

S1. Smiles structure of 170 studied ligands.

Molecule	PubChem ID	SMILES
apigenin	5280443	<chem>C1=CC(=CC=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O</chem>
cannflavin A	10071695	<chem>CC(=CCC/C(=C/CC1=C(C2=C(C=C1O)OC(=CC2=O)C3=C(C(=C(C=C3)O)OC)O)/C)C</chem>
cannflavin B	403815	<chem>CC(=CCC1=C(C2=C(C=C1O)OC(=CC2=O)C3=CC(=C(C=C3)O)OC)O)C</chem>
cannflavin C	25141335	<chem>CC(=CCC/C(=C/CC1=C2C(=C(C=C1O)O)C(=O)C=C(O2)C3=CC(=C(C=C3)O)OC)/C)C</chem>
catechin	9064	<chem>C1[C@@H]([C@H](OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O</chem>
epicatechin	72276	<chem>C1[C@H]([C@H](OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O</chem>
mesuaferone A	101324837	<chem>C1[C@H](OC2=C(C(=CC(=C2C1=O)O)O)C3=C4C(=C(C=C3O)O)C(=O)C[C@H](O4)C5=CC=C(C=C5)O)C6=CC=C(C=C6)O</chem>
mesuaferone B	90472563	<chem>C1[C@H](OC2=C(C(=CC(=C2C1=O)O)O)C3=C(C=C(C4=C3OC(=CC4=O)C5=CC=C(C=C5)O)O)O)C6=CC=C(C=C6)O</chem>
mesuanic acid	5319381	<chem>C[C@H]1[C@H](OC2C(C1=O)C(=O)C(=C2(CC=C(C)C)CC(=C(C)C)CCC(C)C)O)C(CC(=O)O)C3=CC=CC=C3)C</chem>
quercetin	5280343	<chem>C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O</chem>
brachyamide A	14162525	<chem>C1CCN(C1)C(=O)/C=C/C=C/CCCCC/C=C/C2=CC3=C(C=C2)OCO3</chem>
brachystamide B	10047263	<chem>CC(C)CNC(=O)/C=C/C=C/CCCCCCC/C=C/C1=CC2=C(C=C1)OCO2</chem>
dehydropipernonaline	6439947	<chem>C1CCN(CC1)C(=O)/C=C/C=C/CC/C=C/C2=CC3=C(C=C2)OCO3</chem>
ecgonine	91460	<chem>CN1[C@H]2CC[C@@H]1[C@H]([C@H](C2)O)C(=O)O</chem>
guineensine	6442405	<chem>CC(C)CNC(=O)/C=C/C=C/CCCCC/C=C/C1=CC2=C(C=C1)OCO2</chem>
hordenine	68313	<chem>CN(C)CCC1=CC=C(C=C1)O</chem>
neopellitorine B	11118018	<chem>CCCCC/C=C/C=C/C(=O)N1CCCCC1</chem>
pellitorine	5318516	<chem>CCCCC/C=C/C=C/C(=O)NCC(C)C</chem>
piperanine	5320618	<chem>C1CCN(CC1)C(=O)/C=C/CCC2=CC3=C(C=C2)OCO3</chem>
pipercollosine	5372201	<chem>CC(C)CNC(=O)/C=C/C=C/CCCCC1=CC2=C(C=C1)OCO2</chem>
piperchabamide C	44454018	<chem>C1CCN(CC1)C(=O)/C=C/C=C/CCCCC/C=C/C2=CC3=C(C=C2)OCO3</chem>
piperdardine	10086948	<chem>C1CCN(CC1)C(=O)/C=C/C=C/CCC2=CC3=C(C=C2)OCO3</chem>
piperine	638024	<chem>C1CCN(CC1)C(=O)/C=C/C=C/C2=CC3=C(C=C2)OCO3</chem>
piperonaline	9974595	<chem>C1CCN(CC1)C(=O)/C=C/CCCC/C=C/C2=CC3=C(C=C2)OCO3</chem>
