-{4-[2-(4-Chlorobenzamido-d6)ethyl]phenoxy}-2-methylpropanoic Acid

name	category	cas_number	mol_formula	mol_weight	synonym
Perphenazine D4	deuteriumlabeledcom	NA	C21H22ClN3OSD4	407.99	4-[3-(2-Chloro-10H-phenothiazin-10-yl)propyl]-1-(piperazine-d4)ethanol Dihydrochloride; 1-(2-Hydroxyethyl)-4-[3-(2-chloro-10-phenothiazinyl)propyl]piperazine-d4-Dihydrochloride; Chloriprozine-d4
Rac-O-Desvenlafaxine-D6 Succinate Hydrate	deuteriumlabeledcom	NA	C20H27NO7D6	405.52	4-[2-(Dimethylamino)-1-(1-hydroxycyclohexyl)ethyl]-phenol Hydrochloride D6;
Methotrexate13CD3	deuteriumlabeledcom	59-05-2 unlabeled	C1913CH19D3N8O5	458.45	N-[4-[[2,4-Diamino-6-pteridiny]methyl]methylamino-13Cd3]benzoyl]-L-glutamic Acid; (+)-Amethopterin; 4-Amino-N10-methylpteroylglutamic Acid-13Cd3; 4-Amino-N10-methylfolic Acid-13Cd3
25-Hydroxyvitamin D3-d6	deuteriumlabeledcom	NA	C27H38D6O2	406.67	(3β,5Z,7E)- 3-(Hydrogen Butanedioate)-9,10-Secocholesta-5,7,10(19)-triene-3,25-diol-13C4; 25-Hydroxycholecalciferol-3-hemisuccinate D3 D6

name	category	cas_number	mol_formula	mol_weight	synonym
Loratadine D5	deuteriumlabeledcom	1020719-57-6	C22H18D5ClN2O2	387.92	4-(8-chloro-5,6-dihydro-11H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-ylidene-2,3,4,5,5-d5)-1-piperidinecarboxylic Acid Ethyl Ester; Claritin-d5; Sch-29851-d5
2-Pyridylacetic acid D4 HCl	deuteriumlabeledcom	NA	C7H3NO2D4 HCl	177.62	2-Pyridineacetic Acid-d6 Hydrochloride; 2-(Pyridin-2-yl)acetic Acid-d4 Hydrochloride;
Emtricitabine 15N D2	deuteriumlabeledcom	NA	C8H8N2O3SF15ND2	250.25	4-Amino-5-fluoro-1-[(2R,5S)-2-hydroxymethyl)-1,3-oxathiolan-5-yl]-2-(1H-pyrimidinone-d2,15N2; (-)-2',3'-Dideoxy-5-fluoro-3'-thiacytidine-d2,15N2; (-)-2'-Deoxy-5-fluoro-3'-thiacytidine-d2,15N2; BW 1592-d2,15N2; BW 524W91-d2,15N2; Coviracil-d2,15N2; Emtriva-d2,15N2; (-)-FTC-d2,15N2
Etoricoxib D4	deuteriumlabeledcom	NA	C18H11D4ClN2O2S	362.87	Chloro-6'-methyl-3-[4-(methylsulfonyl)phenyl]-2,3'-bipyridine-d4; Algix-d4; Arcoxia-d4

name	category	cas_number	mol_formula	mol_weight	synonym
Diphenhydramine D5HCl	deuteriumlabeledcom	1219795-16-0	C17H16NOD5.HCl	296.85	2-(Diphenylmethoxy)-N,N-dimethylethanamine-d5 Hydrochloride; 2-(Benzhydryloxy)-N,N-dimethylethylamine-d5 Hydrochloride
Desmopressin D5	deuteriumlabeledcom	16679-58-6 unlabeled	C46H59D5N14O12S	1074.24	1-(3-Mercaptopropanoic Acid)-8-d-arginine Vasopressin-d5; 8-d-Arginine-1-(3-mercapto-propanoic Acid)vasopressin-d5; Adiuretin SD-d5; DDAVP-d5; Desmospray-d5; Minirin-d5; Octim-d5; Octostim-d5; Presinex-d5; Stimat-d5
Hydroxy Itraconazole d8	deuteriumlabeledcom	1217516-26-1	C35H30D8Cl2N8O5	729.68	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-d8)-3H-1,2,4-triazol-3-one; R 63373-d8
Vilazodone D8 HCl	deuteriumlabeledcom	NA	C26H20D8N5O2Cl	486.04	5-[4-[4-(5-Cyano-1H-indol-3-yl)butyl]-1-(piperazinyl-d8)]-2-benzofurancarboxamide-d8; EMD 515259-d8

name	category	cas_number	mol_formula	mol_weight	synonym
Descarboxyethoxy Loratadine D5	deuteriumlabeledcom	NA	C19H14D5ClN2	315.85	8-Chloro-6,11-dihydro-11-(4-piperidinylidene)-5H-benzo[5,6]cyclohepta[1,2-b]pyridine-d5; Aerius-d5; Allelex-d5
Darunavir D9	deuteriumlabeledcom	1133378-37-6	C27H28D9N3O7S	556.72	[(1S,2R)-3-[[[4-Aminophenyl)sulfonyl](2-methylpropyl-d9)amino]-2-hydroxy-1-(phenyl-methyl)propyl]carabamic Acid (3R,3aS,6aR)-Hexahydrofuro[2,3-b]-furan-3-yl Ester; TMC-114-d9; UIC-94017-d9
Itraconazole D5	deuteriumlabeledcom	1217510-38-7	C35H33D5Cl2N8O4	710.66	(+/-)-4-[4-[4-[4-[[[(2R,4S)-(2,4-Dichlorophenyl)-2-(1H-1,2,4-triazol-1-yl)methyl]-1,3-dioxolan-4-yl]methoxy]phenyl]-1-piperazinyl]phenyl]-2,4-dihydro-2-(1-methylpropyl-d5)-3H-1,2,4-triazol-3-one; Itrizole-d5; Oriconazole-d5; R-51211-d5; Sporamelt-d5; Sporanox-d5; Triasporin-d5

name	category	cas_number	mol_formula	mol_weight	synonym
Fluconazole D4	deuteriumlabeledcom	1124197-58-5	C13H8D4F2N6O	310.30	α -(2,4-Difluorophenyl)- α -(1H-1,2,4-triazol-1-ylmethyl)-1H-1,2,4-triazol-1-ethanol-d4; 1-(2,4-Difluorophenyl)-1,1-bis[(1H-1,2,4-triazol-1-yl)methyl]methanol-d4; Biozolene-d4; Diflucan-d4; Difluconazole-d4; Elazor-d4; Fluconal-d4; Flucostat-d4; Flumycon-d4; Flunazol-d4; Flusol-d4; Fluzon-d4; Triflucan-d4; UK 49858-d4; Zoltec-d4
Voriconazole D3	deuteriumlabeledcom	1217661-14-7	C16H11D3F3N5O	352.33	(α R, β S)- α -(2,4-Difluorophenyl)-5-fluoro- β -(methyl-d3)- α -(1H-1,2,4-triazol-1-ylmethyl)-4-pyrimidineethanol; DRG 0301; UK-109496-d3; VRC-d3; Vfend-d3; Voriconazol-d3;
Venlafaxine D10	deuteriumlabeledcom	1216539-56-8	C17H17D10NO2.H Cl	287.46	1-[2-(Dimethyloxidoamino)-1-(4-methoxyphenyl)ethyl]cyclohexanol-d10
17-beta - Dihydroequilin D4	deuteriumlabeledcom	NA	C18H18D4O2	274.39	(17 β)-Estra-1,3,5(10),7-tetraene-3,17-diol D4; Estra-1,3,5(10),7-tetraene-3,17 β -diol D4; 7-Dehydroestradiol D4;

name	category	cas_number	mol_formula	mol_weight	synonym
Sodium equilin D4 sulphate	deuteriumlabeledcom	NA	C18H15D4NaO5S	374.42	3-(Sulfooxy)estra-1,3,5(10),7-tetraen-17-one-d4 Sodium Salt; t; 3-Hydroxyestra-1,3,5(10),7-tetraen-17-one-d4 Hydrogen Sulfate Sodium Salt; Sodium Equilin-d4 3-Monosulfate;
Delta 17 beta 8,9 dihydroestradiol D3	deuteriumlabeledcom	NA	C18H19D3O2	273.39	(O-Carboxymethyl)oximinoestradiol D3
Beclomethasone 17 mono propionate D5	deuteriumlabeledcom	NA	C25H28D5ClO6	470.01	(11 β ,16 β)-9-Chloro-11,17,21-trihydroxy-16-methylpregna-1,4-diene-3,20-dione-d5; 9 α -Chloro-16 β -methylprednisolone-d5; Beclometasone-d5; Becolvent-d5;
Mifepristone D6	deuteriumlabeledcom	84371-65-3 unlabeled	C29H29NO2D6	435.59	11 β ,17 β)-11-[4-(Dimethylamino-d6)phenyl]-17-hydroxy-17-(1-propyn-1-yl)estra-4,9-dien-3-one; RU-486-d6;
Tiagabine D6	deuteriumlabeledcom	NA	C20H21NO2S2D6 H	420.07	3R)-1-[4,4-Bis(3-(methyl-d3)-2-thienyl)-3-butenyl]-3-piperidinecarboxylic Acid Hydrochloride; Gabitril-d6;

name	category	cas_number	mol_formula	mol_weight	synonym
Norfloxacin D5 HCl	deuteriumlabeledcom	1015856-57-1	C16H11D5F3NO · H	336.80	1-Ethyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylic Acid-d5; Baccidal-d5; Barazan-d5; Chibroxine-d5; N-Demethylpefloxacin-d5; N-Desmethylpefloxacin-d5; MK-366-d5; Norxacin-d5; Sebercim-d5; Zoroxin-d5;
Clomipramine D3	deuteriumlabeledcom	NA	C19H21Cl2N2D3	354.34	3-Chloro-10,11-dihydro-N,N-(dimethyl-d3)-5H-dibenz[b,f]azepine-5-propanamine Hydrochloride; 3-Chloro-5-[3-(dimethylamino-d3)propyl]-10,11-dihydro-5H-dibenz[b,f]azepine Hydrochloride
Glyburide D3	deuteriumlabeledcompounds		C23H25ClN3O5SD3	497.02	5-Chloro-N-[2-[4-[[[(cyclohexylamino-d11)carbonyl]amino]sulfonyl]phenyl]ethyl]-2-methoxybenzamide; 1-[4-[2-(5-Chloro-2-methoxybenzamido)ethyl]phenylsulfonyl]-3-(cyclohexyl-d3)urea; N-[4-(β-(2-Methoxy-5-chlorobenzamido)ethyl)benzosulfonyl]-N'-(cyclohexyl-d3)urea;

name	category	cas_number	mol_formula	mol_weight	synonym
Piribedil D8	deuteriumlabeledcom	1398044-45-5	C16H10D8N4O2	306.19	2-[4-(1,3-Benzodioxol-5-ylmethyl)-1-piperazinyl]pyrimidine-d8; 2-(4-Piperonyl-1-piperazinyl)pyrimidine-d8; 1-(2-Pyrimidyl)-4-(3,4-methylenedioxybenzyl)piperazine-d8; 1-(2-Pyrimidyl)-4-piperonylpiperazine-d8; 4-[3,4-(Methylenedioxy)benzyl]-1-(2-pyrimidinyl)piperazine-d8; ET 495-d8; EU 4200-d8; Piribedil-d8; Trivastal-d8; Trivastan-d8;
Cefixime 13 C 15N2	deuteriumlabeledcom	NA	C1513CH15N315N2	456.43	(6R,7R)-7-[[[(2Z)-2-(2-Amino-4-thiazolyl-13C,15N2)-2-[(carboxymethoxy)imino]acetyl]amino]-3-ethenyl-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic Acid; FK-027-13C,15N2; FR- 17027-13C,15N2; CL-284635-13C,15N2; Cefixoral-13C,15N2; Cefspan-13C,15N2; Cephoral-13C,15N2; Unixime-13C,15N2;

name	category	cas_number	mol_formula	mol_weight	synonym
Azelnidipine D7	deuteriumlabeledcom	NA	C33H27D7N4O6	589.69	(±)-2-Amino-1,4-dihydro-6-methyl-4-(3-nitrophenyl)-3,5-pyridinedicarboxylic Acid 3-[1-(Diphenylmethyl)-3-azetidiny] 5-(1-methylethyl) Ester-d7; Azelnidipine-d7; CS 905-d7; Calblock 3-[1-(Diphenylmethyl)-3-azetidiny] 5-isopropyl-d7 (±)-2-Amino-1,4-dihydro-6-methyl-4-(m-nitrophenyl)-3,5-pyridinedicarboxylate;
Midodrine D6 HCl	deuteriumlabeledcom	1188265-43-1	C12H12D6N2O4 · H	296.78	ST-1085-d6, Amatine-d6, Gutron-d6, Hipertan-d6, Metligine-d6, ProAmatine-d6,
Ketoprofen D3	deuteriumlabeledcom	159490-55-8	C16H11D3O3	257.30	3-Benzoyl- α -methyl-d3-benzeneacetic Acid; m-Benzoylhydratropic-d3 Acid; 2-(3-Benzoylphenyl)propionic-d3 Acid; RP-19583-d3; Alreumat-d3; Alrheumun-d3; Capisten-d3; Epatec-d3; Fastum-d3; Ketofen-d3; Menamin-d3; Toprec-d3

name	category	cas_number	mol_formula	mol_weight	synonym
Calcitriol D6	deuteriumlabeledcom	78782-99-7	C27H38O3D6	422.67	(1R,3S,5Z)-4-Methylene-5-[(2E)-2- [(1R,3aS,7aS)-octahydro-1-[(1R)-5- hydroxy-1,5-dimethylhexyl]-7a-methyl-4H- inden-4-ylidene]ethylidene]-1,3- cyclohexanediol-d6; (1 α ,3 β ,5Z,7E)- 9,10- Secocholesta-5,7,10(19)-triene-1,3,25- triol-d6; 1 α ,25-Dihydroxycholecalciferol- d6; 1 α ,25-Dihydroxyvitamin D3-d6; Calcijex-d6; Dihydroxyvitamin D3-d6; Panbonis-d6; Ro 21-5535-d6; Rocaltrol-d6; Silkis-d6; Solbone P-d6; Soltriol-d6; Topitriol-d6; Toptriol-d6;
Doxercalciferol D6	deuteriumlabeledcom	NA	C28H38D6O3	434.68	1 α ,3 β ,5Z,7E,22E)- 9,10-Secoergosta- 5,7,10(19),22-tetraene-1,3-diol-d6; 1- Hydroxyergocalciferol-d6
N desmethyl citalopram hydrochloride D4	deuteriumlabeledcom	NA	C19H16D4N2OCIF	350.85	1-(4-Fluoro-phenyl)-1-[3-(methyl- d4)amino-propyl]-1,3-dihydro - isobenzofuran-5-carbonitrile Hydrochloride; 1-[3-(Methylamino- d4)propyl]-1-(4-fluorophenyl)-1,3- dihydroisobenzofuran-5-carbonitrile;

name	category	cas_number	mol_formula	mol_weight	synonym
Olsalazine D3	deuteriumlabeledcom	NA	C14H7D3N2O6	305.24	3,3'-(1,2-Diazenediyl)bis[6-hydroxybenzoic Acid-D3 Sodium Salt; 3,3'-Azobis(6-hydroxybenzoic Acid)-D3 Sodium Salt; Azodisal Sodium-D3; Disodium Azodisalicylate-D3
Nepafenac D5	deuteriumlabeledcom	1246814-53-8	C15H9D5N2O2	259.31	2-Amino-3-benzoylbenzeneacetamide-d5; AHR 9434-d5; AL 6515-d5; Nevanac-d5;
Desethoxy hydroxy ticagrelor D7	deuteriumlabeledcom	NA	C21H17D7F2N6O3S	485.56	AR-C 124910XX-d7;
Prochlorperazine dimaleate D8	deuteriumlabeledcom	1215641-01-2	C28H24D8CIN3O8S	614.14	Buccastem-d8; Compazine-d8; Emetiral-d8; Meterazin-d8 Maleate; Pasotomin-d8; Prochlorperazine-d8 Hydrogen Maleate; Prochloroperazine-d8 Dimaleate; Prochlorperazine-d8 Maleate; Stemetil-d8; Stemetil-d8 Dimaleate; Vertigon-d8
Amfenac D5	deuteriumlabeledcom	NA	C15H7D5NNaO3	282.29	2-Amino-3-(benzoyl-d5)benzeneacetic Acid Sodium Salt Hydrate; [2-Amino-3-(benzoyl-d5)phenyl]acetic Acid

name	category	cas_number	mol_formula	mol_weight	synonym
Beclomethasone dipropionate D10	deuteriumlabeledcom	NA	C28H27D10ClO7	531.10	9 α -Chloro-16 β -methylprednisolone 17,21-Dipropionate-d10; Aerobec-d10; Aldecin-d10; Beclometasone Dipropionate-d10; Beclotide-d10; Clenil A-d10; Entyderma-d10; QVAR-d10; Sanasthmax-d10; Viarox-d10, Ventolair-d10
Ranitidine D6 HCL	deuteriumlabeledcom	1185514-83-3	C13H16D6N4O3S · H	356.90	Label-d6; Midaven-d6; Ulcerit-d6; Zenetac-d6; N-[2-[[[5-[(Dimethyl-d6-amino)methyl]-2-furanyl)methyl]thio]ethyl]-N'-methyl-2-nitro-1,1-ethenediamine
Levomefolate D4	deuteriumlabeledcompounds		C20H21N7O6D4	463.49	N-[4-[[[(6S)-2-Amino-3,4,5,6,7,8-hexahydro-5-methyl-4-oxo-6-pteridiny]methyl]amino]benzoyl]-L-glutamic-D4 Acid Calcium Salt; N-[4-[[[(2-Amino-1,4,5,6,7,8-hexahydro-5-methyl-4-oxo-6-pteridiny]methyl]amino]benzoyl]-L-glutamic-D4 Acid Calcium Salt

name	category	cas_number	mol_formula	mol_weight	synonym
4 hydroxy methyl ambrisentan D10	deuteriumlabeledcom	1261393-98-9	C22H12N2O5D10	404.42	α -[[4-(Hydroxymethyl)-6-(methyl-d10)-2-pyrimidinyl]oxy]- β -methoxy- β -phenylbenzenepropanoic Acid;
GS331007 Sofosbuvir metabolite 13CD3	deuteriumlabeledcom	1256490-42-2	C9H10FN2O513CD3	264.23	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)(phenoxy)phosphoryl)amino)propanoic Acid 13CD3
Sofosbuvir D6	deuteriumlabeledcom	1190307-88-0 unlabeled	C22H23D6FN3O9P	535.49	(2S)-Isopropyl 2-((((2R,3R,4R,5R)-5-(2,4-Dioxo-3,4-dihydropyrimidin-1(2H)-yl)-4-fluoro-3-hydroxy-4-methyltetrahydrofuran-2-yl)methoxy)(phenoxy)phosphoryl)amino)propanoate D6; N-[[P(R),2'R]-2'-Deoxy-2'-fluoro-2'-methyl-P-phenyl-5'-uridylyl]-L-alanine 1-Methylethyl Ester D6
Nor verapamil hydrochloride D7	deuteriumlabeledcom	1216413-74-9	C26H29D7N2O4 · H	484.08	α -[3-[[2-(3,4-Dimethoxyphenyl)ethyl]amino]propyl]-3,4-dimethoxy- α -(1-methylethyl)-benzeneacetonitrile-d7;

name	category	cas_number	mol_formula	mol_weight	synonym
Bortezomib D8	deuteriumlabeledcom	NA	C19H17D8BN4O4	392.29	Velcade-D8, [(1R)-3-Methyl-1-[[[(2S)-1-oxo-3-phenyl-2-[(pyrazinylcarbonyl)amino]propyl]amino]butyl]-boronic Acid-D8
melatonin D4	deuteriumlabeledcom	66521-38-8	C13H12D4N2O2	236.30	N-[2-(5-Methoxy-1H-indol-3-yl)ethyl]acetamide-d4; 5-Methoxy-N-acetyltryptamine-d4; Circadin-d4; Melatol-d4; Melatonine-d4; Melovine-d4; N-Acetyl-5-methoxytryptamine-d4; N-[2-(5-Methoxyindol-3-yl)ethyl]acetamide-d4; NSC 113928-d4; NSC 56423-d4; Regulind4
Sulfadiazine D4	deuteriumlabeledcom	1020719-78-1	C10H6D4N4O2S	254.28	4-Amino-N-2-pyrimidinylbenzenesulfonamide-d4; 2-(4-Aminobenzenesulfonamido-d4)pyrimidine; 2-Sulfanilylaminopyrimidine-d4; Adiazind4; Adiazine-d4; Debenal-d4; Liquadiazine-d4; Microsulfon-d4; Sulfazine-d4; Sulfolex-d4; Sulphadiazine-d4; Theradiazine-d4;

