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Uric acid	C5H4N4O3	O=C1NC(=O)C2=C(N1)NC(=O)N	-2,17
Urea	CH4N2O	NC(N)=O	-2,11
Inosine	C10H12N4O5	OC[C@H]1O[C@H]([C@H](O)[C	-2,10
2-Phenylglycine	C8H9NO2	NC(C(O)=O)c1ccccc1	-2,07
Hexanedioic acid, dihydro	C6H14N4O2	NNC(=O)CCCC(=O)NN	-2,05
5-Methylcytidine	C10H15N3O5	CC1=CN([C@@H]2O[C@H](CO	-2,01
Uridine	C9H12N2O6	OC[C@H]1O[C@H]([C@H](O)[C	-1,98
Guanosine	C10H13N5O5	NC1=Nc2n(cnc2C(=O)N1)[C@@	-1,90
Metrizamide	C18H22I3N3O8	CN(C(C)=O)c1c(I)c(NC(C)=O)c(I)	-1,89
L-Methionine	C5H11NO2S	CSCC[C@H](N)C(O)=O	-1,87
Ascorbic acid	C6H8O6	OCC(O)C1OC(=C(O)C1=O)O	-1,85
Alloxan	C4H2N2O4	O=C1NC(=O)C(=O)C(=O)N1	-1,84
Methyl dopa	C10H13NO4	COC(=O)[C@@H](N)Cc1ccc(O)c	-1,79
Benzenamine, 2-methyl	C7H8N2O3	COc1cc(ccc1N)[N+](=[O-])=O	-1,78
Deoxycytidine	C9H13N3O4	NC1=NC(=O)N(C=C1)[C@H]2C[	-1,77
Glycerol	C3H8O3	OCC(O)CO	-1,76
Creatinine	C4H7N3O	CN1CC(=O)N=C1N	-1,76
Cytosine	C4H5N3O	NC1=NC(=O)NC=C1	-1,73
Deoxyinosine	C10H12N4O4	OC[C@H]1O[C@H](C[C@@H]1	-1,71
L-Alloisoleucine	C6H13NO2	CC[C@@H](C)[C@H](N)C(O)=O	-1,70
L-Isoleucine	C6H13NO2	CC[C@H](C)[C@H](N)C(O)=O	-1,70
Tetrachlorophthalic acid	C8H3Cl4NO3	NC(=O)c1c(Cl)c(Cl)c(Cl)c(Cl)c1C	-1,68
Citric acid	C6H8O7	OC(=O)CC(O)(CC(O)=O)C(O)=O	-1,64
Aciclovir	C8H11N5O3	NC1=NC(=O)c2ncn(COCCO)c2N	-1,56
L-Norleucine	C6H13NO2	CCCC[C@H](N)C(O)=O	-1,53
D-Leucine	C6H13NO2	CC(C)C[C@@H](N)C(O)=O	-1,52
L-Leucine	C6H13NO2	CC(C)C[C@H](N)C(O)=O	-1,52
Formamide	CH3NO	NC=O	-1,51
Deoxyuridine	C9H12N2O5	OC[C@H]1O[C@H](C[C@@H]1	-1,51
Riboflavin	C17H20N4O6	Cc1cc2N=C3C(=O)NC(=O)N=C3	-1,46
Hydroxycotinine	C10H12N2O2	CN1C(CC(O)C1=O)c2cccnc2	-1,45
Diethanolamine	C4H11NO2	OCCNCCO	-1,43
1,3-Diaminopropane	C3H10N2	NCCCN	-1,43
Methylnoradrenaline	C9H13NO3	CC(N)C(O)c1ccc(O)c(O)c1	-1,43
Dimethyl sulfone	C2H6O2S	C[S](C)(=O)=O	-1,41
L-Phenylalanine	C9H11NO2	N[C@@H](Cc1ccccc1)C(O)=O	-1,38
Epinephrine	C9H13NO3	CNC[C@H](O)c1ccc(O)c(O)c1	-1,37
Dimethyl sulfoxide	C2H6OS	C[S](C)=O	-1,35
Diacetyl	C4H6O2	CC(=O)C(C)=O	-1,34
3,7-Dimethyluric acid	C7H8N4O3	CN1C(=O)NC(=O)C2=C1NC(=O)	-1,33
Ethanolamine	C2H7NO	NCCO	-1,31
Deoxyguanosine	C10H13N5O4	NC1=Nc2n(cnc2C(=O)N1)[C@H	-1,30
Acetamide	C2H5NO	CC(N)=O	-1,26
Norepinephrine	C8H11NO3	NCC(O)c1ccc(O)c(O)c1	-1,24
Salicin	C13H18O7	OC[C@H]1O[C@@H](Oc2ccccc	-1,22
Glycolic acid	C2H4O3	OCC(O)=O	-1,11
Hypoxanthine	C5H4N4O	O=C1NC=Nc2nc[nH]c12	-1,11
5-Aminoimidazole-4-carboxamide	C4H6N4O	NC(=O)c1nc[nH]c1N	-1,10
Gabapentin	C9H17NO2	NCC1(CCCCC1)CC(O)=O	-1,10
3-Methyluric acid	C6H6N4O3	CN1C(=O)NC(=O)C2=C1NC(=O)	-1,08
Uracil	C4H4N2O2	O=C1NC=CC(=O)N1	-1,07
1,3,5-Triazine-2,4,6-triamine	C12H15N3O6	O=C1N(CC2CO2)C(=O)N(CC3CC	-1,07

L-Tryptophan	C11H12N2O2	<chem>N[C@@H](Cc1c[nH]c2ccccc12)</chem>	-1,06
Adenosine	C10H13N5O4	<chem>Nc1ncnc2n(cnc12)[C@@H]3O[</chem>	-1,05
N-Methylacetamide	C3H7NO	<chem>CNC(C)=O</chem>	-1,05
Normetanephrine	C9H13NO3	<chem>COc1cc(ccc1O)C(O)CN</chem>	-1,05
N,N-Dimethylformami	C3H7NO	<chem>CN(C)C=O</chem>	-1,01
3,4-Dihydroxyphenylgl	C8H10O4	<chem>OCC(O)c1ccc(O)c(O)c1</chem>	-1,01
Dopamine	C8H11NO2	<chem>NCCc1ccc(O)c(O)c1</chem>	-0,98
N-Methylformamide	C2H5NO	<chem>CNC=O</chem>	-0,97
UDP-D-Xylose	C14H22N2O16P2	<chem>OC1COC(O[P](O)(=O)O[P](O)(=</chem>	-0,96
1-Amino-propan-2-ol	C3H9NO	<chem>CC(O)CN</chem>	-0,96
Thymidine	C10H14N2O5	<chem>CC1=CN([C@H]2C[C@H](O)[C@</chem>	-0,93
Propylene glycol	C3H8O2	<chem>CC(O)CO</chem>	-0,92
2,3-Butanediol	C4H10O2	<chem>CC(O)C(C)O</chem>	-0,92
Guanine	C5H5N5O	<chem>NC1=Nc2nc[nH]c2C(=O)N1</chem>	-0,91
p-Octopamine	C8H11NO2	<chem>C1=CC(=CC=C1[C@H](CN)O)O</chem>	-0,90
7-Methylxanthine	C6H6N4O2	<chem>Cn1cnc2NC(=O)NC(=O)c12</chem>	-0,89
4-Aminohippuric acid	C9H10N2O3	<chem>Nc1ccc(cc1)C(=O)NCC(O)=O</chem>	-0,89
2-Pyrrolidinone	C4H7NO	<chem>O=C1CCCN1</chem>	-0,85
Orotic acid	C5H4N2O4	<chem>OC(=O)C1=CC(=O)NC(=O)N1</chem>	-0,83
Malonic acid	C3H4O4	<chem>OC(=O)CC(O)=O</chem>	-0,81
Theobromine	C7H8N4O2	<chem>Cn1cnc2N(C)C(=O)NC(=O)c12</chem>	-0,78
Acrylamide	C3H5NO	<chem>NC(=O)C=C</chem>	-0,78
N,N-Dimethylacetamic	C4H9NO	<chem>CN(C)C(C)=O</chem>	-0,77
Pyridoxine	C8H11NO3	<chem>Cc1ncc(CO)c(CO)c1O</chem>	-0,77
Methanol	CH4O	<chem>CO</chem>	-0,74
Cefoperazone	C25H27N9O8S2	<chem>CCN1CCN(C(=O)N[C@@H](C(=</chem>	-0,74
Xanthine	C5H4N4O2	<chem>O=C1NC(=O)c2[nH]cnc2N1</chem>	-0,73
Histamine	C5H9N3	<chem>NCCc1c[nH]cn1</chem>	-0,70
Putrescine	C4H12N2	<chem>NCCCCN</chem>	-0,70
Oxoamide	C10H12N2O2	<chem>[N-]=O</chem>	-0,69
Famotidine	C8H15N7O2S3	<chem>NC(N)=Nc1scc(CSCCC(N)=N[S](I</chem>	-0,64
gamma-Butyrolactone	C4H6O2	<chem>O=C1CCCO1</chem>	-0,64
Thymine	C5H6N2O2	<chem>CC1=CNC(=O)NC1=O</chem>	-0,62
Succinic acid	C4H6O4	<chem>OC(=O)CCC(O)=O</chem>	-0,59
Cefazolin	C14H14N8O4S3	<chem>[Na+].Cc1sc(SCC2=C(N3[C@H](</chem>	-0,58
1-Methyluric acid	C6H6N4O3	<chem>CN1C(=O)NC2=C(NC(=O)N2)C1:</chem>	-0,57
Methylamine	CH5N	<chem>CN</chem>	-0,57
Deoxyadenosine	C10H13N5O3	<chem>Nc1ncnc2n(cnc12)[C@H]3C[C@</chem>	-0,55
Allura red AC	C18H16N2O8S2	<chem>[Na+].[Na+].COc1cc(c(C)cc1N\N</chem>	-0,55
Formic acid	CH2O2	<chem>OC=O</chem>	-0,54
1,3-Dimethyluracil	C6H8N2O2	<chem>CN1C=CC(=O)N(C)C1=O</chem>	-0,54
1,3-Dimethyluric acid	C7H8N4O3	<chem>CN1C(=O)N(C)C2=C(NC(=O)N2)</chem>	-0,52
3-Methylxanthine	C6H6N4O2	<chem>CN1C(=O)NC(=O)c2[nH]cnc12</chem>	-0,50
Levulinic acid	C5H8O3	<chem>CC(=O)CCC(O)=O</chem>	-0,49
Maleic acid	C4H4O4	<chem>OC(=O)\C=C/C(O)=O</chem>	-0,48
Acetic anhydride	C4H6O3	<chem>CC(=O)OC(C)=O</chem>	-0,48
2-Piperidinone	C5H9NO	<chem>O=C1CCCN1</chem>	-0,46
Cefacetriple	C13H13N3O6S	<chem>CC(=O)OCC1=C(N2[C@H](SC1)[</chem>	-0,45
p-Synephrine	C9H13NO2	<chem>CNCC(O)c1ccc(O)cc1</chem>	-0,45
Naringin	C27H32O14	<chem>C[C@@H]1O[C@@H](O[C@@@I</chem>	-0,44
Pyrimidine	C4H4N2	<chem>c1cncnc1</chem>	-0,40
Dimethylamine	C2H7N	<chem>CNC</chem>	-0,38

Propargyl alcohol	C3H4O	OCC#C	-0,38
1,3,7-Trimethyluric aci	C8H10N4O3	CN1C(=O)N(C)C2=C(N(C)C(=O)N	-0,37
Purine	C5H4N4	[nH]1cnc2ncnc12	-0,37
Niacinamide	C6H6N2O	NC(=O)c1cccnc1	-0,37
alpha-Hydroxyisobutyri	C4H8O3	CC(C)(O)C(O)=O	-0,36
Acetoin	C4H8O2	CC(O)C(C)=O	-0,36
Acetonitrile	C2H3N	CC#N	-0,34
Nitromethane	CH3NO2	C[N+](=[O-])=O	-0,33
Phenylephrine	C9H13NO2	CNC[C@H](O)c1cccc(O)c1	-0,31
Ethanol	C2H6O	CCO	-0,30
Ethylene oxide	C2H4O	C1CO1	-0,30
Glutaric acid	C5H8O4	OC(=O)CCCC(O)=O	-0,29
1,3-Butanediol	C4H10O2	CC(O)CCO	-0,29
Acetazolamide	C4H6N4O3S2	CC(=O)Nc1sc(nn1)[S](N)(=O)=O	-0,26
Hydrogen cyanide	CHN	C#N	-0,25
Acetone	C3H6O	CC(C)=O	-0,24
Butanamide	C4H9NO	CCCC(N)=O	-0,21
Pymetrozine	C10H11N5O	CC1=NNC(=O)N(C1)N=Cc2cccnc	-0,18
Acetic acid	C2H4O2	CC(O)=O	-0,17
cis-Aconitic acid	C6H6O6	OC(=O)C\C=C/C(O)=O)C(O)=O	-0,14
Acetaldehyde oxime	C2H5NO	CC=NO	-0,13
Ethylamine	C2H7N	CCN	-0,13
Adenine	C5H5N5	Nc1ncnc2nc[nH]c12	-0,09
Imidazole	C3H4N2	[nH]1ccnc1	-0,08
3-Methoxytyramine	C9H13NO2	COc1cc(CCN)ccc1O	-0,08
Hydrochlorothiazide	C7H8ClN3O4S2	N[S](=O)(=O)c1cc2c(NCN[S]2(=	-0,07
Caffeine	C8H10N4O2	Cn1cnc2N(C)C(=O)N(C)C(=O)c1	-0,07
N-Acetyl-L-methionine	C7H13NO3S	CSCC[C@H](NC(C)=O)C(O)=O	-0,03
Theophylline	C7H8N4O2	CN1C(=O)N(C)c2nc[nH]c2C1=O	-0,02
Cefoxitin	C16H17N3O7S2	CO[C@]1(NC(=O)Cc2sccc2)[C@	-0,02
Acrolein	C3H4O	C=CC=O	-0,01
N-Methylnicotinamide	C7H8N2O	CNC(=O)c1cccnc1	0,01
Oxirane, 2,2'-1,4-butari	C10H18O4	C(CCOCC1CO1)COCC2CO2	0,01
Methyloxirane	C3H6O	CC1CO1	0,03
Allylamine	C3H7N	NCC=C	0,03
3-Methylpentane-1,5-di	C6H14O2	CC(CCO)CCO	0,03
4-Aminophenol	C6H7NO	Nc1ccc(O)cc1	0,04
2-Propanol	C3H8O	CC(C)O	0,05
Sulfathiazole	C9H9N3O2S2	Nc1ccc(cc1)[S](=O)(=O)Nc2sccr	0,05
Cotinine	C10H12N2O	CN1C(CCC1=O)c2cccnc2	0,07
Adipic acid	C6H10O4	OC(=O)CCCC(O)=O	0,08
Dimethyl ether	C2H6O	COC	0,10
1,3-Propanediol, 2,2-di	C5H12O2	CC(C)(CO)CO	0,12
4-Hydroxy-4-methyl-2-	C6H12O2	CC(=O)CC(C)(C)O	0,14
Sulfamerazine	C11H12N4O2S	Cc1ccnc(N[S](=O)(=O)c2ccc(N)c	0,14
2-Methyl-2-propenam	C4H7NO	CC(=C)C(N)=O	0,15
Ethylmethylamine	C3H9N	CCNC	0,15
Propanenitrile	C3H5N	CCC#N	0,16
Trimethylamine	C3H9N	CN(C)C	0,16
Atenolol	C14H22N2O3	CC(C)NCC(O)COc1ccc(CC(N)=O)	0,16
Ethanamine, n-ethyl-n	C4H11NO	CCN(O)CC	0,17
Allyl alcohol	C3H6O	OCC=C	0,17

Nornicotine	C9H12N2	C1CNC(C1)c2cccnc2	0,17
Nitroethane	C2H5NO2	CC[N+](O)=O	0,18
Methyl acetate	C3H6O2	COC(C)=O	0,18
1-Butanol, 3-methoxy-	C6H14O2	COC(C)CCO	0,18
Propanoic acid, 3,3'-th	C6H10O4S	OC(=O)CCSCC(O)=O	0,19
Difluoromethane	CH2F2	FCF	0,20
Quinone	C6H4O2	O=C1C=CC(=O)C=C1	0,20
1,3-Propanediol, 2-bro	C3H6BrNO4	OCC(Br)(CO)[N+](O)=O	0,21
Serotonin	C10H12N2O	NCCc1c[nH]c2ccc(O)cc12	0,21
2,4,6,8-Tetramethyl-1,	C8H16O4	CC1OC(C)OC(C)OC(C)O1	0,22
2-Propenamamide, n,n-di	C5H9NO	CN(C)C(=O)C=C	0,24
Gibberellin A3	C19H22O6	CC12[C@@H](O)C=C[C@@]3(C	0,24
1-Propanol	C3H8O	CCCO	0,25
2-Propenenitrile	C3H3N	C=CC#N	0,25
4-Hydroxybenzyl alcoh	C7H8O2	OCc1ccc(O)cc1	0,25
Isopropylamine	C3H9N	CC(C)N	0,26
2-Butanone	C4H8O	CCC(C)=O	0,29
ZINC01055318	C6H6N8O2	N1C2Nc3nonc3NC2Nc4nonc14	0,30
N-Acetylvaline	C7H13NO3	CC(C)[C@H](NC(C)=O)C(O)=O	0,30
Epichlorohydrin	C3H5ClO	ClCC1CO1	0,30
Flonicamid	C9H6F3N3O	FC(F)(F)c1ccncc1C(=O)NCC#N	0,30
Hippuric acid	C9H9NO3	OC(=O)CNC(=O)c1ccccc1	0,31
Propanoic acid	C3H6O2	CCC(O)=O	0,33
Homovanillic acid	C9H10O4	COc1cc(CC(O)=O)ccc1O	0,33
1,3-Propanediol, 2-am	C5H13NO2	CCC(N)(CO)CO	0,34
Butane-1,2-diol	C4H10O2	CCC(O)CO	0,34
Thiocyanic acid, methy	C3H2N2S2	N#CSCSC#N	0,34
Formaldehyde	CH2O	C=O	0,35
2-Methyl-2-propanol	C4H10O	CC(C)(C)O	0,35
Arecoline	C8H13NO2	COC(=O)C1=CCCN(C)C1	0,35
Cis-4-cyclohexene-1,2-	C8H9NO2	O=C1NC(=O)C2=C1CCCC2	0,35
Nicotinic acid	C6H5NO2	OC(=O)c1cccnc1	0,36
Antipyrine	C11H12N2O	CN1N(C(=O)C=C1C)c2ccccc2	0,38
Dimethylmalonic acid	C5H8O4	CC(C)(C(O)=O)C(O)=O	0,39
1,1-Dimethylhydrazine	C2H8N2	CN(C)N	0,40
tert-Butylamine	C4H11N	CC(C)(C)N	0,40
4-Hydroxy-3-methoxy	C8H10O3	COc1cc(CO)ccc1O	0,42
3-Mercaptopropanoic	C3H6O2S	OC(=O)CCS	0,43
Acetaldehyde	C2H4O	CC=O	0,45
2-Hydroxyvaleric acid	C5H10O3	CCCC(O)C(O)=O	0,45
Fumaric acid	C4H4O4	OC(=O)/C=C/C(O)=O	0,46
2,5-Dihydrofuran	C4H6O	C1OCC=C1	0,46
Tetrahydrofuran	C4H8O	C1CCOC1	0,46
Pyrrolidine	C4H9N	C1CCNC1	0,46
Paracetamol	C8H9NO2	CC(=O)Nc1ccc(O)cc1	0,46
2-Pentanone, 4-methc	C7H14O2	COC(C)(C)CC(C)=O	0,46
Propylamine	C3H9N	CCCN	0,48
Cefamandole	C18H18N6O5S2	Cn1nnnc1SCC2=C(N3[C@H](SC	0,50
Fluoromethane	CH3F	CF	0,51
Catechin	C15H14O6	O[C@H]1Cc2c(O)cc(O)cc2O[C@	0,51
ZINC00149819	C13H14O3	O=C1[C@H]2[C@@H]3C[C@H]	0,51
Guanidine, cyano-	C2H4N4	NC(N)=NC#N	0,52



Carbon dioxide	CO2	O=C=O	0,83
Carbon monoxide	CO	C=O	0,83
Propyl formate	C4H8O2	CCCOC=O	0,83
p-Aminobenzoic acid	C7H7NO2	Nc1ccc(cc1)C(O)=O	0,83
Metamitron	C10H10N4O	CC1=NN=C(c2ccccc2)C(=O)N1N	0,83
1-Butanol	C4H10O	CCCCO	0,84
2-Pentanone	C5H10O	CCCC(C)=O	0,84
Piperidine	C5H11N	C1CCNCC1	0,84
Pyrrole-2-carboxylic ac	C5H5NO2	OC(=O)c1[nH]ccc1	0,85
3-Hydroxyphenylacetic	C8H8O3	OC(=O)Cc1cccc(O)c1	0,85
ortho-Hydroxyphenyla	C8H8O3	OC(=O)Cc1cccc1O	0,85
Butanamide, n-(2-met	C11H13NO2	CC(=O)CC(=O)Nc1ccccc1C	0,85
Protocatechuic acid	C7H6O4	OC(=O)c1ccc(O)c(O)c1	0,86
Homogentisic acid	C8H8O4	OC(=O)Cc1cc(O)ccc1O	0,86
Butylamine	C4H11N	CCCCN	0,86
1735-44-0	C5H3F4N3	NNc1c(F)c(F)nc(F)c1F	0,86
Benzenemethanamine	C8H11N	C[C@@H](N)c1ccccc1	0,86
1-Nitropropane	C3H7NO2	CCC[N+](=[O-])=O	0,87
Butanal	C4H8O	CCCC=O	0,88
Pyrocatechol	C6H6O2	Oc1ccccc1O	0,88
Diethyl ether	C4H10O	CCOCC	0,89
2-Methyl-2-butanol	C5H12O	CCC(C)(C)O	0,89
Sulfamethazine	C12H14N4O2S	Cc1cc(C)nc(N[S](=O)(=O)c2ccc(	0,89
Pseudoephedrine	C10H15NO	CN[C@@H](C)[C@@H](O)c1cc	0,89
Aniline	C6H7N	Nc1ccccc1	0,90
Chloromethane	CH3Cl	CCl	0,91
Aminobenzimidazole	C7H7N3	Nc1[nH]c2ccccc2n1	0,91
Methacrylic acid	C4H6O2	CC(=C)C(O)=O	0,93
N-Acetyl-L-phenylalani	C11H13NO3	CC(=O)N[C@@H](Cc1ccccc1)C(	0,93
Sumatriptan	C14H21N3O2S	CN[S](=O)(=O)Cc1ccc2[nH]cc(C	0,93
Isobutyric acid	C4H8O2	CC(C)C(O)=O	0,94
Methyl tert-butyl ethe	C5H12O	COC(C)(C)C	0,94
Pentanenitrile	C5H9N	CCCC#N	0,94
1,3-Propanediol,2-(hyc	C5H12O3	CC(CO)(CO)CO	0,95
3-Hydroxyhippuric aci	C9H9NO4	OC(=O)CNC(=O)c1cccc(O)c1	0,95
Salicyluric acid	C9H9NO4	Oc1ccccc1CN2C(=O)NC3=C(NC(	0,95
2-Propenoic acid, 2-mε	C7H10O3	CC(=C)C(=O)OCC1CO1	0,96
Anabasine	C10H14N2	C1CCC(NC1)c2ccnc2	0,97
3,4-Dihydroxybenzene	C8H8O4	OC(=O)Cc1ccc(O)c(O)c1	0,98
Triamterene	C12H11N7	Nc1nc(N)c2nc(c3ccccc3)c(N)nc.	0,98
Scopolamine	C17H21NO4	CN1[C@@H]2CC(C[C@H]1)[C@	0,98
Mesotrione	C14H13NO7S	C[S](=O)(=O)c1ccc(C(=O)C2C(=	1,00
Aminophenazone	C13H17N3O	NC1C=Cc2nc3ccccc3nc2C1=O	1,00
Hexahydrophthalic aci	C8H12O4	OC(=O)C1CCCC1C(O)=O	1,01
4-Methylaminobenzoi	C8H9NO2	CNc1ccc(cc1)C(O)=O	1,01
5-Hexen-2-one	C6H10O	CC(=O)CCC=C	1,02
3-Furoic acid	C5H4O3	OC(=O)c1cocc1	1,03
Dimethyl adipate	C8H14O4	COC(=O)CCCC(=O)OC	1,03
Syringic acid	C9H10O5	COc1cc(cc(OC)c1O)C(O)=O	1,04
Ethyl vinyl ether	C4H8O	CCOC=C	1,04
N,N'-dipropylpiperazin	C12H24N4O2	CCCNC(=O)N1CCN(CC1)C(=O)N	1,04
Benzyl alcohol	C7H8O	OCc1ccccc1	1,05



Ethene, 1,2-bis(2-chloro	C6H10Cl2O2	ClCCOC=COCCCl	1,07
Aldosterone	C21H28O5	C[C@]12CCC(=O)C=C1CC[C@H]	1,08
Methane	CH4	C	1,09
Benzylamine	C7H9N	NCc1ccccc1	1,09
Pirimicarb	C11H18N4O2	CN(C)C(=O)Oc1nc(nc(C)c1C)N(C	1,10
ZINC00365332	C15H13N5O3S	O=C(C)/N=C2/Sc1c(N2N(C(C)=C	1,10
Amisulpride	C17H27N3O4S	CCN1CCCC1CNC(=O)c2cc(c(N)c	1,10
Codeine	C18H21NO3	COc1ccc2CC3C4C=CC(O)C5Oc1	1,10
Foramsulfuron	C17H20N6O7S	COc1cc(OC)nc(NC(=O)N[S](=O)l	1,11
2-Methylpyridine	C6H7N	Cc1cccn1	1,11
Propamocarb	C9H20N2O2	CCCOC(=O)NCCCN(C)C	1,12
Bis(2-chloroethyl) ethe	C4H8Cl2O	ClCCOCCCl	1,12
Monomethyl phthalat	C9H8O4	COC(=O)c1ccccc1C([O-])=O	1,13
Ephedrine	C10H15NO	CN[C@@H](C)[C@H](O)c1ccccc	1,13
2,3-dimethylpyrazino[	C8H10N6	Cc1nc2c(N)nnc(N)c2nc1C	1,14
Chloridazon	C10H8ClN3O	NC1=C(Cl)C(=O)N(N=C1)c2ccccc	1,14
methyl 2-[(2R)-1-[4-(di	C18H25N3O6S	CCN(CC)[S](=O)(=O)c1ccc(cc1)C	1,14
Atrazine-deisopropyl	C5H8ClN5	CCNc1nc(N)nc(Cl)n1	1,15
Caffeic acid	C9H8O4	OC(=O)\C=C/c1ccc(O)c(O)c1	1,15
Aprobarbital	C10H14N2O3	CC(C)C1(CC=C)C(=O)NC(=O)NC:	1,15
Isovaleric acid	C5H10O2	CC(C)CC(O)=O	1,16
(4aR,8aR)-8a-hydroxy-	C9H14O3	O[C@@]12CCCC[C@@H]1CCCCl	1,16
Desaminotyrosine	C9H10O3	OC(=O)CCc1ccc(O)cc1	1,16
2-Phenoxyethanol	C8H10O2	OCCOc1ccccc1	1,16
N-Acetylarylamine	C8H9NO	CC(=O)Nc1ccccc1	1,16
Nicotine-1'-N-oxide	C10H14N2O	C[N+]1([O-])CCCC1c2cccnc2	1,17
Nicotine	C10H14N2	CN1CCCC1c2cccnc2	1,17
Ethylmethylacetic acid	C5H10O2	CCC(C)C(O)=O	1,18
Quinic acid	C7H12O6	OC1CC(O)(CC(O)C1O)C(O)=O	1,19
Bromomethane	CH3Br	CBr	1,19
Aspirin	C9H8O4	CC(=O)Oc1ccccc1C(O)=O	1,19
Codeine	C18H21NO3	COc1ccc2C[C@@H]3[C@@H]4	1,19
2-Pyrocatechuic acid	C7H6O4	OC(=O)c1ccc(O)c1O	1,20
2-Pentanamine, 4-met	C6H15N	CC(C)CC(C)N	1,20
3-Methylpyridine	C6H7N	Cc1cccnc1	1,20
Diethyl carbonate	C5H10O3	CCOC(=O)OCC	1,21
Ethyl propanoate	C5H10O2	CCOC(=O)CC	1,21
2-Aminobenzoic acid	C7H7NO2	Nc1ccccc1C(O)=O	1,21
3-Pentanol	C5H12O	CCC(O)CC	1,21
Vanillin	C8H8O3	COc1cc(C=O)ccc1O	1,21
1-Methylpyrrole	C5H7N	Cn1cccc1	1,21
4-Methylpyridine	C6H7N	Cc1ccncc1	1,22
Meticillin	C17H20N2O6S	COc1cccc(OC)c1C(=O)N[C@H]2	1,22
Cyclohexanol	C6H12O	OC1CCCCC1	1,23
Aflatoxin B1	C17H12O6	COc1cc2OC3OC=CC3c2c4OC(=C	1,23
Paroxetine	C19H20FNO3	Fc1ccc(cc1)C2CCNCC2COc3ccc	1,23
Propyl acetate	C5H10O2	CCCOC(C)=O	1,24
Dichloromethane	CH2Cl2	ClCCl	1,25
2-Pentanol	C5H12O	CCCC(C)O	1,25
Phenyl formate	C7H6O2	O=COc1ccccc1	1,26
Digoxin	C41H64O14	C[C@H]1O[C@H](C[C@H](O)[C	1,26
Salicylamide	C7H7NO2	NC(=O)c1ccccc1O	1,28

3-Methyl-1-butanol	C5H12O	CC(C)CCO	1,28
3-Methyl-2-butanol	C5H12O	CC(C)C(C)O	1,28
Colchicine	C22H25NO6	COC1=CC=C2C(=CC1=O)[C@H](	1,30
Isosorbide Dinitrate	C6H8N2O8	[O-][N+](=O)O[C@H]1CO[C@@	1,31
S-Allylcysteine	C6H11NO2S	N[C@@H](CSCC=C)C(O)=O	1,31
2,2-Dimethyl-1-propanol	C5H12O	CC(C)(C)CO	1,31
4-Methyl-2-pentanone	C6H12O	CC(C)CC(C)=O	1,31
Ethyl acrylate	C5H8O2	CCOC(=O)C=C	1,32
Guaiacol	C7H8O2	COc1ccccc1O	1,32
N-Acetyl-L-tyrosine	C11H13NO4	CC(=O)N[C@@H](Cc1ccc(O)cc1	1,32
o-Methylaniline	C7H9N	Cc1ccccc1N	1,32
Furan	C4H4O	o1cccc1	1,34
4-Hydroxybenzaldehyde	C7H6O2	Oc1ccc(C=O)cc1	1,35
Benzyl methyl ether	C8H10O	COCc1ccccc1	1,35
Ampicillin	C16H19N3O4S	CC1(C)S[C@@H]2[C@H](NC(=C	1,35
Benzeneethanol	C8H10O	OCCc1ccccc1	1,36
(4-(4-Aminophenyl)(4-	C20H20ClN3	[H+].[Cl-].CC1=CC(C=CC1=N)=C	1,36
Mesosulfuron-methyl	C17H21N5O9S2	COC(=O)c1ccc(CN[S](C)(=O)=O)	1,37
4-Methylcatechol	C7H8O2	Cc1ccc(O)c(O)c1	1,37
Methyl methacrylate	C5H8O2	COC(=O)C(C)=C	1,38
2-Hexanone	C6H12O	CCCCCC(=O)	1,38
Pentanoic acid	C5H10O2	CCCCCC(O)=O	1,39
Guaifenesin	C10H14O4	COc1ccccc1OCC(O)CO	1,39
p-Methylaniline	C7H9N	Cc1ccc(N)cc1	1,39
Cyclohexanamine, N-h	C6H12N2O2	ON=[N+](O)C1CCCCC1	1,40
m-Methylaniline	C7H9N	Cc1ccc(N)c1	1,40
Bromochloromethane	CH2BrCl	ClCBr	1,41
methyl N-[(1R)-1-hydroxy	C10H11NO4	COC(=O)N[C@H](O)C(=O)c1ccc	1,41
Benzeneacetic acid	C8H8O2	OC(=O)Cc1ccccc1	1,41
Indoleacetic acid	C10H9NO2	OC(=O)Cc1[nH]c2ccccc2c1	1,41
Benzeneethanamine	C8H11N	NCCc1ccccc1	1,41
Chenodeoxycholoyl-Cc	C45H74N7O19P3S	C[C@H](CCC(=O)SCCNC(=O)CC	1,41
4-Methoxyphenylacetate	C9H10O3	COc1ccc(CC(O)=O)cc1	1,42
α-Methylbenzyl alcohol	C8H10O	CC(O)c1ccccc1	1,42
Vanillic acid	C8H8O4	COc1cc(ccc1O)C(O)=O	1,43
Carbendazim	C9H9N3O2	COC(=O)Nc1[nH]c2ccccc2n1	1,43
Chloroethane	C2H5Cl	CCCl	1,43
N-[(2R)-1-(butanoylamino	C11H22N2O2	CCCC(=O)NC[C@@H](C)NC(=O)	1,43
1-Phenyl-2-propanone	C9H10O	CC(=O)Cc1ccccc1	1,44
Triethylamine	C6H15N	CCN(CC)CC	1,45
Ethylene chloride	C2H3Cl	ClC=C	1,46
2-Butyne	C4H6	CC#CC	1,46
1-Nitrobutane	C4H9NO2	CCCC[N+](O)=O	1,47
Phenobarbital	C12H12N2O3	CCC1(C(=O)NC(=O)NC1=O)c2cc	1,47
Cortisone	C21H28O5	C[C@]12CCC(=O)C=C1CC[C@H]	1,47
Cortisone	C21H28O5	CC12CCC(=O)C=C1CCC3C4CCC(	1,47
methyl 2-amino-4-methyl	C6H8N2O2S	COC(=O)c1sc(N)nc1C	1,48
1,2-Dichloroethane	C2H4Cl2	ClCCCl	1,48
3,3-Dimethyl-2-butanol	C6H14O	CC(O)C(C)(C)C	1,48
Phenol	C6H6O	Oc1ccccc1	1,48
Benzaldehyde	C7H6O	O=Cc1ccccc1	1,48
ZINC00974316	C11H12O3	O=C1[C@H]2OC[C@H](O2)[C@	1,48

(4S,5S)-N,N,N',N',2,2-hC11H20N2O4	CN(C)C(=O)[C@H]1OC(C)(C)O[C	1,49
Pentylamine	C5H13N CCCCCN	1,49
Cyclohexylamine	C6H13N NC1CCCCC1	1,49
Phenyl acetate	C8H8O2 CC(=O)Oc1ccccc1	1,49
1-Phenylethylamine	C8H11N CC(N)c1ccccc1	1,49
Iodomethane	CH3I CI	1,50
3-Hydroxybenzoic acid	C7H6O3 OC(=O)c1cccc(O)c1	1,50
Prosulfuron	C15H16F3N5O4S COc1nc(C)nc(NC(=O)N[S](=O)=	1,50
1-Pentanol	C5H12O CCCCCCO	1,51
Ferulic acid	C10H10O4 COc1cc(\C=C\C(O)=O)ccc1O	1,51
Diisopropyl ether	C6H14O CC(C)OC(C)C	1,52
Sulfaphenazole	C15H14N4O2S Nc1ccc(cc1)[S](=O)(=O)Nc2ccnr	1,52
Benzamide, n-3-bis(2- yl-	C17H20N2O3 OCCN(CCO)c1cccc(NC(=O)c2ccc	1,54
3-Chloro-1-propene	C3H5Cl ClCC=C	1,55
1-(3-Methoxy-benzyl)-	C11H13N3O COc1cccc(Cn2cc(N)cn2)c1	1,55
Tryptamine	C10H12N2 NCCc1c[nH]c2ccccc12	1,55
N-(3, 4-Dichloropheny	C19H12Cl4N2O5S O[S](=O)(=O)c1cc(Cl)ccc1Oc2cc	1,55
Thifensulfuron-methyl	C12H13N5O6S2 COC(=O)c1sccc1[S](=O)(=O)NC(	1,56
Oprea1_347215	C7H5N5S2 Nc1sc2cc3sc(N)nc3nc2n1	1,56
Benzonitrile	C7H5N N#Cc1ccccc1	1,56
Benzeneacetonitrile	C8H7N N#CCc1ccccc1	1,56
7-(2-methyl-1H-indol-5	C14H13N3O2S2 Cc1[nH]c2ccccc2c1C3=CN4CC[	1,56
Azelaic acid	C9H16O4 OC(=O)CCCCCCC(O)=O	1,57
Fluoxetine	C17H18F3NO CNCCC(Oc1ccc(cc1)C(F)(F)F)c2c	1,57
4-Hydroxybenzoic acid	C7H6O3 OC(=O)c1ccc(O)cc1	1,58
4-Methylbenzenemet	C8H10O Cc1ccc(CO)cc1	1,58
Benzonitrile, 2-amino-	C7H5N3O2 Nc1ccc(cc1C#N)[N+](=[O-])=O	1,60
(4R,5S)-2-tert-butyl-2-	C10H18N2O4 CC(C)(C)C1(C)O[C@H]([C@@	1,60
Bromoethane	C2H5Br CCBr	1,60
Trinexapac-ethyl	C13H16O5 CCOC(=O)[CH]1CC(=O)[C](C(=O	1,60
3-Methylbenzenemet	C8H10O Cc1cccc(CO)c1	1,60
Phenyloxirane	C8H8O C1OC1c2ccccc2	1,61
Cortisol	C21H30O5 C[C@]12CCC(=O)C=C1CC[C@H]	1,61
Hydrocortisone	C21H30O5 CC12CCC(=O)C=C1CCC3C4CCC(	1,61
Amidosulfuron	C9H15N5O7S2 COc1cc(OC)nc(NC(=O)N[S](=O)	1,63
Acetophenone	C8H8O CC(=O)c1ccccc1	1,63
1,3,5-Triazine-2,4,6(1H		
propenyl-	C12H15N3O3 C=CCN1C(=O)N(CC=C)C(=O)N(C	1,64
3-Hexanol	C6H14O CCCC(O)CC	1,65
1-(3,4-Dichlorophenyl)	C7H6Cl2N2O NC(=O)Nc1ccc(Cl)c(Cl)c1	1,65
Metalaxyl	C15H21NO4 COCC(=O)N(C(C)C(=O)OC)c1c(C	1,65
Glycocholic acid	C26H43NO6 CC(CCC(=O)NCC(O)=O)C1CCC2(	1,65
4-Nitrocatechol	C6H5NO4 Oc1ccc(cc1O)[N+](=[O-])=O	1,66
Ethane, 1-chloro-1,1-	C2H3ClF2 CC(F)(F)Cl	1,66
Hexanenitrile	C6H11N CCCCCC#N	1,66
N-Methylaniline	C7H9N CNc1ccccc1	1,66
N,N-Dimethyl-n'-phen	C8H12N2O2S CN(C)[S](=O)(=O)Nc1ccccc1	1,67
Dipropylamine	C6H15N CCCNCCC	1,67
Fosthiazate	C9H18NO3PS2 CCO[P](=O)(SC(C)CC)N1CCSC1=	1,68
Imazamethabenz-met	C16H20N2O3 COC(=O)c1ccc(C)cc1C2=NC(C)(	1,68
Metribuzine	C8H14N4OS CSC1=NN=C(C(=O)N1N)C(C)(C)	1,70