piperolactam C	10881419	<chem>COC1=C(C(=C2C3=C1C4=CC=CC=C4C=C3NC2=O)OC)O</chem>

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piperolein B	21580213	<chem>C1CCN(CC1)C(=O)CCCCC/C=C/C2=CC3=C(C=C2)OC O3</chem>
piperundecalidine	44453654	<chem>C1CCN(CC1)C(=O)/C=C/C=C/CCCC/C=C/C2=CC3=C(C=C2)OCO3</chem>
retrofractamide B	5372162	<chem>CC(C)CNC(=O)/C=C/C=C/CCCC/C=C/C1=CC2=C(C=C1) OCO2</chem>
cannabichromene (CBC)	30219	<chem>CCCCC1=CC(=C2C=CC(OC2=C1)(C)CCC=C(C)C)O</chem>
cannabichromenic acid (CBCA)	3084339	<chem>CCCCC1=CC2=C(C=CC(O2)(C)CCC=C(C)C)C(=C1C(= O)O)O</chem>
cannabichromevarin (CBCV)	6451726	<chem>CCCC1=CC(=C2C=CC(OC2=C1)(C)CCC=C(C)C)O</chem>
cannabichromevarinic acid (CBCVA)	11110322	<chem>CCCC1=CC2=C(C=CC(O2)(C)CCC=C(C)C)C(=C1C(=O)O) O</chem>
cannabidiol (CBD)	644019	<chem>CCCCC1=CC(=C(C(=C1)O)[C@@H]2C=C(CC[C@H]2C(= C)C)C)O</chem>
cannabidiolic acid (CBDA)	160570	<chem>CCCCC1=CC(=C(C(=C1C(=O)O)O)[C@@H]2C=C(CC[C @H]2C(=C)C)C)O</chem>
cannabidivarin (CBDV)	11601669	<chem>CCCC1=CC(=C(C(=C1)O)[C@@H]2C=C(CC[C@H]2C(=C) C)C)O</chem>
cannabidivarinic acid (CBDVA)	59444387	<chem>CCCC1=CC(=C(C(=C1C(=O)O)O)[C@@H]2C=C(CC[C@H] 2C(=C)C)C)O</chem>
cannabigerol (CBG)	5315659	<chem>CCCCC1=CC(=C(C(=C1)O)C/C=C(\C)/CCC=C(C)C)O</chem>
cannabigerovarinic acid (CBGVA)	59444383	<chem>CCCC1=CC(=C(C(=C1C(=O)O)O)C/C=C(\C)/CCC=C(C)C)O</chem>
delta-9-tetrahydrocannabinol (THC)	16078	<chem>CCCCC1=CC(=C2[C@@H]3C=C(CC[C@H]3C(OC2=C1)(C)C)C)O</chem>
delta-9-Tetrahydrocannabivarinic acid (THCVA)	59444416	<chem>CCCC1=CC2=C([C@@H]3C=C(CC[C@H]3C(O2)(C)C)C(=C1C(=O)O)O</chem>
delta-3-carene	26049	<chem>CC1=CCC2C(C1)C2(C)C</chem>
delta-cadinol	3084311	<chem>CC1=C[C@H]2[C@@H](CC[C@@]([C@H]2CC1)(C)O)C(C) C</chem>
beta-caryophyllene	5281515	<chem>C/C1=C\CCC(=C)[C@H]2CC([C@@H]2CC1)(C)C</chem>
alpha-Copaene	19725	<chem>CC1=CCC2C3C1C2(CCC3C(C)C)C</chem>
beta-elemene	6918391	<chem>CC(=C)[C@@H]1CC[C@@]([C@@H](C1)C(=C)C)(C)C=C</chem>
delta-guaiene	94275	<chem>C[C@H]1CCC2=C(CC[C@H](C[C@@H]12)C(=C)C)C</chem>
beta-pinene	14896	<chem>CC1(C2CCC(=C)C1C2)C</chem>
beta-selinene	442393	<chem>CC(=C)[C@@H]1CC[C@]2(CCCC(=C)[C@@H]2C1)C</chem>
gamma-terpinene	7461	<chem>CC1=CCC(=CC1)C(C)C</chem>