name	category	cas_number	mol_formula	mol_weight	synonym
Perfenazine D8	deuteriumlabeledcom	NA	C ₂₁ H ₂₀ D ₈ Cl ₃ N ₃ OS	484.94	4-[3-(2-Chloro-10H-phenothiazin-10-yl)propyl]-1-(piperazine-d8)ethanol Dihydrochloride; 1-(2-Hydroxyethyl)-4-[3-(2-chloro-10-phenothiazinyl)propyl]piperazine-d8-Dihydrochloride; Chloriprozine-d8; Chlorperphenazine-d8; Decentan-d8
Regorafenib 13CD3	deuteriumlabeledcom	NA	C ₂₀ H ₁₃ ClF ₄ N ₃ O ₃	486.83	4-[4-[[[4-Chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]-3-fluorophenoxy]-N-(methyl-13C ₃)-2-pyridinecarboxamide
N desmethyl ivabradine hydrochloride D6	deuteriumlabeledcom	NA	C ₂₆ H ₂₉ D ₆ ClN ₂ O ₅	497.06	3-[3-[[[(7S)-3,4-Dimethoxybicyclo[4.2.0]octa-1,3,5-trien-7-yl]methyl]methylamino-d6]propyl]-1,3,4,5-tetrahydro-7,8-dimethoxy-2H-3-benzazepin-2-one Hydrochloride; Corlantor-d6
Amisulpride D5	deuteriumlabeledcom	1216626-17-3	C ₁₇ H ₂₇ N ₃ O ₄ S	374.51	4-Amino-N-[(1-ethyl-2-pyrrolidinyl)methyl]-5-(ethylsulfonyl)-2-methoxybenzamide-d5; Aminosultopride-d5; DAN-2163-d5; Socian-d5; Solian-d5; Sulamid-d5;

name	category	cas_number	mol_formula	mol_weight	synonym
Oxaprozin D4	deuteriumlabeledcom	21256-18-8 unlabeled	C18H11D4NO3	297.34	4,5-Diphenyl-d4-2-oxazolepropanoic Acid; 4,5-Diphenyl-d4-2-oxazolepropionic Acid; 3-(4,5-Diphenyl-d4-oxazol-2-yl)propionic Acid; Actirin-d4;
Diethyl 1,1,1 1 D4 Stilbestrol D4	deuteriumlabeledcom	NA	C18D8H12O2	276.40	4'[(1E)-1,2-Diethyl-1,2- ethenediyl]bisphenol-d4; Stilbestrol-d4; Stilboestrol-d4;
Sulfamethoxazole D4	deuteriumlabeledcom	1020719-86-1	C10H7D4N3O3S	257.30	4-Amino-N-(5-methyl-3- isoxazolyl)(benzene-d4)sulfonamide; 3-(p- Amino(benzene-d4)sulfonamido)-5- methylisoxazole; Sulfamethoxazole-d4; 3- Sulfanilamido-5-methylisoxazole-d4; 5- Methyl-3-sulfanilamidoisoxazole-d4; Gantanol-d4; MS 53-d4; Radonil-d4; Ro 4- 2130-d4; STX 608-d4; Sinomin-d4
Linezolid D3	deuteriumlabeledcom	1127120-38-0	C16H17D3FN3O4	340.36	N-[[[(5S)-3-[3-Fluoro-4-(4- morpholinyl)phenyl]-2-oxo-5- oxazolidinyl]methyl]- acetamide-d3; Linospan-d3; Linox-d3; PNU 100766-d3; U 100766-d3; Zyvox-d3; Zyvoxid-d3;

name	category	cas_number	mol_formula	mol_weight	synonym
Gefitinib D8	deuteriumlabeledcom	857091-32-8	C22H16D8ClFN4O3	454.95	N-(3-Chloro-4-fluorophenyl)-7-(methoxy-d8)-6-[3-(4-morpholinyl)propoxy]-4-quinazolinamine; Iressa-d8;
Verapamil hydrochloride D7 not in solid form	deuteriumlabeledcom	1188265-55-5	C27H31D7N2O4 · H	498.11	α -[3-[[2-(3,4-Dimethoxyphenyl)ethyl]methylamino]propyl]-3,4-dimethoxy- α -(1-methylethyl-d7)-benzeneacetonitrile Hydrochloride; Berkatens-d7; Calan-d7; Cardibeltin-d7; Dignover-d7; Isoptin-d7; Veracim-d7; Veramex-d7; Zolvera-d7;
Trimethoprim D3	deuteriumlabeledcom	1189923-38-3	C14H15D3N4O3	293.34	5-[(3,4,5-Trimethoxy-d3-phenyl)methyl]-2,4-pyrimidinediamine; 2,4-Diamino-5-(3',4',5'-trimethoxy-d3-benzyl)pyrimidine; Instalac-d3; Monotrim-d3; Proloprim-d3; Syraprim-d3; Tiempe-d3; Trimanyl-d3; Uretrim-d3; Wellcoprim-d3;

name	category	cas_number	mol_formula	mol_weight	synonym
Esomeprazole K+ D3	deuteriumlabeledcom	NA	C17H15D3KN3O3S	386.52	6-(Methoxy-d3)-2-[(S)-[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole Sodium Salt; (-)-Omeprazole-d3 Sodium Salt; (S)-(-)-Omeprazole-d3 Sodium Salt; (S)-5-(Methoxy-d3)-2-[[4-methoxy-3,5-dimethyl-2-pyridyl)methyl]sulfinyl]-1H-benzimidazole Sodium Salt; (S)-Esomeprazole-d3 Sodium Salt; (S)-Omeprazole-d3 Sodium Salt; Escz-d3 Sodium Salt; Esofag-d3 Sodium Salt; IZRA 40-d3 Sodium Salt; Nexiam-d3 Sodium Salt;

name	category	cas_number	mol_formula	mol_weight	synonym
Avanafil 13C5N15D2	deuteriumlabeledcom	NA	C1813C5H24D2CIN6	491.92	(S)-2-(2-Hydroxymethyl-1-pyrrolidinyl)-4-(3-chloro-4-methoxybenzylamino)-5-[(2-pyrimidinylmethyl)carbamoyl]pyrimidine-13C5,15N; 4-[[[(3-Chloro-4-methoxyphenyl)methyl] amino]-2-[(2S)-2-(hydroxymethyl)-1-pyrrolidinyl]-N-(2-pyrimidinylmethyl)-5-pyrimidinecarboxamide-13C5D2,15N; TA 1790-13C5D2,15N;
Dabigatran D4	deuteriumlabeledcom	NA	C25H21D4N7O3	475.51	N-[[2-[[[4-(Aminoiminomethyl)phenyl]amino]methyl]-1-(methyl-d4)-1H-benzimidazol-5-yl]carbonyl]-N-2-pyridinyl-β-alanine; BIBR 953-d4; BIBR 953ZW-d4;

name	category	cas_number	mol_formula	mol_weight	synonym
Tetrabenazine D6	deuteriumlabeledcom	1392826-25-3	C19H21D6NO3	323.24	(3R,11bR)-rel-1,3,4,6,7,11b-Hexahydro-9,10-dimethoxy-3-(2-methylpropyl)-2H-benzo[a]quinolizin-2-one-d6; cis-2-Oxo-3-(isobutyl)-9,10-dimethoxy-1,2,3,4,6,7-hexahydro -11bH-benzo[a]quinolizine-d6; (+/-)-Tetrabenazine-d6; NSC 169886-d6; NSC 172187-d6; Ro 1-9569-d6; Rubigen-d6
Chlorpromazine D6	deuteriumlabeledcom	1228182-46-4	C17H14D6Cl2N2S	361.36	2-Chloro-N,N-(dimethyl-d6)-10H-phenothiazine-10-propanamine Hydrochloride; 2-Chloro-10-[3-(dimethylamino-d6)propyl]phenothiazine Hydrochloride; Klorproman-d6; Marazine-d6; Norcozine-d6; Torazina-d6; Tranzene-d6
N desmethyl enzalutamide D6	deuteriumlabeledcom	NA	C21H10D6F4N4O2S	470.47	4-[3-[4-Cyano-3-(trifluoromethyl)phenyl]-5,5-dimethyl-4-oxo-2-thioxo-1-imidazolidinyl]-2-fluorobenzamide-d6

name	category	cas_number	mol_formula	mol_weight	synonym
N desmethyl clomipramine D3 HCl	deuteriumlabeledcom	1189971-04-7	C18H19D3Cl2N2	340.29	3-Chloro-10,11-dihydro-N-(methyl-d3)-5H-dibenz[b,f]azepine-5-propanamine Hydrochloride; Clordesipramine-d3 Hydrochloride; Demethylchlorimipramine-d3 Hydrochloride; Norchlorimipramine-d3 Hydrochloride; Norclomipramine-d3 Hydrochloride
Monomethyl fumarate D3	deuteriumlabeledcom	NA	C5H3D3O4	133.12	(2E)-2-Butenedioic Acid 1-Methyl Ester-d3; (E)-2-Butenedioic Acid Monomethyl Ester-d3; Fumaric Acid Methyl Ester-d3; Methyl Hydrogen Fumarate-d3
Boceprevir D9	deuteriumlabeledcom	1256751-11-7	C27H36D9N5O5	528.73	(1R,2S,5S)-N-[3-Amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[[2S)-2-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]-6,6-dimethyl-3-azabicyclo[3.1.0]hexane-2-carboxamide; EBP 520; Sch 503034;
Sirolimus 13CD3	deuteriumlabeledcom	53123-88-9 unlabeled	C5013CH76D3NO13	918.18	(-)-Rapamycin-d3; AY 22989-d3; Antibiotic AY 22989-d3; Cypher-d3; NSC 226080-d3; RAPA-d3;

name	category	cas_number	mol_formula	mol_weight	synonym
Apixaban 13CD3	deuteriumlabeledcom	1261393-15-0	C2413CH22D3N5O4	463.51	4,5,6,7-Tetrahydro-1-(4-methoxyphenyl)-7-oxo-6-[4-(2-oxo-1-piperidinyl)phenyl]-1H-pyrazolo[3,4-c]pyridine-3-carboxamide-13C, d3; BMS 562247-01-13C, d3; 1-(4-Methoxyphenyl)-7-oxo-6-[4-(2-oxopiperidin-1-yl)phenyl]-4,5,6,7-tetrahydro-1H-pyrazolo[3,4-c]pyridine-3-carboxylic Acid Amide-13C, d3;
N acetyl dapsone D4	deuteriumlabeledcom	565-20-8 unlabeled	C14H10D4N2O3S	294.36	N-[4-[(4-Aminophenyl)sulfonyl]phenyl]-acetamide-D4; Acetyldapsone-D4; MADDS-D4; Monoacetyldapsone-D4
Raltegravir 13CD3	deuteriumlabeledcom	NA	C20H17FN6O5D3	447.44	N-[(4-Fluorophenyl)methyl]-1,6-dihydro-5-hydroxy-1-methyl-2-[1-methyl-1-[[5-methyl-1,3,4-oxadiazol-2-yl)carbonyl]amino]ethyl]-6-oxo-4-pyrimidinecarboxamide-13Cd3
Baclofen D4	deuteriumlabeledcom	1189938-30-4	C10H8D4ClNO2	217.69	β -(Aminomethyl)-4-chloro-benzenepropanoic Acid-d4; β -(Aminomethyl)-p-chlorohydrocinnamic Acid-d4; β -(4-Chlorophenyl)-GABA-d5; Ba-34647-d4; Baclon-d4; Clofen-d4; Lioresal-d4;

name	category	cas_number	mol_formula	mol_weight	synonym
Axitinib 13CD3	deuteriumlabeledcom	NA	C2113CH15D3N4OS	390.48	N-(Methyl-13Cd3)-2-[[3-[(1E)-2-(2-pyridinyl)ethenyl]-1H-indazol-6-yl]thio]benzamide; AG 013736-13Cd3
Ambrisentan D3	deuteriumlabeledcom	1189479-60-4	C22H19D3N2O4	381.44	α -[(4,6-Dimethyl-2-pyrimidinyl)oxy]- β -(methoxy-d3)- β -phenylbenzenepropanoic Acid; BSF 208075-d3; LU 208075-d3
Acitaminophen D3	deuteriumlabeledcom	60902-28-5	C8H6D3NO2	154.18	N-(4-Hydroxyphenyl)acetamide-d3; N-(4-Hydroxyphenyl)acetamide-2,2,2-d3; 4'-Hydroxyacetanilide-d3; 4-Acetamidophenol-d3; N-Acetyl-4-aminophenol-d3; APAP-d3
O desmethyl geftinib D8	deuteriumlabeledcom	NA	C21H14D8CIFN4O3	440.87	4-[(3-Chloro-4-fluorophenyl)amino]-6-[3-(4-morpholinyl)propoxy]-7-quinazolinol-d6; M523595-d8
Glycopyrronium iodide 13C2D3	deuteriumlabeledcom	873295-32-0 unlabeled	C1813CH25D3NO3	449.33	3-[[2-(4-Chlorophenyl)-2-cyclopentyl-2-hydroxyacetyl]oxy]-1,1-dimethylpyrrolidinium Bromide 13C2D3
21 Beclomethasone propionate D5	deuteriumlabeledcom	NA	C25H28D5ClO6	470.01	(11 β ,16 β)-9-Chloro-11,17-dihydroxy-16-methyl-21-(1-oxopropoxy)-pregna-1,4-diene-3,20-dione-d5; Beclomethasone 21-Monopropionate-d5

name	category	cas_number	mol_formula	mol_weight	synonym
Mirabegron D5	deuteriumlabeledcom	1215807-38-7	C21H19D5N4O2S	401.54	2-Amino-N-[4-[2-[[2-hydroxy-2-phenylethyl]amino]ethyl]phenyl]-4-thiazoleacetamide-d5; 2-(2-Aminothiazol-4-yl)-4'-[2-[(2-hydroxy-2-phenylethyl)amino]ethyl]acetic Acid Anilide-d5
Octreotide D8	deuteriumlabeledcom	NA	C49H58D8N10O10S	1087.34	D-(Phenylalanyl-d8)-L-cysteinyl-L-phenylalanyl-D-tryptophyl -L-lysyl-L-threonyl-N-[(1R,2R)-2-hydroxy-1-(hydroxymethyl)propyl]-L-cysteinamide Cyclic (2-7)-Disulfide di-Trifluoroacetic Acid Salt; SMS 201-995-d8 di-Trifluoroacetic Acid Salt; Sandostatin-d8 di-Trifluoroacetic Acid Salt; Sandostatin LAR-d8 di-Trifluoroacetic Acid Salt;

name	category	cas_number	mol_formula	mol_weight	synonym
Glipizide D11	deuteriumlabeledcom	1189426-07-0	C21H16D11N5O4S	456.60	N-[2-[4[[[(Cyclohexylamino-d11)carbonyl]amino]sulfonyl]phenyl]ethyl]-5-methylpyrazinecarboxamide; 1-(Cyclohexyl-d11)-3-[[p-[2-(5-methylpyrazinecarboxamido) ethyl]phenyl]sulfonyl]urea; Aldiab-d11; Digrin-d11; Dipazide-d11; Glibenese-d11; Glibetin-d11; Glican-d11; Glidiab-d11; Glipid-d11; Glipizid-d11; Gluco-Rite-d11; Glucolip-d11; Glucotrol-d11; Glucozide-d11; Glupitel-d11; Glupizid-d11; Napizide-d11; Ozidia-d11; Semiglynase-d11; Sucrazide-d11; TK 1320-d11;
Erlotinib D6	deuteriumlabeledcom	1189953-78-3	C22H17D6N3O4	399.47	N-(3-Ethynylphenyl)-6,7-bis(2-methoxyethoxy-d6)-4-quinazolinamine Hydrochloride; 6,7-Bis(2-methoxyethoxy-d6)-4-(3-ethynylanilino)quinazoline Hydrochloride; [6,7-Bis(2-methoxyethoxy-d6)quinazolin-4-yl]-(3-ethynylphenyl)amine Hydrochloride;

name	category	cas_number	mol_formula	mol_weight	synonym
Praziquantel D11	deuteriumlabeledcom	1246343-36-1	C19H13N2O2D11	323.48	2-(Cyclohexylcarbonyl)-1,2,3,6,7,11b-hexahydro-4H-(pyrazino-d11)[2,1-a]isoquinolin-4-one; (+/-)-Praziquantel-d11; Azinox-d11; Biltricide-d11; Cesol-d11; Cysticide-d11; Distocide-d11; Droncit-d11; Embay 8440-d11; Prazinon-d11; Pyquidon-d11; Warmnil-d11;
Macitentan D4	deuteriumlabeledcom	1258428-05-5	C19H16D4Br2N6O4S	592.30	N-[5-(4-Bromophenyl)-6-[2-[(5-bromo-2-pyrimidinyl)oxy]ethoxy]-4-pyrimidinyl]-N'-propyl-Sulfamided4; ACT 064992-d4
Enzalutamide carboxylic acid D6	deuteriumlabeledcom	NA	C20H7D6F4N3O3S	457.43	4-[3-[4-Cyano-3-(trifluoromethyl)phenyl]-5,5-dimethyl-4-oxo-2-thioxo-1-imidazolidinyl]-2-fluoro-benzoic Acid D6
Dapagliflozin D5	deuteriumlabeledcom	1204219-80-6	C21H20D5ClO6	413.90	(1S)-1,5-Anhydro-1-C-[4-chloro-3-[(4-ethoxyphenyl)methyl]phenyl]-D-glucitol-D5
Tacrolimus 13CD4	deuteriumlabeledcom	1356841-89-8 unlabeled	C43H13CH65D4NO12	809.57	Prograf-13C,D4; Protopic-13C,D4; TacroBell-13C,D4; Tacrolimus-13C,D4
Alogliptin benzoate 13CD3	deuteriumlabeledcom	NA	C17H18N5O2.C7H5O2	464.50	2-[[6-[(3R)-3-Amino-1-piperidinyl]-3,4-dihydro-3-(methyl-13Cd3)-2,4-dioxo-1(2H)-pyrimidinyl)methyl]benzotrile;

name	category	cas_number	mol_formula	mol_weight	synonym
Riociguat 13CD6	deuteriumlabeledcom	NA	C19H13FN8O2 13C	429.45	[4,6-Diamino-2-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-5-pyrimidinyl]-N-(methyl-d3)carbamic Acid Methyl-13Cd3 Ester; N-[4,6-Diamino-2-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-5-pyrimidinyl]-N-methylcarbamic Acid Methyl Ester-13Cd6; [4,6-Diamino-2-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-5-pyrimidinyl]methylcarbamic Acid Methyl Ester-13Cd6;Methyl [4,6-diamino-2-[1-(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]pyrimidin-5-yl]methylcarbamate-d13C6

name	category	cas_number	mol_formula	mol_weight	synonym
Apremilast D5	deuteriumlabeledcom	1258597-47-5	C22H19D5N2O7S	465.53	(S)-2-[1-(3-Ethoxy-d5-4-methoxyphenyl)-2-methylsulfonylethyl]-4-acetylaminoisoindoline-1,3-dione; (S)-N-(2-(1-(3-Ethoxy-d5-4-methoxyphenyl)-2-(methylsulfonyl)ethyl)-1,3-dioxoisoindolin-4-yl)acetamide; Apremilast-d5; CC 10004-d5
Anagrelide D213C215N	deuteriumlabeledcom	NA	C ₈ ¹³ C ₂ H ₅ D ₂ Cl ₂ N ₂ ¹⁵ N	261.08	6,7-Dichloro-1,5-dihydroimidazo[2,1-b]quinazolin-2(3H)-one-13C3; BL-4162A-D213C215N; BMY-26538-01-D213C215N; Agrylin-D213C215N;
Vildagliptin D3	deuteriumlabeledcom	1217546-82-1	C17H22D3N3O2	306.42	(2S)-1-[2-[(3-Hydroxytricyclo[3.3.1.1 ^{3,7}]dec-1-yl)amino]acetyl]-2-(pyrrolidine-d3)carbonitrile; LAF 237-d3; NVP-LAF 237-d3; Galvus-d3;
Eltrombopag 13C4	deuteriumlabeledcom	1217230-31-3	C2113C4H22N4O4	446.44	3'-[2-[(2Z)-1-(3,4-Dimethylphenyl)-1,5-dihydro-3-methyl-5-oxo-4H-pyrazol-4-ylidene]hydrazinyl]-2'-hydroxy-[1,1'-biphenyl]-3-carboxylic acid-13C4; SB 497115-13C4

name	category	cas_number	mol_formula	mol_weight	synonym
21 Betamethasone acetate D3	deuteriumlabeledcom	NA	C24H28D3FO6	437.52	(11 β ,16 β)-21-(Acetyloxy)-9-fluoro-11,17-dihydroxy-16-methylpregna-1,4-diene-3,20-dione-d3; 9-Fluoro-11 β ,17,21-trihydroxy-16 β -methylpregna-1,4-diene-3,20-dione 21-acetate-d3; Betamethasone Acetate-d3;
17 Betamethasone propionate D5	deuteriumlabeledcom	NA	C25H28D5FO6	453.55	11 β ,16 β)-9-Fluoro-11,21-dihydroxy-16-methyl-17-(1-oxopropoxy)pregna-1,4-diene-3,20-dione-d5; Betamethasone 17 α -Propionate-d5;
Betamethasone D5	deuteriumlabeledcom	NA	C22H24D5FO5	397.49	(11 β ,16 β)-9-Fluoro-11,17,21-trihydroxy-16-methylpregna-1,4-diene-3,20-dione-d5; 9 α -Fluoro-16 β -methylprednisolone-d5; Betadexamethasone-d5; Flubenisolone-d5; Sch-4831-d5; NCS-39470-d5

name	category	cas_number	mol_formula	mol_weight	synonym
Formoterol fumarate D6	deuteriumlabeledcom	NA	C19H18D6N2O4.C4H4O4	466.51	(R*,R*)-(±)-N-[2-Hydroxy-5-[1-hydroxy-2-[[2-(4-methoxyphenyl)-1-methylethyl]amino]ethyl]phenyl]-formamide (E)-2-Butenedioate (2:1) (Salt); Aformoterol; Atock; BD 40A; CGP 25827A; Eformoterol fumarate; Foradil; Foradil Acrolizer; Foradil Certihaler; Formamide, N-[2-hydroxy-5-[1-hydroxy-2-[[2-(4-methoxyphenyl)-1-methylethyl]amino]ethyl]phenyl]-, (R*,R*)-, (E)-2-butenedioate (2:1) (salt); Formoterol fumarate; NSC 299587; Oxis pMDi; YM 08316
Nilotinib D6	deuteriumlabeledcom	1268356-17-7	C28H16F3N7OD6	535.55	4-Methyl-N-[3-(4-methyl-1H-imidazol-1-yl)-5-(trifluoromethyl)phenyl]-3-[[4-(3-pyridinyl)-2-pyrimidinyl]amino]benzamide-d6; AMN 107-d6; Tassigna-d6