Benzenepropanenitrile	C9H9N	N#CCCc1ccccc1	1,72
Butethal	C10H16N2O3	CCCCC1(CC)C(=O)NC(=O)NC1=C	1,73
Gentisic acid	C7H6O4	OC(=O)c1cc(O)ccc1O	1,74
ethyl 2-amino-5-methyl-3-oxopentanoate	C7H10N2O2S	CCOC(=O)c1nc(N)sc1C	1,74
Indole-3-propionic acid	C11H11NO2	OC(=O)CCc1c[nH]c2ccccc12	1,75
2-Hexanol	C6H14O	CCCCC(C)O	1,76
Amphetamine	C9H13N	CC(N)Cc1ccccc1	1,76
Dextroamphetamine	C9H13N	C[C@H](N)Cc1ccccc1	1,76
Dimethyldisulfide	C2H6S2	CSSC	1,77
Hexanal	C6H12O	CCCCCC=O	1,78
Benzeneacetaldehyde	C8H8O	O=CCc1ccccc1	1,78
1,1-Dichloroethane	C2H4Cl2	CC(Cl)Cl	1,79
3-Bromopropene	C3H5Br	BrCC=C	1,79
4-Hydroxycinnamic acid	C9H8O3	OC(=O)C=Cc1ccc(O)cc1	1,79
Alizapride	C16H21N5O2	COc1cc2n[nH]nc2cc1C(=O)NCC	1,79
Nicosulfuron	C15H18N6O6S	COc1cc(OC)nc(NC(=O)N[S](=O)N)cc1	1,80
N-(1-Phenylethyl)metoprolol	C9H13NO2S	CC(N[S](C)(=O)=O)c1ccccc1	1,80
2-Phenylpropanoic acid	C9H10O2	CC(C(O)=O)c1ccccc1	1,80
1-Propanethiol	C3H8S	CCCS	1,81
Thiophene	C4H4S	s1cccc1	1,81
2,5,8,11-tetraoxabicyclo[2.2.1]heptane	C12H16O4	C1COCCOc2ccccc2OCCO1	1,81
Ajmaline	C20H26N2O2	CCC1C(O)N2C3CC1C4C(O)C5(C)CCN4C3	1,81
Butyl acetate	C6H12O2	CCCCOC(C)=O	1,82
Phenyllactic acid	C9H10O3	CC(O)(C(O)=O)c1ccccc1	1,83
3,5-Xylidine	C8H11N	Cc1cc(C)cc(N)c1	1,83
Hydrocinnamic acid	C9H10O2	OC(=O)CCc1ccccc1	1,84
Methylphenobarbital	C13H14N2O3	CCC1(C(=O)NC(=O)N(C)C1=O)c2ccccc2	1,84
2,3-Dimethylbenzenamine	C8H11N	Cc1ccc(N)c1C	1,84
2-Chloro-1-phenylethanol	C8H7ClO	ClCC(=O)c1ccccc1	1,84
Nitrobenzene	C6H5NO2	[O-][N+](=O)c1ccccc1	1,85
2-Methylfuran	C5H6O	Cc1occc1	1,85
2-Methyltetrahydrofuran	C5H10O	CC1CCCO1	1,85
3-(difluoromethyl)sulfamoylurea	C10H10F2N4OS	Nn1c(COc2ccccc2)nnc1SC(F)F	1,85
N-[(1S)-1-phenylethyl]phenethylamine	C12H15NO	C[C@H](NC(=O)C1CC1)c2ccccc2	1,85
Digitoxin	C41H64O13	C[C@H]1O[C@H](C[C@H](O)[C@H]1OC2OC3C(C)OC3O2)O	1,85
cis-1,2-Dichloroethylenediamine	C2H2Cl2	Cl\C=C/Cl	1,86
Benzocaine	C9H11NO2	CCOC(=O)c1ccc(N)cc1	1,86
Imazaquin	C17H17N3O3	CC(C)C1(C)N=C(NC1=O)c2nc3ccc(N)cc32	1,86
ethyl 4-cyanobenzoate	C10H9NO2	CCOC(=O)c1ccc(cc1)C#N	1,87
Benzoic acid	C7H6O2	OC(=O)c1ccccc1	1,88
5-Methyl-2-hexanone	C7H14O	CC(C)CCC(C)=O	1,88
Benzenepropanol	C9H12O	OCCc1ccccc1	1,88
Metoprolol	C15H25NO3	COCCc1ccc(OCC(O)CNC(C)C)cc1	1,88
(2,6-difluorophenyl)-propylamine	C11H11F2NO	Fc1cccc(F)c1C(=O)N2CCCC2	1,88
2-Bromopropane	C3H7Br	CC(C)Br	1,90
2-Chloropropane	C3H7Cl	CC(C)Cl	1,90
Polythiazide	C11H13ClF3N3O4S3	CN1C(CSCC(F)(F)F)Nc2cc(Cl)c(Cl)cc21	1,90
Cinnamaldehyde	C9H8O	O=CC=Cc1ccccc1	1,90
Glutethimide	C13H15NO2	CCC1(CCC(=O)NC1=O)c2ccccc2	1,90
4-Nitrophenol	C6H5NO3	Oc1ccc(cc1)[N+](=O)[O-]	1,91
2,4-Dichloro-6-nitrophenol	C6H3Cl2NO3	Oc1c(Cl)cc(Cl)cc1[N+](=O)[O-]	1,91
Hexanoic acid	C6H12O2	CCCCCC(=O)O	1,92

trans-1,2-Dichloroethy	C2H2Cl2	Cl\C=C\Cl	1,93
Ethyl methacrylate	C6H10O2	CCOC(=O)C(C)=C	1,94
Corticosterone	C21H30O4	C[C@]12C[C@H](O)[C@H]3[C@	1,94
Diethyl sulfide	C4H10S	CCSCC	1,95
3-Methylphenylacetic	C9H10O2	Cc1cccc(CC(O)=O)c1	1,95
p-Anisic acid	C8H8O3	COc1ccc(cc1)C(O)=O	1,96
Benzyl acetate	C9H10O2	CC(=O)OCc1ccccc1	1,96
p-Ethylaniline	C8H11N	CCc1ccc(N)cc1	1,96
Trichloromethane	CHCl3	ClC(Cl)Cl	1,97
p-Cresol	C7H8O	Cc1ccc(O)cc1	1,97
Paraoxon	C10H14NO6P	CCO[P](=O)(OCC)Oc1ccc(cc1)[N	1,98
1-Pentyne	C5H8	CCCC#C	1,98
Hexobarbital	C12H16N2O3	CN1C(=O)NC(=O)C(C)(C1=O)C2:	1,98
2-Heptanone	C7H14O	CCCCCC(C)=O	1,98
m-Cresol	C7H8O	Cc1cccc(O)c1	1,98
o-Cresol	C7H8O	Cc1ccccc1O	1,98
(2R)-1-acetyl-2-(2,4-di	C13H14Cl2N2O4	COCON1[C@@H](N(CC1=O)C(C	1,98
N,N-Dimethylbenzylan	C9H13N	CN(C)Cc1ccccc1	1,98
Acenocoumarol	C19H15NO6	CC(=O)CC(c1ccc(cc1)[N+](O-)=	1,98
Nitroxoline	C9H6N2O3	Oc1ccc(c2cccnc12)[N+](O-)=C	1,99
1,3-Butadiene	C4H6	C=CC=C	1,99
Indole-3-carboxylic aci	C9H7NO2	OC(=O)c1c[nH]c2ccccc12	1,99
Terephthalic acid	C8H6O4	OC(=O)c1ccc(cc1)C(O)=O	2,00
Iodoethane	C2H5I	CCI	2,00
1,2-Dichloropropane	C3H6Cl2	CC(Cl)CCl	2,00
N-[2-(4-morpholin-4-yl	C14H20N2O4S	CC(=O)NCCc1ccc(cc1)[S](=O)(=	2,00
N-(3-methoxypropyl)-2	C12H14F3NO2	COCCNC(=O)c1ccccc1C(F)(F)F	2,00
1-Nitropentane	C5H11NO2	CCCC[N+](O-)=O	2,01
1,3-Propanediol, 2-bu	C9H20O2	CCCC(C)(CO)CO	2,01
Eriodictyol	C15H12O6	Oc1cc(O)c2C(=O)C[C@H](Oc2c	2,02
Cholic acid	C24H40O5	C[C@H](CCC(O)=O)[C@H]1CC[C@	2,02
Glycoursodeoxycholic	C26H43NO5	C[C@H](CCC(=O)NCC(O)=O)[C@	2,02
Furosemide	C12H11ClN2O5S	N[S](=O)(=O)c1cc(C(O)=O)c(NC	2,03
1-Hexanol	C6H14O	CCCCCCO	2,03
Dipropyl ether	C6H14O	CCCOCC	2,03
cis-1,3-Dichloroproper	C3H4Cl2	ClC\C=C/Cl	2,03
Heptabarbital	C13H18N2O3	CCC1(C(=O)NC(=O)NC1=O)C2=C	2,03
Quinoline	C9H7N	c1ccc2ncccc2c1	2,03
Triazoxide	C10H6ClN5O	[O-][n+] <sub>1</sub> nc(nc2ccc(Cl)cc12)n3c	2,04
1-Chloropropane	C3H7Cl	CCCCl	2,04
1,3-Dichloropropene	C3H4Cl2	ClCC=CCl	2,04
methyl 4-[[[(3R)-1,1-dic	C14H12F3NO5S	COC(=O)c1ccc(cc1)N([C@H]2C[	2,05
Bromazepam	C14H10BrN3O	BrC1ccc2NC(=O)CN=C(c3cccn3	2,05
N-ethyl-2-[1-(2-morph	C24H25N3O4	CCN(C(=O)C(=O)c1cn(CC(=O)N2	2,05
Hexylamine	C6H15N	CCCCCCN	2,06
Flunitrazepam	C16H12FN3O3	CN1C(=O)CN=C(c2ccccc2F)c3cc	2,06
Amobarbital	C11H18N2O3	CCC1(CCC(C)C)C(=O)NC(=O)NC:	2,07
Methamphetamine	C10H15N	CN[C@@H](C)Cc1ccccc1	2,07
Isoquinoline	C9H7N	c1ccc2cnccc2c1	2,08
3-amino-7-ethyl-5-oxo	C10H7N5OS	CCC1=C(C#N)C(=O)N2C(=C(SC2	2,09
N-[2-[(3,4-diethoxyph	C19H24N2O5	CCOc1ccc(NC(=O)CN(C)C(=O)c2	2,09
1-Bromopropane	C3H7Br	CCCB	2,10

Oxprenolol	C15H23NO3	CC(C)NCC(O)COc1cccc1OCC=C	2,10
Cortisone acetate	C23H30O6	CC(=O)OCC(=O)[C@@]1(O)CC[	2,10
Bromacil	C9H13BrN2O2	CCC(C)N1C(=O)NC(=C(Br)C1=O)	2,11
Anisole	C7H8O	COc1cccc1	2,11
4-Methylphenyl acetate	C9H10O2	CC(=O)Oc1ccc(C)cc1	2,11
Diethyl maleate	C8H12O4	CCOC(=O)\C=C\C(=O)OCC	2,12
ZINC03435204	C10H14F3N5O2S	CC(C)[C@@H](Sc1nnc(n1C)C(F)	2,12
Metosulam	C14H13Cl2N5O4S	COc1cc(OC)n2nc(nc2n1)[S](=O)	2,12
Chenodeoxycholic acid	C26H43NO5	C[C@H](CCC(=O)NCC(=O)O)[C@	2,12
1,1-Dichloroethylene	C2H2Cl2	ClC(Cl)=C	2,13
Benzene	C6H6	c1ccccc1	2,13
Cinnamic acid	C9H8O2	OC(=O)C=Cc1cccc1	2,13
trans-Cinnamic acid	C9H8O2	OC(=O)\C=C\c1cccc1	2,13
Metazachlor	C14H16ClN3O	Cc1cccc(C)c1N(Cn2cccn2)C(=O)	2,13
Benzoin	C14H12O2	OC(c1cccc1)C(=O)c2cccc2	2,13
2,3-Dihydrobenzofuran	C8H8O	C1Cc2cccc2O1	2,14
Indole	C8H7N	[nH]1ccc2ccccc12	2,14
N-[(4-bromophenyl)methyl]	C11H8BrNO2S2	C1=CSC(=C1)S(=O)(=O)N=CC2=C	2,14
Benzene, 1-chloro-3-(1-fluoro-2-iodoethyl)-	C7H4ClF3	FC(F)(F)c1cccc(Cl)c1	2,14
Allyl isothiocyanate	C4H5NS	C=CCN=C=S	2,15
1-(1-benzofuran-2-yl)ethane	C10H8O2	CC(=O)c1oc2cccc2c1	2,15
Dimethenamid	C12H18ClNO2S	COCC(C)N(C(=O)CCl)c1c(C)sc1	2,15
Dichlorodifluoromethane	CCl2F2	FC(F)(Cl)Cl	2,16
[2-(4-amino-1,3-dimethyl-5-isopropylphenyl)ethyl]amine	C12H15N3O5	CN1C(=C(C(=O)COC(=O)C2CC2)	2,17
Simazine	C7H12ClN5	CCNc1nc(Cl)nc(NCC)n1	2,18
Ethane, 2,2-dichloro-1,1,1-trifluoro-	1C2HCl2F3	FC(F)(F)C(Cl)Cl	2,18
3-Phenylbutyric acid	C10H12O2	CC(CC(O)=O)c1cccc1	2,18
Propachlor	C11H14ClNO	CC(C)N(C(=O)CCl)c1cccc1	2,18
ZINC03467496	C18H17F3N6O2S	C[C@H](Sc1nn2c(C)cc(C)nc2n1	2,18
1-Phenyl-1-propanone	C9H10O	CCC(=O)c1cccc1	2,19
4-Methylacetophenone	C9H10O	CC(=O)c1ccc(C)cc1	2,19
ZINC02915570	C18H20N4O4	COc1cc(OC)c(cc1OC)C2n3ncnc2	2,19
Metsulfuron-methyl	C14H15N5O6S	COC(=O)c1cccc1[S](=O)(=O)N(C	2,20
Salicylic acid	C7H6O3	OC(=O)c1cccc1O	2,20
Fluroxypyr	C7H5Cl2FN2O3	Nc1c(Cl)c(F)nc(OCC(O)=O)c1Cl	2,20
1-Pentene	C5H10	CCCC=C	2,20
2-Bromobenzoic acid	C7H5BrO2	OC(=O)c1cccc1Br	2,20
Methyl benzoate	C8H8O2	COC(=O)c1cccc1	2,20
Menadione	C11H8O2	CC1=CC(=O)c2cccc2C1=O	2,20
4-Heptanol	C7H16O	CCCC(O)CCC	2,22
4-Ethoxybenzaldehyde	C9H10O2	CCOc1ccc(C=O)cc1	2,23
Hydrazine, (2,4,6-trichloro-1,3,5-triazine)-	C6H5Cl3N2	NNc1c(Cl)cc(Cl)cc1Cl	2,23
Omeprazole	C17H19N3O3S	COc1ccc2nc([nH]c2c1)[S](=O)C	2,23
3-Heptanol	C7H16O	CCCCCC(O)CC	2,24
Nitrazepam	C15H11N3O3	[O-][N+](=O)c1ccc2NC(=O)CN=	2,25
Deoxycholic acid glycerate	C26H43NO5	CC(CCCNCC(O)=O)C1CCC2C3CC	2,25
[2-[[4-(dimethylsulfamoyl)phenyl]butyl]amino]propanoic acid	C15H20N2O5S	CN(C)[S](=O)(=O)c1ccc(NC(=O)C	2,26
2-Methylbenzaldehyde	C8H8O	Cc1cccc1C=O	2,26
Fluorobenzene	C6H5F	Fc1ccccc1	2,27
3-chloro-1-[2-[4-(furan-2-yl)butyl]amino]propanoic acid	C17H15ClF3N3O4	FC(F)(F)C1=CN(CC(=O)N2CCN(C	2,27
1-Butanethiol	C4H10S	CCCCS	2,28
(2S,3R,4R,5R,6S)-2-[[3-(13-bromo-1-oxo-2-oxo-1,2,3,4-tetrahydro-1,4-benzodioxin-5-yl)propyl]amino]propanoic acid	C13H18BrNO5	Cc1ccc(N[C@H]2O[C@@H](CO	2,28

(1R,5S)-1,8,8-trimethyl-5-oxo-5-phenyl-1,2,3,4-tetrahydro-1H-benzopyridin-2-one	C <sub>13</sub> H <sub>17</sub> NO <sub>2</sub>	CC1(C)[C@@H]2CC[C@@]1(C)C(=O)C2	2,28
Dichloropropene	C <sub>9</sub> H <sub>8</sub> Cl <sub>2</sub> O <sub>3</sub>	CC(Oc1ccc(Cl)cc1Cl)C(O)=O	2,29
Dibromomethane	CH <sub>2</sub> Br <sub>2</sub>	BrCBr	2,30
1,4-Cyclohexadiene	C <sub>6</sub> H <sub>8</sub>	C1C=CCC=C1	2,30
(Chloromethyl)benzene	C <sub>7</sub> H <sub>7</sub> Cl	ClCc1ccccc1	2,30
3-Indolebutyric acid	C <sub>12</sub> H <sub>13</sub> NO <sub>2</sub>	OC(=O)CCCc1c[nH]c2ccccc12	2,30
(4-phenylsulfonylpiperidin-1-yl)methanesulfonamide	C <sub>16</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub> S	O=C(N1CCN(CC1)[S](=O)(=O)c2ccc(S(=O)(=O)N)cc2)C1=O	2,30
T5263673	C <sub>13</sub> H <sub>12</sub> N <sub>4</sub> O <sub>4</sub> S <sub>3</sub>	O=C(CSc1oc(nn1)c2sccc2)NCCN	2,31
trans-2-Butene	C <sub>4</sub> H <sub>8</sub>	C\C=C\C	2,31
2-Indolecarboxylic acid	C <sub>9</sub> H <sub>7</sub> NO <sub>2</sub>	OC(=O)c1[nH]c2ccccc2c1	2,31
2-Heptanol	C <sub>7</sub> H <sub>16</sub> O	CCCCC(C)O	2,31
N,N-Dimethylaniline	C <sub>8</sub> H <sub>11</sub> N	CN(C)c1ccccc1	2,31
o-Toluic acid	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	Cc1ccccc1C(O)=O	2,32
Carbofuran	C <sub>12</sub> H <sub>15</sub> NO <sub>3</sub>	CNC(=O)Oc1cccc2CC(C)(C)Oc12	2,32
n-Ethyl-p-toluidine	C <sub>9</sub> H <sub>13</sub> N	CCNc1ccc(C)cc1	2,32
Isoxaflutole	C <sub>15</sub> H <sub>12</sub> F <sub>3</sub> NO <sub>4</sub> S	C[S](=O)(=O)c1cc(ccc1C(=O)c2cc(F)(F)F)cc2	2,32
1H-Pyrrole-2,5-dione	C <sub>2</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub>	O=C1C=CC(=O)N1c2ccc(Cc3ccc(N)cc3)cc2	2,32
cis-2-Butene	C <sub>4</sub> H <sub>8</sub>	C\C=C/C	2,33
1-Fluoropentane	C <sub>5</sub> H <sub>11</sub> F	CCCCCF	2,33
5-(3,4-dimethoxyphenyl)pyridin-2-amine	C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub> S	COc1ccc(cc1OC)c2sc(N)nn2	2,34
p-Toluic acid	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	Cc1ccc(cc1)C(O)=O	2,34
2,5-Xylenol	C <sub>8</sub> H <sub>10</sub> O	Cc1ccc(C)c(O)c1	2,34
(4S)-2-amino-5-oxo-4-oxo-4-phenyl-1,2,3,4-tetrahydro-1H-pyridin-2-one	C <sub>17</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> S	NC1=C(C#N)[C@H](c2sccc2)C3=CC(=O)N1C3=O	2,34
Isobutene	C <sub>4</sub> H <sub>8</sub>	CC(C)=C	2,35
2,4-Xylenol	C <sub>8</sub> H <sub>10</sub> O	Cc1ccc(O)c(C)c1	2,35
3,5-Xylenol	C <sub>8</sub> H <sub>10</sub> O	Cc1cc(C)cc(O)c1	2,35
2,6-Xylenol	C <sub>8</sub> H <sub>10</sub> O	Cc1cccc(C)c1O	2,36
Carbaryl	C <sub>12</sub> H <sub>11</sub> NO <sub>2</sub>	CNC(=O)Oc1cccc2ccccc12	2,36
11a-Hydroxyprogesterone	C <sub>21</sub> H <sub>30</sub> O <sub>3</sub>	CC(=O)C1CC[C@@H]2[C@@]1(O)CCC2=O	2,36
m-Toluic acid	C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>	Cc1cccc(c1)C(O)=O	2,37
3,4-Dichloro-1-butene	C <sub>4</sub> H <sub>6</sub> Cl <sub>2</sub>	ClCC(Cl)C=C	2,37
2-Octanone	C <sub>8</sub> H <sub>16</sub> O	CCCCCCC(C)=O	2,37
Cumyl alcohol	C <sub>10</sub> H <sub>14</sub> O	CC(C)c1ccc(CO)cc1	2,37
Tribromomethane	CHBr <sub>3</sub>	BrC(Br)Br	2,38
1,1,2-Trichloroethane	C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub>	ClCC(Cl)Cl	2,38
Metobromuron	C <sub>9</sub> H <sub>11</sub> BrN <sub>2</sub> O <sub>2</sub>	CON(C)C(=O)Nc1ccc(Br)cc1	2,38
Camphor	C <sub>10</sub> H <sub>16</sub> O	CC1(C)C2CCC1(C)C(=O)C2	2,38
1,1,2,2-Tetrachloroethane	C <sub>2</sub> H <sub>2</sub> Cl <sub>4</sub>	ClC(Cl)C(Cl)Cl	2,39
2-Ethylfuran	C <sub>6</sub> H <sub>8</sub> O	CCc1occc1	2,40
Benzenamine, 4-chloro	C <sub>7</sub> H <sub>8</sub> ClN	Cc1cc(Cl)ccc1N	2,40
Phenylacetylene	C <sub>8</sub> H <sub>6</sub>	C#Cc1ccccc1	2,40
Chlortoluron	C <sub>10</sub> H <sub>13</sub> ClN <sub>2</sub> O	CN(C)C(=O)Nc1ccc(C)C(Cl)c1	2,41
(4-cyanophenyl)methylamine	C <sub>20</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub>	CC(=O)N1Cc2ccccc2C[C@H]1CN	2,41
p-Nitrotoluene	C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	Cc1ccc(cc1)[N+](=O)[O-]	2,42
Heptanoic acid	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	CCCCCCC(O)=O	2,42
4-Bromo-2,5-dichloropentanoic acid	C <sub>6</sub> H <sub>3</sub> BrCl <sub>2</sub> NaO	[Na].Oc1cc(Cl)c(Br)cc1Cl	2,42
Benzenebutanoic acid	C <sub>10</sub> H <sub>12</sub> O <sub>2</sub>	OC(=O)CCCc1ccccc1	2,42
CDP	C <sub>9</sub> H <sub>15</sub> N <sub>3</sub> O <sub>11</sub> P <sub>2</sub>	NC1=NC(=O)N(C=C1)C2OC(CO)C2	2,44
(1R,5R)-1,5-diethyl-1,5-dimethyl-1,2,3,4-tetrahydro-1H-benzopyridin-2-one	C <sub>10</sub> H <sub>18</sub> N <sub>4</sub> S <sub>2</sub>	CC[C@]1(C)NC(=S)N2N1C(=S)N2	2,44
N-(3-methoxyphenyl)-N-methylacetamide	C <sub>15</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> S	COc1ccc(NC(=O)CSc2nnc3ccccc23)cc1	2,45
4-Phenylcyclohexanone	C <sub>12</sub> H <sub>14</sub> O	O=C1CCC(CC1)c2ccccc2	2,45
Carbamazepine	C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> O	NC(=O)N1c2ccccc2C=Cc3ccccc13	2,45

Estriol	C18H24O3	C[C@]12CC[C@H]3[C@@H](CC	2,45
4-ethoxy-6-morpholin-	C10H13N5O2	CCOc1nc(nc(n1)N2CCOCC2)C#	2,46
ZINC00367451	C13H11NO4	COC(=O)/C=C/CN1C(=O)c2cccc	2,46
2,4,6-Trimethylphenol	C9H12O	Cc1cc(C)c(O)c(C)c1	2,46
morpholin-4-yl-[(1S,3R)18H30N2O4		CC1(C)[C@@H](CC[C@]1(C)C(=	2,46
o-Ethylphenol	C8H10O	CCc1ccccc1O	2,47
4-(morpholine-4-carboc	C19H17N3O3	O=C(N1CCOCC1)C2=NN(C(=O)c	2,47
1,4-Pentadiene	C5H8	C=CCC=C	2,48
[2-[[[(1R,2R)-2-methylc	C14H21NO5	C[C@@H]1CCCC[C@H]1NC(=O	2,48
[(3R)-1,1-dioxo-2,3-dih	C16H15O6PS	O=[P](O[C@H]1C[S](=O)(=O)C=	2,48
dimethyl (4R,5S)-2-ph	C13H14O6	COC(=O)[C@@H]1OC(O[C@@H]	2,49
1,1,1-Trichloroethane	C2H3Cl3	CC(Cl)(Cl)Cl	2,49
Diiodomethane	CH2I2	ICI	2,50
1-Iodopropane	C3H7I	CCCI	2,50
4-Methyl-1-pentene	C6H12	CC(C)CC=C	2,50
m-Ethylphenol	C8H10O	CCc1cccc(O)c1	2,50
p-Ethylphenol	C8H10O	CCc1ccc(O)cc1	2,50
Azoxystrobin	C22H17N3O5	COC=C(C(=O)OC)c1cccc1Oc2c	2,50
2-[(1,1-dioxo-1,2-benz	C27H25N3O6S	COc1cccc1N(CCOC(=O)[C@H]	2,50
Phenetole	C8H10O	CCOc1cccc1	2,51
Benzenethiol	C6H6S	Sc1cccc1	2,52
Naringenin	C15H12O5	Oc1ccc(cc1)C2CC(=O)c3c(O)cc(	2,52
ZINC01163656	C19H18N2O3S2	CCN1C(=O)/C=C/c2cc(n(c2C)c	2,52
Trichlorofluoromethar	CCl3F	FC(Cl)(Cl)Cl	2,53
Trichloroethylene	C2HCl3	ClC=C(Cl)Cl	2,53
Luteolin	C15H10O6	Oc1cc(O)c2C(=O)C=C(Oc2c1)c3	2,53
2-amino-7-methyl-5-o	C19H19N3O5	COc1cc(cc(OC)c1OC)C2C(=C(N)	2,55
N-[2-(trifluoromethyl)]	C12H12F3NO	FC(F)(F)c1cccc1NC(=O)C2CCC	2,55
Ethane, 1,1,2,2-tetrac	C2Cl4F2	FC(Cl)(Cl)C(F)(Cl)Cl	2,56
2,6-Dimethyl-4-heptar	C9H18O	CC(C)CC(=O)CC(C)C	2,56
2-(4-methoxyphenyl)-	C16H13NO3	COc1ccc(cc1)N2C(=O)Cc3cccc	2,56
Heptylamine	C7H17N	CCCCCCCN	2,57
Benzyl propionate	C10H12O2	CCC(=O)OCc1cccc1	2,57
cyanomethyl 2-(2-oxo-	C15H16N2O3S	O=C(CSc1cccc1C(=O)OCC#N)N	2,57
1-Fluorobutane	C4H9F	CCCCF	2,58
6-amino-5-[2-[3-[2-(4-	C24H24N8O6S2	CN1C(=C(C(=O)CSc2nc3cccc3n	2,59
4-Phenylpyridine	C11H9N	c1ccc(cc1)c2ccncc2	2,59
Aminoparathion	C10H16NO3PS	CCO[P](=S)(OCC)Oc1ccc(N)cc1	2,60
Hesperetin	C16H14O6	COc1ccc(cc1O)[C@@H]2CC(=O	2,60
3-Methylindole	C9H9N	Cc1c[nH]c2cccc12	2,60
N-[(4-methoxyphenyl)]	C14H19NO2	COc1ccc(CNC(=O)C2CCCC2)cc1	2,60
Fenpropimorph	C20H33NO	CC(CN1CC(C)OC(C)C1)Cc2ccc(	2,60
Atrazine	C8H14ClN5	CCNc1nc(Cl)nc(NC(C)C)n1	2,61
cyclopropyl-(4-fluorop	C10H9FO	Fc1ccc(cc1)C(=O)C2CC2	2,61
Prostaglandin F2a	C20H34O5	CCCCC(O)C=CC1C(O)CC(O)C1C	2,61
Lornoxicam	C13H10ClN3O4S2	CN1C(=C(/O)Nc2ccccn2)/C(=O)	2,62
1-Heptanol	C7H16O	CCCCCCCO	2,62
N-Phenylbenzamide	C13H11NO	O=C(Nc1cccc1)c2cccc2	2,62
Nandrolone	C18H26O2	C[C@]12CC[C@H]3[C@@H](CC	2,62
Nandrolone phenprop	C27H34O3	C[C@]12CC[C@H]3[C@@H](CC	2,62
Nandrolone decanoat	C28H44O3	CCCCCCCCC(=O)O[C@H]1CC[	2,62
1,2,3-Trichloropropan	C3H5Cl3	ClCC(Cl)CCl	2,63



1,3,5-Cycloheptatriene	C7H8	C1C=CC=CC=C1	2,63
azepan-1-yl-(4-bromo-	C11H16BrN3O	Cn1ncc(Br)c1C(=O)N2CCCCC2	2,63
Dimethomorph	C21H22ClNO4	COc1ccc(cc1OC)C(=CC(=O)N2C	2,63
ZINC00273616	C8H7N3O2S	Cc1cc2c(c(c1C)[N+](=O)[O-])nsr	2,64
Tetrachloromethane	CCl4	ClC(Cl)(Cl)Cl	2,64
1-Chlorobutane	C4H9Cl	CCCCCl	2,64
Methabenzthiazuron	C10H11N3OS	CNC(=O)N(C)c1sc2ccccc2n1	2,64
Ethyl benzoate	C9H10O2	CCOC(=O)c1ccccc1	2,64
3-Methylanisole	C8H10O	COc1ccc(C)c1	2,66
(1R,4S)-N,N-diethyl-1,7-	C14H23NO3	CCN(CC)C(=O)[C@@]12CC[C@]	2,66
Benzofuran	C8H6O	o1ccc2ccccc12	2,67
2,3,6-Trimethylphenol	C9H12O	Cc1ccc(C)c(O)c1C	2,67
N-phenylbenzene-1,2-	C12H12N2	Nc1ccccc1Nc2ccccc2	2,67
Di-2-(ethylhexyl)phosph	C16H35O4P	CCCCC(CC)CO[P](O)(=O)OCC(CC	2,67
Diphenylmethanol	C13H12O	OC(c1ccccc1)c2ccccc2	2,67
ZINC00081634	C11H13N3O2	CNC1=C(C=O)C(=O)[nH]2cccc(C	2,68
m-Chlorobenzoic acid	C7H5ClO2	OC(=O)c1cccc(Cl)c1	2,68
4-Methoxycinnamic ac	C10H10O3	COc1ccc(C=CC(O)=O)cc1	2,68
4-Octanol	C8H18O	CCCCC(O)CCC	2,68
Diuron	C9H10Cl2N2O	CN(C)C(=O)Nc1ccc(Cl)c(Cl)c1	2,68
(3S)-1-(4-propoxyphen	C16H19N3O3S	CCCOc1ccc(cc1)N2C(=O)C[C@H]	2,68
2-[4-(3,4-dihydro-2H-1C	C14H12N2O2S	N#CCc1scc(n1)c2ccc3OCCCOc3	2,68
ZINC02942705	C18H19N3O3	CCc1noc(c1C)c2[nH]c3ccccc3c2	2,68
Canrenone	C22H28O3	CC12CCC(=O)C=C1C=CC3C2CCC	2,68
2-[(5-amino-1,3,4-thia	C11H11BrN4OS2	Cc1cc(Br)ccc1NC(=O)CSc2sc(N)	2,69
ZINC02475899	C14H26N4O2	CCCCN1[C@H]2[C@@H](N(C)C	2,69
4-[bis(2,2,2-trifluoroet	C8H12F6NO4P	FC(F)(F)CO[P](=O)(OCC(F)(F)F)N	2,69
(3E,6Z)-3,6-Nonadien-	C9H16O	CC\C=C/C/C=C/CCO	2,69
1-(3-butanoyl-1,5-dim	C17H30N2O2	CCCC(=O)N1CC2(C)CN(CC(C)(C1	2,69
3-(2,3-dimethylphenyl	C12H18N2O	CC(C)NC(=O)Nc1cccc(C)c1C	2,70
2-Naphthol	C10H8O	Oc1ccc2ccccc2c1	2,70
Warfarin	C19H16O4	CC(=O)CC(c1ccccc1)C2=C(O)Oc	2,70
ethyl 1-[(5,7-dimethyl-	C15H21N5O4S	CCOC(=O)C1CCN(CC1)[S](=O)(=	2,71
1-tert-butyl-3-(4-fluor	C11H15FN2S	CC(C)(C)NC(=S)Nc1ccc(F)cc1	2,71
4-(Diethylamino)benz	C11H15NO	CCN(CC)c1ccc(C=O)cc1	2,72
1,4-Dibromobutane	C4H8Br2	BrCCCCBr	2,73
1-Hexyne	C6H10	CCCCC#C	2,73
Toluene	C7H8	Cc1ccccc1	2,73
1-methylbicyclo[3.3.1]	C11H19NO	CC12CCCC(CCC1)(C2)C(N)=O	2,73
Yohimbine	C21H26N2O3	COC(=O)[C@H]1[C@@H](O)CC	2,73
(4-amino-6-dimethylar	C15H16N8O2	CN(C)c1nc(N)nc(COC(=O)c2ccc(	2,74
2-Methylanisole	C8H10O	COc1ccccc1C	2,74
Eucalyptol	C10H18O	CC12CCC(CC1)C(C)(C)O2	2,74
Triclopyr	C7H4Cl3NO3	OC(=O)COc1nc(Cl)c(Cl)cc1Cl	2,75
1-Bromobutane	C4H9Br	CCCCBr	2,75
Valproic acid	C8H16O2	CCCC(CCC)C(O)=O	2,75
Octanenitrile	C8H15N	CCCCCCCC#N	2,75
[(2R)-1-amino-1-oxopr	C11H10F3NO3	C[C@@H](OC(=O)c1cccc(c1)C(F	2,75
Fludiazepam	C16H12ClFN2O	CN1C(=O)CN=C(c2ccccc2F)c3cc	2,75
Androstenedione	C19H26O2	C[C@]12CC[C@H]3[C@@H](CC	2,75
Androstenedione	C19H26O2	CC12CCC3C(CCC4=CC(=O)CCC3	2,75
1-[4-(furan-2-carbonyl	C18H20N2O5	COc1ccc(OCC(=O)N2CCN(CC)C	2,76

Chlorantraniliprole	C18H14BrCl2N5O2	CNC(=O)c1cc(Cl)cc(C)c1NC(=O)C	2,76
4-[5-(4-chloro-2-methyl-2-propylamino)oxy]phenol	C8H8ClN7O2	Cn1ncc(Cl)c1c2onc(n2)c3nonc3	2,77
methyl 4,5-dimethoxy-2-(2S)-1-(2,3-dihydro-1,4-benzodioxin-5-yl)butane-2-carboxylate	C15H18N4O5S	COC(=O)c1cc(OC)c(OC)cc1NC(=O)C	2,78
[(2S)-1-(2,3-dihydro-1,4-benzodioxin-5-yl)butane-2-carboxylate]	C17H18N2O6	C[C@H](OC(=O)c1c(C)onc1C)C1=CC2C3CC(C=C3)C12	2,78
3a,4,7,7a-Tetrahydro-2H-piperidin-2-one	C10H12	O=C(CN1N(CC(=O)N2CCCCC2)CCN(CCC)CCC	2,78
1,2-bis(2-oxo-2-piperidinyl)ethane	C22H29N5O4	O=C(CN1N(CC(=O)N2CCCCC2)CCN(CCC)CCC	2,79
Tripropylamine	C9H21N	CCCN(CCC)CCC	2,79
(2S)-2-hydroxy-7-methyl-2-(2S)-1-(2,3-dihydro-1,4-benzodioxin-5-yl)butane-2-carboxylate	C11H9F3O4	COc1ccc2C(=O)C[C@](O)(Oc2c1)C(C)(C)C(=O)Nc1ccc(NC(=O)C(C)C	2,79
N-[4-(2,2-dimethylpropyl)phenyl]acetamide	C16H24N2O2	CC(C)(C)C(=O)Nc1ccc(NC(=O)C(C)C	2,80
Isobutane	C4H10	CC(C)C	2,80
Irgarol	C11H19N5S	CSc1nc(NC2CC2)nc(NC(C)(C)C)rc1	2,80
1,5-Hexadiene	C6H10	C=CCCC=C	2,80
(2R,6R)-N-(3-methoxyphenyl)acetamide	C12H24N2OS	COCCCN(C(=S)N1[C@H](C)CCC[C@H]1C)C(=O)Nc1ccc(C)cc1	2,80
4-Methylanisole	C8H10O	COc1ccc(C)cc1	2,81
ZINC00171218	C14H15BrN2O2	CCCN1C(=O)N(C=C(Br)C1=O)c2ccc(C)cc2	2,82
Prostaglandin E2	C20H32O5	CCCC[C@H](O)/C=C/[C@H]1[C@@H](O)C=CC1	2,82
Prostaglandin E2	C20H32O5	CCCCC(O)C=CC1C(O)CC(=O)C1	2,82
14-Hydroxy-E4-neurosporin	C22H32O5	CC/C=C\C/C=C\C\CC(/C=C/C/C1C(C)C(=O)C1	2,82
17-Hydroxy-E4-neurosporin	C22H32O5	CC/C=C\C\CC(/C=C/C/C1C(C)C(=O)C1	2,82
20-Hydroxy-E4-neurosporin	C22H32O5	CCC(/C=C/C/C1C(C)C(=O)C1C/C=C\C/C1C(C)C(=O)C1	2,82
4-Hydroxy-D4-neurosporin	C22H32O5	CC/C=C\C/C=C\C\C/C=C\C\CC1C(C)C(=O)C1	2,82
7-Hydroxy-D4-neurosporin	C22H32O5	CC/C=C\C/C=C\C\CC1C(C)C(=O)C1	2,82
Dichlone	C10H4Cl2O2	ClC1=C(Cl)C(=O)c2ccccc2C1=O	2,83
Chlorobenzene	C6H5Cl	Clc1ccccc1	2,84
Pyrimethanil	C12H13N3	Cc1cc(C)nc(Nc2ccccc2)n1	2,84
1-[(2S)-butan-2-yl]-3-(1,1,1-trifluoroethyl)urea	C8H12F6N2O	CC[C@H](C)NC(=O)NC(C(F)(F)F)C(=O)N	2,84
Cyclohexaneacetic acid	C8H14O2	OC(=O)CC1CCCCC1	2,85
(1R,2S)-2-(4-methoxyphenyl)propanoic acid	C13H18O2	COc1ccc(cc1)[C@@H](C)C(=O)O	2,85
3-Cresotinic acid	C8H8O3	CC1=C(C(=CC=C1)C(=O)O)O	2,86
4-Bromobenzoic acid	C7H5BrO2	OC(=O)c1ccc(Br)cc1	2,86
Cyclohexene	C6H10	C1CCC=CC1	2,86
4-Aminobiphenyl	C12H11N	Nc1ccc(cc1)c2ccccc2	2,86
(3aR,6aR)-3-(4-ethylphenyl)propanoic acid	C16H20N2O2S2	CCc1ccc(cc1)N2[C@H]3C[S](=O)(=O)C3	2,86
3-Bromobenzoic acid	C7H5BrO2	OC(=O)c1ccc(Br)c1	2,87
Hexyl acetate	C8H16O2	CCCCCCOC(=O)C	2,87
Isoproturon	C12H18N2O	CC(C)c1ccc(NC(=O)N(C)C)cc1	2,87
Isocyclocitral	C10H16O	CC1CC(=CC(C)C1C=O)C.CC2C=C	2,87
ZINC02916975	C19H22N4O4	Cn1c2Nc3cccc[nH]3C(=O)c2cc1	2,87
Butyl methacrylate	C8H14O2	CCCCOC(=O)C(C)=C	2,88
Tetrachloroethylene	C2Cl4	ClC(Cl)=C(Cl)Cl	2,88
Deoxycorticosterone	C21H30O3	C[C@]12CC[C@H]3[C@@H](CC1)C(=O)C2	2,88
4-Chloro-6-methoxy-N-(2,3-dihydro-1,4-benzodioxin-5-yl)butane-2-carboxylate	C10H9ClN4O	COc1nc(Cl)nc(Nc2ccccc2)n1	2,89
4-Ethylbenzoic acid	C9H10O2	CCc1ccc(cc1)C(=O)O	2,89
Pentachloroethane	C2HCl5	ClC(Cl)C(Cl)(Cl)Cl	2,89
[2,6-diacetyloxy-4-[[4-(2,3-dihydro-1,4-benzodioxin-5-yl)butane-2-carboxylate]]phenyl]acetamide	C25H21NO8	CC(=O)Oc1cc(cc(OC(=O)C)O)c1OC	2,89
2-Octanol	C8H18O	CCCCCCC(O)C	2,90
2-Octanol	C8H18O	CCCCCCC(O)C	2,90
Phenol, 4-(1-methylethyl)-	C9H10O	CC(=C)c1ccc(O)cc1	2,90
Triadimenol	C14H18ClN3O2	CC(C)(C)C(O)C(Oc1ccc(Cl)cc1)n1	2,90
5-Methyl-2-octanone	C9H18O	CCCC(C)CCC(C)=O	2,92
(Bromomethyl)benzene	C7H7Br	BrCc1ccccc1	2,92
2-[4-(2,3-dihydro-1,4-benzodioxin-5-yl)butane-2-carboxylate]phenyl acetamide	C13H10N2O2S2	N#CCc1sc(n1)c2ccc3OCCOc3c	2,92