alpha-terpineol	17100	<chem>CC1=CCC(CC1)C(C)(C)O</chem>
gamma-terpineol	11467	<chem>CC(=C1CCC(CC1)(C)O)C</chem>
alpha-trans-bergamotene	86608	<chem>CC1=CCC2CC1C2(C)CCC=C(C)C</chem>
alpha-zingiberene	11127403	<chem>CC1=CC[C@H](C=C1)[C@H](C)CCC=C(C)C</chem>

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α -humulene	5281520	<chem>C/C/1=C\CC(/C=C/C/C(=C/CC1)/C)(C)C</chem>
α -selinene	10856614	<chem>CC1=CCC[C@]2([C@H]1C[C@@H])(CC2)C(=C)C</chem>
α -terpinene	7462	<chem>CC1=CC=C(CC1)C(C)C</chem>
α -cadinol	10398656	<chem>CC1=C[C@H]2[C@@H](CC[C@@]([C@@H]2CC1)(C)O)C(C)C</chem>
α -panasinsene	578929	<chem>CC1=CCCC2(C13CC(C3CC2)(C)C)C</chem>
α -phellandrene	7460	<chem>CC1=CCC(C=C1)C(C)C</chem>
α -pinene	6654	<chem>CC1=CCC2CC1C2(C)C</chem>
α -terpineol	17100	<chem>CC1=CCC(CC1)C(C)(C)O</chem>
α -thujene	17868	<chem>CC1=CCC2(C1C2)C(C)C</chem>
1,8-cineole	2758	<chem>CC1(C2CCC(O1)(CC2)C)C</chem>
13-epi-manoyl oxide	6432025	<chem>C[C@@]1(CC[C@H]2[C@]3(CCCC([C@@H]3CC[C@]2(O1)C)(C)C)C=C</chem>
4-terpineol	11230	<chem>CC1=CCC(CC1)(C(C)C)O</chem>
7-epi- α -selinene	10726905	<chem>CC1=CCC[C@]2([C@H]1C[C@H])(CC2)C(=C)C</chem>
anethole	637563	<chem>C/C=C/C1=CC=C(C=C1)OC</chem>
borneol	64685	<chem>CC1(C2CCC1(C(C2)O)C)C</chem>
camphene	6616	<chem>CC1(C2CCC(C2)C1=C)C</chem>
camphor	2537	<chem>CC1(C2CCC1(C(=O)C2)C)C</chem>
carvacrol	10364	<chem>CC1=C(C=C(C=C1)C(C)C)O</chem>
caryophyllene	5281515	<chem>C/C/1=C\CCC(=C)[C@H]2CC([C@@H]2CC1)(C)C</chem>
cis-piperitol	85567	<chem>CC1=C[C@@H]([C@@H](CC1)C(C)C)O</chem>
dithymoquinone	398941	<chem>CC(C)C1=CC(=O)C2(C(C1=O)C3(C2C(=O)C(=CC3=O)C(C)C)C)C</chem>
E- β -ocimene	5281553	<chem>CC(=CC/C=C(\C)/C=C)C</chem>
endo-fenchol	6997371	<chem>C[C@@]12CC[C@@H](C1)C([C@@H]2O)(C)C</chem>
epi- α -cadinol	160799	<chem>CC1=C[C@H]2[C@@H](CC[C@]([C@@H]2CC1)(C)O)C(C)C</chem>
geraniol	637566	<chem>CC(=CCC/C(=C/CO)/C)C</chem>
geranyl acetate	1549026	<chem>CC(=CCC/C(=C/COC(=O)C)/C)C</chem>
germacrene-D	91723653	<chem>C/C/1=C/CCC(=C)/C=C\[C@@H](CC1)C(C)C</chem>
guaiol	227829	<chem>C[C@H]1CC[C@H](CC2=C1CC[C@@H]2C)C(C)(C)O</chem>
isoborneol	6321405	<chem>C[C@@]12CC[C@H](C1(C)C)C[C@H]2O</chem>
isoelemicin	5318557	<chem>C/C=C/C1=CC(=C(C(=C1)OC)OC)OC</chem>