name	category	cas_number	mol_formula	mol_weight	synonym
Agomelatin D6	deuteriumlabeledcom	1079389-42-6	C15H11NO2D6	249.34	N-[2-(7-Methoxy-1-naphthalenyl)ethyl]acetamide-d6; N-[2-(7-Methoxy-1-naphthyl) ethyl]acetamide-d6; S 20098-d6; Valdoxan-d6
Thalidomide D4	deuteriumlabeledcom	1219177-18-0	C13H6D4N2O4	262.25	2-(2,6-Dioxo-3-piperidiny)-1H-iso-indole-1,3(2H)-dione-d4; α -Phthalimidoglutaramide-d4; 3-Phthalimidoglutaramide-d4; Celgene-d4; Contergan-d4; Distaval-d4; K 17-d4; Kevadon-d4; Myrin-d4; N-(2,6-Dioxo-3-piperidyl)phthalimide-d4; NSC 527179-d4; NSC 66847-d4;
Zileuton D4	deuteriumlabeledcom	1189878-76-9	C11H8D4N2O2S	240.31	N-(1-Benzo[b]thien-2-yl-ethyl)-N-hydroxyurea-d4; A-64077-d4; Abbott 64077-d4; Leutrol-d4; Zyflo-d4;
Erythromycin 13CD3	deuteriumlabeledcom	959119-26-7	C3613CH64D3NO13	737.94	E-Base-13C,d3; E-Mycin-13C,d3; Erytromycin A-13C,d3; Aknemycin-13C,d3; Aknin-13C,d3; Eemgel-13C,d3; Ery-Derm-13C,d3; Erymax-13C,d3; Ery-Tab-13C,d3; Erythromid-13C,d3; ERYC-13C,d3;

name	category	cas_number	mol_formula	mol_weight	synonym
Dolutegravir D6 Sodium salt	deuteriumlabeledcom	NA	C20H13F2N3O5D6	425.38	(4R,12aS)-N-[(2,4-Difluorophenyl)methyl]-3,4,6,8,12,12a-hexahydro-7-hydroxy-4-methyl-6,8-dioxo-2H-pyrido[1',2':4,5]pyrazino[2,1-b][1,3]oxazine-9-carboxamide-d6; GSK 1349572-d6;
GS56650013 Sofosbuvir met 13CD15N2	deuteriumlabeledcom	NA	C9 ¹³ CH12DF15N2O5	264.2	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)(phenoxy)phosphoryl)amino)propanoic Acid 15N2D
Dasatinib D8	deuteriumlabeledcom	1132093-70-9	C22H18D8ClN7O2S	496.01	N-[2-Chloro-6-methylphenyl]-2-[[6-[4-(2-hydroxyethyl)-1-piperazinyl-d8]-2-methyl-4-pyrimidinyl]amino]-5-thiazolecarboxamide
Bosutinib D8	deuteriumlabeledcom	380843-75-4 unlabeled	C26H21D8Cl2N5O3	538.50	4-[(2,4-Dichloro-5-methoxyphenyl)amino]-6-methoxy-7-[3-(4-methyl-1-piperazinyl)propoxy]-3-quinolinecarbonitrile-d8
Dapsone D8	deuteriumlabeledcom	557794-38-4	C12H4D8N2O2S	256.35	4,4'-Sulfonylbisbenzeneamine-D8; 4,4'-Sulfonylbis-benzen-2,3,5,6-d4-amine

name	category	cas_number	mol_formula	mol_weight	synonym
4,6,7 Chlorzoxazone D3	deuteriumlabeledcom	1185173-60-7	C7HD3CINO2	172.58	5-Chloro-2(3H)-benzoxazolone-d3; 5-Chloro-2-benzoxazolol-d3; paraflex-d3; Biomioran-d3; Solaxin-d3
Tofacitinib 13C315N	deuteriumlabeledcom	477600-75-2 unlabeled	C1313C3H20N5 15N	316.37	rac CP-690550 Citrate- 13C3-15N
Piperaquine D6	deuteriumlabeledcom	1261394-71-1	C29H26D6Cl2N6	541.55	4,4'-(1,3-Propanediyl)di-4,1-piperazinediyl]bis[7-chloroquinoline]-d6
Bazedoxefene hydrochloride D4	deuteriumlabeledcom	NA	C30H30D4N2O3.HC	511.10	1-[[4-[2-(Hexahydro-1H-azepin-1-yl)ethoxy-1,1,2,2-d4]phenyl]methyl]-2-(4-hydroxyphenyl)-3-methyl-1H-Indol-5-ol
Scopalamine oxalate 13CD3	deuteriumlabeledcom	NA	C1613CH18D3NO4	397.17	(α S)- α -(Hydroxymethyl)benzeneacetic Acid (1 α ,2 β ,4 β ,5 α ,7 β)-9-(Methyl-13Cd3)-3-oxa-9-azatricyclo[3.3.1.0 ^{2,4}]non-7-yl Ester; Hydrobromide; Scopolammonium-13Cd3 Bromide
Rilpivirine D6	deuteriumlabeledcom	1312424-26-2	C22H12D6N6	372.46	4-[[4-[[4-[(1E)-2-Cyanoethenyl]-2,6-(dimethyl-d6)phenyl]amino]-2-pyrimidinyl]amino]benzotrile

name	category	cas_number	mol_formula	mol_weight	synonym
3 Hydroxy anagrelide 15N13C2D2	deuteriumlabeledcom	NA	C813C2H5D2CI3N2	313.56	6,7-Dichloro-1,5-dihydro-3-hydroxyimidazo[2,1-b]quinazolin-2(3H)-one-15N13C2D2; BCH 24426-15N13C2D2;
Sunitinib D10	deuteriumlabeledcom	NA	C22H17D10FN4O2	408.47	N-[2-(Diethyl-d10)aminoethyl]-5-[(Z)-(5-fluoro-1,2-dihydro-2-oxo-3H-indol-3-ylidene)methyl]-2,4-dimethyl-1H-pyrrole-3-carboxamide; Sutent-d10; SU-11248-d10
Vortioxetine dihydrobromide D8	deuteriumlabeledcom	NA	C18H16D8Br2N2S	468.32	1-[2-[(2,4-Dimethylphenyl)thio]phenyl]-piperazine Hydrobromide-D8; Lu AA 21004 Hydrobromide-D8
Regorafenib D3	deuteriumlabeledcom	NA	C21H12D3CIF4N4O3	485.83	4-[4-[[[4-Chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]-3-fluorophenoxy]-N-(methyl-d3)-2-pyridinecarboxamide
Atomoxetine D7 HCl	deuteriumlabeledcom	NA	C17H14NOD7 HCl	298.86	(R)-N-(Methyl-d3)-(2-methylphenoxy)benzenepropanamine HydrochlorideD7; R-Tomoxetine-d3 HydrochlorideD7; Tomoxetine-d7 Hydrochloride; 3

name	category	cas_number	mol_formula	mol_weight	synonym
Zidovudine D4	deuteriumlabeledcom	NA	C10H9D4N5O4	271.27	1-[(2R,4S,5S)-4-azido-5-(hydroxymethyl)oxolan-2-yl]-5-methylpyrimidine-2,4-dione[1] D4
Phenindione D5	deuteriumlabeledcom	70711-53-4	C15H5D5O2	227.27	2-Phenyl-1H-indene-1,3(2H)-dione-d5; -Phenyl-1,3-diketohydrindene-d5; 2-Phenyl-1,3-indandione-d5; 2-Phenyl-1,3-indanedione-d5; 2-Phenyl-1H-indene-1,3(2H)-dione-d5; 2-Phenylindandionev; Athrombon-d5; Bindan-d5; Cronodione-d5; Danedion-d5; Danilon-d5; Danilone-d5; Diadilan-d5; Dindevan-d5; Dineval-d5; Diophindane-d5; Emandion-d5; Emandione-d5; Fenhydren-d5; Fenilin-d5; Fenindion-d5; Hedulin-d5; Hemolidione-d5; Indema-d5; Indion-d5; Indon-d5; NSC 41693-d5; PID-d5; Phenhydren-d5; Phenillin-d5; Phenindione-d5; Phenylen-d5; Phenylin-d5; Phenylindione-d5; Pindione-d5; Rectadione-d5; Theradione-d5; Thrombasal-d5; Tromazal-d5; Trombol-d5

name	category	cas_number	mol_formula	mol_weight	synonym
Trifluoperazine dihydrochloride D8	deuteriumlabeledcom	440-17-5 unlabeled	C ₂₁ H ₁₆ D ₈ F ₃ N ₃ S · 2	488.47	10-[3-[4-(Methyl-d3)-1-piperazinyl]propyl]-2-(trifluoromethyl)-10H-phenothiazine Dihydrochloride; Triftazin-d8; Triphthasine-d8; Eskazinyl-d8; Eskazine-d3; Modalina-d8;
Methenamide D12	deuteriumlabeledcom	23304-08-7	C ₆ D ₁₂ N ₄	152.26	1,3,5,7-Tetraazatricyclodecane-d12; Aceto HMT-d12; Aminoform-d12; Ammoform-d12; Antihydral-d12; Cystogen-d12; Duirexol-d12; Ekagom H-d12; Formamine-d12; Formin-d12; HMTA-d12; Heksa K-d12; Herax UTS-d12; Heterin-d12; Hexa-d12; Hexa B-d12; Hexaform-d12; Hexamethylenamine-d12; Hexamine-d12; Hexasan-d12; Methenamide-d12; Methenamin-d12; Methenamine-d12; NSC 26346-d12; Nocceler H-d12; Nocceler H-PO-d12; Preparation AF-d12; Sanceler H-d12; Sanceler HT-d12; Thixon 715B-d12; Uramin-d12; Uratrine-d12; Uritone-d12; Urodeine-d12; Urotropin-d12; Urotropine-d12; Vulkacit H-d12; Vulkacit H 30-d12; Xametrin-d12

name	category	cas_number	mol_formula	mol_weight	synonym
Lorcaserine D6	deuteriumlabeledcompounds		C11H8D6NCI HCl	238.19	(1R)-8-Chloro-2,3,4,5-tetrahydro-1-methyl-1H-3-benzazepine-d6 Hydrochloride; (R)-8-Chloro-1-methyl-2,3,4,5-tetrahydro-1H-3-benzazepine-d6 Hydrochloride; (R)-8-Chloro-1-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine-d6
Daclatasvir D6	deuteriumlabeledcom	NA	C40H44D6N8O6 . 2H	817.83	N,N'-[[[1,1'-biphenyl]-4,4'-diylbis[1H-imidazole-5,2-diyl-(2S)-2,1-pyrrolidinediyl[(1S)-1-(1-methylethyl)-2-oxo-2,1-ethanediy]]]]bis-carbamic Acid C,C'-Dimethyl Ester-d6
Nateglinide D5	deuteriumlabeledcom	1227666-13-8	C19H22D5NO3	322.45	N-[[trans-4-(1-Methylethyl)cyclohexyl]carbonyl]-D-phenylalanine-d5; A 4166; AY 4166-d5; D-Nateglinide-d5; DJN 608-d5; Fastic-d5; Glinat-d5; Natelide-d5; SDZ-DJN 608-d5; Senaglinide-d5; Starlix-d5; Starlix DS-d5; Starsis-d5

name	category	cas_number	mol_formula	mol_weight	synonym
17 Medroxyprogesterone acetate D3	deuteriumlabeledcom	NA	C24H31O4D3	389.54	(6 α)-17-(Acetyloxy)-6-methyl-pregn-4-ene-3,20-dione-d6; 17 α -Acetoxy-6 α -methylpregn-4-ene-3,20-dione-d6; 17 α -Acetoxy-6 α -methyl- progesterone-d6; 17 α -Hydroxy-6 α -methylprogesterone-d6 Acetate; Meprate-d6; Metigestrona-d6; NSC 26386-d6; Nadigest-d6; Nidaxin-d6; Novo-Medrone-d6; Oragest-d6; Prodasone-d6; Progespon-d6; Progestalfa-d6; Progoston-d6; Progevera-d6; Provera-d6; Ralovera-d6; Repromap-d6; Repromix-d6; Sirprogen-d6; Sodelut G-d6; U 8839-d6; Veramix-d6
Roflumilast N oxide D4	deuteriumlabeledcom	1794760-31-8	C17H10D4Cl2F2N2O	423.23	3-(Cyclopropylmethoxy-d4)-N-(3,5-dichloro-1-oxido-4-pyridinyl)-4-(difluoromethoxy)benzamide; N-(3,5-Dichloro-1-oxopyridin-4-yl)-4-difluoromethoxy-3-(cyclopropyl-d4) methoxybenzamide

name	category	cas_number	mol_formula	mol_weight	synonym
Ponatinib D8	deuteriumlabeledcom	NA	C29H19D8F3N6O	540.61	3-(2-Imidazo[1,2-b]pyridazin-3-ylethynyl)-4-methyl-N-[4-[(4-methyl-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]benzamide-d8
5 Pyridoxal Phosphate D3	deuteriumlabeledcom	853645-22-4 unlabeled	C8H7D3NO6P	250.16	5-Hydroxy-6-methyl-3,4-pyridinedimethanol 3-(Dihydrogen phosphate); Pyridoxol 5-(Dihydrogen phosphate); NSC 83119; Pyridoxine 5-Phosphate; Pyridoxine 5'-Phosphate;
Tranlycypromine D5	deuteriumlabeledcom	107077-98-5	C9H6D5N·HCl	174.68	(1S-trans)-2-Phenyl-cyclopropanamine Hydrochloride; trans-(+)-2-Phenyl-cyclopropylamine Hydrochloride; (1S,2R)-2-Phenylcyclopropanamine Hydrochloride; 1-(S)-Amino-2-(R)-phenylcyclopropane Hydrochloride D5;
Risperidone D4	deuteriumlabeledcom	1020719-76-9	C23H23D4FN4O2	414.52	3-[2-4-(6-Fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]ethyl-6,7,8,9-tetrahydro-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one-d4

name	category	cas_number	mol_formula	mol_weight	synonym
Chlorthalidone D4	deuteriumlabeledcom	1794941-44-8	C14H7D4ClN2O4S	342.80	2-Chloro-5-(2,3-dihydro-1-hydroxy-3-oxo-1H-isoindol-1-yl)-benzenesulfonamide-d4; 3-Hydroxy-3-[4-chloro-3-sulfamylphenyl]phthalimidine-d4; Chlorthalidon-d4; Chlorthalidone-d4; Hygroton-d4; Igroton-d4; Phthalamudine-d4; Zambesil-d4
Cyclophosphamide D8	deuteriumlabeledcom	NA	C7H15Cl2N2O2P · H	287.15	N,N-Bis(2-chloroethyl)tetrahydro-4,5-d8-2H-1,3,2-oxazaphosphorin-2-amine 2-Oxide; Cyclostin-d8; Cytoxan-d8; Endoxan-d8; Genoxal-d8; Hexadrin-d8;
ACT132577 Macitentan metabolite D4	deuteriumlabeledcom	NA	C16H10D4Br2N6O4	550.22	N-[5-(4-Bromophenyl)-6-[2-[(5-bromo-2-pyrimidinyl)oxy]ethoxy]-4-pyrimidinyl]-sulfamide-d4

name	category	cas_number	mol_formula	mol_weight	synonym
Alverine D5 Citrate	deuteriumlabeledcom	1215327-00-6	C ₂₆ H ₃₀ D ₅ NO ₇	478.59	N-(Ethyl-d5)-N-(3-phenylpropyl)benzenepropanamine 2-Hydroxy-1,2,3- propanetricarboxylate; N-(Ethyl-d5)-3,3'-diphenyldipropylamine Citrate; Antispasmin-d5; Calmabel-d5; Gamatran-d5; NSC 35459-d5; Profenine-d5; Prophelan-d5; Proverine-d5; Spacolin-d5; Spasmaverine-d5; Spasmonal-d5
Azacitidine 13C5	deuteriumlabeledcom	320-67-2 unlabeled	C ₈ H ₁₂ N ₄ O ₅	249.17	4-Amino-1-β-D-ribofuranosyl-1,3,5-triazin-2(1H)-one-15N4; 5-AC-13C5; 5-AZC-13C5; 5-AZCR-13C5; 5-AzaC-13C5
Dofetilide D4	deuteriumlabeledcom	1189700-56-8	C ₁₉ H ₂₃ D ₄ N ₃ O ₅ S ₂	445.59	N-[4-[2-[Methyl[2-[4-[(methylsulfonyl)amino]phenoxy]ethyl]amino]ethyl]phenyl]-methanesulfonamide-d4; UK-68798-d4; Tikosyn-d4

name	category	cas_number	mol_formula	mol_weight	synonym
Nicardipine hydrochloride D3	deuteriumlabeledcom	1432061-50-1	C ₂₆ H ₂₇ D ₃ CIN ₃ O ₆	519.00	1,4-Dihydro-2,6-dimethyl-4-(3-nitrophenyl)-3,5-pyridinedicarboxylic Acid Methyl 2-[Methyl-d ₃ (phenylmethyl)amino]ethyl Ester Hydrochloride; RS-69216-d ₃ ; YC-93-d ₃ ; Antagonyl-d ₃ ; Barizin-d ₃ ; Bionicard-d ₃ ; Cardene-d ₃ ; Dacarel-d ₃ ; Vasonase-d ₃
Ledipasvir dihydrochloride D6	deuteriumlabeledcom	NA	C ₄₉ H ₄₈ D ₆ F ₂ N ₈ O ₆	967.96	N-[(1S)-1-[[[(6S)-6-[5-[9,9-Difluoro-7-[2-[(1R,3S,4S)-2-[(2S)-2-[(methoxycarbonyl)amino]-3-methyl-1-oxobutyl]-2-azabicyclo[2.2.1]hept-3-yl]-1H-benzimidazol-6-yl]-9H-fluoren-2-yl]-1H-imidazol-2-yl]-5-azaspiro[2.4]hept-5-yl]carbonyl]-2-methylpropyl]-carbamic Acid Methyl Ester-d ₆
Dimethyl fumarate D6	deuteriumlabeledcom	NA	C ₆ H ₂ O ₄ D ₆	150.16	Fumaric-d ₂ Acid Dimethyl Ester; Dimethyl Fumarate-d ₆ ; (2E)-2-Butenedioic-2,3-d ₆ Acid Dimethyl Ester; (E)-2-Butenedioic-2,3-d ₆ Acid Dimethyl Ester

name	category	cas_number	mol_formula	mol_weight	synonym
Pitavastatin sodium salt D4	deuteriumlabeledcom	NA	C25H19D4FNNaO4	447.47	(3R,5S,6E)-7-[2-Cyclopropyl-4-(4-fluorophenyl)-3-quinolinyl]-3,5-dihydroxy-6-heptenoic Acid-d4 Calcium Salt; Flovas-d4; Livalo-d4; NK 104-d4; NK 104 (acid)-d4; Pitava-d4
Afatinib D6	deuteriumlabeledcom	1313874-96-2	C24H19D6CIFN5O3	491.98	(2E)-N-[4-[(3-Chloro-4-fluorophenyl)amino]-7-[[3S)-tetrahydro-3-furanyl]oxy]-6-quinazolinyl]-4-(dimethylamino)-2-butenamide-d6
N1 Acetyl triethylenetetramine D4	deuteriumlabeledcom	NA	C8H16D4N4O · HCl	228.76	N-[2-[[2-[(2-Aminoethyl)amino]ethyl]amino]ethyl]acetamide-d4; N1-Acetyltriethylenetetramine-d4
Doxylamine D5	deuteriumlabeledcom	1173020-59-1	C17H17D5N2O	275.40	N,N-Dimethyl-2-[1-(phenyl-d5)-1-(2-pyridinyl)ethoxy]ethanamine Succinate Salt; 2-[α-(2-Dimethylaminoethoxy)-α-methyl(benzyl-d5)]pyridine Succinate; Alsodorm-d5; Decamium-d5; Decapryn-d5 Succinate; Gittalun-d5; Meraprina-d5; Mereprine-d5; NSC 74772-d5

name	category	cas_number	mol_formula	mol_weight	synonym
Perampanel D5	deuteriumlabeledcom	NA	C23H10D5N3O	354.42	2-(1',6'-Dihydro-6'-oxo-1'-phenyl[2,3'-bipyridin]-5'-yl)benzotrile-d5; 3-(2-Cyanophenyl)-1-phenyl-5-(2-pyridyl)-1,2-dihydropyridin-2-one-d5; 3-(2-Cyanophenyl)-5-(2-pyridyl)-1-phenyl-1,2-dihydropyridin-2-one-d5
Rotigotine D7	deuteriumlabeledcom	NA	C19H19D7CINOS	358.98	5,6,7,8-Tetrahydro-6-[propyl-[2-(2-thienyl)ethyl]amino]-1-naphthalenol-d7 Hydrochloride; rac-N 0437-d7; rac-N 0923-d7; rac-Neupro-d7 Hydrochloride; rac-Rotigotine-d7 Hydrochloride
Pemetrexed D5	deuteriumlabeledcom	NA	C20H16D5N5O6	432.44	N-[4-[2-(2-Amino-4,7-dihydro-4-oxo-3H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoyl]-L-glutamic Acid-d5;N-[4-[(2-Amino-4,7-dihydro-4-oxo-1H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoyl]-L-glutamic Acid-d5
4 Hydroxy alverine hydrochloride salt D5	deuteriumlabeledcom	NA	C20H22D5NO .HCl	338.93	4-[3-[Ethyl-d5(3-phenylpropyl)amino]propyl]phenol D5;