Indene	C9H8	C1C=Cc2ccccc12	2,92
8-(2-hydroxyethylamir	C14H23N5O3	CC(C)CCn1c(NCCO)nc2N(C)C(=C	2,93
1-(4-chlorophenyl)sulf	C10H9ClN2O2S	Cc1nccn1[S](=O)(=O)c2ccc(Cl)c	2,93
2-Propylphenol	C9H12O	CCCc1ccccc1O	2,93
[1-(hydroxymethyl)-2,4	C11H20O2	CC1CC(=CC(C)C1(CO)CO)C	2,93
5-bromo-N-(3-methox	C14H20BrNO2	COCCCN(C=O)c1cc(Br)c(C)c(C)c	2,93
1-(3,4-Dichlorophenyl)	C8H8Cl2N2O	CNC(=O)Nc1ccc(Cl)c(Cl)c1	2,94
5-Phenylvaleric acid	C11H14O2	OC(=O)CCCCc1ccccc1	2,94
ZINC02592096	C18H19N3O4S	COc1ccc(cc1OC)N2C(=O)C[C@H]	2,95
ZINC02842393	C20H14N4O4	c1cc(c(cc1)[N+](=O)[O-])/C=N/c	2,95
1-(3,4-dimethylphenyl)	C15H17NO	CC1=CC(=O)C=C(C)N1c2ccc(C)c	2,95
Boscalid	C18H12Cl2N2O	Clc1ccc(cc1)c2ccccc2NC(=O)c3c	2,96
Ametryn	C9H17N5S	CCNc1nc(NC(C)C)nc(SC)n1	2,98
ethyl 2-(3-thiophen-2-	C12H12N4O2S2	CCOC(=O)CC1=Nn2c(SC1)nnc2c	2,98
alpha-Terpineol	C10H18O	CC1=CCC(CC1)C(C)(C)O	2,98
3-(4-methylphenoxy)-1	C18H22N2O4S2	Cc1ccc(OCCC(=O)N2CCN(CC2)[S]	2,98
Bromobenzene	C6H5Br	Brc1ccccc1	2,99
2-Chloro-4-nitrotoluen	C7H6ClNO2	Cc1ccc(cc1Cl)[N+](=O)[O-]=O	3,00
Disulphide, diethyl	C4H10S2	CCSSCC	3,00
1-Iodobutane	C4H9I	CCCCI	3,00
Cyclopentane	C5H10	C1CCCC1	3,00
Iprodione	C13H13Cl2N3O3	CC(C)NC(=O)N1CC(=O)N(C1=O)	3,00
Amlodipine	C20H25ClN2O5	CCOC(=O)C1=C(COCCN)NC(=C(C	3,00
Tebutame	C15H23NO	CC(C)N(Cc1ccccc1)C(=O)C(C)(C)	3,00
Bevantolol	C20H27NO4	COc1ccc(CCNCC(O)COc2cccc(C	3,00
Ursodeoxycholic acid	C24H40O4	C[C@H](CCC(O)=O)[C@H]1CC[C@H]	3,00
Apigenin	C15H10O5	Oc1ccc(cc1)C2=CC(=O)c3c(O)cc	3,02
[2-[(2-chloro-4-fluorop	C12H13ClFNO3	CCCC(=O)OCC(=O)Nc1ccc(F)cc1	3,02
Acetochlor	C14H20ClNO2	CCOCCN(C(=O)CCl)c1c(C)cccc1C	3,03
Finasteride	C23H36N2O2	CC(C)(C)NC(=O)[C@H]1CC[C@H]	3,03
ZINC00346783	C11H9NO6S	CC1(OC(=O)C(=Cc2ccc(s2)[N+](=	3,04
ZINC02064506	C11H13FN2O3	CCCCC(=O)Nc1ccc(c1)[N+](=C	3,04
Isoeugenol	C10H12O2	COc1cc(C=CC)ccc1O	3,04
Octanoic acid	C8H16O2	CCCCCCCC(O)=O	3,05
Styrene	C8H8	C=Cc1ccccc1	3,05
Erythromycin	C37H67NO13	CC[C@H]1OC(=O)[C@H](C)[C@H]	3,06
1-Octanol	C8H18O	CCCCCCCCO	3,07
(4S,7R)-2-amino-4-(2-f	C22H17FN2O2	NC1=C(C#N)[C@H](c2ccccc2F)C	3,07
ZINC02776618	C12H15ClF3N3O2	C[C@H](n1nc(c(Cl)c1C)C(F)(F)F	3,08
ZINC00116611	C16H15N3O2	Cc1cc(n(c(=O)c1C#N)/N=C/c2cc	3,08
(6-oxo-7,8,9,10-tetra	C24H25NO6S	CC[C@@H](N[S](=O)(=O)c1ccc(	3,08
Cortexolone	C21H30O4	CC12CCC(=O)C=C1CCC3C2CCC4	3,08
Hyodeoxycholic acid	C24H40O4	CC(CCC(O)=O)C1CCC2C3CC(O)C	3,08
Murocholic acid	C24H40O4	C[C@H](CCC(=O)O)[C@H]1CC[C@H]	3,08
2-Phenylphenol	C12H10O	Oc1ccccc1c2ccccc2	3,09
ZINC02555316	C16H10F2N2O3	CC1=CC2=C([C@@H](c3ccccc(F	3,10
Neopentane	C5H12	CC(C)(C)C	3,11
ZINC01038169	C17H18N2O4S3	CN1c2ccccc2-c3c(c(sc3C(=O)N4	3,11
ZINC03575851	C17H21N3O2	C[C@H]1CCCC[C@@H]1NC(=O	3,11
ZINC01322675	C13H18F3NO2	C[C@]12CO[C@@]3(C[C@H]1C	3,11
o-Xylene	C8H10	Cc1ccccc1C	3,12
Benzo[b]thiophene	C8H6S	s1ccc2ccccc12	3,12

(-)-trans-Carveol	C10H16O	CC(=C)[C@@H]1CC=C(C)[C@@	3,12
ZINC02778289	C15H20BrF2N5O	C[C@@H](n1nc(C(F)F)c(Br)c1C	3,12
N-(2-acetamido-[1,3]thiazol-5-yl)acetamide	C12H10N4O2S2	CC(=O)Nc1sc2cc3nc(NC(C)=O)s	3,13
Metolachlor	C15H22ClNO2	CCc1cccc(C)c1N(C(C)COC)C(=O)	3,13
Estrone	C18H22O2	C[C@]12CC[C@H]3[C@@H](CC	3,13
Estrone	C18H22O2	CC12CCC3C(CCc4cc(O)ccc34)C1	3,13
6-(6-ethoxypyridazin-3-yl)pyridine	C14H21N7O2	CCNc1nc(NC(C)C)nc(Oc2ccc(OC	3,14
(3R)-1-(benzoyl)-3-phenylpropan-1-ol	C19H18N4O2S	O=C1[C@@H](CCCCN1C(=O)c2	3,14
Ethylbenzene	C8H10	CCc1ccccc1	3,15
p-Xylene	C8H10	Cc1ccc(C)cc1	3,15
2,6-Dimethylbenzene	C8H10S	Cc1cccc(C)c1S	3,15
1,1,2-Trichlorotrifluoroethane	C2Cl3F3	FC(F)(Cl)C(F)(Cl)Cl	3,16
2-Nonanone	C9H18O	CCCCCCCC(C)=O	3,16
Cuminaldehyde	C10H12O	CC(C)c1ccc(C=O)cc1	3,17
Perillyl alcohol	C10H16O	CC(=C)[C@H]1CCC(=CC1)CO	3,17
beta-Carboline	C11H8N2	[nH]1c2ccccc2c3ccncc13	3,17
17-Hydroxyprogesterone	C21H30O3	CC(=O)[C@@]1(O)CC[C@H]2[C	3,17
ZINC00450333	C14H15N7O4	c1cc(ccc1/C=N/Oc2nc(nc(n2)N:	3,18
Isopropyl benzoate	C10H12O2	CC(C)OC(=O)c1ccccc1	3,18
Naproxen	C14H14O3	COc1ccc2cc(ccc2c1)C(C)C(O)=C	3,18
[2-oxo-2-(phenylamino)ethyl]phosphonic acid	C15H12FNO3	Fc1ccccc1C(=O)OCC(=O)Nc2ccc	3,18
Benzophenone	C13H10O	O=C(c1ccccc1)c2ccccc2	3,18
2-Phenylacetophenone	C14H12O	O=C(Cc1ccccc1)c2ccccc2	3,18
Clotiazepam	C16H15ClN2OS	CCc1sc2N(C)C(=O)CN=C(c3cccc	3,18
N-(2,3-dihydro-1,4-benzodioxin-5-yl)acetamide	C17H17NO5S	O=C(C[S](=O)(=O)Cc1ccccc1)Nc	3,19
2-(2-hydroxyethyl)-5-oxo-1,4-dihydro-2H-pyridin-4-ylideneacetamide	C20H16N2O6	OCCN1C(=O)c2ccc(cc2C1=O)c3	3,19
n-(4-Methoxyphenyl)acetamide	C14H15NO2	COc1ccc(Nc2ccc(OC)cc2)cc1	3,19
N-(2,3-dimethylphenyl)acetamide	C15H16N2OS	Cc1cccc(NC(=O)CSc2cccn2)c1C	3,19
N,N'-bis(2-hydroxyethyl)acetamide	C19H22N2O8S2	CN(CCO)[S](=O)(=O)c1ccc2c(OC	3,20
Linuron	C9H10Cl2N2O2	CON(C)C(=O)Nc1ccc(Cl)c(Cl)c1	3,20
Bromocyclohexane	C6H11Br	BrC1CCCCC1	3,20
4-Propylphenol	C9H12O	CCCc1ccc(O)cc1	3,20
2-[[4-amino-5,6,7,8-tetrahydro-2H-pyridin-2-yl]methyl]propanoic acid	C16H22N4O3S2	Nc1nc(SCC(=O)N(CCO)CCO)nc2	3,20
m-Xylene	C8H10	Cc1cccc(C)c1	3,20
N-tert-butyl-2-[[5-cyclohexylidene-2,3-dihydro-1,4-benzodioxin-5-yl]methyl]propanoic acid	C16H28N4OS	CCn1c(SCC(=O)NC(C)(C)C)nn1C	3,20
Flufenacet	C14H13F4N3O2S	CC(C)N(C(=O)COc1sc(nn1)C(F)(F)F)C(=O)N	3,20
Prostaglandin E1	C20H34O5	CCCC[C@H](O)/C=C/[C@H]1[C@@H](O)CC1	3,20
Fencamfamine	C15H21N	CCNC1C2CCC(C2)C1c3ccccc3	3,20
N-[2-methyl-3-(tetrazol-5-yl)propyl]acetamide	C23H21N5O	Cc1c(NC(=O)CC(c2ccccc2)c3ccc	3,20
Paclobutrazol	C30H40Cl2N6O2	CC(C)(C)C(O)C(Cc1ccc(Cl)cc1)n2	3,20
Terbutylazine	C9H16ClN5	CCNc1nc(Cl)nc(NC(C)(C)C)n1	3,21
Dibutyl ether	C8H18O	CCCCOCCCC	3,21
1,2-Dibromotetrafluoroethane	C2Br2F4	FC(F)(Br)C(F)(F)Br	3,22
Azulene	C10H8	c1ccc2cccc2cc1	3,22
2,4-Dichlorophenol	C6H4Cl2O	Oc1ccc(Cl)cc1Cl	3,23
3,4-Xylenol	C8H10O	Cc1ccc(O)cc1C	3,23
Dehydroepiandrosterone	C19H28O2	C[C@]12CC[C@H]3[C@@H](CC	3,23
7-ethyl-8-[[[(2S)-2-hydroxypropanoate]methyl]amino]octahydroindole	C17H21N5O3	CCn1c(NC[C@@H](O)c2ccccc2)	3,24
ZINC00551538	C18H17N5O2	CC1CN(C3=C/C=C(C#N)/C#N)C	3,24
2-amino-7,7-dimethyl-2,3,4,5-tetrahydro-1H-benzodiazepin-5-one	C19H24N2O4	CC1(C)CC(=O)C2=C(C1)OC(=C(C	3,24
2,5-bis(diethoxyphosphoryl)benzene	C14H26O7P2	CCO[P](=O)(Cc1oc(C[P](=O)(OC	3,25
2,4-dichlorophenol	C9H9ClO3	Cc1cc(Cl)ccc1OCC(O)=O	3,25

Isoamyl butyrate	C9H18O2	CCCC(=O)OCCC(C)C	3,25
ZINC02871160	C18H19N3O3	C[C@]12CC[C@@H]3[C@]1(CN	3,25
5-[1,3-dioxo-2-(1,3-thi	C23H10N4O5S2	O=C1N(c2scn2)C(=O)c3cc(ccc1	3,25
6-bromo-N-[(1-ethyl-3	C18H18BrN3O3	CCn1cc(CN(C)C(=O)C2=Cc3cc(B	3,27
5-methyl-2,4-di(pheny	C16H15N3	Cc1nn(c2ccccc2)c(N)c1c3ccccc:	3,27
Iodobenzene	C6H5I	Ic1ccccc1	3,28
(2S)-N-(1,3-benzodiox	C16H13NO5	O=C(Nc1ccc2OCOc2c1)[C@@H	3,28
m-Chlorotoluene	C7H7Cl	Cc1cccc(Cl)c1	3,28
ZINC03766933	C22H26N4O4S2	OC[C@@H](O)Cn1c(SCCSc2nc3	3,29
Triticonazole	C17H20ClN3O	CC1(C)CCC(=Cc2ccc(Cl)cc2)C1(C	3,29
5-(chloromethyl)-3-(2-	C10H9ClN2O	Cc1ccccc1c2noc(CCl)n2	3,30
Thymol	C10H14O	CC(C)c1ccc(C)cc1O	3,30
(3S,6R)-4-oxo-6-propa	C16H18N4O	CCC[C@@H]1C(=O)C[C@H](C(C	3,30
2-[2-(trifluoromethyls	C15H8F3NO3S	FC(F)(F)[S](=O)c1ccccc1N2C(=O	3,30
2-[2-(3,4-diethoxypher	C22H29NO4	CCOc1ccc(CC(=O)C2=C(CCCC2=	3,30
2-Aminoanthraquinon	C14H9NO2	Nc1ccc2C(=O)c3ccccc3C(=O)c2:	3,31
(1S,4R)-N-(2-ethylpher	C18H23NO3	CCc1ccccc1NC(=O)[C@]23CC[C	3,31
Pentyl butanoate	C9H18O2	CCCCCOC(=O)CCC	3,32
Benzene, 1-chloro-2-(	C7H6Cl2	ClCc1ccccc1Cl	3,32
ZINC03433862	C20H23ClN2O6S2	COc1ccc(cc1)N(CC(=O)N[C@@I	3,32
19-Oxotestosterone	C19H26O3	C[C@]12CC[C@H]3[C@H]([C@	3,32
Testosterone	C19H28O2	C[C@]12CC[C@H]3[C@@H](CC	3,32
Testosterone	C19H28O2	CC12CCC3C(CCC4=CC(=O)CCC3	3,32
[2-(3,3-dimethyl-2-oxo	C15H23N3O4S	COCc1cc(OC(=O)N(C)C)nc(SCC(:	3,33
p-Chlorotoluene	C7H7Cl	Cc1ccc(Cl)cc1	3,33
4-methyl-7-propan-2-yl	C13H14O3	CC(C)Oc1ccc2C(=CC(=O)Oc2c1)	3,33
Indan	C9H10	C1Cc2ccccc2C1	3,33
1,3-Dicyclohexylurea	C13H24N2O	O=C(NC1CCCCC1)NC2CCCCC2	3,33
5-cyclopropyl-N-[[[(2R)	C16H17F3N4O2	FC(F)(F)c1cc(nc2cc(nn12)C(=O)	3,33
1H-Isoindole-1,3(2H)-c	C14H15NO2S	O=C1N(SC2CCCCC2)C(=O)c3ccc	3,34
Naphthalene	C10H8	c1ccc2ccccc2c1	3,34
O4-[2-[[[(3R)-1,1-dioxo	C17H24N2O7S	CCOC(=O)c1[nH]c(C)c(C(=O)OC	3,35
1-Bromopentane	C5H11Br	CCCCCBr	3,37
Methylcyclopentane	C6H12	CC1CCCC1	3,37
ZINC01125223	C20H24N2O2S	CC1=C(C(c2sccc2)C3=C(O)CCCC	3,37
ZINC03372338	C25H25N3O4S	CN(C)[S](=O)(=O)c1cccc(CN2C(:	3,37
(1R,2S,3aR)-1-(2,2-dim	C23H21N3OS	CC(C)(C)C(=O)[C@H]1[C@H](c2	3,37
o-Dichlorobenzene	C6H4Cl2	Clc1ccccc1Cl	3,38
p-Dichlorobenzene	C6H4Cl2	Clc1ccc(Cl)cc1	3,38
ZINC03409607	C17H15FN4OS	CC(Sc1nnc(n1c2ccccc2)c3ccc(F)	3,38
ZINC02690652	C24H31N3O9	CC(=O)c1ccc(NC(=O)CNC(=O)C	3,39
methyl 3-[3-(1,3-dioxo	C19H16N2O5	COC(=O)c1cccc(NC(=O)CCN2C(:	3,39
p-t-Butyl-alpha-methy	C14H20O2	CC(Cc1ccc(cc1)C(C)(C)C)C(O)=O	3,39
1-Hexene	C6H12	CCCCCC=C	3,40
Menthol	C10H20O	CC(C)C1CCC(C)CC1O	3,40
Piperidine, 1,1'-(tetra	C12H20N2S6	S=C(SSSSC(=S)N1CCCCC1)N2CC	3,40
[(2R)-1-(ethyl-phenyla	C21H25NO6	CCN(C(=O)[C@@H](C)OC(=O)c:	3,40
Acridine	C13H9N	c1ccc2nc3ccccc3cc2c1	3,40
1-(2,3-dichlorophenyl)	C22H25Cl2N3O4S	Cc1cccc(C)c1NC(=O)CNC(=O)C2	3,41
Pelargonic acid	C9H18O2	CCCCCCCCC(O)=O	3,42
3,5,5-Trimethyl-1-hex	C9H20O	CC(CCO)CC(C)(C)C	3,42
o-Chlorotoluene	C7H7Cl	Cc1ccccc1Cl	3,42

1,3,5-Trimethylbenzen	C9H12	Cc1cc(C)cc(C)c1	3,42
ZINC02750654	C18H32N2O2	C[C@@H]1CCCCN1C(=O)CCCC	3,42
2-(3-oxo-2,4-dihydro-1C26H24N6O4		O=C(CC1Nc2ccccc2NC1=O)Nc3	3,42
methyl 2-[(4-methoxy)C16H17NO5S		COC(=O)CN(c1ccccc1)[S](=O)=	3,43
Propyzamide	C12H11Cl2NO	CC(C)(NC(=O)c1cc(Cl)cc(Cl)c1)C	3,43
6-[(1R)-1-(4-methoxy)C19H23NO		COc1ccc(cc1)[C@@H](C)n2c(C)	3,43
Cyclohexane	C6H12	C1CCCCC1	3,44
N-(3-cyanophenyl)-3,4C17H16N2O4		COc1cc(cc(OC)c1OC)C(=O)Nc2c	3,44
Diphenylamine	C12H11N	N(c1ccccc1)c2ccccc2	3,44
Pentane	C5H12	CCCCC	3,45
Geranial	C10H16O	CC(C)=CCC\C(C)=C\C=O	3,45
7-methoxy-3,4,8-trimeC13H14O3		COc1ccc2C(=C(C)C(=O)Oc2c1C)	3,45
ZINC06506520	C19H21N5O2S	COCCn1c(C)cc(C(=O)CSc2nnc3[	3,45
N-tert-butyl-2,3,4,5,6-C12H12F5NO		CN(C(=O)c1c(F)c(F)c(F)c(F)c1F)(	3,45
2,2,3,3,4,4,5,5,6,6,7,7-C7H4F12O		OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C	3,46
Acetal R	C13H20O2	CCCOC(C)OCCc1ccccc1	3,46
1-Isothiocyanato-2-phC9H9NS		S=C=NCCc1ccccc1	3,47
Geraniol	C10H18O	CC(C)=CCC\C(C)=C\C=O	3,47
(10bR)-8,9-dimethoxy-C19H25NO4		COc1cc2CCN3C(=O)OC4(CCCCC	3,47
2-[3-(cyclopropanecarC22H22N2O2		Cc1ccc(C)c1NC(=O)Cn2cc(C(=C	3,47
Terbutryne	C10H19N5S	CCNc1nc(NC(C)(C)C)nc(SC)n1	3,48
m-Dichlorobenzene	C6H4Cl2	Clc1ccc(Cl)c1	3,48
(2R)-2-[(4-chlorophenC15H21ClN2O3S		C[C@@H](N(c1ccc(Cl)cc1)[S](C	3,48
Propranolol	C16H21NO2	CC(C)NCC(O)COc1cccc2ccccc12	3,48
1-(4-fluorobenzoyl)-N-C21H23FN2O2		C[C@@H](NC(=O)C1CCN(CC1)C	3,48
7-[4-(2,5-dimethylpyrrC17H15N5		Cc1ccc(C)n1c2ccc(cc2)c3ccnc4r	3,50
Deoxycholic acid	C24H40O4	C[C@H](CCC(O)=O)[C@H]1CC[O	3,50
ZINC03443597	C20H19N3O8S	c1ccc2c(c1)C(=NS2(=O)=O)NCC	3,52
Alachlor	C14H20ClNO2	CCc1cccc(CC)c1N(COC)C(=O)CC	3,52
Deferasirox	C21H15N3O4	OC(=O)c1ccc(cc1)N\2N\C(NC2=	3,52
Propericiazine	C21H23N3OS	OC1CCN(CCCN2c3ccccc3Sc4ccc	3,52
2-[[5-[2-(4-bromo-3,5-C16H23BrN6OS		CCn1c(CCn2nc(C)c(Br)c2C)nnc1	3,53
o-Ethyltoluene	C9H12	CCc1ccccc1C	3,53
(4S)-4-(5-methylfuran-C21H18O3		Cc1oc(cc1)[C@@H](O)C#CC(O)	3,53
N-cyclopropyl-5-[(2,3,5C15H11F4NO3		Fc1cc(F)c(F)c(OCc2oc(cc2)C(=O	3,54
N-[5-(4-amino-1,3-dioC21H15N3O5		Cc1ccc(cc1NC(=O)c2occc2)C(=C	3,55
2-[2-(trifluoromethyl)C15H8F3NO2		FC(F)(F)c1ccccc1N2C(=O)c3cccc	3,55
Dihydrotestosterone	C19H30O2	C[C@]12CC[C@H]3[C@@H](CC	3,55
3-chloro-N-[[[(2S)-oxolC14H14ClNO2S		Clc1c(sc2ccccc12)C(=O)NC[C@	3,56
Flavone	C15H10O2	O=C1C=C(Oc2ccccc12)c3ccccc3	3,56
ZINC01126453	C18H17ClN2O3S	Cc1ccc(cc1)N2[C@H]3C[S](=O)(	3,56
methyl 2-[(4R)-4,6-bis(C19H14Cl2N2O4		COC(=O)C(=O)C1=C(NC(=O)N[C	3,56
ZINC03542779	C22H34N4O3S2	COC1CCCC(C1)N2C(NC3CCCCC3	3,56
[2-(4-amino-1,3-dimetC17H18N4O6		CN1C(=C(C(=O)COC(=O)c2cccc(	3,57
ZINC00218005	C16H31N3O3S	CCN(CC)[S](=O)(=O)N1CCC[C@	3,58
9H-Fluoren-9-one	C13H8O	O=C1c2ccccc2c3ccccc13	3,58
ethyl (4S)-4-(1,3-benzC17H20N2O5		CCCC1=C([C@@H](NC(=O)N1)c	3,59
Phenyl benzoate	C13H10O2	O=C(Oc1ccccc1)c2ccccc2	3,59
3-Methylpentane	C6H14	CCC(C)CC	3,60
1,2,3-TrimethylbenzenC9H12		Cc1ccc(C)c1C	3,60
4-chloro-N-pentan-3-yC16H23ClN2O3S		CCC(CC)NC(=O)c1ccc(Cl)c(c1)[S	3,60
ZINC00118751	C16H7N7	Cn1c2ccccc2n3c4nc(C#N)c(nc4	3,61

2-(4,6-dimethylpyrimidin-2-yl)-N-(2-tert-butylphenyl)acetamide	C <sub>15</sub> H <sub>23</sub> N <sub>3</sub> O <sub>5</sub>	CC[C@@H]1CCCCN1C(=O)CSc2	3,61
N-(2-tert-butylphenyl)acetamide	C <sub>20</sub> H <sub>25</sub> N <sub>3</sub> O <sub>4</sub>	COc1cc(cc(OC)c1OC)C(=O)Nc2c	3,61
1,1-bis(4-fluorophenyl)ethane-2,2-diol	C <sub>16</sub> H <sub>12</sub> F <sub>2</sub> O <sub>2</sub>	OCC#CC(O)(c1ccc(F)cc1)c2ccc(F	3,61
7-dimethylamino-5-methyl-2-oxo-1,2,3,4-tetrahydroquinoline	C <sub>14</sub> H <sub>14</sub> N <sub>4</sub> S <sub>2</sub>	CN(C)c1nc(C)nc2N(C(=S)Sc12)c	3,62
[2-[[2-(2R)-3-methylbutanoate]]-1,2,3,4-tetrahydroquinolin-2(1H)-one	C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O <sub>5</sub>	CCCCN1C(=O)c2ccc(cc2C1=O)C	3,62
N-[(1R)-2-oxo-2-phenylethyl]acetamide	C <sub>19</sub> H <sub>15</sub> N <sub>3</sub> O <sub>2</sub> S	O=C(N[C@H](Sc1ncccc1)C(=O)O	3,62
ZINC00707994	C <sub>23</sub> H <sub>27</sub> N <sub>3</sub> O <sub>5</sub>	COc1cccc(c1)[C@H]2C(C(=O)O)C	3,62
1,2,4-Trimethylbenzene	C <sub>9</sub> H <sub>12</sub>	Cc1ccc(C)c(C)c1	3,63
p-Ethyltoluene	C <sub>9</sub> H <sub>12</sub>	CCc1ccc(C)cc1	3,63
ethyl 4-[2-(4-fluoro-3-iodophenyl)ethyl]piperazine-1-carboxylate	C <sub>22</sub> H <sub>25</sub> F <sub>2</sub> N <sub>2</sub> O <sub>8</sub> S	CCOC(=O)c1c(C)[nH]c(C)c1C(=C	3,63
[2-[[1,5-dimethyl-3-oxo-1,2,3,4-tetrahydroquinolin-2(1H)-one]]-1,2,3,4-tetrahydroquinolin-2(1H)-one	C <sub>20</sub> H <sub>20</sub> N <sub>4</sub> O <sub>4</sub> S	CSc1ncccc1C(=O)OCC(=O)NC2=	3,63
N-(3-fluorophenyl)-4-methylpiperazine-1-carboxamide	C <sub>18</sub> H <sub>19</sub> F <sub>2</sub> N <sub>2</sub> O <sub>5</sub> S	COc1ccc(cc1[S](=O)(=O)N2CCO	3,64
(E)-5-(4-chlorophenyl)-4-methylpiperazine-1-carboxamide	C <sub>13</sub> H <sub>10</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	C1SC(=C(C(=O))/C=C/C2=CC=C(C	3,64
4-Butylphenol	C <sub>10</sub> H <sub>14</sub> O	CCCCc1ccc(O)cc1	3,65
2-(1,3-dioxoisindol-2-yl)acetamide	C <sub>21</sub> H <sub>19</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>7</sub> S	O[C@H]1C[C@H](N(C1)[S](=O)O	3,65
4-(4-chlorophenyl)-2-methylpiperazine-1-carboxamide	C <sub>10</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>2</sub>	Cc1scc(n1)c2ccc(Cl)cc2	3,65
(1R,2R,5S)-2-[3,4-diphenylbutyl]piperazine-1-carboxamide	C <sub>20</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub> S	O=C1C[C@H]([C@@H]2CO[C@H]2	3,65
methyl 4-bromo-3-piperidylacetate	C <sub>13</sub> H <sub>16</sub> Br <sub>2</sub> N <sub>2</sub> O <sub>4</sub> S	COC(=O)c1ccc(Br)c(c1)[S](=O)(=	3,66
Isopropylbenzene	C <sub>9</sub> H <sub>12</sub>	CC(C)c1ccccc1	3,66
ZINC03621394	C <sub>27</sub> H <sub>26</sub> F <sub>2</sub> N <sub>2</sub> O <sub>6</sub>	COc1ccc(cc1OC)[C@H]2[C@H](O)C	3,66
O3-ethyl O5-methyl 4-ethylpiperazine-1-carboxylate	C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> O <sub>5</sub>	CCOC(=O)C1=C(C)NC(=C(C1c2oc	3,67
17a-Ethynylestradiol	C <sub>20</sub> H <sub>24</sub> O <sub>2</sub>	C[C@]12CC[C@H]3[C@@H](CC[C@]1	3,67
1-[[2-(2R,4R)-2-(2,4-dichlorophenyl)ethyl]oxy]propan-1-ol	C <sub>13</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>	C[C@]1(OC[C@@H](Cn2cncn2)O)C	3,68
(4-formyl-2-methoxyphenyl)acetamide	C <sub>14</sub> H <sub>10</sub> F <sub>2</sub> O <sub>5</sub> S	COc1cc(C=O)ccc1O[S](=O)(=O)c	3,68
ZINC00731980	C <sub>13</sub> H <sub>14</sub> Cl <sub>3</sub> N <sub>3</sub> O <sub>3</sub>	CC(C)C(=O)N[C@H](Oc1ccc(C(=O)N	3,68
Maybridge4_002663	C <sub>16</sub> H <sub>11</sub> F <sub>2</sub> N <sub>5</sub> O <sub>5</sub>	Cn1c(SCc2cc(F)cc(F)c2)nnc1c3c	3,68
1-[[3-(5S)-3,5-dimethylpiperidin-2-yl]oxy]propan-1-ol	C <sub>18</sub> H <sub>24</sub> N <sub>4</sub> O <sub>5</sub>	C[C@H]1C[C@H](C)CN(C1)C(=C	3,68
ZINC13154025	C <sub>20</sub> H <sub>23</sub> N <sub>3</sub> O <sub>3</sub>	NC(=O)c1cc(ccc1N2CCCC2)N3	3,68
Propylbenzene	C <sub>9</sub> H <sub>12</sub>	CCCC1CCCC1	3,69
Maybridge3_003470	C <sub>10</sub> H <sub>7</sub> N <sub>3</sub> S	CSc1scc(c2sccc2)c1C#N	3,69
N-(2-hydroxyethyl)-4-methylpiperazine-1-carboxamide	C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> O <sub>3</sub> S	Cc1ccc(cc1)[S](=O)(=O)N(CCO)C	3,69
Androsterone	C <sub>19</sub> H <sub>30</sub> O <sub>2</sub>	C[C@]12CC[C@@H](O)C[C@@]12	3,69
Tebuconazole	C <sub>16</sub> H <sub>22</sub> Cl <sub>2</sub> N <sub>3</sub> O	CC(C)(C)C(O)(CCc1ccc(Cl)cc1)Cr	3,70
4-chloro-N-(2-phenylethyl)acetamide	C <sub>15</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>2</sub> O	Clc1ccc(cc1)C(=O)NCCc2ccccc2	3,71
1-phenyl-5-[2-(1-phenylethoxy)ethyl]piperazine-1-carboxamide	C <sub>16</sub> H <sub>14</sub> N <sub>8</sub> O <sub>2</sub>	C(COc1nnnn1c2ccccc2)Oc3nnn	3,72
ZINC00045256	C <sub>17</sub> H <sub>13</sub> N <sub>3</sub> O <sub>5</sub>	c1cc2c(cc1/C=C/C(=O)Nc3ccc4c	3,72
methyl 3-[[4-methylbenzoyl]oxy]propanoate	C <sub>16</sub> H <sub>15</sub> N <sub>3</sub> O <sub>3</sub>	COC(=O)c1cccc(NC(=O)c2ccc(C)cc	3,72
Propiconazole	C <sub>15</sub> H <sub>17</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub>	CCCC1COC(Cn2cncn2)(O1)c3ccc	3,72
Carbazole	C <sub>12</sub> H <sub>9</sub> N	[nH]1c2ccccc2c3ccccc13	3,72
5-[[3-ethoxy-5-iodo-4-methylphenyl]oxy]propanoic acid	C <sub>18</sub> H <sub>17</sub> I <sub>2</sub> N <sub>2</sub> O <sub>4</sub> S	CCOc1cc(cc(I)c1OCC#C)C=C2C(=O	3,72
Oryzalin	C <sub>12</sub> H <sub>18</sub> N <sub>4</sub> O <sub>6</sub> S	CCCN(CCC)c1c(cc(cc1[N+])([O-])O	3,73
(2-chlorophenyl)-[(5R)-1,2,3,4-tetrahydroquinolin-2(1H)-one]	C <sub>17</sub> H <sub>14</sub> Cl <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	CC1=NN(C(=O)c2ccccc2Cl)[C@H]1	3,73
Prazepam	C <sub>19</sub> H <sub>17</sub> Cl <sub>2</sub> N <sub>2</sub> O	Clc1ccc2N(CC3CC3)C(=O)CN=C1	3,73
ZINC02774982	C <sub>13</sub> H <sub>15</sub> Cl <sub>2</sub> F <sub>2</sub> N <sub>2</sub> O <sub>2</sub> S	FC(F)Oc1ccc(NC(=S)NC[C@@H]1C	3,74
ethyl 4-[4-[[3a,7a]-1,2,3,4-tetrahydroquinolin-2(1H)-one]]-1,2,3,4-tetrahydroquinolin-2(1H)-one	C <sub>22</sub> H <sub>27</sub> N <sub>3</sub> O <sub>5</sub>	CCOC(=O)N1CCN(CC1)C(=O)c2c	3,74
2-[3-cyano-6-(difluoromethyl)pyridin-2-yl]acetamide	C <sub>17</sub> H <sub>17</sub> F <sub>2</sub> N <sub>5</sub> O <sub>3</sub>	Cn1cc(c(C)n1)c2cc(nc(SCC(=O)N)C	3,74
methyl 2-[[4-(2-methylpropanoate)oxy]phenyl]acetamide	C <sub>14</sub> H <sub>23</sub> N <sub>5</sub> O <sub>3</sub> S	COC(=O)CSc1nc(NCC(C)C)nc(n1	3,75
propan-2-yl (4R)-4-[4-(1,2,3,4-tetrahydroquinolin-2(1H)-one)]acetamide	C <sub>17</sub> H <sub>20</sub> F <sub>2</sub> N <sub>2</sub> O <sub>5</sub>	COc1cc(ccc1OC(F)F)[C@H]2NC1	3,75
ZINC05163260	C <sub>20</sub> H <sub>17</sub> N <sub>5</sub> O <sub>3</sub>	c1ccc2c(c1)nc3c(n2)n(c(n3)c4cc	3,75
Biphenyl	C <sub>12</sub> H <sub>10</sub>	c1ccc(cc1)c2ccccc2	3,76
ZINC03614715	C <sub>28</sub> H <sub>27</sub> N <sub>3</sub> O <sub>5</sub>	COc1ccc(cc1)[C@H](N(C)C(=O)O)C	3,76
ZINC02807950	C <sub>14</sub> H <sub>14</sub> N <sub>6</sub> S	CCn1cc(cn1)c2nn3cnc4sc(C)c(C	3,77

ZINC01105326	C21H18ClNO9	COC(=O)c1cc(ccc1Cl)N2C(=O)[C	3,77
2-Decanone	C10H20O	CCCCCCCCC(C)=O	3,77
[2-oxo-2-(propan-2-yl)ac	C18H26N2O5S	CC(C)NC(=O)COC(=O)c1ccc(cc1	3,78
Oxybenzone	C14H12O3	COc1ccc(c(O)c1)C(=O)c2ccccc2	3,79
Benzyl phenyl ether	C13H12O	C(Oc1ccccc1)c2ccccc2	3,79
ZINC00438087	C20H16N2O4	c1cc(c(cc1)NC(=O)/C=C/c2occc	3,79
2-[[5-(2-fluorophenyl)-C	C22H23FN4O2S	Fc1ccccc1c2nnc(SCC(=O)N3CCC	3,79
ZINC00678637	C28H31NO6	CCOC(=O)C1=C(C)NC2=C([C@H	3,79
Verapamil	C27H38N2O4	COc1ccc(CCN(C)CCCC(C#N))(C(C	3,79
1-Bromohexane	C6H13Br	CCCCCBr	3,80
ethyl 2-(1-naphthalen-C	C15H14N4O2S	CCOC(=O)CSc1nnnn1c2cccc3cc	3,80
ZINC01133653	C21H25NO6	CC(=O)N[C@@H]1[C@@H](O)[	3,80
N-(2-adamantyl)penta	C15H25NO	CCCCC(=O)NC1C2CC3CC(C2)CC	3,80
Diazinon	C12H21N2O3PS	CCO[P](=S)(OCC)Oc1cc(C)nc(n1	3,81
ZINC03468009	C20H19NO6	COc1cccc(NC(=O)[C@H])(OC(=C	3,81
(2S)-2-[[5-[3-(dimethyl	C20H23N5O3S2	C[C@H](Sc1nnc(n1c2cccc(C)c2]	3,81
ZINC03587776	C19H18N2O8	Cc1c(c([nH])c1C(=O)COC(=O)c2c	3,82
2,2-Dimethylbutane	C6H14	CCC(C)(C)C	3,82
Azobenzene	C12H10N2	c1ccc(cc1)N=Nc2ccccc2	3,82
Fentin fluoride	C18H15FSn	[F]([Sn](c1ccccc1)(c2ccccc2)c3c	3,82
1H-Indene, 3a,4,7,7a-C	C9H12	C1C=CCC2C=CCC12	3,83
(4R)-6-amino-4-(2-met	C15H16N4OS	CCc1[nH]nc2OC(=C(C#N))[C@	3,83
ZINC03369081	C21H19NO3S2	Cc1ccc(c(c1)C)NC(=O)COC(=O)/	3,83
ZINC01067643	C21H14N2O2S	O=C1[C@@H]2[C@@H](C3c4c	3,83
2,3-Dimethylbutane	C6H14	CC(C)C(C)C	3,85
ZINC02802544	C17H16F3N11S	CCn1c(SCc2nn3cnc4n(C)ncc4c3	3,85
ZINC00936899	C19H21BrN4O2	CCOc1ccc(Br)cc1[C@@H]2n3nc	3,85
1,1-Dimethoxyoctane	C10H22O2	CCCCCCCC(OC)OC	3,85
EU-0081523	C14H15NO2S2	CC(=O)c1sc(SCCOc2ccccc2)nc1	3,86
1-Methylnaphthalene	C11H10	Cc1cccc2ccccc12	3,87
5-[[3,5-bis(trifluorome	C17H11F6N3O3	NC(=O)c1cc(NC(=O)c2cc(cc(c2)N	3,87
Progesterone	C21H30O2	CC(=O)[C@H]1CC[C@H]2[C@@	3,87
Progesterone	C21H30O2	CC(=O)C1CCC2C3CCC4=CC(=O)N	3,87
Methylcyclohexane	C7H14	CC1CCCCC1	3,88
Bicyclo 2.2.1 hept-5-ε	C9H4Cl6O4	OC(=O)C1C(C(O)=O)C2(Cl)C(=C	3,88
(2S)-1-(4-chlorophenyl	C23H25ClN4O4S	CN1N(C(=O)C(=C1C)NC(=O)[C@	3,89
ZINC02801329	C22H27NO4	CCOCCOC(=O)C1=C(C)NC2=C([C	3,89
propyl 5-carbamoyl-4-	C17H25N3O6S2	CCCOC(=O)c1c(C)c(sc1NC(=O)C	3,90
methyl 2-[6-methyl-3-	C17H15NO5S	COC(=O)COc1cc2OC=C(C(=O)c2	3,90
1-Chloronaphthalene	C10H7Cl	Clc1cccc2ccccc12	3,90
tert-butyl (2S)-2-[(3,4-	C18H26N2O3	Cc1ccc(NC(=O)[C@@H]2CCCN2	3,90
N-propan-2-yl-4-[3-(tri	C15H20F3N3O2S2	CC(C)NC(=S)N1CCN(CC1)[S](=O	3,90
[(3S)-1-(5-phenylthien	C18H19N3OS	OC[C@H]1CCCN(C1)c2ncnc3sc	3,90
ethyl 4-chloro-5-formy	C13H14ClNO3	CCOC(=O)c1[nH]c2CCC(=C(Cl)c:	3,92
ZINC18324649	C18H19N5O	Cc1ccc2c(C)nc(NC3=NC4=C(CCC	3,92
3-Chlorodiphenylamin	C12H10ClN	Clc1cccc(Nc2ccccc2)c1	3,92
ethyl (4S)-4-(2-bromo-	C17H20BrNO5	CCOC(=O)C1=C(C)NC(=O)C[C@	3,93
[7,8-bis(propylsulfonyl	C21H24N2O5S2	CCC[S](=O)(=O)c1c2cncnc2c(C	3,93
(3aS,7aS)-2-(3-bromo	C16H16BrNO2	CC1=C(C)C[C@H]2[C@H](C1)C	3,93
Methadone	C21H27NO	CCC(=O)C(CC(C)N(C)C)(c1ccccc:	3,93
Isoxaben	C18H24N2O4	CCC(C)(CC)c1cc(NC(=O)c2c(OC	3,94
ZINC01446574	C18H18Cl3N3O2S	COc1ccccc1NC(=S)N[C@H](NC	3,95