limonene	22311	<chem>CC1=CCC(CC1)C(=C)C</chem>
linalool	6549	<chem>CC(=CCCC(C)(C=C)O)C</chem>
myrcene	31253	<chem>CC(=CCCC(=C)C=C)C</chem>
nerol	643820	<chem>CC(=CCC/C(=C\CO)/C)C</chem>
neryl acetate	1549025	<chem>CC(=CCC/C(=C\COC(=O)C)/C)C</chem>
p-cymene	7463	<chem>CC1=CC=C(C=C1)C(C)C</chem>
phytol	5280435	<chem>C[C@@H](CCC[C@H](C)CCC/C(=C/CO)/C)CCCC(C)C</chem>
sabinene	18818	<chem>CC(C)C12CCC(=C)C1C2</chem>
sclareolide	929262	<chem>C[C@]12CCCC([C@@H]1CC[C@@]3([C@@H]2CC(=O)O3)C)(C)C</chem>
spathulenol	92231	<chem>C[C@@]1(CC[C@H]2[C@@H]1[C@H]3[C@H](C3(C)C)CC2=C)O</chem>
terpinen-4-ol	11230	<chem>CC1=CCC(CC1)(C(C)C)O</chem>
terpinolene	11463	<chem>CC1=CCC(=C(C)C)CC1</chem>
tetradecanoic acid	11005	<chem>CCCCCCCCCCCCCCCC(=O)O</chem>

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thymohydroquinone	95779	<chem>CC1=CC(=C(C=C1O)C(C)C)O</chem>
thymol	6989	<chem>CC1=CC(=C(C=C1)C(C)C)O</chem>
thymoquinone	10281	<chem>CC1=CC(=O)C(=CC1=O)C(C)C</chem>
α -amyrin	73170	<chem>C[C@@H]1CC[C@@]2(CC[C@@]3(C(=CC[C@H]4[C@]3(CC[C@@H]5[C@@]4(CC[C@@H](C5(C)C)O)C)C)[C@@H]2[C@H]1C)C)C</chem>
α -terpinene	7462	<chem>CC1=CC=C(CC1)C(C)C</chem>
α -terpineol	17100	<chem>CC1=CCC(CC1)C(C)(C)O</chem>
β -sitosterol	222284	<chem>CC[C@H](CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C(C)C</chem>
β -amyrin	73145	<chem>C[C@@]12CC[C@@]3(C(=CC[C@H]4[C@]3(CC[C@@H]5[C@@]4(CC[C@@H](C5(C)C)O)C)C)[C@@H]1CC(CC2)(C)C</chem>
cannabisin D	71448965	<chem>COC1=C(C=CC(=C1)[C@@H]2[C@H](C(=CC3=CC(=C(C=C23)O)OC)C(=O)NCCC4=CC=C(C=C4)O)C(=O)NCCC5=CC=C(C=C5)O)O</chem>
<i>N-trans</i> -caffeoyltyramine	9994897	<chem>C1=CC(=CC=C1CCNC(=O)/C=C/C2=CC(=C(C=C2)O)O)O</chem>
<i>N-trans</i> -coumaroyltyramine	5372945	<chem>C1=CC(=CC=C1CCNC(=O)/C=C/C2=CC=C(C=C2)O)O</chem>
<i>N-trans</i> -feruloyltyramine	5280537	<chem>COC1=C(C=CC(=C1)/C=C/C(=O)NCCC2=CC=C(C=C2)O)O</chem>
cannabispiradienone	90475437	<chem>COC1=CC2=C(C(=C1)O)C3(CC2)C=CC(=O)C=C3</chem>
cannabispiran	162936	<chem>COC1=CC2=C(C(=C1)O)C3(CCC(=O)CC3)CC2</chem>
cannabistilbene I	146349	<chem>CC(=CCC1=C(C=CC(=C1)CCC2=CC(=CC(=C2)OC)O)O)C</chem>
denbinobin	10423984	<chem>COC1=CC(=C2C(=C1)C=CC3=C2C(=O)C(=CC3=O)OC)O</chem>