name	category	cas_number	mol_formula	mol_weight	synonym
3 Hydroxy methyl tolcapone D7	deuteriumlabeledcom	NA	C15H6D7NO5	294.30	4-Hydroxy-3-methoxy-5-nitrophenyl)(4-methylphenyl)methanone-d7; 4-Hydroxy-3-methoxy-4'-methyl-5-nitrobenzophenone-d7
Tolcapone D7	deuteriumlabeledcom	134308-13-7 unlabeled	C14H4D7NO6	280.30	(3,4-Dihydroxy-5-nitrophenyl)(4-methylphenyl-d7)methanone; Ro-40-7592-d7;
7 Hydroxy chlorpromazine D6	deuteriumlabeledcom	NA	C17H13D6ClN2OS	340.90	8-Chloro-10-[3-(dimethylamino)propyl]-10H-phenothiazin-3-ol-d6 Hydrochloride; 8-Chloro-10-[3-(dimethylamino)propyl]phenothiazin-3-ol-d6 Hydrochloride; 7-Hydroxy-2-chloropromazine-d6 Hydrochloride
Regorafenib n oxide13CD3	deuteriumlabeledcom	NA	C2013CH12D3ClF4N	502.83	4-[4-[[[4-Chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]-3-fluorophenoxy]-N-methyl-2-pyridinecarboxamide 1-Oxide-13Cd3

name	category	cas_number	mol_formula	mol_weight	synonym
Leuprolide trifluoroacetate D10	deuteriumlabeledcom	NA	C ₅₉ H ₇₄ D ₁₀ N ₁₆ O ₁ 2 C ₂ H ₀ 2F ₃	1333.42	6-D-Leucine-9-(N-ethyl-L-prolinamide)- 10-deglycinamideluteinizing-d10 TFA Salt; Hormone-Releasing Factor (Pig) TFA Salt; A 43818-d10 TFA Salt; Abbott 43818-d10 TFA Salt; Leuprorelin-d10 TFA Salt; Lupron-d10 TFA Salt; Procren Depot-d10 TFA Salt; Procrin-d10 TFA Salt; Prostag- d10 TFA Salt; TAP 144-d10 TFA Salt; TAP 144SR-d10 TFA Salt;
Bivalirudin D4	deuteriumlabeledcom	NA	C ₉₈ H ₁₃₄ D ₄ N ₂₄ O ₃₃	2184.29	D-Phenylalanyl-L-prolyl-L-arginyl-L- prolylglycylglycylglycyl(d2)glycyl(d2)-L- asparaginylglycyl-L- α -aspartyl-L- phenylalanyl-L- α -glutamyl-L- α -glutamyl- L-isoleucyl-L-prolyl-L- α -glutamyl-L- α - glutamyl-L-tyrosyl-L-leucine

name	category	cas_number	mol_formula	mol_weight	synonym
Lymecycline D8	deuteriumlabeledcom	992-21-2	C ₂₉ H ₃₀ D ₈ N ₄ O ₁₀	610.68	N6-[[[(4S,4aS,5aS,6S,12aS)-4-(Dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-2-naphthaceny]carbonyl]amino]methyl]-L-lysine-d8; Armyl-d8; Ciclisin-d8; Ciclolysal-d8; Ciclolysine-d8; Infaciclina-d8; Lisinbiotic-d8; Lisinciclina-d8; Mucomycin-d8; N-Lysinomethyltetracycline-d8; Tetramyl-d8
Nadolol D9	deuteriumlabeledcom	1246820-10-9	C ₁₇ H ₁₈ D ₉ N ₁ O ₄	318.40	5-[3-[(1,1-Dimethylethyl-d9)amino]-2-hydroxypropoxy]-1,2,3,4-tetrahydro-2,3-naphthalenediol; Anabet-d9; Corgard-d9; SQ 11725-d9; Solgol-d9
E10 hydroxynortriptylin e D3	deuteriumlabeledcom	NA	C ₁₉ H ₁₈ D ₃ N ₁ O	282.40	(5Z)-10,11-Dihydro-5-[3-(methylamino)propylidene]-5H-dibenzo[a,d]cyclohepten-10-ol-D3

name	category	cas_number	mol_formula	mol_weight	synonym
Ospemifene D4	deuteriumlabeledcom	NA	C24H19D4ClO2	382.92	2-[4-[(1Z)-4-Chloro-1,2-diphenyl-1-buten-1-yl]phenoxy]-ethanol-d4; (Z)-2-[4-(4-chloro-1,2-diphenyl-1-butenyl)phenoxy]-ethanol-d4; 2-[4-[(1Z)-4-Chloro-1,2-diphenyl-1-butenyl]phenoxy]-ethanol-d4
S Desmethyl venlafaxine D6	deuteriumlabeledcom	NA	C16H19D6NO2	269.41	1-[1-(4-Methoxyphenyl)-2-(methyl-d6-amino)ethyl]cyclohexanol; Norvenlafaxine-d6
R Praziquantel d11	deuteriumlabeledcom	1399880-38-6	C19H13N2O2D11	323.48	(R)-2-(Cyclohexylcarbonyl)-1,2,3,6,7,11b-hexahydro-4H-(pyrazino-d11)[2,1-a]isoquinolin-4-one; 1; (R)-Azinox-d11
S Praziquantel d11	deuteriumlabeledcom	57452-97-8 (non-labelled)	C19H13N2O2D11	323.48	(S)-2-(Cyclohexylcarbonyl)-1,2,3,6,7,11b-hexahydro-4H-(pyrazino-d11)[2,1-a]isoquinolin-4-one; 1; (S)-Azinox-d11
Liothyronine sodium 15N13C9	deuteriumlabeledcom	NA	C613C9H11I315NNa	682.88	O-(4-Hydroxy-3,5-diiodophenyl)-3,5-diiodo-L-tyrosine; (-)-Thyroxine; 3,3',5,5'-Tetraiodo-L-thyronine15N13C9; Henning15N13C9;; L-T4 15N13C9;; L-Thyroxin15N13C9;

name	category	cas_number	mol_formula	mol_weight	synonym
S Apremilast D5	deuteriumlabeledcom	1258597-47-5	C22H19D5N2O7S	465.53	(S)-2-[1-(3-Ethoxy-d5-4-methoxyphenyl)-2-methylsulfonyl ethyl]-4-acetylaminoisoindoline-1,3-dione; (S)-N-(2-(1-(3-Ethoxy-d5-4-methoxyphenyl)-2-(methylsulfonyl)ethyl)-1,3-dioxoisoindolin-4-yl)acetamide; Apremilast-d5
Methimazole D3	deuteriumlabeledcom	1160932-07-9	C4H3D3N2S	117.19	1,3-Dihydro-1-(methyl-d3)-2H-imidazole-2-thione; 1-Methylimidazole-d3-2-thiol; Mercazolyl-d3; Thiamazole-d3; Basolan-d3; Mercazole-d3; Metazolo-d3; Tapazole-d3
Nabilone D6	deuteriumlabeledcom	NA	C24H30D6O3	378.58	Cesamet D6; Nabilona D6; Nabilonum D6;
Tapentadol D5	deuteriumlabeledcom	NA	C14H18D5NO	226.34	3-[(1R,2R)-3-(Dimethylamino)-1-ethyl-2-methylpropyl]phenol Hydrochloride D5;
Ivacaftor D18	deuteriumlabeledcom	1413431-05-6	C24H10N2O3D18	410.60	N-[2,4-Bis[1,1-di(methyl-d3)ethyl-2,2,2-d3]-5-hydroxyphenyl]-1,4-dihydro-4-oxo-3-quinolinecarboxamide-d18; Kalydeco-d18

name	category	cas_number	mol_formula	mol_weight	synonym
Eslicarbazepine D4	deuteriumlabeledcom	NA	C17H12D4N2O3	300.35	(10S)-10-(Acetyloxy)-10,11-dihydro-5H-dibenz[b,f]azepine-5-carboxamide-D4; (S)-(-)-10-Acetoxy-10,11-dihydro-5H-dibenz[b,f]azepine-5-carboxamide-D4
Nitisinone 13C6	deuteriumlabeledcom	1246815-63-3	C813C6H10F3NO5	335.18	2-[2-Nitro-4-(trifluoromethyl)benzoyl]-1,3-cyclohexanedione-13C6; NTBC-13C6; Nitisonone-13C6; Orfadin-13C6
Trazodone hydrochloride salt D6	deuteriumlabeledcom	1181578-71-1	C19H16D6ClN5O · H	414.36	1,4:3,6-Dianhydro-D-glucitol-13C6 Dinitrate; Dinitrosorbide-13C6; 1,4:3,6-Dianhydrosorbitol-13C6 2,5-Dinitrate; Carvasin-13C6; Cedocard-13C6; Corovliss-13C6; Dignonitrat-13C6; Dilatrate-13C6; Diniket-13C6; ISDN-13C6
Isosorbide-13C6 2,5-Dinitrate	deuteriumlabeledcom	NA	13C6H8N2O8	242.09	(+/-)-1,2-Dithiolane-3-pentanoic Acid-d5; (+/-)-1,2-Dithiolane-3-valeric Acid-d5; (+/-)-Thioctic Acid-d5; (RS)- α -Lipoic Acid-d5; DL-Thioctic Acid-d5; Liposan-d5; Lipothion-d5; NSC 628502-d5; NSC 90788-d5; Protogen A-d5; Thioctsan-d5; Tioctacid-d5

name	category	cas_number	mol_formula	mol_weight	synonym
Rac alpha lipoic acid D5	deuteriumlabeledcom	1189471-66-6	C8H9D5O2S2	211.35	2-[(2,6-Dichlorophenyl)-amino]benzeneacetic Acid Carboxymethyl-d4,13C2 Ester; Glycolic Acid [o-(2,6-Dichloroanilino)phenyl]acetate-d4,13C2 Ester; PR-82/3-d4,13C2; Airtal-d4,13C2; Aceclofar-d4,13C2; Falcol-d4,13C2; Gerbin-d4,13C2; Preservex-d4,13C2; Tresquim-d4,13C2; Zerodol-d4,13C2
Aceclofenac 13C2D4	deuteriumlabeledcom	1795019-63-4	C14H9D4Cl2NO4 13	360.19	N-[2,4-Bis[1,1-di(methyl-d3)ethyl-2,2,2-d3]-5-hydroxyphenyl]-1,4-dihydro-4-oxo-3-quinolinecarboxamide-13C6
Ivacaftor 13C6	deuteriumlabeledcom	873054-44-5 unlabeled	C1813C6H28N2O3	398.45	(8S,10S)-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 Hydrochloride 13CD3; Adriamycinol Hydrochloride 13CD3; 13-Dihydrodoxorubicin Hydrochloride 13CD3

name	category	cas_number	mol_formula	mol_weight	synonym
Doxorubicinol 13CD3	deuteriumlabeledcom	54193-28-1 unlabeled	C2613CH28D3NO11	663.57	N1-(5-Chloro-2-pyridinyl)-N2-[(1S,2R,4S)-4-[[di(methyl-d3)amino]carbonyl]-2-[[[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]amino]cyclohexyl]ethanediamide; DU 176-d6
Edoxaban hydrochloride D6	deuteriumlabeledcom	1304701-57-2 free base	C24H24D6ClN7O4S	590.56	4-[1-(5,6,7,8-Tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)ethenyl)benzoic Acid-d4; LG 100069-d3;; RO 26-4455-d4
Bexarotene D4	deuteriumlabeledcom	NA	C24H24O2D4	352.51	(1R,2S)-2-(Aminomethyl)-N,N-diethyl-1-phenylcyclopropanecarboxamide-d10 Hydrochloride; Levomilnacipran-d10; Savella-d10; cis-(-)-Milnacipran Hydrochloride-d10;

name	category	cas_number	mol_formula	mol_weight	synonym
Levomilnacipran D10 HCl	deuteriumlabeledcom	NA	C15H12D10N2O.HC	292.87	N, α , α -Trimethyl-N-[4-(2-methylphenyl)-6-(4-methyl-1-piperazinyl)-3-pyridinyl]-3,5-bis(trifluoromethyl)-benzeneacetamide-d6; 2-[3,5-Bis(trifluoromethyl)phenyl]-N-[6-(4-methylpiperazin-1-yl)-4-o-tolylpyridin-3-yl]-N-methylisobutyramide-d6
Netupitant D6	deuteriumlabeledcom	NA	C30H26F6N4OD6	584.64	3,4,5,6-Tetrahydro-5-(methyl-d5)-1-phenyl-1H-2,5-benzoxazocine Hydrochloride; (+/-)-Nefopam-d5 Hydrochloride;
Desmethyl nefopam D5 HCl	deuteriumlabeledcom	NA	C16H13D5ClNO	280.80	N'-[trans-4-[2-[4-(2,3-Dichlorophenyl)-1-piperazinyl]ethyl]cyclohexyl]-N,N-dimethylurea D6; RGH 188 D6

name	category	cas_number	mol_formula	mol_weight	synonym
Cariprazine D6	deuteriumlabeledcom	NA	C21H26Cl2N4OD6	433.46	N-[4-[1-Hydroxy-2-[(1-methylethyl-d6)amino]ethyl]phenyl]methanesulfonamide Hydrochloride; 4'-[1-Hydroxy-2-(isopropylamino-d6)ethyl]methanesulfonanilide Hydrochloride; Betapace-d6; DL-MJ 1999-d6; Darob-d6; MJ 1999-d6; Sotacor-d6; Sotalex-d6; dl-Sotalol-d6 Hydrochloride
Sotalol D6	deuteriumlabeledcom	1246820-85-8	C12H14D6N2O3S H	314.86	[(S)-1-(5-Fluoro-4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)propyl]amino D5
Idelalisib D5	deuteriumlabeledcom	870281-82-6 unlabeled	C22H13D5FN7O	420.46	N1,N2-Bis(2-aminoethyl)-1,2-ethanediamine-d4 Tetrahydrochloride; 1,2-Bis(2-aminoethylamino)ethane-d4 Tetrahydrochloride; 1,4,7,10-Tetraazadecane-d4 Tetrahydrochloride; 1,8-Diamino-3,6-diazaoctane-d4 Tetrahydrochloride; 3,6-Diazaoctane-1,8-diamine-d4 Tetrahydrochloride; Ancamine TETA-d4 Tetrahydrochloride; EpoxySet 145-20020-d4

name	category	cas_number	mol_formula	mol_weight	synonym
Trientine hydrochloride D4	deuteriumlabeledcom	NA	C6H14D4N4 HCl	186.72	5-[Bis(2-chloroethyl)-amino]-1-methyl-1H-benzimidazole-2-butanoic Acid-d8 Hydrochloride; Cytostasan-d8; Ribomustin-d8; Treanda-d8;
Bendamustine d8	deuteriumlabeledcom	NA	C16H21Cl2N3O2 · H	402.77	(10S)-10,11-Dihydro-10-hydroxy-5H-Dibenz[b,f]azepine-5-carboxamide-D3; S-(+)-10,11-Dihydro-10-hydroxy-5H-dibenz[b,f]azepine-5-carboxamide-D3; (S)-Licarbazepine-D3; BIA 2-194-D3; CGP 13751-D3; Erelib-D3; Pazzul-D3; Stedesa-D3
Eslicarbazepine D3	deuteriumlabeledcom	NA	C15H11D3N2O2	257.30	(α S)- α -[[2-(4-Morpholinyl)acetyl]amino]benzenebutanoyl-L-leucyl-N-[(1S)-3-methyl-1-[[2-(2-methyl-2-oxiranyl)carbonyl]butyl]-L-phenylalaninamide-d8; (α S)- α -[(4-Morpholinylacetyl)amino]benzenebutanoyl-L-leucyl-N-[(1S)-3-methyl-1-[[2-(2-methyloxiranyl)carbonyl]butyl]-L-phenylalaninamide-d8

name	category	cas_number	mol_formula	mol_weight	synonym
Carfilzomib D8	deuteriumlabeledcom	1537187-53-3	C40H49D8N5O7	727.96	2-[(R)-[[3-Methyl-4-(2,2,2-trifluoroethoxy)-2-pyridinyl]methyl]sulfinyl]-1H-benzimidazole-d4; Dextralansoprazole-d4; R-(+)-Lansoprazole-d4; T 168390-d4; TAK 390-d4;
Dextralansoprazole D4	deuteriumlabeledcom	934294-22-1	C16H10D4F3N3O2S	373.39	(3S,5R)-7-[3-(4-Fluorophenyl)-1-(1-methylethyl)-1H-indol-2-yl]-3,5-dihydroxy-6-heptenoic Acid-d6
(-)-3S 5R Fluvastatin sodium salt D6	deuteriumlabeledcom	NA	C24H19D6FNNaO4	439.48	(2R,3R,11bR)-1,3,4,6,7,11b-Hexahydro-9,10-dimethoxy-3-(2-methylpropyl)-2H-benzo[a]quinolizin-2-ol-13C2D6; [2R-(2 α ,3 β ,11b β)]-1,3,4,6,7,11b-Hexahydro-9,10-dimethoxy-3-(2-methylpropyl)-2H-benzo[a]quinolizin-2-ol-13C2D6; (+)-(2R,3R,11bR)-Dihydrotrabenazine-13C2D6; (+)-DTBZ-13C2D6; (+)-Dihydrotrabenazine-13C2D6; (2R,3R,11bR)-DHTBZ-13C2D6

name	category	cas_number	mol_formula	mol_weight	synonym
Dihydratetabenazine 13C2D6 racemic	deuteriumlabeledcom	NA	$C_{17}^{13}C_2H_{23}D_6NO_3$	327.46	L-Histidyl-L-alanyl-L- α -glutamylglycyl-L-threonyl-L-phenylalanyl-L-threonyl-L-seryl-L- α -aspartyl-L-valyl-L-seryl-L-seryl-L-tyrosyl-L-leucyl-L- α -glutamylglycyl-L-glutamyl-L-alanyl-L-alanyl-N6-[N-(1-oxohexadecyl)-L- γ -glutamyl]-L-lysyl-L- α -glutamyl-L-phenylalanyl-L-isoleucyl-L-alanyl-L-tryptophyl-L-leucyl-L-valyl-L-arginylglycyl-L-arginyl-glycine; 10: PN: WO2012006598 SEQID: 10 claimed protein; 1: PN: WO02069994 PAGE: 16 claimed protein; 31: PN: US20050009742 PAGE: 40 claimed sequence; 3: PN: WO2014000058 SEQID: 6 claimed protein; 3: PN: WO2014096145 SEQID: 3 claimed protein; 3: PN: WO2014096148 SEQID: 3 claimed protein; 3: PN: WO2014096149 SEQID: 3 claimed protein; 3: PN: WO2014096150 SEQID: 3 claimed protein; 55: PN: WO2004005342 PAGE: 46 claimed protein; 6: PN: WO2009030499 SEQID: 6 D4

name	category	cas_number	mol_formula	mol_weight	synonym
Liraglutide D4	deuteriumlabeledcom	NA	C172H261D4N43O5	3755.23	5-Chloro-N4-[2-[(1-methylethyl)sulfonyl]phenyl]-N2-[5-methyl-2-[1-(methyl-d3)ethoxy-1,2,2,2-d4]-4-(4-piperidinyl)phenyl]-2,4-pyrimidinediamine
Ceritinib D7	deuteriumlabeledcom	1632484-77-5	C28H36ClN5O3S	282.40	11-(3-Dimethylaminopropylidene-d3)-6,11-dihydrodibenz[b,e]oxepin Hydrochloride; Adapin-d3; Aponal-d3; Curatin-d3; Quitaxon-d3; Sinequan-d3
Doxepin D3 HCl	deuteriumlabeledcom	347840-07-7	C19H18D3NO · HCl	441.53	Votrient-13Cd3 Hydrochloride; 5-[[4-[(2,3-Dimethyl-2H-indazol-6-yl)methylamino]-2-pyrimidinyl]amino]-2-methylbenzenesulfonamide-13Cd3 Hydrochloride;
Pazopanib 13CD3	deuteriumlabeledcom	NA	C2013CH20 D3N7O3	216.21	(β S)-rel-β,3-Dihydroxy-D-tyrosine-D3 Hydrochloride; DL-threo-3-(3,4-Dihydroxyphenyl)serine-D3 DL-DOPS-13C2,15N; L-Threodops-D3; DL-threo-3,4-Dihydroxyphenylserine- D3

name	category	cas_number	mol_formula	mol_weight	synonym
Droxidopa D3	deuteriumlabeledcom	NA	C9H8D3NO5	355.48	(2E)-3-[6-[(1E)-1-(4-Methylphenyl)-3-(1-pyrrolidinyl)-1-propen-1-yl]-2-pyridinyl]-2-propenoic Acid-d7; BW 0270C-d7; BW 825C-d7; BW A825C-d7; Semprex-d8; (E,E)-3-[6-[1-(4-Methylphenyl)-3-(1-pyrrolidinyl)-1-propenyl]-2-pyridinyl]-2-propenoic Acid-d8; (2E)-3-[6-[1-(4-Methylphenyl)-3-(1-pyrrolidinyl)-1-propenyl]-2-pyridinyl]-2-propenoic Acid-d7
Acrivastine D7	deuteriumlabeledcom	172165-56-9	C22H17D7N2O2	439.48	3R,5S)-7-[3-(4-Fluorophenyl)-1-(1-methylethyl-d6)-1H-indol-2-yl]-3,5-dihydroxy-6-heptenoic Acid Sodium Salt;
(+)-3R,5S-Fluvastatin D6 Sodium salt	deuteriumlabeledcom	NA	C24H19D6FNNaO4	753.95	(2R,3aR,10Z,11aS,12aR,14aR)-N-(Cyclopropylsulfonyl)-2,3,3a,4,5,6,7,8,9,11a,12,13,14,14a-tetradecahydro-2-[[7-methoxy-8-methyl-2-[4-(1-methylethyl)-2-thiazolyl]-4-quinolinyl]oxy]-5-methyl-4,14-dioxo-cyclopenta[c]cyclopropa[g][1,6]diazacyclotetradecine-12a(1H)-carboxamide-13Cd3