N-cyclopentyl-9H-xant	C19H19NO2	O=C(NC1CCCC1)C2c3cccc3Oc	3,95
ZINC02964424	C25H26N4O3S	CC[C@@H](SC1=Nc2cccc2C3=	3,95
2-furan-2-yl-5-(3,4,5-tr	C18H20N2O5	CCOc1cc(cc(OCC)c1OCC)c2oc(n	3,96
Acenaphthene	C12H10	C1Cc2cccc3cccc1c23	3,96
(9R)-9-(2-chloro-6-fluo	C17H13ClFNO3	Fc1cccc(Cl)c1[C@@H]2CC(=O)F	3,96
ZINC02767247	C18H20N2O4	Cc1oc(cc1)/C=C/C(=O)NCCNC(=	3,97
Ibuprofen	C13H18O2	CC(C)Cc1ccc(cc1)C(C)C(O)=O	3,97
Benzyl benzoate	C14H12O2	O=C(OCC1CCCCC1)c2cccc2	3,97
methyl (2S)-2-[(7,7-din	C24H28N2O5S	COC(=O)[C@H](CCSC)NC(=O)C1	3,97
1,2,4-Trichlorobenzene	C6H3Cl3	Clc1ccc(Cl)c(Cl)c1	3,98
2-Chloronaphthalene	C10H7Cl	Clc1ccc2cccc2c1	3,98
1-Chloroanthraquinon	C14H7ClO2	Clc1cccc2C(=O)c3cccc3C(=O)c	3,98
1-Heptene	C7H14	CCCCCC=C	3,99
Pyraclostrobin	C19H18ClN3O4	CON(C(=O)OC)c1cccc1COc2cc	3,99
Hexane	C6H14	CCCCCC	4,00
Hexachloroethane	C2Cl6	ClC(Cl)(Cl)C(Cl)(Cl)Cl	4,00
1,2,3,4-Tetramethylbe	C10H14	Cc1ccc(C)c(C)c1C	4,00
Cyprodinil	C14H15N3	Cc1cc(nc(Nc2cccc2)n1)C3CC3	4,00
2-Methylnaphthalene	C11H10	Cc1ccc2cccc2c1	4,00
1-cyclohexyl-3-[2-(trifl	C14H17F3N2O	FC(F)(F)c1cccc1NC(=O)NC2CC(	4,00
3,6-dichloro-N-(2,4-dir	C16H15Cl2NO2	COc1c(Cl)ccc(Cl)c1C(=O)Nc2ccc	4,00
N-[2-(3,4-dimethoxyph	C26H28FN5O5S	COc1ccc(CCNC(=O)CSc2nc3N(C	4,00
(3R,3aS,6aR)-3,5-di(ph	C26H17NO5	O=C1[C@@H]2[C@@H](OC3([I	4,00
Isobutylbenzene	C10H14	CC(C)Cc1cccc1	4,01
1-(3,4-dihydro-2H-1,5-C	C23H28N2O5S	Cc1ccc(CNC(=O)C2CCN(CC2)[S]	4,01
Estradiol	C18H24O2	C[C@]12CC[C@H]3[C@@H](CC	4,01
1-Nonanol	C9H20O	CCCCCCCCO	4,02
1,3,5-Trichlorobenzene	C6H3Cl3	Clc1cc(Cl)cc(Cl)c1	4,02
Azithromycin	C38H72N2O12	CC[C@H]1OC(=O)[C@H](C)[C@	4,02
ZINC00160197	C15H8ClN3O4	O=C(N2/N=C/c3c(Cl)ccc([N+])([C	4,03
ZINC02835695	C16H14O2S2	c1ccc(cc1)S/C=C/C=C/S(=O)(=O	4,03
Quazepam	C17H11ClF4N2S	Fc1cccc1C2=NCC(=S)N(CC(F)(F	4,03
1,2,3-Trichlorobenzene	C6H3Cl3	Clc1ccc(Cl)c1Cl	4,04
2-(1,3-benzothiazol-2-yl	C13H9NOS3	O=C(CSc1sc2cccc2n1)c3sccc3	4,04
(3-methoxyphenyl)-[3C	C19H21NO2	COc1cccc(c1)C(=O)N2CCC[C@@	4,04
2-(4-bromophenyl)-N-yl	C16H16BrNO	Cc1cccc(NC(=O)Cc2ccc(Br)cc2)c	4,05
4-[5-chloro-4-[[[(4S)-2,	C15H19ClF2N2O4	CC1(C)OC[C@H](COc2c(F)c(nc(	4,07
methyl 7-(trifluoromet	C18H16F3N3O5	COC(=O)c1cnn2c1nc(cc2C(F)(F	4,08
Phenol, 2-(1,1-dimeth	C12H18O	Cc1cc(C)c(O)c(c1)C(C)(C)C	4,08
Decanoic acid	C10H20O2	CCCCCCCCC(O)=O	4,09
ZINC03531368	C17H24N2O5S	CCCCNc1cccc1C(=O)OCC(=O)N	4,09
2-Undecanone	C11H22O	CCCCCCCCC(C)=O	4,09
2-[[5-(phenylmethyl)an	C17H24N4OS2	CC(C)N(C(C)C)C(=O)CSc1sc(NC	4,09
ZINC04713445	C20H24N4O2	CCOCc1c(C)cc(C)c([C@@H]2C(=	4,09
(2S)-N-[[5-(4-chloroph	C21H20ClN3O4	CC(C)N(Cc1oc(nn1)c2ccc(Cl)cc2	4,09
(2S)-2-[3-chloro-5-(trif	C13H8ClF3N2S	FC(F)(F)c1cnc([C@H](Cc2sccc2)	4,09
(2-oxo-2-pyrrolidin-1-yl	C21H19NO3	O=C(COC(=O)c1c2cccc2cc3ccc	4,09
ZINC03325954	C14H18ClN3O2S	CCCN(CC1CC1)C(=S)Nc2cc(ccc2	4,10
1,2,3,5-Tetramethylbe	C10H14	Cc1cc(C)c(C)c(C)c1	4,10
1,2,4,5-Tetramethylbe	C10H14	Cc1cc(C)c(C)cc1C	4,10
p-Cymene	C10H14	CC(C)c1ccc(C)cc1	4,10
Cyclododecanone	C12H22O	O=C1CCCCCCCCCCC1	4,10

Prochloraz	C15H16Cl3N3O2	CCCN(CCOc1c(Cl)cc(Cl)cc1Cl)C(=O)Nc1ccc(c(O)c1)C(C)(C)C	4,10
Phenol, 2-(1,1-dimethyl-2-propylphenyl)-	C11H16O	Cc1ccc(c(O)c1)C(C)(C)C	4,11
tert-Butylbenzene	C10H14	CC(C)(C)c1ccccc1	4,11
N-(3,4-dimethoxyphenyl)-2-propylbenzamide	C21H27NO6	CCOc1cc(cc(OCC)c1OCC)C(=O)Nc2ccc(cc2)C	4,11
ZINC13959247	C19H21F3N6O2	C[C@H]1CN(C[C@@H](C)O1)C(F)(F)F	4,11
Dibenzofuran	C12H8O	c1ccc2c(c1)ccc3ccccc23	4,12
T5257341	C23H26N4O4S2	Cc1c(sc2N=C3CCCCN3C(=O)c1)S(=O)(=O)N	4,13
ZINC00137750	C17H22N4S	Cn1c(CC#N)nnc1SCc2c(C)c(C)c(C)c2	4,14
Diphenylmethane	C13H12	C(c1ccccc1)c2ccccc2	4,14
N-[4-(benzoylamino)-3-methylphenyl]-2-propanamide	C22H20N2O2	Cc1ccc(c1)C(=O)Nc2ccc(NC(=O)C)cc2	4,14
5-[[2-[1-(2-methoxy-5-methylphenyl)ethyl]oxy]ethyl]oxy-2-propanamide	C19H19N7O4S	COc1ccc(C)cc1n2nnnc2SCC(=O)N	4,15
1-Chloroheptane	C7H15Cl	CCCCCCCCl	4,15
1,3-divinylbenzene	C10H10	C=Cc1ccc(C=C)c1	4,15
AP-853/42160273	C17H14N2O3S	COc1ccc(cc1)C(=O)CSc2oc(nn2)S	4,15
T5889711	C20H18N2O3S	Cc1cc(SCC(=O)N)Cc2ccc3OCOC3	4,15
Penbutolol	C18H29NO2	CC(C)(C)NC[C@@H](O)COc1ccc(cc1)C	4,15
ZINC01868102	C27H22N2O6	CC[C@@H](OC(=O)CNC(=O)c1ccc(cc1)C)C(=O)N	4,15
Chenodeoxycholic acid	C24H40O4	C[C@H](CCC(O)=O)[C@H]1CC[C@@H](C(=O)O)CC[C@H]1C	4,15
7-(3-methoxyphenyl)-2-propylbenzamide	C23H21N5O3	COc1ccc(c1)c2cn3c(nc4N(C)C(=O)N4)cc32	4,16
2,6-dimethoxy-N-[4-[4-(2-methoxyphenyl)butyl]piperidin-1-yl]acetamide	C27H29N3O4	COc1ccc(OC)c1C(=O)Nc2ccc(cc2)C(=O)N	4,16
Dibutyl adipate	C14H26O4	CCCCOC(=O)CCCC(=O)OCCCC	4,17
N-cyclopentyl-5,6,7,8-tetrahydro-2H-benzothiazine-2-thione	C15H19N3S	C1CCC(C1)Nc2ncnc3sc4CCCCc4	4,17
(4R)-4-(2-methoxyphenyl)-2-propylbenzamide	C18H19NO3	COc1ccccc1[C@@H]2CC(=O)Nc2ccc(cc2)C	4,17
2-[3-[4-(difluoromethyl)phenyl]butyl]piperidine	C17H11F2N3O2S	FC(F)Oc1ccc(cc1)N2C(=O)c3ccc(cc3)N2	4,17
T0507-5626	C33H34N2O6S	CCCN(CCC)[S](=O)(=O)c1ccc(cc1)S(=O)(=O)N	4,17
Benzene, 1,4-diethenyl-	C10H10	C=Cc1ccc(C=C)cc1	4,18
ZINC02617139	C22H27NO6	COc1ccc(C(=O)OCC(=O)c2cc(C)cc2)cc1	4,18
ZINC00766498	C21H17N3O3	Cc1ccc(cc1)N2[C@@H](Nc3ccc(O)cc3)C2	4,18
4-[(2R)-oxolane-2-carboxamide]piperidine	C22H25N3O3S	O=C([C@H]1CCCCO1)N2CCN(CC2)C1	4,18
Disperse yellow 163	C18H14Cl2N6O2	[O-][N+](=O)c1cc(Cl)c(N=Nc2ccc(cc2)C)cc1	4,19
ZINC01457114	C23H22N2O4	C[C@H]1CN(C[C@H](C)O1)C(=O)N	4,19
9H-Fluorene	C13H10	C1c2ccccc2c3ccccc13	4,20
(6,7-dimethoxy-3,4-dihydroquinolin-2(1H)-ylidene)acetamide	C23H28N2O5S	COc1cc2CCN(Cc2cc1OC)C(=O)c1ccccc1	4,20
Diphenyl ether	C12H10O	O(c1ccccc1)c2ccccc2	4,21
2-Phenylindole	C14H11N	[nH]1c2ccccc2cc1c3ccccc3	4,21
2-[[5-(4-chlorophenyl)butyl]oxy]acetamide	C18H23ClN4O5	Cn1c(SCC(=O)N)CC(CCCCl)cc1	4,21
ZINC03380609	C24H25N3O5S	C[C@@H](C(=O)OCC(=O)C)C(=O)N	4,21
ZINC02801315	C22H27NO4	CCCCOC(=O)C1=C(C)NC2=C([C@H]1)C(=O)N	4,21
ZINC09313347	C27H32N2O5	COc1cc(cc(OC)c1OC(C)=O)[C@@H]2CCN(C2)C	4,21
dimethyl (4R)-4-(3-chlorophenyl)-2-piperidinecarboxylate	C17H18ClNO4	COC(=O)C1[C@H](c2ccccc2Cl)c2ccccc12	4,22
N-[2-(3,4-dimethoxyphenyl)ethyl]acetamide	C20H25NO4	CCc1ccc(OCC(=O)N)CCc2ccc(OC)cc2	4,22
(2-chloro-6-fluorophenyl)acetamide	C18H17ClFNO4S	Fc1ccc(Cl)c1COC(=O)c2ccccc2	4,22
Pregnenolone	C21H32O2	CC(=O)[C@H]1CC[C@H]2[C@@H](C)CC[C@H]2C1	4,22
methyl 4-[[2-[(4-ethylphenyl)oxy]ethyl]oxy]acetate	C20H20N4O3S	CCn1c(SCC(=O)N)Cc2ccc(cc2)C(=O)OC	4,24
4-methoxy-3-[[2,3,5,6-tetrahydro-2H-pyridin-4-yl]oxy]acetamide	C15H10F4O3	COc1ccc(C=O)cc1COc2c(F)c(F)c(F)c2	4,24
1-[[4-amino-5-(4-methylphenyl)butyl]oxy]acetamide	C23H18N4O3S	COc1ccc(cc1)c2nnc(SCC3=CC(=O)N3)cc2	4,24
ZINC02944542	C23H36O5	C[C@@H]1CCC2[C@@]3(C)COC(=O)C3	4,24
2-ethoxyethyl (2S)-2-[(1S)-1-(2-ethoxyethyl)pyrrolidine-2-carboxylate]	C18H24N2O4S	CCOCCOC(=O)[C@H](C)N1C=N1	4,25
ZINC00989373	C25H22N2O8	COC(=O)CC1=C(C(=O)OC)[C@@H]2CCN(C2)C	4,25
2-(2-methylphenoxy)-1-(2-methylphenoxy)ethane	C20H24N2O4	Cc1ccccc1OCC(=O)NCCNC(=O)C	4,25
ZINC00647320	C23H27F3N6O3	COc1ccc(cc1OC)[C@H]2C[C@@H](F)N2	4,25
Butylbenzene	C10H14	CCCCc1ccccc1	4,26

ZINC04978849	C21H19N5O2S	CC(=O)Nc1ccc(cc1)[C@@H]2C(	4,26
[4-[(1,1-dioxo-1,2-ben:	C21H16N2O4S	CN(c1ccc(OC(=O)c2ccccc2)cc1)	4,26
T5256547	C15H21NO4S	CN(C)[S](=O)(=O)c1ccc(cc1)C(=	4,27
ZINC03428301	C22H25NO4	COc1cc(cc(c1OC)OC)/C=C/C(=O	4,27
ZINC02741252	C18H16F7N3O2	FC(F)C(F)(F)COCC1CCCC(c1)C(=O	4,27
Methadyl Acetate	C23H31NO2	CCC(OC(C)=O)C(CC(C)N(C)C)(c1	4,27
ZINC00125686	C14H15F3N2O3S	CC(C)(C)S(=O)(=O)/C(=C/Nc1ccc	4,28
ZINC02464437	C14H27NO	CCCCC(=O)NC1(CCC)CCCC1	4,28
ZINC18162323	C18H13Cl2N5O3	Clc1ccc(N2C(=O)[C@H]3N=NN(	4,30
ZINC03495716	C20H22N2O3	Cc1ccc(o1)/C=C/C(=O)N2CCN(C	4,30
2-[(4-methylphenyl)-(4	C21H26N2O4S2	CSc1ccc(cc1)[S](=O)(=O)N(CC(=	4,30
1,2-Dimethylnaphthalen	C12H12	Cc1ccc2ccccc2c1C	4,31
2,4-dichloro-N-(2-cyan	C22H23Cl2N3O6S	CCOc1cc(NC(=O)c2cc(c(Cl)cc2C	4,31
ZINC01042205	C24H20N4O3	CCc1ccc2nc3c(cc2c1)C(=O)N(c4	4,31
ZINC01145594	C22H23N3O5S	Cc1ccc(cc1)N(CC(=O)Nc2ccccc2	4,32
N-(furan-2-ylmethyl)-2	C13H13N5O2S	O=C(Cn1cnnn1)N(Cc2occc2)Cc:	4,33
2-[(3,4-dichlorophenyl	C11H8Cl2N2S	Clc1ccc(CSc2ncccn2)cc1Cl	4,33
N-(4-ethoxyphenyl)-2-	C22H19N3O3S2	CCOc1ccc(NC(=O)CSC2=Nc3ccs	4,33
ZINC03538275	C16H18Cl2N2O3	CCOC(=O)N1CCN(CC1)C(=O)/C=	4,34
ZINC03017635	C18H25N3O2S	C[C@@H]1CCC[C@@H](NC(=O	4,34
ZINC03226116	C19H28N2O3S	CCN(CC)S(=O)(=O)c1ccc(cc1)/C:	4,34
[4-(3-chlorophenyl)pi	C21H24ClN3O4S	Clc1cccc(c1)N2CCN(CC2)C(=O)c	4,34
N-(2,6-difluorophenyl)	C15H11Cl3F2N2O3S	C[S](=O)(=O)N(CC(=O)Nc1c(F)c	4,34
N-(3-quinoxalin-2-ylph	C19H13N3OS	O=C(Nc1cccc(c1)c2cnc3ccccc3r	4,34
6-amino-8-[2-[(2-chlor	C23H17ClN2O5	NC1=C(C#N)C(C2=C(O1)C(=O)C	4,34
ZINC03241789	C23H25N5O2	Cc1cc(C)nc(n1)n2nc(C)c3[C@H]	4,34
3-(4-chloro-2-methylp	C18H18ClN3S	Cc1cc(Cl)ccc1NC(=S)NCCc2c[nH]	4,34
ZINC00705483	C26H26ClN3O3	COc1ccc(cc1OC)[C@H]2C(=C(N	4,34
6-[[4-amino-5-[4-(diflu	C21H21F2N9OS	CCc1ccccc1Nc2nc(N)nc(CSc3nn	4,35
ZINC00062144	C14H18N2	CC(C)(C)c1[nH]nc(Cc2ccccc2)c1	4,35
Ketoconazole	C26H28Cl2N4O4	CC(=O)N1CCN(CC1)c2ccc(OC[C]	4,35
1-Bromoheptane	C7H15Br	CCCCCBr	4,36
N-[(1R)-1-phenylethyl]	C22H23N5OS	CCc1c2ccccc2c3nnc(SCC(=O)N	4,36
Isoamyl salicylate	C12H16O3	CC(C)CCOC(=O)c1ccccc1O	4,37
1,4-Dimethylnaphthalen	C12H12	Cc1ccc(C)c2ccccc12	4,37
ZINC03462024	C21H17N3O4S	CC(=O)N(c1ccccc1)c2nc(cs2)/C:	4,37
(3S,4S)-4-(1,3-benzodi	C25H21NO6	Cc1ccccc1O[C@H]2[C@@H](N	4,37
(+)-Limonene	C10H16	CC(=C)[C@@H]1CCC(=CC1)C	4,38
[2-[(2R,6R)-2,6-dimeth	C20H22ClFN2O4	C[C@@H]1CCC[C@@H](C)N1C	4,38
(3aR,7aR)-2-[2-[1-(1,3-	C24H24N2O5	Cc1cc(C(=O)CN2C(=O)[C@@H]:	4,38
ZINC01404771	C25H18ClF3N4O6	CCOC(=O)[C@H]1N=C([C@H]2[	4,38
(6R)-6-(6-chloro-1,3-b	C24H25ClN2O3	Cc1cc2N[C@@H](c3cc4OCOc4	4,38
Prostaglandin F2a	C20H34O5	CCCC[C@H](O)/C=C/[C@H]1[	4,39
Prostaglandin F2b	C20H34O5	CCCC[C@H](O)/C=C/[C@H]1[	4,39
[2-[(2S,6R)-2,6-dimeth	C23H23NO6S	C[C@@H]1CCC[C@@H](C)N1C(=	4,39
(2E)-5,5-dichloro-1-(4-	C12H10Cl2O2	COc1=CC=C(C=C1)C(=O)/C=C/C	4,40
1-Ethyl-naphthalene	C12H12	CCc1cccc2ccccc12	4,40
Methyl decanoate	C11H22O2	CCCCCCCCC(=O)OC	4,41
ZINC00132954	C14H13NO3	Cc1c(ccccc1OCc2ccccc2)[N+](=O	4,41
2-[[4-amino-5-[4-(diflu	C20H21F2N5O2S	Cc1cc(C)c(NC(=O)CSc2nnc(n2N	4,41
4-[2-amino-3-cyano-6-	C16H12F6N4O	CC1=CC(C(=C(N)N1c2ccc(cc2)C]	4,41
ZINC05841926	C16H16F3NO	CN1c2ccccc2C(C)(C)C1=CC=CC	4,41

ZINC00721789	C23H19ClN2O2	c1ccc(cc1)CNC(=O)/C=C/c2ccc	4,41
Undecanoic acid	C11H22O2	CCCCCCCCCCC(O)=O	4,42
8-(azepan-1-yl)-7-[2-(4C22H27N5O4		COc1ccc(cc1)C(=O)Cn2c(nc3N(C	4,42
ZINC04114722	C22H19FN4O3	COc1cc(ccc1OCc2cccc(F)c2)[C@	4,42
2-[4-(trifluoromethyl)phenyl]piperidine	C14H9F3N2	FC(F)(F)c1ccc(cc1)n2cc3cccc3r	4,42
Niflumic Acid	C13H9F3N2O2	OC(=O)c1cccn1Nc2cccc(c2)C(F	4,43
2,5-Cyclohexadiene-1,4-diene	C6H8		
ime)	C20H14N2O4	O=C(O\N=C1\C=C\C(C=C1)=N/C	4,43
ZINC01048892	C15H17F6N3O3S	C[C@H]1CN(C[C@@H](C)O1)Cl	4,43
[(1S)-2-oxocyclohexyl]piperidine	C19H20O4	O=C(Cc1coc2cc3CCCc3cc12)O(=	4,43
2-(3-acetyl-5-oxo-2-sulfamoyl)phenyl	C23H20N4O3S2	CC(=O)N1CC(=O)N(CC(=O)N(Cc	4,43
ZINC03379013	C21H22BrN5OS	CCn1c(SCC2=CC(=O)[nH]3cc(B	4,43
[4-[(5,7-dimethyl-1,2,4-triazol-3-yl)amino]phenyl]piperidine	C21H18N4OS	Cc1cc(C)n2c(SCc3ccc(cc3)C(=O)	4,43
2-[(2,4-difluorophenoxy)methyl]piperidine	C21H21F2N3O2	CCn1ccc(CN(C)C(=O)c2cccc2Cl	4,43
(+)-alpha-Pinene	C10H16	CC1=CC[C@@H]2C[C@H]1C2(C	4,44
(S)-bis(2-methylpropoxy)benzene	C16H27O4P	CC(C)CO[P](=O)(OCC(C)C)[C@H	4,44
ZINC01456961	C29H26N2O5	COC(=O)c1ccc(cc1)[C@H]2N(C(	4,44
Cyclooctane	C8H16	C1CCCCCCC1	4,45
ZINC01779942	C16H23NO2	CCCCOc1ccc(cc1)/C=C/C(=O)NC	4,45
Diphenyl sulfide	C12H10S	S(c1ccccc1)c2ccccc2	4,45
(5-acetyl-2-methoxyphenyl)methyl	C17H14Cl2O4	COc1ccc(cc1COC(=O)c2cc(Cl)cc	4,45
N-[2-[4-(3-chlorophenyl)butyl]phenyl]piperidine	C24H25ClN4O3	CC1=Cc2cccc2C(=O)N1CC(=O)N	4,45
ZINC03639569	C28H33NO6S	COc1ccc(cc1OC)[C@@H]2C(=C	4,45
Benzene, 1-methyl-3-(2-methylphenyl)-	C13H12O	Cc1cccc(Oc2ccccc2)c1	4,46
2-Chloroanthraquinone	C14H7ClO2	Clc1ccc2C(=O)c3ccccc3C(=O)c2	4,46
ZINC03621212	C17H12FNO3	COc1cc(ccc1OC(=O))/C=C/c2ccc	4,46
N,4-dimethyl-N-[4-[2-(2,4-dichlorophenyl)butyl]phenyl]piperidine	C24H27N5O4S	CN(c1ccc(OCC(=O)N2CCN(CC2)	4,46
N-[4-[4-(thiophene-2-yl)butyl]phenyl]piperidine	C22H16N2O4S3	O=C(Nc1ccc(cc1)[S](=O)(=O)c2c	4,46
O4-[2-(2,3-dihydroindolizin-5(1H)-yl)ethyl]piperidine	C20H22N2O5	CCOC(=O)c1[nH]c(C)c(C(=O)OC	4,47
ZINC02880968	C22H14FN3O5	c1ccc(c(c1)CN(C(=O)c2cccc(c2)	4,47
1-[4-(2,3-dihydro-1,4-benzodioxin-5-yl)butyl]piperidine	C24H24N2O6S	O=C(COCc1ccc2ccccc2c1)N3CCN	4,47
ZINC00865825	C16H16BrF3N4OS	FC(F)(F)[C@@H]1C[C@H](Nc2r	4,47
1,4-Benzenediamine, N,N'-bis(2-phenyl-1-methyl-4-ethyl-6-amino-5-ethyl)phenyl-	C18H24N2	CC(C)CC(C)Nc1ccc(Nc2ccccc2)c	4,47
methyl (4R)-6-amino-1-ethyl-4-ethyl-6-amino-5-ethylphenyl	C20H21N5O5	CCCc1[nH]nc2OC(=C(C(=O)OC)	4,48
ethyl (4R)-6-amino-5-ethyl-4-ethyl-6-amino-1-ethylphenyl	C16H15N2O3	CCOC(=O)C1=C(C)OC(=C(C#N))[(	4,48
ZINC05130489	C21H20N4O4	CCOc1ccc(c(OCC)c1)C2=NN=C3	4,48
N-[2-(2,4-dichlorophenyl)ethyl]piperidine	C17H18Cl2N2O3S	CN(C)[S](=O)(=O)c1cccc(c1)C(=	4,48
N-(3-fluoro-4-methylphenyl)piperidine	C18H17FN4OS2	Cc1ccc(NC(=O)CSc2nnc(n2CC(=	4,48
N-(2-ethyl-6-methylphenyl)piperidine	C24H31N3O3	CCc1cccc(C)c1N([C@@H](C)CO	4,48
[1,2-bis(propylsulfonyl)ethyl]piperidine	C25H25NO5S2	CCC[S](=O)(=O)c1c(n2ccc3cccc	4,48
methyl 4,5-dimethoxy-2-(6-(diethylsulfamoyl)phenyl)piperidine	C18H22N4O8	COC(=O)c1cc(OC)c(OC)cc1NC(=	4,49
2-[6-(diethylsulfamoyl)phenyl]piperidine	C25H27N5O4S	CCN(CC)[S](=O)(=O)c1ccc2nnn(	4,49
1-(2,6-dimethylpiperidin-1-yl)ethane	C22H26N4O2S	CC1CCCC(C)N1C(=O)CSc2nnc(n	4,49
Heptane	C7H16	CCCCCCC	4,50
gamma-Terpinene	C10H16	CC(C)C1=CCC(=CC1)C	4,50
ZINC01061488	C18H13ClN4S	NC1=C(C#N)C2=CCSC[C@H]2[C	4,50
(2R)-N-[4-(trifluoromethyl)phenyl]piperidine	C17H14F3NO2	FC(F)(F)c1ccc(NC(=O)[C@H]2CC	4,50
1,2,4,5-Tetrachlorobenzene	C6H2Cl4	Clc1cc(Cl)c(Cl)cc1Cl	4,51
Diclofenac	C14H11Cl2NO2	OC(=O)Cc1ccccc1Nc2c(Cl)cccc2	4,51
(1,3-dioxoisindol-2-yl)ethane	C27H19N5O4S	O=C(CSc1nnc2c3ccccc3n(Cc4cc	4,51
(4R)-2-amino-3-(benzylamino)butane	C32H29F3N2O5	COc1cc(cc(OC)c1OC)[C@H]2C(=	4,51

ZINC02803312	C19H29N3O4	CCOC(=O)N1CCN(CC1)C(=O)c2r	4,52
tert-butyl 2-(4-ethyl-8-	C18H22O5	CCC1=CC(=O)Oc2c(C)c(OCC(=O	4,52
ZINC03493467	C18H14ClF3N6O2S	C[C@@H](Sc1nnnn1c2ccc(Cl)c	4,52
ZINC09210816	C22H19BrN4O4	COc1cccc(c1)C2=NN=C3OC(=C(	4,52
2-Chlorobiphenyl	C12H9Cl	Clc1ccccc1c2ccccc2	4,52
Phenanthrene	C14H10	c1ccc2c(c1)ccc3ccccc23	4,52
(1R)-2-(5-methyl-1,3,4	C23H17N3O4S	Cc1sc(nn1)N2[C@H](c3cccc(OC	4,52
(Z)-2,2'-(4-((2-Chloro- propionamidophenyl)-	C23H26ClN5O7	CCC(=O)Nc1cc(ccc1N=Nc2ccc(c	4,53
tert-butyl (4S,5R)-4-[5-	C22H24N2O4S	CC(=O)c1ccc(cc1)c2oc(cc2)[C@	4,53
ZINC03303526	C23H21ClN2O5S	COc1ccc(NC(=O)[C@H](OC(=O)	4,54
N-[2-(benzoyl)-4-meth	C25H24N2O5S	Cc1ccc(NC(=O)c2ccc(cc2)[S](=C	4,54
[2-(4-amino-1,3-dimet	C24H20N4O7	CN1C(=C(C(=O)COC(=O)c2ccc3(	4,55
1,2,3,4-Tetrachlorober	C6H2Cl4	Clc1ccc(Cl)c(Cl)c1Cl	4,55
[(5R)-3-(5-chloro-2,4-d	C19H25ClN2O4	CC[C@@H]1CCCCN1C(=O)[C@	4,55
ZINC03599705	C18H25N3O2S	CCC[C@@H](C)NC(=O)COc1ncr	4,55
4-[(4aR)-9-oxo1,3,4,4a	C24H29N3O4S	CCCN(CCC)[S](=O)(=O)c1ccc(cc:	4,55
[7-(difluoromethyl)-5-	C19H18F2N4OS	Cc1ccc(cc1)c2cc(C(F)F)n3ncc(Cl	4,55
(4R)-2-amino-7,7-dime	C19H17F3N2O2	CC1(C)CC(=O)C2=C(C1)OC(=C(C	4,55
ZINC01430778	C26H26N2O4S	COc1ccc([C@@H]2CC(=O)N(C3	4,55
1,8-Dichlorooctane	C8H16Cl2	ClCCCCCCCCl	4,56
Pentamethylbenzene	C11H16	Cc1cc(C)c(C)c(C)c1C	4,56
ethyl 2-[(3aR,7aR)-5,6-	C19H23NO4S	CCOC(=O)c1c(C)c(C)sc1N2C(=O	4,56
Anthracene	C14H10	c1ccc2cc3ccccc3cc2c1	4,56
1-Octene	C8H16	CCCCCCC=C	4,57
1-Decanol	C10H22O	CCCCCCCCCO	4,57
(-)-Limonene	C10H16	CC(=C)[C@H]1CCC(=CC1)C	4,57
N-(3-propan-2-yloxypr	C18H28N2O3	CC(C)OCCNC(=O)C(=O)NCc1cc	4,57
ZINC08763282	C18H25Cl2F3N6O	Cc1nnc2n1C3CC(Cl)CCC3N(CCN	4,57
3-Chlorobiphenyl	C12H9Cl	Clc1cccc(c1)c2ccccc2	4,58
ZINC00308399	C17H22N2O5S2	O=C1[C@@H](CSCc2ccccc2)NC	4,58
[2-(4-amino-1,3-dimet	C22H28N4O8S	COc1ccc(cc1C(=O)OCC(=O)C2=(	4,59
2-(5,6-dimethylthieno	C19H23N3O2S2	COCCn1c(C)cc(C(=O)CSc2ncnc3	4,59
Dodecanoic acid	C12H24O2	CCCCCCCCCCCC(O)=O	4,60
2-(2-hydroxyethyl)-5-:	C26H20N2O8	OCCN1C(=O)c2ccc(Oc3ccccc(Oc	4,61
ZINC02459574	C15H15BrN2OS2	CCCSC1=NC2=C(SCC2)C(=O)N1c	4,61
4-Chlorobiphenyl	C12H9Cl	Clc1ccc(cc1)c2ccccc2	4,61
4-Chloro-alpha-methyl	C9H9Cl	CC(=C)c1ccc(Cl)cc1	4,62
2-Naphthalenecarboxy	C17H13NO2	Oc1cc2ccccc2cc1C(=O)Nc3cccc	4,62
3-[(2-methyl-1-prop-2-	C22H23NO4	Cc1n(CC=C)c2ccccc2c1C=C3C(=	4,62
1-[1-[2-(azepan-1-yl)-2	C18H18BrF3N2O2	FC(F)(F)C(=O)c1cn(CC(=O)N2CC	4,62
4-acetamido-N-[1-[(2,(	C29H33N3O4	CC(=O)Nc1ccc(cc1)C(=O)N(Cc2c	4,62
(6R,9S)-9-furan-2-yl-6-	C26H21F3N2O4	COc1ccc(cc1)[C@H]2N(C(=O)C(	4,62
4-Methylbiphenyl	C13H12	Cc1ccc(cc1)c2ccccc2	4,63
[3-(4-methoxyphenoxy	C22H18F3NO7	COc1ccc(OC2=C(Oc3cc(OC(=O)	4,63
N-(1,3-benzodioxol-5-)	C25H20FN3O4S	CC(SC1=Nc2ccccc2C(=O)N1c3cc	4,63
4-amino-2-[2-(2-chloro	C24H14ClN3O3	Nc1cccc2C(=O)N(C(=O)c3cc(nc	4,63
(4-methoxycarbonylph	C17H16O6	COC(=O)c1ccc(OC(=O)c2cc(OC)	4,64
ZINC00549477	C17H18N4OS	NC1=C(C#N)[C@@H](C2CCCC	4,64
ZINC03562644	C22H23N3O3S2	CCOc1ccc(cc1)N2C(=O)c3c4CCC	4,64
1-[4-(benzoyl)piperazi	C27H25N5O2S	O=C(CSc1nnc(n1c2ccccc2)c3ccc	4,64
1,2,3,5-Tetrachlorober	C6H2Cl4	Clc1cc(Cl)c(Cl)c(Cl)c1	4,65

ZINC01239456	C30H27N3O4	COc1ccc(cc1COc2ccc(NC(C)=O)	4,65
ethyl 2-[2-[(5-ethoxyca	C16H22N4O4S2	CCOC(=O)c1sc(NCCNc2sc(C(=O	4,66
ZINC02719029	C26H23FN6O2S	COc1ccccc1NC(=O)C2=C(C)Nc3	4,66
ZINC01112071	C13H10INOS	c1cc(sc1)/C=C/C(=O)Nc2ccc(cc	4,67
Methotrimeprazine	C19H24N2OS	COc1ccc2Sc3ccccc3N(C[C@H])(	4,68
[2-(4-fluorophenyl)-2-(	C23H14FNO5	Fc1ccc(cc1)C(=O)COC(=O)c2ccc	4,68
Simvastatin	C25H38O5	CCC(C)(C)C(=O)O[C@H]1C[C@	4,68
N-(4-acetylphenyl)-2-[	C19H19N5O2S	CCc1ccc(cc1)n2nnc2SCC(=O)N	4,69
methyl 3-[(2-pyridin-3-	C19H20N4O2S	COC(=O)CCNc1nc(nc2sc3CCCC	4,69
Hexamethylbenzene	C12H18	Cc1c(C)c(C)c(C)c(C)c1C	4,69
T0509-5688	C17H14FN3OS2	Fc1ccc(NC(=O)CSc2ncnc3sc4CC	4,69
ZINC00170706	C19H17NO	CN(C)/C=C/C(=O)c1ccc(cc1)C#C	4,69
1-Iodoheptane	C7H15I	CCCCCCI	4,70
Naphthalene, decahyC	C10H18	C1CCC2CCCCC2C1	4,70
1,2-Diphenylethane	C14H14	C(Cc1ccccc1)c2ccccc2	4,70
CD 08571	C16H14F6N4O2S	Cc1cc(C)n(n1)C2=NCCN2[S](=O	4,70
Rotigotine	C19H25NOS	CCCN(CCc1sc1)C2CCc3c(O)cc	4,70
6-amino-5-[2-(2,3-dihy	C22H22N4O3S	CN1C(=O)N(Cc2ccccc2)C(=C(C(=	4,71
ZINC02996352	C25H25NO4	Cc1ccc(cc1C)C(=O)COc2cccc(c2	4,71
Benzene, 1-chloro-4-(	C9H7ClO	Clc1ccc(OCC#C)cc1	4,73
N-[4-(azepan-1-ylsulfo	C21H23N3O6S2	O=C(CN1C(=O)c2ccccc2[S]1(=O	4,73
ZINC00634239	C21H15F3N4O6	CCOC(=O)C1=NN[C@@]2([C@	4,73
[2-(4-acetyl-3,5-dimet	C22H20N2O6	CC(=O)c1c(C)[nH]c(C(=O)COC(=	4,73
ZINC02622674	C21H28N4O3S2	CC(=C)CSc1nnc(n1C2CCCC2)c3c	4,73
N-[(1S)-1-phenylethyl]	C21H19N5OS	C[C@H](NC(=O)CSc1ncnc2n(nc	4,73
2-(2-ethoxyphenoxy)-	C20H19NO3	CCOc1ccccc1OCC(=O)Nc2ccc3c	4,73
TULIP024483	C26H21N3O5S	CCN1C(=O)c2cccc3c(ccc1c23)[S	4,74
ZINC02502884	C20H24N2O3S	CCc1ccc(cc1)[C@H]2N3C(=O)C	4,75
ZINC01024189	C21H23N3O2S	Cc1cccc(c1)NC(=O)C[C@H]2C(=	4,75
2-(3,5-dimethylpyrazol	C15H20Cl2N2O2	Cc1cc(C)n(CCOC(=O)[C@H]2[C	4,76
1,3-benzodioxol-5-yl 4	C19H20O6	CCCCOc1ccc(cc1OC)C(=O)Oc2c	4,77
methyl 4-[2,5-dimethy	C23H21N5O4	COC(=O)c1ccc(cc1)n2c(C)cc(C(=	4,77
(2R)-2-(phenoxy)-N-[4-	C16H14F3NO3	C[C@@H](Oc1ccccc1)C(=O)Nc2	4,77
ZINC00627547	C23H20N2O5S2	CC1=C(C(OCC)=O)C(C2=CC=CS2	4,77
Bifonazole	C22H18N2	c1ccc(cc1)C(n2ccnc2)c3ccc(cc3	4,77
methyl 3-[2-(6,7-dihy	C22H21NO4	COC(=O)c1ccc(C)c(NC(=O)Cc2c	4,78
3,4-difluoro-N-[(6S)-6-	C15H14F2N2OS	C[C@H]1CCc2nc(NC(=O)c3ccc(l	4,79
N'-[[[(2R)-2,3-dihydro-1	C21H24N2O4	C[C@@H](CCc1ccccc1)NC(=O)C	4,80
Imipramine	C19H24N2	CN(C)CCCN1c2ccccc2CCc3ccccc	4,80
trans-Stilbene	C14H12	c1ccc(cc1)\C=C\c2ccccc2	4,81
N-(2,6-dimethylphenyl	C18H16F3N5O2S	Cc1cccc(C)c1NC(=O)CSc2nnnn2	4,82
Pencycuron	C19H21ClN2O	Clc1ccc(CN(C2CCCC2)C(=O)Nc3	4,82
STOCK3S-55473	C23H25N3O4S2	CCOC(=O)c1ccc(CNC(=O)CSC2=	4,83
ZINC02778755	C19H21Cl2N3O2S2	Clc1ccc2c(Cl)c(sc2c1)C(=O)N3C	4,83
ZINC00808563	C26H38N2O4	CC1CCC(CC1C)N2C(=O)C3CC4C	4,83
prop-2-enyl 2-[3-(4-ch	C21H17ClO5	CC1=C(C(=O)c2ccc(OCC(=O)OC	4,84
N-(3-chloro-4-methylp	C18H16ClN3O2S	Cc1ccc(NC(=O)CSc2oc(Cc3ccccc	4,85
ZINC02964517	C25H26N4O4S	CC[C@@H](SC1=Nc2ccccc2C3=	4,85
ZINC03536278	C23H19F2N5O2S	Nn1c(SCC(=O)Nc2ccccc2c3ccccc	4,85
6-amino-5-[(4-fluorop	C21H13FN6O2S	Nc1n(Cc2ccc(F)cc2)c3nc(C#N)c	4,86
Aprindine	C22H30N2	CCN(CC)CCCN(C1Cc2ccccc2C1)	4,86
9-(4-methoxyphenyl)-	C31H29F3N2O6	COc1ccc(cc1)C2CC(=O)C3=C(C2	4,87