dihydroresveratrol	185914	<chem>C1=CC(=CC=C1CCC2=CC(=CC(=C2)O)O)O</chem>
chlorogenic acid	1794427	<chem>C1[C@H]([C@H]([C@@H](C[C@@]1(C(=O)O)O)OC(=O)/C=C/C2=CC(=C(C=C2)O)O)O)O</chem>
ferulic acid	445858	<chem>COC1=C(C=CC(=C1)/C=C/C(=O)O)O</chem>
gallic acid	370	<chem>C1=C(C=C(C(=C1O)O)O)C(=O)O</chem>
<i>p</i> -coumaric acid	637542	<chem>C1=CC(=CC=C1/C=C/C(=O)O)O</chem>
vanillic acid	8468	<chem>COC1=C(C=CC(=C1)C(=O)O)O</chem>
3-acetyl-11keto- β -boswellic acid	11168203	<chem>C[C@@H]1CC[C@@]2(CC[C@@]3(C(=CC(=O)[C@H]4[C@]3(CC[C@@H]5[C@@]4(CC[C@@H]([C@]5(C)C(=O)O)OC(=O)C)C)C)[C@@H]2[C@H]1C)C)C</chem>
betulin	72326	<chem>CC(=C)[C@@H]1CC[C@]2([C@H]1[C@H]3CC[C@@H]4[C@@]5(CC[C@@H](C([C@@H]5CC[C@]4([C@@]3(CC2)C)C)(C)C)O)C)CO</chem>
caryophyllene oxide	1742210	<chem>C[C@@]12CC[C@@H]3[C@H](CC3(C)C)C(=C)CC[C@H]1O2</chem>

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lupeol	259846	<chem>CC(=C)[C@@H]1CC[C@]2([C@H]1[C@H]3CC[C@@H]4[C@@]5(CC[C@@H](C([C@@H]5CC[C@]4([C@@]3(CC2)C)C)(C)C)O)C</chem>
α -amyl cinnamyl alcohol	7584	<chem>CCCCC(=CC1=CC=CC=C1)CO</chem>
1-Hexanol	8103	<chem>CCCCCCO</chem>
3,7dimethyloct-6-en-1yn-3ol	62842	<chem>CC(=CCCC(C)(C#C)O)C</chem>
3,7dimethylocta-1,6dien-3ol	6549	<chem>CC(=CCCC(C)(C=C)O)C</chem>
3-methylhexan-2-ol	16835	<chem>CCCC(C)C(C)O</chem>
4-isopropylbenzyl alcohol	325	<chem>CC(C)C1=CC=C(C=C1)CO</chem>
cineole	2758	<chem>CC1(C2CCC(O1)(CC2)C)C</chem>
elemol	92138	<chem>CC(=C)[C@@H]1C[C@@H](CC[C@@]1(C)C=C)C(C)(C)O</chem>
<i>trans</i> -nerolidol	5284507	<chem>CC(=CCC/C(=C/CCC(C)(C=C)O)/C)C</chem>
β -Eudesmol	91457	<chem>C[C@]12CCCC(=C)[C@@H]1C[C@@H](CC2)C(C)(C)O</chem>
costunolide	5281437	<chem>C/C1=C\CC/C(=C/[C@@H]2[C@@H](CC1)C(=C)C(=O)O2)/C</chem>
cynaropicrin	119093	<chem>C=C1C[C@@H]([C@@H]2[C@@H]([C@@H]3[C@H]1C[C@@H](C3=C)O)OC(=O)C2=C)OC(=O)C(=C)CO</chem>
dehydrocostus lactone	73174	<chem>C=C1CC[C@@H]2[C@@H]([C@@H]3[C@H]1CCC3=C)OC(=O)C2=C</chem>
dihydrocostunolide	5367639	<chem>CC1C2CC/C(=C\CC/C(=C\C2OC1=O)/C)/C</chem>
mokko lactone	167495	<chem>C[C@H]1[C@@H]2CCC(=C)[C@@H]3CCC(=C)[C@@H]3[C@@H]2OC1=O</chem>
allo-aromadendrene	42608158	<chem>C[C@@H]1CC[C@H]2[C@@H]1C3C(C3(C)C)CCC2=C</chem>
α -cedrene	6431015	<chem>C[C@@H]1CC[C@@H]2[C@]13CC=C([C@H](C3)C2(C)C)C</chem>