name	category	cas_number	mol_formula	mol_weight	synonym
Simeprevir 13CD3	deuteriumlabeledcom	923604-59-5 unlabeled	C3713CH44D3N5O7	315.42	(±)-N-[3-Acetyl-4-[2-hydroxy-3-[(1-methylethyl-d7)amino]propoxy]phenyl]acetamide; DL-3'-Acetyl-4'-[2-hydroxy-3-[(isopropyl-d7)amino]propoxy]acetanilide; (±)-Diacetolol-d7; Diacetolol-d7; Acetylacetolol-d7; M and B 16942-d7; 1-(4-Acetamido-2-acetylphenoxy)-2-hydroxy-3-(isopropyl-d7)aminopropane; DL-1-(2-Acetyl-4-acetamidophenoxy)-2-hydroxy-3-(isopropyl-d7)aminopropane
Diacetolol D7	deuteriumlabeledcom	1346604-19-0	C16H17D7N2O4	343.47	N-[3-Acetyl-4-[2-hydroxy-3-[(1-methylethyl)amino](propoxy)]phenyl]butanamide-d7
Acebutolol D7	deuteriumlabeledcom	28197-63-9 unlabeled	C18H21D7N2O4	412.90	2-[(4-Clorophenyl)-2-pyridinylmethoxy]-N,N-dimethyl-d6-ethanamine Maleate Salt; Allergefon-d6; Clistin-d6; Ciberon-d6; Lergefin-d6

name	category	cas_number	mol_formula	mol_weight	synonym
Carbinoxamine D6 Maleate	deuteriumlabeledcom	1216872-59-1	C ₁₆ H ₁₃ D ₆ CIN ₂ O · C	345.43	(5 α)-17-(Cyclopropyl-methyl-d ₃)-4,5-epoxy-3,14-dihydroxymorphinan-6-one; Antaxone-D3; Depade-D3; EN 1639A-D4; NIH 8503-D4; Nalorex-D4; Trexan-D4;
Naltrexone D4	deuteriumlabeledcom	NA	C ₂₀ H ₁₉ N ₄ O ₄ D ₄	347.45	6beta-hydroxynaltrexone D4
6-beta-naltrexol D4	deuteriumlabeledcom	1279034-32-0 free base	C ₂₀ H ₂₁ D ₄ N ₄ O ₄	241.14	1-[[[(5-Nitro-2-furanyl)methylene]amino]-2,4-imidazolidinedione-13C ₃]; 1-(5-Nitro-2-furfurylideneamino)hydantoin-13C ₃ ; 5-Nitrofurantoin-13C ₃ ; Berkfurin-13C ₃ ; Chemiofuran-13C ₃ ; Cyantin-13C ₃ ; Cystit-13C ₃ ; Furadantoin-13C ₃ ; Furadoin-13C ₃ ; Furadoine-13C ₃ ; Nifurantoin-13C ₃ ; Nitoin-13C ₃ ; Nitrofurantoin-13C ₃ ; Novofuran-13C ₃
Nitrofurantoin 13C ₃	deuteriumlabeledcom	1217226-46-4	C ₅ ¹³ C ₃ H ₆ N ₄ O ₅	329.47	(4S,6S)-4-(Ethylamino)-5,6-dihydro-6-methyl-4H-thieno[2,3-b]thiopyran-2-sulfonamide 7,7-Dioxide-d ₅ L 671152-d ₅ ; MK 507-d ₅ ; Trusopt-d ₅
Dorzolamide D5	deuteriumlabeledcom	1227097-70-2	C ₁₀ H ₁₁ D ₅ N ₂ O ₄ S ₃	1206.64	Cyclosporine-d ₄ ; Ciclosporin-d ₄ ; Atopica-d ₄ ; Sandimmun(e)-d ₄ ; Neoral-d ₄ ; Optimune-d ₄

name	category	cas_number	mol_formula	mol_weight	synonym
Cyclosporin A D4	deuteriumlabeledcom	NA	C62H107D4N11O12	467.84	4-[4-[[[4-Chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenoxy]-N-(methyl-d3)-2-pyridinecarboxamide
Sorafenib D3	deuteriumlabeledcom	1130115-44-4	C21H13D3ClF3N4O	497.61	N-[(1R,3aR,4aR,6R,8aR,9S,9aS)-9-[(1E)-2-[5-(3-Fluorophenyl)-2-pyridinyl]ethenyl]dodecahydro-1-methyl-3-oxonaphtho[2,3-c]furan-6-yl]carbamic Acid Ethyl Ester-d5
Vorapaxar D5	deuteriumlabeledcom	618385-01-6 unlabeled	C29H33FN2O4	263.33	5-Benzoyl- α -methyl-2-thiopheneacetic Acid D3; (RS)-Tiaprofenic Acid D3
Tiaprofenic Acid D3	deuteriumlabeledcom	NA	C14H9D3O3S	701.77	N-(2,2,2-Trifluoroethyl)-9-[4-[4-[[[4'-(trifluoromethyl)[1,1'-biphenyl]-2-yl]carbonyl]amino]-1-piperidinyl]butyl]-9H-fluorene-9-carboxamide-d8
Lomitapide D8	deuteriumlabeledcom	NA	C39H29D8F6N3O2	168.62	(+/-)-4-Amino-5-hexenoic Acid-13C,d2; (+/-)- γ -Vinyl GABA-13C,d2; GVG-13C,d2; MDL 71754-13C,d2; RMI 71754-13C,d2; Sabril-13C,d2;
Vigabatrin 13 C D2 HCl salt	deuteriumlabeledcom	NA	13C C5H9D2NO2. H	298.27	S 3341-3; N-(Dicyclopropylmethyl)-4,5-dihydro-2-oxazolamine D4 Trifluoroacetate

name	category	cas_number	mol_formula	mol_weight	synonym
Rilmenidine-D4 trifluoroacetate	deuteriumlabeledcom	NA	C12H13D4F3N2O3	539.99	(2E)-2-[1-[2-Cyclopropyl-1-(2-fluorophenyl)-2-oxoethyl]-4-[[2-(3-(methoxy-d3)phenyl)-2-oxoethyl]thio]-3-piperidinylidene]acetic Acid
Prasugrel derivative HCl(trans R- 138727MP) D3	deuteriumlabeledcom	NA	C21H28FN05S 13C6	469.65	4-[2-[4-[1-(2-Ethoxyethyl)-1H-benzimidazol-2-yl]-1-piperidinyl]ethyl]- α , α -(dimethyl-d6)benzeneacetic Acid;
Bilastine D6	deuteriumlabeledcom	1215358-58-9	C28H31D6N3O3	441.62	7-[4-(4-(Benzo[b]thien-4-yl)-piperazin-1-yl)butoxy]-1H-quinolin-2-one-d8; OPC 34712-d8
Brexpirazole D8	deuteriumlabeledcom	1427049-19-1	C25H19D8N3O2S	232.3	N-[2-(7-Hydroxy-1-naphthalenyl)ethyl]acetamide D3; O-Demethylagomelatine; S 21517 D3
7-Desmethyl- Agomelatine D3	deuteriumlabeledcom	NA	C14H12D3NO2	573.67	5-[[[(2S)-2-Amino-3-[4-(aminocarbonyl)-2,6-dimethylphenyl]-1-oxopropyl]][(1S)-1-(5-phenyl-1H-imidazol-2-yl)ethyl]amino]methyl]-2-methoxybenzoic Acid13C,d3 Hydrochloride; MuDelta13C,d3

name	category	cas_number	mol_formula	mol_weight	synonym
Eluxadoline 13CD3	deuteriumlabeledcom	NA	C32H32N5O5D3	228.34	(2R,3R,4R,5S)-1-Butyl-2-(hydroxymethyl)-,3,4,5-Piperidinetriol D9Hydrochloride-
Miglustat D9	deuteriumlabeledcom	72599-27-0 unlabeled	C10H12NO4D9	375.56	2-(4-[Ethyl-d5]-1-piperazinyl)-4-(4-fluorophenyl)-5,6,7,8,9,10-hexahydro-cycloocta[b]pyridine D8; Lonasen-d8
Blonanserin D8	deuteriumlabeledcom	132810-10-7 unlabeled	C23H22FN3D8	245.31	N-2,3-Xylylanthranilic-d4 Acid; 2-(2,3-Dimethylanilino)benzoic-d4 Acid; 2-[(2,3-Dimethylphenyl)amino]benzoic-d4 Acid; 2',3'-Dimethyl-N-phenylanthranilic-d4 Acid; Bafameritin M-d4; Baphameritin M-d4; Bonabol-d4; C.I. 473-d4; CN 35355-d4; Coslan-d4; INF 3355-d4; In-M-d4; Lysalgo-d4; Mefacit-d4; Mefenacid-d4; Mefenamic-d4 Acid; Mephenamic-d4 Acid; N-(2,3-Dimethylphenyl)anthranilic-d4 Acid; N-(2,3-Xylyl)-2-aminobenzoic-d4 Acid; N-(2,3-Xylyl)anthranilic-d4 Acid; NSC 94437-d4; Namphen-d4; Parkemed-d4; Ponalar-d4; Ponstan-d4; Ponstel-d4; Ponstil-d4; Ponstyl-d4; Pontal-d4; Relafan-d4; Tanston-d4; Vialidon-d4

name	category	cas_number	mol_formula	mol_weight	synonym
Mefenamic acid D4	deuteriumlabeledcom	1216745-79-7	C15H11D4NO2	245.31	N-2,3-Xylylanthranilic-d4 Acid; 2-(2,3-Dimethylanilino)benzoic-d4 Acid; 2-[(2,3-Dimethylphenyl)amino]benzoic-d4 Acid; 2',3'-Dimethyl-N-phenylanthranilic-d4 Acid; Bafameritin M-d4; Baphameritin M-d4; Bonabol-d4; C.I. 473-d4; CN 35355-d4; Coslan-d4; INF 3355-d4; In-M-d4; Lysalgo-d4; Mefacit-d4; Mefenacid-d4; Mefenamic-d4 Acid; Mephenamic-d4 Acid; N-(2,3-Dimethylphenyl)anthranilic-d4 Acid; N-(2,3-Xylyl)-2-aminobenzoic-d4 Acid; N-(2,3-Xylyl)anthranilic-d4 Acid; NSC 94437-d4; Namphen-d4; Parkemed-d4; Ponalar-d4; Ponstan-d4; Ponstel-d4; Ponstil-d4; Ponstyl-d4; Pontal-d4; Relafan-d4; Tanston-d4; Vialidon-d4
5-OH-2 Chloro Pyridine 15 N D3	deuteriumlabeledcompounds		15NC5HD3ClO	133.56	N-(6-Chloro-3-pyridinyl)acetamide; 5-(Acetamido)-2-chloropyridine 15ND3
3 OH Agomelatin D3	deuteriumlabeledcom	NA	C15H14D3NO3	262.32	S 21540; N-[2-(3-Hydroxy-7-methoxy-1-naphthalenyl)ethyl]acetamide d3;

name	category	cas_number	mol_formula	mol_weight	synonym
Nintedanib 13CD3	deuteriumlabeledcom	NA	C3013CH30D3N5O4	543.64	(3Z)-2,3-Dihydro-3-[[[4-[methyl[2-(4-methyl-1-piperazinyl)acetyl]amino]phenyl]amino]phenylmethylene]-2-oxo-H-Indole-6-carboxylic Acid Methyl Ester-13CD3;
25-Hydroxyvitamin D2-d6	deuteriumlabeledcom	1262843-46-8	C28H38D6O2	418.68	(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]cyclohexanol-d6; (3β,5Z,7E,22E)-9,10-Secoergosta-5,7,10(19),22-tetraene-3,25-diol-d6; 25-Hydroxycalciferol-d6; 25-Hydroxyergocalciferol-d6; Ercalcidiol-d6;
Levothyroxine-13C915N	deuteriumlabeledcom	NA	C6H12ClI4O4 13C9	823.33	O-(4-Hydroxy-3,5-diiodophenyl)-3,5-diiodo-L-tyrosine; (-)-Thyroxine; 3,3',5,5'-Tetraiodo-L-thyronine 13C915N

name	category	cas_number	mol_formula	mol_weight	synonym
Sacubitril 13C4	deuteriumlabeledcom	149709-44-4 unlabeled	C2013C4H29NO5	415.51	[S-(R*,S*)]-[1,1'-Biphenyl]-4-pentanoic Acid, γ -[(3-carboxy-1-oxopropyl)amino]- α -methyl-Ethyl Ester-13C4;(2R,4S)-4-[(3-Carboxy-1-oxopropyl)amino]-4-[(p-phenylphenyl)methyl]-2-methylbutanoic Acid Ethyl Ester-13C4;(2R,4S)-5-(Biphenyl-4-yl)-4-[(3-carboxypropionyl)amino]-2-methylpentanoic Acid Ethyl Ester-13C4
15 OH Lubiprostone D4	deuteriumlabeledcom	NA	C20H30D4F2O5	396.50	(11 α)-16,16-Difluoro-11,15-dihydroxy-9-oxoprostan-1-oic Acid-d4
Fenpiverinium D3 bromide	deuteriumlabeledcom	NA	C22H26D3N2OBr	420.41	1-(4-Amino-4-oxo-3,3-diphenylbutyl)-1-methylpiperidinium Bromide d3; 1-(3-Carbamoyl-3,3-diphenylpropyl)-1-methylpiperidinium Bromide d3; 2,2-Diphenyl-2-(2-piperidinoethyl)acetamide Methyl Bromide d3;

name	category	cas_number	mol_formula	mol_weight	synonym
Micafungin-d11 sodium Salt	deuteriumlabeledcom	NA	C ₅₆ H ₅₉ D ₁₁ N ₉ NaO ₂	1303.32	1-[(4R,5R)-4,5-Dihydroxy-N ² -[4-[5-[4-(pentyloxy)phenyl]-3-isoxazolyl]benzoyl]-L-ornithine]-4-[(4S)-4-hydroxy-4-[4-hydroxy-3-(sulfoxy)phenyl]-L-threonine]pneumocandin A0 Monosodium Salt-d11; Funguard-d11
Caspofungin-d4 acetate	deuteriumlabeledcom	1131958-73-0	C ₅₆ H ₉₂ D ₄ N ₁₀ O ₁₉	1217.44	1-[(4R,5S)-5-[(2-Aminoethyl)amino]-N ² -[(10R,12S)-10,12-dimethyl-1-oxotetradecyl]-4-hydroxy-L-ornithine]-5-(threo-3-hydroxy-L-ornithine)pneumocandin B0 Diacetate-d4; Cancidas-d4; Caspofungin Diacetate-d4; L 743872-d4; L 743873-d4; MK 0991-d4; 1-[(4R,5S)-5-[(2-Aminoethyl)amino]-N ² -[(10R,12S)-10,12-dimethyl-1-oxotetradecyl]-4-hydroxy-L-ornithine]-5-[(3R)-3-hydroxy-L-ornithine]pneumocandin B0 Diacetate-d4
Elvitegravir-13CD3	deuteriumlabeledcom	NA	C ₂₂ H ₂₀ CIFNO ₅ 13C	451.88	6-[(3-Chloro-2-fluorophenyl)methyl]-1,4-dihydro-1-[(1S)-1-hydroxymethyl-2-methylpropyl]-7-methoxy-4-oxo-3-quinolinecarboxylic Acid-13cD3

name	category	cas_number	mol_formula	mol_weight	synonym
Clavulanic Acid methyl d3 Ester	deuteriumlabeledcom	NA	C ₉ H ₈ D ₃ NO ₅	216.21	(2R,3Z,5R)-3-(2-Hydroxyethylidene)-7-oxo-4-oxa-1-azabicyclo[3.2.0]heptane-2-carboxylic Acid Methyl-d3 Ester; [2R-(2 α ,3Z,5 α)]-3-(2-Hydroxyethylidene)-7-oxo-4-oxa-1-azabicyclo[3.2.0]heptane-2-carboxylic Acid Methyl-d3 Ester; Methyl-d3 Clavulanate
Pitofenone D4	deuteriumlabeledcom	NA	C ₂₂ H ₂₂ D ₄ ClNO ₄	407.93	4'-(β -Piperidinoethoxy)-2-(carbomethoxy)benzophenone Hydrochloride D4; 2-[4-[2-(1-Piperidinyl)ethoxy]benzoyl]benzoic Acid Methyl Ester Hydrochloride D4;
Olaparib D5	deuteriumlabeledcom	NA	C ₂₄ H ₁₈ D ₅ FN ₄ O ₃	439.5	4-[[3-[[4-(Cyclopropylcarbonyl)-1-piperazinyl]carbonyl]-4-fluorophenyl]methyl]-1(2H)-phthalazinone D5;
Mexiletine D6	deuteriumlabeledcom	1329835-60-0	C ₁₁ H ₁₁ D ₆ NO · HCl	221.76	1-(2,6-Dimethylphenoxy)-2-propanamine-d6 Hydrochloride; 1-Methyl-2-(2,6-xylyloxy)ethylamine-d6 Hydrochloride; Katen-d6; Ko 1173-d6; Ko 1173Cl-d6; Mexilitene-d6; Mexitil-d6; Ritalmex-d6

name	category	cas_number	mol_formula	mol_weight	synonym
Acotiamide D6	deuteriumlabeledcom	NA	C21H24D6N4O5S	456.59	N-[2-[Bis(1-methylethyl)amino]ethyl]-2-[(2-hydroxy-4,5-dimethoxybenzoyl)amino]-4-thiazolecarboxamide -D6
Teneligliptin D8	deuteriumlabeledcom	1391012-95-5	C22H22D8N6OS	434.63	[(2S,4S)-4-[4-(3-Methyl-1-phenyl-1H-pyrazol-5-yl)-1-piperazinyl]-2-pyrrolidinyl]-3-thiazolidinylmethanone-d8; 3-[[[(2S,4S)-4-[4-(3-Methyl-1-phenyl-1H-pyrazol-5-yl)-1-piperazinyl]-2-pyrrolidinyl]carbonyl]thiazolidine-d8; Tenelia-d8
Carbocysteine-13C3	deuteriumlabeledcom	NA		182.17	S-Carboxymethyl-L-cysteine-13C3; (2R)-2-Amino-3-[(carboxymethyl)thio]propionic Acid-13C3; (R)-S-(Carboxymethyl)cysteine-13C3;
Obeticholic Acid Glycine D4	deuteriumlabeledcom	NA	C28H42D4NNaO5	503.68	2-[[[(3 α ,5 β ,6 α ,7 α)-6-Ethyl-3,7-dihydroxy-24-oxocholan-24-yl]amino]ethanesulfonic Acid-d4 Sodium Salt

name	category	cas_number	mol_formula	mol_weight	synonym
Obeticholic Acid Taurine D4	deuteriumlabeledcom	NA	C28H44D4NNaO6S	553.76	2-[[[(3 α ,5 β ,6 α ,7 α)-6-Ethyl-3,7-dihydroxy-24-oxocholan-24-yl]amino]ethanesulfonic Acid-d4 Sodium Salt A3
Obeticholic Acid D4	deuteriumlabeledcom	459789-99-2 unlabeled	C26H44O4	424.66	3 α ,5 β ,6 α ,7 α)-6-Ethyl-3,7-dihydroxycholan-24-oic Acid-d4; 3 α ,7 β -Dihydroxy-6 α -ethyl-5 β -cholan-24-oic Acid-d4
Velpatasvir D6	deuteriumlabeledcom	NA	C49H48D6N8O8	889.04	Methyl [(2S)-1-[(2S,5S)-2-[9-[2-[(2S,4S)-1-[(2R)-2-[(Methoxycarbonyl)amino]-2-phenylacetyl]-4-(methoxymethyl)pyrrolidin-2-yl]-1H-imidazol-5-yl]-1,11-dihydroisochromeno[4',3':6,7]naphtho[1,2-d]imidazol-2-yl]-5-methylpyrrolidin-1-yl]-3-methyl-1-oxobutan-2-yl]carbamate—D6
7 Desbutyl Dronedarone D7	deuteriumlabeledcom	NA	C27H30D7CIN2O5S	544.16	N-[2-Butyl-3-[4-[3-(butylamino)propoxybenzoyl]-5-benzofuranyl]-methanesulfonamide-d7 Hydrochloride; SR 35021-d7;