3,4-diamino-N,N'-bis(3C24H24N4O6S2	COc1ccc(NC(=O)c2sc3sc(C(=O)F	4,88
1-Bromooctane C8H17Br	CCCCCCCCBr	4,89
6-amino-5-[2-[[5-(4-mC24H21F3N6O4S	COc1ccc(cc1)c2nnc(SCC(=O)C3:	4,89
2-[2-(6,7-dimethoxy-3,C27H31N3O4S	CCc1c(C#N)c(SCC(=O)N2CCc3cc	4,89
[3-(4-fluorobenzoyl)-5-C21H14F2O3	COc1cc(cc(c1)C(=O)c2ccc(F)cc2	4,89
Pentylbenzene C11H16	CCCCC1CCCC1	4,90
2-(cyclohexyl-phenyl)C22H28N2O3S	C[C@@H](NC(=O)CN(C1CCCCC	4,90
ZINC13464795 C20H21ClN4O3S	CCN(C(=O)CN1C(=O))[C@@H]2(	4,91
N-[2-(3,4-dihydro-1H-iC25H26N2O4S	C[S](=O)(=O)N(CC(=O)N1CCc2c	4,91
ZINC02381831 C18H22N2O3S3	c1cc(sc1)/C=C/2\C(=O)N(C(=S)S	4,92
ZINC03060391 C20H31N3O3S	CC1CCN(CC1)[S](=O)(=O)N2CCC	4,92
5-methyl-7-(trifluoromC17H9F6N5O	Cc1cc(n2nc(cc2n1)c3oc(nn3)c4	4,92
ZINC03287055 C30H22N4O6	O=C(NCc1cccc(CNC(=O)C(=Cc2c	4,92
2-[3-(4-chlorophenyl)-C22H22ClN3O2S	Clc1ccc(cc1)N2C(=O)c3cccc3N	4,92
ID11_013473 C20H18F3N3OS	FC(F)(F)c1ccc(nc1)N2CCCN(CC2	4,92
9-[4-[(2-fluorophenyl)C26H23FO4	Fc1cccc1COc2ccc(cc2)C3C4=C	4,92
ZINC01183526 C22H22N4O6S	O=C/C(S4)=C/C3=C([N+])([O-])=	4,93
N-[4-[(4R)-6-amino-1-(C22H18ClN5O2	CC(=O)Nc1ccc(cc1)[C@H]2C(=C	4,93
1,4-benzenediamine, rC18H16N2	N(c1cccc1)c2ccc(Nc3cccc3)cc	4,93
(2S)-2-phenyl-1-[4-[(2C25H32N2O2	CC[C@H](C(=O)N1CCCN(CC1)Cl	4,93
9-(3-ethoxy-4-prop-2-ylC28H32O5	CCOc1cc(ccc1OCC#C)C2C3=C(C	4,93
(7S,7aS)-3,7-bis(4-chloC17H14Cl2N4S2	C[C@]1(NC(=S)N2[C@@H]1NC	4,94
ZINC01263811 C24H23N3O2S	c1ccc(cc1)/C=C/C(=O)Nc2ccc(cc	4,94
Chlorpyrifos C9H11Cl3NO3PS	CCO[P](=S)(OCC)Oc1nc(Cl)c(Cl)nc	4,96
ZINC05950541 C23H23N3O3S	CC[C@H]1CS/C(=N)\c2cccc(c2)C	4,96
Silanol, triphenyl-C18H16OSi	O[Si](c1cccc1)(c2cccc2)c3ccc	4,96
[2-[(3S)-3-methylpiperC16H18Cl3NO4	C[C@H]1CCCN(C1)C(=O)COC(=O	4,97
propan-2-yl 6,7,8,9-tetC16H19NO2	CC(C)OC(=O)c1ccc2[nH]c3CCCC	4,97
1-Methylfluorene C14H12	Cc1cccc2c1Cc3cccc23	4,97
Ethanol, 2,2'-(1-methylC19H20Br4O4	CC(C)(c1cc(Br)c(OCCO)c(Br)c1)C	4,97
ZINC08934271 C23H20ClN3O2S	CC(=O)C1=C(C)NC(=C(C#N))[C@	4,97
[2-oxo-2-[4-(phenylmeC21H29NO3	O=C(COC(=O)C1CCCCC1)N2CCC	4,98
ZINC01250844 C29H36N2O5S	CCOc1ccc(C[C@@H]2N(CCc3ccc	4,98
ZINC02731613 C21H18ClN9S	Cc1cccc(Cl)c1Cn2ccc(Nc3sc(Cc4	4,99
[2-(dicyclohexylamino)C20H27ClN2O3	Clc1ccc(cn1)C(=O)OCC(=O)N(C2	4,99
2-amino-6-[(3-methyl-C24H18N6OS	Cc1ccc(cc1)c2c(C#N)c(N)nc(SC2	4,99
(4R)-2-amino-4-anthraC26H22N2O2	CC1(C)CC(=O)C2=C(C1)OC(=C(C	4,99
[(3R,4S)-4-(benzoyloxyC22H19NO8	CCOC(=O)CN1C(=O)[C@@H](O	5,00
2,6-Dichlorobiphenyl C12H8Cl2	Clc1ccc(Cl)c1c2cccc2	5,00
ZINC02771743 C26H27NO5S2	CCSCCOC(=O)C1=C(C)NC2=C([C	5,00
1,4-bis[[2,4-dimethylpC21H28N2O4S2	Cc1ccc(c(C)c1)[S](=O)(=O)N2CC	5,01
ZINC03661324 C30H31FN2O3	COc1ccc(cc1)[C@@H]2[C@H](F	5,01
(5S)-5-methyl-3,5-bis(4C17H28N2O	CC(C)=CCCC1=NN(C=O)[C@@H](	5,02
ethyl 2-[[2-[(5-methyl-C17H21N3O3S3	CCOC(=O)c1c(NC(=O)CS2sc(C)	5,03
Pentachlorobenzene C6HCl5	Clc1cc(Cl)c(Cl)c(Cl)c1Cl	5,03
mo-4,1-phenylene)oxy		
2-Ethylhexyl vinyl ethC10H20O	CCCC(CC)COC=C	5,04
methyl 2-[[1(R)-1-acet.C14H17Cl3N2O3S	COC(=O)c1c2CCCCc2sc1N[C@@	5,04
ZINC00719771 C24H20ClF2N3O	CC1(C)CC(=O)C2=C(C1)N(C(=C(C	5,04
7-[2-(1,3-benzothiazol-C22H26N6O2S2	C[C@@H]1CCCN(C1)c2nc3N(C)	5,05
ethyl 2-[[1(R,4S,6R)-biC21H30N2O4S	CCOC(=O)c1c(C)c(sc1NC(=O))[C	5,05
2-[(4-diethylamino-2-nC21H21NO3	CCN(CC)c1ccc(C=C2C(=O)c3ccc	5,05

(1S,2S,3aR)-1-(benzoylC25H16BrN3OS	BrC1sc(cc1)[C@@H]2[C@H](N	5,05	
ZINC01426971	C15H11BrN2O3S2	COC(=O)c1c(C)sc2[C@@H](c3s	5,06
Pentachlorophenol	C6HCl5O	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	5,07
ZINC04754751	C18H19N3O2S	CC/C(=N\N=C/1\N(C(=O)[C@@	5,07
9-Methylanthracene	C15H12	Cc1c2ccccc2cc3ccccc13	5,07
Diethylstilbestrol	C18H20O2	CC\C(c1ccc(O)cc1)=C(CC)/c2ccc	5,07
N-(2,3-dihydro-1,4-berC25H27N3O4		CC1CCC2(CC1)N=C(C(=O)N2CC(	5,07
Fluoranthene	C16H10	c1ccc2c(c1)c3cccc4cccc2c34	5,07
ZINC02722701	C29H33NO6	COc1cc2CCN([C@@H])(COc3ccc	5,07
60063 p-EthylbiphenylC14H14		CCc1ccc(cc1)c2ccccc2	5,08
Pyrene	C16H10	c1cc2ccc3cccc4ccc(c1)c2c34	5,08
2-(4-methylphenyl)sulic26H28N2O2S2		Cc1ccc(SCC(=O)NCc2ccccc(CNC(	5,08
ethyl 4-[[[4-ethoxycartC19H24N2O4		CCOC(=O)c1[nH]c(C)c(CNc2cccd	5,09
4,4'-Dimethylbiphenyl C14H14		Cc1ccc(cc1)c2ccc(C)cc2	5,09
ZINC01074408	C18H21NO2S3	CC(C)CC(=O)N1c2c(cccc2OC)-c	5,09
1,2-Bis(2-chlorophenylC12H10Cl2N2		Clc1ccccc1NNc2ccccc2Cl	5,10
2,5-Dichlorobiphenyl C12H8Cl2		Clc1ccc(Cl)c(c1)c2ccccc2	5,10
(5R)-5-butyl-2-(4-methC19H23N3S		CCCC[C@@]1(NN(C(=S)N1)c2cc	5,10
2-(phenylmethylsulfanC18H16N2OS		C=CCN1C(=O)c2ccccc2N=C1SCc	5,11
1-Dodecanol	C12H26O	CCCCCCCCCCCCO	5,13
N-(2-acetyl-5-tert-butylC19H21NO2		CC(=O)c1ccc(cc1NC(=O)c2ccccc	5,13
[3-[5-[2-(3-acetyloxyplC33H20N2O9		CC(=O)Oc1cccc(c1)N2C(=O)c3c	5,13
ZINC02715265	C21H22N2O5S	C=CCN2C1=C(OC)C=CC=C1S/C2	5,14
1-MethylphenanthrenC15H12		Cc1cccc2c1ccc3ccccc23	5,14
2-(4-fluorophenyl)-N-[C22H21FN2O3S		CN(Cc1ccccc1)[S](=O)(=O)c2ccc	5,14
[4-[4-(benzoyl)-2-fluorC24H19F3N2O2		Fc1cccc(F)c1C(=O)N2CCN(CC2)	5,14
Octane	C8H18	CCCCCCCC	5,15
2-Methylanthracene C15H12		Cc1ccc2cc3ccccc3cc2c1	5,15
ZINC01457198	C16H18F4N2O3	CC(C)COc1ccc(cc1)C(=O)N2N=C	5,16
3-cyclohexyl-5,6-dimeic20H27N3O2S2		Cc1sc2N=C(SCC(=O)N3CCCC3)N	5,16
ZINC00087965	C15H17N3O3	c1cc(cc(c1)[N+](=O)[O-])c2nc(o	5,17
Trinitro-t-butyl xyleneC12H15N3O6		Cc1c(c(C)c(c(c1[N+](=[O-])=O)C(	5,20
ZINC03424333	C22H22N2O5	Cc1cc(c(n1c2cc(on2)C)C)C(=O)C	5,20
Loratadine	C22H23ClN2O2	CCOC(=O)N1CCC(CC1)=C2c3ccc	5,20
T5294172	C24H23N5O4S2	CN1C(=C(C(=O)C)SC2=Nc3sc4CC	5,21
1,3-bis[[4-methoxypheC21H18N2O7S2		COc1ccc(cc1)[S](=O)(=O)N2C(=	5,22
Benzene, 1,4-bis(1-meC12H18		CC(C)c1ccc(cc1)C(C)C	5,23
ZINC02716446	C25H29ClN2O3	CC[C@@H]1CCCCN1C(=O)COc	5,23
2-methoxyethyl 7-(3-nC31H31NO7		COCCOC(=O)C1=C(C)NC2=C(C1	5,23
Naphthalene, 1-butoxC14H16O		CCCCOc1cccc2ccccc12	5,24
ZINC03640152	C27H29NO5S2	CCSCCOC(=O)C1=C(C)NC2=C([C	5,24
ZINC16676346	C21H16Cl2N2O2S2	CC(=O)C1=C(C)NC(=C(C#N)[C@	5,25
ZINC01052739	C26H26N2O5S	COc1ccc(cc1)N(C(=O)C2CCCC	5,26
ZINC01022529	C25H23NO	Cc1ccc(C)c(NC(=O)[C@H]2CC3c	5,26
N-(2-methoxyphenyl)-C14H12F6N4O3		COc1ccccc1Nc2nc(OCC(F)(F)F)r	5,27
1(3H)-Isobenzofuranoc26H29N3O2		CN(C)c1ccc(cc1)C2(OC(=O)c3cc	5,27
ZINC06567055	C24H19N3OS	Cn1c(nc2ccccc12)[C@@H](C#N	5,28
ZINC18247170	C24H20BrNO5	C[C@@H]1C=CC[C@H]2[C@@	5,29
Bis(2,3,3,3-tetrachloroC6H6Cl8O		ClC(CC(Cl)(Cl)Cl)OC(Cl)CC(Cl)(Cl	5,30
4-[1-(4-dimethylaminoC18H22N2		CN(C)c1ccc(cc1)C(=C)c2ccc(cc2	5,30
ZINC00956989	C23H25ClN2O4S	CCOC(=O)C1=C(C)NC(=S)N[C@	5,31
ZINC01015500	C18H15ClF3NO3	COc1ccc(cc1OC)C(=O)/C=C/Nc	5,31





9,10-Anthracenedione	C19H18O2	CCCCC1ccc2C(=O)c3ccccc3C(=	5,59
5-(benzoylamino)-N,N'	C29H25N3O5	COc1ccc(NC(=O)c2cc(NC(=O)c3	5,59
phenylmethyl 2-[[4-cy	C22H18N2O4S3	O=C(CSc1snc(SCC(=O)OCc2cccc	5,60
2,4,5-Trichlorobipheny	C12H7Cl3	Clc1cc(Cl)c(cc1Cl)c2ccccc2	5,60
ZINC03040513	C24H31BrN2O2	BrC1cccc(c1)[C@H]2N(CCC3=C	5,60
N-[(R)-di(propan-2-yl	C20H27FNO3P	CC(C)O[P](=O)(OC(C)C)[C@H]	5,63
3-[(2-chloro-6-fluorop	C20H16Cl2FNO2	CC1=C(OCc2c(F)cccc2Cl)C(=O)C	5,63
N-[2,2-bis[(4-methylp	C24H25NO5S2	CCOc1ccc(NC=C([S](=O)(=O)c2c	5,64
Nonane	C9H20	CCCCCCCCC	5,65
ZINC01095206	C16H11BrF3NO	c1cc(cc(c1)N/C=C/C(=O)c2ccc(c	5,65
N-[4-(azepan-1-ylsulfo	C22H23FN2O4S	Cc1c(oc2ccc(F)cc12)C(=O)Nc3c	5,68
Vitamin A	C20H30O	CC(=C\CO)/C=C/C=C(C)/C=C/C1	5,68
ZINC02038455	C10H6Cl6	ClC1=C(Cl)[C@]2(Cl)[C@]3C	5,69
9,10-Dimethylanthrac	C16H14	Cc1c2ccccc2c(C)c3ccccc13	5,69
[3-(1,3-benzothiazol-2	C23H13NO4S	O=C(Oc1ccc2C=C(C(=O)Oc2c1)c	5,70
2,3,4,5-Tetrachlorobip	C12H6Cl4	Clc1cc(c2ccccc2)c(Cl)c(Cl)c1Cl	5,72
ZINC01060140	C27H22BrN5O2S	BrC1=CC=C(/C=C3\SC2=NC(N(C	5,72
9-(1,3-benzodioxol-5-y	C31H33NO5	COc1ccc(cc1)N2C3=C(C(c4ccc5	5,72
2,2',4',5-Tetrachlorobi	C12H6Cl4	Clc1ccc(c(Cl)c1)c2cc(Cl)ccc2Cl	5,73
Chrysene	C18H12	c1ccc2c(c1)ccc3c4ccccc4ccc23	5,73
Phenol, 4,4'-thiobis 2			
yl-	C22H30O2S	Cc1cc(O)c(cc1Sc2cc(c(O)cc2C)C	5,73
Triphenylamine	C18H15N	c1ccc(cc1)N(c2ccccc2)c3ccccc3	5,74
11H-Benzo[b]fluorene	C17H12	C1c2ccccc2c3ccc4ccccc4cc13	5,75
methyl 2-[[1,1,1,3,3,3-	C20H19F6N3O3S	COC(=O)c1c(NC(NC(=O)c2cccnc	5,75
ethyl (6R)-2-[[1,3-dime	C20H25N3O5S	CCOC(=O)c1c(NC=C2C(=O)N(C)	5,76
Naphthacene	C18H12	c1ccc2cc3cc4ccccc4cc3cc2c1	5,76
N-(4-methylpyridin-2-y	C24H24N2O2S2	Cc1ccnc(c1)N(C(=O)c2sc3CCCC	5,76
O1-tert-butyl O2-[3-(4	C25H24FNO6	CC(C)(C)OC(=O)N1CCC[C@H]1C	5,77
N-[2-[4-tert-butyl-6-(tr	C18H26F3N3OS	CC(C)(C)c1cc(nc(SCCN(C(=O)C2C	5,77
(9R,12S)-12-(1,3-benz	C31H25NO4	COc1ccc(cc1)[C@H]2CC(=O)C3:	5,77
ZINC01803312	C23H23N3O5S2	COC(=O)c1ccc(C(=O)OC)c(NC(=	5,79
ZINC01023102	C15H8F3NOS3	c1cc(cc(c1)N2C(=O)/C(=C/c3ccc	5,80
Cycloprothrin	C26H21Cl2NO4	CCOc1ccc(cc1)C2(CC2(Cl)Cl)C(=	5,80
N,N-dicyclohexyl-5-(1,	C25H31F3N6O	Cn1cc(c(C)n1)c2cc(n3ncc(C(=O)	5,81
ZINC01439744	C31H33NO6	COc1cccc1[C@H]2CC(=O)C3=C	5,81
ZINC01403863	C18H12F5N3O3	C[C@]@H](Oc1ccc(F)cc1F)C(=O)	5,83
ZINC01245439	C28H33N5O4	CCOc1cc(ccc1OC(C)C)[C@H]2[C	5,83
ZINC08741738	C28H25N3O4S	COc1ccc(cc1)[C@@]@H]2[C@@]@H	5,83
4-chloro-N-[1-[2-[[3-cl	C24H19Cl2F3N4O3	FC(F)(F)c1cnc(NCCN2C(=O)C(=C	5,83
N-[3-chloro-4-[4-(furar	C22H15ClF5N3O3	Fc1c(F)c(F)c(c(F)c1F)C(=O)Nc2c	5,85
3-ethyl-2-[[2-fluoroph	C17H17FN2OS2	CCN1C(=O)c2c(C)c(C)sc2N=C1S	5,86
3-amino-N-(3,4-difluor	C21H15F2N3O2S	COc1cccc(c1)c2ccc3c(N)c(sc3n:	5,86
Fluspirilene	C29H31F2N3O	Fc1ccc(cc1)C(CCCN2CCC3(CC2)	5,86
[4-[[2,5-dimethylphen	C23H21NO6S	CN(c1ccc(OC(=O)c2ccc3OCOC3	5,87
(4aS,6R,6aR,10bS)-6-p	C16H26O	CC(C)[C@H]1O[C@H]2CCCC[C@	5,87
methyl 2-[[5-[(2-meth	C24H25NO6	CCCC1ccc(OCc2oc(cc2)C(=O)Nc	5,89
Benz[a]anthracene	C18H12	c1ccc2cc3c(ccc4ccccc34)cc2c1	5,91
ethyl 4-[6,8-dimethyl-	C18H21F3N4O2	CCOC(=O)N1CCN(CC1)c2nc(nc3	5,92
ZINC00673948	C20H16ClF3N4O	FC(F)(F)[C@@]@H]1C[C@H](Nc2c	5,92
1,2,4-Benzenetricarbo	C33H54O6	CCCC(CC)COC(=O)c1ccc(C(=O)	5,94
4-[[4-chloro-1-cyclohe	C25H26ClN3O5	COc1ccc(OC)c(NC(=O)c2ccc(NC	5,96

ZINC02972969	C26H24N6O	CN1N(c2ccccc2)C(=O)C(=C1C)N	5,96
2-(2-phenylethyl)-N-[(C27H27N3O2		CC(C)N(Cc1onc(n1)c2ccccc2)C(	5,98
(3S,3aS,6aS)-3-(4-methylC25H19F3N2O3S		CSc1ccc(cc1)[C@@H]2[C@H]3	5,98
N-[4-(difluoromethoxyC19H14F2INO4		FC(F)Oc1ccc(NC(=O)c2oc(COc3	5,99
ZINC12376491	C24H20FN3O2S	c1ccc(cc1)CN\2C(=O)C[C@@H]	6,00
ZINC03329891	C25H22N2O8S	C[C@H]1Cc2ccccc2N1S(=O)(=O	6,01
ZINC01134578	C24H28N2O3S2	CCOC(=O)c1c(C)nc(SC[C@@]2(	6,01
ZINC02172513	C24H22F3N3O	CC1(C)[C@@]2(C)CC[C@]1(C(=	6,01
Tetradecanol	C14H30O	CCCCCCCCCCCCCO	6,03
ZINC03294668	C23H31N3O2S2	CCc1sc2N=C(SCC(=O)N3C[C@@	6,04
ZINC01042477	C20H16F6N2O4	CCOC(=O)C1=C(C)NC(=O)N[C@	6,04
5-(trifluoromethyl)-3-[C12H4F6N4O2		FC(F)(F)c1onc(n1)c2ccc(cc2)c3r	6,06
ZINC00959448	C21H23NO6S2	CS(=O)(=O)c1ccc(c(c1)[N+](=O)	6,08
methyl 3-[[3-(1,3-dioxoC32H23N3O8		COC(=O)c1cccc(NC(=O)c2cc(cc(	6,09
4'-Hexyl[1,1'-biphenyl]C19H21N		CCCCCCc1ccc(cc1)c2ccc(cc2)C#	6,09
Tetradecanoic acid	C14H28O2	CCCCCCCCCCCCC(O)=O	6,10
(4-methyl-2-oxochromC23H24O7		CCOc1cc(cc(OCC)c1OCC)C(=O)C	6,15
2-(2-methoxyphenyl)-C30H20N4O5		COc1ccccc1N2C(=O)c3ccc(cc3C	6,17
3-(1-benzothiophen-3-C19H26N2S2		C[C@H]1C[C@@H](CC(C)(C)C1	6,21
Decane	C10H22	CCCCCCCCC	6,25
ZINC01132042	C32H27NO3	Cc1ccc(cc1)C(c2ccc(C)cc2)=C3[	6,25
ZINC01164511	C18H19NOS2	Cc1ccc(cc1)CN2C(=O)/C=C/[C@	6,26
ZINC00710587	C28H25ClN4O4S	COc1ccccc1NC(=O)C2=C(C)NC(	6,27
ZINC01812703	C32H42N2O6	COC(=O)[C@@H](NC(=O)CONC	6,27
ZINC12616401	C28H27NO3	CN1c2ccccc2C(C)(C)C1=CC(=O)N	6,27
5-cyano-6-hexylsulfanC25H29N3O2S2		CCCCCSC1=C(C#N)C(c2sccc2)C	6,28
3-Hydroxyisovaleric acC5H10O3		CC(C)(O)CC(O)=O	6,30
Octylbenzene	C14H22	CCCCCCCCc1cccc1	6,30
2,3,4,5,6-PentachlorokC12H5Cl5		Clc1c(Cl)c(Cl)c(c2ccccc2)c(Cl)c1	6,30
9,13-cis-Retinoic acid	C20H28O2	CC1=C(C(CCC1)(C)C)/C=C/C(=C\	6,30
all-trans-Retinoic acid	C20H28O2	CC1=C(C\C=C\C(C)=C\C=C\C(C)=	6,30
2,2',4,5,5'-PentachloroC12H5Cl5		Clc1ccc(Cl)c(c1)c2cc(Cl)c(Cl)cc2	6,40
alpha-Linolenic acid	C18H30O2	CC\C=C/C/C=C\C\C=C/C/CCCCC	6,46
Linolenic acid	C18H30O2	CC/C=C/C/C=C/C/C=C/C/CCCCC	6,46
[2-[(3S,3aR,6aS)-5-(4-cC29H21ClN2O6S		Clc1ccc(cc1)N2C(=O)[C@H]3ON	6,47
Permethrin	C21H20Cl2O3	CC1(C)[C@@H](C=C(Cl)Cl)[C@H	6,50
Peroxide, (3,3,5-trimetC17H34O4		CC1CC(C)(C)CC(C1)(OOC(C)(C)C	6,53
2-[5-[5-tert-butyl-2-(p)C22H20F3N5O		CC(C)(C)c1cc(n(Cc2ccccc2)n1)c:	6,58
ZINC02312992	C21H17N3O2S	CCc1ccc(cc1)c2csc(n2)/C=C/Nc	6,59
ZINC02782138	C20H14ClF6N3O3	C[C@H](n1nc(c(Cl)c1C2CC2)C(F	6,63
1-[(5R)-5-(2,3-dimethoC34H38N4O6		CCC(=O)N1N=C(C[C@@H]1c2c	6,65
ZINC01181998	C14H19NOS2	CC(C)CN1C(=O)/C(=C/[C@H]2C	6,66
2,2',3,3',6,6'-HexachlorC12H4Cl6		Clc1ccc(Cl)c(c1Cl)c2c(Cl)ccc(Cl)c	6,70
2,2',3,3',4,4',6-HeptachlorC12H3Cl7		Clc1ccc(c(Cl)c1Cl)c2c(Cl)cc(Cl)c	6,70
ZINC01038638	C25H26F3N3O6	CCOC(=O)C1=C(Nc2ccc(OC(=O)	6,72
ZINC03315666	C21H26ClN3O2S	CCCCNC(=S)N(C)/N=C/c1ccc(c(c	6,80
5-(1,3-dioxoisindol-2-C32H19N3O4		O=C(Nc1cccc(c1)C#C)c2cc(cc(c:	6,85
Arachidonic acid	C20H32O2	CCCCC/C=C\C\C=C/C/C/C=C\C\C=C	6,98
2,2',3,3',4,4'-HexachlorC12H4Cl6		Clc1ccc(c(Cl)c1Cl)c2ccc(Cl)c(Cl)c	7,00
2,2',4,4',6,6'-HexachlorC12H4Cl6		Clc1cc(Cl)c(c(Cl)c1)c2c(Cl)cc(Cl)	7,00
Linoleic acid	C18H32O2	CCCCC/C=C\C\C=C/C/CCCCCCC	7,05
2,2',3,3',5,5',6,6'-OctacC12H2Cl8		Clc1cc(Cl)c(Cl)c(c1Cl)c2c(Cl)c(Cl	7,10

Hexadecanoic acid	C16H32O2	CCCCCCCCCCCCCCCC(O)=O	7,17
2,2',3,3',4,5,5',6,6'-Nor	C12HCl9	Clc1cc(Cl)c(Cl)c(c1Cl)c2c(Cl)c(Cl)c2	8,16
Stearic acid	C18H36O2	CCCCCCCCCCCCCCCC(O)=O	8,23
Decachlorobiphenyl	C12Cl10	Clc1c(Cl)c(Cl)c(c(Cl)c1Cl)c2c(Cl)c(Cl)c2	8,26
Arachidic acid	C20H40O2	CCCCCCCCCCCCCCCC(O)=O	9,29

## Experimental database and model performance

Calculated logP - Mannhold 2009	Squared error	Calculated logP - Chaker 2023	Squared error
-1,83	10,56	0,47	30,80
0,42	28,84	1,75	44,89
-0,48	18,66	-0,11	22,00
-0,93	13,76	0,57	27,14
-0,48	13,99	0,82	25,40
-0,93	10,69	0,51	22,18
-1,38	6,30	0,13	16,16
-1,38	5,95	0,21	16,24
-0,48	10,37	-0,11	12,89
-0,93	7,62	0,38	16,56
-0,93	7,34	0,46	16,81
-0,48	8,07	0,79	16,89
-0,93	5,34	0,19	11,76
-1,38	3,35	0,35	12,67
-0,93	5,11	0,43	13,10
-0,48	7,24	0,74	15,29
-0,48	7,24	0,85	16,16
-0,48	7,24	0,85	16,16
-0,93	4,71	0,19	10,82
-0,93	4,71	0,19	10,82
-1,38	2,86	0,24	10,96
-0,93	4,49	0,60	13,32
-0,03	9,12	1,07	16,97
0,87	15,37	2,21	27,67
-0,93	4,37	0,30	11,02
-1,83	1,28	-0,21	7,56
0,42	11,36	1,35	18,49
-0,93	4,04	0,49	11,76
-1,38	2,37	0,21	9,80
-0,48	5,90	0,85	14,14
-0,93	3,69	0,60	11,90
-0,93	3,42	0,60	11,42
-0,03	6,76	1,10	13,91
-0,93	2,79	0,35	8,70
-1,38	1,42	-0,17	5,76
-0,48	4,37	0,96	12,46
-0,03	6,30	1,10	13,25
-0,48	4,12	0,46	8,82
-0,93	2,50	1,71	17,81
-1,38	1,23	0,66	9,92
0,87	10,63	1,38	14,21
-0,93	1,93	0,30	6,86
0,42	7,45	1,35	13,40
-0,93	1,85	0,41	7,29
-0,03	4,97	1,10	11,29
1,32	12,82	1,74	16,00
-0,03	4,93	1,23	12,11
-0,93	1,61	0,19	5,71

-1,83	0,12	-0,10	4,28
-1,83	0,08	0,18	5,24
-0,48	2,62	0,43	6,40
1,32	11,49	1,85	15,37
-0,93	1,25	0,51	6,55
-0,03	3,92	0,71	7,40
-0,48	2,25	0,38	5,57
-0,93	0,94	0,15	4,20
0,87	7,62	2,32	17,72
-0,48	1,93	1,16	9,18
-0,93	0,85	0,19	4,16
-1,83	0,00	-0,15	2,86
1,32	9,67	1,63	11,70
-0,03	3,06	0,96	7,51
-0,03	3,03	0,82	6,71
-0,93	0,69	0,52	5,20
-0,93	0,69	0,65	5,81
-0,93	0,64	0,65	5,66
-0,03	2,82	0,79	6,25
0,42	4,49	1,35	9,30
0,42	4,49	1,35	9,30
-0,93	0,56	2,41	16,73
-1,38	0,07	-0,17	2,16
-0,93	0,40	0,37	3,72
0,42	3,80	1,35	8,29
0,42	3,76	1,35	8,24
0,42	3,76	1,35	8,24
-1,38	0,02	0,46	3,88
-0,03	2,19	0,74	5,06
2,22	13,54	1,82	10,76
1,77	10,37	2,07	12,39
-0,48	0,90	0,85	5,20
-0,48	0,90	1,04	6,10
1,32	7,56	1,74	10,05
-1,38	0,00	0,69	4,41
1,77	9,92	2,10	12,11
1,32	7,24	1,74	9,67
-0,93	0,18	1,05	5,76
-0,03	1,72	1,13	6,10
-0,93	0,16	0,40	2,99
-0,93	0,14	0,71	4,08
-0,48	0,67	0,51	3,28
-0,93	0,11	0,71	3,88
0,87	4,45	1,49	7,45
1,77	8,94	1,58	7,84
-1,38	0,07	0,27	1,90
-0,93	0,03	0,62	2,99
-1,38	0,08	0,37	2,16
1,77	8,24	2,10	10,24
-1,38	0,09	0,15	1,51
-0,93	0,02	0,57	2,69
0,42	2,22	0,85	3,69

2,22	10,76	2,32	11,42
-0,48	0,32	0,51	2,43
-0,48	0,32	0,96	4,04
1,32	5,62	1,74	7,78
-0,48	0,28	0,96	3,88
0,87	3,53	1,41	5,86
1,32	5,29	1,85	8,01
-0,93	0,00	0,71	2,82
-3,63	7,13	-1,97	1,02
-0,48	0,23	0,96	3,69
0,42	1,82	0,99	3,69
-0,48	0,19	0,88	3,24
-0,03	0,79	1,13	4,20
-1,38	0,22	0,34	1,56
1,32	4,93	1,85	7,56
-0,93	0,00	0,51	1,96
0,87	3,10	1,46	5,52
-0,03	0,67	1,21	4,24
-1,38	0,30	0,10	0,86
-1,38	0,32	0,16	0,94
-0,48	0,09	0,76	2,37
-0,48	0,09	0,96	3,03
-0,03	0,55	1,21	3,92
0,87	2,69	1,49	5,11
-0,93	0,04	0,74	2,19
1,77	6,30	1,82	6,55
-1,38	0,42	0,26	0,98
-0,03	0,45	1,26	3,84
-0,03	0,45	1,29	3,96
1,77	6,05	2,07	7,62
-2,73	4,37	0,35	0,98
-0,03	0,37	1,13	3,13
-0,48	0,02	0,82	2,07
-0,93	0,12	0,41	1,00
-1,38	0,64	0,85	2,04
-1,38	0,66	0,15	0,52
-0,93	0,13	0,82	1,93
-0,03	0,27	0,87	2,02
1,77	5,38	2,03	6,66
-1,38	0,71	0,38	0,85
-0,03	0,26	1,07	2,59
-0,93	0,17	0,40	0,85
-0,93	0,18	0,51	1,02
-0,03	0,21	1,02	2,28
-0,93	0,20	0,41	0,79
-0,48		0,77	1,56
0,42	0,77	1,46	3,69
0,42	0,76	1,16	2,59
1,77	4,93	2,10	6,50
4,92	28,73	2,56	9,00
-0,03	0,14	1,29	2,86
-0,48	0,01	1,07	2,10

-0,03	0,12	1,24	2,62
-0,48	0,01	0,65	1,04
-0,48	0,01	0,98	1,82
0,42	0,62	1,43	3,24
-0,48	0,01	0,77	1,28
-0,03	0,11	1,13	2,22
-0,48	0,02	1,07	1,99
-1,83	2,25	0,10	0,18
1,77	4,33	2,10	5,81
-0,48	0,03	0,99	1,66
-0,48	0,03	0,99	1,66
-0,48	0,04	0,66	0,90
-0,03	0,07	1,13	2,02
-3,18	8,53	-0,23	0,00
-0,93	0,46	0,82	1,14
-0,03	0,04	1,24	2,19
-0,03	0,03	1,21	2,02
0,87	1,10	1,59	3,13
-0,93	0,58	0,63	0,64
-0,93	0,62	0,19	0,11
-0,93	0,64	0,71	0,71
-0,48	0,12	1,07	1,44
-0,93	0,71	0,70	0,62
-0,48	0,16	1,04	1,25
1,77	3,42	2,10	4,75
-2,28	4,88	0,67	0,55
-0,03	0,00	1,01	1,17
-0,03	0,00	1,30	1,77
-0,48	0,21	0,76	0,61
0,87	0,79	1,61	2,66
-0,03	0,00	1,24	1,56
0,87	0,76	1,68	2,82
1,77	3,10	1,91	3,61
-0,03	0,00	1,24	1,46
-0,03	0,00	1,32	1,66
0,87	0,71	1,63	2,56
0,87	0,69	1,71	2,79
-0,03	0,01	1,24	1,42
-0,03	0,01	1,66	2,59
2,22	4,62	2,43	5,57
-0,03	0,01	0,91	0,69
-0,48	0,34	0,99	0,79
0,42	0,09	1,38	1,59
0,87	0,53	1,63	2,22
0,87	0,53	1,82	2,82
-0,03	0,03	1,21	1,12
-0,03	0,03	1,32	1,37
-0,03	0,04	1,32	1,35
-0,03	0,04	1,32	1,35
3,12	8,76	2,71	6,50
-0,03	0,04	1,21	1,08
-0,03	0,04	1,24	1,14



2,22	4,20	2,54	5,62
-1,38	2,43	0,35	0,03
-0,48	0,44	0,88	0,49
0,87	0,48	1,63	2,10
-0,03	0,05	0,91	0,52
-1,38	2,50	1,56	1,85
0,87	0,45	1,63	2,04
-2,28	6,20	0,11	0,01
2,22	4,04	2,43	4,93
0,87	0,42	1,41	1,42
0,42	0,03	1,46	1,49
4,92	21,90	3,44	10,24
-0,03	0,08	1,24	0,98
-0,03	0,08	1,32	1,14
1,32	1,14	1,88	2,66
-0,03	0,08	1,32	1,12
0,42	0,02	1,49	1,44
-2,73	9,18	-0,61	0,83
0,42	0,01	1,24	0,88
-0,48	0,61	1,47	1,37
-0,03	0,11	2,59	5,24
1,32	1,02	1,74	2,04
-0,48	0,66	0,88	0,30
1,32	0,98	1,66	1,77
-0,03	0,14	1,10	0,58
-0,03	0,14	1,13	0,62
-1,38	2,96	1,16	0,67
-0,93	1,64	0,74	0,15
0,42	0,00	1,49	1,30
1,32	0,94	1,85	2,25
1,32	0,94	1,85	2,25
0,42	0,00	1,35	0,98
2,67	5,24	2,68	5,29
-0,48	0,76	0,66	0,07
-0,93	1,77	0,79	0,15
0,42	0,00	1,57	1,37
1,32	0,81	1,77	1,82
-0,93	1,85	0,94	0,26
-0,48	0,86	0,99	0,29
-0,03	0,23	1,02	0,32
-0,93	1,93	0,41	0,00
0,42	0,00	1,49	1,06
0,42	0,00	1,49	1,06
0,42	0,00	1,57	1,23
1,32	0,74	1,85	1,93
1,32	0,74	1,88	2,02
-0,03	0,26	1,32	0,71
1,32	0,67	1,99	2,22
-0,93	2,07	1,33	0,67
3,12	6,81	2,44	3,72
3,57	9,36	3,02	6,30
-1,83	5,52	0,23	0,08