β -sesquiphellandrene	12315492	<chem>C[C@@H](CCC=C(C)C)[C@H]1CCC(=C)C=C1</chem>
β -thujene	520384	<chem>CC1C=CC2(C1C2)C(C)C</chem>
2,6dimethylhept-5-enal	61016	<chem>CC(CCC=C(C)C)C=O</chem>
2-heptanone	8051	<chem>CCCCCC(=O)C</chem>
butanal	261	<chem>CCCC=O</chem>
germacrone	6436348	<chem>C/C1=C\CC(=C(C)C)C(=O)C/C(=C/CC1)/C</chem>
endo-bornyl acetate	93009	<chem>CC(=O)O[C@@H]1C[C@@H]2CC[C@]1(C2(C)C)C</chem>
geranyl propionate	5355853	<chem>CCC(=O)OC/C=C(\C)/CCC=C(C)C</chem>
neryl acetate	1549025	<chem>CC(=CCC/C(=C\COC(=O)C)/C)C</chem>
sec-butyl acetate	7758	<chem>CCC(C)OC(=O)C</chem>
lauric acid	3893	<chem>CCCCCCCCCCCC(=O)O</chem>
linoleic acid	5280450	<chem>CCCC/C=C\C/C=C\CCCCCCCC(=O)O</chem>

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linolenic acid	5280934	<chem>CC/C=C\C/C=C\C/C=C\CCCCCCCC(=O)O</chem>
myristic acid	11005	<chem>CCCCCCCCCCCCCCCC(=O)O</chem>
oleic acid	445639	<chem>CCCCCCCC/C=C\CCCCCCCC(=O)O</chem>
palmitic acid	985	<chem>CCCCCCCCCCCCCCCC(=O)O</chem>
stearic acid	5281	<chem>CCCCCCCCCCCCCCCC(=O)O</chem>
hexanal	6184	<chem>CCCCCC=O</chem>
limonene	110923	<chem>CC1=CCC(CC1)C(C)CC=O</chem>
aldehyde		
tetradecanal	31291	<chem>CCCCCCCCCCCCCCCC=O</chem>
Z-	6428995	<chem>C1=CC=C(C=C1)/C=C\C=O</chem>
cinnamaldehyde		
eugenol	3314	<chem>COC1=C(C=CC(=C1)CC=C)O</chem>
methyl eugenol	7127	<chem>COC1=C(C=C(C=C1)CC=C)OC</chem>
<i>trans</i> -isoeugenol	853433	<chem>C/C=C/C1=CC(=C(C=C1)O)OC</chem>
Kleinhospitine A		<chem>CC1=C[C@@]2(C=C(C(=O)N2)[C@H]3CC[C@@]4([C@@]3(CC[C@]56[C@H]4CC[C@@H]7[C@]5(C6)C=CC(=O)C7(C)C)C)OC1=O</chem>
Kleinhospitine B		<chem>CC1=C[C@]2(C=C(C(=O)N2)[C@H]3CC[C@@]4([C@@]3(C[C@]56[C@H]4CC[C@@H]7[C@]5(C6)C=CC(=O)C7(C)C)C)OC1=O</chem>
Kleinhospitine C		<chem>CC1=C[C@@]2(C=C(C(=O)N2)[C@H]3CC[C@@]4([C@@]3(CC[C@]56[C@H]4CC[C@@H]7[C@@]5(C6)C=CC(=O)C7(C)C)C)OC1=O</chem>
Kleinhospitine D		<chem>CC1=C[C@]2(C=C(C(=O)N2)[C@H]3CC[C@@]4([C@@]3(C[C@]56[C@H]4CC[C@@H]7[C@@]5(C6)C=CC(=O)C7(C)C)C)OC1=O</chem>
Donepezil	3152	<chem>COC1=C(C=C2C(=C1)CC(C2=O)CC3CCN(CC3)CC4=CC=CC=C4)OC</chem>
Galantamine	9651	<chem>CN1CC[C@@]23C=C[C@@H](C[C@@H]2OC4=C(C=CC(=C34)C1)OC)O</chem>
Rivastigmine	77991	<chem>CCN(C)C(=O)OC1=CC=CC(=C1)[C@H](C)N(C)C</chem>