name	category	cas_number	mol_formula	mol_weight	synonym
Domperidone D6	deuteriumlabeledcom	1329614-18-7	C ₂₂ H ₁₈ D ₆ N ₅ O ₂ Cl	431.95	5-Chloro-1-[1-[3-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)propyl]-4-piperidinyl]-1,3-dihydro-2H-benzimidazol-2-one-d ₆ ; Euciton-d ₆ ; Evoxin-d ₆ ; Gastronorm-d ₆ ; KW 5338-d ₆ ; Mod-d ₆ ; Motilium-d ₆ ; NSC 299589-d ₆ ; Nauzelin-d ₆ ; Nauzelin Ds-d ₆ ; Peridon-d ₆ ; Peridys-d ₆
Piracetam D6	deuteriumlabeledcom	7491-74-9 (non-labelled)	C ₆ H ₄ N ₂ O ₂ D ₆	148.19	2-Oxo-1-pyrrolidineacetamide-d ₆ ; (2-Oxopyrrolidino)acetamide-d ₆ ; 2-(2-Oxopyrrolidin-1-yl)acetamide-d ₆ ;
Brexpiprazole Metabolite DM-3411 D8	deuteriumlabeledcom	NA	C ₂₅ H ₁₉ D ₈ N ₃ O ₃ S	457.62	7-[4-[4-(1-Oxidobenzo[b]thien-4-yl)-1-piperazinyl]butoxy]-2(1H)-quinolinone- D8
Droxidopa 13C215N HCl	deuteriumlabeledcom	NA	C ₇ ¹³ C ₂ H ₁₂ Cl ¹⁵ NO ₅	252.63	3-Dihydroxy-D-tyrosine-13C215N; 3-(3,4-Dihydroxyphenyl)serine-c;

name	category	cas_number	mol_formula	mol_weight	synonym
Ibrutinib D5	deuteriumlabeledcom	1553977-17-5	C ₂₅ H ₁₉ D ₅ N ₆ O ₂	445.54	1-[(3R)-3-[4-Amino-3-(4-phenoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl]-1-piperidinyl]-2-propen-1-one-d5; PCI 32765-d5; PCI 32765-00-d5; CRA 032765-d5; (R)-1-(3-(4-Amino-3-(4-phenoxyphenyl)-1H-pyrazolo[3,4-d]pyrimidin-1-yl)piperidin-1-yl)prop-2-en-1-one-d5
Brexipiprazole DH-3,411 D8	deuteriumlabeledcom	1427049-19-1	C ₂₅ H ₁₉ D ₈ N ₃ O ₃ S	457.62	7-[4-(4-(Benzo[b]thien-4-yl)-piperazin-1-yl)butoxy]-1H-quinolin-2-one-d8; OPC 34712-d8
Dolutegravir D6	deuteriumlabeledcom	1407166-95-3	C ₂₀ H ₁₂ D ₆ F ₂ N ₃ O ₅ N	447.4	(4R,12aS)-N-[(2,4-Difluorophenyl)methyl-d2]-3,4,6,8,12,12a-hexahydro-7-hydroxy-4-(methyl-d3)-6,8-dioxo-2H-pyrido[1',2':4,5]pyrazino[2,1-b][1,3]oxazine-4-d-9-carboxamide
Pomalidomide D4	deuteriumlabeledcom	1416575-78-4	C ₁₃ H ₇ D ₄ N ₃ O ₄	277.27	4-Amino-2-(2,6-dioxo-3-piperidinyl)isoindole-1,3-dione-d4; 4-Amino-2-(2,6-dioxo-3-piperidyl)isoindoline-1,3-dione-d4; Actimid-d4

name	category	cas_number	mol_formula	mol_weight	synonym
7 Hydroxy Dronedarone D7	deuteriumlabeledcom	197431-02-0(unlabelled)	C27H30D7CIN2O5S	507.7	N-[2-Butyl-3-[4-[3-(butylamino)propoxybenzoyl]-5-benzofuranyl]-methanesulfonamide-d7 Hydrochloride; SR 35021-d7;
Deferasirox D4	deuteriumlabeledcom	1133425-75-8	C21H11D4N3O4	377.39	4-[3,5-Bis(2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]benzoic Acid-d4; Exjade-d4
Erlotinib HCl 13C6	deuteriumlabeledcom	1210610-07-3	C1613C6H23N3O4	435.82	N-(3-Ethynylphenyl)-6,7-bis(2-methoxyethoxy-13C6)-4-quinazolinamine Hydrochloride
LBQ sacubitrilat 13C4	deuteriumlabeledcom	149709-44-4 (unlabeled)	C1813C4H25NO5	387.41 g/mol	[S-(R*,S*)]-γ-[(3-Carboxy-1-oxopropyl)amino]-α-methyl-[1,1'-Biphenyl]-4-pentanoic Acid-13C4; (2R,4S)-4-[(3-Carboxy-1-oxopropyl)amino]-4-[(p-phenylphenyl)methyl]-2-methylbutanoic Acid-13C4; (2R,4S)-5-(Biphenyl-4-yl)-4-[(3-carboxypropionyl)amino]-2-methylpentanoic Acid-13C4; Sacubitrilat-13C4; LBQ 657-13C4

name	category	cas_number	mol_formula	mol_weight	synonym
Norethindrone D6	deuteriumlabeledcom	68-22-4 (unlabelled)	C20H20D6O2	304.47	(17 α)-17-Hydroxy-19-norpregn-4-en-20-yn-3-one; 19-Nor-17 α - -ethynyl-4-androsten-17 β -ol-3-one; 17 α -Ethinyl-19-nortestosterone; 19-Norethisterone-D6
Omeprazole D3	deuteriumlabeledcom	922731-01-9	C17H16D3N3O3S	384.43	6-(Methoxy-d3)-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole-4,5,7-d3; rac-Esomeprazole-d3; 6-(methoxy-d3)-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-1H-Benzimidazole
R cinacalcet D3 HCL	deuteriumlabeledcom	364752-34-3 (unlabelled)	C22H20D3ClF3N	396.89	α -(Methyl-d3)-N-[3-[3-(trifluoromethyl)phenyl]propyl]-1-naphthalenemethanamine Hydrochloride; N-(3-(3-(trifluoromethyl)phenyl)propyl)-1-(1-naphthyl)ethylamine-d3 Hydrochloride

name	category	cas_number	mol_formula	mol_weight	synonym
Domperidone D6 HCl	deuteriumlabeledcom	1329614-18-7	C ₂₂ H ₁₈ D ₆ N ₅ O ₂ Cl.H	468.41	5-Chloro-1-[1-[3-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)propyl]-4-piperidinyl]-1,3-dihydro-2H-benzimidazol-2-one-d ₆ ; Euciton-d ₆ ; Evoxin-d ₆ ; Gastronorm-d ₆ ; KW 5338-d ₆ ; Mod-d ₆ ; Motilium-d ₆ ; NSC 299589-d ₆ ; Nauzelin-d ₆ ; Nauzelin Ds-d ₆ ; Peridon-d ₆ ; Peridys-d ₆
5-Hydroxy Saxagliptin-15N,D2 Hydrochloride	deuteriumlabeledcom	N/A	C ₁₈ H ₂₃ D ₂ N ₂ 15NO ₃	370.88	(1S,3S,5S)-2-[(2S)-2-Amino-2-(3-hydroxytricyclo[3.3.1.1 ^{3,7}]dec-1-yl)acetyl]-2-azabicyclo[3.1.0]hexane-3-carbonitrile-15N,D2 Hydrochloride; BMS 477118-15N,D2 Hydrochloride; BMS 477118-11-15N,D2 Hydrochloride; Onglyza-15N,D2 Hydrochloride

name	category	cas_number	mol_formula	mol_weight	synonym
Pyridoxal D3	deuteriumlabeledcom	1173023-49-8	C8H8D3NO3	172.2	3-Hydroxy-5-(hydroxymethyl)-2-methyl-4-pyridinecarboxaldehyde-d3 Hydrochloride; 2-Methyl-3-hydroxy-4-formyl-5-hydroxymethylpyridine-d3 Hydrochloride; 3-Hydroxy-5-(hydroxymethyl)-2-methyl-4-pyridinecarboxaldehyde-d3 Hydrochloride; 3-Hydroxy-5-hydroxymethyl-2-methylisonicotinaldehyde-d3 Hydrochloride
Pyridoxine D3	deuteriumlabeledcom	NA	C8H6D3NO3	172.2	5-Hydroxy-6-(methyl-d3)-3,4-pyridinedimethanol Hydrochloride; Pyridoxol-d3 Hydrochloride; Aderomine-d3 Hydrochloride; Aderoxin-d3; Hexobion-d3; Pyridox-d3

name	category	cas_number	mol_formula	mol_weight	synonym
Lanreotide-D8	deuteriumlabeledcom	NA	C ₅₄ H ₆₁ D ₈ N ₁₁ O ₁₀ S	1104.319	3-(2-Naphthalenyl)-D-alanyl-L-cysteinyl-L-tyrosyl-D-tryptophyl-L-lysyl-L-valyl-L-cysteinyl-, cyclic (2→7)-disulfide L-Threoninamide-d8; 1,2-Dithia-5,8,11,14,17-pentaazacycloeicosane, cyclic peptide deri-d8.; 2: PN: WO0006185 PAGE: 8 Claimed Protein-d8; BIM 23014C-d8; Somatulina-d8; Somatuline-d8
Pramlintide-D10	deuteriumlabeledcom	NA		3959.741	5-L-Proline-28-L-proline-29-L-proline-amylin (human)-d3 Trifluoroacetate; Tripo-amylin-d3
Cysteamine D4 Hcl	deuteriumlabeledcom	1219805-04-5	C ₂ H ₄ D ₄ CINS	117.63	2-Aminoethane-d4-thiol; 2-Mercaptoethylamine-d4 Hydrochloride
Ipratropium D3 Bromide	deuteriumlabeledcom	NA	C ₂₀ H ₂₇ N ₃ O ₃ D ₃ Br	335.51	(3-endo,8-syn)-3-(3-Hydroxy-1-oxo-2-phenylpropoxy)-8-(methyl-d3)-8-(1-methylethyl)-8-azoniabicyclo[3.2.1]octane Iodide

name	category	cas_number	mol_formula	mol_weight	synonym
Nefopam D3	deuteriumlabeledcom	1346603-30-2	C17H16NOD3.HCl	292.5	3,4,5,6-Tetrahydro-5-(methyl-d3)-1-phenyl-1H-2,5-benzoxazocine Hydrochloride; (+/-)-Nefopam-d3 Hydrochloride; Acupan-d3; Ajan-d3; Fenazoxine-d3; Fenazoxine-d3 Hydrochloride;
Tenofovir D5 Alafenamide	deuteriumlabeledcom	379270-36-7 (unlabelled)	C21H24D5N6O5P	481.5	1-Methylethyl Ester N-[[[(1R)-2-(6-Amino-9H-purin-9-yl)-1-methylethoxy)methyl]phenoxyphosphinyl]-L-alanine-d5
Sitagliptin D4 HCL	deuteriumlabeledcom	486460-32-6 (unlabelled)	C16H12D4ClF6N5O	447.8	7-[3-Amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-5,6,7,8-tetrahydro-3-(trifluoromethyl)-1,2,4-triazolo[4,3-a]pyrazine-d4 Hydrochloride
Palbociclib D8	deuteriumlabeledcom	1628752-83-9	C24H21D8N7O2	455.58	6-Acetyl-8-cyclopentyl-5-methyl-2-[[5-(piperazin-1-yl)pyridin-2-yl]amino]-8H-pyrido[2,3-d]pyrimidin-7-one-d8
Eliglustat D4	deuteriumlabeledcom	491833-29-5 (Unlabelled)	C23H32D4N2O4	408.57	N-[(1R,2R)-1-(2,3-Dihydro-1,4-benzodioxin-6-yl)-1-hydroxy-3-pyrrolidin-1-ylpropan-2-yl]octanamide-d4

name	category	cas_number	mol_formula	mol_weight	synonym
Rifaximin D6	deuteriumlabeledcom	1262992-43-7	C43H45D6N3O11	791.92	4-Deoxy-4'-methylpyridol[1',2'-1,2]imidazo[5,4-c]rifamycin SV-d6; Rifamycin L 105-d6; Rifaxidin-d6; L-105-d6; Fatroximin-d6; Normix-d6; Rifacol-d6; Xifaxan-d6
Sildenafil D3	deuteriumlabeledcom	1126745-90-1	C22H27D3N6O4S	477.6	1-[[3-(4,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo[4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl]sulfonyl]-4-methylpiperazine-d3; 5-[2-Ethoxy-5-[[4-(methyl-d3)-1-piperazinyl]sulfonyl]phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one
17 Desacetyl Norgestimate D8	deuteriumlabeledcom	53016-31-2 (<i>of the unlabelled compound</i>)	C21H21D8NO2	335.52	(17 α)-13-Ethyl-17-hydroxy-18,19-dinorpregn-4-en-20-yn-3-one-d8 Oxime; 17-Deacetylnorgestimate-d8; 18-Methylnorethindrone-d8 Oxime; D-Norgestrel-d8 3-Oxime; Levonorgestrel-d8 3-Oxime; Norelgestromin-d8

name	category	cas_number	mol_formula	mol_weight	synonym
Efavirenz D5	deuteriumlabeledcom	1132642-95-5	C14H4D5ClF3NO2	320.71	6-Chloro-4-(2-cyclopropyl-d5-ethynyl)-1,4-dihydro-4-(trifluoromethyl)-2H-3,1-benzoxazin-2-one; DMP 266-d5; L 743726-d5; Stocrin-d5; Sustiva-d5;
Ticagrelor D7	deuteriumlabeledcom	1265911-55-4	C23H21D7F2N6O4S	529.38	(1S,2S,3R,5S)-3-[7-[[[(1R,2S)-2-(3,4-D1,2-Cyclopentane diolifluorophenyl)cyclopropyl]amino]-5-(propylthio-d7)-3H-1,2,3-triazolo[4,5-d]pyrimidin-3-yl]-5-(2-hydroxyethoxy)-1,2-cyclopentane diol
Levetiracetam D6	deuteriumlabeledcom	1133229-29-4	C8H8D6N2O2	176.25	(α S)- α -(Ethyl-1,1,2,2,2-d5)-2-oxo-1-pyrrolidineacetamide- α -d; (-)-Levetiracetam-d6; Keppra-d6; Levesam 500-d6
Lamotrigine 13CD3	deuteriumlabeledcom	84057-84-1 (non-labelled)	C813CH4D3Cl2N5	262.09	6-(2,3-Dichlorophenyl)-1,2,4-triazine-3,5-diamine-13C3; 3,5-Diamino-6-(2,3-dichlorophenyl)-1,2,4-triazine-13C3; BW 430C-13C3; LTG-13C3; Lamictal-13C3; Lamictal XR-13C3;

name	category	cas_number	mol_formula	mol_weight	synonym
9-OH Risperidone D4	deuteriumlabeledcom	1020719-55-4	C ₂₃ H ₂₃ D ₄ FN ₄ O ₃	430.51	3-[2-[4-(6-Fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]ethyl-d ₄]-6,7,8,9-tetrahydro-9-hydroxy-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one; Invega-d ₄ ; Paliperidone-d ₄ ; R 76477-d ₄ ; RO 76477-d ₄ ; Risperidone Imp. C (EP)-d ₄
Lumefantrine D9	deuteriumlabeledcom	NA	C ₃₀ H ₂₃ D ₉ Cl ₃ NO	538	Benflumelol-d ₉ ; Benflumetol-d ₉ ; dl-Benflumelol-d ₉
Pimobendan D3	deuteriumlabeledcom	N/A	C ₁₉ H ₁₅ D ₃ N ₄ O ₂	337.39	4,5-Dihydro-6-[2-(4-methoxyphenyl)-1H-benzimidazol-6-yl]-5-methyl-3(2H)-pyridazinone-d ₃ ; 4,5Dihydro-6-[2-(4-methoxyphenyl)-1H-benzimidazol-5-yl]-5-methyl-3(2H)-pyridazinone; Acardi-d ₃ ; Pimobendan-d ₃ ;UD-CG 115-d ₃ ; UD-CG 115BS-d ₃ ; Vetmedin-d ₃ ; dl-Pimobendan-d ₃
Tadalafil D3	deuteriumlabeledcom	960226-55-5	C ₂₂ H ₁₆ D ₃ N ₃ O ₄	392.42	(6R,12aR)-6-(1,3-Benzodioxol-5-yl)-2,3,6,7,12,12a-hexahydro-2-(methyl-d ₃)pyrazino[1',2':1,6]pyrido[3,4-b]indole-1,4-dione; Cialis-d ₃ ; GF 196960-d ₃ ; IC 351-d ₃ ; ICOS 351-d ₃ ; Tildenafil-d ₃

name	category	cas_number	mol_formula	mol_weight	synonym
Deracoxib D3	deuteriumlabeledcom	N/A	C17H11D3F3N3O3S	400.39	4-[3-(Difluoromethyl)-5-(3-fluoro-4-methoxyphenyl)-1H-pyrazol-1-yl]benzenesulfonamide-d3; Deram-d3; Deramaxx-d3; 4-[5-(3-Fluoro-4-methoxyphenyl)-3-(difluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide-d3
Ritonavir D6	deuteriumlabeledcom	1217720-20-1	C37H42D6N6O5S2	726.98	(3S,4S,6S,9S)-4-Hydroxy-12-methyl-9-(1-methylethyl-d6)-13-[2-(1-methylethyl)-4-thiazolyl]-8,11-dioxo-3,6-bis(phenylmethyl)-2,7,10,12-tetraazatridecanoic Acid 5-thiazolylmethyl Ester
Clonidine D4 HCl	deuteriumlabeledcom	67151-02-4	C9H6D4Cl3N3	270.58	N-(2,6-Dichlorophenyl)-4,5-dihydro-1H-(imidazol-d4)-2-amine Hydrochloride; 2-(2,6-Dichloroanilino)-2-(imidazoline-d4) Hydrochloride; Atensina-d4; Capresin-d4; Catapres-d4; Haemiton-d4; Hemiton-d4; Isoglaucon-d4; Katapresan-d4; Neuclon-d4; Normopresan-d4
Exemestane 13CD4	deuteriumlabeledcom	107868-30-4 (unlabelled)	C1913CH20D4O2	301.4	6-Methyleneandrosta-1,4-diene-3,17-dione-19-13C,D4; Aromasin-19-13C,D4

name	category	cas_number	mol_formula	mol_weight	synonym
Isotretinoine D5	deuteriumlabeledcom	4759-48-2 unlabeled	C20H23D5O2	305.47	3,7-Dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2Z,4E,6E,8E-nonatetranenoic Acid-d5; Isotretinoin-d5; 13-cis-Vitamin A Acid-d5; Accutane-d5; Isotretinoin-d5
Pirfenidone D5	deuteriumlabeledcom	53179-13-8 (unlabeled)	C12H6D5NO	190.25	5-Methyl-N-phenyl-2-1H-pyridone-d5
Canagliflozin D4	deuteriumlabeledcom	842133-18-0 (unlabeled)	C24H21D4FO5S	448.54	(1S)-1,5-Anhydro-1-C-[3-[[5-(4-fluorophenyl)-2-thienyl]methyl]-4-methylphenyl]-D-glucitol-D4
Ondansetron D6	deuteriumlabeledcom	1132757-82-4	C18H13D6N3O	299.41	1,2,3,9-Tetrahydro-9-(methyl-d3)-3-[(2-methyl-1H-imidazol-1-yl)methyl]-4H-carbazol-4-one; Ondansetron-d6; Setron-d6; Yatrox-d6; Zofran-d6; Zophren-d6; Zudan-d6
Paclitaxel D5	deuteriumlabeledcom	33069-62-4 (unlabeled)	C47H46D5NO14	858.94	Abraxane-d5; Genaxol-d5; Genetaxyl-d5; OncoGel-d5; Onxal-d5; Pacliex-d5; (-)-Paclitaxel-d5; Taxol-d5; Yewtaxan-d5

name	category	cas_number	mol_formula	mol_weight	synonym
Venetoclax D8	deuteriumlabeledcom	N/A	C45H42D8CIN7O7S	876.5	4-[4-[[2-(4-Chlorophenyl)-4,4-dimethyl-1-cyclohexen-1-yl]methyl]-1-piperazinyl]-N-[[3-nitro-4-[[tetrahydro-2H-pyran-4-yl)methyl]amino]phenyl]sulfonyl]-D82-(1H-
Venlafaxine D6 HCl	deuteriumlabeledcom	N/A	C17H22D6CINO2	319.9	1-[2-(Dimethylamino)-1-(4-methoxyphenyl)ethyl]cyclohexanol-d6
Clidinium Iodide D3	deuteriumlabeledcom	N/A	C22H23D3INO3	482.38	3-[(Hydroxyphenylacetyl)oxy]-1-methyl-1-azoniabicyclo[2,2,2]octane Iodide D3
Hydroxy Risperidone D4	deuteriumlabeledcom	1020719-55-4	C23H23D4FN4O3	430.51	3-[2-[4-(6-Fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]ethyl-d4]-6,7,8,9-tetrahydro-9-hydroxy-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one; 9-Hydroxyrisperidone-d4; R 76477-
Prasugrel Trans R-138727	deuteriumlabeledcom	NA	C2113C6H29CIFNO3	540	(2E)-2-[1-[2-Cyclopropyl-1-(2-fluorophenyl)-2-oxoethyl]-4-mercapto-3-piperidinylidene]acetic Acid

name	category	cas_number	mol_formula	mol_weight	synonym
Saxagliptin metabolite 15ND2	deuteriumlabeledcom	1309934-06-2	C ₁₈ H ₂₃ D ₂ N ₂ 15NO ₃	370.88	(1S,3S,5S)-2-[(2S)-2-Amino-2-(3-hydroxytricyclo[3.3.1.1 ^{3,7}]dec-1-yl)acetyl]-2-azabicyclo[3.1.0]hexane-3-carbonitrile-15N,D2 ; BMS 477118-15N,D2; ; Onglyza-15N,D2
Ebastine D5	deuteriumlabeledcom	158641-28-2 (unlabelled) 1216953-13-7 (d5-unlabelled)	C ₃₂ H ₃₄ D ₅ NO ₂	474.70g/mol	1-[4-(1,1-Dimethylethyl)phenyl]-4-[4-(diphenyl-d5-methoxy)]-1-piperidinyl]-1-butan- one; Estivan-d5; Ebastel-d5; Ebastin-d5; Kestine-d5
Carbozantinib D4	deuteriumlabeledcom	NA	C ₂₈ H ₂₀ D ₄ FN ₃ O ₅	505.54	N-[4-[(6,7-Dimethoxy-4-quinolinyl)oxy]phenyl]-N'-(4-fluorophenyl)-1,1-cyclopropanedicarboxamide-d4 (2S)-2-Hydroxybutanedioic Acid; Cabozantini-d4 S-Malate; XL 184-d4;
Fenofibric acid D6	deuteriumlabeledcom	1092484-69-9	C ₁₇ H ₉ D ₆ ClO ₄	324.79	2-[4-(4-Chlorobenzoyl)phenoxy]-2-methylpropanoic-d6 Acid; FNF Acid-d6; NSC 281318-d6; Procetofenic Acid-d6