0,87	0,12	1,74	1,49
0,87	0,11	1,52	0,96
1,32	0,59	1,93	1,90
0,87	0,10	1,74	1,39
3,12	6,55	2,69	4,54
-0,48	1,10	1,21	0,41
0,42	0,03	1,57	0,98
1,32	0,55	1,99	1,99
-0,03	0,38	1,24	0,42
0,87	0,08	1,63	1,08
-1,38	3,92	0,27	0,11
0,42	0,03	1,57	0,94
0,42	0,04	1,16	0,30
-0,03	0,41	1,58	0,94
1,32	0,50	1,99	1,90
1,32	0,49	1,77	1,32
1,77	1,30	2,13	2,25
-0,03	0,45	1,02	0,14
0,42	0,05	1,49	0,71
0,87	0,05	1,60	0,90
0,87	0,05	1,82	1,37
-0,93	2,53	0,71	0,00
0,87	0,04	1,60	0,85
-2,28	8,88	0,52	0,03
-0,03	0,53	0,80	0,01
0,42	0,08	1,35	0,42
0,87	0,03	1,52	0,66
-0,03	0,56	1,13	0,17
0,42	0,09	1,35	0,40
-0,03	0,58	1,13	0,16
-0,03	0,58	1,13	0,16
0,87	0,02	1,41	0,46
1,77	1,08	2,29	2,43
2,67	3,76	2,32	2,53
0,42	0,10	1,49	0,56
0,42	0,11	1,57	0,67
1,32	0,32	1,77	1,04
2,22	2,16	2,51	3,10
0,42	0,12	1,49	0,53
-0,93	2,89	1,25	0,23
2,22	2,07	2,83	4,20
-0,03	0,67	1,13	0,12
0,87	0,01	1,49	0,49
3,12	5,43	2,71	3,69
-2,28	9,49	-0,09	0,79
-0,03	0,69	1,13	0,11
1,32	0,27	2,46	2,76
-0,03	0,71	1,72	0,83
1,32	0,26	1,99	1,39
0,87	0,00	1,74	0,85
0,87	0,00	1,74	0,85
1,77	0,90	2,45	2,66

-1,38	4,88	0,38	0,20
-0,93	3,10	0,74	0,01
-0,03	0,74	1,13	0,09
0,87	0,00	1,60	0,59
1,32	0,24	1,87	1,08
0,42	0,18	1,49	0,42
0,87	0,00	1,74	0,81
0,87	0,00	1,82	0,96
-0,03	0,77	1,10	0,06
1,32	0,22	1,77	0,85
1,32	0,22	1,77	0,85
2,67	3,31	2,60	3,06
0,42	0,19	1,16	0,09
0,87	0,00	1,41	0,30
0,42	0,19	1,57	0,50
-1,83	7,24	2,18	1,74
2,22	1,85	2,57	2,92
-0,93	3,24	0,60	0,07
0,42	0,21	1,49	0,37
0,87	0,00	1,63	0,56
0,42	0,22	1,49	0,36
0,87	0,00	1,74	0,72
1,32	0,18	2,07	1,39
2,67	3,17	2,71	3,31
1,32	0,18	2,07	1,37
-0,93	3,39	1,33	0,18
0,87	0,00	1,76	0,72
-0,03	0,92	1,13	0,04
2,22	1,66	2,24	1,72
2,67	3,03	2,85	3,69
-0,03	0,94	1,13	0,04
0,87	0,00	1,74	0,64
0,87	0,00	1,82	0,77
-0,03	0,96	1,02	0,00
0,87	0,01	1,38	0,18
0,87	0,01	1,38	0,18
0,87	0,01	1,52	0,31
2,67	2,89	2,79	3,31
0,87	0,01	1,41	0,18
1,32	0,12	1,89	0,83
4,47	12,18	3,38	5,76
1,32	0,10	1,61	0,37
3,12	4,49	2,90	3,61
0,87	0,02	1,41	0,16
1,32	0,10	1,85	0,71
1,32	0,09	1,99	0,94
-0,03	1,12	1,02	0,00
0,87	0,03	1,41	0,14
0,87	0,03	1,30	0,07
0,42	0,38	1,49	0,20
1,77	0,53	2,01	0,94
1,77	0,52	2,24	1,42

-0,03	1,21	2,09	1,04
6,27	26,94	4,30	10,37
-0,48	2,46	1,10	0,00
1,77	0,46	2,32	1,51
1,32	0,05	1,76	0,44
1,77	0,45	2,18	1,17
3,12	4,08	2,88	3,17
5,37	18,23	3,99	8,35
0,42	0,48	0,96	0,02
1,32	0,04	2,07	0,92
1,32	0,04	1,82	0,49
-0,48	2,56	1,95	0,69
1,32	0,04	1,66	0,28
2,67	2,37	2,71	2,50
-0,03	1,37	1,17	0,00
1,32	0,03	2,38	1,54
2,67	2,34	2,41	1,61
-1,38	6,40	0,93	0,05
1,32	0,03	1,66	0,26
1,32	0,03	1,71	0,31
0,42	0,55	1,38	0,05
1,77	0,37	2,02	0,74
1,77	0,37	2,02	0,74
1,77	0,37	2,13	0,94
1,77	0,37	2,21	1,10
2,22	1,10	2,43	1,59
2,67	2,25	2,79	2,62
0,42	0,58	1,38	0,04
-0,48	2,79	0,44	0,56
-0,93	4,49	1,33	0,02
1,32	0,02	1,66	0,22
5,37	17,47	3,99	7,84
0,42	0,61	1,16	0,00
1,32	0,01	2,07	0,76
1,32	0,01	2,07	0,76
-0,03	1,54	1,02	0,04
0,42	0,62	1,38	0,03
0,87	0,12	1,60	0,15
0,87	0,12	1,74	0,28
1,32	0,01	1,77	0,31
0,87	0,12	1,82	0,37
1,32	0,01	2,07	0,72
2,67	2,10	2,44	1,49
1,32	0,01	1,99	0,58
4,02	7,78	2,94	2,92
5,37	17,14	4,47	10,50
0,42	0,67	1,38	0,02
-1,38	6,92	1,56	0,10
0,87	0,14	1,74	0,24
1,32	0,00	1,88	0,38
11,22	99,20	6,06	23,04
0,87	0,17	1,60	0,10

0,87	0,17	1,74	0,21
0,87	0,17	1,74	0,21
5,82	20,43	3,91	6,81
-2,73	16,32	-1,09	5,76
-0,03	1,80	1,41	0,01
0,87	0,19	1,74	0,18
1,32	0,00	1,99	0,46
0,42	0,81	1,38	0,00
1,32		1,88	0,31
1,77	0,20	1,88	0,31
1,77	0,20	2,32	1,00
0,42	0,85	1,49	0,02
1,32	0,00	1,88	0,28
2,22	0,76	2,49	1,30
2,67	1,74	2,63	1,64
2,22	0,74	2,49	1,28
6,27	24,11	5,24	15,05
-0,48	3,42	0,58	0,62
1,32	0,00	1,88	0,26
0,42	0,92	1,38	
1,32	0,00	1,99	0,37
0,42	0,94	1,38	0,00
1,77	0,14	1,91	0,27
1,77	0,14	2,32	0,86
-0,03	2,04	1,07	0,11
1,77	0,14	2,32	0,85
-1,38	7,78	1,56	0,02
1,32	0,01	1,63	0,05
1,77	0,13	2,13	0,52
2,22	0,66	2,35	0,88
2,22	0,66	2,57	1,35
5,82	19,45	3,36	3,80
1,77	0,12	2,02	0,36
2,22	0,64	2,49	1,14
0,87	0,31	1,41	0,00
0,87	0,31	1,54	0,01
-0,48	3,65	1,58	0,02
2,22	0,62	2,32	0,79
2,67	1,51	2,74	1,69
1,32	0,02	2,07	0,38
-0,48	3,76	1,58	0,01
0,87	0,35	1,85	0,15
-0,48	3,80	0,85	0,38
2,22	0,56	2,21	0,55
6,27	23,04	4,30	8,01
6,27	23,04	4,30	8,01
-0,48	3,84	1,13	0,12
-0,93	5,81	1,81	0,11
1,32	0,03	1,99	0,26
1,32	0,03	1,99	0,26
1,77	0,08	2,24	0,58
2,67	1,42	2,52	1,08

1,32	0,03	1,60	0,01
0,87	0,38	1,82	0,11
1,32	0,03	2,07	0,34
1,77	0,08	2,13	0,41
2,22	0,53	2,57	1,17
-0,93	5,90	1,33	0,03
0,87	0,40	1,52	0,00
-0,03	2,34	2,51	1,02
0,87	0,41	1,74	0,05
1,77	0,07	1,91	0,16
1,32	0,04	1,99	0,22
2,67	1,32	2,82	1,69
4,47	8,58	3,46	3,69
-0,03	2,50	1,83	0,08
2,22	0,45	2,40	0,72
2,67	1,25	2,79	1,54
2,67	1,25	4,16	6,81
-1,38	8,64	0,41	1,32
-0,93	6,20	1,32	0,06
1,77	0,04	2,32	0,58
2,22	0,44	2,57	1,02
2,22	0,44	2,91	1,82
1,32	0,06	1,66	0,01
4,47	8,41	5,15	12,82
0,87	0,50	1,52	0,00
2,22	0,41	2,49	0,83
-0,03	2,66	1,04	0,31
0,87	0,53	1,35	0,06
-0,48	4,33	1,58	0,00
2,67	1,14	2,30	0,49
2,22	0,38	2,49	0,79
2,22	0,37	2,49	0,77
6,27	21,72	4,30	7,24
6,27	21,72	4,30	7,24
-3,18	23,14	-0,70	5,43
2,22	0,35	2,49	0,74
1,77	0,02	1,93	0,08
1,32	0,11	1,99	0,12
-0,03	2,82	2,14	0,24
3,57	3,69	2,88	1,51
7,62	35,64	4,91	10,63
-0,48	4,58	0,63	1,06
-1,38	9,24	2,04	0,14
1,32	0,12	2,07	0,17
1,77	0,01	2,32	0,44
0,87	0,64	1,57	0,01
1,32	0,12	2,07	0,16
-0,03	2,92	1,86	0,03
4,02	5,48	3,21	2,34
-0,03	2,99	1,43	0,07

2,67	0,90	2,82	1,21
1,32	0,17	1,71	0,00
0,42	1,74	1,16	0,34
-0,03	3,13	1,38	0,13
2,67	0,85	2,60	0,72
1,32	0,19	1,99	0,05
2,67	0,83	2,82	1,12
2,67	0,83	2,82	1,12
-0,93	7,29	1,47	0,09
1,32	0,21	1,99	0,04
2,22	0,19	2,49	0,50
-0,93	7,40	1,81	0,00
-0,03	3,31	1,83	0,00
1,77	0,00	2,02	0,05
3,12	1,77	2,73	0,88
-0,03	3,35	0,82	0,96
1,32	0,23	2,16	0,13
2,22	0,18	2,38	0,34
-0,03	3,39	1,66	0,02
0,42	1,93	1,91	0,01
2,67	0,74	2,41	0,36
6,27	19,89	4,57	7,62
0,87	0,90	1,63	0,04
1,77	0,00	2,02	0,04
2,22	0,15	2,57	0,55
2,22	0,14	2,38	0,29
2,67	0,69	2,46	0,38
2,22	0,14	2,57	0,53
1,77	0,00	2,72	0,77
0,42	2,04	1,35	0,25
0,87	0,96	1,74	0,01
0,87	0,96	1,74	0,01
-0,03	3,53	2,39	0,29
3,57	2,96	3,21	1,85
11,67	96,43	6,42	20,88
-0,93	7,78	1,81	0,00
1,77	0,01	2,10	0,06
4,02	4,67	3,18	1,74
2,22	0,12	2,35	0,23
1,32	0,31	1,88	
1,77	0,01	2,24	0,13
2,67	0,62	2,74	0,74
4,02	4,58	3,24	1,85
2,22	0,12	3,42	2,37
-0,03	3,72	1,83	0,00
-0,03	3,72	1,83	0,00
-2,28	17,47	2,42	0,27
2,67	0,59	2,74	0,71
3,57	2,79	3,10	1,44
-0,03	3,76	0,99	0,85
-0,93	8,07	1,45	0,21
0,87	1,10	1,63	0,08

-0,93	8,18	1,81	0,01
0,87	1,14	1,63	0,10
6,72	22,85	4,66	7,40
0,42	2,34	1,91	0,00
2,22	0,07	2,38	0,18
1,32	0,41	1,77	0,04
2,22	0,07	2,38	0,18
2,22	0,07	2,57	0,37
-1,83	14,44	1,79	0,03
1,77	0,04	2,24	0,07
-0,03	4,04	0,91	1,14
1,32	0,44	2,10	0,01
2,22	0,06	2,21	0,05
1,77	0,04	2,24	0,07
1,77	0,04	2,24	0,07
1,77	0,04	2,24	0,07
1,32	0,44	2,56	0,34
2,67	0,48	2,82	0,71
4,47	6,20	3,16	1,39
0,87	1,25	1,46	0,28
0,87	1,25	1,85	0,02
1,77	0,05	2,10	0,01
0,87	1,28	1,41	0,35
-0,48	6,15	1,58	0,18
-0,48	6,15	2,06	0,00
2,22	0,05	2,41	0,17
1,77	0,05	3,54	2,37
-0,03	4,16	1,10	0,83
2,22	0,04	2,38	0,14
3,12	1,21	2,44	0,18
7,62	31,36	5,05	9,18
8,07	36,60	5,27	10,56
0,42	2,59	1,78	0,06
1,32	0,50	1,99	0,00
1,32	0,50	1,99	0,00
-0,48	6,30	2,06	0,00
2,67	0,41	2,46	0,18
2,67	0,41	2,82	0,62
0,42	2,62	1,82	0,05
-0,03	4,28	1,83	0,04
-0,48	6,35	2,06	0,00
0,87	1,39	3,02	0,94
3,12	1,14	3,38	1,77
6,72	21,81	4,57	6,35
1,32	0,55	2,07	0,00
3,12	1,12	3,16	1,21
1,77	0,09	1,96	0,01
3,12	1,10	3,07	1,00
2,67	0,35	2,82	0,55
0,42	2,79	1,65	0,19
4,47	5,66	3,24	1,32
-0,03	4,54	1,83	0,07



4,02	3,69	3,24	1,30
6,72	21,34	4,44	5,48
0,87	1,54	2,05	0,00
1,77	0,12	2,24	0,02
2,22	0,01	2,38	0,07
0,87	1,56	1,41	0,50
-1,38	12,25	1,98	0,02
-0,03	4,62	2,03	0,01
8,07	35,40	5,27	9,92
-0,93	9,36	1,81	0,10
1,77	0,13	2,35	0,05
2,22	0,01	2,38	0,06
2,22	0,01	2,38	0,06
3,12	0,98	3,38	1,56
4,47	5,48	3,63	2,25
2,22	0,01	2,49	0,12
2,22	0,01	2,57	0,18
1,32	0,67	2,95	0,66
0,42	2,96	3,52	1,90
-0,03	4,75	1,63	0,27
2,67	0,27	2,63	0,23
2,22	0,00	3,14	0,98
-2,28	19,71	2,02	0,02
0,87	1,69	1,21	0,92
-0,48	7,08	1,43	0,56
-2,28	19,89	2,50	0,10
2,67	0,24	2,63	0,20
2,67	0,24	3,19	1,02
1,77	0,17	3,70	2,31
2,67	0,23	2,74	0,30
2,67	0,23	2,74	0,30
3,57	1,90	2,79	0,36
-0,03	4,97	0,85	1,82
0,87	1,77	1,52	0,46
-1,38	12,82	1,65	0,30
1,32	0,77	2,10	0,01
0,87	1,77	2,11	0,01
1,77	0,18	2,13	0,00
3,12	0,85	2,88	0,46
1,77	0,20	2,24	0,00
2,22	0,00	2,38	0,02
-0,48	7,34	2,48	0,06
3,57	1,80	3,24	1,02
1,77	0,22	2,24	
3,12	0,76	2,68	0,18
8,07	33,87	5,27	9,12
2,22	0,00	2,30	0,00
2,22	0,00	2,49	0,05
1,32	0,90	2,58	0,10
1,77	0,25	3,74	2,16
0,42	3,46	1,91	0,14
1,77	0,26	2,25	0,00

3,57	1,66	3,10	0,67
0,87	2,02	2,48	0,04
-1,38	13,54	1,56	0,55
1,77	0,28	2,35	0,00
1,77	0,28	2,83	0,28
3,12	0,67	2,85	0,30
3,12	0,67	2,99	0,48
-0,03	5,48	1,72	0,35
0,87	2,07	1,85	0,21
1,77	0,29	2,10	0,04
1,77	0,29	2,24	0,00
2,22	0,01	2,57	0,07
1,77	0,30	2,13	0,04
2,67	0,12	2,49	0,03
2,67	0,12	2,82	0,25
1,77	0,30	3,63	1,72
5,82	12,25	4,10	3,17
0,87	2,13	1,85	0,23
0,87	2,13	2,33	
0,87	2,16	1,85	0,24
1,77	0,32	2,13	0,04
2,22	0,01	2,49	0,02
4,02	2,82	3,52	1,39
0,87	2,19	1,85	0,25
2,22	0,02	2,49	0,02
2,22	0,02	2,49	0,02
2,22	0,02	2,49	0,02
3,12	0,58	2,85	0,24
7,17	23,14	5,02	7,08
1,77	0,36	2,13	0,06
-0,03	5,76	2,31	0,00
2,22	0,02	2,49	0,01
3,12	0,56	2,99	0,38
-1,83	17,72	1,79	0,35
-1,38	14,14	2,04	0,12
0,87	2,28	2,05	0,11
3,12	0,55	2,99	0,37
-1,83	17,81	2,27	0,01
1,32	1,17	1,99	0,17
1,32	1,17	2,55	0,02
2,67	0,07	2,85	0,20
1,77	0,41	2,66	0,06
5,82	11,63	4,21	3,24
0,87	2,40	1,60	0,67
1,32	1,21	1,88	0,29
-0,93	11,22	2,40	0,00
2,67	0,06	2,63	0,04
-4,08	42,51	-1,70	17,14
0,87	2,46	2,35	0,01
2,67	0,05	2,82	0,14
4,02	2,46	3,49	1,08
4,47	4,08	3,68	1,51

5,82	11,36	4,27	3,31
0,42	4,16	1,23	1,51
2,67	0,04	2,38	0,01
2,67	0,04	2,74	0,08
4,47	4,04	3,35	0,79
2,22	0,06	2,49	0,00
4,92	6,00	3,68	1,46
1,32	1,35	2,10	0,14
2,67	0,04	2,27	0,04
3,12	0,41	2,75	0,07
2,22	0,07	1,94	0,30
-1,38	14,98	2,04	0,20
-1,38	15,05	1,56	0,88
-0,03	6,40	1,83	0,45
1,77	0,53	2,35	0,02
2,22	0,08	2,49	0,00
2,22	0,08	2,49	0,00
5,37	8,24	3,71	1,46
6,72	17,81	4,66	4,67
2,22	0,08	2,49	0,00
1,32	1,44	2,41	0,01
3,57	1,10	2,80	0,08
4,47	3,80	4,08	2,43
-2,28	23,14	2,02	0,26
-1,38	15,29	2,04	0,24
3,12	0,35	2,44	0,01
4,02	2,16	2,96	0,17
2,22	0,11	3,90	1,82
-2,73	27,98	2,73	0,03
2,67	0,01	2,74	0,03
4,47	3,65	3,49	0,86
1,77	0,64	2,32	0,06
2,67	0,01	2,63	0,00
3,12	0,30	3,02	0,20
0,42	4,67	2,08	0,25
2,67	0,01	2,57	0,00
3,57	0,96	3,32	0,53
0,87	2,99	2,05	0,30
3,57	0,94	2,69	0,01
2,67	0,00	2,82	0,05
4,02	2,02	3,35	0,56
7,17	20,88	5,21	6,81
-0,03	6,97	1,68	0,86
2,67	0,00	3,22	0,37
5,82	10,30	4,05	2,07
0,42	4,84	2,17	0,20
1,77	0,72	2,24	0,14
4,02	1,96	3,46	0,71
6,27	13,32	4,63	4,04
9,87	52,56	6,52	15,21
10,32	59,29	6,77	17,22
-0,93	12,67	2,29	0,12

2,22	0,17	2,60	0,00
1,77	0,74	2,63	
5,82	10,18	4,61	3,92
-0,03	7,13	1,35	1,66
-2,28	24,21	2,02	0,38
0,42	4,93	2,08	0,31
1,32	1,74	2,21	0,18
2,22	0,18	2,38	0,07
2,22	0,19	2,49	0,03
3,57	0,83	2,99	0,11
2,22	0,20	2,49	0,03
2,67		2,74	0,00
3,57	0,81	3,29	0,38
4,47	3,24	3,41	0,55
4,47	3,24	3,74	1,14
1,77	0,83	2,04	0,41
0,87	3,28	2,11	0,32
2,22	0,21	2,27	0,17
2,22	0,21	2,49	0,04
0,87	3,28	2,64	0,00
3,12	0,19	2,99	0,10
3,12	0,19	3,13	0,20
4,47	3,20	3,43	0,56
7,62	24,40	5,27	6,71
0,42	5,15	2,47	0,05
2,67	0,00	2,51	0,03
-2,28	24,70	2,51	0,03
2,67	0,00	2,74	0,00
4,92	4,97	3,82	1,28
3,12	0,18	2,93	0,05
3,12	0,18	2,99	0,08
5,82	9,73	4,16	2,13
1,32	1,93	1,82	0,79
2,22	0,24	3,33	0,38
3,12	0,16	2,96	0,06
-0,03	7,62	2,31	0,18
1,77	0,92	2,35	0,14
2,22	0,26	2,60	0,02
3,12	0,15	2,96	0,05
6,27	12,53	4,46	2,99
1,32	2,02	1,64	1,21
2,22	0,27	2,49	0,06
3,12	0,14	2,99	0,06
-0,93	13,54	1,93	0,67
0,42	5,43	2,08	0,45
1,77	0,96	2,13	0,38
2,22	0,28	2,57	0,03
0,87	3,53	2,93	0,03
4,02	1,61	4,39	2,69
6,72	15,76	4,88	4,54
6,72	15,76	4,88	4,54
4,02	1,59	2,99	0,05

2,67	0,01	3,92	1,35
-1,83	21,16	0,40	5,62
1,32	2,13	1,74	1,08
3,12	0,12	2,38	0,16
3,57	0,62	3,35	0,32
4,92	4,58	3,51	0,53
2,67	0,01	2,82	0,00
0,87	3,69	2,85	0,00
4,47	2,82	3,57	0,61
0,87	3,72	1,85	0,90
1,32	2,19	2,26	0,29
1,77	1,06	2,35	0,20
2,67	0,02	2,99	0,04
2,22	0,35	2,49	0,10
3,12	0,09	3,30	0,23
5,82	9,00	4,05	1,51
5,82	9,00	4,05	1,51
6,72	15,21	4,55	2,99
6,72	15,21	4,55	2,99
6,72	15,21	4,55	2,99
6,72	15,21	4,55	2,99
6,72	15,21	4,55	2,99
1,77	1,12	3,09	0,07
1,32	2,31	2,58	0,07
3,12	0,08	3,01	0,03
-1,38	17,81	3,31	0,22
1,77	1,17	2,13	0,52
4,02	1,37	3,38	0,28
1,32	2,37	1,77	1,19
0,87	3,96	2,11	0,56
1,77	1,19	2,35	0,26
4,02	1,35	3,57	0,50
3,57	0,50	3,69	0,69
0,87	4,00	2,11	0,58
1,77	1,21	2,13	0,55
3,12	0,06	2,93	0,00
3,12	0,06	2,99	0,01
4,02	1,32	3,04	0,03
1,77	1,23	2,13	0,56
-1,83	22,18	2,27	0,37
7,17	18,40	5,02	4,58
0,87	4,08	2,10	0,62
2,22	0,45	2,38	0,26
-2,28	26,73	2,50	0,15
6,27	11,42	3,94	1,10
2,22	0,46	2,49	0,17
2,22	0,46	2,49	0,17
2,67	0,05	2,74	0,03
2,67	0,05	3,02	0,01
2,67	0,06	2,74	0,03
1,77	1,32	2,83	0,01
2,67	0,06	2,88	0,00

3,12	0,04	3,10	0,03
1,77	1,35	1,87	1,12
0,87	4,24	2,36	0,32
2,67	0,07	2,74	0,04
3,12	0,04	2,88	0,00
3,57	0,41	3,58	0,42
0,42	6,35	2,39	0,30
3,12	0,03	2,88	0,00
3,57	0,38	3,13	0,03
4,47	2,31	3,29	0,12
4,92	3,88	3,96	1,02
4,92	3,84	4,89	3,72
0,42	6,55	1,76	1,49
0,87	4,45	2,13	0,72
3,12	0,02	2,99	0,00
3,57	0,35	3,47	0,24
1,32	2,79	2,58	0,17
0,42	6,66	1,83	1,37
-0,03	9,18	1,97	1,06
0,42	6,66	2,08	0,85
1,32	2,82	2,10	0,81
1,32	2,82	2,64	0,13
4,47	2,16	3,72	0,52
4,92	3,69	3,96	0,92
5,82	7,95	4,13	1,28
8,07	25,70	5,41	5,81
3,57	0,30	2,80	0,05
1,77	1,56	2,95	0,00
3,57	0,29	3,58	0,30
7,62	21,07	5,32	5,24
0,42	6,86	1,22	3,31
1,32	2,96	2,19	0,72
2,67	0,14	2,63	0,17
1,77	1,64	2,13	0,85
2,67	0,14	2,85	0,04
9,42	40,45	5,14	4,33
2,22	0,72	2,49	0,34
6,72	13,32	5,30	4,97
0,42	7,08	3,21	0,02
4,02	0,88	3,29	0,04
6,27	10,18	4,47	1,93
6,72	13,25	4,66	2,50
8,07	24,90	5,41	5,43
8,07	24,90	5,41	5,43
4,02	0,86	3,49	0,16
3,12	0,00	3,67	0,32
1,32	3,20	2,10	1,02
2,67	0,19	3,28	0,03
4,47	1,85	3,54	0,18
2,22	0,79	3,79	0,46
2,67	0,20	2,85	0,07
2,22	0,81	2,91	0,04

3,12		2,99	0,02
1,77	1,82	3,53	0,17
0,87	5,11	2,13	1,00
4,02	0,79	3,83	0,49
6,27	9,86	4,63	2,25
6,27	9,86	4,63	2,25
1,32	3,31	1,67	2,16
4,47	1,77	3,82	0,46
2,67	0,23	2,85	0,09
2,67	0,23	2,85	0,09
2,22	0,86	2,91	0,06
-2,73	34,69	2,73	0,18
2,67	0,24	2,74	0,18
3,12	0,00	2,99	0,03
3,12	0,00	2,99	0,03
3,12	0,00	3,04	0,02
7,17	16,00	5,02	3,42
0,42	7,62	0,95	4,97
2,67	0,26	2,63	0,30
4,02	0,71	3,27	0,01
3,57	0,15	3,47	0,08
4,47	1,66	3,74	0,31
4,92	3,03	3,99	0,66
4,02	0,71	4,22	1,08
3,57	0,14	3,08	0,01
4,47	1,64	3,13	0,00
4,02	0,69	3,35	0,03
4,02	0,69	3,74	0,30
2,22	0,96	2,28	0,85
0,42	7,73	2,28	0,85
1,32	3,53	2,58	0,38
2,67	0,28	2,74	0,21
2,22	0,96	2,77	0,18
2,67	0,28	2,85	0,12
3,57	0,14	3,43	0,05
0,87	5,43	3,77	0,32
5,82	6,86	4,05	0,72
5,37	4,71	4,32	1,25
6,72	12,39	4,84	2,69
8,07	23,72	6,41	10,30
0,42	7,78	1,93	1,64
2,22	0,98	2,49	0,52
-2,73	35,40	2,73	0,24
3,57	0,12	3,35	0,02
0,42	7,90	2,45	0,61
2,22	1,02	2,49	0,55
6,72	12,18	4,88	2,72
3,12	0,01	2,62	0,38
4,02	0,61	3,23	0,00
4,92	2,82	3,60	0,13
2,22	1,06	1,83	2,02
1,32	3,72	2,25	1,00

2,22	1,06	2,38	0,76
4,47	1,49	3,43	0,03
4,47	1,49	3,80	0,30
4,02	0,56	3,66	0,15
4,92	2,72	4,01	0,55
1,32	3,84	2,58	0,49
3,57	0,08	2,77	0,26
1,77	2,28	2,83	0,20
4,47	1,39	3,91	0,38
4,47	1,39	4,13	0,71
1,77	2,34	2,66	0,41
3,12	0,03	2,99	0,10
4,02	0,52	3,37	0,00
2,22	1,17	3,99	0,48
6,72	11,70	4,63	1,77
4,02	0,50	3,35	0,00
5,37	4,24	3,99	0,46
2,22	1,21	2,38	0,88
1,32	4,00	3,06	0,07
3,12	0,04	3,48	0,03
6,27	8,70	4,52	1,44
6,72	11,56	4,88	2,43
6,72	11,56	4,88	2,43
2,22	1,23	2,38	0,90
1,77	2,43	2,83	0,25
3,57	0,06	3,02	0,10
3,12	0,04	3,10	0,05
3,57	0,06	3,18	0,02
2,22	1,23	3,70	0,14
4,02	0,46	3,35	0,00
3,57	0,05	3,35	0,00
2,22	1,28	2,08	1,61
0,87	6,25	2,33	1,08
1,77	2,56	2,35	1,04
5,82	6,00	4,63	1,59
6,72	11,22	4,88	2,28
7,17	14,44	5,46	4,37
0,87	6,30	2,81	0,32
0,87	6,30	2,81	0,32
3,57	0,04	3,91	0,28
4,47	1,17	2,77	0,38
4,47	1,17	3,24	0,02
4,47	1,17	3,63	0,06
1,77	2,66	2,35	1,10
3,12	0,08	2,99	0,17
0,87	6,40	3,65	0,06
5,37	3,88	3,66	0,07
4,47	1,14	3,82	0,18
4,47	1,12	4,59	1,39
2,22	1,44	2,38	1,08
2,67	0,56	2,74	0,46
1,77	2,72	2,83	0,35



3,12	0,09	3,10	0,10
5,37	3,80	4,07	0,42
6,27	8,12	4,23	0,66
3,12	0,10	2,83	0,36
2,67	0,58	3,67	0,06
5,82	5,71	4,40	0,94
1,77	2,79	2,35	1,19
4,02	0,34	3,10	0,12
4,02	0,34	3,57	0,02
1,32	4,54	2,10	1,82
3,12	0,11	2,99	0,21
3,57	0,01	3,02	0,18
4,02	0,32	3,54	0,01
1,32	4,54	4,36	0,83
-3,63	50,27	5,00	2,37
4,02	0,31	3,38	0,01
2,22	1,56	2,88	0,35
3,12	0,12	2,99	0,23
5,37	3,61	3,88	0,17
7,17	13,69	5,07	2,56
0,87	6,81	2,01	2,16
0,87	6,81	2,81	0,45
2,67	0,66	3,25	0,05
4,92	2,07	3,85	0,14
6,27	7,78	5,05	2,46
4,47	0,94	3,70	0,04
8,07	20,88	5,41	3,65
2,67	0,72	2,19	1,77
3,57	0,00	3,58	0,00
5,37	3,42	3,82	0,09
6,27	7,56	4,96	2,07
2,22	1,72	3,10	0,18
3,12	0,17	3,10	0,18
7,17	13,25	5,02	2,22
2,22	1,74	4,16	0,38
4,92	1,88	3,46	0,01
3,12	0,18	4,29	0,55
6,72	10,05	4,88	1,77
3,12	0,19	3,64	0,01
4,92	1,85	3,88	0,10
4,02	0,21	4,00	0,19
4,02	0,21	4,06	0,25
4,92	1,85	4,27	0,50
2,22	1,82	1,82	3,06
3,12	0,21	2,99	0,35
4,47	0,79	3,74	0,03
3,57	0,00	2,74	0,72
4,02	0,18	3,38	0,04
1,77	3,35	2,35	1,56
3,12	0,23	3,10	0,25
3,12	0,23	3,50	0,01
3,12	0,24	2,89	0,52

3,57	0,00	3,46	0,02
5,82	4,88	4,13	0,27
4,47	0,74	4,59	0,96
2,67	0,90	3,35	0,07
4,92	1,69	3,49	0,02
4,92	1,69	4,10	0,23
6,72	9,61	4,52	0,81
3,12	0,26	3,10	0,28
3,12	0,26	3,10	0,28
3,57	0,00	3,20	0,18
4,02	0,15	3,35	0,08
3,12	0,27	3,28	0,13
2,22	2,02	3,45	0,04
3,12	0,28	2,99	0,44
3,57	0,01	3,31	0,12
2,22	2,04	3,36	0,08
4,92	1,61	3,99	0,12
1,77	3,57	2,67	0,98
3,12	0,29	3,10	0,31
6,72	9,36	5,34	2,82
3,57	0,01	2,77	0,81
7,17	12,25	5,13	2,13
1,77	3,65	3,00	0,46
1,77	3,65	3,07	0,37
1,77	3,65	3,43	0,06
2,22	2,13	3,61	0,00
4,47	0,62	3,93	0,06
5,37	2,86	3,93	0,06
3,12	0,32	3,10	0,35
1,77	3,69	3,25	0,19
4,02	0,11	3,55	0,02
6,72	9,18	4,88	1,42
4,02	0,10	3,88	0,03
4,47	0,58	4,19	0,23
1,77	3,80	1,89	3,35
4,02	0,09	3,02	0,49
4,47	0,56	3,49	0,05
2,67	1,10	3,50	0,05
4,02	0,09	3,57	0,02
3,57	0,02	3,64	0,01
-0,48	17,72	0,63	9,61
4,02	0,08	4,28	0,30
5,82	4,37	4,91	1,39
1,32	5,86	3,57	0,03
5,37	2,66	3,71	0,00
2,67	1,14	3,86	0,01
1,32	5,90	1,93	3,31
2,67	1,17	3,20	0,30
4,47	0,52	3,37	0,14
4,47	0,50	3,85	0,01
8,07	18,58	5,21	2,10
2,22	2,40	2,73	1,08

3,57	0,04	2,81	0,92
3,12	0,42	2,99	0,61
3,57	0,04	3,05	0,53
4,02	0,05	3,27	0,27
4,47	0,46	3,74	0,00
5,37	2,50	3,85	0,00
5,37	2,50	4,80	1,02
8,52	22,37	5,41	2,62
8,52	22,37	5,60	3,28
1,32	6,15	2,58	1,49
2,67	1,28	2,82	0,96
5,37	2,46	3,66	0,02
4,92	1,25	3,96	0,03
1,32	6,20	2,27	2,37
4,92	1,23	3,41	0,16
3,57	0,06	3,49	0,10
3,12	0,49	2,16	2,76
1,77	4,20	2,35	2,16
3,57	0,06	3,29	0,28
5,82	4,00	5,30	2,19
3,12	0,50	3,10	0,53
3,12	0,50	3,18	0,42
5,82	3,96	4,86	1,06
6,27	5,95	4,88	1,10
1,77	4,33	2,35	2,25
-0,03	15,05	2,77	1,17
4,47	0,38	3,99	0,02
2,67	1,40	2,63	1,50
3,12	0,55	3,47	0,15
4,02	0,02	3,60	0,07
1,32	6,50	4,56	0,48
7,62	14,06	5,38	2,28
7,62	14,06	5,38	2,28
2,22	2,76	2,60	1,64
-1,38	27,67	3,04	0,71
4,92	1,06	4,33	0,19
6,72	8,01	4,63	0,55
1,77	4,54	2,22	2,82
3,57	0,11	3,08	0,67
3,12	0,61	3,58	0,10
4,92	1,04	3,71	0,04
1,32	6,66	3,85	0,00
4,92	1,04	4,21	0,10
2,67	1,56	2,97	0,90
4,47	0,30	3,59	0,11
3,57	0,12	3,80	0,01
3,57	0,13	3,25	0,46
4,47	0,29	3,86	0,00
4,47	0,29	4,08	0,02
7,62	13,62	5,46	2,34
4,47	0,28	3,35	0,35
3,12	0,69	4,54	0,35

6,27	5,38	4,60	0,42
6,72	7,67	4,96	1,02
4,02	0,00	2,99	0,94
4,47	0,26	3,85	0,01
4,02	0,00	4,20	0,06
4,47	0,25	3,35	0,38
4,02	0,00	3,38	0,35
4,47	0,25	3,63	0,12
6,27	5,29	4,55	0,34
0,42	12,67	3,04	0,88
3,12	0,74	3,58	0,16
4,02	0,00	3,86	0,01
2,22	3,13	2,60	1,93
4,02	0,00	3,55	0,19
1,77	4,97	2,35	2,72
-2,73	45,29	2,73	1,61
3,57	0,18	3,35	0,42
4,02	0,00	3,51	0,24
4,02	0,00	3,60	0,16
2,67	1,77	4,12	0,01
4,02	0,00	4,31	0,10
5,37	1,88	4,44	0,19
8,07	16,56	5,27	1,61
3,57	0,19	3,35	0,44
5,82	3,28	4,30	0,08
6,27	5,11	4,63	0,38
2,67	1,82	2,74	1,64
0,42	12,96	3,04	0,96
9,87	34,22	5,47	2,10
2,22	3,28	2,55	2,19
4,47	0,19	4,25	0,05
3,12	0,83	5,75	2,96
0,42	13,10	3,04	1,00
2,67	1,88	3,64	0,16
6,27	4,97	4,60	0,31
4,92	0,76	4,44	0,15
1,77	5,29	3,29	0,61
2,22	3,46	3,40	0,46
4,02	0,00	3,49	0,35
2,67	2,02	2,63	2,13
3,12	0,94	2,80	1,66
3,57	0,27	3,24	0,72
3,57	0,27	3,74	0,12
5,37	1,64	4,01	0,01
4,92	0,69	4,05	0,00
1,77	5,38	4,52	0,18
6,72	6,92	4,74	0,42
2,22	3,53	3,08	1,04
3,57	0,28	3,35	0,56
3,57	0,28	3,35	0,56
3,57	0,28	3,35	0,56
4,02	0,01	3,49	0,37

2,22	3,53	3,73	0,14
3,57	0,29	3,24	0,76
3,57	0,29	3,35	0,58
5,37	1,59	3,66	0,20
2,67	2,07	3,89	0,05
4,02	0,01	3,49	0,40
4,92	0,62	4,16	0,00
4,47	0,11	4,04	0,01
4,92	0,61	4,10	0,00
7,17	9,18	5,07	0,86
2,22	3,72	2,26	3,57
1,77	5,66	2,83	1,74
3,57	0,34	3,35	0,64
4,02	0,02	3,52	0,40
5,37	1,49	4,27	0,01
5,82	2,79	4,35	0,04
7,62	12,04	4,88	0,53
8,07	15,37	5,41	1,59
5,82	2,76	4,12	0,00
8,07	15,29	5,32	1,35
3,57	0,36	2,91	1,59
4,02	0,02	3,82	0,12
5,37	1,44	3,99	0,03
3,12	1,10	4,06	0,01
9,87	32,49	6,44	5,15
3,57	0,37	3,35	0,69
5,82	2,69	3,91	0,07
5,82	2,69	4,18	
5,82	2,69	4,49	0,10
2,67	2,31	3,41	0,61
6,72	6,40	4,60	0,17
4,92	0,52	4,10	0,01
5,82	2,62	4,30	0,01
4,02	0,04	3,49	0,52
4,92	0,50	4,07	0,02
4,02	0,04	4,16	0,00
5,82	2,59	4,27	0,00
6,72	6,30	4,63	0,18
8,07	14,90	5,24	1,06
4,02	0,04	3,61	0,37
5,82	2,56	4,13	0,01
3,57	0,42	4,15	0,00
7,62	11,56	5,38	1,35
4,47	0,05	3,71	0,28
2,67	2,46	4,44	0,04
5,82	2,50	4,46	0,05
7,17	8,58	4,80	0,31
4,02	0,05	3,41	0,71
5,82	2,46	3,66	0,35
5,37	1,25	3,85	0,16
4,02	0,05	4,53	0,08
3,57	0,48	3,35	0,83

4,92	0,44	4,04	0,05
5,37	1,23	4,16	0,01
3,12	1,32	2,94	1,77
6,72	6,00	4,63	0,13
1,77	6,25	5,40	1,28
8,07	14,44	5,60	1,77
1,32	8,76	3,46	0,67
4,47	0,04	3,71	0,32
2,67	2,66	3,33	0,94
5,82	2,31	4,21	0,01
4,92	0,38	4,22	0,01
4,47	0,03	3,85	0,21
3,57	0,55	3,87	0,19
6,72	5,81	4,65	0,12
4,92	0,36	3,77	0,30
1,32	9,06	2,04	5,24
1,77	6,55	3,56	0,59
5,37	1,08	4,55	0,05
3,12	1,49	3,67	0,45
4,47	0,02	3,85	0,24
4,92	0,34	4,02	0,10
4,47	0,02	4,11	0,05
0,87	12,04	4,17	0,03
5,37	1,06	4,46	0,01
5,82	2,19	4,47	0,02
6,27	3,72	4,48	0,02
4,92	0,34	4,80	0,21
7,62	10,76	5,66	1,74
2,67	2,82	3,74	0,37
4,47	0,01	3,79	0,31
6,27	3,69	5,25	0,81
1,77	6,71	2,83	2,34
5,82	2,13	4,65	0,08
3,12	1,56	2,77	2,56
4,47	0,01	3,85	0,27
4,92	0,30	3,88	0,24
7,17	7,84	4,66	0,08
3,57	0,66	3,35	1,06
4,47	0,01	4,31	0,00
6,72	5,48	4,49	0,01
4,02	0,13	4,74	0,13
7,17	7,78	5,44	1,12
5,82	2,04	4,05	0,12
5,82	2,04	4,05	0,12
5,82	2,04	4,22	0,03
2,67	2,99	3,59	0,66
4,47	0,00	3,85	0,30
3,12	1,66	2,88	2,34
3,57	0,71	2,99	2,02
3,57	0,71	4,25	0,03
1,32	9,55	4,75	0,12
4,02	0,15	4,90	0,24

7,17	7,62	5,55	1,30
3,12	1,69	2,88	2,37
4,92	0,25	3,51	0,83
5,37	0,90	4,38	0,00
3,12	1,69	4,48	0,00
1,77	7,08	3,51	0,85
5,37	0,88	3,85	0,34
-0,03	19,89	4,12	0,10
5,82	1,93	4,16	0,07
5,37	0,88	4,52	0,01
4,92	0,24	4,63	0,04
5,82	1,93	4,68	0,06
5,37	0,88	5,00	0,32
3,57	0,76	3,35	1,19
4,47	0,00	3,41	1,06
8,97	20,52	5,74	1,69
2,67	3,17	2,85	2,56
4,92	0,22	3,85	0,36
4,02	0,18	3,91	0,29
4,02	0,18	4,12	0,11
6,27	3,31	4,88	0,18
8,07	13,10	5,47	1,04
4,47	0,00	3,74	0,52
4,02	0,19	3,86	0,36
4,47	0,00	3,97	0,24
5,37	0,83	4,07	0,15
4,92	0,21	4,53	0,00
4,92	0,20	3,49	0,96
4,92	0,20	3,94	0,28
5,82	1,82	4,19	0,08
1,77	7,29	4,35	0,01
6,27	3,24	4,79	0,10
3,57	0,83	2,65	3,35
3,57	0,83	3,44	1,08
4,92	0,19	3,54	0,88
3,12	1,85	3,98	0,25
3,57	0,83	4,22	0,07
7,17	7,24	4,93	0,20
6,72	5,02	5,14	0,44
1,77	7,40	1,35	9,86
5,82	1,77	4,32	0,03
5,82	1,77	4,57	0,01
2,22	5,20	2,60	3,61
3,57	0,86	3,35	1,32
4,47	0,00	4,52	0,00
4,02	0,23	4,79	0,08
-0,03	20,61	3,27	1,54
3,12	1,93	3,81	0,49
6,72	4,88	4,82	0,10
8,97	19,89	7,18	7,13

4,47	0,00	3,32	1,44
4,92	0,16	3,55	0,94
1,32	10,24	3,93	0,35
4,92	0,16	4,02	0,25
4,02	0,25	4,08	0,19
5,37	0,72	4,35	0,03
5,82	1,69	4,38	0,02
3,57	0,92	2,91	2,62
5,82	1,66	4,41	0,01
5,37	0,69	4,53	0,00
6,72	4,75	4,80	0,07
4,92	0,14	3,21	1,80
-0,03	20,98	3,27	1,64
4,47	0,01	3,83	0,52
4,47	0,01	3,85	0,49
6,27	2,96	4,63	0,01
4,02	0,28	4,64	0,01
4,47	0,01	5,01	0,21
7,62	9,42	5,41	0,74
1,77	7,78	3,31	1,56
4,02	0,29	3,60	0,92
4,92	0,13	3,94	0,38
5,37	0,66	4,35	0,04
2,67	3,61	2,85	2,96
3,12	2,10	2,99	2,50
3,57	1,00	3,35	1,49
4,92	0,12	3,71	0,74
1,77	7,84	4,46	0,01
4,02	0,31	4,08	0,25
4,47	0,01	4,30	0,08
3,12	2,16	2,41	4,75
4,47	0,01	4,16	0,18
3,57	1,06	3,13	2,16
6,27	2,76	3,91	0,49
3,12	2,22	4,03	0,34
4,02	0,35	4,08	0,28
2,67	3,80	3,33	1,66
5,37	0,56	4,10	0,27
6,72	4,41	4,63	0,00
3,57	1,10	4,99	0,14
8,97	18,92	5,82	1,44
6,72	4,41	6,04	2,02
4,92	0,08	4,10	0,28
4,02	0,37	4,24	0,15
6,27	2,69	5,11	0,23
6,72	4,37	5,16	0,28
4,02	0,38	2,94	2,89
4,02	0,38	3,68	0,92
5,37	0,53	4,55	0,01
7,62	8,88	5,54	0,81
-0,03	21,90	3,27	1,90



9,42	22,75	6,07	2,02
1,77	8,35	2,41	5,06
6,27	2,59	5,24	0,34
3,12	2,40	3,75	0,85
5,82	1,30	4,74	0,00
6,27	2,53	4,75	0,00
8,07	11,49	5,30	0,38
4,02	0,45	3,54	1,32
4,47	0,05	3,82	0,76
4,47	0,05	3,85	0,71
3,57	1,25	4,25	0,19
6,72	4,12	4,96	0,07
1,77	8,58	2,83	3,50
3,57	1,28	3,35	1,82
5,37	0,45	4,35	0,12
0,42	18,32	4,45	0,06
6,27	2,46	5,02	0,10
5,37	0,44	4,21	0,25
8,07	11,29	5,38	0,45
2,22	6,30	2,97	3,10
3,57	1,35	3,22	2,28
2,67	4,24	3,51	1,49
5,37	0,41	3,63	1,21
4,47	0,07	4,02	0,50
5,37	0,41	4,40	0,11
6,27	2,37	4,49	0,06
6,72	3,92	4,77	0,00
5,37	0,38	4,27	0,23
5,82	1,14	4,60	0,02
3,12	2,69	3,78	0,96
4,92	0,02	3,44	1,77
5,37	0,36	3,76	1,02
3,12	2,72	4,18	0,35
5,37	0,36	4,36	0,17
8,07	10,89	5,79	1,04
6,72	3,76	4,63	0,02
3,12	2,79	4,20	0,35
5,82	1,04	4,10	0,49
6,72	3,69	5,04	0,06
5,37	0,31	4,35	0,21
2,22	6,76	3,98	0,71
5,82	1,00	4,91	0,01
5,37	0,29	4,44	0,15
3,57	1,59	4,62	0,04
8,07	10,50	5,35	0,27
5,82	0,96	4,53	0,10
4,02	0,69	4,08	0,59
6,27	2,02	4,60	0,06
4,92	0,00	5,00	0,02
4,02	0,71	3,99	0,76
8,07	10,30	5,79	0,86
8,07	10,24	6,57	2,89

4,47	0,17	3,69	1,42
2,22	7,13	3,08	3,28
3,57	1,74	4,48	0,17
7,62	7,45	5,38	0,24
6,27	1,90	5,48	0,35
4,02	0,77	3,60	1,69
6,27	1,88	4,77	0,02
4,02	0,79	3,94	0,94
7,17	5,11	5,16	0,06
3,57	1,82	3,89	1,06
4,92		3,99	0,86
1,32	12,96	4,72	0,04
8,07	9,92	5,07	0,02
5,82	0,81	5,08	0,03
4,47	0,20	5,40	0,23
8,52	12,96	6,14	1,49
4,02	0,83	3,13	3,24
5,37	0,19	4,46	0,22
6,27	1,80	4,79	0,02
8,52	12,89	5,82	0,79
9,42	20,16	6,05	1,25
3,12	3,31	4,56	0,14
7,17	4,97	5,35	0,17
-0,93	34,69	2,49	6,10
6,27	1,72	4,74	0,05
6,27	1,72	4,99	0,00
2,67	5,29	3,82	1,32
4,92	0,00	3,85	1,25
5,37	0,16	4,35	0,38
4,02	0,90	5,08	0,01
6,27	1,69	5,33	0,13
6,72	3,03	4,74	0,06
8,52	12,53	5,80	0,67
3,57	2,02	3,87	1,25
5,37	0,14	4,44	0,30
6,27	1,64	4,87	0,01
8,97	15,84	6,07	1,17
4,92	0,01	3,19	3,28
3,57	2,04	4,31	0,48
7,17	4,71	5,39	0,15
4,92	0,01	4,22	0,62
9,87	23,62	6,94	3,72
5,37	0,12	4,18	0,71
2,67	5,57	3,36	2,79
-0,48	30,36	3,50	2,34
3,12	3,69	2,99	4,20
1,32	13,84	3,46	2,50
6,72	2,82	6,34	1,69
4,47	0,34	4,07	0,96
5,37	0,10	4,16	0,79
6,72	2,79	4,74	0,10

7,62	6,60	6,19	1,30
2,22	8,07	3,31	3,06
-0,93	36,00	3,14	3,72
4,47	0,36	3,85	1,49
5,82	0,56	4,60	0,22
6,27	1,44	4,63	0,19
7,17	4,41	4,82	0,06
6,27	1,44	4,85	0,05
8,97	15,21	5,66	0,35
5,37	0,08	4,35	0,53
6,27	1,42	4,85	0,05
8,07	8,94	6,19	1,23
4,92	0,03	3,60	2,22
5,37	0,08	4,35	0,55
4,47	0,38	4,53	0,31
2,67	5,90	3,75	1,82
3,57	2,34	4,31	0,62
5,82	0,52	4,82	0,08
5,37	0,07	4,49	0,38
4,02	1,23	3,49	2,69
6,27	1,30	4,60	0,28
8,97	14,75	5,30	0,03
4,92	0,05	3,80	1,80
5,82	0,46	4,60	0,29
5,82	0,46	5,00	0,02
6,72	2,50	6,26	1,25
2,67	6,15	2,85	5,29
5,82	0,45	4,60	0,30
2,22	8,64	4,13	1,06
4,92	0,06	4,41	0,56
3,12	4,20	2,68	6,20
0,42	22,85	0,85	18,92
5,82	0,38	3,99	1,46
6,72	2,31	5,30	0,01
4,92	0,08	4,13	1,17
3,57	2,72	3,14	4,33
4,47	0,58	3,85	1,90
7,62	5,71	5,69	0,21
9,42	17,56	5,80	0,32
4,92	0,10	3,99	1,56
7,62	5,66	5,64	0,16
4,92	0,11	5,40	0,02
7,17	3,65	5,05	0,04
9,42	17,31	6,46	1,44
-0,48	33,06	3,53	3,03
8,52	10,56	5,79	0,27
7,62	5,48	5,71	0,18
6,72	2,04	5,00	0,08
-2,28	57,46	3,83	2,16
6,27	0,94	4,79	0,26
5,82	0,26	4,89	0,18
3,57	3,03	4,91	0,16

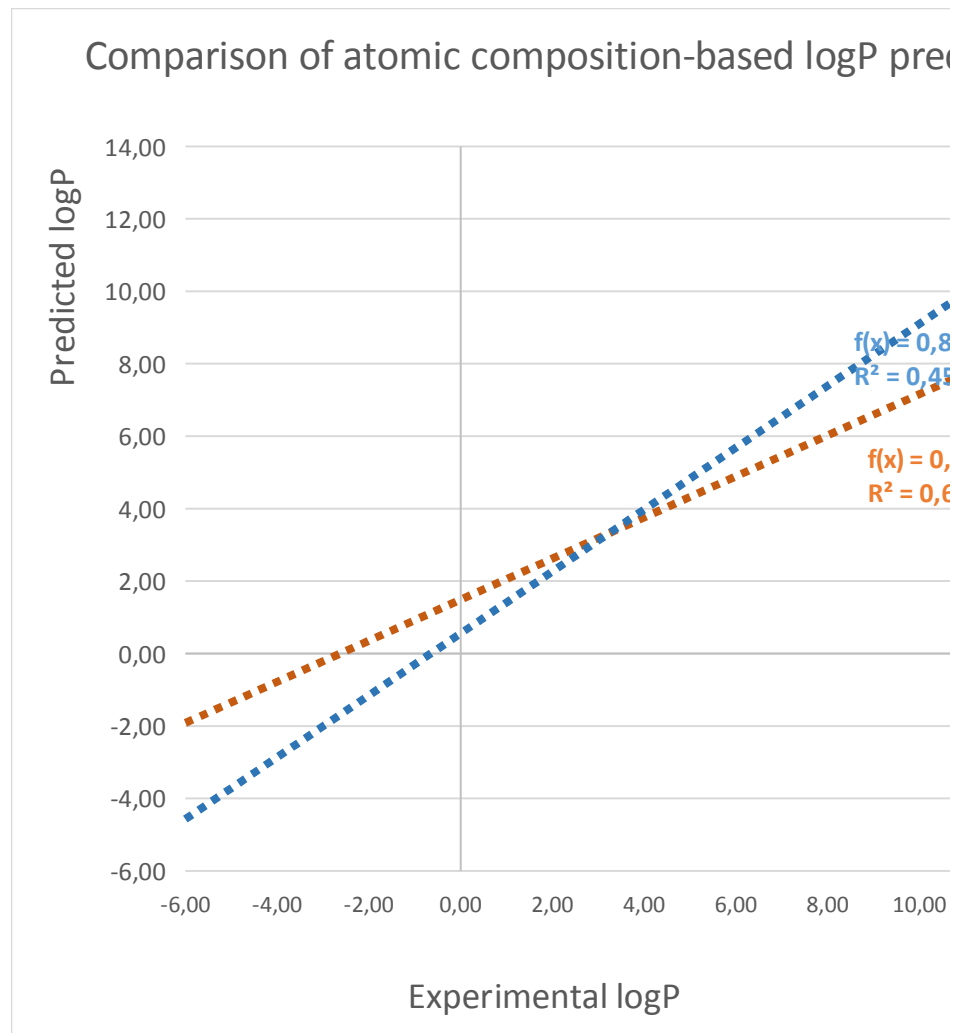
4,47	0,71	4,99	0,10
7,17	3,46	4,99	0,10
7,17	3,46	5,24	0,00
4,47	0,72	3,63	2,86
5,37	0,00	4,19	1,28
2,67	7,13	4,39	0,90
8,97	13,18	5,52	0,03
8,52	10,05	5,49	0,02
10,32	24,70	6,79	2,07
5,82	0,21	5,17	0,04
5,37	0,00	4,17	1,46
5,82	0,19	4,52	0,74
2,22	10,05	4,46	0,86
6,27	0,77	4,85	0,29
8,52	9,80	5,68	0,08
9,42	16,24	5,85	0,21
3,12	5,20	3,10	5,29
6,72	1,74	5,10	0,09
5,82	0,17	4,97	0,19
7,62	4,84	5,37	0,00
3,57	3,46	3,35	4,33
-0,03	29,81	3,75	2,82
7,17	3,03	4,41	1,04
7,17	3,03	5,18	0,06
9,42	15,84	6,33	0,79
4,92	0,28	4,33	1,25
6,72	1,61	4,99	0,21
8,07	6,86	7,26	3,28
4,47	1,00	3,44	4,12
-0,93	40,96	3,73	3,03
3,12	5,52	4,54	0,86
7,62	4,62	5,75	0,08
3,57	3,65	3,39	4,37
7,17	2,86	5,23	0,06
8,07	6,71	5,97	0,24
3,57	3,69	4,01	2,19
5,37	0,01	4,81	0,46
7,17	2,82	5,35	0,02
5,37	0,02	5,45	0,00
11,22	32,72	6,94	2,07
2,67	8,07	3,80	2,92
5,37	0,02	4,07	2,07
5,37	0,02	5,40	0,01
4,47	1,10	3,85	2,79
6,72	1,42	5,30	0,05
2,67	8,24	5,33	0,04
6,72	1,35	4,81	0,56
6,27	0,50	5,24	0,10
7,17	2,59	5,27	0,08
6,72	1,30	4,97	0,37
7,17	2,53	5,17	0,17
4,47	1,25	4,04	2,40

6,72	1,28	4,88	0,50
8,52	8,58	5,46	0,02
4,92	0,46	4,53	1,14
3,12	6,15	4,54	1,12
7,62	4,08	5,80	0,04
5,82	0,04	4,72	0,83
5,37	0,07	5,54	0,01
6,27	0,40	4,89	0,56
3,12	6,40	3,10	6,50
3,57	4,33	5,13	0,27
5,37	0,10	4,64	1,08
7,62	3,76	5,49	0,04
0,87	23,23	4,73	0,92
6,27	0,34	4,85	0,71
6,72	1,04	4,94	0,58
2,67	9,30	4,77	0,90
7,17	2,10	5,77	0,00
10,32	21,16	6,52	0,64
2,67	9,36	4,77	0,92
7,17	2,07	5,35	0,14
8,07	5,48	5,63	0,01
6,72	0,96	5,07	0,45
6,72	0,94	5,10	0,42
2,22	12,46	5,37	0,14
4,02	3,03	3,27	6,20
7,17	1,99	5,35	0,17
7,17	1,99	5,69	0,00
6,72	0,90	4,89	0,77
3,57	4,84	4,90	0,76
10,77	25,00	6,88	1,23
4,92	0,76	4,08	2,92
2,22	12,82	4,83	0,94
7,62	3,31	6,09	0,08
5,82	0,00	5,75	0,00
9,87	16,48	6,16	0,12
2,22	13,03	4,58	1,56
7,62	3,20	5,01	0,67
8,07	5,02	5,63	0,04
4,47	1,85	5,80	0,00
3,57	5,20	5,81	0,00
4,02	3,39	4,53	1,77
4,92	0,88	5,06	0,64
9,42	12,67	7,36	2,25
5,82	0,00	4,22	2,72
5,82	0,00	4,49	1,90
6,72	0,69	4,41	2,19
7,17	1,59	5,35	0,31
3,12	7,84	4,20	2,96
4,02	3,61	5,29	0,40
11,22	27,88	6,94	1,00
6,27	0,10	4,69	1,61

7,62	2,76	5,31	0,42
8,97	8,94	6,04	0,00
6,27	0,08	6,21	0,05
4,02	3,88	4,57	2,02
6,72	0,52	5,58	0,18
5,37	0,41	3,72	5,24
6,72	0,50	5,33	0,46
6,72	0,50	6,34	0,11
4,92	1,23	3,99	4,16
6,27	0,05	5,16	0,77
2,67	11,36	5,23	0,66
-0,93	48,86	3,39	7,13
4,47	2,59	3,78	5,29
8,52	5,90	5,13	0,92
7,17	1,17	5,32	0,59
4,47	2,66	3,63	6,10
6,27	0,01	4,08	4,28
8,52	5,52	5,43	0,55
5,82	0,15	5,16	1,10
3,57	7,18	3,35	8,41
11,67	29,38	7,49	1,54
5,37	0,79	4,83	2,04
7,17	0,81	5,58	0,48
9,87	12,96	6,13	0,02
9,87	12,96	6,49	0,05
7,17	0,79	5,66	0,38
-0,03	40,07	1,02	27,88
5,37	0,86	4,35	3,80
2,22	16,65	5,00	1,69
7,17	0,76	5,13	1,37
7,17	0,76	5,13	1,37
2,22	17,47	5,00	1,96
6,27	0,04	4,63	3,35
6,27	0,04	4,63	3,35
7,62	1,32	5,67	0,64
6,27	0,05	5,48	1,04
4,92	2,59	3,66	8,24
4,92	2,76	5,28	1,69
5,82	0,59	4,60	3,96
2,22	19,45	5,54	1,19
9,87	10,37	6,07	0,34
3,57	9,55	3,83	8,01
1,77	24,30	5,23	2,16
1,32	28,94	5,46	1,54
4,92	3,24	4,79	3,72
5,37	2,04	4,83	3,88
10,32	12,04	6,57	0,08
7,17	0,04	5,13	3,42
1,77	27,35	5,23	3,13
1,77	27,35	5,23	3,13
6,27	0,61	4,63	5,86
0,87	38,81	5,69	1,99

5,37	3,24	4,13	9,24
0,42	59,91	5,92	5,02
6,27	3,84	4,63	12,96
4,02	17,98	4,08	17,47
7,17	4,49	5,13	17,31

	Mannhold 2009	Chaker 2023
RMSE	#NOM ?	#NOM ?
BIC	4553	766









































































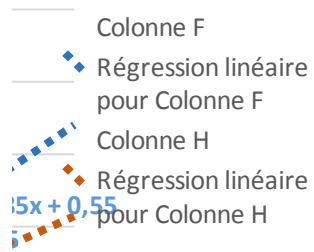








## dictive models



$$57x + 1,49$$

55

12,00













































































# Supporting information : A2 - Parameter tolerance

## 1. Mass-to-charge ratio

*(computed if at least one sample has abundance > 100)*

	<u>m/z ≤ 200 Da</u>	<u>m/z &gt; 200 Da</u>
<u>Δm/z (ppm)</u>	15	10

## 2. Retention time

*(filtered out if CI of high)*

<u>ΔRt (min)</u>
Experimental Rt
RTI-predicted Rt
Retip-predicted Rt
logP-predicted Rt

*Note : these are def*

## 3. Isotopic mass-to-charge differences

*(computed if at least one sample has abundance of M0 > 100)*

	<u>All m/z</u>
<u>Δm/z (ppm)</u>	25

## 4. Isotopic retenti

<u>ΔRt (min)</u>
------------------

## Δ values for annotation using Scannotation

(best ranked available Rt is < 0.3)

Rt < 15 mn	15 ≤ Rt < 30 mn	30 ≤ Rt < 45 mn	Rt ≥ 45 mn
0,74	3,22	4,35	3,02
15,43	10,87	10,83	5,81
16,54	13,04	6,82	2,61
12,65	11,32	13,37	8,98

Default values, that can be adapted by Scannotation based on user's data (Screening tab, section "Chromatog)

### on time difference

All Rt
0,06

*raphic parameters")*



## Supporting information : A3

---

CI

$m/z + Rt + Is\_M2$

$m/z + Rt + Is\_M1$

$m/z + Is\_M2$

$m/z + Is\_M1$

$m/z + Rt$

$m/z$

---

### 3 - Codification of global confidence

---

#### Neutral loss not detected

---

G3<sup>b</sup>

G3<sup>a</sup>

G2<sup>b</sup>

G2<sup>a</sup>

G2

G1

---

*(1, 2, 3 refer to number of predictors used **and** "a" or "b" refer to the isotopologue considered)*

# ce index

---

## Neutral loss detected

---

G4cb

G4ca

G3cb

G3ca

G3c

G2c

---

*(Number of predictors used raised by 1 **and** "c" indicates one of the predictors is neutral loss)*

---

**Abundance ratio [metabolite/parent compound]\*  $\geq 1$**

---

G4db

G4da

G3db

G3da

G3d

G2d

---

*("d" indicates one of the predictors is neutral loss **and** metabolite is more abundant than parent compound)*

## Supporting information : A4 - Prioritization process of Sci

---

	<b>Total pre-annotations</b>	<b>Number of pre-annotations with at least one area ratio sample/blank &gt; 10</b>
<b>Phree (ESI +)</b>	10460 (2826)	4554 (1588)
<b>Phree (ESI -)</b>	9570 (2410)	3295 (1254)
<b>PPT (ESI +)</b>	7137 (3016)	4735 (1675)
<b>PPT (ESI -)</b>	5622 (1975)	2492 (892)

Values are presented as:                      Number of pre-annotations (*Number of unique pre-anno*

\*Unique pre-annotations group together adducts from the same compound and multiple features

# annotation pre-annotations

---

**Number of pre-annotations scored as  
Clg > 0,7 (G2 + G3)**

264 (123) + 66 (55)

193 (80) + 73 (52)

203 (89) + 63 (55)

101 (79) + 57 (49)

*tations\*)*

; assigned to the same compound

---

**Number of pre-annotations scored as  
Clg > 0,7 (G2 + G3)  
excluding internal standards**

---

259 (121) + 47 (36)

188 (77) + 61 (46)

194 (86) + 42 (35)

95 (77) + 46 (44)

---

Pre-annotations manually curated to obt

ain 89 confirmed compounds



**Sup**





## porting information : A5 - Annotations performed in cohort sei

Compound name
(2-oxo-2,3-dihydro-1H-indol-3-yl)acetic acid
1,3,5-tris(2,2-dimethylpropionylamino)benzene
13-Hydroxy-7,14-labdadien-6-one
2-((3-dodecanamidopropyl)dimethylammonio)acetate
2-chlorophenol
2-hydroxybenzoic acid
2-Naphthalenesulfonic acid
2-Naphthol
2-naphthylamine
3-(4-Hydroxyphenyl)lactic acid
3,5-dibromo-4-hydroxybenzoic acid
3-Formylindole
3-hydroxybenzoic acid
4-chlorophenol
4-hydroxy-2,5,6-trichloroisophthalonitrile
4-hydroxybenzoic acid
4-quinolone
5-acetylsalicylamide
5-hydroxytryptophan
Acesulfame
Acetaminophen glucuronide
Acetaminophen sulfate
Aminoacetophenone
Arabinosylhypoxanthine
Aspartame
Auraptene
Azelaic acid
Benzothiazole
Benzothiazole sulfonic acid
Benzylbutylphthalate
Bis(2-(tert-butyl)-6-(3-(tert-butyl)-2-hydroxy-5-methylbenzyl)-4-methylphenyl) terephthalate
Bromoxynil

Caffeine  
Carveol  
Caryophyllene oxide  
Chavicol sulfate  
Cinchonidine  
Cinnamaldehyde  
CMPF  
Cocamidopropyl Betaine  
Coumaraldehyde  
Coumaric acid  
Cresol sulfate  
Di(ethylhexyl) phthalate  
Dioctyl phthalate  
Diphenylphosphate  
Diphenylsulfone  
Docosahexaenoic acid  
Dodecylbenzenesulfonic acid  
Eicosapentaenoic acid  
Ferulic acid  
Fipronil sulfone  
Ibuprofen  
Indole-3-acetaldehyde  
Indole-3-carbinol  
Indoxyl sulfate  
Ioxynil  
Isobutylparaben  
Isopropylparaben  
Lenticin  
Lidocaine  
Lumichrome  
Mercaptobenzothiazole  
Methionine  
Methylperfluorooctanesulfonamidoacetic acid  
Paracetamol  
Paraxanthine  
Pentachlorophenol  
Perfluoroheptanesulfonic acid  
Perfluorohexanesulfonic acid  
Perfluorooctanesulfonic acid

Phenol sulfate

Piperidone

Piperine

Propylparaben

Propylparaben sulfate

Reserpine

Solanidine

Sucralose

Theobromine

Theophylline

Thymol

Triclosan glucuronide

Triclosan sulfate

Triethylphosphate

Triphenylphosphine oxide

Tris(2-butoxyethyl)phosphate

Tritosulfuron

Tryptophan

---

# rum samples

	Gut microbiota
SMILES	Gut microbiota metabolites
<chem>C1=CC=C2C(=C1)C(C(=O)N2)CC(=O)O</chem>	
<chem>CC(C)(C)C(=O)NC1=CC(=CC(=C1)NC(=O)C(C)(C)C)NC(=O)C(C)(C)C</chem>	
<chem>CC1=CC(=O)C2C(CCCC2(C1CCC(C)(C=C)O)C)(C)C</chem>	
<chem>CCCCCCCCC(=O)NCCC[N+](C)(C)CC(=O)[O-]</chem>	
<chem>C1=CC=C(C(=C1)O)Cl</chem>	
<chem>C1=CC=C(C(=C1)C(=O)O)O</chem>	
<chem>C1=CC=C2C=C(C=CC2=C1)S(=O)(=O)O</chem>	
<chem>C1=CC=C2C=C(C=CC2=C1)O</chem>	
<chem>C1=CC=C2C=C(C=CC2=C1)N</chem>	
<chem>C1=CC(=CC=C1CC(C(=O)O)O)O</chem>	P
<chem>C1=C(C=C(C(=C1Br)O)Br)C(=O)O</chem>	
<chem>C1=CC=C2C(=C1)C(=CN2)C=O</chem>	P
<chem>C1=CC(=CC(=C1)O)C(=O)O</chem>	
<chem>C1=CC(=CC=C1O)Cl</chem>	
<chem>C(#N)C1=C(C(=C(C(=C1Cl)C#N)Cl)Cl)O</chem>	
<chem>C1=CC(=CC=C1C(=O)O)O</chem>	
<chem>C1=CC=C2C(=C1)C(=O)C=CN2</chem>	
<chem>CC(=O)C1=CC(=C(C=C1)O)C(=O)N</chem>	
<chem>C1=CC2=C(C=C1O)C(=CN2)CC(C(=O)O)N</chem>	P
<chem>CC1=CC(=O)NS(=O)(=O)O1</chem>	
<chem>CC(=O)NC1=CC=C(C=C1)OC2C(C(C(O2)C(=O)O)O)O</chem>	
<chem>CC(=O)NC1=CC=C(C=C1)OS(=O)(=O)O</chem>	
<chem>C1=CC=C(C=C1)C(=O)CN</chem>	
<chem>C1=NC2=C(C(=O)N1)N=CN2C3C(C(C(O3)CO)O)O</chem>	
<chem>COC(=O)C(CC1=CC=CC=C1)NC(=O)C(CC(=O)O)N</chem>	
<chem>CC(=CCCC(=CCOC1=CC2=C(C=C1)C=CC(=O)O2)C)C</chem>	
<chem>C(CCCC(=O)O)CCCC(=O)O</chem>	
<chem>C1=CC=C2C(=C1)N=CS2</chem>	
<chem>C1=CC=C2C(=C1)N=C(S2)S(=O)(=O)O</chem>	
<chem>CCCCOC(=O)C1=CC=CC=C1C(=O)OCC2=CC=CC=C2</chem>	
<chem>CC1=CC(=C(C=C1)C(C)(C)O)CC2=C(C(=CC(=C2)C)C(C)(C)OC(=O)C3=CC=C(C=C3)C(=O)OC4=C(C=C(C=C4C(C)(C)C)CC5=C(C(=CC(=C5)C)C(C)(C)O</chem>	
<chem>C1=C(C=C(C(=C1Br)O)Br)C#N</chem>	

CN1C=NC2=C1C(=O)N(C(=O)N2C)C  
CC1=CCC(CC1O)C(=C)C  
CC1(CC2C1CCC3(C(O3)CC2=C)C)C  
C=CCC1=CC=C(C=C1)OS(=O)(=O)O  
C=CC1CN2CCC1CC2C(C3=CC=NC4=CC=CC=C34)O  
C1=CC=C(C=C1)C=CC=O  
CCCC1=C(C(=C(O1)CCC(=O)O)C(=O)O)C  
CCCCCCCCC(=O)NCCC[N+](C)(C)CC(=O)[O-]  
C1=CC(=CC=C1C=CC=O)O  
C1=CC(=CC=C1C=CC(=O)O)O  
CC1=CC=CC=C1OS(=O)(=O)O  
CCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC  
CCCCCCCCOC(=O)C1=CC=CC=C1C(=O)OCCCCCCCC  
C1=CC=C(C=C1)OP(=O)([O-])OC2=CC=CC=C2  
C1=CC=C(C=C1)S(=O)(=O)C2=CC=CC=C2  
CCC=CCC=CCC=CCC=CCC=CCC=CCCC(=O)O  
CCCCCCCCCCCCC1=CC=CC=C1S(=O)(=O)O  
CCC=CCC=CCC=CCC=CCC=CCCC(=O)O  
COC1=C(C=CC(=C1)C=CC(=O)O)O  
C1=C(C=C(C(=C1Cl)N2C(=C(C(=N2)C#N)S(=O)(=O)C(F)  
(F)F)N)Cl)C(F)(F)F  
CC(C)CC1=CC=C(C=C1)C(C)C(=O)O  
C1=CC=C2C(=C1)C(=CN2)CC=O  
C1=CC=C2C(=C1)C(=CN2)CO  
C1=CC=C2C(=C1)C(=CN2)OS(=O)(=O)O  
C1=C(C=C(C(=C1I)O)I)C#N  
CC(C)COC(=O)C1=CC=C(C=C1)O  
CC(C)OC(=O)C1=CC=C(C=C1)O  
C[N+](C)(C)C(CC1=CNC2=CC=CC=C21)C(=O)[O-]  
CCN(CC)CC(=O)NC1=C(C=CC=C1C)C  
CC1=CC2=C(C=C1C)N=C3C(=N2)C(=O)NC(=O)N3  
C1=CC=C2C(=C1)NC(=S)S2  
CSCCC(C(=O)O)N  
CN(CC(=O)O)S(=O)(=O)C(C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F  
(F)F)(F)F)(F)F  
CC(=O)NC1=CC=C(C=C1)O  
CN1C=NC2=C1C(=O)N(C(=O)N2)C  
C1(=C(C(=C(C(=C1Cl)Cl)Cl)Cl)Cl)O  
C(C(C(C(F)(F)F)(F)F)(F)F)(C(C(C(F)(F)S(=O)(=O)O)(F)F)(F)F)(F)F  
C(C(C(C(F)(F)S(=O)(=O)O)(F)F)(F)F)(C(C(F)(F)F)(F)F)(F)F  
C(C(C(C(C(F)(F)S(=O)(=O)O)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)F)(F)F)  
(F)F

P

P



C1=CC=C(C=C1)OS(=O)(=O)O  
C1CCNC(=O)C1  
C1CCN(CC1)C(=O)C=CC=CC2=CC3=C(C=C2)OCO3  
CCCOC(=O)C1=CC=C(C=C1)O  
CCCOC(=O)C1=CC=C(C=C1)OS(=O)(=O)O  
COC1C(CC2CN3CCC4=C(C3CC2C1C(=O)OC)NC5=C4C=CC(=C5)OC  
)OC(=O)C6=CC(=C(C(=C6)OC)OC)OC  
CC1CCC2C(C3C(N2C1)CC4C3(CCC5C4CC=C6C5(CCC(C6)O)C)C)C  
C(C1C(C(C(C(O1)OC2(C(C(C(O2)C(Cl)O)O)C(Cl)O)O)Cl)O  
CN1C=NC2=C1C(=O)NC(=O)N2C  
CN1C2=C(C(=O)N(C1=O)C)NC=N2  
CC1=CC(=C(C=C1)C(C)C)O  
C1=CC(=C(C=C1Cl)OC2C(C(C(C(O2)C(=O)O)O)O)OC3=C(C=C(C  
=C3)Cl)Cl  
C1=CC(=C(C=C1Cl)OS(=O)(=O)O)OC2=C(C=C(C=C2)Cl)Cl  
CCOP(=O)(OCC)OCC  
C1=CC=C(C=C1)P(=O)(C2=CC=CC=C2)C3=CC=CC=C3  
CCCCOCCOP(=O)(OCCOCCCC)OCCOCCCC  
COC1=NC(=NC(=N1)NC(=O)NS(=O)(=O)C2=CC=CC=C2C(F)  
(F)F)C(F)(F)F  
C1=CC=C2C(=C1)C(=CN2)CC(C(=O)O)N

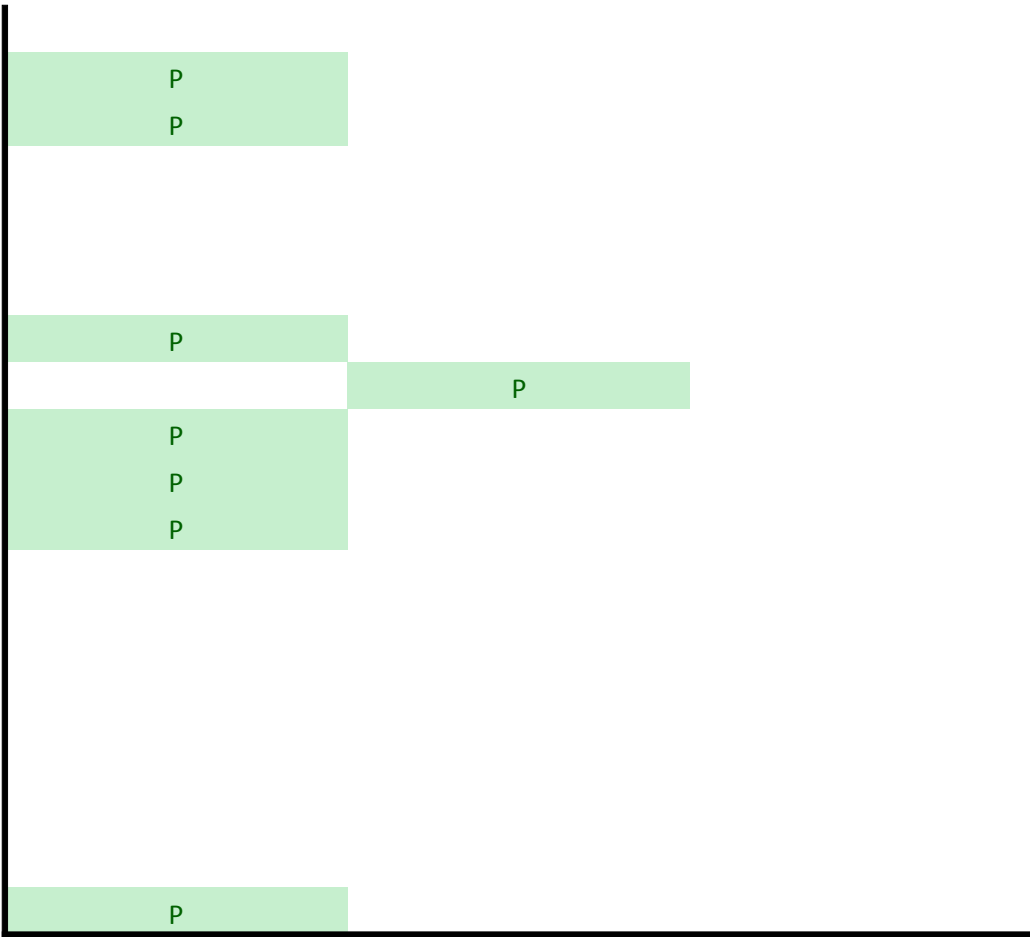
P

Food compounds

Natural compound	Flavoring agent	Preservatives and other stabilizers
------------------	-----------------	-------------------------------------

P		
P	S	
S		
		P
S		
S		
	P	
		S
P		
	P	
P		
P		
	P	
	P	





**Classification** (P = primary use, S =

**Medication and personal care**

Indirect food additive	Medication	Personal care and cosmetics products
------------------------	------------	--------------------------------------