name	category	cas_number	mol_formula	mol_weight	synonym
Nizatidine D3	deuteriumlabeledcom	1246833-99-7	C12H18D3N5O2S2	334.47	N-[2-[[[2-[(Dimethylamino)methyl]-4-thiazolyl]methyl]thio]ethyl]-N'-(methyl-d3)-2-nitro-1,1-ethenediamine; LY-139037-d3; ZE-101-d3; ZL-101-d3; Axid-d3; Calmaxid-d3; Cronizat-d3; Distaxid-d3; Gastrax-d3; Nizax-d3; Nizaxid-d3
Piperazine N desmethylsildenafil D8	deuteriumlabeledcom	1185168-06-2	C21H20D8N6O4S	468.6	5-[2-Ethoxy-5-(1-piperazinylsulfonyl)phenyl]-1,6-dihydro-1-methyl-3-propyl-7H-pyrazolo[4,3-d]pyrimidin-7-one-d8; Desmethylsildenafil-d8
Olanzapine D3	deuteriumlabeledcom	786686-79-1	C17H17D3N4S	315.44	2-Methyl-4-(4-methyl-d3-1-piperazinyl)-10H-thieno[2,3-b][1,5]benzodiazepine; Integrol-d3; LY 170053-d3; Lanzac-d3; Oleanz-d3; Oliza-d3; Oltal-d3; Zyprexa-d3
R-Nicardipine D3	deuteriumlabeledcom	N/A	C26H29N3O6	479.53	R-1,4-Dihydro-2,6-dimethyl-4-(3-nitrophenyl)-3,5-pyridinedicarboxylic Acid Methyl 2-[Methyl-d3(phenylmethyl)amino]ethyl Ester HydrochlorideAntagonyl-d3; Barizin-d3; Bionicard-d3; Cardene-d3; Dacarel-d3; Vasonase-d3;

name	category	cas_number	mol_formula	mol_weight	synonym
S-Nicardipine D3	deuteriumlabeledcom	N/A	C26H29N3O6	479.53	S-1,4-Dihydro-2,6-dimethyl-4-(3-nitrophenyl)-3,5-pyridinedicarboxylic Acid Methyl 2-[Methyl-d3(phenylmethyl)amino]ethyl Ester HydrochlorideAntagonyl-d3; Barizin-d3;
Lenvatinib D4	deuteriumlabeledcom	417716-92-8 (unlabeled)	C21 H15 D4 Cl N4 O	430.88	4-[3-Chloro-4-[[[(cyclopropylamino)carbonyl]amino]phenoxy]-7-methoxy-6-quinolinecarboxamide-d5; 4-[3-Chloro-4-[(cyclopropylaminocarbonyl)amino]phenoxy]-7-methoxy-6-quinolinecarboxamide-d4
Metaxolone D6	deuteriumlabeledcom	1189944-95-3	C12H9D6NO3	227.29	5-[(3,5-Dimethylphenoxy)methyl]oxazolidin-2-one-d6; AHR-438-d6; Skelaxin-d6
Osimertinib 13C D3	deuteriumlabeledcom	1421373-65-0 unlabeled	C2713CH30D3N7O2	503.63	N-[2-[[2-(Dimethylamino)ethyl]methylamino]-4-methoxy-5-[[4-(1-methyl-1H-indol-3-yl)-2-pyrimidinyl]amino]phenyl]-2-propenamide 13CD3; AZD9291 13

name	category	cas_number	mol_formula	mol_weight	synonym
Crizotinib D9 HCl	deuteriumlabeledcom	877399-54-7 unlabeled	C21H14D9N5OFCl3	495.85	3-[(1R)-1-(2,6-Dichloro-3-fluorophenyl)ethoxy]-5-[1-(4-piperidinyl-d4)-1H-pyrazol-4-yl]-2-pyridinamine-d9; (R)-3-[1-(2,6-Dichloro-3-fluorophenyl)ethoxy]-5-[1-(piperidin-4-yl-d4)-1H-pyrazol-4-yl]pyridin-2-ylamine-d9; PF 02341066-d5; PF 2341066-d5; [3-[[[(R)-1-(2,6-Dichloro-3-fluorophenyl)ethyl]oxy]-5-[1-(piperidin-4-yl-d4)-1H-pyrazol-4-yl]pyridin-2-yl]amine-d9
Perindopril D4 HCl	deuteriumlabeledcom	1356929-58-2	C19H29D4N2O5Cl	408.95	(2S,3aS,7aS)-1-[(2S)-2-[[[(1S)-1-(Ethoxycarbonyl)butyl]amino]-1-oxopropyl-d4]octahydro-1H-indole-2-carboxylic Acid; [2S-[1[R*(R*)],2 α ,3a β ,7a β]]-1-[2-[[1-(Ethoxycarbonyl) butyl]amino]-1-oxopropyl-d4]octahydro-1H-indole-2-carboxylic Acid
Oseltamivir D5	deuteriumlabeledcom	NA	C16H23D5N2O4	317.44	(3R,4R,5S)-4-(Acetyl-2,2,2-d3-amino)-5-amino-3-(1-ethylpropoxy)-1-cyclohexene-1-carboxylic Acid Ethyl Ester

name	category	cas_number	mol_formula	mol_weight	synonym
Bendroflumethiazid e D5	deuteriumlabeledcom	1330183-13-5	C15H9D5F3N3O4S2	426.45	3,4-Dihydro-3-(phenylmethyl-d5)-6-(trifluoromethyl)-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-Dioxide
Digoxin D3	deuteriumlabeledcom	127299-95-0	C41H64O14	783.45	(3 β ,5 β ,12 β)-3-[(O-2,6-Dideoxy- β -D-ribo-hexopyranosyl-(1-4)-O-2,6-dideoxy- β -D-ribo-hexopyranosyl-(1-4)-2,6-dideoxy- β -D-ribo-hexopyranosyl)oxyl]-12,14-dihydroxycard-20(22)-enolide-d3
Ciprofloxacin D8 HCl	deuteriumlabeledcom	1216659-54-9	C17H11D8ClFN3O3	375.85	1-Cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl-d8)-3-quinolinecarboxylic Acid Hydrochloride
Glycoursodeoxycho lic Acid D4	deuteriumlabeledcom	2044276-17-5	C26H39D4NO5	453.65	N-[(3.alpha.,5.beta.,7.beta.)-3,7-dihydroxy-24-oxocholan-24-yl]Glycine D4; 3.alpha.,7.beta.-Dihydroxy-5.beta.-cholanoylglycine D4;
Tauroursodeoxych olic Acid D4 Sodium	deuteriumlabeledcom	14605-22-2 (unlabelled)	C26H41D4NO6S	503.72	2-[[[(3 α ,5 β ,7 α ,12 α)-3,7,12-Trihydroxy-24-oxocholan-24-yl]amino]-ethanesulfonic Acid-d4 Sodium Salt; 3 α ,7 α ,12 α -Trihydroxy-5 β -cholanic Acid-24-aurine-d5 Sodium Salt; Cholaic Acid-d4 Sodium Salt;

name	category	cas_number	mol_formula	mol_weight	synonym
Doxazosin D8	deuteriumlabeledcom	1126484-44-9	C23H17D8N5O5	459.42	(R)-1-(4-Amino-6,7-dimethoxy-2-quinazolinyl)-4-[(2,3-dihydro-1,4-benzodioxin-2-yl)carbonyl]-piperazine-d8;
Nifedipine D6	deuteriumlabeledcom	1188266-14-9	C17H12D6N2O6	352.38	1,4-Dihydro-2,6-dimethyl-4-(2-nitrophenyl)-3,5-pyridinedicarboxylic Acid Dimethyl Ester-d6
Cobicistat D8	deuteriumlabeledcom	NA	C40H45D8N7O5S2	783.41	(3R,6R,9S)-2-Methyl-13-[2-(1-methylethyl)-4-thiazolyl]-9-[2-(4-morpholinyl)ethyl]-8,11-dioxo-3,6-bis(phenylmethyl)-2,7,10,12-tetraazatridecanoic-d8 Acid 5-Thiazolylmethyl Ester
Retigabine D4	deuteriumlabeledcom	NA	C16H14D4FN3O2	307.36	N-[2-Amino-4-[4-(fluorobenzyl-d4)amino]phenyl]carbamic Acid Ethyl Ester ; Ethyl [2-Amino-4-[[4-(fluorophenyl-d4)methyl]amino]phenyl] carbamat
Diclofenac D4	deuteriumlabeledcom	153466-65-0	C14H7D4Cl2NO2	300.17	2-((2,6-Dichlorophenyl)aminobenzeneacetic Acid-d4,

name	category	cas_number	mol_formula	mol_weight	synonym
Rufinamide 15N,D2	deuteriumlabeledcom	106308-44-5(unlabelled) 1795037-48-7 (15N,d2-labelled)	C10H6D2F2N315NC	241.2	1-[(2,6-Difluorophenyl)methyl]-1H-1,2,3-triazole-4-carboxamide-15N,d2
Carebastine D5	deuteriumlabeledcom	1189661-02-6	C32H32D5NO4	504.3	4-[4-[4-(Diphenylmethoxy-d5)-1-piperidiny]-1-oxobutyl]- α , α -dimethylbenzeneacetic Acid
Carbamazepine D10	deuteriumlabeledcom	298-46-4(unlabelled) 132183-78-9 (d10-labelled)	C15H2D10N2O	246.34	5H-Dibenz[b,f]azepine-5-carboxamide-d10; 5-Carbamoyl-5H-dibenz[b,f]azepine - d10; Amizepin-d10; Biston-d10; ; Calepsin-d10; Carbamazepen-d10; Carbamazepin-d10; Tegretol-d10
Thiothixene D8	deuteriumlabeledcom	NA	C23H21D8N3O2S2	451.67	N,N-Dimethyl-9-[3-(4-methyl-1-piperaziny)propylidene]- thioxanthene-2-sulfonamide-d8 (7Cl,8Cl)

name	category	cas_number	mol_formula	mol_weight	synonym
Alimemazine D6	deuteriumlabeledcom	1346603-88-0	C18H16D6N2S	304.48	β -Methyl-(N,N-Dimethyl-d6)-10H-phenothiazine-10-propanamine Tartrate; 10-(2-Methyl-3-(dimethyl-d6)aminopropyl)phenothiazine Tartrate; 10-[3-[(Dimethyl-d6)amino]-2-methylpropyl]phenothiazine Tartrate
Clidinium bromide D5	deuteriumlabeledcom	NA	C22H21D5BrNO3	437.39	3-[(Hydroxyphenylacetyl)oxy]-1-methyl-1-azoniabicyclo[2,2,2]octane Bromide D5
Desmethyl-Doxepin HCl D3	deuteriumlabeledcom	N/A	C18H17D3ClNO	304.83	3-(Dibenz[b,e]oxepin-11(6H)-ylidene)-N-ethyl-N-methyl-1-propanamine-d3; Dibenz[b,e]oxepin 1-Propanamine Deriv-d3.
Metformin D6 HCl	deuteriumlabeledcom	1185166-01-1	C4H6D6ClN6	171.66	N,N-Dimethylimidodicarbonimidic Diamide-d6, Hydrochloride; Diabetosan-d6; Diabex-d6, Glucophage-d6; Metiguanide-d6
Halobetasol-17-propionate D5	deuteriumlabeledcom	NA	C25H26D5ClF2O5	489.99	(6 α ,11 β ,16 β)-21-Chloro-6,9-difluoro-11-hydroxy-16-methyl-17-(1-oxopropoxy)pregna-1,4-diene-3,20-dione; Miracorten; Ulobetasol propionate; Ultravate;

name	category	cas_number	mol_formula	mol_weight	synonym
Azithromycin 13C-D3	deuteriumlabeledcom	NA	C37H13CH69D3N2O1	753	; Azitrocin-13Cd3; Ribotrex-13Cd3; Sumamed- Cd3; Trozocina-d3; Zithromaz-13Cd3; Zitromax-13Cd3
(S)-Empagliflozin D4	deuteriumlabeledcom	N/A	C23H23D4ClO7	454.94	(1S)-1,5-Anhydro-1-C-[4-chloro-3-[[4-[[[(3S)-tetrahydro-3-furanyl]oxy]phenyl]methyl]phenyl]-D-glucitol-d4
Carbamazepine-10,11-epoxide-d10	deuteriumlabeledcom	36507-30-9(unlabelled) 1219804-16-6(d10-labelled)	C15H2D10N2O	246.33	1a,10b-Dihydro-6H-dibenzo[b,f]oxireno[d]azepine-6-carboxamide-d10; 10,11-Dihydro-10,11-epoxycarbamazepine-d10; 10,11-Epoxycarbamazepine-d10; Carbamazepine-d10 10,11-Oxide
Valproic acid D4	deuteriumlabeledcom	87745-17-3	C8H12D4O2	148.24	3,3,3',3'-Tetradeuterovalproic Acid; 2-(Propyl-1,1-d2)-pentanoic-3,3-d2 Acid
Dothiepin D6 HCl	deuteriumlabeledcom	NA	C19H15D6NS HCl	337.94	3-Dibenzo[b,e]thiepin-11(6H)-ylidene-N-methyl-N-(methyl-d6)-1-propanamine HCl; Prothiadene-d6 HCl
Ursodeoxycholic-2,2,4,4-D4 Acid	deuteriumlabeledcom	NA	C24H36O4D4	396.6	$\alpha, 5\beta, 7\beta$ -3,7-Dihydroxycholan-24-oic Acid-d4; Ursodiol-d4;

name	category	cas_number	mol_formula	mol_weight	synonym
(+)-Oxybutynin-D11 HCl	deuteriumlabeledcom	NA	C22H20NO3D11.HC	405.02	α -Phenylcyclohexaneglycolic Acid 4-(Diethyl-d11-amino)-2-butynyl Ester, Hydrochloride
Pyridoxine D3 HCL	deuteriumlabeledcom	1189921-12-7	C8H8D3NO3.HCl	'208.66	5-Hydroxy-6-(methyl-d3)-3,4-pyridinedimethanol Hydrochloride
Glycochenodeoxycholic acid D4	deuteriumlabeledcom	1201918-16-2	C26H39D4NO5	453.65	N-[(3 α ,5 β ,7 α)-3,7-Dihydroxy-24-oxocholan-24-yl-2,2,4,4-d4]glycine
Prilocaine D7 HCL	deuteriumlabeledcom	NA	C13H14D7N2OCl	263.81	N-(2-Methylphenyl)-2-(propylamino)propanamide-d7 Hydrochloride; 2-(Propylamino-d7)-o-propionotoluidide Hydrochloride

name	category	cas_number	mol_formula	mol_weight	synonym
Clarithromycin-13CD3	deuteriumlabeledcom	81103-11-9 unlabeled	C3713CH66D3NO13	751.96	6-O-Methylerythromycin-13C, d3; 6-O-Methylerythromycin A-13C, d3; A 56268-13C, d3; Abbott 56268-13C, d3; Antibiotic A 56268-13C, d3; Antibiotic TE 31-13C, d3; BIAXIN XL-13C, d3; Biacin-13C, d3; CRIXAN OD-13C, d3; Clamicin-13C, d3; Claric-13C, d3; Claris-d3; Claritek-13C, d3; Clarith-13C, d3; Clarithro-13C, d3; Clathromycin-13C, d3; Crixan-13C, d3; Fascar-13C, d3; Fromilid-13C, d3; Kelamycin-13C, d3; Klacid-13C, d3; Klaribac-13C, d3; Klaricid-13C, d3; Klarithran eclar-13C, d3;
Exenatide D10	deuteriumlabeledcom	NA		4196.601	Exendin-4-d10; His-Gly-Glu-Gly-Thr-Phe-Thr-Ser-Asp-Leu(d10)-Ser-Lys-Gln-Met-Glu-Glu-Glu-Ala-Val-Arg-Leu-Phe-Ile-Glu-Trp-Leu-Lys-Asn-Gly-Gly-Pro-Ser-Ser-Gly-Ala-Pro-

name	category	cas_number	mol_formula	mol_weight	synonym
Ethosuximide D5	deuteriumlabeledcom	77-67-8 (unlabeled)	C7H6D5NO2	146.2	3-(Ethyl-d3)-3-methyl-2,5-pyrrolidinedione; 2-(Ethyl-d3)-2-methylsuccinimide; Atysmal-d5; Capitus-d5; Emeside-d5; Etosuximid-d5; Mesentol-d5; d3; Simatin-Succimal-d5; Succimitin-d5; Suxilep-d5; Suximal-d5
Linaclotide D4	deuteriumlabeledcom	NA	C ₅₉ H ₇₅ D ₄ N ₁₅ O ₂₁ S ₆	1373.601	L-Cysteinyl-L-cysteinyl-L-α-glutamyl-L-tyrosyl-L-cysteinyl-L-cysteinyl-L-asparaginyl-L-prolyl-L-alanyl-d4-L-cysteinyl-L-threonylglycyl-L-cysteinyl-L-tyrosine Cyclic (1→6),(2→10),(5→13)-Tris(disulfide)
rac- Clopidogrel D3 Bisulfate	deuteriumlabeledcom	120202-66-6	C16H15D3ClNO6S2	422.92	(±)-Methyl-d3 2-(2-Chlorophenyl)-2-(6,7-dihydro-4H-thieno[3,2-c]pyridin-5-yl)acetate Hydrogen Sulfate; (±)-Clopidogrel-d3 Bisulfate; Clopidogrel-d3 Hemisulfate; Iscover-d3 ;
Ganciclovir D5	deuteriumlabeledcom	82410-32-0 (unlabeled)	C9H8D5N5O4	260.26	2-Amino-1,9-dihydro-9-[[2-hydroxy-1-(hydroxymethyl)ethoxy-d5]methyl]-6H-purin-6-one
6-Mercaptopurine 13C2 15N1	deuteriumlabeledcom	NA	C313C2H4N315N1S	155.02	1,9-Dihydro-6H-purine-13C2,15N-6-thione

name	category	cas_number	mol_formula	mol_weight	synonym
Rivastgmine D6 Oxalate	deuteriumlabeledcom	194929-99-2 free base	C16H18D6N2O6	346.41	N-Ethyl-N-methylcarbamic Acid 3-[1-(Dimethylamino-d6)ethyl]phenyl Ester Oxalate Salt
Enzalutamide D6	deuteriumlabeledcom	144331-94-9	C21H10D6F4N4O2S	470.48	4-[3-[4-Cyano-3-(trifluoromethyl)phenyl]-5,5-dimethyl-4-oxo-2-thioxo-1-imidazolidinyl]-2-fluoro-N-methylbenzamide-d6
Dicycloverine D4 HCl	deuteriumlabeledcom	NA	C19H32D4ClNO2	349.98	[1,1'-Bicyclohexyl]-1-carboxylic Acid 2-(Diethylamino) Ethyl-d4 Ester Hydrochloride; Bentlyl-d4; Bentlyl-d4; Dicycloverin-d4; Dicycloverine-d4; Diocyl-d4; Wyovin-d4
Prasugrel Metabolite M3 D3	deuteriumlabeledcom	1226870-93-4 (without HCl)	C27H25D3FNO5S.H	500,6 * 36,5	2-(1-(2-cyclopropyl-1-(2-fluorophenyl)-2-oxoethyl)-4-((2-(3-(methoxy-d3)phenyl)-2-oxoethyl)thio)piperidin-3-ylidene)acetic acid hydrochloride
Azilsartan D4	deuteriumlabeledcom	1794817-45-0	C25H16D4N4O5	460.47	1-[[2'-(2,5-Dihydro-5-oxo-1,2,4-oxadiazol-3-yl)[1,1'-biphenyl]-4-yl]methyl]-2-ethoxy-1H-benzimidazole-7-carboxylic Acid-d4; 2-Ethoxy-1-[[2'-(4,5-dihydro-5-oxo-1,2,4-oxadiazol-3-yl)biphenyl-4-yl]methyl]benzimidazole-7-carboxylic Acid-d4

name	category	cas_number	mol_formula	mol_weight	synonym
Perindoprilate D4 HCL	deuteriumlabeledcom	NA	C17H24D4N2O5.HC	380.90 (free base 344.44)	(3aS,7aS)-1-(2-((1-Carboxybutyl)amino)propanoyl)octahydro-1H-indole-2-carboxylic Acid-d4
Catechol D6	deuteriumlabeledcom	202656-22-2	DOC6D40D	116.15	1,2-Benzenediol-d6; Pyrocatechol-d6; 1,2-Dihydroxybenzene-d6; 2-Hydroxyphenol-d6; Oxyphenic Acid-d6; Phthalhydroquinone-d6; Phthalic Alcohol-d6; Pyrocatechin-d6; o-Benzenediol-d6; o-Dihydroxybenzene-d6; o-Dioxybenzene-d6; o-Hydroquinone-d6; o-Hydroxyphenol-d6; o-Phenylenediol-d6;
Cefpodoxime D3	deuteriumlabeledcom	NA	C15H14D3N5O6S2	430.47	6R,7R)-7-[[[(2Z)-2-(2-Amino-4-thiazolyl)-2-(methoxyimino-d3)acetyl]amino]-3-(methoxymethyl)-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic Acid;
Mometasone furoate D3	deuteriumlabeledcom	NA	C27H27D3C12O6	524.45	(11 β ,16 α)-9,21-Dichloro-11,17-dihydroxy-16-methylpregna-1,4-diene-3,20-dione-d3;
Rifampicin D4	deuteriumlabeledcom	13292-46-1(unlabeled)	C43H54D4N4O12	826.98	3-[[[(4-Methyl-d4-1-piperazin-yl)imino]methyl]rifamycin; Rifampin-d4;