P

P

S

S

S

P

S

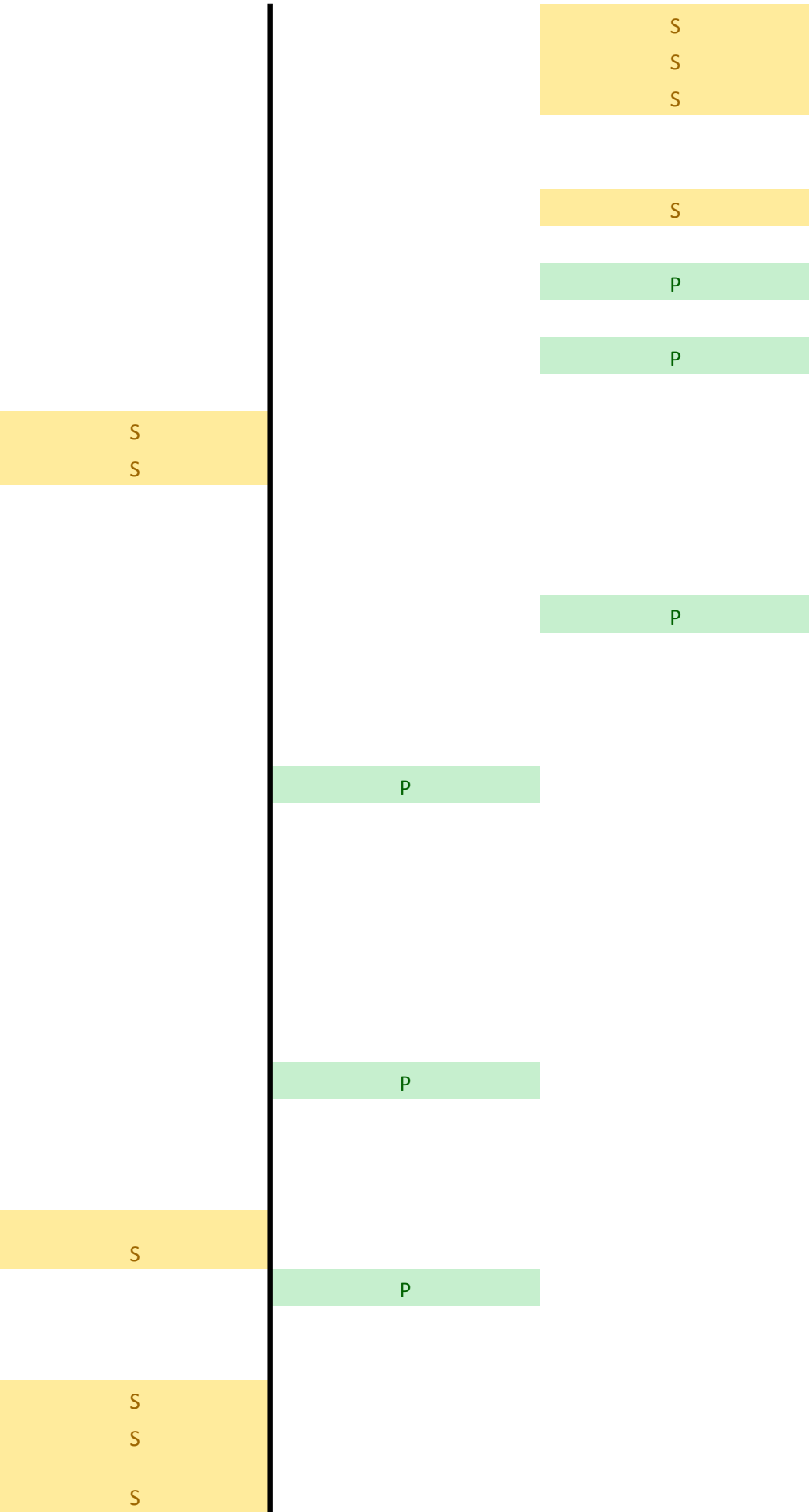
P  
P

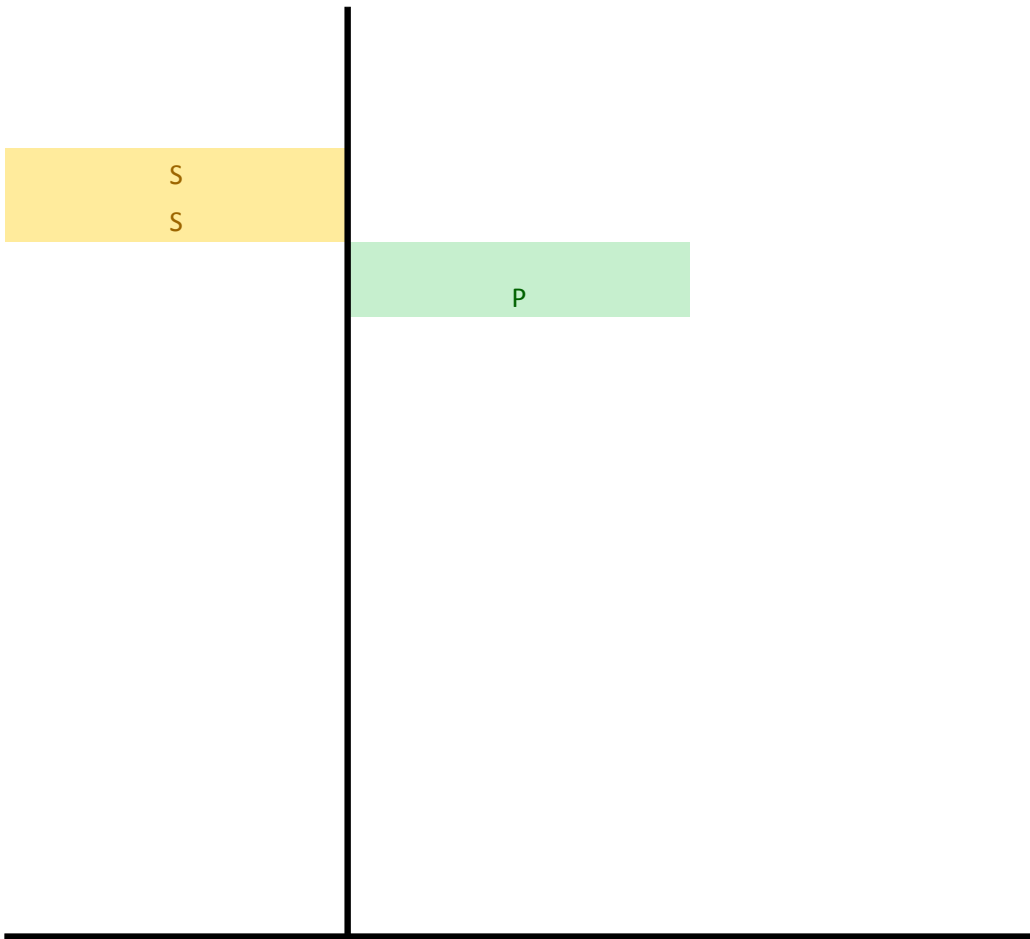
S S

S

S

P





secondary use)

products

Preservatives and other stabilizers	Pesticides	Plasticizers
-------------------------------------	------------	--------------

S

P

S

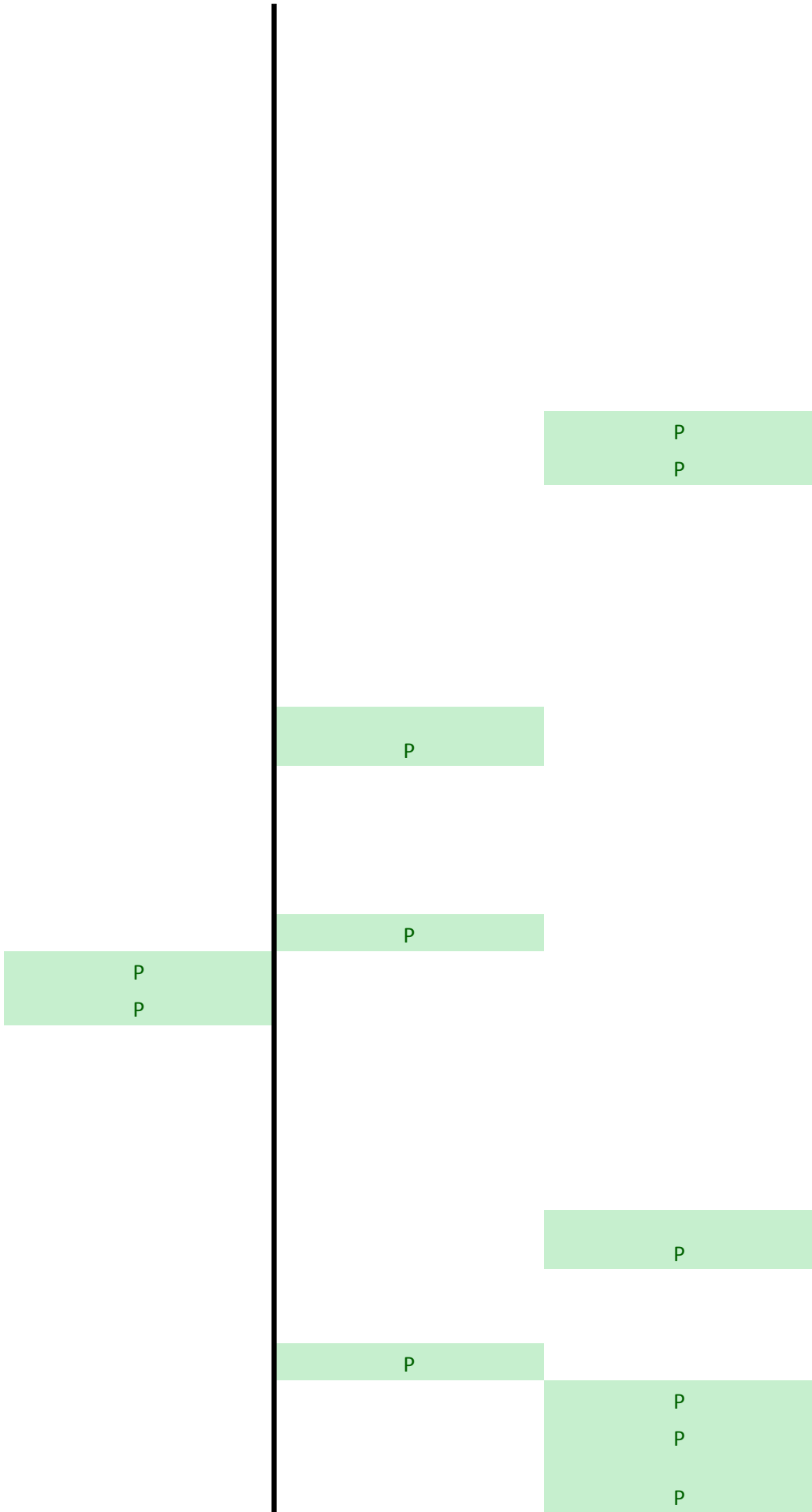
P

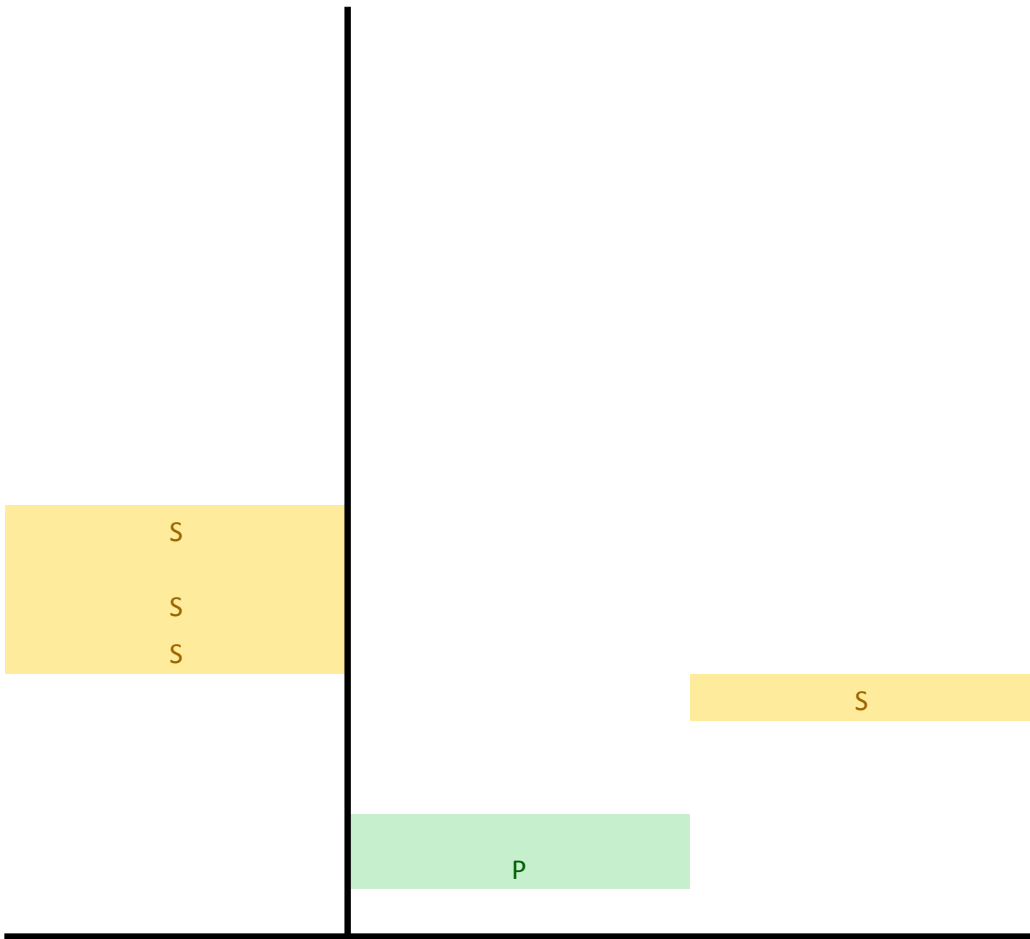
P

P

P







Industrial compounds			m
Organophosphate flame retardant	Synthesis intermediate	Preservatives and other stabilizers	(+)
			192,06
			n.a.
			305,25
			n.a.
	P		n.a.
	S		n.a.
	P		n.a.
	P		n.a.
	P		144,08
			n.a.
			n.a.
			146,06
	P		n.a.
			n.a.
			n.a.
			146,06
	S		180,07
			n.a.
			n.a.
			n.a.
			136,08
			n.a.
			295,13
			n.a.
		S	n.a.
			n.a.
			n.a.
			313,14
			811,49
			n.a.

		195,09
		153,13
		207,17
		n.a.
		n.a.
		133,06
		n.a.
		343,29
		149,06
		n.a.
		n.a.
		391,28
		391,28
P	S	251,05
P		219,05
		n.a.
		n.a.
		n.a.
		n.a.
		n.a.
		n.a.
		160,07
		130,06
		n.a.
		n.a.
		195,1
		181,09
		247,15
		235,18
		243,09
		n.a.
		150,06
	S	n.a.
		152,07
		n.a.
	S	n.a.
S		n.a.
S		n.a.
S		n.a.

			n.a.
	S		100,08
			286,14
		P	n.a.
		P	n.a.
			609,28
			398,34
			n.a.
			181,07
			181,07
			151,11
		P	n.a.
		P	n.a.
P	S		183,08
	P		279,09
P			399,25
			n.a.
			205,1

## SOFTNAM

/z	Rt (min)	Cl m/z		Cl			
				Experimental		RTI-predicted	
		(+)	(-)	(+)	(-)	(+)	(-)
n.a.	2,7	0,95	n.a.	n.a.	n.a.	n.a.	n.a.
410,22	34,11	n.a.	0,86	n.a.	n.a.	n.a.	<b>0,66</b>
n.a.	46,63	0,87	n.a.	n.a.	n.a.	n.a.	n.a.
377,26	29,19	n.a.	0,88	n.a.	n.a.	n.a.	<b>0,77</b>
127	14,01	n.a.	0,92	n.a.	n.a.	n.a.	<b>0,5</b>
137,02	21,9	n.a.	0,95	n.a.	n.a.	n.a.	<b>0,6</b>
207,01	7,25	n.a.	0,95	n.a.	n.a.	n.a.	<b>0,69</b>
143,05	22,93	n.a.	0,94	n.a.	n.a.	n.a.	<b>0,87</b>
n.a.	14,41	0,97	n.a.	n.a.	n.a.	<b>0,75</b>	n.a.
181,05	4,07	n.a.	0,91	n.a.	n.a.	n.a.	<b>0,55</b>
292,85	19,22	n.a.	0,88	n.a.	n.a.	n.a.	<b>0,96</b>
n.a.	4,24	0,95	n.a.	n.a.	n.a.	<b>0,68</b>	n.a.
137,02	5,38	n.a.	0,95	n.a.	n.a.	n.a.	<b>0,55</b>
127	11,81	n.a.	0,94	n.a.	n.a.	n.a.	<b>0,76</b>
244,91	27,74	n.a.	0,86	n.a.	n.a.	n.a.	n.a.
137,02	8,69	n.a.	1	n.a.	n.a.	n.a.	<b>0,8</b>
n.a.	6,27	0,95	n.a.	n.a.	n.a.	<b>0,71</b>	n.a.
n.a.	6,21	0,81	n.a.	<b>0,93</b>	n.a.	0,5	n.a.
219,08	4,52	n.a.	0,91	n.a.	n.a.	n.a.	<b>0,89</b>
161,99	3,12	n.a.	0,9	n.a.	<b>0,96</b>	n.a.	0,28
362,06	4,09	n.a.	0,79	n.a.	<b>0,61</b>	n.a.	0,99
230,01	3,61	n.a.	0,97	n.a.	<b>0,91</b>	n.a.	0,84
n.a.	2,07	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
303,05	2,98	n.a.	0,99	n.a.	n.a.	n.a.	n.a.
n.a.	5,8	0,97	n.a.	<b>0,96</b>	n.a.	0,22	n.a.
297,15	44,08	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
187,1	9,41	n.a.	0,94	n.a.	n.a.	n.a.	<b>0,91</b>
136,02	46,77	n.a.	0,91	n.a.	n.a.	n.a.	<b>0,83</b>
213,96	6,68	n.a.	0,99	n.a.	n.a.	n.a.	<b>0,83</b>
n.a.	44,94	0,87	n.a.	<b>0,95</b>	n.a.	0,36	n.a.
n.a.	12,55	0,85	n.a.	n.a.	n.a.	<b>0,78</b>	n.a.
275,9	20,2	n.a.	0,84	n.a.	n.a.	n.a.	<b>0,42</b>

n.a.	5,53	0,95	n.a.	n.a.	n.a.	<b>0,67</b>	n.a.
n.a.	38,1	0,79	n.a.	n.a.	n.a.	<b>0,81</b>	n.a.
n.a.	44,42	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
213,02	11,38	n.a.	0,97	n.a.	<b>0,88</b>	n.a.	0,61
293,18	32,49	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	14,33	0,82	n.a.	n.a.	n.a.	n.a.	n.a.
239,09	22,08	n.a.	0,98	n.a.	n.a.	n.a.	<b>0,97</b>
n.a.	35,78	0,79	n.a.	n.a.	n.a.	<b>0,9</b>	n.a.
n.a.	3,36	0,92	n.a.	n.a.	n.a.	<b>0,96</b>	n.a.
163,04	5,1	n.a.	0,9	n.a.	n.a.	n.a.	<b>0,74</b>
187,01	7,35	n.a.	0,85	n.a.	<b>0,63</b>	n.a.	1
n.a.	45,67	0,91	n.a.	n.a.	n.a.	<b>0,79</b>	n.a.
n.a.	49,09	0,95	n.a.	n.a.	n.a.	<b>0,86</b>	n.a.
n.a.	46,2	0,99	n.a.	<b>0,94</b>	n.a.	0,8	n.a.
n.a.	26,77	0,89	n.a.	n.a.	n.a.	<b>0,74</b>	n.a.
327,23	46,43	n.a.	0,97	n.a.	<b>1</b>	n.a.	0,79
325,19	48,41	n.a.	0,93	n.a.	n.a.	n.a.	<b>0,98</b>
301,22	45,99	n.a.	0,91	n.a.	n.a.	n.a.	<b>0,88</b>
193,05	6,5	n.a.	0,97	n.a.	n.a.	n.a.	<b>0,63</b>
450,93	44,56	n.a.	0,89	n.a.	n.a.	n.a.	<b>0,73</b>
205,12	41,19	n.a.	0,99	n.a.	<b>0,97</b>	n.a.	n.a.
n.a.	9,52	0,86	n.a.	n.a.	n.a.	<b>0,94</b>	n.a.
n.a.	10,5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
212	5,92	n.a.	0,96	n.a.	<b>0,86</b>	n.a.	n.a.
369,82	28,48	n.a.	0,95	n.a.	n.a.	n.a.	<b>0,6</b>
n.a.	40,82	0,88	n.a.	n.a.	n.a.	<b>0,72</b>	n.a.
n.a.	8,43	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	5,26	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	5,94	0,93	n.a.	n.a.	n.a.	<b>0,81</b>	n.a.
n.a.	10,08	0,93	n.a.	n.a.	n.a.	<b>0,52</b>	n.a.
165,98	15,22	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	1,53	0,78	n.a.	n.a.	n.a.	<b>0,78</b>	n.a.
569,97	44,87	n.a.	0,95	n.a.	n.a.	n.a.	n.a.
n.a.	4,24	0,83	n.a.	n.a.	n.a.	n.a.	n.a.
179,06	5,23	n.a.	0,96	n.a.	n.a.	n.a.	<b>0,82</b>
262,84	43,01	n.a.	0,85	n.a.	n.a.	n.a.	<b>0,84</b>
448,93	33,49	n.a.	0,84	n.a.	n.a.	n.a.	<b>0,73</b>
398,94	35,31	n.a.	0,89	n.a.	n.a.	n.a.	n.a.
498,93	43,18	n.a.	0,93	n.a.	n.a.	n.a.	n.a.

172,99	4,74	n.a.	0,97	n.a.	<b>0,62</b>	n.a.	n.a.
n.a.	3,78	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	37,81	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
179,07	21,58	n.a.	0,95	n.a.	<b>0,76</b>	n.a.	0,46
259,03	17,12	n.a.	0,98	n.a.	<b>0,81</b>	n.a.	0,23
n.a.	15,39	0,96	n.a.	n.a.	n.a.	<b>0,99</b>	n.a.
n.a.	26,15	0,91	n.a.	n.a.	n.a.	<b>0,63</b>	n.a.
430,98	6,78	n.a.	0,9	n.a.	n.a.	n.a.	<b>0,59</b>
n.a.	3,86	0,95	n.a.	n.a.	n.a.	<b>0,45</b>	n.a.
n.a.	5,91	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	19,52	0,93	n.a.	n.a.	n.a.	n.a.	n.a.
462,98	27,17	n.a.	0,86	n.a.	n.a.	n.a.	<b>0,91</b>
366,9	36,32	n.a.	0,94	n.a.	<b>0,97</b>	n.a.	
n.a.	12,57	0,89	n.a.	n.a.	n.a.	<b>0,77</b>	n.a.
n.a.	2,76	0,8	n.a.	n.a.	n.a.	<b>0,55</b>	n.a.
n.a.	44,69	0,93	n.a.	n.a.	n.a.	n.a.	n.a.
444,02	34,47	n.a.	0,91	n.a.	<b>0,96</b>	n.a.	0,86
n.a.	4,61	0,83	n.a.	n.a.	n.a.	<b>0,9</b>	n.a.



E pre-annotation							
Rt				Isotopic fit		Global CI	
Retip-predicted		logP-predicted		CI overall			
(+)	(-)	(+)	(-)	(+)	(-)	(+)	(-)
<b>0,99</b>	n.a.	n.a.	n.a.	n.a.	n.a.	G2_0.97	n.a.
n.a.	0,66	n.a.		n.a.	0,54	n.a.	G3_0.76
<b>0,67</b>	n.a.	0,42	n.a.	n.a.	n.a.	G2_0.77	n.a.
n.a.	0,65	n.a.	n.a.	n.a.	0,61	n.a.	G3_0.75
n.a.	0,19	n.a.	0,5	n.a.	0,91	n.a.	G3_0.78
n.a.	n.a.	n.a.	0,97	n.a.	n.a.	n.a.	G2_0.78
n.a.	0,35	n.a.	0,37	n.a.	n.a.	n.a.	G2_0.82
n.a.	0,4	n.a.	0,81	n.a.	0,65	n.a.	G3_0.82
0,23	n.a.	0,41	n.a.	n.a.	n.a.	G2_0.86	n.a.
n.a.	0,83	n.a.	0,63	n.a.	n.a.	n.a.	G2_0.73
n.a.		n.a.	0,59	n.a.	0,78	n.a.	G3_0.87
0,11	n.a.	0,14	n.a.	0,76	n.a.	G3_0.8	n.a.
n.a.	0,55	n.a.	0,41	n.a.	n.a.	n.a.	G2_0.75
n.a.	0,05	n.a.	0,35	n.a.	n.a.	n.a.	G2_0.85
n.a.	<b>0,92</b>	n.a.	0,88	n.a.	0,96	n.a.	G3_0.91
n.a.	0,72	n.a.	0,64	n.a.	0,88	n.a.	G3_0.89
0,29	n.a.	0,22	n.a.	0,76	n.a.	G3_0.81	n.a.
	n.a.	0,81	n.a.	0,94	n.a.	G3_0.88	n.a.
n.a.	0,27	n.a.	0,16	n.a.	n.a.	n.a.	G2_0.9
n.a.	0,97	n.a.	0,64	n.a.	n.a.	n.a.	G2_0.95
n.a.	0,97	n.a.	n.a.	n.a.	n.a.	n.a.	G2_0.7
n.a.	0,7	n.a.	0,8	n.a.	n.a.	n.a.	G2_0.94
n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	<b>0,77</b>	n.a.	n.a.	n.a.	0,31	n.a.	G3_0.70
0,95	n.a.	0,28	n.a.	0,94	n.a.	G3_0.96	n.a.
n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	0,79	n.a.	0,78	n.a.	0,91	n.a.	G3_0.92
n.a.	n.a.	n.a.	0,68	n.a.	n.a.	n.a.	G2_0.87
n.a.	0,62	n.a.	0,89	n.a.	n.a.	n.a.	G2_0.91
0,72	n.a.	0,04	n.a.	0,77	n.a.	G3_0.86	n.a.
0,32	n.a.	n.a.	n.a.	n.a.	n.a.	G2_0.82	n.a.
n.a.		n.a.	0,6	n.a.	0,79	n.a.	G3_0.70

0,53	n.a.	0,77	n.a.	n.a.	n.a.	G2_0.81	n.a.
	n.a.	n.a.	n.a.	0,77	n.a.	G3_0.79	n.a.
n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	0,54	n.a.	0,44	n.a.	0,91	n.a.	G3_0.92
n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
<b>0,68</b>	n.a.	0,76	n.a.	n.a.	n.a.	G2_0.75	n.a.
n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	G2_0.98
0,47	n.a.	n.a.	n.a.	0,9	n.a.	G3_0.86	n.a.
0,86	n.a.	0,59	n.a.	0,91	n.a.	G3_0.93	n.a.
n.a.	0,23	n.a.	0,25	n.a.	n.a.	n.a.	G2_0.82
n.a.	0,62	n.a.	0,26	n.a.	0,86	n.a.	G3_0.78
0,69	n.a.	n.a.	n.a.	n.a.	n.a.	G2_0.85	n.a.
0,78	n.a.	n.a.	n.a.	n.a.	n.a.	G2_0.91	n.a.
0,02	n.a.	0,01	n.a.	0,93	n.a.	G3_0.95	n.a.
n.a.	n.a.	0,87	n.a.	0,82	n.a.	G3_0.82	n.a.
n.a.	0,89	n.a.	0,6	n.a.	0,98	n.a.	G3_0.98
n.a.	0,22	n.a.	0,69	n.a.	0,9	n.a.	G3_0.94
n.a.	0,96	n.a.	0,82	n.a.	0,92	n.a.	G3a_0.9
n.a.	0,4	n.a.	0,39	n.a.	n.a.	n.a.	G2_0.8
n.a.	0,79	n.a.	n.a.	n.a.	0,95	n.a.	G3_0.86
n.a.	0,36	n.a.	0,46	n.a.	n.a.	n.a.	G2_0.98
0,62	n.a.	0,91	n.a.	0,89	n.a.	G3_0.90	n.a.
n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	n.a.	n.a.	0,41	n.a.	0,85	n.a.	G3_0.89
n.a.	0,43	n.a.	0,33	n.a.	0,9	n.a.	G3_0.82
0,38	n.a.	n.a.	n.a.	n.a.	n.a.	G2_0.8	n.a.
n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
0,72	n.a.	0,8	n.a.	0,87	n.a.	G3_0.87	n.a.
	n.a.	0,01	n.a.	n.a.	n.a.	G2_0.73	n.a.
n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
0,51	n.a.	0,1	n.a.	0,87	n.a.	G3_0.81	n.a.
n.a.	<b>0,79</b>	n.a.	0,8	n.a.	0,7	n.a.	G3_0.81
<b>0,74</b>	n.a.	0,69	n.a.	0,95	n.a.	G3_0.84	n.a.
n.a.	0,78	n.a.	n.a.	n.a.	0,83	n.a.	G3_0.87
n.a.		n.a.	0,72	n.a.	0,91	n.a.	G3_0.87
n.a.	0,13	n.a.	0,93	n.a.	n.a.	n.a.	G2_0.78
n.a.	<b>0,84</b>	n.a.	0,84	n.a.	n.a.	n.a.	G2_0.87
n.a.	<b>0,76</b>	n.a.	0,79	n.a.	0,77	n.a.	G3_0.82

n.a.	0,55	n.a.	0,36	n.a.	0,87	n.a.	G3_0.82
n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
n.a.	0,04	n.a.	0,19	n.a.	n.a.	n.a.	G2_0.86
n.a.	0,73	n.a.	0,65	n.a.	0,9	n.a.	G3_0.9
0,48	n.a.		n.a.	0,9	n.a.	G3_0.95	n.a.
0,78	n.a.	0,75	n.a.	n.a.	n.a.	G2_0.77	n.a.
n.a.	0,97	n.a.	n.a.	n.a.	0,98	n.a.	G3_0.82
n.a.	n.a.		n.a.	n.a.	n.a.	G2_0.7	n.a.
n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
<b>0,93</b>	n.a.	0,91	n.a.	0,98	n.a.	G3_0.95	n.a.
n.a.	n.a.	n.a.	0,85	n.a.	1	n.a.	G3_0.92
n.a.	n.a.	n.a.	0,98	n.a.	0,88	n.a.	G3_0.93
0,82	n.a.	0,92	n.a.	n.a.	n.a.	G2_0.83	n.a.
0,7	n.a.	0,59	n.a.	n.a.	n.a.	G2_0.72	n.a.
<b>0,66</b>	n.a.	0,82	n.a.	n.a.	n.a.	G2_0.8	n.a.
n.a.	0,69	n.a.	0,33	n.a.	n.a.	n.a.	G2_0.94
0,83	n.a.	0,51	n.a.	n.a.	n.a.	G2_0.87	n.a.

Detection frequency (%)	MS/	
	Theoretical fragments	
	(+)	(-)
100	77.0391, 91.0555, 103.0545	n.a.
45	n.a.	232.1091, 290.1874, 316.1667
68	195.0648, 397.2115	n.a.
1	n.a.	102.0561, 238.2177, 283.2756
8	n.a.	91,02
88	n.a.	93,03
39	n.a.	79.9574, 114.0553, 143.0503
85	n.a.	98.9055, 115.0553
8	91.0556, 115.0542, 117.0699, 127.0	n.a.
87	n.a.	72.9921, 93.0301, 107.0480, 119.04
97	n.a.	248,86
100	65.0400, 77.0389, 91.0560, 117.059	n.a.
50	n.a.	93,03
80	n.a.	n.a.
74	n.a.	146.9765, 174.9704, 181.9447, 209
88	n.a.	93,03
88	77.0415, 91.0555, 104.0494, 128.04	n.a.
95	165.0694, 179.0726, 194.0958	n.a.
96	n.a.	132.0447, 144.0456, 158.0622
97	n.a.	67.0065, 77.9655, 82.0298
20	n.a.	113.0252, 150.0561, 175.0252
14	n.a.	107.0365, 108.0445, 150.0551
100	167.0729, 180.0807, 182.0963, 193.	n.a.
98	n.a.	92.0241, 108.0190, 135.0301
100	115.0543, 135.0446, 143.0485, 171.	n.a.
100	n.a.	170.0038, 183.0014, 197.0272
35	n.a.	57.0331, 95.0488, 97.0645, 123.080
97	n.a.	65.0382, 105.0448, 109.0108
3	n.a.	57.9751, 134.0069, 150.0019
3	380,33	n.a.
86	91.0546, 115.0548, 130.0655, 143.0	n.a.
61	n.a.	78,92

94	149,02	n.a.
20	283.1693, 431.1844, 589.2939	n.a.
91	51.0233, 53.0389, 77.0382, 95.0493	n.a.
100	n.a.	105.0710, 133.0659
99	n.a.	96.9588, 221.1544, 236.1056
75	79.0548, 81.0701, 91.0546, 95.0854	n.a.
59	n.a.	96.9588, 135.0810, 151.1119, 177.0
97	67.0282, 108.0554, 110.0713, 122.0	n.a.
100	77.0386, 105.0335	n.a.
100	n.a.	145,9
100	n.a.	92.0279, 107.0493
97	69.0454, ,96.0561, 124.0507, 142.0	n.a.
10	77.0380, 79.0550, 9.0540, 95.0490,	n.a.
17	58.0652, 86.0968	n.a.
45	91.0553, 117.0564, 118.0657, 130.0	n.a.
100	n.a.	229.1958, 283.2446
81	n.a.	170.0042, 183.0121, 197.0277, 255
100	n.a.	203.1802, 229.1957, 257.2274
65	n.a.	133.0299, 149.0608
29	n.a.	246.0120, 281.9913, 414.9496
25	n.a.	91.0549, 105.0701, 119.0855
98	69.0442, 83.0606, 110.0718, 123.04	n.a.
100	167.0730, 180.0808, 182.0964, 210.	n.a.
100	n.a.	79.9578, 132.0460
92	n.a.	126.9051, 230.9182
72	71.0851, 149.0232, 261.1485	n.a.
96	55.0195, 77.0392, 91.0541, 103.054	n.a.
94	60.0815, 118.0653, 146.0600, 170.0	n.a.
93	77.0380, 103.0560, 128.0500, 130.0	n.a.
95	121.0284, 139.0389, 163.0754	n.a.
98	n.a.	57.9752, 134.0069
97	51.0237, 65.0364, 91.0539, 117.057	n.a.
100	n.a.	418.9773, 482.9356, 511.9607
5	91.0543, 149.02335, 239.0708	n.a.
91	n.a.	122.0365, 164.0341
92	n.a.	n.a.
2	n.a.	168,99
57	n.a.	98.9538, 118.9930, 168.9892
98	n.a.	98.9538, 118.9930, 168.9892

100	n.a.	79.9551, 93.0325
82	91.0543, 118.0662, 128.0511, 132.0	n.a.
86	56.0493, 72.0444, 82.0651, 94.0650	n.a.
99	n.a.	92.0266, 121.0300, 136.0167
95	n.a.	121.0297, 137.0239, 179.0716
67	57.0701, 83.0855, 101.0971, 143.01	n.a.
8	127.0164, 155.0480	n.a.
13	n.a.	146.9399, 359.0325
100	79.0544, 91.0543, 107.0856, 119.08	n.a.
100	67.0544, 81.0699, 91.0543, 105.071	n.a.
2	103.0542, 120.0808, 130.0651, 131.	n.a.
25	n.a.	n.a.
13	n.a.	286,94
16	183.1745, 240.2315	n.a.
77	110.0598, 134.0593	n.a.
26	149.0219, 173.0513, 201.0465, 219.	n.a.
91	n.a.	193.0347, 223.9999
100	77.0386, 95.0492, 152.0633, 175.01	n.a.

Manual curation		
MS		Confidence level (Schymanski 2014)
Experimental fragments		
(+)	(-)	
77.0390, 91.0554, 103.0548	n.a.	2a
n.a.	232.1089, 290.1875, 316.1671	2b
195.0655, 397.2110	n.a.	2a
n.a.	102.0558, 238.2182, 283.2751	2b
n.a.	91,02	2a
n.a.	93,03	2a
n.a.	79.9577, 115.0546, 143.0500	2a
n.a.	98.9057, 115.0557	2a
91.0549, 115.0543, 117.0690, 127.0	n.a.	2a
n.a.	72.9922, 93.0304, 107.0482, 119.04	2a
n.a.	248,85	2a
65.0396, 77.0384, 91.0551, 117.058	n.a.	2a
n.a.	93,03	2a
n.a.	n.a.	4
n.a.	146.9765, 174.9710, 181.9447, 209	2a
n.a.	93,03	2a
77.0415, 91.0548, 104.0490, 128.04	n.a.	2a
165.0697, 179.0720, 194.0963	n.a.	1
n.a.	132.0453, 144.0450, 158.0630	2a
n.a.	67.0063, 77.9654, 82.0299	2a
n.a.	113.0245, 150.0562, 175.0247	1
n.a.	107.0367, 108.0452, 150.0556	1
167.0730, 180.0803, 182.0966, 193.	n.a.	2a
n.a.	92.0247, 108.0199, 135.0305	2a
115.0551, 135.0450, 143.0495, 171.	n.a.	1
n.a.	170.0040, 183.0114, 197.0244	2a
n.a.	57.0339, 95.0486, 97.0652, 123.080	2a
n.a.	65.0382, 105.0448, 109.0109	2a
n.a.	57.9749, 134.0071, 150.0023	2a
380,33	n.a.	1
91.0543, 115.0543, 130.0654, 143.0	n.a.	2b
n.a.	78,92	2a

149,02	n.a.	2a
283.1700, 431.1849, 589.2947	n.a.	2a
51.0229, 53.0388, 77.0375, 95.0491	n.a.	2a
n.a.	105.0710, 133.0657	2b
n.a.	96.9590, 221.1546, 236.1055	2a
79.0539, 81.0705, 91.0537, 95.0844	n.a.	2a
n.a.	96.9584, 135.0818, 151.1121, 177.0	2a
67.0288, 108.0556, 110.0711, 122.0	n.a.	2a
77.0388, 105.0337	n.a.	2b
n.a.	145,9	2a
n.a.	92.0275, 107.0500	1
69.0451, 96.0563, 124.0502, 142.06	n.a.	2a
77.0386, 79.0552, 9.0544, 95.0485,	n.a.	2a
58.0655, 86.0965	n.a.	2a
91.0549, 117.0568, 118.0658, 130.0	n.a.	2a
n.a.	229.1953, 283.2439	1
n.a.	170.0041, 183.0128, 197.0287, 255	2a
n.a.	203.1807, 229.1951, 257.2275	2a
n.a.	133.0305, 149.0609	2b
n.a.	246.0117, 281.9920, 414.9500	2a
n.a.	91.0555, 105.0708, 119.0848	1
69.0448, 83.0603, 110.0712, 123.04	n.a.	2a
167.0721, 180.0812, 182.0966, 210.	n.a.	2a
n.a.	79.9570, 132.0457	1
n.a.	126.9041, 230.9178	2a
71.0858, 149.0234, 261.1490	n.a.	2a
55.0199, 77.0386, 91.0544, 103.055	n.a.	2a
60.0810, 118.0651, 146.0597, 170.0	n.a.	2a
77.0388, 103.0555, 128.0501, 130.0	n.a.	2a
121.0282, 139.0393, 163.0751	n.a.	2b
n.a.	57.9750, 134.0063	2a
51.0236, 65.0365, 91.0541, 117.057	n.a.	2a
n.a.	418.9771, 482.9356, 511.9617	2a
91.0542, 149.0234, 239.0707	n.a.	2a
n.a.	122.0361, 164.0341	2a
n.a.	n.a.	4
n.a.	168,99	2a
n.a.	98.9535, 118.9937, 168.9882	2a
n.a.	98.9533, 118.9931, 168.9985	2a



n.a.	79.9558, 93.0331	2a
91.0546, 118.0660, 128.0519, 132.0	n.a.	2a
56.0494, 72.0451, 82.0651, 94.0649	n.a.	2a
n.a.	92.0263, 121.0302, 136.0166	2a
n.a.	121.0296, 137.0244, 179.0712	1
57.0702, 83.0850, 101.0972, 143.01	n.a.	2a
127.0155, 155.0472	n.a.	2a
n.a.	146.9391, 359.0319	2a
79.0551, 91.0544, 107.0853, 119.08	n.a.	2a
67.0545, 81.0701, 91.0547, 105.072	n.a.	2a
103.0542, 120.0811, 130.0655, 131.	n.a.	2a
n.a.	n.a.	4
n.a.	286,94	1
183.1751, 240.2326	n.a.	2a
110.0602, 134.0596	n.a.	2a
149.0220, 173.0515, 201.0472, 219.	n.a.	2a
n.a.	193.0344, 223.9998	1
77.0387, 95.0484, 152.0627, 175.01	n.a.	2a

## Supporting information : A6 - Quality controls

	Repeatability Features in composite QCs with CV < 30% (%)	Median area CV in composite QCs All features (%)
	Threshold : > 80%	Threshold : < 20%
Phree (ESI +)	81,2	11,6
Phree (ESI -)	81,6	10,8
PPT (ESI +)	80,4	11,1
PPT (ESI -)	81,1	9,9

<b>Median area CV in composite QCs Internal standards (%)</b>	<b>Median area CV in cohort samples Internal standards (%)</b>	<b>Median Rt CV in composite QCs Internal standards (%)</b>
Threshold : < 20%	Threshold : < 20%	Threshold : < 15%
12,0	8,0	1,4
13,0	9,6	1,7
9,3	7,8	9,4
9,5	7,2	10,6