name	category	cas_number	mol_formula	mol_weight	synonym
Rifampicin D8	deuteriumlabeledcom	13292-46-1(unlabeled)	C43H50D8N4O12	831	3-[[[(4-Methyl-d8-1-piperazin-yl)imino]methyl]rifamycin; Rifampin-d8;
Ethacrynic 13C2 D5	deuteriumlabeledcom	58-54-8(unlabeled)	C13H7D5C12O4	310.18	cervonic acid d5; Efalex D5
Lamivudine 13C15N2D2	deuteriumlabeledcom	NA	C7H9NO3S 13C 15N	234.25	(2R-cis)-5-(4-amino-2-oxo-1(2H)-pyrimidinyl)-1,3-oxathiolane-2-carboxylic Acid-13C,15N2
Ritonavir 13CD3	deuteriumlabeledcom	155213-67-5 unlabeled	C3613CH45D3N6O5S2	724.96	3S,4S,6S,9S)-4-Hydroxy-12-methyl-9-(1-methylethyl)-13-[2-(1-methylethyl)-4-thiazolyl]-8,11-dioxo-3,6-bis(phenylmethyl)-2,7,10,12-tetraazatridecanoic Acid 5-Thiazolylmethyl-13C3 Ester;
Triamcinolone Acetonide D6	deuteriumlabeledcom	352431-33-5	C24H25FD6O6	440.5	3-(Dibenz[b,e]oxepin-11(6H)-ylidene)-N-ethyl-N-methyl-1-propanamine-d3;
Dihydroartemisinin 13C D4	deuteriumlabeledcom	NA	C14H20O5 13C D4	289.34	3R,5aS,6R,8aS,9R,10S,12R,12aR)-Decahydro-3,6,9-trimethyl-3,12-epoxy-12H-pyrano[4,3-j]-1,2-benzodioxepin-10-ol-13C,d4; (13C,2H4)-Dihydroartemisinin
Benzbromarone D5	deuteriumlabeledcom	3562-84-3	C17H7D5Br2O3	429.12	N,N-Dimethylimidodicarbonimidic Diamide-d6, Hydrochloride

name	category	cas_number	mol_formula	mol_weight	synonym
Methyl Dopa D3	deuteriumlabeledcom	555-30-6(unlabelled)	C10H10D3NO4	214.24	3-Hydroxy-N-(methyl-d3)-L-tyrosine; 3-(3,4-Dihydroxyphenyl)-N-(methyl-d3)alanine;
Diosmetin D3	deuteriumlabeledcom	1189728-54-8	C16H9D3O6	303.08	5,7-Dihydroxy-2-[3-hydroxy-4-(methoxy-d3)yphenyl]-4H-1-benzopyran-4-one;
Ethambutol D4	deuteriumlabeledcom	NA	C10H20D4N2O2	208.33	(S,S)-2,2'-(1,2-Ethanediyldiimino)-bis-1-butanol-d4 Dihydrochloride
Hycoscine Butyl Bromide D9	deuteriumlabeledcom	NA	C21H21D9BrNO4	449.43	α S)- α -(Hydroxymethyl)benzeneacetic Acid (1 α , 2 β , 4 β , 5 α , 7 β)-9-(Methyl-d9)-3-oxa-9-azatricyclo[3.3.1.0 _{2,4}]non-7-yl Ester;
Verapamil D7	deuteriumlabeledcom	NA	C27H31D7N2O4	461.33	4-[(3,4-Dimethoxyphenethyl)methylamino]-2-(3,4-dimethoxyphenyl)-2-(isopropyl-d7)butyronitrile Monohydrochloride;
Norverapamil D7	deuteriumlabeledcom	NA	C26H29D7N2O4	447.31	α -[3-[[2-(3,4-Dimethoxyphenyl)ethyl]amino]propyl]-3,4-dimethoxy- α -(1-methylethyl)-benzeneacetonitrile-d7;
Esomeprazole D3	deuteriumlabeledcom	NA	C17H16D3N3O3S	348.44	6-(Methoxy-d3)-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole-4,5,7-d3];

name	category	cas_number	mol_formula	mol_weight	synonym
Quetiapine D4 Fumarate	deuteriumlabeledcom	1331636-50-0	C21H21N3O2SD4.C	503.61	2-[2-(4-Dibenzo[b,f][1,4]thiazepin-11-yl-1-piperazinyloxy)ethoxy]ethanol-d4 (2E)-2-Butenedioate;
Raltegravir 13CD3 Potassium Salt	deuteriumlabeledcom	NA	C1913CH17D3FKN6	485.48	N-[(4-Fluorophenyl)methyl]-1,6-dihydro-5-hydroxy-1-methyl-2-[1-methyl-1-[(5-methyl-1,3,4-oxadiazol-2-yl)carbonyl]amino]ethyl]-6-oxo-4-pyrimidinecarboxamide-13Cd3 Potassium Salt
Labetalol D5	deuteriumlabeledcom	NA	C19H19D5N2O3	333.44	2-Hydroxy-5-[1-hydroxy-2-[(1-methyl-3-phenylpropyl)amino]ethyl]benzamide-d5 Hydrochloride;
Hesperetin D3	deuteriumlabeledcom	NA	C16H11D3O6	305.1	3-[(Hydroxyphenylacetyl)oxy]-1-methyl-1-azoniabicyclo[2,2,2]octane Bromide D5;
Ulipristal D8	deuteriumlabeledcom	NA	C28H27D8NO3	441	11 β)-11-[4-(Dimethylamino)phenyl]-17-hydroxy-19-norpregna-4,9-diene-3,20-dione;
Linagliptin D4	deuteriumlabeledcom	NA	C25H24D4N8O2	476.57	8-[(3R)-3-Amino-1-piperidinyl]-7-(2-butyn-1-yl)-3,7-dihydro-3-methyl-1-[(4-methyl-2-quinazolinyloxy)methyl]-1H-purine-2,6-dione-d4;

name	category	cas_number	mol_formula	mol_weight	synonym
Isosorbide-13C6-2-Mononitrate	deuteriumlabeledcom	NA	13C6H9NO6	197.09	1,4:3,6-Dianhydro-D-glucitol-13C6 5-Nitrate; 6-Nitrooxyhexahydro-furo[3,2-b]furan-3-ol-13C6; Isosorbide-13C6 5-Nitrate
Varenicline D4	deuteriumlabeledcom	249296-44-4(non Labelled)	C13H9N3D4	215.29	Azitrocin-13Cd3; Ribotrex-13Cd3; Sumamed-Cd3; Trozocina-d3; Zithromaz-13Cd3; Zitromax-13Cd3;
Rizatriptan D6 Benzoate	deuteriumlabeledcom	1216984-85-8	C15H13N5D6.C7H6O	275.39	N,N-(Dimethyl-d6)-5-(1H-1,2,4-triazol-1-ylmethyl)-1H-indole-3-ethanamine Benzoate
Selexipag D7	deuteriumlabeledcom	NA	C25H23D7N4O4S	489.64	2-[4-[(5,6-Diphenyl-2-pyrazinyl)(1-methylethyl)amino]butoxy]-N-(methylsulfonyl)acetamide-d7
Enalaprilat D5 Sodium Salt	deuteriumlabeledcom	1356922-29-6	C18H17D5N2Na2O5	397.39	N-[(1S)-1-(Carboxy)-(3-phenyl-d5)propyl]-L-alanyl]-L-proline Dihydrate
Selexipag Active Metabolite D7	deuteriumlabeledcom	NA	C25H22D7N3O3	412.54	Selexipag Hydroxy Impurity; 5,6-Diphenyl-2(1H)-pyrazinone D7;
Enalapril D5 Maleate Salt	deuteriumlabeledcom	349554-02-5	C20H23D5N2O5	381.48	Acapril-d5; Acetensil-d5; Alphrin-d5

name	category	cas_number	mol_formula	mol_weight	synonym
Indomethacin D4	deuteriumlabeledcom	NA	C19H12D4ClNO4	361.81	1-(4-Chlorobenzoyl-d4)-5-methoxy-2-methyl-1H-indole-3-acetic Acid; Indometacin-d4; Bonidon-d4; Catlep-d4; Indomethine-d4; Inacid-d4; Indomod-d4
Venlafaxine D10 HCl	deuteriumlabeledcom	NA	C17H18D10ClNO2	323.93	1-[2-(Dimethyloxidoamino)-1-(4-methoxyphenyl)ethyl]cyclohexanol-d10
Paroxetine D6 HCl	deuteriumlabeledcom	NA	C19H15D6ClFNO3	371.16	rac-3-[(1,3-Benzod-d4-ioxol-5-yloxy)methyl]-4-(4-fluorophenyl-d6)piperidine Hydrochloride; rac-Aropax-d6; rac-Deroxat-d6; rac-Paxil-d6; rac-Seroxat-d6
Primaquine Phosphate 13CD3	deuteriumlabeledcom	63-45-6(unlabeled)	C15H18D3N3O5P	361.36	N4-(6-Methoxy-8-quinolinyl)-1,4-pentanediamine-13Cd3 Phosphate
Sacubitril D4	deuteriumlabeledcom	NA	C24H24D4NO-5(1/2	434.52	[S-(R*,S*)]-[1,1'-Biphenyl]-4-pentanoic Acid, γ -[(3-carboxy-1-oxopropyl)amino]- α -methyl-Ethyl Ester-d4; (2R,4S)-4-[(3-Carboxy-1-oxopropyl)amino]-4-[(p-phenylphenyl)methyl]-2-methylbutanoic Acid Ethyl Ester-d4; (2R,4S)-5-(Biphenyl-4-yl)-4-[(3-carboxypropionyl)amino]-2-methylpentanoic Acid Ethyl Ester-d4

name	category	cas_number	mol_formula	mol_weight	synonym
6 α -Methylprednisolone-D6	deuteriumlabeledcom	NA	C22H24D6O5	380.51	(6 α ,11 β)-21-(3-Carboxy-1-oxopropoxy)-11,17-dihydroxy-6-methyl-pregna-1,4-diene-3,20-dione, Monosodium Salt;
Sulfasalazine D4	deuteriumlabeledcompounds		C18H10D4N4O5S	402.42	2-Hydroxy-5-[[4-[(2-pyridinylamino-d4)sulfonyl]phenyl]azo]benzoic Acid;
Prazosin D8 Hcl	deuteriumlabeledcom	NA	C19H14D8ClN5O4	427.91	4-(4-Amino-6,7-dimethoxy-2-quinazolinyl)-1-piperazinyl-D8]-2-furanylmethanone;
Bimatoprost D5	deuteriumlabeledcom	NA	C25H32D5NO4	420.6	5Z)-7-[(1R,2R,3R,5S)-3,5-Dihydroxy-2-[(1E,3S)-3-hydroxy-5-phenyl-1-penten-1-yl]cyclopentyl]-N-(ethyl-d5)-5-heptenamide;
Fluvastatin D6 sodium salt	deuteriumlabeledcom	NA	C24H19D6FNNaO4	417.5	(3R,5S,6E)-rel-7-[3-(4-Fluorophenyl)-1-(1-methylethyl-d6)-1H-indol-2-yl]-3,5-dihydroxy-6-heptenoic Acid Sodium Salt;
Amphotericin B Methyl ester D3	deuteriumlabeledcom	36148-89-7(unlabeled)	C48H72D3NO17	941.1	Amphotericin B Monomethyl Ester-d3
Tiotropium D3 Bromide	deuteriumlabeledcom	NA	C18H17D5N2Na2O5	475.43	1 α ,2 β ,4 β ,5 α ,7 β)-7-[(2-Hydroxy-2,2-di-2-thienylacetyl)oxy]-9,9-dimethyl-3-oxa-9-azoniatricyclo[3.3.1.0 ^{2,4}]nonane-d3 Bromide;

name	category	cas_number	mol_formula	mol_weight	synonym
Suvorexant D6	deuteriumlabeledcom	NA	C23H17D6ClN6O2	456	(7R)-4-(5-Chloro-2-benzoxazolyl)hexahydro-7-methyl-1H-1,4-diazepin-1-yl][5-methyl-d3-2-(2H-1,2,3-triazol-2-yl)phenyl-d3]-methanone;
Sulfapyridine D4	deuteriumlabeledcom	NA	C11H7D4N3O2S	253.31	4-Amino-N-2-pyridinyl-d4-benzenesulfonamide;
Tiopronin 13CD3	deuteriumlabeledcom	NA	C413CH6D3NO3S	167.2	N-(2-Mercapto-1-oxopropyl)glycine-13C,d3
Tizoxanide D4	deuteriumlabeledcom	NA	C10H3D4N3O4S	269.27	2-Hydroxy-N-(5-nitro-2-thiazolyl)benzamide-d4
Etravirine D4	deuteriumlabeledcom	NA	C20H11D4BrN6O	439.31	4-[[6-Amino-5-bromo-2-[(4-cyanophenyl)amino]-4-pyrimidinyl]oxy]-3,5-(dimethyl)benzonitrate-d4;
Nitazoxanide D4	deuteriumlabeledcom	NA	C12H5D4N3O5S	311.3	2-(Acetyloxy)-N-(5-nitro-2-thiazolyl)benzamide-d4;
Felbamate D4	deuteriumlabeledcom	NA	C11H10D4N2O4	242.27	2-Phenyl-1,3-propanedioldicarbamate-d4;
Zafirlukast D7	deuteriumlabeledcom	NA	C31H26N3O6SD7	582.73	[3-[[2-Methoxy-4-[[[(2-methylphenyl-d7)sulfonyl]amino]carbonyl]phenyl]methyl]-1-methyl-1H-indol-5-yl]carbamic Acid Cyclopentyl Ester;

name	category	cas_number	mol_formula	mol_weight	synonym
Theophylline D6	deuteriumlabeledcom	NA	C7H2D6N4O2	186.2	3,9-Dihydro-1,3-dimethyl-1H-purine-2,6-dione-d6;
Mebeverine acid d5	deuteriumlabeledcom	NA	C16H21D5ClNO3 HCl	284.41	4-[Ethyl[2-(4-methoxyphenyl)-1-methylethyl]amino]butanoic Acid-d5;
O-demethyl Mebeverine acid d5	deuteriumlabeledcom	NA	C15H19D5ClNO3	270.38	4-[Ethyl[2-(4-hydroxyphenyl)-1-methylethyl-d5]amino]butanoic Acid
O-demethyl Mebeverine alcohol d5	deuteriumlabeledcom	NA	C15H21D5ClNO2	256.4	4-[2-[Ethyl(4-hydroxybutyl)amino]propyl]phenol-d5;
Enclomiphene D4 HCL	deuteriumlabeledcom	NA	C26H24D4ClNO.HCl	409.99	(E)-2-[p-[2-chloro-(1,2-diphenyl-d5)vinyl]phenoxy]-triethylamine Hydrochloride;
Ezetimibe D4 Phenoxy Glucuronide	deuteriumlabeledcom	NA	C30H25D4F2NO9	589.57	4-[(2S,3R)-1-(4-Fluorophenyl-d4)-3-[(3S)-3-(4-fluorophenyl)-3-hydroxypropyl]-4-oxo-2-azetidiny]phenyl β-D-Glucopyranosiduronic Acid;
3-hydroxy repaglinide D5	deuteriumlabeledcom	1352792-15-4	C27H31D5N2O5	473.62	2-(Ethoxy-d5)-4-[2-[[1-[2-(3-hydroxy-1-piperidiny]phenyl]-3-methylbutyl]amino]-2-oxoethyl]benzoic Acid;

name	category	cas_number	mol_formula	mol_weight	synonym
Naloxone glucuronide D5	deuteriumlabeledcom	NA	C ₂₅ H ₂₄ D ₅ N ₁ O ₁₀	508.53	(3S,4S,5S,6S)-6-[[[(4R,4aS,7aR,12bS)-4a-hydroxy-7-oxo-3-prop-2-enyl-2,4,5,6,7a,13-hexahydro-1H-4,12-methanobenzofuro[3,2-e]isoquinoline-9-yl]oxy]-3,4,5-trihydroxyoxaneta-D-8G1586 D5;
Minoxidil D10	deuteriumlabeledcom	1020718-66-4	C ₉ H ₅ D ₁₀ N ₅ O	219.31	6-(1-Piperidinyl-d10)-2,4-pyrimidinediamine 3-Oxide; 2,4-Diamino-6-(piperidino-d10) pyrimidine 3-N-Oxide;
Ezetimibe D4 Glucuronide (Phenolic) Na	deuteriumlabeledcom	NA	C ₃₀ H ₂₄ D ₄ F ₂ NNaO ₉	611.19	4-[(2S,3R)-1-(4-Fluorophenyl-d4)-3-[(3S)-3-(4-fluorophenyl)-3-hydroxypropyl]-4-oxo-2-azetidiny]phenyl β-D-Glucopyranosiduronic Acid sodium salt;
Methocarbamol D5	deuteriumlabeledcom	1189699-70-4	C ₁₁ H ₁₀ D ₅ N ₁ O ₅	245.29	3-(2-Methoxyphenoxy)-1,2-propanediol-d5 1-Carbamate; 3-(o-Methoxyphenoxy) -2-hydroxypropyl-d5 Carbamate;
Rifapentine D9	deuteriumlabeledcom	61379-65-5 (non-labelled)	C ₄₇ H ₅₅ D ₉ N ₄ O ₁₂	886.09	3-[[[(4-Cyclopentyl-1-piperazinyl)imino]methyl]rifamycin D9;

name	category	cas_number	mol_formula	mol_weight	synonym
Abacavir D4 HCl	deuteriumlabeledcom	1260619-56-4	C14H14D4N6O.HCl	326.82	(1R,4R)-rel-4-[2-Amino-6-[cyclopropyl-d4]amino]-9H-purin-9-yl]-2-cyclopentene-1-methanol Hydrochloride
Ambroxol D5 HCl	deuteriumlabeledcom	1246818-80-3 (free base)	C13H13Br2N2OD5. HCl	383.14 36.46	4-[[[(2-Amino-3,5-dibromophenyl)methyl]amino]cycophexano]l-d5 HCL;
Penicillamine D3	deuteriumlabeledcom	52-67-5(non-labelled)	C5H8D3NO2S	152.23	(2S)-2-Amino-3-methyl-3-sulfanylbutanoic acid-D3
Aminocaproic D6 Acid	deuteriumlabeledcom	60-32-2(non-labelled)	C6H7D6NO2	137.21	6-amino(3,3,4,4,5,5-D6)hexanoic acid
Emtricitabine 15ND2	deuteriumlabeledcom	43491-57-0 (Unlabeled)	C8H8D2N2 15NO3SF.HCL	286.71	4-Amino-5-fluoro-1-[(2R,5S)-2-hydroxymethyl]-1,3-oxathiolan-5-yl]-2-(1H-pyrimidinone-d2,15N2 HCL;
Miltefosin D4	deuteriumlabeledcom	NA	C21H42D4NO4P	411.59	hexadecyl (2-(trimethylammonio) ethyl) phosphate-D4
Bupivacaine D9	deuteriumlabeledcom	474668-57-0	C18H19N2OD9	297.49	N-(2,6-dimethylphenyl)-1-(1,1,2,2,3,3,4,4,4-nonadeuteriobutyl)piperidine-2-carboxamide
Monohydroxylated ramelteon	deuteriumlabeledcom	896736-21-3 (Unlabeled)	C16H18D3NO3	278.37	Monohydroxylated ramelteon (M-II) D3
Crisaborole D4	deuteriumlabeledcom	906673-24-3 (unlabelled)	C14H6D4BNO3	255.07	4-((1-Hydroxy-1,3-dihydrobenzo[c][1,2]oxaborol-5-yl)oxy)benzotrile-d4;

name	category	cas_number	mol_formula	mol_weight	synonym
9-cis Retinoic acid D ₅	deuteriumlabeledcom	NA	C ₂₀ H ₂₃ D ₅ O ₂	305.47	(2E,4E,6Z,8E)-3,7-Dimethyl-9-(2,6,6-trimethylcyclohex-1-enyl)nona-2,4,6,8-tetraenoic Acid-d ₅ ; 9-cis-Tretinoin-d ₅ ;
Albendazole D ₃	deuteriumlabeledcom	1353867-92-1	C ₁₂ H ₁₂ D ₃ N ₃ O ₂ S	268.35	N-[6-(Propylthio)-1H-benzimidazol-2-yl]carbamic Acid Methyl-d ₃ Ester; [5-(Propylthio)-1H-benzimidazol-2-yl]carbamic Acid Methyl-d ₃ Ester;
Sacubitril 13C ₄ Calcium	deuteriumlabeledcom	1369773-39-6 (unlabelled); 149709-62-6 (free acid, unlabelled)	C ₂₀ 13C ₄ H ₂₈ N ₅ O ₅ .1 /2Ca	434.5	[S-(R*,S*)]-[1,1'-Biphenyl]-4-pentanoic Acid, γ -[(3-carboxy-1-oxopropyl)amino]-α -methyl-Ethyl Ester-13C ₄ Calcium,